Electronic Supplementary Information (ESI)

Syntheses and Tautomeric Equilibria in Mono- and Di-azaderivatives of Malonaldehyde. Tailoring Electronic Delocalization and Aromatic Transition Structures with Computational Studies.

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Table S1. Free energy values (hartrees) calculated for structures **13a-l**, **14a-l**, and **31**-**33a-l** in gas-phase, chloroform, dimethyl sulfoxide and ethanol

	Medium	a	b	c	d	e	f	g	h	i	j	k	l
13[a]	Gas-phase	-800.462434	-800.455411	-800.457939	-800.450189	-800.446854	-800.448436	-800.452830	-800.429701	-800.436789	-800.436752	-800.436852	-800.435836
	$CHCl_3$	-800.485304	-800.480279	-800.482823	-800.477170	-800.473552	-800.472705	-800.473126	-800.455521	-800.461828	-800.461449	-800.460957	-800.459751
	DMSO	-800.484706	-800.480645	-800.484090	-800.478603	-800.474330	-800.472716	-800.471266	-800.453971	-800.457536	-800.461070	-800.458714	-800.458281
	EtOH	-800.484111	-800.483701	-800.486019	-800.482296	-800.476364	-800.476408	-800.471820	-800.459630	-800.462040	-800.464805	-800.463098	-800.462644
14[a]	Gas-phase	-952.842799	-952.838739	-952.839106	-952.833424	-952.828949	-952.831178	-952.833375	-952.812505	-952.817069	-952.819497	-952.820815	-952.817830
	$CHCl_3$	-952.869873	-952.868247	-952.873636	-952.863305	-952.859093	-952.861018	-952.859105	-952.841938	-952.847293	-952.849007	-952.849517	-952.846193
	DMSO	-952.869162	-952.868154	-952.870670	-952.865053	-952.860022	-952.859184	-952.858840	-952.839676	-952.844603	-952.848695	-952.846658	-952.843210
	EtOH	-952.870502	-952.870886	-952.873636	-952.866676	-952.862331	-952.861435	-952.859190	-952.845773	-952.848871	-952.853572	-952.850839	-952.847581
31[a]	Gas-phase	-517.412421	-517.406853	-517.407706	-517.399505	-517.395872	-517.398235	-517.403459	-517.381932	-517.387049	-517.386230	-517.387896	-517.386223
	$CHCl_3$	-517.430112	-517.426669	-517.428136	-517.421318	-517.418409	-517.417849	-517.419449	-517.402675	-517.406886	-517.407157	-517.407153	-517.404925
	DMSO	-517.428484	-517.427175	-517.428481	-517.422598	-517.419466	-517.420781	-517.416293	-517.400019	-517.403702	-517.405738	-517.404757	-517.403087
	EtOH	-517.431492	-517.429731	-517.432314	-517.425971	-517.422949	-517.420781	-517.418427	-517.407505	-517.409407	-517.411603	-517.409672	-517.407429
32[a]	Gas-phase	-631.894424	-631.889904	-631.890903	-631.882701	-631.879163	-631.881327	-631.886107	-631.864754	-631.870761	-631.870129	-631.869851	-631.869637
	$CHCl_3$	-631.912841	-631.910500	-631.913568	-631.905155	-631.901222	-631.901057	-631.901673	-631.886150	-631.889414	-631.891600	-631.892100	-631.889247
	DMSO	-631.912296	-631.910380	-631.915052	-631.907117	-631.903802	-631.901674	-631.900141	-631.883946	-631.888119	-631.891936	-631.889957	-631.888618
	EtOH	-631.915290	-631.914676	-631.918434	-631.910550	-631.908028	-631.905491	-631.902325	-631.890834	-631.894278	-631.897109	-631.894783	-631.893865
32[b]	Gas-phase	-632.173563	-632.167411	-632.168054	-632.160385	-632.155783	-632.158059	-632.162542	-632.139768	-632.145322	-632.145291	-632.145380	-632.144781
	$CHCl_3$	-632.191188	-632.188582	-632.190202	-632.182960	-632.178937	-632.177600	-632.177480	-632.159766	-632.164508	-632.166158	-632.165511	-632.163385
	DMSO	-632.190226	-632.188723	-632.191643	-632.184631	-632.179924	-632.178193	-632.175163	-632.158201	-632.161366	-632.164959	-632.163591	-632.162602
	EtOH	-632.194666	-632.192873	-632.195487	-632.188030	-632.183804	-632.181842	-632.177337	-632.164220	-632.167594	-632.171146	-632.168244	-632.167520
33[a]	Gas-phase	-721.904952	-721.898607	-721.900759	-721.893753	-721.889814	-721.891362	-721.895593	-721.873326	-721.879591	-721.880821	-721.880029	-721.879245
	$CHCl_3$	-721.925191	-721.922168	-721.924757	-721.917885	-721.914289	-721.913751	-721.912974	-721.895997	-721.900809	-721.902543	-721.902203	-721.899209
	DMSO	-721.925694	-721.923185	-721.926196	-721.922095	-721.917107	-721.915081	-721.912347	-721.896084	-721.899155	-721.901672	-721.902007	-721.900273
	EtOH	-721.927268	-721.924533	-721.927550	-721.921394	-721.918655	-721.917294	-721.912803	-721.901398	-721.903233	-721.906772	-721.904752	-721.902520
33[b]	Gas-phase	-722.213704	-722.206228	-722.206946	-722.201053	-722.196502	-722.197520	-722.202056	-722.179117	-722.184723	-722.185363	-722.185191	-722.184251
	$CHCl_3$	-722.233879	-722.229073	-722.230419	-722.226834	-722.220721	-722.219731	-722.219256	-722.201182	-722.205596	-722.206925	-722.206348	-722.203739
	DMSO	-722.234512	-722.230540	-722.232734	-722.228517	-722.223393	-722.221203	-722.218803	-722.200990	-722.203254	-722.206537	-722.205584	-722.204364
	EtOH	-722.236519	-722.232049	-722.234430	-722.230218	-722.225672	-722.224049	-722.220364	-722.205454	-722.207764	-722.211149	-722.208607	-722.206817

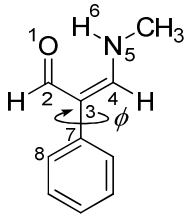
[a] At M06-2X/6-311++G(d,p) level. [b] At B3LYP/6-311++G(d,p) level.

Table S2. Solvation free energies (ΔG_{solv}, kcal mol^{-1}) in $CHCl_3$, DMSO, and C_2H_5OH for conformers and tautomers **a-l** of structures **13**, **14**, and **31-33** at the M06-2X/6-311++G(d,p) and B3LYP/6-311++G(d,p) levels of theory.

		a	**b**	**c**	**d**	**e**	**f**	**g**	**h**	**i**	**j**	**k**	**l**
13[a]	$CHCl_3$	-14.4	-15.6	-15.6	-16.9	-16.8	-15.2	-12.7	-16.2	-15.7	-15.5	-15.1	-15.0
	DMSO	-14.0	-15.8	-16.4	-17.8	-17.2	-15.2	-11.6	-15.2	-13.0	-15.3	-13.7	-14.1
	C_2H_5OH	-13.6	-17.8	-17.6	-20.1	-18.5	-17.6	-11.9	-18.8	-15.8	-17.6	-16.5	-16.8
14[a]	$CHCl_3$	-17.0	-18.5	-21.7	-18.8	-18.9	-18.7	-16.1	-18.5	-19.0	-18.5	-18.0	-17.8
	DMSO	-16.5	-18.5	-19.8	-19.8	-19.5	-17.6	-16.0	-17.1	-17.3	-18.3	-16.2	-15.9
	C_2H_5OH	-17.4	-20.2	-21.7	-20.9	-20.9	-19.0	-16.2	-20.9	-20.0	-21.4	-18.8	-18.7
31[a]	$CHCl_3$	-11.1	-12.4	-12.8	-13.7	-14.1	-12.3	-10.0	-13.0	-12.4	-13.1	-12.1	-11.7
	DMSO	-10.1	-12.8	-13.0	-14.5	-14.8	-14.1	-8.1	-11.3	-10.4	-12.2	-10.6	-10.6
	C_2H_5OH	-12.0	-14.4	-15.4	-16.6	-17.0	-14.1	-9.4	-16.0	-14.0	-15.9	-13.7	-13.3
32[a]	$CHCl_3$	-11.6	-12.9	-14.2	-14.1	-13.8	-12.4	-9.8	-13.4	-11.7	-13.5	-14.0	-12.3
	DMSO	-11.2	-12.8	-15.2	-15.3	-15.5	-12.8	-8.8	-12.0	-10.9	-13.7	-12.6	-11.9
	C_2H_5OH	-13.1	-15.5	-17.3	-17.5	-18.1	-15.2	-10.2	-16.4	-14.8	-16.9	-15.6	-15.2
32[b]	$CHCl_3$	-11.1	-13.3	-13.9	-14.2	-14.5	-12.3	-9.4	-12.5	-12.0	-13.1	-12.6	-11.7
	DMSO	-10.5	-13.4	-14.8	-15.2	-15.1	-12.6	-7.9	-11.6	-10.1	-12.3	-11.4	-11.2
	C_2H_5OH	-13.2	-16.0	-17.2	-17.3	-17.6	-14.9	-9.3	-15.3	-14.0	-16.2	-14.3	-14.3
33[a]	$CHCl_3$	-12.7	-14.8	-15.1	-15.1	-15.4	-14.0	-10.9	-14.2	-13.3	-13.6	-13.9	-12.5
	DMSO	-13.0	-15.4	-16.0	-17.8	-17.1	-14.9	-10.5	-14.3	-12.3	-13.1	-13.8	-13.2
	C_2H_5OH	-14.0	-16.3	-16.8	-17.3	-18.1	-16.3	-10.8	-17.6	-14.8	-16.3	-15.5	-14.6
33[b]	$CHCl_3$	-12.7	-14.3	-14.7	-16.2	-15.2	-13.9	-10.8	-13.8	-13.1	-13.5	-13.3	-12.2
	DMSO	-13.1	-15.3	-16.2	-17.2	-16.9	-14.9	-10.5	-13.7	-11.6	-13.3	-12.8	-12.6
	C_2H_5OH	-14.3	-16.2	-17.2	-18.3	-18.3	-16.6	-11.5	-16.5	-14.5	-16.2	-14.7	-14.2

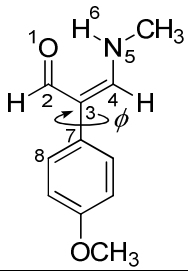
[a] M06-2X/6-311++G(d,p). [b] B3LYP/6-311++G(d,p).

Table S3. Selected geometric and delocalization parameters for isomers **31a-l**



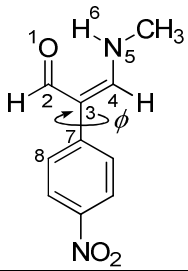
	Medium	Bond distances (Å)							ϕ (°)	Q	$\langle\lambda\rangle$	HOMA index
		O_1-C_2	C_2-C_3	C_3-C_4	C_4-N_5	O_1-N_5	O_1-H_6	N_5-H_6				
31a	Gas phase	1.227	1.444	1.377	1.334	2.682	1.910	1.017	43.58	0.174	0.333	0.93
31b		1.213	1.464	1.362	1.347	4.136	4.738	1.011	49.00	0.236	0.262	0.82
31c		1.210	1.460	1.361	1.351	4.778	5.004	1.011	45.81	0.240	0.256	0.82
31d		1.210	1.460	1.365	1.355	4.185	3.845	1.007	40.42	0.240	0.257	0.82
31e		1.212	1.464	1.368	1.355	4.291	5.269	1.005	40.44	0.239	0.260	0.82
31f		1.216	1.461	1.372	1.344	3.051	3.981	1.006	36.37	0.217	0.285	0.85
31g		1.319	1.360	1.455	1.280	2.579	1.002	1.683	43.06	-0.134	0.316	0.57
31h		1.346	1.343	1.475	1.266	2.835	0.959	3.771	41.51	-0.212	0.231	0.22
31i		1.353	1.341	1.479	1.266	4.168	0.959	4.560	37.84	-0.225	0.218	0.13
31j		1.353	1.343	1.470	1.265	4.772	0.959	5.470	44.08	-0.215	0.227	0.17
31k		1.359	1.342	1.471	1.267	4.064	0.959	5.005	46.17	-0.221	0.222	0.11
31l		1.350	1.347	1.467	1.266	4.214	0.961	3.764	46.87	-0.204	0.240	0.22
31a	$CHCl_3$	1.235	1.435	1.386	1.326	2.704	1.948	1.017	41.45	0.140	0.372	0.96
31b		1.224	1.450	1.374	1.333	4.138	4.755	1.013	48.04	0.185	0.320	0.91
31c		1.221	1.445	1.373	1.335	4.773	5.028	1.012	47.98	0.186	0.317	0.91
31d		1.221	1.446	1.378	1.339	4.195	3.877	1.010	40.97	0.186	0.318	0.91
31e		1.222	1.451	1.379	1.340	4.297	5.280	1.009	41.34	0.190	0.315	0.90
31f		1.224	1.451	1.381	1.335	3.060	3.989	1.009	34.12	0.181	0.326	0.91
31g		1.324	1.359	1.458	1.280	2.558	1.009	1.649	40.66	-0.143	0.307	0.52
31h		1.344	1.345	1.474	1.269	2.855	0.964	3.799	39.09	-0.204	0.240	0.25
31i		1.348	1.343	1.478	1.268	4.186	0.964	4.590	37.00	-0.215	0.229	0.19
31j		1.347	1.345	1.468	1.268	4.678	0.964	5.471	46.95	-0.202	0.241	0.24
31k		1.353	1.345	1.469	1.269	4.064	0.963	5.015	46.67	-0.208	0.236	0.19
31l		1.348	1.348	1.468	1.269	4.215	0.965	3.778	47.33	-0.199	0.246	0.24
31a	DMSO	1.235	1.434	1.389	1.323	2.713	1.961	1.016	37.20	0.133	0.380	0.96
31b		1.225	1.447	1.378	1.328	4.140	4.764	1.013	45.87	0.172	0.335	0.92
31c		1.224	1.442	1.377	1.330	4.774	5.037	1.013	48.38	0.171	0.335	0.93
31d		1.224	1.443	1.383	1.332	4.199	3.883	1.012	41.48	0.168	0.339	0.93
31e		1.225	1.449	1.383	1.334	4.320	5.304	1.010	42.84	0.175	0.332	0.92
31f		1.233	1.440	1.388	1.328	3.054	3.980	1.011	33.46	0.147	0.365	0.95
31g		1.322	1.361	1.458	1.281	2.542	1.014	1.621	37.14	-0.138	0.313	0.54
31h		1.345	1.345	1.475	1.269	2.900	0.965	3.847	36.21	-0.206	0.238	0.24
31i		1.348	1.344	1.478	1.269	4.191	0.965	4.599	37.27	-0.213	0.232	0.20
31j		1.346	1.345	1.466	1.270	4.762	0.965	5.469	51.68	-0.197	0.247	0.27
31k		1.350	1.346	1.468	1.271	4.061	0.965	5.014	46.13	-0.201	0.244	0.23
31l		1.346	1.349	1.468	1.270	4.212	0.966	3.767	47.29	-0.195	0.250	0.27
31a	EtOH	1.243	1.426	1.392	1.321	2.721	1.974	1.016	39.99	0.112	0.405	0.97
31b		1.235	1.436	1.382	1.324	4.139	4.759	1.014	47.64	0.143	0.369	0.95
31c		1.234	1.431	1.381	1.326	4.769	5.024	1.013	51.61	0.142	0.369	0.96
31d		1.233	1.433	1.387	1.328	4.203	3.890	1.012	43.16	0.141	0.370	0.96
31e		1.234	1.439	1.386	1.331	4.321	5.306	1.010	45.67	0.150	0.361	0.95
31f		1.233	1.440	1.388	1.328	3.054	3.980	1.011	33.46	0.147	0.365	0.95
31g		1.329	1.358	1.460	1.280	2.552	1.012	1.638	38.05	-0.151	0.299	0.48
31h		1.345	1.346	1.473	1.270	2.865	0.965	3.813	39.24	-0.202	0.243	0.25
31i		1.349	1.344	1.477	1.270	4.205	0.965	4.623	40.05	-0.212	0.233	0.20
31j		1.347	1.345	1.465	1.270	4.764	0.965	5.476	53.69	-0.197	0.247	0.26
31k		1.351	1.346	1.468	1.271	4.063	0.964	5.016	46.92	-0.202	0.243	0.22
31l		1.349	1.348	1.468	1.271	4.218	0.966	3.790	48.14	-0.198	0.248	0.24

Table S4. Selected geometric and delocalization parameters for isomers **32a-l**



	Medium	Bond distances (Å)							ϕ (°)	Q	$\langle\lambda\rangle$	HOMA index
		O_1-C_2	C_2-C_3	C_3-C_4	C_4-N_5	O_1-N_5	O_1-H_6	N_5-H_6				
32a	Gas phase	1.227	1.444	1.376	1.335	2.683	1.912	1.017	45.65	0.176	0.331	0.93
32b		1.214	1.464	1.361	1.348	4.141	4.738	1.011	50.71	0.237	0.261	0.82
32c		1.210	1.460	1.361	1.353	4.777	4.998	1.011	45.47	0.242	0.254	0.82
32d		1.211	1.460	1.365	1.358	4.183	3.838	1.007	40.26	0.242	0.255	0.82
32e		1.212	1.464	1.367	1.356	4.286	5.264	1.005	39.68	0.241	0.258	0.81
32f		1.216	1.461	1.371	1.345	3.055	3.986	1.006	37.82	0.219	0.282	0.85
32g		1.321	1.359	1.456	1.279	2.583	1.000	1.690	45.36	-0.139	0.311	0.55
32h		1.348	1.343	1.475	1.266	2.837	0.959	3.770	44.13	-0.214	0.229	0.20
32i		1.355	1.340	1.479	1.266	4.172	0.959	4.564	36.14	-0.228	0.215	0.11
32j		1.354	1.343	1.470	1.265	4.772	0.959	5.470	43.60	-0.216	0.226	0.16
32k		1.361	1.342	1.471	1.268	4.061	0.959	5.003	44.76	-0.222	0.222	0.09
32l		1.351	1.347	1.467	1.266	4.216	0.961	3.766	46.18	-0.205	0.239	0.21
32a	$CHCl_3$	1.235	1.434	1.385	1.327	2.704	1.948	1.017	42.38	0.141	0.371	0.96
32b		1.225	1.449	1.374	1.333	4.138	4.752	1.012	48.96	0.183	0.323	0.91
32c		1.222	1.445	1.373	1.336	4.772	5.021	1.012	48.65	0.186	0.318	0.91
32d		1.222	1.446	1.378	1.340	4.180	3.851	1.010	38.99	0.186	0.319	0.91
32e		1.223	1.450	1.378	1.341	4.295	5.278	1.008	41.84	0.190	0.315	0.90
32f		1.224	1.451	1.380	1.337	3.065	3.997	1.009	36.13	0.184	0.322	0.91
32g		1.326	1.359	1.458	1.280	2.562	1.007	1.654	42.02	-0.145	0.305	0.51
32h		1.346	1.345	1.475	1.269	2.867	0.964	3.810	40.14	-0.207	0.237	0.23
32i		1.350	1.343	1.478	1.269	4.189	0.963	4.594	36.03	-0.216	0.228	0.18
32j		1.349	1.345	1.468	1.268	4.767	0.964	5.471	46.99	-0.204	0.240	0.22
32k		1.354	1.345	1.469	1.270	4.061	0.963	5.011	45.99	-0.208	0.237	0.18
32l		1.349	1.348	1.468	1.269	4.215	0.965	3.773	47.87	-0.200	0.245	0.23
32a	DMSO	1.236	1.433	1.388	1.325	2.718	1.969	1.016	41.05	0.134	0.379	0.96
32b		1.226	1.447	1.377	1.329	4.142	4.761	1.013	47.78	0.173	0.334	0.92
32c		1.225	1.440	1.377	1.330	4.770	5.022	1.013	50.28	0.168	0.338	0.93
32d		1.225	1.442	1.382	1.334	4.182	3.851	1.011	41.81	0.169	0.338	0.93
32e		1.226	1.448	1.383	1.336	4.315	5.300	1.010	42.52	0.175	0.333	0.92
32f		1.225	1.449	1.382	1.334	3.072	4.008	1.010	34.38	0.176	0.331	0.91
32g		1.325	1.359	1.459	1.281	2.551	1.011	1.636	40.24	-0.144	0.306	0.51
32h		1.347	1.345	1.476	1.269	2.910	0.964	3.856	37.27	-0.209	0.236	0.22
32i		1.350	1.343	1.478	1.269	4.191	0.964	4.601	35.77	-0.216	0.228	0.18
32j		1.347	1.345	1.466	1.270	4.761	0.965	5.469	51.98	-0.198	0.246	0.26
32k		1.352	1.346	1.469	1.271	4.057	0.964	5.010	46.81	-0.204	0.241	0.21
32l		1.347	1.348	1.468	1.270	4.204	0.966	3.754	47.93	-0.197	0.248	0.26
32a	EtOH	1.243	1.425	1.391	1.322	2.721	1.977	1.016	42.14	0.113	0.403	0.98
32b		1.236	1.435	1.381	1.325	4.140	4.755	1.014	49.21	0.143	0.369	0.96
32c		1.235	1.429	1.381	1.326	4.764	5.007	1.014	53.55	0.139	0.372	0.97
32d		1.233	1.432	1.386	1.330	4.188	3.862	1.012	44.44	0.143	0.368	0.96
32e		1.234	1.438	1.386	1.332	4.315	5.300	1.010	45.30	0.150	0.361	0.95
32f		1.233	1.439	1.387	1.330	3.060	3.988	1.011	34.82	0.149	0.362	0.95
32g		1.331	1.357	1.460	1.280	2.557	1.011	1.645	40.73	-0.154	0.296	0.46
32h		1.347	1.346	1.473	1.271	2.872	0.965	3.821	40.43	-0.203	0.242	0.24
32i		1.350	1.343	1.477	1.270	4.204	0.965	4.620	37.87	-0.214	0.231	0.19
32j		1.348	1.345	1.465	1.271	4.763	0.965	5.477	53.72	-0.197	0.247	0.25
32k		1.353	1.346	1.468	1.271	4.064	0.964	5.017	48.58	-0.204	0.241	0.20
32l		1.350	1.348	1.468	1.271	4.211	0.966	3.775	49.03	-0.199	0.247	0.23

Table S5. Selected geometric and delocalization parameters for isomers **33a-l**



	Medium	Bond distances (Å)							ϕ (°)	Q	$\langle\lambda\rangle$	HOMA index
		O_1-C_2	C_2-C_3	C_3-C_4	C_4-N_5	O_1-N_5	O_1-H_6	N_5-H_6				
33a	Gas phase	1.225	1.446	1.381	1.329	2.675	1.900	1.019	38.92	0.169	0.338	0.92
33b		1.212	1.467	1.366	1.342	4.118	4.736	1.011	44.29	0.231	0.268	0.82
33c		1.209	1.461	1.364	1.347	4.779	5.020	1.011	42.63	0.235	0.261	0.82
33d		1.210	1.460	1.369	1.349	4.182	3.846	1.008	37.10	0.230	0.268	0.83
33e		1.211	1.465	1.370	1.350	4.292	5.270	1.006	37.59	0.234	0.265	0.82
33f		1.214	1.462	1.376	1.339	3.046	3.968	1.007	32.67	0.211	0.291	0.85
33g		1.313	1.363	1.456	1.278	2.562	1.007	1.660	39.32	-0.128	0.323	0.60
33h		1.342	1.345	1.477	1.264	2.843	0.960	3.773	38.33	-0.210	0.233	0.24
33i		1.349	1.342	1.480	1.265	4.161	0.960	4.557	36.25	-0.222	0.221	0.16
33j		1.350	1.343	1.471	1.264	4.767	0.960	5.474	43.46	-0.214	0.228	0.19
33k		1.354	1.343	1.472	1.267	4.063	0.959	5.007	44.07	-0.216	0.630	0.16
33l		1.345	1.348	1.468	1.265	4.218	0.961	3.776	45.00	-0.200	0.243	0.26
33a	$CHCl_3$	1.232	1.437	1.391	1.321	2.694	1.931	1.018	35.56	0.135	0.377	0.95
33b		1.222	1.452	1.379	1.327	4.117	4.750	1.012	42.57	0.178	0.328	0.90
33c		1.220	1.447	1.377	1.331	4.776	5.045	1.012	43.84	0.181	0.323	0.91
33d		1.220	1.448	1.383	1.331	4.167	3.830	1.011	33.43	0.176	0.330	0.91
33e		1.221	1.452	1.383	1.335	4.291	5.274	1.009	36.34	0.183	0.323	0.90
33f		1.222	1.453	1.386	1.329	3.052	3.974	1.010	29.61	0.174	0.333	0.90
33g		1.316	1.364	1.459	1.279	2.538	1.016	1.619	35.91	-0.132	0.319	0.58
33h		1.339	1.348	1.476	1.267	2.854	0.964	3.794	35.50	-0.200	0.245	0.29
33i		1.343	1.345	1.479	1.267	4.176	0.964	4.585	35.85	-0.210	0.234	0.24
33j		1.344	1.346	1.468	1.267	4.762	0.964	5.475	46.26	-0.199	0.244	0.27
33k		1.348	1.346	1.470	1.269	4.060	0.964	5.013	43.49	-0.203	0.241	0.23
33l		1.343	1.349	1.469	1.268	4.202	0.965	3.759	43.64	-0.195	0.250	0.28
33a	DMSO	1.233	1.436	1.394	1.318	2.709	1.953	1.017	34.81	0.127	0.387	0.95
33b		1.224	1.450	1.383	1.323	4.121	4.759	1.013	43.32	0.166	0.342	0.91
33c		1.223	1.443	1.382	1.325	4.776	5.050	1.013	45.13	0.163	0.344	0.93
33d		1.223	1.445	1.389	1.325	4.169	3.833	1.012	32.41	0.158	0.350	0.92
33e		1.224	1.449	1.388	1.329	4.288	5.273	1.011	35.14	0.166	0.342	0.92
33f		1.223	1.452	1.390	1.325	3.063	3.988	1.011	27.67	0.164	0.345	0.91
33g		1.316	1.365	1.459	1.280	2.527	1.020	1.598	34.94	-0.130	0.322	0.58
33h		1.340	1.348	1.476	1.268	2.892	0.965	3.836	33.69	-0.200	0.245	0.28
33i		1.343	1.346	1.479	1.268	4.179	0.965	4.589	34.88	-0.208	0.237	0.24
33j		1.343	1.346	1.467	1.269	4.760	0.965	5.472	48.18	-0.195	0.249	0.29
33k		1.346	1.347	1.469	1.270	4.058	0.965	5.012	43.12	-0.198	0.247	0.26
33l		1.341	1.350	1.469	1.269	4.206	0.967	3.761	44.52	-0.191	0.254	0.31
33a	EtOH	1.239	1.430	1.397	1.316	2.711	1.959	1.017	34.97	0.110	0.406	0.96
33b		1.232	1.440	1.386	1.320	4.119	4.755	1.014	44.88	0.142	0.370	0.94
33c		1.231	1.434	1.385	1.322	4.772	5.041	1.013	46.64	0.140	0.371	0.95
33d		1.230	1.437	1.393	1.322	4.171	3.836	1.013	33.80	0.136	0.376	0.95
33e		1.231	1.441	1.391	1.327	4.294	5.279	1.011	37.59	0.146	0.365	0.94
33f		1.230	1.443	1.394	1.322	3.045	3.965	1.012	28.06	0.141	0.371	0.94
33g		1.321	1.362	1.460	1.279	2.535	1.019	1.613	35.34	-0.140	0.311	0.54
33h		1.340	1.349	1.475	1.269	2.863	0.965	3.805	34.86	-0.197	0.248	0.29
33i		1.342	1.347	1.478	1.269	4.191	0.965	4.611	35.65	-0.204	0.241	0.26
33j		1.343	1.347	1.466	1.269	4.762	0.965	5.478	48.21	-0.193	0.251	0.29
33k		1.346	1.348	1.469	1.270	4.056	0.965	5.011	43.54	-0.197	0.248	0.26
33l		1.343	1.350	1.469	1.269	4.195	0.966	3.754	43.43	-0.193	0.252	0.29

Table S6. Free energy values (hartrees) calculated at M06-2X/6-31++G(d,p) level in gas-phase, chloroform, dimethyl sulfoxide and ethanol for structures **34-36a-f**

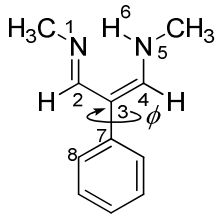
	Medium	a	b	c	d	e	f
34	Gas-phase	-536.788463	-536.779812	-536.781562	-536.775614	-536.771873	-536.770741
	$CHCl_3$	-536.804881	-536.798737	-536.802346	-536.796137	-536.792681	-536.790494
	DMSO	-536.800662	-536.796456	-536.800112	-536.793875	-536.791668	-536.787683
	EtOH	-536.803821	-536.798835	-536.802995	-536.797061	-536.794475	-536.790190
35	Gas-phase	-651.270762	-651.263207	-651.263974	-651.259004	-651.254176	-651.253909
	$CHCl_3$	-651.289026	-651.283763	-651.285048	-651.280669	-651.276914	-651.274087
	DMSO	-651.285530	-651.281496	-651.284337	-651.280238	-651.276647	-651.271673
	EtOH	-651.288829	-651.284978	-651.288077	-651.283696	-651.279876	-651.274913
36	Gas-phase	-741.282731	-741.273412	-741.275243	-741.270692	-741.267246	-741.264650
	$CHCl_3$	-741.302916	-741.295575	-741.297297	-741.294001	-741.289710	-741.286462
	DMSO	-741.301507	-741.293327	-741.297104	-741.294197	-741.289549	-741.285492
	EtOH	-741.303289	-741.295934	-741.298491	-741.295676	-741.291670	-741.286864

Table S7. Relative free energies (ΔG, kcal/mol)[a] in gas-phase, chloroform, dimethyl sulfoxide and ethanol for **34-36a-f**

	Medium	a	b	c	d	e	f
34	Gas-phase	0.0	5.4	4.3	8.1	10.4	11.1
	$CHCl_3$	0.0	3.9	1.6	5.5	7.7	9.0
	DMSO	0.0	2.6	0.4	4.3	5.6	8.1
	EtOH	0.0	3.1	0.5	4.2	5.9	8.6
35	Gas-phase	0.0	4.7	4.3	7.4	10.4	10.6
	$CHCl_3$	0.0	3.3	2.5	5.2	7.6	9.4
	DMSO	0.0	2.5	0.8	3.3	5.6	8.7
	EtOH	0.0	2.4	0.5	3.2	5.6	8.7
36	Gas-phase	0.0	5.9	4.7	7.6	9.7	11.4
	$CHCl_3$	0.0	4.6	3.5	5.6	8.3	10.3
	DMSO	0.0	5.1	2.8	4.6	7.5	10.1
	EtOH	0.0	4.6	3.0	4.8	7.3	10.3

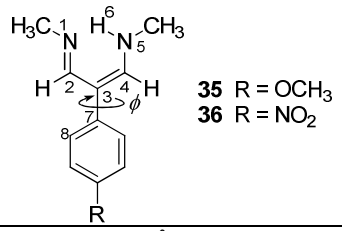
[a] Relative in every case to the free energy of the most stable form

Table S8. Selected geometric parameters and delocalization parameters for structures **34a-f**



	Medium	Bond distances (Å)							ϕ (°)	Q	$\langle\lambda\rangle$	HOMA index
		N_1-C_2	C_2-C_3	C_3-C_4	C_4-N_5	N_1-N_5	N_1-H_6	N_5-H_6				
34a	Gas-phase	1.281	1.450	1.371	1.341	2.723	1.933	1.021	40.81	0.139	0.344	0.85
34b		1.269	1.470	1.356	1.362	4.192	4.775	1.011	43.68	0.207	0.270	0.71
34c		1.268	1.461	1.355	1.366	4.833	5.023	1.012	50.58	0.204	0.271	0.72
34d		1.269	1.462	1.358	1.369	4.224	3.862	1.008	42.73	0.204	0.273	0.72
34e		1.270	1.466	1.359	1.370	4.270	5.257	1.005	41.20	0.207	0.271	0.71
34f		1.271	1.466	1.360	1.359	3.170	4.151	1.005	54.70	0.194	0.284	0.74
34a	$CHCl_3$	1.283	1.449	1.376	1.337	2.739	1.960	1.019	38.12	0.127	0.358	0.86
34b		1.273	1.467	1.363	1.352	4.205	4.801	1.012	41.98	0.183	0.297	0.76
34c		1.273	1.457	1.362	1.355	4.833	5.051	1.012	53.66	0.177	0.302	0.78
34d		1.273	1.459	1.365	1.356	4.216	3.868	1.009	42.14	0.177	0.303	0.78
34e		1.274	1.462	1.367	1.355	4.319	5.305	1.007	42.96	0.176	0.305	0.78
34f		1.273	1.466	1.364	1.356	3.167	4.147	1.008	52.27	0.185	0.295	0.75
34a	DMSO	1.284	1.449	1.378	1.335	2.743	1.970	1.019	36.57	0.122	0.364	0.87
34b		1.275	1.465	1.367	1.346	4.207	4.812	1.012	41.22	0.169	0.312	0.78
34c		1.276	1.453	1.366	1.348	4.829	5.059	1.012	54.23	0.159	0.321	0.81
34d		1.275	1.457	1.370	1.349	4.218	3.880	1.010	41.88	0.161	0.320	0.80
34e		1.276	1.460	1.371	1.349	4.327	5.315	1.008	43.82	0.162	0.320	0.80
34f		1.274	1.467	1.365	1.355	3.165	4.146	1.009	49.20	0.183	0.298	0.76
34a	EtOH	1.285	1.449	1.378	1.336	2.751	1.979	1.018	37.21	0.122	0.364	0.87
34b		1.275	1.465	1.366	1.348	4.217	4.817	1.012	41.64	0.172	0.309	0.78
34c		1.276	1.453	1.365	1.350	4.830	5.056	1.012	56.55	0.162	0.318	0.81
34d		1.276	1.457	1.368	1.352	4.217	3.876	1.010	43.50	0.165	0.316	0.80
34e		1.277	1.460	1.370	1.351	4.325	5.313	1.008	45.00	0.164	0.318	0.80
34f		1.274	1.467	1.364	1.357	3.182	4.168	1.009	50.06	0.186	0.294	0.75

Table S9. Most significant geometric parameters and delocalization parameters for structures **35a-f** and **36a-f**

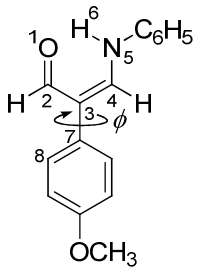


	Medium	Bond distances (Å)							ϕ (º)	Q	$\langle\lambda\rangle$	HOMA index
		N_1-C_2	C_2-C_3	C_3-C_4	C_4-N_5	N_1-N_5	N_1-H_6	N_5-H_6				
35a	Gas-phase	1.281	1.450	1.369	1.344	2.729	1.941	1.020	43.43	0.144	0.339	0.84
35b		1.269	1.469	1.355	1.364	4.202	4.778	1.011	46.86	0.209	0.267	0.71
35c		1.268	1.461	1.355	1.368	4.834	5.020	1.012	49.88	0.206	0.270	0.72
35d		1.269	1.462	1.357	1.371	4.229	3.864	1.008	44.36	0.207	0.270	0.72
35e		1.270	1.465	1.359	1.371	4.266	5.252	1.005	40.49	0.207	0.271	0.71
35f		1.271	1.466	1.359	1.362	3.177	4.163	1.005	57.32	0.198	0.667	0.73
35a	$CHCl_3$	1.284	1.449	1.374	1.339	2.746	1.972	1.018	41.18	0.130	0.355	0.86
35b		1.273	1.466	1.361	1.354	4.210	4.803	1.012	45.43	0.186	0.293	0.75
35c		1.273	1.457	1.362	1.357	4.834	5.053	1.012	53.48	0.179	0.300	0.78
35d		1.273	1.459	1.364	1.360	4.227	3.877	1.010	43.97	0.182	0.297	0.77
35e		1.274	1.462	1.367	1.358	4.316	5.302	1.007	43.26	0.179	0.302	0.77
35f		1.273	1.466	1.362	1.359	3.174	4.159	1.007	54.82	0.190	0.289	0.75
35a	DMSO	1.285	1.449	1.376	1.337	2.751	1.983	1.018	39.68	0.125	0.361	0.87
35b		1.275	1.465	1.365	1.349	4.214	4.816	1.012	43.27	0.174	0.307	0.77
35c		1.276	1.453	1.365	1.350	4.831	5.062	1.012	54.41	0.162	0.318	0.81
35d		1.276	1.457	1.368	1.354	4.227	3.886	1.011	44.70	0.167	0.314	0.80
35e		1.278	1.459	1.371	1.350	4.360	5.345	1.008	46.74	0.160	0.323	0.81
35f		1.274	1.467	1.363	1.359	3.165	4.151	1.009	51.22	0.189	0.291	0.75
35a	EtOH	1.285	1.449	1.375	1.338	2.760	1.994	1.018	39.99	0.127	0.358	0.87
35b		1.275	1.465	1.364	1.351	4.221	4.818	1.012	44.08	0.177	0.303	0.77
35c		1.276	1.453	1.364	1.352	4.832	5.056	1.012	58.19	0.165	0.315	0.81
35d		1.276	1.457	1.367	1.356	4.223	3.877	1.011	45.49	0.170	0.311	0.80
35e		1.277	1.460	1.370	1.352	4.328	5.316	1.008	45.61	0.165	0.317	0.80
35f		1.274	1.467	1.362	1.360	3.181	4.171	1.009	52.27	0.191	0.289	0.75
36a	Gas-phase	1.280	1.451	1.376	1.335	2.712	1.915	1.022	36.14	0.130	0.355	0.85
36b		1.268	1.471	1.360	1.355	4.174	4.776	1.011	40.96	0.198	0.280	0.72
36c		1.267	1.463	1.358	1.361	4.835	5.048	1.011	46.74	0.199	0.277	0.73
36d		1.268	1.463	1.361	1.361	4.224	3.872	1.007	40.32	0.195	0.282	0.74
36e		1.269	1.466	1.363	1.362	4.288	5.273	1.005	38.78	0.196	0.282	0.73
36f		1.270	1.467	1.364	1.353	3.171	4.147	1.006	49.90	0.186	0.293	0.75
36a	$CHCl_3$	1.282	1.451	1.382	1.329	2.725	1.939	1.021	34.10	0.116	0.371	0.86
36b		1.272	1.468	1.370	1.341	4.168	4.789	1.011	35.58	0.167	0.315	0.77
36c		1.272	1.458	1.366	1.348	4.837	5.086	1.012	46.85	0.168	0.312	0.79
36d		1.272	1.460	1.371	1.346	4.201	3.855	1.010	35.83	0.163	0.318	0.79
36e		1.273	1.463	1.372	1.348	4.313	5.301	1.008	38.16	0.166	0.316	0.78
36f		1.272	1.467	1.369	1.347	3.169	4.142	1.008	45.99	0.173	0.308	0.77
36a	DMSO	1.283	1.451	1.385	1.327	2.727	1.945	1.021	31.42	0.110	0.378	0.86
36b		1.274	1.466	1.375	1.335	4.165	4.795	1.012	34.34	0.152	0.332	0.79
36c		1.275	1.455	1.372	1.340	4.834	5.096	1.012	47.05	0.148	0.334	0.82
36d		1.275	1.459	1.377	1.339	4.190	3.842	1.011	34.93	0.146	0.338	0.81
36e		1.275	1.462	1.376	1.342	4.310	5.300	1.009	37.08	0.153	0.330	0.80
36f		1.273	1.469	1.371	1.346	3.166	4.138	1.009	41.41	0.171	0.311	0.76
36a	EtOH	1.283	1.451	1.386	1.326	2.732	1.951	1.021	30.67	0.108	0.380	0.86
36b		1.274	1.466	1.376	1.335	4.167	4.795	1.012	33.77	0.151	0.333	0.79
36c		1.275	1.455	1.370	1.342	4.837	5.099	1.012	48.70	0.152	0.330	0.82
36d		1.274	1.459	1.376	1.339	4.179	3.825	1.011	34.39	0.148	0.335	0.81
36e		1.275	1.462	1.376	1.342	4.304	5.294	1.009	36.88	0.153	0.330	0.80
36f		1.273	1.471	1.372	1.345	3.178	4.149	1.009	36.85	0.171	0.312	0.76

Table S10. Free energy values (hartrees) calculated at M06-2X/6-31++G(d,p) level for structures **26a-g** and **28a-g** in gas-phase, chloroform, dimethyl sulfoxide and ethanol

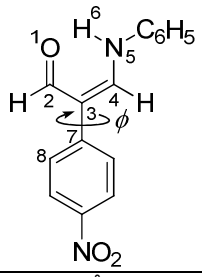
	Medium	a	b	c	d	e	f	g
26	Gas-phase	-823.560695	-823.556530	-823.557175	-823.549121	-823.543214	-823.541826	-823.552029
	$CHCl_3$	-823.584504	-823.583004	-823.583933	-823.576647	-823.569847	-823.569222	-823.573457
	DMSO	-823.582475	-823.583004	-823.583936	-823.576657	-823.570422	-823.568889	-823.570503
	EtOH	-823.584991	-823.584551	-823.587485	-823.580247	-823.573814	-823.572602	-823.572840
28	Gas-phase	-913.570550	-913.564277	-913.565799	-913.558766	-913.552792	-913.551088	-913.561144
	$CHCl_3$	-913.596805	-913.591437	-913.594358	-913.586867	-913.581575	-913.580473	-913.584766
	DMSO	-913.596895	-913.591352	-913.597192	-913.588608	-913.582328	-913.580525	-913.582679
	EtOH	-913.596285	-913.592465	-913.597192	-913.589052	-913.583645	-913.583445	-913.582360

Table S11. Selected geometric parameters and delocalization parameters for isomers **26a-g**



	Medium	Bond distances (Å)							ϕ (°)	Q	$\langle\lambda\rangle$	HOMA index
		O_1-C_2	C_2-C_3	C_3-C_4	C_4-N_5	O_1-N_5	O_1-H_6	N_5-H_6				
26a	Gas-phase	1.224	1.451	1.370	1.347	2.684	1.901	1.019	45.15	0.204	0.300	0.89
26b		1.211	1.469	1.357	1.356	4.147	4.721	1.012	52.80	0.257	0.239	0.78
26c		1.209	1.463	1.358	1.358	4.761	4.953	1.012	48.42	0.254	0.759	0.79
26d		1.209	1.464	1.361	1.365	4.163	3.828	1.008	44.08	0.259	0.763	0.78
26e		1.208	1.475	1.357	1.376	4.173	5.118	1.008	37.03	0.286	0.210	0.71
26f		1.211	1.466	1.365	1.360	2.996	3.909	1.009	40.42	0.250	0.752	0.80
26g		1.318	1.363	1.448	1.288	2.580	1.000	1.689	44.43	-0.115	0.338	0.62
26a	$CHCl_3$	1.230	1.445	1.375	1.343	2.695	1.919	1.018	42.10	0.183	0.324	0.92
26b		1.220	1.459	1.363	1.349	4.152	4.732	1.014	52.21	0.225	0.276	0.85
26c		1.218	1.452	1.364	1.350	4.761	4.972	1.014	51.16	0.220	0.720	0.87
26d		1.218	1.455	1.367	1.356	4.170	3.852	1.011	45.88	0.226	0.725	0.86
26e		1.216	1.462	1.365	1.364	4.195	5.150	1.011	38.72	0.245	0.255	0.81
26f		1.219	1.457	1.371	1.355	3.014	3.925	1.012	38.34	0.222	0.720	0.86
26g		1.322	1.362	1.449	1.289	2.569	1.003	1.673	43.10	-0.120	0.333	0.59
26a	DMSO	1.230	1.445	1.375	1.343	2.708	1.943	1.018	40.89	0.183	0.324	0.92
26b		1.220	1.459	1.365	1.347	4.149	4.740	1.015	48.58	0.221	0.280	0.86
26c		1.220	1.451	1.366	1.348	4.760	4.968	1.015	55.92	0.213	0.712	0.88
26d		1.220	1.453	1.370	1.351	4.174	3.840	1.012	43.00	0.214	0.712	0.87
26e		1.219	1.459	1.368	1.359	4.202	5.164	1.012	38.39	0.231	0.271	0.84
26f		1.220	1.456	1.372	1.353	3.028	3.940	1.013	37.10	0.217	0.714	0.87
26g		1.322	1.363	1.448	1.290	2.559	1.006	1.655	41.70	-0.117	0.336	0.59
26a	EtOH	1.236	1.438	1.378	1.340	2.707	1.945	1.018	41.50	0.164	0.346	0.95
26b		1.228	1.449	1.369	1.343	4.149	4.736	1.015	49.85	0.195	0.310	0.90
26c		1.228	1.441	1.369	1.344	4.757	4.972	1.015	54.50	0.188	0.683	0.92
26d		1.227	1.444	1.373	1.347	4.179	3.852	1.013	47.86	0.191	0.686	0.92
26e		1.227	1.448	1.373	1.352	4.226	5.194	1.013	41.07	0.200	0.305	0.90
26f		1.227	1.448	1.376	1.349	3.023	3.935	1.013	37.28	0.194	0.688	0.91
26g		1.327	1.360	1.450	1.288	2.571	1.004	1.676	42.06	-0.129	0.323	0.54

Table S12. Selected geometric parameters and delocalization parameters for structures **28a-g**

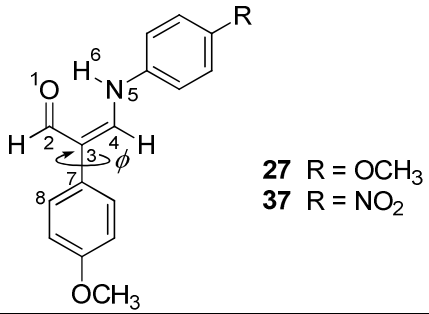


	Medium	Bond distances (Å)							ϕ (°)	Q	$\langle\lambda\rangle$	HOMA index
		O_1-C_2	C_2-C_3	C_3-C_4	C_4-N_5	O_1-N_5	O_1-H_6	N_5-H_6				
28a	Gas-phase	1.223	1.451	1.375	1.340	2.679	1.895	1.019	40.25	0.193	0.312	0.90
28b		1.210	1.471	1.361	1.350	4.128	4.724	1.012	46.63	0.250	0.247	0.79
28c		1.208	1.464	1.360	1.353	4.766	4.982	1.012	45.06	0.249	0.754	0.80
28d		1.208	1.464	1.364	1.357	4.173	3.836	1.008	41.51	0.249	0.753	0.80
28e		1.209	1.474	1.363	1.365	4.196	5.155	1.009	33.47	0.267	0.230	0.75
28f		1.210	1.467	1.370	1.352	2.997	3.912	1.009	35.28	0.239	0.740	0.81
28g		1.311	1.366	1.449	1.286	2.564	1.005	1.667	39.44	-0.108	0.345	0.66
28a	$CHCl_3$	1.228	1.446	1.380	1.336	2.693	1.917	1.019	39.26	0.174	0.334	0.92
28b		1.218	1.461	1.368	1.343	4.127	4.731	1.014	43.04	0.218	0.283	0.85
28c		1.217	1.454	1.367	1.346	4.766	4.995	1.014	47.32	0.216	0.716	0.87
28d		1.217	1.455	1.372	1.347	4.172	3.838	1.012	40.45	0.213	0.712	0.87
28e		1.217	1.462	1.372	1.352	4.212	5.179	1.012	33.00	0.225	0.277	0.84
28f		1.217	1.459	1.376	1.346	3.016	3.929	1.012	32.91	0.212	0.709	0.86
28g		1.314	1.366	1.450	1.287	2.551	1.009	1.645	37.00	-0.111	0.343	0.64
28a	DMSO	1.229	1.446	1.381	1.335	2.705	1.933	1.019	37.10	0.171	0.337	0.93
28b		1.219	1.460	1.370	1.341	4.128	4.734	1.015	41.97	0.212	0.290	0.86
28c		1.226	1.444	1.372	1.339	4.763	4.997	1.015	49.02	0.185	0.680	0.92
28d		1.219	1.453	1.375	1.343	4.172	3.838	1.013	39.80	0.202	0.699	0.89
28e		1.218	1.459	1.376	1.348	4.201	5.172	1.013	32.57	0.213	0.290	0.86
28f		1.219	1.457	1.378	1.345	3.025	3.939	1.014	31.23	0.205	0.701	0.87
28g		1.314	1.368	1.449	1.289	2.538	1.013	1.623	35.07	-0.106	0.348	0.65
28a	EtOH	1.234	1.440	1.384	1.333	2.705	1.935	1.019	36.67	0.155	0.356	0.95
28b		1.226	1.451	1.373	1.337	4.130	4.735	1.016	42.83	0.189	0.317	0.90
28c		1.226	1.444	1.372	1.339	4.763	4.997	1.015	49.02	0.185	0.680	0.92
28d		1.225	1.446	1.378	1.340	4.178	3.848	1.013	41.69	0.183	0.677	0.92
28e		1.225	1.451	1.379	1.344	4.221	5.195	1.013	33.93	0.191	0.315	0.90
28f		1.225	1.450	1.382	1.341	3.023	3.939	1.014	31.44	0.184	0.677	0.91
28g		1.318	1.365	1.451	1.287	2.551	1.010	1.645	35.26	-0.117	0.336	0.61

Table S13. Free energy values (hartrees) calculated at M06-2X/6-31++G(d,p) level for structures **27a-g**, **29a-g**, **37a-g** and **39a-g** in gas-phase, chloroform, dimethyl sulfoxide and ethanol

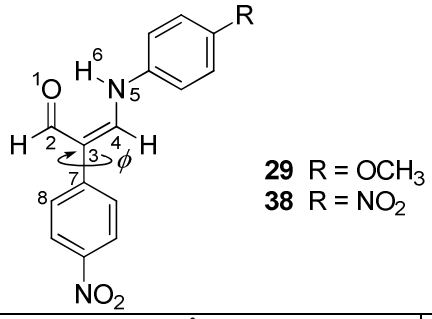
	Medium	a	b	c	d	g
27	Gas-phase	-938.042538	-938.038806	-938.039095	-938.030099	-938.035698
	$CHCl_3$	-938.065965	-938.065110	-938.067545	-938.058262	-938.057619
	DMSO	-938.066146	-938.065129	-938.068435	-938.059850	-938.056502
	EtOH	-938.068493	-938.067615	-938.071623	-938.062661	-938.058423
29	Gas-phase	-1028.052225	-1028.046997	-1028.048385	-1028.042263	-1028.044828
	$CHCl_3$	-1028.078218	-1028.075077	-1028.077705	-1028.070164	-1028.068067
	DMSO	-1028.077811	-1028.076288	-1028.079238	-1028.072639	-1028.067640
	EtOH	-1028.080596	-1028.077747	-1028.080093	-1028.074424	-1028.067707
37	Gas-phase	-1028.053189	-1028.048625	-1028.049618	-1028.040116	-1028.044208
	$CHCl_3$	-1028.079635	-1028.077996	-1028.079942	-1028.069928	-1028.068309
	DMSO	-1028.079204	-1028.078478	-1028.082255	-1028.073296	-1028.067839
	EtOH	-1028.080411	-1028.080125	-1028.083971	-1028.073774	-1028.067911
38	Gas-phase	-1118.060823	-1118.054938	-1118.056710	-1118.047641	-1118.052197
	$CHCl_3$	-1118.088726	-1118.085422	-1118.088629	-1118.081061	-1118.077821
	DMSO	-1118.090309	-1118.088891	-1118.091961	-1118.085154	-1118.078822
	EtOH	-1118.089372	-1118.088179	-1118.091578	-1118.084570	-1118.076966

Table S14. Selected geometric parameters and delocalization parameters for structures **27a-d**, **27g**, **37a-d** and **37g**



	Medium	Bond distances (Å)							ϕ (°)	Q	⟨λ⟩	HOMA index
		O_1-C_2	C_2-C_3	C_3-C_4	C_4-N_5	O_1-N_5	O_1-H_6	N_5-H_6				
27a	Gas-phase	1.226	1.448	1.373	1.344	2.678	1.898	1.019	44.11	0.193	0.312	0.91
27b		1.212	1.467	1.358	1.353	4.143	4.724	1.012	52.39	0.250	0.754	0.80
27c		1.209	1.462	1.358	1.356	4.764	4.970	1.012	47.90	0.251	0.244	0.80
27d		1.210	1.461	1.363	1.361	4.174	3.840	1.008	43.74	0.249	0.753	0.81
27g		1.319	1.362	1.449	1.287	2.584	0.999	1.694	44.20	-0.119	0.333	0.60
27a	$CHCl_3$	1.232	1.441	1.378	1.340	2.694	1.926	1.018	43.26	0.171	0.337	0.94
27b		1.221	1.457	1.365	1.345	4.148	4.738	1.014	50.57	0.216	0.286	0.87
27c		1.219	1.451	1.365	1.347	4.763	4.986	1.014	51.81	0.214	0.714	0.88
27d		1.219	1.452	1.370	1.351	4.189	3.869	1.011	46.28	0.214	0.288	0.88
27g		1.323	1.361	1.451	1.288	2.568	1.004	1.670	42.29	-0.125	0.327	0.57
27a	DMSO	1.232	1.441	1.379	1.339	2.704	1.942	1.018	41.40	0.169	0.340	0.94
27b		1.222	1.455	1.367	1.344	4.159	4.748	1.015	50.50	0.210	0.708	0.88
27c		1.221	1.448	1.368	1.345	4.764	4.990	1.015	53.57	0.204	0.298	0.89
27d		1.221	1.450	1.373	1.347	4.194	3.881	1.012	46.32	0.203	0.700	0.89
27g		1.323	1.362	1.450	1.289	2.559	1.006	1.653	40.17	-0.122	0.331	0.58
27a	EtOH	1.238	1.434	1.381	1.336	2.707	1.948	1.018	42.37	0.151	0.360	0.96
27b		1.230	1.446	1.371	1.340	4.152	4.743	1.015	51.27	0.185	0.321	0.92
27c		1.229	1.439	1.371	1.340	4.758	4.982	1.015	54.60	0.179	0.673	0.93
27d		1.229	1.441	1.376	1.344	4.200	3.894	1.013	49.05	0.180	0.327	0.93
27g		1.329	1.360	1.452	1.288	2.570	1.005	1.672	41.01	-0.133	0.319	0.52
37a	Gas-phase	1.222	1.458	1.365	1.355	2.680	1.894	1.019	47.36	0.226	0.276	0.85
37b		1.209	1.476	1.352	1.364	4.146	4.717	1.012	54.26	0.279	0.785	0.73
37c		1.206	1.469	1.353	1.367	4.761	4.944	1.013	49.08	0.277	0.215	0.74
37d		1.207	1.469	1.357	1.372	4.168	3.821	1.008	44.66	0.277	0.783	0.74
37g		1.317	1.364	1.443	1.291	2.598	0.994	1.720	46.28	-0.105	0.349	0.64
37a	$CHCl_3$	1.226	1.453	1.368	1.353	2.700	1.931	1.018	43.90	0.212	0.292	0.88
37b		1.216	1.468	1.357	1.358	4.148	4.731	1.014	49.69	0.253	0.245	0.79
37c		1.214	1.460	1.358	1.360	4.761	4.964	1.015	52.96	0.248	0.751	0.81
37d		1.215	1.462	1.362	1.365	4.185	3.857	1.011	47.06	0.250	0.249	0.81
37g		1.320	1.364	1.444	1.292	2.581	0.999	1.695	42.16	-0.108	0.346	0.62
37a	DMSO	1.227	1.453	1.369	1.352	2.708	1.941	1.018	42.97	0.209	0.296	0.88
37b		1.217	1.467	1.359	1.357	4.158	4.745	1.015	48.72	0.248	0.749	0.80
37c		1.217	1.457	1.360	1.358	4.761	4.974	1.016	54.17	0.238	0.260	0.84
37d		1.217	1.461	1.364	1.362	4.189	3.864	1.013	47.16	0.242	0.742	0.82
37g		1.320	1.365	1.444	1.293	2.567	1.002	1.672	41.00	-0.106	0.348	0.62
37a	EtOH	1.231	1.448	1.370	1.351	2.712	1.952	1.018	43.21	0.198	0.308	0.90
37b		1.223	1.459	1.361	1.354	4.152	4.739	1.016	49.74	0.229	0.272	0.85
37c		1.223	1.450	1.362	1.355	4.756	4.962	1.016	55.80	0.220	0.719	0.87
37d		1.223	1.454	1.365	1.359	4.194	3.875	1.013	49.08	0.225	0.277	0.86
37g		1.325	1.362	1.445	1.292	2.589	0.998	1.708	41.13	-0.116	0.337	0.58

Table S15. Selected geometric parameters and delocalization parameters for structures **29a-d**, **29g**, **38a-d** and **38g**

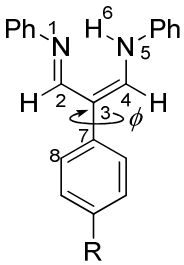


	Medium	Bond distances (Å)							ϕ (°)	*Q*	$\langle\lambda\rangle$	HOMA index
		O_1-C_2	C_2-C_3	C_3-C_4	C_4-N_5	O_1-N_5	O_1-H_6	N_5-H_6				
29a	Gas-phase	1.224	1.449	1.378	1.337	2.671	1.886	1.020	38.38	0.184	0.322	0.91
29b		1.211	1.469	1.363	1.347	4.125	4.727	1.012	45.96	0.242	0.744	0.80
29c		1.208	1.463	1.362	1.351	4.769	4.997	1.012	44.18	0.244	0.251	0.81
29d		1.209	1.462	1.366	1.354	4.173	3.839	1.008	40.79	0.241	0.744	0.81
29g		1.313	1.365	1.451	1.286	2.568	1.005	1.669	39.46	-0.113	0.340	0.64
29a	$CHCl_3$	1.230	1.443	1.384	1.332	2.684	1.912	1.019	35.04	0.161	0.349	0.94
29b		1.219	1.459	1.370	1.340	4.129	4.739	1.014	45.05	0.210	0.292	0.87
29c		1.217	1.453	1.369	1.342	4.769	5.014	1.014	44.90	0.209	0.708	0.88
29d		1.218	1.453	1.375	1.343	4.180	3.847	1.012	41.42	0.203	0.300	0.88
29g		1.315	1.366	1.451	1.287	2.546	1.011	1.637	36.19	-0.113	0.341	0.63
29a	DMSO	1.230	1.443	1.384	1.332	2.698	1.930	1.019	34.87	0.161	0.349	0.94
29b		1.220	1.458	1.373	1.337	4.125	4.740	1.015	40.98	0.202	0.698	0.88
29c		1.220	1.451	1.371	1.339	4.770	5.020	1.015	46.48	0.199	0.304	0.89
29d		1.221	1.451	1.378	1.340	4.184	3.856	1.013	41.22	0.192	0.687	0.90
29g		1.315	1.367	1.450	1.288	2.533	1.016	1.612	35.30	-0.110	0.344	0.63
29a	EtOH	1.236	1.437	1.387	1.329	2.699	1.939	1.019	35.26	0.143	0.369	0.95
29b		1.227	1.449	1.376	1.334	4.123	4.739	1.015	41.84	0.180	0.327	0.91
29c		1.227	1.442	1.374	1.336	4.765	5.010	1.015	49.00	0.177	0.671	0.93
29d		1.227	1.444	1.381	1.337	4.187	3.864	1.013	42.10	0.173	0.334	0.93
29g		1.320	1.365	1.452	1.287	2.548	1.012	1.639	36.10	-0.120	0.333	0.59
38a	Gas-phase	1.221	1.458	1.369	1.348	2.672	1.882	1.020	40.80	0.216	0.287	0.86
38b		1.208	1.477	1.355	1.358	4.129	4.722	1.012	48.49	0.272	0.777	0.74
38c		1.205	1.470	1.355	1.362	4.765	4.968	1.012	46.27	0.272	0.221	0.75
38d		1.206	1.469	1.359	1.365	4.171	3.823	1.008	43.71	0.269	0.775	0.76
38g		1.311	1.366	1.445	1.288	2.587	0.998	1.704	41.93	-0.102	0.352	0.67
38a	$CHCl_3$	1.225	1.454	1.373	1.345	2.686	1.913	1.019	36.42	0.201	0.304	0.89
38b		1.215	1.468	1.360	1.353	4.138	4.733	1.014	47.65	0.246	0.252	0.80
38c		1.214	1.461	1.360	1.355	4.765	4.987	1.014	48.33	0.242	0.745	0.82
38d		1.214	1.462	1.365	1.357	4.184	3.847	1.012	44.60	0.240	0.259	0.82
38g		1.314	1.367	1.445	1.290	2.571	1.002	1.680	39.30	-0.102	0.352	0.66
38a	DMSO	1.226	1.453	1.373	1.345	2.703	1.931	1.019	37.60	0.199	0.306	0.89
38b		1.216	1.467	1.362	1.351	4.147	4.746	1.015	45.93	0.240	0.741	0.82
38c		1.216	1.458	1.362	1.352	4.766	4.994	1.015	49.66	0.232	0.267	0.84
38d		1.217	1.460	1.367	1.354	4.187	3.856	1.013	44.66	0.230	0.730	0.84
38g		1.313	1.368	1.445	1.291	2.554	1.007	1.651	37.38	-0.099	0.356	0.67
38a	EtOH	1.230	1.448	1.375	1.343	2.698	1.932	1.019	36.67	0.186	0.321	0.91
38b		1.222	1.459	1.364	1.349	4.143	4.741	1.016	47.35	0.222	0.280	0.86
38c		1.222	1.451	1.364	1.350	4.761	4.983	1.016	51.47	0.215	0.714	0.88
38d		1.222	1.454	1.369	1.352	4.193	3.868	1.014	45.60	0.215	0.288	0.87
38g		1.318	1.366	1.446	1.290	2.580	1.001	1.695	37.65	-0.108	0.346	0.63

Table S16. Free energy values (hartrees) calculated at M06-2X/6-31++G(d,p) level for structures **30a-f** and **39a-f** in gas phase, chloroform, dimethyl sulfoxide and ethanol

		a	**b**	**c**	**d**	**e**	**f**
30	Gas-phase	-1124.616128	-1124.607767	-1124.610130	-1124.605532	-1124.599885	-1124.595077
	$CHCl_3$	-1124.647701	-1124.642549	-1124.644299	-1124.640001	-1124.634437	-1124.629424
	DMSO	-1124.641999	-1124.638609	-1124.640932	-1124.637450	-1124.631134	-1124.627743
	EtOH	-1124.643764	-1124.640851	-1124.642649	-1124.639449	-1124.633340	-1124.628866
39	Gas-phase	-1034.606967	-1034.599318	-1034.600724	-1034.594759	-1034.589540	-1034.585299
	$CHCl_3$	-1034.635849	-1034.631779	-1034.633756	-1034.630011	-1034.623677	-1034.617279
	DMSO	-1034.630220	-1034.626335	-1034.630002	-1034.627279	-1034.618663	-1034.613745
	EtOH	-1034.633988	-1034.632347	-1034.634069	-1034.630470	-1034.622452	-1034.617594

Table S17. Selected geometric parameters and delocalization parameters for structures **30a-f** and **39a-f**



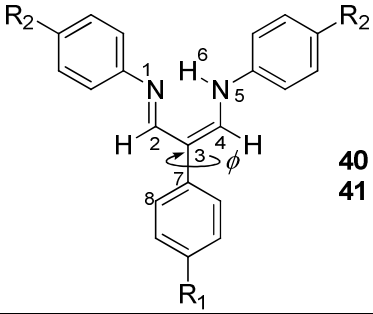
30 R = NO_2
39 R = OCH_3

	Medium	Bond distances (Å)							ϕ (°)	Q	$\langle\lambda\rangle$	HOMA index
		N_1-C_2	C_2-C_3	C_3-C_4	C_4-N_5	N_1-N_5	N_1-H_6	N_5-H_6				
30a	Gas-phase	1.286	1.447	1.373	1.343	2.711	1.904	1.024	39.37	0.131	0.354	0.87
30b		1.276	1.463	1.360	1.357	4.164	4.744	1.011	43.18	0.184	0.295	0.77
30c		1.274	1.456	1.358	1.360	4.814	5.016	1.011	47.86	0.184	0.294	0.77
30d		1.275	1.458	1.361	1.365	4.160	3.821	1.008	38.42	0.187	0.292	0.77
30e		1.274	1.464	1.359	1.374	4.185	5.152	1.008	36.20	0.205	0.274	0.72
30f		1.275	1.460	1.364	1.362	3.022	3.960	1.008	47.87	0.183	0.297	0.77
30a	$CHCl_3$	1.288	1.446	1.377	1.340	2.718	1.920	1.023	37.11	0.121	0.365	0.88
30b		1.280	1.460	1.365	1.351	4.159	4.736	1.013	38.50	0.166	0.316	0.80
30c		1.279	1.451	1.364	1.354	4.810	5.013	1.013	50.95	0.162	0.319	0.82
30d		1.279	1.455	1.367	1.356	4.170	3.819	1.011	38.01	0.165	0.317	0.81
30e		1.280	1.458	1.368	1.359	4.185	5.167	1.012	35.10	0.169	0.313	0.80
30f		1.278	1.457	1.368	1.358	3.047	3.979	1.011	46.16	0.169	0.313	0.80
30a	DMSO	1.289	1.446	1.378	1.340	2.722	1.929	1.023	35.68	0.119	0.368	0.88
30b		1.282	1.457	1.367	1.348	4.166	4.755	1.014	41.22	0.156	0.327	0.82
30c		1.283	1.447	1.366	1.350	4.810	5.024	1.014	51.74	0.148	0.334	0.85
30d		1.281	1.452	1.370	1.352	4.171	3.819	1.013	36.98	0.153	0.330	0.83
30e		1.280	1.457	1.368	1.359	4.185	5.165	1.013	33.52	0.168	0.314	0.80
30f		1.281	1.455	1.370	1.356	3.052	3.981	1.013	45.05	0.160	0.323	0.82
30a	EtOH	1.289	1.446	1.378	1.340	2.725	1.933	1.023	35.32	0.119	0.368	0.88
30b		1.282	1.457	1.368	1.348	4.165	4.749	1.014	39.58	0.155	0.328	0.82
30c		1.282	1.448	1.366	1.351	4.805	4.812	1.014	51.48	0.151	0.331	0.84
30d		1.281	1.453	1.370	1.352	4.169	3.815	1.013	36.97	0.154	0.329	0.83
30e		1.280	1.458	1.368	1.359	4.185	5.167	1.012	34.28	0.169	0.313	0.80
30f		1.281	1.456	1.370	1.356	3.060	3.990	1.013	44.99	0.161	0.322	0.82
39a	Gas-phase	1.288	1.446	1.368	1.350	2.723	1.928	1.022	45.15	0.140	0.344	0.86
39b		1.277	1.461	1.356	1.362	4.178	4.744	1.012	50.71	0.190	0.289	0.76
39c		1.276	1.454	1.357	1.364	4.806	4.983	1.012	49.79	0.185	0.293	0.78
39d		1.276	1.457	1.358	1.373	4.167	3.846	1.008	42.51	0.196	0.283	0.75
39e		1.275	1.464	1.355	1.384	4.170	5.125	1.008	39.13	0.218	0.261	0.69
39f		1.276	1.459	1.360	1.370	3.009	3.937	1.008	54.11	0.193	0.287	0.75
39a	$CHCl_3$	1.290	1.445	1.371	1.349	2.733	1.947	1.021	43.17	0.133	0.352	0.88
39b		1.282	1.458	1.361	1.357	4.183	4.763	1.013	46.49	0.172	0.309	0.80
39c		1.280	1.449	1.361	1.358	4.805	4.990	1.013	55.51	0.166	0.314	0.82
39d		1.280	1.454	1.362	1.366	4.176	3.851	1.011	44.23	0.178	0.303	0.79
39e		1.278	1.460	1.359	1.377	4.174	5.137	1.011	38.93	0.200	0.280	0.74
39f		1.279	1.457	1.363	1.368	3.034	3.962	1.011	50.20	0.183	0.298	0.78
39a	DMSO	1.291	1.444	1.372	1.348	2.732	1.949	1.021	41.21	0.129	0.357	0.88
39b		1.284	1.456	1.363	1.355	4.185	4.762	1.014	45.66	0.164	0.318	0.82
39c		1.284	1.446	1.364	1.355	4.803	4.993	1.014	56.26	0.153	0.329	0.84
39d		1.283	1.452	1.364	1.361	4.182	3.836	1.012	45.57	0.166	0.316	0.82
39e		1.280	1.457	1.361	1.371	4.175	5.142	1.012	40.58	0.187	0.294	0.77
39f		1.281	1.455	1.365	1.366	3.043	3.968	1.012	48.83	0.175	0.307	0.79
39a	EtOH	1.291	1.444	1.371	1.348	2.743	1.963	1.021	42.50	0.130	0.355	0.88
39b		1.284	1.456	1.362	1.355	4.186	4.762	1.014	45.85	0.165	0.317	0.81
39c		1.284	1.446	1.363	1.355	4.806	5.004	1.014	58.20	0.154	0.328	0.84
39d		1.282	1.452	1.364	1.361	4.181	3.839	1.012	46.33	0.167	0.315	0.81
39e		1.280	1.457	1.361	1.371	4.177	5.146	1.012	41.08	0.187	0.294	0.77
39f		1.281	1.455	1.364	1.366	3.053	3.979	1.012	49.56	0.176	0.306	0.79

Table S18. Free energy values (hartrees) calculated at M06-2X/6-31++G(d,p) level for structures **40-43a-d** in gas-phase, chloroform, dimethyl sulfoxide and ethanol

		a	**b**	**c**	**d**
40	Gas-phase	-1263.570283	-1263.562752	-1263.563985	-1263.558365
	$CHCl_3$	-1263.602452	-1263.596752	-1263.598948	-1263.595076
	DMSO	-1263.597062	-1263.594392	-1263.596986	-1263.591575
	EtOH	-1263.601462	-1263.598108	-1263.600622	-1263.597308
41	Gas-phase	-1443.592468	-1443.585989	-1443.587141	-1443.579641
	$CHCl_3$	-1443.627190	-1443.625027	-1443.624933	-1443.618972
	DMSO	-1443.626052	-1443.622743	-1443.624643	-1443.620374
	EtOH	-1443.627210	-1443.622765	-1443.626110	-1443.620444
42	Gas-phase	-1353.580406	-1353.571589	-1353.572497	-1353.568698
	$CHCl_3$	-1353.614649	-1353.607658	-1353.609515	-1353.608668
	DMSO	-1353.610096	-1353.604029	-1353.607995	-1353.604943
	EtOH	-1353.612591	-1353.607212	-1353.609628	-1353.606352
43	Gas-phase	-1533.598436	-1533.590847	-1533.592383	-1533.586062
	$CHCl_3$	-1533.637265	-1533.632519	-1533.635105	-1533.629895
	DMSO	-1533.638663	-1533.632858	-1533.635847	-1533.630957
	EtOH	-1533.637223	-1533.630421	-1533.635619	-1533.629661

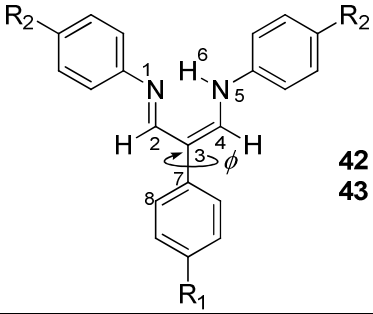
Table S19. Selected geometric parameters and delocalization parameters for structures **40a-d** and **41a-d**



40 $R_1 = R_2 = OCH_3$
41 $R_1 = OCH_3$; $R_2 = NO_2$

	Medium	Bond distances (Å)							ϕ (º)	Q	$\langle\lambda\rangle$	HOMA index
		N_1-C_2	C_2-C_3	C_3-C_4	C_4-N_5	N_1-N_5	N_1-H_6	N_5-H_6				
40a	Gas-phase	1.289	1.445	1.369	1.348	2.718	1.922	1.022	44.67	0.135	0.349	0.87
40b		1.278	1.460	1.357	1.361	4.176	4.744	1.011	47.79	0.186	0.293	0.77
40c		1.276	1.454	1.358	1.363	4.811	5.001	1.011	48.87	0.183	0.295	0.78
40d		1.276	1.457	1.359	1.371	4.160	3.835	1.008	41.54	0.193	0.286	0.76
40a	$CHCl_3$	1.291	1.444	1.373	1.346	2.725	1.938	1.022	43.08	0.126	0.360	0.88
40b		1.282	1.457	1.362	1.355	4.176	4.749	1.013	46.86	0.168	0.313	0.81
40c		1.281	1.449	1.363	1.356	4.811	5.012	1.013	54.26	0.161	0.320	0.83
40d		1.280	1.454	1.364	1.363	4.175	3.842	1.010	42.55	0.173	0.308	0.80
40a	DMSO	1.291	1.444	1.374	1.346	2.722	1.931	1.022	40.90	0.125	0.361	0.89
40b		1.284	1.456	1.364	1.352	4.177	4.757	1.014	43.33	0.160	0.322	0.82
40c		1.284	1.446	1.365	1.352	4.810	5.020	1.014	55.18	0.149	0.333	0.85
40d		1.283	1.451	1.367	1.358	4.183	3.848	1.012	43.17	0.159	0.324	0.83
40a	EtOH	1.291	1.443	1.373	1.346	2.741	1.960	1.021	42.08	0.125	0.361	0.89
40b		1.284	1.455	1.364	1.353	4.182	4.759	1.014	44.76	0.160	0.322	0.82
40c		1.284	1.445	1.365	1.353	4.809	5.016	1.014	56.54	0.149	0.333	0.85
40d		1.283	1.451	1.366	1.359	4.180	3.842	1.012	44.55	0.161	0.321	0.82
41a	Gas-phase	1.289	1.446	1.365	1.356	2.724	1.928	1.021	46.36	0.148	0.335	0.86
41b		1.278	1.460	1.354	1.366	4.174	4.735	1.012	50.54	0.194	0.284	0.76
41c		1.276	1.453	1.356	1.368	4.796	4.950	1.013	53.25	0.189	0.289	0.77
41d		1.277	1.458	1.356	1.378	4.146	3.821	1.008	42.33	0.203	0.276	0.73
41a	$CHCl_3$	1.291	1.445	1.368	1.355	2.728	1.941	1.022	44.02	0.141	0.344	0.87
41b		1.283	1.456	1.358	1.362	4.182	4.745	1.015	49.75	0.177	0.303	0.80
41c		1.282	1.448	1.359	1.363	4.794	4.963	1.015	55.70	0.170	0.310	0.81
41d		1.281	1.453	1.360	1.372	4.163	3.836	1.012	42.74	0.184	0.297	0.78
41a	DMSO	1.291	1.444	1.369	1.354	2.724	1.937	1.023	42.21	0.138	0.347	0.87
41b		1.284	1.455	1.360	1.360	4.176	4.748	1.016	46.80	0.171	0.310	0.81
41c		1.285	1.445	1.361	1.360	4.795	4.977	1.016	55.77	0.159	0.322	0.84
41d		1.284	1.451	1.363	1.367	4.161	3.814	1.013	43.59	0.171	0.311	0.81
41a	EtOH	1.291	1.446	1.368	1.355	2.738	1.953	1.021	41.72	0.142	0.343	0.86
41b		1.285	1.455	1.359	1.361	4.184	4.751	1.016	48.12	0.172	0.309	0.81
41c		1.285	1.445	1.360	1.361	4.795	4.975	1.016	57.69	0.161	0.320	0.83
41d		1.283	1.451	1.362	1.369	4.155	3.808	1.013	43.91	0.175	0.307	0.80

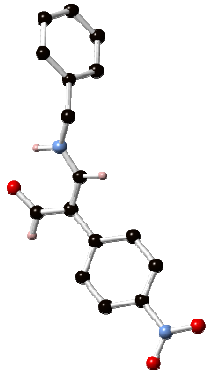
Table S20. Selected geometric parameters and delocalization parameters for structures **42a-d** and **43a-d**



42 $R_1 = NO_2$; $R_2 = OCH_3$
43 $R_1 = R_2 = NO_2$

	Medium	Bond distances (Å)							ϕ (º)	Q	$\langle\lambda\rangle$	HOMA index
		N_1-C_2	C_2-C_3	C_3-C_4	C_4-N_5	N_1-N_5	N_1-H_6	N_5-H_6				
42a	Gas-phase	1.287	1.446	1.375	1.340	2.701	1.900	1.024	37.37	0.124	0.362	0.88
42b		1.276	1.463	1.361	1.355	4.156	4.739	1.011	41.12	0.181	0.299	0.77
42c		1.275	1.456	1.360	1.359	4.816	5.024	1.011	47.54	0.180	0.299	0.78
42d		1.275	1.458	1.362	1.363	4.176	3.848	1.008	38.96	0.184	0.295	0.77
42a	$CHCl_3$	1.289	1.445	1.378	1.338	2.721	1.938	1.023	35.00	0.116	0.371	0.89
42b		1.280	1.460	1.367	1.348	4.155	4.747	1.013	38.88	0.161	0.321	0.81
42c		1.279	1.451	1.365	1.352	4.816	5.037	1.013	49.00	0.159	0.322	0.82
42d		1.279	1.455	1.368	1.354	4.181	3.851	1.011	38.44	0.162	0.320	0.81
42a	DMSO	1.290	1.445	1.381	1.336	2.713	1.924	1.023	33.41	0.110	0.378	0.89
42b		1.282	1.458	1.370	1.345	4.157	4.752	1.014	37.46	0.151	0.333	0.83
42c		1.283	1.447	1.368	1.348	4.815	5.042	1.014	50.35	0.144	0.339	0.85
42d		1.282	1.452	1.372	1.349	4.191	3.848	1.013	39.17	0.147	0.337	0.84
42a	EtOH	1.289	1.446	1.381	1.336	2.719	1.932	1.023	33.65	0.112	0.376	0.89
42b		1.282	1.458	1.370	1.345	4.154	4.750	1.014	36.77	0.151	0.333	0.83
42c		1.283	1.448	1.368	1.348	4.816	5.042	1.014	49.96	0.145	0.338	0.85
42d		1.281	1.453	1.371	1.350	4.181	3.833	1.013	39.94	0.151	0.332	0.83
43a	Gas-phase	1.287	1.447	1.369	1.348	2.715	1.910	1.023	41.68	0.139	0.345	0.86
43b		1.277	1.462	1.357	1.361	4.161	4.740	1.012	46.81	0.189	0.290	0.76
43c		1.275	1.455	1.356	1.364	4.805	4.988	1.012	50.39	0.188	0.290	0.77
43d		1.276	1.458	1.358	1.371	4.169	3.845	1.009	41.05	0.195	0.284	0.75
43a	$CHCl_3$	1.289	1.446	1.371	1.348	2.729	1.940	1.022	39.08	0.134	0.351	0.87
43b		1.281	1.458	1.361	1.356	4.163	4.750	1.014	45.44	0.172	0.309	0.80
43c		1.280	1.449	1.361	1.359	4.804	5.002	1.014	51.71	0.167	0.313	0.82
43d		1.280	1.454	1.363	1.364	4.180	3.859	1.012	39.59	0.175	0.306	0.80
43a	DMSO	1.290	1.445	1.374	1.346	2.708	1.912	1.024	36.38	0.127	0.359	0.88
43b		1.282	1.457	1.362	1.354	4.163	4.765	1.015	43.58	0.167	0.314	0.81
43c		1.284	1.446	1.362	1.356	4.803	5.003	1.015	56.35	0.156	0.325	0.84
43d		1.282	1.451	1.365	1.359	4.191	3.846	1.013	41.06	0.163	0.319	0.82
43a	EtOH	1.290	1.445	1.374	1.347	2.710	1.915	1.024	41.05	0.128	0.358	0.88
43b		1.282	1.457	1.361	1.355	4.178	4.780	1.015	44.96	0.169	0.312	0.81
43c		1.283	1.446	1.362	1.357	4.803	5.010	1.015	52.49	0.158	0.323	0.84
43d		1.282	1.452	1.364	1.360	4.188	3.841	1.013	41.79	0.166	0.316	0.82

Table S21. Crystal data and structure refinement details for **14**.



Empirical formula	$C_{16}H_{14}N_2O_3$	
Formula weight	282.29	
Temperature	100(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 4.1847(19) Å	
	b = 13.013(6) Å	β = 93.169(8)°
	c = 24.919(11) Å	
Volume	1354.9(10) Å^3	
Z	4	
Density (calculated)	1.384 Mg / m^3	
Absorption coefficient	0.097 mm^{-1}	
F(000)	592	
Crystal	Fragment; Yellow	
Crystal size	$0.23 \times 0.21 \times 0.07$ mm^3	
θ range for data collection	2.91 – 25.02°	
Index ranges	$-4 \le h \le 4$, $-14 \le k \le 15$, $-29 \le l \le 29$	
Reflections collected	6477	
Independent reflections	2360 [R_{int} = 0.0338]	
Completeness to θ = 25.02°	99.2 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	0.9932 and 0.9780	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2360 / 0 / 194	
Goodness-of-fit on F^2	1.119	
Final R indices [$F^2 > 2\sigma(F^2)$]	$R1$ = 0.0440, $wR2$ = 0.1033	
R indices (all data)	$R1$ = 0.0553, $wR2$ = 0.1089	
Largest diff. peak and hole	0.162 and –0.239 e Å^{-3}	

Diffractometer: *Rigaku AFC12* goniometer equipped with an enhanced sensitivity (HG) *Saturn724+* detector mounted at the window of an *FR-E+ SuperBright* molybdenum rotating anode generator with HF *Varimax* optics (100µm focus). **Cell determination, Data collection, Data reduction and cell refinement & Absorption correction**: CrystalClear-SM Expert 2.0 r7 (Rigaku, 2011) , **Structure solution**: SHELXS97 (G. M. Sheldrick, Acta Cryst. (1990) A**46** 467–473). S**tructure refinement**: SHELXL97 (G. M. Sheldrick (1997), University of Göttingen, Germany). **Graphics:** CrystalMaker: a crystal and molecular structures program for Mac and Windows. CrystalMaker Software Ltd, Oxford, England (www.crystalmaker.com)

Special details: All hydrogen atoms were placed in idealised positions and refined using a riding model, except the NH which was freely refined.

Table S22. Atomic coordinates [$\times 10^4$], equivalent isotropic displacement parameters [$Å^2 \times 10^3$] and site occupancy factors for **14**.

Atom	***x***	***y***	***z***	U_{eq} [a]	***S.o.f.***
O1	826(3)	9045(1)	320(1)	21(1)	1
O2	−6036(4)	4660(1)	2383(1)	36(1)	1
O3	−7782(4)	5843(1)	2901(1)	38(1)	1
N1	−3207(4)	10387(1)	752(1)	18(1)	1
N2	−6436(4)	5570(1)	2497(1)	25(1)	1
C1	−3623(5)	12953(1)	322(1)	22(1)	1
C2	−2081(5)	13898(1)	353(1)	26(1)	1
C3	−375(5)	14180(2)	821(1)	27(1)	1
C4	−263(5)	13530(2)	1260(1)	27(1)	1
C5	−1823(5)	12594(1)	1229(1)	23(1)	1
C6	−3515(4)	12293(1)	758(1)	18(1)	1
C7	−5295(5)	11286(1)	728(1)	20(1)	1
C8	−3649(4)	9614(1)	1078(1)	18(1)	1
C9	−2164(4)	8651(1)	1072(1)	17(1)	1
C10	18(4)	8435(1)	671(1)	18(1)	1
C11	−3133(4)	7856(1)	1450(1)	18(1)	1
C12	−4427(5)	8115(1)	1941(1)	21(1)	1
C13	−5549(5)	7379(1)	2277(1)	22(1)	1
C14	−5265(5)	6352(1)	2143(1)	20(1)	1
C15	−3937(5)	6056(1)	1673(1)	22(1)	1
C16	−2919(5)	6802(1)	1328(1)	21(1)	1

[a] U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table S23. Bond lengths [Å] and angles [°]for **14**.

Bond lengths [Å]

O1–C10	1.241(2)	C5–C6	1.393(3)
O2–N2	1.231(2)	C6–C7	1.508(3)
O3–N2	1.234(2)	C8–C9	1.399(3)
N1–C8	1.311(2)	C9–C10	1.419(3)
N1–C7	1.460(2)	C9–C11	1.471(3)
N2–C14	1.450(2)	C11–C12	1.405(3)
C1–C6	1.384(3)	C11–C16	1.409(3)
C1–C2	1.388(3)	C12–C13	1.372(3)
C2–C3	1.384(3)	C13–C14	1.385(3)
C3–C4	1.380(3)	C14–C15	1.379(3)
C4–C5	1.382(3)	C15–C16	1.380(3)

Angles [°]

C8–N1–C7	122.38(17)	C8–C9–C10	119.20(17)
O2–N2–O3	122.65(17)	C8–C9–C11	119.04(18)
O2–N2–C14	118.68(17)	C10–C9–C11	121.50(17)
O3–N2–C14	118.68(16)	O1–C10–C9	125.44(18)
C6–C1–C2	120.71(18)	C12–C11–C16	116.94(17)
C3–C2–C1	119.94(19)	C12–C11–C9	121.45(17)
C4–C3–C2	119.82(19)	C16–C11–C9	121.56(17)
C3–C4–C5	120.11(19)	C13–C12–C11	121.73(18)
C4–C5–C6	120.72(18)	C12–C13–C14	119.29(18)
C1–C6–C5	118.71(17)	C15–C14–C13	121.24(18)
C1–C6–C7	120.41(17)	C15–C14–N2	119.14(17)
C5–C6–C7	120.84(17)	C13–C14–N2	119.61(18)
N1–C7–C6	113.69(16)	C14–C15–C16	119.02(17)
N1–C8–C9	127.08(19)	C15–C16–C11	121.71(18)

Table S24. Anisotropic displacement parameters [$Å^2 \times 10^3$] for **14**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O1	24(1)	20(1)	19(1)	3(1)	3(1)	−2(1)
O2	54(1)	17(1)	36(1)	3(1)	12(1)	−4(1)
O3	61(1)	30(1)	24(1)	2(1)	18(1)	−8(1)
N1	21(1)	14(1)	18(1)	2(1)	4(1)	0(1)
N2	32(1)	22(1)	21(1)	2(1)	3(1)	−4(1)
C1	21(1)	23(1)	22(1)	1(1)	4(1)	2(1)
C2	30(1)	20(1)	30(1)	7(1)	11(1)	2(1)
C3	28(1)	15(1)	38(1)	−4(1)	10(1)	−2(1)
C4	27(1)	22(1)	30(1)	−8(1)	−1(1)	1(1)
C5	27(1)	19(1)	23(1)	2(1)	1(1)	5(1)
C6	16(1)	15(1)	23(1)	0(1)	6(1)	3(1)
C7	20(1)	17(1)	23(1)	2(1)	4(1)	2(1)
C8	19(1)	20(1)	17(1)	0(1)	2(1)	−4(1)
C9	20(1)	15(1)	17(1)	0(1)	−1(1)	−1(1)
C10	18(1)	18(1)	19(1)	0(1)	−1(1)	−1(1)
C11	16(1)	18(1)	19(1)	1(1)	0(1)	0(1)
C12	28(1)	16(1)	20(1)	0(1)	2(1)	0(1)
C13	29(1)	22(1)	14(1)	−1(1)	2(1)	−1(1)
C14	24(1)	19(1)	18(1)	5(1)	2(1)	−1(1)
C15	26(1)	15(1)	25(1)	0(1)	4(1)	2(1)
C16	25(1)	19(1)	18(1)	0(1)	6(1)	2(1)

Table S25. Hydrogen coordinates [$\times 10^4$] and isotropic displacement parameters [$Å^2 \times 10^3$] for **14**.

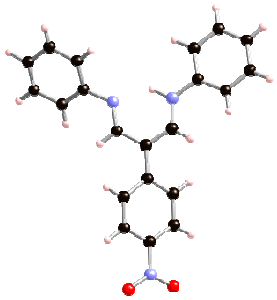
Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
H901	−1760(50)	10263(16)	478(9)	38(7)	1
H1	−4765	12758	−2	26	1
H2	−2196	14349	53	31	1
H3	716	14821	841	32	1
H4	889	13726	1583	32	1
H5	−1740	12151	1532	27	1
H7A	−6741	11252	1029	24	1
H7B	−6639	11264	389	24	1
H8	−5139	9720	1346	22	1
H10	936	7767	670	22	1
H12	−4528	8817	2042	25	1
H13	−6509	7573	2599	26	1
H15	−3726	5348	1587	26	1
H16	−2051	6601	1000	25	1

Table S26. Hydrogen bonds [Å and °] for **14**.

D–H···*A*	*d*(*D*–H)	*d*(H···*A*)	*d*(*D*···*A*)	∠(*DHA*)
N1–H901···O1	0.95(2)	1.97(2)	2.694(2)	131.1(18)
N1–H901···O1^{i}	0.95(2)	2.24(2)	2.996(2)	136.1(18)

Symmetry transformations used to generate equivalent atoms: (i) −x,−y+2,−z

Table S27. Crystal data and structure refinement details for **30**.



Empirical formula	$C_{21}H_{17}N_3O_2$
Formula weight	343.38
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	*P*21/*c*
Unit cell dimensions	a = 8.649(7) Å b = 21.553(15) Å β = 109.782(9)° c = 9.886(8) Å
Volume	1734(2) Å^3
Z	4
Density (calculated)	1.315 Mg / m^3
Absorption coefficient	0.087 mm^{-1}
F(000)	720
Crystal	Slab; Orange
Crystal size	0.11 × 0.08 × 0.05 mm^3
θ range for data collection	3.14 – 25.02°
Index ranges	$-10 \le h \le 7$, $-25 \le k \le 23$, $-8 \le l \le 11$
Reflections collected	6840
Independent reflections	3031 [R_{int} = 0.0581]
Completeness to θ = 25.02°	99.1 %
Absorption correction	Semi–empirical from equivalents
Max. and min. transmission	0.9957 and 0.9905
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3031 / 0 / 239
Goodness-of-fit on F^2	1.208
Final *R* indices [$F^2 > 2\sigma(F^2)$]	*R1* = 0.0889, *wR2* = 0.1428
R indices (all data)	*R1* = 0.1207, *wR2* = 0.1557
Largest diff. peak and hole	0.185 and –0.205 e Å^{-3}

Diffractometer: *Rigaku AFC11 and Saturn944+ mounted at the window of RA-Micro7 HFM with Varimax optics.* **Cell determination, Data collection, Data reduction and cell refinement & Absorption correction**: CrystalClear-SM Expert 2.0 r7 (Rigaku, 2011) , **Structure solution**: *SHELXS97* (G. M. Sheldrick, Acta Cryst. (1990) A**46** 467–473). S**tructure refinement**: *SHELXL97* (G. M. Sheldrick (1997), University of Göttingen, Germany). **Graphics:** CrystalMaker: a crystal and molecular structures program for Mac and Windows. CrystalMaker Software Ltd, Oxford, England (www.crystalmaker.com)

Special details: All hydrogen atoms were placed in idealised positions and refined using a riding model, except the NH hydrogen which was freely refined.

Table S28. Atomic coordinates [$\times 10^4$], equivalent isotropic displacement parameters [$Å^2 \times 10^3$] and site occupancy factors for **30**.

Atom	*x*	*y*	*z*	U_{eq} [a]	*S.o.f.*
O1	–3695(3)	10275(1)	7303(3)	47(1)	1
O2	–3275(3)	10674(1)	5443(3)	52(1)	1
N1	–3190(3)	10238(1)	6282(3)	36(1)	1
N2	–587(3)	6824(1)	5445(3)	27(1)	1
N3	1379(3)	7397(1)	4287(3)	28(1)	1
C1	–2460(4)	9655(2)	6039(4)	29(1)	1
C2	–2323(4)	9162(2)	6984(3)	28(1)	1
C3	–1633(4)	8614(2)	6734(3)	29(1)	1
C4	–1099(4)	8538(2)	5541(3)	26(1)	1
C5	–1243(4)	9056(2)	4639(3)	31(1)	1
C6	–1908(4)	9610(2)	4877(4)	35(1)	1
C7	–455(4)	7937(2)	5243(3)	25(1)	1
C8	–1064(4)	7379(2)	5652(3)	26(1)	1
C9	–1396(4)	6290(2)	5748(3)	27(1)	1
C10	–3035(4)	6296(2)	5700(3)	27(1)	1
C11	–3758(4)	5753(2)	5964(3)	30(1)	1
C12	–2878(4)	5199(2)	6243(3)	33(1)	1
C13	–1267(4)	5191(2)	6273(3)	31(1)	1
C14	–526(4)	5729(2)	6031(3)	30(1)	1
C15	728(4)	7921(2)	4586(3)	28(1)	1
C16	2614(4)	7343(2)	3651(3)	29(1)	1
C17	2883(4)	6755(2)	3181(3)	32(1)	1
C18	4037(4)	6682(2)	2497(4)	39(1)	1
C19	4920(4)	7181(2)	2289(4)	41(1)	1
C20	4680(4)	7762(2)	2790(4)	40(1)	1
C21	3524(4)	7849(2)	3461(4)	35(1)	1

[a] U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table S29. Bond lengths [Å] and angles [°] for **30**.

Bond lengths [Å]

O1–N1	1.231(3)	C7–C15	1.385(4)
O2–N1	1.240(3)	C7–C8	1.426(4)
N1–C1	1.462(4)	C9–C14	1.401(4)
N2–C8	1.302(4)	C9–C10	1.402(4)
N2–C9	1.431(4)	C10–C11	1.393(4)
N3–C15	1.339(4)	C11–C12	1.392(4)
N3–C16	1.416(4)	C12–C13	1.383(5)
C1–C6	1.388(4)	C13–C14	1.385(4)
C1–C2	1.393(4)	C16–C21	1.394(4)
C2–C3	1.384(4)	C16–C17	1.395(4)
C3–C4	1.414(4)	C17–C18	1.392(4)
C4–C5	1.408(4)	C18–C19	1.376(5)
C4–C7	1.478(4)	C19–C20	1.387(5)
C5–C6	1.379(4)	C20–C21	1.387(4)

Angles [°]

O1–N1–O2	122.8(3)	N2–C8–C7	124.3(3)
O1–N1–C1	119.0(3)	C14–C9–C10	118.9(3)
O2–N1–C1	118.2(3)	C14–C9–N2	117.9(3)
C8–N2–C9	120.1(3)	C10–C9–N2	123.1(3)
C15–N3–C16	127.3(3)	C11–C10–C9	120.0(3)
C6–C1–C2	121.8(3)	C10–C11–C12	120.5(3)
C6–C1–N1	118.9(3)	C13–C12–C11	119.6(3)
C2–C1–N1	119.2(3)	C12–C13–C14	120.5(3)
C3–C2–C1	118.4(3)	C13–C14–C9	120.6(3)
C2–C3–C4	122.0(3)	N3–C15–C7	123.9(3)
C5–C4–C3	116.9(3)	C21–C16–C17	120.0(3)
C5–C4–C7	121.9(3)	C21–C16–N3	122.7(3)
C3–C4–C7	121.2(3)	C17–C16–N3	117.3(3)
C6–C5–C4	122.1(3)	C18–C17–C16	119.5(3)
C5–C6–C1	118.7(3)	C19–C18–C17	120.6(4)
C15–C7–C8	120.9(3)	C18–C19–C20	119.7(3)
C15–C7–C4	120.1(3)	C19–C20–C21	120.8(3)
C8–C7–C4	118.9(3)	C20–C21–C16	119.4(3)

Table S30. Anisotropic displacement parameters [$Å^2 \times 10^3$] for **30**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

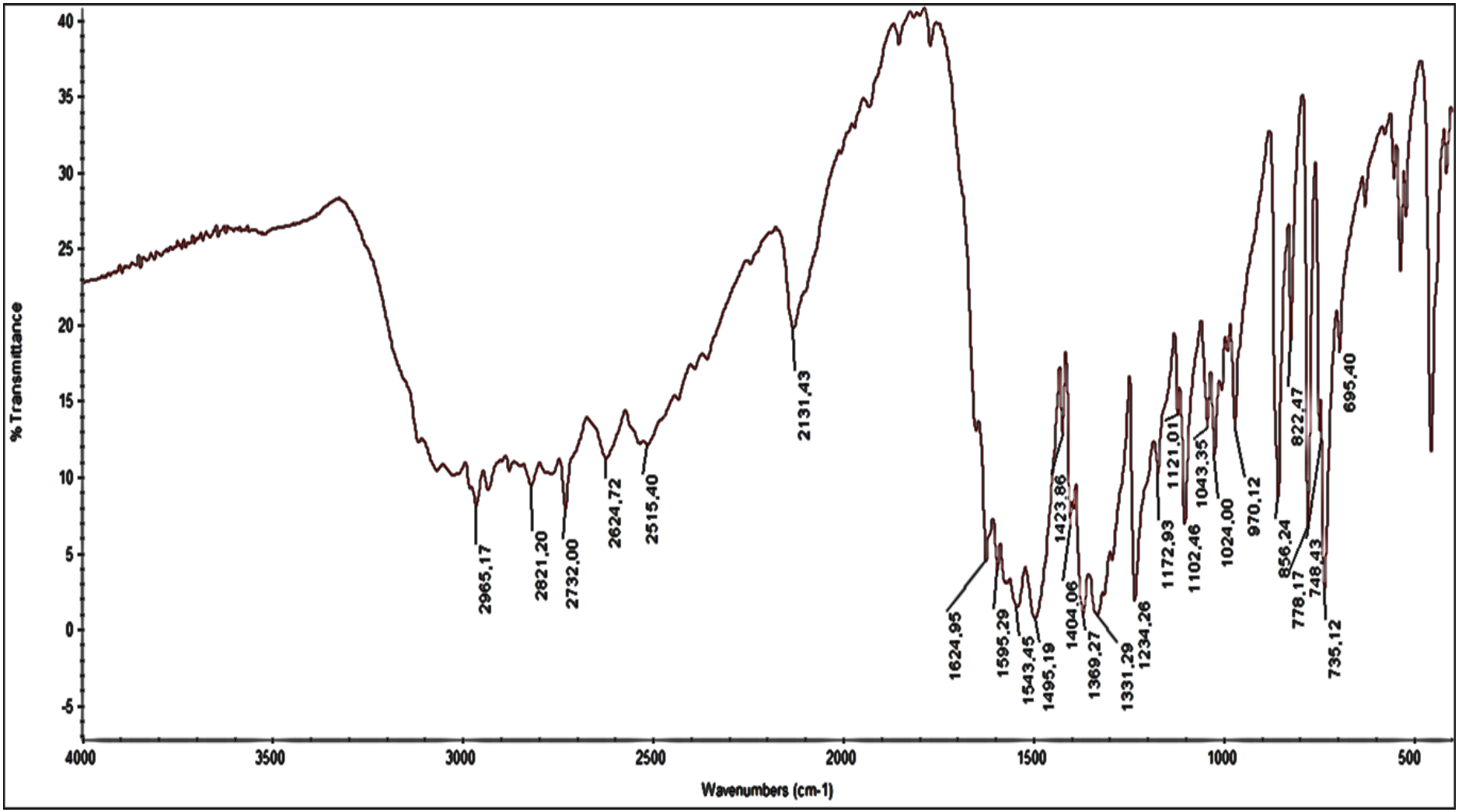
Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O1	57(2)	47(2)	50(2)	–3(1)	35(2)	8(1)
O2	79(2)	36(2)	45(2)	8(1)	29(2)	14(2)
N1	34(2)	41(2)	34(2)	–5(2)	13(2)	–1(2)
N2	26(2)	33(2)	24(2)	0(1)	13(1)	–2(1)
N3	26(2)	34(2)	31(2)	–1(1)	17(1)	–1(1)
C1	26(2)	30(2)	31(2)	–4(2)	10(2)	0(2)
C2	24(2)	40(2)	24(2)	–4(2)	14(2)	–4(2)
C3	30(2)	34(2)	27(2)	–1(2)	15(2)	–3(2)
C4	22(2)	34(2)	24(2)	–3(2)	11(2)	–5(2)
C5	32(2)	41(2)	25(2)	2(2)	16(2)	0(2)
C6	35(2)	41(2)	30(2)	1(2)	15(2)	–2(2)
C7	24(2)	32(2)	20(2)	1(1)	7(2)	–3(2)
C8	23(2)	37(2)	20(2)	–1(2)	9(2)	3(2)
C9	30(2)	31(2)	21(2)	–1(2)	11(2)	3(2)
C10	24(2)	33(2)	25(2)	–5(2)	10(2)	0(2)
C11	30(2)	37(2)	25(2)	–5(2)	12(2)	–6(2)
C12	41(2)	34(2)	24(2)	–4(2)	10(2)	–7(2)
C13	37(2)	29(2)	28(2)	–4(2)	11(2)	4(2)
C14	30(2)	40(2)	23(2)	–4(2)	11(2)	3(2)
C15	26(2)	31(2)	27(2)	2(2)	8(2)	–3(2)
C16	19(2)	46(2)	22(2)	2(2)	8(2)	1(2)
C17	24(2)	43(2)	29(2)	–1(2)	8(2)	2(2)
C18	26(2)	60(3)	30(2)	0(2)	9(2)	12(2)
C19	29(2)	68(3)	31(2)	9(2)	18(2)	13(2)
C20	32(2)	52(3)	41(2)	12(2)	20(2)	3(2)
C21	33(2)	45(2)	34(2)	6(2)	20(2)	3(2)

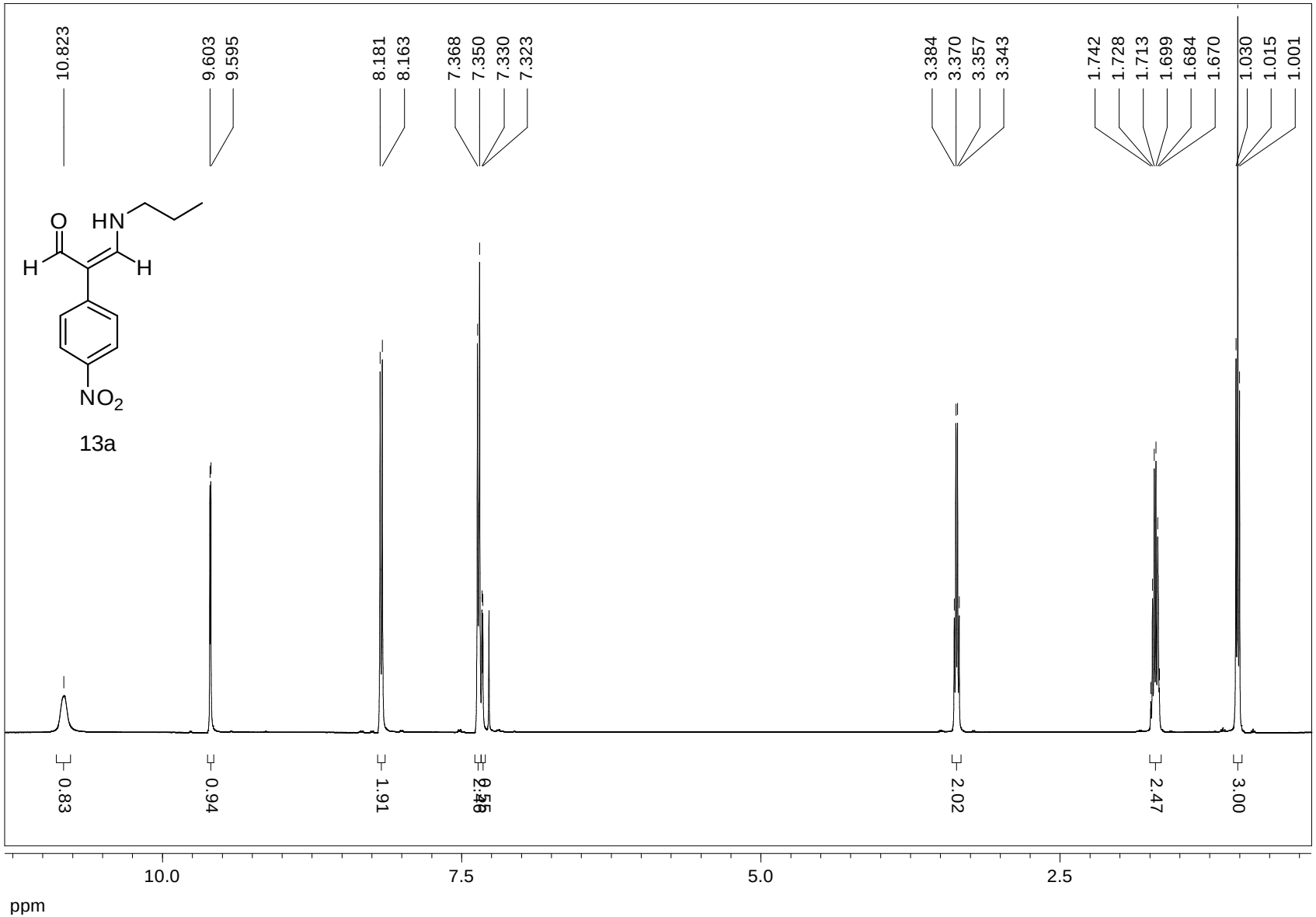
Table 31. Hydrogen coordinates [$\times 10^4$] and isotropic displacement parameters [$Å^2 \times 10^3$] for **30**.

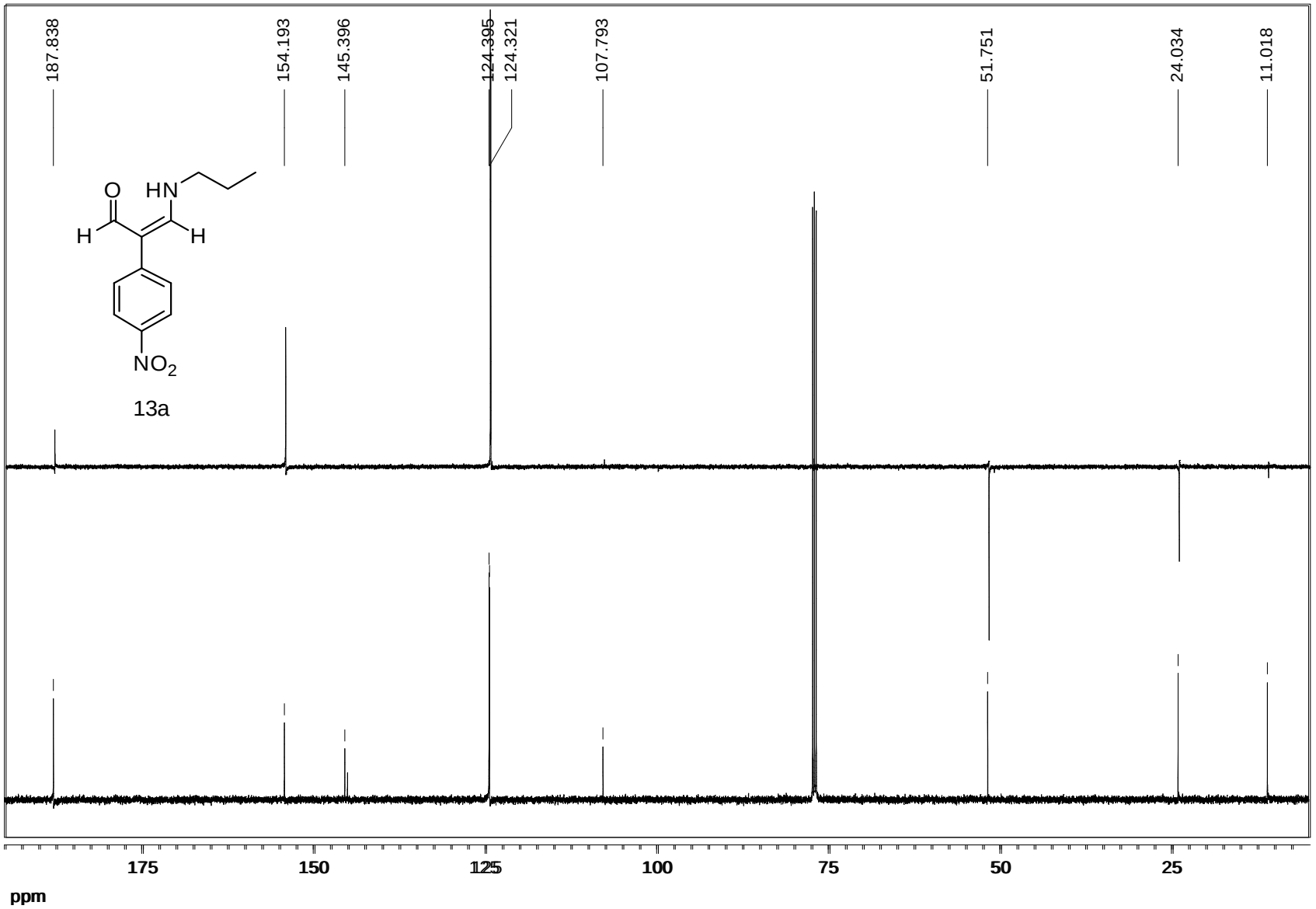
Atom	x	y	z	U_{eq}	*S.o.f.*
H93	940(40)	7032(16)	4590(40)	56(12)	1
H2	–2694	9201	7781	33	1
H3	–1514	8278	7383	35	1
H5	–871	9024	3841	37	1
H6	–1986	9955	4258	41	1
H8	–1870	7413	6104	32	1
H10	–3651	6670	5488	32	1
H11	–4861	5760	5953	36	1
H12	–3380	4829	6411	40	1
H13	–665	4813	6461	37	1
H14	582	5718	6058	36	1
H15	1098	8305	4333	34	1
H17	2282	6408	3328	38	1
H18	4216	6282	2170	47	1
H19	5690	7129	1804	49	1
H20	5315	8104	2673	48	1
H21	3353	8249	3788	42	1

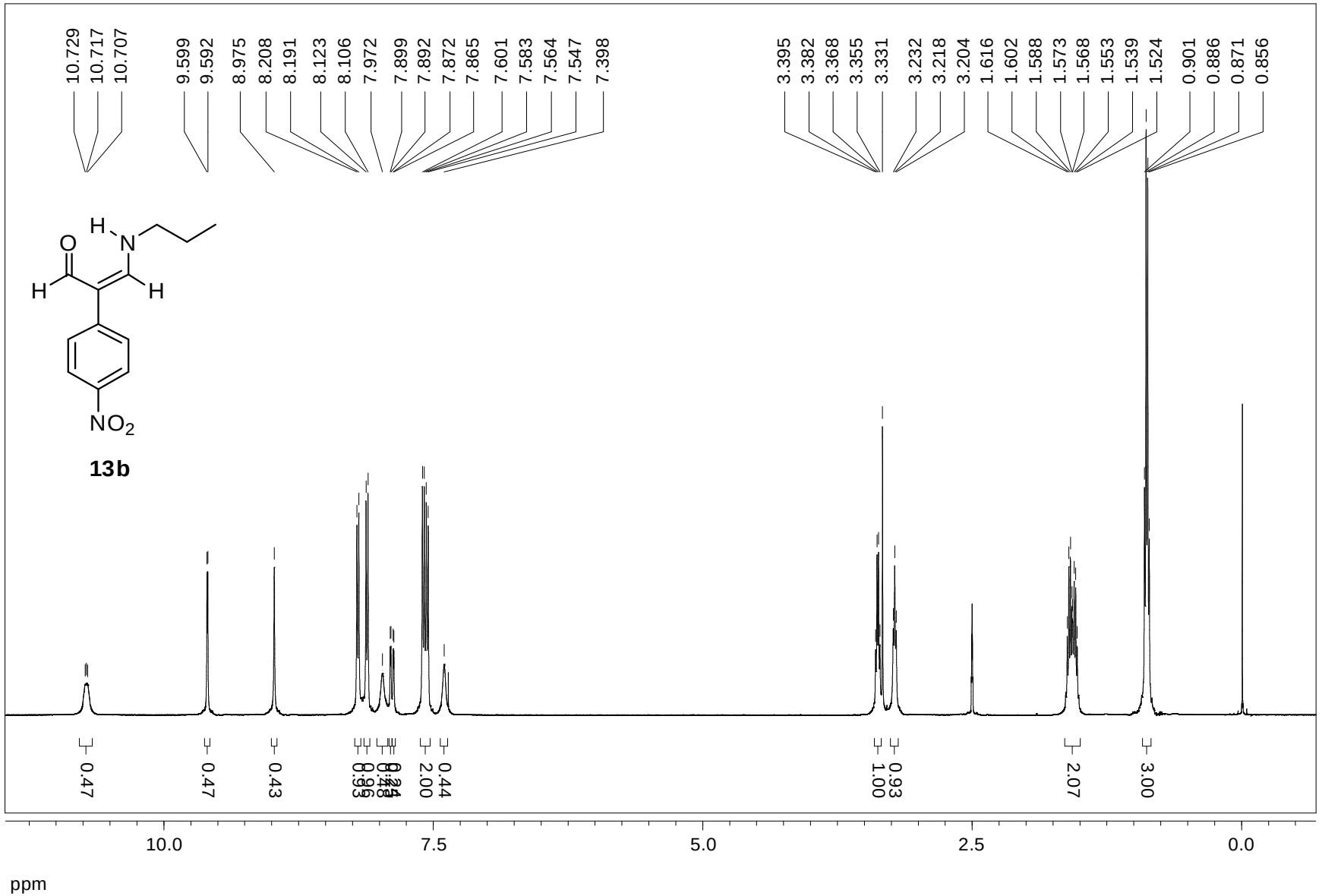
2. Copies of IR, ^{1}HNMR and ^{13}CNMR spectra for all prepared compounds:

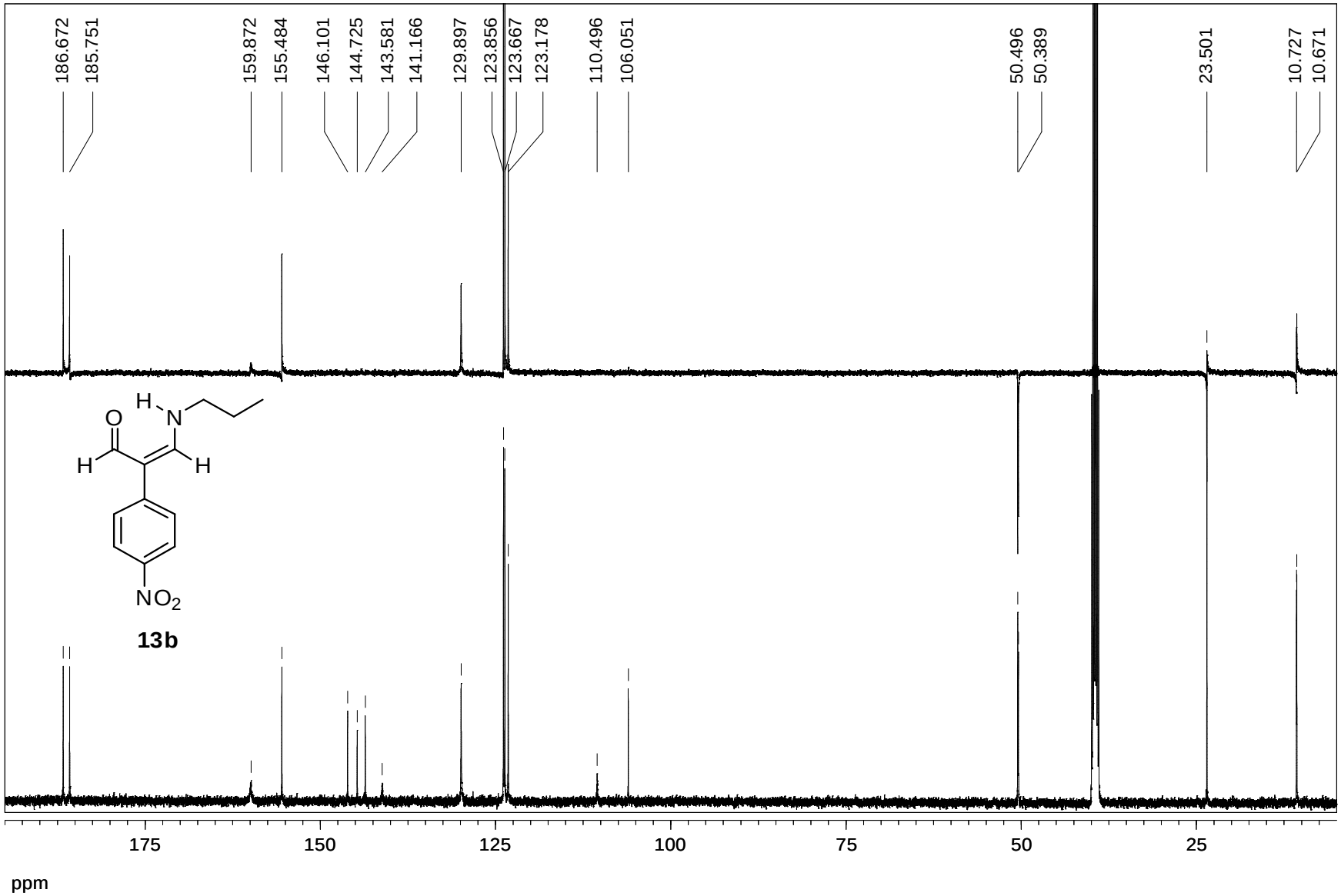
Compound **13**:



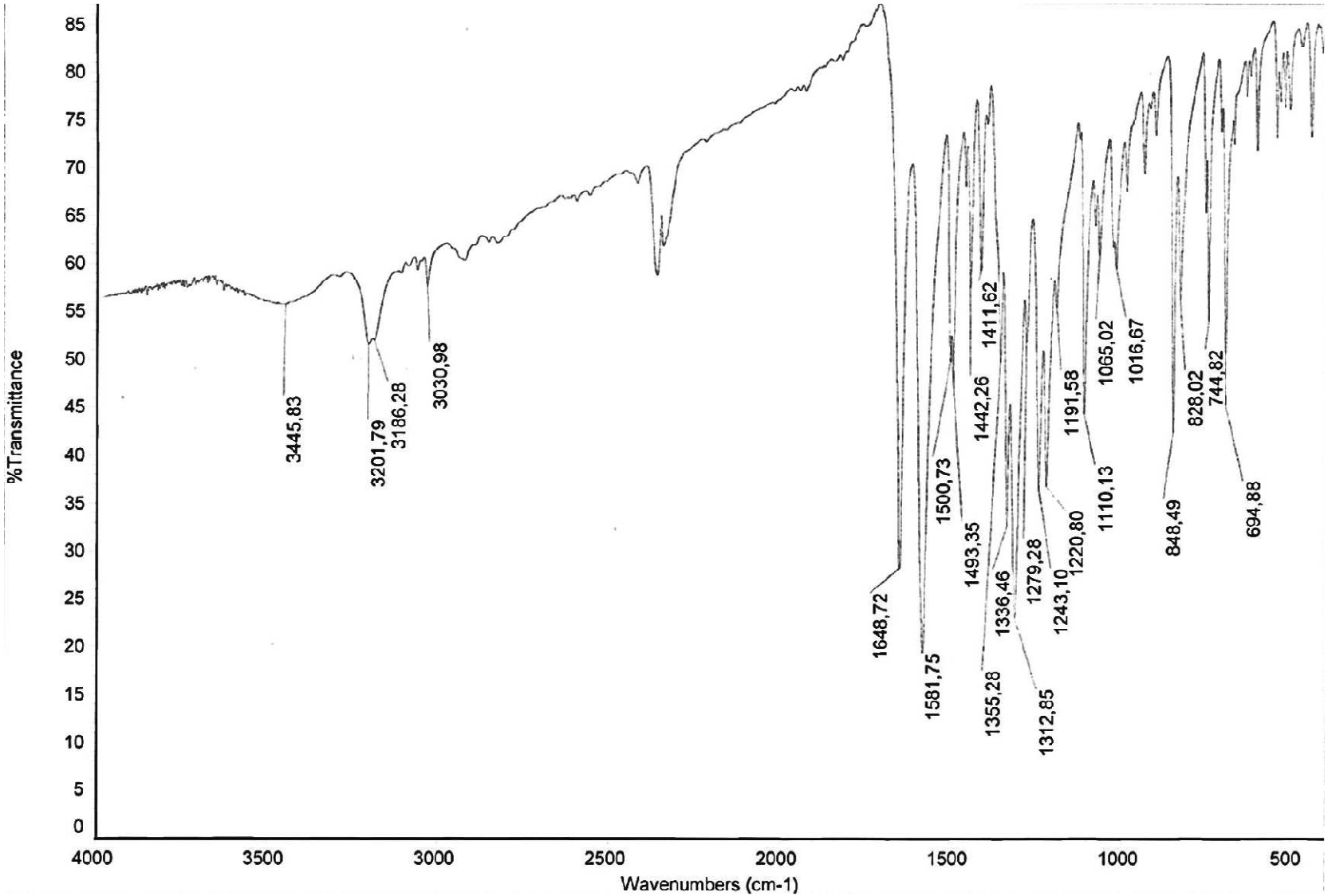

10.823
9.603
9.595
8.181
8.163
7.368
7.350
7.330
7.323
3.384
3.370
3.357
3.343
1.742
1.728
1.713
1.699
1.684
1.670
1.030
1.015
1.001
O
HN
H
H
NO2
13a
0.83
0.94
1.91
2.45
2.02
2.47
3.00
10.0
7.5
5.0
2.5
ppm

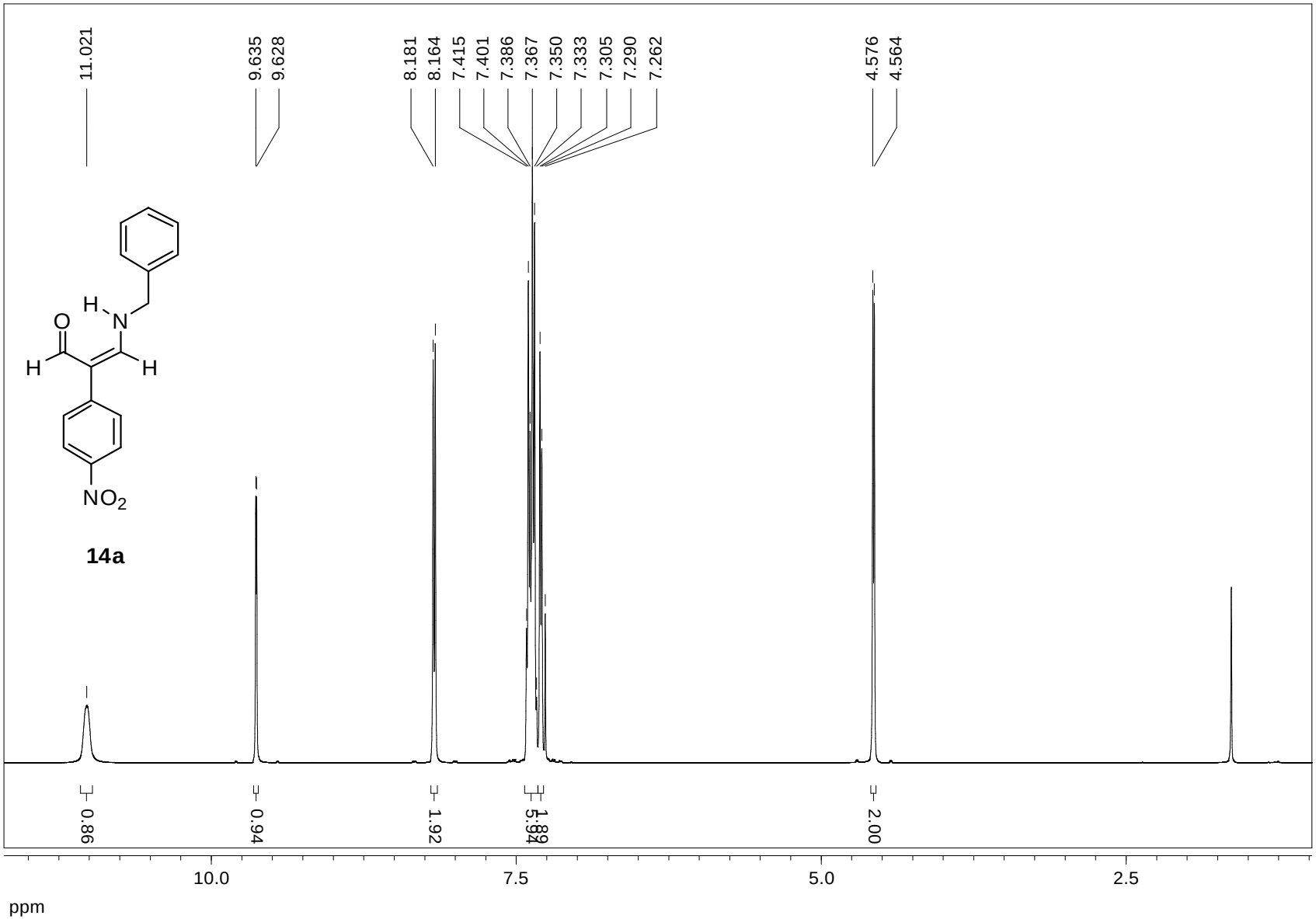

187.838
154.193
145.396
124.395
124.321
107.793
51.751
24.034
11.018
O
HN
H
H
NO2
13a
175
150
125
100
75
50
25
ppm

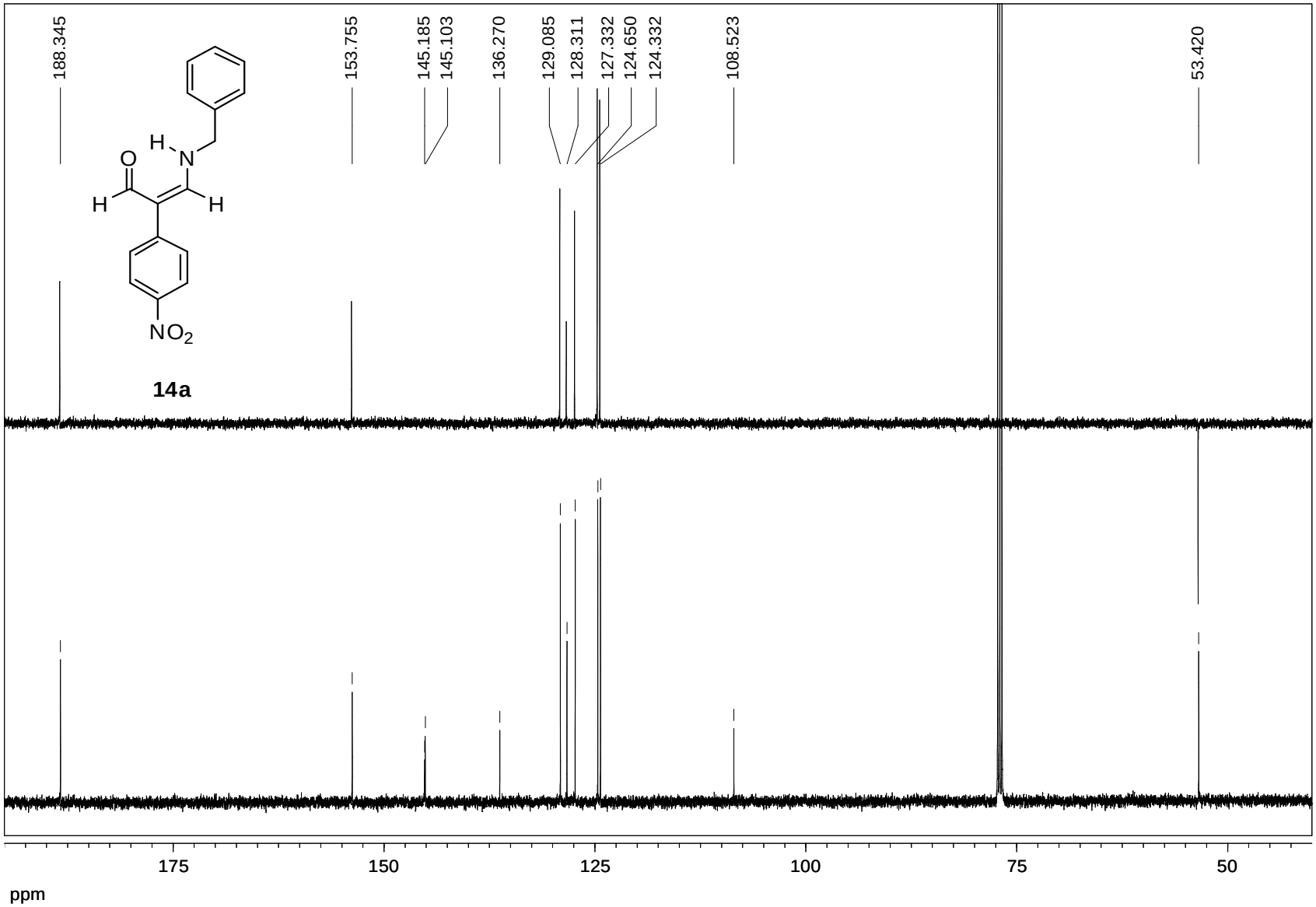

10.729
10.717
10.707
9.599
9.592
8.975
8.208
8.191
8.123
8.106
7.972
7.899
7.892
7.872
7.865
7.601
7.583
7.564
7.547
7.398
3.395
3.382
3.368
3.355
3.331
3.232
3.218
3.204
1.616
1.602
1.588
1.573
1.568
1.553
1.539
1.524
0.901
0.886
0.871
0.856
H
N
O
H
H
NO2
13b
0.47
0.47
0.43
2.00
0.44
1.00
0.93
2.07
3.00
10.0
7.5
5.0
2.5
0.0
ppm

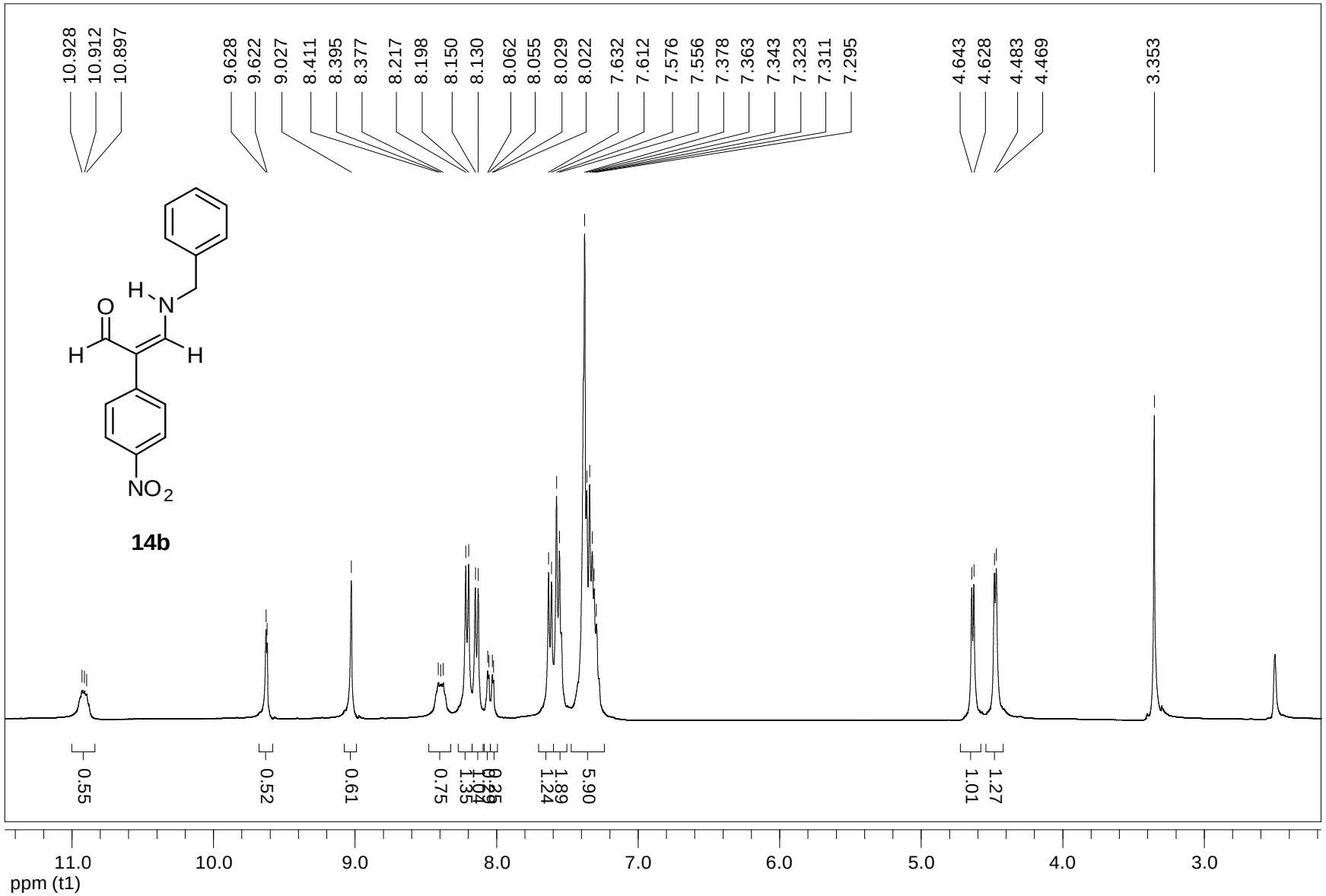

186.672
185.751
159.872
155.484
146.101
144.725
143.581
141.166
129.897
123.856
123.667
123.178
110.496
106.051
50.496
50.389
23.501
10.727
10.671
O
H
N
H
H
NO2
13b
175
150
125
100
75
50
25
ppm

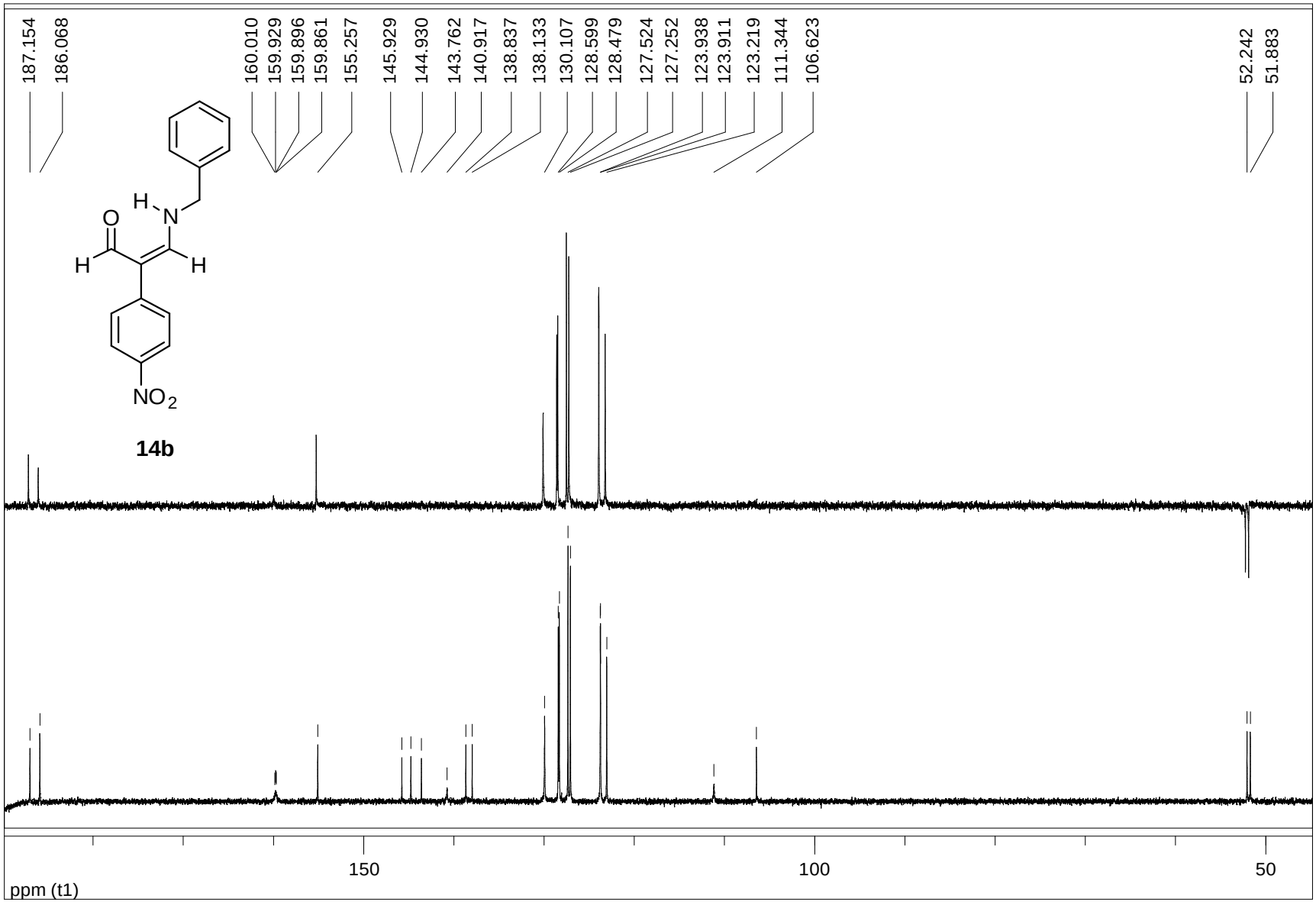
Compound **14**:


%Transmittance
Wavenumbers (cm-1)
3445,83
3201,79
3186,28
3030,98
1648,72
1581,75
1500,73
1493,35
1442,26
1411,62
1355,28
1336,46
1312,85
1279,28
1243,10
1220,80
1191,58
1110,13
1065,02
1016,67
848,49
828,02
744,82
694,88

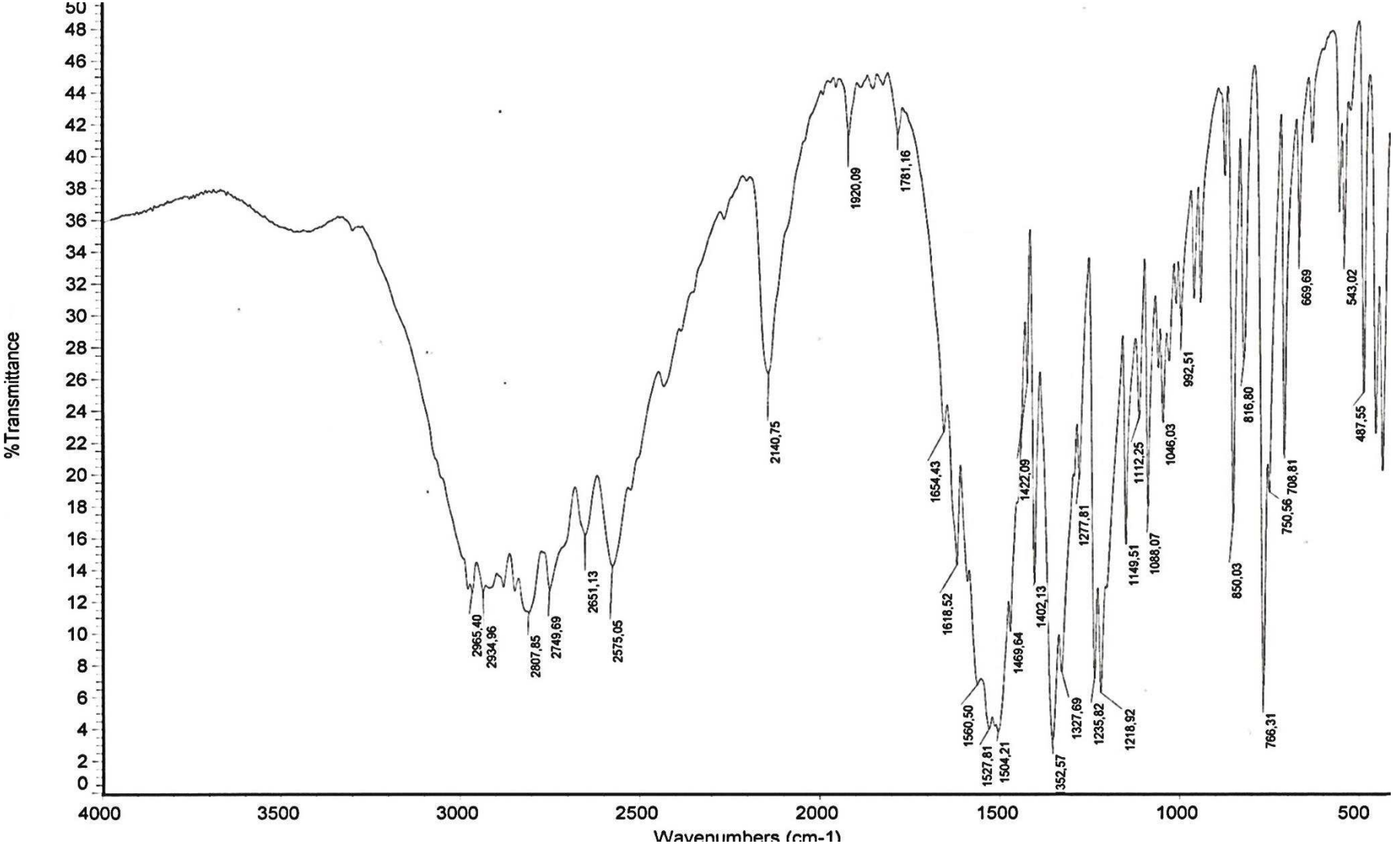

11.021
9.635
9.628
8.181
8.164
7.415
7.401
7.386
7.367
7.350
7.333
7.305
7.290
7.262
4.576
4.564
H
N
O
H
H
NO2
14a
0.86
0.94
1.92
5.94
1.89
2.00
10.0
7.5
5.0
2.5
ppm

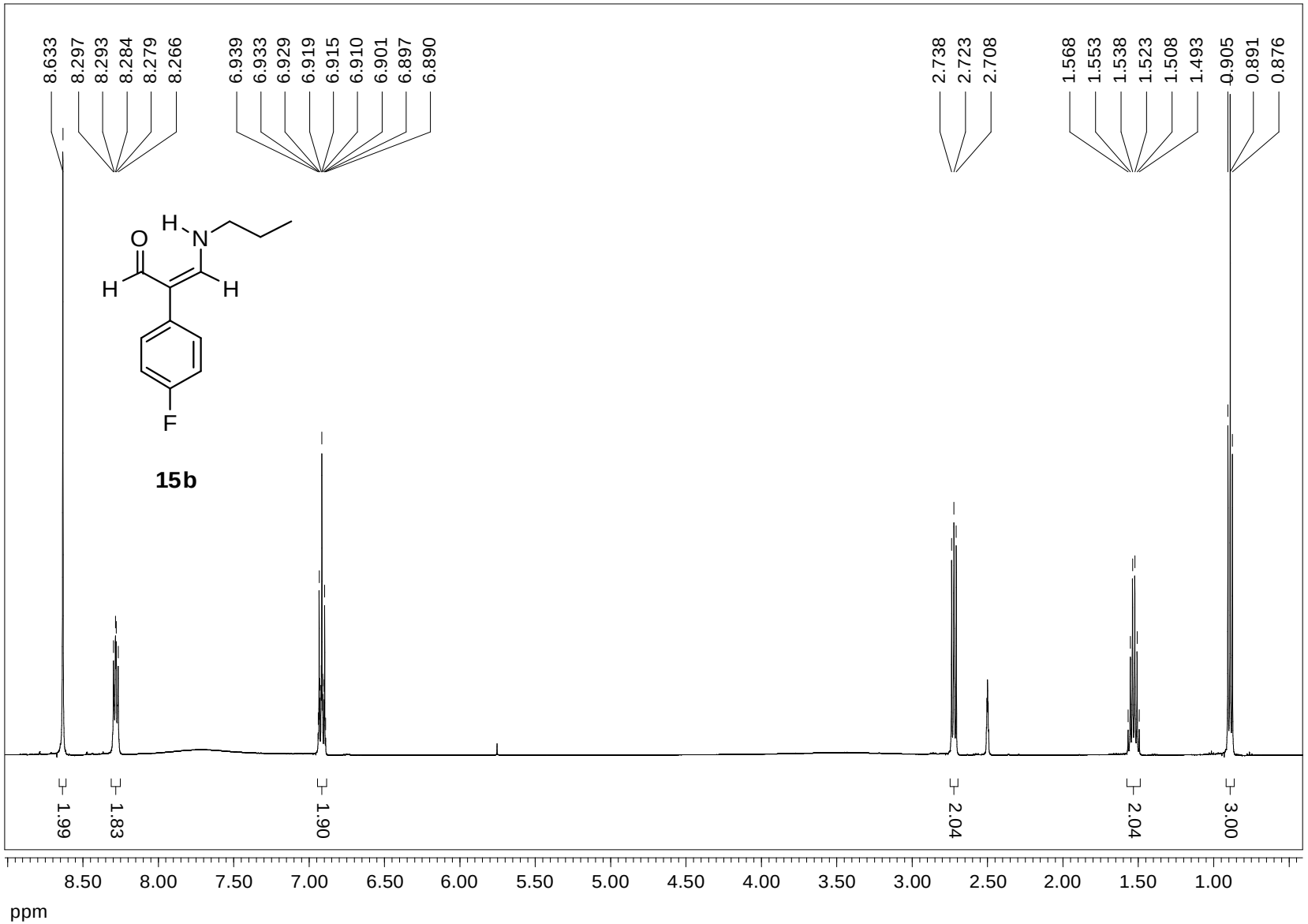

188.345
153.755
145.185
145.103
136.270
129.085
128.311
127.332
124.650
124.332
108.523
53.420
H
N
O
H
H
NO2
14a
175
150
125
100
75
50
ppm

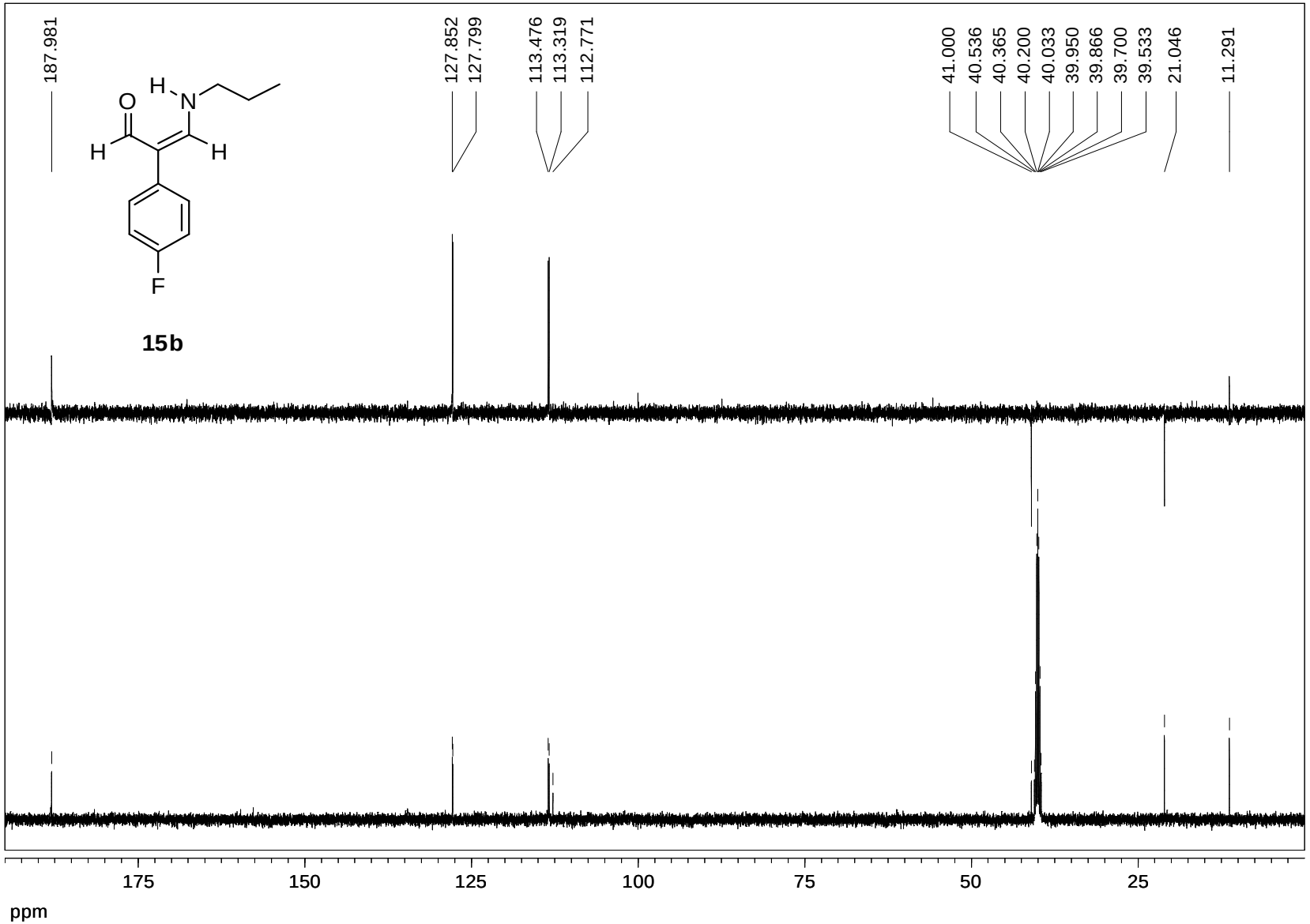

10.928
10.912
10.897
9.628
9.622
9.027
8.411
8.395
8.377
8.217
8.198
8.150
8.130
8.062
8.055
8.029
8.022
7.632
7.612
7.576
7.556
7.378
7.363
7.343
7.323
7.311
7.295
4.643
4.628
4.483
4.469
3.353
H
N
O
H
H
NO2
14b
0.55
0.52
0.61
0.75
1.35
1.24
1.89
5.90
1.01
1.27
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
ppm (t1)


187.154
186.068
160.010
159.929
159.896
159.861
155.257
145.929
144.930
143.762
140.917
138.837
138.133
130.107
128.599
128.479
127.524
127.252
123.938
123.911
123.219
111.344
106.623
52.242
51.883
H
N
O
H
H
NO2
14b
150
100
50
ppm (t1)

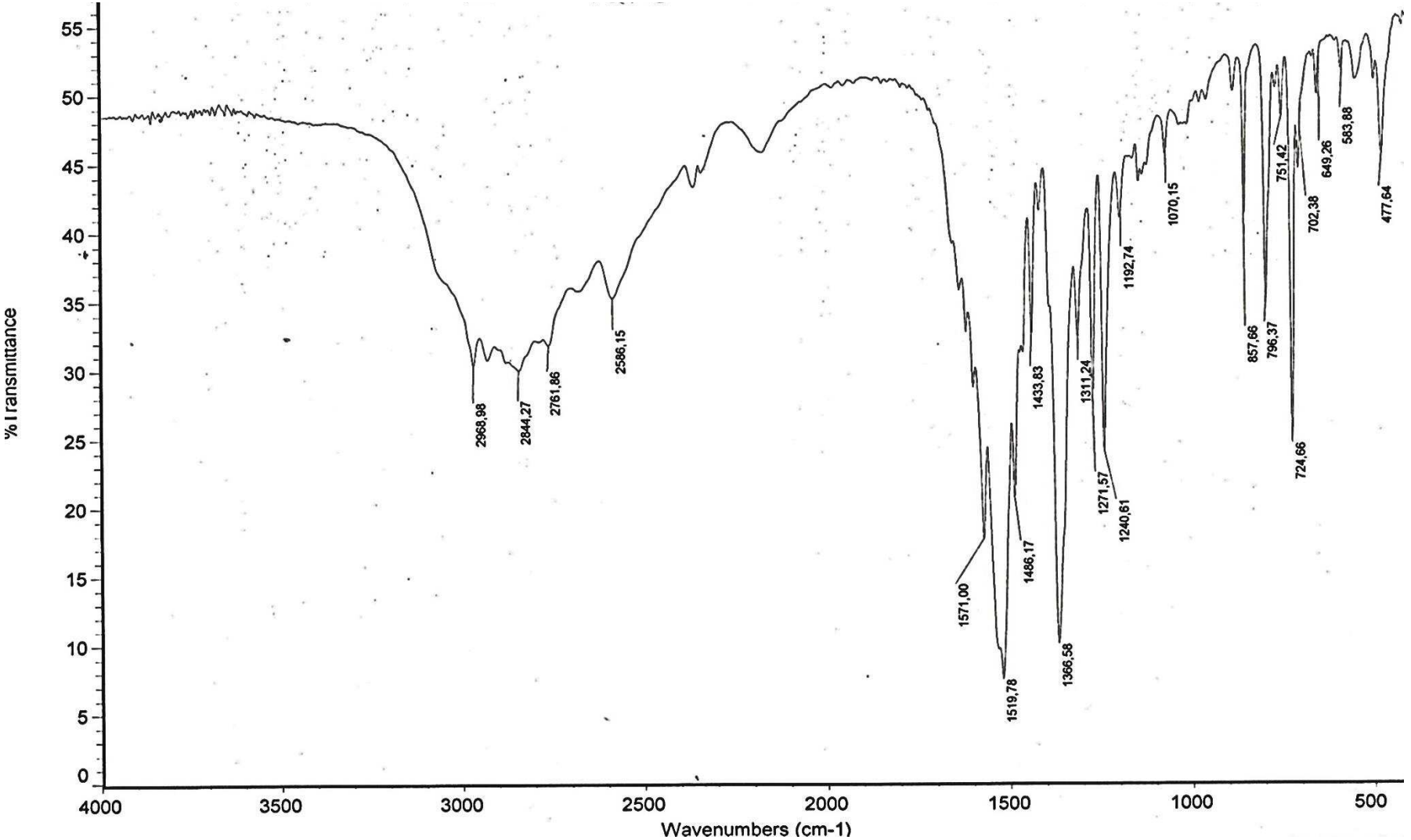
Compound **15**:

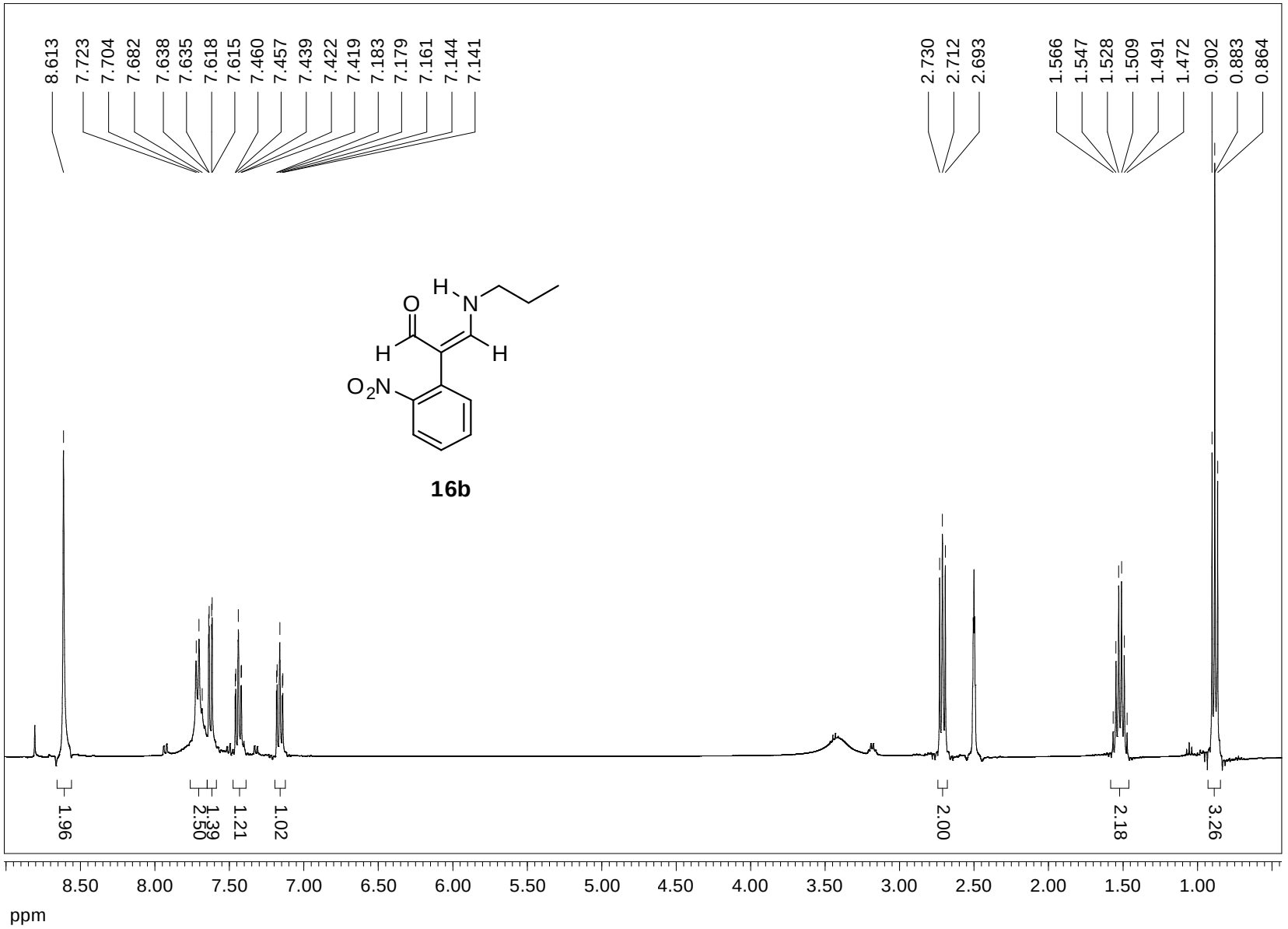

%Transmittance
Wavenumbers (cm-1)
4000
3500
3000
2500
2000
1500
1000
500
2965,40
2934,96
2807,85
2749,69
2651,13
2575,05
2140,75
1920,09
1781,16
1654,43
1618,52
1560,50
1527,81
1504,21
1469,64
1422,09
1402,13
1352,57
1327,69
1277,81
1235,82
1218,92
1149,51
1112,25
1088,07
1046,03
992,51
850,03
816,80
766,31
750,56
708,81
669,69
543,02
487,55

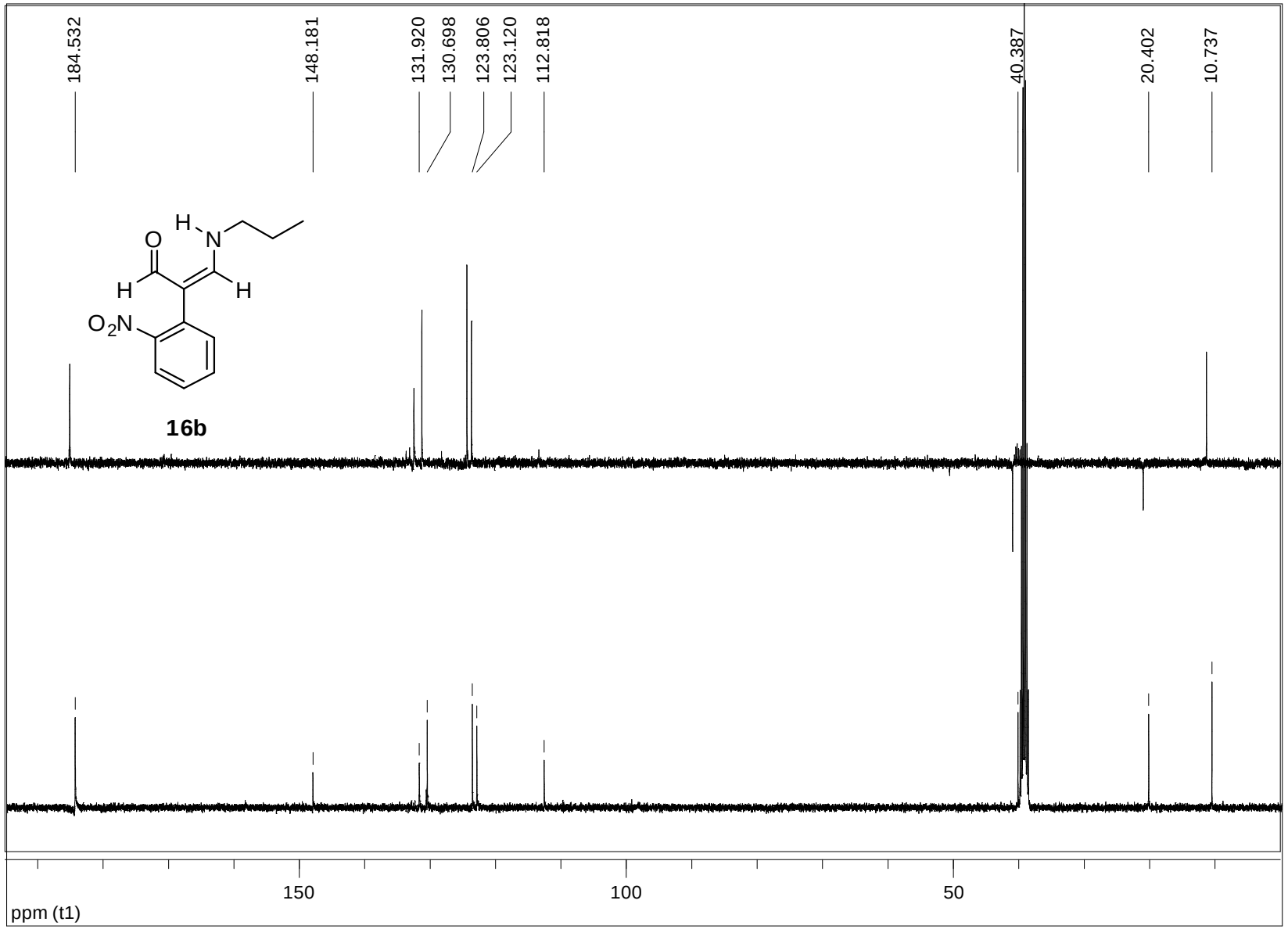

8.633
8.297
8.293
8.284
8.279
8.266
6.939
6.933
6.929
6.919
6.915
6.910
6.901
6.897
6.890
2.738
2.723
2.708
1.568
1.553
1.538
1.523
1.508
1.493
0.905
0.891
0.876
O
H
N
H
H
F
15b
1.99
1.83
1.90
2.04
2.04
3.00
8.50
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
4.00
3.50
3.00
2.50
2.00
1.50
1.00
ppm


187.981
127.852
127.799
113.476
113.319
112.771
41.000
40.536
40.365
40.200
40.033
39.950
39.866
39.700
39.533
21.046
11.291
O
H
N
H
H
F
15b
175
150
125
100
75
50
25
ppm

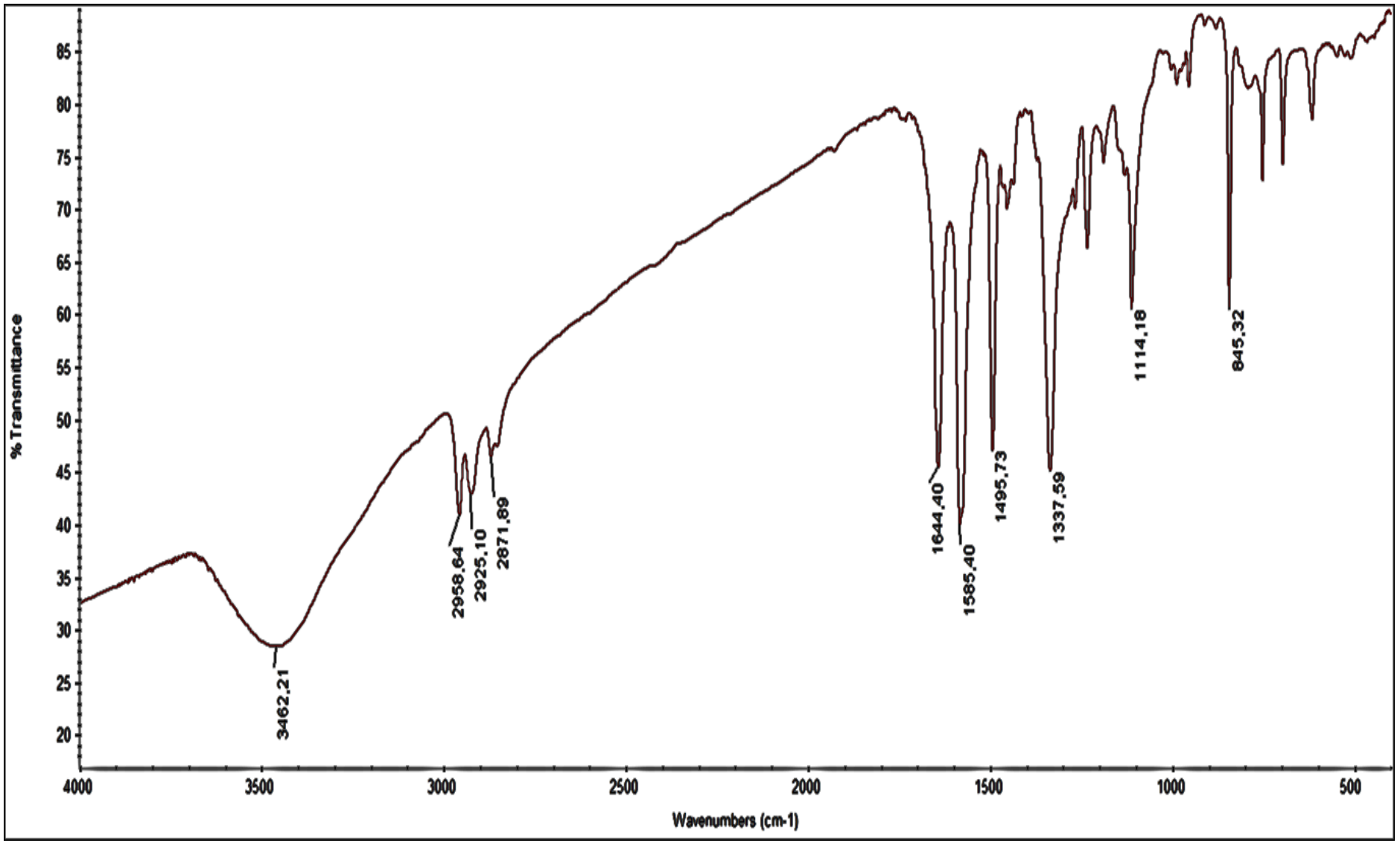
Compound **16**:


% Transmittance
Wavenumbers (cm-1)
4000
3500
3000
2500
2000
1500
1000
500
0
5
10
15
20
25
30
35
40
45
50
55
2968,98
2844,27
2761,86
2586,15
1571,00
1519,78
1486,17
1433,83
1366,58
1311,24
1271,57
1240,61
1192,74
1070,15
857,66
796,37
751,42
724,66
702,38
649,26
583,88
477,64


8.613
7.723
7.704
7.682
7.638
7.635
7.618
7.615
7.460
7.457
7.439
7.422
7.419
7.183
7.179
7.161
7.144
7.141
2.730
2.712
2.693
1.566
1.547
1.528
1.509
1.491
1.472
0.902
0.883
0.864
H
N
O
H
H
O2N
16b
1.96
2.50
1.39
1.21
1.02
2.00
2.18
3.26
8.50
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
4.00
3.50
3.00
2.50
2.00
1.50
1.00
ppm


184.532
148.181
131.920
130.698
123.806
123.120
112.818
40.387
20.402
10.737
H
N
O
H
H
O2N
16b
150
100
50
ppm (t1)

Compound **17**:


% Transmittance
Wavenumbers (cm-1)
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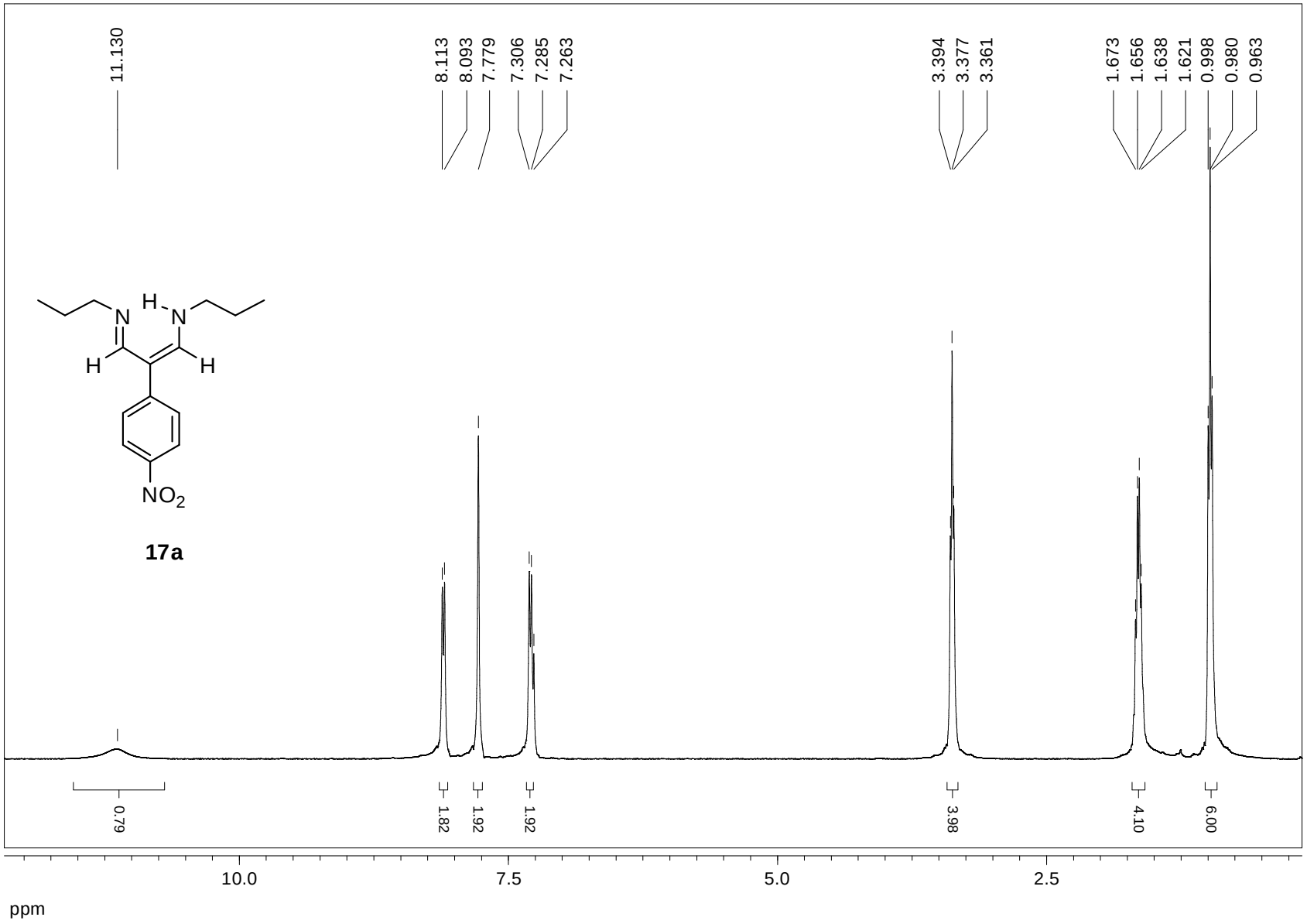
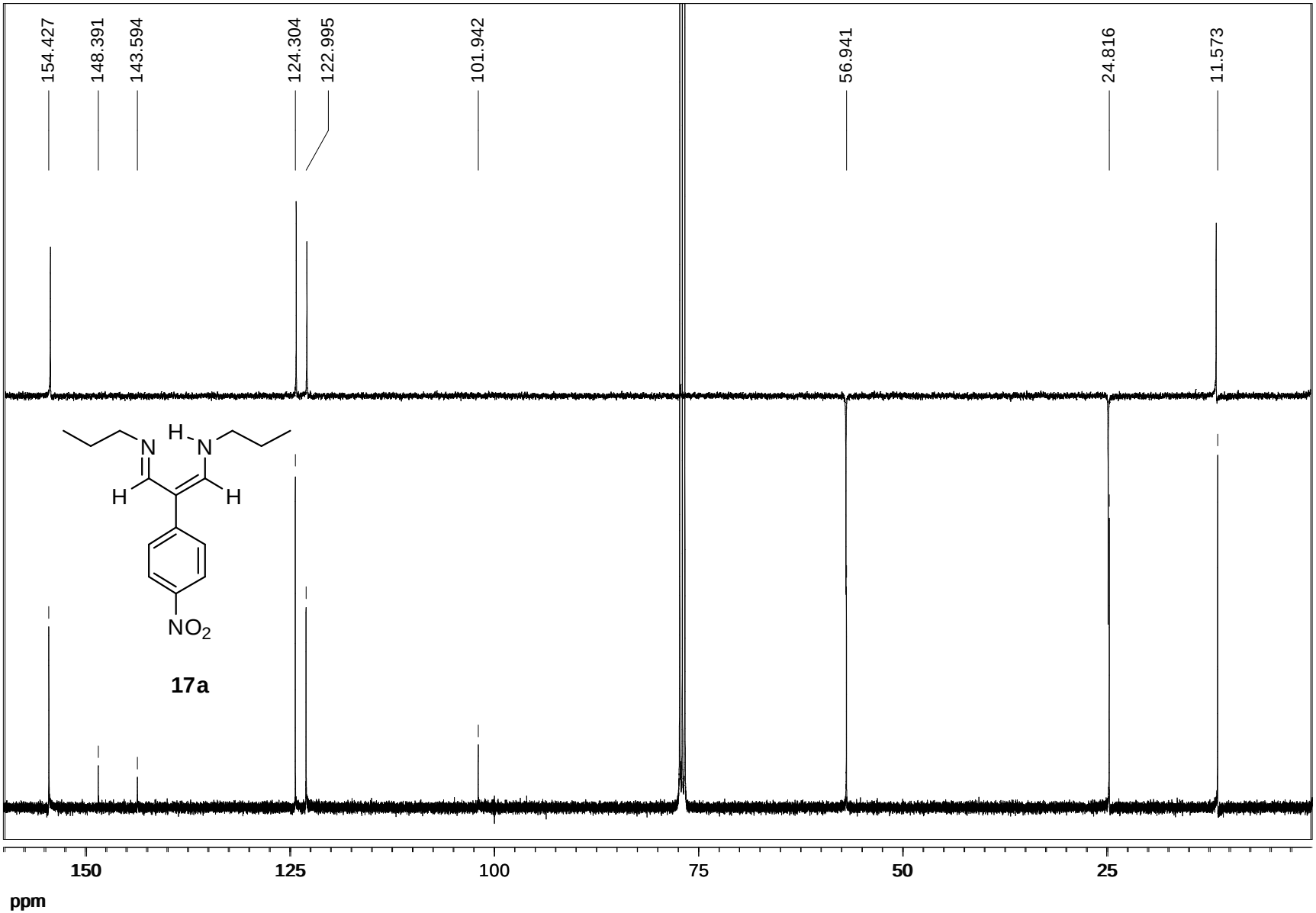
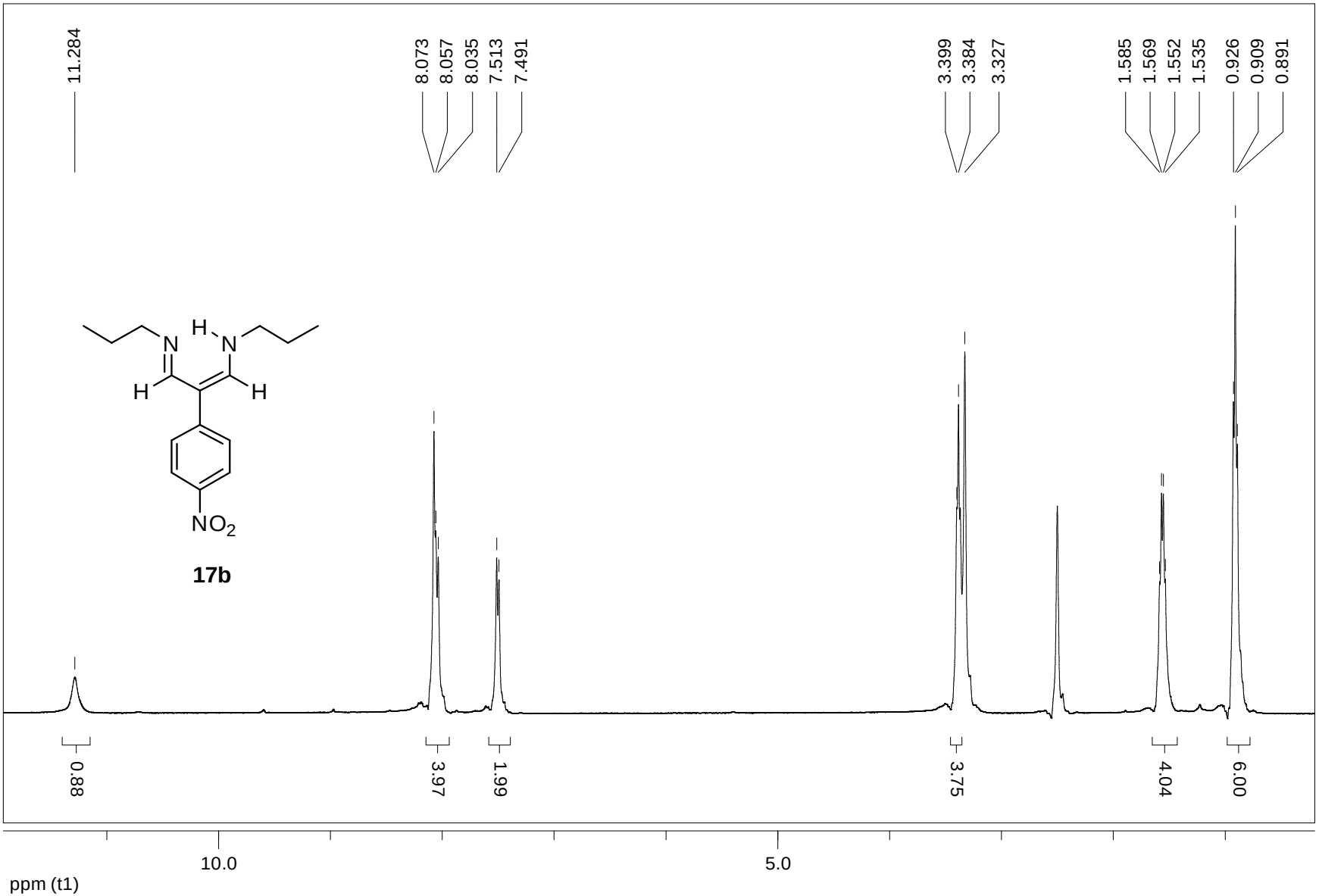
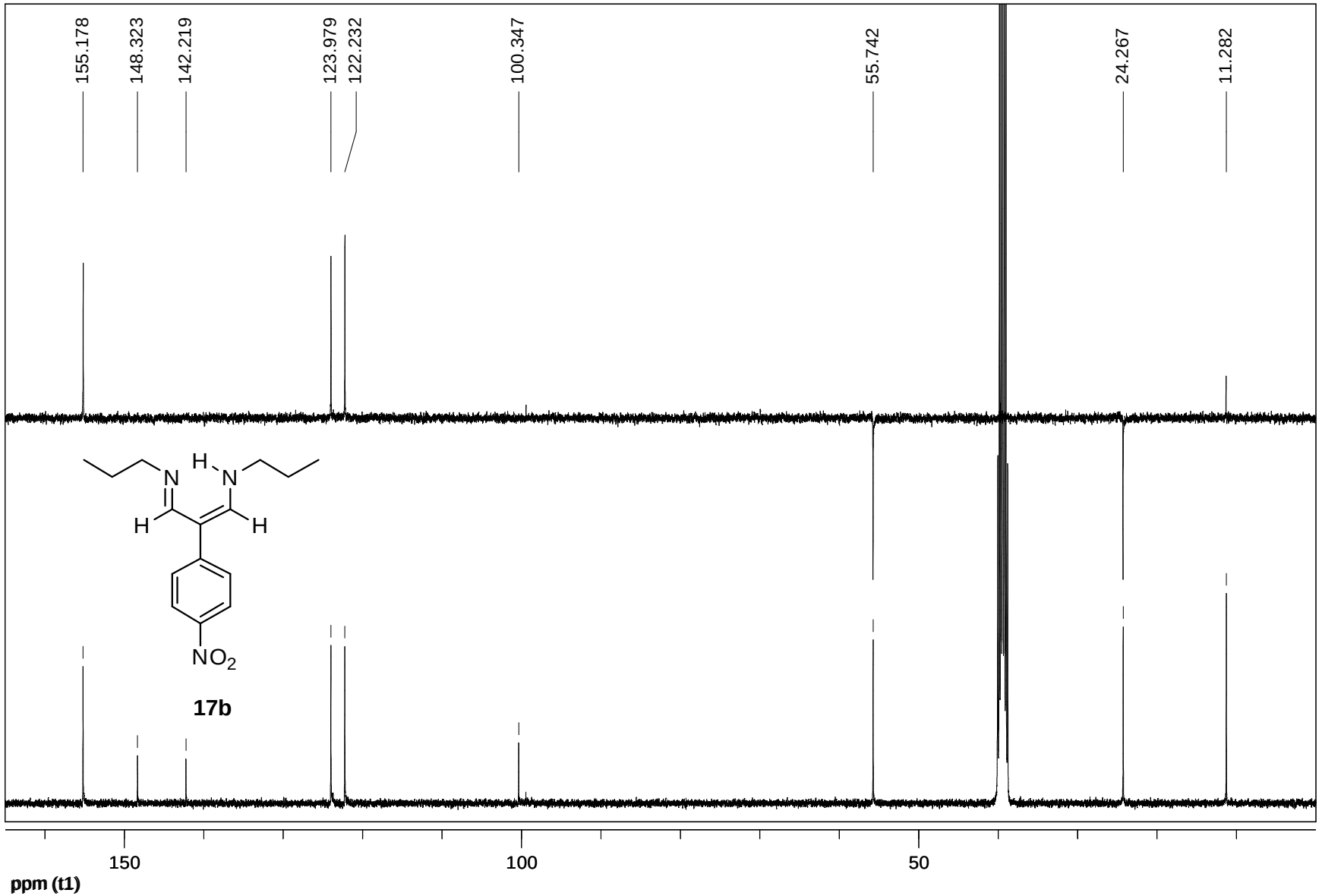
2958,64
2925,10
2871,89
1644,40
1585,40
1495,73
1337,59
1114,18
845,32

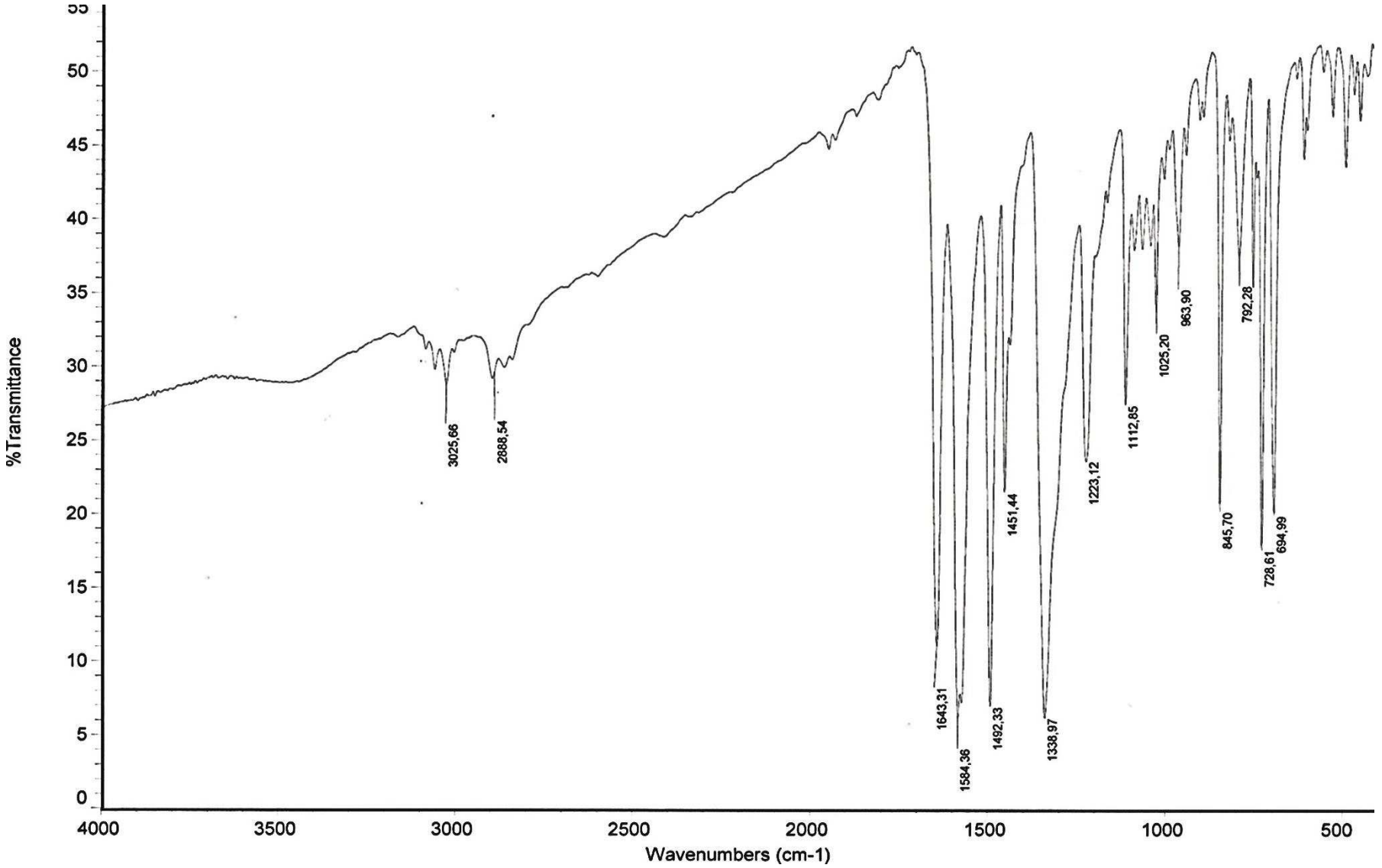

11.130
8.113
8.093
7.779
7.306
7.285
7.263
3.394
3.377
3.361
1.673
1.656
1.638
1.621
0.998
0.980
0.963
N
H
N
H
H
NO2
17a
0.79
1.82
1.92
1.92
3.98
4.10
6.00
10.0
7.5
5.0
2.5
ppm

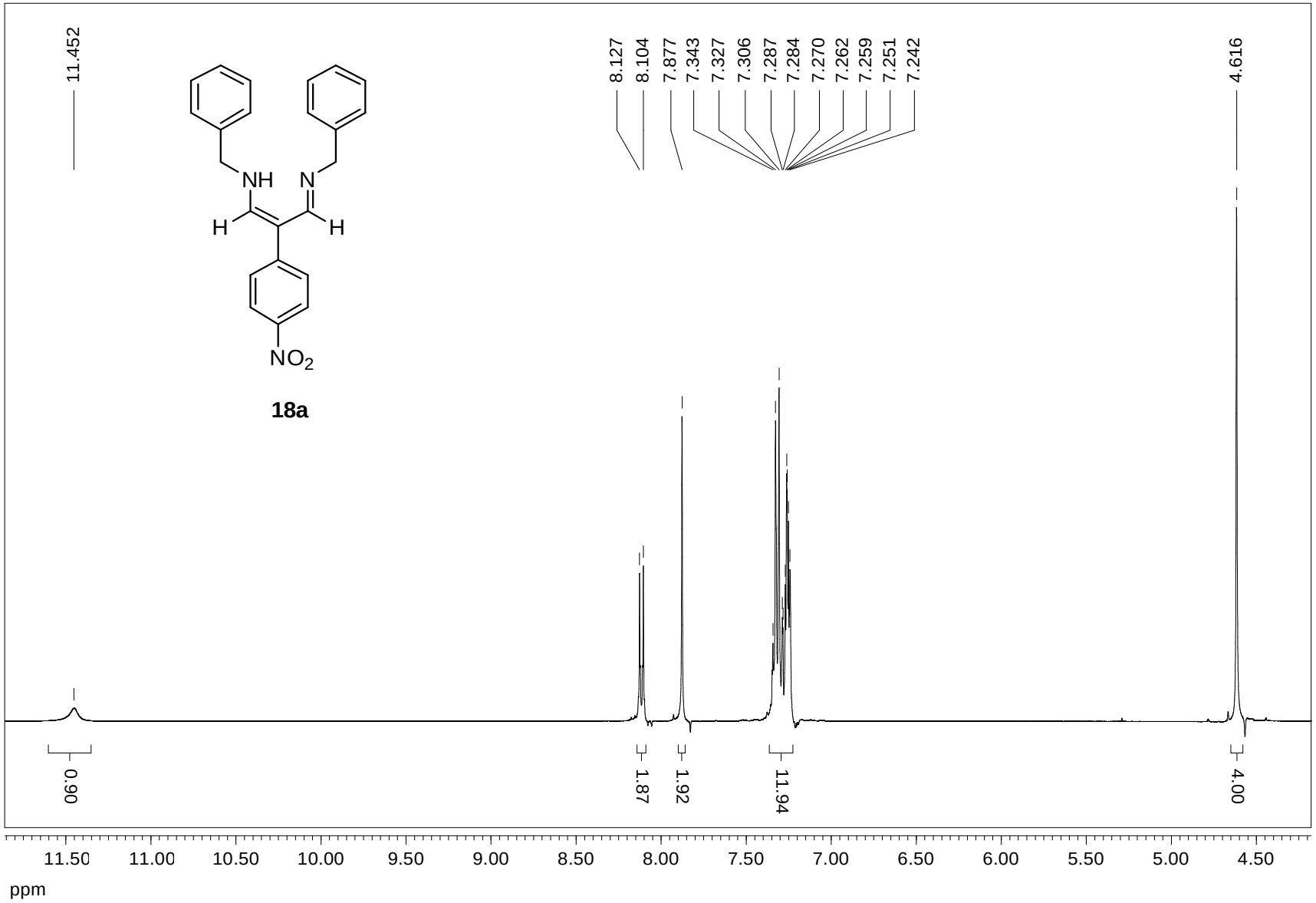

154.427
148.391
143.594
124.304
122.995
101.942
56.941
24.816
11.573
H
N
N
H
H
NO2
17a
150
125
100
75
50
25
ppm

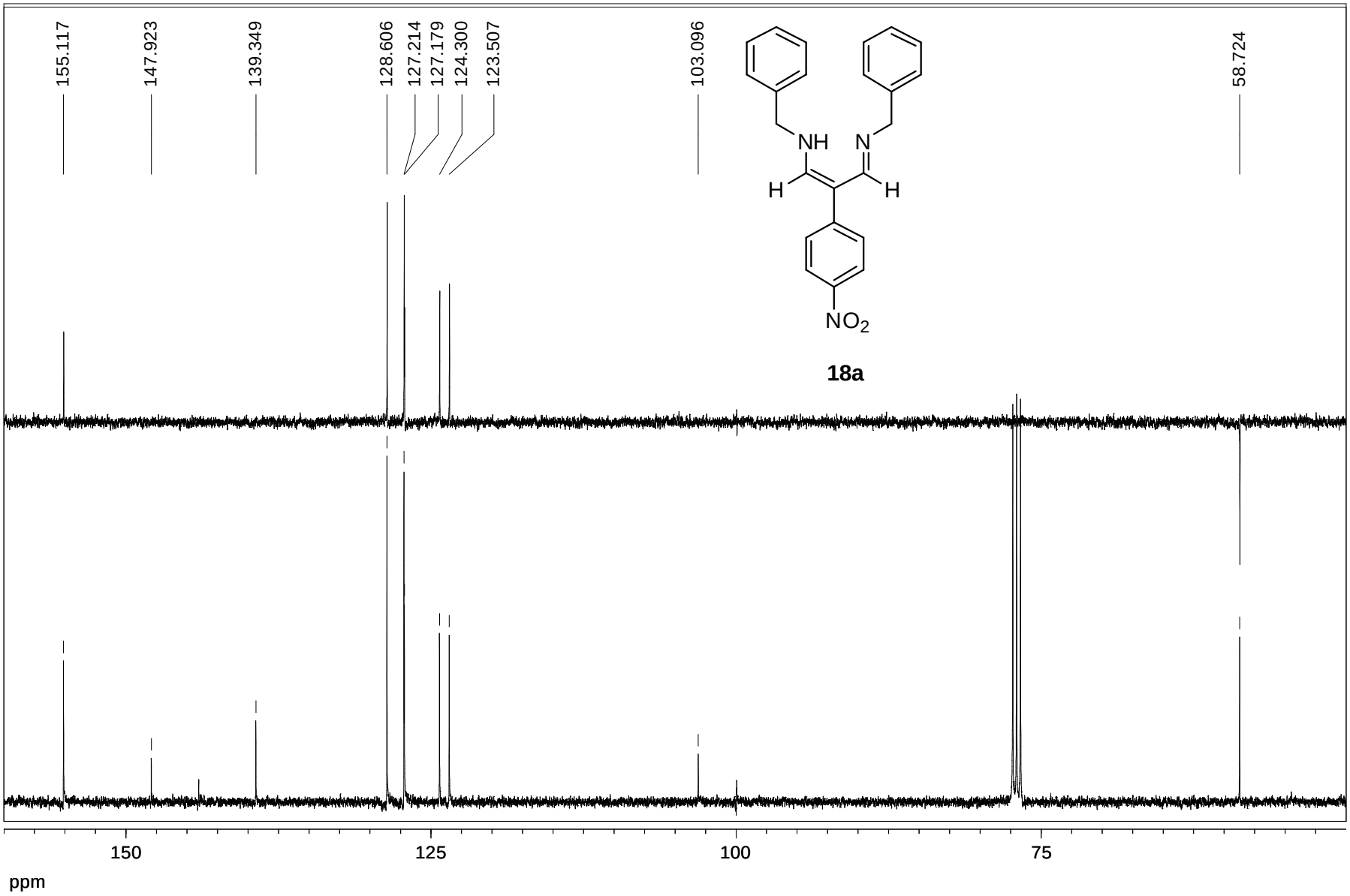

11.284
8.073
8.057
8.035
7.513
7.491
3.399
3.384
3.327
1.585
1.569
1.552
1.535
0.926
0.909
0.891
H
N
N
H
H
NO2
17b
0.88
3.67
1.69
3.75
4.04
6.00
10.0
5.0
ppm (t1)

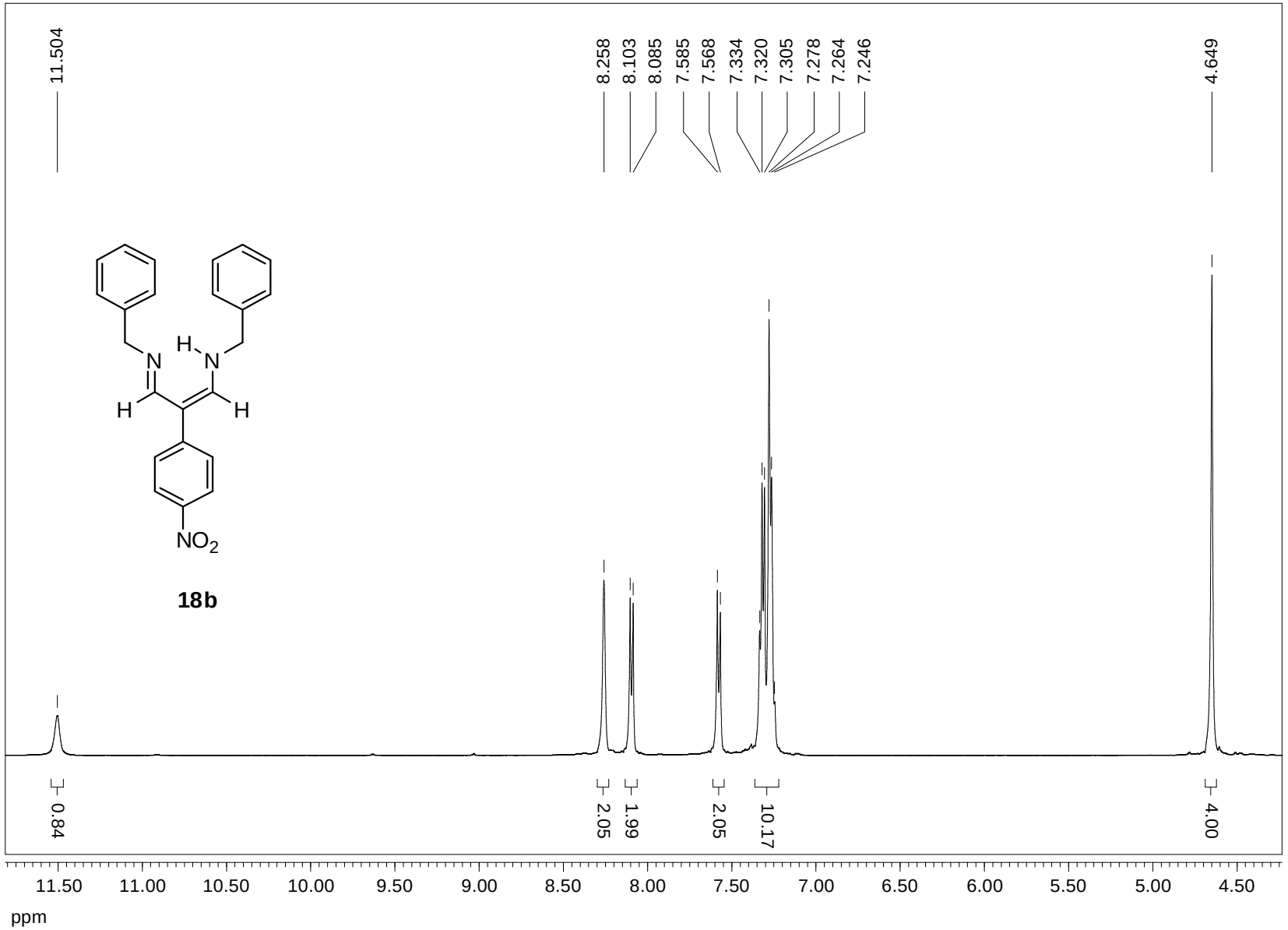

155.178
148.323
142.219
123.979
122.232
100.347
55.742
24.267
11.282
H
N
N
H
H
NO2
17b
150
100
50
ppm (t1)

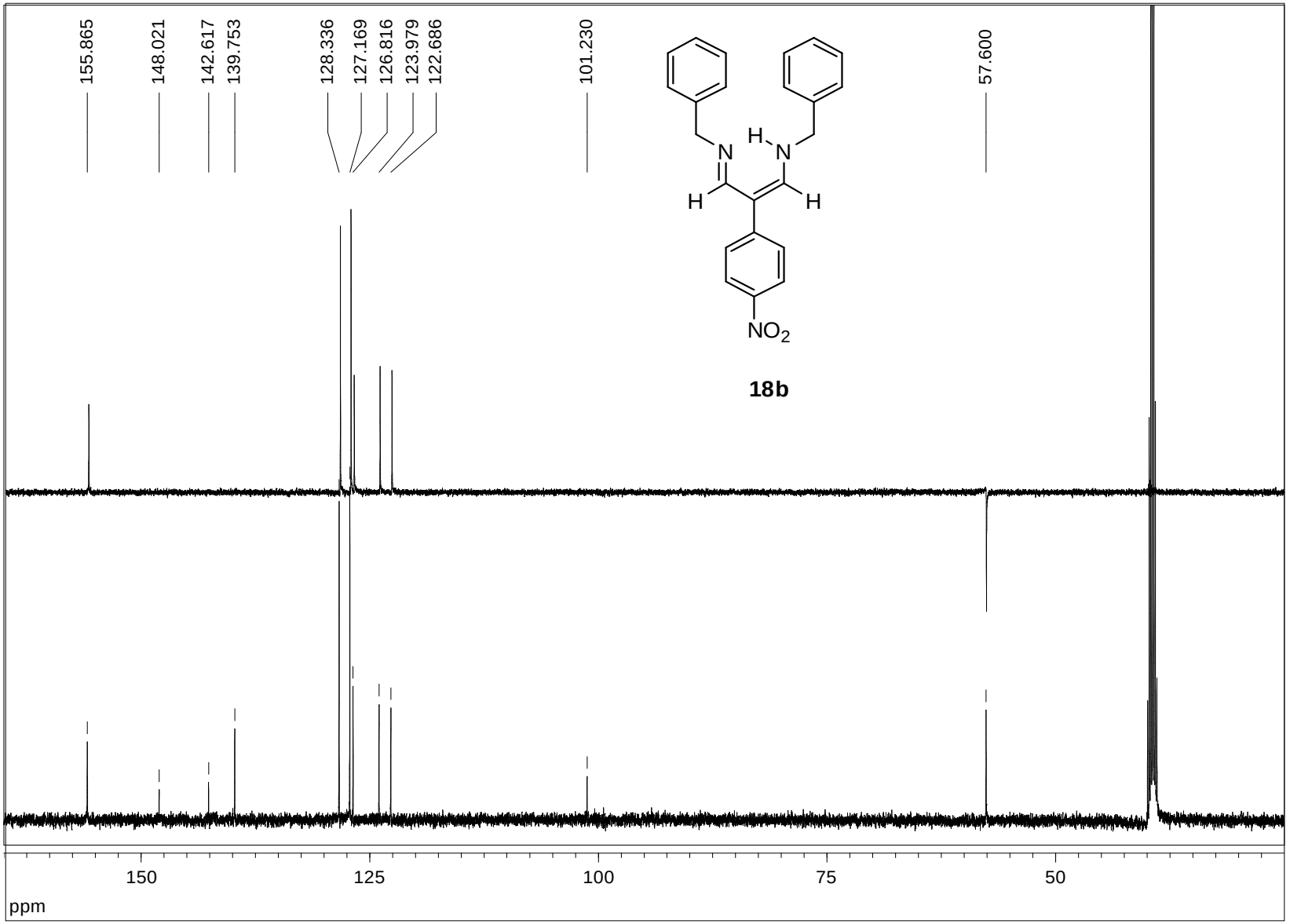
Compound **18**:


%Transmittance
Wavenumbers (cm-1)
4000
3500
3000
2500
2000
1500
1000
500
0
5
10
15
20
25
30
35
40
45
50
3025,66
2888,54
1643,31
1584,36
1492,33
1451,44
1338,97
1223,12
1112,85
1025,20
963,90
845,70
792,28
728,61
694,99

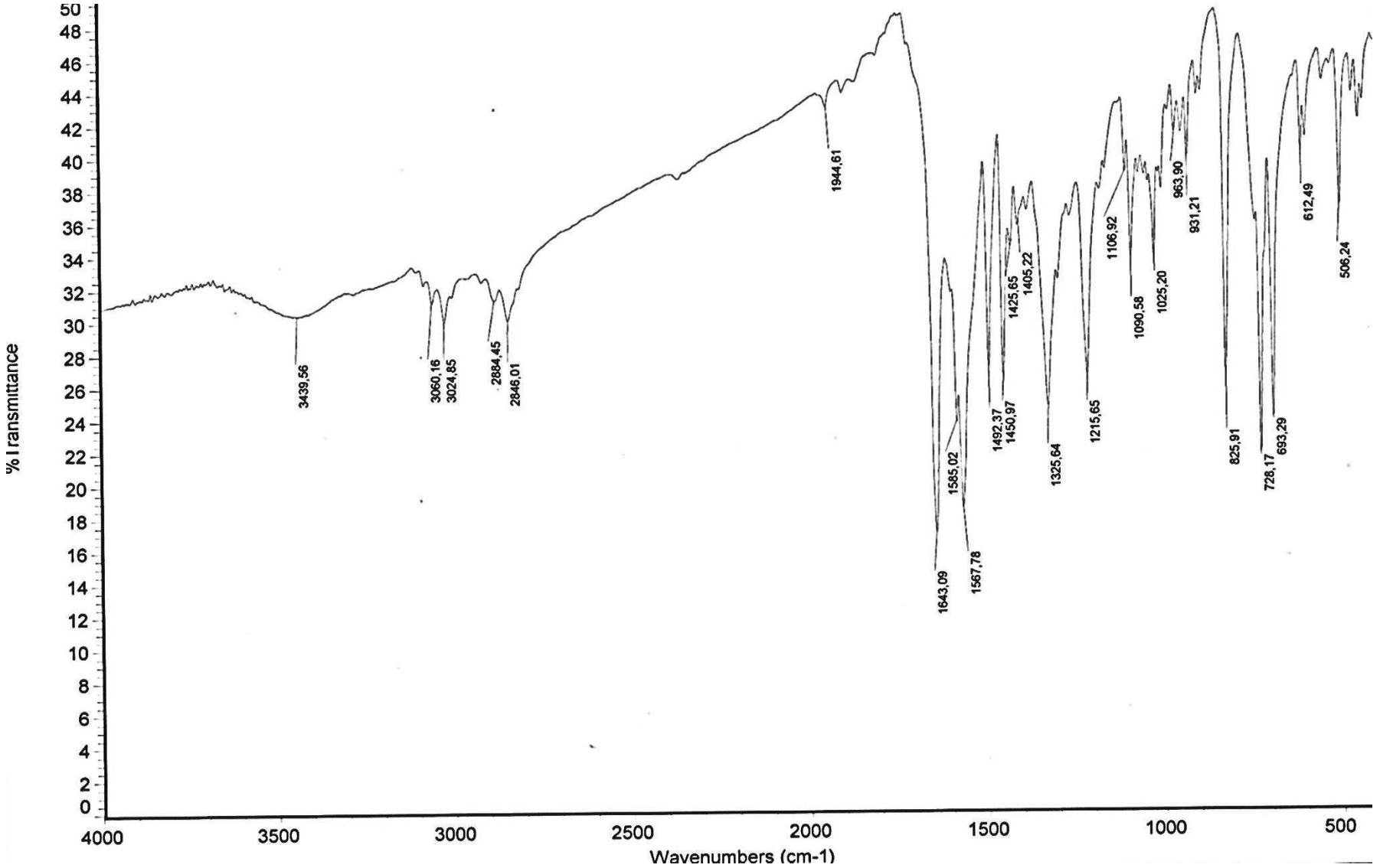

11.452
8.127
8.104
7.877
7.343
7.327
7.306
7.287
7.284
7.270
7.262
7.259
7.251
7.242
4.616
NH
N
H
H
NO2
18a
0.90
1.87
1.92
11.94
4.00
11.50
11.00
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
ppm

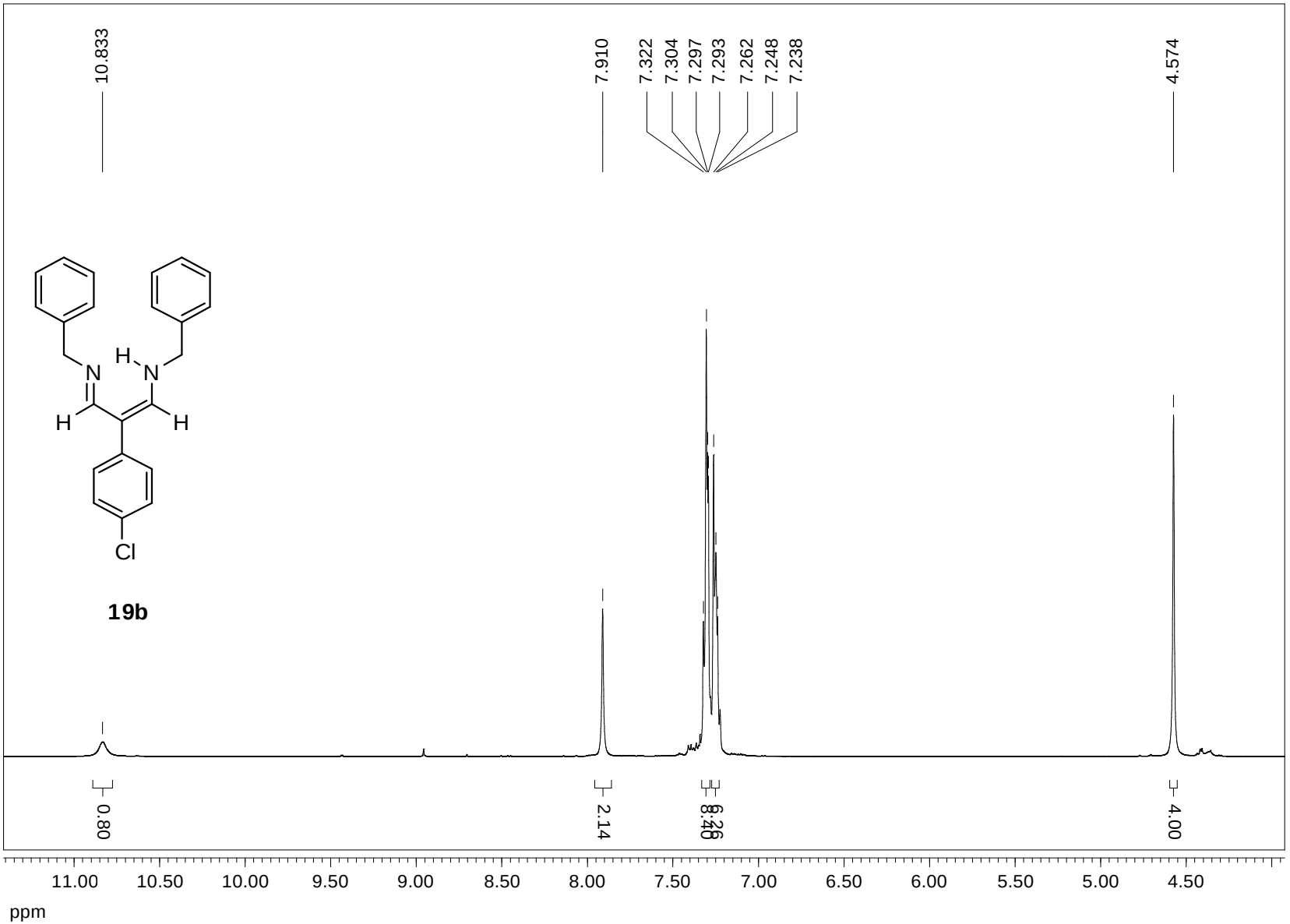

155.117
147.923
139.349
128.606
127.214
127.179
124.300
123.507
103.096
58.724
NH
N
H
H
NO2
18a
150
125
100
75
ppm

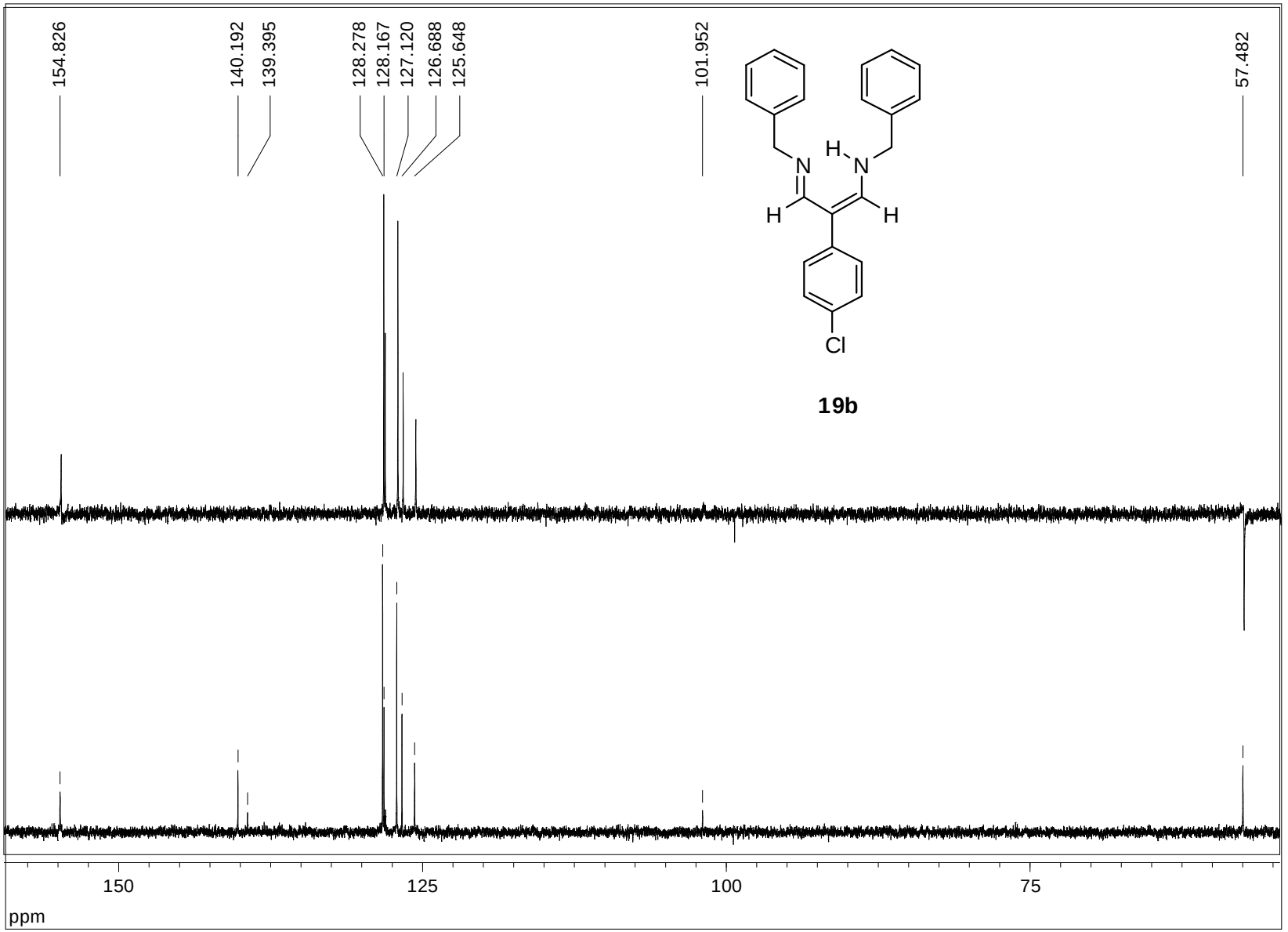

11.504
8.258
8.103
8.085
7.585
7.568
7.334
7.320
7.305
7.278
7.264
7.246
4.649
N
H
N
H
H
NO2
18b
0.84
2.05
1.99
2.05
10.17
4.00
11.50
11.00
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
ppm


155.865
148.021
142.617
139.753
128.336
127.169
126.816
123.979
122.686
101.230
57.600
H
N
N
H
H
NO2
18b
150
125
100
75
50
ppm

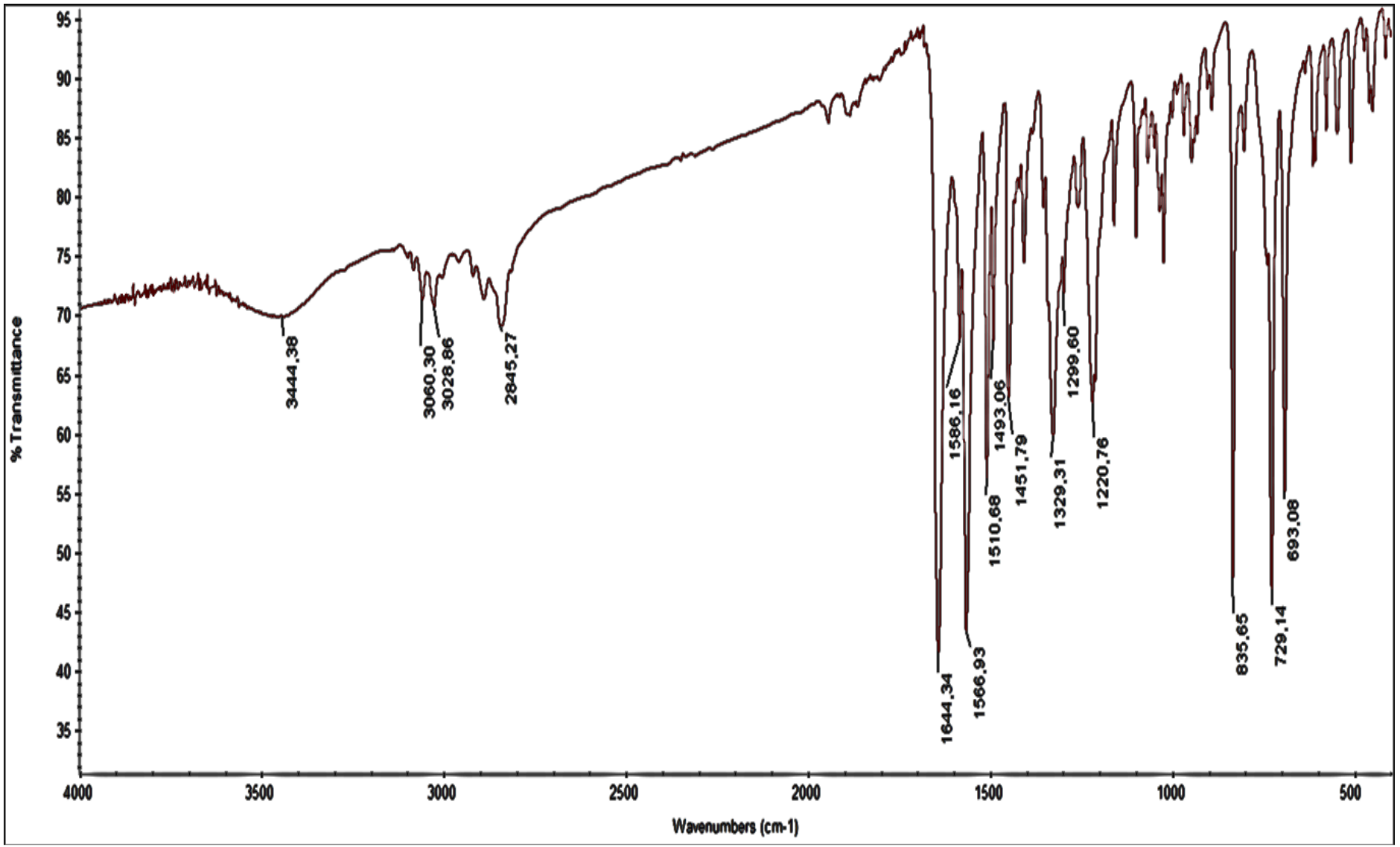
Compound **19**:

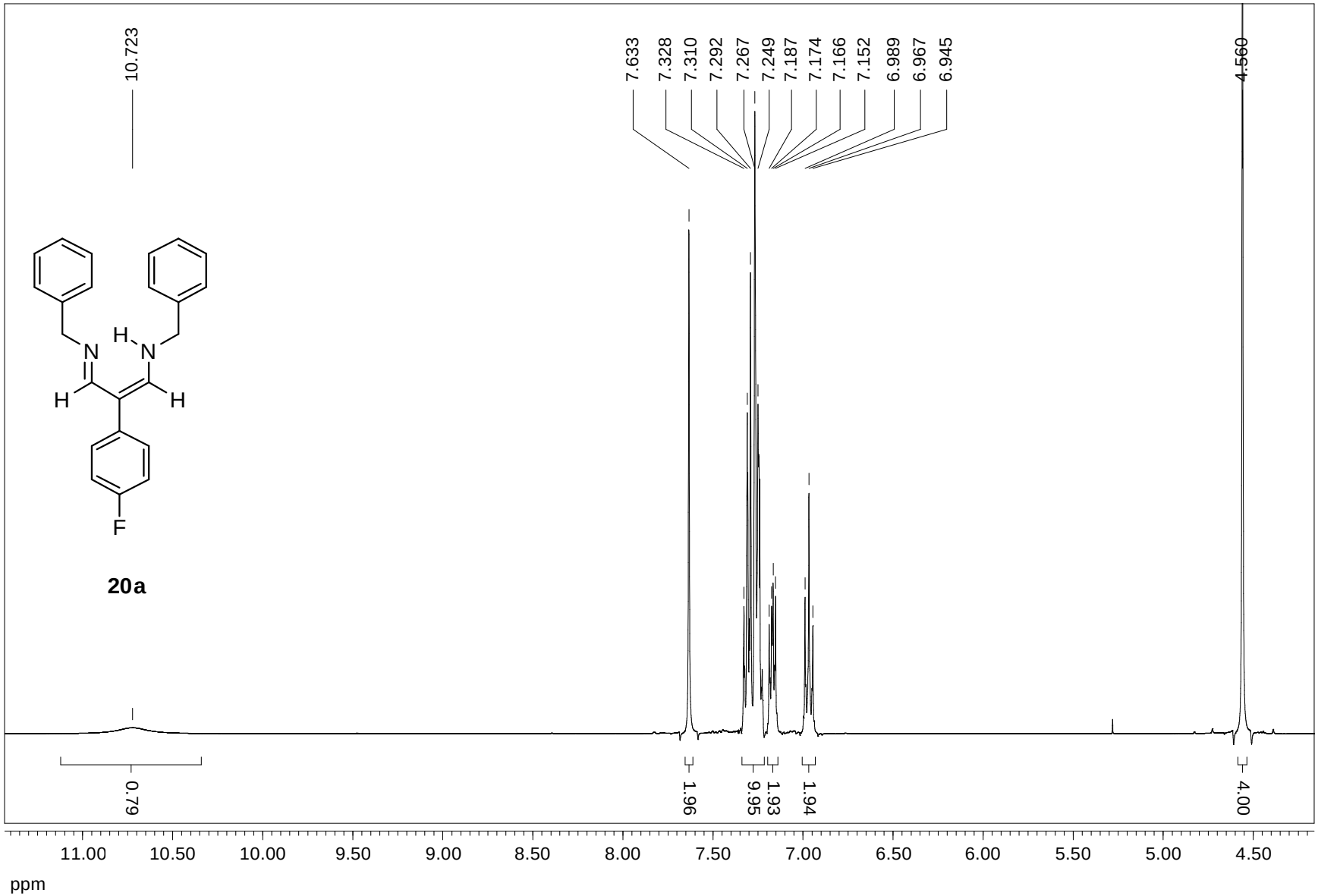

% Transmittance
Wavenumbers (cm-1)
4000
3500
3000
2500
2000
1500
1000
500
3439,56
3060,16
3024,85
2884,45
2846,01
1944,61
1643,09
1585,02
1567,78
1492,37
1450,97
1425,65
1405,22
1325,64
1215,65
1106,92
1090,58
1025,20
963,90
931,21
825,91
728,17
693,29
612,49
506,24

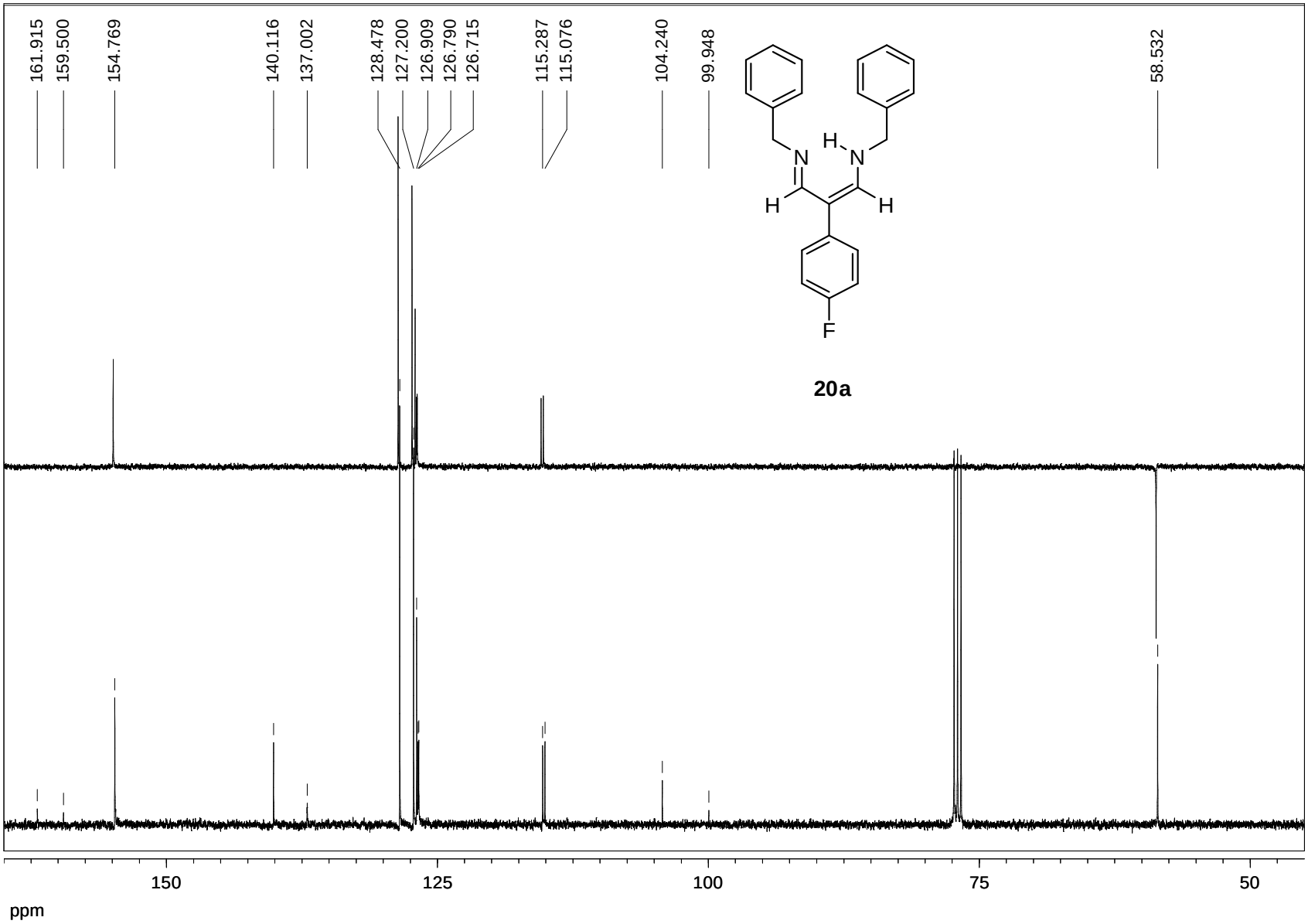

10.833
7.910
7.322
7.304
7.297
7.293
7.262
7.248
7.238
4.574
H
N
N
H
H
Cl
19b
0.80
2.14
8.40
6.26
4.00
11.00
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
ppm

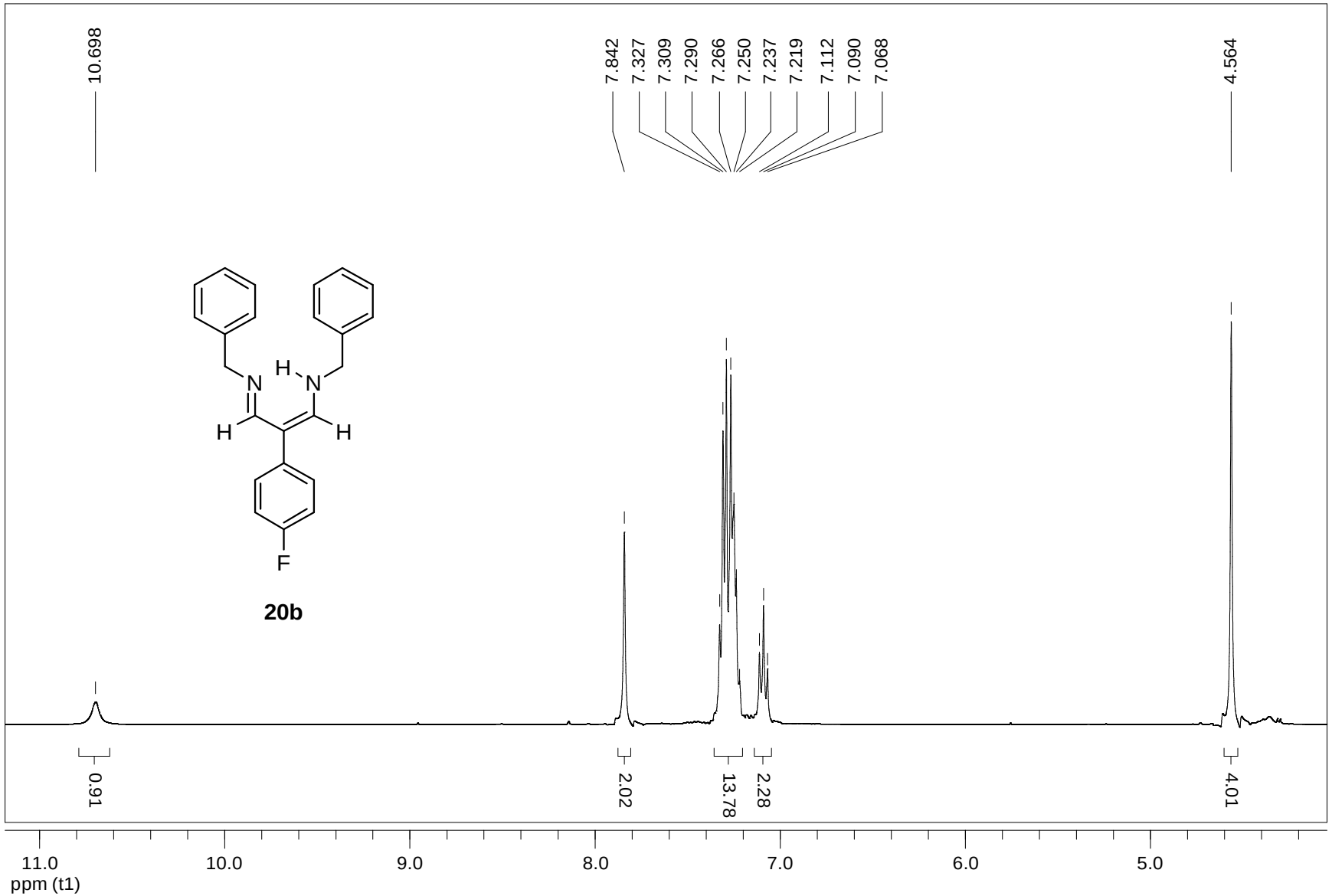

154.826
140.192
139.395
128.278
128.167
127.120
126.688
125.648
101.952
57.482
N
H
N
H
H
Cl
19b
150
125
100
75
ppm

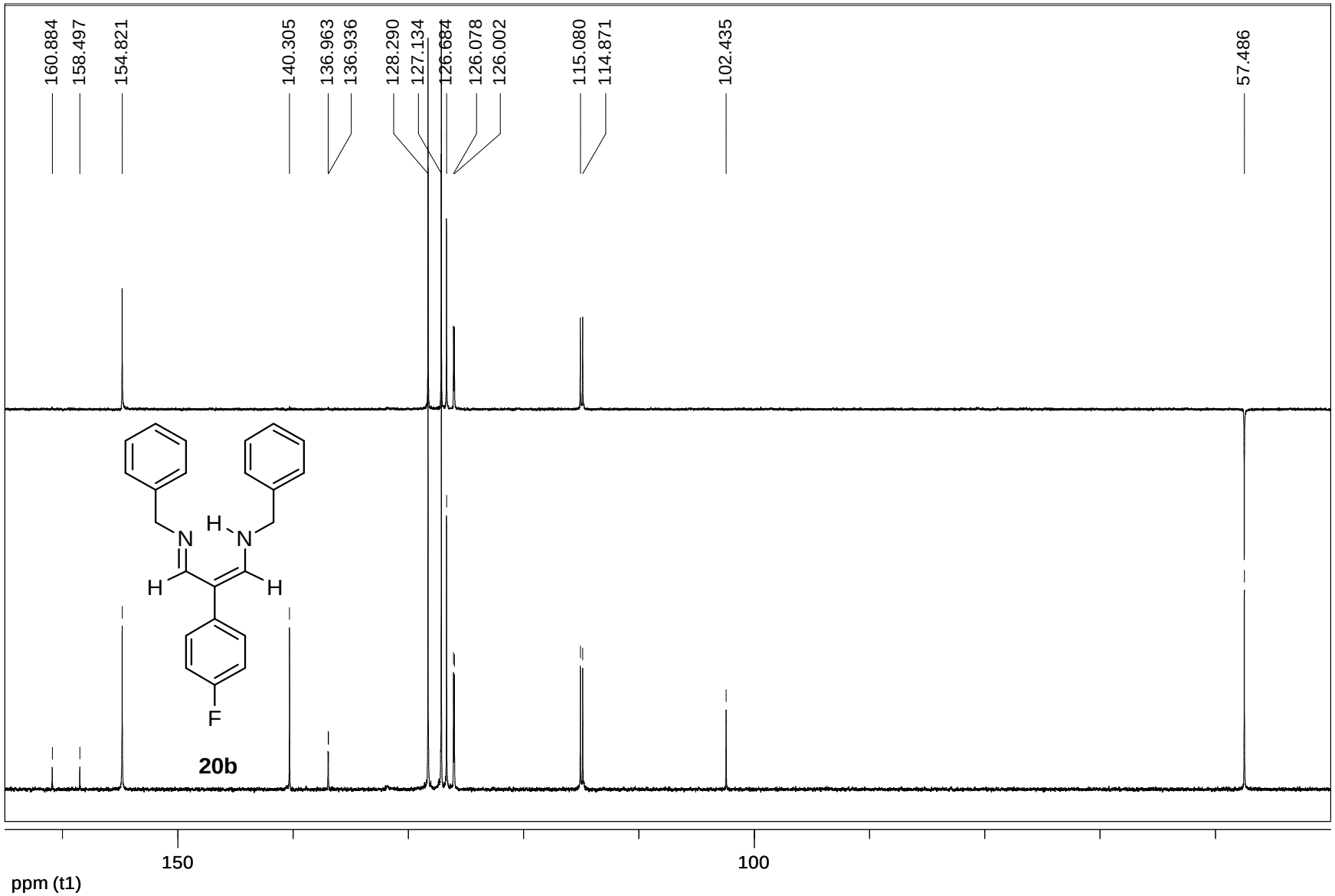
Compound **20**:


% Transmittance
Wavenumbers (cm-1)
4000
3500
3000
2500
2000
1500
1000
500
95
90
85
80
75
70
65
60
55
50
45
40
35
3444.38
3060.30
3028.86
2845.27
1644.34
1586.16
1566.93
1510.68
1493.06
1451.79
1329.31
1299.60
1220.76
835.65
729.14
693.08

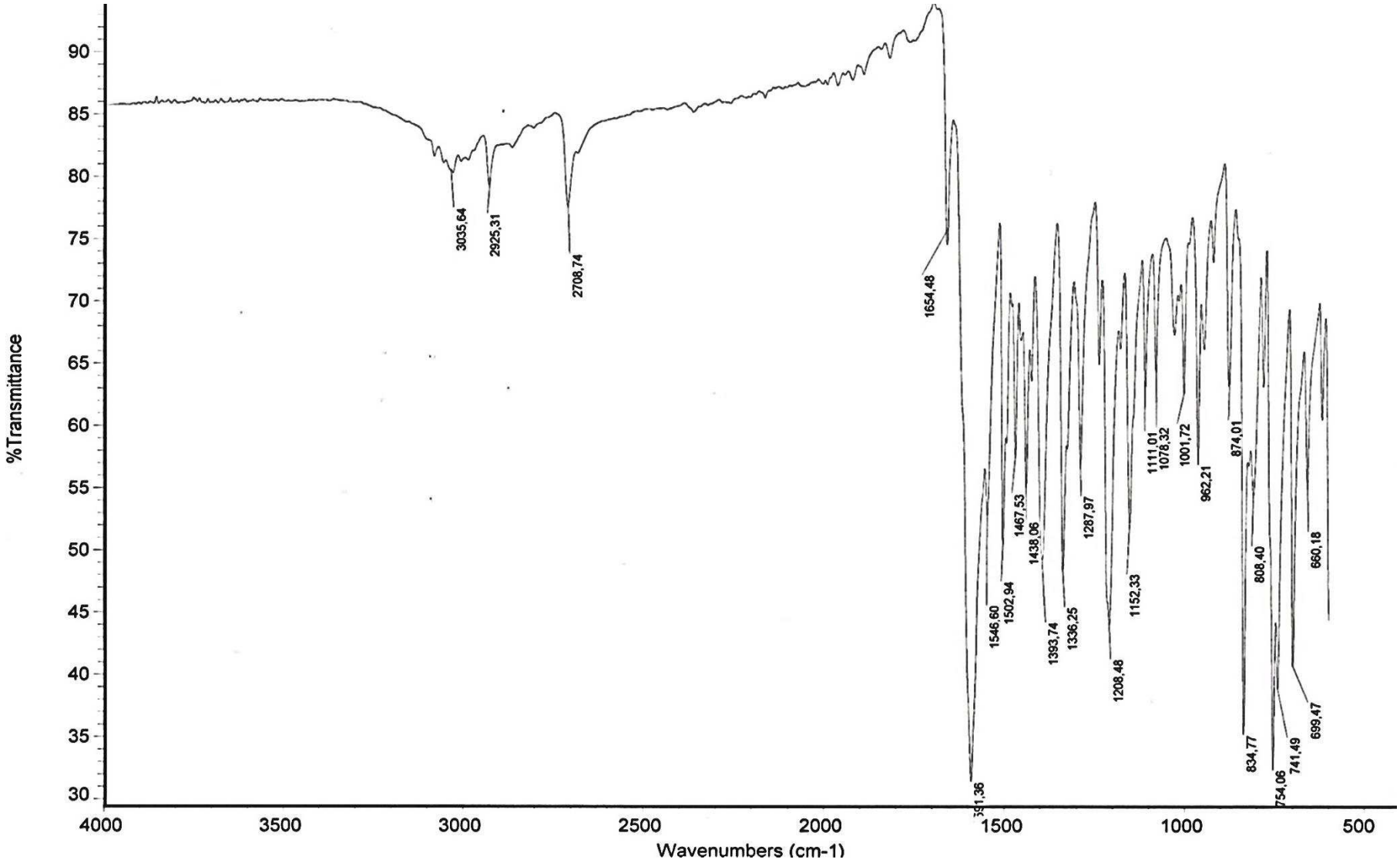

10.723
7.633
7.328
7.310
7.292
7.267
7.249
7.187
7.174
7.166
7.152
6.989
6.967
6.945
4.560
H
N
N
H
H
F
20a
0.79
1.96
9.95
1.93
1.94
4.00
11.00
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
ppm

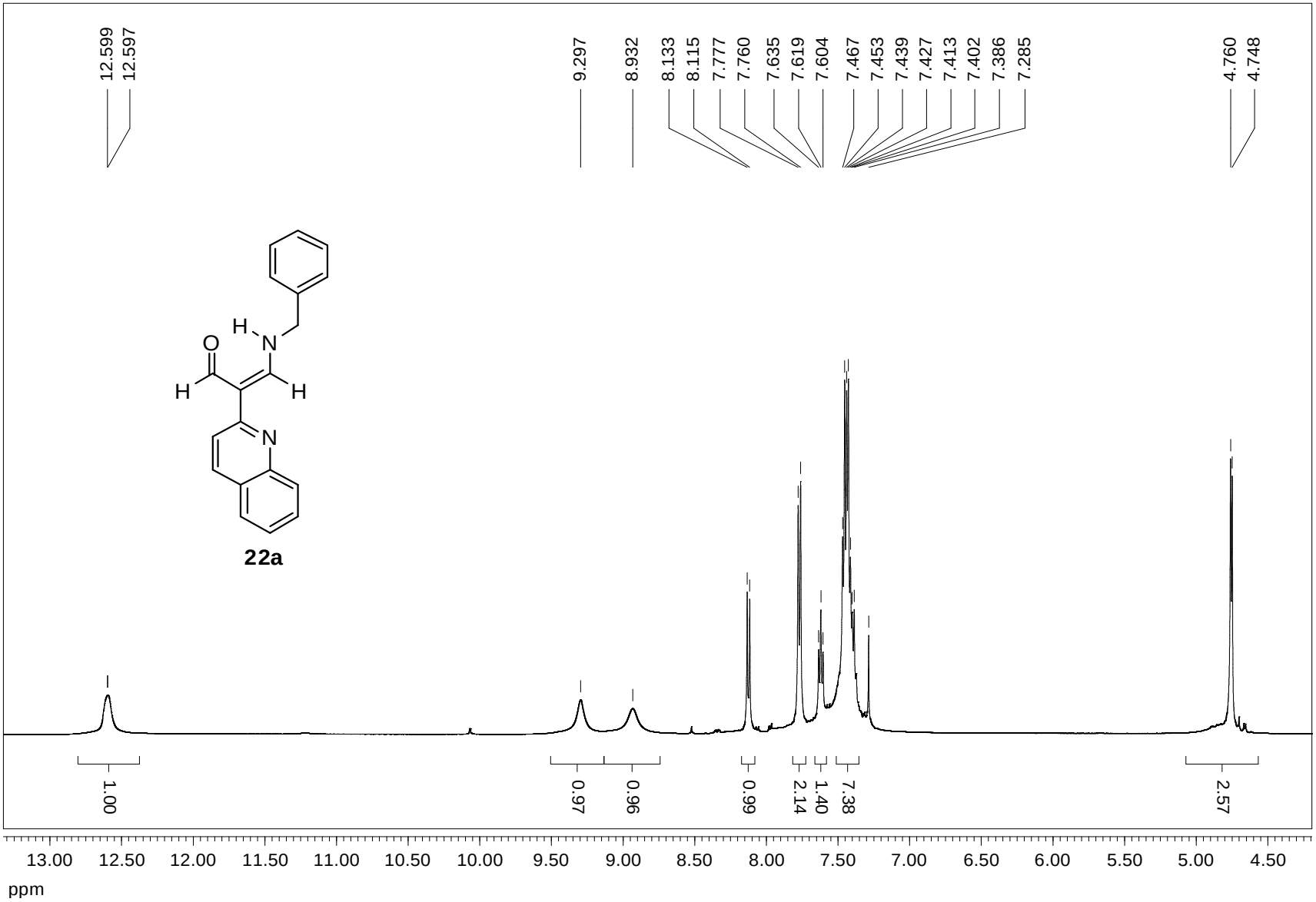

161.915
159.500
154.769
140.116
137.002
128.478
127.200
126.909
126.790
126.715
115.287
115.076
104.240
99.948
58.532
N
H
N
H
H
F
20a
150
125
100
75
50
ppm

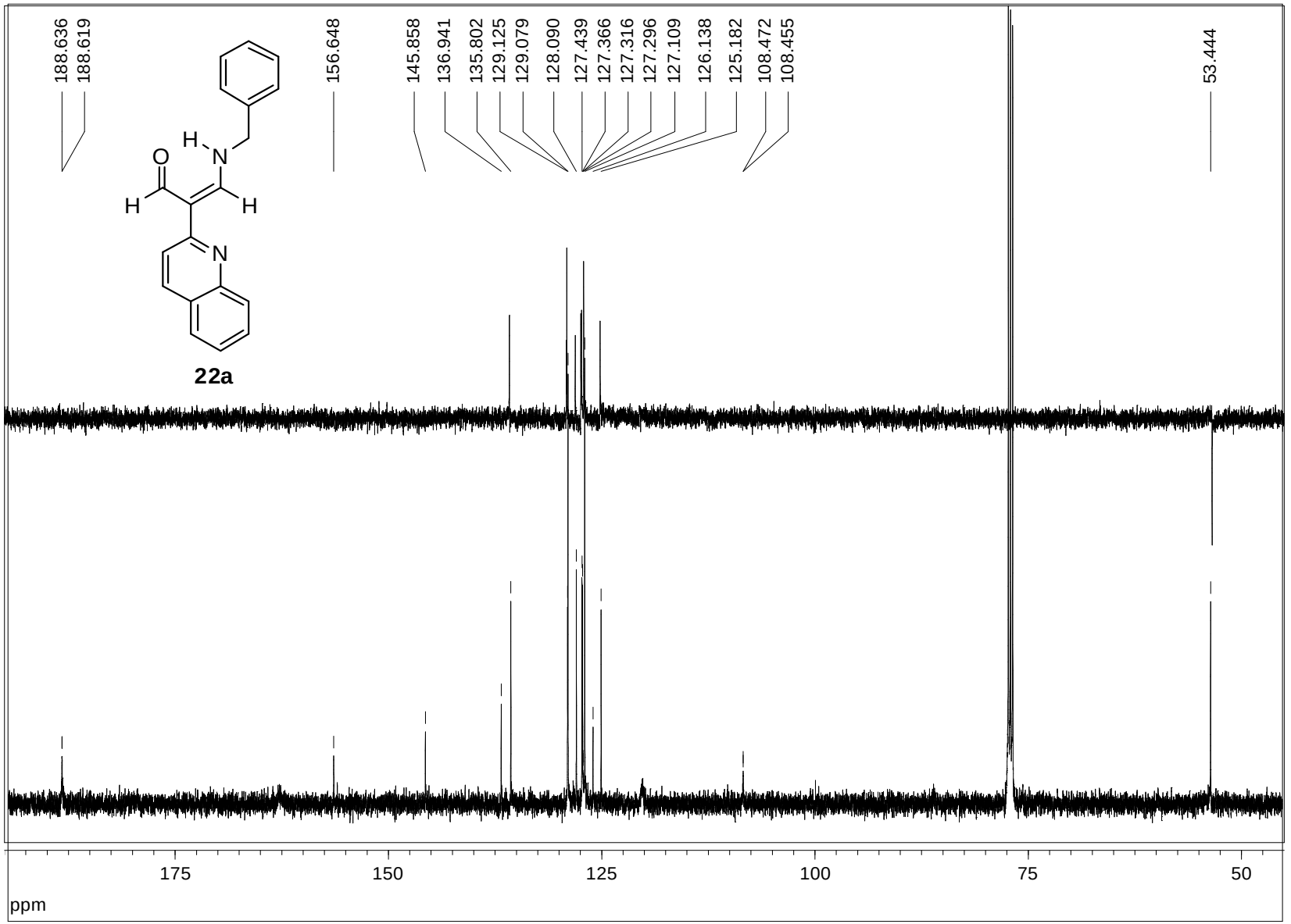

10.698
7.842
7.327
7.309
7.290
7.266
7.250
7.237
7.219
7.112
7.090
7.068
4.564
H
N
N
H
H
F
20b
0.91
2.02
13.78
2.28
4.01
11.0
10.0
9.0
8.0
7.0
6.0
5.0
ppm (t1)

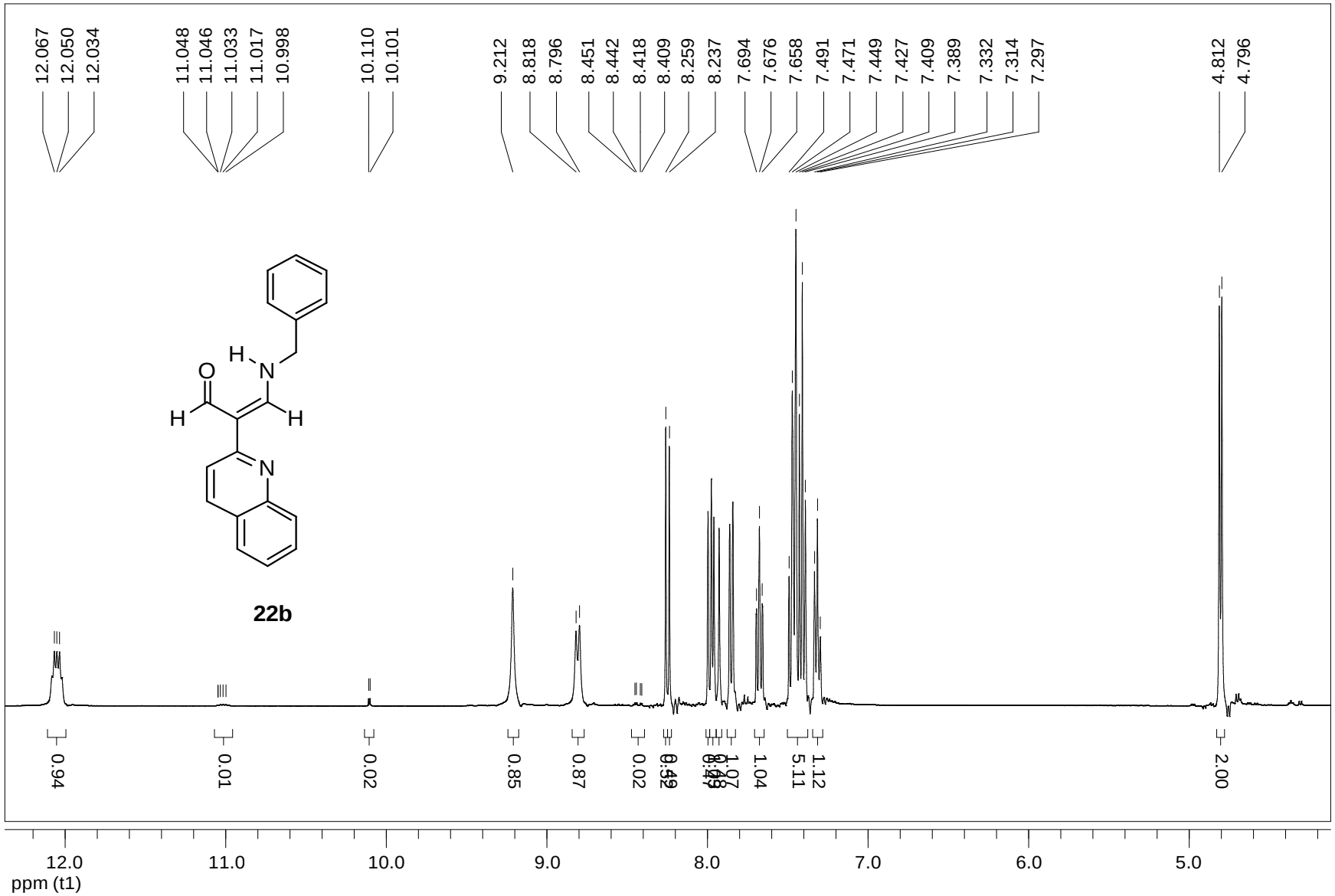

160.884
158.497
154.821
140.305
136.963
136.936
128.290
127.134
126.684
126.078
126.002
115.080
114.871
102.435
57.486
H
N
N
H
H
F
20b
150
100
ppm (t1)

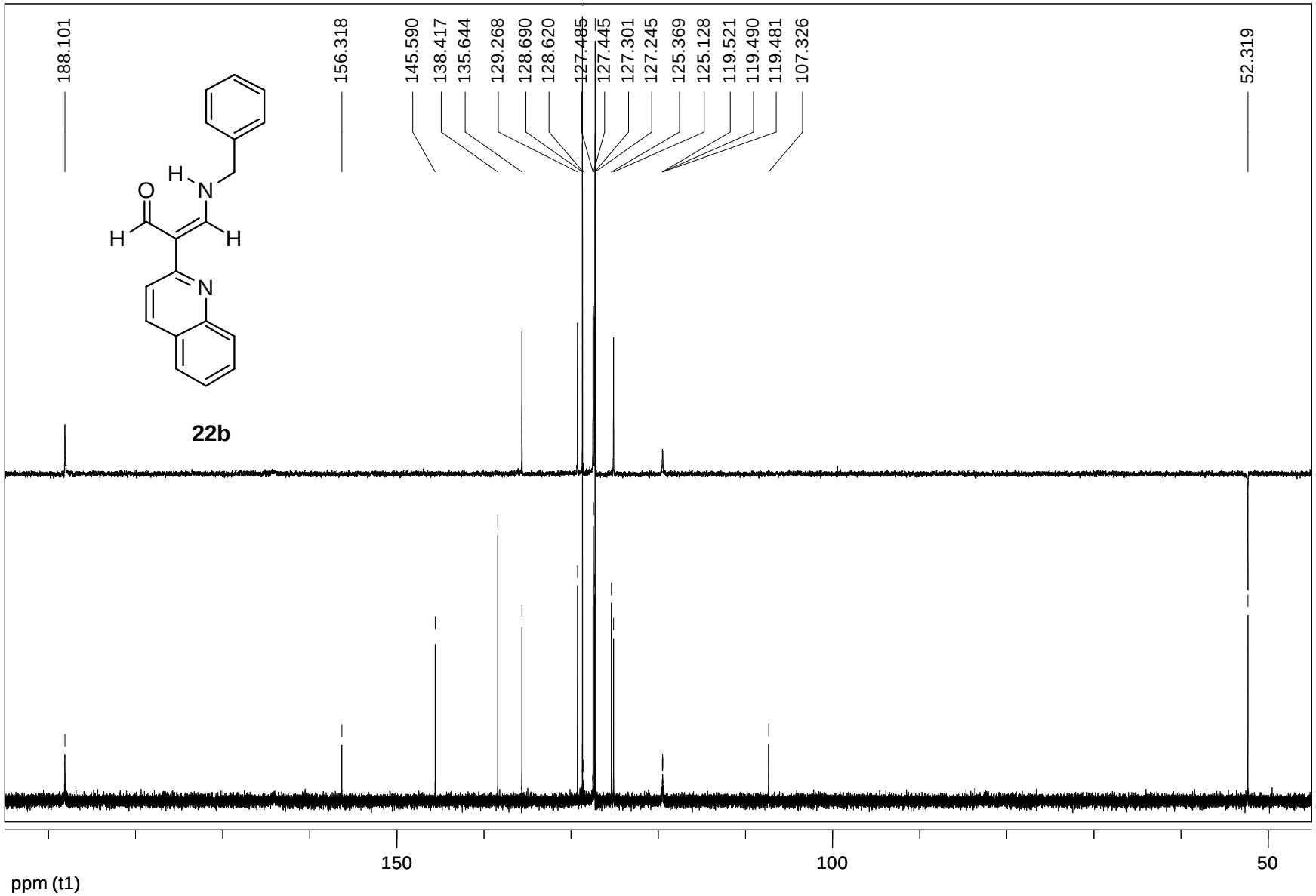
Compound **22**:


%Transmittance
Wavenumbers (cm-1)
3035,64
2925,31
2708,74
1654,48
1546,60
1502,94
1467,53
1438,06
1393,74
1336,25
1287,97
1208,48
1152,33
1111,01
1078,32
1001,72
962,21
874,01
834,77
808,40
754,06
741,49
699,47
660,18

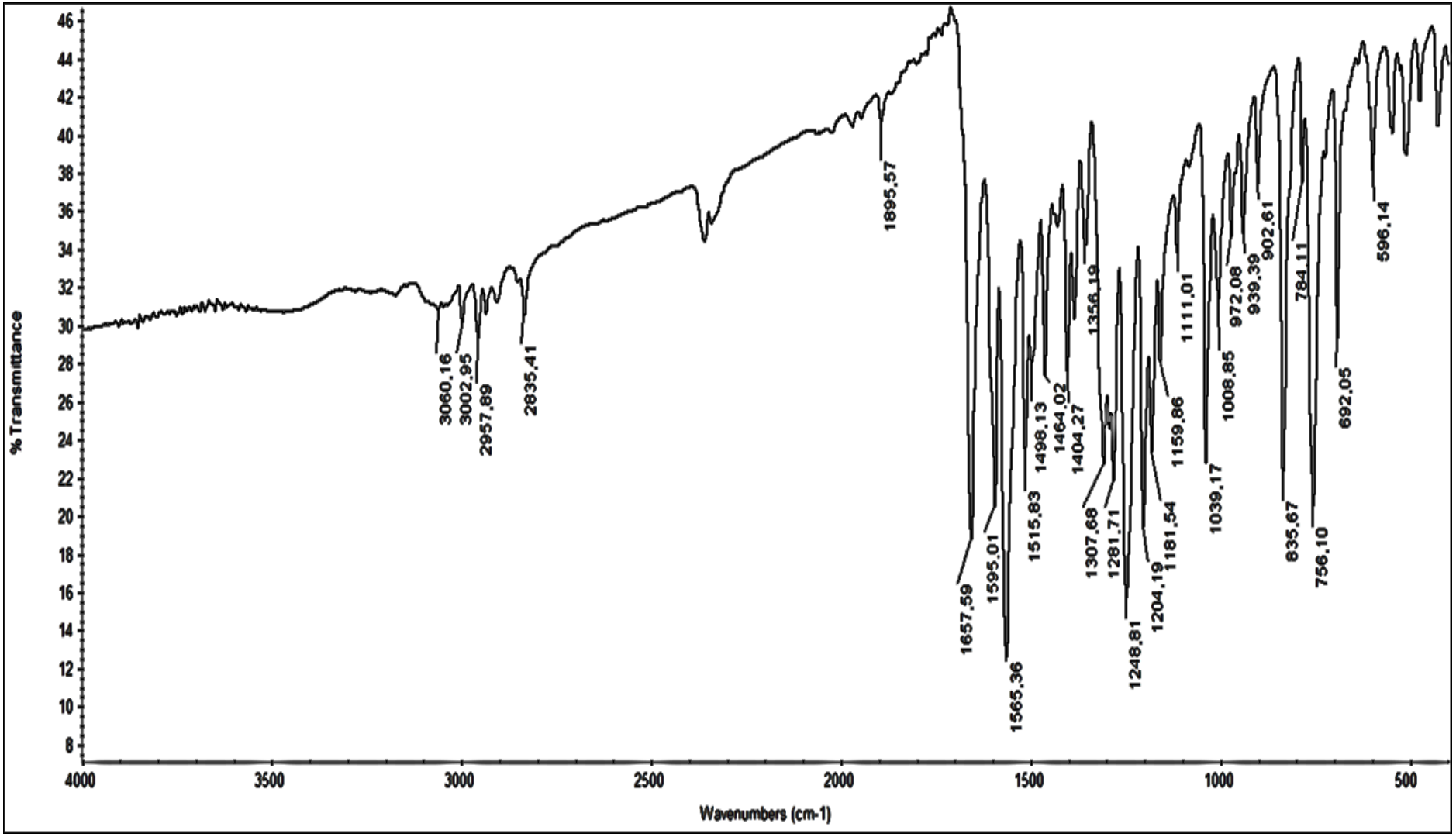

12.599
12.597
9.297
8.932
8.133
8.115
7.777
7.760
7.635
7.619
7.604
7.467
7.453
7.439
7.427
7.413
7.402
7.386
7.285
4.760
4.748
22a
1.00
0.97
0.96
0.99
2.14
1.40
7.38
2.57
13.00
12.50
12.00
11.50
11.00
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
ppm

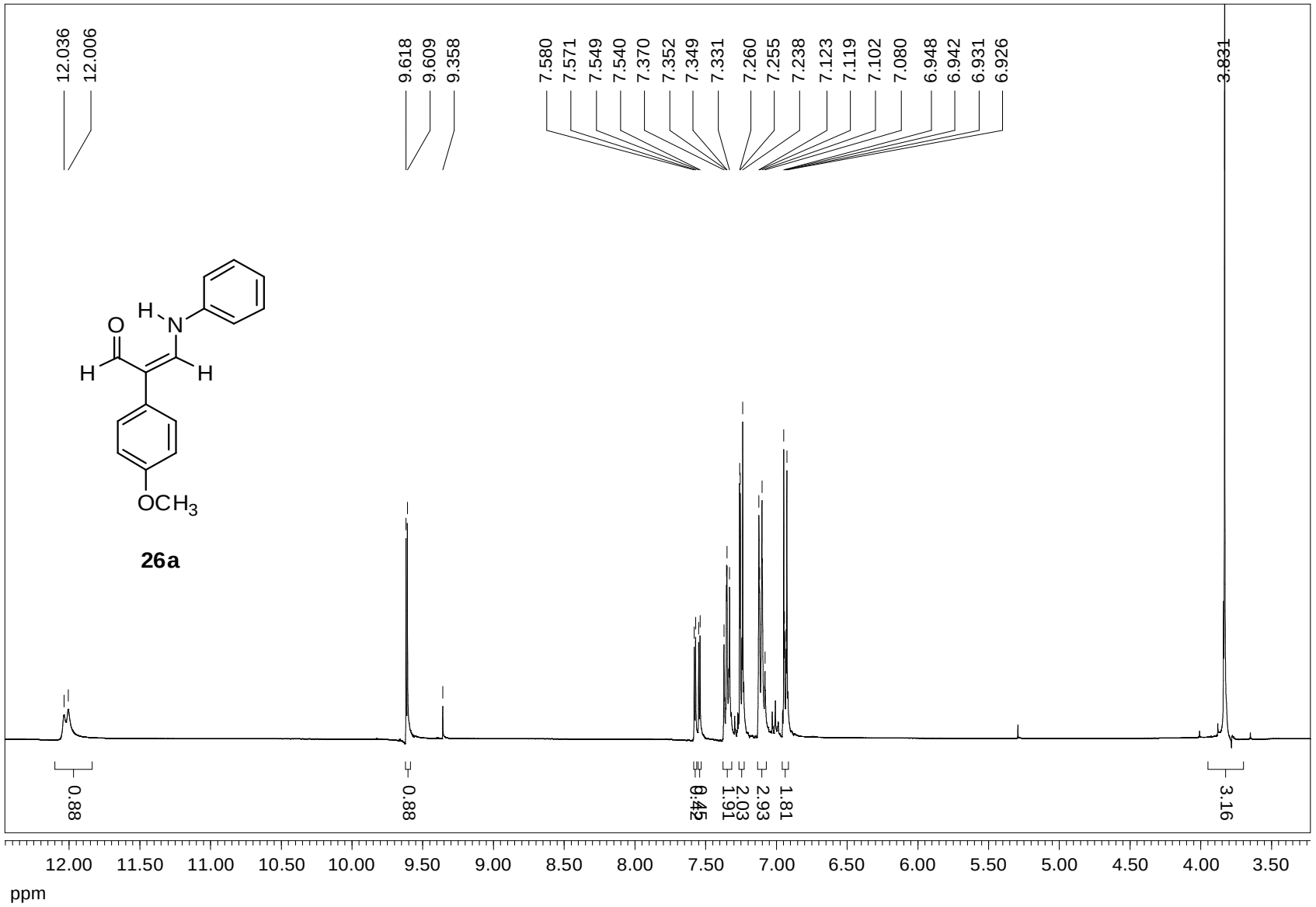

188.636
188.619
156.648
145.858
136.941
135.802
129.125
129.079
128.090
127.439
127.366
127.316
127.296
127.109
126.138
125.182
108.472
108.455
53.444
H
N
O
H
H
N
22a
175
150
125
100
75
50
ppm

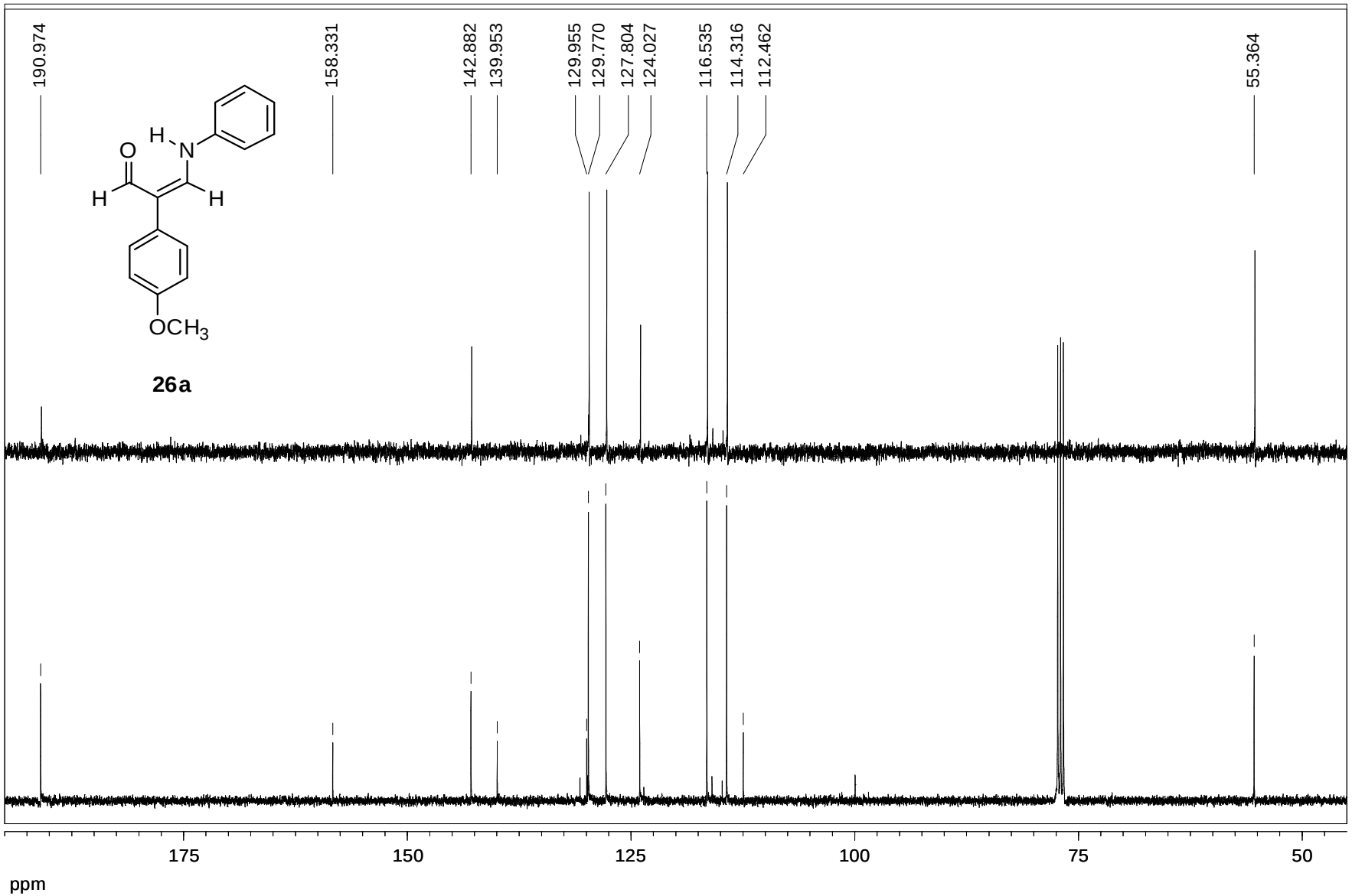

12.067
12.050
12.034
11.048
11.046
11.033
11.017
10.998
10.110
10.101
9.212
8.818
8.796
8.451
8.442
8.418
8.409
8.259
8.237
7.694
7.676
7.658
7.491
7.471
7.449
7.427
7.409
7.389
7.332
7.314
7.297
4.812
4.796
H
N
O
H
H
N
22b
0.94
0.01
0.02
0.85
0.87
0.02
1.04
5.11
1.12
2.00
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
ppm (t1)

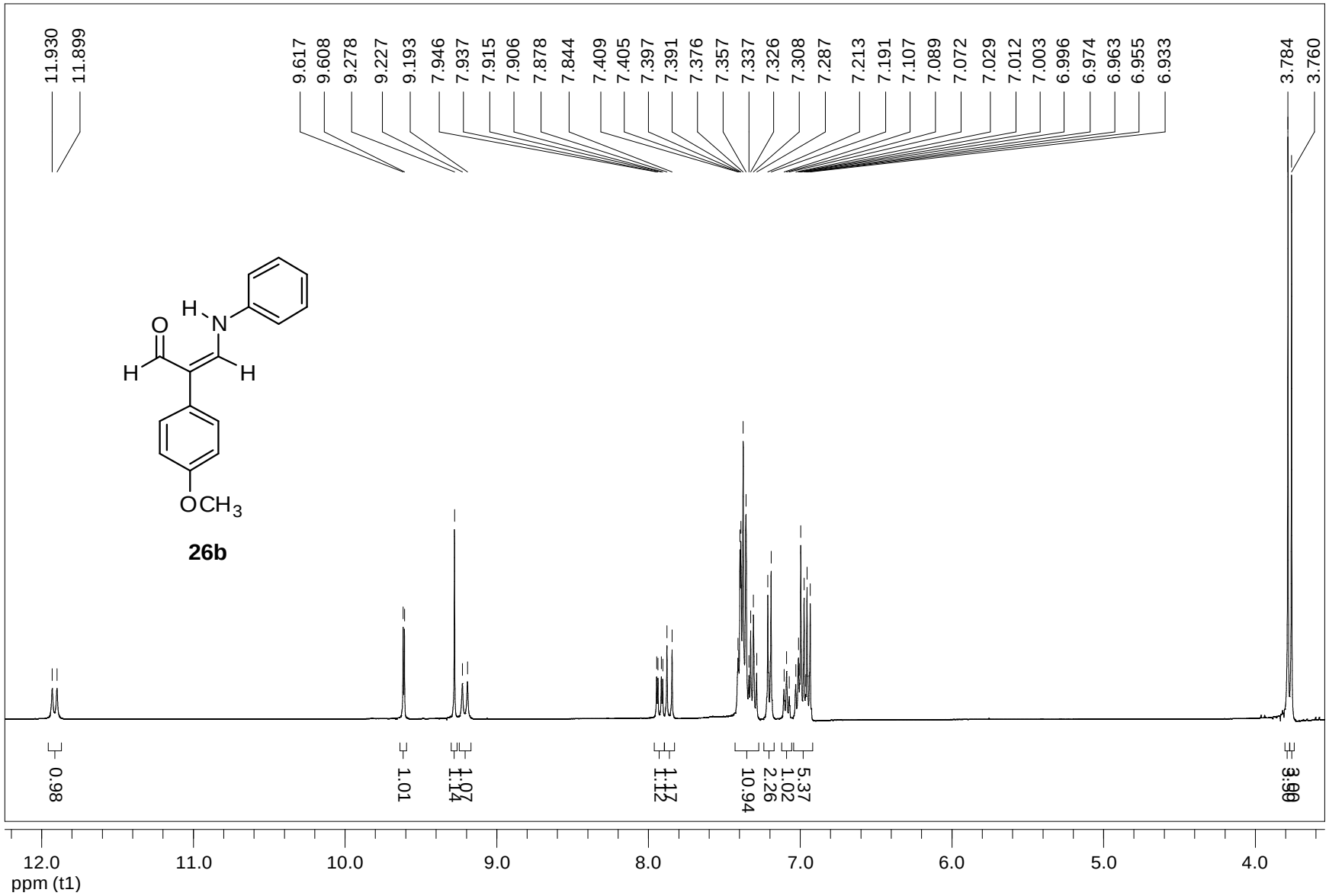

188.101
156.318
145.590
138.417
135.644
129.268
128.690
128.620
127.485
127.445
127.301
127.245
125.369
125.128
119.521
119.490
119.481
107.326
52.319
22b
150
100
50
ppm (t1)

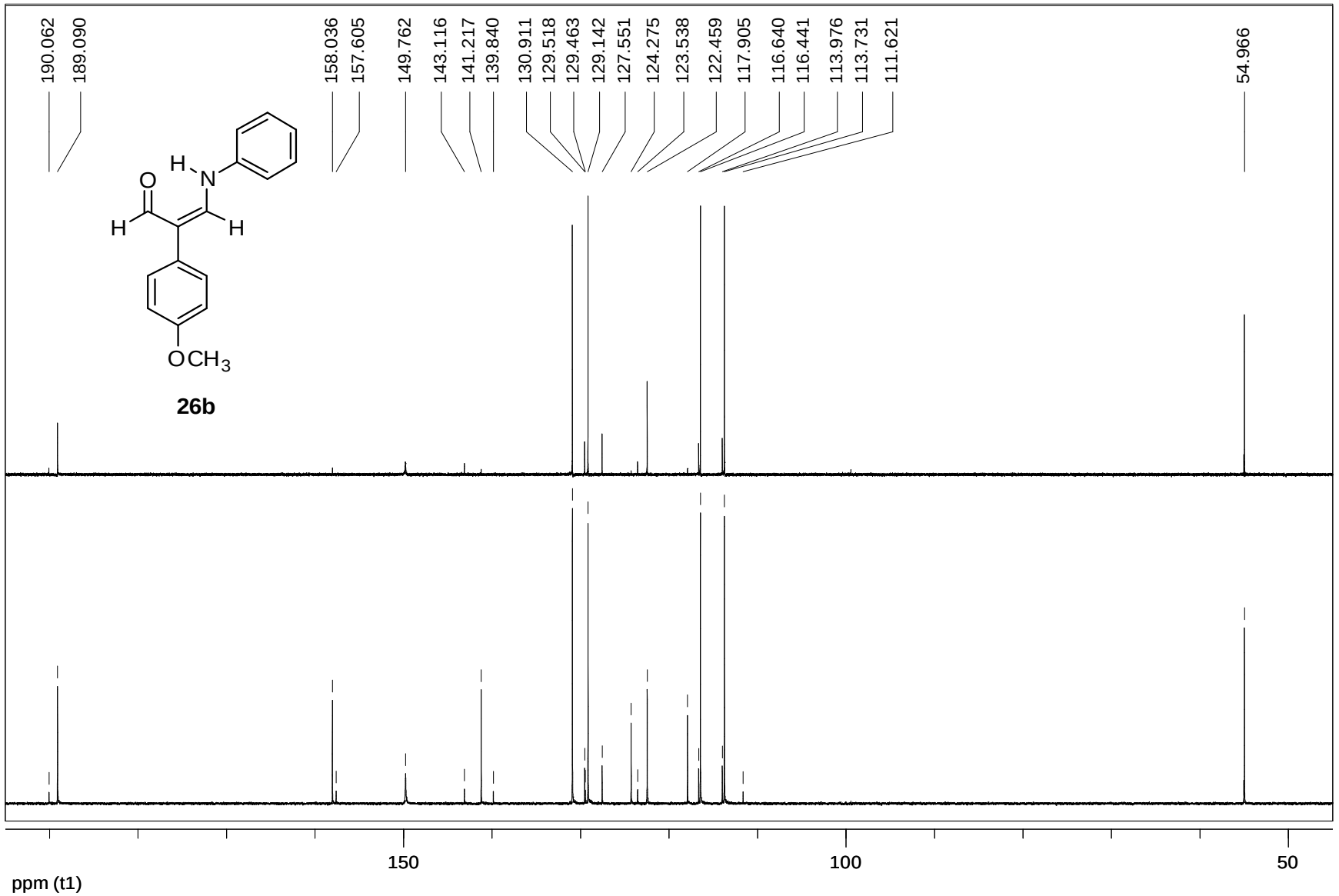
Compound **26**:


% Transmittance
Wavenumbers (cm-1)
4000
3500
3000
2500
2000
1500
1000
500
3060.16
3002.95
2957.89
2835.41
1895.57
1657.59
1595.01
1565.36
1515.83
1498.13
1464.02
1404.27
1356.19
1307.68
1281.71
1248.81
1204.19
1181.54
1159.86
1111.01
1039.17
1008.85
972.08
939.39
902.61
835.67
784.11
756.10
692.05
596.14

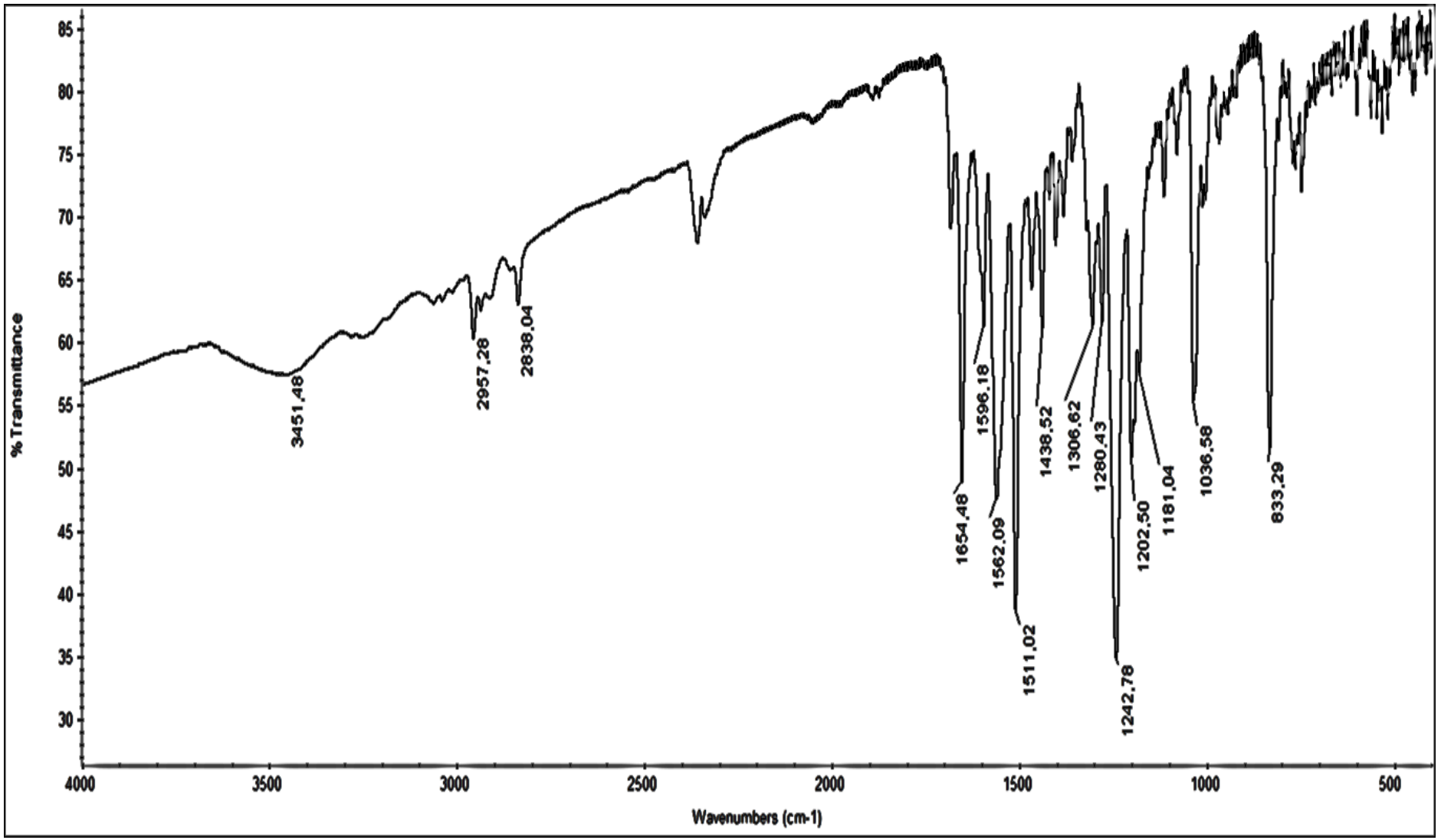

12.036
12.006
9.618
9.609
9.358
7.580
7.571
7.549
7.540
7.370
7.352
7.349
7.331
7.260
7.255
7.238
7.123
7.119
7.102
7.080
6.948
6.942
6.931
6.926
3.831
H
N
O
H
H
OCH3
26a
0.88
0.88
0.45
2.03
1.91
2.93
1.81
3.16
12.00
11.50
11.00
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
4.00
3.50
ppm

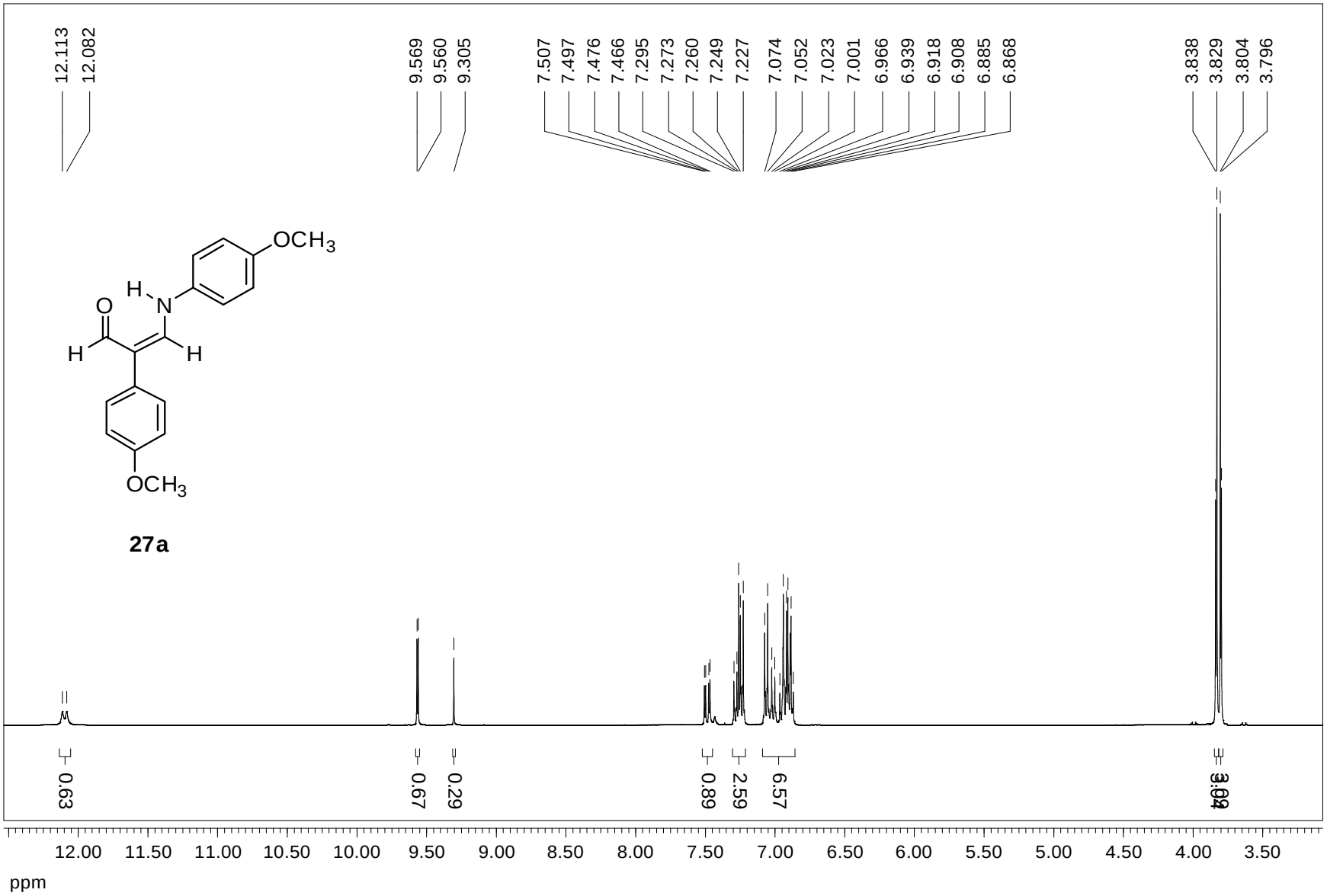

190.974
158.331
142.882
139.953
129.955
129.770
127.804
124.027
116.535
114.316
112.462
55.364
H
N
O
H
H
OCH3
26a
175
150
125
100
75
50
ppm

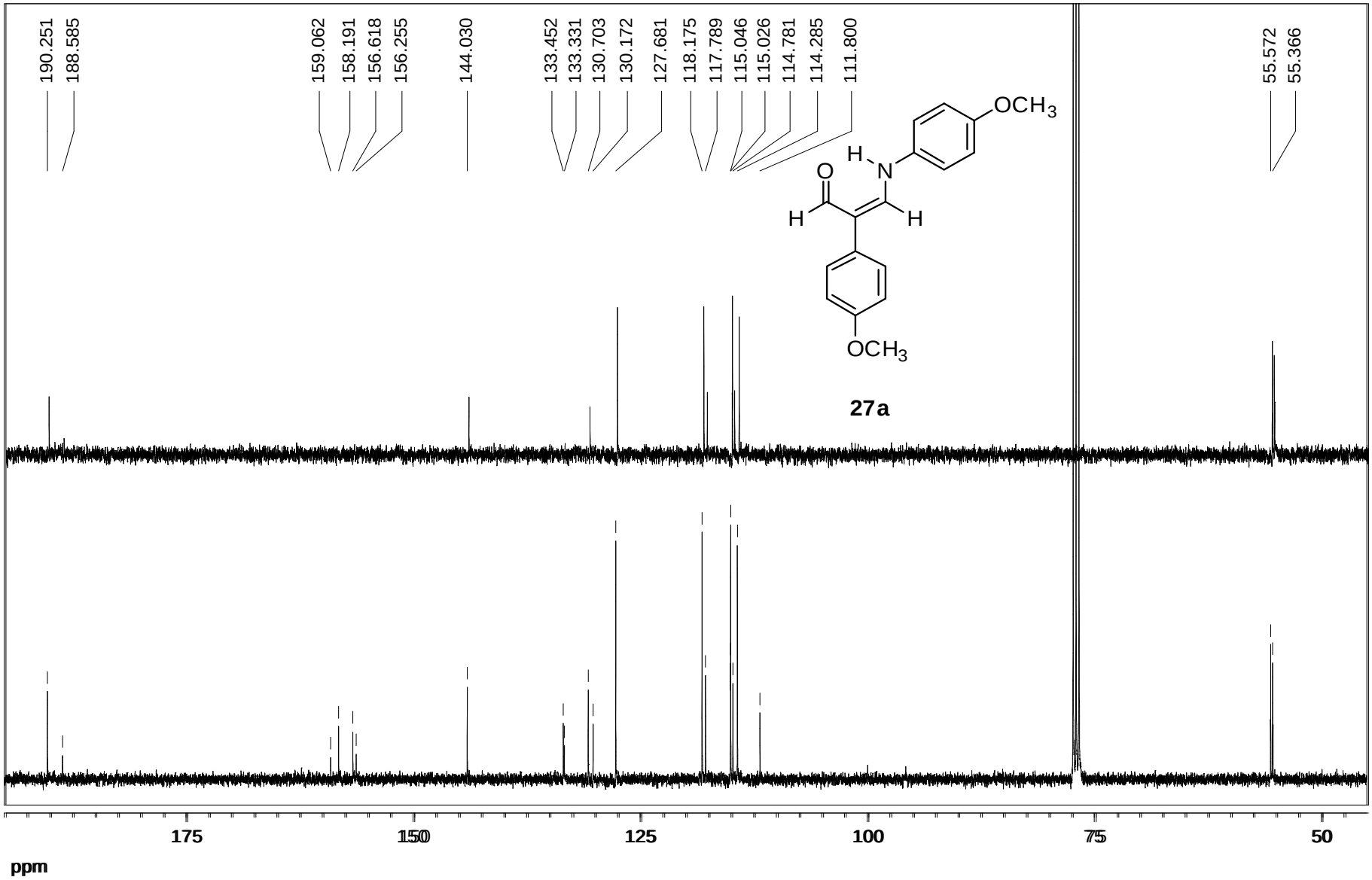

11.930
11.899
9.617
9.608
9.278
9.227
9.193
7.946
7.937
7.915
7.906
7.878
7.844
7.409
7.405
7.397
7.391
7.376
7.357
7.337
7.326
7.308
7.287
7.213
7.191
7.107
7.089
7.072
7.029
7.012
7.003
6.996
6.974
6.963
6.955
6.933
3.784
3.760
H
N
O
H
H
OCH3
26b
0.98
1.01
1.07
1.14
1.12
1.17
10.94
2.26
1.02
5.37
3.00
3.00
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
ppm (t1)

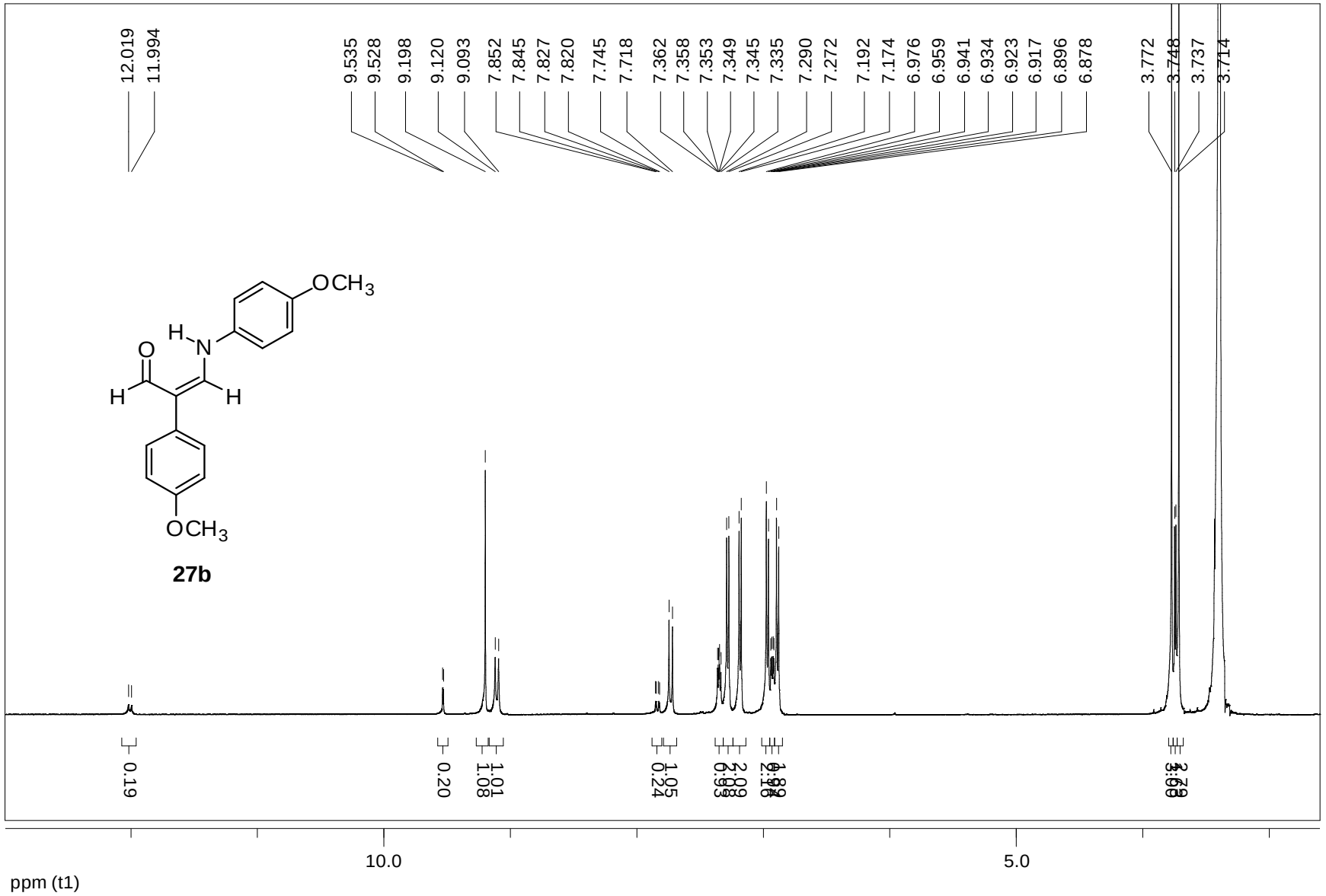

190.062
189.090
158.036
157.605
149.762
143.116
141.217
139.840
130.911
129.518
129.463
129.142
127.551
124.275
123.538
122.459
117.905
116.640
116.441
113.976
113.731
111.621
54.966
H
N
O
H
H
OCH3
26b
150
100
50
ppm (t1)

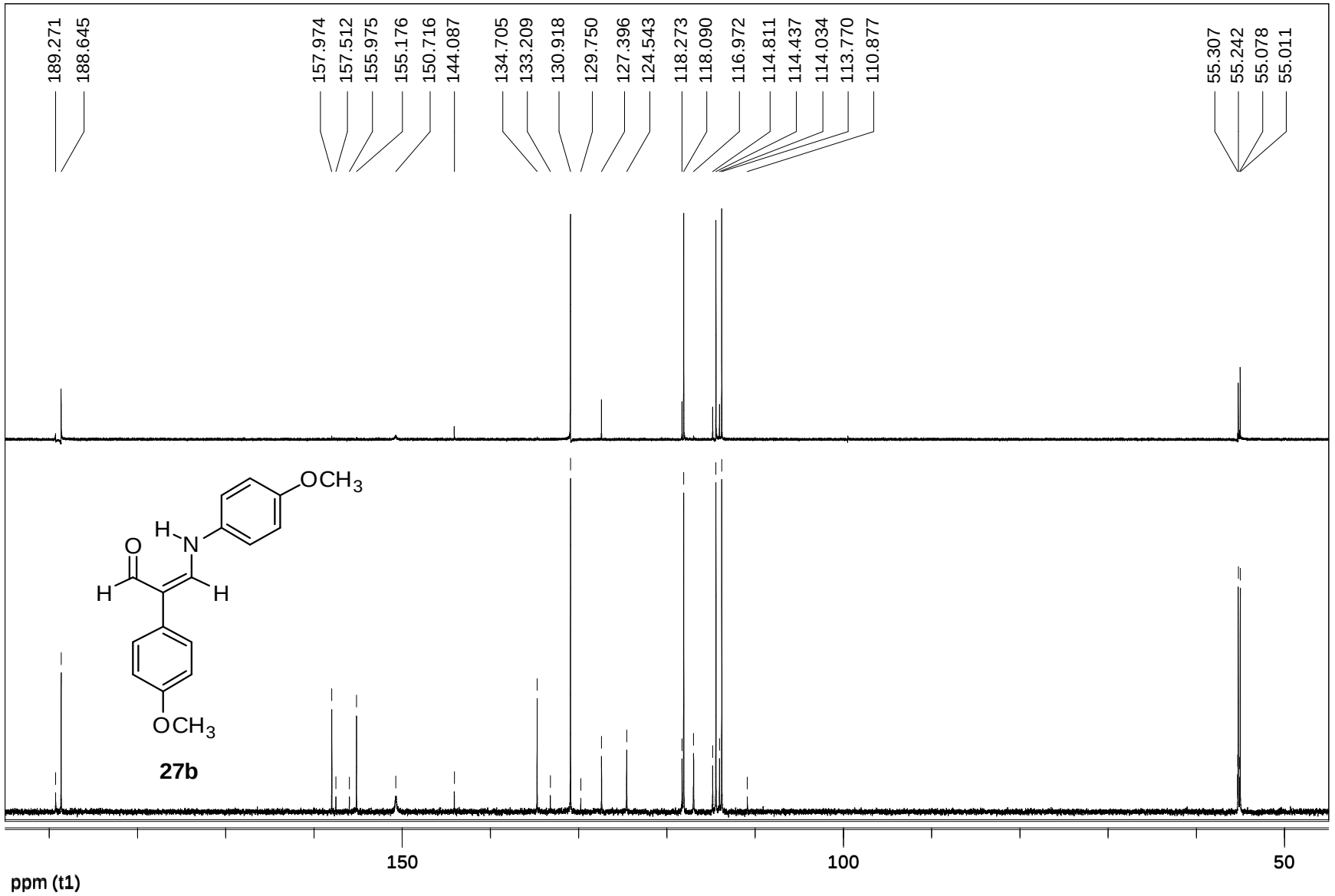
Compound **27**:


% Transmittance
Wavenumbers (cm-1)
3451.48
2957.28
2838.04
1654.48
1596.18
1562.09
1511.02
1438.52
1306.62
1280.43
1242.78
1202.50
1181.04
1036.58
833.29

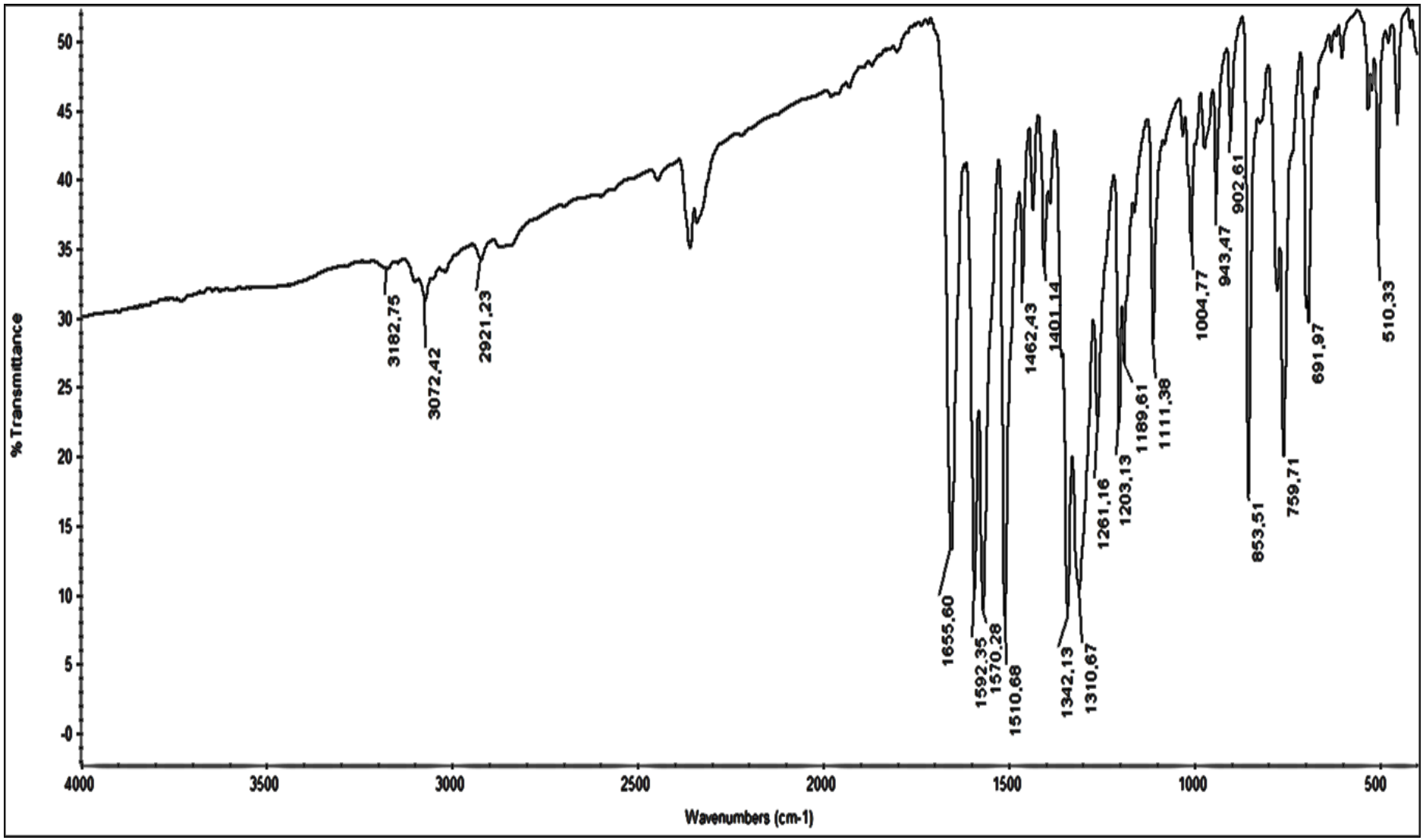

12.113
12.082
9.569
9.560
9.305
7.507
7.497
7.476
7.466
7.295
7.273
7.260
7.249
7.227
7.074
7.052
7.023
7.001
6.966
6.939
6.918
6.908
6.885
6.868
3.838
3.829
3.804
3.796
OCH3
H
N
O
H
H
OCH3
27a
0.63
0.67
0.29
0.89
2.59
6.57
3.00
3.04
12.00
11.50
11.00
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
4.00
3.50
ppm

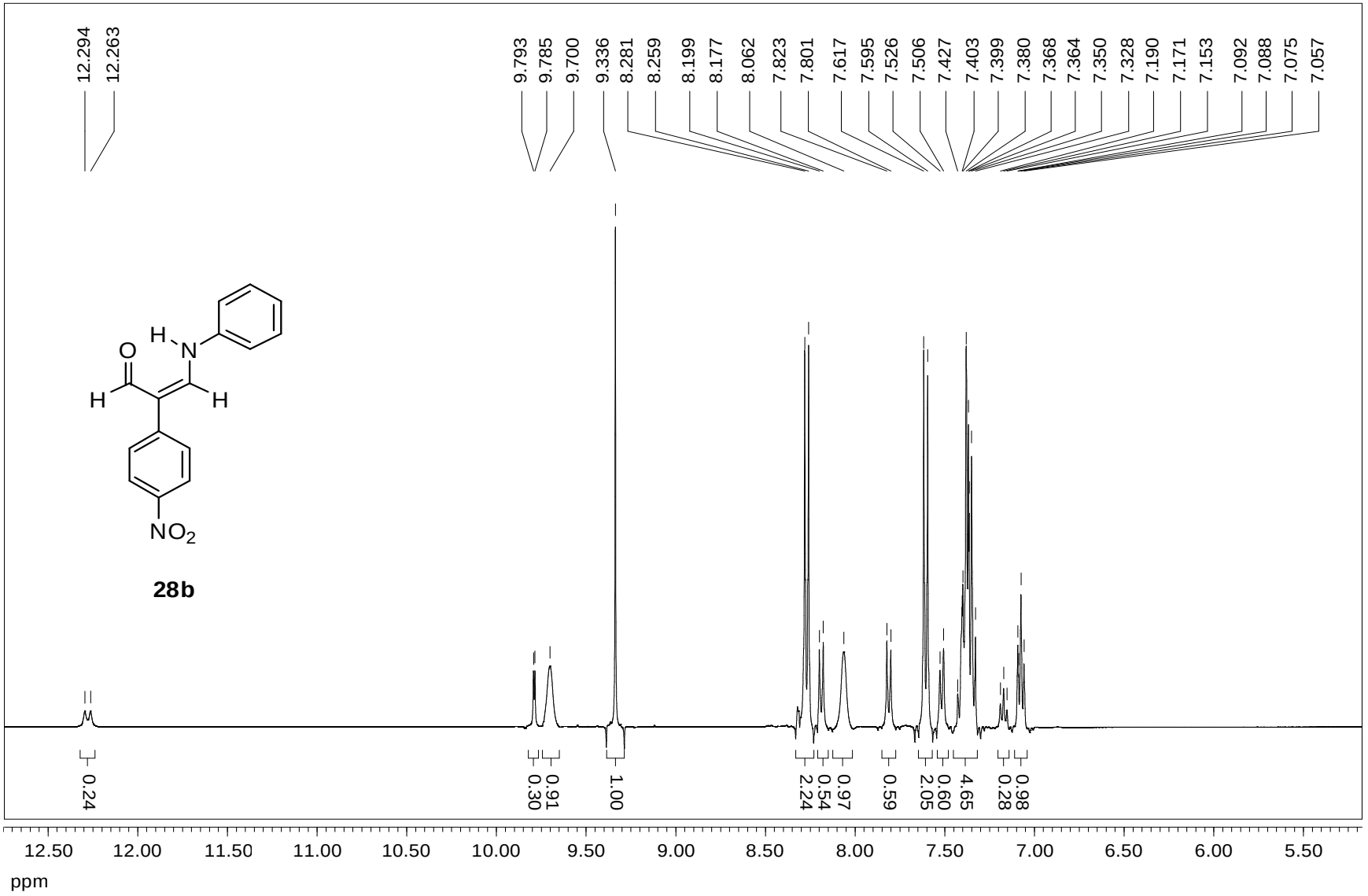

190.251
188.585
159.062
158.191
156.618
156.255
144.030
133.452
133.331
130.703
130.172
127.681
118.175
117.789
115.046
115.026
114.781
114.285
111.800
55.572
55.366
OCH3
H
N
O
H
H
OCH3
27a
175
150
125
100
75
50
ppm

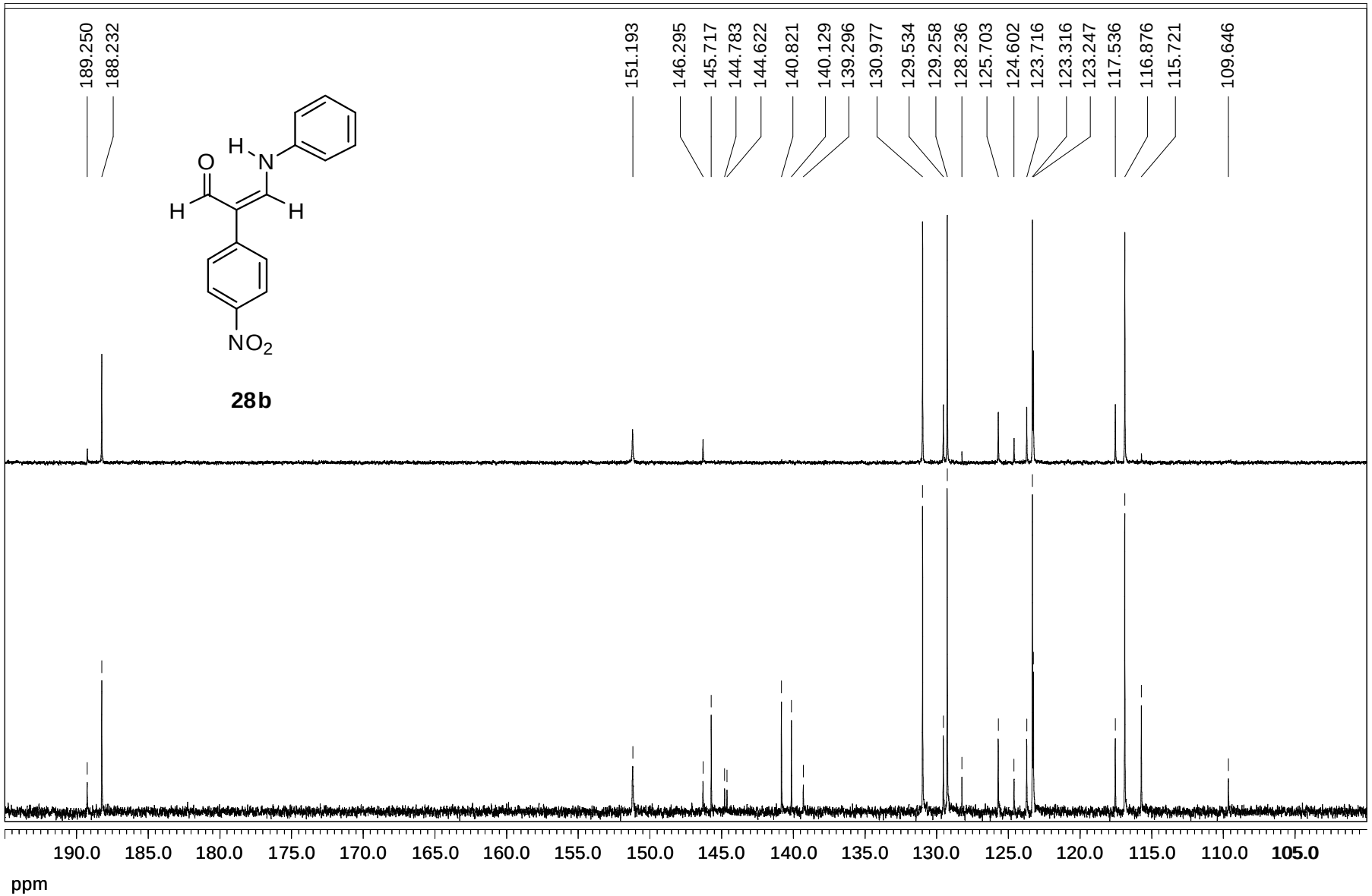

12.019
11.994
9.535
9.528
9.198
9.120
9.093
7.852
7.845
7.827
7.820
7.745
7.718
7.362
7.358
7.353
7.349
7.345
7.335
7.290
7.272
7.192
7.174
6.976
6.959
6.941
6.934
6.923
6.917
6.896
6.878
3.772
3.748
3.737
3.714
OCH3
H
N
O
H
H
OCH3
27b
0.19
0.20
1.08
1.01
0.24
1.05
0.63
2.09
10.0
5.0
ppm (t1)


189.271
188.645
157.974
157.512
155.975
155.176
150.716
144.087
134.705
133.209
130.918
129.750
127.396
124.543
118.273
118.090
116.972
114.811
114.437
114.034
113.770
110.877
55.307
55.242
55.078
55.011
OCH3
H
N
O
H
H
OCH3
27b
150
100
50
ppm (t1)

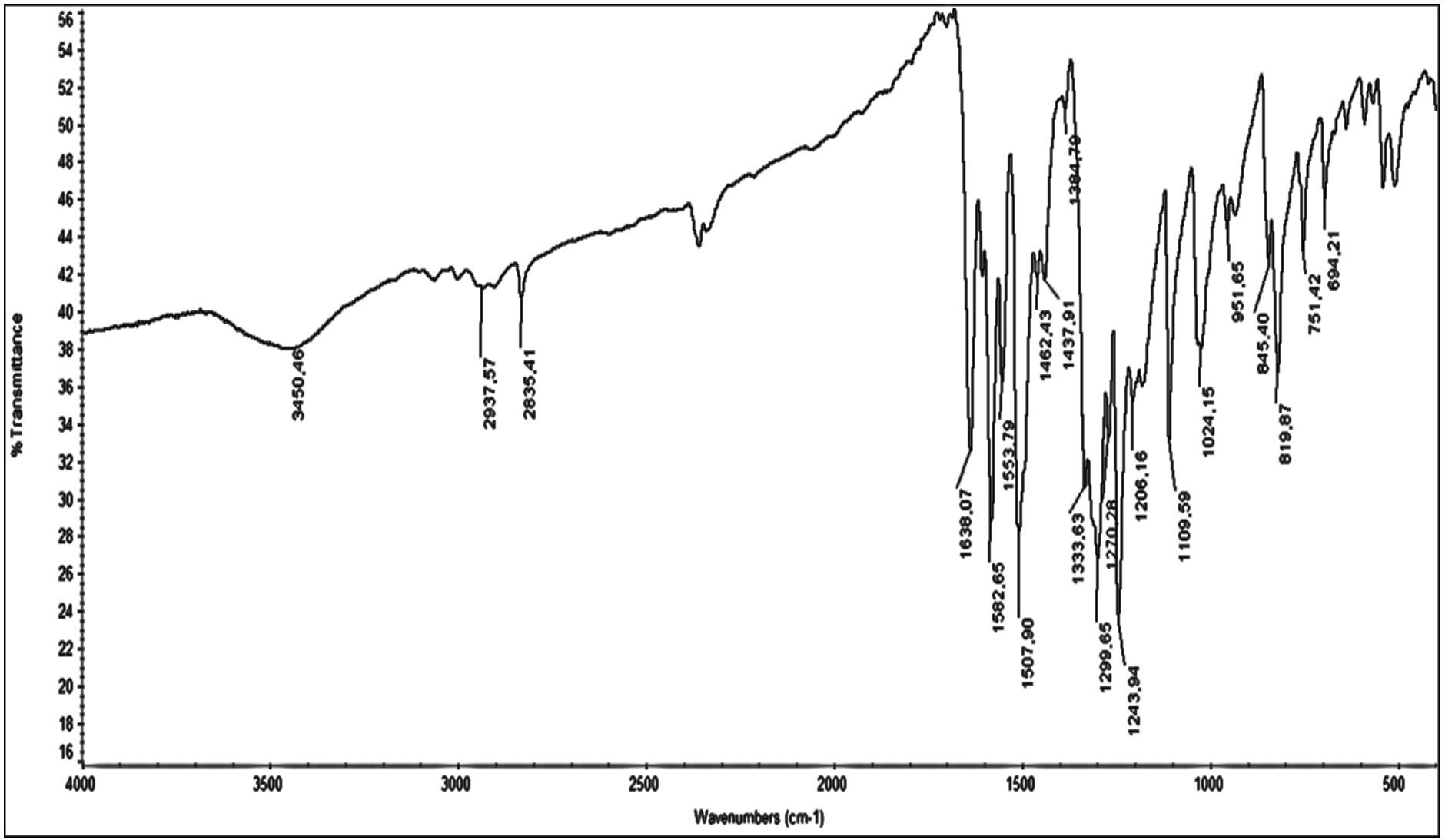
Compound **28**:

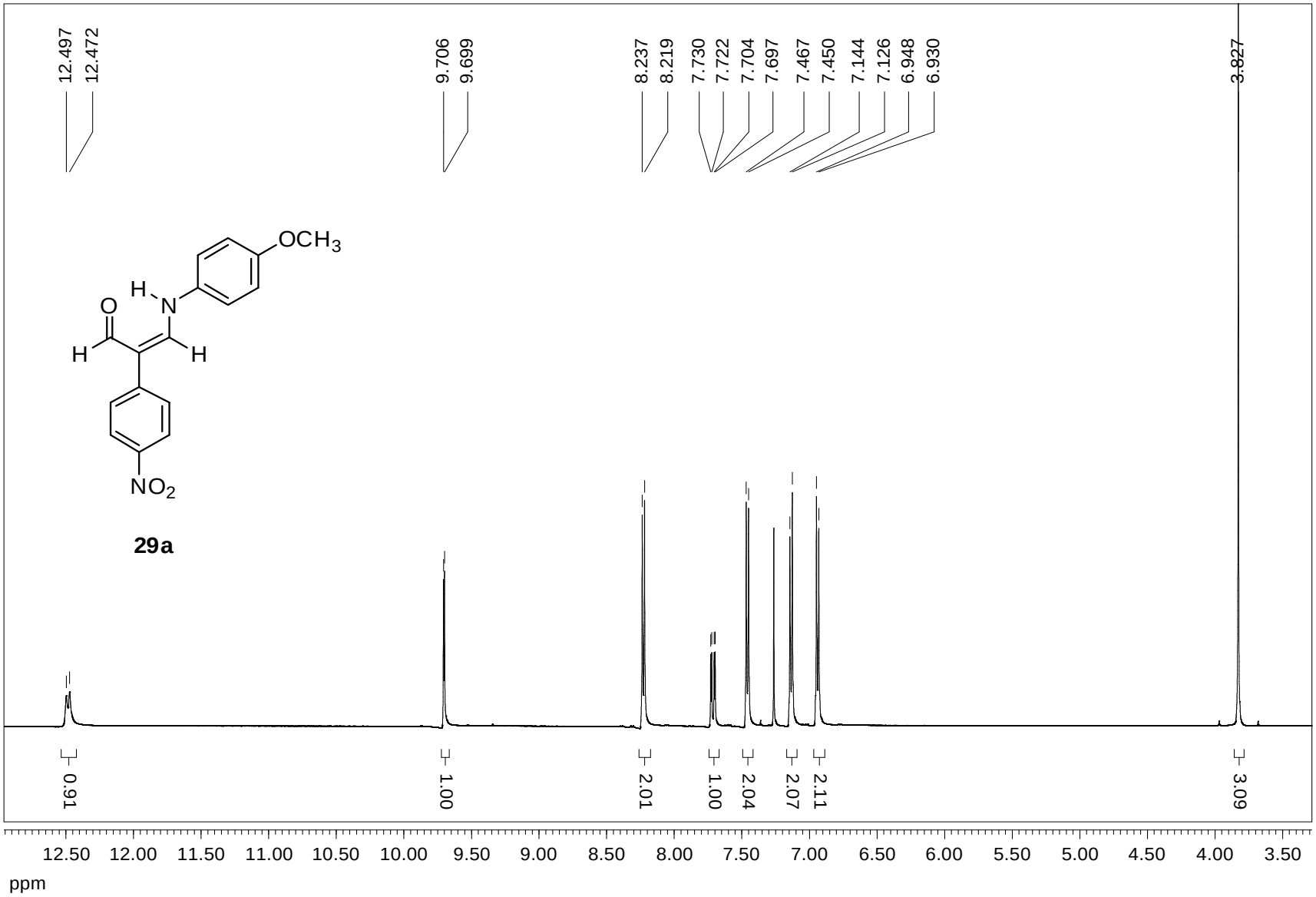

% Transmittance
Wavenumbers (cm-1)
3182,75
3072,42
2921,23
1655,60
1592,35
1570,28
1510,68
1462,43
1401,14
1342,13
1310,67
1261,16
1203,13
1189,61
1111,38
1004,77
943,47
902,61
853,51
759,71
691,97
510,33

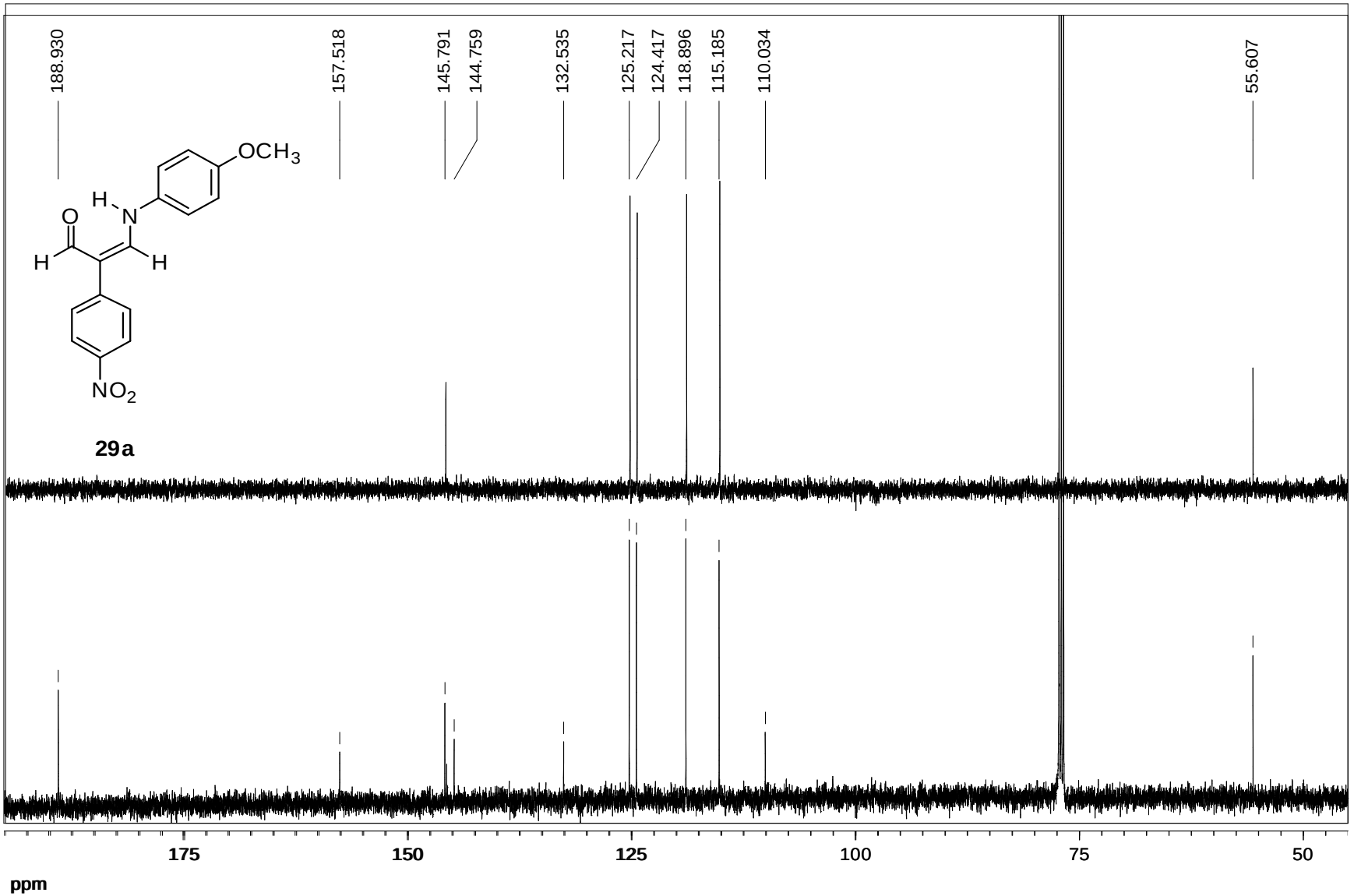

12.294
12.263
9.793
9.785
9.700
9.336
8.281
8.259
8.199
8.177
8.062
7.823
7.801
7.617
7.595
7.526
7.506
7.427
7.403
7.399
7.380
7.368
7.364
7.350
7.328
7.190
7.171
7.153
7.092
7.088
7.075
7.057
O
H
N
H
H
NO2
28b
0.24
0.30
0.61
1.00
2.24
0.54
0.97
0.59
2.05
0.60
4.65
0.28
0.68
12.50
12.00
11.50
11.00
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
6.00
5.50
ppm

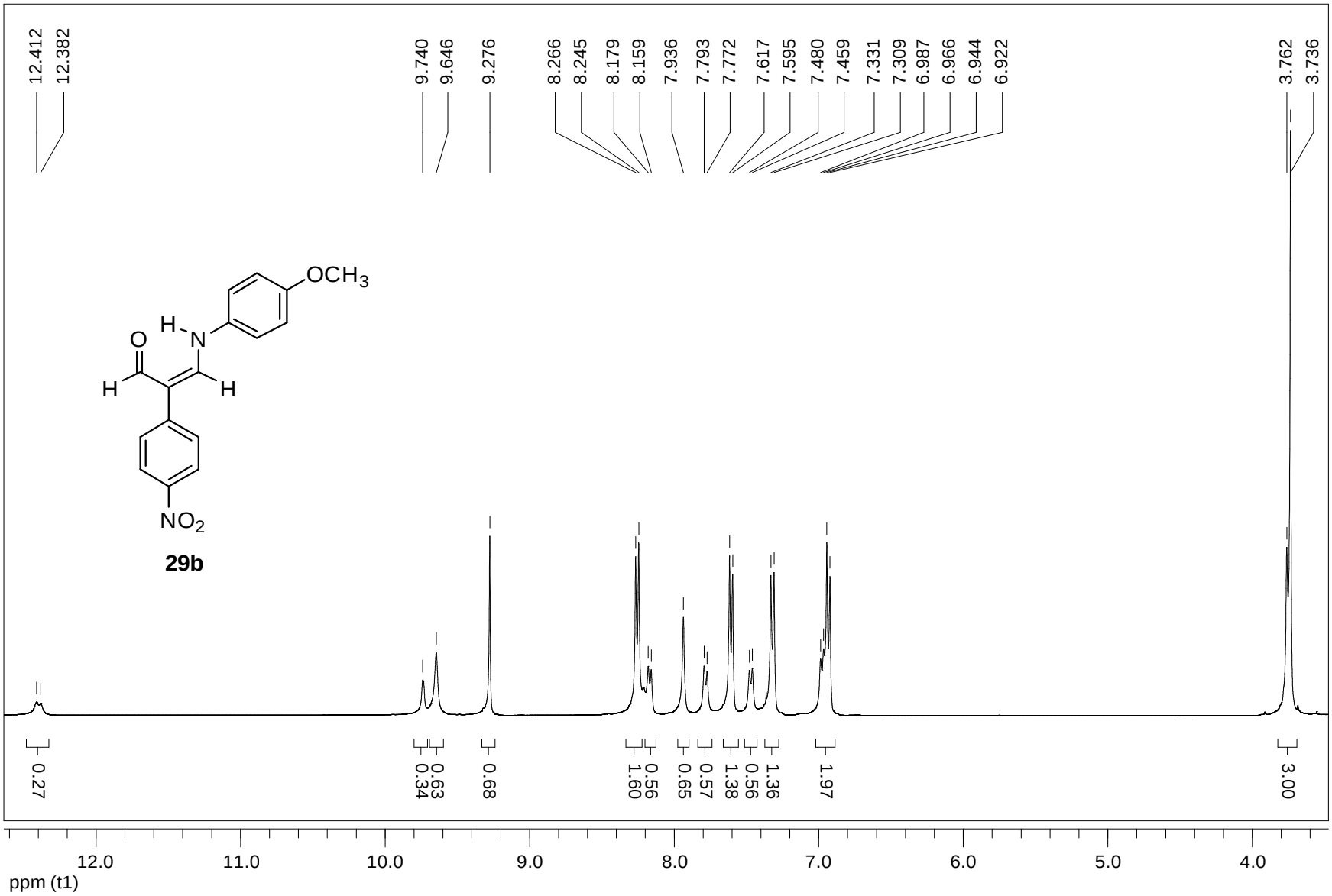

189.250
188.232
151.193
146.295
145.717
144.783
144.622
140.821
140.129
139.296
130.977
129.534
129.258
128.236
125.703
124.602
123.716
123.316
123.247
117.536
116.876
115.721
109.646
O
H
N
H
H
NO2
28b
190.0
185.0
180.0
175.0
170.0
165.0
160.0
155.0
150.0
145.0
140.0
135.0
130.0
125.0
120.0
115.0
110.0
105.0
ppm

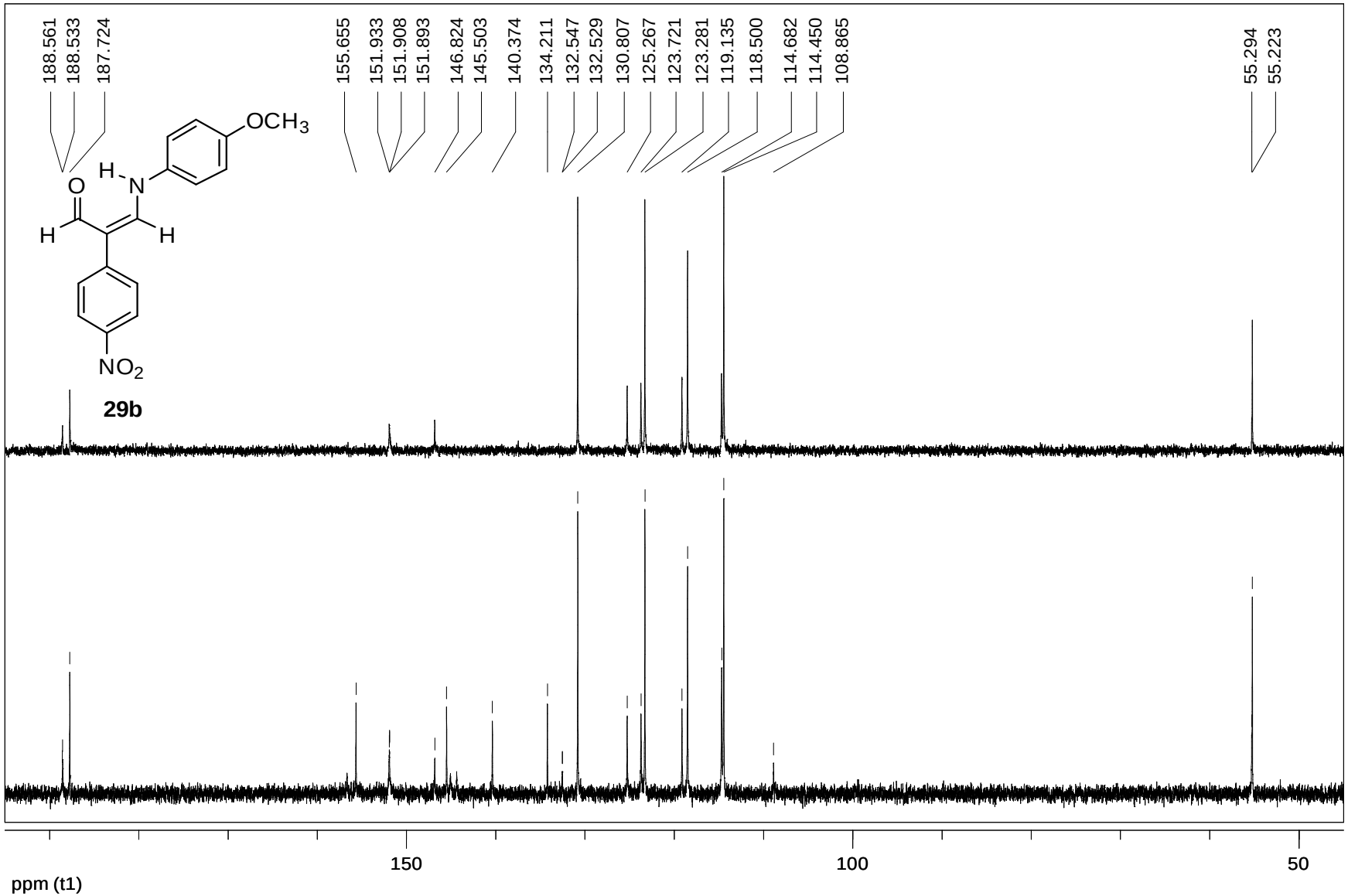
Compound **29**:


% Transmittance
Wavenumbers (cm-1)
3450,46
2937,57
2835,41
1638,07
1582,65
1553,79
1507,90
1462,43
1437,91
1384,79
1333,63
1299,65
1270,28
1243,94
1206,16
1109,59
1024,15
951,65
845,40
819,87
751,42
694,21

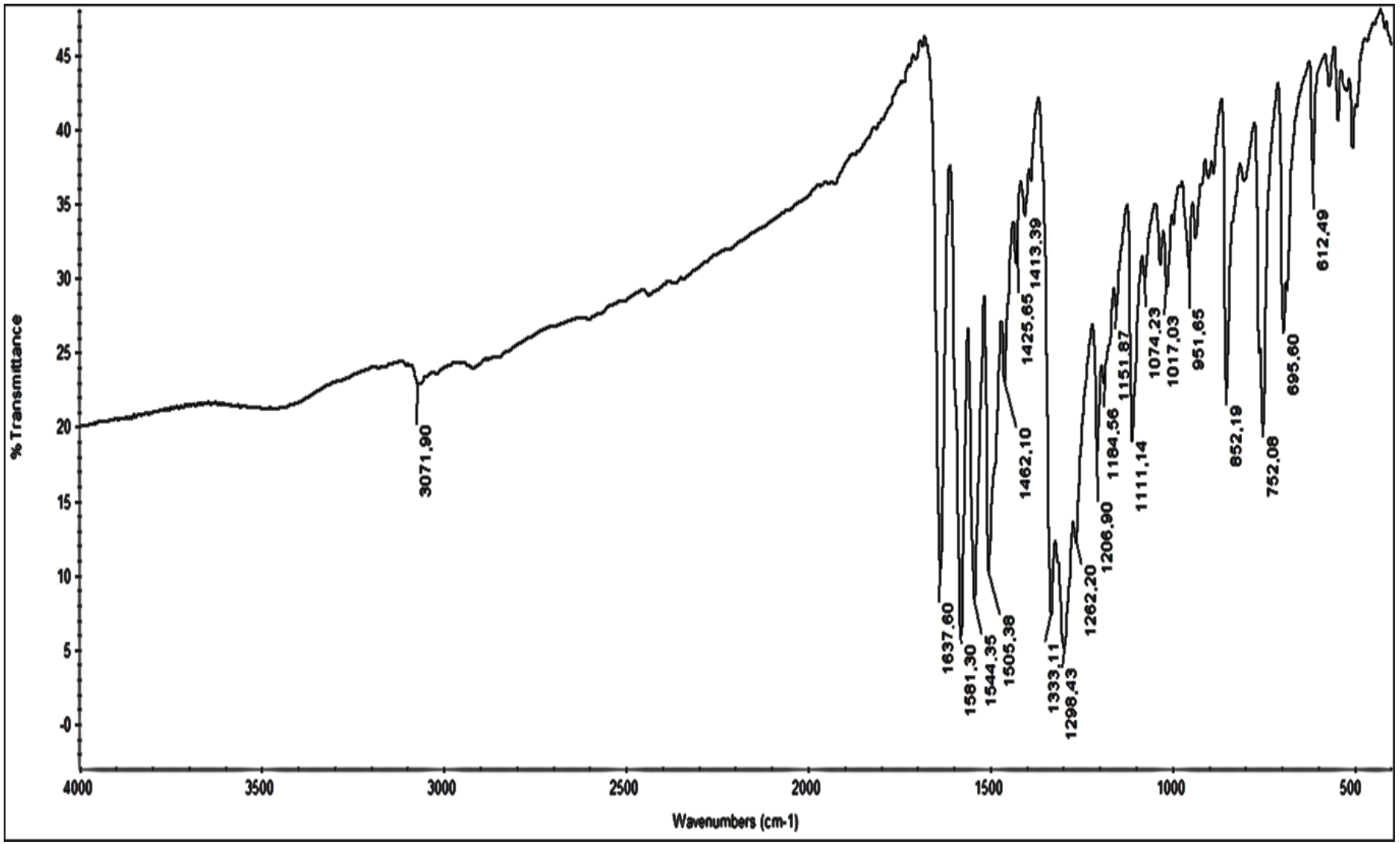

12.497
12.472
9.706
9.699
8.237
8.219
7.730
7.722
7.704
7.697
7.467
7.450
7.144
7.126
6.948
6.930
3.827
OCH3
H
N
O
H
H
NO2
29a
0.91
1.00
2.01
1.00
2.04
2.07
2.11
3.09
12.50 12.00 11.50 11.00 10.50 10.00 9.50 9.00 8.50 8.00 7.50 7.00 6.50 6.00 5.50 5.00 4.50 4.00 3.50
ppm

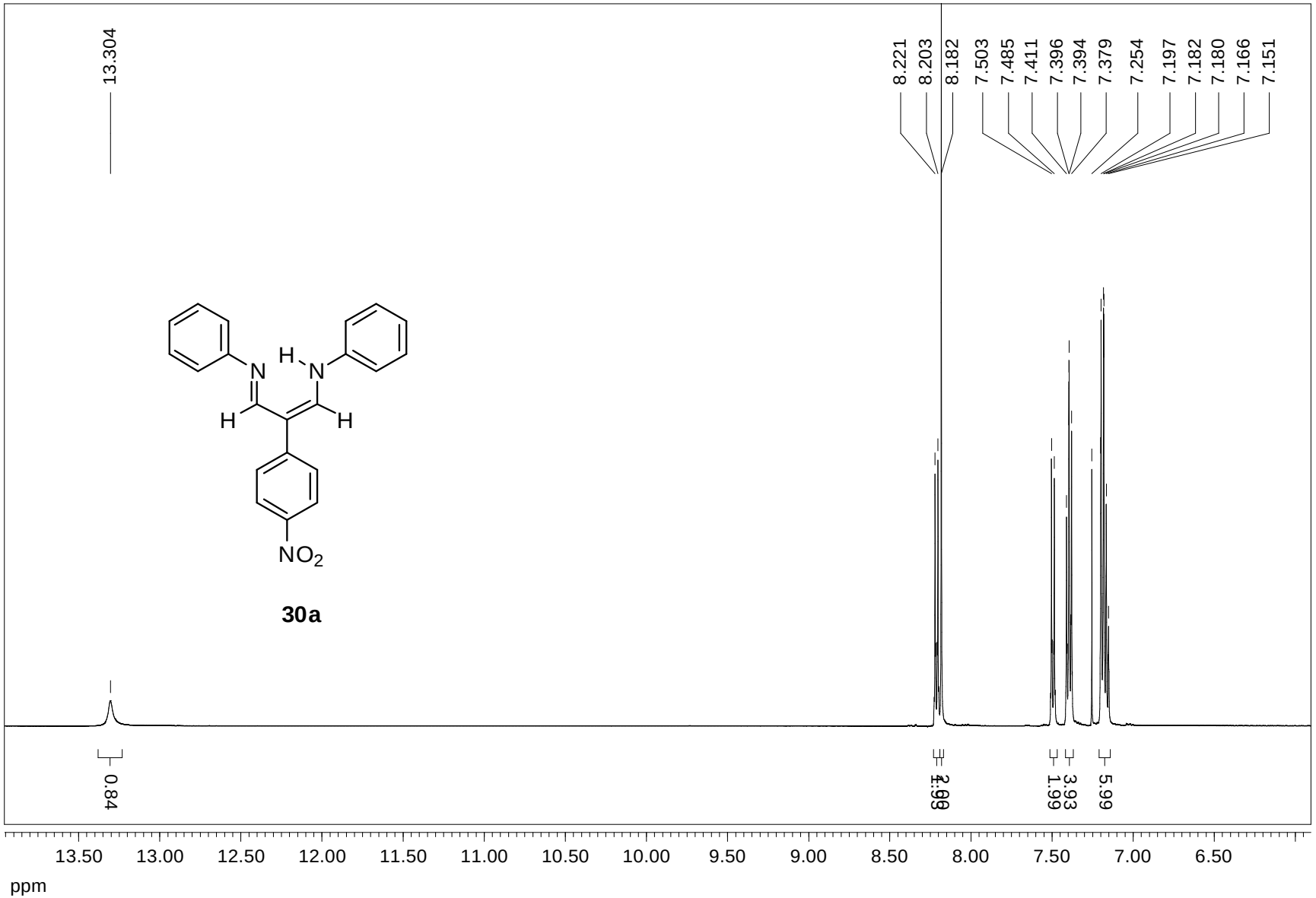

188.930
157.518
145.791
144.759
132.535
125.217
124.417
118.896
115.185
110.034
55.607
OCH3
H
N
O
H
H
NO2
29a
175
150
125
100
75
50
ppm


12.412
12.382
9.740
9.646
9.276
8.266
8.245
8.179
8.159
7.936
7.793
7.772
7.617
7.595
7.480
7.459
7.331
7.309
6.987
6.966
6.944
6.922
3.762
3.736
OCH3
H
N
O
H
H
NO2
29b
0.27
0.34
0.63
0.68
1.60
0.56
0.65
0.57
1.38
0.56
1.36
1.97
3.00
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
ppm (t1)

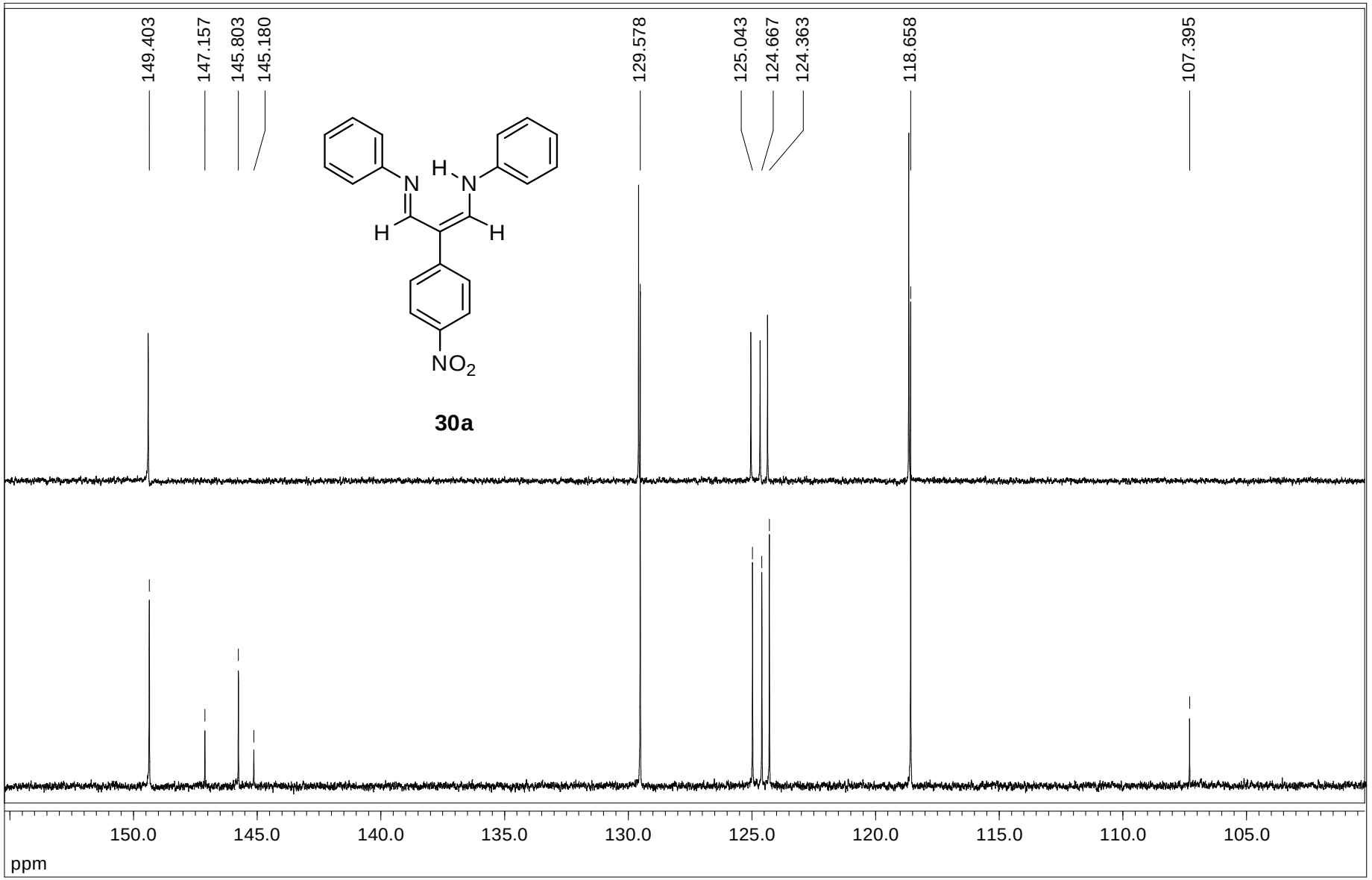

188.561
188.533
187.724
155.655
151.933
151.908
151.893
146.824
145.503
140.374
134.211
132.547
132.529
130.807
125.267
123.721
123.281
119.135
118.500
114.682
114.450
108.865
55.294
55.223
OCH3
H
N
O
H
H
NO2
29b
150
100
50
ppm (t1)

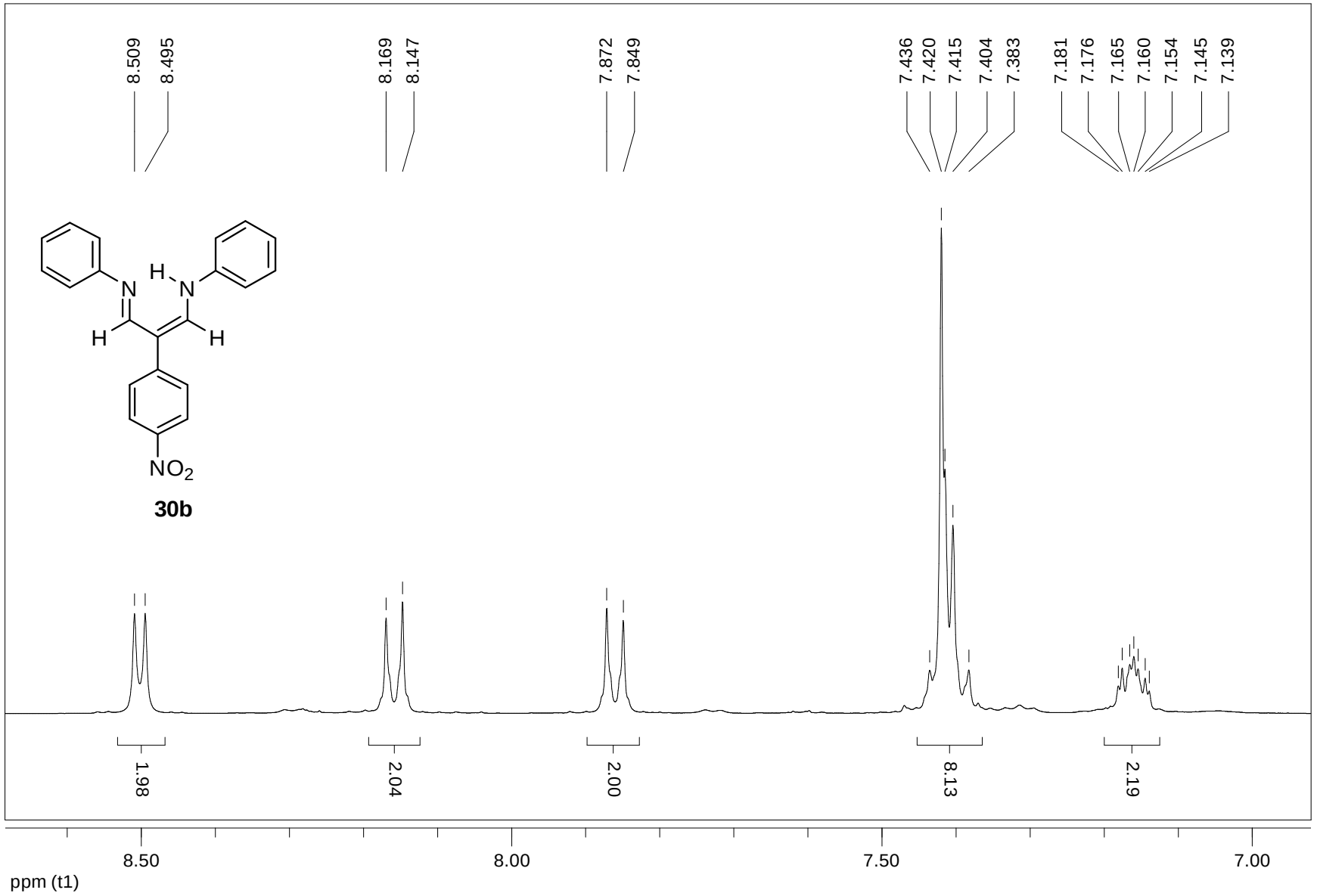
Compound **30**:

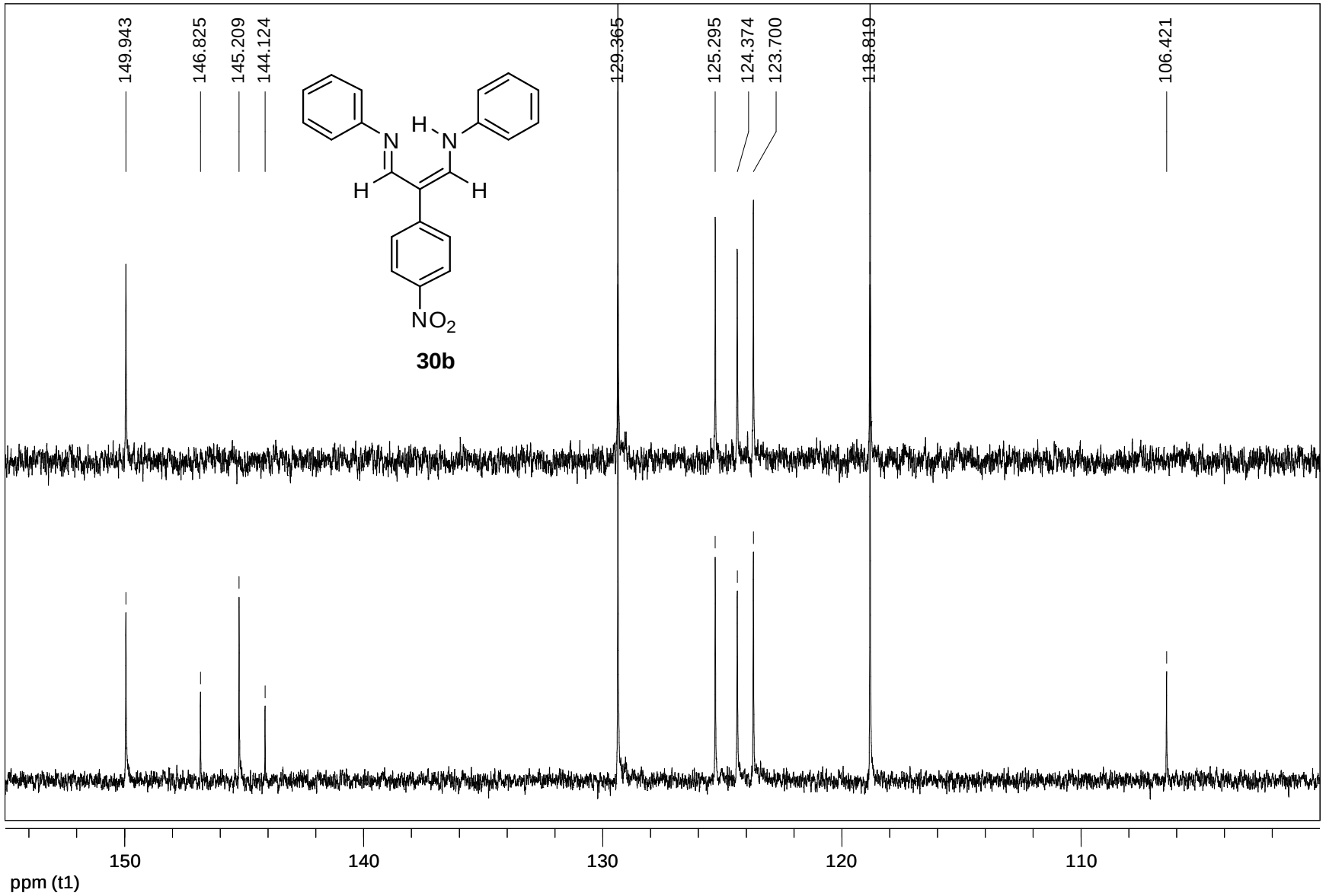

% Transmittance
45
40
35
30
25
20
15
10
5
-0
4000
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)
3071.90
1637.60
1581.30
1544.35
1505.38
1462.10
1425.65
1413.39
1333.11
1298.43
1262.20
1206.90
1184.56
1151.87
1111.14
1074.23
1017.03
951.65
852.19
752.08
695.60
612.49


13.304
8.221
8.203
8.182
7.503
7.485
7.411
7.396
7.394
7.379
7.254
7.197
7.182
7.180
7.166
7.151
N
H
N
H
H
NO2
0.84
2.00
1.69
3.93
5.99
13.50
13.00
12.50
12.00
11.50
11.00
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
ppm

30a


149.403
147.157
145.803
145.180
129.578
125.043
124.667
124.363
118.658
107.395
H
N
N
H
H
NO2
30a
150.0
145.0
140.0
135.0
130.0
125.0
120.0
115.0
110.0
105.0
ppm


8.509
8.495
8.169
8.147
7.872
7.849
7.436
7.420
7.415
7.404
7.383
7.181
7.176
7.165
7.160
7.154
7.145
7.139
N
H
N
H
H
NO2
30b
1.98
2.04
2.00
8.13
2.19
8.50
8.00
7.50
7.00
ppm (t1)


149.943
146.825
145.209
144.124
129.365
125.295
124.374
123.700
118.819
106.421
H
N
N
H
H
NO2
30b
150
140
130
120
110
ppm (t1)

3. Computational data: cartesian coordinates for all optimized structures at M06-2X/6311++G(d,p) level:

Structure 13a (vacuum)

Energy (Hartrees): -800.667055513
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.473495	1.172295	0.727029
2	6	0	-2.796270	0.773444	0.829588
3	6	0	-3.233286	-0.290110	0.053273
4	6	0	-2.390054	-0.952396	-0.826556
5	6	0	-1.075939	-0.527521	-0.931583
6	6	0	-0.585827	0.532337	-0.152491
7	1	0	-1.115233	1.972950	1.362776
8	1	0	-3.483997	1.256642	1.510551
9	1	0	-2.774422	-1.766533	-1.426031
10	1	0	-0.424272	-1.004703	-1.654274
11	6	0	0.817958	0.963884	-0.251796
12	6	0	1.821888	0.028866	-0.409834
13	6	0	1.153670	2.369178	-0.189944
14	1	0	1.562289	-1.029004	-0.413878
15	1	0	0.302548	3.065754	-0.089498
16	8	0	2.289769	2.820712	-0.266551
17	7	0	3.119253	0.285166	-0.548399
18	1	0	3.383118	1.267822	-0.506846
19	7	0	-4.634252	-0.727760	0.164812
20	8	0	-4.986893	-1.664172	-0.521140
21	8	0	-5.351594	-0.126800	0.936460
22	6	0	4.140876	-0.748288	-0.543445
23	6	0	4.732063	-0.992714	0.843881
24	1	0	4.928437	-0.454072	-1.242234
25	1	0	3.695366	-1.669960	-0.930132
26	6	0	5.816592	-2.065089	0.808559
27	1	0	5.138855	-0.052071	1.226445
28	1	0	3.924644	-1.286403	1.521623
29	1	0	6.232583	-2.235747	1.802220
30	1	0	5.418337	-3.015853	0.444866
31	1	0	6.637418	-1.771902	0.149274

Structure 13a ($CHCl_3$)

Energy (Hartrees): -800.690274576
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.513457	1.224696	0.647343
2	6	0	-2.837904	0.836283	0.754395
3	6	0	-3.262576	-0.288707	0.058519
4	6	0	-2.398743	-1.022238	-0.745390
5	6	0	-1.082682	-0.609195	-0.856160
6	6	0	-0.605729	0.514831	-0.158710
7	1	0	-1.171886	2.074532	1.225688
8	1	0	-3.529883	1.381134	1.382870
9	1	0	-2.760304	-1.886454	-1.286812
10	1	0	-0.418959	-1.154625	-1.516688
11	6	0	0.799190	0.936766	-0.262564
12	6	0	1.800429	-0.020096	-0.389355
13	6	0	1.137549	2.333961	-0.235612
14	1	0	1.530178	-1.074282	-0.371000
15	1	0	0.292085	3.039284	-0.168872
16	8	0	2.281462	2.785311	-0.310438
17	7	0	3.094515	0.216464	-0.512760
18	1	0	3.381261	1.193339	-0.504310
19	7	0	-4.657354	-0.714734	0.177714
20	8	0	-5.006628	-1.709689	-0.428619
21	8	0	-5.400592	-0.054672	0.878326
22	6	0	4.114126	-0.823503	-0.505445
23	6	0	4.885729	-0.856750	0.810844
24	1	0	4.798253	-0.642681	-1.338969
25	1	0	3.617494	-1.780810	-0.682060
26	6	0	5.960424	-1.938289	0.798409
27	1	0	5.339470	0.124693	0.979888
28	1	0	4.178710	-1.029284	1.627734
29	1	0	6.513017	-1.952010	1.739582
30	1	0	5.519630	-2.928758	0.655124
31	1	0	6.678722	-1.770337	-0.008641

Structure 13a (DMSO)

Energy (Hartrees): -800.689628259
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.523234	1.237942	0.625909
2	6	0	-2.848279	0.851973	0.729449
3	6	0	-3.266718	-0.291467	0.059061
4	6	0	-2.392658	-1.046653	-0.714566
5	6	0	-1.075539	-0.637411	-0.822263
6	6	0	-0.605881	0.507222	-0.152129
7	1	0	-1.190162	2.104879	1.183589
8	1	0	-3.543914	1.415925	1.336830
9	1	0	-2.744077	-1.926524	-1.237186
10	1	0	-0.406206	-1.204920	-1.457946
11	6	0	0.797178	0.931059	-0.256186
12	6	0	1.802704	-0.026424	-0.376886
13	6	0	1.128456	2.328934	-0.241323
14	1	0	1.538640	-1.081781	-0.355222
15	1	0	0.278025	3.028937	-0.187398
16	8	0	2.270470	2.788550	-0.314687
17	7	0	3.093550	0.216047	-0.498211
18	1	0	3.379595	1.193035	-0.496267
19	7	0	-4.661078	-0.713022	0.173116
20	8	0	-5.006016	-1.724686	-0.410328
21	8	0	-5.414334	-0.034059	0.847142
22	6	0	4.118462	-0.819611	-0.502800
23	6	0	4.903304	-0.844829	0.804970
24	1	0	4.792067	-0.632180	-1.343209
25	1	0	3.624153	-1.779024	-0.671787
26	6	0	5.980705	-1.923174	0.781482
27	1	0	5.355596	0.138811	0.965809
28	1	0	4.205340	-1.020288	1.629152
29	1	0	6.543909	-1.936075	1.716691
30	1	0	5.539224	-2.913858	0.641492
31	1	0	6.688535	-1.751928	-0.034209

Structure 13a (C_2H_5OH)

Energy (Hartrees): -800.689688188
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.644942	1.329705	0.429036
2	6	0	-2.982044	0.978739	0.479732
3	6	0	-3.359715	-0.279630	0.024985
4	6	0	-2.434985	-1.183892	-0.486542
5	6	0	-1.105052	-0.809932	-0.546853
6	6	0	-0.675644	0.448105	-0.084567
7	1	0	-1.346200	2.293118	0.823859
8	1	0	-3.718451	1.660147	0.885294
9	1	0	-2.756715	-2.152250	-0.846973
10	1	0	-0.390906	-1.499924	-0.980843
11	6	0	0.741257	0.835742	-0.133667
12	6	0	1.729040	-0.135540	0.030285
13	6	0	1.101484	2.200869	-0.370469
14	1	0	1.430867	-1.163919	0.224401
15	1	0	0.271980	2.901316	-0.556433
16	8	0	2.261237	2.632960	-0.411877
17	7	0	3.031125	0.058603	-0.001227
18	1	0	3.363702	1.005367	-0.166980
19	7	0	-4.763150	-0.663571	0.091064
20	8	0	-5.080154	-1.777074	-0.289316
21	8	0	-5.566151	0.142902	0.526416
22	6	0	4.003445	-1.017482	0.203796
23	6	0	5.420800	-0.478127	0.105861
24	1	0	3.839957	-1.790668	-0.552494
25	1	0	3.836216	-1.464947	1.187871
26	6	0	6.444962	-1.590145	0.300355
27	1	0	5.558304	-0.007585	-0.872907
28	1	0	5.560787	0.299658	0.863204
29	1	0	7.462125	-1.198823	0.235913
30	1	0	6.327958	-2.064309	1.278682
31	1	0	6.333465	-2.363184	-0.464945

Structure 13b (vacuum)

Energy (Hartrees): -800.660297675
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.275257	1.204781	0.866348
2	6	0	-2.539070	0.644247	0.963342
3	6	0	-2.910452	-0.318325	0.036562
4	6	0	-2.066585	-0.721841	-0.987617
5	6	0	-0.811115	-0.140567	-1.078385
6	6	0	-0.386979	0.824506	-0.151244
7	1	0	-0.960361	1.934436	1.603200
8	1	0	-3.228391	0.927654	1.747223
9	1	0	-2.406835	-1.460926	-1.700673
10	1	0	-0.161637	-0.406291	-1.905257
11	6	0	0.944837	1.443866	-0.244826
12	6	0	2.099445	0.746346	-0.460102
13	6	0	1.083329	2.893946	-0.073077
14	1	0	3.017014	1.330483	-0.500500
15	1	0	0.128089	3.435193	0.074302
16	8	0	2.128251	3.506932	-0.097848
17	7	0	2.255670	-0.577208	-0.622412
18	1	0	1.449536	-1.169473	-0.471924
19	7	0	-4.246733	-0.932032	0.139848
20	8	0	-4.527572	-1.802098	-0.657110
21	8	0	-4.982291	-0.531074	1.016041
22	6	0	3.565426	-1.213717	-0.586174
23	6	0	4.020304	-1.580608	0.824991
24	1	0	4.279230	-0.523686	-1.044307
25	1	0	3.533023	-2.105424	-1.217995
26	6	0	5.401911	-2.227863	0.816291
27	1	0	4.026283	-0.674102	1.437972
28	1	0	3.286973	-2.259997	1.270951
29	1	0	5.716630	-2.496107	1.825394
30	1	0	5.405902	-3.138499	0.211779
31	1	0	6.150117	-1.547289	0.402473

Structure 13b ($CHCl_3$)

Energy (Hartrees): -800.685336998
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.335579	1.251513	0.821995
2	6	0	-2.592367	0.676224	0.909202
3	6	0	-2.915990	-0.348421	0.029698
4	6	0	-2.028050	-0.798248	-0.938747
5	6	0	-0.780544	-0.201376	-1.021338
6	6	0	-0.404063	0.827413	-0.140838
7	1	0	-1.063090	2.029962	1.524996
8	1	0	-3.305803	1.001210	1.654959
9	1	0	-2.320997	-1.584408	-1.622051
10	1	0	-0.103044	-0.511617	-1.809067
11	6	0	0.916247	1.471322	-0.228894
12	6	0	2.100112	0.791353	-0.414857
13	6	0	1.011498	2.915452	-0.095311
14	1	0	3.004661	1.393228	-0.471620
15	1	0	0.041939	3.436049	0.013262
16	8	0	2.041821	3.571744	-0.112713
17	7	0	2.293400	-0.519538	-0.514439
18	1	0	1.504851	-1.141374	-0.380677
19	7	0	-4.238517	-0.974595	0.123650
20	8	0	-4.480117	-1.913765	-0.609471
21	8	0	-5.027782	-0.524696	0.930677
22	6	0	3.616492	-1.132393	-0.555870
23	6	0	4.081555	-1.614349	0.815339
24	1	0	4.311291	-0.389234	-0.953815
25	1	0	3.585582	-1.966444	-1.261972
26	6	0	5.461844	-2.257714	0.738058
27	1	0	4.096478	-0.760689	1.500050
28	1	0	3.352946	-2.329994	1.209333
29	1	0	5.794532	-2.591820	1.722514
30	1	0	5.455420	-3.126913	0.074699
31	1	0	6.202761	-1.549935	0.356347

Structure 13b (DMSO)

Energy (Hartrees): -800.685553531
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.351911	1.266642	0.799666
2	6	0	-2.609214	0.693895	0.887212
3	6	0	-2.924130	-0.353379	0.030315
4	6	0	-2.023157	-0.828296	-0.914732
5	6	0	-0.774295	-0.234964	-0.997591
6	6	0	-0.407921	0.818106	-0.141321
7	1	0	-1.090179	2.062684	1.486876
8	1	0	-3.327987	1.040763	1.617735
9	1	0	-2.301570	-1.633954	-1.581257
10	1	0	-0.087937	-0.573703	-1.765538
11	6	0	0.911037	1.462461	-0.230122
12	6	0	2.101598	0.784401	-0.409076
13	6	0	0.998603	2.905626	-0.105853
14	1	0	3.003534	1.390029	-0.466633
15	1	0	0.024828	3.419595	-0.004743
16	8	0	2.023838	3.572919	-0.124056
17	7	0	2.304968	-0.521384	-0.499125
18	1	0	1.524015	-1.156669	-0.378760
19	7	0	-4.246993	-0.974348	0.123876
20	8	0	-4.489609	-1.921545	-0.600512
21	8	0	-5.041624	-0.514504	0.922476
22	6	0	3.633624	-1.122002	-0.551456
23	6	0	4.108056	-1.598007	0.817780
24	1	0	4.319522	-0.372740	-0.952822
25	1	0	3.601311	-1.958283	-1.254243
26	6	0	5.493108	-2.229119	0.732023
27	1	0	4.120505	-0.742408	1.500294
28	1	0	3.386878	-2.319371	1.214726
29	1	0	5.835143	-2.561429	1.714222
30	1	0	5.488368	-3.097511	0.067428
31	1	0	6.224529	-1.514028	0.345132

Structure 13b (C_2H_5OH)

Energy (Hartrees): -800.687787107
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.352933	1.259737	0.820330
2	6	0	-2.604469	0.673868	0.901182
3	6	0	-2.909835	-0.361867	0.026299
4	6	0	-2.008092	-0.813356	-0.929539
5	6	0	-0.766423	-0.205322	-1.005783
6	6	0	-0.409173	0.835808	-0.131430
7	1	0	-1.095236	2.046133	1.520048
8	1	0	-3.324339	0.999256	1.640515
9	1	0	-2.281168	-1.607862	-1.611303
10	1	0	-0.078534	-0.521375	-1.781841
11	6	0	0.905246	1.492000	-0.216984
12	6	0	2.102753	0.817173	-0.393154
13	6	0	0.980769	2.926078	-0.096697
14	1	0	3.003542	1.422856	-0.458708
15	1	0	0.008771	3.438623	0.006585
16	8	0	2.007543	3.606275	-0.118688
17	7	0	2.306404	-0.485794	-0.471231
18	1	0	1.524314	-1.120842	-0.351594
19	7	0	-4.223934	-0.993563	0.112039
20	8	0	-4.455575	-1.949059	-0.606037
21	8	0	-5.034429	-0.538444	0.897947
22	6	0	3.633253	-1.091456	-0.539849
23	6	0	4.085780	-1.644218	0.807398
24	1	0	4.326595	-0.325846	-0.893776
25	1	0	3.605049	-1.888951	-1.286672
26	6	0	5.459554	-2.296384	0.698515
27	1	0	4.107848	-0.826221	1.534133
28	1	0	3.349060	-2.372562	1.160549
29	1	0	5.784680	-2.689583	1.663786
30	1	0	5.444470	-3.125118	-0.014657
31	1	0	6.208773	-1.575541	0.359779

Structure 13c (vacuum)

Energy (Hartrees):
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.221786	1.185777	0.806657
2	6	0	-2.446201	0.548693	0.931592
3	6	0	-2.767074	-0.461358	0.036267
4	6	0	-1.913989	-0.841216	-0.987800
5	6	0	-0.693112	-0.192226	-1.101919
6	6	0	-0.321198	0.816416	-0.201812
7	1	0	-0.959019	1.984546	1.486591
8	1	0	-3.149096	0.819884	1.707577
9	1	0	-2.216761	-1.616377	-1.678773
10	1	0	-0.034204	-0.443711	-1.925832
11	6	0	0.986108	1.489408	-0.319504
12	6	0	2.160441	0.827490	-0.529805
13	6	0	1.096433	2.937951	-0.160239
14	1	0	3.071008	1.420835	-0.599578
15	7	0	2.361155	-0.497401	-0.666303
16	1	0	1.575596	-1.106681	-0.478477
17	8	0	0.190592	3.694097	0.103716
18	1	0	2.125385	3.329902	-0.302790
19	7	0	-4.065523	-1.149302	0.168318
20	8	0	-4.307234	-2.046434	-0.611684
21	8	0	-4.810288	-0.778935	1.049718
22	6	0	3.690554	-1.086637	-0.582669
23	6	0	4.146405	-1.358803	0.849551
24	1	0	4.387669	-0.403532	-1.076994
25	1	0	3.691622	-2.013034	-1.162737
26	6	0	5.547051	-1.962985	0.886202
27	1	0	4.119373	-0.420545	1.412432
28	1	0	3.430064	-2.033993	1.327992
29	1	0	5.859547	-2.170541	1.910232
30	1	0	5.583581	-2.902216	0.328555
31	1	0	6.279453	-1.282505	0.444567

Structure 13c ($CHCl_3$)

Energy (Hartrees): -800.687595866
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.258271	1.177168	-0.820490
2	6	0	2.478289	0.530604	-0.929711
3	6	0	2.774468	-0.486391	-0.031253
4	6	0	1.897717	-0.864238	0.975472
5	6	0	0.683125	-0.202498	1.073975
6	6	0	0.337412	0.817927	0.175259
7	1	0	1.012039	1.970281	-1.513864
8	1	0	3.187931	0.801083	-1.700266
9	1	0	2.170674	-1.646761	1.670883
10	1	0	0.008702	-0.460377	1.883056
11	6	0	-0.957431	1.515780	0.277889
12	6	0	-2.160250	0.874603	0.466374
13	6	0	-1.037052	2.956412	0.153289
14	1	0	-3.055121	1.491424	0.531204
15	7	0	-2.394051	-0.433063	0.569097
16	1	0	-1.624879	-1.076996	0.427969
17	8	0	-0.104847	3.718400	-0.041729
18	1	0	-2.061678	3.363295	0.259160
19	7	0	4.061912	-1.182982	-0.145493
20	8	0	4.279110	-2.110226	0.609960
21	8	0	4.845418	-0.800009	-0.991069
22	6	0	-3.738156	-1.000089	0.568291
23	6	0	-4.209007	-1.395324	-0.828734
24	1	0	-4.411944	-0.255712	1.000098
25	1	0	-3.742201	-1.869463	1.230506
26	6	0	-5.611906	-1.991988	-0.795231
27	1	0	-4.187565	-0.508785	-1.470498
28	1	0	-3.501927	-2.115453	-1.252439
29	1	0	-5.942839	-2.271987	-1.797005
30	1	0	-5.642950	-2.888985	-0.170494
31	1	0	-6.333584	-1.276366	-0.391621

Structure 13c (DMSO)

Energy (Hartrees): -800.688554241
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.276641	1.182922	0.817922
2	6	0	-2.494841	0.532707	0.922360
3	6	0	-2.779031	-0.495434	0.031497
4	6	0	-1.887699	-0.882981	-0.959454
5	6	0	-0.674845	-0.217825	-1.052718
6	6	0	-0.342424	0.816823	-0.164417
7	1	0	-1.040083	1.980779	1.509228
8	1	0	-3.210051	0.809090	1.685466
9	1	0	-2.142808	-1.676281	-1.649336
10	1	0	0.011236	-0.490674	-1.846758
11	6	0	0.948916	1.518842	-0.264161
12	6	0	2.159907	0.880347	-0.444461
13	6	0	1.024262	2.957712	-0.159176
14	1	0	3.049895	1.503122	-0.515073
15	7	0	2.401183	-0.421935	-0.530910
16	1	0	1.639176	-1.077613	-0.399589
17	8	0	0.089305	3.727166	0.009898
18	1	0	2.050191	3.361495	-0.259527
19	7	0	-4.066465	-1.189429	0.138051
20	8	0	-4.273615	-2.131151	-0.603494
21	8	0	-4.866008	-0.790873	0.963535
22	6	0	3.748444	-0.981657	-0.561069
23	6	0	4.234722	-1.396216	0.823981
24	1	0	4.411958	-0.225995	-0.987664
25	1	0	3.744046	-1.841323	-1.235350
26	6	0	5.638392	-1.988530	0.763930
27	1	0	4.219537	-0.518118	1.477196
28	1	0	3.533529	-2.124207	1.243764
29	1	0	5.984126	-2.281048	1.757402
30	1	0	5.662427	-2.876342	0.125952
31	1	0	6.351366	-1.264733	0.359396

Structure 13c (C_2H_5OH)

Energy (Hartrees): -800.691088888
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.256036	1.150967	0.853250
2	6	0	-2.475144	0.502367	0.954126
3	6	0	-2.773387	-0.494463	0.032865
4	6	0	-1.898316	-0.854033	-0.983034
5	6	0	-0.685932	-0.188131	-1.073078
6	6	0	-0.341187	0.816945	-0.157163
7	1	0	-1.003820	1.920209	1.572133
8	1	0	-3.176855	0.754101	1.738295
9	1	0	-2.167084	-1.624096	-1.694111
10	1	0	-0.011105	-0.434596	-1.885263
11	6	0	0.949197	1.524120	-0.255306
12	6	0	2.163520	0.886001	-0.436701
13	6	0	1.021004	2.954289	-0.153879
14	1	0	3.054693	1.507915	-0.500097
15	7	0	2.398932	-0.413447	-0.531691
16	1	0	1.631496	-1.066469	-0.416947
17	8	0	0.074099	3.724917	0.001521
18	1	0	2.041198	3.368870	-0.242139
19	7	0	-4.058542	-1.186982	0.133550
20	8	0	-4.274710	-2.117756	-0.620144
21	8	0	-4.857560	-0.802859	0.966809
22	6	0	3.744761	-0.978965	-0.564472
23	6	0	4.228549	-1.403189	0.818059
24	1	0	4.411186	-0.223591	-0.987249
25	1	0	3.736069	-1.834035	-1.244592
26	6	0	5.631319	-1.997137	0.754864
27	1	0	4.214313	-0.529036	1.476983
28	1	0	3.526228	-2.133206	1.232755
29	1	0	5.975454	-2.296063	1.747066
30	1	0	5.654631	-2.881802	0.112228
31	1	0	6.346148	-1.272242	0.355243

Structure 13d (vacuum)

Energy (Hartrees): -800.654545454
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.366685	1.149685	0.709385
2	6	0	-2.659529	0.667239	0.832810
3	6	0	-3.053402	-0.404969	0.044567
4	6	0	-2.199768	-0.995751	-0.873218
5	6	0	-0.912552	-0.495263	-0.992267
6	6	0	-0.464811	0.566870	-0.193650
7	1	0	-1.050711	1.987119	1.315439
8	1	0	-3.360852	1.103032	1.531560
9	1	0	-2.551698	-1.814129	-1.486310
10	1	0	-0.251943	-0.917971	-1.740389
11	6	0	0.929454	1.044294	-0.298259
12	6	0	1.931170	0.133083	-0.501333
13	6	0	1.240526	2.463325	-0.154866
14	1	0	1.669247	-0.923772	-0.479516
15	7	0	3.240514	0.338231	-0.751931
16	1	0	3.592743	1.282579	-0.775851
17	1	0	2.319591	2.719944	-0.184985
18	8	0	0.438044	3.354684	0.004961
19	7	0	-4.425544	-0.924719	0.177540
20	8	0	-4.739357	-1.868654	-0.517329
21	8	0	-5.158582	-0.381280	0.976092
22	6	0	4.222074	-0.726625	-0.596595
23	6	0	4.656336	-0.952244	0.850373
24	1	0	5.086547	-0.482512	-1.218983
25	1	0	3.785914	-1.644232	-1.004112
26	6	0	5.684965	-2.074081	0.957176
27	1	0	5.068433	-0.019804	1.248638
28	1	0	3.771100	-1.187171	1.449890
29	1	0	5.987928	-2.232944	1.992651
30	1	0	5.279325	-3.016125	0.579643
31	1	0	6.582075	-1.839966	0.378521

Structure 13d ($CHCl_3$)

Energy (Hartrees): -800.681581534
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.407975	1.185643	0.662538
2	6	0	-2.700877	0.705509	0.784106
3	6	0	-3.074127	-0.411411	0.046196
4	6	0	-2.192849	-1.049109	-0.815845
5	6	0	-0.906232	-0.550179	-0.933339
6	6	0	-0.478788	0.561709	-0.187962
7	1	0	-1.109986	2.048586	1.241572
8	1	0	-3.410719	1.179363	1.449120
9	1	0	-2.515420	-1.905421	-1.393100
10	1	0	-0.228053	-1.018636	-1.636677
11	6	0	0.911352	1.043322	-0.286287
12	6	0	1.925837	0.120403	-0.462138
13	6	0	1.225301	2.451842	-0.165376
14	1	0	1.666714	-0.936124	-0.419079
15	7	0	3.223333	0.325487	-0.689646
16	1	0	3.581289	1.269168	-0.753448
17	1	0	2.302939	2.699757	-0.165037
18	8	0	0.422216	3.363964	-0.058335
19	7	0	-4.437910	-0.929034	0.177982
20	8	0	-4.740090	-1.917150	-0.463746
21	8	0	-5.202354	-0.349117	0.924640
22	6	0	4.212505	-0.742685	-0.584535
23	6	0	4.740790	-0.918859	0.836373
24	1	0	5.030712	-0.510075	-1.269675
25	1	0	3.743384	-1.667549	-0.932505
26	6	0	5.799646	-2.013450	0.905424
27	1	0	5.156892	0.032594	1.182083
28	1	0	3.899749	-1.158922	1.494830
29	1	0	6.168675	-2.138684	1.924991
30	1	0	5.395207	-2.974143	0.575235
31	1	0	6.654985	-1.773071	0.267948

Structure 13d (DMSO)

Energy (Hartrees): -800.683028097
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.416147	1.187780	0.662409
2	6	0	-2.709059	0.707606	0.780056
3	6	0	-3.077185	-0.416259	0.048475
4	6	0	-2.187180	-1.061776	-0.800136
5	6	0	-0.900705	-0.562767	-0.914276
6	6	0	-0.479621	0.559450	-0.178734
7	1	0	-1.121454	2.052459	1.240855
8	1	0	-3.420896	1.186869	1.439295
9	1	0	-2.500598	-1.924745	-1.372682
10	1	0	-0.216668	-1.041213	-1.605293
11	6	0	0.906076	1.046298	-0.276863
12	6	0	1.924356	0.118763	-0.447103
13	6	0	1.216015	2.454283	-0.173013
14	1	0	1.665102	-0.937511	-0.399359
15	7	0	3.217404	0.324473	-0.666405
16	1	0	3.578659	1.268175	-0.731110
17	1	0	2.292840	2.702363	-0.176842
18	8	0	0.410500	3.369983	-0.082783
19	7	0	-4.440217	-0.931230	0.173143
20	8	0	-4.733744	-1.937457	-0.446238
21	8	0	-5.218715	-0.331899	0.892076
22	6	0	4.206551	-0.745949	-0.579787
23	6	0	4.771354	-0.902900	0.828568
24	1	0	5.006502	-0.521009	-1.288428
25	1	0	3.723482	-1.672624	-0.900839
26	6	0	5.822312	-2.005396	0.883168
27	1	0	5.203843	0.050804	1.146820
28	1	0	3.946112	-1.128233	1.511775
29	1	0	6.220108	-2.120344	1.893445
30	1	0	5.397897	-2.965843	0.577660
31	1	0	6.659828	-1.781655	0.216515

Structure 13d (C_2H_5OH)

Energy (Hartrees): -800.685275572
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.419980	1.176840	0.677090
2	6	0	-2.716350	0.707285	0.795472
3	6	0	-3.093679	-0.410449	0.058580
4	6	0	-2.210692	-1.063035	-0.792513
5	6	0	-0.920548	-0.574661	-0.905333
6	6	0	-0.491950	0.543580	-0.169010
7	1	0	-1.117002	2.033654	1.263602
8	1	0	-3.422286	1.189953	1.458541
9	1	0	-2.531010	-1.922729	-1.366328
10	1	0	-0.239078	-1.056591	-1.596613
11	6	0	0.897355	1.019944	-0.275699
12	6	0	1.911023	0.078704	-0.426077
13	6	0	1.215696	2.419474	-0.206724
14	1	0	1.645560	-0.973287	-0.334466
15	7	0	3.197948	0.271244	-0.672814
16	1	0	3.558114	1.211143	-0.788731
17	1	0	2.290790	2.666938	-0.212989
18	8	0	0.410558	3.346697	-0.138802
19	7	0	-4.458218	-0.911292	0.179209
20	8	0	-4.774345	-1.893775	-0.467952
21	8	0	-5.227960	-0.329074	0.922352
22	6	0	4.192343	-0.793046	-0.563723
23	6	0	4.861570	-0.819904	0.806297
24	1	0	4.936833	-0.639673	-1.348102
25	1	0	3.685818	-1.740720	-0.761884
26	6	0	5.908484	-1.924709	0.888884
27	1	0	5.324189	0.154257	0.993790
28	1	0	4.090948	-0.965649	1.569974
29	1	0	6.395076	-1.931167	1.866297
30	1	0	5.454409	-2.907579	0.734249
31	1	0	6.683865	-1.789127	0.129632

Structure 13e (vacuum)

Energy (Hartrees): -800.651732725
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.787630	1.043729	-0.314022
2	6	0	-1.421252	1.252107	-0.399971
3	6	0	-0.515710	0.215882	-0.125793
4	6	0	-1.027087	-1.028248	0.268546
5	6	0	-2.392771	-1.255603	0.352507
6	6	0	-3.252418	-0.211125	0.055385
7	1	0	-3.494378	1.833067	-0.531460
8	1	0	-1.049543	2.227085	-0.681887
9	1	0	-0.344286	-1.823643	0.543754
10	1	0	-2.793540	-2.212015	0.659607
11	6	0	0.945330	0.413546	-0.265777
12	6	0	1.676926	-0.610125	-0.810036
13	1	0	1.115423	-1.431534	-1.249349
14	6	0	1.532882	1.709467	0.081422
15	1	0	2.584215	1.856032	-0.216688
16	1	0	3.305547	-1.607789	-1.417396
17	7	0	3.010258	-0.798261	-0.894013
18	8	0	0.938011	2.621454	0.612660
19	7	0	-4.705628	-0.437857	0.147520
20	8	0	-5.438235	0.487905	-0.128831
21	8	0	-5.082728	-1.538957	0.490800
22	6	0	4.060946	-0.117537	-0.151889
23	6	0	5.245932	-1.049320	0.069069
24	1	0	3.644075	0.199602	0.810225
25	1	0	4.395277	0.782043	-0.680419
26	6	0	6.376870	-0.346653	0.814865
27	1	0	4.909919	-1.926760	0.629537
28	1	0	5.608766	-1.404722	-0.902002
29	1	0	7.218737	-1.021228	0.973450
30	1	0	6.739058	0.517191	0.252812
31	1	0	6.039819	0.005563	1.792397

Structure 13e ($CHCl_3$)

Energy (Hartrees): -800.678578641
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.787987	1.052484	-0.298484
2	6	0	-1.422287	1.256303	-0.390965
3	6	0	-0.513663	0.214184	-0.136531
4	6	0	-1.029402	-1.036476	0.239911
5	6	0	-2.394188	-1.260244	0.330235
6	6	0	-3.255270	-0.207249	0.057803
7	1	0	-3.486309	1.852418	-0.505823
8	1	0	-1.054251	2.232406	-0.674597
9	1	0	-0.350016	-1.842282	0.492118
10	1	0	-2.785694	-2.224665	0.625206
11	6	0	0.944400	0.410885	-0.277366
12	6	0	1.681991	-0.635573	-0.800572
13	1	0	1.123546	-1.457423	-1.242764
14	6	0	1.537408	1.697571	0.043238
15	1	0	2.582196	1.838837	-0.271356
16	1	0	3.297431	-1.655596	-1.364445
17	7	0	3.000756	-0.834111	-0.854502
18	8	0	0.957175	2.627359	0.581880
19	7	0	-4.700438	-0.428907	0.157100
20	8	0	-5.441329	0.504659	-0.082198
21	8	0	-5.089801	-1.537480	0.471268
22	6	0	4.058929	-0.119967	-0.149218
23	6	0	5.243591	-1.044692	0.095182
24	1	0	3.651144	0.235226	0.803007
25	1	0	4.382706	0.754690	-0.722335
26	6	0	6.374076	-0.315530	0.813309
27	1	0	4.911039	-1.902524	0.687310
28	1	0	5.600559	-1.430422	-0.865967
29	1	0	7.219625	-0.983099	0.987863
30	1	0	6.731184	0.533024	0.224063
31	1	0	6.040649	0.064056	1.782690

Structure 13e (DMSO)

Energy (Hartrees): -800.679848019
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.786053	1.050034	-0.316104
2	6	0	-1.419483	1.247265	-0.404669
3	6	0	-0.513714	0.205511	-0.133488
4	6	0	-1.036374	-1.041389	0.249225
5	6	0	-2.402306	-1.258310	0.336192
6	6	0	-3.260075	-0.204414	0.052903
7	1	0	-3.478065	1.851489	-0.538641
8	1	0	-1.047419	2.217554	-0.702895
9	1	0	-0.362588	-1.850840	0.505107
10	1	0	-2.794420	-2.220690	0.637282
11	6	0	0.943432	0.400236	-0.266352
12	6	0	1.683475	-0.660557	-0.769189
13	1	0	1.125288	-1.489216	-1.198474
14	6	0	1.534950	1.686989	0.044641
15	1	0	2.581056	1.823186	-0.265283
16	1	0	3.290969	-1.697410	-1.307413
17	7	0	2.996668	-0.862286	-0.816026
18	8	0	0.955448	2.624257	0.576922
19	7	0	-4.704439	-0.417648	0.152537
20	8	0	-5.441719	0.523357	-0.076691
21	8	0	-5.102409	-1.526616	0.458604
22	6	0	4.060271	-0.123535	-0.144903
23	6	0	5.256378	-1.033518	0.094559
24	1	0	3.667367	0.248210	0.807328
25	1	0	4.364447	0.740745	-0.743719
26	6	0	6.393554	-0.278243	0.772684
27	1	0	4.943120	-1.881026	0.711555
28	1	0	5.595419	-1.437047	-0.865418
29	1	0	7.248809	-0.934355	0.945205
30	1	0	6.730004	0.559777	0.156396
31	1	0	6.075513	0.120761	1.739709

Structure 13e (C_2H_5OH)

Energy (Hartrees): -800.682336342
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.788155	1.038859	-0.365208
2	6	0	-1.421635	1.236746	-0.450630
3	6	0	-0.517010	0.208059	-0.134038
4	6	0	-1.035417	-1.028698	0.282384
5	6	0	-2.400871	-1.247486	0.368163
6	6	0	-3.258220	-0.204474	0.045138
7	1	0	-3.480639	1.829675	-0.621785
8	1	0	-1.050635	2.195707	-0.787141
9	1	0	-0.358541	-1.826579	0.565728
10	1	0	-2.791639	-2.201226	0.697522
11	6	0	0.942524	0.404701	-0.254410
12	6	0	1.684123	-0.652656	-0.768857
13	1	0	1.123242	-1.470714	-1.214652
14	6	0	1.527616	1.674715	0.094398
15	1	0	2.580393	1.821404	-0.178938
16	1	0	3.286163	-1.693775	-1.307658
17	7	0	2.993940	-0.860905	-0.810681
18	8	0	0.931331	2.606142	0.634886
19	7	0	-4.699103	-0.418036	0.145452
20	8	0	-5.442733	0.505879	-0.130178
21	8	0	-5.099819	-1.512151	0.499627
22	6	0	4.059683	-0.124480	-0.139242
23	6	0	5.270575	-1.024155	0.058807
24	1	0	3.677200	0.221341	0.827017
25	1	0	4.342395	0.755645	-0.725387
26	6	0	6.407212	-0.272569	0.742242
27	1	0	4.978234	-1.892437	0.657045
28	1	0	5.601528	-1.396443	-0.916535
29	1	0	7.273339	-0.921885	0.883898
30	1	0	6.724267	0.587067	0.145585
31	1	0	6.098058	0.094465	1.724732

Structure 13f (vacuum)

Energy (Hartrees): -800.653622720
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.842564	1.133914	-0.076829
2	6	0	-1.474130	1.323846	-0.175477
3	6	0	-0.579560	0.242835	-0.100488
4	6	0	-1.113363	-1.043668	0.078814
5	6	0	-2.480796	-1.254396	0.155011
6	6	0	-3.325562	-0.157294	0.081023
7	1	0	-3.536646	1.961054	-0.140405
8	1	0	-1.095159	2.324169	-0.346592
9	1	0	-0.442027	-1.886798	0.191499
10	1	0	-2.898263	-2.242877	0.292166
11	6	0	0.875242	0.455127	-0.214609
12	6	0	1.613357	-0.467879	-0.920504
13	1	0	1.063299	-1.188737	-1.522712
14	6	0	1.420548	1.713284	0.294001
15	1	0	0.760260	2.241513	1.008300
16	1	0	3.271274	-1.327338	-1.631215
17	7	0	2.939441	-0.639760	-0.971604
18	8	0	2.475271	2.218534	-0.033081
19	7	0	-4.779611	-0.369852	0.176414
20	8	0	-5.494976	0.608399	0.133360
21	8	0	-5.174669	-1.511173	0.291299
22	6	0	3.932268	-0.144950	-0.025864
23	6	0	5.112550	-1.105530	0.039056
24	1	0	3.447069	-0.065966	0.952442
25	1	0	4.253437	0.861714	-0.300643
26	6	0	6.184753	-0.598904	0.999707
27	1	0	4.762727	-2.094187	0.352649
28	1	0	5.541242	-1.216888	-0.963679
29	1	0	7.029901	-1.286909	1.043904
30	1	0	6.559181	0.377475	0.684647
31	1	0	5.783425	-0.493321	2.010291

Structure 13f ($CHCl_3$)

Energy (Hartrees): -800.678204301
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.833061	1.140457	-0.004556
2	6	0	-1.467877	1.335023	-0.121652
3	6	0	-0.570246	0.250564	-0.126065
4	6	0	-1.104976	-1.046141	-0.012349
5	6	0	-2.469504	-1.259804	0.080994
6	6	0	-3.316513	-0.158842	0.090118
7	1	0	-3.518697	1.977352	-0.008253
8	1	0	-1.096187	2.345087	-0.244075
9	1	0	-0.437752	-1.898952	0.031075
10	1	0	-2.875082	-2.258960	0.168997
11	6	0	0.879891	0.467903	-0.251800
12	6	0	1.625538	-0.465842	-0.954906
13	1	0	1.087870	-1.179628	-1.575687
14	6	0	1.424852	1.725312	0.234421
15	1	0	0.789638	2.254052	0.968178
16	1	0	3.283501	-1.339918	-1.625257
17	7	0	2.942056	-0.645504	-0.973089
18	8	0	2.470531	2.243032	-0.127130
19	7	0	-4.760105	-0.374344	0.201590
20	8	0	-5.486043	0.601017	0.213380
21	8	0	-5.165306	-1.518832	0.275535
22	6	0	3.922084	-0.142843	-0.017657
23	6	0	5.076430	-1.128189	0.108731
24	1	0	3.415517	-0.018584	0.944501
25	1	0	4.278943	0.843637	-0.322284
26	6	0	6.135043	-0.612219	1.077700
27	1	0	4.693475	-2.095191	0.449562
28	1	0	5.523739	-1.284936	-0.879113
29	1	0	6.959292	-1.321736	1.170709
30	1	0	6.546991	0.340785	0.736175
31	1	0	5.711682	-0.458073	2.073802

Structure 13f (DMSO)

Energy (Hartrees): -800.678318453
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.829175	1.141759	0.010456
2	6	0	-1.465115	1.337851	-0.112644
3	6	0	-0.565852	0.253345	-0.134632
4	6	0	-1.102040	-1.045147	-0.035036
5	6	0	-2.465756	-1.259218	0.062769
6	6	0	-3.314081	-0.158579	0.091831
7	1	0	-3.511323	1.981484	0.019373
8	1	0	-1.097718	2.350435	-0.226588
9	1	0	-0.437661	-1.900792	-0.007370
10	1	0	-2.865889	-2.261529	0.139896
11	6	0	0.882242	0.469882	-0.265033
12	6	0	1.627365	-0.477776	-0.957225
13	1	0	1.091699	-1.196160	-1.574113
14	6	0	1.427741	1.732036	0.204190
15	1	0	0.797194	2.265190	0.938618
16	1	0	3.280931	-1.373803	-1.600599
17	7	0	2.939773	-0.662878	-0.964493
18	8	0	2.469123	2.252666	-0.169729
19	7	0	-4.754703	-0.373695	0.210860
20	8	0	-5.479542	0.603006	0.267164
21	8	0	-5.164943	-1.519642	0.247078
22	6	0	3.916186	-0.148040	-0.012447
23	6	0	5.068885	-1.132323	0.133276
24	1	0	3.406244	-0.008377	0.945955
25	1	0	4.277061	0.832385	-0.331732
26	6	0	6.119437	-0.601744	1.102237
27	1	0	4.682721	-2.093963	0.484802
28	1	0	5.520065	-1.302638	-0.850191
29	1	0	6.943310	-1.309575	1.212445
30	1	0	6.534142	0.346417	0.749664
31	1	0	5.687616	-0.433578	2.092732

Structure 13f (C_2H_5OH)

Energy (Hartrees): -800.680756688
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.834404	1.139553	0.047005
2	6	0	-1.475382	1.363084	-0.079629
3	6	0	-0.559618	0.294425	-0.145461
4	6	0	-1.071484	-1.015788	-0.086988
5	6	0	-2.429605	-1.257552	0.017750
6	6	0	-3.294993	-0.172106	0.090555
7	1	0	-3.530434	1.967012	0.090346
8	1	0	-1.125354	2.384852	-0.162088
9	1	0	-0.391876	-1.859837	-0.094756
10	1	0	-2.810948	-2.269079	0.064315
11	6	0	0.885045	0.531910	-0.277094
12	6	0	1.631922	-0.378362	-1.024134
13	1	0	1.097947	-1.047233	-1.696314
14	6	0	1.426941	1.766465	0.238054
15	1	0	0.786482	2.292681	0.966016
16	1	0	3.286281	-1.240796	-1.703997
17	7	0	2.940090	-0.571497	-1.025739
18	8	0	2.491888	2.285440	-0.093096
19	7	0	-4.726184	-0.415166	0.216632
20	8	0	-5.476336	0.543769	0.260262
21	8	0	-5.117761	-1.567708	0.272927
22	6	0	3.905203	-0.140969	-0.019867
23	6	0	5.002861	-1.186237	0.123665
24	1	0	3.367698	-0.011935	0.923840
25	1	0	4.329024	0.828875	-0.290405
26	6	0	6.039471	-0.750515	1.153499
27	1	0	4.557263	-2.141463	0.417284
28	1	0	5.482814	-1.336124	-0.849499
29	1	0	6.823498	-1.502617	1.261949
30	1	0	6.513362	0.189353	0.858018
31	1	0	5.578832	-0.602498	2.134148

Structure 13g (vacuum)

Energy (Hartrees): -800.657442810
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.997496	-0.794771	-0.416742
2	6	0	-2.320568	-1.206790	-0.405383
3	6	0	-3.292281	-0.304212	-0.000143
4	6	0	-2.978846	0.985600	0.401364
5	6	0	-1.649267	1.375688	0.400038
6	6	0	-0.636827	0.500633	-0.018911
7	1	0	-0.235723	-1.480454	-0.769029
8	1	0	-2.610389	-2.201096	-0.717333
9	1	0	-3.767128	1.651978	0.724694
10	1	0	-1.386976	2.365202	0.754730
11	6	0	0.773396	0.928894	-0.046696
12	6	0	1.111256	2.184297	-0.457309
13	6	0	1.828204	0.005891	0.349512
14	1	0	0.356437	2.893131	-0.788027
15	1	0	1.525039	-0.986053	0.707401
16	8	0	2.338998	2.645344	-0.524245
17	1	0	2.945048	1.899714	-0.221348
18	7	0	3.062873	0.337275	0.317275
19	7	0	-4.702686	-0.731734	0.010771
20	8	0	-5.531192	0.076399	0.372154
21	8	0	-4.948410	-1.865474	-0.342405
22	6	0	4.070597	-0.620147	0.735086
23	6	0	5.018224	-0.950184	-0.415934
24	1	0	3.605678	-1.540425	1.116787
25	1	0	4.643092	-0.172875	1.554509
26	6	0	6.136727	-1.889535	0.026195
27	1	0	4.441206	-1.400915	-1.228961
28	1	0	5.434850	-0.016657	-0.804033
29	1	0	6.805516	-2.123220	-0.803409
30	1	0	6.734608	-1.437445	0.821512
31	1	0	5.733555	-2.832003	0.405692

Structure 13g ($CHCl_3$)

Energy (Hartrees): -800.677163327
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.994614	-0.804869	-0.390434
2	6	0	-2.317534	-1.215669	-0.382607
3	6	0	-3.293194	-0.304024	-0.002410
4	6	0	-2.982396	0.995729	0.374947
5	6	0	-1.653504	1.385081	0.376552
6	6	0	-0.637509	0.499509	-0.015222
7	1	0	-0.231771	-1.500881	-0.719284
8	1	0	-2.593821	-2.218921	-0.678715
9	1	0	-3.765799	1.677005	0.679223
10	1	0	-1.397410	2.384635	0.707211
11	6	0	0.772752	0.925395	-0.037200
12	6	0	1.111705	2.184230	-0.437036
13	6	0	1.827677	-0.001928	0.355030
14	1	0	0.363319	2.901829	-0.763675
15	1	0	1.531570	-0.997066	0.705507
16	8	0	2.347591	2.633464	-0.496172
17	1	0	2.944840	1.868462	-0.193501
18	7	0	3.060674	0.338930	0.322162
19	7	0	-4.697413	-0.728540	0.006167
20	8	0	-5.541990	0.095475	0.297050
21	8	0	-4.947362	-1.883313	-0.278379
22	6	0	4.079487	-0.613115	0.731998
23	6	0	5.010841	-0.945209	-0.431268
24	1	0	3.620973	-1.531029	1.123206
25	1	0	4.661319	-0.157030	1.539682
26	6	0	6.133188	-1.884070	-0.000581
27	1	0	4.423374	-1.400411	-1.234773
28	1	0	5.426138	-0.013556	-0.826870
29	1	0	6.790556	-2.122214	-0.839217
30	1	0	6.743201	-1.429707	0.784966
31	1	0	5.733390	-2.825206	0.387335

Structure 13g (DMSO)

Energy (Hartrees): -800.675454892
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.109135	-0.702911	-0.748440
2	6	0	-2.440405	-1.073351	-0.654694
3	6	0	-3.306352	-0.264307	0.069379
4	6	0	-2.874874	0.892109	0.707201
5	6	0	-1.538621	1.241903	0.613749
6	6	0	-0.633922	0.460836	-0.123508
7	1	0	-0.436566	-1.316405	-1.336267
8	1	0	-2.804684	-1.967089	-1.143721
9	1	0	-3.568310	1.494389	1.279085
10	1	0	-1.189425	2.123421	1.138574
11	6	0	0.781177	0.850263	-0.246832
12	6	0	1.138037	2.165242	-0.323967
13	6	0	1.823863	-0.168107	-0.299742
14	1	0	0.398610	2.962052	-0.304154
15	1	0	1.529437	-1.216224	-0.181813
16	8	0	2.379227	2.582972	-0.452876
17	1	0	2.957491	1.741075	-0.482215
18	7	0	3.055674	0.150747	-0.444754
19	7	0	-4.717445	-0.645800	0.169156
20	8	0	-5.457167	0.060358	0.828093
21	8	0	-5.082901	-1.650011	-0.412472
22	6	0	4.070670	-0.890003	-0.420400
23	6	0	5.047881	-0.659611	0.729198
24	1	0	4.616863	-0.854855	-1.368836
25	1	0	3.605815	-1.880206	-0.330680
26	6	0	6.137458	-1.725347	0.759319
27	1	0	5.492673	0.334395	0.620504
28	1	0	4.489491	-0.661665	1.670563
29	1	0	6.834480	-1.552221	1.581928
30	1	0	5.707418	-2.722526	0.888389
31	1	0	6.711172	-1.725614	-0.171722

Structure 13g (C_2H_5OH)

Energy (Hartrees): -800.676027909
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.105028	-0.690675	-0.758413
2	6	0	-2.434180	-1.067664	-0.667290
3	6	0	-3.302170	-0.266927	0.064337
4	6	0	-2.876654	0.888627	0.708597
5	6	0	-1.542552	1.244726	0.616334
6	6	0	-0.634912	0.470698	-0.124885
7	1	0	-0.429801	-1.297122	-1.350492
8	1	0	-2.794402	-1.959557	-1.162814
9	1	0	-3.572376	1.484706	1.284286
10	1	0	-1.197171	2.124425	1.146763
11	6	0	0.779548	0.864720	-0.242790
12	6	0	1.129166	2.179372	-0.319581
13	6	0	1.824577	-0.153077	-0.293440
14	1	0	0.389493	2.975496	-0.306349
15	1	0	1.527851	-1.201161	-0.180969
16	8	0	2.374084	2.603427	-0.443300
17	1	0	2.961404	1.769181	-0.469423
18	7	0	3.056770	0.164625	-0.431999
19	7	0	-4.706185	-0.656761	0.168052
20	8	0	-5.450806	0.036415	0.836470
21	8	0	-5.074428	-1.658411	-0.417787
22	6	0	4.064927	-0.884204	-0.416983
23	6	0	5.047210	-0.679714	0.732669
24	1	0	4.609861	-0.842679	-1.365882
25	1	0	3.592109	-1.871744	-0.340091
26	6	0	6.126581	-1.756671	0.742111
27	1	0	5.502241	0.310995	0.637577
28	1	0	4.493182	-0.691079	1.676604
29	1	0	6.831299	-1.600804	1.561697
30	1	0	5.688284	-2.751434	0.862450
31	1	0	6.694060	-1.751008	-0.192795

Structure 13h (vacuum)

Energy (Hartrees): -800.633413082
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.346734	-1.073616	-0.638463
2	6	0	1.026746	-0.655534	-0.698577
3	6	0	0.611828	0.529113	-0.074239
4	6	0	1.560689	1.279557	0.633455
5	6	0	2.887532	0.882921	0.693632
6	6	0	3.257698	-0.290875	0.054842
7	1	0	2.679864	-1.980850	-1.124149
8	1	0	0.308178	-1.243265	-1.257992
9	1	0	1.249157	2.168138	1.169464
10	1	0	3.628409	1.451735	1.239038
11	6	0	-0.803777	0.948869	-0.169054
12	6	0	-1.085068	2.253326	-0.333762
13	1	0	-0.275271	2.973003	-0.427412
14	6	0	-1.830345	-0.108011	-0.073482
15	1	0	-1.505755	-1.016538	0.458308
16	7	0	-2.997644	-0.009049	-0.551114
17	8	0	-2.330757	2.747930	-0.396106
18	1	0	-2.299446	3.696961	-0.535338
19	7	0	4.665153	-0.725450	0.122719
20	8	0	5.439923	-0.025050	0.738842
21	8	0	4.961989	-1.755744	-0.443156
22	6	0	-3.905826	-1.116710	-0.324333
23	6	0	-5.104926	-0.664780	0.507703
24	1	0	-3.407844	-1.965630	0.170993
25	1	0	-4.263359	-1.459675	-1.301224
26	6	0	-6.114541	-1.792404	0.701360
27	1	0	-4.743590	-0.307004	1.476576
28	1	0	-5.570404	0.189353	0.009465
29	1	0	-6.967390	-1.462281	1.296810
30	1	0	-6.495011	-2.146232	-0.260386
31	1	0	-5.659806	-2.644445	1.213474

Structure 13h ($CHCl_3$)

Energy (Hartrees): -800.658866320
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.330901	-1.088895	-0.616761
2	6	0	1.013267	-0.664913	-0.676030
3	6	0	0.608338	0.535939	-0.073798
4	6	0	1.566757	1.297703	0.611824
5	6	0	2.890945	0.895083	0.671098
6	6	0	3.251213	-0.295749	0.054461
7	1	0	2.646165	-2.008994	-1.090477
8	1	0	0.290882	-1.263764	-1.218616
9	1	0	1.269436	2.202700	1.128276
10	1	0	3.631121	1.479360	1.201337
11	6	0	-0.805627	0.960830	-0.170054
12	6	0	-1.081628	2.271793	-0.312657
13	1	0	-0.275541	2.996926	-0.389045
14	6	0	-1.834179	-0.093934	-0.083671
15	1	0	-1.521605	-0.997855	0.459922
16	7	0	-2.997758	-0.004414	-0.579189
17	8	0	-2.323427	2.768757	-0.372607
18	1	0	-2.282806	3.726736	-0.475375
19	7	0	4.650658	-0.734083	0.120667
20	8	0	5.446171	-0.021285	0.700131
21	8	0	4.944682	-1.787437	-0.408790
22	6	0	-3.902617	-1.118244	-0.345208
23	6	0	-5.097182	-0.674867	0.497718
24	1	0	-3.394198	-1.960743	0.147162
25	1	0	-4.265815	-1.464927	-1.318667
26	6	0	-6.085201	-1.816033	0.716542
27	1	0	-4.729054	-0.303728	1.459584
28	1	0	-5.588891	0.164961	-0.001569
29	1	0	-6.936064	-1.492024	1.319643
30	1	0	-6.472943	-2.186860	-0.236506
31	1	0	-5.610319	-2.654856	1.233331

Structure 13h (DMSO)

Energy (Hartrees): -800.657048028
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.313361	-1.093312	-0.608935
2	6	0	0.998470	-0.660621	-0.665619
3	6	0	0.605256	0.548103	-0.071268
4	6	0	1.571039	1.309308	0.604591
5	6	0	2.892018	0.896596	0.662844
6	6	0	3.241854	-0.301596	0.053227
7	1	0	2.615886	-2.020126	-1.077956
8	1	0	0.270327	-1.261405	-1.198608
9	1	0	1.283982	2.223080	1.111268
10	1	0	3.635847	1.482422	1.186365
11	6	0	-0.807054	0.980244	-0.166799
12	6	0	-1.073615	2.294788	-0.299954
13	1	0	-0.261622	3.014874	-0.359549
14	6	0	-1.832377	-0.077515	-0.082045
15	1	0	-1.517268	-0.977167	0.465831
16	7	0	-2.995477	-0.001450	-0.583128
17	8	0	-2.311032	2.803414	-0.369925
18	1	0	-2.254260	3.764729	-0.436776
19	7	0	4.637593	-0.748430	0.116845
20	8	0	5.438257	-0.045723	0.703672
21	8	0	4.927901	-1.799353	-0.422060
22	6	0	-3.889168	-1.125435	-0.344828
23	6	0	-5.093820	-0.690782	0.487483
24	1	0	-3.372321	-1.955593	0.157928
25	1	0	-4.243131	-1.485222	-1.317139
26	6	0	-6.062813	-1.846199	0.714454
27	1	0	-4.736287	-0.304376	1.447518
28	1	0	-5.600559	0.134086	-0.022649
29	1	0	-6.922679	-1.530313	1.309320
30	1	0	-6.437959	-2.234097	-0.236925
31	1	0	-5.574675	-2.669921	1.242948

Structure 13h (C_2H_5OH)

Energy (Hartrees): -800.663006819
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.307756	-1.113066	-0.576286
2	6	0	0.993651	-0.679351	-0.633814
3	6	0	0.606955	0.545954	-0.068336
4	6	0	1.581133	1.324083	0.577224
5	6	0	2.902204	0.914409	0.629898
6	6	0	3.243995	-0.302159	0.051569
7	1	0	2.604762	-2.053412	-1.021629
8	1	0	0.260672	-1.292946	-1.145147
9	1	0	1.300548	2.249494	1.065709
10	1	0	3.651053	1.514346	1.129885
11	6	0	-0.804531	0.976572	-0.159286
12	6	0	-1.079075	2.291424	-0.280564
13	1	0	-0.278749	3.023661	-0.338488
14	6	0	-1.832432	-0.078930	-0.083062
15	1	0	-1.526969	-0.978888	0.469023
16	7	0	-2.991124	0.001549	-0.595645
17	8	0	-2.322048	2.787423	-0.340737
18	1	0	-2.284915	3.750594	-0.391182
19	7	0	4.635413	-0.745912	0.112453
20	8	0	5.461922	0.006668	0.594009
21	8	0	4.910693	-1.848734	-0.322614
22	6	0	-3.891154	-1.118621	-0.360203
23	6	0	-5.091462	-0.684066	0.477536
24	1	0	-3.376323	-1.953252	0.136427
25	1	0	-4.248278	-1.472912	-1.333068
26	6	0	-6.062396	-1.838193	0.703861
27	1	0	-4.729788	-0.302119	1.437913
28	1	0	-5.598284	0.143943	-0.027478
29	1	0	-6.919744	-1.521803	1.302226
30	1	0	-6.441558	-2.222803	-0.247336
31	1	0	-5.574859	-2.664546	1.228997

Structure 13i (vacuum)

Energy (Hartrees): -800.640229757
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.219804	-1.166786	-0.650388
2	6	0	0.912619	-0.711791	-0.728406
3	6	0	0.519907	0.478984	-0.102280
4	6	0	1.478410	1.211363	0.611261
5	6	0	2.788991	0.769810	0.699253
6	6	0	3.136994	-0.414601	0.066584
7	1	0	2.535691	-2.079896	-1.136213
8	1	0	0.189670	-1.280186	-1.301846
9	1	0	1.190412	2.129540	1.104652
10	1	0	3.538057	1.321139	1.251202
11	6	0	-0.886472	0.920106	-0.196432
12	6	0	-1.264689	2.203343	-0.302694
13	1	0	-2.321438	2.441004	-0.376392
14	6	0	-1.950079	-0.110091	-0.178706
15	1	0	-1.642070	-1.096776	0.197279
16	7	0	-3.141972	0.112854	-0.541378
17	8	0	-0.390608	3.230091	-0.346955
18	1	0	-0.860064	4.056977	-0.477383
19	7	0	4.530086	-0.890149	0.159852
20	8	0	5.312268	-0.216682	0.796064
21	8	0	4.808739	-1.926218	-0.405339
22	6	0	-4.107666	-0.960083	-0.397170
23	6	0	-5.213167	-0.564882	0.580270
24	1	0	-3.633762	-1.896366	-0.063419
25	1	0	-4.554966	-1.142778	-1.380256
26	6	0	-6.285059	-1.645308	0.690086
27	1	0	-4.764101	-0.374919	1.560083
28	1	0	-5.652440	0.378133	0.243950
29	1	0	-7.071032	-1.352380	1.388003
30	1	0	-6.751966	-1.832086	-0.280442
31	1	0	-5.859544	-2.588245	1.043020

Structure 13i ($CHCl_3$)

Energy (Hartrees): -800.663408923
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.196723	-1.195304	-0.597381
2	6	0	0.890486	-0.737669	-0.664258
3	6	0	0.516621	0.482513	-0.081314
4	6	0	1.495007	1.237537	0.583503
5	6	0	2.805273	0.794518	0.659394
6	6	0	3.134524	-0.417023	0.065925
7	1	0	2.488431	-2.130773	-1.055612
8	1	0	0.153081	-1.329569	-1.194179
9	1	0	1.225630	2.173499	1.053901
10	1	0	3.561284	1.370783	1.175828
11	6	0	-0.889075	0.925756	-0.167536
12	6	0	-1.265992	2.212449	-0.280254
13	1	0	-2.320567	2.465223	-0.327241
14	6	0	-1.949483	-0.104907	-0.128997
15	1	0	-1.665003	-1.057770	0.338978
16	7	0	-3.120219	0.077611	-0.580221
17	8	0	-0.394522	3.231131	-0.363088
18	1	0	-0.870833	4.065145	-0.450679
19	7	0	4.522290	-0.890976	0.142749
20	8	0	5.335520	-0.189321	0.710782
21	8	0	4.788880	-1.961764	-0.365982
22	6	0	-4.088575	-0.991182	-0.394994
23	6	0	-5.207993	-0.551831	0.547260
24	1	0	-3.615308	-1.904957	-0.007077
25	1	0	-4.521249	-1.223991	-1.373850
26	6	0	-6.295829	-1.614074	0.667076
27	1	0	-4.776629	-0.340043	1.531136
28	1	0	-5.632753	0.385123	0.175151
29	1	0	-7.081858	-1.296550	1.355461
30	1	0	-6.760543	-1.809865	-0.303267
31	1	0	-5.887337	-2.557750	1.039518

Structure 13i (DMSO)

Energy (Hartrees): -800.660379743
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.185347	-1.190154	-0.600598
2	6	0	0.881088	-0.726013	-0.662456
3	6	0	0.515805	0.494607	-0.075311
4	6	0	1.498359	1.242540	0.591025
5	6	0	2.806443	0.792303	0.663441
6	6	0	3.128492	-0.418268	0.063213
7	1	0	2.466764	-2.126910	-1.062727
8	1	0	0.138633	-1.315288	-1.188641
9	1	0	1.235728	2.176438	1.069410
10	1	0	3.563590	1.363887	1.183554
11	6	0	-0.889688	0.940555	-0.155592
12	6	0	-1.266458	2.227256	-0.270328
13	1	0	-2.320166	2.487550	-0.300160
14	6	0	-1.944636	-0.094130	-0.098083
15	1	0	-1.666211	-1.021547	0.420410
16	7	0	-3.103942	0.055561	-0.591069
17	8	0	-0.391244	3.241208	-0.373612
18	1	0	-0.868206	4.078265	-0.433704
19	7	0	4.513417	-0.899178	0.136581
20	8	0	5.329724	-0.208333	0.715442
21	8	0	4.777788	-1.964940	-0.385735
22	6	0	-4.065110	-1.016448	-0.374614
23	6	0	-5.243858	-0.526597	0.463275
24	1	0	-3.597465	-1.882664	0.114608
25	1	0	-4.435912	-1.339631	-1.353375
26	6	0	-6.264702	-1.635177	0.696197
27	1	0	-4.864702	-0.157225	1.421690
28	1	0	-5.714411	0.320824	-0.044648
29	1	0	-7.109603	-1.276145	1.287838
30	1	0	-6.656215	-2.011920	-0.253123
31	1	0	-5.814782	-2.476639	1.230508

Structure 13i (C_2H_5OH)

Energy (Hartrees): -800.665332764
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.171990	-1.201148	-0.579255
2	6	0	0.869949	-0.732561	-0.637958
3	6	0	0.513446	0.499249	-0.067159
4	6	0	1.505042	1.254567	0.578817
5	6	0	2.812244	0.802221	0.644701
6	6	0	3.123967	-0.420061	0.061961
7	1	0	2.446205	-2.146210	-1.028985
8	1	0	0.121293	-1.326325	-1.150285
9	1	0	1.249113	2.194699	1.048952
10	1	0	3.575586	1.379709	1.149242
11	6	0	-0.890683	0.946406	-0.144514
12	6	0	-1.267708	2.234337	-0.256323
13	1	0	-2.320279	2.497519	-0.283250
14	6	0	-1.945368	-0.087315	-0.088189
15	1	0	-1.679366	-1.000536	0.461019
16	7	0	-3.092729	0.045661	-0.614336
17	8	0	-0.395680	3.249580	-0.358824
18	1	0	-0.869183	4.088513	-0.422409
19	7	0	4.503206	-0.903212	0.129261
20	8	0	5.342648	-0.187730	0.643125
21	8	0	4.753678	-2.000803	-0.332446
22	6	0	-4.054567	-1.023761	-0.383470
23	6	0	-5.230548	-0.528285	0.454236
24	1	0	-3.585131	-1.885309	0.111754
25	1	0	-4.428489	-1.357467	-1.357156
26	6	0	-6.255031	-1.633060	0.690902
27	1	0	-4.849252	-0.157619	1.411498
28	1	0	-5.700083	0.319210	-0.054672
29	1	0	-7.096508	-1.270288	1.285314
30	1	0	-6.651634	-2.008469	-0.256922
31	1	0	-5.807190	-2.476471	1.224098

Structure 13j (vacuum)

Energy (Hartrees): -800.641025525
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.720966	-0.946043	-0.927241
2	6	0	0.537734	-0.225753	-0.977054
3	6	0	0.319378	0.849849	-0.109063
4	6	0	1.305129	1.181962	0.825812
5	6	0	2.490537	0.465355	0.893921
6	6	0	2.677006	-0.585617	0.009998
7	1	0	1.910040	-1.774997	-1.595305
8	1	0	-0.228878	-0.500656	-1.687599
9	1	0	1.140342	2.006563	1.506696
10	1	0	3.261228	0.705052	1.613633
11	6	0	-0.935529	1.632865	-0.188862
12	6	0	-0.955457	2.974997	-0.143825
13	1	0	-1.897125	3.513142	-0.215995
14	6	0	-2.242369	0.973257	-0.333127
15	1	0	-3.103224	1.657817	-0.398817
16	7	0	-2.396829	-0.281282	-0.373474
17	8	0	0.157967	3.727884	-0.017593
18	1	0	-0.057790	4.659653	-0.095457
19	7	0	3.938415	-1.349880	0.071385
20	8	0	4.754475	-1.022168	0.906514
21	8	0	4.083889	-2.258747	-0.717820
22	6	0	-3.748507	-0.795648	-0.486099
23	6	0	-4.107620	-1.636426	0.737472
24	1	0	-3.791848	-1.431792	-1.376964
25	1	0	-4.487907	0.010902	-0.614908
26	6	0	-5.488572	-2.271358	0.601909
27	1	0	-3.341383	-2.404891	0.867135
28	1	0	-4.068090	-0.998241	1.625577
29	1	0	-5.741338	-2.860635	1.484822
30	1	0	-6.262480	-1.509498	0.475889
31	1	0	-5.529474	-2.934678	-0.265925

Structure 13j ($CHCl_3$)

Energy (Hartrees): -800.665687876
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.755996	-0.895242	-0.978314
2	6	0	0.574452	-0.173060	-1.028734
3	6	0	0.323954	0.857543	-0.114242
4	6	0	1.282372	1.147572	0.863491
5	6	0	2.467762	0.431310	0.932372
6	6	0	2.682058	-0.579412	0.006362
7	1	0	1.958914	-1.688569	-1.685040
8	1	0	-0.162241	-0.407325	-1.785560
9	1	0	1.095530	1.936465	1.581140
10	1	0	3.210465	0.643307	1.689757
11	6	0	-0.935680	1.633168	-0.188322
12	6	0	-0.958248	2.977648	-0.136118
13	1	0	-1.898375	3.518625	-0.206960
14	6	0	-2.236720	0.968501	-0.334416
15	1	0	-3.095872	1.649164	-0.422237
16	7	0	-2.389749	-0.289948	-0.347738
17	8	0	0.153149	3.723821	-0.016036
18	1	0	-0.072021	4.660894	-0.050232
19	7	0	3.934034	-1.346766	0.074779
20	8	0	4.743053	-1.046387	0.930137
21	8	0	4.097701	-2.243972	-0.727593
22	6	0	-3.743882	-0.802746	-0.476808
23	6	0	-4.121034	-1.652278	0.734590
24	1	0	-3.779886	-1.432206	-1.373084
25	1	0	-4.476358	0.007944	-0.607301
26	6	0	-5.506976	-2.270869	0.580923
27	1	0	-3.367488	-2.434694	0.862468
28	1	0	-4.084587	-1.024855	1.631020
29	1	0	-5.769341	-2.873755	1.452924
30	1	0	-6.273836	-1.499442	0.466004
31	1	0	-5.550443	-2.919072	-0.298958

Structure 13j (DMSO)

Energy (Hartrees): -800.663965910
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.770884	-0.849866	-1.015050
2	6	0	0.592542	-0.122162	-1.062112
3	6	0	0.320449	0.866439	-0.108077
4	6	0	1.254020	1.110594	0.905404
5	6	0	2.437216	0.389641	0.970480
6	6	0	2.672958	-0.579709	0.005702
7	1	0	1.987203	-1.609503	-1.754180
8	1	0	-0.122421	-0.316936	-1.851169
9	1	0	1.050163	1.865931	1.654361
10	1	0	3.159831	0.569891	1.755199
11	6	0	-0.937542	1.644932	-0.179344
12	6	0	-0.954740	2.989670	-0.126269
13	1	0	-1.891868	3.536607	-0.191695
14	6	0	-2.236499	0.979281	-0.326225
15	1	0	-3.096821	1.655916	-0.419948
16	7	0	-2.383139	-0.281721	-0.334945
17	8	0	0.163927	3.725586	-0.017542
18	1	0	-0.060177	4.664322	-0.034328
19	7	0	3.922759	-1.350008	0.070139
20	8	0	4.717133	-1.079574	0.949900
21	8	0	4.101459	-2.220436	-0.759358
22	6	0	-3.735709	-0.800734	-0.471992
23	6	0	-4.105053	-1.675475	0.723114
24	1	0	-3.769895	-1.413796	-1.379962
25	1	0	-4.471938	0.008058	-0.585459
26	6	0	-5.489286	-2.294964	0.560915
27	1	0	-3.350222	-2.460065	0.833395
28	1	0	-4.068831	-1.065908	1.631941
29	1	0	-5.747194	-2.917602	1.420456
30	1	0	-6.257426	-1.522275	0.465311
31	1	0	-5.533327	-2.923018	-0.333541

Structure 13j (C_2H_5OH)

Energy (Hartrees): -800.668564223
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.776932	-0.860502	-1.008860
2	6	0	0.597440	-0.135899	-1.057736
3	6	0	0.326731	0.860975	-0.111369
4	6	0	1.265957	1.119385	0.894134
5	6	0	2.450886	0.402392	0.961288
6	6	0	2.682622	-0.577631	0.005817
7	1	0	1.991812	-1.627491	-1.741121
8	1	0	-0.119741	-0.338781	-1.842555
9	1	0	1.063693	1.882100	1.636262
10	1	0	3.176657	0.592755	1.740834
11	6	0	-0.934029	1.634110	-0.182847
12	6	0	-0.953524	2.979619	-0.129940
13	1	0	-1.889271	3.527926	-0.197427
14	6	0	-2.232330	0.968337	-0.329659
15	1	0	-3.089996	1.647341	-0.431167
16	7	0	-2.386334	-0.292170	-0.327976
17	8	0	0.161925	3.718965	-0.019473
18	1	0	-0.059503	4.658283	-0.037099
19	7	0	3.928506	-1.345828	0.073683
20	8	0	4.724538	-1.080292	0.954483
21	8	0	4.113435	-2.218144	-0.753469
22	6	0	-3.743350	-0.799818	-0.468279
23	6	0	-4.130813	-1.666005	0.726732
24	1	0	-3.779002	-1.415105	-1.374613
25	1	0	-4.470911	0.015475	-0.590056
26	6	0	-5.522380	-2.267769	0.558315
27	1	0	-3.387694	-2.460702	0.843998
28	1	0	-4.092186	-1.054714	1.634498
29	1	0	-5.791105	-2.887750	1.416607
30	1	0	-6.280965	-1.485781	0.460622
31	1	0	-5.571021	-2.894976	-0.336630

Structure 13k (vacuum)

Energy (Hartrees): -800.640585529
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.924734	-0.813671	-0.918110
2	6	0	0.683492	-0.199916	-0.958347
3	6	0	0.375892	0.850210	-0.083967
4	6	0	1.334596	1.250169	0.854051
5	6	0	2.584376	0.649677	0.904026
6	6	0	2.856838	-0.373319	0.011233
7	1	0	2.181291	-1.620465	-1.591128
8	1	0	-0.059134	-0.534019	-1.668971
9	1	0	1.089638	2.024893	1.571015
10	1	0	3.333481	0.948946	1.624411
11	6	0	-0.927142	1.550317	-0.161200
12	6	0	-0.945929	2.891900	-0.096488
13	1	0	-0.025395	3.464825	-0.031250
14	6	0	-2.193429	0.815595	-0.313875
15	1	0	-3.092514	1.439961	-0.381065
16	7	0	-2.252164	-0.449361	-0.359117
17	8	0	-2.098537	3.602535	-0.118758
18	1	0	-1.910194	4.541290	-0.176096
19	7	0	4.181051	-1.022128	0.055839
20	8	0	4.978901	-0.614662	0.873363
21	8	0	4.392847	-1.921383	-0.729166
22	6	0	-3.565266	-1.054656	-0.482899
23	6	0	-3.867281	-1.933763	0.728998
24	1	0	-3.561622	-1.681586	-1.381434
25	1	0	-4.356746	-0.298943	-0.604142
26	6	0	-5.210588	-2.644115	0.589156
27	1	0	-3.057885	-2.659311	0.843195
28	1	0	-3.859902	-1.307879	1.626503
29	1	0	-5.423105	-3.264848	1.461062
30	1	0	-6.026894	-1.924591	0.484305
31	1	0	-5.220682	-3.290340	-0.292432

Structure 13k ($CHCl_3$)

Energy (Hartrees): -800.664580150
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.942671	-0.820805	-0.922213
2	6	0	0.702733	-0.205614	-0.968115
3	6	0	0.388875	0.846366	-0.095928
4	6	0	1.346907	1.252356	0.842175
5	6	0	2.596013	0.652624	0.897750
6	6	0	2.871687	-0.376876	0.010752
7	1	0	2.192861	-1.627637	-1.598054
8	1	0	-0.029372	-0.537941	-1.691680
9	1	0	1.105228	2.035667	1.550867
10	1	0	3.336648	0.964233	1.622097
11	6	0	-0.916876	1.540113	-0.176530
12	6	0	-0.941947	2.884099	-0.092644
13	1	0	-0.027826	3.464814	-0.008488
14	6	0	-2.177520	0.803332	-0.346838
15	1	0	-3.068997	1.424033	-0.495026
16	7	0	-2.252936	-0.463281	-0.314759
17	8	0	-2.091124	3.586811	-0.119203
18	1	0	-1.900104	4.531630	-0.123164
19	7	0	4.188909	-1.024204	0.064852
20	8	0	4.996999	-0.607770	0.871252
21	8	0	4.406835	-1.942220	-0.700534
22	6	0	-3.570298	-1.058132	-0.472207
23	6	0	-3.925795	-1.913612	0.741499
24	1	0	-3.544810	-1.699782	-1.360329
25	1	0	-4.345137	-0.293825	-0.631209
26	6	0	-5.283369	-2.589081	0.575625
27	1	0	-3.143008	-2.663886	0.884757
28	1	0	-3.926364	-1.278246	1.632869
29	1	0	-5.529769	-3.200193	1.446541
30	1	0	-6.079202	-1.849316	0.451128
31	1	0	-5.292133	-3.240350	-0.303042

Structure 13k (DMSO)

Energy (Hartrees): -800.662543619
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.944409	-0.820970	-0.925086
2	6	0	0.705764	-0.203198	-0.972943
3	6	0	0.392110	0.849315	-0.100473
4	6	0	1.350598	1.256810	0.836835
5	6	0	2.598509	0.654916	0.893683
6	6	0	2.872756	-0.378228	0.009760
7	1	0	2.191632	-1.626736	-1.603583
8	1	0	-0.022703	-0.531418	-1.702668
9	1	0	1.112883	2.046044	1.540469
10	1	0	3.337119	0.970936	1.618161
11	6	0	-0.913873	1.541460	-0.180394
12	6	0	-0.938543	2.886107	-0.090986
13	1	0	-0.024320	3.465671	0.000959
14	6	0	-2.172483	0.803346	-0.350360
15	1	0	-3.062907	1.419610	-0.518492
16	7	0	-2.252100	-0.463331	-0.295914
17	8	0	-2.086286	3.587420	-0.118611
18	1	0	-1.891227	4.532349	-0.104823
19	7	0	4.187054	-1.029344	0.067248
20	8	0	5.003331	-0.602414	0.861126
21	8	0	4.396985	-1.963464	-0.682443
22	6	0	-3.570691	-1.056070	-0.463654
23	6	0	-3.931932	-1.923010	0.739553
24	1	0	-3.543226	-1.688978	-1.358198
25	1	0	-4.342858	-0.288863	-0.617958
26	6	0	-5.299008	-2.577068	0.568605
27	1	0	-3.160182	-2.687587	0.870524
28	1	0	-3.922645	-1.299886	1.639725
29	1	0	-5.548129	-3.203365	1.428065
30	1	0	-6.084663	-1.823328	0.464966
31	1	0	-5.321375	-3.208522	-0.324298

Structure 13k (C_2H_5OH)

Energy (Hartrees): -800.666893927
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.953459	-0.824878	-0.926830
2	6	0	0.714667	-0.208650	-0.975713
3	6	0	0.396787	0.840541	-0.100357
4	6	0	1.352246	1.246242	0.841436
5	6	0	2.600901	0.647399	0.899414
6	6	0	2.878612	-0.382656	0.012118
7	1	0	2.203622	-1.627109	-1.608460
8	1	0	-0.010188	-0.533874	-1.710352
9	1	0	1.110758	2.031691	1.547982
10	1	0	3.336565	0.962636	1.627456
11	6	0	-0.908370	1.532933	-0.182934
12	6	0	-0.929917	2.878296	-0.093743
13	1	0	-0.016233	3.458143	-0.001286
14	6	0	-2.168143	0.798323	-0.356091
15	1	0	-3.052820	1.417827	-0.542295
16	7	0	-2.257420	-0.467229	-0.284054
17	8	0	-2.073793	3.585721	-0.122705
18	1	0	-1.878021	4.530567	-0.111507
19	7	0	4.191158	-1.026644	0.068314
20	8	0	5.010830	-0.599403	0.859775
21	8	0	4.410089	-1.960947	-0.679946
22	6	0	-3.580030	-1.049969	-0.459235
23	6	0	-3.960856	-1.910126	0.742225
24	1	0	-3.551021	-1.685335	-1.351969
25	1	0	-4.344113	-0.276974	-0.623753
26	6	0	-5.332750	-2.551699	0.560682
27	1	0	-3.198113	-2.682123	0.882143
28	1	0	-3.953970	-1.285466	1.641482
29	1	0	-5.593906	-3.174801	1.419024
30	1	0	-6.111239	-1.791341	0.450484
31	1	0	-5.354140	-3.184224	-0.331596

Structure 13l (vacuum)

Energy (Hartrees): -800.639343435
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.923284	-0.799703	-0.932881
2	6	0	0.685469	-0.179691	-0.974739
3	6	0	0.374525	0.858952	-0.088499
4	6	0	1.326865	1.244043	0.861218
5	6	0	2.573826	0.637313	0.913240
6	6	0	2.848970	-0.375731	0.010284
7	1	0	2.182434	-1.597864	-1.615103
8	1	0	-0.050451	-0.500484	-1.698784
9	1	0	1.081031	2.014221	1.582723
10	1	0	3.318770	0.925319	1.642503
11	6	0	-0.926626	1.567132	-0.166940
12	6	0	-0.922681	2.913857	-0.098928
13	1	0	0.008621	3.465458	-0.039432
14	6	0	-2.177758	0.816285	-0.328434
15	1	0	-3.099976	1.406378	-0.462303
16	7	0	-2.242617	-0.447957	-0.328342
17	8	0	-1.973216	3.753740	-0.111789
18	1	0	-2.806902	3.274727	-0.110413
19	7	0	4.169440	-1.032593	0.058206
20	8	0	4.962443	-0.639144	0.886841
21	8	0	4.381980	-1.924238	-0.735208
22	6	0	-3.547420	-1.063099	-0.477035
23	6	0	-3.875077	-1.930331	0.736681
24	1	0	-3.518222	-1.699202	-1.368501
25	1	0	-4.340870	-0.313433	-0.627603
26	6	0	-5.215724	-2.640871	0.574796
27	1	0	-3.068756	-2.655132	0.873381
28	1	0	-3.885215	-1.297096	1.628959
29	1	0	-5.445071	-3.254965	1.446940
30	1	0	-6.029825	-1.922211	0.449101
31	1	0	-5.208901	-3.293655	-0.301851

Structure 13l ($CHCl_3$)

Energy (Hartrees): -800.662668044
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.932222	-0.805639	-0.935900
2	6	0	0.696157	-0.183232	-0.980013
3	6	0	0.382573	0.856924	-0.094063
4	6	0	1.335188	1.243917	0.856300
5	6	0	2.581100	0.636446	0.910690
6	6	0	2.856997	-0.380621	0.010019
7	1	0	2.183040	-1.602708	-1.622937
8	1	0	-0.032401	-0.500649	-1.714107
9	1	0	1.093669	2.019779	1.573195
10	1	0	3.318947	0.933530	1.643920
11	6	0	-0.919528	1.562588	-0.176840
12	6	0	-0.913449	2.910128	-0.095666
13	1	0	0.018154	3.460894	-0.021328
14	6	0	-2.169782	0.812810	-0.356575
15	1	0	-3.075248	1.397939	-0.574550
16	7	0	-2.242137	-0.451097	-0.278931
17	8	0	-1.961275	3.748987	-0.110609
18	1	0	-2.804191	3.278613	-0.114345
19	7	0	4.170762	-1.035879	0.062196
20	8	0	4.976859	-0.634576	0.877917
21	8	0	4.386966	-1.945036	-0.714113
22	6	0	-3.544773	-1.067741	-0.466009
23	6	0	-3.922887	-1.909693	0.750321
24	1	0	-3.481950	-1.722934	-1.342256
25	1	0	-4.326402	-0.318428	-0.661902
26	6	0	-5.263055	-2.610970	0.554169
27	1	0	-3.132133	-2.643920	0.927922
28	1	0	-3.960400	-1.261151	1.631368
29	1	0	-5.524156	-3.213208	1.426863
30	1	0	-6.067875	-1.887793	0.395015
31	1	0	-5.234407	-3.275627	-0.313871

Structure 13l (DMSO)

Energy (Hartrees): -800.661009085
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.937468	-0.799947	-0.942814
2	6	0	0.702103	-0.175970	-0.989470
3	6	0	0.385598	0.860686	-0.099681
4	6	0	1.335909	1.246028	0.854030
5	6	0	2.581104	0.637515	0.910387
6	6	0	2.858806	-0.378967	0.008894
7	1	0	2.187463	-1.593206	-1.634831
8	1	0	-0.021149	-0.486833	-1.732126
9	1	0	1.094904	2.023245	1.569836
10	1	0	3.314475	0.935949	1.647506
11	6	0	-0.917661	1.562296	-0.180865
12	6	0	-0.916602	2.909699	-0.091059
13	1	0	0.012272	3.463883	-0.006784
14	6	0	-2.166642	0.811224	-0.358953
15	1	0	-3.072703	1.392167	-0.580900
16	7	0	-2.239457	-0.453148	-0.271320
17	8	0	-1.969586	3.739668	-0.104753
18	1	0	-2.807966	3.259193	-0.129401
19	7	0	4.170427	-1.036432	0.065111
20	8	0	4.982065	-0.626511	0.872392
21	8	0	4.382022	-1.958245	-0.699035
22	6	0	-3.545590	-1.066163	-0.460391
23	6	0	-3.917855	-1.926014	0.744462
24	1	0	-3.489513	-1.707266	-1.347657
25	1	0	-4.325461	-0.312002	-0.638867
26	6	0	-5.273913	-2.597425	0.555189
27	1	0	-3.139843	-2.680366	0.895432
28	1	0	-3.931488	-1.294846	1.638864
29	1	0	-5.530077	-3.219276	1.415765
30	1	0	-6.066469	-1.854007	0.431798
31	1	0	-5.273590	-3.236644	-0.332397

Structure 13l (C_2H_5OH)

Energy (Hartrees): -800.664806763
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.950287	-0.785764	-0.958978
2	6	0	0.715292	-0.162538	-1.008117
3	6	0	0.387062	0.857552	-0.103224
4	6	0	1.326280	1.228065	0.867484
5	6	0	2.571924	0.621703	0.926747
6	6	0	2.860236	-0.379095	0.010483
7	1	0	2.209884	-1.565251	-1.663114
8	1	0	0.001868	-0.459077	-1.766027
9	1	0	1.074988	1.991116	1.594890
10	1	0	3.295702	0.907887	1.678259
11	6	0	-0.917234	1.557069	-0.186177
12	6	0	-0.914547	2.903966	-0.088196
13	1	0	0.015846	3.454995	0.002098
14	6	0	-2.163507	0.802891	-0.370291
15	1	0	-3.065299	1.384421	-0.602873
16	7	0	-2.235917	-0.461276	-0.270378
17	8	0	-1.964743	3.740510	-0.100121
18	1	0	-2.810498	3.274347	-0.123173
19	7	0	4.168778	-1.032256	0.068253
20	8	0	4.985022	-0.620435	0.871137
21	8	0	4.386696	-1.958248	-0.690342
22	6	0	-3.542859	-1.072640	-0.462419
23	6	0	-3.931242	-1.916086	0.748615
24	1	0	-3.482033	-1.724734	-1.341236
25	1	0	-4.318351	-0.318263	-0.658102
26	6	0	-5.288770	-2.583693	0.554880
27	1	0	-3.158616	-2.672502	0.916241
28	1	0	-3.950621	-1.274613	1.635713
29	1	0	-5.554989	-3.194093	1.420746
30	1	0	-6.077476	-1.838767	0.415957
31	1	0	-5.283758	-3.233931	-0.324731

Structure 14a (vacuum)

Energy (Hartrees): -953.069476715
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.770801	1.444405	-0.025800
2	6	0	-4.011462	0.827875	-0.003151
3	6	0	-4.064266	-0.557289	0.039166
4	6	0	-2.916965	-1.337352	0.049880
5	6	0	-1.685162	-0.705164	0.007704
6	6	0	-1.584677	0.694197	-0.022058
7	1	0	-2.720909	2.526622	-0.017843
8	1	0	-4.929799	1.399431	-0.000365
9	1	0	-3.003586	-2.415431	0.068665
10	1	0	-0.784774	-1.307590	-0.033828
11	6	0	-0.274266	1.367142	-0.057520
12	6	0	0.783044	0.874460	0.676918
13	6	0	-0.086333	2.539981	-0.886192
14	1	0	0.633546	-0.009490	1.295292
15	1	0	-0.957295	2.846841	-1.491817
16	8	0	0.957996	3.172127	-0.974327
17	7	0	2.009176	1.393869	0.734684
18	1	0	2.181464	2.203651	0.142315
19	7	0	-5.377931	-1.221873	0.070037
20	8	0	-5.393361	-2.434420	0.100905
21	8	0	-6.364853	-0.517258	0.062935
22	6	0	3.104137	0.742156	1.421175
23	1	0	2.687994	0.176742	2.260920
24	1	0	3.752704	1.510358	1.848228
25	6	0	3.925875	-0.186531	0.543160
26	6	0	3.497108	-0.584131	-0.719664
27	6	0	5.139481	-0.671026	1.034081
28	6	0	4.268867	-1.461604	-1.478599
29	1	0	2.565782	-0.202718	-1.123533
30	6	0	5.907557	-1.546973	0.278996
31	1	0	5.484839	-0.357389	2.014614
32	6	0	5.472082	-1.946111	-0.982331
33	1	0	3.927369	-1.761752	-2.462104
34	1	0	6.848499	-1.914955	0.670900
35	1	0	6.071868	-2.626089	-1.575181

Structure 14a ($CHCl_3$)

Energy (Hartrees): -953.095846834
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.749144	1.352497	0.283670
2	6	0	-4.104398	1.082800	0.373503
3	6	0	-4.553848	-0.191367	0.051199
4	6	0	-3.685921	-1.192375	-0.366791
5	6	0	-2.336739	-0.901049	-0.466873
6	6	0	-1.835898	0.370173	-0.137657
7	1	0	-2.391548	2.333339	0.574005
8	1	0	-4.803395	1.838741	0.706314
9	1	0	-4.067877	-2.170562	-0.627191
10	1	0	-1.662452	-1.665819	-0.834386
11	6	0	-0.398170	0.669278	-0.228664
12	6	0	0.533746	-0.303431	0.102141
13	6	0	0.039457	1.969409	-0.666393
14	1	0	0.184760	-1.272309	0.455516
15	1	0	-0.755938	2.677313	-0.954627
16	8	0	1.214638	2.320218	-0.764172
17	7	0	1.850179	-0.172126	0.059385
18	1	0	2.223907	0.722432	-0.248723
19	7	0	-5.984314	-0.487829	0.148569
20	8	0	-6.360490	-1.602512	-0.159720
21	8	0	-6.727600	0.394303	0.532966
22	6	0	2.766833	-1.240714	0.470428
23	1	0	2.571718	-2.128391	-0.137061
24	1	0	2.577072	-1.491428	1.517305
25	6	0	4.193903	-0.789865	0.296217
26	6	0	4.849265	-0.974834	-0.921179
27	6	0	4.857331	-0.141404	1.338072
28	6	0	6.153264	-0.521263	-1.094140
29	1	0	4.335169	-1.477713	-1.734487
30	6	0	6.161316	0.312657	1.167282
31	1	0	4.349381	0.006022	2.286011
32	6	0	6.810967	0.122346	-0.049138
33	1	0	6.656132	-0.672099	-2.042547
34	1	0	6.670260	0.812634	1.983508
35	1	0	7.827597	0.474315	-0.181984

Structure 14a (DMSO)

Energy (Hartrees): -953.094319172
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.754107	1.360679	0.272458
2	6	0	-4.108653	1.086064	0.353519
3	6	0	-4.550670	-0.194400	0.043460
4	6	0	-3.673153	-1.197305	-0.352002
5	6	0	-2.324729	-0.901797	-0.444445
6	6	0	-1.832078	0.377041	-0.128778
7	1	0	-2.405867	2.346877	0.555223
8	1	0	-4.810091	1.845778	0.672409
9	1	0	-4.044377	-2.182463	-0.601632
10	1	0	-1.644712	-1.671558	-0.790286
11	6	0	-0.395666	0.680226	-0.211439
12	6	0	0.535032	-0.300956	0.108637
13	6	0	0.040103	1.985818	-0.630254
14	1	0	0.184643	-1.275197	0.444038
15	1	0	-0.756298	2.694673	-0.912409
16	8	0	1.215177	2.343673	-0.721381
17	7	0	1.849650	-0.170089	0.074428
18	1	0	2.228442	0.727618	-0.216027
19	7	0	-5.978392	-0.495914	0.133601
20	8	0	-6.344594	-1.627141	-0.128008
21	8	0	-6.735676	0.397877	0.464842
22	6	0	2.763327	-1.242906	0.484476
23	1	0	2.557138	-2.130351	-0.118414
24	1	0	2.579671	-1.484870	1.534036
25	6	0	4.189244	-0.795652	0.295324
26	6	0	4.832596	-0.983777	-0.928513
27	6	0	4.863277	-0.144592	1.329176
28	6	0	6.134910	-0.529541	-1.115736
29	1	0	4.310887	-1.490921	-1.734377
30	6	0	6.165604	0.310245	1.144003
31	1	0	4.364979	0.002659	2.282387
32	6	0	6.802927	0.118440	-0.079326
33	1	0	6.628765	-0.683673	-2.068599
34	1	0	6.682895	0.811942	1.954181
35	1	0	7.818073	0.470716	-0.223717

Structure 14a (C_2H_5OH)

Energy (Hartrees): -953.096123410
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.753793	1.362261	0.278641
2	6	0	-4.106536	1.084627	0.369492
3	6	0	-4.548119	-0.193702	0.047770
4	6	0	-3.673875	-1.191163	-0.369647
5	6	0	-2.327088	-0.892417	-0.468105
6	6	0	-1.834833	0.383391	-0.140450
7	1	0	-2.403673	2.345814	0.568729
8	1	0	-4.806091	1.839690	0.703477
9	1	0	-4.045350	-2.173765	-0.629171
10	1	0	-1.648204	-1.656280	-0.829084
11	6	0	-0.398838	0.687540	-0.230693
12	6	0	0.533971	-0.296571	0.086662
13	6	0	0.031595	1.986557	-0.652490
14	1	0	0.181985	-1.267800	0.429184
15	1	0	-0.762384	2.698941	-0.927496
16	8	0	1.212245	2.343684	-0.754716
17	7	0	1.846210	-0.170355	0.043189
18	1	0	2.228836	0.722180	-0.259209
19	7	0	-5.969311	-0.499665	0.152738
20	8	0	-6.345939	-1.617507	-0.151949
21	8	0	-6.724570	0.373292	0.541956
22	6	0	2.758692	-1.250723	0.440319
23	1	0	2.564729	-2.123735	-0.187272
24	1	0	2.556475	-1.518869	1.479852
25	6	0	4.186571	-0.797512	0.285452
26	6	0	4.854298	-0.972168	-0.926979
27	6	0	4.839514	-0.158416	1.340145
28	6	0	6.160174	-0.516202	-1.083087
29	1	0	4.348706	-1.469918	-1.748923
30	6	0	6.145407	0.297777	1.186155
31	1	0	4.322384	-0.021391	2.284879
32	6	0	6.807169	0.119393	-0.026102
33	1	0	6.672813	-0.659638	-2.027724
34	1	0	6.646614	0.789988	2.012209
35	1	0	7.825131	0.473135	-0.145763

Structure 14b (vacuum)

Energy (Hartrees): -953.062952189
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.100008	0.893273	1.118574
2	6	0	-3.153538	-0.006354	1.167695
3	6	0	-3.467609	-0.722678	0.022174
4	6	0	-2.773521	-0.556413	-1.166895
5	6	0	-1.729490	0.355087	-1.201229
6	6	0	-1.367147	1.089558	-0.061093
7	1	0	-1.825161	1.438568	2.013934
8	1	0	-3.719737	-0.170829	2.074560
9	1	0	-3.065699	-1.122880	-2.041016
10	1	0	-1.208270	0.531564	-2.135763
11	6	0	-0.257678	2.057406	-0.097586
12	6	0	0.963481	1.796043	-0.649590
13	6	0	-0.427778	3.381446	0.510841
14	1	0	1.697294	2.598762	-0.609643
15	1	0	-1.436695	3.573118	0.926070
16	8	0	0.425024	4.239924	0.570528
17	7	0	1.383805	0.657925	-1.227262
18	1	0	0.778743	-0.151844	-1.167294
19	7	0	-4.578603	-1.691005	0.067580
20	8	0	-4.826153	-2.308558	-0.946184
21	8	0	-5.175837	-1.810657	1.115664
22	6	0	2.779974	0.399796	-1.542741
23	1	0	3.279272	1.370273	-1.607227
24	1	0	2.846898	-0.061234	-2.531208
25	6	0	3.472624	-0.480848	-0.522095
26	6	0	3.261615	-0.289997	0.843711
27	6	0	4.350078	-1.477787	-0.941670
28	6	0	3.924884	-1.081637	1.773558
29	1	0	2.573016	0.477034	1.183337
30	6	0	5.016386	-2.269972	-0.011679
31	1	0	4.512713	-1.638579	-2.002674
32	6	0	4.804432	-2.073086	1.347915
33	1	0	3.754191	-0.925185	2.832047
34	1	0	5.694223	-3.044349	-0.350588
35	1	0	5.318295	-2.691553	2.073839

Structure 14b ($CHCl_3$)

Energy (Hartrees): -953.093237638
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.344037	0.990767	1.015763
2	6	0	-3.349418	0.039095	1.052996
3	6	0	-3.456940	-0.853408	-0.005443
4	6	0	-2.600998	-0.809691	-1.098120
5	6	0	-1.612756	0.160592	-1.127366
6	6	0	-1.458389	1.075431	-0.071680
7	1	0	-2.231321	1.670258	1.852406
8	1	0	-4.029039	-0.025048	1.892374
9	1	0	-2.724325	-1.509906	-1.913671
10	1	0	-0.975479	0.231829	-2.001949
11	6	0	-0.424502	2.123108	-0.099389
12	6	0	0.876015	1.928489	-0.506920
13	6	0	-0.766613	3.466472	0.342331
14	1	0	1.526094	2.800129	-0.489710
15	1	0	-1.828908	3.610126	0.613835
16	8	0	-0.000299	4.414919	0.409806
17	7	0	1.458692	0.798737	-0.896799
18	1	0	0.931590	-0.066339	-0.869350
19	7	0	-4.511485	-1.872290	0.027866
20	8	0	-4.532830	-2.702510	-0.859770
21	8	0	-5.311581	-1.836180	0.941784
22	6	0	2.864997	0.686442	-1.261157
23	1	0	3.311100	1.677304	-1.145911
24	1	0	2.949801	0.406321	-2.314236
25	6	0	3.594679	-0.326402	-0.405976
26	6	0	3.456339	-0.313980	0.983549
27	6	0	4.424437	-1.275632	-0.999074
28	6	0	4.140805	-1.236912	1.765925
29	1	0	2.807298	0.418919	1.452933
30	6	0	5.113970	-2.198542	-0.216203
31	1	0	4.530564	-1.294495	-2.079165
32	6	0	4.971556	-2.182000	1.167089
33	1	0	4.026069	-1.220179	2.843761
34	1	0	5.755882	-2.933563	-0.688393
35	1	0	5.503043	-2.903283	1.777106

Structure 14b (DMSO)

Energy (Hartrees): -953.092842635
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.281477	1.015782	1.017346
2	6	0	-3.321773	0.104594	1.083663
3	6	0	-3.497673	-0.780198	0.027029
4	6	0	-2.676093	-0.764367	-1.092969
5	6	0	-1.652433	0.167027	-1.151424
6	6	0	-1.426311	1.068847	-0.097500
7	1	0	-2.114870	1.683289	1.854766
8	1	0	-3.972171	0.065566	1.947564
9	1	0	-2.849376	-1.453810	-1.908738
10	1	0	-1.042959	0.214033	-2.046990
11	6	0	-0.344243	2.063397	-0.147637
12	6	0	0.928051	1.810358	-0.617774
13	6	0	-0.597157	3.403982	0.352058
14	1	0	1.630558	2.640521	-0.600967
15	1	0	-1.641856	3.591183	0.661734
16	8	0	0.219155	4.310439	0.433257
17	7	0	1.427237	0.668162	-1.072821
18	1	0	0.854469	-0.168872	-1.060099
19	7	0	-4.583433	-1.760425	0.093651
20	8	0	-4.650287	-2.603150	-0.781506
21	8	0	-5.366701	-1.686773	1.021790
22	6	0	2.824780	0.486909	-1.441922
23	1	0	3.284114	1.477613	-1.465215
24	1	0	2.879346	0.067646	-2.448558
25	6	0	3.559909	-0.413448	-0.471961
26	6	0	3.484081	-0.183501	0.903676
27	6	0	4.333769	-1.471886	-0.943406
28	6	0	4.176050	-0.998666	1.792423
29	1	0	2.879140	0.636238	1.279815
30	6	0	5.030202	-2.288416	-0.054398
31	1	0	4.388757	-1.659877	-2.011037
32	6	0	4.952024	-2.053747	1.314431
33	1	0	4.111707	-0.811435	2.858450
34	1	0	5.628416	-3.110102	-0.432054
35	1	0	5.490525	-2.690296	2.007393

Structure 14b (C_2H_5OH)

Energy (Hartrees): -953.094950804
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.175159	0.942805	1.081809
2	6	0	-3.211110	0.026549	1.144903
3	6	0	-3.464775	-0.763844	0.030592
4	6	0	-2.725078	-0.654476	-1.140274
5	6	0	-1.700811	0.276801	-1.189266
6	6	0	-1.401699	1.087031	-0.081470
7	1	0	-1.946393	1.541300	1.956278
8	1	0	-3.798348	-0.087069	2.046496
9	1	0	-2.959633	-1.270946	-1.998192
10	1	0	-1.147283	0.398278	-2.113984
11	6	0	-0.318477	2.084179	-0.127767
12	6	0	0.946452	1.827709	-0.623089
13	6	0	-0.557129	3.399474	0.413406
14	1	0	1.665924	2.642907	-0.593896
15	1	0	-1.580375	3.567514	0.792451
16	8	0	0.253936	4.323576	0.467555
17	7	0	1.414754	0.688667	-1.109618
18	1	0	0.819028	-0.133034	-1.117134
19	7	0	-4.547847	-1.743717	0.093110
20	8	0	-4.725231	-2.474079	-0.864415
21	8	0	-5.227994	-1.788537	1.101308
22	6	0	2.811246	0.477312	-1.473126
23	1	0	3.290625	1.458200	-1.499197
24	1	0	2.857112	0.053448	-2.477953
25	6	0	3.522042	-0.434805	-0.496143
26	6	0	3.499601	-0.158219	0.873141
27	6	0	4.218120	-1.551449	-0.953696
28	6	0	4.166481	-0.985941	1.768970
29	1	0	2.957498	0.709208	1.238985
30	6	0	4.889769	-2.380975	-0.057309
31	1	0	4.233797	-1.774031	-2.016041
32	6	0	4.863932	-2.100494	1.304693
33	1	0	4.144167	-0.762297	2.829815
34	1	0	5.426951	-3.248787	-0.423763
35	1	0	5.382460	-2.746944	2.003857

Structure 14c (vacuum)

Energy (Hartrees): -953.064696156
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.995676	0.859596	1.066285
2	6	0	-3.048922	-0.039099	1.135611
3	6	0	-3.398996	-0.745642	-0.005994
4	6	0	-2.743766	-0.571739	-1.214657
5	6	0	-1.692440	0.331596	-1.268644
6	6	0	-1.292875	1.047265	-0.131310
7	1	0	-1.717596	1.431466	1.941372
8	1	0	-3.596735	-0.200060	2.054197
9	1	0	-3.065633	-1.126599	-2.085546
10	1	0	-1.195811	0.511776	-2.215885
11	6	0	-0.159469	1.990287	-0.195992
12	6	0	1.030576	1.695776	-0.791479
13	6	0	-0.242137	3.303280	0.443819
14	1	0	1.810815	2.455185	-0.777665
15	7	0	1.391403	0.549671	-1.407546
16	1	0	0.760976	-0.237885	-1.322119
17	8	0	-1.177783	3.718648	1.086133
18	1	0	0.660236	3.933201	0.298669
19	7	0	-4.513618	-1.710203	0.063636
20	8	0	-4.796953	-2.313934	-0.949298
21	8	0	-5.076203	-1.841916	1.128850
22	6	0	2.781317	0.237569	-1.683436
23	1	0	2.825472	-0.394530	-2.573494
24	1	0	3.283457	1.174893	-1.940899
25	6	0	3.517966	-0.441235	-0.541412
26	6	0	4.755614	-1.032741	-0.799711
27	6	0	3.005993	-0.476324	0.752788
28	6	0	5.473611	-1.643052	0.219851
29	1	0	5.157404	-1.016499	-1.808383
30	6	0	3.724487	-1.092313	1.775424
31	1	0	2.043251	-0.028141	0.972793
32	6	0	4.957549	-1.674669	1.513075
33	1	0	6.432448	-2.100356	0.006266
34	1	0	3.314629	-1.116901	2.778092
35	1	0	5.513108	-2.155553	2.309172

Structure 14c ($CHCl_3$)

Energy (Hartrees): -953.096035611
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.088521	0.860188	1.058976
2	6	0	-3.127889	-0.052883	1.133650
3	6	0	-3.434836	-0.803425	0.006020
4	6	0	-2.746495	-0.661518	-1.190267
5	6	0	-1.711763	0.259698	-1.248577
6	6	0	-1.359923	1.026034	-0.127775
7	1	0	-1.834445	1.452644	1.928311
8	1	0	-3.689407	-0.188958	2.048181
9	1	0	-3.024649	-1.250438	-2.054004
10	1	0	-1.188254	0.406092	-2.186939
11	6	0	-0.253579	2.000311	-0.195237
12	6	0	0.980363	1.715405	-0.725555
13	6	0	-0.410013	3.339030	0.336940
14	1	0	1.726248	2.508458	-0.733379
15	7	0	1.406476	0.554587	-1.232003
16	1	0	0.799766	-0.254749	-1.168448
17	8	0	-1.407127	3.785547	0.877303
18	1	0	0.481958	3.983203	0.212004
19	7	0	-4.529792	-1.780147	0.080284
20	8	0	-4.741262	-2.475833	-0.893390
21	8	0	-5.166970	-1.846334	1.112143
22	6	0	2.791133	0.306208	-1.591589
23	1	0	2.814284	-0.293927	-2.503392
24	1	0	3.247309	1.269873	-1.832066
25	6	0	3.596488	-0.388348	-0.508431
26	6	0	4.760767	-1.070072	-0.868467
27	6	0	3.226488	-0.341302	0.834471
28	6	0	5.547348	-1.686624	0.097590
29	1	0	5.049496	-1.119387	-1.913950
30	6	0	4.012803	-0.962026	1.803173
31	1	0	2.320352	0.174732	1.133098
32	6	0	5.174228	-1.634355	1.438906
33	1	0	6.447500	-2.214451	-0.196092
34	1	0	3.713057	-0.920239	2.844126
35	1	0	5.783277	-2.118890	2.193176

Structure 14c (DMSO)

Energy (Hartrees): -953.096068258
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.115888	0.867536	1.051612
2	6	0	-3.123785	-0.079590	1.124582
3	6	0	-3.388771	-0.854543	0.001797
4	6	0	-2.684864	-0.705853	-1.184946
5	6	0	-1.680682	0.248722	-1.240567
6	6	0	-1.374333	1.043561	-0.126156
7	1	0	-1.891190	1.475724	1.918543
8	1	0	-3.688686	-0.222946	2.036176
9	1	0	-2.925973	-1.314600	-2.046295
10	1	0	-1.144025	0.393381	-2.172024
11	6	0	-0.302049	2.054303	-0.183998
12	6	0	0.956452	1.803295	-0.684394
13	6	0	-0.512787	3.389823	0.327170
14	1	0	1.676274	2.619980	-0.681492
15	7	0	1.429166	0.655703	-1.164612
16	1	0	0.841935	-0.170759	-1.138862
17	8	0	-1.543884	3.821793	0.820571
18	1	0	0.367390	4.054070	0.230625
19	7	0	-4.451565	-1.863870	0.070949
20	8	0	-4.640779	-2.565181	-0.904548
21	8	0	-5.091485	-1.952250	1.101357
22	6	0	2.821019	0.451074	-1.529370
23	1	0	2.864356	-0.070097	-2.487619
24	1	0	3.271289	1.436567	-1.671006
25	6	0	3.603457	-0.330047	-0.491954
26	6	0	4.643732	-1.164401	-0.902325
27	6	0	3.330380	-0.205434	0.870670
28	6	0	5.407231	-1.856177	0.033698
29	1	0	4.854203	-1.274684	-1.961753
30	6	0	4.091427	-0.899155	1.807835
31	1	0	2.518651	0.432325	1.205216
32	6	0	5.132499	-1.725164	1.392451
33	1	0	6.211741	-2.502741	-0.298571
34	1	0	3.869176	-0.794864	2.864037
35	1	0	5.722618	-2.266777	2.122984

Structure 14c (C_2H_5OH)

Energy (Hartrees): -953.098525560
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.087637	0.841414	1.074319
2	6	0	-3.096269	-0.105170	1.145997
3	6	0	-3.389995	-0.846676	0.007924
4	6	0	-2.715607	-0.667635	-1.192123
5	6	0	-1.709308	0.284072	-1.244582
6	6	0	-1.374713	1.046344	-0.115941
7	1	0	-1.838556	1.421594	1.954250
8	1	0	-3.640149	-0.271537	2.066485
9	1	0	-2.977432	-1.252405	-2.064089
10	1	0	-1.192010	0.451725	-2.182952
11	6	0	-0.297662	2.054065	-0.175748
12	6	0	0.959045	1.797648	-0.686451
13	6	0	-0.497108	3.382072	0.333407
14	1	0	1.682252	2.611364	-0.690334
15	7	0	1.419144	0.648810	-1.167166
16	1	0	0.826196	-0.173831	-1.133681
17	8	0	-1.531597	3.817878	0.835695
18	1	0	0.378497	4.048701	0.237574
19	7	0	-4.449093	-1.855654	0.075494
20	8	0	-4.731982	-2.464541	-0.938978
21	8	0	-5.001066	-2.043542	1.143143
22	6	0	2.807506	0.433137	-1.543695
23	1	0	2.835564	-0.099780	-2.495830
24	1	0	3.260289	1.414621	-1.703700
25	6	0	3.595859	-0.338988	-0.504448
26	6	0	4.611359	-1.202644	-0.915905
27	6	0	3.354707	-0.175902	0.860292
28	6	0	5.381437	-1.886343	0.020816
29	1	0	4.798534	-1.342384	-1.976331
30	6	0	4.121732	-0.862012	1.797909
31	1	0	2.564174	0.486531	1.197945
32	6	0	5.137741	-1.718042	1.381253
33	1	0	6.166596	-2.555763	-0.312770
34	1	0	3.923653	-0.727751	2.855630
35	1	0	5.732668	-2.253583	2.112492

Structure 14d (vacuum)

Energy (Hartrees): -953.057158684
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.231216	0.802497	0.986425
2	6	0	-3.474481	0.205671	1.117572
3	6	0	-3.984548	-0.520120	0.050745
4	6	0	-3.296866	-0.653990	-1.144547
5	6	0	-2.058081	-0.042472	-1.263948
6	6	0	-1.494660	0.676756	-0.200583
7	1	0	-1.825528	1.372341	1.810423
8	1	0	-4.047376	0.288617	2.031146
9	1	0	-3.740369	-1.209439	-1.959780
10	1	0	-1.532486	-0.099978	-2.210123
11	6	0	-0.148602	1.273403	-0.327712
12	6	0	0.822437	0.585968	-1.003727
13	6	0	0.154597	2.558639	0.298594
14	1	0	0.595478	-0.425818	-1.335468
15	7	0	2.066213	0.985352	-1.348352
16	1	0	2.377856	1.902843	-1.065807
17	1	0	1.211429	2.888325	0.224839
18	8	0	-0.630896	3.260556	0.892662
19	7	0	-5.304639	-1.161571	0.186944
20	8	0	-5.717449	-1.804212	-0.755679
21	8	0	-5.897629	-1.010913	1.233717
22	6	0	3.110615	0.039812	-1.699568
23	1	0	3.745916	0.488222	-2.466867
24	1	0	2.623575	-0.825993	-2.158577
25	6	0	3.966574	-0.409851	-0.529744
26	6	0	5.276222	-0.827302	-0.763749
27	6	0	3.463751	-0.446206	0.769696
28	6	0	6.069493	-1.285449	0.281458
29	1	0	5.678918	-0.790994	-1.771248
30	6	0	4.259191	-0.900722	1.817497
31	1	0	2.449627	-0.119040	0.972498
32	6	0	5.561417	-1.322717	1.576438
33	1	0	7.086231	-1.605304	0.086544
34	1	0	3.858610	-0.923549	2.823928
35	1	0	6.179832	-1.673666	2.393682

Structure 14d ($CHCl_3$)

Energy (Hartrees): -953.090070200
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.370074	1.010634	0.821468
2	6	0	-3.628999	0.469771	1.020168
3	6	0	-4.095927	-0.487288	0.127399
4	6	0	-3.342309	-0.907471	-0.959702
5	6	0	-2.088168	-0.350469	-1.148831
6	6	0	-1.568003	0.603861	-0.258568
7	1	0	-1.997991	1.750197	1.516881
8	1	0	-4.240430	0.775388	1.858825
9	1	0	-3.739768	-1.639486	-1.650085
10	1	0	-1.512712	-0.644368	-2.019080
11	6	0	-0.210903	1.148933	-0.450566
12	6	0	0.778222	0.312878	-0.931047
13	6	0	0.095080	2.524806	-0.112948
14	1	0	0.545316	-0.744498	-1.041688
15	7	0	2.026905	0.614122	-1.293949
16	1	0	2.347414	1.572618	-1.247779
17	1	0	1.157092	2.817262	-0.211819
18	8	0	-0.701540	3.363885	0.272946
19	7	0	-5.426734	-1.064518	0.333871
20	8	0	-5.820490	-1.896633	-0.460968
21	8	0	-6.073311	-0.686730	1.291469
22	6	0	3.044785	-0.388382	-1.567790
23	1	0	3.563671	-0.123147	-2.491275
24	1	0	2.529716	-1.336688	-1.741792
25	6	0	4.051552	-0.536805	-0.444573
26	6	0	5.400773	-0.718851	-0.743834
27	6	0	3.646459	-0.519387	0.890938
28	6	0	6.334245	-0.889504	0.275028
29	1	0	5.724350	-0.723759	-1.780053
30	6	0	4.578508	-0.687248	1.910156
31	1	0	2.600114	-0.368221	1.137596
32	6	0	5.924595	-0.873344	1.604372
33	1	0	7.381151	-1.027884	0.029878
34	1	0	4.253708	-0.671125	2.944407
35	1	0	6.650869	-1.000517	2.398924

Structure 14d (DMSO)

Energy (Hartrees): -953.090381718
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.403507	-1.072991	-0.760590
2	6	0	-3.671511	-0.559858	-0.972910
3	6	0	-4.129904	0.460385	-0.146746
4	6	0	-3.356166	0.969577	0.887616
5	6	0	-2.094261	0.437913	1.093468
6	6	0	-1.581873	-0.579125	0.268823
7	1	0	-2.037528	-1.856160	-1.410052
8	1	0	-4.293984	-0.934014	-1.775003
9	1	0	-3.741396	1.751229	1.528698
10	1	0	-1.504487	0.806296	1.924761
11	6	0	-0.218357	-1.095615	0.476472
12	6	0	0.765315	-0.210527	0.890873
13	6	0	0.102568	-2.484293	0.228344
14	1	0	0.519330	0.849018	0.919980
15	7	0	2.012173	-0.468973	1.271563
16	1	0	2.340868	-1.425715	1.323057
17	1	0	1.172342	-2.748399	0.311593
18	8	0	-0.689929	-3.366008	-0.069788
19	7	0	-5.467110	1.009848	-0.370488
20	8	0	-5.832697	1.936053	0.329904
21	8	0	-6.151911	0.517738	-1.248363
22	6	0	3.014188	0.563367	1.497817
23	1	0	3.490893	0.388889	2.464270
24	1	0	2.490795	1.520984	1.549544
25	6	0	4.067208	0.596602	0.410343
26	6	0	5.418524	0.651326	0.746477
27	6	0	3.699917	0.590050	-0.937094
28	6	0	6.393133	0.704240	-0.248003
29	1	0	5.709844	0.648995	1.792273
30	6	0	4.671361	0.640008	-1.931000
31	1	0	2.649895	0.542757	-1.210403
32	6	0	6.021508	0.698020	-1.588526
33	1	0	7.441535	0.743688	0.026096
34	1	0	4.375756	0.634056	-2.974331
35	1	0	6.778130	0.735509	-2.364202

Structure 14d (C_2H_5OH)

Energy (Hartrees): -953.092522899
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.376400	0.886287	0.967601
2	6	0	-3.631435	0.314118	1.077938
3	6	0	-4.081735	-0.511372	0.053657
4	6	0	-3.313260	-0.771974	-1.073690
5	6	0	-2.064362	-0.182515	-1.172732
6	6	0	-1.563843	0.647765	-0.155096
7	1	0	-2.013286	1.511724	1.771733
8	1	0	-4.247247	0.493793	1.949472
9	1	0	-3.692619	-1.406367	-1.863864
10	1	0	-1.478667	-0.354914	-2.068453
11	6	0	-0.218972	1.242689	-0.256384
12	6	0	0.795723	0.495489	-0.840095
13	6	0	0.045415	2.568482	0.234913
14	1	0	0.572006	-0.531554	-1.120692
15	7	0	2.043325	0.853300	-1.112664
16	1	0	2.366190	1.788848	-0.896259
17	1	0	1.093240	2.907043	0.172893
18	8	0	-0.783495	3.346475	0.702314
19	7	0	-5.402732	-1.120400	0.164440
20	8	0	-5.767416	-1.881481	-0.714054
21	8	0	-6.088200	-0.844738	1.132566
22	6	0	3.058252	-0.076950	-1.592176
23	1	0	3.576874	0.379046	-2.437220
24	1	0	2.537754	-0.965673	-1.956696
25	6	0	4.057593	-0.454725	-0.519797
26	6	0	5.424871	-0.356445	-0.769240
27	6	0	3.622785	-0.926165	0.721295
28	6	0	6.349500	-0.730355	0.204107
29	1	0	5.768780	0.015123	-1.729578
30	6	0	4.543743	-1.297275	1.694361
31	1	0	2.559205	-1.002385	0.928387
32	6	0	5.910729	-1.200992	1.437300
33	1	0	7.411102	-0.649015	-0.001466
34	1	0	4.195832	-1.663506	2.653960
35	1	0	6.627952	-1.490894	2.196972

Structure 14e (vacuum)

Energy (Hartrees): -953.054860620
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.049647	0.900026	-0.105492
2	6	0	-2.741537	1.353601	-0.138994
3	6	0	-1.665768	0.453881	-0.087249
4	6	0	-1.947755	-0.914491	0.031558
5	6	0	-3.251927	-1.385509	0.057130
6	6	0	-4.284311	-0.465106	-0.014694
7	1	0	-4.885879	1.584243	-0.153419
8	1	0	-2.549451	2.415087	-0.204645
9	1	0	-1.132752	-1.621233	0.135490
10	1	0	-3.475697	-2.439492	0.149911
11	6	0	-0.264336	0.921967	-0.177023
12	6	0	0.618786	0.166044	-0.903610
13	1	0	0.202242	-0.633388	-1.512277
14	6	0	0.108957	2.215989	0.398837
15	1	0	1.106255	2.593833	0.115267
16	1	0	2.399730	-0.388834	-1.653954
17	7	0	1.964087	0.232780	-0.989915
18	8	0	-0.606454	2.902106	1.094838
19	7	0	-5.674838	-0.952505	0.018901
20	8	0	-6.561711	-0.128180	-0.043922
21	8	0	-5.849183	-2.150277	0.103758
22	6	0	2.884069	0.884797	-0.062944
23	1	0	2.384043	0.943648	0.909800
24	1	0	3.114290	1.905032	-0.382536
25	6	0	4.158114	0.082971	0.047869
26	6	0	4.127375	-1.191018	0.617991
27	6	0	5.366026	0.589249	-0.423949
28	6	0	5.288760	-1.945748	0.716550
29	1	0	3.187224	-1.585400	0.991721
30	6	0	6.532229	-0.165818	-0.325982
31	1	0	5.397056	1.579588	-0.866108
32	6	0	6.494433	-1.432608	0.243116
33	1	0	5.256589	-2.930648	1.166829
34	1	0	7.467955	0.236925	-0.695036
35	1	0	7.401645	-2.019844	0.319982

Structure 14e ($CHCl_3$)

Energy (Hartrees): -953.086801615
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.058971	0.912836	-0.138467
2	6	0	-2.742777	1.339345	-0.160595
3	6	0	-1.681074	0.423240	-0.065898
4	6	0	-1.991054	-0.938837	0.076245
5	6	0	-3.303611	-1.384573	0.089303
6	6	0	-4.320350	-0.447159	-0.019046
7	1	0	-4.875014	1.618136	-0.223238
8	1	0	-2.533344	2.394939	-0.263736
9	1	0	-1.192781	-1.661250	0.201764
10	1	0	-3.537663	-2.434961	0.200006
11	6	0	-0.273870	0.871114	-0.144897
12	6	0	0.611892	0.069984	-0.839431
13	1	0	0.186395	-0.741441	-1.424876
14	6	0	0.107370	2.162894	0.401291
15	1	0	1.105101	2.530972	0.117912
16	1	0	2.361687	-0.554442	-1.568641
17	7	0	1.945345	0.101601	-0.921327
18	8	0	-0.603935	2.873038	1.093690
19	7	0	-5.712803	-0.904820	0.001613
20	8	0	-6.591699	-0.065599	-0.025249
21	8	0	-5.921999	-2.102124	0.042045
22	6	0	2.890044	0.848464	-0.094632
23	1	0	2.438455	0.975228	0.894675
24	1	0	3.077124	1.840885	-0.512943
25	6	0	4.187985	0.086049	0.019292
26	6	0	4.210582	-1.155857	0.658265
27	6	0	5.368121	0.603456	-0.509889
28	6	0	5.398773	-1.868040	0.767998
29	1	0	3.292374	-1.559658	1.074815
30	6	0	6.560970	-0.108267	-0.398660
31	1	0	5.354369	1.567188	-1.008563
32	6	0	6.577158	-1.343593	0.239142
33	1	0	5.409213	-2.828271	1.270832
34	1	0	7.475121	0.303276	-0.811105
35	1	0	7.505109	-1.896931	0.327074

Structure 14e (DMSO)

Energy (Hartrees): -953.086782424
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.054643	0.914452	-0.104247
2	6	0	-2.741242	1.347810	-0.140714
3	6	0	-1.671510	0.435907	-0.087249
4	6	0	-1.973957	-0.931960	0.023663
5	6	0	-3.283719	-1.384031	0.051229
6	6	0	-4.308328	-0.449980	-0.011487
7	1	0	-4.873109	1.620093	-0.159527
8	1	0	-2.540440	2.406633	-0.226647
9	1	0	-1.170990	-1.654789	0.110809
10	1	0	-3.505650	-2.439444	0.137831
11	6	0	-0.269732	0.891478	-0.174112
12	6	0	0.616109	0.092292	-0.879545
13	1	0	0.191195	-0.712196	-1.474897
14	6	0	0.114084	2.178303	0.375917
15	1	0	1.103588	2.553373	0.074397
16	1	0	2.359190	-0.529404	-1.611974
17	7	0	1.944922	0.122525	-0.957401
18	8	0	-0.585105	2.880385	1.092695
19	7	0	-5.695916	-0.914392	0.028327
20	8	0	-6.581829	-0.079906	0.014860
21	8	0	-5.900066	-2.113560	0.071431
22	6	0	2.889013	0.864789	-0.126438
23	1	0	2.427391	1.004683	0.856281
24	1	0	3.093659	1.850401	-0.551639
25	6	0	4.174303	0.085325	0.012988
26	6	0	4.159258	-1.179447	0.606049
27	6	0	5.380760	0.610909	-0.443977
28	6	0	5.336020	-1.906833	0.741263
29	1	0	3.220178	-1.590305	0.965381
30	6	0	6.562295	-0.115823	-0.306520
31	1	0	5.395567	1.591968	-0.907775
32	6	0	6.541316	-1.374502	0.284720
33	1	0	5.315530	-2.886345	1.205510
34	1	0	7.496555	0.301096	-0.665679
35	1	0	7.460125	-1.940193	0.390325

Structure 14e (C_2H_5OH)

Energy (Hartrees): -953.088676304
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.040118	0.903807	-0.433831
2	6	0	-2.705800	1.259609	-0.350080
3	6	0	-1.732816	0.334773	0.063083
4	6	0	-2.147142	-0.959288	0.412244
5	6	0	-3.479007	-1.335361	0.333136
6	6	0	-4.406119	-0.393424	-0.090819
7	1	0	-4.784471	1.613169	-0.770966
8	1	0	-2.410547	2.261904	-0.632152
9	1	0	-1.419028	-1.679736	0.767959
10	1	0	-3.793101	-2.334048	0.606811
11	6	0	-0.298849	0.706824	0.097947
12	6	0	0.593576	-0.218492	-0.423570
13	1	0	0.151231	-1.096280	-0.887975
14	6	0	0.074766	1.995420	0.628019
15	1	0	1.127277	2.287874	0.541301
16	1	0	2.316548	-1.045144	-0.970460
17	7	0	1.921111	-0.253343	-0.478998
18	8	0	-0.705525	2.787138	1.156231
19	7	0	-5.813156	-0.776787	-0.181781
20	8	0	-6.612381	0.048050	-0.585077
21	8	0	-6.129328	-1.905827	0.146202
22	6	0	2.884592	0.677000	0.104849
23	1	0	2.601978	0.856799	1.147580
24	1	0	2.859081	1.629415	-0.430740
25	6	0	4.270488	0.088054	0.028617
26	6	0	4.616452	-1.001026	0.832052
27	6	0	5.209859	0.606880	-0.860754
28	6	0	5.885498	-1.563071	0.744570
29	1	0	3.889022	-1.406029	1.529578
30	6	0	6.482656	0.047131	-0.947060
31	1	0	4.943873	1.453294	-1.486063
32	6	0	6.821141	-1.038867	-0.146033
33	1	0	6.147101	-2.407543	1.372414
34	1	0	7.207107	0.458675	-1.641065
35	1	0	7.811055	-1.476145	-0.213824

Structure 14f (vacuum)

Energy (Hartrees): -953.057282363
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.107051	0.964597	-0.000856
2	6	0	2.785073	1.376892	0.031227
3	6	0	1.730926	0.447788	0.036703
4	6	0	2.054898	-0.918046	0.007428
5	6	0	3.372229	-1.348200	-0.001660
6	6	0	4.379812	-0.395808	-0.010931
7	1	0	4.923376	1.674120	0.002192
8	1	0	2.568100	2.436757	0.087076
9	1	0	1.259316	-1.652245	-0.040384
10	1	0	3.628269	-2.398792	-0.024508
11	6	0	0.326505	0.895444	0.080410
12	6	0	-0.557174	0.188047	0.863456
13	1	0	-0.139006	-0.533180	1.563064
14	6	0	-0.006636	2.156698	-0.580251
15	1	0	0.742446	2.496362	-1.320599
16	1	0	-2.351591	-0.314285	1.603338
17	7	0	-1.894709	0.233012	0.888946
18	8	0	-0.977845	2.848834	-0.349528
19	7	0	5.783099	-0.842986	-0.035475
20	8	0	6.644543	0.010224	-0.053833
21	8	0	5.992159	-2.037863	-0.034881
22	6	0	-2.775352	0.755583	-0.154014
23	1	0	-2.256621	0.627832	-1.109488
24	1	0	-2.938838	1.824948	-0.020080
25	6	0	-4.075038	-0.010217	-0.143158
26	6	0	-4.102846	-1.355266	-0.518507
27	6	0	-5.257722	0.606814	0.256957
28	6	0	-5.293448	-2.070199	-0.494096
29	1	0	-3.184338	-1.838127	-0.838351
30	6	0	-6.453299	-0.106826	0.280795
31	1	0	-5.241942	1.652016	0.546678
32	6	0	-6.472133	-1.445088	-0.093253
33	1	0	-5.305764	-3.111525	-0.793208
34	1	0	-7.368063	0.383913	0.590974
35	1	0	-7.402002	-2.000825	-0.076564

Structure 14f ($CHCl_3$)

Energy (Hartrees): -953.086794711
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.096493	0.952459	-0.108992
2	6	0	2.779271	1.375815	-0.073469
3	6	0	1.718077	0.458376	0.041627
4	6	0	2.036019	-0.909574	0.121640
5	6	0	3.348915	-1.348570	0.107789
6	6	0	4.363408	-0.407716	-0.013346
7	1	0	4.909371	1.662122	-0.188565
8	1	0	2.575612	2.439463	-0.100411
9	1	0	1.239488	-1.643056	0.170153
10	1	0	3.586966	-2.402263	0.168126
11	6	0	0.320371	0.918929	0.089383
12	6	0	-0.568624	0.230757	0.898505
13	1	0	-0.157322	-0.466568	1.625277
14	6	0	-0.008214	2.166586	-0.582085
15	1	0	0.717889	2.484347	-1.351890
16	1	0	-2.352542	-0.251380	1.650009
17	7	0	-1.898109	0.274980	0.914911
18	8	0	-0.964711	2.884909	-0.334580
19	7	0	5.755157	-0.862696	-0.037062
20	8	0	6.631756	-0.021871	-0.090471
21	8	0	5.967564	-2.059642	-0.000546
22	6	0	-2.780540	0.792727	-0.129532
23	1	0	-2.255419	0.689405	-1.083413
24	1	0	-2.974876	1.854738	0.023374
25	6	0	-4.063540	-0.000960	-0.143352
26	6	0	-4.073822	-1.309063	-0.632604
27	6	0	-5.244085	0.550370	0.351135
28	6	0	-5.248401	-2.052547	-0.631979
29	1	0	-3.155971	-1.739563	-1.022376
30	6	0	-6.422763	-0.192912	0.353252
31	1	0	-5.240846	1.567682	0.728959
32	6	0	-6.425914	-1.494245	-0.137372
33	1	0	-5.248513	-3.064522	-1.020477
34	1	0	-7.336840	0.245889	0.736905
35	1	0	-7.343115	-2.072046	-0.139454

Structure 14f (DMSO)

Energy (Hartrees): -953.085631886
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.076308	0.952217	-0.159319
2	6	0	2.766318	1.390521	-0.077729
3	6	0	1.698405	0.486088	0.082145
4	6	0	2.005849	-0.885503	0.163734
5	6	0	3.312815	-1.337783	0.112186
6	6	0	4.333721	-0.409984	-0.055941
7	1	0	4.889360	1.656720	-0.275278
8	1	0	2.577404	2.456625	-0.105359
9	1	0	1.205969	-1.612268	0.245217
10	1	0	3.537141	-2.394384	0.176319
11	6	0	0.308312	0.957627	0.172874
12	6	0	-0.568704	0.256931	0.990204
13	1	0	-0.151428	-0.443339	1.710424
14	6	0	-0.029901	2.221244	-0.460200
15	1	0	0.679308	2.555243	-1.238530
16	1	0	-2.344574	-0.233429	1.749113
17	7	0	-1.894900	0.300381	1.014759
18	8	0	-0.977765	2.939407	-0.175184
19	7	0	5.716093	-0.880452	-0.125436
20	8	0	6.590809	-0.064829	-0.352751
21	8	0	5.929466	-2.066529	0.048151
22	6	0	-2.775168	0.819673	-0.025995
23	1	0	-2.225445	0.767915	-0.970883
24	1	0	-3.014524	1.868327	0.154409
25	6	0	-4.031050	-0.014274	-0.105574
26	6	0	-3.948231	-1.391652	-0.325613
27	6	0	-5.284869	0.579984	0.022831
28	6	0	-5.102453	-2.161220	-0.416907
29	1	0	-2.973492	-1.859487	-0.429987
30	6	0	-6.443444	-0.189067	-0.072282
31	1	0	-5.354076	1.648761	0.198081
32	6	0	-6.354107	-1.559893	-0.290890
33	1	0	-5.027999	-3.228849	-0.590660
34	1	0	-7.413864	0.283800	0.030289
35	1	0	-7.255022	-2.158975	-0.361293

Structure 14f (C_2H_5OH)

Energy (Hartrees): -953.087908191
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.075178	0.942176	-0.162147
2	6	0	2.773338	1.402580	-0.082394
3	6	0	1.692160	0.516120	0.087112
4	6	0	1.975977	-0.859417	0.182726
5	6	0	3.274299	-1.334678	0.129922
6	6	0	4.308780	-0.423996	-0.050088
7	1	0	4.899932	1.631802	-0.284274
8	1	0	2.601679	2.471255	-0.118701
9	1	0	1.163983	-1.571543	0.274026
10	1	0	3.481192	-2.394356	0.202638
11	6	0	0.308062	1.006114	0.174256
12	6	0	-0.573217	0.327812	1.012089
13	1	0	-0.156255	-0.343894	1.759434
14	6	0	-0.021384	2.254291	-0.474359
15	1	0	0.698428	2.590689	-1.239358
16	1	0	-2.349997	-0.147193	1.772972
17	7	0	-1.896949	0.367018	1.026032
18	8	0	-0.984960	2.972531	-0.214580
19	7	0	5.678794	-0.915734	-0.125471
20	8	0	6.573272	-0.113893	-0.328091
21	8	0	5.875964	-2.109493	0.016716
22	6	0	-2.774153	0.840276	-0.041286
23	1	0	-2.210175	0.779544	-0.976747
24	1	0	-3.043866	1.885534	0.113689
25	6	0	-4.011040	-0.022116	-0.114610
26	6	0	-3.900398	-1.398804	-0.326126
27	6	0	-5.276295	0.547334	0.014078
28	6	0	-5.039087	-2.192303	-0.407364
29	1	0	-2.916918	-1.847841	-0.431859
30	6	0	-6.419114	-0.245685	-0.071473
31	1	0	-5.367030	1.615862	0.181252
32	6	0	-6.302332	-1.615827	-0.280673
33	1	0	-4.943158	-3.259448	-0.574120
34	1	0	-7.398689	0.208223	0.030419
35	1	0	-7.190901	-2.234036	-0.343640

Structure 14g (vacuum)

Energy (Hartrees): -953.059292820
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.279267	-0.125189	-1.126206
2	6	0	-3.589282	-0.569505	-1.041718
3	6	0	-4.303647	-0.310457	0.118294
4	6	0	-3.745811	0.367628	1.191706
5	6	0	-2.429666	0.790850	1.096692
6	6	0	-1.676833	0.564185	-0.063927
7	1	0	-1.725647	-0.290070	-2.043243
8	1	0	-4.066736	-1.094097	-1.858398
9	1	0	-4.333594	0.536685	2.083786
10	1	0	-1.967928	1.280157	1.945950
11	6	0	-0.285615	1.040297	-0.171863
12	6	0	0.072977	2.259233	0.322228
13	6	0	0.722427	0.210806	-0.816308
14	1	0	-0.656010	2.913621	0.793155
15	1	0	0.417697	-0.790531	-1.145257
16	8	0	1.281627	2.768819	0.262247
17	1	0	1.860638	2.094893	-0.207023
18	7	0	1.928440	0.608920	-0.967864
19	7	0	-5.699303	-0.774299	0.213985
20	8	0	-6.302852	-0.530930	1.237006
21	8	0	-6.158924	-1.370541	-0.736623
22	6	0	2.903597	-0.295029	-1.562035
23	1	0	3.309319	0.188838	-2.454817
24	1	0	2.429811	-1.236314	-1.868595
25	6	0	4.022609	-0.569040	-0.583389
26	6	0	3.985948	-1.694808	0.236169
27	6	0	5.079794	0.330346	-0.455239
28	6	0	4.993062	-1.922435	1.168771
29	1	0	3.165145	-2.399150	0.143284
30	6	0	6.086029	0.108176	0.477529
31	1	0	5.111589	1.210538	-1.089526
32	6	0	6.044097	-1.020001	1.291423
33	1	0	4.958049	-2.804250	1.797707
34	1	0	6.903462	0.813556	0.568750
35	1	0	6.828930	-1.195349	2.017570

Structure 14g ($CHCl_3$)

Energy (Hartrees): -953.085372308
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.214381	-0.000007	-1.141643
2	6	0	-3.511280	-0.485468	-1.098462
3	6	0	-4.236091	-0.340298	0.076487
4	6	0	-3.698451	0.264314	1.205078
5	6	0	-2.396004	0.731101	1.149580
6	6	0	-1.633845	0.619317	-0.023964
7	1	0	-1.656594	-0.080609	-2.067255
8	1	0	-3.962337	-0.955725	-1.962000
9	1	0	-4.283541	0.345852	2.111489
10	1	0	-1.955211	1.166147	2.038556
11	6	0	-0.256086	1.139619	-0.084245
12	6	0	0.081298	2.290425	0.566641
13	6	0	0.765335	0.430632	-0.843548
14	1	0	-0.652132	2.867432	1.123992
15	1	0	0.483409	-0.507776	-1.333642
16	8	0	1.285066	2.820696	0.559966
17	1	0	1.869257	2.205075	0.003497
18	7	0	1.966693	0.868462	-0.914323
19	7	0	-5.609494	-0.852886	0.130945
20	8	0	-6.231653	-0.711579	1.165287
21	8	0	-6.057178	-1.394307	-0.860790
22	6	0	2.968428	0.082558	-1.624905
23	1	0	3.461852	0.736515	-2.347461
24	1	0	2.496208	-0.744091	-2.168755
25	6	0	3.988544	-0.454870	-0.645461
26	6	0	3.719009	-1.625839	0.064051
27	6	0	5.177023	0.230266	-0.399015
28	6	0	4.623356	-2.106366	1.005001
29	1	0	2.793475	-2.162739	-0.122411
30	6	0	6.084254	-0.247227	0.543818
31	1	0	5.393010	1.141800	-0.947431
32	6	0	5.808374	-1.415585	1.247558
33	1	0	4.404931	-3.018624	1.548645
34	1	0	7.006157	0.292762	0.728152
35	1	0	6.514343	-1.788949	1.980733

Structure 14g (DMSO)

Energy (Hartrees): -953.083332846
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.210836	-0.190880	-1.098145
2	6	0	-3.508544	-0.672612	-1.042708
3	6	0	-4.287014	-0.362961	0.064857
4	6	0	-3.800225	0.405261	1.115081
5	6	0	-2.496830	0.866747	1.050937
6	6	0	-1.680949	0.589593	-0.058351
7	1	0	-1.613995	-0.409755	-1.975464
8	1	0	-3.914194	-1.267957	-1.849947
9	1	0	-4.423371	0.621916	1.972545
10	1	0	-2.100817	1.432341	1.885969
11	6	0	-0.302473	1.104974	-0.131374
12	6	0	0.019326	2.315494	0.412559
13	6	0	0.736891	0.334329	-0.800590
14	1	0	-0.725433	2.943058	0.895347
15	1	0	0.470659	-0.643353	-1.214476
16	8	0	1.224740	2.840581	0.379216
17	1	0	1.812938	2.169288	-0.112681
18	7	0	1.938602	0.772352	-0.884338
19	7	0	-5.661670	-0.865338	0.130443
20	8	0	-6.324843	-0.593216	1.113456
21	8	0	-6.075784	-1.529329	-0.801064
22	6	0	2.948825	-0.054378	-1.528487
23	1	0	3.401236	0.523964	-2.337533
24	1	0	2.488395	-0.950023	-1.964091
25	6	0	4.026876	-0.457354	-0.544890
26	6	0	3.686317	-1.135936	0.627859
27	6	0	5.367679	-0.173133	-0.797770
28	6	0	4.670594	-1.526187	1.529092
29	1	0	2.643612	-1.359012	0.834562
30	6	0	6.356841	-0.564483	0.102949
31	1	0	5.639310	0.358843	-1.704030
32	6	0	6.010369	-1.240912	1.268108
33	1	0	4.394717	-2.055376	2.434485
34	1	0	7.396445	-0.336955	-0.105491
35	1	0	6.777979	-1.545731	1.970457

Structure 14g (C_2H_5OH)

Energy (Hartrees): -953.083854816
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.208130	-0.168463	-1.106278
2	6	0	-3.502659	-0.657293	-1.052646
3	6	0	-4.276791	-0.367024	0.063492
4	6	0	-3.789814	0.386303	1.124774
5	6	0	-2.488251	0.852151	1.062550
6	6	0	-1.677312	0.596904	-0.055616
7	1	0	-1.615578	-0.367391	-1.991239
8	1	0	-3.910869	-1.239026	-1.868575
9	1	0	-4.408899	0.584257	1.989905
10	1	0	-2.088685	1.402211	1.906222
11	6	0	-0.301058	1.118777	-0.127901
12	6	0	0.013450	2.327004	0.420055
13	6	0	0.739878	0.350168	-0.799929
14	1	0	-0.730353	2.951694	0.907388
15	1	0	0.473597	-0.631031	-1.205720
16	8	0	1.220708	2.860008	0.386727
17	1	0	1.816946	2.199608	-0.106497
18	7	0	1.939131	0.790847	-0.892950
19	7	0	-5.645023	-0.874746	0.125829
20	8	0	-6.341529	-0.544985	1.068087
21	8	0	-6.032952	-1.606495	-0.766452
22	6	0	2.946155	-0.045127	-1.531302
23	1	0	3.405893	0.528117	-2.339695
24	1	0	2.481240	-0.937534	-1.968870
25	6	0	4.018032	-0.456325	-0.544753
26	6	0	3.670403	-1.134654	0.626013
27	6	0	5.361495	-0.182770	-0.795264
28	6	0	4.650384	-1.535289	1.527358
29	1	0	2.625707	-1.350111	0.831355
30	6	0	6.346300	-0.584553	0.105525
31	1	0	5.638947	0.348955	-1.700003
32	6	0	5.992806	-1.260892	1.268561
33	1	0	4.369150	-2.064518	2.431195
34	1	0	7.388076	-0.365195	-0.101378
35	1	0	6.756932	-1.574468	1.971040

Structure 14h (vacuum)

Energy (Hartrees): -953.036981391
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.551287	-1.118057	-0.517004
2	6	0	2.226191	-0.742663	-0.674486
3	6	0	1.748720	0.467095	-0.151280
4	6	0	2.637571	1.287254	0.556832
5	6	0	3.969040	0.935003	0.710404
6	6	0	4.402898	-0.265765	0.169219
7	1	0	3.933504	-2.045463	-0.922087
8	1	0	1.554532	-1.384748	-1.232756
9	1	0	2.274097	2.197527	1.018434
10	1	0	4.664057	1.558857	1.255977
11	6	0	0.331485	0.841063	-0.347905
12	6	0	0.017002	2.127110	-0.579280
13	1	0	0.804394	2.872428	-0.660010
14	6	0	-0.677645	-0.233133	-0.262581
15	1	0	-0.398671	-1.085485	0.376309
16	7	0	-1.788784	-0.192216	-0.864771
17	8	0	-1.241991	2.575250	-0.720363
18	1	0	-1.236206	3.520647	-0.886320
19	7	0	5.815847	-0.653312	0.338285
20	8	0	6.544891	0.124297	0.916190
21	8	0	6.161736	-1.724541	-0.111348
22	6	0	-2.710537	-1.286300	-0.649165
23	1	0	-2.301669	-2.047439	0.033134
24	1	0	-2.880544	-1.768294	-1.618541
25	6	0	-4.047381	-0.805828	-0.118097
26	6	0	-5.040372	-1.746854	0.158955
27	6	0	-4.310840	0.544212	0.099004
28	6	0	-6.278608	-1.348375	0.645133
29	1	0	-4.839845	-2.801126	-0.008142
30	6	0	-5.553694	0.943029	0.586950
31	1	0	-3.540645	1.274608	-0.121104
32	6	0	-6.539136	0.002780	0.861106
33	1	0	-7.040505	-2.090233	0.854661
34	1	0	-5.750745	1.996016	0.753188
35	1	0	-7.504166	0.317932	1.240000

Structure 14h ($CHCl_3$)

Energy (Hartrees): -953.068027076
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.518649	-1.157523	-0.449872
2	6	0	2.198856	-0.769919	-0.617967
3	6	0	1.746825	0.481108	-0.171108
4	6	0	2.659365	1.332808	0.470340
5	6	0	3.985095	0.968147	0.633250
6	6	0	4.392806	-0.276243	0.170502
7	1	0	3.870609	-2.118381	-0.801204
8	1	0	1.513658	-1.440013	-1.124598
9	1	0	2.322238	2.281835	0.869853
10	1	0	4.690034	1.622787	1.128231
11	6	0	0.332448	0.861756	-0.370683
12	6	0	0.019384	2.151986	-0.598417
13	1	0	0.799658	2.904054	-0.681735
14	6	0	-0.681422	-0.205562	-0.271882
15	1	0	-0.420822	-1.038951	0.396510
16	7	0	-1.784185	-0.187424	-0.896297
17	8	0	-1.237701	2.596882	-0.728852
18	1	0	-1.230034	3.549354	-0.879881
19	7	0	5.793435	-0.675549	0.352061
20	8	0	6.548206	0.115214	0.882745
21	8	0	6.129429	-1.776230	-0.037665
22	6	0	-2.700174	-1.284210	-0.652776
23	1	0	-2.279724	-2.026117	0.041608
24	1	0	-2.876349	-1.790548	-1.607979
25	6	0	-4.035893	-0.805721	-0.118111
26	6	0	-5.063116	-1.736819	0.059054
27	6	0	-4.267059	0.527933	0.213168
28	6	0	-6.298450	-1.344262	0.559123
29	1	0	-4.889780	-2.777774	-0.198671
30	6	0	-5.507929	0.922500	0.713080
31	1	0	-3.476893	1.256730	0.069148
32	6	0	-6.525211	-0.008617	0.888468
33	1	0	-7.085253	-2.078781	0.690603
34	1	0	-5.677695	1.963657	0.965004
35	1	0	-7.488902	0.301855	1.275918

Structure 14h (DMSO)

Energy (Hartrees): -953.065411639
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.490015	-1.198210	-0.360638
2	6	0	2.172421	-0.807446	-0.539074
3	6	0	1.742367	0.481209	-0.186926
4	6	0	2.675842	1.368818	0.372378
5	6	0	3.998583	0.999614	0.544890
6	6	0	4.385575	-0.282651	0.174554
7	1	0	3.818886	-2.190061	-0.641029
8	1	0	1.472928	-1.510463	-0.977135
9	1	0	2.361709	2.352372	0.700186
10	1	0	4.714933	1.686102	0.976634
11	6	0	0.330621	0.864908	-0.399627
12	6	0	0.030357	2.149930	-0.673678
13	1	0	0.817218	2.891276	-0.782797
14	6	0	-0.688224	-0.192813	-0.255629
15	1	0	-0.439384	-0.987685	0.461316
16	7	0	-1.782384	-0.214275	-0.897352
17	8	0	-1.221734	2.604618	-0.818220
18	1	0	-1.197189	3.556651	-0.975908
19	7	0	5.783014	-0.683599	0.363815
20	8	0	6.549481	0.124204	0.853003
21	8	0	6.109760	-1.804102	0.021788
22	6	0	-2.694913	-1.305466	-0.606347
23	1	0	-2.269961	-2.011009	0.122083
24	1	0	-2.868205	-1.857440	-1.535616
25	6	0	-4.032118	-0.809543	-0.093831
26	6	0	-5.133002	-1.670167	-0.123488
27	6	0	-4.190037	0.470339	0.436780
28	6	0	-6.365348	-1.264325	0.375864
29	1	0	-5.018982	-2.665720	-0.542469
30	6	0	-5.426879	0.880061	0.934205
31	1	0	-3.346024	1.151269	0.452456
32	6	0	-6.516228	0.015803	0.907680
33	1	0	-7.209940	-1.943901	0.346408
34	1	0	-5.537246	1.878961	1.342157
35	1	0	-7.477406	0.336653	1.293250

Structure 14h (C_2H_5OH)

Energy (Hartrees): -953.071298098
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.478868	-1.206783	-0.317503
2	6	0	2.161439	-0.826856	-0.514405
3	6	0	1.726103	0.473346	-0.213358
4	6	0	2.654669	1.385003	0.315502
5	6	0	3.977204	1.026475	0.507694
6	6	0	4.369201	-0.268045	0.186709
7	1	0	3.811534	-2.207235	-0.560872
8	1	0	1.465621	-1.547028	-0.930083
9	1	0	2.336969	2.379859	0.603648
10	1	0	4.689528	1.731023	0.916437
11	6	0	0.314572	0.839748	-0.450277
12	6	0	0.006239	2.109661	-0.783338
13	1	0	0.783361	2.857613	-0.911067
14	6	0	-0.696678	-0.219539	-0.270440
15	1	0	-0.452012	-0.974775	0.489319
16	7	0	-1.781862	-0.283151	-0.925664
17	8	0	-1.247576	2.542402	-0.972389
18	1	0	-1.238900	3.486394	-1.173461
19	7	0	5.763910	-0.654315	0.390102
20	8	0	6.530774	0.169644	0.853358
21	8	0	6.102189	-1.783061	0.085268
22	6	0	-2.696459	-1.359581	-0.580992
23	1	0	-2.258552	-2.041316	0.162183
24	1	0	-2.895246	-1.939708	-1.486369
25	6	0	-4.014151	-0.827674	-0.055397
26	6	0	-5.195357	-1.530092	-0.302159
27	6	0	-4.071184	0.339978	0.707044
28	6	0	-6.409402	-1.080595	0.209087
29	1	0	-5.163566	-2.434650	-0.902161
30	6	0	-5.285813	0.794102	1.215669
31	1	0	-3.163278	0.901364	0.901382
32	6	0	-6.458481	0.085651	0.969181
33	1	0	-7.318306	-1.636357	0.005757
34	1	0	-5.314828	1.704751	1.804146
35	1	0	-7.404386	0.441652	1.362083

Structure 14i (vacuum)

Energy (Hartrees): -953.042581203
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.461358	-1.124029	-0.609265
2	6	0	2.129801	-0.752130	-0.711173
3	6	0	1.650361	0.407764	-0.087126
4	6	0	2.544936	1.191314	0.655044
5	6	0	3.878404	0.832120	0.767536
6	6	0	4.314472	-0.320485	0.130659
7	1	0	3.845311	-2.011145	-1.094323
8	1	0	1.455245	-1.360065	-1.303331
9	1	0	2.190117	2.085492	1.148528
10	1	0	4.578402	1.424366	1.341116
11	6	0	0.224071	0.762025	-0.222717
12	6	0	-0.245675	2.017962	-0.282857
13	1	0	-1.314180	2.181919	-0.383653
14	6	0	-0.770654	-0.330861	-0.292168
15	1	0	-0.487483	-1.262904	0.218393
16	7	0	-1.889947	-0.203430	-0.869305
17	8	0	0.548460	3.107616	-0.244653
18	1	0	0.020150	3.904451	-0.329182
19	7	0	5.733967	-0.705103	0.244085
20	8	0	6.457693	0.007677	0.905931
21	8	0	6.090587	-1.711093	-0.331573
22	6	0	-2.833383	-1.307034	-0.778129
23	1	0	-2.448773	-2.137521	-0.170407
24	1	0	-2.997934	-1.681421	-1.794555
25	6	0	-4.153025	-0.824662	-0.216020
26	6	0	-4.742915	-1.451468	0.877393
27	6	0	-4.796915	0.267264	-0.801123
28	6	0	-5.963333	-1.001746	1.377861
29	1	0	-4.247227	-2.296615	1.343958
30	6	0	-6.011691	0.718785	-0.302890
31	1	0	-4.331075	0.762185	-1.646140
32	6	0	-6.599222	0.084214	0.789559
33	1	0	-6.412960	-1.499124	2.229267
34	1	0	-6.503829	1.565827	-0.766721
35	1	0	-7.547354	0.436488	1.178453

Structure 14i ($CHCl_3$)

Energy (Hartrees): -953.071998775
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.445197	-1.124672	-0.604862
2	6	0	2.114779	-0.752217	-0.712696
3	6	0	1.634743	0.414774	-0.099297
4	6	0	2.529670	1.201727	0.641725
5	6	0	3.862198	0.842995	0.760158
6	6	0	4.298915	-0.315286	0.130788
7	1	0	3.819486	-2.018611	-1.085562
8	1	0	1.443646	-1.368061	-1.300712
9	1	0	2.177075	2.096006	1.137435
10	1	0	4.553473	1.443925	1.335835
11	6	0	0.209479	0.771814	-0.239130
12	6	0	-0.251820	2.033916	-0.308934
13	1	0	-1.318303	2.216234	-0.398420
14	6	0	-0.783605	-0.321235	-0.301639
15	1	0	-0.512921	-1.240921	0.234662
16	7	0	-1.892099	-0.212909	-0.908038
17	8	0	0.548365	3.112435	-0.291922
18	1	0	0.019412	3.915943	-0.362308
19	7	0	5.711034	-0.699677	0.251338
20	8	0	6.443118	0.014502	0.907074
21	8	0	6.077280	-1.713212	-0.310141
22	6	0	-2.828828	-1.326269	-0.803912
23	1	0	-2.426429	-2.147930	-0.198317
24	1	0	-3.006176	-1.701987	-1.816884
25	6	0	-4.139853	-0.846900	-0.220839
26	6	0	-4.592411	-1.310610	1.012653
27	6	0	-4.906476	0.092925	-0.914240
28	6	0	-5.795459	-0.848504	1.544935
29	1	0	-4.003423	-2.039238	1.560777
30	6	0	-6.103761	0.558327	-0.384750
31	1	0	-4.555592	0.459804	-1.873622
32	6	0	-6.552207	0.087095	0.848687
33	1	0	-6.138810	-1.219628	2.504214
34	1	0	-6.690085	1.286847	-0.933524
35	1	0	-7.487366	0.448652	1.261350

Structure 14i (DMSO)

Energy (Hartrees): -953.068259803
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.440696	-1.123870	-0.608236
2	6	0	2.111336	-0.748023	-0.717363
3	6	0	1.633866	0.418032	-0.100530
4	6	0	2.527957	1.198359	0.648430
5	6	0	3.859695	0.836875	0.767270
6	6	0	4.295421	-0.318682	0.131476
7	1	0	3.809296	-2.018123	-1.092865
8	1	0	1.440186	-1.362743	-1.306609
9	1	0	2.177018	2.088730	1.152537
10	1	0	4.547741	1.434724	1.350114
11	6	0	0.209990	0.780217	-0.242480
12	6	0	-0.246067	2.044532	-0.313522
13	1	0	-1.312175	2.233854	-0.394936
14	6	0	-0.783728	-0.312444	-0.302818
15	1	0	-0.510150	-1.234923	0.225633
16	7	0	-1.894963	-0.202194	-0.905735
17	8	0	0.559056	3.119226	-0.307934
18	1	0	0.027637	3.924019	-0.353054
19	7	0	5.706503	-0.704591	0.250260
20	8	0	6.447676	0.023048	0.882538
21	8	0	6.066381	-1.733073	-0.289700
22	6	0	-2.826637	-1.322197	-0.805519
23	1	0	-2.419760	-2.141331	-0.200725
24	1	0	-3.002529	-1.695056	-1.819672
25	6	0	-4.138578	-0.848367	-0.221180
26	6	0	-4.562479	-1.277581	1.035277
27	6	0	-4.933586	0.053758	-0.933220
28	6	0	-5.765263	-0.819095	1.571973
29	1	0	-3.950169	-1.975731	1.597491
30	6	0	-6.130879	0.516037	-0.399227
31	1	0	-4.608626	0.392510	-1.912141
32	6	0	-6.550486	0.079180	0.857041
33	1	0	-6.085967	-1.163925	2.548797
34	1	0	-6.740220	1.213957	-0.962757
35	1	0	-7.485511	0.437535	1.273057

Structure 14i (C_2H_5OH)

Energy (Hartrees): -953.073836389
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.382091	-1.200965	-0.503847
2	6	0	2.074172	-0.812232	-0.743930
3	6	0	1.586392	0.419893	-0.281637
4	6	0	2.447771	1.255639	0.445915
5	6	0	3.756566	0.881542	0.698218
6	6	0	4.202977	-0.342221	0.214786
7	1	0	3.758918	-2.146987	-0.869743
8	1	0	1.427833	-1.468817	-1.315730
9	1	0	2.086192	2.199212	0.832193
10	1	0	4.417681	1.522496	1.266357
11	6	0	0.182815	0.790433	-0.548373
12	6	0	-0.231063	2.050822	-0.784641
13	1	0	-1.283222	2.260644	-0.948707
14	6	0	-0.829577	-0.283861	-0.536077
15	1	0	-0.572299	-1.168679	0.060619
16	7	0	-1.940360	-0.208124	-1.148086
17	8	0	0.604169	3.098025	-0.851200
18	1	0	0.107749	3.909180	-1.017139
19	7	0	5.587178	-0.740241	0.473559
20	8	0	6.279147	-0.011208	1.159289
21	8	0	5.988885	-1.783268	-0.007349
22	6	0	-2.883762	-1.301775	-0.940641
23	1	0	-2.413272	-2.136193	-0.403947
24	1	0	-3.211520	-1.663374	-1.917928
25	6	0	-4.089735	-0.815529	-0.165868
26	6	0	-3.934371	-0.363863	1.147152
27	6	0	-5.359388	-0.800288	-0.739711
28	6	0	-5.029642	0.087678	1.874800
29	1	0	-2.946542	-0.367987	1.599657
30	6	0	-6.460134	-0.348160	-0.013262
31	1	0	-5.488681	-1.145793	-1.760613
32	6	0	-6.297623	0.096190	1.294818
33	1	0	-4.896893	0.432655	2.894377
34	1	0	-7.443125	-0.342899	-0.471288
35	1	0	-7.153076	0.446897	1.861441

Structure 14j (vacuum)

Energy (Hartrees): -953.044416638
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.796742	-1.241385	-0.506928
2	6	0	0.952970	-0.142365	-0.533657
3	6	0	1.386265	1.101569	-0.059836
4	6	0	2.681036	1.223324	0.452698
5	6	0	3.534731	0.130704	0.493321
6	6	0	3.074423	-1.083643	0.009849
7	1	0	1.481797	-2.208219	-0.875132
8	1	0	-0.051755	-0.246726	-0.920983
9	1	0	3.021249	2.181001	0.824547
10	1	0	4.537574	0.206189	0.890810
11	6	0	0.482457	2.274002	-0.112021
12	6	0	0.881061	3.480375	-0.545715
13	1	0	0.181247	4.311330	-0.582154
14	6	0	-0.922376	2.160638	0.304942
15	1	0	-1.532599	3.065529	0.157837
16	7	0	-1.410000	1.106747	0.805178
17	8	0	2.140145	3.735317	-0.958584
18	1	0	2.205827	4.627866	-1.305024
19	7	0	3.976555	-2.251253	0.046686
20	8	0	5.090735	-2.086972	0.496155
21	8	0	3.549664	-3.304947	-0.374726
22	6	0	-2.815224	1.107052	1.165733
23	1	0	-3.314048	2.054010	0.913498
24	1	0	-2.874172	0.980927	2.253098
25	6	0	-3.540050	-0.045637	0.502906
26	6	0	-4.824686	0.125836	-0.006207
27	6	0	-2.936023	-1.301045	0.414377
28	6	0	-5.503739	-0.940545	-0.589878
29	1	0	-5.298843	1.100537	0.051068
30	6	0	-3.611714	-2.365262	-0.170440
31	1	0	-1.932158	-1.429916	0.803406
32	6	0	-4.898371	-2.188571	-0.673541
33	1	0	-6.502506	-0.793237	-0.984112
34	1	0	-3.134288	-3.336326	-0.234531
35	1	0	-5.422578	-3.018888	-1.131743

Structure 14j ($CHCl_3$)

Energy (Hartrees): -953.074829411
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.851947	-1.235753	-0.517926
2	6	0	0.977422	-0.161206	-0.533847
3	6	0	1.372904	1.092502	-0.050111
4	6	0	2.666009	1.248113	0.461383
5	6	0	3.552579	0.182065	0.489663
6	6	0	3.127180	-1.043024	-0.003411
7	1	0	1.555183	-2.204677	-0.896398
8	1	0	-0.021741	-0.292338	-0.928102
9	1	0	2.979911	2.210496	0.845546
10	1	0	4.551934	0.293531	0.888302
11	6	0	0.434551	2.237595	-0.092986
12	6	0	0.792517	3.449848	-0.554497
13	1	0	0.071990	4.263340	-0.589742
14	6	0	-0.955055	2.096326	0.355725
15	1	0	-1.582418	2.988747	0.220667
16	7	0	-1.412854	1.034372	0.875527
17	8	0	2.027267	3.722946	-1.006994
18	1	0	2.067834	4.627417	-1.338960
19	7	0	4.061675	-2.177348	0.018538
20	8	0	5.177980	-1.990084	0.460156
21	8	0	3.671894	-3.246916	-0.405591
22	6	0	-2.814600	1.023591	1.266384
23	1	0	-3.311328	1.982366	1.067621
24	1	0	-2.854079	0.842403	2.346243
25	6	0	-3.555095	-0.089479	0.555530
26	6	0	-4.752857	0.164774	-0.109235
27	6	0	-3.045486	-1.390699	0.559826
28	6	0	-5.438013	-0.862761	-0.756320
29	1	0	-5.152645	1.173763	-0.123305
30	6	0	-3.724805	-2.415944	-0.088041
31	1	0	-2.110132	-1.592763	1.071155
32	6	0	-4.924546	-2.154644	-0.748643
33	1	0	-6.368624	-0.650166	-1.270651
34	1	0	-3.319974	-3.421795	-0.077660
35	1	0	-5.452699	-2.954901	-1.254709

Structure 14j (DMSO)

Energy (Hartrees): -953.072251941
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.932100	-1.250415	-0.493760
2	6	0	0.993665	-0.230536	-0.473719
3	6	0	1.333632	1.046482	-0.009003
4	6	0	2.636069	1.281901	0.445734
5	6	0	3.587173	0.273025	0.434421
6	6	0	3.214844	-0.977988	-0.036984
7	1	0	1.676522	-2.236154	-0.858922
8	1	0	-0.011037	-0.423229	-0.827686
9	1	0	2.906063	2.262109	0.818701
10	1	0	4.593462	0.449679	0.790049
11	6	0	0.331086	2.135901	-0.001195
12	6	0	0.593475	3.363103	-0.489987
13	1	0	-0.167922	4.138900	-0.474462
14	6	0	-1.016233	1.929760	0.536915
15	1	0	-1.684544	2.798278	0.465679
16	7	0	-1.403240	0.839163	1.061659
17	8	0	1.775017	3.692655	-1.034579
18	1	0	1.746304	4.603944	-1.351752
19	7	0	4.215979	-2.053506	-0.052766
20	8	0	5.349115	-1.785457	0.296798
21	8	0	3.862908	-3.158982	-0.414978
22	6	0	-2.787204	0.781897	1.525234
23	1	0	-3.262572	1.770608	1.501985
24	1	0	-2.784439	0.419193	2.556291
25	6	0	-3.568532	-0.179214	0.656852
26	6	0	-4.215508	0.285764	-0.488953
27	6	0	-3.608380	-1.542503	0.951499
28	6	0	-4.896205	-0.594952	-1.324794
29	1	0	-4.187458	1.345830	-0.724063
30	6	0	-4.285965	-2.427097	0.116105
31	1	0	-3.108367	-1.910693	1.842212
32	6	0	-4.931845	-1.954615	-1.023744
33	1	0	-5.399766	-0.220739	-2.209319
34	1	0	-4.311924	-3.484324	0.356256
35	1	0	-5.462845	-2.641787	-1.672880

Structure 14j (C_2H_5OH)

Energy (Hartrees): -953.077139267
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.897828	-1.269785	-0.518485
2	6	0	0.999054	-0.215668	-0.510240
3	6	0	1.367097	1.036165	-0.000248
4	6	0	2.656294	1.210446	0.516178
5	6	0	3.566976	0.165175	0.523320
6	6	0	3.168381	-1.058058	0.002286
7	1	0	1.620171	-2.235773	-0.918862
8	1	0	0.003144	-0.360702	-0.910008
9	1	0	2.946684	2.171124	0.923815
10	1	0	4.562118	0.294504	0.927637
11	6	0	0.406191	2.162273	-0.018026
12	6	0	0.732590	3.378261	-0.497358
13	1	0	0.004972	4.185553	-0.513983
14	6	0	-0.964958	2.001105	0.470057
15	1	0	-1.610449	2.880428	0.343015
16	7	0	-1.395844	0.936664	1.015330
17	8	0	1.945653	3.659645	-0.996689
18	1	0	1.971377	4.569394	-1.318106
19	7	0	4.124953	-2.167907	0.002488
20	8	0	5.221899	-1.984824	0.495369
21	8	0	3.782648	-3.225726	-0.490877
22	6	0	-2.797867	0.919500	1.415611
23	1	0	-3.258042	1.911491	1.310601
24	1	0	-2.853697	0.627888	2.467285
25	6	0	-3.566624	-0.085618	0.584317
26	6	0	-3.678153	0.099049	-0.796299
27	6	0	-4.161467	-1.203570	1.165936
28	6	0	-4.376342	-0.813392	-1.579024
29	1	0	-3.213354	0.965228	-1.259050
30	6	0	-4.862305	-2.121200	0.384253
31	1	0	-4.075994	-1.358352	2.237030
32	6	0	-4.971297	-1.928092	-0.988837
33	1	0	-4.458391	-0.656530	-2.649057
34	1	0	-5.320431	-2.986943	0.849837
35	1	0	-5.515874	-2.640926	-1.597955

Structure 14k (vacuum)

Energy (Hartrees): -953.044049711
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.901969	-1.160636	-0.525081
2	6	0	0.997770	-0.111901	-0.537843
3	6	0	1.368537	1.158654	-0.077271
4	6	0	2.661317	1.345914	0.422240
5	6	0	3.581117	0.306422	0.437759
6	6	0	3.182329	-0.930582	-0.039802
7	1	0	1.634079	-2.144429	-0.885762
8	1	0	-0.005719	-0.273576	-0.908476
9	1	0	2.942930	2.310792	0.827188
10	1	0	4.582976	0.436385	0.823668
11	6	0	0.417017	2.291869	-0.145685
12	6	0	0.840879	3.478425	-0.608392
13	1	0	1.857923	3.614608	-0.964839
14	6	0	-0.989079	2.121305	0.253592
15	1	0	-1.657070	2.961268	0.029461
16	7	0	-1.397631	1.062945	0.816396
17	8	0	0.030813	4.562353	-0.660325
18	1	0	0.458799	5.277855	-1.135017
19	7	0	4.150831	-2.043499	-0.024799
20	8	0	5.266204	-1.812253	0.391603
21	8	0	3.774017	-3.121614	-0.431470
22	6	0	-2.810487	0.961372	1.133335
23	1	0	-3.380141	1.842726	0.807568
24	1	0	-2.896826	0.891085	2.223742
25	6	0	-3.395320	-0.291250	0.515232
26	6	0	-4.625304	-0.258976	-0.135475
27	6	0	-2.704327	-1.501678	0.602985
28	6	0	-5.166724	-1.418946	-0.684922
29	1	0	-5.164597	0.679318	-0.216618
30	6	0	-3.242363	-2.658785	0.053958
31	1	0	-1.739929	-1.522422	1.098395
32	6	0	-4.476460	-2.621226	-0.591032
33	1	0	-6.124827	-1.379286	-1.189907
34	1	0	-2.699135	-3.593770	0.128922
35	1	0	-4.894363	-3.524459	-1.019543

Structure 14k ($CHCl_3$)

Energy (Hartrees): -953.073707763
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.942461	-1.175121	-0.509430
2	6	0	1.014409	-0.147555	-0.510756
3	6	0	1.364261	1.138349	-0.073363
4	6	0	2.667509	1.363238	0.387176
5	6	0	3.612082	0.347534	0.388295
6	6	0	3.230429	-0.907104	-0.062147
7	1	0	1.679054	-2.166142	-0.854070
8	1	0	0.008629	-0.340566	-0.860296
9	1	0	2.940729	2.340128	0.768452
10	1	0	4.619211	0.517184	0.744991
11	6	0	0.383009	2.246414	-0.121784
12	6	0	0.775515	3.449752	-0.580241
13	1	0	1.782868	3.616176	-0.950778
14	6	0	-1.009437	2.048776	0.303511
15	1	0	-1.698720	2.871885	0.083990
16	7	0	-1.396800	0.994544	0.894699
17	8	0	-0.055350	4.509437	-0.615893
18	1	0	0.374766	5.254904	-1.050270
19	7	0	4.222874	-1.990034	-0.062345
20	8	0	5.357639	-1.725187	0.282529
21	8	0	3.861353	-3.096549	-0.409928
22	6	0	-2.808987	0.900213	1.240870
23	1	0	-3.364701	1.804800	0.963125
24	1	0	-2.873917	0.777766	2.326720
25	6	0	-3.421832	-0.308856	0.568146
26	6	0	-4.386082	-0.160787	-0.426716
27	6	0	-3.001402	-1.593920	0.920199
28	6	0	-4.933611	-1.278539	-1.054669
29	1	0	-4.713651	0.834193	-0.711238
30	6	0	-3.542836	-2.710032	0.293528
31	1	0	-2.244445	-1.713143	1.689031
32	6	0	-4.512840	-2.554402	-0.696174
33	1	0	-5.687236	-1.150353	-1.823727
34	1	0	-3.211983	-3.702749	0.577630
35	1	0	-4.938145	-3.425013	-1.182375

Structure 14k (DMSO)

Energy (Hartrees): -953.070855638
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.945804	-1.179771	-0.501983
2	6	0	1.010868	-0.158321	-0.503384
3	6	0	1.355567	1.133461	-0.077798
4	6	0	2.662082	1.370894	0.368005
5	6	0	3.613085	0.361359	0.369299
6	6	0	3.235417	-0.900501	-0.065401
7	1	0	1.684214	-2.173675	-0.839869
8	1	0	0.005652	-0.360408	-0.850450
9	1	0	2.935239	2.354241	0.732680
10	1	0	4.621439	0.545606	0.715261
11	6	0	0.367717	2.234917	-0.122412
12	6	0	0.757983	3.443745	-0.571584
13	1	0	1.766840	3.616488	-0.935466
14	6	0	-1.021625	2.031732	0.306505
15	1	0	-1.719157	2.844741	0.078161
16	7	0	-1.401995	0.984226	0.916435
17	8	0	-0.075102	4.499321	-0.600968
18	1	0	0.363190	5.251129	-1.018031
19	7	0	4.231898	-1.978457	-0.060497
20	8	0	5.367607	-1.707218	0.279164
21	8	0	3.874124	-3.090602	-0.397812
22	6	0	-2.815573	0.890624	1.265792
23	1	0	-3.367771	1.797636	0.991585
24	1	0	-2.880616	0.758341	2.350139
25	6	0	-3.425915	-0.311853	0.580400
26	6	0	-4.311618	-0.151273	-0.483769
27	6	0	-3.074365	-1.603161	0.982194
28	6	0	-4.844756	-1.262466	-1.135303
29	1	0	-4.587666	0.848916	-0.803109
30	6	0	-3.601216	-2.713616	0.331724
31	1	0	-2.383170	-1.733707	1.809357
32	6	0	-4.489473	-2.545054	-0.729870
33	1	0	-5.537791	-1.124521	-1.957799
34	1	0	-3.322731	-3.711115	0.653262
35	1	0	-4.903928	-3.410354	-1.234842

Structure 14k (C_2H_5OH)

Energy (Hartrees): -953.075477634
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.933972	-1.210867	-0.489036
2	6	0	1.013792	-0.176949	-0.494714
3	6	0	1.369669	1.106621	-0.053091
4	6	0	2.673378	1.324224	0.411361
5	6	0	3.611369	0.303286	0.415465
6	6	0	3.221488	-0.950308	-0.033479
7	1	0	1.663637	-2.198258	-0.839435
8	1	0	0.010474	-0.361115	-0.857729
9	1	0	2.953278	2.300331	0.790098
10	1	0	4.617213	0.470403	0.777601
11	6	0	0.394514	2.218506	-0.101124
12	6	0	0.799542	3.423082	-0.550661
13	1	0	1.810768	3.588703	-0.910665
14	6	0	-0.999484	2.028891	0.317645
15	1	0	-1.691138	2.839237	0.062051
16	7	0	-1.392866	0.998113	0.949719
17	8	0	-0.021158	4.487923	-0.587415
18	1	0	0.424729	5.236620	-1.002204
19	7	0	4.201418	-2.036751	-0.022378
20	8	0	5.350052	-1.775051	0.282320
21	8	0	3.828292	-3.155885	-0.320469
22	6	0	-2.814299	0.918323	1.268814
23	1	0	-3.342412	1.840011	0.992768
24	1	0	-2.913781	0.772303	2.347336
25	6	0	-3.430450	-0.261742	0.549630
26	6	0	-3.670592	-0.186054	-0.824357
27	6	0	-3.730425	-1.443565	1.224880
28	6	0	-4.207111	-1.270687	-1.509871
29	1	0	-3.436095	0.731158	-1.357780
30	6	0	-4.267177	-2.533119	0.541233
31	1	0	-3.543610	-1.511071	2.292114
32	6	0	-4.506627	-2.448657	-0.826832
33	1	0	-4.394710	-1.198613	-2.575601
34	1	0	-4.498294	-3.446320	1.078657
35	1	0	-4.926766	-3.294724	-1.359265

Structure 14l (vacuum)

Energy (Hartrees): -953.041634846
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.543646	-0.674185	-1.147765
2	6	0	1.565802	0.306224	-1.115257
3	6	0	1.415976	1.131344	0.006430
4	6	0	2.256604	0.935166	1.107033
5	6	0	3.244781	-0.039523	1.089177
6	6	0	3.369181	-0.827344	-0.042517
7	1	0	2.678378	-1.313882	-2.009215
8	1	0	0.910256	0.437575	-1.964946
9	1	0	2.120386	1.538176	1.996941
10	1	0	3.900012	-0.203123	1.933752
11	6	0	0.400969	2.213208	0.027395
12	6	0	0.776022	3.432407	0.464184
13	1	0	1.804514	3.629648	0.743962
14	6	0	-0.971134	1.947430	-0.418017
15	1	0	-1.668281	2.800930	-0.435266
16	7	0	-1.374929	0.802402	-0.775304
17	8	0	0.023933	4.537849	0.604677
18	1	0	-0.901822	4.362006	0.412917
19	7	0	4.412209	-1.871509	-0.070956
20	8	0	5.125540	-1.978964	0.903477
21	8	0	4.492619	-2.556970	-1.067402
22	6	0	-2.756849	0.664037	-1.186540
23	1	0	-2.755609	0.384304	-2.246804
24	1	0	-3.313828	1.608839	-1.098436
25	6	0	-3.476552	-0.420205	-0.408637
26	6	0	-2.780777	-1.443251	0.232536
27	6	0	-4.870481	-0.411735	-0.360054
28	6	0	-3.473331	-2.444461	0.907441
29	1	0	-1.698122	-1.446315	0.202690
30	6	0	-5.561881	-1.413429	0.311397
31	1	0	-5.419634	0.386035	-0.850789
32	6	0	-4.863180	-2.434563	0.948289
33	1	0	-2.922510	-3.234434	1.404529
34	1	0	-6.644951	-1.393689	0.342031
35	1	0	-5.399258	-3.214373	1.475868

Structure 14l ($CHCl_3$)

Energy (Hartrees): -953.070519880
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.613781	-0.747425	-1.056870
2	6	0	1.592016	0.186060	-1.108022
3	6	0	1.383908	1.081525	-0.049713
4	6	0	2.215119	1.001125	1.074447
5	6	0	3.247781	0.077762	1.139894
6	6	0	3.427858	-0.783392	0.068445
7	1	0	2.785885	-1.434737	-1.874279
8	1	0	0.953675	0.227821	-1.980180
9	1	0	2.040826	1.659005	1.917595
10	1	0	3.889704	0.015570	2.008341
11	6	0	0.331812	2.125021	-0.121287
12	6	0	0.654187	3.370020	0.291833
13	1	0	1.662320	3.602800	0.618174
14	6	0	-1.008069	1.809678	-0.629592
15	1	0	-1.707087	2.649354	-0.752021
16	7	0	-1.380965	0.633596	-0.927478
17	8	0	-0.125991	4.459465	0.351541
18	1	0	-1.040780	4.268971	0.108778
19	7	0	4.515238	-1.769730	0.126176
20	8	0	5.216508	-1.788430	1.118099
21	8	0	4.662062	-2.515689	-0.821456
22	6	0	-2.743218	0.465493	-1.420592
23	1	0	-2.681375	0.038797	-2.425533
24	1	0	-3.272270	1.425951	-1.486300
25	6	0	-3.507210	-0.483400	-0.524730
26	6	0	-3.575533	-1.845240	-0.815005
27	6	0	-4.123331	-0.005368	0.632028
28	6	0	-4.251500	-2.716259	0.035058
29	1	0	-3.096804	-2.224526	-1.712273
30	6	0	-4.800574	-0.871990	1.483654
31	1	0	-4.073280	1.054298	0.865425
32	6	0	-4.865533	-2.230935	1.185821
33	1	0	-4.298974	-3.773191	-0.202021
34	1	0	-5.277624	-0.487912	2.378313
35	1	0	-5.393717	-2.908070	1.847401

Structure 14l (DMSO)

Energy (Hartrees): -953.069171902
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.709674	-0.649689	-1.118416
2	6	0	1.694840	0.290530	-1.169927
3	6	0	1.398927	1.090361	-0.056829
4	6	0	2.137267	0.915657	1.118605
5	6	0	3.161018	-0.019086	1.187342
6	6	0	3.426537	-0.787742	0.064478
7	1	0	2.949344	-1.260847	-1.978437
8	1	0	1.134225	0.416547	-2.087498
9	1	0	1.899540	1.506996	1.995255
10	1	0	3.729295	-0.157022	2.097530
11	6	0	0.338163	2.124397	-0.131307
12	6	0	0.625538	3.361638	0.325447
13	1	0	1.615250	3.598138	0.702457
14	6	0	-0.980593	1.789815	-0.679823
15	1	0	-1.678390	2.617207	-0.865222
16	7	0	-1.334564	0.596749	-0.936881
17	8	0	-0.178137	4.433816	0.376857
18	1	0	-1.073754	4.227031	0.077450
19	7	0	4.500309	-1.787831	0.127398
20	8	0	5.145269	-1.871775	1.154630
21	8	0	4.692034	-2.484005	-0.850722
22	6	0	-2.680713	0.395094	-1.460433
23	1	0	-2.595165	-0.091623	-2.435575
24	1	0	-3.206465	1.349705	-1.596342
25	6	0	-3.470519	-0.499661	-0.530244
26	6	0	-3.863246	-1.778665	-0.920318
27	6	0	-3.804271	-0.048145	0.748740
28	6	0	-4.583130	-2.595204	-0.049388
29	1	0	-3.604565	-2.137841	-1.911309
30	6	0	-4.522760	-0.859593	1.620026
31	1	0	-3.498245	0.946418	1.060683
32	6	0	-4.914275	-2.137359	1.221584
33	1	0	-4.884025	-3.587983	-0.365035
34	1	0	-4.779993	-0.497186	2.609155
35	1	0	-5.475330	-2.770352	1.899905

Structure 14l (C_2H_5OH)

Energy (Hartrees): -953.072899211
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.716663	-0.590483	-1.119023
2	6	0	1.693066	0.339954	-1.160717
3	6	0	1.371399	1.106506	-0.031343
4	6	0	2.093145	0.907866	1.150919
5	6	0	3.122004	-0.021134	1.212897
6	6	0	3.413317	-0.755553	0.072989
7	1	0	2.974963	-1.175341	-1.991959
8	1	0	1.145038	0.485335	-2.082985
9	1	0	1.838099	1.476194	2.037910
10	1	0	3.676909	-0.178244	2.128334
11	6	0	0.302385	2.133334	-0.096571
12	6	0	0.590620	3.366057	0.372542
13	1	0	1.579195	3.592890	0.758972
14	6	0	-1.012569	1.794585	-0.652100
15	1	0	-1.725557	2.616990	-0.790611
16	7	0	-1.344849	0.605920	-0.957112
17	8	0	-0.202585	4.447374	0.427986
18	1	0	-1.097081	4.270432	0.109616
19	7	0	4.491477	-1.745388	0.127060
20	8	0	5.045388	-1.939625	1.192645
21	8	0	4.789118	-2.331036	-0.896697
22	6	0	-2.693704	0.405459	-1.479426
23	1	0	-2.605300	-0.053990	-2.467544
24	1	0	-3.230581	1.356596	-1.586969
25	6	0	-3.463936	-0.522087	-0.567031
26	6	0	-3.551608	-1.887548	-0.836025
27	6	0	-4.063465	-0.018921	0.589033
28	6	0	-4.229556	-2.738053	0.034547
29	1	0	-3.088175	-2.286532	-1.733086
30	6	0	-4.743180	-0.864761	1.459775
31	1	0	-3.997426	1.043685	0.805578
32	6	0	-4.827126	-2.228099	1.183569
33	1	0	-4.291579	-3.798118	-0.185848
34	1	0	-5.207871	-0.461271	2.352710
35	1	0	-5.357144	-2.888798	1.860584

Structure 26a (vacuum)

Energy (Hartrees): -823.79115479
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.593797	1.022985	0.582554
2	6	0	-3.870691	0.467398	0.637988
3	6	0	-4.137339	-0.712485	-0.052692
4	6	0	-3.123947	-1.315458	-0.801696
5	6	0	-1.867945	-0.740289	-0.860589
6	6	0	-1.569706	0.438199	-0.160722
7	1	0	-2.392005	1.922758	1.154003
8	1	0	-4.633272	0.955208	1.229949
9	1	0	-3.355805	-2.223372	-1.344947
10	1	0	-1.104253	-1.197372	-1.481076
11	6	0	-0.220267	1.045426	-0.209624
12	6	0	0.898096	0.266240	-0.067191
13	6	0	-0.091152	2.476753	-0.411128
14	1	0	0.777852	-0.797144	0.114691
15	1	0	-1.039436	3.021975	-0.565593
16	8	0	0.966570	3.093055	-0.432646
17	7	0	2.167113	0.715415	-0.101121
18	1	0	2.264752	1.724713	-0.196694
19	6	0	3.326438	-0.063830	0.032363
20	6	0	4.517245	0.584884	0.370709
21	6	0	3.333042	-1.444150	-0.178979
22	6	0	5.692252	-0.138831	0.508045
23	1	0	4.509301	1.657101	0.532753
24	6	0	4.514187	-2.160310	-0.025504
25	1	0	2.433036	-1.961936	-0.485032
26	6	0	5.698205	-1.517717	0.318058
27	1	0	6.607003	0.378799	0.770978
28	1	0	4.507181	-3.230891	-0.192384
29	1	0	6.615472	-2.081990	0.429055
30	8	0	-5.340824	-1.343037	-0.063614
31	6	0	-6.393589	-0.759662	0.674298
32	1	0	-7.256810	-1.405662	0.530689
33	1	0	-6.149708	-0.709935	1.740339
34	1	0	-6.625256	0.244778	0.305847

Structure 26a ($CHCl_3$)

Energy (Hartrees): -823.81550574
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.615119	1.043098	0.545661
2	6	0	-3.893359	0.488460	0.594960
3	6	0	-4.142998	-0.722892	-0.047477
4	6	0	-3.109742	-1.359026	-0.742012
5	6	0	-1.851691	-0.785012	-0.796759
6	6	0	-1.571523	0.426494	-0.146264
7	1	0	-2.430696	1.969669	1.079635
8	1	0	-4.671791	1.001526	1.144289
9	1	0	-3.321056	-2.293169	-1.249847
10	1	0	-1.072528	-1.275789	-1.370985
11	6	0	-0.221904	1.037515	-0.193586
12	6	0	0.900370	0.254980	-0.057941
13	6	0	-0.102060	2.463632	-0.393721
14	1	0	0.781401	-0.810949	0.109188
15	1	0	-1.048863	3.005695	-0.558338
16	8	0	0.955497	3.091755	-0.409251
17	7	0	2.165363	0.705019	-0.089262
18	1	0	2.271762	1.713719	-0.179680
19	6	0	3.332260	-0.068261	0.036031
20	6	0	4.525419	0.602432	0.320771
21	6	0	3.342843	-1.454982	-0.131177
22	6	0	5.712004	-0.106363	0.444710
23	1	0	4.510578	1.679687	0.449059
24	6	0	4.536933	-2.154654	0.005532
25	1	0	2.437872	-1.992974	-0.384067
26	6	0	5.725447	-1.490703	0.292823
27	1	0	6.629234	0.427414	0.665541
28	1	0	4.534846	-3.230404	-0.128055
29	1	0	6.651812	-2.043516	0.391594
30	8	0	-5.346187	-1.353372	-0.055510
31	6	0	-6.426285	-0.720029	0.610195
32	1	0	-7.289104	-1.367742	0.467136
33	1	0	-6.224657	-0.616118	1.680674
34	1	0	-6.634417	0.262632	0.176306

Structure 26a (DMSO)

Energy (Hartrees): -823.81330327
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.623443	1.057509	0.518177
2	6	0	-3.899568	0.497236	0.569172
3	6	0	-4.137177	-0.731529	-0.045967
4	6	0	-3.091853	-1.377379	-0.714788
5	6	0	-1.835550	-0.798656	-0.771513
6	6	0	-1.568652	0.430650	-0.148377
7	1	0	-2.451305	1.998415	1.030986
8	1	0	-4.684644	1.020540	1.099535
9	1	0	-3.287869	-2.326727	-1.200492
10	1	0	-1.047948	-1.303963	-1.321435
11	6	0	-0.221204	1.047107	-0.192292
12	6	0	0.902080	0.265396	-0.055452
13	6	0	-0.108509	2.473581	-0.394873
14	1	0	0.783702	-0.802230	0.101598
15	1	0	-1.057869	3.008510	-0.567643
16	8	0	0.944556	3.109474	-0.405262
17	7	0	2.167131	0.715316	-0.077638
18	1	0	2.282975	1.723551	-0.155107
19	6	0	3.330803	-0.064503	0.039673
20	6	0	4.526795	0.598108	0.332548
21	6	0	3.333734	-1.449530	-0.143156
22	6	0	5.709912	-0.118545	0.451133
23	1	0	4.516624	1.674264	0.471001
24	6	0	4.524602	-2.156534	-0.012461
25	1	0	2.425972	-1.980106	-0.401816
26	6	0	5.716403	-1.501713	0.284425
27	1	0	6.629633	0.408270	0.678891
28	1	0	4.517001	-3.230789	-0.158280
29	1	0	6.639912	-2.060517	0.378160
30	8	0	-5.335394	-1.368019	-0.049202
31	6	0	-6.420906	-0.726723	0.604500
32	1	0	-7.279642	-1.382880	0.476774
33	1	0	-6.219009	-0.597207	1.671795
34	1	0	-6.635543	0.245171	0.150721

Structure 26a (C_2H_5OH)

Energy (Hartrees): -823.81571433
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.620138	1.053266	0.532996
2	6	0	-3.895592	0.491867	0.582373
3	6	0	-4.131014	-0.730858	-0.043032
4	6	0	-3.089429	-1.372530	-0.719194
5	6	0	-1.833612	-0.792145	-0.774472
6	6	0	-1.567646	0.432376	-0.142536
7	1	0	-2.446599	1.990014	1.052988
8	1	0	-4.680904	1.009190	1.118219
9	1	0	-3.288369	-2.317830	-1.212173
10	1	0	-1.046806	-1.291050	-1.331445
11	6	0	-0.221751	1.052731	-0.191329
12	6	0	0.905416	0.271453	-0.052628
13	6	0	-0.113205	2.471373	-0.399931
14	1	0	0.786333	-0.794337	0.116613
15	1	0	-1.060660	3.008680	-0.568304
16	8	0	0.944783	3.110607	-0.419424
17	7	0	2.167738	0.718421	-0.085481
18	1	0	2.287555	1.725506	-0.175408
19	6	0	3.331601	-0.064460	0.036821
20	6	0	4.524667	0.595231	0.344061
21	6	0	3.333089	-1.447146	-0.158190
22	6	0	5.705879	-0.124045	0.467035
23	1	0	4.514701	1.670361	0.490434
24	6	0	4.521534	-2.157120	-0.022447
25	1	0	2.426842	-1.973644	-0.430869
26	6	0	5.711267	-1.505726	0.289950
27	1	0	6.624592	0.399711	0.705913
28	1	0	4.514267	-3.230148	-0.177478
29	1	0	6.633366	-2.066505	0.387244
30	8	0	-5.333889	-1.370231	-0.049461
31	6	0	-6.424857	-0.729758	0.599952
32	1	0	-7.282266	-1.385759	0.462195
33	1	0	-6.227620	-0.606517	1.668525
34	1	0	-6.632998	0.243309	0.146416

Structure 26b (vacuum)

Energy (Hartrees): -823.786478494
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.389092	1.161342	0.972742
2	6	0	3.516408	0.362010	1.030014
3	6	0	3.672582	-0.698634	0.133702
4	6	0	2.689131	-0.941686	-0.823711
5	6	0	1.564754	-0.119782	-0.874221
6	6	0	1.384975	0.936293	0.019120
7	1	0	2.272693	1.969618	1.686964
8	1	0	4.292226	0.531434	1.766675
9	1	0	2.789775	-1.745367	-1.540500
10	1	0	0.818904	-0.294268	-1.643551
11	6	0	0.185328	1.801219	-0.048440
12	6	0	-1.083231	1.318861	-0.026207
13	6	0	0.342565	3.258474	-0.141219
14	1	0	-1.898229	2.031007	-0.101166
15	1	0	1.394175	3.603640	-0.190731
16	8	0	-0.564184	4.061138	-0.176532
17	8	0	4.807569	-1.429622	0.271626
18	6	0	5.004876	-2.512729	-0.612943
19	1	0	5.052253	-2.171548	-1.651789
20	1	0	5.957180	-2.958635	-0.335082
21	1	0	4.210082	-3.258112	-0.508344
22	7	0	-1.425479	0.015651	0.125979
23	1	0	-0.675195	-0.630065	0.336775
24	6	0	-2.723058	-0.514532	0.093041
25	6	0	-2.942849	-1.775130	0.655713
26	6	0	-3.786706	0.166267	-0.503618
27	6	0	-4.208973	-2.341082	0.629160
28	1	0	-2.117753	-2.301215	1.124372
29	6	0	-5.052854	-0.405841	-0.510658
30	1	0	-3.629232	1.125169	-0.980614
31	6	0	-5.275099	-1.658060	0.051677
32	1	0	-4.362901	-3.318437	1.071248
33	1	0	-5.870377	0.131366	-0.976839
34	1	0	-6.263980	-2.098207	0.035059

Structure 26b ($CHCl_3$)

Energy (Hartrees): -823.812711279
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.396184	1.163555	0.970750
2	6	0	3.525905	0.365433	1.028867
3	6	0	3.680031	-0.701985	0.139108
4	6	0	2.691680	-0.954590	-0.812000
5	6	0	1.564161	-0.136733	-0.861071
6	6	0	1.387868	0.928299	0.023731
7	1	0	2.285436	1.979901	1.677367
8	1	0	4.303131	0.546488	1.762447
9	1	0	2.789911	-1.764734	-1.522379
10	1	0	0.812678	-0.326553	-1.621496
11	6	0	0.186270	1.793488	-0.045441
12	6	0	-1.088546	1.310311	-0.031756
13	6	0	0.351366	3.239916	-0.138378
14	1	0	-1.905039	2.019371	-0.121416
15	1	0	1.402056	3.580670	-0.196152
16	8	0	-0.549729	4.061350	-0.167970
17	8	0	4.816149	-1.430574	0.275246
18	6	0	5.033360	-2.497208	-0.634508
19	1	0	5.077891	-2.132505	-1.664911
20	1	0	5.993634	-2.931202	-0.362480
21	1	0	4.253259	-3.259058	-0.544398
22	7	0	-1.434678	0.015603	0.122543
23	1	0	-0.695372	-0.640398	0.349272
24	6	0	-2.737577	-0.509010	0.087871
25	6	0	-2.963832	-1.753183	0.684538
26	6	0	-3.791590	0.157714	-0.542031
27	6	0	-4.232372	-2.315915	0.663807
28	1	0	-2.141273	-2.267547	1.170520
29	6	0	-5.060119	-0.411994	-0.544358
30	1	0	-3.627208	1.100753	-1.048664
31	6	0	-5.291250	-1.646242	0.055364
32	1	0	-4.393357	-3.279894	1.133034
33	1	0	-5.871644	0.112219	-1.036248
34	1	0	-6.281954	-2.084069	0.042534

Structure 26b (DMSO)

Energy (Hartrees): -823.811173854
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.441076	1.214220	0.905648
2	6	0	3.581578	0.430190	0.955156
3	6	0	3.708258	-0.683272	0.118178
4	6	0	2.679967	-0.994370	-0.772056
5	6	0	1.543802	-0.188185	-0.816474
6	6	0	1.394440	0.921560	0.017709
7	1	0	2.354182	2.064910	1.574141
8	1	0	4.386255	0.659986	1.644364
9	1	0	2.751677	-1.842787	-1.439901
10	1	0	0.765740	-0.427588	-1.534761
11	6	0	0.188787	1.780294	-0.046358
12	6	0	-1.088802	1.300137	-0.025404
13	6	0	0.352944	3.226149	-0.147510
14	1	0	-1.900607	2.014073	-0.117063
15	1	0	1.403066	3.565620	-0.219753
16	8	0	-0.547176	4.050032	-0.171513
17	8	0	4.855787	-1.393782	0.239699
18	6	0	5.002831	-2.554305	-0.567211
19	1	0	4.996814	-2.300051	-1.630876
20	1	0	5.968191	-2.982157	-0.303732
21	1	0	4.213672	-3.281973	-0.357410
22	7	0	-1.444600	0.010743	0.135472
23	1	0	-0.713434	-0.657102	0.358211
24	6	0	-2.750699	-0.503358	0.096395
25	6	0	-2.974980	-1.765946	0.654870
26	6	0	-3.808941	0.187285	-0.500523
27	6	0	-4.245905	-2.323816	0.628686
28	1	0	-2.146766	-2.297707	1.111954
29	6	0	-5.079610	-0.378722	-0.508586
30	1	0	-3.649393	1.146632	-0.977208
31	6	0	-5.309089	-1.631500	0.052892
32	1	0	-4.404647	-3.302956	1.066604
33	1	0	-5.894004	0.163735	-0.975640
34	1	0	-6.301377	-2.065997	0.034805

Structure 26b (C_2H_5OH)

Energy (Hartrees): -823.814163948
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.422525	1.201961	0.921209
2	6	0	3.558365	0.411478	0.975202
3	6	0	3.692528	-0.684013	0.117690
4	6	0	2.683137	-0.971846	-0.799876
5	6	0	1.552116	-0.158674	-0.848857
6	6	0	1.392852	0.932736	0.007190
7	1	0	2.325282	2.038000	1.606577
8	1	0	4.351199	0.620691	1.684739
9	1	0	2.765023	-1.806337	-1.483901
10	1	0	0.785978	-0.377718	-1.586348
11	6	0	0.187108	1.793096	-0.053694
12	6	0	-1.091594	1.305250	-0.031422
13	6	0	0.349605	3.230353	-0.139266
14	1	0	-1.911436	2.010909	-0.117436
15	1	0	1.395167	3.575786	-0.220934
16	8	0	-0.554212	4.062209	-0.138359
17	8	0	4.837053	-1.407356	0.249678
18	6	0	4.993284	-2.561269	-0.567399
19	1	0	5.008744	-2.293221	-1.627181
20	1	0	5.951376	-2.995472	-0.287941
21	1	0	4.195232	-3.284203	-0.377425
22	7	0	-1.434685	0.016039	0.123434
23	1	0	-0.696268	-0.647362	0.336985
24	6	0	-2.740281	-0.507544	0.089593
25	6	0	-2.961920	-1.754906	0.680131
26	6	0	-3.794858	0.163778	-0.533606
27	6	0	-4.231357	-2.316910	0.661741
28	1	0	-2.135218	-2.271974	1.156436
29	6	0	-5.064074	-0.405162	-0.533173
30	1	0	-3.632456	1.108876	-1.037469
31	6	0	-5.292567	-1.642665	0.061774
32	1	0	-4.390549	-3.284285	1.125026
33	1	0	-5.877468	0.121485	-1.019790
34	1	0	-6.283740	-2.080248	0.050635

Structure 26c (vacuum)

Energy (Hartrees): -823.787721553
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.369229	1.093586	0.918384
2	6	0	-3.439435	0.223306	0.997552
3	6	0	-3.520449	-0.877269	0.139109
4	6	0	-2.518325	-1.090951	-0.804645
5	6	0	-1.444003	-0.204636	-0.871882
6	6	0	-1.340531	0.887528	-0.012632
7	1	0	-2.325978	1.953869	1.574672
8	1	0	-4.236738	0.375714	1.714535
9	1	0	-2.563635	-1.920844	-1.496595
10	1	0	-0.682916	-0.359643	-1.630498
11	6	0	-0.186024	1.809815	-0.089090
12	6	0	1.104215	1.387929	-0.072224
13	6	0	-0.384921	3.258682	-0.135009
14	1	0	1.901311	2.121046	-0.146757
15	8	0	-4.609016	-1.673113	0.295541
16	6	0	-4.747781	-2.775921	-0.574865
17	1	0	-3.915257	-3.477805	-0.461495
18	1	0	-5.675657	-3.268239	-0.292757
19	1	0	-4.810894	-2.450354	-1.617998
20	7	0	1.510441	0.100870	0.081974
21	1	0	0.791054	-0.573915	0.309428
22	6	0	2.833248	-0.360739	0.072189
23	6	0	3.115547	-1.589677	0.675876
24	6	0	3.864354	0.355031	-0.540489
25	6	0	4.409686	-2.088256	0.674304
26	1	0	2.315646	-2.143466	1.155971
27	6	0	5.159912	-0.148313	-0.521109
28	1	0	3.659340	1.284667	-1.055901
29	6	0	5.443390	-1.367850	0.082831
30	1	0	4.611336	-3.041801	1.147749
31	1	0	5.951416	0.415695	-1.000395
32	1	0	6.454212	-1.755143	0.087193
33	8	0	-1.450910	3.825293	-0.078734
34	1	0	0.555159	3.843097	-0.225226

Structure 26c ($CHCl_3$)

Energy (Hartrees): -823.815370540
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.345970	1.063796	0.966145
2	6	0	-3.424162	0.200663	1.042283
3	6	0	-3.534392	-0.871343	0.150355
4	6	0	-2.553186	-1.063681	-0.821179
5	6	0	-1.471841	-0.185398	-0.883395
6	6	0	-1.341173	0.882139	0.004108
7	1	0	-2.275862	1.893440	1.660041
8	1	0	-4.199785	0.338999	1.786774
9	1	0	-2.618716	-1.874332	-1.534688
10	1	0	-0.722717	-0.332541	-1.655602
11	6	0	-0.180591	1.799898	-0.071251
12	6	0	1.114390	1.371750	-0.066633
13	6	0	-0.363170	3.239697	-0.125472
14	1	0	1.909827	2.106364	-0.149148
15	8	0	-4.623612	-1.665464	0.305873
16	6	0	-4.809966	-2.722617	-0.621292
17	1	0	-3.986944	-3.442061	-0.573614
18	1	0	-5.735668	-3.216020	-0.331338
19	1	0	-4.906756	-2.338024	-1.640870
20	7	0	1.517226	0.090556	0.073780
21	1	0	0.806769	-0.597149	0.299026
22	6	0	2.845646	-0.367275	0.063225
23	6	0	3.132474	-1.578854	0.698876
24	6	0	3.867766	0.335332	-0.579617
25	6	0	4.429066	-2.074185	0.701865
26	1	0	2.334396	-2.120054	1.196443
27	6	0	5.165324	-0.165263	-0.556886
28	1	0	3.655670	1.251100	-1.117775
29	6	0	5.455860	-1.367316	0.080687
30	1	0	4.637527	-3.013361	1.201416
31	1	0	5.952246	0.386063	-1.058931
32	1	0	6.468381	-1.751980	0.087977
33	8	0	-1.430773	3.824754	-0.103910
34	1	0	0.579677	3.817275	-0.192795

Structure 26c (DMSO)

Energy (Hartrees): -823.814916633
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.294348	1.043246	1.007939
2	6	0	-3.367823	0.175488	1.106662
3	6	0	-3.515344	-0.872249	0.189960
4	6	0	-2.575085	-1.034931	-0.827036
5	6	0	-1.499168	-0.151211	-0.911754
6	6	0	-1.333189	0.893202	-0.002765
7	1	0	-2.192281	1.848483	1.726841
8	1	0	-4.107731	0.291721	1.890585
9	1	0	-2.666199	-1.829049	-1.556320
10	1	0	-0.780242	-0.280798	-1.715275
11	6	0	-0.181036	1.820412	-0.103027
12	6	0	1.119093	1.402202	-0.106116
13	6	0	-0.380197	3.254630	-0.188653
14	1	0	1.904647	2.144651	-0.201842
15	8	0	-4.594899	-1.671782	0.367689
16	6	0	-4.801931	-2.717329	-0.571969
17	1	0	-3.969283	-3.426416	-0.564591
18	1	0	-5.711942	-3.225872	-0.259386
19	1	0	-4.936814	-2.317107	-1.580893
20	7	0	1.524048	0.122950	0.023946
21	1	0	0.807686	-0.577877	0.183850
22	6	0	2.844978	-0.351014	0.043496
23	6	0	3.044523	-1.685951	0.411461
24	6	0	3.943760	0.442364	-0.297980
25	6	0	4.325958	-2.217844	0.445028
26	1	0	2.186256	-2.296322	0.673907
27	6	0	5.223294	-0.102562	-0.253064
28	1	0	3.816182	1.471607	-0.607778
29	6	0	5.426198	-1.428623	0.116870
30	1	0	4.463820	-3.253792	0.733311
31	1	0	6.069021	0.521420	-0.519587
32	1	0	6.427047	-1.842287	0.146002
33	8	0	-1.456666	3.828101	-0.194363
34	1	0	0.555923	3.841441	-0.257347

Structure 26c (C_2H_5OH)

Energy (Hartrees): -823.818424304
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.311845	1.030574	1.012966
2	6	0	-3.395117	0.172375	1.087560
3	6	0	-3.535003	-0.865336	0.160208
4	6	0	-2.581754	-1.030628	-0.843108
5	6	0	-1.497116	-0.156357	-0.904464
6	6	0	-1.337072	0.879276	0.015876
7	1	0	-2.213132	1.828320	1.741233
8	1	0	-4.147127	0.289041	1.860088
9	1	0	-2.669739	-1.817814	-1.580344
10	1	0	-0.767628	-0.285130	-1.698421
11	6	0	-0.177457	1.799843	-0.060667
12	6	0	1.123712	1.373453	-0.057114
13	6	0	-0.361734	3.227384	-0.131572
14	1	0	1.915805	2.111675	-0.138371
15	8	0	-4.628012	-1.660156	0.314967
16	6	0	-4.834580	-2.695738	-0.638365
17	1	0	-4.008366	-3.411857	-0.625927
18	1	0	-5.753171	-3.196992	-0.339441
19	1	0	-4.954132	-2.282028	-1.643367
20	7	0	1.523583	0.097410	0.073887
21	1	0	0.813082	-0.600506	0.271261
22	6	0	2.853252	-0.364385	0.060224
23	6	0	3.122715	-1.600897	0.653153
24	6	0	3.886121	0.356764	-0.542661
25	6	0	4.416986	-2.103549	0.656886
26	1	0	2.313127	-2.156445	1.115364
27	6	0	5.180630	-0.152788	-0.520143
28	1	0	3.690057	1.294549	-1.048350
29	6	0	5.456053	-1.379342	0.077083
30	1	0	4.612480	-3.062875	1.122862
31	1	0	5.977235	0.412260	-0.991074
32	1	0	6.466818	-1.769511	0.084037
33	8	0	-1.441909	3.810990	-0.142070
34	1	0	0.572223	3.814882	-0.185117

Structure 26d (vacuum)

Energy (Hartrees): -823.777790106
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.552767	1.007633	0.529871
2	6	0	-3.776356	0.346293	0.601788
3	6	0	-3.931502	-0.892050	-0.018012
4	6	0	-2.859495	-1.451050	-0.716247
5	6	0	-1.653336	-0.777984	-0.785818
6	6	0	-1.468110	0.457768	-0.150577
7	1	0	-2.447011	1.971612	1.010169
8	1	0	-4.592183	0.809156	1.140449
9	1	0	-3.005161	-2.404029	-1.209980
10	1	0	-0.842839	-1.208667	-1.364972
11	6	0	-0.156379	1.148575	-0.199476
12	6	0	0.985638	0.430352	-0.021023
13	6	0	-0.095417	2.588842	-0.455954
14	1	0	0.896459	-0.636112	0.159478
15	7	0	2.273556	0.880982	0.011068
16	1	0	2.442608	1.873184	0.058172
17	6	0	3.411356	0.061325	0.069647
18	6	0	4.600395	0.597196	0.572561
19	6	0	3.389992	-1.261182	-0.377719
20	6	0	5.745061	-0.183431	0.638321
21	1	0	4.618201	1.624043	0.922351
22	6	0	4.538620	-2.038976	-0.288301
23	1	0	2.493704	-1.677263	-0.819935
24	6	0	5.720411	-1.509788	0.217036
25	1	0	6.659132	0.245830	1.031084
26	1	0	4.509126	-3.064370	-0.637252
27	1	0	6.613388	-2.119300	0.273255
28	8	0	-5.078412	-1.620947	-0.007415
29	6	0	-6.188500	-1.087986	0.682784
30	1	0	-6.988843	-1.816605	0.574101
31	1	0	-5.964741	-0.948745	1.745295
32	1	0	-6.503755	-0.133636	0.249022
33	1	0	0.921948	3.008168	-0.599349
34	8	0	-1.044413	3.333028	-0.542916

Structure 26d ($CHCl_3$)

Energy (Hartrees): -823.806246669
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.552906	1.001785	0.544075
2	6	0	-3.781652	0.347314	0.609358
3	6	0	-3.937969	-0.891065	-0.012096
4	6	0	-2.862184	-1.454800	-0.702737
5	6	0	-1.651469	-0.786342	-0.767007
6	6	0	-1.465454	0.451159	-0.133961
7	1	0	-2.445368	1.960194	1.037044
8	1	0	-4.598511	0.811830	1.146079
9	1	0	-3.002091	-2.409868	-1.196090
10	1	0	-0.836889	-1.226604	-1.333465
11	6	0	-0.153293	1.145316	-0.179513
12	6	0	0.992920	0.423565	0.005791
13	6	0	-0.091559	2.569158	-0.474068
14	1	0	0.902432	-0.647721	0.159638
15	7	0	2.269720	0.876571	0.063305
16	1	0	2.440226	1.869585	0.144309
17	6	0	3.412625	0.059609	0.094425
18	6	0	4.600647	0.595435	0.601150
19	6	0	3.395854	-1.251645	-0.386091
20	6	0	5.752914	-0.177707	0.637340
21	1	0	4.610256	1.616123	0.969236
22	6	0	4.553351	-2.021100	-0.328076
23	1	0	2.497853	-1.666964	-0.826670
24	6	0	5.735613	-1.493669	0.180917
25	1	0	6.667490	0.249656	1.032362
26	1	0	4.529272	-3.037745	-0.703330
27	1	0	6.635306	-2.096286	0.212093
28	8	0	-5.087656	-1.614815	-0.003877
29	6	0	-6.210744	-1.060601	0.660889
30	1	0	-7.014659	-1.785895	0.548911
31	1	0	-6.005957	-0.908776	1.724901
32	1	0	-6.510611	-0.112797	0.203921
33	1	0	0.921640	2.995142	-0.594383
34	8	0	-1.049667	3.304272	-0.629880

Structure 26d (DMSO)

Energy (Hartrees): -823.806455738
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.543015	0.971013	0.596785
2	6	0	-3.771992	0.314906	0.650301
3	6	0	-3.941593	-0.890478	-0.032150
4	6	0	-2.874738	-1.421692	-0.762679
5	6	0	-1.663676	-0.750830	-0.814355
6	6	0	-1.467039	0.457209	-0.128855
7	1	0	-2.425807	1.900925	1.139922
8	1	0	-4.577885	0.749830	1.226976
9	1	0	-3.018382	-2.353278	-1.298305
10	1	0	-0.856383	-1.167170	-1.408505
11	6	0	-0.156689	1.153487	-0.167043
12	6	0	0.990644	0.416120	-0.035045
13	6	0	-0.095937	2.588439	-0.385044
14	1	0	0.888640	-0.655026	0.107121
15	7	0	2.269132	0.853498	-0.030695
16	1	0	2.452550	1.848954	-0.025350
17	6	0	3.411105	0.038328	0.049890
18	6	0	4.614789	0.635408	0.439404
19	6	0	3.385225	-1.322499	-0.266855
20	6	0	5.773385	-0.124218	0.527393
21	1	0	4.629973	1.694298	0.676242
22	6	0	4.551232	-2.074554	-0.160590
23	1	0	2.475524	-1.796730	-0.613660
24	6	0	5.748733	-1.486517	0.235683
25	1	0	6.698468	0.352098	0.831607
26	1	0	4.519927	-3.129884	-0.406828
27	1	0	6.652671	-2.079203	0.308615
28	8	0	-5.094402	-1.605990	-0.046528
29	6	0	-6.212454	-1.059899	0.638390
30	1	0	-7.032406	-1.758582	0.483918
31	1	0	-6.013032	-0.966514	1.709609
32	1	0	-6.485560	-0.083341	0.228546
33	1	0	0.916504	3.026411	-0.440569
34	8	0	-1.055175	3.328163	-0.530453

Structure 26d (C_2H_5OH)

Energy (Hartrees): -823.809531464
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.523638	0.961376	0.617076
2	6	0	-3.749776	0.300992	0.675341
3	6	0	-3.931208	-0.875195	-0.050841
4	6	0	-2.886956	-1.372694	-0.833643
5	6	0	-1.677810	-0.698464	-0.887611
6	6	0	-1.466589	0.478352	-0.155407
7	1	0	-2.392432	1.866860	1.198300
8	1	0	-4.541237	0.708103	1.290907
9	1	0	-3.045264	-2.283196	-1.401051
10	1	0	-0.883879	-1.087521	-1.517411
11	6	0	-0.154957	1.174469	-0.189195
12	6	0	0.994430	0.433390	-0.063377
13	6	0	-0.093341	2.602736	-0.390085
14	1	0	0.890086	-0.639759	0.065379
15	7	0	2.270140	0.866401	-0.048447
16	1	0	2.458731	1.860961	-0.026428
17	6	0	3.406815	0.039523	0.042962
18	6	0	4.594688	0.606656	0.512725
19	6	0	3.381314	-1.303697	-0.338180
20	6	0	5.740970	-0.169609	0.618801
21	1	0	4.608127	1.653445	0.799077
22	6	0	4.533145	-2.073759	-0.212150
23	1	0	2.483255	-1.747586	-0.750552
24	6	0	5.715734	-1.516909	0.265730
25	1	0	6.655964	0.280507	0.987168
26	1	0	4.504475	-3.116475	-0.508248
27	1	0	6.610212	-2.122394	0.352386
28	8	0	-5.084295	-1.600089	-0.060404
29	6	0	-6.159927	-1.141125	0.748529
30	1	0	-6.964160	-1.862333	0.614809
31	1	0	-5.871215	-1.109132	1.802759
32	1	0	-6.499797	-0.152968	0.426419
33	1	0	0.914072	3.048577	-0.441577
34	8	0	-1.060117	3.345322	-0.529204

Structure 26e (vacuum)

Energy (Hartrees): -823.773378318
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.199962	1.307029	-0.579144
2	6	0	3.563784	1.202424	-0.394456
3	6	0	4.125676	0.015536	0.087519
4	6	0	3.298544	-1.060781	0.393050
5	6	0	1.921447	-0.938062	0.206774
6	6	0	1.346702	0.227337	-0.295669
7	1	0	1.784604	2.234742	-0.950551
8	1	0	4.225869	2.029805	-0.618593
9	1	0	3.698371	-1.984038	0.790058
10	1	0	1.282682	-1.769419	0.485708
11	6	0	-0.108273	0.302880	-0.552147
12	6	0	-0.744591	-0.764294	-1.098412
13	6	0	-0.840880	1.562476	-0.322155
14	1	0	-0.136555	-1.579592	-1.484642
15	7	0	-2.096476	-0.967803	-1.257181
16	1	0	-2.343196	-1.662986	-1.944284
17	6	0	-3.162715	-0.605768	-0.403903
18	6	0	-2.970103	-0.271707	0.938513
19	6	0	-4.457484	-0.642853	-0.923822
20	6	0	-4.066294	0.025399	1.737131
21	1	0	-1.970682	-0.243773	1.354540
22	6	0	-5.546909	-0.353990	-0.111945
23	1	0	-4.604935	-0.890771	-1.969613
24	6	0	-5.358998	-0.012606	1.222220
25	1	0	-3.903569	0.285882	2.776220
26	1	0	-6.545578	-0.386608	-0.531033
27	1	0	-6.206719	0.224942	1.852437
28	1	0	-1.862491	1.597226	-0.739977
29	8	0	-0.379742	2.533485	0.229878
30	8	0	5.476400	0.013941	0.231228
31	6	0	6.084584	-1.169553	0.701116
32	1	0	7.153610	-0.970539	0.726880
33	1	0	5.737354	-1.420572	1.708526
34	1	0	5.886593	-2.009893	0.027736

Structure 26e ($CHCl_3$)

Energy (Hartrees): -823.800663906
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.193093	1.263809	-0.672349
2	6	0	3.561309	1.184165	-0.495125
3	6	0	4.138523	0.034386	0.056312
4	6	0	3.323614	-1.030470	0.430801
5	6	0	1.942962	-0.931416	0.251865
6	6	0	1.350642	0.199117	-0.309647
7	1	0	1.767609	2.161114	-1.104615
8	1	0	4.209533	2.004923	-0.780093
9	1	0	3.738196	-1.926470	0.873374
10	1	0	1.315809	-1.754621	0.578307
11	6	0	-0.111680	0.255328	-0.540092
12	6	0	-0.748384	-0.843029	-1.040969
13	6	0	-0.843838	1.504249	-0.333101
14	1	0	-0.136747	-1.656473	-1.424856
15	7	0	-2.085244	-1.089372	-1.157356
16	1	0	-2.324906	-1.837461	-1.793815
17	6	0	-3.166130	-0.641327	-0.362188
18	6	0	-3.001032	-0.257874	0.971658
19	6	0	-4.443280	-0.658905	-0.923287
20	6	0	-4.109077	0.113901	1.721701
21	1	0	-2.014806	-0.252882	1.420714
22	6	0	-5.546639	-0.293870	-0.159322
23	1	0	-4.564524	-0.957702	-1.959038
24	6	0	-5.386218	0.100612	1.164444
25	1	0	-3.970620	0.410136	2.755206
26	1	0	-6.533366	-0.311764	-0.607757
27	1	0	-6.244675	0.392895	1.757258
28	1	0	-1.866639	1.530332	-0.744111
29	8	0	-0.388632	2.499563	0.197495
30	8	0	5.489517	0.052040	0.192166
31	6	0	6.106645	-1.081844	0.778260
32	1	0	7.173684	-0.868090	0.797801
33	1	0	5.749380	-1.240333	1.800236
34	1	0	5.928641	-1.981815	0.181835

Structure 26e (DMSO)

Energy (Hartrees): -823.800450544
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.177996	1.248653	-0.697369
2	6	0	3.548381	1.187994	-0.522274
3	6	0	4.140946	0.055859	0.050940
4	6	0	3.336551	-1.009931	0.448017
5	6	0	1.954005	-0.929034	0.272273
6	6	0	1.346253	0.184382	-0.308601
7	1	0	1.743329	2.130817	-1.151461
8	1	0	4.183847	2.010981	-0.829601
9	1	0	3.760461	-1.894768	0.904200
10	1	0	1.338716	-1.755844	0.612294
11	6	0	-0.117772	0.222911	-0.533258
12	6	0	-0.745874	-0.901206	-0.996265
13	6	0	-0.858634	1.467070	-0.356832
14	1	0	-0.127814	-1.718892	-1.359790
15	7	0	-2.074223	-1.171818	-1.092977
16	1	0	-2.307732	-1.956428	-1.688577
17	6	0	-3.160398	-0.673698	-0.334803
18	6	0	-3.008259	-0.268879	0.994525
19	6	0	-4.425056	-0.664778	-0.922248
20	6	0	-4.117051	0.157957	1.713396
21	1	0	-2.031320	-0.293137	1.463630
22	6	0	-5.530475	-0.244180	-0.189163
23	1	0	-4.534020	-0.988049	-1.952027
24	6	0	-5.382622	0.175876	1.128573
25	1	0	-3.991017	0.469178	2.744284
26	1	0	-6.508682	-0.241268	-0.656523
27	1	0	-6.242873	0.508647	1.697329
28	1	0	-1.880880	1.473251	-0.769798
29	8	0	-0.417209	2.483412	0.150507
30	8	0	5.490436	0.088490	0.182911
31	6	0	6.116517	-1.037098	0.781657
32	1	0	7.182280	-0.817123	0.797407
33	1	0	5.760356	-1.186998	1.804964
34	1	0	5.942053	-1.944242	0.195745

Structure 26e (C_2H_5OH)

Energy (Hartrees): -823.803629262
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.163100	1.248278	-0.710290
2	6	0	3.535397	1.195026	-0.546294
3	6	0	4.133940	0.070952	0.033771
4	6	0	3.340595	-0.994982	0.448262
5	6	0	1.956428	-0.920755	0.284477
6	6	0	1.340276	0.185593	-0.300392
7	1	0	1.720568	2.121979	-1.174553
8	1	0	4.167151	2.015754	-0.867853
9	1	0	3.773467	-1.873701	0.907814
10	1	0	1.346352	-1.746666	0.636422
11	6	0	-0.128037	0.216432	-0.507168
12	6	0	-0.745425	-0.909598	-0.993812
13	6	0	-0.873813	1.436947	-0.279142
14	1	0	-0.112810	-1.700178	-1.390675
15	7	0	-2.060023	-1.215061	-1.074836
16	1	0	-2.283702	-2.006147	-1.666020
17	6	0	-3.157131	-0.697185	-0.337195
18	6	0	-3.033443	-0.385975	1.018972
19	6	0	-4.389474	-0.572834	-0.973824
20	6	0	-4.141428	0.069506	1.720390
21	1	0	-2.077557	-0.500535	1.518069
22	6	0	-5.497321	-0.127126	-0.257881
23	1	0	-4.473301	-0.822219	-2.026144
24	6	0	-5.377414	0.202734	1.087503
25	1	0	-4.041334	0.310049	2.772834
26	1	0	-6.453570	-0.031759	-0.759930
27	1	0	-6.238629	0.555727	1.642778
28	1	0	-1.909486	1.450506	-0.650947
29	8	0	-0.421817	2.452230	0.239783
30	8	0	5.489668	0.110909	0.154949
31	6	0	6.129002	-1.005789	0.760644
32	1	0	7.192830	-0.775898	0.766821
33	1	0	5.779333	-1.146309	1.787125
34	1	0	5.956532	-1.917627	0.182128

Structure 26f (vacuum)

Energy (Hartrees): -823.772539811
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.281718	1.429956	-0.285353
2	6	0	3.652309	1.313163	-0.155096
3	6	0	4.233277	0.064328	0.083862
4	6	0	3.420313	-1.060089	0.196437
5	6	0	2.037747	-0.921752	0.078257
6	6	0	1.439106	0.311346	-0.173552
7	1	0	1.855193	2.402871	-0.504078
8	1	0	4.303299	2.173984	-0.246574
9	1	0	3.838656	-2.038183	0.392295
10	1	0	1.410631	-1.797227	0.209111
11	6	0	-0.029381	0.437419	-0.327868
12	6	0	-0.673545	-0.457635	-1.132887
13	6	0	-0.680480	1.605296	0.273330
14	1	0	-0.044644	-1.105635	-1.740354
15	1	0	-0.022048	2.202801	0.933281
16	8	0	-1.822436	1.957991	0.075245
17	7	0	-1.999799	-0.675121	-1.343640
18	1	0	-2.208914	-1.221152	-2.165508
19	6	0	-3.107312	-0.500303	-0.484735
20	6	0	-2.971625	-0.482706	0.901255
21	6	0	-4.375970	-0.430061	-1.058770
22	6	0	-4.102598	-0.390264	1.700722
23	1	0	-1.986911	-0.546279	1.346549
24	6	0	-5.501296	-0.341416	-0.250988
25	1	0	-4.474617	-0.430772	-2.139105
26	6	0	-5.370826	-0.318590	1.133495
27	1	0	-3.988639	-0.374032	2.778100
28	1	0	-6.482179	-0.280758	-0.707271
29	1	0	-6.247951	-0.242981	1.764127
30	8	0	5.587322	0.049942	0.193406
31	6	0	6.209490	-1.188824	0.460021
32	1	0	6.020171	-1.908384	-0.342971
33	1	0	7.276276	-0.984955	0.518070
34	1	0	5.865624	-1.606116	1.411829

Structure 26f ($CHCl_3$)

Energy (Hartrees): -823.799919847
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.281989	1.412726	-0.357578
2	6	0	3.653336	1.304712	-0.213026
3	6	0	4.235165	0.069645	0.089589
4	6	0	3.422483	-1.050039	0.251307
5	6	0	2.039959	-0.919779	0.119442
6	6	0	1.439110	0.300076	-0.193965
7	1	0	1.858314	2.374359	-0.627067
8	1	0	4.299202	2.165159	-0.345450
9	1	0	3.842768	-2.016563	0.496273
10	1	0	1.417315	-1.792465	0.287760
11	6	0	-0.030767	0.416514	-0.359858
12	6	0	-0.677830	-0.544092	-1.093114
13	6	0	-0.672412	1.627323	0.137215
14	1	0	-0.055185	-1.231489	-1.661743
15	1	0	-0.025358	2.265183	0.767023
16	8	0	-1.808726	1.987824	-0.114932
17	7	0	-1.998318	-0.788846	-1.271601
18	1	0	-2.205111	-1.407264	-2.045047
19	6	0	-3.106490	-0.542302	-0.435056
20	6	0	-2.976253	-0.350543	0.939770
21	6	0	-4.376952	-0.579730	-1.012868
22	6	0	-4.113374	-0.191674	1.722307
23	1	0	-1.994253	-0.337793	1.395527
24	6	0	-5.506967	-0.419042	-0.222338
25	1	0	-4.470216	-0.731043	-2.083284
26	6	0	-5.381819	-0.219528	1.149888
27	1	0	-4.003025	-0.042770	2.790464
28	1	0	-6.487846	-0.445298	-0.682952
29	1	0	-6.263262	-0.087028	1.765871
30	8	0	5.587598	0.060561	0.209209
31	6	0	6.214186	-1.171706	0.524250
32	1	0	6.034706	-1.917554	-0.255841
33	1	0	7.280487	-0.960916	0.580829
34	1	0	5.868530	-1.555048	1.488833

Structure 26f (DMSO)

Energy (Hartrees): -823.799638739
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.279399	1.412559	-0.362419
2	6	0	3.650868	1.305658	-0.211579
3	6	0	4.233362	0.072036	0.098173
4	6	0	3.419439	-1.048028	0.259763
5	6	0	2.037409	-0.919264	0.120950
6	6	0	1.436471	0.299567	-0.199470
7	1	0	1.857526	2.374232	-0.635129
8	1	0	4.293824	2.168400	-0.344804
9	1	0	3.838566	-2.014313	0.508362
10	1	0	1.415574	-1.793434	0.285013
11	6	0	-0.032644	0.413457	-0.373143
12	6	0	-0.677965	-0.567763	-1.082549
13	6	0	-0.671324	1.636858	0.092091
14	1	0	-0.057188	-1.270886	-1.633439
15	1	0	-0.029488	2.278578	0.722860
16	8	0	-1.799295	2.008054	-0.186316
17	7	0	-1.996911	-0.818821	-1.252424
18	1	0	-2.202980	-1.463311	-2.006376
19	6	0	-3.102444	-0.551499	-0.421246
20	6	0	-2.971425	-0.312312	0.946987
21	6	0	-4.374902	-0.621771	-0.994064
22	6	0	-4.109080	-0.139992	1.727049
23	1	0	-1.989594	-0.276200	1.402406
24	6	0	-5.505041	-0.444829	-0.206259
25	1	0	-4.467388	-0.818100	-2.057365
26	6	0	-5.379197	-0.198834	1.159173
27	1	0	-3.997741	0.041097	2.790335
28	1	0	-6.486819	-0.500693	-0.662848
29	1	0	-6.260662	-0.057738	1.773544
30	8	0	5.583837	0.062372	0.222724
31	6	0	6.206126	-1.176799	0.530841
32	1	0	6.019023	-1.917608	-0.251776
33	1	0	7.273757	-0.972313	0.585111
34	1	0	5.861327	-1.563642	1.494014

Structure 26f (C_2H_5OH)

Energy (Hartrees): -823.803228661
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.280327	1.425278	-0.347234
2	6	0	3.651086	1.311411	-0.193629
3	6	0	4.225338	0.071798	0.102632
4	6	0	3.409868	-1.047477	0.250970
5	6	0	2.028840	-0.911542	0.111355
6	6	0	1.434281	0.313405	-0.197371
7	1	0	1.862566	2.391023	-0.611750
8	1	0	4.299259	2.172202	-0.315646
9	1	0	3.826171	-2.017516	0.489486
10	1	0	1.402555	-1.784511	0.265483
11	6	0	-0.034881	0.429846	-0.371629
12	6	0	-0.676423	-0.545385	-1.099788
13	6	0	-0.676558	1.637317	0.103986
14	1	0	-0.050863	-1.225668	-1.673444
15	1	0	-0.039966	2.286509	0.729326
16	8	0	-1.818368	1.998924	-0.160854
17	7	0	-1.989327	-0.810758	-1.262507
18	1	0	-2.194378	-1.446379	-2.024663
19	6	0	-3.096522	-0.554778	-0.425645
20	6	0	-2.961886	-0.344192	0.946418
21	6	0	-4.367821	-0.604271	-1.000920
22	6	0	-4.097899	-0.174720	1.729501
23	1	0	-1.978959	-0.326441	1.401355
24	6	0	-5.496342	-0.432246	-0.209616
25	1	0	-4.461980	-0.778856	-2.067823
26	6	0	-5.367807	-0.211760	1.159604
27	1	0	-3.985303	-0.012716	2.795717
28	1	0	-6.478662	-0.470021	-0.666827
29	1	0	-6.248142	-0.072385	1.776136
30	8	0	5.580888	0.055101	0.229418
31	6	0	6.202313	-1.191959	0.513928
32	1	0	6.008996	-1.915570	-0.282686
33	1	0	7.270208	-0.988685	0.567584
34	1	0	5.858127	-1.592235	1.471420

Structure 26g (vacuum)

Energy (Hartrees): -823.78286338
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.917891	-0.467806	-0.733354
2	6	0	-3.200494	-1.011619	-0.691717
3	6	0	-4.169862	-0.423801	0.117884
4	6	0	-3.838673	0.694502	0.886828
5	6	0	-2.556602	1.210700	0.846920
6	6	0	-1.569173	0.646864	0.026791
7	1	0	-1.183683	-0.914950	-1.395546
8	1	0	-3.428211	-1.875269	-1.301863
9	1	0	-4.602050	1.127949	1.521211
10	1	0	-2.304791	2.057053	1.476804
11	6	0	-0.204335	1.219403	-0.032995
12	6	0	-0.018493	2.566139	-0.125560
13	6	0	0.947852	0.343699	-0.001924
14	1	0	-0.864242	3.246541	-0.176896
15	1	0	0.759464	-0.731821	0.087636
16	8	0	1.151354	3.170204	-0.179569
17	1	0	1.849297	2.454774	-0.156751
18	7	0	2.151644	0.794789	-0.076337
19	6	0	3.245717	-0.089044	0.018819
20	6	0	3.264121	-1.176354	0.897256
21	6	0	4.366395	0.171368	-0.773411
22	6	0	4.376276	-2.009164	0.949611
23	1	0	2.423574	-1.347892	1.559942
24	6	0	5.470231	-0.667726	-0.720523
25	1	0	4.347642	1.030905	-1.432981
26	6	0	5.479231	-1.763645	0.138834
27	1	0	4.384980	-2.845908	1.638243
28	1	0	6.329672	-0.462107	-1.347716
29	1	0	6.345138	-2.412782	0.185307
30	8	0	-5.450148	-0.863815	0.229765
31	6	0	-5.825382	-1.992345	-0.530872
32	1	0	-5.233906	-2.870910	-0.254085
33	1	0	-6.872936	-2.175791	-0.302934
34	1	0	-5.714616	-1.801441	-1.603097

Structure 26g ($CHCl_3$)

Energy (Hartrees): -823.80509819
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.922148	-0.484888	-0.715198
2	6	0	-3.207783	-1.022274	-0.671317
3	6	0	-4.178925	-0.417340	0.125116
4	6	0	-3.845613	0.710998	0.880122
5	6	0	-2.560469	1.222970	0.837084
6	6	0	-1.572666	0.642493	0.028139
7	1	0	-1.187197	-0.949883	-1.364613
8	1	0	-3.437181	-1.895122	-1.268273
9	1	0	-4.606947	1.161880	1.506311
10	1	0	-2.311049	2.081504	1.452121
11	6	0	-0.204934	1.210961	-0.037597
12	6	0	-0.017009	2.557242	-0.124392
13	6	0	0.944524	0.329307	-0.012452
14	1	0	-0.856320	3.246145	-0.169684
15	1	0	0.753337	-0.745206	0.068116
16	8	0	1.161908	3.152793	-0.178503
17	1	0	1.854760	2.427485	-0.158609
18	7	0	2.148660	0.782730	-0.081389
19	6	0	3.248410	-0.095624	0.013510
20	6	0	3.254437	-1.211862	0.856810
21	6	0	4.388287	0.204278	-0.738111
22	6	0	4.374956	-2.034093	0.912260
23	1	0	2.395320	-1.420515	1.484802
24	6	0	5.501107	-0.624693	-0.681512
25	1	0	4.380214	1.084648	-1.371167
26	6	0	5.499061	-1.748528	0.142315
27	1	0	4.373564	-2.894489	1.572036
28	1	0	6.375660	-0.388342	-1.277067
29	1	0	6.371284	-2.389879	0.191352
30	8	0	-5.460921	-0.851137	0.234093
31	6	0	-5.845015	-1.975947	-0.539731
32	1	0	-5.271289	-2.864075	-0.258340
33	1	0	-6.898118	-2.145309	-0.323211
34	1	0	-5.721862	-1.779190	-1.609037

Structure 26g (DMSO)

Energy (Hartrees): -823.80209392
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.920461	-0.500536	-0.695928
2	6	0	-3.207942	-1.034153	-0.652924
3	6	0	-4.185638	-0.411848	0.123154
4	6	0	-3.855928	0.732539	0.856809
5	6	0	-2.569267	1.242151	0.813931
6	6	0	-1.575004	0.641548	0.027467
7	1	0	-1.180592	-0.984111	-1.325914
8	1	0	-3.432122	-1.919128	-1.233973
9	1	0	-4.619708	1.201071	1.467252
10	1	0	-2.325178	2.114926	1.410962
11	6	0	-0.205564	1.205918	-0.036609
12	6	0	-0.013915	2.552689	-0.122296
13	6	0	0.941613	0.321921	-0.010719
14	1	0	-0.851034	3.244616	-0.165727
15	1	0	0.751683	-0.752419	0.067009
16	8	0	1.168240	3.140881	-0.176701
17	1	0	1.853305	2.404997	-0.158050
18	7	0	2.146063	0.778517	-0.076076
19	6	0	3.248472	-0.097057	0.015485
20	6	0	3.252220	-1.227100	0.841009
21	6	0	4.393088	0.219667	-0.722521
22	6	0	4.377548	-2.043278	0.894153
23	1	0	2.387874	-1.452751	1.455873
24	6	0	5.510925	-0.603494	-0.667937
25	1	0	4.387560	1.109151	-1.343198
26	6	0	5.507227	-1.740467	0.138021
27	1	0	4.373929	-2.914744	1.539485
28	1	0	6.389227	-0.353894	-1.252719
29	1	0	6.382210	-2.378446	0.185073
30	8	0	-5.466870	-0.843115	0.230302
31	6	0	-5.842936	-1.981420	-0.531748
32	1	0	-5.270706	-2.864628	-0.233177
33	1	0	-6.897898	-2.149002	-0.323176
34	1	0	-5.708581	-1.799858	-1.602082

Structure 26g (C_2H_5OH)

Energy (Hartrees): -823.81571433
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.913554	-0.492671	-0.700888
2	6	0	-3.198389	-1.032173	-0.658154
3	6	0	-4.174787	-0.417033	0.123341
4	6	0	-3.851062	0.723768	0.863031
5	6	0	-2.566452	1.239006	0.820820
6	6	0	-1.572229	0.646984	0.028482
7	1	0	-1.172954	-0.968648	-1.335958
8	1	0	-3.420985	-1.914909	-1.243215
9	1	0	-4.616667	1.185100	1.477010
10	1	0	-2.324767	2.108993	1.422889
11	6	0	-0.204863	1.217042	-0.036439
12	6	0	-0.021124	2.562296	-0.122379
13	6	0	0.944490	0.332718	-0.010828
14	1	0	-0.858746	3.253001	-0.166096
15	1	0	0.752682	-0.741150	0.070494
16	8	0	1.163089	3.159703	-0.176898
17	1	0	1.857495	2.435219	-0.159657
18	7	0	2.148248	0.786697	-0.079962
19	6	0	3.246219	-0.095320	0.013604
20	6	0	3.249734	-1.210359	0.858712
21	6	0	4.385287	0.200175	-0.741064
22	6	0	4.369193	-2.034389	0.915071
23	1	0	2.390025	-1.417017	1.486873
24	6	0	5.496919	-0.631167	-0.683906
25	1	0	4.380821	1.079283	-1.376394
26	6	0	5.492988	-1.753638	0.142098
27	1	0	4.365958	-2.893906	1.576346
28	1	0	6.371296	-0.398285	-1.281487
29	1	0	6.363763	-2.397340	0.191685
30	8	0	-5.459312	-0.856086	0.230626
31	6	0	-5.833914	-1.992928	-0.537670
32	1	0	-5.257632	-2.873905	-0.241668
33	1	0	-6.888165	-2.163189	-0.327537
34	1	0	-5.700822	-1.802934	-1.606362

Structure 27a (vacuum)

Energy (Hartrees): -938.302373751
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.479855	0.925267	0.621016
2	6	0	-4.694460	0.245758	0.698027
3	6	0	-4.859103	-0.948454	0.000721
4	6	0	-3.808809	-1.440474	-0.777697
5	6	0	-2.617883	-0.742569	-0.859067
6	6	0	-2.420450	0.453180	-0.152464
7	1	0	-3.355178	1.834346	1.199555
8	1	0	-5.486792	0.649780	1.313438
9	1	0	-3.961997	-2.363107	-1.324093
10	1	0	-1.828000	-1.116807	-1.501869
11	6	0	-1.139309	1.191297	-0.222500
12	6	0	0.055564	0.521696	-0.131793
13	6	0	-1.151006	2.630522	-0.383894
14	1	0	0.048536	-0.553933	0.020559
15	1	0	-2.149011	3.088965	-0.502247
16	8	0	-0.155543	3.345416	-0.409396
17	7	0	1.271714	1.090372	-0.183389
18	1	0	1.272970	2.106836	-0.247746
19	6	0	2.498616	0.403704	-0.109123
20	6	0	3.614556	1.069832	0.384704
21	6	0	2.635900	-0.919965	-0.539413
22	6	0	4.850724	0.435298	0.465453
23	1	0	3.515845	2.096027	0.720585
24	6	0	3.857226	-1.561299	-0.443527
25	1	0	1.794673	-1.444305	-0.976119
26	6	0	4.974697	-0.891599	0.059112
27	1	0	5.696792	0.985120	0.854450
28	1	0	3.977053	-2.584645	-0.776746
29	8	0	-5.993109	-1.697666	0.011341
30	6	0	-7.084513	-1.223790	0.770629
31	1	0	-7.880593	-1.953838	0.642446
32	1	0	-6.826793	-1.150400	1.832114
33	1	0	-7.424098	-0.247722	0.409532
34	8	0	6.128291	-1.607800	0.102830
35	6	0	7.283325	-0.960059	0.592284
36	1	0	7.148800	-0.643751	1.631671
37	1	0	8.085533	-1.692494	0.538214
38	1	0	7.541845	-0.092345	-0.023037

Structure 27a ($CHCl_3$)

Energy (Hartrees): -938.327778814
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.478975	0.928495	0.611219
2	6	0	-4.690069	0.242906	0.697481
3	6	0	-4.854481	-0.951627	-0.001088
4	6	0	-3.808204	-1.434924	-0.792038
5	6	0	-2.619266	-0.731689	-0.881418
6	6	0	-2.421973	0.463316	-0.172434
7	1	0	-3.356576	1.837977	1.190111
8	1	0	-5.479220	0.641336	1.321308
9	1	0	-3.955179	-2.358874	-1.339748
10	1	0	-1.830819	-1.107466	-1.525531
11	6	0	-1.140697	1.205977	-0.239756
12	6	0	0.058021	0.530160	-0.173460
13	6	0	-1.160861	2.641606	-0.367695
14	1	0	0.050102	-0.549648	-0.054354
15	1	0	-2.159369	3.100016	-0.470439
16	8	0	-0.165634	3.367257	-0.385440
17	7	0	1.271676	1.095780	-0.211566
18	1	0	1.288482	2.113223	-0.240227
19	6	0	2.500128	0.405285	-0.136067
20	6	0	3.600422	1.055894	0.412283
21	6	0	2.648088	-0.900915	-0.612568
22	6	0	4.835269	0.419638	0.504239
23	1	0	3.491121	2.070252	0.780852
24	6	0	3.869306	-1.543691	-0.508338
25	1	0	1.818686	-1.411781	-1.087552
26	6	0	4.971639	-0.891973	0.051310
27	1	0	5.669433	0.953675	0.939315
28	1	0	3.994129	-2.555146	-0.876725
29	8	0	-5.983602	-1.706966	0.022543
30	6	0	-7.057282	-1.262815	0.835039
31	1	0	-7.844651	-2.006590	0.726634
32	1	0	-6.758560	-1.203314	1.886009
33	1	0	-7.430363	-0.289991	0.501291
34	8	0	6.125052	-1.606241	0.102676
35	6	0	7.264209	-0.979583	0.669527
36	1	0	7.087236	-0.713684	1.716107
37	1	0	8.067608	-1.711842	0.614979
38	1	0	7.548035	-0.087362	0.103289

Structure 27a (DMSO)

Energy (Hartrees): -938.326416165
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.492059	0.943252	0.585683
2	6	0	-4.702972	0.256456	0.671282
3	6	0	-4.856368	-0.954371	-0.002837
4	6	0	-3.795827	-1.453549	-0.765884
5	6	0	-2.606311	-0.750110	-0.854495
6	6	0	-2.422284	0.462906	-0.172062
7	1	0	-3.382714	1.866742	1.144861
8	1	0	-5.500716	0.668253	1.275468
9	1	0	-3.927955	-2.391274	-1.293939
10	1	0	-1.806225	-1.143574	-1.473322
11	6	0	-1.140994	1.205577	-0.237136
12	6	0	0.056550	0.525076	-0.178299
13	6	0	-1.162826	2.641759	-0.356400
14	1	0	0.044478	-0.556005	-0.073033
15	1	0	-2.162020	3.098142	-0.460225
16	8	0	-0.169532	3.370619	-0.366798
17	7	0	1.271023	1.087515	-0.213028
18	1	0	1.296401	2.104839	-0.230442
19	6	0	2.499402	0.396440	-0.140631
20	6	0	3.604623	1.061267	0.380922
21	6	0	2.643861	-0.919243	-0.591944
22	6	0	4.841966	0.429965	0.474295
23	1	0	3.496727	2.084111	0.726460
24	6	0	3.868973	-1.556154	-0.487276
25	1	0	1.810792	-1.444857	-1.044014
26	6	0	4.976751	-0.891180	0.047148
27	1	0	5.679263	0.976216	0.887934
28	1	0	3.988494	-2.575346	-0.836349
29	8	0	-5.984541	-1.708346	0.021681
30	6	0	-7.061481	-1.251067	0.826633
31	1	0	-7.849113	-1.995896	0.728753
32	1	0	-6.763508	-1.174762	1.876501
33	1	0	-7.433579	-0.282940	0.479063
34	8	0	6.132152	-1.599358	0.102169
35	6	0	7.264386	-0.962854	0.677625
36	1	0	7.071355	-0.685449	1.718076
37	1	0	8.070355	-1.693369	0.642224
38	1	0	7.553808	-0.075766	0.107033

Structure 27a (C_2H_5OH)

Energy (Hartrees): -938.329178386
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.491428	0.941390	0.594627
2	6	0	-4.699489	0.249378	0.676416
3	6	0	-4.845048	-0.957238	-0.004559
4	6	0	-3.785126	-1.449698	-0.770808
5	6	0	-2.598573	-0.740635	-0.855885
6	6	0	-2.420887	0.468867	-0.166558
7	1	0	-3.384939	1.862385	1.158486
8	1	0	-5.499659	0.653357	1.282687
9	1	0	-3.915212	-2.385266	-1.303654
10	1	0	-1.797095	-1.126070	-1.478082
11	6	0	-1.142557	1.217773	-0.231413
12	6	0	0.058533	0.538777	-0.161901
13	6	0	-1.169665	2.645327	-0.366162
14	1	0	0.045954	-0.541387	-0.047165
15	1	0	-2.167416	3.101067	-0.473632
16	8	0	-0.173495	3.380896	-0.386552
17	7	0	1.270470	1.099402	-0.196402
18	1	0	1.299479	2.116597	-0.220326
19	6	0	2.498140	0.403695	-0.128111
20	6	0	3.603324	1.058514	0.405245
21	6	0	2.637631	-0.904885	-0.599428
22	6	0	4.838230	0.421751	0.491449
23	1	0	3.498093	2.076480	0.765602
24	6	0	3.860161	-1.547567	-0.502066
25	1	0	1.803579	-1.418902	-1.063093
26	6	0	4.966837	-0.892289	0.044026
27	1	0	5.677188	0.957757	0.914999
28	1	0	3.978801	-2.561628	-0.866531
29	8	0	-5.974467	-1.719316	0.015902
30	6	0	-7.057898	-1.271907	0.820969
31	1	0	-7.839080	-2.022774	0.716920
32	1	0	-6.760721	-1.199086	1.870933
33	1	0	-7.433433	-0.305451	0.473559
34	8	0	6.124171	-1.607373	0.088589
35	6	0	7.264183	-0.982700	0.666128
36	1	0	7.076768	-0.720019	1.711060
37	1	0	8.065435	-1.717578	0.614603
38	1	0	7.551096	-0.090274	0.103134

Structure 27b (vacuum)

Energy (Hartrees): -938.297520617
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.258885	0.996789	0.984219
2	6	0	4.309898	0.100866	1.053363
3	6	0	4.395438	-0.952882	0.139623
4	6	0	3.418885	-1.090345	-0.845382
5	6	0	2.371650	-0.171958	-0.907003
6	6	0	2.263655	0.880469	0.001887
7	1	0	3.194982	1.799570	1.711192
8	1	0	5.078390	0.189705	1.811520
9	1	0	3.466547	-1.886857	-1.575594
10	1	0	1.634272	-0.267181	-1.698148
11	6	0	1.153830	1.857815	-0.065313
12	6	0	-0.157794	1.504505	-0.057526
13	6	0	1.453280	3.293077	-0.108531
14	1	0	-0.894186	2.300291	-0.106204
15	1	0	2.534649	3.534226	-0.126831
16	8	0	0.631126	4.183676	-0.133713
17	8	0	5.457788	-1.784785	0.288607
18	6	0	5.591229	-2.850618	-0.628230
19	1	0	5.702009	-2.478968	-1.651799
20	1	0	6.491823	-3.387223	-0.338938
21	1	0	4.732480	-3.527577	-0.576691
22	7	0	-0.637117	0.243447	0.045004
23	1	0	0.038906	-0.490572	0.213246
24	6	0	-1.993890	-0.128099	0.064080
25	6	0	-2.346974	-1.355860	0.635804
26	6	0	-2.993284	0.672446	-0.476341
27	6	0	-3.666148	-1.762021	0.674115
28	1	0	-1.576618	-1.989103	1.062958
29	6	0	-4.328786	0.274973	-0.421391
30	1	0	-2.747392	1.608030	-0.962341
31	6	0	-4.672579	-0.944217	0.154416
32	1	0	-3.947292	-2.709597	1.116551
33	1	0	-5.080365	0.925963	-0.846676
34	8	0	-5.940417	-1.424708	0.251698
35	6	0	-6.983613	-0.627251	-0.266883
36	1	0	-6.861185	-0.466304	-1.342859
37	1	0	-7.903762	-1.178149	-0.086111
38	1	0	-7.033507	0.340012	0.243526

Structure 27b ($CHCl_3$)

Energy (Hartrees): -938.324955991
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.271307	1.015065	0.973481
2	6	0	4.329968	0.126853	1.049094
3	6	0	4.411380	-0.946755	0.157278
4	6	0	3.422244	-1.112909	-0.812022
5	6	0	2.367284	-0.203798	-0.879490
6	6	0	2.264387	0.869791	0.006503
7	1	0	3.214186	1.835276	1.681971
8	1	0	5.105078	0.242393	1.798024
9	1	0	3.464257	-1.927121	-1.523427
10	1	0	1.620649	-0.327395	-1.658203
11	6	0	1.153222	1.847103	-0.073668
12	6	0	-0.166260	1.497066	-0.076594
13	6	0	1.462041	3.269894	-0.119743
14	1	0	-0.899639	2.294408	-0.137431
15	1	0	2.542955	3.504710	-0.138324
16	8	0	0.649584	4.180619	-0.149385
17	8	0	5.479962	-1.769289	0.309631
18	6	0	5.635840	-2.829476	-0.619869
19	1	0	5.738016	-2.445773	-1.639286
20	1	0	6.549774	-3.347076	-0.335110
21	1	0	4.795167	-3.527863	-0.570038
22	7	0	-0.652109	0.246251	0.022059
23	1	0	0.012380	-0.502173	0.184487
24	6	0	-2.011882	-0.123146	0.040152
25	6	0	-2.348691	-1.377990	0.560876
26	6	0	-3.022758	0.698607	-0.447029
27	6	0	-3.666933	-1.789832	0.607008
28	1	0	-1.565675	-2.026982	0.939460
29	6	0	-4.356050	0.292840	-0.386643
30	1	0	-2.794189	1.657951	-0.894840
31	6	0	-4.685431	-0.952026	0.143252
32	1	0	-3.931708	-2.759610	1.011869
33	1	0	-5.117905	0.958196	-0.770664
34	8	0	-5.950742	-1.437053	0.243218
35	6	0	-7.010796	-0.603312	-0.194180
36	1	0	-6.928007	-0.385877	-1.263369
37	1	0	-7.927424	-1.160841	-0.010731
38	1	0	-7.036809	0.331958	0.373054

Structure 27b (DMSO)

Energy (Hartrees): -938.324354927
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.264809	1.008918	0.978998
2	6	0	4.318923	0.114603	1.058058
3	6	0	4.402371	-0.956071	0.161828
4	6	0	3.418789	-1.112672	-0.815623
5	6	0	2.367671	-0.199225	-0.884803
6	6	0	2.263277	0.871231	0.005223
7	1	0	3.208979	1.827247	1.690058
8	1	0	5.088375	0.226647	1.813647
9	1	0	3.460010	-1.924405	-1.530056
10	1	0	1.622489	-0.321688	-1.665159
11	6	0	1.156011	1.853270	-0.077940
12	6	0	-0.166173	1.506512	-0.089315
13	6	0	1.476998	3.272052	-0.114429
14	1	0	-0.899928	2.303321	-0.155996
15	1	0	2.560899	3.494251	-0.120947
16	8	0	0.677144	4.194841	-0.146913
17	8	0	5.463777	-1.784793	0.317083
18	6	0	5.616046	-2.841285	-0.620777
19	1	0	5.727831	-2.450871	-1.636415
20	1	0	6.523163	-3.369718	-0.333957
21	1	0	4.768119	-3.531008	-0.582412
22	7	0	-0.652106	0.257270	0.007169
23	1	0	0.009604	-0.495563	0.166239
24	6	0	-2.011456	-0.113387	0.031772
25	6	0	-2.339420	-1.373227	0.546948
26	6	0	-3.029189	0.708438	-0.441861
27	6	0	-3.656395	-1.789658	0.601188
28	1	0	-1.550203	-2.022552	0.912003
29	6	0	-4.360798	0.296756	-0.375120
30	1	0	-2.808992	1.673231	-0.882463
31	6	0	-4.682295	-0.953628	0.148848
32	1	0	-3.910566	-2.764344	1.001527
33	1	0	-5.127553	0.961995	-0.749838
34	8	0	-5.944340	-1.442790	0.252576
35	6	0	-7.006225	-0.610622	-0.190300
36	1	0	-6.914587	-0.386895	-1.257120
37	1	0	-7.922155	-1.172679	-0.017836
38	1	0	-7.041048	0.322027	0.380390

Structure 27b (C_2H_5OH)

Energy (Hartrees): -938.327682027
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.252893	1.000407	0.994194
2	6	0	4.309203	0.108319	1.071116
3	6	0	4.401508	-0.949204	0.161868
4	6	0	3.428649	-1.098691	-0.825882
5	6	0	2.376183	-0.186835	-0.893651
6	6	0	2.262122	0.871954	0.008977
7	1	0	3.187386	1.809357	1.715115
8	1	0	5.072402	0.211900	1.834529
9	1	0	3.479477	-1.901600	-1.549684
10	1	0	1.639116	-0.300384	-1.682978
11	6	0	1.152523	1.852640	-0.072564
12	6	0	-0.171724	1.499182	-0.084024
13	6	0	1.465952	3.263503	-0.104821
14	1	0	-0.911078	2.291201	-0.146167
15	1	0	2.545407	3.496849	-0.109173
16	8	0	0.657407	4.189723	-0.136308
17	8	0	5.468898	-1.779160	0.315835
18	6	0	5.636894	-2.823139	-0.635684
19	1	0	5.754539	-2.416058	-1.643658
20	1	0	6.545499	-3.347951	-0.346955
21	1	0	4.792920	-3.517839	-0.611055
22	7	0	-0.649615	0.251004	0.007805
23	1	0	0.015696	-0.500394	0.161362
24	6	0	-2.010223	-0.123415	0.027097
25	6	0	-2.341585	-1.367659	0.574320
26	6	0	-3.020239	0.685177	-0.483078
27	6	0	-3.659832	-1.780600	0.628921
28	1	0	-1.556567	-2.006393	0.965932
29	6	0	-4.352733	0.278661	-0.414963
30	1	0	-2.792107	1.634017	-0.953633
31	6	0	-4.677733	-0.954205	0.145024
32	1	0	-3.920954	-2.742193	1.056049
33	1	0	-5.116028	0.932263	-0.816172
34	8	0	-5.946278	-1.437734	0.255631
35	6	0	-7.009634	-0.603263	-0.185950
36	1	0	-6.931974	-0.401805	-1.257959
37	1	0	-7.925995	-1.155886	0.013003
38	1	0	-7.023994	0.338272	0.370148

Structure 27c (vacuum)

Energy (Hartrees): -938.298623435
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.238699	0.976675	0.922682
2	6	0	-4.259080	0.048750	0.998162
3	6	0	-4.284263	-1.045037	0.127678
4	6	0	-3.275161	-1.194694	-0.820789
5	6	0	-2.250729	-0.250000	-0.884079
6	6	0	-2.205626	0.839224	-0.016268
7	1	0	-3.239239	1.831885	1.586831
8	1	0	-5.060359	0.150528	1.719701
9	1	0	-3.277589	-2.019669	-1.520104
10	1	0	-1.485670	-0.356346	-1.647128
11	6	0	-1.115005	1.836550	-0.086059
12	6	0	0.202436	1.505419	-0.073610
13	6	0	-1.410885	3.267793	-0.105608
14	1	0	0.944818	2.296197	-0.131487
15	8	0	-5.328556	-1.900013	0.277814
16	6	0	-5.424211	-2.984081	-0.621319
17	1	0	-4.559555	-3.650114	-0.534555
18	1	0	-6.325808	-3.526652	-0.346345
19	1	0	-5.511091	-2.632866	-1.654468
20	7	0	0.708470	0.253615	0.051177
21	1	0	0.049406	-0.485881	0.258509
22	6	0	2.076154	-0.075296	0.074415
23	6	0	2.490057	-1.218366	0.768261
24	6	0	3.029984	0.692679	-0.582865
25	6	0	3.824532	-1.570334	0.811300
26	1	0	1.755192	-1.823975	1.287561
27	6	0	4.381477	0.353651	-0.523324
28	1	0	2.731833	1.553104	-1.169328
29	6	0	4.785483	-0.780756	0.173885
30	1	0	4.152908	-2.451574	1.348312
31	1	0	5.097005	0.975980	-1.042865
32	8	0	-2.512180	3.763040	-0.040297
33	1	0	-0.511774	3.915422	-0.182975
34	8	0	6.072620	-1.202080	0.286267
35	6	0	7.072339	-0.424087	-0.336875
36	1	0	8.017195	-0.918013	-0.122364
37	1	0	6.922801	-0.381861	-1.420529
38	1	0	7.092757	0.592423	0.069203

Structure 27c ($CHCl_3$)

Energy (Hartrees): -938.327310149
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.218069	0.942224	0.974210
2	6	0	-4.249107	0.022680	1.038067
3	6	0	-4.297137	-1.044792	0.135231
4	6	0	-3.297152	-1.180480	-0.826575
5	6	0	-2.263605	-0.244900	-0.876465
6	6	0	-2.200913	0.824757	0.015623
7	1	0	-3.197459	1.771178	1.672336
8	1	0	-5.036432	0.115129	1.777395
9	1	0	-3.313707	-1.989337	-1.545191
10	1	0	-1.503806	-0.345499	-1.645799
11	6	0	-1.113125	1.828054	-0.054689
12	6	0	0.213067	1.505466	-0.027815
13	6	0	-1.412303	3.245544	-0.128676
14	1	0	0.945492	2.304339	-0.098251
15	8	0	-5.348956	-1.892370	0.268446
16	6	0	-5.486655	-2.926993	-0.691747
17	1	0	-4.638332	-3.617014	-0.657277
18	1	0	-6.395812	-3.464170	-0.428723
19	1	0	-5.587123	-2.515325	-1.700469
20	7	0	0.722973	0.266612	0.114576
21	1	0	0.074921	-0.488765	0.307624
22	6	0	2.093903	-0.062175	0.116005
23	6	0	2.507752	-1.219845	0.784577
24	6	0	3.042327	0.715714	-0.538650
25	6	0	3.842598	-1.577834	0.805978
26	1	0	1.773324	-1.834127	1.294894
27	6	0	4.392527	0.368060	-0.504145
28	1	0	2.743596	1.593173	-1.099439
29	6	0	4.799053	-0.781313	0.168833
30	1	0	4.168070	-2.472815	1.323197
31	1	0	5.105195	0.995626	-1.022121
32	8	0	-2.525499	3.741179	-0.141273
33	1	0	-0.519403	3.899710	-0.180951
34	8	0	6.086171	-1.207911	0.253637
35	6	0	7.077620	-0.441982	-0.410243
36	1	0	8.022889	-0.950236	-0.229511
37	1	0	6.889026	-0.401973	-1.487381
38	1	0	7.130334	0.573517	-0.005961

Structure 27c (DMSO)

Energy (Hartrees): -938.327860739
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.178053	0.926584	1.007228
2	6	0	-4.198989	-0.003029	1.095588
3	6	0	-4.280655	-1.050492	0.170410
4	6	0	-3.326343	-1.150939	-0.841406
5	6	0	-2.303637	-0.204331	-0.915968
6	6	0	-2.205864	0.843035	-0.000709
7	1	0	-3.127181	1.732332	1.731010
8	1	0	-4.947603	0.064400	1.876995
9	1	0	-3.365990	-1.944647	-1.575899
10	1	0	-1.575728	-0.285793	-1.717749
11	6	0	-1.120959	1.849093	-0.082026
12	6	0	0.208329	1.527949	-0.086110
13	6	0	-1.419266	3.265692	-0.127892
14	1	0	0.934219	2.332863	-0.146418
15	8	0	-5.313347	-1.913074	0.334000
16	6	0	-5.458510	-2.952207	-0.624029
17	1	0	-4.593035	-3.620820	-0.617209
18	1	0	-6.346372	-3.509890	-0.332281
19	1	0	-5.600471	-2.542964	-1.628423
20	7	0	0.719584	0.287856	0.006771
21	1	0	0.073182	-0.479970	0.156784
22	6	0	2.088041	-0.048917	0.032177
23	6	0	2.449612	-1.299867	0.546241
24	6	0	3.083897	0.800142	-0.440094
25	6	0	3.777484	-1.680883	0.599854
26	1	0	1.678348	-1.970744	0.910682
27	6	0	4.426035	0.424699	-0.373305
28	1	0	2.839021	1.758948	-0.880621
29	6	0	4.780906	-0.817382	0.148580
30	1	0	4.057796	-2.649178	0.998230
31	1	0	5.174166	1.111126	-0.747528
32	8	0	-2.532829	3.766100	-0.127192
33	1	0	-0.525622	3.917838	-0.173095
34	8	0	6.055997	-1.272450	0.250751
35	6	0	7.092960	-0.417906	-0.208475
36	1	0	8.023976	-0.957727	-0.046076
37	1	0	6.982021	-0.200517	-1.274773
38	1	0	7.113695	0.517695	0.358115

Structure 27c (C_2H_5OH)

Energy (Hartrees): -938.331708004
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.175704	0.907698	1.018256
2	6	0	-4.204331	-0.015528	1.087394
3	6	0	-4.287487	-1.045640	0.144947
4	6	0	-3.329400	-1.141616	-0.862601
5	6	0	-2.300037	-0.201789	-0.918342
6	6	0	-2.201567	0.831936	0.012369
7	1	0	-3.121889	1.702101	1.755063
8	1	0	-4.957730	0.044938	1.865018
9	1	0	-3.372836	-1.923523	-1.609581
10	1	0	-1.569241	-0.275134	-1.718201
11	6	0	-1.114290	1.837290	-0.058076
12	6	0	0.217508	1.512764	-0.045759
13	6	0	-1.408105	3.244379	-0.114446
14	1	0	0.949213	2.312879	-0.109768
15	8	0	-5.333870	-1.903591	0.287644
16	6	0	-5.488522	-2.922937	-0.692487
17	1	0	-4.629798	-3.599704	-0.694540
18	1	0	-6.383253	-3.475654	-0.412691
19	1	0	-5.623433	-2.489891	-1.687417
20	7	0	0.720749	0.275875	0.071167
21	1	0	0.072891	-0.488190	0.236098
22	6	0	2.093235	-0.056222	0.088191
23	6	0	2.486934	-1.227992	0.742396
24	6	0	3.054419	0.731754	-0.534937
25	6	0	3.820528	-1.591214	0.783226
26	1	0	1.739141	-1.849261	1.224279
27	6	0	4.402141	0.377368	-0.482530
28	1	0	2.769886	1.621780	-1.083592
29	6	0	4.789442	-0.786234	0.177318
30	1	0	4.131251	-2.497563	1.290381
31	1	0	5.127382	1.011123	-0.975275
32	8	0	-2.531343	3.743705	-0.125631
33	1	0	-0.522916	3.904375	-0.155773
34	8	0	6.077261	-1.219106	0.276680
35	6	0	7.079213	-0.461795	-0.390144
36	1	0	8.018156	-0.981856	-0.209971
37	1	0	6.885879	-0.420851	-1.465764
38	1	0	7.141799	0.551907	0.015361

Structure 27d (vacuum)

Energy (Hartrees): -938.288802913
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.436671	0.874923	0.611351
2	6	0	-4.581176	0.084625	0.687157
3	6	0	-4.631453	-1.129650	0.005842
4	6	0	-3.534881	-1.536631	-0.756041
5	6	0	-2.409144	-0.735924	-0.828917
6	6	0	-2.327764	0.478461	-0.134255
7	1	0	-3.413434	1.818588	1.140604
8	1	0	-5.418457	0.429699	1.278430
9	1	0	-3.599622	-2.472362	-1.297595
10	1	0	-1.581857	-1.047174	-1.458605
11	6	0	-1.097443	1.304341	-0.194873
12	6	0	0.118539	0.696697	-0.095243
13	6	0	-1.194794	2.751718	-0.370916
14	1	0	0.138330	-0.378662	0.052448
15	7	0	1.357101	1.260156	-0.118554
16	1	0	1.438796	2.264211	-0.100223
17	6	0	2.568427	0.541049	-0.078940
18	6	0	3.700282	1.143550	0.458768
19	6	0	2.672024	-0.758049	-0.587361
20	6	0	4.919304	0.472738	0.502888
21	1	0	3.631465	2.148636	0.861039
22	6	0	3.874714	-1.437740	-0.523199
23	1	0	1.819253	-1.232430	-1.057222
24	6	0	5.008767	-0.830903	0.020164
25	1	0	5.777913	0.974400	0.927646
26	1	0	3.966889	-2.443435	-0.914171
27	8	0	-5.698265	-1.972923	0.013621
28	6	0	-6.841561	-1.573956	0.738880
29	1	0	-7.575721	-2.365561	0.606287
30	1	0	-6.616157	-1.462132	1.804319
31	1	0	-7.246784	-0.633392	0.352351
32	1	0	-0.230282	3.286082	-0.500339
33	8	0	-2.218507	3.396157	-0.399236
34	8	0	6.141344	-1.580680	0.024865
35	6	0	7.314689	-0.991639	0.544413
36	1	0	7.191322	-0.728827	1.599944
37	1	0	8.096573	-1.741366	0.447660
38	1	0	7.594345	-0.099445	-0.025004

Structure 27d ($CHCl_3$)

Energy (Hartrees): -938.318523165
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.426619	0.859058	0.641914
2	6	0	-4.570702	0.066053	0.712435
3	6	0	-4.629309	-1.127935	-0.005194
4	6	0	-3.541551	-1.510579	-0.793734
5	6	0	-2.416286	-0.705974	-0.860176
6	6	0	-2.326931	0.489815	-0.133784
7	1	0	-3.394856	1.781717	1.208446
8	1	0	-5.399340	0.388789	1.329052
9	1	0	-3.604965	-2.433077	-1.359338
10	1	0	-1.592940	-1.004691	-1.501294
11	6	0	-1.097952	1.322148	-0.184566
12	6	0	0.123353	0.706776	-0.096084
13	6	0	-1.197110	2.759070	-0.364979
14	1	0	0.135836	-0.372932	0.019428
15	7	0	1.354719	1.262406	-0.100539
16	1	0	1.448266	2.267843	-0.055373
17	6	0	2.565799	0.536915	-0.073717
18	6	0	3.695285	1.134321	0.476342
19	6	0	2.669250	-0.753396	-0.603642
20	6	0	4.914540	0.463573	0.515595
21	1	0	3.622820	2.135994	0.887057
22	6	0	3.874416	-1.432307	-0.547423
23	1	0	1.818245	-1.224630	-1.081020
24	6	0	5.006101	-0.833017	0.011414
25	1	0	5.771446	0.958884	0.952154
26	1	0	3.963555	-2.432259	-0.955728
27	8	0	-5.694844	-1.971644	-0.004115
28	6	0	-6.823026	-1.605069	0.772163
29	1	0	-7.556939	-2.396299	0.630800
30	1	0	-6.566748	-1.535988	1.833716
31	1	0	-7.245259	-0.654838	0.431795
32	1	0	-0.238989	3.302607	-0.466018
33	8	0	-2.232542	3.398675	-0.435101
34	8	0	6.140410	-1.579938	0.010274
35	6	0	7.311473	-1.000183	0.561261
36	1	0	7.171697	-0.759624	1.619506
37	1	0	8.093488	-1.750851	0.463283
38	1	0	7.603067	-0.099850	0.011881

Structure 27d (DMSO)

Energy (Hartrees): -938.319521200
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.424062	0.854883	0.648542
2	6	0	-4.571447	0.065201	0.715043
3	6	0	-4.633794	-1.125344	-0.010005
4	6	0	-3.544339	-1.506365	-0.798284
5	6	0	-2.415477	-0.705293	-0.859633
6	6	0	-2.324218	0.488722	-0.129494
7	1	0	-3.389519	1.772555	1.223410
8	1	0	-5.398103	0.386174	1.335635
9	1	0	-3.604766	-2.427061	-1.367636
10	1	0	-1.589787	-1.008647	-1.495686
11	6	0	-1.096360	1.322675	-0.177940
12	6	0	0.126225	0.703183	-0.099828
13	6	0	-1.198292	2.758456	-0.354021
14	1	0	0.135733	-0.378335	-0.000752
15	7	0	1.354904	1.256229	-0.102261
16	1	0	1.454004	2.262166	-0.047258
17	6	0	2.565223	0.529931	-0.077026
18	6	0	3.699012	1.139643	0.451581
19	6	0	2.665405	-0.769342	-0.585636
20	6	0	4.919451	0.470877	0.494513
21	1	0	3.628188	2.150379	0.840069
22	6	0	3.873388	-1.444579	-0.528059
23	1	0	1.811403	-1.252508	-1.045791
24	6	0	5.009488	-0.834656	0.011244
25	1	0	5.778749	0.976662	0.914536
26	1	0	3.956743	-2.451408	-0.920939
27	8	0	-5.701385	-1.963462	-0.014585
28	6	0	-6.824905	-1.597863	0.772951
29	1	0	-7.562076	-2.386094	0.632247
30	1	0	-6.560704	-1.534604	1.832571
31	1	0	-7.246554	-0.644359	0.441702
32	1	0	-0.242829	3.306471	-0.439913
33	8	0	-2.238359	3.392939	-0.439067
34	8	0	6.145082	-1.577825	0.014014
35	6	0	7.313353	-0.986557	0.563942
36	1	0	7.168459	-0.736574	1.619060
37	1	0	8.099865	-1.733743	0.475433
38	1	0	7.602269	-0.089339	0.008909

Structure 27d (C_2H_5OH)

Energy (Hartrees): -938.323037423
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.412514	0.838985	0.683348
2	6	0	-4.558299	0.046747	0.742517
3	6	0	-4.622532	-1.125523	-0.009359
4	6	0	-3.541207	-1.489959	-0.814675
5	6	0	-2.414930	-0.684905	-0.869965
6	6	0	-2.321623	0.493315	-0.115823
7	1	0	-3.372310	1.740231	1.284501
8	1	0	-5.379953	0.351449	1.377668
9	1	0	-3.606201	-2.399657	-1.401335
10	1	0	-1.593847	-0.971997	-1.519309
11	6	0	-1.097032	1.333943	-0.163827
12	6	0	0.129628	0.717295	-0.072005
13	6	0	-1.200732	2.756988	-0.368130
14	1	0	0.138405	-0.363301	0.037944
15	7	0	1.354683	1.269056	-0.074113
16	1	0	1.455377	2.275941	-0.035800
17	6	0	2.564861	0.538401	-0.058594
18	6	0	3.698478	1.134085	0.484879
19	6	0	2.659314	-0.749154	-0.595499
20	6	0	4.916292	0.460140	0.515135
21	1	0	3.630407	2.136301	0.895176
22	6	0	3.864301	-1.430365	-0.550493
23	1	0	1.803752	-1.217085	-1.068530
24	6	0	4.999334	-0.834028	0.003835
25	1	0	5.777638	0.952392	0.946710
26	1	0	3.947143	-2.428779	-0.964911
27	8	0	-5.693036	-1.968290	-0.024509
28	6	0	-6.823100	-1.612346	0.761847
29	1	0	-7.559923	-2.397036	0.600995
30	1	0	-6.564372	-1.569276	1.823424
31	1	0	-7.237058	-0.652498	0.440721
32	1	0	-0.252507	3.315672	-0.438798
33	8	0	-2.248596	3.385608	-0.496198
34	8	0	6.136161	-1.583844	-0.008388
35	6	0	7.311747	-1.007713	0.547071
36	1	0	7.169415	-0.774052	1.605841
37	1	0	8.091582	-1.759973	0.443564
38	1	0	7.601535	-0.104943	0.002126

Structure 27g (vacuum)

Energy (Hartrees): -938.294907935
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.634063	-0.512780	-0.728895
2	6	0	-3.840877	-1.209254	-0.694777
3	6	0	-4.882677	-0.738329	0.100905
4	6	0	-4.698154	0.416894	0.864012
5	6	0	-3.488286	1.085927	0.831752
6	6	0	-2.431805	0.641981	0.023951
7	1	0	-1.843835	-0.871892	-1.379950
8	1	0	-3.954546	-2.099222	-1.298833
9	1	0	-5.515103	0.756998	1.488601
10	1	0	-3.347488	1.960072	1.458172
11	6	0	-1.146566	1.375794	-0.035201
12	6	0	-1.123422	2.733377	-0.136462
13	6	0	0.102284	0.642349	0.007859
14	1	0	-2.044018	3.308559	-0.185909
15	1	0	0.039503	-0.444830	0.128591
16	8	0	-0.032086	3.471755	-0.197992
17	1	0	0.744794	2.843477	-0.175039
18	7	0	1.244878	1.227967	-0.084408
19	6	0	2.433270	0.478565	0.040894
20	6	0	2.566212	-0.590486	0.936888
21	6	0	3.532464	0.843537	-0.730282
22	6	0	3.755338	-1.290757	1.025121
23	1	0	1.742183	-0.850691	1.591352
24	6	0	4.730377	0.139098	-0.655469
25	1	0	3.437117	1.683263	-1.408537
26	6	0	4.843617	-0.937089	0.223703
27	1	0	3.874927	-2.109307	1.724114
28	1	0	5.560209	0.442286	-1.279358
29	8	0	-6.100592	-1.331988	0.204763
30	6	0	-6.325478	-2.502995	-0.550721
31	1	0	-5.632667	-3.299765	-0.261388
32	1	0	-7.344730	-2.812871	-0.331040
33	1	0	-6.228243	-2.306955	-1.623351
34	8	0	5.966537	-1.685587	0.382183
35	6	0	7.096422	-1.344818	-0.392525
36	1	0	7.876243	-2.050851	-0.116203
37	1	0	6.885034	-1.436969	-1.462679
38	1	0	7.433664	-0.326591	-0.173836

Structure 27g ($CHCl_3$)

Energy (Hartrees): -938.318215649
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.642373	-0.530467	-0.709783
2	6	0	-3.855599	-1.216630	-0.674471
3	6	0	-4.902036	-0.721380	0.101628
4	6	0	-4.716279	0.449105	0.842654
5	6	0	-3.500486	1.109467	0.808811
6	6	0	-2.439159	0.639955	0.021071
7	1	0	-1.846851	-0.913795	-1.340678
8	1	0	-3.970561	-2.120155	-1.258651
9	1	0	-5.534251	0.812919	1.453808
10	1	0	-3.363673	1.998376	1.415486
11	6	0	-1.145892	1.362654	-0.037177
12	6	0	-1.111926	2.720733	-0.125175
13	6	0	0.097880	0.617129	-0.000660
14	1	0	-2.023908	3.310314	-0.165199
15	1	0	0.032365	-0.468926	0.118242
16	8	0	-0.006242	3.445292	-0.182401
17	1	0	0.762750	2.800041	-0.170065
18	7	0	1.241505	1.202369	-0.093419
19	6	0	2.434623	0.459022	0.032431
20	6	0	2.564906	-0.624729	0.911352
21	6	0	3.540042	0.848393	-0.719646
22	6	0	3.761722	-1.313061	1.003474
23	1	0	1.733497	-0.909642	1.546389
24	6	0	4.745460	0.156189	-0.640935
25	1	0	3.447388	1.698475	-1.386479
26	6	0	4.857921	-0.933544	0.222660
27	1	0	3.875454	-2.142967	1.691218
28	1	0	5.580910	0.477555	-1.248605
29	8	0	-6.123358	-1.305978	0.204171
30	6	0	-6.351880	-2.488772	-0.543720
31	1	0	-5.673812	-3.289445	-0.233503
32	1	0	-7.378133	-2.784129	-0.333334
33	1	0	-6.239896	-2.304694	-1.616395
34	8	0	5.986936	-1.670342	0.382406
35	6	0	7.124460	-1.307515	-0.382849
36	1	0	7.910540	-2.006658	-0.104171
37	1	0	6.923436	-1.396639	-1.454642
38	1	0	7.447218	-0.288288	-0.150901

Structure 27g (DMSO)

Energy (Hartrees): -938.316108508
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.634536	-0.554323	-0.677388
2	6	0	-3.850730	-1.235902	-0.642440
3	6	0	-4.912547	-0.711369	0.094126
4	6	0	-4.736619	0.485021	0.796763
5	6	0	-3.518000	1.141133	0.764454
6	6	0	-2.441784	0.640917	0.016392
7	1	0	-1.828630	-0.965602	-1.276803
8	1	0	-3.954824	-2.159381	-1.197061
9	1	0	-5.563488	0.877520	1.377771
10	1	0	-3.394102	2.052465	1.340097
11	6	0	-1.145480	1.358135	-0.037860
12	6	0	-1.106021	2.716685	-0.128423
13	6	0	0.095255	0.608277	0.005852
14	1	0	-2.015119	3.310367	-0.176369
15	1	0	0.026768	-0.478246	0.113361
16	8	0	0.004714	3.433723	-0.176693
17	1	0	0.766756	2.777113	-0.156501
18	7	0	1.240169	1.195354	-0.072825
19	6	0	2.434667	0.452745	0.046439
20	6	0	2.557654	-0.663404	0.885497
21	6	0	3.549419	0.875942	-0.673304
22	6	0	3.756355	-1.350499	0.966629
23	1	0	1.719306	-0.979102	1.496593
24	6	0	4.757414	0.186259	-0.604593
25	1	0	3.464706	1.751698	-1.307707
26	6	0	4.862777	-0.937630	0.216077
27	1	0	3.859041	-2.207483	1.622489
28	1	0	5.599491	0.536001	-1.187237
29	8	0	-6.135615	-1.289622	0.191497
30	6	0	-6.347121	-2.498648	-0.523564
31	1	0	-5.674913	-3.286745	-0.172349
32	1	0	-7.377303	-2.789249	-0.326770
33	1	0	-6.210411	-2.349777	-1.598540
34	8	0	5.990784	-1.676311	0.358520
35	6	0	7.132119	-1.281683	-0.389489
36	1	0	7.916190	-1.995171	-0.143530
37	1	0	6.931729	-1.318967	-1.464073
38	1	0	7.457634	-0.275181	-0.111208

Structure 27g (C_2H_5OH)

Energy (Hartrees): -938.317957677
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.626468	-0.546032	-0.685084
2	6	0	-3.838422	-1.234876	-0.651873
3	6	0	-4.897081	-0.721963	0.095106
4	6	0	-4.727154	0.466090	0.810924
5	6	0	-3.512497	1.129913	0.779530
6	6	0	-2.438484	0.643313	0.020059
7	1	0	-1.820542	-0.945220	-1.292712
8	1	0	-3.941431	-2.153333	-1.214966
9	1	0	-5.554812	0.844606	1.400545
10	1	0	-3.390142	2.035499	1.364447
11	6	0	-1.146636	1.368962	-0.036364
12	6	0	-1.118908	2.725064	-0.131715
13	6	0	0.098416	0.623269	0.008830
14	1	0	-2.030051	3.314755	-0.180721
15	1	0	0.032283	-0.462669	0.124321
16	8	0	-0.009064	3.453681	-0.185277
17	1	0	0.762658	2.810717	-0.164300
18	7	0	1.241215	1.211115	-0.077008
19	6	0	2.433734	0.464527	0.044840
20	6	0	2.558943	-0.629342	0.911626
21	6	0	3.541916	0.861830	-0.699606
22	6	0	3.754408	-1.322070	0.997176
23	1	0	1.725158	-0.922110	1.540281
24	6	0	4.745691	0.165493	-0.627772
25	1	0	3.455486	1.720599	-1.356421
26	6	0	4.851644	-0.935238	0.221936
27	1	0	3.861760	-2.161986	1.674369
28	1	0	5.583231	0.492434	-1.229899
29	8	0	-6.122005	-1.308850	0.190850
30	6	0	-6.333531	-2.513928	-0.534190
31	1	0	-5.657572	-3.301243	-0.189449
32	1	0	-7.362789	-2.806538	-0.335107
33	1	0	-6.200269	-2.352842	-1.607451
34	8	0	5.981372	-1.679479	0.371386
35	6	0	7.119335	-1.312785	-0.398845
36	1	0	7.902284	-2.020261	-0.132675
37	1	0	6.907796	-1.388068	-1.469044
38	1	0	7.446584	-0.298327	-0.155293

Structure 28a (vacuum)

Energy (Hartrees): -913.769748913
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.319443	1.335734	0.555380
2	6	0	-3.608300	0.833280	0.642919
3	6	0	-3.883459	-0.395673	0.062271
4	6	0	-2.914968	-1.126046	-0.610242
5	6	0	-1.636455	-0.600729	-0.703681
6	6	0	-1.309733	0.630316	-0.116315
7	1	0	-2.086717	2.275435	1.041989
8	1	0	-4.391633	1.366289	1.164868
9	1	0	-3.175884	-2.072677	-1.063742
10	1	0	-0.884601	-1.139021	-1.269115
11	6	0	0.057797	1.173894	-0.205072
12	6	0	1.141554	0.338799	-0.067230
13	6	0	0.254950	2.592407	-0.440261
14	1	0	0.972531	-0.711630	0.148287
15	1	0	-0.662984	3.189164	-0.583388
16	8	0	1.345350	3.141910	-0.509675
17	7	0	2.424169	0.719117	-0.134633
18	1	0	2.573068	1.718766	-0.267521
19	6	0	3.545476	-0.119465	0.012619
20	6	0	4.766211	0.471632	0.343241
21	6	0	3.475391	-1.499317	-0.181642
22	6	0	5.900396	-0.313053	0.493455
23	1	0	4.815101	1.544960	0.489840
24	6	0	4.615013	-2.276623	-0.014162
25	1	0	2.549761	-1.970710	-0.486821
26	6	0	5.830447	-1.692442	0.323708
27	1	0	6.841850	0.157225	0.750372
28	1	0	4.551475	-3.347391	-0.166551
29	1	0	6.715523	-2.304048	0.444979
30	7	0	-5.248757	-0.941567	0.158909
31	8	0	-5.460550	-2.017381	-0.359219
32	8	0	-6.076631	-0.282719	0.751011

Structure 28a ($CHCl_3$)

Energy (Hartrees): -913.795948036
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.325654	1.334033	0.554914
2	6	0	-3.616245	0.836782	0.635735
3	6	0	-3.892520	-0.393234	0.053666
4	6	0	-2.920721	-1.129229	-0.611566
5	6	0	-1.640004	-0.609960	-0.697048
6	6	0	-1.313658	0.623772	-0.111697
7	1	0	-2.094844	2.273391	1.043761
8	1	0	-4.393383	1.380702	1.156170
9	1	0	-3.172370	-2.077106	-1.068227
10	1	0	-0.887354	-1.159410	-1.250753
11	6	0	0.055020	1.166485	-0.192759
12	6	0	1.138483	0.320774	-0.071073
13	6	0	0.245326	2.583711	-0.405967
14	1	0	0.962694	-0.734041	0.113318
15	1	0	-0.671172	3.180073	-0.547947
16	8	0	1.337424	3.143058	-0.465875
17	7	0	2.418419	0.699819	-0.124656
18	1	0	2.578426	1.699392	-0.242899
19	6	0	3.547926	-0.131310	0.016155
20	6	0	4.776510	0.487557	0.258728
21	6	0	3.481348	-1.521211	-0.094799
22	6	0	5.925754	-0.278137	0.398784
23	1	0	4.820242	1.568489	0.341178
24	6	0	4.638224	-2.277382	0.057302
25	1	0	2.547055	-2.021927	-0.314416
26	6	0	5.863262	-1.665778	0.304368
27	1	0	6.872881	0.214467	0.586049
28	1	0	4.577913	-3.356129	-0.030756
29	1	0	6.760446	-2.262653	0.415587
30	7	0	-5.253147	-0.932803	0.142458
31	8	0	-5.470996	-2.017861	-0.360138
32	8	0	-6.095894	-0.269648	0.714244

Structure 28a (DMSO)

Energy (Hartrees): -913.794681634
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.345481	1.337973	-0.556334
2	6	0	3.635865	0.837339	-0.607625
3	6	0	3.894814	-0.397777	-0.027087
4	6	0	2.903000	-1.135588	0.607344
5	6	0	1.622561	-0.612923	0.665316
6	6	0	1.314456	0.626752	0.080533
7	1	0	2.132343	2.282352	-1.043131
8	1	0	4.424769	1.385029	-1.105988
9	1	0	3.135238	-2.088523	1.063959
10	1	0	0.855720	-1.166746	1.194627
11	6	0	-0.053111	1.173531	0.131606
12	6	0	-1.134519	0.320665	0.036381
13	6	0	-0.241273	2.596923	0.302705
14	1	0	-0.953228	-0.738902	-0.106876
15	1	0	0.676259	3.194854	0.426989
16	8	0	-1.332321	3.160687	0.347250
17	7	0	-2.415233	0.696067	0.083012
18	1	0	-2.583733	1.694678	0.195007
19	6	0	-3.545431	-0.137608	-0.027637
20	6	0	-4.797136	0.483967	-0.021339
21	6	0	-3.462698	-1.527633	-0.135160
22	6	0	-5.954440	-0.276025	-0.124933
23	1	0	-4.852397	1.564300	0.063962
24	6	0	-4.630178	-2.276420	-0.240749
25	1	0	-2.509385	-2.040006	-0.134437
26	6	0	-5.878921	-1.661957	-0.236875
27	1	0	-6.917978	0.220526	-0.118381
28	1	0	-4.555976	-3.354900	-0.323576
29	1	0	-6.781942	-2.255313	-0.317013
30	7	0	5.254648	-0.937913	-0.082209
31	8	0	5.453030	-2.041102	0.391322
32	8	0	6.122239	-0.258553	-0.598276

Structure 28a (C_2H_5OH)

Energy (Hartrees): -913.795195207
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.339512	1.336132	-0.552217
2	6	0	3.630180	0.839532	-0.613290
3	6	0	3.895511	-0.394187	-0.031442
4	6	0	2.911286	-1.133370	0.614261
5	6	0	1.630488	-0.613919	0.681386
6	6	0	1.315443	0.623772	0.095168
7	1	0	2.118939	2.277768	-1.040766
8	1	0	4.412931	1.388568	-1.119628
9	1	0	3.150325	-2.084336	1.071549
10	1	0	0.869673	-1.167805	1.219165
11	6	0	-0.051885	1.169306	0.152789
12	6	0	-1.135866	0.314856	0.056350
13	6	0	-0.237253	2.587710	0.318914
14	1	0	-0.954814	-0.744095	-0.091504
15	1	0	0.677260	3.187780	0.443922
16	8	0	-1.332063	3.155830	0.358002
17	7	0	-2.413720	0.689679	0.102642
18	1	0	-2.584373	1.687930	0.216774
19	6	0	-3.546169	-0.141522	-0.020798
20	6	0	-4.792002	0.489363	-0.064306
21	6	0	-3.468681	-1.533621	-0.091140
22	6	0	-5.951399	-0.265102	-0.183196
23	1	0	-4.840790	1.571739	-0.006258
24	6	0	-4.638059	-2.277093	-0.212747
25	1	0	-2.518815	-2.050640	-0.046755
26	6	0	-5.881744	-1.653662	-0.260497
27	1	0	-6.911380	0.237143	-0.217187
28	1	0	-4.570130	-3.357715	-0.266226
29	1	0	-6.786039	-2.243078	-0.354450
30	7	0	5.250920	-0.932210	-0.099662
31	8	0	5.464989	-2.024806	0.393099
32	8	0	6.112154	-0.267862	-0.646714

Structure 28b (vacuum)

Energy (Hartrees): -913.763477532
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.189917	1.288556	-0.809318
2	6	0	3.356493	0.537992	-0.809783
3	6	0	3.448255	-0.543930	0.052387
4	6	0	2.422513	-0.888783	0.919993
5	6	0	1.267665	-0.121818	0.914796
6	6	0	1.126492	0.972082	0.047206
7	1	0	2.092703	2.121606	-1.495859
8	1	0	4.182252	0.769295	-1.469165
9	1	0	2.545817	-1.728981	1.589899
10	1	0	0.473305	-0.349778	1.617065
11	6	0	-0.100277	1.790088	0.052165
12	6	0	-1.357984	1.270794	0.017108
13	6	0	0.005726	3.256379	0.090413
14	1	0	-2.185358	1.973054	0.045234
15	1	0	1.040565	3.644720	0.159581
16	8	0	-0.931604	4.021275	0.072285
17	7	0	-1.685195	-0.033713	-0.102549
18	1	0	-0.936529	-0.688902	-0.287051
19	6	0	-2.990963	-0.560201	-0.095637
20	6	0	-3.213021	-1.801562	-0.694797
21	6	0	-4.049637	0.115301	0.512562
22	6	0	-4.485063	-2.355764	-0.694204
23	1	0	-2.388852	-2.322276	-1.170939
24	6	0	-5.321792	-0.442993	0.491717
25	1	0	-3.883658	1.057113	1.020150
26	6	0	-5.548809	-1.676792	-0.108135
27	1	0	-4.645152	-3.319247	-1.163175
28	1	0	-6.138527	0.088038	0.965926
29	1	0	-6.541947	-2.107539	-0.113098
30	7	0	4.681010	-1.355023	0.049827
31	8	0	4.721293	-2.313893	0.790435
32	8	0	5.575007	-1.013888	-0.693764

Structure 28b ($CHCl_3$)

Energy (Hartrees): -913.791655336
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.235346	1.326368	-0.746970
2	6	0	3.404946	0.582379	-0.740503
3	6	0	3.463067	-0.553642	0.054820
4	6	0	2.397890	-0.957617	0.848761
5	6	0	1.240422	-0.196265	0.838944
6	6	0	1.133372	0.952175	0.037521
7	1	0	2.170661	2.201507	-1.383299
8	1	0	4.253367	0.865727	-1.349279
9	1	0	2.483814	-1.838107	1.471382
10	1	0	0.418909	-0.480125	1.487043
11	6	0	-0.092263	1.771317	0.039208
12	6	0	-1.360587	1.260184	0.000903
13	6	0	0.026718	3.226528	0.100627
14	1	0	-2.183680	1.966153	0.055685
15	1	0	1.059284	3.605012	0.210594
16	8	0	-0.901903	4.013640	0.063034
17	7	0	-1.703132	-0.029774	-0.146098
18	1	0	-0.972298	-0.697286	-0.366999
19	6	0	-3.015854	-0.542701	-0.111753
20	6	0	-3.263983	-1.765522	-0.739441
21	6	0	-4.048792	0.122771	0.551210
22	6	0	-4.540457	-2.310820	-0.716166
23	1	0	-2.455274	-2.278160	-1.249849
24	6	0	-5.325732	-0.427646	0.554247
25	1	0	-3.860548	1.047627	1.082909
26	6	0	-5.580589	-1.641818	-0.075931
27	1	0	-4.722245	-3.259442	-1.208037
28	1	0	-6.123515	0.093629	1.070850
29	1	0	-6.577091	-2.066216	-0.060994
30	7	0	4.693923	-1.354462	0.058932
31	8	0	4.700530	-2.385473	0.701662
32	8	0	5.642881	-0.946268	-0.580033

Structure 28b (DMSO)

Energy (Hartrees): -913.791200679
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.243535	1.339944	-0.726610
2	6	0	3.412285	0.595189	-0.721950
3	6	0	3.462005	-0.555586	0.053419
4	6	0	2.388043	-0.972726	0.829144
5	6	0	1.231733	-0.210307	0.822116
6	6	0	1.133703	0.952995	0.041282
7	1	0	2.187503	2.225515	-1.349173
8	1	0	4.264124	0.891885	-1.319695
9	1	0	2.461626	-1.865689	1.435439
10	1	0	0.403890	-0.509819	1.454939
11	6	0	-0.090939	1.772574	0.044590
12	6	0	-1.361520	1.262789	0.006038
13	6	0	0.030613	3.226496	0.107382
14	1	0	-2.182630	1.970269	0.067395
15	1	0	1.062860	3.601289	0.229913
16	8	0	-0.895072	4.018290	0.056882
17	7	0	-1.706038	-0.024146	-0.146541
18	1	0	-0.978310	-0.695782	-0.370196
19	6	0	-3.017202	-0.536880	-0.111401
20	6	0	-3.253988	-1.774465	-0.715554
21	6	0	-4.059698	0.137681	0.528011
22	6	0	-4.528822	-2.324285	-0.694182
23	1	0	-2.435219	-2.293587	-1.203075
24	6	0	-5.334591	-0.418470	0.529567
25	1	0	-3.882639	1.073968	1.043230
26	6	0	-5.578754	-1.646577	-0.078396
27	1	0	-4.701012	-3.284634	-1.166897
28	1	0	-6.139267	0.109608	1.028682
29	1	0	-6.573833	-2.074875	-0.064417
30	7	0	4.690525	-1.356925	0.055519
31	8	0	4.691088	-2.401277	0.678828
32	8	0	5.649370	-0.938372	-0.564425

Structure 28b (C_2H_5OH)

Energy (Hartrees): -913.792200281
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.236668	1.331489	-0.742959
2	6	0	3.403483	0.584304	-0.737733
3	6	0	3.456444	-0.554351	0.055647
4	6	0	2.389039	-0.957666	0.848072
5	6	0	1.234550	-0.193247	0.838350
6	6	0	1.133124	0.957783	0.040127
7	1	0	2.176520	2.207918	-1.378008
8	1	0	4.250555	0.869403	-1.347860
9	1	0	2.465825	-1.840418	1.468819
10	1	0	0.411720	-0.480778	1.483086
11	6	0	-0.091381	1.778922	0.042044
12	6	0	-1.364017	1.264465	0.004749
13	6	0	0.032707	3.223785	0.100855
14	1	0	-2.190058	1.966151	0.066424
15	1	0	1.063734	3.601243	0.209389
16	8	0	-0.895171	4.024596	0.061221
17	7	0	-1.701059	-0.020762	-0.146198
18	1	0	-0.968971	-0.691185	-0.360589
19	6	0	-3.012920	-0.539051	-0.111824
20	6	0	-3.249822	-1.766229	-0.734897
21	6	0	-4.050475	0.123605	0.546309
22	6	0	-4.523845	-2.318291	-0.714437
23	1	0	-2.433856	-2.276270	-1.236530
24	6	0	-5.324612	-0.433987	0.546696
25	1	0	-3.869843	1.051095	1.076417
26	6	0	-5.570156	-1.652094	-0.080530
27	1	0	-4.698254	-3.270798	-1.202002
28	1	0	-6.127078	0.084285	1.059554
29	1	0	-6.564584	-2.082232	-0.067389
30	7	0	4.679831	-1.356926	0.058230
31	8	0	4.698839	-2.377571	0.720412
32	8	0	5.626352	-0.970929	-0.601427

Structure 28c (vacuum)

Energy (Hartrees): -913.765236685
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.150906	1.228315	-0.787012
2	6	0	3.265732	0.403722	-0.802456
3	6	0	3.300729	-0.685092	0.055922
4	6	0	2.269742	-0.967652	0.938264
5	6	0	1.161511	-0.133541	0.942401
6	6	0	1.078117	0.962697	0.072723
7	1	0	2.110383	2.090535	-1.438961
8	1	0	4.100183	0.591553	-1.464504
9	1	0	2.350657	-1.813205	1.607762
10	1	0	0.361098	-0.316307	1.651120
11	6	0	-0.115610	1.832333	0.076002
12	6	0	-1.389081	1.355806	0.038798
13	6	0	0.024667	3.290005	0.070186
14	1	0	-2.210440	2.065988	0.058642
15	7	0	-1.758621	0.059154	-0.078430
16	1	0	-1.027827	-0.614866	-0.266839
17	6	0	-3.079726	-0.424004	-0.086071
18	6	0	-3.339134	-1.648980	-0.704051
19	6	0	-4.120423	0.275643	0.526199
20	6	0	-4.628351	-2.161363	-0.718206
21	1	0	-2.529257	-2.189658	-1.182283
22	6	0	-5.410757	-0.239648	0.489271
23	1	0	-3.926544	1.200191	1.055408
24	6	0	-5.673868	-1.456260	-0.129782
25	1	0	-4.816257	-3.112758	-1.201144
26	1	0	-6.212690	0.310034	0.967542
27	1	0	-6.680344	-1.854394	-0.147026
28	8	0	1.068712	3.895168	0.020037
29	1	0	-0.939545	3.837241	0.119341
30	7	0	4.480977	-1.571724	0.037567
31	8	0	4.476084	-2.526636	0.784858
32	8	0	5.379876	-1.293313	-0.725664

Structure 28c ($CHCl_3$)

Energy (Hartrees): -913.794322506
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.137808	1.201865	-0.821839
2	6	0	3.257683	0.385203	-0.833456
3	6	0	3.310122	-0.681054	0.054182
4	6	0	2.290916	-0.947986	0.956924
5	6	0	1.177767	-0.121046	0.955182
6	6	0	1.079242	0.955332	0.062365
7	1	0	2.079018	2.038016	-1.506761
8	1	0	4.074676	0.565106	-1.519346
9	1	0	2.375794	-1.775021	1.648999
10	1	0	0.385275	-0.299763	1.673637
11	6	0	-0.116148	1.823094	0.058547
12	6	0	-1.396751	1.346078	0.028716
13	6	0	0.018403	3.270659	0.059853
14	1	0	-2.214206	2.061033	0.055253
15	7	0	-1.765742	0.056983	-0.083162
16	1	0	-1.043131	-0.629268	-0.271035
17	6	0	-3.091087	-0.422505	-0.085248
18	6	0	-3.354388	-1.637397	-0.722020
19	6	0	-4.124415	0.269024	0.549409
20	6	0	-4.644850	-2.149137	-0.733789
21	1	0	-2.545918	-2.169706	-1.212223
22	6	0	-5.415614	-0.246847	0.516484
23	1	0	-3.925051	1.186727	1.089487
24	6	0	-5.684524	-1.453558	-0.121795
25	1	0	-4.837904	-3.092185	-1.232042
26	1	0	-6.213433	0.294407	1.012029
27	1	0	-6.691838	-1.851539	-0.135646
28	8	0	1.067260	3.887168	0.048829
29	1	0	-0.943841	3.817210	0.081124
30	7	0	4.492387	-1.554558	0.044817
31	8	0	4.512358	-2.495561	0.812959
32	8	0	5.389014	-1.293151	-0.731309

Structure 28c (DMSO)

Energy (Hartrees): -913.795816754
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.126631	1.183146	-0.847604
2	6	0	3.250931	0.373597	-0.855028
3	6	0	3.313461	-0.678398	0.049923
4	6	0	2.298911	-0.940900	0.960176
5	6	0	1.183481	-0.117784	0.955975
6	6	0	1.077265	0.947387	0.050950
7	1	0	2.055372	2.001210	-1.553766
8	1	0	4.058874	0.547696	-1.553255
9	1	0	2.386145	-1.758410	1.663387
10	1	0	0.395518	-0.293555	1.680077
11	6	0	-0.115164	1.819386	0.048697
12	6	0	-1.403043	1.347009	0.018509
13	6	0	0.021658	3.256366	0.069403
14	1	0	-2.215254	2.067656	0.047337
15	7	0	-1.772789	0.064191	-0.090450
16	1	0	-1.052177	-0.631523	-0.257130
17	6	0	-3.099339	-0.415852	-0.086452
18	6	0	-3.350043	-1.654000	-0.681918
19	6	0	-4.140681	0.294456	0.513042
20	6	0	-4.639310	-2.169826	-0.692472
21	1	0	-2.531985	-2.200677	-1.139597
22	6	0	-5.429926	-0.227306	0.482458
23	1	0	-3.953945	1.231867	1.023168
24	6	0	-5.688292	-1.456112	-0.117821
25	1	0	-4.822878	-3.131134	-1.159066
26	1	0	-6.234813	0.328214	0.950476
27	1	0	-6.694811	-1.857052	-0.130148
28	8	0	1.080062	3.874555	0.090927
29	1	0	-0.933040	3.810987	0.077923
30	7	0	4.496682	-1.542413	0.046734
31	8	0	4.512454	-2.501385	0.794632
32	8	0	5.412047	-1.265013	-0.704364

Structure 28c (C_2H_5OH)

Energy (Hartrees): -913.795816754
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.126631	1.183146	-0.847604
2	6	0	3.250931	0.373597	-0.855028
3	6	0	3.313461	-0.678398	0.049923
4	6	0	2.298911	-0.940900	0.960176
5	6	0	1.183481	-0.117784	0.955975
6	6	0	1.077265	0.947387	0.050950
7	1	0	2.055372	2.001210	-1.553766
8	1	0	4.058874	0.547696	-1.553255
9	1	0	2.386145	-1.758410	1.663387
10	1	0	0.395518	-0.293555	1.680077
11	6	0	-0.115164	1.819386	0.048697
12	6	0	-1.403043	1.347009	0.018509
13	6	0	0.021658	3.256366	0.069403
14	1	0	-2.215254	2.067656	0.047337
15	7	0	-1.772789	0.064191	-0.090450
16	1	0	-1.052177	-0.631523	-0.257130
17	6	0	-3.099339	-0.415852	-0.086452
18	6	0	-3.350043	-1.654000	-0.681918
19	6	0	-4.140681	0.294456	0.513042
20	6	0	-4.639310	-2.169826	-0.692472
21	1	0	-2.531985	-2.200677	-1.139597
22	6	0	-5.429926	-0.227306	0.482458
23	1	0	-3.953945	1.231867	1.023168
24	6	0	-5.688292	-1.456112	-0.117821
25	1	0	-4.822878	-3.131134	-1.159066
26	1	0	-6.234813	0.328214	0.950476
27	1	0	-6.694811	-1.857052	-0.130148
28	8	0	1.080062	3.874555	0.090927
29	1	0	-0.933040	3.810987	0.077923
30	7	0	4.496682	-1.542413	0.046734
31	8	0	4.512454	-2.501385	0.794632
32	8	0	5.412047	-1.265013	-0.704364

Structure 28d (vacuum)

Energy (Hartrees): -913.756795244
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.270306	1.302826	0.546128
2	6	0	-3.515146	0.702740	0.654268
3	6	0	-3.707225	-0.546474	0.083041
4	6	0	-2.700248	-1.206565	-0.603635
5	6	0	-1.463436	-0.589890	-0.709618
6	6	0	-1.221262	0.660432	-0.125208
7	1	0	-2.108414	2.277900	0.983937
8	1	0	-4.331320	1.184609	1.175440
9	1	0	-2.897527	-2.170018	-1.053812
10	1	0	-0.680251	-1.076168	-1.280166
11	6	0	0.118999	1.282524	-0.214781
12	6	0	1.225311	0.499910	-0.057863
13	6	0	0.243263	2.717243	-0.477992
14	1	0	1.080077	-0.557291	0.139946
15	7	0	2.529901	0.873114	-0.065277
16	1	0	2.758838	1.854909	-0.083720
17	6	0	3.623915	-0.008997	0.033272
18	6	0	4.834852	0.481795	0.525864
19	6	0	3.530323	-1.341986	-0.367090
20	6	0	5.934998	-0.357193	0.628903
21	1	0	4.905705	1.517932	0.839363
22	6	0	4.633794	-2.177679	-0.240561
23	1	0	2.615379	-1.724782	-0.801692
24	6	0	5.839013	-1.694148	0.255357
25	1	0	6.868857	0.035328	1.013206
26	1	0	4.551240	-3.211770	-0.552859
27	1	0	6.696376	-2.349473	0.341264
28	1	0	1.277262	3.090261	-0.626123
29	8	0	-0.673212	3.499821	-0.566758
30	7	0	-5.028576	-1.190597	0.199471
31	8	0	-5.170426	-2.278831	-0.317232
32	8	0	-5.892184	-0.595527	0.807158

Structure 28d ($CHCl_3$)

Energy (Hartrees): -913.787072534
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.277302	1.307044	0.538661
2	6	0	-3.524022	0.711664	0.641170
3	6	0	-3.712542	-0.545014	0.080904
4	6	0	-2.695499	-1.216033	-0.584179
5	6	0	-1.457464	-0.602802	-0.684969
6	6	0	-1.219559	0.658042	-0.116831
7	1	0	-2.119299	2.281394	0.980491
8	1	0	-4.337526	1.206963	1.154474
9	1	0	-2.877539	-2.186982	-1.025431
10	1	0	-0.668598	-1.104603	-1.233791
11	6	0	0.117730	1.283570	-0.200432
12	6	0	1.229901	0.491969	-0.061007
13	6	0	0.247344	2.710213	-0.453546
14	1	0	1.081452	-0.569482	0.111863
15	7	0	2.523959	0.864943	-0.067562
16	1	0	2.757959	1.849149	-0.084468
17	6	0	3.622747	-0.014333	0.030058
18	6	0	4.829130	0.489201	0.522042
19	6	0	3.536196	-1.348491	-0.369488
20	6	0	5.935960	-0.342369	0.626373
21	1	0	4.888479	1.528180	0.829287
22	6	0	4.647467	-2.175122	-0.243866
23	1	0	2.620993	-1.740142	-0.796701
24	6	0	5.849679	-1.680824	0.252238
25	1	0	6.867497	0.057281	1.010320
26	1	0	4.572959	-3.210679	-0.555120
27	1	0	6.712729	-2.329826	0.337876
28	1	0	1.281086	3.088628	-0.550110
29	8	0	-0.672444	3.494759	-0.592503
30	7	0	-5.028170	-1.184205	0.193398
31	8	0	-5.171088	-2.288526	-0.294404
32	8	0	-5.910131	-0.580649	0.771620

Structure 28d (DMSO)

Energy (Hartrees): -913.787929590
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.277982	1.306408	0.538030
2	6	0	-3.524590	0.711651	0.640284
3	6	0	-3.713387	-0.544865	0.078248
4	6	0	-2.694218	-1.215594	-0.585112
5	6	0	-1.455663	-0.603510	-0.684890
6	6	0	-1.218135	0.658698	-0.117418
7	1	0	-2.120155	2.278168	0.985434
8	1	0	-4.335830	1.208214	1.156204
9	1	0	-2.871423	-2.187597	-1.026254
10	1	0	-0.666035	-1.109599	-1.228635
11	6	0	0.117305	1.285115	-0.197376
12	6	0	1.229809	0.486882	-0.070572
13	6	0	0.250457	2.712997	-0.433192
14	1	0	1.078217	-0.576209	0.088523
15	7	0	2.520977	0.858076	-0.077956
16	1	0	2.758533	1.842857	-0.093076
17	6	0	3.619123	-0.020372	0.023498
18	6	0	4.832075	0.498310	0.483759
19	6	0	3.528777	-1.365222	-0.340159
20	6	0	5.941639	-0.328983	0.596955
21	1	0	4.893086	1.546658	0.757033
22	6	0	4.643944	-2.186131	-0.206879
23	1	0	2.609101	-1.771417	-0.743866
24	6	0	5.852360	-1.677740	0.260662
25	1	0	6.877637	0.082569	0.957271
26	1	0	4.566954	-3.229930	-0.489377
27	1	0	6.717406	-2.323582	0.352755
28	1	0	1.284659	3.090667	-0.512474
29	8	0	-0.667946	3.502105	-0.575442
30	7	0	-5.028136	-1.181622	0.187924
31	8	0	-5.175848	-2.283049	-0.307523
32	8	0	-5.910097	-0.580536	0.771922

Structure 28d (C_2H_5OH)

Energy (Hartrees): -913.789002672
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.268073	1.292176	0.572364
2	6	0	-3.515761	0.700153	0.671004
3	6	0	-3.710302	-0.545150	0.085238
4	6	0	-2.697014	-1.209222	-0.594342
5	6	0	-1.457929	-0.598422	-0.690704
6	6	0	-1.216563	0.654222	-0.105143
7	1	0	-2.102356	2.252344	1.042959
8	1	0	-4.321687	1.190023	1.201463
9	1	0	-2.879046	-2.172574	-1.052363
10	1	0	-0.671527	-1.095625	-1.247456
11	6	0	0.116971	1.284230	-0.191942
12	6	0	1.234520	0.489090	-0.062056
13	6	0	0.241819	2.701413	-0.448300
14	1	0	1.084241	-0.573024	0.106084
15	7	0	2.521671	0.862035	-0.077847
16	1	0	2.758214	1.847100	-0.104464
17	6	0	3.622591	-0.016488	0.024454
18	6	0	4.830257	0.499342	0.499141
19	6	0	3.534744	-1.356291	-0.355279
20	6	0	5.939645	-0.328571	0.611397
21	1	0	4.888205	1.544559	0.784976
22	6	0	4.649223	-2.178103	-0.222973
23	1	0	2.617771	-1.757029	-0.770816
24	6	0	5.853389	-1.673314	0.259247
25	1	0	6.872884	0.079266	0.983079
26	1	0	4.575732	-3.218685	-0.518173
27	1	0	6.718466	-2.319438	0.350329
28	1	0	1.269316	3.093203	-0.523912
29	8	0	-0.688233	3.481263	-0.615919
30	7	0	-5.024741	-1.175727	0.185400
31	8	0	-5.178968	-2.275860	-0.312603
32	8	0	-5.912027	-0.575988	0.763870

Structure 28e (vacuum)

Energy (Hartrees): -913.752369425
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.921966	1.144751	-0.627087
2	6	0	3.291570	1.055158	-0.442766
3	6	0	3.820133	-0.107937	0.099967
4	6	0	3.020950	-1.175185	0.474949
5	6	0	1.650402	-1.067041	0.292286
6	6	0	1.078411	0.079069	-0.277613
7	1	0	1.501022	2.047778	-1.046242
8	1	0	3.952392	1.866391	-0.716413
9	1	0	3.470041	-2.055367	0.914477
10	1	0	1.009875	-1.875417	0.625075
11	6	0	-0.377747	0.139895	-0.521055
12	6	0	-1.020347	-0.985617	-0.941579
13	6	0	-1.094002	1.424900	-0.424033
14	1	0	-0.412765	-1.835205	-1.245040
15	7	0	-2.360094	-1.217256	-1.065238
16	1	0	-2.610630	-2.017389	-1.625800
17	6	0	-3.434412	-0.661141	-0.322688
18	6	0	-3.268428	-0.248034	1.000084
19	6	0	-4.689520	-0.589448	-0.921827
20	6	0	-4.356171	0.247741	1.704165
21	1	0	-2.293811	-0.311289	1.469241
22	6	0	-5.776222	-0.105838	-0.201401
23	1	0	-4.808430	-0.903174	-1.953107
24	6	0	-5.614142	0.320983	1.110633
25	1	0	-4.219807	0.572146	2.728709
26	1	0	-6.748810	-0.052590	-0.675740
27	1	0	-6.458088	0.708379	1.667375
28	1	0	-2.116587	1.430087	-0.838214
29	8	0	-0.618078	2.442298	0.022024
30	7	0	5.278067	-0.208427	0.295368
31	8	0	5.711490	-1.236883	0.770711
32	8	0	5.955981	0.741072	-0.033666

Structure 28e ($CHCl_3$)

Energy (Hartrees): -913.781281111
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.907870	1.115574	-0.656253
2	6	0	3.279817	1.051556	-0.485651
3	6	0	3.830732	-0.089218	0.086248
4	6	0	3.048208	-1.158571	0.496138
5	6	0	1.675273	-1.075287	0.324921
6	6	0	1.078950	0.050377	-0.265160
7	1	0	1.474548	1.997871	-1.106707
8	1	0	3.918131	1.868354	-0.795082
9	1	0	3.504631	-2.025446	0.954994
10	1	0	1.052900	-1.888174	0.680328
11	6	0	-0.379974	0.092784	-0.485017
12	6	0	-1.020967	-1.064360	-0.849670
13	6	0	-1.101979	1.362622	-0.419639
14	1	0	-0.408614	-1.913961	-1.141542
15	7	0	-2.344000	-1.331837	-0.930749
16	1	0	-2.583224	-2.174544	-1.436677
17	6	0	-3.435235	-0.702693	-0.272645
18	6	0	-3.313942	-0.243096	1.040105
19	6	0	-4.654156	-0.609342	-0.938856
20	6	0	-4.410831	0.331822	1.666858
21	1	0	-2.367235	-0.330939	1.561091
22	6	0	-5.751531	-0.044025	-0.295657
23	1	0	-4.735268	-0.971740	-1.957888
24	6	0	-5.632800	0.435500	1.003923
25	1	0	-4.312260	0.692997	2.683977
26	1	0	-6.697731	0.028353	-0.819401
27	1	0	-6.484462	0.886109	1.499343
28	1	0	-2.121577	1.353466	-0.836525
29	8	0	-0.642890	2.404534	0.008783
30	7	0	5.283567	-0.160794	0.274025
31	8	0	5.744642	-1.156439	0.797729
32	8	0	5.956570	0.777433	-0.104851

Structure 28e (DMSO)

Energy (Hartrees): -913.781632659
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.898828	1.101643	-0.678181
2	6	0	3.269776	1.048450	-0.499054
3	6	0	3.825134	-0.084083	0.086364
4	6	0	3.046279	-1.157539	0.495071
5	6	0	1.673937	-1.085369	0.314980
6	6	0	1.072766	0.034624	-0.282565
7	1	0	1.464845	1.976067	-1.143407
8	1	0	3.901853	1.867662	-0.814912
9	1	0	3.501899	-2.021621	0.960241
10	1	0	1.056483	-1.903878	0.666149
11	6	0	-0.383998	0.071524	-0.504570
12	6	0	-1.026483	-1.094915	-0.849014
13	6	0	-1.108975	1.337007	-0.456289
14	1	0	-0.418786	-1.948974	-1.137064
15	7	0	-2.346791	-1.360518	-0.910430
16	1	0	-2.594816	-2.210984	-1.401690
17	6	0	-3.427991	-0.710088	-0.258043
18	6	0	-3.294950	-0.235749	1.048948
19	6	0	-4.648958	-0.611564	-0.919654
20	6	0	-4.381242	0.362106	1.673293
21	1	0	-2.348146	-0.334191	1.568254
22	6	0	-5.735691	-0.022218	-0.278963
23	1	0	-4.740528	-0.991946	-1.931189
24	6	0	-5.604661	0.474960	1.013284
25	1	0	-4.274516	0.732716	2.686431
26	1	0	-6.683718	0.053680	-0.799224
27	1	0	-6.448515	0.942781	1.506619
28	1	0	-2.120361	1.319824	-0.892799
29	8	0	-0.666293	2.386043	-0.022744
30	7	0	5.274929	-0.141636	0.286903
31	8	0	5.743589	-1.135231	0.810286
32	8	0	5.943294	0.806839	-0.079587

Structure 28e (C_2H_5OH)

Energy (Hartrees): -913.782933983
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.897802	1.109534	-0.672638
2	6	0	3.268988	1.054210	-0.499003
3	6	0	3.823039	-0.080005	0.084998
4	6	0	3.044408	-1.151792	0.499818
5	6	0	1.671886	-1.075385	0.327202
6	6	0	1.071699	0.045401	-0.269710
7	1	0	1.464659	1.981195	-1.144415
8	1	0	3.901331	1.871113	-0.820628
9	1	0	3.499883	-2.016720	0.963719
10	1	0	1.053349	-1.891118	0.683229
11	6	0	-0.386852	0.083437	-0.484832
12	6	0	-1.023626	-1.085756	-0.845659
13	6	0	-1.111914	1.337932	-0.408870
14	1	0	-0.405958	-1.926174	-1.152205
15	7	0	-2.335286	-1.370915	-0.902366
16	1	0	-2.572693	-2.228432	-1.387064
17	6	0	-3.426789	-0.718963	-0.262657
18	6	0	-3.316455	-0.284936	1.059474
19	6	0	-4.626328	-0.579684	-0.953312
20	6	0	-4.406481	0.316891	1.673123
21	1	0	-2.383343	-0.415683	1.596439
22	6	0	-5.718191	0.012282	-0.323284
23	1	0	-4.698584	-0.929587	-1.977349
24	6	0	-5.609944	0.470376	0.985198
25	1	0	-4.319425	0.657770	2.698537
26	1	0	-6.651833	0.120517	-0.863481
27	1	0	-6.457681	0.939870	1.470501
28	1	0	-2.134484	1.329532	-0.813854
29	8	0	-0.657124	2.389796	0.023418
30	7	0	5.270139	-0.144354	0.271615
31	8	0	5.747030	-1.151466	0.762359
32	8	0	5.941763	0.810840	-0.072936

Structure 28f (vacuum)

Energy (Hartrees): -913.751187170
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.021483	1.270848	-0.393578
2	6	0	3.394096	1.153181	-0.247466
3	6	0	3.923014	-0.082680	0.095533
4	6	0	3.122176	-1.194376	0.305026
5	6	0	1.749430	-1.054650	0.173160
6	6	0	1.172094	0.171386	-0.189426
7	1	0	1.606803	2.222187	-0.704483
8	1	0	4.057230	1.991797	-0.411848
9	1	0	3.574872	-2.135876	0.585525
10	1	0	1.108502	-1.902593	0.384796
11	6	0	-0.288545	0.298336	-0.360509
12	6	0	-0.949637	-0.712441	-1.007123
13	6	0	-0.919889	1.564069	0.028232
14	1	0	-0.333179	-1.462135	-1.499300
15	1	0	-0.269316	2.240483	0.614935
16	8	0	-2.044474	1.904232	-0.262216
17	7	0	-2.271383	-0.939105	-1.181788
18	1	0	-2.491666	-1.625950	-1.887530
19	6	0	-3.383204	-0.558737	-0.390752
20	6	0	-3.262358	-0.333670	0.977504
21	6	0	-4.633552	-0.501393	-1.001398
22	6	0	-4.394571	-0.042192	1.725668
23	1	0	-2.289721	-0.392204	1.450444
24	6	0	-5.761155	-0.214715	-0.243861
25	1	0	-4.716095	-0.667086	-2.070134
26	6	0	-5.646396	0.019715	1.122140
27	1	0	-4.295514	0.136387	2.789596
28	1	0	-6.729928	-0.165030	-0.726150
29	1	0	-6.524845	0.252570	1.711105
30	7	0	5.382922	-0.218111	0.246183
31	8	0	5.816281	-1.308163	0.554034
32	8	0	6.061214	0.767916	0.052353

Structure 28f ($CHCl_3$)

Energy (Hartrees): -913.780309429
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.029405	1.262060	-0.436891
2	6	0	3.399569	1.144690	-0.274905
3	6	0	3.923236	-0.086550	0.097820
4	6	0	3.116365	-1.194093	0.319227
5	6	0	1.746261	-1.054111	0.171525
6	6	0	1.173876	0.168282	-0.216962
7	1	0	1.624383	2.210144	-0.770112
8	1	0	4.057675	1.984899	-0.452475
9	1	0	3.554108	-2.135489	0.623868
10	1	0	1.104746	-1.899645	0.390970
11	6	0	-0.285650	0.294869	-0.392098
12	6	0	-0.956928	-0.753370	-0.979685
13	6	0	-0.902350	1.578769	-0.076112
14	1	0	-0.351786	-1.525467	-1.449733
15	1	0	-0.258210	2.277406	0.487664
16	8	0	-2.022517	1.924665	-0.402279
17	7	0	-2.274321	-0.993494	-1.119415
18	1	0	-2.496958	-1.722323	-1.785796
19	6	0	-3.383630	-0.573517	-0.348737
20	6	0	-3.258670	-0.222669	0.994042
21	6	0	-4.642334	-0.612036	-0.947434
22	6	0	-4.395215	0.096950	1.726646
23	1	0	-2.283507	-0.210877	1.465282
24	6	0	-5.772365	-0.290239	-0.206496
25	1	0	-4.726905	-0.889942	-1.992744
26	6	0	-5.653915	0.069327	1.133110
27	1	0	-4.293112	0.368861	2.770919
28	1	0	-6.746659	-0.318046	-0.680500
29	1	0	-6.534953	0.324558	1.709964
30	7	0	5.373134	-0.219309	0.272432
31	8	0	5.813624	-1.308560	0.583921
32	8	0	6.063088	0.765816	0.097518

Structure 28f (DMSO)

Energy (Hartrees): -913.780864937
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.029955	1.272408	-0.427115
2	6	0	3.397906	1.147609	-0.253570
3	6	0	3.914530	-0.090963	0.106693
4	6	0	3.100610	-1.198634	0.304687
5	6	0	1.732924	-1.051867	0.146181
6	6	0	1.168046	0.178339	-0.231253
7	1	0	1.634088	2.227557	-0.750633
8	1	0	4.057459	1.990290	-0.413503
9	1	0	3.527720	-2.148424	0.598132
10	1	0	1.087714	-1.899957	0.343608
11	6	0	-0.288425	0.307879	-0.419149
12	6	0	-0.958160	-0.752653	-0.990338
13	6	0	-0.902879	1.596992	-0.128597
14	1	0	-0.355532	-1.531171	-1.452406
15	1	0	-0.263773	2.298701	0.436149
16	8	0	-2.016868	1.948275	-0.475757
17	7	0	-2.274407	-0.996209	-1.117219
18	1	0	-2.499588	-1.741607	-1.766354
19	6	0	-3.374753	-0.573190	-0.339202
20	6	0	-3.235377	-0.172642	0.989085
21	6	0	-4.644116	-0.662784	-0.912447
22	6	0	-4.367317	0.141391	1.732124
23	1	0	-2.253601	-0.119651	1.443457
24	6	0	-5.768747	-0.342128	-0.162187
25	1	0	-4.739466	-0.987201	-1.943453
26	6	0	-5.636100	0.064482	1.163281
27	1	0	-4.253433	0.447915	2.765770
28	1	0	-6.750609	-0.413393	-0.616206
29	1	0	-6.513035	0.315974	1.748369
30	7	0	5.360844	-0.232424	0.288072
31	8	0	5.795742	-1.325620	0.598706
32	8	0	6.059678	0.749341	0.119794

Structure 28f (C_2H_5OH)

Energy (Hartrees): -913.782601479
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.023968	1.273260	-0.426684
2	6	0	3.392382	1.154086	-0.258192
3	6	0	3.913547	-0.081736	0.106655
4	6	0	3.104648	-1.191540	0.315880
5	6	0	1.736274	-1.049291	0.162521
6	6	0	1.166973	0.177231	-0.220493
7	1	0	1.624044	2.224634	-0.756351
8	1	0	4.048116	1.997712	-0.428664
9	1	0	3.535610	-2.138216	0.614163
10	1	0	1.094263	-1.897951	0.368532
11	6	0	-0.290439	0.299260	-0.406834
12	6	0	-0.954346	-0.769918	-0.977762
13	6	0	-0.909152	1.579076	-0.123227
14	1	0	-0.344348	-1.540002	-1.444319
15	1	0	-0.275799	2.295355	0.426298
16	8	0	-2.036165	1.918126	-0.461914
17	7	0	-2.264622	-1.028363	-1.098759
18	1	0	-2.485746	-1.779842	-1.742755
19	6	0	-3.371619	-0.589912	-0.333448
20	6	0	-3.240123	-0.218015	1.003332
21	6	0	-4.631251	-0.630710	-0.929945
22	6	0	-4.373043	0.122106	1.732982
23	1	0	-2.263824	-0.206987	1.473275
24	6	0	-5.757573	-0.287310	-0.191800
25	1	0	-4.719662	-0.932390	-1.968380
26	6	0	-5.633470	0.093720	1.141675
27	1	0	-4.267101	0.408029	2.773350
28	1	0	-6.733558	-0.319018	-0.662568
29	1	0	-6.511859	0.362691	1.716890
30	7	0	5.357334	-0.218548	0.277009
31	8	0	5.803889	-1.312348	0.571329
32	8	0	6.056056	0.765788	0.117439

Structure 28g (vacuum)

Energy (Hartrees): -913.761064382
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.593567	-0.526378	-0.750556
2	6	0	-2.871377	-1.063226	-0.752558
3	6	0	-3.864736	-0.412243	-0.036718
4	6	0	-3.616776	0.747100	0.682573
5	6	0	-2.329594	1.260064	0.689015
6	6	0	-1.299531	0.641981	-0.033589
7	1	0	-0.820082	-1.006409	-1.338656
8	1	0	-3.111212	-1.960206	-1.307483
9	1	0	-4.418723	1.215969	1.236766
10	1	0	-2.112097	2.138224	1.285387
11	6	0	0.063685	1.206911	-0.042534
12	6	0	0.253266	2.558171	-0.104075
13	6	0	1.216439	0.328905	-0.011938
14	1	0	-0.588477	3.243269	-0.161651
15	1	0	1.034425	-0.748874	0.052233
16	8	0	1.421734	3.152614	-0.130360
17	1	0	2.118625	2.429331	-0.105129
18	7	0	2.416217	0.790300	-0.050118
19	6	0	3.518832	-0.085393	0.046007
20	6	0	3.525615	-1.198105	0.891451
21	6	0	4.653117	0.210316	-0.712869
22	6	0	4.643542	-2.022881	0.943033
23	1	0	2.672795	-1.397268	1.530416
24	6	0	5.762643	-0.621388	-0.661067
25	1	0	4.641559	1.089053	-1.346881
26	6	0	5.761372	-1.743129	0.164196
27	1	0	4.644674	-2.880389	1.605526
28	1	0	6.633990	-0.389921	-1.262115
29	1	0	6.631425	-2.386675	0.209581
30	7	0	-5.228320	-0.972629	-0.037559
31	8	0	-6.081416	-0.372947	0.580747
32	8	0	-5.412788	-1.998922	-0.656195

Structure 28g ($CHCl_3$)

Energy (Hartrees): -913.784878794
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.594015	-0.566072	-0.709670
2	6	0	-2.875461	-1.092841	-0.713148
3	6	0	-3.874718	-0.411979	-0.031344
4	6	0	-3.627940	0.767388	0.658579
5	6	0	-2.337807	1.270600	0.666860
6	6	0	-1.302302	0.622717	-0.024048
7	1	0	-0.819172	-1.073705	-1.272286
8	1	0	-3.105242	-2.003798	-1.249673
9	1	0	-4.427450	1.265826	1.190518
10	1	0	-2.123726	2.167420	1.236191
11	6	0	0.061501	1.185760	-0.037040
12	6	0	0.246022	2.538364	-0.093317
13	6	0	1.216420	0.309540	-0.012559
14	1	0	-0.593055	3.227289	-0.142323
15	1	0	1.041533	-0.768038	0.051151
16	8	0	1.419659	3.129020	-0.123792
17	1	0	2.115618	2.398153	-0.105246
18	7	0	2.413535	0.780963	-0.054109
19	6	0	3.525926	-0.083335	0.039648
20	6	0	3.536689	-1.210464	0.867369
21	6	0	4.665610	0.239929	-0.701529
22	6	0	4.665164	-2.021933	0.918144
23	1	0	2.675412	-1.436666	1.486334
24	6	0	5.786118	-0.579055	-0.650035
25	1	0	4.652177	1.128446	-1.322924
26	6	0	5.790035	-1.714297	0.157866
27	1	0	4.668640	-2.891787	1.565277
28	1	0	6.661317	-0.326904	-1.238002
29	1	0	6.668085	-2.347948	0.202123
30	7	0	-5.237634	-0.955843	-0.042119
31	8	0	-6.113178	-0.312761	0.502117
32	8	0	-5.423093	-2.021265	-0.596102

Structure 28g (DMSO)

Energy (Hartrees): -913.782699947
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.586232	-0.580699	-0.675245
2	6	0	-2.866892	-1.108828	-0.681095
3	6	0	-3.877064	-0.409579	-0.034044
4	6	0	-3.639798	0.791791	0.621799
5	6	0	-2.351372	1.298391	0.631428
6	6	0	-1.304932	0.629767	-0.023381
7	1	0	-0.802240	-1.107909	-1.206195
8	1	0	-3.082577	-2.038103	-1.191364
9	1	0	-4.443740	1.308365	1.129048
10	1	0	-2.152024	2.215585	1.172963
11	6	0	0.060441	1.187305	-0.032130
12	6	0	0.254031	2.540042	-0.085738
13	6	0	1.210217	0.305417	-0.009024
14	1	0	-0.579859	3.235509	-0.131214
15	1	0	1.032685	-0.771172	0.050059
16	8	0	1.433418	3.117987	-0.116827
17	1	0	2.118643	2.372292	-0.101450
18	7	0	2.409094	0.776470	-0.048023
19	6	0	3.522401	-0.086899	0.040210
20	6	0	3.528692	-1.231823	0.844021
21	6	0	4.668700	0.255931	-0.682373
22	6	0	4.661375	-2.038015	0.891165
23	1	0	2.661110	-1.477115	1.446687
24	6	0	5.793848	-0.557654	-0.633852
25	1	0	4.659054	1.156426	-1.286792
26	6	0	5.793961	-1.709751	0.150167
27	1	0	4.660869	-2.921821	1.519417
28	1	0	6.674191	-0.289542	-1.207166
29	1	0	6.674487	-2.340427	0.191810
30	7	0	-5.236734	-0.957134	-0.042653
31	8	0	-6.116834	-0.314916	0.498302
32	8	0	-5.420503	-2.026798	-0.591790

Structure 28g (C_2H_5OH)

Energy (Hartrees): -913.782594512
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.579442	-0.568095	-0.687139
2	6	0	-2.856647	-1.103037	-0.692981
3	6	0	-3.868066	-0.412291	-0.037876
4	6	0	-3.637290	0.788014	0.623108
5	6	0	-2.351711	1.300584	0.632242
6	6	0	-1.303155	0.639555	-0.027391
7	1	0	-0.794372	-1.087474	-1.224283
8	1	0	-3.068858	-2.029746	-1.209618
9	1	0	-4.442708	1.297494	1.135680
10	1	0	-2.154950	2.215457	1.178632
11	6	0	0.060472	1.201513	-0.032791
12	6	0	0.246928	2.553262	-0.081375
13	6	0	1.211918	0.319022	-0.010292
14	1	0	-0.587361	3.247833	-0.125770
15	1	0	1.032184	-0.757254	0.049761
16	8	0	1.427432	3.139450	-0.109149
17	1	0	2.121861	2.405742	-0.096438
18	7	0	2.410817	0.786668	-0.049758
19	6	0	3.518169	-0.085238	0.039710
20	6	0	3.520894	-1.218144	0.860022
21	6	0	4.661210	0.236972	-0.697049
22	6	0	4.646210	-2.034526	0.909170
23	1	0	2.656231	-1.445482	1.474100
24	6	0	5.778593	-0.587145	-0.647250
25	1	0	4.655497	1.129279	-1.313611
26	6	0	5.774882	-1.727865	0.153289
27	1	0	4.643270	-2.908958	1.550566
28	1	0	6.656556	-0.335392	-1.231718
29	1	0	6.649935	-2.366197	0.196394
30	7	0	-5.219271	-0.968618	-0.041671
31	8	0	-6.109400	-0.329830	0.488268
32	8	0	-5.398770	-2.048014	-0.574627

Structure 29a (vacuum)

Energy (Hartrees): -1028.28159041
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.225624	1.251910	0.581115
2	6	0	-4.456164	0.625455	0.693757
3	6	0	-4.622843	-0.622060	0.110762
4	6	0	-3.601824	-1.249672	-0.587915
5	6	0	-2.384048	-0.600371	-0.707633
6	6	0	-2.166018	0.655030	-0.119441
7	1	0	-3.075190	2.206780	1.070465
8	1	0	-5.275333	1.077209	1.236854
9	1	0	-3.778028	-2.216174	-1.040864
10	1	0	-1.596792	-1.060805	-1.293320
11	6	0	-0.865125	1.337002	-0.229778
12	6	0	0.306869	0.616999	-0.148722
13	6	0	-0.819642	2.773725	-0.413092
14	1	0	0.262510	-0.454540	0.025558
15	1	0	-1.796205	3.276605	-0.523725
16	8	0	0.206793	3.438381	-0.473844
17	7	0	1.536343	1.135484	-0.225408
18	1	0	1.575807	2.150418	-0.316138
19	6	0	2.740160	0.403256	-0.136952
20	6	0	3.870850	1.030330	0.371493
21	6	0	2.831271	-0.923310	-0.567800
22	6	0	5.081168	0.350509	0.468428
23	1	0	3.804859	2.059374	0.706732
24	6	0	4.026187	-1.609390	-0.456612
25	1	0	1.976415	-1.414292	-1.017095
26	6	0	5.161005	-0.980141	0.061535
27	1	0	5.942060	0.867313	0.869516
28	1	0	4.113876	-2.635744	-0.790310
29	8	0	6.285040	-1.736365	0.117567
30	6	0	7.462874	-1.128774	0.607792
31	1	0	7.338665	-0.808475	1.646993
32	1	0	8.238486	-1.889049	0.553480
33	1	0	7.750252	-0.271149	-0.008436
34	7	0	-5.924406	-1.299699	0.234104
35	8	0	-6.040421	-2.392164	-0.279934
36	8	0	-6.801351	-0.724972	0.843436

Structure 29a ($CHCl_3$)

Energy (Hartrees): -1028.30877342
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.247461	1.276409	0.525403
2	6	0	-4.475262	0.646710	0.637340
3	6	0	-4.619868	-0.629711	0.109598
4	6	0	-3.574212	-1.282142	-0.532114
5	6	0	-2.359061	-0.630313	-0.652376
6	6	0	-2.164655	0.656386	-0.121584
7	1	0	-3.119682	2.253677	0.975452
8	1	0	-5.303689	1.125299	1.142592
9	1	0	-3.720592	-2.271979	-0.944063
10	1	0	-1.555185	-1.121081	-1.188557
11	6	0	-0.867750	1.345688	-0.227774
12	6	0	0.310512	0.623701	-0.159074
13	6	0	-0.833013	2.778427	-0.399935
14	1	0	0.268683	-0.451707	-0.011943
15	1	0	-1.808190	3.278074	-0.522616
16	8	0	0.192522	3.455815	-0.446760
17	7	0	1.535319	1.143588	-0.219188
18	1	0	1.588678	2.159477	-0.283148
19	6	0	2.741026	0.408546	-0.142317
20	6	0	3.864794	1.024690	0.395738
21	6	0	2.835467	-0.904937	-0.609747
22	6	0	5.075052	0.343610	0.488338
23	1	0	3.793974	2.045610	0.755410
24	6	0	4.031917	-1.591760	-0.505786
25	1	0	1.984432	-1.385772	-1.077400
26	6	0	5.160163	-0.975841	0.044288
27	1	0	5.930469	0.849278	0.915718
28	1	0	4.118991	-2.609359	-0.867857
29	8	0	6.285183	-1.731042	0.094640
30	6	0	7.455273	-1.139755	0.637639
31	1	0	7.304517	-0.858291	1.684118
32	1	0	8.231456	-1.900306	0.577438
33	1	0	7.760235	-0.263486	0.057867
34	7	0	-5.911394	-1.308637	0.235469
35	8	0	-6.015072	-2.431606	-0.219230
36	8	0	-6.817521	-0.717209	0.789750

Structure 29a (DMSO)

Energy (Hartrees): -1028.30837106
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.256469	1.279230	0.529433
2	6	0	-4.491192	0.660546	0.623410
3	6	0	-4.641001	-0.612874	0.088426
4	6	0	-3.592788	-1.272879	-0.542254
5	6	0	-2.370074	-0.632545	-0.645019
6	6	0	-2.171547	0.651081	-0.107153
7	1	0	-3.126578	2.254221	0.984153
8	1	0	-5.319644	1.147446	1.120760
9	1	0	-3.739399	-2.259788	-0.961196
10	1	0	-1.563948	-1.130374	-1.171379
11	6	0	-0.867978	1.328607	-0.198503
12	6	0	0.301006	0.590503	-0.127160
13	6	0	-0.823914	2.761621	-0.364217
14	1	0	0.240587	-0.483635	0.018986
15	1	0	-1.796724	3.265394	-0.486622
16	8	0	0.204549	3.435811	-0.403927
17	7	0	1.531343	1.095862	-0.189260
18	1	0	1.600212	2.109845	-0.264497
19	6	0	2.737085	0.364306	-0.108256
20	6	0	3.896464	1.050123	0.238104
21	6	0	2.806926	-1.004336	-0.383638
22	6	0	5.119091	0.390453	0.326752
23	1	0	3.844381	2.113695	0.446917
24	6	0	4.018140	-1.666794	-0.284488
25	1	0	1.927872	-1.558080	-0.690760
26	6	0	5.183286	-0.979398	0.071174
27	1	0	6.000924	0.955699	0.598172
28	1	0	4.080736	-2.727586	-0.498203
29	8	0	6.317847	-1.717862	0.132174
30	6	0	7.520849	-1.046851	0.480404
31	1	0	7.452434	-0.612490	1.481919
32	1	0	8.302403	-1.804186	0.467466
33	1	0	7.760242	-0.264706	-0.245720
34	7	0	-5.939462	-1.278393	0.193587
35	8	0	-6.044601	-2.407283	-0.249244
36	8	0	-6.854540	-0.672229	0.719450

Structure 29a (C_2H_5OH)

Energy (Hartrees): -1028.30919811
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.248676	1.276737	0.536295
2	6	0	-4.472769	0.640809	0.645245
3	6	0	-4.611238	-0.632763	0.106148
4	6	0	-3.562958	-1.276227	-0.542402
5	6	0	-2.350867	-0.619085	-0.656985
6	6	0	-2.163806	0.665058	-0.115990
7	1	0	-3.126045	2.251907	0.992734
8	1	0	-5.300181	1.115194	1.156340
9	1	0	-3.700597	-2.263163	-0.964522
10	1	0	-1.544552	-1.104049	-1.195039
11	6	0	-0.869888	1.359525	-0.218756
12	6	0	0.309769	0.632924	-0.154949
13	6	0	-0.843545	2.786524	-0.385352
14	1	0	0.262307	-0.442735	-0.013590
15	1	0	-1.819389	3.284235	-0.498850
16	8	0	0.182907	3.472714	-0.438218
17	7	0	1.533876	1.146591	-0.215153
18	1	0	1.601491	2.161676	-0.274684
19	6	0	2.737214	0.405752	-0.142800
20	6	0	3.873035	1.035088	0.353519
21	6	0	2.815949	-0.920995	-0.573820
22	6	0	5.082357	0.352179	0.445966
23	1	0	3.813188	2.068051	0.680053
24	6	0	4.012864	-1.608425	-0.470972
25	1	0	1.954780	-1.414665	-1.008895
26	6	0	5.151747	-0.980159	0.040794
27	1	0	5.948257	0.867626	0.839701
28	1	0	4.086968	-2.637371	-0.803995
29	8	0	6.278690	-1.739343	0.095586
30	6	0	7.451212	-1.142973	0.637405
31	1	0	7.289538	-0.838871	1.675309
32	1	0	8.221982	-1.910512	0.599231
33	1	0	7.764363	-0.281442	0.041468
34	7	0	-5.894595	-1.315255	0.227028
35	8	0	-6.003755	-2.434767	-0.240349
36	8	0	-6.806527	-0.738485	0.791924

Structure 29b (vacuum)

Energy (Hartrees): -1028.27502628
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.070535	1.177997	-0.811635
2	6	0	-4.164104	0.325868	-0.824346
3	6	0	-4.178167	-0.746345	0.054980
4	6	0	-3.145697	-0.982078	0.950773
5	6	0	-2.064466	-0.114047	0.957294
6	6	0	-2.001447	0.973451	0.072235
7	1	0	-3.031491	2.003533	-1.512743
8	1	0	-4.990205	0.470578	-1.507384
9	1	0	-3.208740	-1.819644	1.632497
10	1	0	-1.270698	-0.257721	1.682325
11	6	0	-0.852502	1.896238	0.070701
12	6	0	0.448386	1.490571	0.048688
13	6	0	-1.087067	3.346046	0.049928
14	1	0	1.206964	2.267869	0.041230
15	1	0	-2.153213	3.643173	0.090771
16	8	0	-0.221597	4.191939	0.012073
17	7	0	0.898263	0.222410	-0.016678
18	1	0	0.215141	-0.512371	-0.147670
19	6	0	2.255253	-0.166344	-0.054305
20	6	0	2.591291	-1.379455	-0.663341
21	6	0	3.260163	0.611586	0.505470
22	6	0	3.907068	-1.793810	-0.720782
23	1	0	1.813550	-1.993295	-1.105115
24	6	0	4.592217	0.207599	0.430463
25	1	0	3.019797	1.532207	1.022576
26	6	0	4.922346	-0.997522	-0.183611
27	1	0	4.179112	-2.729829	-1.192199
28	1	0	5.351632	0.838591	0.871283
29	8	0	6.183249	-1.483233	-0.303132
30	6	0	7.239518	-0.709040	0.227224
31	1	0	7.129567	-0.579035	1.308546
32	1	0	8.152074	-1.263047	0.020454
33	1	0	7.292132	0.271481	-0.256503
34	7	0	-5.330514	-1.666778	0.040643
35	8	0	-5.303275	-2.610983	0.800782
36	8	0	-6.232553	-1.423498	-0.731503

Structure 29b ($CHCl_3$)

Energy (Hartrees): -1028.30410560
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.073305	1.187989	-0.802050
2	6	0	-4.168208	0.339172	-0.825667
3	6	0	-4.185931	-0.742033	0.045046
4	6	0	-3.157073	-0.986482	0.944752
5	6	0	-2.074562	-0.121261	0.961819
6	6	0	-2.007077	0.972860	0.084667
7	1	0	-3.032133	2.018464	-1.497808
8	1	0	-4.985341	0.498127	-1.516636
9	1	0	-3.214249	-1.827600	1.622907
10	1	0	-1.282974	-0.278940	1.686340
11	6	0	-0.853678	1.891349	0.085835
12	6	0	0.454524	1.484655	0.079844
13	6	0	-1.094022	3.329556	0.047665
14	1	0	1.212861	2.262078	0.073888
15	1	0	-2.158947	3.623237	0.090594
16	8	0	-0.234290	4.192187	-0.006553
17	7	0	0.907159	0.224731	0.031022
18	1	0	0.232825	-0.522548	-0.089570
19	6	0	2.265253	-0.164624	-0.010330
20	6	0	2.580893	-1.407883	-0.567708
21	6	0	3.285660	0.636372	0.488086
22	6	0	3.895182	-1.827559	-0.643661
23	1	0	1.787219	-2.039628	-0.952965
24	6	0	4.614673	0.224229	0.396805
25	1	0	3.065728	1.582965	0.966991
26	6	0	4.926105	-1.007996	-0.173773
27	1	0	4.147237	-2.787086	-1.079624
28	1	0	5.387634	0.871770	0.788594
29	8	0	6.184577	-1.496965	-0.308366
30	6	0	7.259924	-0.678601	0.122972
31	1	0	7.204605	-0.486634	1.198689
32	1	0	8.168060	-1.236691	-0.096741
33	1	0	7.276325	0.269324	-0.423033
34	7	0	-5.332564	-1.658636	0.014388
35	8	0	-5.299969	-2.638086	0.732505
36	8	0	-6.255462	-1.393131	-0.729498

Structure 29b (DMSO)

Energy (Hartrees): -1028.30448153
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.136954	1.242000	-0.709661
2	6	0	-4.238232	0.402160	-0.722117
3	6	0	-4.203720	-0.748013	0.055844
4	6	0	-3.111501	-1.070125	0.851148
5	6	0	-2.022717	-0.213827	0.859849
6	6	0	-2.008578	0.951466	0.075264
7	1	0	-3.143640	2.125916	-1.337213
8	1	0	-5.101449	0.626148	-1.334975
9	1	0	-3.120909	-1.964586	1.459753
10	1	0	-1.183082	-0.443887	1.506231
11	6	0	-0.857178	1.870180	0.074220
12	6	0	0.456834	1.475163	0.039219
13	6	0	-1.105021	3.307076	0.091997
14	1	0	1.207412	2.259526	0.063905
15	1	0	-2.166066	3.591910	0.212910
16	8	0	-0.255386	4.178711	0.005647
17	7	0	0.923457	0.226312	-0.063702
18	1	0	0.262175	-0.527979	-0.216927
19	6	0	2.284330	-0.151464	-0.078404
20	6	0	2.617791	-1.387626	-0.642226
21	6	0	3.289465	0.645148	0.458252
22	6	0	3.934646	-1.805834	-0.683004
23	1	0	1.835166	-2.016059	-1.054630
24	6	0	4.620997	0.233700	0.403391
25	1	0	3.057045	1.586330	0.941952
26	6	0	4.950875	-0.993713	-0.168806
27	1	0	4.196581	-2.762252	-1.120507
28	1	0	5.380316	0.877420	0.827261
29	8	0	6.212803	-1.481816	-0.261230
30	6	0	7.267750	-0.663245	0.223683
31	1	0	7.160007	-0.473089	1.295410
32	1	0	8.186477	-1.219310	0.047209
33	1	0	7.308826	0.286475	-0.317563
34	7	0	-5.357538	-1.652080	0.037935
35	8	0	-5.298989	-2.669688	0.701761
36	8	0	-6.317554	-1.342765	-0.641721

Structure 29b (C_2H_5OH)

Energy (Hartrees): -1028.30575914
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.123377	1.226142	-0.741259
2	6	0	-4.226615	0.389558	-0.750717
3	6	0	-4.204433	-0.744478	0.051584
4	6	0	-3.122237	-1.056484	0.864853
5	6	0	-2.031734	-0.202756	0.869652
6	6	0	-2.007142	0.948211	0.064652
7	1	0	-3.119504	2.097604	-1.385996
8	1	0	-5.081431	0.604114	-1.378417
9	1	0	-3.140117	-1.938834	1.490809
10	1	0	-1.200492	-0.421118	1.530845
11	6	0	-0.855107	1.867314	0.067699
12	6	0	0.461482	1.468264	0.044194
13	6	0	-1.102331	3.295495	0.079473
14	1	0	1.216471	2.248427	0.070523
15	1	0	-2.163155	3.586270	0.166978
16	8	0	-0.246389	4.173342	0.021411
17	7	0	0.922168	0.220119	-0.050133
18	1	0	0.258601	-0.533803	-0.197595
19	6	0	2.284341	-0.159911	-0.065632
20	6	0	2.617991	-1.387893	-0.644965
21	6	0	3.285766	0.631680	0.484374
22	6	0	3.935915	-1.802642	-0.690872
23	1	0	1.836840	-2.011599	-1.067215
24	6	0	4.617843	0.224485	0.424378
25	1	0	3.049315	1.564904	0.981555
26	6	0	4.947578	-0.993400	-0.165938
27	1	0	4.201928	-2.751517	-1.142499
28	1	0	5.376598	0.862821	0.857230
29	8	0	6.215238	-1.477868	-0.266774
30	6	0	7.275177	-0.652843	0.201605
31	1	0	7.186779	-0.471541	1.276297
32	1	0	8.192745	-1.202928	0.001575
33	1	0	7.295212	0.298639	-0.337004
34	7	0	-5.361472	-1.638527	0.041635
35	8	0	-5.323684	-2.641927	0.729245
36	8	0	-6.314336	-1.341925	-0.654643

Structure 29c (vacuum)

Energy (Hartrees): -1028.27652650
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.029481	1.136938	-0.787588
2	6	0	4.088510	0.242775	-0.802652
3	6	0	4.058469	-0.839176	0.064915
4	6	0	3.015904	-1.047839	0.954121
5	6	0	1.963117	-0.144427	0.957493
6	6	0	1.946674	0.949493	0.080829
7	1	0	3.039907	1.994381	-1.446766
8	1	0	4.928587	0.370298	-1.471706
9	1	0	3.046413	-1.892624	1.628880
10	1	0	1.157308	-0.269724	1.672630
11	6	0	0.817111	1.900410	0.077315
12	6	0	-0.489222	1.517628	0.049105
13	6	0	1.059062	3.342863	0.035945
14	1	0	-1.254419	2.289231	0.048901
15	7	0	-0.962745	0.255299	-0.032074
16	1	0	-0.292129	-0.485753	-0.189215
17	6	0	-2.328324	-0.100451	-0.069220
18	6	0	-2.709696	-1.258049	-0.755400
19	6	0	-3.300530	0.659231	0.568160
20	6	0	-4.037059	-1.633301	-0.811543
21	1	0	-1.957607	-1.856998	-1.257504
22	6	0	-4.645090	0.297650	0.493992
23	1	0	-3.022229	1.529447	1.150357
24	6	0	-5.019586	-0.851909	-0.196127
25	1	0	-4.343887	-2.526165	-1.341793
26	1	0	-5.378284	0.912567	0.997281
27	8	0	2.141870	3.875298	-0.030599
28	1	0	0.135123	3.956731	0.072351
29	8	0	-6.295098	-1.295940	-0.320809
30	6	0	-7.319579	-0.531463	0.280971
31	1	0	-8.250540	-1.047295	0.058379
32	1	0	-7.185374	-0.475812	1.365840
33	1	0	-7.354862	0.479682	-0.136879
34	7	0	5.179319	-1.799307	0.049926
35	8	0	5.121529	-2.740927	0.812092
36	8	0	6.086764	-1.589949	-0.725389

Structure 29c ($CHCl_3$)

Energy (Hartrees): -1028.30637666
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.053177	1.047367	-0.854565
2	6	0	4.076127	0.113150	-0.853871
3	6	0	4.010049	-0.941724	0.046646
4	6	0	2.967425	-1.082533	0.951313
5	6	0	1.954660	-0.135676	0.941105
6	6	0	1.975298	0.934932	0.035043
7	1	0	3.085586	1.874004	-1.552268
8	1	0	4.906918	0.190948	-1.542448
9	1	0	2.960278	-1.907022	1.651859
10	1	0	1.150491	-0.213959	1.664815
11	6	0	0.891859	1.937860	0.018588
12	6	0	-0.440506	1.622981	0.039348
13	6	0	1.193339	3.357401	-0.052108
14	1	0	-1.157354	2.439565	0.042519
15	7	0	-0.981779	0.395342	0.011866
16	1	0	-0.368827	-0.397114	-0.142975
17	6	0	-2.368456	0.119586	0.041682
18	6	0	-2.848719	-1.013407	-0.605096
19	6	0	-3.262760	0.950677	0.722298
20	6	0	-4.207783	-1.317461	-0.596200
21	1	0	-2.157672	-1.663427	-1.131267
22	6	0	-4.616278	0.663284	0.716845
23	1	0	-2.904675	1.812156	1.274125
24	6	0	-5.100890	-0.469941	0.058098
25	1	0	-4.549178	-2.205722	-1.110771
26	1	0	-5.318695	1.301314	1.240008
27	8	0	2.305138	3.850554	-0.106383
28	1	0	0.300216	4.011824	-0.045343
29	8	0	-6.442216	-0.664969	0.117351
30	6	0	-6.971005	-1.817058	-0.519368
31	1	0	-8.045430	-1.788076	-0.349108
32	1	0	-6.773568	-1.799233	-1.595338
33	1	0	-6.560263	-2.732080	-0.082289
34	7	0	5.083451	-1.945183	0.043882
35	8	0	4.960726	-2.914049	0.766970
36	8	0	6.037259	-1.757898	-0.684225

Structure 29c (DMSO)

Energy (Hartrees): -1028.30767651
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.009057	1.118420	-0.823478
2	6	0	4.074397	0.233883	-0.850060
3	6	0	4.073115	-0.831801	0.041365
4	6	0	3.049984	-1.032556	0.957148
5	6	0	1.992150	-0.135651	0.971421
6	6	0	1.949080	0.944034	0.077953
7	1	0	2.990823	1.950326	-1.515647
8	1	0	4.887126	0.361491	-1.552567
9	1	0	3.086694	-1.864189	1.648271
10	1	0	1.200089	-0.266396	1.700712
11	6	0	0.819855	1.894665	0.077530
12	6	0	-0.499459	1.520475	0.069539
13	6	0	1.058150	3.325287	0.047506
14	1	0	-1.248662	2.307103	0.066172
15	7	0	-0.980344	0.271237	0.022214
16	1	0	-0.324684	-0.495027	-0.089629
17	6	0	-2.346177	-0.086638	-0.018743
18	6	0	-2.684642	-1.336321	-0.548689
19	6	0	-3.353822	0.746192	0.454805
20	6	0	-4.007485	-1.730930	-0.621564
21	1	0	-1.901045	-1.993813	-0.910916
22	6	0	-4.690879	0.358447	0.366804
23	1	0	-3.120296	1.700090	0.912359
24	6	0	-5.025013	-0.881201	-0.175192
25	1	0	-4.273149	-2.697675	-1.033358
26	1	0	-5.451533	1.031096	0.740610
27	8	0	2.148593	3.871570	0.035527
28	1	0	0.136606	3.937449	0.049870
29	8	0	-6.292667	-1.347359	-0.300665
30	6	0	-7.347557	-0.502141	0.135439
31	1	0	-8.269596	-1.047472	-0.056707
32	1	0	-7.268313	-0.291090	1.205750
33	1	0	-7.358480	0.436677	-0.425959
34	7	0	5.195548	-1.777628	0.017713
35	8	0	5.162869	-2.725189	0.779067
36	8	0	6.104139	-1.567625	-0.762574

Structure 29c (C_2H_5OH)

Energy (Hartrees): -1028.30929611
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.985272	1.089807	-0.860765
2	6	0	4.049674	0.204242	-0.881867
3	6	0	4.064409	-0.831927	0.043345
4	6	0	3.061589	-1.003861	0.987467
5	6	0	2.007412	-0.102947	0.998182
6	6	0	1.948204	0.947676	0.072053
7	1	0	2.948251	1.894356	-1.584983
8	1	0	4.845898	0.306018	-1.607436
9	1	0	3.112814	-1.812452	1.704790
10	1	0	1.230714	-0.207476	1.748194
11	6	0	0.821118	1.902946	0.069218
12	6	0	-0.500671	1.528114	0.061367
13	6	0	1.058850	3.324887	0.042469
14	1	0	-1.251257	2.313259	0.053921
15	7	0	-0.974961	0.279503	0.019951
16	1	0	-0.314644	-0.484819	-0.080548
17	6	0	-2.340822	-0.084727	-0.016872
18	6	0	-2.675666	-1.333128	-0.550249
19	6	0	-3.347534	0.743963	0.464908
20	6	0	-3.997985	-1.730113	-0.621727
21	1	0	-1.891545	-1.987416	-0.917055
22	6	0	-4.683755	0.354545	0.378008
23	1	0	-3.113430	1.695257	0.927767
24	6	0	-5.013660	-0.882513	-0.170141
25	1	0	-4.264329	-2.695489	-1.036782
26	1	0	-5.445778	1.022922	0.756611
27	8	0	2.158050	3.870267	0.041473
28	1	0	0.145099	3.944990	0.037040
29	8	0	-6.285219	-1.350871	-0.298307
30	6	0	-7.346104	-0.505186	0.128592
31	1	0	-8.264706	-1.052074	-0.075537
32	1	0	-7.276190	-0.298283	1.200039
33	1	0	-7.348219	0.433053	-0.433149
34	7	0	5.180760	-1.779864	0.022206
35	8	0	5.124968	-2.754657	0.747538
36	8	0	6.115294	-1.552238	-0.722191

Structure 29d (vacuum)

Energy (Hartrees): -1028.26811538
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.178647	1.195662	0.599784
2	6	0	-4.342179	0.453036	0.725106
3	6	0	-4.408781	-0.792326	0.118352
4	6	0	-3.356447	-1.310531	-0.619923
5	6	0	-2.202691	-0.552708	-0.742245
6	6	0	-2.085144	0.699202	-0.122808
7	1	0	-3.113665	2.169771	1.063802
8	1	0	-5.190520	0.820313	1.286538
9	1	0	-3.458747	-2.276664	-1.095308
10	1	0	-1.389165	-0.927675	-1.352702
11	6	0	-0.828967	1.474799	-0.225741
12	6	0	0.366138	0.819327	-0.131248
13	6	0	-0.875261	2.922341	-0.424406
14	1	0	0.351536	-0.255911	0.021078
15	7	0	1.617056	1.336513	-0.153350
16	1	0	1.737059	2.337419	-0.147577
17	6	0	2.801547	0.565513	-0.109578
18	6	0	3.930424	1.083093	0.512829
19	6	0	2.867708	-0.700520	-0.697817
20	6	0	5.115835	0.354785	0.563054
21	1	0	3.885694	2.062346	0.977101
22	6	0	4.034582	-1.438904	-0.628626
23	1	0	2.013973	-1.100164	-1.231938
24	6	0	5.168544	-0.918845	0.000225
25	1	0	5.976670	0.788161	1.053101
26	1	0	4.101682	-2.421378	-1.079089
27	1	0	0.105794	3.414544	-0.585510
28	8	0	-1.874651	3.602854	-0.448960
29	8	0	6.264450	-1.716889	0.002308
30	6	0	7.429954	-1.233217	0.638383
31	1	0	7.248045	-1.041396	1.700458
32	1	0	8.177083	-2.016285	0.534169
33	1	0	7.792319	-0.319278	0.157179
34	7	0	-5.642588	-1.588297	0.251677
35	8	0	-5.675918	-2.669528	-0.297553
36	8	0	-6.548721	-1.115881	0.904000

Structure 29d ($CHCl_3$)

Energy (Hartrees): -1028.29934584
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.164155	1.181253	0.633703
2	6	0	-4.333208	0.449453	0.760614
3	6	0	-4.425481	-0.777635	0.116700
4	6	0	-3.389706	-1.285847	-0.654774
5	6	0	-2.230434	-0.537550	-0.777296
6	6	0	-2.088674	0.698247	-0.127779
7	1	0	-3.078384	2.133461	1.138850
8	1	0	-5.159470	0.815143	1.355605
9	1	0	-3.500238	-2.237132	-1.158102
10	1	0	-1.429055	-0.908529	-1.405842
11	6	0	-0.829062	1.465657	-0.229436
12	6	0	0.365219	0.786067	-0.179812
13	6	0	-0.862650	2.909055	-0.391658
14	1	0	0.332404	-0.294209	-0.073338
15	7	0	1.610762	1.289197	-0.198791
16	1	0	1.742771	2.291393	-0.162434
17	6	0	2.797645	0.521983	-0.135538
18	6	0	3.936028	1.098406	0.416453
19	6	0	2.862475	-0.784131	-0.628263
20	6	0	5.130210	0.387902	0.496414
21	1	0	3.891211	2.113356	0.797225
22	6	0	4.042321	-1.501460	-0.532962
23	1	0	2.002196	-1.238718	-1.104734
24	6	0	5.184695	-0.924579	0.029129
25	1	0	5.996359	0.865851	0.933766
26	1	0	4.104099	-2.514911	-0.911600
27	1	0	0.116788	3.401516	-0.533036
28	8	0	-1.865650	3.599782	-0.416667
29	8	0	6.291865	-1.707753	0.067942
30	6	0	7.474702	-1.150800	0.619010
31	1	0	7.330294	-0.881056	1.669487
32	1	0	8.234245	-1.927029	0.547874
33	1	0	7.798832	-0.273041	0.051909
34	7	0	-5.660174	-1.558335	0.248546
35	8	0	-5.710327	-2.645942	-0.292436
36	8	0	-6.572852	-1.080870	0.893542

Structure 29d (DMSO)

Energy (Hartrees): -1028.30108677
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.166893	1.183133	0.631481
2	6	0	-4.337753	0.453709	0.753040
3	6	0	-4.426877	-0.777300	0.114975
4	6	0	-3.382577	-1.291905	-0.641966
5	6	0	-2.221443	-0.545824	-0.759727
6	6	0	-2.084515	0.696337	-0.119229
7	1	0	-3.084120	2.135303	1.137124
8	1	0	-5.165909	0.825475	1.341592
9	1	0	-3.483949	-2.247054	-1.140131
10	1	0	-1.414529	-0.926837	-1.375106
11	6	0	-0.828357	1.466962	-0.219054
12	6	0	0.367802	0.784982	-0.168766
13	6	0	-0.862660	2.907788	-0.389598
14	1	0	0.332390	-0.295838	-0.068969
15	7	0	1.610048	1.286864	-0.182859
16	1	0	1.746849	2.289701	-0.143614
17	6	0	2.796032	0.518206	-0.128444
18	6	0	3.942139	1.102537	0.400196
19	6	0	2.854066	-0.794427	-0.605404
20	6	0	5.137132	0.392511	0.476285
21	1	0	3.902148	2.124085	0.763677
22	6	0	4.036405	-1.509780	-0.515788
23	1	0	1.988260	-1.257816	-1.063487
24	6	0	5.186300	-0.926611	0.025083
25	1	0	6.008495	0.877845	0.895209
26	1	0	4.089300	-2.527884	-0.883722
27	1	0	0.116903	3.400320	-0.519883
28	8	0	-1.868265	3.597994	-0.435399
29	8	0	6.294609	-1.707412	0.060806
30	6	0	7.476610	-1.140964	0.608751
31	1	0	7.329841	-0.862497	1.656427
32	1	0	8.240034	-1.914014	0.544569
33	1	0	7.797598	-0.265891	0.036530
34	7	0	-5.662838	-1.553644	0.240461
35	8	0	-5.714044	-2.643614	-0.298005
36	8	0	-6.580580	-1.072412	0.878291

Structure 29d (C_2H_5OH)

Energy (Hartrees): -1028.30242553
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.168698	1.182473	0.639166
2	6	0	-4.337869	0.450508	0.757516
3	6	0	-4.421394	-0.778844	0.114847
4	6	0	-3.375738	-1.289941	-0.643225
5	6	0	-2.217290	-0.540198	-0.757798
6	6	0	-2.085457	0.699961	-0.112895
7	1	0	-3.086965	2.130672	1.153353
8	1	0	-5.166532	0.818095	1.348331
9	1	0	-3.474403	-2.243645	-1.144975
10	1	0	-1.408530	-0.915591	-1.374287
11	6	0	-0.830358	1.473284	-0.211133
12	6	0	0.369400	0.792577	-0.152166
13	6	0	-0.866259	2.904435	-0.396232
14	1	0	0.334106	-0.287617	-0.044829
15	7	0	1.608317	1.294569	-0.166699
16	1	0	1.745843	2.297980	-0.138939
17	6	0	2.795223	0.524090	-0.117789
18	6	0	3.938565	1.099849	0.424975
19	6	0	2.852084	-0.779414	-0.617511
20	6	0	5.132479	0.387566	0.493288
21	1	0	3.897808	2.115131	0.805435
22	6	0	4.033170	-1.497599	-0.535879
23	1	0	1.986937	-1.231727	-1.087883
24	6	0	5.179268	-0.922626	0.019457
25	1	0	6.003474	0.863644	0.923379
26	1	0	4.089123	-2.509462	-0.920777
27	1	0	0.107872	3.406959	-0.514169
28	8	0	-1.880608	3.590435	-0.468676
29	8	0	6.290513	-1.707698	0.045405
30	6	0	7.476026	-1.153244	0.602927
31	1	0	7.327274	-0.892178	1.654382
32	1	0	8.234871	-1.929666	0.525913
33	1	0	7.797606	-0.271472	0.041973
34	7	0	-5.650722	-1.558415	0.238586
35	8	0	-5.700023	-2.651776	-0.294735
36	8	0	-6.576201	-1.083643	0.871081

Structure 29g (vacuum)

Energy (Hartrees): -1028.27343382
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.316087	-0.513769	-0.747689
2	6	0	-3.527494	-1.186569	-0.757524
3	6	0	-4.589937	-0.648847	-0.047063
4	6	0	-4.472950	0.528917	0.675537
5	6	0	-3.249808	1.180383	0.688310
6	6	0	-2.155284	0.680277	-0.030460
7	1	0	-1.491076	-0.905881	-1.330900
8	1	0	-3.664487	-2.104614	-1.312823
9	1	0	-5.323657	0.904705	1.227955
10	1	0	-3.134080	2.076760	1.285929
11	6	0	-0.861431	1.389252	-0.040227
12	6	0	-0.816294	2.751787	-0.105340
13	6	0	0.377873	0.635957	-0.004875
14	1	0	-1.725471	3.345179	-0.154328
15	1	0	0.306161	-0.452748	0.087875
16	8	0	0.285353	3.464616	-0.141743
17	1	0	1.052890	2.816578	-0.122132
18	7	0	1.523518	1.216566	-0.063452
19	6	0	2.710238	0.462074	0.057658
20	6	0	2.822437	-0.644723	0.909263
21	6	0	3.824444	0.860927	-0.673241
22	6	0	4.008954	-1.348971	0.991872
23	1	0	1.986011	-0.932027	1.536204
24	6	0	5.020104	0.152532	-0.604368
25	1	0	3.744381	1.729903	-1.315765
26	6	0	5.114119	-0.961788	0.228715
27	1	0	4.113810	-2.197180	1.656950
28	1	0	5.862909	0.481499	-1.196819
29	8	0	6.230907	-1.717489	0.377029
30	6	0	7.381535	-1.340388	-0.350737
31	1	0	8.153754	-2.059648	-0.087987
32	1	0	7.198019	-1.381612	-1.428940
33	1	0	7.711314	-0.334152	-0.073837
34	7	0	-5.883857	-1.354980	-0.056005
35	8	0	-6.796578	-0.861608	0.571230
36	8	0	-5.956009	-2.385542	-0.690789

Structure 29g ($CHCl_3$)

Energy (Hartrees): -1028.29826692
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.308221	-0.573481	-0.664594
2	6	0	-3.527325	-1.231101	-0.684125
3	6	0	-4.610206	-0.640680	-0.046943
4	6	0	-4.504131	0.575073	0.615473
5	6	0	-3.274928	1.212348	0.637563
6	6	0	-2.159851	0.659182	-0.010508
7	1	0	-1.468551	-1.013454	-1.189792
8	1	0	-3.644769	-2.177302	-1.195392
9	1	0	-5.364600	1.000782	1.114240
10	1	0	-3.175227	2.143275	1.182958
11	6	0	-0.861546	1.359141	-0.020265
12	6	0	-0.811324	2.721435	-0.104009
13	6	0	0.375886	0.601898	0.022527
14	1	0	-1.714491	3.323482	-0.159181
15	1	0	0.308800	-0.483940	0.135055
16	8	0	0.300565	3.422172	-0.151514
17	1	0	1.063390	2.758518	-0.130234
18	7	0	1.518680	1.188269	-0.055225
19	6	0	2.715538	0.448933	0.064649
20	6	0	2.845884	-0.651201	0.922228
21	6	0	3.819677	0.857512	-0.678204
22	6	0	4.044106	-1.338161	1.001436
23	1	0	2.014282	-0.951076	1.550084
24	6	0	5.026298	0.166523	-0.612786
25	1	0	3.725410	1.720795	-1.327634
26	6	0	5.139778	-0.940905	0.228153
27	1	0	4.159189	-2.182051	1.671655
28	1	0	5.861508	0.502296	-1.212826
29	8	0	6.268509	-1.679343	0.371995
30	6	0	7.404295	-1.304160	-0.390606
31	1	0	8.188802	-2.012164	-0.130767
32	1	0	7.197848	-1.369059	-1.463015
33	1	0	7.731718	-0.291484	-0.137718
34	7	0	-5.907225	-1.325999	-0.070015
35	8	0	-6.837398	-0.808510	0.516124
36	8	0	-5.987560	-2.376650	-0.675442

Structure 29g (DMSO)

Energy (Hartrees): -1028.29689417
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.346018	-0.585259	-0.682385
2	6	0	-3.577144	-1.220462	-0.686741
3	6	0	-4.643226	-0.609231	-0.039799
4	6	0	-4.509152	0.608669	0.614719
5	6	0	-3.269326	1.224330	0.620704
6	6	0	-2.170008	0.647408	-0.034535
7	1	0	-1.519658	-1.046319	-1.210684
8	1	0	-3.712623	-2.167612	-1.191982
9	1	0	-5.354179	1.055773	1.121071
10	1	0	-3.149455	2.156844	1.159394
11	6	0	-0.859792	1.323679	-0.045444
12	6	0	-0.788719	2.687632	-0.106537
13	6	0	0.364831	0.547239	-0.011183
14	1	0	-1.682724	3.303601	-0.159544
15	1	0	0.279960	-0.540258	0.053749
16	8	0	0.335986	3.367650	-0.133006
17	1	0	1.083018	2.679956	-0.105737
18	7	0	1.514570	1.127863	-0.043414
19	6	0	2.714245	0.391111	0.058047
20	6	0	2.824012	-0.815709	0.762920
21	6	0	3.852658	0.921744	-0.543877
22	6	0	4.036123	-1.479919	0.826622
23	1	0	1.967098	-1.226076	1.285311
24	6	0	5.075185	0.257674	-0.490469
25	1	0	3.774575	1.865599	-1.072665
26	6	0	5.169144	-0.954306	0.194972
27	1	0	4.128891	-2.409045	1.377319
28	1	0	5.935895	0.695731	-0.978010
29	8	0	6.308338	-1.678547	0.312199
30	6	0	7.483317	-1.152025	-0.289084
31	1	0	8.276799	-1.866816	-0.079871
32	1	0	7.360174	-1.052182	-1.371330
33	1	0	7.744614	-0.181686	0.142769
34	7	0	-5.949800	-1.272954	-0.042206
35	8	0	-6.860693	-0.747618	0.569389
36	8	0	-6.061449	-2.317399	-0.655836

Structure 29g (C_2H_5OH)

Energy (Hartrees): -1028.29694477
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.309017	-0.570847	-0.677694
2	6	0	-3.527108	-1.229495	-0.691849
3	6	0	-4.606505	-0.641125	-0.045056
4	6	0	-4.499053	0.574304	0.619625
5	6	0	-3.271138	1.212777	0.634920
6	6	0	-2.159785	0.660954	-0.021454
7	1	0	-1.471759	-1.010783	-1.206912
8	1	0	-3.642351	-2.174678	-1.205768
9	1	0	-5.354247	1.001476	1.126386
10	1	0	-3.170357	2.143519	1.180607
11	6	0	-0.862093	1.361308	-0.031352
12	6	0	-0.816933	2.723180	-0.105119
13	6	0	0.374833	0.601995	0.009831
14	1	0	-1.719239	3.326131	-0.158806
15	1	0	0.304530	-0.485055	0.102867
16	8	0	0.299086	3.426307	-0.144007
17	1	0	1.063902	2.763695	-0.120097
18	7	0	1.517948	1.191022	-0.047404
19	6	0	2.713325	0.447721	0.068559
20	6	0	2.830581	-0.678132	0.894082
21	6	0	3.829852	0.881299	-0.641652
22	6	0	4.028435	-1.367301	0.970402
23	1	0	1.989524	-0.999518	1.498555
24	6	0	5.036499	0.189347	-0.578466
25	1	0	3.748483	1.765830	-1.264059
26	6	0	5.135053	-0.944306	0.227800
27	1	0	4.130108	-2.233851	1.614111
28	1	0	5.881503	0.544940	-1.153199
29	8	0	6.265371	-1.688943	0.364196
30	6	0	7.407740	-1.299015	-0.388071
31	1	0	8.185100	-2.022289	-0.149439
32	1	0	7.198034	-1.328683	-1.460757
33	1	0	7.741660	-0.297722	-0.102411
34	7	0	-5.898467	-1.323906	-0.063569
35	8	0	-6.838005	-0.800023	0.505813
36	8	0	-5.982623	-2.387192	-0.649915

Structure 30a (vacuum)

Energy (Hartrees): -1124.90165526
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.536010	0.809990	-0.792404
2	6	0	3.921146	0.791957	-0.802575
3	6	0	4.579188	-0.152849	-0.029064
4	6	0	3.892832	-1.067015	0.756574
5	6	0	2.508196	-1.024126	0.768239
6	6	0	1.801393	-0.096081	-0.011725
7	1	0	2.014334	1.518727	-1.424547
8	1	0	4.494569	1.481140	-1.407746
9	1	0	4.445451	-1.776159	1.358024
10	1	0	1.964853	-1.699528	1.418620
11	6	0	0.326400	-0.065813	-0.017843
12	6	0	-0.371222	-1.248026	0.008258
13	6	0	-0.341548	1.217762	-0.043337
14	1	0	0.180940	-2.180962	0.022861
15	1	0	0.305812	2.101316	-0.002476
16	1	0	-2.202327	-0.452625	0.002384
17	7	0	-1.619604	1.357599	-0.085963
18	7	0	-1.709890	-1.350067	0.004466
19	7	0	6.051087	-0.182976	-0.037581
20	8	0	6.599678	-1.039532	0.623445
21	8	0	6.626606	0.650073	-0.705389
22	6	0	-2.161260	2.655614	0.005943
23	6	0	-3.262266	2.974351	-0.793937
24	6	0	-1.666012	3.611259	0.899350
25	6	0	-3.829225	4.239608	-0.731331
26	1	0	-3.649173	2.221126	-1.470362
27	6	0	-2.244734	4.873503	0.963409
28	1	0	-0.850909	3.350531	1.564811
29	6	0	-3.322273	5.195861	0.145720
30	1	0	-4.674269	4.480653	-1.365622
31	1	0	-1.857983	5.603409	1.665165
32	1	0	-3.772822	6.179295	0.200968
33	6	0	-2.461571	-2.534763	-0.015444
34	6	0	-3.832381	-2.434981	0.239234
35	6	0	-1.904074	-3.785435	-0.289175
36	6	0	-4.629922	-3.569485	0.231046
37	1	0	-4.262738	-1.461971	0.450282
38	6	0	-2.712214	-4.916523	-0.283645
39	1	0	-0.853470	-3.888739	-0.527479
40	6	0	-4.074582	-4.819760	-0.024509
41	1	0	-5.690520	-3.474842	0.431037
42	1	0	-2.268052	-5.881776	-0.496233
43	1	0	-4.696406	-5.706103	-0.027287

Structure 30a ($CHCl_3$)

Energy (Hartrees): -1124.93460596
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.541228	0.845238	-0.759328
2	6	0	3.925666	0.828086	-0.769000
3	6	0	4.584735	-0.147406	-0.032233
4	6	0	3.896472	-1.094468	0.715324
5	6	0	2.512875	-1.054641	0.724868
6	6	0	1.804858	-0.094264	-0.017622
7	1	0	2.024560	1.583465	-1.361077
8	1	0	4.489843	1.546482	-1.348686
9	1	0	4.438963	-1.831439	1.292412
10	1	0	1.974082	-1.762890	1.343131
11	6	0	0.330389	-0.063462	-0.022955
12	6	0	-0.366432	-1.250478	0.000833
13	6	0	-0.334978	1.220333	-0.043816
14	1	0	0.186823	-2.182528	0.012893
15	1	0	0.311946	2.102405	0.009395
16	1	0	-2.206634	-0.464619	-0.009774
17	7	0	-1.614423	1.359902	-0.095747
18	7	0	-1.702722	-1.355213	-0.005241
19	7	0	6.049010	-0.175898	-0.039655
20	8	0	6.607899	-1.053212	0.590084
21	8	0	6.635350	0.678582	-0.675552
22	6	0	-2.161107	2.654766	0.004367
23	6	0	-3.281135	2.962246	-0.775652
24	6	0	-1.657775	3.618781	0.886264
25	6	0	-3.860584	4.222542	-0.704631
26	1	0	-3.676428	2.204902	-1.443664
27	6	0	-2.248658	4.875795	0.958390
28	1	0	-0.823936	3.370680	1.533685
29	6	0	-3.346669	5.186194	0.161382
30	1	0	-4.721012	4.453337	-1.322824
31	1	0	-1.854833	5.611350	1.651052
32	1	0	-3.806632	6.165452	0.224104
33	6	0	-2.455629	-2.540897	-0.017975
34	6	0	-3.835740	-2.425268	0.175660
35	6	0	-1.892151	-3.802743	-0.223965
36	6	0	-4.639285	-3.556774	0.174924
37	1	0	-4.267941	-1.442040	0.330974
38	6	0	-2.707933	-4.929275	-0.215282
39	1	0	-0.831079	-3.920406	-0.403944
40	6	0	-4.080378	-4.818078	-0.016096
41	1	0	-5.707056	-3.450370	0.328340
42	1	0	-2.259746	-5.903573	-0.374291
43	1	0	-4.706592	-5.702068	-0.014243

Structure 30a (DMSO)

Energy (Hartrees): -1124.92889797
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.540020	0.862401	-0.734155
2	6	0	3.924261	0.845078	-0.744695
3	6	0	4.584012	-0.149803	-0.033934
4	6	0	3.894363	-1.116832	0.687675
5	6	0	2.511000	-1.077268	0.698784
6	6	0	1.802886	-0.095730	-0.016644
7	1	0	2.025795	1.618196	-1.315688
8	1	0	4.484033	1.580959	-1.306549
9	1	0	4.432453	-1.872498	1.244563
10	1	0	1.974386	-1.805742	1.294969
11	6	0	0.328759	-0.062652	-0.020031
12	6	0	-0.368075	-1.251158	0.000801
13	6	0	-0.333798	1.221945	-0.038130
14	1	0	0.185881	-2.182697	0.010881
15	1	0	0.313439	2.103142	0.017380
16	1	0	-2.213760	-0.469098	-0.008710
17	7	0	-1.614137	1.362682	-0.092843
18	7	0	-1.703905	-1.356241	-0.007046
19	7	0	6.046640	-0.177809	-0.042403
20	8	0	6.608288	-1.066534	0.571054
21	8	0	6.634350	0.688877	-0.662830
22	6	0	-2.158002	2.658786	0.006063
23	6	0	-3.289570	2.960594	-0.760517
24	6	0	-1.642969	3.630226	0.873930
25	6	0	-3.868957	4.221548	-0.690744
26	1	0	-3.696343	2.198815	-1.416841
27	6	0	-2.233562	4.887770	0.944745
28	1	0	-0.798364	3.389869	1.510378
29	6	0	-3.343069	5.192217	0.160436
30	1	0	-4.738082	4.446867	-1.298931
31	1	0	-1.830087	5.628771	1.626137
32	1	0	-3.802379	6.172026	0.221971
33	6	0	-2.456055	-2.543005	-0.019534
34	6	0	-3.839506	-2.424763	0.151520
35	6	0	-1.889044	-3.807477	-0.201704
36	6	0	-4.643078	-3.556764	0.153384
37	1	0	-4.274169	-1.439441	0.286879
38	6	0	-2.705606	-4.933774	-0.191470
39	1	0	-0.825310	-3.929247	-0.362648
40	6	0	-4.081236	-4.820681	-0.012878
41	1	0	-5.713174	-3.448236	0.289528
42	1	0	-2.254800	-5.909896	-0.331858
43	1	0	-4.707462	-5.704908	-0.008630

Structure 30a (C_2H_5OH)

Energy (Hartrees): -1124.93066285
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.537625	0.867925	-0.727776
2	6	0	3.921165	0.851590	-0.737621
3	6	0	4.580518	-0.149036	-0.033193
4	6	0	3.891075	-1.121370	0.682784
5	6	0	2.508595	-1.080293	0.695415
6	6	0	1.800133	-0.094606	-0.015232
7	1	0	2.023519	1.625184	-1.307534
8	1	0	4.480783	1.589874	-1.296734
9	1	0	4.428460	-1.879486	1.237114
10	1	0	1.972431	-1.809524	1.291023
11	6	0	0.327163	-0.061711	-0.018772
12	6	0	-0.368727	-1.251100	0.002937
13	6	0	-0.336000	1.222844	-0.038154
14	1	0	0.185701	-2.182274	0.013586
15	1	0	0.310771	2.103898	0.024083
16	1	0	-2.214800	-0.471549	-0.010232
17	7	0	-1.615840	1.364162	-0.100701
18	7	0	-1.704014	-1.357885	-0.006326
19	7	0	6.037912	-0.177433	-0.042279
20	8	0	6.604018	-1.102181	0.513307
21	8	0	6.632260	0.724511	-0.605649
22	6	0	-2.157871	2.661484	0.000411
23	6	0	-3.279640	2.972093	-0.776559
24	6	0	-1.650473	3.624453	0.881769
25	6	0	-3.856527	4.233994	-0.703477
26	1	0	-3.681234	2.216756	-1.443564
27	6	0	-2.238446	4.883074	0.955755
28	1	0	-0.814416	3.376548	1.526683
29	6	0	-3.337985	5.196655	0.161256
30	1	0	-4.718402	4.466197	-1.319542
31	1	0	-1.840775	5.617649	1.647643
32	1	0	-3.795708	6.177162	0.225423
33	6	0	-2.454576	-2.546450	-0.018297
34	6	0	-3.836829	-2.431276	0.161568
35	6	0	-1.886070	-3.808681	-0.208866
36	6	0	-4.638260	-3.564817	0.163703
37	1	0	-4.272809	-1.447381	0.303311
38	6	0	-2.700194	-4.936722	-0.197851
39	1	0	-0.823192	-3.927565	-0.377827
40	6	0	-4.074924	-4.826901	-0.010699
41	1	0	-5.707803	-3.458989	0.306706
42	1	0	-2.248266	-5.911465	-0.344714
43	1	0	-4.699418	-5.712468	-0.006153

Structure 30b (vacuum)

Energy (Hartrees): -1124.89269357
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.902482	-2.145609	-0.838499
2	6	0	1.967805	-3.033102	-0.824079
3	6	0	3.041550	-2.767041	0.012090
4	6	0	3.076091	-1.653643	0.839236
5	6	0	2.000283	-0.780369	0.817152
6	6	0	0.899337	-1.003266	-0.024709
7	1	0	0.065229	-2.329822	-1.501933
8	1	0	1.983382	-3.913943	-1.451967
9	1	0	3.923589	-1.496444	1.492739
10	1	0	1.992701	0.070772	1.488756
11	6	0	-0.253304	-0.081210	-0.033763
12	6	0	-0.125879	1.272396	-0.056659
13	6	0	-1.600756	-0.651323	-0.024875
14	1	0	-1.659183	-1.727572	0.185435
15	1	0	-1.035509	1.862906	-0.025189
16	7	0	-2.655899	0.035770	-0.230883
17	7	0	1.033108	1.966592	-0.180553
18	1	0	1.869390	1.446984	-0.411307
19	7	0	4.181473	-3.702044	0.028431
20	8	0	5.117192	-3.431701	0.750755
21	8	0	4.113842	-4.682401	-0.681200
22	6	0	1.172769	3.359949	-0.086561
23	6	0	2.312783	3.953959	-0.634569
24	6	0	0.223050	4.155159	0.557589
25	6	0	2.494867	5.326109	-0.546185
26	1	0	3.048387	3.335898	-1.138434
27	6	0	0.409796	5.530796	0.624358
28	1	0	-0.643789	3.707307	1.026388
29	6	0	1.541391	6.125275	0.077590
30	1	0	3.383809	5.772573	-0.975371
31	1	0	-0.333458	6.138828	1.126111
32	1	0	1.682629	7.196655	0.142037
33	6	0	-3.906095	-0.588648	-0.065607
34	6	0	-4.923600	-0.280816	-0.973587
35	6	0	-4.178394	-1.462753	0.992536
36	6	0	-6.171690	-0.875574	-0.854594
37	1	0	-4.708925	0.419209	-1.772205
38	6	0	-5.435111	-2.045717	1.113162
39	1	0	-3.413864	-1.655901	1.736805
40	6	0	-6.433327	-1.762067	0.188045
41	1	0	-6.948223	-0.641402	-1.573442
42	1	0	-5.637178	-2.715171	1.941280
43	1	0	-7.412318	-2.215324	0.286472

Structure 30b ($CHCl_3$)

Energy (Hartrees): -1124.92736721
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.850392	-2.199914	-0.744204
2	6	0	1.906728	-3.096512	-0.734932
3	6	0	3.033138	-2.787538	0.015598
4	6	0	3.125534	-1.620983	0.763946
5	6	0	2.057633	-0.739739	0.749192
6	6	0	0.904998	-1.004147	-0.010346
7	1	0	-0.025217	-2.423623	-1.342845
8	1	0	1.868414	-4.014229	-1.306636
9	1	0	4.008158	-1.420221	1.356660
10	1	0	2.103766	0.151739	1.364336
11	6	0	-0.241320	-0.075699	-0.014734
12	6	0	-0.115336	1.283614	-0.043712
13	6	0	-1.587291	-0.640431	0.008495
14	1	0	-1.654637	-1.698633	0.289963
15	1	0	-1.021573	1.876419	0.025521
16	7	0	-2.641438	0.028849	-0.272019
17	7	0	1.030673	1.980275	-0.202868
18	1	0	1.864056	1.474195	-0.478906
19	7	0	4.158152	-3.729129	0.027173
20	8	0	5.146341	-3.429466	0.667993
21	8	0	4.047107	-4.760917	-0.604952
22	6	0	1.168330	3.373617	-0.097807
23	6	0	2.299540	3.970413	-0.662631
24	6	0	0.229964	4.162019	0.572183
25	6	0	2.482518	5.342725	-0.566851
26	1	0	3.025689	3.353179	-1.181350
27	6	0	0.418816	5.537857	0.647411
28	1	0	-0.629142	3.709525	1.051901
29	6	0	1.540583	6.136835	0.082833
30	1	0	3.363595	5.793412	-1.009032
31	1	0	-0.314762	6.141921	1.168965
32	1	0	1.683650	7.208258	0.153732
33	6	0	-3.894374	-0.586035	-0.086356
34	6	0	-4.887510	-0.363086	-1.047114
35	6	0	-4.194936	-1.367965	1.035526
36	6	0	-6.139341	-0.948632	-0.911583
37	1	0	-4.653215	0.263227	-1.900768
38	6	0	-5.455575	-1.941779	1.171142
39	1	0	-3.447953	-1.501553	1.810633
40	6	0	-6.429814	-1.741615	0.197690
41	1	0	-6.895101	-0.780863	-1.670820
42	1	0	-5.680062	-2.539143	2.047931
43	1	0	-7.411017	-2.188535	0.307917

Structure 30b (DMSO)

Energy (Hartrees): -1124.92247776
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.862764	-2.170023	-0.764747
2	6	0	1.916013	-3.069629	-0.770067
3	6	0	3.034155	-2.785304	0.002808
4	6	0	3.120765	-1.641238	0.786020
5	6	0	2.056616	-0.754841	0.783383
6	6	0	0.912408	-0.996137	0.004362
7	1	0	-0.006799	-2.374257	-1.378773
8	1	0	1.877788	-3.969073	-1.369889
9	1	0	3.996135	-1.457595	1.394533
10	1	0	2.103069	0.119843	1.422166
11	6	0	-0.233885	-0.068028	0.007936
12	6	0	-0.110299	1.293453	-0.000307
13	6	0	-1.574921	-0.638467	0.011973
14	1	0	-1.634427	-1.704858	0.258794
15	1	0	-1.019327	1.881292	0.063135
16	7	0	-2.637898	0.029385	-0.248771
17	7	0	1.033029	1.995914	-0.125932
18	1	0	1.883918	1.494809	-0.358411
19	7	0	4.157243	-3.727958	-0.002503
20	8	0	5.129334	-3.465251	0.679705
21	8	0	4.062621	-4.727827	-0.688588
22	6	0	1.154838	3.393022	-0.060492
23	6	0	2.333934	3.970317	-0.543633
24	6	0	0.156768	4.206685	0.482713
25	6	0	2.504749	5.347144	-0.496607
26	1	0	3.107331	3.331967	-0.958111
27	6	0	0.337129	5.585834	0.511775
28	1	0	-0.745751	3.777233	0.898968
29	6	0	1.505093	6.165692	0.025194
30	1	0	3.423060	5.781208	-0.875285
31	1	0	-0.443063	6.208988	0.933995
32	1	0	1.638393	7.240297	0.058386
33	6	0	-3.882981	-0.605654	-0.077265
34	6	0	-4.896398	-0.333950	-1.004600
35	6	0	-4.158993	-1.454496	1.002825
36	6	0	-6.144278	-0.931255	-0.877942
37	1	0	-4.684788	0.340724	-1.827007
38	6	0	-5.414147	-2.042488	1.128409
39	1	0	-3.397669	-1.630572	1.754955
40	6	0	-6.409479	-1.789907	0.188384
41	1	0	-6.915553	-0.721546	-1.610648
42	1	0	-5.616969	-2.692619	1.972309
43	1	0	-7.386713	-2.246988	0.291650

Structure 30b (C_2H_5OH)

Energy (Hartrees): -1124.92447459
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.831746	-2.197959	-0.779248
2	6	0	1.876716	-3.106919	-0.761907
3	6	0	2.991631	-2.819877	0.015451
4	6	0	3.083343	-1.663994	0.781940
5	6	0	2.028297	-0.769029	0.755078
6	6	0	0.888181	-1.011409	-0.030158
7	1	0	-0.035669	-2.405384	-1.395622
8	1	0	1.834934	-4.015567	-1.347945
9	1	0	3.954968	-1.476656	1.394946
10	1	0	2.076460	0.116230	1.379026
11	6	0	-0.245463	-0.068044	-0.042001
12	6	0	-0.098053	1.291454	-0.058372
13	6	0	-1.595231	-0.616531	-0.023736
14	1	0	-1.670901	-1.680005	0.232028
15	1	0	-0.993949	1.898983	0.017536
16	7	0	-2.648692	0.068177	-0.279876
17	7	0	1.056176	1.970910	-0.210759
18	1	0	1.889038	1.456634	-0.476949
19	7	0	4.103500	-3.768220	0.034051
20	8	0	5.066909	-3.514212	0.733358
21	8	0	4.021541	-4.771745	-0.649854
22	6	0	1.212305	3.361922	-0.096436
23	6	0	2.360445	3.942131	-0.644846
24	6	0	0.277808	4.162532	0.564848
25	6	0	2.562932	5.311660	-0.543817
26	1	0	3.085073	3.312804	-1.151311
27	6	0	0.487203	5.535488	0.646048
28	1	0	-0.594433	3.724003	1.033857
29	6	0	1.624662	6.118997	0.095959
30	1	0	3.457279	5.749405	-0.972825
31	1	0	-0.243219	6.149457	1.160957
32	1	0	1.783148	7.188217	0.171582
33	6	0	-3.902313	-0.544587	-0.087765
34	6	0	-4.924498	-0.258827	-1.000439
35	6	0	-4.176927	-1.382963	1.000384
36	6	0	-6.179844	-0.835802	-0.854114
37	1	0	-4.714290	0.409733	-1.828337
38	6	0	-5.439299	-1.950579	1.146078
39	1	0	-3.408390	-1.566244	1.743805
40	6	0	-6.443374	-1.686327	0.218786
41	1	0	-6.958251	-0.617060	-1.576873
42	1	0	-5.641536	-2.593224	1.996113
43	1	0	-7.426354	-2.127752	0.337664

Structure 30c (vacuum)

Energy (Hartrees): -1124.89426737
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.775181	1.702573	-0.859143
2	6	0	0.698454	3.086194	-0.886550
3	6	0	-0.157737	3.722556	0.000176
4	6	0	-0.928457	3.025045	0.916742
5	6	0	-0.842129	1.640158	0.929420
6	6	0	-0.001657	0.960173	0.038619
7	1	0	1.448359	1.187274	-1.530733
8	1	0	1.286720	3.674446	-1.577692
9	1	0	-1.566608	3.564219	1.603623
10	1	0	-1.414991	1.076746	1.657795
11	6	0	0.062956	-0.518858	0.050732
12	6	0	-1.050737	-1.296077	0.019196
13	6	0	1.344659	-1.209573	0.057986
14	1	0	-0.935996	-2.374807	0.040841
15	1	0	1.286233	-2.307337	0.060285
16	7	0	2.468715	-0.609857	0.083744
17	7	0	-2.334923	-0.862730	-0.096479
18	1	0	-2.479064	0.116285	-0.304741
19	7	0	-0.248552	5.195639	-0.027435
20	8	0	-1.004508	5.725325	0.759072
21	8	0	0.434708	5.785234	-0.836361
22	6	0	3.642388	-1.385658	0.038738
23	6	0	4.707399	-1.026692	0.870069
24	6	0	3.796089	-2.462448	-0.840913
25	6	0	5.884339	-1.762053	0.854913
26	1	0	4.585626	-0.174063	1.527285
27	6	0	4.983838	-3.185451	-0.861520
28	1	0	2.995899	-2.707692	-1.530366
29	6	0	6.028525	-2.845013	-0.009708
30	1	0	6.698391	-1.483663	1.513922
31	1	0	5.095725	-4.010580	-1.555339
32	1	0	6.953119	-3.408946	-0.028559
33	6	0	-3.477411	-1.675843	-0.055810
34	6	0	-4.656604	-1.208981	-0.642932
35	6	0	-3.470132	-2.921370	0.575449
36	6	0	-5.806694	-1.984059	-0.607930
37	1	0	-4.662406	-0.242613	-1.135708
38	6	0	-4.624386	-3.696011	0.587373
39	1	0	-2.582084	-3.275978	1.083186
40	6	0	-5.796787	-3.236466	-0.000992
41	1	0	-6.713576	-1.608896	-1.066921
42	1	0	-4.606348	-4.660901	1.079995
43	1	0	-6.693878	-3.842205	0.019133

Structure 30c ($CHCl_3$)

Energy (Hartrees): -1124.92964833
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.726562	1.658389	0.912045
2	6	0	-0.666316	3.041255	0.963272
3	6	0	0.124267	3.704706	0.033828
4	6	0	0.846182	3.034266	-0.942231
5	6	0	0.775218	1.648841	-0.977200
6	6	0	-0.001560	0.942513	-0.049902
7	1	0	-1.340120	1.123069	1.625258
8	1	0	-1.216844	3.599819	1.708307
9	1	0	1.437389	3.585284	-1.661344
10	1	0	1.312120	1.110309	-1.750692
11	6	0	-0.059246	-0.537383	-0.082844
12	6	0	1.057069	-1.320634	-0.080336
13	6	0	-1.335984	-1.226200	-0.086824
14	1	0	0.929627	-2.397142	-0.111731
15	1	0	-1.276867	-2.321759	-0.068649
16	7	0	-2.464747	-0.626225	-0.135279
17	7	0	2.336735	-0.886311	-0.003375
18	1	0	2.487524	0.107048	0.125385
19	7	0	0.194656	5.172525	0.083478
20	8	0	0.887466	5.738773	-0.738267
21	8	0	-0.441467	5.745173	0.944959
22	6	0	-3.639534	-1.398998	-0.074284
23	6	0	-4.723684	-1.021223	-0.875006
24	6	0	-3.782700	-2.488154	0.794312
25	6	0	-5.908867	-1.744616	-0.839106
26	1	0	-4.614419	-0.162157	-1.527506
27	6	0	-4.976826	-3.200970	0.833858
28	1	0	-2.967136	-2.754805	1.457493
29	6	0	-6.041971	-2.838202	0.014899
30	1	0	-6.736737	-1.448951	-1.473842
31	1	0	-5.077610	-4.035930	1.518368
32	1	0	-6.971863	-3.393526	0.050508
33	6	0	3.494947	-1.677817	0.012856
34	6	0	4.708866	-1.043531	0.298103
35	6	0	3.483129	-3.049280	-0.254684
36	6	0	5.890419	-1.770296	0.322815
37	1	0	4.716883	0.022416	0.501690
38	6	0	4.674509	-3.766719	-0.219383
39	1	0	2.564377	-3.564617	-0.502469
40	6	0	5.882206	-3.139528	0.068558
41	1	0	6.821278	-1.261210	0.545025
42	1	0	4.652394	-4.830144	-0.428877
43	1	0	6.804135	-3.707696	0.089310

Structure 30c (DMSO)

Energy (Hartrees): -1124.92612573
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.716620	1.672591	0.931606
2	6	0	-0.664310	3.055862	0.977364
3	6	0	0.109813	3.720501	0.034117
4	6	0	0.825299	3.049844	-0.946773
5	6	0	0.762535	1.663958	-0.975788
6	6	0	-0.000819	0.957021	-0.038191
7	1	0	-1.311679	1.137153	1.660885
8	1	0	-1.207042	3.610456	1.731215
9	1	0	1.409474	3.597287	-1.674273
10	1	0	1.300089	1.127127	-1.749898
11	6	0	-0.055173	-0.522564	-0.066646
12	6	0	1.062683	-1.307849	-0.068248
13	6	0	-1.325899	-1.215548	-0.070734
14	1	0	0.930628	-2.383868	-0.095119
15	1	0	-1.260489	-2.309910	-0.042052
16	7	0	-2.461536	-0.623078	-0.135501
17	7	0	2.340168	-0.875835	-0.002679
18	1	0	2.501678	0.118660	0.113221
19	7	0	0.171871	5.187768	0.076540
20	8	0	0.840665	5.756928	-0.764100
21	8	0	-0.447870	5.761404	0.951022
22	6	0	-3.627096	-1.409904	-0.075173
23	6	0	-4.713657	-1.050327	-0.882118
24	6	0	-3.760754	-2.497868	0.797792
25	6	0	-5.890058	-1.789175	-0.848694
26	1	0	-4.615459	-0.194312	-1.540958
27	6	0	-4.945623	-3.226699	0.833820
28	1	0	-2.944002	-2.754599	1.463665
29	6	0	-6.012451	-2.882191	0.008063
30	1	0	-6.718228	-1.506771	-1.489316
31	1	0	-5.037290	-4.061828	1.519628
32	1	0	-6.934438	-3.451052	0.039881
33	6	0	3.494278	-1.674157	0.009229
34	6	0	4.712889	-1.046135	0.290149
35	6	0	3.471467	-3.045998	-0.257049
36	6	0	5.889691	-1.781651	0.313461
37	1	0	4.725822	0.020205	0.491331
38	6	0	4.658312	-3.771512	-0.223432
39	1	0	2.547872	-3.555073	-0.500251
40	6	0	5.871249	-3.151768	0.061366
41	1	0	6.824833	-1.278912	0.532966
42	1	0	4.628384	-4.835266	-0.430958
43	1	0	6.789412	-3.726526	0.081415

Structure 30c (C_2H_5OH)

Energy (Hartrees): -1124.92763776
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.710869	1.683021	0.923314
2	6	0	-0.647772	3.065358	0.969184
3	6	0	0.141593	3.722077	0.032614
4	6	0	0.857691	3.046045	-0.944720
5	6	0	0.778098	1.661554	-0.977392
6	6	0	0.003398	0.961362	-0.043446
7	1	0	-1.312786	1.152702	1.650633
8	1	0	-1.189296	3.624363	1.720765
9	1	0	1.449827	3.588371	-1.669932
10	1	0	1.310587	1.120263	-1.751996
11	6	0	-0.063137	-0.517284	-0.070897
12	6	0	1.048500	-1.311069	-0.068554
13	6	0	-1.339317	-1.201003	-0.073846
14	1	0	0.907934	-2.386058	-0.093080
15	1	0	-1.281591	-2.295581	-0.038931
16	7	0	-2.470972	-0.602398	-0.145605
17	7	0	2.329782	-0.889962	0.000919
18	1	0	2.498827	0.103424	0.114244
19	7	0	0.220575	5.183978	0.079012
20	8	0	0.994330	5.744445	-0.673931
21	8	0	-0.489251	5.775245	0.869966
22	6	0	-3.639716	-1.385010	-0.080485
23	6	0	-4.718967	-1.040700	-0.903162
24	6	0	-3.781867	-2.453793	0.814117
25	6	0	-5.896950	-1.776615	-0.862820
26	1	0	-4.614397	-0.199439	-1.579768
27	6	0	-4.968294	-3.179749	0.856973
28	1	0	-2.970479	-2.696365	1.492026
29	6	0	-6.028102	-2.850802	0.016207
30	1	0	-6.719835	-1.506305	-1.515489
31	1	0	-5.067052	-3.999575	1.560198
32	1	0	-6.951789	-3.416767	0.053509
33	6	0	3.477357	-1.698324	0.012504
34	6	0	4.701558	-1.080689	0.291122
35	6	0	3.442432	-3.069991	-0.252566
36	6	0	5.872108	-1.826178	0.313386
37	1	0	4.724452	-0.014248	0.491269
38	6	0	4.623016	-3.805766	-0.219752
39	1	0	2.514439	-3.571725	-0.494604
40	6	0	5.841583	-3.196247	0.062696
41	1	0	6.811935	-1.330954	0.530548
42	1	0	4.583764	-4.869470	-0.426563
43	1	0	6.755075	-3.778674	0.081739

Structure 30d (vacuum)

Energy (Hartrees): -1124.88957826
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.212126	-0.310655	0.722044
2	6	0	-3.443637	-0.939900	0.780507
3	6	0	-3.644899	-2.084901	0.021727
4	6	0	-2.658157	-2.610661	-0.795601
5	6	0	-1.431524	-1.964648	-0.847433
6	6	0	-1.181026	-0.818473	-0.081389
7	1	0	-2.042783	0.584302	1.304336
8	1	0	-4.243579	-0.562937	1.402997
9	1	0	-2.864110	-3.493585	-1.385475
10	1	0	-0.666194	-2.338697	-1.517146
11	6	0	0.152109	-0.179322	-0.104153
12	6	0	1.260832	-0.966740	-0.149794
13	6	0	0.291260	1.271519	-0.054202
14	1	0	1.298255	1.656421	0.158738
15	1	0	2.700610	0.369358	-0.730220
16	1	0	1.153889	-2.042742	-0.050722
17	7	0	-0.678982	2.080092	-0.229394
18	7	0	2.545922	-0.546118	-0.336705
19	7	0	-4.954920	-2.758324	0.078317
20	8	0	-5.103849	-3.756777	-0.594506
21	8	0	-5.804634	-2.275419	0.796062
22	6	0	-0.440036	3.459046	-0.077590
23	6	0	-1.059849	4.332383	-0.976145
24	6	0	0.346552	3.982689	0.954162
25	6	0	-0.850935	5.700349	-0.876646
26	1	0	-1.692293	3.913599	-1.749611
27	6	0	0.538286	5.356190	1.057157
28	1	0	0.774699	3.315162	1.693806
29	6	0	-0.050214	6.218696	0.138952
30	1	0	-1.323174	6.368060	-1.587711
31	1	0	1.140395	5.753096	1.866195
32	1	0	0.099752	7.288175	0.222918
33	6	0	3.689481	-1.327374	-0.113169
34	6	0	4.879599	-0.976141	-0.756503
35	6	0	3.668079	-2.430422	0.742375
36	6	0	6.027708	-1.726649	-0.555456
37	1	0	4.895633	-0.118574	-1.420898
38	6	0	4.821378	-3.186593	0.919555
39	1	0	2.769254	-2.680911	1.291919
40	6	0	6.004549	-2.842949	0.276654
41	1	0	6.943445	-1.442614	-1.059936
42	1	0	4.794399	-4.042265	1.583723
43	1	0	6.900950	-3.430494	0.428803

Structure 30d ($CHCl_3$)

Energy (Hartrees): -1124.92613701
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.214847	-0.334161	0.723998
2	6	0	-3.437215	-0.980165	0.775311
3	6	0	-3.613999	-2.134635	0.021756
4	6	0	-2.609248	-2.650319	-0.783315
5	6	0	-1.393153	-1.985933	-0.829275
6	6	0	-1.166359	-0.828737	-0.068820
7	1	0	-2.065743	0.561324	1.311894
8	1	0	-4.241686	-0.606056	1.394296
9	1	0	-2.785093	-3.540920	-1.371976
10	1	0	-0.617015	-2.358859	-1.487370
11	6	0	0.154306	-0.166008	-0.079888
12	6	0	1.278503	-0.942345	-0.116669
13	6	0	0.267532	1.283100	-0.024895
14	1	0	1.260830	1.686121	0.208636
15	1	0	2.722147	0.438681	-0.562509
16	1	0	1.173299	-2.019523	-0.039507
17	7	0	-0.711754	2.078210	-0.234935
18	7	0	2.556657	-0.511493	-0.257724
19	7	0	-4.906436	-2.825674	0.074293
20	8	0	-5.032935	-3.853646	-0.562592
21	8	0	-5.788065	-2.338566	0.754599
22	6	0	-0.496916	3.462118	-0.087150
23	6	0	-1.123326	4.321816	-0.996056
24	6	0	0.273046	4.005572	0.948498
25	6	0	-0.940149	5.694973	-0.901613
26	1	0	-1.740630	3.892042	-1.776919
27	6	0	0.441325	5.383302	1.044485
28	1	0	0.712288	3.349550	1.692188
29	6	0	-0.155602	6.232507	0.117529
30	1	0	-1.418067	6.350408	-1.621048
31	1	0	1.032845	5.794406	1.854988
32	1	0	-0.023443	7.305287	0.196300
33	6	0	3.708055	-1.296183	-0.082690
34	6	0	4.914136	-0.817683	-0.605594
35	6	0	3.687423	-2.512855	0.603433
36	6	0	6.080922	-1.551979	-0.451816
37	1	0	4.924846	0.128013	-1.137570
38	6	0	4.861980	-3.246985	0.735150
39	1	0	2.775362	-2.880135	1.057374
40	6	0	6.062101	-2.775973	0.213259
41	1	0	7.008595	-1.167503	-0.860167
42	1	0	4.835472	-4.189734	1.269549
43	1	0	6.973623	-3.349277	0.330499

Structure 30d (DMSO)

Energy (Hartrees): -1124.92255469
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.220852	-0.337638	0.710123
2	6	0	-3.436857	-0.995722	0.757701
3	6	0	-3.592820	-2.165246	0.021837
4	6	0	-2.569423	-2.686736	-0.756676
5	6	0	-1.359901	-2.010915	-0.799047
6	6	0	-1.155837	-0.834175	-0.060782
7	1	0	-2.088645	0.565862	1.290081
8	1	0	-4.250206	-0.617475	1.362552
9	1	0	-2.721610	-3.592115	-1.329215
10	1	0	-0.569376	-2.394010	-1.433688
11	6	0	0.155913	-0.156755	-0.070016
12	6	0	1.288688	-0.926206	-0.101512
13	6	0	0.257262	1.291158	-0.020176
14	1	0	1.244162	1.703363	0.220438
15	1	0	2.723318	0.467756	-0.532652
16	1	0	1.188616	-2.003560	-0.019752
17	7	0	-0.726971	2.079700	-0.246200
18	7	0	2.560015	-0.488188	-0.240612
19	7	0	-4.878904	-2.864937	0.065791
20	8	0	-4.991054	-3.901550	-0.561697
21	8	0	-5.775033	-2.377014	0.728851
22	6	0	-0.522164	3.464843	-0.095304
23	6	0	-1.147190	4.323321	-1.007297
24	6	0	0.234817	4.012042	0.948828
25	6	0	-0.978292	5.698420	-0.906287
26	1	0	-1.751393	3.893494	-1.798898
27	6	0	0.389323	5.391145	1.050697
28	1	0	0.678238	3.357841	1.691834
29	6	0	-0.208250	6.239410	0.122376
30	1	0	-1.454809	6.351844	-1.628700
31	1	0	0.972154	5.804202	1.866666
32	1	0	-0.085945	7.313134	0.206235
33	6	0	3.714614	-1.270610	-0.074700
34	6	0	4.915676	-0.785825	-0.603858
35	6	0	3.700774	-2.489767	0.607925
36	6	0	6.084556	-1.520841	-0.464134
37	1	0	4.919140	0.164196	-1.128112
38	6	0	4.877652	-3.222824	0.727320
39	1	0	2.792324	-2.861925	1.065493
40	6	0	6.072739	-2.748362	0.195623
41	1	0	7.008537	-1.133264	-0.878319
42	1	0	4.856732	-4.167415	1.258969
43	1	0	6.985927	-3.321747	0.301148

Structure 30d (C_2H_5OH)

Energy (Hartrees): -1124.92429665
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.222232	-0.337238	0.718834
2	6	0	-3.441249	-0.988530	0.761660
3	6	0	-3.599525	-2.156650	0.022941
4	6	0	-2.575835	-2.683956	-0.752353
5	6	0	-1.364370	-2.012747	-0.791400
6	6	0	-1.158081	-0.836586	-0.052013
7	1	0	-2.086247	0.563826	1.301696
8	1	0	-4.254291	-0.607899	1.365729
9	1	0	-2.730588	-3.587150	-1.327973
10	1	0	-0.574892	-2.396681	-1.426910
11	6	0	0.153510	-0.160721	-0.061786
12	6	0	1.285790	-0.930663	-0.095539
13	6	0	0.256040	1.287485	-0.013283
14	1	0	1.242189	1.697706	0.233411
15	1	0	2.719706	0.461940	-0.533991
16	1	0	1.186243	-2.007985	-0.012757
17	7	0	-0.724316	2.078008	-0.248451
18	7	0	2.557023	-0.492889	-0.238069
19	7	0	-4.886345	-2.844935	0.058271
20	8	0	-4.996638	-3.901225	-0.537852
21	8	0	-5.798776	-2.334939	0.682992
22	6	0	-0.513492	3.462946	-0.097073
23	6	0	-1.124109	4.324638	-1.015503
24	6	0	0.235425	4.006068	0.954695
25	6	0	-0.947235	5.698674	-0.913603
26	1	0	-1.723920	3.899165	-1.812752
27	6	0	0.398213	5.384186	1.057329
28	1	0	0.665606	3.349549	1.703583
29	6	0	-0.183935	6.235532	0.122128
30	1	0	-1.412519	6.354760	-1.641076
31	1	0	0.974794	5.794042	1.879475
32	1	0	-0.055391	7.308597	0.206314
33	6	0	3.711742	-1.276980	-0.074986
34	6	0	4.909554	-0.799767	-0.617346
35	6	0	3.699784	-2.489753	0.618451
36	6	0	6.077751	-1.536268	-0.479884
37	1	0	4.911723	0.145548	-1.150199
38	6	0	4.875567	-3.225018	0.735064
39	1	0	2.793903	-2.854666	1.087063
40	6	0	6.067668	-2.758069	0.190319
41	1	0	6.999709	-1.154406	-0.903989
42	1	0	4.856521	-4.165061	1.274959
43	1	0	6.980354	-3.332765	0.294143

Structure 30e (vacuum)

Energy (Hartrees): -1124.88497700
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.325764	0.619256	-0.729492
2	6	0	3.669654	0.899515	-0.553536
3	6	0	4.471063	-0.040814	0.080693
4	6	0	3.966186	-1.241909	0.549900
5	6	0	2.615562	-1.504737	0.370908
6	6	0	1.777899	-0.593949	-0.286373
7	1	0	1.690580	1.344486	-1.219047
8	1	0	4.104175	1.826738	-0.901672
9	1	0	4.619736	-1.938226	1.057501
10	1	0	2.198452	-2.420165	0.773583
11	6	0	0.360248	-0.928100	-0.536934
12	6	0	0.038397	-2.204581	-0.872552
13	6	0	-0.674216	0.107516	-0.499817
14	1	0	-1.613479	-0.131348	-1.010599
15	1	0	-1.260944	-3.602306	-1.542896
16	1	0	0.842614	-2.900472	-1.096503
17	7	0	-0.509374	1.227654	0.084537
18	7	0	-1.215257	-2.750097	-1.006038
19	7	0	5.902899	0.252216	0.270790
20	8	0	6.579095	-0.585171	0.830745
21	8	0	6.320081	1.311782	-0.145731
22	6	0	-1.541382	2.183485	-0.002417
23	6	0	-1.830237	2.936660	1.139024
24	6	0	-2.246304	2.432169	-1.184382
25	6	0	-2.841690	3.886259	1.111215
26	1	0	-1.254550	2.752106	2.038124
27	6	0	-3.246673	3.397238	-1.209644
28	1	0	-1.986646	1.891317	-2.087485
29	6	0	-3.554818	4.120367	-0.062394
30	1	0	-3.068945	4.454716	2.005505
31	1	0	-3.780139	3.591094	-2.132898
32	1	0	-4.334406	4.872090	-0.086293
33	6	0	-2.386951	-2.462367	-0.266875
34	6	0	-3.619980	-2.801655	-0.823582
35	6	0	-2.337152	-1.897138	1.009422
36	6	0	-4.792731	-2.575550	-0.113427
37	1	0	-3.656117	-3.232016	-1.818668
38	6	0	-3.516964	-1.658637	1.701350
39	1	0	-1.383565	-1.643612	1.455493
40	6	0	-4.749425	-1.994082	1.148286
41	1	0	-5.743712	-2.843681	-0.557997
42	1	0	-3.467606	-1.212862	2.687696
43	1	0	-5.664237	-1.802838	1.694780

Structure 30e ($CHCl_3$)

Energy (Hartrees): -1124.92005343
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.328788	0.616187	-0.726787
2	6	0	3.669863	0.914268	-0.564554
3	6	0	4.488650	-0.013399	0.070086
4	6	0	4.001088	-1.220566	0.547923
5	6	0	2.653329	-1.500658	0.382137
6	6	0	1.796034	-0.601539	-0.270333
7	1	0	1.686429	1.330546	-1.224342
8	1	0	4.081810	1.846664	-0.927328
9	1	0	4.659841	-1.913664	1.054016
10	1	0	2.255059	-2.423141	0.787933
11	6	0	0.379073	-0.948148	-0.498313
12	6	0	0.061385	-2.240362	-0.802178
13	6	0	-0.657958	0.079669	-0.473685
14	1	0	-1.587187	-0.161025	-0.999548
15	1	0	-1.203038	-3.690163	-1.399855
16	1	0	0.866895	-2.934250	-1.026480
17	7	0	-0.516306	1.204071	0.115932
18	7	0	-1.174399	-2.807181	-0.908187
19	7	0	5.910404	0.297080	0.247871
20	8	0	6.609175	-0.521712	0.813420
21	8	0	6.322903	1.357170	-0.180397
22	6	0	-1.560020	2.146298	0.009765
23	6	0	-1.880096	2.900150	1.144061
24	6	0	-2.251653	2.379483	-1.184468
25	6	0	-2.905797	3.835240	1.095734
26	1	0	-1.322231	2.729008	2.057966
27	6	0	-3.268057	3.328125	-1.229178
28	1	0	-1.974091	1.835807	-2.080890
29	6	0	-3.604684	4.053851	-0.090209
30	1	0	-3.155458	4.403578	1.984783
31	1	0	-3.791744	3.506554	-2.161722
32	1	0	-4.396281	4.793108	-0.129468
33	6	0	-2.372147	-2.469037	-0.232827
34	6	0	-3.588500	-2.778607	-0.841100
35	6	0	-2.358617	-1.886932	1.037564
36	6	0	-4.784187	-2.499575	-0.187568
37	1	0	-3.591065	-3.230590	-1.827398
38	6	0	-3.559009	-1.598460	1.673763
39	1	0	-1.416052	-1.661447	1.522568
40	6	0	-4.776791	-1.898808	1.066791
41	1	0	-5.723535	-2.742677	-0.670908
42	1	0	-3.539672	-1.142726	2.657130
43	1	0	-5.708365	-1.670117	1.570294

Structure 30e (DMSO)

Energy (Hartrees): -1124.91640249
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.321007	0.632880	-0.697288
2	6	0	3.660013	0.940156	-0.536730
3	6	0	4.492819	0.005224	0.069777
4	6	0	4.019249	-1.219144	0.519345
5	6	0	2.672831	-1.507310	0.359689
6	6	0	1.800998	-0.599671	-0.263292
7	1	0	1.671348	1.349841	-1.182028
8	1	0	4.058164	1.884081	-0.884965
9	1	0	4.685441	-1.922792	1.000603
10	1	0	2.288663	-2.444997	0.743674
11	6	0	0.386838	-0.952283	-0.486388
12	6	0	0.074380	-2.248827	-0.793050
13	6	0	-0.655184	0.066453	-0.464923
14	1	0	-1.574737	-0.175869	-1.006349
15	1	0	-1.184300	-3.705281	-1.377214
16	1	0	0.880157	-2.938038	-1.029642
17	7	0	-0.533575	1.189634	0.136009
18	7	0	-1.154486	-2.820486	-0.885831
19	7	0	5.911637	0.323684	0.241650
20	8	0	6.632777	-0.517500	0.745114
21	8	0	6.304200	1.414100	-0.129404
22	6	0	-1.582652	2.124146	0.014583
23	6	0	-1.915116	2.886315	1.140578
24	6	0	-2.267387	2.345025	-1.186942
25	6	0	-2.942127	3.820046	1.077390
26	1	0	-1.366734	2.725191	2.062370
27	6	0	-3.286398	3.290724	-1.245702
28	1	0	-1.982942	1.795811	-2.077959
29	6	0	-3.633542	4.026089	-0.115459
30	1	0	-3.199565	4.394338	1.960508
31	1	0	-3.804198	3.459181	-2.183527
32	1	0	-4.426909	4.762822	-0.167162
33	6	0	-2.354528	-2.471146	-0.221613
34	6	0	-3.568488	-2.770033	-0.839850
35	6	0	-2.344903	-1.892438	1.050912
36	6	0	-4.766779	-2.476330	-0.196897
37	1	0	-3.566003	-3.225671	-1.824287
38	6	0	-3.547567	-1.591238	1.677496
39	1	0	-1.403432	-1.682615	1.545499
40	6	0	-4.763728	-1.876462	1.058510
41	1	0	-5.704690	-2.710581	-0.687633
42	1	0	-3.532174	-1.141959	2.664147
43	1	0	-5.697355	-1.639135	1.554619

Structure 30e (C_2H_5OH)

Energy (Hartrees): -1124.91857659
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.325246	0.622719	-0.723423
2	6	0	3.663402	0.931061	-0.563186
3	6	0	4.491182	0.005552	0.065533
4	6	0	4.015694	-1.212712	0.531222
5	6	0	2.671341	-1.503768	0.365038
6	6	0	1.802805	-0.603340	-0.273267
7	1	0	1.677384	1.333452	-1.219761
8	1	0	4.063541	1.870109	-0.922648
9	1	0	4.678927	-1.910430	1.025357
10	1	0	2.284843	-2.436971	0.757673
11	6	0	0.388893	-0.956095	-0.493564
12	6	0	0.076528	-2.254641	-0.791193
13	6	0	-0.652572	0.063811	-0.470755
14	1	0	-1.572446	-0.176790	-1.012262
15	1	0	-1.181830	-3.717410	-1.362880
16	1	0	0.882432	-2.944891	-1.024563
17	7	0	-0.530068	1.184539	0.134318
18	7	0	-1.151842	-2.828089	-0.880005
19	7	0	5.902851	0.327915	0.246118
20	8	0	6.599730	-0.448949	0.874110
21	8	0	6.328595	1.360680	-0.238848
22	6	0	-1.581457	2.117861	0.018016
23	6	0	-1.915037	2.873644	1.147694
24	6	0	-2.266554	2.343562	-1.182112
25	6	0	-2.944723	3.804710	1.089691
26	1	0	-1.365646	2.709990	2.068519
27	6	0	-3.288299	3.286563	-1.235890
28	1	0	-1.980030	1.800481	-2.076317
29	6	0	-3.637300	4.014855	-0.101694
30	1	0	-3.203012	4.374219	1.975783
31	1	0	-3.806818	3.458563	-2.172785
32	1	0	-4.432771	4.749778	-0.149138
33	6	0	-2.353146	-2.468607	-0.221820
34	6	0	-3.566719	-2.758815	-0.844354
35	6	0	-2.343434	-1.890437	1.050705
36	6	0	-4.765125	-2.456588	-0.205440
37	1	0	-3.564676	-3.213956	-1.829129
38	6	0	-3.545876	-1.580278	1.673183
39	1	0	-1.401826	-1.687170	1.548157
40	6	0	-4.761851	-1.856767	1.049885
41	1	0	-5.703162	-2.683746	-0.699504
42	1	0	-3.530665	-1.130721	2.659785
43	1	0	-5.695425	-1.612658	1.543007

Structure 30f (vacuum)

Energy (Hartrees): -1124.88052872
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.532078	0.451685	0.856881
2	6	0	-3.878312	0.754584	0.988802
3	6	0	-4.771499	0.220158	0.072368
4	6	0	-4.356321	-0.594051	-0.970734
5	6	0	-3.005450	-0.876713	-1.092991
6	6	0	-2.069802	-0.373268	-0.177725
7	1	0	-1.831465	0.841359	1.586062
8	1	0	-4.244330	1.381065	1.790969
9	1	0	-5.083753	-0.975141	-1.674946
10	1	0	-2.665022	-1.477037	-1.928549
11	6	0	-0.625112	-0.695068	-0.300794
12	6	0	-0.288475	-1.991588	-0.558715
13	6	0	0.313749	0.419221	-0.212003
14	1	0	-1.109097	-2.679137	-0.745589
15	1	0	-0.071679	1.352287	0.218695
16	1	0	0.899430	-3.549924	-0.991030
17	7	0	1.499952	0.351535	-0.675217
18	7	0	0.921835	-2.614398	-0.615679
19	7	0	-6.205121	0.529878	0.209128
20	8	0	-6.963252	0.055856	-0.610259
21	8	0	-6.540643	1.239066	1.133873
22	6	0	2.374546	1.434728	-0.498045
23	6	0	3.235881	1.766194	-1.548292
24	6	0	2.460016	2.143356	0.705368
25	6	0	4.126535	2.821284	-1.415112
26	1	0	3.181762	1.186897	-2.462258
27	6	0	3.365421	3.190640	0.837216
28	1	0	1.839937	1.846311	1.544314
29	6	0	4.195016	3.539496	-0.222690
30	1	0	4.778277	3.080279	-2.241353
31	1	0	3.429391	3.728518	1.776117
32	1	0	4.901168	4.353998	-0.116551
33	6	0	2.136309	-2.274653	0.029059
34	6	0	3.338802	-2.599725	-0.591971
35	6	0	2.141387	-1.671335	1.284226
36	6	0	4.543498	-2.298480	0.030840
37	1	0	3.324328	-3.058522	-1.574388
38	6	0	3.349103	-1.361757	1.894634
39	1	0	1.200032	-1.437101	1.767803
40	6	0	4.554666	-1.668477	1.270657
41	1	0	5.475929	-2.542481	-0.463924
42	1	0	3.348132	-0.878713	2.864704
43	1	0	5.494171	-1.418526	1.747522

Structure 30f ($CHCl_3$)

Energy (Hartrees): -1124.91564468
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.515967	0.450708	0.852987
2	6	0	-3.864485	0.735865	0.994860
3	6	0	-4.759022	0.187977	0.085393
4	6	0	-4.340061	-0.622917	-0.961325
5	6	0	-2.987881	-0.889498	-1.092522
6	6	0	-2.050304	-0.371198	-0.184834
7	1	0	-1.818211	0.854367	1.577364
8	1	0	-4.222361	1.359811	1.803077
9	1	0	-5.059791	-1.018796	-1.665661
10	1	0	-2.652373	-1.490313	-1.929559
11	6	0	-0.602459	-0.675173	-0.316908
12	6	0	-0.255542	-1.961513	-0.628846
13	6	0	0.319793	0.446050	-0.197212
14	1	0	-1.066178	-2.643343	-0.869358
15	1	0	-0.078855	1.361855	0.254818
16	1	0	0.927890	-3.495242	-1.121255
17	7	0	1.508035	0.415053	-0.667955
18	7	0	0.951181	-2.581029	-0.689574
19	7	0	-6.188227	0.478273	0.231695
20	8	0	-6.956609	-0.007694	-0.575197
21	8	0	-6.535724	1.190291	1.153603
22	6	0	2.347931	1.526328	-0.483909
23	6	0	3.179503	1.906196	-1.543632
24	6	0	2.427613	2.220491	0.729437
25	6	0	4.037380	2.989051	-1.407947
26	1	0	3.131575	1.343099	-2.468922
27	6	0	3.300502	3.296116	0.862902
28	1	0	1.826875	1.896424	1.572789
29	6	0	4.101938	3.690054	-0.204335
30	1	0	4.666036	3.282095	-2.241333
31	1	0	3.361206	3.821545	1.809610
32	1	0	4.783086	4.525902	-0.095961
33	6	0	2.158587	-2.296991	-0.014669
34	6	0	3.353276	-2.742453	-0.580543
35	6	0	2.173900	-1.651894	1.221262
36	6	0	4.557643	-2.520670	0.076177
37	1	0	3.332107	-3.247319	-1.540702
38	6	0	3.383376	-1.429241	1.867978
39	1	0	1.243248	-1.329935	1.673259
40	6	0	4.580331	-1.855624	1.299040
41	1	0	5.481970	-2.863347	-0.374800
42	1	0	3.388233	-0.919579	2.824890
43	1	0	5.520981	-1.674074	1.805204

Structure 30f (DMSO)

Energy (Hartrees): -1124.91315682
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.515757	0.476418	0.836189
2	6	0	-3.862621	0.768880	0.976804
3	6	0	-4.763658	0.202045	0.084808
4	6	0	-4.351632	-0.637531	-0.942615
5	6	0	-3.001194	-0.912243	-1.073389
6	6	0	-2.057605	-0.372116	-0.184043
7	1	0	-1.815349	0.894976	1.549340
8	1	0	-4.210806	1.413410	1.773039
9	1	0	-5.072419	-1.051638	-1.635420
10	1	0	-2.674353	-1.540210	-1.893810
11	6	0	-0.611598	-0.681692	-0.316799
12	6	0	-0.268099	-1.974813	-0.611495
13	6	0	0.315742	0.434304	-0.205931
14	1	0	-1.076628	-2.659655	-0.849643
15	1	0	-0.061531	1.343902	0.274510
16	1	0	0.916413	-3.518281	-1.071011
17	7	0	1.492587	0.404480	-0.710049
18	7	0	0.936613	-2.596181	-0.652835
19	7	0	-6.189543	0.501074	0.229909
20	8	0	-6.966421	-0.008570	-0.555812
21	8	0	-6.531032	1.244918	1.130351
22	6	0	2.351126	1.499076	-0.512648
23	6	0	3.182813	1.886197	-1.570649
24	6	0	2.454782	2.164355	0.716075
25	6	0	4.064291	2.948522	-1.417552
26	1	0	3.117023	1.349024	-2.510666
27	6	0	3.349515	3.220250	0.865429
28	1	0	1.851918	1.835441	1.556217
29	6	0	4.151990	3.621483	-0.199155
30	1	0	4.692391	3.247310	-2.249502
31	1	0	3.426866	3.723499	1.823044
32	1	0	4.850568	4.441112	-0.077612
33	6	0	2.143253	-2.290437	0.010931
34	6	0	3.339043	-2.738822	-0.552440
35	6	0	2.161252	-1.614067	1.231039
36	6	0	4.546757	-2.482811	0.086638
37	1	0	3.314478	-3.276341	-1.494663
38	6	0	3.373815	-1.358088	1.860348
39	1	0	1.231609	-1.290667	1.684533
40	6	0	4.572155	-1.782174	1.290308
41	1	0	5.471128	-2.828727	-0.362154
42	1	0	3.379415	-0.823983	2.804062
43	1	0	5.515086	-1.575979	1.783129

Structure 30f (C_2H_5OH)

Energy (Hartrees): -1124.91485130
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.517491	0.475963	0.843922
2	6	0	-3.863552	0.771924	0.978886
3	6	0	-4.762401	0.204450	0.084041
4	6	0	-4.348926	-0.639574	-0.940004
5	6	0	-2.999316	-0.916988	-1.064610
6	6	0	-2.057307	-0.376335	-0.173081
7	1	0	-1.818999	0.894085	1.559210
8	1	0	-4.213132	1.419134	1.772543
9	1	0	-5.066869	-1.053363	-1.635920
10	1	0	-2.670286	-1.545320	-1.883849
11	6	0	-0.612722	-0.688578	-0.303590
12	6	0	-0.272464	-1.983020	-0.596680
13	6	0	0.317189	0.425977	-0.193761
14	1	0	-1.083009	-2.667180	-0.830081
15	1	0	-0.053541	1.331887	0.298526
16	1	0	0.907878	-3.532842	-1.048646
17	7	0	1.486654	0.400464	-0.714694
18	7	0	0.930213	-2.607557	-0.638129
19	7	0	-6.183016	0.508154	0.220558
20	8	0	-6.964370	-0.010790	-0.556166
21	8	0	-6.531177	1.267767	1.106534
22	6	0	2.348611	1.492574	-0.514588
23	6	0	3.171921	1.887971	-1.575826
24	6	0	2.463165	2.147603	0.718550
25	6	0	4.055411	2.948378	-1.421262
26	1	0	3.098534	1.358830	-2.519874
27	6	0	3.359806	3.201583	0.869493
28	1	0	1.868280	1.811864	1.561743
29	6	0	4.153655	3.611288	-0.198247
30	1	0	4.677213	3.253229	-2.255893
31	1	0	3.445791	3.696454	1.830887
32	1	0	4.854123	4.429283	-0.075597
33	6	0	2.142002	-2.291792	0.014145
34	6	0	3.337493	-2.717849	-0.565404
35	6	0	2.162008	-1.626114	1.239671
36	6	0	4.547870	-2.450102	0.064093
37	1	0	3.311812	-3.246352	-1.512753
38	6	0	3.376752	-1.357501	1.859062
39	1	0	1.231720	-1.321161	1.705102
40	6	0	4.575089	-1.759576	1.273320
41	1	0	5.472666	-2.778058	-0.397374
42	1	0	3.384597	-0.831614	2.807479
43	1	0	5.519894	-1.543801	1.758622

Structure 31a (vacuum)

Energy (Hartrees): -517.564821965
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.118577	0.688634	0.659265
2	6	0	1.756707	0.959387	0.602519
3	6	0	0.873571	0.081580	-0.038303
4	6	0	1.403087	-1.076822	-0.619258
5	6	0	2.762192	-1.358858	-0.544939
6	6	0	3.627645	-0.474651	0.090749
7	1	0	3.782653	1.382084	1.162144
8	1	0	1.367266	1.850680	1.082305
9	1	0	0.743615	-1.749236	-1.157914
10	1	0	3.149049	-2.262760	-1.001293
11	1	0	4.688524	-0.688372	0.140021
12	6	0	-0.574530	0.377365	-0.095687
13	6	0	-1.496677	-0.616808	0.144331
14	1	0	-1.141182	-1.611460	0.408301
15	6	0	-1.027857	1.713324	-0.403851
16	1	0	-0.233711	2.454472	-0.604819
17	1	0	-3.163914	0.448746	-0.119036
18	7	0	-2.823405	-0.484903	0.098863
19	6	0	-3.749970	-1.536857	0.458878
20	1	0	-4.508914	-1.657599	-0.315801
21	1	0	-3.206361	-2.476798	0.558533
22	1	0	-4.247650	-1.320644	1.407696
23	8	0	-2.202750	2.060930	-0.471800

Structure 31a ($CHCl_3$)

Energy (Hartrees): -517.582821953
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.132541	0.699316	0.611454
2	6	0	1.770201	0.975512	0.566599
3	6	0	0.871065	0.080608	-0.030476
4	6	0	1.387031	-1.103436	-0.575255
5	6	0	2.746470	-1.389920	-0.510860
6	6	0	3.627905	-0.487251	0.078016
7	1	0	3.807890	1.408335	1.077458
8	1	0	1.395357	1.887647	1.018867
9	1	0	0.718452	-1.797108	-1.074699
10	1	0	3.120901	-2.313816	-0.938063
11	1	0	4.688824	-0.705317	0.118509
12	6	0	-0.576035	0.388323	-0.084019
13	6	0	-1.507280	-0.610223	0.153867
14	1	0	-1.156189	-1.609668	0.403659
15	6	0	-1.012275	1.719701	-0.393119
16	1	0	-0.214232	2.449649	-0.614010
17	1	0	-3.182006	0.451350	-0.093925
18	7	0	-2.825934	-0.474841	0.127386
19	6	0	-3.757203	-1.550902	0.409054
20	1	0	-4.381086	-1.755147	-0.463374
21	1	0	-3.199014	-2.451489	0.664037
22	1	0	-4.400783	-1.285542	1.249887
23	8	0	-2.188887	2.089328	-0.448953

Structure 31a (DMSO)

Energy (Hartrees): -517.581584171
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.148422	0.716798	0.546416
2	6	0	1.786214	0.998169	0.514147
3	6	0	0.869702	0.080063	-0.021266
4	6	0	1.371377	-1.133525	-0.515356
5	6	0	2.730604	-1.423723	-0.461977
6	6	0	3.628877	-0.497715	0.063459
7	1	0	3.835435	1.444553	0.964604
8	1	0	1.426918	1.934552	0.928063
9	1	0	0.691844	-1.851885	-0.962195
10	1	0	3.091239	-2.370794	-0.848771
11	1	0	4.689474	-0.719549	0.094613
12	6	0	-0.576054	0.393330	-0.066644
13	6	0	-1.511970	-0.609326	0.154333
14	1	0	-1.166494	-1.614644	0.386991
15	6	0	-1.006073	1.727701	-0.366506
16	1	0	-0.204544	2.452625	-0.590286
17	1	0	-3.185916	0.458367	-0.080986
18	7	0	-2.827541	-0.470085	0.125731
19	6	0	-3.764144	-1.553493	0.364821
20	1	0	-4.373869	-1.729390	-0.523412
21	1	0	-3.209797	-2.460700	0.603218
22	1	0	-4.420123	-1.306400	1.201306
23	8	0	-2.180389	2.108024	-0.415229

Structure 31a (C_2H_5OH)

Energy (Hartrees): -517.584239656
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.140965	0.702757	0.582743
2	6	0	1.779164	0.985420	0.545442
3	6	0	0.869543	0.083225	-0.025458
4	6	0	1.373720	-1.116107	-0.548823
5	6	0	2.732571	-1.408070	-0.491396
6	6	0	3.625150	-0.497495	0.069046
7	1	0	3.824470	1.417775	1.027852
8	1	0	1.414476	1.909216	0.982612
9	1	0	0.697541	-1.820481	-1.022591
10	1	0	3.097349	-2.343838	-0.901332
11	1	0	4.685491	-0.720657	0.103834
12	6	0	-0.576850	0.398339	-0.076409
13	6	0	-1.511984	-0.606480	0.155112
14	1	0	-1.159768	-1.606708	0.399197
15	6	0	-1.001734	1.725209	-0.379896
16	1	0	-0.202804	2.451999	-0.600448
17	1	0	-3.193012	0.446784	-0.093894
18	7	0	-2.825929	-0.475381	0.124844
19	6	0	-3.755484	-1.560146	0.389969
20	1	0	-4.371401	-1.752803	-0.490258
21	1	0	-3.194985	-2.460474	0.639110
22	1	0	-4.405526	-1.301375	1.227438
23	8	0	-2.182586	2.108540	-0.433426

Structure 31b (vacuum)

Energy (Hartrees): -517.558987889
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.880759	0.478647	0.836225
2	6	0	1.553849	0.890419	0.786024
3	6	0	0.637979	0.260881	-0.064814
4	6	0	1.096252	-0.791928	-0.867546
5	6	0	2.420122	-1.212675	-0.808686
6	6	0	3.317905	-0.578162	0.043812
7	1	0	3.573459	0.978921	1.502975
8	1	0	1.215215	1.699977	1.423759
9	1	0	0.410637	-1.260654	-1.566623
10	1	0	2.754652	-2.026242	-1.441993
11	1	0	4.350972	-0.901800	0.087160
12	6	0	-0.769886	0.709517	-0.124710
13	6	0	-1.832502	-0.136137	-0.016642
14	1	0	-2.825063	0.305513	-0.072919
15	6	0	-1.073875	2.132982	-0.283915
16	1	0	-0.181984	2.784779	-0.372015
17	1	0	-0.895042	-1.894856	0.314478
18	7	0	-1.799107	-1.471601	0.153816
19	6	0	-2.975135	-2.249226	0.496639
20	1	0	-3.121004	-2.322698	1.578659
21	1	0	-3.853241	-1.775828	0.057544
22	1	0	-2.887347	-3.253905	0.082685
23	8	0	-2.185040	2.617761	-0.331093

Structure 31b ($CHCl_3$)

Energy (Hartrees): -517.579053273
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.899476	0.474048	0.810265
2	6	0	1.573228	0.891897	0.765751
3	6	0	0.642727	0.248078	-0.060128
4	6	0	1.085595	-0.828912	-0.840562
5	6	0	2.408495	-1.255534	-0.786832
6	6	0	3.321776	-0.604500	0.037976
7	1	0	3.602620	0.987231	1.456841
8	1	0	1.248518	1.720633	1.386803
9	1	0	0.390886	-1.318639	-1.516309
10	1	0	2.729085	-2.088607	-1.402514
11	1	0	4.354060	-0.932910	0.076219
12	6	0	-0.761101	0.715109	-0.120336
13	6	0	-1.844681	-0.119873	0.005622
14	1	0	-2.831849	0.332156	-0.056452
15	6	0	-1.033384	2.128083	-0.295247
16	1	0	-0.130620	2.757828	-0.410487
17	1	0	-0.944023	-1.899514	0.332448
18	7	0	-1.836258	-1.436443	0.211051
19	6	0	-3.031405	-2.225695	0.452716
20	1	0	-3.101498	-2.517597	1.503456
21	1	0	-3.907674	-1.632914	0.191788
22	1	0	-3.020360	-3.125299	-0.164510
23	8	0	-2.137462	2.654566	-0.336249

Structure 31b (DMSO)

Energy (Hartrees): -517.578486433
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.920496	0.489931	0.762995
2	6	0	1.595882	0.914595	0.723463
3	6	0	0.645325	0.241365	-0.056534
4	6	0	1.068441	-0.873517	-0.795031
5	6	0	2.389727	-1.306265	-0.745309
6	6	0	3.322792	-0.625494	0.032914
7	1	0	3.637767	1.026892	1.373974
8	1	0	1.289926	1.772324	1.314158
9	1	0	0.360557	-1.394390	-1.432672
10	1	0	2.692458	-2.170221	-1.326866
11	1	0	4.353309	-0.960088	0.068583
12	6	0	-0.754874	0.718516	-0.113103
13	6	0	-1.849683	-0.107786	0.019481
14	1	0	-2.832753	0.351649	-0.051830
15	6	0	-1.012542	2.130171	-0.299802
16	1	0	-0.102673	2.745629	-0.435672
17	1	0	-0.973347	-1.898857	0.357944
18	7	0	-1.856901	-1.416246	0.244519
19	6	0	-3.063347	-2.206447	0.420002
20	1	0	-3.119246	-2.601085	1.436565
21	1	0	-3.931228	-1.574418	0.235155
22	1	0	-3.074056	-3.039148	-0.285385
23	8	0	-2.109463	2.675628	-0.332507

Structure 31b (C_2H_5OH)

Energy (Hartrees): -517.581906803
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.909525	0.479056	0.786746
2	6	0	1.584005	0.901459	0.748732
3	6	0	0.642874	0.246795	-0.056442
4	6	0	1.072557	-0.846849	-0.821363
5	6	0	2.394319	-1.278095	-0.772904
6	6	0	3.319369	-0.615579	0.030173
7	1	0	3.621324	1.001458	1.416560
8	1	0	1.270377	1.743189	1.358225
9	1	0	0.369749	-1.350648	-1.478298
10	1	0	2.703925	-2.125614	-1.374719
11	1	0	4.350635	-0.948405	0.064454
12	6	0	-0.759599	0.721934	-0.113625
13	6	0	-1.851984	-0.113434	0.024588
14	1	0	-2.840907	0.331944	-0.053083
15	6	0	-1.018463	2.121694	-0.303529
16	1	0	-0.115960	2.743444	-0.442188
17	1	0	-0.951348	-1.886927	0.371915
18	7	0	-1.842325	-1.415630	0.263446
19	6	0	-3.038630	-2.227825	0.415439
20	1	0	-3.089098	-2.647363	1.421852
21	1	0	-3.915545	-1.604719	0.244258
22	1	0	-3.033661	-3.042568	-0.310725
23	8	0	-2.124632	2.670087	-0.336159

Structure 31c (vacuum)

Energy (Hartrees): -517.559860179
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.755543	-0.080005	0.850411
2	6	0	1.545813	0.597302	0.765885
3	6	0	0.528507	0.131398	-0.073851
4	6	0	0.765845	-1.014585	-0.841467
5	6	0	1.977305	-1.693014	-0.754378
6	6	0	2.974488	-1.229670	0.096624
7	1	0	3.533330	0.293845	1.505965
8	1	0	1.384077	1.501125	1.339482
9	1	0	0.005276	-1.356608	-1.536504
10	1	0	2.146501	-2.574712	-1.361689
11	1	0	3.920260	-1.754187	0.164201
12	6	0	-0.765836	0.843566	-0.155003
13	6	0	-1.970597	0.216028	-0.067688
14	1	0	-2.873597	0.820013	-0.136622
15	6	0	-0.816093	2.297057	-0.284718
16	1	0	-1.845356	2.707858	-0.364336
17	1	0	-1.393975	-1.683818	0.294735
18	7	0	-2.199594	-1.105726	0.095879
19	6	0	-3.500310	-1.617877	0.485846
20	1	0	-3.673643	-1.540339	1.564025
21	1	0	-4.277432	-1.056906	-0.034689
22	1	0	-3.584210	-2.663034	0.189415
23	8	0	0.135993	3.043206	-0.303137

Structure 31c ($CHCl_3$)

Energy (Hartrees): -517.581162894
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.770890	-0.096475	0.851980
2	6	0	1.556497	0.576903	0.787465
3	6	0	0.533033	0.126521	-0.055216
4	6	0	0.766586	-1.010612	-0.838529
5	6	0	1.980969	-1.687643	-0.770094
6	6	0	2.987013	-1.233498	0.077232
7	1	0	3.551471	0.267976	1.510479
8	1	0	1.394576	1.462749	1.390055
9	1	0	-0.000321	-1.353693	-1.526356
10	1	0	2.144952	-2.563633	-1.387898
11	1	0	3.934774	-1.757210	0.129003
12	6	0	-0.758350	0.849017	-0.122148
13	6	0	-1.978867	0.228847	-0.019000
14	1	0	-2.874416	0.843388	-0.087101
15	6	0	-0.804292	2.284972	-0.278824
16	1	0	-1.829410	2.703379	-0.329829
17	1	0	-1.428291	-1.686880	0.315606
18	7	0	-2.218128	-1.070936	0.169514
19	6	0	-3.542922	-1.614883	0.412761
20	1	0	-3.719482	-1.774851	1.479698
21	1	0	-4.288951	-0.917727	0.031099
22	1	0	-3.654905	-2.564544	-0.111213
23	8	0	0.154195	3.037339	-0.359237

Structure 31c (DMSO)

Energy (Hartrees): -517.581616964
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.774445	-0.097923	0.852076
2	6	0	1.559287	0.575596	0.790299
3	6	0	0.533912	0.128640	-0.053110
4	6	0	0.766714	-1.007502	-0.838729
5	6	0	1.981623	-1.684742	-0.773620
6	6	0	2.989911	-1.232616	0.072612
7	1	0	3.554845	0.262164	1.513539
8	1	0	1.396820	1.456428	1.400421
9	1	0	-0.002989	-1.355074	-1.521131
10	1	0	2.142317	-2.561452	-1.391381
11	1	0	3.936752	-1.758331	0.123260
12	6	0	-0.757421	0.850902	-0.115904
13	6	0	-1.980943	0.227300	-0.008345
14	1	0	-2.876284	0.842490	-0.073531
15	6	0	-0.807154	2.282855	-0.275387
16	1	0	-1.834026	2.696600	-0.317323
17	1	0	-1.430099	-1.692436	0.310022
18	7	0	-2.217144	-1.067426	0.183119
19	6	0	-3.543532	-1.620992	0.399642
20	1	0	-3.719753	-1.818245	1.459869
21	1	0	-4.288000	-0.911146	0.039989
22	1	0	-3.647548	-2.552865	-0.156689
23	8	0	0.148366	3.041842	-0.370761

Structure 31c (C_2H_5OH)

Energy (Hartrees): -517.585476984
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.754491	-0.123694	0.890824
2	6	0	1.536603	0.545879	0.836962
3	6	0	0.531556	0.132691	-0.045886
4	6	0	0.781569	-0.967597	-0.875000
5	6	0	1.998230	-1.641988	-0.816714
6	6	0	2.989071	-1.221437	0.065867
7	1	0	3.521287	0.211226	1.580861
8	1	0	1.356919	1.394708	1.487533
9	1	0	0.023150	-1.288505	-1.582848
10	1	0	2.174907	-2.490542	-1.468571
11	1	0	3.938042	-1.744087	0.109933
12	6	0	-0.761667	0.854835	-0.106594
13	6	0	-1.985669	0.224782	0.002533
14	1	0	-2.885285	0.833394	-0.062845
15	6	0	-0.815175	2.274921	-0.275093
16	1	0	-1.835851	2.697357	-0.312060
17	1	0	-1.413558	-1.688022	0.306666
18	7	0	-2.207661	-1.068446	0.194096
19	6	0	-3.530464	-1.641400	0.387353
20	1	0	-3.713830	-1.855569	1.442774
21	1	0	-4.279545	-0.935599	0.029719
22	1	0	-3.616402	-2.566529	-0.182950
23	8	0	0.149065	3.036168	-0.386549

Structure 31d (vacuum)

Energy (Hartrees): -517.551218220
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.995038	0.351002	0.722393
2	6	0	1.676128	0.777570	0.639584
3	6	0	0.720466	0.009337	-0.036081
4	6	0	1.134593	-1.179402	-0.646116
5	6	0	2.453838	-1.610253	-0.555282
6	6	0	3.389840	-0.846148	0.131284
7	1	0	3.719892	0.957696	1.252570
8	1	0	1.380184	1.712681	1.096982
9	1	0	0.420650	-1.759859	-1.220910
10	1	0	2.752296	-2.533989	-1.037404
11	1	0	4.420467	-1.174240	0.196545
12	6	0	-0.699497	0.429405	-0.093463
13	6	0	-1.677698	-0.509577	0.067238
14	1	0	-1.371634	-1.519322	0.335201
15	6	0	-1.047967	1.833124	-0.289977
16	1	0	-2.132632	2.066603	-0.244561
17	1	0	-3.398254	0.511348	-0.330566
18	7	0	-3.018553	-0.390519	-0.091196
19	6	0	-3.940257	-1.355844	0.479328
20	1	0	-4.872364	-1.347927	-0.084939
21	1	0	-3.503770	-2.352535	0.399345
22	1	0	-4.159769	-1.154271	1.532556
23	8	0	-0.269012	2.741520	-0.471238

Structure 31d ($CHCl_3$)

Energy (Hartrees): -517.573600113
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.004285	0.334546	0.715256
2	6	0	1.685754	0.768291	0.645210
3	6	0	0.716078	0.012070	-0.027791
4	6	0	1.119019	-1.181563	-0.639814
5	6	0	2.437296	-1.621032	-0.560861
6	6	0	3.387246	-0.863569	0.116168
7	1	0	3.736721	0.934351	1.244161
8	1	0	1.399925	1.698757	1.119781
9	1	0	0.395760	-1.764265	-1.201111
10	1	0	2.723595	-2.548392	-1.044543
11	1	0	4.416834	-1.198337	0.170752
12	6	0	-0.699487	0.450431	-0.078671
13	6	0	-1.691419	-0.490461	0.091175
14	1	0	-1.387842	-1.500172	0.362069
15	6	0	-1.034164	1.842844	-0.282355
16	1	0	-2.111106	2.090809	-0.226602
17	1	0	-3.414586	0.527119	-0.300764
18	7	0	-3.017810	-0.365072	-0.042427
19	6	0	-3.946487	-1.377022	0.433374
20	1	0	-4.837943	-1.376750	-0.193119
21	1	0	-3.472746	-2.356840	0.363782
22	1	0	-4.240671	-1.198530	1.471404
23	8	0	-0.244000	2.750068	-0.492371

Structure 31d (DMSO)

Energy (Hartrees): -517.574577397
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.009759	0.327152	0.711583
2	6	0	1.691923	0.765980	0.648008
3	6	0	0.714857	0.016244	-0.023599
4	6	0	1.111074	-1.179649	-0.637646
5	6	0	2.428576	-1.624248	-0.565489
6	6	0	3.385876	-0.871294	0.107369
7	1	0	3.746491	0.920964	1.241788
8	1	0	1.411295	1.693141	1.132377
9	1	0	0.381488	-1.762876	-1.190400
10	1	0	2.708006	-2.553740	-1.049467
11	1	0	4.414085	-1.211253	0.158072
12	6	0	-0.698538	0.460183	-0.069376
13	6	0	-1.691903	-0.486384	0.105907
14	1	0	-1.383613	-1.494197	0.378607
15	6	0	-1.032097	1.848352	-0.279204
16	1	0	-2.108171	2.094975	-0.220229
17	1	0	-3.413691	0.525959	-0.294491
18	7	0	-3.012486	-0.360977	-0.019649
19	6	0	-3.948375	-1.386572	0.411170
20	1	0	-4.754758	-1.477915	-0.316720
21	1	0	-3.423881	-2.339401	0.480067
22	1	0	-4.375667	-1.145026	1.387651
23	8	0	-0.242636	2.757204	-0.502756

Structure 31d (C_2H_5OH)

Energy (Hartrees): -517.578041441
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.007392	0.312540	0.728302
2	6	0	1.690069	0.753903	0.670666
3	6	0	0.715052	0.018328	-0.018089
4	6	0	1.109020	-1.166890	-0.652565
5	6	0	2.425531	-1.614756	-0.585539
6	6	0	3.382207	-0.874935	0.102647
7	1	0	3.743930	0.895273	1.270950
8	1	0	1.409232	1.669990	1.177072
9	1	0	0.378713	-1.738283	-1.216934
10	1	0	2.704753	-2.535893	-1.085409
11	1	0	4.409942	-1.217209	0.149057
12	6	0	-0.698163	0.466813	-0.062661
13	6	0	-1.694831	-0.480320	0.121080
14	1	0	-1.384607	-1.485020	0.402434
15	6	0	-1.028429	1.843654	-0.284259
16	1	0	-2.099872	2.101688	-0.227486
17	1	0	-3.412997	0.528361	-0.290546
18	7	0	-3.011443	-0.355380	-0.004655
19	6	0	-3.950934	-1.389381	0.400819
20	1	0	-4.736876	-1.485460	-0.348492
21	1	0	-3.421957	-2.338249	0.483958
22	1	0	-4.405425	-1.149171	1.364869
23	8	0	-0.230778	2.753486	-0.521161

Structure 31e (vacuum)

Energy (Hartrees): -517.548977006
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.958566	0.734700	-0.520680
2	6	0	-1.584787	0.933206	-0.539047
3	6	0	-0.716847	-0.039247	-0.026994
4	6	0	-1.272358	-1.197963	0.524773
5	6	0	-2.648932	-1.400376	0.536407
6	6	0	-3.497867	-0.433589	0.012060
7	1	0	-3.614079	1.497221	-0.925106
8	1	0	-1.177449	1.847834	-0.949644
9	1	0	-0.618137	-1.938719	0.972646
10	1	0	-3.056269	-2.306328	0.970161
11	1	0	-4.570937	-0.583153	0.026138
12	6	0	0.757764	0.134894	-0.087297
13	6	0	1.506169	-0.941388	-0.477044
14	1	0	0.956004	-1.800951	-0.852839
15	6	0	1.333032	1.453846	0.182195
16	1	0	2.409080	1.566251	-0.031249
17	1	0	3.146834	-2.023899	-0.874472
18	7	0	2.843349	-1.158189	-0.463215
19	6	0	3.851006	-0.392842	0.243036
20	1	0	4.693454	-1.047554	0.465445
21	1	0	4.217652	0.456969	-0.337977
22	1	0	3.436072	-0.023384	1.184422
23	8	0	0.707831	2.419449	0.563816

Structure 31e ($CHCl_3$)

Energy (Hartrees): -517.571578077
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.960996	0.733079	-0.536358
2	6	0	-1.585509	0.926892	-0.556466
3	6	0	-0.716182	-0.039467	-0.030716
4	6	0	-1.276152	-1.193544	0.529836
5	6	0	-2.654279	-1.392498	0.542482
6	6	0	-3.503365	-0.428561	0.010177
7	1	0	-3.614584	1.491714	-0.952603
8	1	0	-1.177309	1.832108	-0.988508
9	1	0	-0.624528	-1.937016	0.977494
10	1	0	-3.063268	-2.295579	0.981969
11	1	0	-4.577102	-0.576494	0.025181
12	6	0	0.759291	0.138425	-0.086167
13	6	0	1.516062	-0.952027	-0.459185
14	1	0	0.968846	-1.814829	-0.831693
15	6	0	1.329908	1.443555	0.189915
16	1	0	2.403739	1.560565	-0.017028
17	1	0	3.139243	-2.051818	-0.823323
18	7	0	2.837576	-1.172947	-0.431004
19	6	0	3.865434	-0.369719	0.202918
20	1	0	4.723875	-1.010600	0.400495
21	1	0	4.190152	0.462051	-0.426745
22	1	0	3.493769	0.024709	1.152102
23	8	0	0.703606	2.416127	0.585133

Structure 31e (DMSO)

Energy (Hartrees): -517.572616403
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.950984	0.726440	-0.579426
2	6	0	-1.573800	0.914007	-0.585408
3	6	0	-0.713776	-0.042169	-0.025032
4	6	0	-1.286336	-1.182959	0.551088
5	6	0	-2.665924	-1.376307	0.549808
6	6	0	-3.505345	-0.420782	-0.013371
7	1	0	-3.596148	1.476782	-1.023633
8	1	0	-1.156013	1.806339	-1.035371
9	1	0	-0.644142	-1.924044	1.016288
10	1	0	-3.083170	-2.270355	1.000107
11	1	0	-4.579776	-0.565378	-0.010051
12	6	0	0.762993	0.135577	-0.062192
13	6	0	1.519573	-0.970142	-0.406432
14	1	0	0.965318	-1.844805	-0.738556
15	6	0	1.322032	1.440476	0.227234
16	1	0	2.400417	1.561928	0.058437
17	1	0	3.124643	-2.096531	-0.746531
18	7	0	2.834964	-1.194883	-0.395869
19	6	0	3.888362	-0.338001	0.112766
20	1	0	4.784483	-0.943889	0.236059
21	1	0	4.112500	0.482818	-0.572635
22	1	0	3.599868	0.073142	1.083813
23	8	0	0.680812	2.411416	0.611120

Structure 31e (C_2H_5OH)

Energy (Hartrees): -517.576248345
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.949454	0.706932	-0.614408
2	6	0	-1.572470	0.896399	-0.623515
3	6	0	-0.714029	-0.038627	-0.028016
4	6	0	-1.283392	-1.162145	0.582430
5	6	0	-2.662519	-1.357728	0.584438
6	6	0	-3.501720	-0.422206	-0.011738
7	1	0	-3.595007	1.440708	-1.084884
8	1	0	-1.154067	1.772578	-1.105505
9	1	0	-0.639150	-1.886377	1.071074
10	1	0	-3.080092	-2.237535	1.061781
11	1	0	-4.575950	-0.568916	-0.006190
12	6	0	0.763655	0.140783	-0.064290
13	6	0	1.520204	-0.963999	-0.423570
14	1	0	0.963370	-1.831063	-0.771011
15	6	0	1.322238	1.430912	0.242272
16	1	0	2.399553	1.559712	0.084285
17	1	0	3.121922	-2.088692	-0.771500
18	7	0	2.832019	-1.190816	-0.410520
19	6	0	3.884468	-0.340216	0.112606
20	1	0	4.780511	-0.947242	0.229678
21	1	0	4.110130	0.488613	-0.562341
22	1	0	3.593206	0.056612	1.088584
23	8	0	0.676194	2.404587	0.637801

Structure 31f (vacuum)

Energy (Hartrees): -517.552301808
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.036015	1.002709	-0.296005
2	6	0	-1.651354	1.112520	-0.324176
3	6	0	-0.833940	0.022281	0.005035
4	6	0	-1.456812	-1.179071	0.365532
5	6	0	-2.842076	-1.296164	0.373198
6	6	0	-3.638639	-0.203779	0.047124
7	1	0	-3.646451	1.858874	-0.559256
8	1	0	-1.196938	2.047212	-0.634440
9	1	0	-0.844953	-2.022218	0.668177
10	1	0	-3.300183	-2.237700	0.653459
11	1	0	-4.718426	-0.290552	0.062461
12	6	0	0.642383	0.137925	-0.037440
13	6	0	1.359049	-0.896384	-0.583969
14	1	0	0.798945	-1.656338	-1.125728
15	6	0	1.231209	1.409968	0.374789
16	1	0	0.556345	2.047762	0.977427
17	1	0	2.997047	-1.931314	-1.075797
18	7	0	2.678123	-1.148874	-0.529790
19	6	0	3.621976	-0.600291	0.428325
20	1	0	4.424733	-1.324896	0.563913
21	1	0	4.022925	0.359687	0.105604
22	1	0	3.112359	-0.449454	1.382996
23	8	0	2.334130	1.822846	0.071904

Structure 31f ($CHCl_3$)

Energy (Hartrees): -517.571906192
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.038290	1.010285	-0.256457
2	6	0	-1.652936	1.122343	-0.289787
3	6	0	-0.830331	0.023889	0.004798
4	6	0	-1.452103	-1.189855	0.331378
5	6	0	-2.838045	-1.308209	0.342431
6	6	0	-3.638860	-0.206947	0.053942
7	1	0	-3.650377	1.873776	-0.492746
8	1	0	-1.203321	2.067020	-0.576979
9	1	0	-0.841297	-2.045167	0.601283
10	1	0	-3.293487	-2.259557	0.594368
11	1	0	-4.718939	-0.295804	0.071644
12	6	0	0.645978	0.143307	-0.043043
13	6	0	1.368689	-0.899592	-0.587151
14	1	0	0.820555	-1.655100	-1.146581
15	6	0	1.230580	1.412337	0.349778
16	1	0	0.568602	2.052669	0.961736
17	1	0	3.002622	-1.949091	-1.035504
18	7	0	2.675961	-1.156850	-0.502584
19	6	0	3.608610	-0.603137	0.461848
20	1	0	4.400335	-1.334927	0.619662
21	1	0	4.033078	0.342892	0.126143
22	1	0	3.087842	-0.426708	1.406382
23	8	0	2.330364	1.837677	0.022782

Structure 31f (DMSO)

Energy (Hartrees): -517.574736227
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.048095	1.004898	-0.229202
2	6	0	-1.663885	1.129835	-0.280088
3	6	0	-0.828262	0.034918	-0.008304
4	6	0	-1.434723	-1.189690	0.307966
5	6	0	-2.819673	-1.320100	0.335964
6	6	0	-3.634097	-0.221605	0.074560
7	1	0	-3.670932	1.865883	-0.446808
8	1	0	-1.227447	2.082688	-0.561050
9	1	0	-0.813288	-2.044641	0.554802
10	1	0	-3.262991	-2.279498	0.579848
11	1	0	-4.713289	-0.320219	0.105706
12	6	0	0.647124	0.163073	-0.062827
13	6	0	1.373027	-0.883109	-0.614918
14	1	0	0.833788	-1.619734	-1.207159
15	6	0	1.229696	1.420659	0.327308
16	1	0	0.564972	2.076266	0.916545
17	1	0	3.002435	-1.943812	-1.032408
18	7	0	2.668352	-1.153680	-0.497443
19	6	0	3.579679	-0.627965	0.503343
20	1	0	4.319307	-1.399024	0.716377
21	1	0	4.081229	0.279705	0.167455
22	1	0	3.022175	-0.398368	1.414123
23	8	0	2.347604	1.838879	0.018982

Structure 31f (C_2H_5OH)

Energy (Hartrees): -517.574736227
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.048095	1.004898	-0.229202
2	6	0	-1.663885	1.129835	-0.280088
3	6	0	-0.828262	0.034918	-0.008304
4	6	0	-1.434723	-1.189690	0.307966
5	6	0	-2.819673	-1.320100	0.335964
6	6	0	-3.634097	-0.221605	0.074560
7	1	0	-3.670932	1.865883	-0.446808
8	1	0	-1.227447	2.082688	-0.561050
9	1	0	-0.813288	-2.044641	0.554802
10	1	0	-3.262991	-2.279498	0.579848
11	1	0	-4.713289	-0.320219	0.105706
12	6	0	0.647124	0.163073	-0.062827
13	6	0	1.373027	-0.883109	-0.614918
14	1	0	0.833788	-1.619734	-1.207159
15	6	0	1.229696	1.420659	0.327308
16	1	0	0.564972	2.076266	0.916545
17	1	0	3.002435	-1.943812	-1.032408
18	7	0	2.668352	-1.153680	-0.497443
19	6	0	3.579679	-0.627965	0.503343
20	1	0	4.319307	-1.399024	0.716377
21	1	0	4.081229	0.279705	0.167455
22	1	0	3.022175	-0.398368	1.414123
23	8	0	2.347604	1.838879	0.018982

Structure 31g (vacuum)

Energy (Hartrees): -517.556667801
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.751661	-1.354921	-0.540097
2	6	0	1.390815	-1.077060	-0.588569
3	6	0	0.876561	0.096142	-0.024813
4	6	0	1.767512	0.979760	0.593751
5	6	0	3.130742	0.710605	0.627628
6	6	0	3.628605	-0.459418	0.063893
7	1	0	3.129893	-2.267541	-0.985975
8	1	0	0.720927	-1.765930	-1.092336
9	1	0	1.382305	1.874272	1.070595
10	1	0	3.804040	1.409519	1.110167
11	1	0	4.690036	-0.673436	0.097596
12	6	0	-0.572103	0.392092	-0.087410
13	6	0	-1.017248	1.640476	-0.392114
14	1	0	-0.323867	2.447019	-0.614732
15	6	0	-1.539181	-0.662296	0.178569
16	1	0	-1.141423	-1.646145	0.459535
17	7	0	-2.801854	-0.463884	0.119819
18	6	0	-3.698643	-1.556910	0.433427
19	1	0	-4.329630	-1.277523	1.280218
20	1	0	-4.356727	-1.743713	-0.417996
21	1	0	-3.161098	-2.480260	0.679585
22	8	0	-2.286001	1.993333	-0.467802
23	1	0	-2.825790	1.173446	-0.268561

Structure 31g ($CHCl_3$)

Energy (Hartrees): -517.571313023
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.748309	-1.376290	-0.506769
2	6	0	1.386315	-1.098523	-0.550690
3	6	0	0.878995	0.094323	-0.020110
4	6	0	1.778083	0.998232	0.559316
5	6	0	3.141823	0.727702	0.587897
6	6	0	3.633282	-0.462177	0.058397
7	1	0	3.120428	-2.304875	-0.925261
8	1	0	0.712253	-1.805933	-1.022305
9	1	0	1.401895	1.911993	1.006780
10	1	0	3.821129	1.442578	1.038659
11	1	0	4.695208	-0.676799	0.088595
12	6	0	-0.570399	0.391481	-0.080563
13	6	0	-1.013538	1.641589	-0.378270
14	1	0	-0.326811	2.454616	-0.598368
15	6	0	-1.541367	-0.665588	0.175519
16	1	0	-1.153505	-1.654499	0.447093
17	7	0	-2.802344	-0.454962	0.116455
18	6	0	-3.711635	-1.544661	0.412313
19	1	0	-4.358031	-1.261536	1.246381
20	1	0	-4.353394	-1.726943	-0.452900
21	1	0	-3.181665	-2.468673	0.668251
22	8	0	-2.289837	1.985800	-0.450260
23	1	0	-2.821620	1.151882	-0.252273

Structure 31g (DMSO)

Energy (Hartrees): -517.568963630
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.741489	-1.404738	-0.458053
2	6	0	1.378526	-1.127546	-0.493343
3	6	0	0.880327	0.090921	-0.012690
4	6	0	1.790793	1.020258	0.508900
5	6	0	3.154740	0.748909	0.528064
6	6	0	3.637177	-0.466281	0.047925
7	1	0	3.104984	-2.353425	-0.837630
8	1	0	0.697714	-1.858511	-0.916513
9	1	0	1.425042	1.956803	0.916697
10	1	0	3.841614	1.483433	0.934085
11	1	0	4.699486	-0.680852	0.070925
12	6	0	-0.568648	0.389394	-0.067605
13	6	0	-1.010883	1.644629	-0.352143
14	1	0	-0.322911	2.459847	-0.560973
15	6	0	-1.543964	-0.668673	0.169327
16	1	0	-1.167806	-1.667274	0.416808
17	7	0	-2.803688	-0.444726	0.113129
18	6	0	-3.726321	-1.532604	0.374941
19	1	0	-4.364631	-1.271722	1.222673
20	1	0	-4.375246	-1.672864	-0.492851
21	1	0	-3.206476	-2.471673	0.592119
22	8	0	-2.286657	1.985504	-0.422206
23	1	0	-2.812116	1.139685	-0.231540

Structure 31g (C_2H_5OH)

Energy (Hartrees): -517.570503198
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.738969	-1.398088	-0.473919
2	6	0	1.376768	-1.117836	-0.511415
3	6	0	0.879426	0.094551	-0.015434
4	6	0	1.788086	1.014820	0.523878
5	6	0	3.151454	0.740355	0.545990
6	6	0	3.633530	-0.468565	0.050308
7	1	0	3.103030	-2.341890	-0.865242
8	1	0	0.695938	-1.840944	-0.948231
9	1	0	1.421452	1.945932	0.943287
10	1	0	3.838062	1.467509	0.965702
11	1	0	4.695411	-0.685678	0.075420
12	6	0	-0.569689	0.394760	-0.072686
13	6	0	-1.008376	1.648033	-0.358087
14	1	0	-0.323672	2.465397	-0.567026
15	6	0	-1.542914	-0.665134	0.172202
16	1	0	-1.159982	-1.656606	0.437532
17	7	0	-2.803311	-0.451027	0.106645
18	6	0	-3.713960	-1.545055	0.388335
19	1	0	-4.365419	-1.270140	1.221339
20	1	0	-4.351344	-1.719410	-0.481800
21	1	0	-3.184148	-2.470177	0.638113
22	8	0	-2.290555	1.990865	-0.427416
23	1	0	-2.821465	1.149219	-0.241323

Structure 31h (vacuum)

Energy (Hartrees): -517.532613746
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.634584	-1.416386	-0.540609
2	6	0	1.284014	-1.089350	-0.542832
3	6	0	0.836664	0.120647	0.000403
4	6	0	1.782782	0.983729	0.563623
5	6	0	3.135444	0.663201	0.554756
6	6	0	3.567205	-0.538277	0.002745
7	1	0	2.961013	-2.355673	-0.971847
8	1	0	0.566007	-1.768644	-0.990204
9	1	0	1.450663	1.901460	1.036424
10	1	0	3.852035	1.346334	0.996065
11	1	0	4.620595	-0.792021	0.003243
12	6	0	-0.608466	0.456190	-0.030249
13	6	0	-0.978122	1.712226	-0.328886
14	1	0	-0.219899	2.451761	-0.574973
15	6	0	-1.559419	-0.625806	0.286357
16	1	0	-1.127388	-1.457728	0.865224
17	7	0	-2.776853	-0.632133	-0.060239
18	6	0	-3.579270	-1.758906	0.365269
19	1	0	-4.027799	-2.228572	-0.513338
20	1	0	-3.012161	-2.513152	0.928279
21	1	0	-4.401303	-1.394801	0.986468
22	8	0	-2.254557	2.140216	-0.343863
23	1	0	-2.279831	3.070641	-0.576225

Structure 31h ($CHCl_3$)

Energy (Hartrees): -517.553424866
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.624116	-1.437315	-0.513638
2	6	0	1.273869	-1.103923	-0.516222
3	6	0	0.834135	0.121145	0.001751
4	6	0	1.789372	0.995897	0.534676
5	6	0	3.140955	0.668696	0.524628
6	6	0	3.564804	-0.549835	0.001558
7	1	0	2.943310	-2.389263	-0.923137
8	1	0	0.553088	-1.793538	-0.943685
9	1	0	1.467937	1.930813	0.981013
10	1	0	3.863086	1.361464	0.942464
11	1	0	4.617598	-0.808211	0.001810
12	6	0	-0.611198	0.462659	-0.028145
13	6	0	-0.973729	1.726842	-0.311746
14	1	0	-0.217514	2.473037	-0.540760
15	6	0	-1.562255	-0.621598	0.277125
16	1	0	-1.131020	-1.459930	0.843989
17	7	0	-2.783999	-0.631652	-0.064276
18	6	0	-3.574410	-1.774429	0.350456
19	1	0	-4.014166	-2.243971	-0.533381
20	1	0	-2.998326	-2.525024	0.907428
21	1	0	-4.404166	-1.429817	0.973349
22	8	0	-2.245837	2.159464	-0.330927
23	1	0	-2.259094	3.101457	-0.534402

Structure 31h (DMSO)

Energy (Hartrees): -517.551193572
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.597112	-1.468925	-0.469823
2	6	0	1.249542	-1.122389	-0.465207
3	6	0	0.830044	0.129331	0.004397
4	6	0	1.801870	1.017797	0.484026
5	6	0	3.149814	0.675966	0.467116
6	6	0	3.554124	-0.569134	-0.008872
7	1	0	2.900348	-2.441434	-0.841508
8	1	0	0.515932	-1.825213	-0.847607
9	1	0	1.498492	1.977189	0.889309
10	1	0	3.884840	1.378912	0.843688
11	1	0	4.604527	-0.837550	-0.013718
12	6	0	-0.613410	0.479329	-0.017823
13	6	0	-0.973790	1.746315	-0.292093
14	1	0	-0.217637	2.492252	-0.521390
15	6	0	-1.563605	-0.603516	0.300172
16	1	0	-1.155796	-1.395995	0.944189
17	7	0	-2.760222	-0.663025	-0.117710
18	6	0	-3.555717	-1.795667	0.320595
19	1	0	-3.915693	-2.339391	-0.557106
20	1	0	-3.004411	-2.486269	0.971138
21	1	0	-4.437938	-1.430956	0.853760
22	8	0	-2.244846	2.185199	-0.294948
23	1	0	-2.248252	3.133396	-0.472134

Structure 31h (C_2H_5OH)

Energy (Hartrees): -517.557992963
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.623194	-1.433638	-0.521972
2	6	0	1.272921	-1.098692	-0.529087
3	6	0	0.832606	0.123092	-0.003377
4	6	0	1.784972	0.993351	0.542174
5	6	0	3.136448	0.663595	0.537943
6	6	0	3.561751	-0.551575	0.007101
7	1	0	2.943651	-2.382803	-0.937521
8	1	0	0.553530	-1.785702	-0.963831
9	1	0	1.462710	1.927479	0.990135
10	1	0	3.857292	1.352385	0.964976
11	1	0	4.614438	-0.811404	0.011400
12	6	0	-0.613357	0.465050	-0.035541
13	6	0	-0.972017	1.733111	-0.311515
14	1	0	-0.218098	2.484669	-0.528020
15	6	0	-1.559129	-0.623916	0.263948
16	1	0	-1.117343	-1.475275	0.800220
17	7	0	-2.790530	-0.629380	-0.048439
18	6	0	-3.564038	-1.788961	0.359048
19	1	0	-4.017922	-2.245126	-0.524651
20	1	0	-2.968881	-2.544533	0.886545
21	1	0	-4.383680	-1.466626	1.006729
22	8	0	-2.244778	2.168434	-0.337871
23	1	0	-2.253874	3.116612	-0.516274

Structure 31i (vacuum)

Energy (Hartrees): -517.538941162
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.323466	-1.711482	-0.515623
2	6	0	1.013548	-1.246793	-0.526062
3	6	0	0.688123	0.001091	0.017125
4	6	0	1.713967	0.772988	0.573508
5	6	0	3.022944	0.307679	0.583766
6	6	0	3.334117	-0.935078	0.040308
7	1	0	2.554298	-2.678168	-0.947830
8	1	0	0.235292	-1.852073	-0.978876
9	1	0	1.479783	1.739304	1.001251
10	1	0	3.803856	0.917927	1.022495
11	1	0	4.356088	-1.294926	0.050349
12	6	0	-0.718678	0.460898	0.002042
13	6	0	-1.097806	1.730171	-0.203416
14	1	0	-2.154337	1.979493	-0.199469
15	6	0	-1.783151	-0.541327	0.227769
16	1	0	-1.447865	-1.482114	0.688999
17	7	0	-3.001078	-0.349365	-0.060671
18	6	0	-3.944395	-1.395521	0.273657
19	1	0	-4.490078	-1.688145	-0.626398
20	1	0	-3.469991	-2.283879	0.711744
21	1	0	-4.679841	-1.003462	0.980822
22	8	0	-0.223760	2.735560	-0.439672
23	1	0	-0.702393	3.551372	-0.599456

Structure 31i ($CHCl_3$)

Energy (Hartrees): -517.557739606
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.298542	-1.730836	-0.505136
2	6	0	0.991562	-1.255039	-0.504929
3	6	0	0.683722	0.005172	0.023217
4	6	0	1.724763	0.774287	0.558411
5	6	0	3.030833	0.297883	0.557594
6	6	0	3.324480	-0.954941	0.025285
7	1	0	2.514540	-2.706457	-0.926066
8	1	0	0.202061	-1.863131	-0.934797
9	1	0	1.506340	1.746062	0.983413
10	1	0	3.822581	0.906930	0.979316
11	1	0	4.343966	-1.323068	0.025116
12	6	0	-0.720271	0.477627	0.017830
13	6	0	-1.089069	1.753326	-0.184233
14	1	0	-2.139141	2.027063	-0.158207
15	6	0	-1.785633	-0.518201	0.259126
16	1	0	-1.472525	-1.414883	0.812222
17	7	0	-2.988354	-0.371530	-0.116140
18	6	0	-3.936058	-1.402049	0.263317
19	1	0	-4.437650	-1.777981	-0.631864
20	1	0	-3.470625	-2.241568	0.794852
21	1	0	-4.707621	-0.964100	0.902602
22	8	0	-0.211737	2.744342	-0.441458
23	1	0	-0.686775	3.573734	-0.564839

Structure 31i (DMSO)

Energy (Hartrees): -517.554686748
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.291361	-1.731359	-0.510766
2	6	0	0.985772	-1.250366	-0.509633
3	6	0	0.683131	0.010093	0.021633
4	6	0	1.726559	0.773306	0.561514
5	6	0	3.031088	0.291354	0.560312
6	6	0	3.320282	-0.960893	0.022897
7	1	0	2.503174	-2.707609	-0.932613
8	1	0	0.193226	-1.856486	-0.937044
9	1	0	1.513384	1.743496	0.993160
10	1	0	3.824608	0.894795	0.987044
11	1	0	4.338370	-1.333219	0.023529
12	6	0	-0.720487	0.484484	0.019786
13	6	0	-1.090356	1.761000	-0.178544
14	1	0	-2.138998	2.039309	-0.136902
15	6	0	-1.782609	-0.512376	0.271233
16	1	0	-1.474201	-1.391523	0.853224
17	7	0	-2.979217	-0.384940	-0.131590
18	6	0	-3.928024	-1.410162	0.265076
19	1	0	-4.410564	-1.819265	-0.626225
20	1	0	-3.465611	-2.227152	0.832029
21	1	0	-4.714051	-0.955956	0.874853
22	8	0	-0.215516	2.749253	-0.451183
23	1	0	-0.690996	3.583677	-0.541519

Structure 31i (C_2H_5OH)

Energy (Hartrees): -517.560405069
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.292566	-1.713028	-0.549381
2	6	0	0.987343	-1.231024	-0.549405
3	6	0	0.678654	0.009552	0.022899
4	6	0	1.713720	0.750702	0.607018
5	6	0	3.018174	0.268280	0.606464
6	6	0	3.314074	-0.963272	0.026575
7	1	0	2.510454	-2.672980	-1.004473
8	1	0	0.199769	-1.818841	-1.010829
9	1	0	1.492839	1.702415	1.075700
10	1	0	3.806017	0.853841	1.067600
11	1	0	4.332110	-1.336043	0.027259
12	6	0	-0.724320	0.488166	0.016269
13	6	0	-1.080795	1.766399	-0.195150
14	1	0	-2.123824	2.064123	-0.161869
15	6	0	-1.786609	-0.505639	0.271479
16	1	0	-1.473209	-1.386309	0.848596
17	7	0	-2.987024	-0.379844	-0.122069
18	6	0	-3.926667	-1.411053	0.281767
19	1	0	-4.423708	-1.814617	-0.603793
20	1	0	-3.453449	-2.231602	0.834129
21	1	0	-4.703358	-0.965030	0.909112
22	8	0	-0.190269	2.740869	-0.472203
23	1	0	-0.649157	3.582496	-0.580532

Structure 31j (vacuum)

Energy (Hartrees): -517.538843644
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.870768	-1.808292	-0.707593
2	6	0	0.664678	-1.119383	-0.739277
3	6	0	0.510757	0.072410	-0.025779
4	6	0	1.585243	0.549606	0.729188
5	6	0	2.788514	-0.144991	0.766086
6	6	0	2.936177	-1.325174	0.045472
7	1	0	1.976403	-2.729412	-1.268782
8	1	0	-0.167294	-1.506699	-1.311884
9	1	0	1.475006	1.470699	1.288102
10	1	0	3.610818	0.236401	1.360122
11	1	0	3.874260	-1.867183	0.072704
12	6	0	-0.765814	0.825273	-0.075593
13	6	0	-0.820006	2.157770	-0.231175
14	1	0	-1.777545	2.671389	-0.261744
15	6	0	-2.066529	0.150864	0.047209
16	1	0	-2.941809	0.818345	-0.014497
17	7	0	-2.208545	-1.094096	0.220403
18	6	0	-3.557683	-1.604166	0.341046
19	1	0	-3.723783	-2.367097	-0.423337
20	1	0	-3.668158	-2.094448	1.311308
21	1	0	-4.328706	-0.827139	0.243699
22	8	0	0.279068	2.935909	-0.362299
23	1	0	0.021442	3.843045	-0.537628

Structure 31j ($CHCl_3$)

Energy (Hartrees): -517.559548899
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.911836	-1.760640	-0.753551
2	6	0	0.699016	-1.081637	-0.790074
3	6	0	0.509163	0.076894	-0.029847
4	6	0	1.557622	0.530711	0.776246
5	6	0	2.769105	-0.151752	0.816380
6	6	0	2.950954	-1.299119	0.050332
7	1	0	2.044482	-2.655376	-1.351528
8	1	0	-0.108970	-1.448511	-1.411001
9	1	0	1.419772	1.422947	1.375831
10	1	0	3.570186	0.212514	1.449786
11	1	0	3.894630	-1.831984	0.081008
12	6	0	-0.775948	0.817690	-0.083714
13	6	0	-0.838844	2.152461	-0.238757
14	1	0	-1.797571	2.663299	-0.275257
15	6	0	-2.068178	0.131915	0.034745
16	1	0	-2.948923	0.785136	-0.054510
17	7	0	-2.198395	-1.112774	0.239537
18	6	0	-3.548201	-1.630399	0.351991
19	1	0	-3.703688	-2.403932	-0.404831
20	1	0	-3.669314	-2.109887	1.327022
21	1	0	-4.320583	-0.858716	0.236667
22	8	0	0.252791	2.931135	-0.368984
23	1	0	-0.012734	3.848108	-0.500577

Structure 31j (DMSO)

Energy (Hartrees): -517.558271033
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.955325	-1.683965	-0.826911
2	6	0	0.738519	-1.011169	-0.867289
3	6	0	0.503916	0.085946	-0.031720
4	6	0	1.511969	0.489466	0.848696
5	6	0	2.728331	-0.186131	0.892052
6	6	0	2.953996	-1.274384	0.053859
7	1	0	2.124631	-2.529167	-1.484827
8	1	0	-0.035656	-1.333650	-1.554077
9	1	0	1.338556	1.334413	1.505619
10	1	0	3.498972	0.138220	1.582569
11	1	0	3.900772	-1.801672	0.087297
12	6	0	-0.787568	0.815934	-0.087427
13	6	0	-0.857715	2.150309	-0.241859
14	1	0	-1.818275	2.657826	-0.280774
15	6	0	-2.069402	0.114193	0.031373
16	1	0	-2.960029	0.750358	-0.068583
17	7	0	-2.176082	-1.132332	0.249044
18	6	0	-3.518745	-1.673959	0.356575
19	1	0	-3.656161	-2.455531	-0.395736
20	1	0	-3.640030	-2.147663	1.334679
21	1	0	-4.301581	-0.915852	0.229277
22	8	0	0.233383	2.928317	-0.370361
23	1	0	-0.037435	3.845063	-0.499966

Structure 31j (C_2H_5OH)

Energy (Hartrees): -517.563722162
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.976478	-1.653564	-0.853483
2	6	0	0.757208	-0.985424	-0.893919
3	6	0	0.503167	0.084647	-0.029805
4	6	0	1.494564	0.466641	0.878480
5	6	0	2.714151	-0.203305	0.920911
6	6	0	2.958771	-1.265179	0.054799
7	1	0	2.160445	-2.478400	-1.533125
8	1	0	-0.003782	-1.289983	-1.603587
9	1	0	1.305811	1.291413	1.557271
10	1	0	3.472461	0.105002	1.632274
11	1	0	3.907960	-1.788374	0.087669
12	6	0	-0.790733	0.811698	-0.085962
13	6	0	-0.857832	2.146005	-0.242879
14	1	0	-1.813518	2.661450	-0.284671
15	6	0	-2.071614	0.109688	0.031824
16	1	0	-2.961480	0.746521	-0.070082
17	7	0	-2.181101	-1.137001	0.249920
18	6	0	-3.526369	-1.673505	0.351997
19	1	0	-3.665714	-2.451104	-0.403912
20	1	0	-3.652227	-2.151489	1.327265
21	1	0	-4.306549	-0.912560	0.226542
22	8	0	0.237585	2.920221	-0.370884
23	1	0	-0.023125	3.838552	-0.509793

Structure 31k (vacuum)

Energy (Hartrees): -517.538957001
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.443168	-1.225642	-0.754808
2	6	0	1.101223	-0.870393	-0.772238
3	6	0	0.648568	0.230057	-0.037159
4	6	0	1.570331	0.945865	0.730780
5	6	0	2.915968	0.591412	0.745634
6	6	0	3.357171	-0.495076	0.000530
7	1	0	2.777727	-2.078330	-1.334317
8	1	0	0.393642	-1.445758	-1.354400
9	1	0	1.224614	1.773177	1.341147
10	1	0	3.614479	1.157768	1.350578
11	1	0	4.403271	-0.777947	0.014215
12	6	0	-0.772373	0.654041	-0.092600
13	6	0	-1.057026	1.951362	-0.283337
14	1	0	-0.268115	2.681943	-0.436746
15	6	0	-1.872702	-0.310272	0.059785
16	1	0	-2.882583	0.111629	-0.016791
17	7	0	-1.680054	-1.544680	0.271752
18	6	0	-2.849819	-2.385316	0.416034
19	1	0	-2.817390	-3.176490	-0.337244
20	1	0	-2.816024	-2.874351	1.392607
21	1	0	-3.796970	-1.837507	0.321125
22	8	0	-2.330424	2.427165	-0.293470
23	1	0	-2.335938	3.345081	-0.570392

Structure 31k ($CHCl_3$)

Energy (Hartrees): -517.558668101
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.451690	-1.215390	-0.774433
2	6	0	1.109499	-0.857248	-0.792019
3	6	0	0.650348	0.227988	-0.036066
4	6	0	1.569647	0.929725	0.749589
5	6	0	2.915909	0.573359	0.764287
6	6	0	3.361951	-0.500078	0.001335
7	1	0	2.788837	-2.055263	-1.371684
8	1	0	0.408888	-1.417084	-1.399390
9	1	0	1.223514	1.751737	1.367320
10	1	0	3.612127	1.130243	1.381447
11	1	0	4.408570	-0.782716	0.014456
12	6	0	-0.772005	0.652101	-0.095580
13	6	0	-1.055231	1.954093	-0.278328
14	1	0	-0.268697	2.690002	-0.418667
15	6	0	-1.871660	-0.312564	0.041462
16	1	0	-2.879449	0.097715	-0.093686
17	7	0	-1.691379	-1.540756	0.306878
18	6	0	-2.870178	-2.377495	0.416082
19	1	0	-2.805608	-3.185048	-0.318378
20	1	0	-2.886858	-2.845831	1.403673
21	1	0	-3.808822	-1.829722	0.263555
22	8	0	-2.322031	2.427508	-0.303293
23	1	0	-2.316420	3.364239	-0.528417

Structure 31k (DMSO)

Energy (Hartrees): -517.556629655
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.452653	-1.212256	-0.776056
2	6	0	1.110519	-0.852032	-0.798510
3	6	0	0.648559	0.231660	-0.040606
4	6	0	1.565861	0.933152	0.748152
5	6	0	2.912153	0.575409	0.766492
6	6	0	3.360476	-0.498914	0.005333
7	1	0	2.792100	-2.050147	-1.375065
8	1	0	0.413668	-1.407191	-1.415510
9	1	0	1.220808	1.759353	1.360987
10	1	0	3.606777	1.133730	1.384295
11	1	0	4.407040	-0.781857	0.021707
12	6	0	-0.774281	0.652328	-0.102893
13	6	0	-1.061533	1.956205	-0.273047
14	1	0	-0.276791	2.696645	-0.400886
15	6	0	-1.867704	-0.319650	0.020968
16	1	0	-2.875174	0.070961	-0.163249
17	7	0	-1.684440	-1.538013	0.331577
18	6	0	-2.859885	-2.384709	0.418837
19	1	0	-2.752958	-3.220261	-0.278412
20	1	0	-2.921669	-2.812053	1.423374
21	1	0	-3.793022	-1.852016	0.198393
22	8	0	-2.328590	2.422155	-0.298214
23	1	0	-2.321898	3.364537	-0.502997

Structure 31k (C_2H_5OH)

Energy (Hartrees): -517.561767139
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.460065	-1.201511	-0.787783
2	6	0	1.117797	-0.842186	-0.812191
3	6	0	0.650783	0.230548	-0.042226
4	6	0	1.563241	0.922568	0.760141
5	6	0	2.909896	0.566068	0.780576
6	6	0	3.363078	-0.497656	0.007576
7	1	0	2.803578	-2.030949	-1.396298
8	1	0	0.424880	-1.389227	-1.440920
9	1	0	1.213525	1.739511	1.382776
10	1	0	3.600990	1.116682	1.409383
11	1	0	4.409959	-0.779785	0.025634
12	6	0	-0.772767	0.649524	-0.105357
13	6	0	-1.060645	1.953551	-0.275249
14	1	0	-0.279376	2.697241	-0.402183
15	6	0	-1.866070	-0.322097	0.018120
16	1	0	-2.872420	0.068630	-0.172203
17	7	0	-1.688069	-1.539622	0.337131
18	6	0	-2.870064	-2.378607	0.420568
19	1	0	-2.766301	-3.216924	-0.273646
20	1	0	-2.940703	-2.803588	1.425329
21	1	0	-3.798666	-1.840993	0.193999
22	8	0	-2.328230	2.421231	-0.300293
23	1	0	-2.325029	3.365695	-0.494488

Structure 31l (vacuum)

Energy (Hartrees): -517.537977589
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.433970	-1.219221	-0.766245
2	6	0	1.094517	-0.855880	-0.790672
3	6	0	0.640906	0.235762	-0.043898
4	6	0	1.558813	0.937380	0.740536
5	6	0	2.902522	0.575747	0.761904
6	6	0	3.344593	-0.503659	0.007318
7	1	0	2.769446	-2.065109	-1.355021
8	1	0	0.390901	-1.419220	-1.389794
9	1	0	1.212574	1.761668	1.354560
10	1	0	3.598856	1.132198	1.378303
11	1	0	4.389127	-0.791804	0.026083
12	6	0	-0.779855	0.667340	-0.103467
13	6	0	-1.044959	1.974303	-0.293486
14	1	0	-0.243504	2.686485	-0.451909
15	6	0	-1.861883	-0.312987	0.040229
16	1	0	-2.892927	0.055545	-0.097824
17	7	0	-1.670209	-1.536896	0.301132
18	6	0	-2.829511	-2.393646	0.419276
19	1	0	-2.748803	-3.207147	-0.305588
20	1	0	-2.833503	-2.849831	1.411946
21	1	0	-3.781564	-1.867546	0.262228
22	8	0	-2.245942	2.589674	-0.330287
23	1	0	-2.956289	1.974817	-0.127576

Structure 31l ($CHCl_3$)

Energy (Hartrees): -517.556901991
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.442002	-1.200045	-0.786120
2	6	0	1.101853	-0.836293	-0.813014
3	6	0	0.638792	0.240156	-0.047236
4	6	0	1.551442	0.928988	0.756185
5	6	0	2.896331	0.566950	0.780619
6	6	0	3.346235	-0.498587	0.009377
7	1	0	2.782654	-2.033065	-1.390864
8	1	0	0.406213	-1.386384	-1.435380
9	1	0	1.201892	1.745649	1.378969
10	1	0	3.588013	1.113573	1.411826
11	1	0	4.391436	-0.785881	0.030478
12	6	0	-0.785153	0.665221	-0.111519
13	6	0	-1.053407	1.974272	-0.289998
14	1	0	-0.253156	2.690940	-0.440211
15	6	0	-1.861540	-0.325016	0.013144
16	1	0	-2.883178	0.014231	-0.211674
17	7	0	-1.663853	-1.532806	0.347500
18	6	0	-2.818859	-2.404904	0.419707
19	1	0	-2.682397	-3.238742	-0.274021
20	1	0	-2.882766	-2.832046	1.423660
21	1	0	-3.762765	-1.896074	0.185656
22	8	0	-2.253877	2.586425	-0.323758
23	1	0	-2.974120	1.981592	-0.107734

Structure 31l (DMSO)

Energy (Hartrees): -517.555316209
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.443321	-1.193249	-0.795631
2	6	0	1.102792	-0.828472	-0.823158
3	6	0	0.637353	0.240414	-0.046980
4	6	0	1.548089	0.922797	0.764616
5	6	0	2.893328	0.560372	0.788587
6	6	0	3.345478	-0.499111	0.009543
7	1	0	2.786532	-2.019196	-1.408813
8	1	0	0.409839	-1.369210	-1.457477
9	1	0	1.199058	1.737506	1.390349
10	1	0	3.583636	1.103498	1.424468
11	1	0	4.390972	-0.785692	0.030115
12	6	0	-0.786351	0.665276	-0.112978
13	6	0	-1.052449	1.976461	-0.281821
14	1	0	-0.250458	2.695421	-0.411944
15	6	0	-1.863128	-0.325447	0.005782
16	1	0	-2.885374	0.007111	-0.224789
17	7	0	-1.662392	-1.530642	0.351893
18	6	0	-2.816753	-2.406308	0.424722
19	1	0	-2.668757	-3.251353	-0.253173
20	1	0	-2.892008	-2.816266	1.435335
21	1	0	-3.757419	-1.903135	0.169970
22	8	0	-2.252012	2.584410	-0.324772
23	1	0	-2.973255	1.964119	-0.155214

Structure 31l (C_2H_5OH)

Energy (Hartrees): -517.559800602
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.450003	-1.180648	-0.806300
2	6	0	1.109540	-0.816416	-0.837147
3	6	0	0.638410	0.241990	-0.050268
4	6	0	1.543763	0.915605	0.774316
5	6	0	2.889268	0.553951	0.801818
6	6	0	3.346670	-0.495819	0.012894
7	1	0	2.797747	-1.998790	-1.427500
8	1	0	0.420852	-1.349060	-1.483151
9	1	0	1.189724	1.721632	1.408539
10	1	0	3.575588	1.089481	1.448606
11	1	0	4.392251	-0.782303	0.036640
12	6	0	-0.787033	0.662067	-0.116621
13	6	0	-1.055370	1.972503	-0.285634
14	1	0	-0.254054	2.691268	-0.422161
15	6	0	-1.859619	-0.333543	-0.002273
16	1	0	-2.874787	-0.004256	-0.260792
17	7	0	-1.661228	-1.533027	0.366691
18	6	0	-2.818125	-2.407702	0.424011
19	1	0	-2.658873	-3.258477	-0.243990
20	1	0	-2.914063	-2.811012	1.435384
21	1	0	-3.753449	-1.906759	0.147032
22	8	0	-2.256536	2.585390	-0.321846
23	1	0	-2.985095	1.984417	-0.119447

Structure 32a (vacuum)
Energy (Hartrees): -632.076987300
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.262297	0.791247	0.502311
2	6	0	0.886611	1.016295	0.496377
3	6	0	-0.001443	0.132453	-0.115575
4	6	0	0.541540	-1.004666	-0.731839
5	6	0	1.901952	-1.254886	-0.716970
6	6	0	2.774207	-0.354578	-0.101399
7	1	0	2.911356	1.505132	0.991240
8	1	0	0.500192	1.894653	1.002156
9	1	0	-0.117777	-1.692714	-1.250630
10	1	0	2.320403	-2.133069	-1.193397
11	6	0	-1.459253	0.389606	-0.113222
12	6	0	-2.343914	-0.621856	0.184643
13	1	0	-1.951522	-1.602632	0.448968
14	6	0	-1.960783	1.705549	-0.430391
15	1	0	-1.194175	2.460544	-0.683089
16	1	0	-4.050157	0.394568	-0.025388
17	7	0	-3.675729	-0.526049	0.191714
18	6	0	-4.557207	-1.599248	0.598476
19	1	0	-5.346363	-1.744091	-0.141157
20	1	0	-3.985227	-2.524358	0.677028
21	1	0	-5.017803	-1.391876	1.567912
22	8	0	-3.145960	2.024396	-0.451001
23	8	0	4.094399	-0.679201	-0.145203
24	6	0	5.006480	0.211013	0.460539
25	1	0	4.809174	0.311667	1.532710
26	1	0	5.993904	-0.221247	0.314095
27	1	0	4.967654	1.198632	-0.010504

Structure 32a ($CHCl_3$)
Energy (Hartrees): -632.095877894
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.274453	0.806025	0.469117
2	6	0	0.899457	1.040499	0.468684
3	6	0	-0.004093	0.136849	-0.094202
4	6	0	0.525283	-1.032424	-0.663203
5	6	0	1.885087	-1.291731	-0.651066
6	6	0	2.772107	-0.370426	-0.087340
7	1	0	2.934924	1.536170	0.918060
8	1	0	0.528791	1.945359	0.938926
9	1	0	-0.141463	-1.743733	-1.139836
10	1	0	2.286628	-2.197093	-1.091883
11	6	0	-1.461546	0.405711	-0.093819
12	6	0	-2.354417	-0.612625	0.196866
13	1	0	-1.965485	-1.596418	0.453402
14	6	0	-1.947720	1.716072	-0.414167
15	1	0	-1.178518	2.462729	-0.679178
16	1	0	-4.068458	0.393240	-0.020395
17	7	0	-3.678103	-0.517404	0.207300
18	6	0	-4.566831	-1.619771	0.520972
19	1	0	-5.199037	-1.858253	-0.336906
20	1	0	-3.974482	-2.497823	0.777752
21	1	0	-5.204604	-1.364650	1.369401
22	8	0	-3.135779	2.053452	-0.430875
23	8	0	4.089160	-0.706149	-0.128814
24	6	0	5.022545	0.224116	0.393242
25	1	0	4.853395	0.399117	1.459963
26	1	0	6.005017	-0.223490	0.253939
27	1	0	4.977015	1.174480	-0.147338

Structure 32a (DMSO)
Energy (Hartrees): -632.095486858
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.279722	0.815552	0.440981
2	6	0	0.904632	1.052286	0.443605
3	6	0	-0.005548	0.136279	-0.090141
4	6	0	0.519062	-1.049006	-0.631626
5	6	0	1.879179	-1.309663	-0.622099
6	6	0	2.773163	-0.375947	-0.088474
7	1	0	2.943493	1.556344	0.867337
8	1	0	0.540581	1.970693	0.892666
9	1	0	-0.150425	-1.775229	-1.081334
10	1	0	2.271677	-2.229130	-1.042053
11	6	0	-1.462437	0.409184	-0.088667
12	6	0	-2.358521	-0.613130	0.190268
13	1	0	-1.972421	-1.600926	0.435098
14	6	0	-1.941296	1.723722	-0.398464
15	1	0	-1.166409	2.466953	-0.656811
16	1	0	-4.076764	0.391819	-0.018211
17	7	0	-3.680037	-0.517684	0.200917
18	6	0	-4.568598	-1.625574	0.501486
19	1	0	-5.192344	-1.859077	-0.363702
20	1	0	-3.974653	-2.502017	0.759150
21	1	0	-5.214372	-1.373154	1.344375
22	8	0	-3.127103	2.071021	-0.414169
23	8	0	4.088445	-0.712269	-0.129072
24	6	0	5.020097	0.226736	0.386588
25	1	0	4.844992	0.414451	1.449980
26	1	0	6.003945	-0.220459	0.256621
27	1	0	4.975491	1.170865	-0.164341

Structure 32a (C_2H_5OH)
Energy (Hartrees): -632.098457608
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.276326	0.809027	0.458713
2	6	0	0.901569	1.046076	0.460558
3	6	0	-0.005708	0.138472	-0.091331
4	6	0	0.517910	-1.039224	-0.648384
5	6	0	1.878036	-1.300564	-0.638477
6	6	0	2.767717	-0.374006	-0.088317
7	1	0	2.940013	1.542176	0.898219
8	1	0	0.535401	1.957222	0.922530
9	1	0	-0.151155	-1.757606	-1.111281
10	1	0	2.273863	-2.213354	-1.070231
11	6	0	-1.462799	0.413488	-0.092896
12	6	0	-2.359333	-0.610975	0.193395
13	1	0	-1.968829	-1.595316	0.444885
14	6	0	-1.936643	1.720179	-0.406897
15	1	0	-1.165735	2.464091	-0.668637
16	1	0	-4.081181	0.385117	-0.022788
17	7	0	-3.678194	-0.519913	0.204135
18	6	0	-4.563262	-1.629725	0.511804
19	1	0	-5.189434	-1.864643	-0.351005
20	1	0	-3.966975	-2.504483	0.769043
21	1	0	-5.205883	-1.375245	1.356292
22	8	0	-3.129352	2.070628	-0.422541
23	8	0	4.088080	-0.711602	-0.130718
24	6	0	5.023770	0.224159	0.388845
25	1	0	4.850033	0.403107	1.453543
26	1	0	6.005709	-0.225454	0.252516
27	1	0	4.976212	1.170114	-0.158030

Structure 32b (vacuum)
Energy (Hartrees): -632.071648570
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.053171	0.740599	-0.657763
2	6	0	-0.689708	1.031062	-0.676904
3	6	0	0.217694	0.354318	0.136380
4	6	0	-0.291030	-0.639195	0.988343
5	6	0	-1.638635	-0.950512	1.010006
6	6	0	-2.530665	-0.260752	0.184776
7	1	0	-2.719666	1.293285	-1.306050
8	1	0	-0.325957	1.797362	-1.353341
9	1	0	0.385158	-1.154983	1.663009
10	1	0	-2.032953	-1.711865	1.672020
11	6	0	1.659111	0.687098	0.117048
12	6	0	2.639749	-0.242669	-0.047688
13	1	0	3.668324	0.110784	-0.042153
14	6	0	2.086869	2.079290	0.264319
15	1	0	1.256997	2.798407	0.416136
16	1	0	1.536204	-1.910964	-0.333143
17	7	0	2.480761	-1.571126	-0.213192
18	6	0	3.565402	-2.445540	-0.617147
19	1	0	3.646323	-2.529783	-1.705351
20	1	0	4.503102	-2.048440	-0.228199
21	1	0	3.416758	-3.440045	-0.195743
22	8	0	3.233550	2.475672	0.236752
23	8	0	-3.833988	-0.632723	0.276180
24	6	0	-4.769126	0.048295	-0.533532
25	1	0	-4.546923	-0.089923	-1.596506
26	1	0	-5.739080	-0.389201	-0.307929
27	1	0	-4.789041	1.117683	-0.300893

Structure 32b ($CHCl_3$)
Energy (Hartrees): -632.092588569
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.071347	0.764716	-0.616953
2	6	0	-0.708545	1.061746	-0.636740
3	6	0	0.214041	0.347899	0.129229
4	6	0	-0.280627	-0.693845	0.931306
5	6	0	-1.627311	-1.013044	0.951215
6	6	0	-2.534000	-0.284410	0.175191
7	1	0	-2.748684	1.348080	-1.226804
8	1	0	-0.359003	1.866536	-1.275637
9	1	0	0.400909	-1.248490	1.569386
10	1	0	-2.003705	-1.814434	1.576651
11	6	0	1.653628	0.697431	0.111538
12	6	0	2.653544	-0.223341	-0.086826
13	1	0	3.679368	0.136434	-0.064699
14	6	0	2.055809	2.077393	0.291492
15	1	0	1.220504	2.774972	0.494366
16	1	0	1.577729	-1.907427	-0.386574
17	7	0	2.513695	-1.526577	-0.327166
18	6	0	3.620458	-2.444238	-0.528114
19	1	0	3.522902	-2.953484	-1.488688
20	1	0	4.552501	-1.880250	-0.523589
21	1	0	3.655109	-3.191508	0.268019
22	8	0	3.199255	2.513544	0.248173
23	8	0	-3.833915	-0.668653	0.258727
24	6	0	-4.787634	0.059218	-0.497335
25	1	0	-4.583778	-0.016978	-1.569777
26	1	0	-5.752961	-0.395360	-0.282331
27	1	0	-4.807575	1.111656	-0.199372

Structure 32b (DMSO)
Energy (Hartrees): -632.092922719
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.080327	0.771978	-0.598222
2	6	0	-0.717380	1.069639	-0.620647
3	6	0	0.212050	0.340191	0.123391
4	6	0	-0.276890	-0.720643	0.904303
5	6	0	-1.623924	-1.039807	0.927002
6	6	0	-2.538074	-0.294232	0.175008
7	1	0	-2.761139	1.367948	-1.192123
8	1	0	-0.375079	1.889592	-1.244279
9	1	0	0.407723	-1.295331	1.521061
10	1	0	-1.990911	-1.859131	1.534963
11	6	0	1.649724	0.698182	0.107446
12	6	0	2.659784	-0.216469	-0.091627
13	1	0	3.682909	0.150603	-0.063460
14	6	0	2.037409	2.079162	0.295065
15	1	0	1.193126	2.764829	0.502620
16	1	0	1.604279	-1.913668	-0.396206
17	7	0	2.534202	-1.516199	-0.337990
18	6	0	3.651707	-2.427245	-0.513707
19	1	0	3.561755	-2.954087	-1.465069
20	1	0	4.578680	-1.854994	-0.511389
21	1	0	3.681899	-3.159507	0.296117
22	8	0	3.175573	2.533024	0.255753
23	8	0	-3.836388	-0.678383	0.258935
24	6	0	-4.789150	0.060542	-0.491712
25	1	0	-4.577272	0.004497	-1.563538
26	1	0	-5.754796	-0.399929	-0.291485
27	1	0	-4.813635	1.107652	-0.176592

Structure 32b (C_2H_5OH)
Energy (Hartrees): -632.096571804
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.069791	0.759510	-0.620978
2	6	0	-0.706531	1.054680	-0.642243
3	6	0	0.214627	0.345893	0.130658
4	6	0	-0.279215	-0.690839	0.939157
5	6	0	-1.626952	-1.007692	0.961358
6	6	0	-2.531500	-0.282772	0.180118
7	1	0	-2.746239	1.338401	-1.236292
8	1	0	-0.356888	1.854882	-1.287070
9	1	0	0.401044	-1.246875	1.577481
10	1	0	-2.001624	-1.807022	1.591120
11	6	0	1.654413	0.699398	0.114000
12	6	0	2.659760	-0.226303	-0.087893
13	1	0	3.687772	0.126685	-0.063403
14	6	0	2.045133	2.069229	0.291168
15	1	0	1.210466	2.765174	0.490763
16	1	0	1.579626	-1.905035	-0.383355
17	7	0	2.516003	-1.520420	-0.331829
18	6	0	3.621009	-2.443801	-0.530965
19	1	0	3.517103	-2.951706	-1.491063
20	1	0	4.555445	-1.884391	-0.523504
21	1	0	3.643397	-3.190503	0.265437
22	8	0	3.193938	2.522291	0.249106
23	8	0	-3.835789	-0.664590	0.265504
24	6	0	-4.786896	0.056319	-0.508098
25	1	0	-4.573441	-0.036548	-1.576736
26	1	0	-5.753368	-0.395211	-0.291892
27	1	0	-4.804854	1.111763	-0.223249

Structure 32c (vacuum)
Energy (Hartrees): -632.072980383
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.966355	0.631229	-0.631759
2	6	0	-0.626361	1.009512	-0.635458
3	6	0	0.320059	0.340214	0.138623
4	6	0	-0.123870	-0.715968	0.947925
5	6	0	-1.451792	-1.105655	0.959911
6	6	0	-2.382492	-0.435005	0.163972
7	1	0	-2.668581	1.178775	-1.245595
8	1	0	-0.315332	1.851017	-1.241745
9	1	0	0.581802	-1.219947	1.600993
10	1	0	-1.798492	-1.915264	1.590373
11	6	0	1.742921	0.742549	0.124151
12	6	0	2.767172	-0.142881	-0.015133
13	1	0	3.786883	0.237339	-0.002972
14	6	0	2.129574	2.146952	0.216249
15	1	0	3.228163	2.312932	0.230131
16	1	0	1.749043	-1.858227	-0.317571
17	7	0	2.675770	-1.484272	-0.162356
18	6	0	3.800261	-2.286735	-0.606201
19	1	0	3.924930	-2.267669	-1.693787
20	1	0	4.713192	-1.909684	-0.143617
21	1	0	3.661836	-3.318809	-0.285126
22	8	0	1.374881	3.091781	0.265449
23	8	0	-3.662365	-0.885216	0.237956
24	6	0	-4.639030	-0.215611	-0.531195
25	1	0	-4.416475	-0.284368	-1.600840
26	1	0	-5.581707	-0.717589	-0.325270
27	1	0	-4.716306	0.837271	-0.242239

Structure 32c ($CHCl_3$)
Energy (Hartrees): -632.095054360
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.973449	0.594089	-0.667765
2	6	0	-0.632094	0.970384	-0.682311
3	6	0	0.316145	0.333996	0.118473
4	6	0	-0.126493	-0.699852	0.957136
5	6	0	-1.455104	-1.091369	0.978970
6	6	0	-2.388558	-0.445145	0.164605
7	1	0	-2.675960	1.117776	-1.302568
8	1	0	-0.320794	1.783232	-1.328003
9	1	0	0.578541	-1.189912	1.621969
10	1	0	-1.795515	-1.885659	1.633384
11	6	0	1.735870	0.754664	0.097785
12	6	0	2.780325	-0.122002	-0.059876
13	1	0	3.793034	0.276191	-0.052551
14	6	0	2.105216	2.146192	0.215922
15	1	0	3.198083	2.330205	0.196542
16	1	0	1.792441	-1.867028	-0.314147
17	7	0	2.708897	-1.445195	-0.229816
18	6	0	3.857364	-2.280721	-0.533596
19	1	0	3.904256	-2.519899	-1.599285
20	1	0	4.767489	-1.752020	-0.250641
21	1	0	3.804093	-3.209564	0.035472
22	8	0	1.340175	3.091985	0.329261
23	8	0	-3.668670	-0.890478	0.253462
24	6	0	-4.654581	-0.223699	-0.517800
25	1	0	-4.452104	-0.321536	-1.588636
26	1	0	-5.599253	-0.711611	-0.284956
27	1	0	-4.716475	0.834910	-0.248910

Structure 32c (DMSO)
Energy (Hartrees): -632.096281838
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.979933	0.594460	-0.667635
2	6	0	-0.637463	0.969247	-0.694893
3	6	0	0.318042	0.340276	0.103888
4	6	0	-0.119170	-0.688645	0.952055
5	6	0	-1.448183	-1.078834	0.987516
6	6	0	-2.389872	-0.438551	0.176444
7	1	0	-2.685942	1.110767	-1.304944
8	1	0	-0.331643	1.773368	-1.354563
9	1	0	0.591538	-1.182898	1.607831
10	1	0	-1.777990	-1.873174	1.647560
11	6	0	1.738047	0.761655	0.070882
12	6	0	2.782574	-0.119667	-0.101187
13	1	0	3.797066	0.273922	-0.088993
14	6	0	2.109398	2.146381	0.210919
15	1	0	3.201480	2.329024	0.172052
16	1	0	1.782796	-1.859402	-0.344140
17	7	0	2.700145	-1.432042	-0.301986
18	6	0	3.845036	-2.310460	-0.466503
19	1	0	3.775758	-2.848647	-1.413393
20	1	0	4.755846	-1.712417	-0.465629
21	1	0	3.894204	-3.033988	0.350046
22	8	0	1.348599	3.093177	0.368216
23	8	0	-3.668086	-0.881530	0.277670
24	6	0	-4.651001	-0.239463	-0.521939
25	1	0	-4.433680	-0.360122	-1.587230
26	1	0	-5.595193	-0.728343	-0.289580
27	1	0	-4.724194	0.824639	-0.279492

Structure 32c (C_2H_5OH)
Energy (Hartrees): -632.100543597
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.963117	0.564945	-0.708609
2	6	0	-0.618807	0.932081	-0.738951
3	6	0	0.321187	0.347007	0.109774
4	6	0	-0.128733	-0.630529	1.009618
5	6	0	-1.459724	-1.013179	1.048580
6	6	0	-2.384666	-0.415732	0.188375
7	1	0	-2.659402	1.043920	-1.384645
8	1	0	-0.298152	1.692433	-1.443222
9	1	0	0.572773	-1.087546	1.701273
10	1	0	-1.805945	-1.766638	1.747503
11	6	0	1.744791	0.759416	0.070607
12	6	0	2.782753	-0.134930	-0.103292
13	1	0	3.801267	0.247584	-0.102098
14	6	0	2.126865	2.130685	0.200498
15	1	0	3.215468	2.315729	0.155371
16	1	0	1.754363	-1.856864	-0.315814
17	7	0	2.679467	-1.443461	-0.291732
18	6	0	3.810175	-2.338037	-0.478325
19	1	0	3.724897	-2.859804	-1.433016
20	1	0	4.730146	-1.754639	-0.473958
21	1	0	3.850516	-3.074702	0.326404
22	8	0	1.365270	3.089396	0.358703
23	8	0	-3.669963	-0.850249	0.298871
24	6	0	-4.644632	-0.259013	-0.551794
25	1	0	-4.408530	-0.439922	-1.604003
26	1	0	-5.588808	-0.740563	-0.304339
27	1	0	-4.723864	0.815778	-0.366802

Structure 32d (vacuum)
Energy (Hartrees): -632.063876786
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.151987	0.675535	0.530938
2	6	0	0.791678	0.970536	0.513923
3	6	0	-0.128491	0.132433	-0.115384
4	6	0	0.366385	-1.011178	-0.756799
5	6	0	1.714768	-1.323566	-0.740339
6	6	0	2.618201	-0.480272	-0.093291
7	1	0	2.829948	1.353722	1.031199
8	1	0	0.444777	1.875093	0.996450
9	1	0	-0.316570	-1.655373	-1.300637
10	1	0	2.097126	-2.205442	-1.239523
11	6	0	-1.580228	0.428244	-0.098930
12	6	0	-2.468722	-0.588794	0.098886
13	1	0	-2.069664	-1.570689	0.347964
14	6	0	-2.054896	1.798657	-0.263305
15	1	0	-3.150846	1.941114	-0.156664
16	1	0	-4.281283	0.288150	-0.225037
17	7	0	-3.821994	-0.581969	-0.008309
18	6	0	-4.633768	-1.604164	0.626356
19	1	0	-5.598562	-1.667687	0.123921
20	1	0	-4.134110	-2.568704	0.523495
21	1	0	-4.799227	-1.409150	1.690868
22	8	0	-1.364726	2.771002	-0.473210
23	8	0	3.923732	-0.860444	-0.133890
24	6	0	4.869157	-0.021235	0.493287
25	1	0	4.668671	0.069542	1.565716
26	1	0	5.837973	-0.493523	0.345554
27	1	0	4.877246	0.975090	0.039599

Structure 32d ($CHCl_3$)
Energy (Hartrees): -632.086944133
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.170322	0.683660	0.510007
2	6	0	0.811156	0.989571	0.501887
3	6	0	-0.130087	0.143379	-0.089371
4	6	0	0.348394	-1.028589	-0.695151
5	6	0	1.694892	-1.354733	-0.683560
6	6	0	2.617699	-0.498060	-0.080361
7	1	0	2.861535	1.369634	0.981736
8	1	0	0.481849	1.908447	0.970590
9	1	0	-0.346159	-1.690818	-1.201664
10	1	0	2.055608	-2.261322	-1.155795
11	6	0	-1.579613	0.454149	-0.065856
12	6	0	-2.478376	-0.569329	0.140921
13	1	0	-2.081157	-1.545823	0.412364
14	6	0	-2.051448	1.810029	-0.236196
15	1	0	-3.138366	1.960153	-0.090983
16	1	0	-4.284657	0.287482	-0.255501
17	7	0	-3.813655	-0.558792	0.031216
18	6	0	-4.652685	-1.637005	0.525546
19	1	0	-5.517601	-1.755023	-0.126806
20	1	0	-4.081245	-2.565717	0.518562
21	1	0	-4.998800	-1.444402	1.544648
22	8	0	-1.365011	2.787475	-0.494184
23	8	0	3.918817	-0.891513	-0.123257
24	6	0	4.890754	-0.012531	0.417416
25	1	0	4.730281	0.146169	1.487814
26	1	0	5.853329	-0.498004	0.267143
27	1	0	4.884470	0.949853	-0.102796

Structure 32d (DMSO)
Energy (Hartrees): -632.088672113
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.167047	0.675783	0.523685
2	6	0	0.805327	0.972476	0.523935
3	6	0	-0.131186	0.146145	-0.102759
4	6	0	0.354682	-1.000087	-0.750291
5	6	0	1.704623	-1.316379	-0.751058
6	6	0	2.623144	-0.478782	-0.114072
7	1	0	2.853261	1.344900	1.026571
8	1	0	0.469894	1.868564	1.031920
9	1	0	-0.336799	-1.653724	-1.272487
10	1	0	2.067028	-2.206403	-1.253306
11	6	0	-1.581547	0.454922	-0.067888
12	6	0	-2.477809	-0.574704	0.148710
13	1	0	-2.073190	-1.555393	0.393959
14	6	0	-2.054491	1.805665	-0.246623
15	1	0	-3.141778	1.952982	-0.108041
16	1	0	-4.289543	0.298329	-0.161648
17	7	0	-3.810146	-0.557541	0.083477
18	6	0	-4.643420	-1.657514	0.539818
19	1	0	-5.472932	-1.800622	-0.152836
20	1	0	-4.046328	-2.569017	0.569228
21	1	0	-5.043161	-1.463692	1.538546
22	8	0	-1.370419	2.784541	-0.519174
23	8	0	3.925749	-0.859261	-0.170525
24	6	0	4.874099	-0.051420	0.510297
25	1	0	4.655062	-0.004593	1.581126
26	1	0	5.841046	-0.528435	0.360787
27	1	0	4.903006	0.961021	0.096907

Structure 32d (C_2H_5OH)
Energy (Hartrees): -632.092460920
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.162437	0.659057	0.557288
2	6	0	0.800777	0.955336	0.563618
3	6	0	-0.131739	0.151769	-0.097073
4	6	0	0.353591	-0.972700	-0.780659
5	6	0	1.703282	-1.289302	-0.787371
6	6	0	2.616895	-0.472574	-0.119127
7	1	0	2.847569	1.308133	1.087032
8	1	0	0.463684	1.829707	1.108738
9	1	0	-0.337755	-1.607255	-1.326226
10	1	0	2.068620	-2.162175	-1.317272
11	6	0	-1.582955	0.460887	-0.062857
12	6	0	-2.478955	-0.572053	0.163148
13	1	0	-2.069249	-1.546142	0.425407
14	6	0	-2.053938	1.799848	-0.254593
15	1	0	-3.137691	1.958628	-0.118591
16	1	0	-4.289374	0.286589	-0.179449
17	7	0	-3.806874	-0.561155	0.089011
18	6	0	-4.640264	-1.663864	0.542337
19	1	0	-5.459646	-1.815815	-0.160170
20	1	0	-4.039072	-2.571880	0.586698
21	1	0	-5.053974	-1.463076	1.533623
22	8	0	-1.361955	2.780031	-0.540165
23	8	0	3.923976	-0.854387	-0.183516
24	6	0	4.876727	-0.065971	0.517937
25	1	0	4.657570	-0.048891	1.589204
26	1	0	5.841257	-0.542920	0.353107
27	1	0	4.904858	0.955425	0.128383

Structure 32e (vacuum)
Energy (Hartrees): -632.061674106
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.124069	0.786910	0.417435
2	6	0	0.744441	0.963853	0.461627
3	6	0	-0.132703	-0.019614	0.003429
4	6	0	0.426322	-1.188184	-0.531215
5	6	0	1.796327	-1.383955	-0.574234
6	6	0	2.656095	-0.394761	-0.097141
7	1	0	2.765958	1.575669	0.785549
8	1	0	0.347830	1.889480	0.858128
9	1	0	-0.227695	-1.949627	-0.943267
10	1	0	2.225883	-2.286146	-0.992150
11	6	0	-1.606002	0.145215	0.093291
12	6	0	-2.341066	-0.926685	0.518314
13	1	0	-1.780717	-1.773753	0.907444
14	6	0	-2.199285	1.454034	-0.183895
15	1	0	-3.272754	1.557394	0.047509
16	1	0	-3.970937	-2.012369	0.953763
17	7	0	-3.677987	-1.153222	0.521879
18	6	0	-4.693845	-0.420544	-0.206742
19	1	0	-5.525833	-1.092710	-0.416706
20	1	0	-5.075786	0.438098	0.351053
21	1	0	-4.279592	-0.067783	-1.154956
22	8	0	-1.591087	2.423292	-0.584702
23	8	0	3.986166	-0.666383	-0.184354
24	6	0	4.887607	0.323220	0.262674
25	1	0	4.747617	0.534614	1.327714
26	1	0	5.884466	-0.082234	0.103338
27	1	0	4.775080	1.249718	-0.309378

Structure 32e ($CHCl_3$)
Energy (Hartrees): -632.085087469
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.126907	0.780458	0.436454
2	6	0	0.746018	0.954124	0.482202
3	6	0	-0.133898	-0.015605	-0.004109
4	6	0	0.426815	-1.172574	-0.563505
5	6	0	1.798574	-1.366516	-0.608793
6	6	0	2.659469	-0.388862	-0.107460
7	1	0	2.769752	1.557555	0.828314
8	1	0	0.349382	1.865749	0.912236
9	1	0	-0.225805	-1.930186	-0.985322
10	1	0	2.223946	-2.263436	-1.044280
11	6	0	-1.608690	0.151353	0.086864
12	6	0	-2.345546	-0.934024	0.509092
13	1	0	-1.781806	-1.778926	0.898028
14	6	0	-2.200598	1.443717	-0.200487
15	1	0	-3.271520	1.551498	0.027623
16	1	0	-3.950756	-2.041641	0.929378
17	7	0	-3.665990	-1.170292	0.509106
18	6	0	-4.709410	-0.406583	-0.147624
19	1	0	-5.555801	-1.069320	-0.324594
20	1	0	-5.049666	0.438343	0.455898
21	1	0	-4.345230	-0.033860	-1.108594
22	8	0	-1.594511	2.418682	-0.621907
23	8	0	3.989394	-0.657761	-0.195948
24	6	0	4.892922	0.313916	0.302775
25	1	0	4.737038	0.487212	1.371931
26	1	0	5.890148	-0.093643	0.146464
27	1	0	4.797810	1.258918	-0.240429

Structure 32e (DMSO)
Energy (Hartrees): -632.086839648
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.122597	0.772016	0.453354
2	6	0	0.740011	0.939614	0.489894
3	6	0	-0.135016	-0.024415	-0.017952
4	6	0	0.434984	-1.173284	-0.585752
5	6	0	1.808523	-1.362418	-0.621289
6	6	0	2.664416	-0.388780	-0.101484
7	1	0	2.759007	1.545222	0.863685
8	1	0	0.338269	1.843178	0.932296
9	1	0	-0.210096	-1.932364	-1.016827
10	1	0	2.235917	-2.256446	-1.061314
11	6	0	-1.611316	0.144694	0.062320
12	6	0	-2.351359	-0.956305	0.451724
13	1	0	-1.783607	-1.819865	0.790340
14	6	0	-2.190524	1.439882	-0.228855
15	1	0	-3.262937	1.555903	-0.021163
16	1	0	-3.941823	-2.086736	0.849416
17	7	0	-3.666311	-1.191426	0.472618
18	6	0	-4.735222	-0.357437	-0.040948
19	1	0	-5.625236	-0.976269	-0.143373
20	1	0	-4.963408	0.474171	0.630102
21	1	0	-4.461615	0.038623	-1.022737
22	8	0	-1.572150	2.411232	-0.648587
23	8	0	3.994471	-0.650530	-0.180789
24	6	0	4.886988	0.327876	0.331183
25	1	0	4.720809	0.495029	1.399446
26	1	0	5.889059	-0.069595	0.180918
27	1	0	4.786775	1.274862	-0.207283

Structure 32e (C_2H_5OH)
Energy (Hartrees): -632.090821326
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.121730	0.759324	-0.484838
2	6	0	-0.739642	0.927851	-0.526626
3	6	0	0.135260	-0.018244	0.013285
4	6	0	-0.429779	-1.151646	0.614322
5	6	0	-1.802826	-1.341950	0.655614
6	6	0	-2.657502	-0.384719	0.106487
7	1	0	-2.760770	1.517287	-0.918815
8	1	0	-0.338839	1.815901	-1.001815
9	1	0	0.218606	-1.895549	1.066561
10	1	0	-2.231090	-2.222393	1.121796
11	6	0	1.612063	0.151255	-0.067596
12	6	0	2.350082	-0.947409	-0.478618
13	1	0	1.779156	-1.798614	-0.842315
14	6	0	2.193239	1.429931	0.241562
15	1	0	3.264825	1.552100	0.042576
16	1	0	3.936813	-2.073295	-0.890587
17	7	0	3.660761	-1.186422	-0.493658
18	6	0	4.727630	-0.369084	0.052538
19	1	0	5.611618	-0.995802	0.157837
20	1	0	4.972329	0.472338	-0.599916
21	1	0	4.439889	0.009174	1.037054
22	8	0	1.571723	2.404232	0.674573
23	8	0	-3.991908	-0.648230	0.194445
24	6	0	-4.891436	0.316148	-0.337359
25	1	0	-4.729378	0.454519	-1.409929
26	1	0	-5.890725	-0.081929	-0.170839
27	1	0	-4.788450	1.274467	0.179231

Structure 32f (vacuum)
Energy (Hartrees): -632.064678260
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.203775	0.909160	0.265560
2	6	0	0.817336	1.042888	0.302527
3	6	0	-0.034993	-0.015980	-0.014757
4	6	0	0.560300	-1.233927	-0.377578
5	6	0	1.934533	-1.390963	-0.398371
6	6	0	2.767849	-0.316686	-0.080233
7	1	0	2.821925	1.758313	0.524414
8	1	0	0.396855	1.993133	0.613946
9	1	0	-0.071636	-2.065543	-0.670674
10	1	0	2.391787	-2.331910	-0.679433
11	6	0	-1.508123	0.139868	0.037587
12	6	0	-2.248695	-0.859252	0.614749
13	1	0	-1.706204	-1.621882	1.170547
14	6	0	-2.064729	1.415606	-0.405402
15	1	0	-1.376513	2.015957	-1.031588
16	1	0	-3.912719	-1.839809	1.135317
17	7	0	-3.575527	-1.078127	0.571571
18	6	0	-4.506322	-0.526466	-0.396575
19	1	0	-5.332338	-1.228454	-0.509718
20	1	0	-4.875500	0.454103	-0.098391
21	1	0	-3.996784	-0.416548	-1.357203
22	8	0	-3.150866	1.871667	-0.102245
23	8	0	4.103846	-0.561355	-0.139209
24	6	0	4.979490	0.507599	0.148454
25	1	0	5.986368	0.111406	0.036937
26	1	0	4.834530	1.336269	-0.552120
27	1	0	4.842543	0.868270	1.172830

Structure 32f ($CHCl_3$)
Energy (Hartrees): -632.085194200
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.206656	0.914663	0.242226
2	6	0	0.819883	1.051989	0.280832
3	6	0	-0.038405	-0.011512	-0.012692
4	6	0	0.553953	-1.239651	-0.349332
5	6	0	1.929083	-1.399596	-0.370772
6	6	0	2.767074	-0.320447	-0.078482
7	1	0	2.828802	1.766609	0.483601
8	1	0	0.404930	2.010601	0.574858
9	1	0	-0.076929	-2.080765	-0.617892
10	1	0	2.378411	-2.351248	-0.630963
11	6	0	-1.512079	0.148418	0.042989
12	6	0	-2.257736	-0.860033	0.617561
13	1	0	-1.724678	-1.616650	1.190015
14	6	0	-2.064180	1.420585	-0.382997
15	1	0	-1.384656	2.026358	-1.011450
16	1	0	-3.914999	-1.860682	1.095976
17	7	0	-3.573044	-1.086742	0.546461
18	6	0	-4.495053	-0.534199	-0.428295
19	1	0	-5.306937	-1.248224	-0.563742
20	1	0	-4.892250	0.431769	-0.116671
21	1	0	-3.974856	-0.396976	-1.379811
22	8	0	-3.150527	1.886694	-0.064855
23	8	0	4.102025	-0.568824	-0.132216
24	6	0	4.986013	0.508094	0.130034
25	1	0	5.991117	0.103274	0.026310
26	1	0	4.845989	1.318650	-0.591631
27	1	0	4.854133	0.891651	1.146304

Structure 32f (DMSO)
Energy (Hartrees): -632.085480567
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.209352	0.917297	0.225560
2	6	0	0.822585	1.057041	0.272842
3	6	0	-0.040841	-0.010260	0.005274
4	6	0	0.548301	-1.246429	-0.310091
5	6	0	1.923469	-1.408318	-0.338945
6	6	0	2.766945	-0.324505	-0.077093
7	1	0	2.833433	1.773976	0.444961
8	1	0	0.413806	2.023309	0.550020
9	1	0	-0.084647	-2.093672	-0.553772
10	1	0	2.365582	-2.367927	-0.582661
11	6	0	-1.514052	0.152298	0.058885
12	6	0	-2.265221	-0.865917	0.615851
13	1	0	-1.741742	-1.628192	1.189457
14	6	0	-2.062762	1.427151	-0.358173
15	1	0	-1.381654	2.034488	-0.983541
16	1	0	-3.924202	-1.881622	1.045434
17	7	0	-3.575888	-1.092596	0.519522
18	6	0	-4.478412	-0.532993	-0.468539
19	1	0	-5.285532	-1.247431	-0.625587
20	1	0	-4.884591	0.429061	-0.156028
21	1	0	-3.938767	-0.384409	-1.407845
22	8	0	-3.147365	1.898176	-0.037056
23	8	0	4.099763	-0.572827	-0.140928
24	6	0	4.983678	0.511217	0.103915
25	1	0	5.989500	0.107967	0.001623
26	1	0	4.838585	1.312312	-0.626783
27	1	0	4.854011	0.908034	1.115024

Structure 32f (C_2H_5OH)
Energy (Hartrees): -632.089112465
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.212931	0.919538	0.228677
2	6	0	0.827302	1.066130	0.279833
3	6	0	-0.040526	0.002910	0.011212
4	6	0	0.539868	-1.236175	-0.306614
5	6	0	1.914238	-1.404975	-0.338865
6	6	0	2.760465	-0.324716	-0.077359
7	1	0	2.843324	1.771473	0.448333
8	1	0	0.423085	2.033128	0.561065
9	1	0	-0.098481	-2.079535	-0.550196
10	1	0	2.352884	-2.366041	-0.584208
11	6	0	-1.513509	0.168810	0.065869
12	6	0	-2.263916	-0.847287	0.638374
13	1	0	-1.742047	-1.586165	1.243283
14	6	0	-2.064728	1.430573	-0.353267
15	1	0	-1.383300	2.054525	-0.958171
16	1	0	-3.917833	-1.866353	1.068033
17	7	0	-3.565976	-1.091666	0.522421
18	6	0	-4.461848	-0.562676	-0.489869
19	1	0	-5.223883	-1.316172	-0.686186
20	1	0	-4.937074	0.366617	-0.175071
21	1	0	-3.898485	-0.369229	-1.405742
22	8	0	-3.169557	1.888051	-0.050833
23	8	0	4.097126	-0.581014	-0.143988
24	6	0	4.991953	0.498530	0.091484
25	1	0	5.993278	0.085992	-0.018308
26	1	0	4.844983	1.297030	-0.641178
27	1	0	4.871445	0.896114	1.103130

Structure 32g (vacuum)
Energy (Hartrees): -632.069047103
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.892896	-1.251395	-0.703800
2	6	0	0.532930	-1.002588	-0.704837
3	6	0	0.000700	0.147566	-0.103468
4	6	0	0.891446	1.031617	0.500744
5	6	0	2.267223	0.804966	0.496453
6	6	0	2.771964	-0.344855	-0.105161
7	1	0	2.306287	-2.136704	-1.171136
8	1	0	-0.131931	-1.702287	-1.200555
9	1	0	0.505637	1.910901	1.005006
10	1	0	2.921242	1.518997	0.978388
11	6	0	-1.456906	0.406558	-0.115615
12	6	0	-1.948412	1.635288	-0.424980
13	1	0	-1.287147	2.454019	-0.695438
14	6	0	-2.382063	-0.667912	0.213121
15	1	0	-1.943418	-1.636527	0.487428
16	7	0	-3.651308	-0.506495	0.209698
17	6	0	-4.500324	-1.621189	0.575464
18	1	0	-5.108879	-1.346260	1.439951
19	1	0	-5.182929	-1.843912	-0.247648
20	1	0	-3.925217	-2.522811	0.817450
21	8	0	-3.229665	1.956513	-0.445312
22	1	0	-3.737995	1.129265	-0.204468
23	8	0	4.089917	-0.672891	-0.156560
24	6	0	5.009878	0.218669	0.436312
25	1	0	4.821019	0.326285	1.509230
26	1	0	5.994510	-0.217892	0.284613
27	1	0	4.969981	1.203054	-0.041125

Structure 32g ($CHCl_3$)
Energy (Hartrees): -632.084725068
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.884889	-1.286471	-0.640834
2	6	0	0.524680	-1.031776	-0.643492
3	6	0	0.002212	0.147924	-0.091175
4	6	0	0.903639	1.056369	0.463893
5	6	0	2.278386	0.822801	0.459909
6	6	0	2.773619	-0.357578	-0.091156
7	1	0	2.285134	-2.197499	-1.070767
8	1	0	-0.144640	-1.754076	-1.099393
9	1	0	0.529747	1.963107	0.927622
10	1	0	2.940596	1.555002	0.902698
11	6	0	-1.455635	0.410954	-0.104867
12	6	0	-1.944991	1.642843	-0.403064
13	1	0	-1.290278	2.470567	-0.662427
14	6	0	-2.385835	-0.667813	0.207731
15	1	0	-1.958009	-1.640181	0.479622
16	7	0	-3.654365	-0.497301	0.191330
17	6	0	-4.516826	-1.611005	0.533774
18	1	0	-5.150759	-1.333402	1.379235
19	1	0	-5.174933	-1.833129	-0.309823
20	1	0	-3.949129	-2.511490	0.792856
21	8	0	-3.233410	1.953580	-0.423604
22	1	0	-3.733414	1.109464	-0.194601
23	8	0	4.089084	-0.693411	-0.133960
24	6	0	5.025226	0.237453	0.383223
25	1	0	4.857722	0.416149	1.449517
26	1	0	6.006453	-0.212693	0.243881
27	1	0	4.980487	1.185736	-0.160874

Structure 32g (DMSO)
Energy (Hartrees): -632.083281951
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.884278	-1.302194	-0.617212
2	6	0	0.523207	-1.048246	-0.618414
3	6	0	0.003221	0.143649	-0.089614
4	6	0	0.908045	1.064392	0.441076
5	6	0	2.282923	0.830787	0.435815
6	6	0	2.776842	-0.361870	-0.091936
7	1	0	2.278138	-2.224245	-1.029812
8	1	0	-0.147205	-1.782931	-1.052437
9	1	0	0.538073	1.983043	0.884579
10	1	0	2.946378	1.573268	0.859422
11	6	0	-1.454420	0.408119	-0.103207
12	6	0	-1.941250	1.643846	-0.393048
13	1	0	-1.284781	2.472999	-0.643850
14	6	0	-2.388462	-0.670197	0.201342
15	1	0	-1.968881	-1.648553	0.461939
16	7	0	-3.656318	-0.489336	0.188194
17	6	0	-4.527123	-1.600502	0.521764
18	1	0	-5.162349	-1.323574	1.366574
19	1	0	-5.183879	-1.814064	-0.325241
20	1	0	-3.964214	-2.504513	0.777267
21	8	0	-3.229713	1.953091	-0.412782
22	1	0	-3.724666	1.101300	-0.187154
23	8	0	4.091197	-0.695399	-0.133033
24	6	0	5.023204	0.244497	0.381895
25	1	0	4.847261	0.433260	1.444868
26	1	0	6.006756	-0.203442	0.252825
27	1	0	4.978935	1.187591	-0.170579

Structure 32g (C_2H_5OH)
Energy (Hartrees): -632.085059759
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.883111	-1.297858	-0.625227
2	6	0	0.521953	-1.043755	-0.627194
3	6	0	0.002587	0.144583	-0.090752
4	6	0	0.905648	1.061612	0.449140
5	6	0	2.280292	0.827801	0.445094
6	6	0	2.771997	-0.360463	-0.091415
7	1	0	2.279919	-2.216385	-1.043432
8	1	0	-0.148103	-1.774570	-1.068362
9	1	0	0.534481	1.976578	0.899136
10	1	0	2.944059	1.566152	0.875385
11	6	0	-1.455059	0.410163	-0.105552
12	6	0	-1.937588	1.644700	-0.396717
13	1	0	-1.284088	2.474921	-0.650031
14	6	0	-2.388631	-0.669446	0.202387
15	1	0	-1.965529	-1.644725	0.468533
16	7	0	-3.656341	-0.492248	0.187661
17	6	0	-4.521669	-1.606313	0.527071
18	1	0	-5.158409	-1.328162	1.370248
19	1	0	-5.177589	-1.827028	-0.318647
20	1	0	-3.955316	-2.506622	0.787439
21	8	0	-3.232001	1.956083	-0.414919
22	1	0	-3.732175	1.107594	-0.188999
23	8	0	4.091484	-0.695306	-0.133127
24	6	0	5.027267	0.243287	0.382256
25	1	0	4.851937	0.427952	1.445648
26	1	0	6.008874	-0.207967	0.249496
27	1	0	4.981006	1.185920	-0.170223

Structure 32h (vacuum)
Energy (Hartrees): -632.045063017
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.814404	-1.259240	-0.676858
2	6	0	0.460086	-0.984592	-0.647152
3	6	0	-0.034050	0.190719	-0.061286
4	6	0	0.887987	1.065554	0.508208
5	6	0	2.258591	0.810159	0.477420
6	6	0	2.725533	-0.358794	-0.117655
7	1	0	2.198578	-2.163113	-1.133610
8	1	0	-0.234071	-1.683314	-1.102440
9	1	0	0.532697	1.958427	1.010988
10	1	0	2.938234	1.516651	0.934527
11	6	0	-1.492219	0.466614	-0.055412
12	6	0	-1.923193	1.701636	-0.358330
13	1	0	-1.204585	2.466084	-0.644426
14	6	0	-2.385030	-0.649405	0.308687
15	1	0	-1.893150	-1.461476	0.867635
16	7	0	-3.616220	-0.706545	0.019210
17	6	0	-4.351269	-1.863178	0.484162
18	1	0	-4.819382	-2.356105	-0.371228
19	1	0	-3.728831	-2.590235	1.024249
20	1	0	-5.158827	-1.529726	1.140690
21	8	0	-3.216140	2.080901	-0.325289
22	1	0	-3.289072	2.999680	-0.590649
23	8	0	4.035308	-0.713553	-0.194849
24	6	0	4.986009	0.165331	0.366726
25	1	0	4.821700	0.291485	1.441711
26	1	0	5.957897	-0.294249	0.201313
27	1	0	4.957925	1.144102	-0.123179

Structure 32h ($CHCl_3$)
Energy (Hartrees): -632.066894100
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.800636	-1.295361	-0.611320
2	6	0	0.446445	-1.011816	-0.585006
3	6	0	-0.037653	0.193266	-0.052003
4	6	0	0.896227	1.092199	0.463530
5	6	0	2.264991	0.828337	0.433299
6	6	0	2.721901	-0.373187	-0.105437
7	1	0	2.171072	-2.225407	-1.027256
8	1	0	-0.251310	-1.731089	-1.001833
9	1	0	0.554512	2.014837	0.920602
10	1	0	2.952778	1.553410	0.848095
11	6	0	-1.495894	0.477004	-0.048084
12	6	0	-1.918864	1.721374	-0.333626
13	1	0	-1.201633	2.492566	-0.602458
14	6	0	-2.391103	-0.640690	0.304355
15	1	0	-1.910599	-1.445046	0.880770
16	7	0	-3.617063	-0.716489	-0.013451
17	6	0	-4.345654	-1.883425	0.444467
18	1	0	-4.785988	-2.391341	-0.417604
19	1	0	-3.723104	-2.595012	1.002509
20	1	0	-5.174423	-1.561746	1.080938
21	8	0	-3.207958	2.106940	-0.301078
22	1	0	-3.266020	3.044003	-0.517733
23	8	0	4.028845	-0.736304	-0.173240
24	6	0	4.994437	0.176412	0.321764
25	1	0	4.846240	0.368589	1.388549
26	1	0	5.962492	-0.298536	0.173233
27	1	0	4.965513	1.120424	-0.230747

Structure 32h (DMSO)
Energy (Hartrees): -632.065628884
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.786186	-1.317176	-0.567078
2	6	0	0.432766	-1.025929	-0.540530
3	6	0	-0.040629	0.203360	-0.055120
4	6	0	0.902586	1.119190	0.413791
5	6	0	2.269359	0.847028	0.382755
6	6	0	2.717069	-0.379794	-0.107918
7	1	0	2.144005	-2.267855	-0.946211
8	1	0	-0.270909	-1.761325	-0.918066
9	1	0	0.571339	2.064446	0.830890
10	1	0	2.963427	1.586390	0.760517
11	6	0	-1.498111	0.490433	-0.045175
12	6	0	-1.922680	1.737522	-0.316808
13	1	0	-1.208600	2.512129	-0.583633
14	6	0	-2.389971	-0.626756	0.320651
15	1	0	-1.930908	-1.384758	0.971907
16	7	0	-3.591734	-0.752830	-0.067775
17	6	0	-4.322777	-1.908420	0.420643
18	1	0	-4.686722	-2.488427	-0.431741
19	1	0	-3.721132	-2.558701	1.067957
20	1	0	-5.202544	-1.569501	0.974631
21	8	0	-3.211199	2.125221	-0.262232
22	1	0	-3.262399	3.070116	-0.447808
23	8	0	4.020723	-0.748453	-0.169517
24	6	0	4.986596	0.172195	0.317545
25	1	0	4.826201	0.386616	1.378063
26	1	0	5.954519	-0.308490	0.188535
27	1	0	4.967297	1.105118	-0.253168

Structure 32h (C_2H_5OH)
Energy (Hartrees): -632.072677545
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.805579	-1.289718	-0.634335
2	6	0	0.449802	-1.009116	-0.612163
3	6	0	-0.038619	0.186190	-0.062227
4	6	0	0.889963	1.078909	0.474684
5	6	0	2.259375	0.817823	0.449697
6	6	0	2.720175	-0.374016	-0.106180
7	1	0	2.178456	-2.212924	-1.064135
8	1	0	-0.242994	-1.724261	-1.044558
9	1	0	0.544664	1.995762	0.940941
10	1	0	2.943335	1.538083	0.879275
11	6	0	-1.497733	0.470986	-0.061288
12	6	0	-1.910509	1.722802	-0.335070
13	1	0	-1.189870	2.496789	-0.583839
14	6	0	-2.391256	-0.649980	0.278691
15	1	0	-1.896072	-1.485269	0.792957
16	7	0	-3.634966	-0.700119	0.022741
17	6	0	-4.347303	-1.885335	0.465895
18	1	0	-4.842520	-2.348891	-0.391258
19	1	0	-3.697974	-2.626242	0.948225
20	1	0	-5.133464	-1.591824	1.166761
21	8	0	-3.198065	2.118227	-0.315435
22	1	0	-3.243290	3.064228	-0.499693
23	8	0	4.032212	-0.733057	-0.170389
24	6	0	4.992973	0.182774	0.340322
25	1	0	4.834773	0.362195	1.407237
26	1	0	5.963773	-0.286470	0.191759
27	1	0	4.958082	1.130393	-0.204421

Structure 32i (vacuum)
Energy (Hartrees): -632.051681198
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.625315	-1.403110	-0.591465
2	6	0	0.283232	-1.072744	-0.554026
3	6	0	-0.155558	0.148850	-0.021115
4	6	0	0.810445	1.024126	0.473608
5	6	0	2.165921	0.706262	0.442596
6	6	0	2.578075	-0.513248	-0.091300
7	1	0	1.965761	-2.342935	-1.008678
8	1	0	-0.441005	-1.768876	-0.964154
9	1	0	0.502640	1.973346	0.892873
10	1	0	2.881121	1.413918	0.840031
11	6	0	-1.600514	0.463390	0.008359
12	6	0	-2.117774	1.685641	-0.176932
13	1	0	-3.193134	1.825165	-0.135004
14	6	0	-2.549164	-0.642180	0.266069
15	1	0	-2.113550	-1.526825	0.754305
16	7	0	-3.780351	-0.594651	-0.026715
17	6	0	-4.603121	-1.727165	0.343376
18	1	0	-5.102761	-2.114130	-0.547863
19	1	0	-4.036388	-2.538883	0.818917
20	1	0	-5.385559	-1.393859	1.029890
21	8	0	-1.360548	2.779581	-0.434065
22	1	0	-1.927886	3.540723	-0.570557
23	8	0	3.872420	-0.921398	-0.167520
24	6	0	4.865155	-0.047600	0.325267
25	1	0	4.724592	0.149111	1.392940
26	1	0	5.816120	-0.553192	0.172900
27	1	0	4.865450	0.900194	-0.222531

Structure 32i ($CHCl_3$)
Energy (Hartrees): -632.071615107
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.612157	-1.406845	-0.584212
2	6	0	0.270566	-1.069344	-0.544468
3	6	0	-0.160110	0.158512	-0.017671
4	6	0	0.814668	1.031977	0.467911
5	6	0	2.168993	0.707638	0.433933
6	6	0	2.572938	-0.518403	-0.093906
7	1	0	1.940792	-2.354222	-0.995930
8	1	0	-0.458120	-1.767255	-0.944465
9	1	0	0.516404	1.983746	0.889565
10	1	0	2.889788	1.413053	0.826188
11	6	0	-1.605551	0.477649	0.021471
12	6	0	-2.117104	1.705454	-0.162036
13	1	0	-3.188231	1.867687	-0.099733
14	6	0	-2.548640	-0.629256	0.287546
15	1	0	-2.122359	-1.488063	0.825177
16	7	0	-3.769227	-0.616532	-0.057641
17	6	0	-4.587980	-1.748473	0.332137
18	1	0	-5.050414	-2.180939	-0.558795
19	1	0	-4.026242	-2.529432	0.860088
20	1	0	-5.400029	-1.401334	0.976833
21	8	0	-1.356890	2.786083	-0.440496
22	1	0	-1.920092	3.559855	-0.551469
23	8	0	3.864139	-0.931963	-0.169699
24	6	0	4.867502	-0.055930	0.317116
25	1	0	4.730096	0.147759	1.383156
26	1	0	5.814895	-0.570786	0.168751
27	1	0	4.875474	0.884819	-0.241244

Structure 32i (DMSO)
Energy (Hartrees): -632.069584610
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.607587	-1.408792	-0.581873
2	6	0	0.266113	-1.069244	-0.539114
3	6	0	-0.160665	0.162788	-0.018125
4	6	0	0.817500	1.035906	0.462585
5	6	0	2.171534	0.709700	0.425698
6	6	0	2.572808	-0.520027	-0.098414
7	1	0	1.929251	-2.360780	-0.988832
8	1	0	-0.464787	-1.770945	-0.928861
9	1	0	0.524551	1.989113	0.884883
10	1	0	2.893777	1.415605	0.814724
11	6	0	-1.605854	0.482979	0.024815
12	6	0	-2.119984	1.711144	-0.154201
13	1	0	-3.189892	1.876991	-0.075861
14	6	0	-2.545226	-0.625341	0.298722
15	1	0	-2.124938	-1.469268	0.862805
16	7	0	-3.758735	-0.629017	-0.072635
17	6	0	-4.578615	-1.757785	0.329180
18	1	0	-5.027657	-2.209778	-0.559017
19	1	0	-4.019072	-2.524303	0.879189
20	1	0	-5.400275	-1.401339	0.956689
21	8	0	-1.363835	2.790109	-0.446527
22	1	0	-1.928454	3.568821	-0.517530
23	8	0	3.861332	-0.934032	-0.174662
24	6	0	4.863732	-0.057501	0.320937
25	1	0	4.716054	0.147881	1.384936
26	1	0	5.811924	-0.573163	0.181313
27	1	0	4.877105	0.882700	-0.237724

Structure 32i (C_2H_5OH)
Energy (Hartrees): -632.075386353
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.604560	-1.396472	-0.608488
2	6	0	0.262916	-1.056874	-0.564111
3	6	0	-0.164166	0.161329	-0.012852
4	6	0	0.811037	1.019022	0.500009
5	6	0	2.165143	0.693100	0.461611
6	6	0	2.565214	-0.520517	-0.096349
7	1	0	1.929805	-2.336591	-1.040186
8	1	0	-0.467433	-1.746040	-0.976936
9	1	0	0.515138	1.958047	0.952272
10	1	0	2.886653	1.385892	0.874715
11	6	0	-1.608947	0.486196	0.026308
12	6	0	-2.110680	1.717570	-0.165348
13	1	0	-3.177591	1.901514	-0.094968
14	6	0	-2.550267	-0.618290	0.302700
15	1	0	-2.129279	-1.459936	0.869589
16	7	0	-3.764126	-0.626152	-0.069327
17	6	0	-4.577628	-1.757796	0.338698
18	1	0	-5.024466	-2.217649	-0.546396
19	1	0	-4.014471	-2.518733	0.892342
20	1	0	-5.401535	-1.403882	0.964329
21	8	0	-1.341172	2.785929	-0.465439
22	1	0	-1.895044	3.568748	-0.569002
23	8	0	3.859336	-0.934360	-0.179655
24	6	0	4.865359	-0.060748	0.318255
25	1	0	4.728314	0.125420	1.386886
26	1	0	5.812732	-0.572118	0.158410
27	1	0	4.865515	0.886711	-0.227605

Structure 32j (vacuum)
Energy (Hartrees): -632.051879836
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.416737	-1.198398	-0.863548
2	6	0	0.087107	-0.824940	-0.821923
3	6	0	-0.324825	0.294025	-0.084589
4	6	0	0.641616	1.010340	0.615290
5	6	0	1.984678	0.639785	0.590865
6	6	0	2.375125	-0.469701	-0.154761
7	1	0	1.741843	-2.059585	-1.434379
8	1	0	-0.649465	-1.408007	-1.358221
9	1	0	0.347399	1.875936	1.196174
10	1	0	2.702574	1.220531	1.153660
11	6	0	-1.746428	0.707412	-0.055972
12	6	0	-2.141067	1.985268	-0.177013
13	1	0	-3.196458	2.243263	-0.143089
14	6	0	-2.829787	-0.270980	0.118335
15	1	0	-3.845850	0.157111	0.120664
16	7	0	-2.647583	-1.514219	0.266140
17	6	0	-3.818393	-2.345811	0.446527
18	1	0	-3.847456	-3.104242	-0.339696
19	1	0	-3.736188	-2.875252	1.398729
20	1	0	-4.760961	-1.780881	0.432335
21	8	0	-1.279250	3.016512	-0.343857
22	1	0	-1.764778	3.829670	-0.494903
23	8	0	3.655150	-0.919067	-0.250429
24	6	0	4.650379	-0.216530	0.460923
25	1	0	4.453422	-0.232418	1.537741
26	1	0	5.587427	-0.730307	0.257460
27	1	0	4.723510	0.821340	0.120022

Structure 32j ($CHCl_3$)
Energy (Hartrees): -632.073564481
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.430957	-1.153490	0.925073
2	6	0	-0.099355	-0.781292	0.883119
3	6	0	0.327465	0.290426	0.086233
4	6	0	-0.628942	0.964477	-0.669401
5	6	0	-1.974242	0.598760	-0.642751
6	6	0	-2.378423	-0.466198	0.160108
7	1	0	-1.761596	-1.979035	1.544813
8	1	0	0.623588	-1.325886	1.477818
9	1	0	-0.323919	1.794854	-1.295904
10	1	0	-2.683953	1.147419	-1.247487
11	6	0	1.751006	0.704042	0.059706
12	6	0	2.139201	1.986085	0.183129
13	1	0	3.192149	2.254361	0.156010
14	6	0	2.834063	-0.271290	-0.112442
15	1	0	3.848926	0.153010	-0.082579
16	7	0	2.651965	-1.513188	-0.294327
17	6	0	3.829769	-2.342800	-0.457950
18	1	0	3.845055	-3.106765	0.324305
19	1	0	3.769802	-2.867727	-1.414896
20	1	0	4.769207	-1.775707	-0.420477
21	8	0	1.270356	3.003409	0.353162
22	1	0	1.752788	3.829396	0.469186
23	8	0	-3.659678	-0.906209	0.261528
24	6	0	-4.654154	-0.218931	-0.478930
25	1	0	-4.462328	-0.283358	-1.554282
26	1	0	-5.595689	-0.715621	-0.251760
27	1	0	-4.715801	0.831034	-0.177339

Structure 32j (DMSO)
Energy (Hartrees): -632.073289352
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.446024	-1.058050	1.023088
2	6	0	-0.111280	-0.696104	0.971661
3	6	0	0.334183	0.301858	0.093345
4	6	0	-0.605399	0.914388	-0.731982
5	6	0	-1.954009	0.558877	-0.696889
6	6	0	-2.378125	-0.433458	0.186332
7	1	0	-1.789679	-1.825849	1.707060
8	1	0	0.599402	-1.188650	1.625653
9	1	0	-0.284614	1.685843	-1.423430
10	1	0	-2.650166	1.056955	-1.358888
11	6	0	1.762613	0.698469	0.054012
12	6	0	2.166362	1.976419	0.169981
13	1	0	3.221631	2.234071	0.132816
14	6	0	2.824419	-0.296946	-0.120950
15	1	0	3.848495	0.100944	-0.088288
16	7	0	2.607955	-1.534457	-0.307547
17	6	0	3.765350	-2.395570	-0.468373
18	1	0	3.756388	-3.161944	0.311903
19	1	0	3.697741	-2.915648	-1.427782
20	1	0	4.717325	-1.852067	-0.422924
21	8	0	1.307265	2.998325	0.349961
22	1	0	1.799771	3.823283	0.435349
23	8	0	-3.661489	-0.855319	0.302536
24	6	0	-4.632837	-0.245574	-0.535821
25	1	0	-4.405000	-0.415191	-1.592100
26	1	0	-5.581793	-0.719028	-0.291316
27	1	0	-4.702918	0.828593	-0.341635

Structure 32j (C_2H_5OH)
Energy (Hartrees): -632.078887657
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.457125	-1.021322	1.059913
2	6	0	-0.121021	-0.663690	1.009733
3	6	0	0.334122	0.302444	0.101763
4	6	0	-0.595631	0.888882	-0.753463
5	6	0	-1.945393	0.537841	-0.719538
6	6	0	-2.376709	-0.422794	0.192612
7	1	0	-1.812248	-1.764965	1.764901
8	1	0	0.582462	-1.134600	1.687388
9	1	0	-0.264681	1.634187	-1.469015
10	1	0	-2.635151	1.013065	-1.404722
11	6	0	1.764718	0.693442	0.059689
12	6	0	2.166590	1.972603	0.167763
13	1	0	3.219419	2.238739	0.131571
14	6	0	2.824246	-0.303004	-0.115895
15	1	0	3.848072	0.095242	-0.081478
16	7	0	2.609888	-1.540329	-0.309712
17	6	0	3.773260	-2.393670	-0.475451
18	1	0	3.773053	-3.162064	0.302660
19	1	0	3.707461	-2.912837	-1.435245
20	1	0	4.721737	-1.844352	-0.432015
21	8	0	1.301937	2.993490	0.335941
22	1	0	1.784511	3.824609	0.420452
23	8	0	-3.666809	-0.841060	0.311255
24	6	0	-4.632901	-0.263545	-0.558088
25	1	0	-4.391519	-0.469279	-1.604565
26	1	0	-5.581516	-0.733687	-0.305657
27	1	0	-4.706769	0.815680	-0.398082

Structure 32k (vacuum)
Energy (Hartrees): -632.051738231
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.842949	0.714341	-0.592926
2	6	0	-0.457025	0.603374	-0.656171
3	6	0	0.219911	-0.428082	-0.007618
4	6	0	-0.537493	-1.342149	0.735299
5	6	0	-1.916883	-1.247832	0.805150
6	6	0	-2.579396	-0.217380	0.137451
7	1	0	-2.329492	1.528586	-1.112813
8	1	0	0.107328	1.337418	-1.215841
9	1	0	-0.031577	-2.126833	1.287590
10	1	0	-2.503451	-1.949111	1.385791
11	6	0	1.691320	-0.576886	-0.115937
12	6	0	2.210190	-1.790319	-0.359971
13	1	0	1.569140	-2.650852	-0.528153
14	6	0	2.600012	0.568892	0.045741
15	1	0	3.668198	0.339099	-0.053968
16	7	0	2.193037	1.745151	0.285574
17	6	0	3.197872	2.777507	0.431464
18	1	0	3.020250	3.559272	-0.311446
19	1	0	3.089440	3.241727	1.414710
20	1	0	4.225263	2.405460	0.321301
21	8	0	3.550521	-2.018416	-0.409457
22	1	0	3.719860	-2.915110	-0.702850
23	8	0	-3.933338	-0.197924	0.265003
24	6	0	-4.637782	0.843403	-0.376160
25	1	0	-4.492446	0.811045	-1.460745
26	1	0	-5.689081	0.682017	-0.147891
27	1	0	-4.328811	1.822725	0.002997

Structure 32k ($CHCl_3$)
Energy (Hartrees): -632.072286824
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.853840	0.695607	-0.622756
2	6	0	-0.468057	0.579331	-0.695201
3	6	0	0.218085	-0.427302	-0.015106
4	6	0	-0.532921	-1.317758	0.763538
5	6	0	-1.912738	-1.219737	0.842337
6	6	0	-2.582893	-0.210752	0.147803
7	1	0	-2.347273	1.490293	-1.166805
8	1	0	0.087794	1.288533	-1.296320
9	1	0	-0.024087	-2.090999	1.329544
10	1	0	-2.490469	-1.906872	1.449819
11	6	0	1.691077	-0.574352	-0.128235
12	6	0	2.210793	-1.793154	-0.359518
13	1	0	1.574092	-2.660082	-0.511684
14	6	0	2.598456	0.571338	0.023578
15	1	0	3.662526	0.351832	-0.124107
16	7	0	2.205299	1.743236	0.314267
17	6	0	3.221727	2.769396	0.444075
18	1	0	3.018995	3.571083	-0.271380
19	1	0	3.157773	3.210730	1.442205
20	1	0	4.240686	2.395048	0.282329
21	8	0	3.544362	-2.019581	-0.419514
22	1	0	3.707466	-2.935344	-0.669432
23	8	0	-3.934262	-0.185692	0.285910
24	6	0	-4.648624	0.836307	-0.389125
25	1	0	-4.506604	0.770062	-1.471994
26	1	0	-5.699029	0.674476	-0.154020
27	1	0	-4.346142	1.827225	-0.037537

Structure 32k (DMSO)
Energy (Hartrees): -632.071245651
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.857639	0.678745	-0.642412
2	6	0	-0.472333	0.558522	-0.721258
3	6	0	0.219472	-0.426929	-0.015303
4	6	0	-0.525370	-1.294005	0.795094
5	6	0	-1.905259	-1.192343	0.880527
6	6	0	-2.582206	-0.204446	0.160891
7	1	0	-2.353948	1.455783	-1.209019
8	1	0	0.076702	1.245602	-1.354927
9	1	0	-0.013522	-2.055525	1.374317
10	1	0	-2.475801	-1.865444	1.510474
11	6	0	1.691551	-0.574399	-0.139733
12	6	0	2.211712	-1.796068	-0.358330
13	1	0	1.575529	-2.668107	-0.483727
14	6	0	2.593400	0.577262	-0.008237
15	1	0	3.649129	0.381039	-0.227645
16	7	0	2.204822	1.733020	0.349915
17	6	0	3.215845	2.769332	0.453784
18	1	0	2.935200	3.613209	-0.182369
19	1	0	3.243758	3.140916	1.481817
20	1	0	4.218358	2.426092	0.169899
21	8	0	3.543443	-2.016367	-0.430565
22	1	0	3.706342	-2.938532	-0.660094
23	8	0	-3.930537	-0.174567	0.304640
24	6	0	-4.647623	0.816597	-0.417690
25	1	0	-4.497487	0.705306	-1.495372
26	1	0	-5.698599	0.659650	-0.182520
27	1	0	-4.351973	1.822732	-0.106830

Structure 32k (C_2H_5OH)
Energy (Hartrees): -632.076582328
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.859075	0.665617	-0.661266
2	6	0	-0.474095	0.543804	-0.739770
3	6	0	0.219212	-0.422348	-0.009235
4	6	0	-0.522070	-1.268267	0.825580
5	6	0	-1.902230	-1.164948	0.911490
6	6	0	-2.578179	-0.197125	0.166797
7	1	0	-2.358232	1.426512	-1.246967
8	1	0	0.073534	1.213129	-1.393677
9	1	0	-0.007726	-2.013713	1.423205
10	1	0	-2.473167	-1.820793	1.559506
11	6	0	1.690927	-0.573700	-0.136797
12	6	0	2.203724	-1.797032	-0.363201
13	1	0	1.565216	-2.666441	-0.490725
14	6	0	2.595185	0.575669	-0.008674
15	1	0	3.647274	0.380853	-0.246257
16	7	0	2.213582	1.729602	0.363952
17	6	0	3.228599	2.764223	0.449497
18	1	0	2.939261	3.607031	-0.183999
19	1	0	3.275067	3.139428	1.475354
20	1	0	4.225778	2.419432	0.149851
21	8	0	3.534461	-2.028053	-0.444007
22	1	0	3.692163	-2.949969	-0.678881
23	8	0	-3.931886	-0.164932	0.312852
24	6	0	-4.655586	0.803576	-0.436152
25	1	0	-4.505951	0.659159	-1.509676
26	1	0	-5.704929	0.647089	-0.193000
27	1	0	-4.362430	1.818136	-0.152762

Structure 32l (vacuum)
Energy (Hartrees): -632.050685667
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.836496	0.699600	-0.613645
2	6	0	-0.451495	0.583627	-0.684024
3	6	0	0.227943	-0.431880	-0.014438
4	6	0	-0.524557	-1.327097	0.755116
5	6	0	-1.903174	-1.228265	0.832279
6	6	0	-2.568785	-0.212739	0.145182
7	1	0	-2.325693	1.501242	-1.150319
8	1	0	0.109580	1.302215	-1.267363
9	1	0	-0.015837	-2.102747	1.317340
10	1	0	-2.487134	-1.916114	1.431297
11	6	0	1.700710	-0.585944	-0.127202
12	6	0	2.201894	-1.812043	-0.373823
13	1	0	1.543506	-2.655847	-0.545078
14	6	0	2.586454	0.572591	0.033906
15	1	0	3.667743	0.398013	-0.101574
16	7	0	2.179129	1.740363	0.305900
17	6	0	3.168888	2.786831	0.439392
18	1	0	2.958358	3.575374	-0.287259
19	1	0	3.079740	3.235089	1.431666
20	1	0	4.200178	2.435018	0.295885
21	8	0	3.495757	-2.191436	-0.456311
22	1	0	4.084512	-1.458487	-0.256922
23	8	0	-3.921241	-0.187687	0.282289
24	6	0	-4.630296	0.833223	-0.386225
25	1	0	-4.489559	0.768829	-1.469996
26	1	0	-5.680280	0.676714	-0.148754
27	1	0	-4.321661	1.823728	-0.037160

Structure 32l ($CHCl_3$)
Energy (Hartrees): -632.070537612
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.846378	0.672296	-0.651930
2	6	0	-0.461628	0.552534	-0.731341
3	6	0	0.229537	-0.427399	-0.019150
4	6	0	-0.513572	-1.287869	0.798668
5	6	0	-1.892917	-1.186529	0.885170
6	6	0	-2.568744	-0.204951	0.158346
7	1	0	-2.344259	1.445822	-1.221696
8	1	0	0.088296	1.238429	-1.365060
9	1	0	0.000618	-2.041661	1.385546
10	1	0	-2.465855	-1.851660	1.521028
11	6	0	1.703023	-0.581655	-0.143533
12	6	0	2.196640	-1.814420	-0.375589
13	1	0	1.533356	-2.658706	-0.530234
14	6	0	2.590507	0.580485	-0.009700
15	1	0	3.651324	0.432883	-0.262282
16	7	0	2.191794	1.725452	0.364916
17	6	0	3.177008	2.784802	0.448435
18	1	0	2.864183	3.617867	-0.186437
19	1	0	3.209911	3.161439	1.474067
20	1	0	4.184971	2.468038	0.150418
21	8	0	3.486554	-2.199815	-0.458528
22	1	0	4.089738	-1.478673	-0.243138
23	8	0	-3.918846	-0.175281	0.305396
24	6	0	-4.640608	0.814164	-0.409147
25	1	0	-4.501610	0.702819	-1.488687
26	1	0	-5.689448	0.656753	-0.164179
27	1	0	-4.342660	1.820502	-0.100068

Structure 32l (DMSO)
Energy (Hartrees): -632.069923447
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.847784	0.660449	-0.659576
2	6	0	-0.463377	0.536783	-0.742456
3	6	0	0.229980	-0.437137	-0.022588
4	6	0	-0.511574	-1.290391	0.804383
5	6	0	-1.891271	-1.185797	0.893704
6	6	0	-2.569907	-0.208391	0.161817
7	1	0	-2.345293	1.429052	-1.236475
8	1	0	0.083689	1.213550	-1.389131
9	1	0	0.002200	-2.043121	1.393288
10	1	0	-2.459973	-1.848213	1.536507
11	6	0	1.703862	-0.583501	-0.147915
12	6	0	2.211604	-1.812862	-0.368738
13	1	0	1.558532	-2.668866	-0.503515
14	6	0	2.581303	0.586510	-0.020065
15	1	0	3.637277	0.454732	-0.294102
16	7	0	2.178172	1.722382	0.379706
17	6	0	3.157572	2.789909	0.456233
18	1	0	2.831885	3.622322	-0.173427
19	1	0	3.200056	3.163510	1.482760
20	1	0	4.162487	2.478430	0.145630
21	8	0	3.505467	-2.177583	-0.458509
22	1	0	4.097481	-1.434564	-0.283626
23	8	0	-3.917315	-0.173167	0.311683
24	6	0	-4.635252	0.812761	-0.417126
25	1	0	-4.492484	0.688969	-1.494404
26	1	0	-5.685327	0.662430	-0.173769
27	1	0	-4.333885	1.821097	-0.119111

Structure 32l (C_2H_5OH)
Energy (Hartrees): -632.074535326
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.850604	0.657237	-0.669891
2	6	0	-0.466283	0.533306	-0.753210
3	6	0	0.228771	-0.427688	-0.017858
4	6	0	-0.509425	-1.266440	0.826280
5	6	0	-1.889221	-1.161388	0.916876
6	6	0	-2.567195	-0.198537	0.167894
7	1	0	-2.351356	1.414290	-1.259168
8	1	0	0.079263	1.198036	-1.413775
9	1	0	0.006742	-2.008090	1.427020
10	1	0	-2.457957	-1.812191	1.571826
11	6	0	1.701987	-0.581215	-0.148365
12	6	0	2.195004	-1.815008	-0.375154
13	1	0	1.531845	-2.662570	-0.513699
14	6	0	2.587536	0.583033	-0.024606
15	1	0	3.637351	0.444799	-0.317161
16	7	0	2.195677	1.718411	0.389790
17	6	0	3.185155	2.778578	0.451576
18	1	0	2.857342	3.614103	-0.172644
19	1	0	3.247392	3.152874	1.476699
20	1	0	4.182772	2.460114	0.125573
21	8	0	3.486363	-2.197379	-0.468154
22	1	0	4.096438	-1.474594	-0.274009
23	8	0	-3.920018	-0.163629	0.319763
24	6	0	-4.646244	0.801155	-0.431690
25	1	0	-4.501505	0.650407	-1.504975
26	1	0	-5.694607	0.646777	-0.183030
27	1	0	-4.351101	1.817040	-0.155179

Structure 33a (vacuum)

Energy (Hartrees): -722.056855450
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.943691	1.101695	0.475084
2	6	0	0.566243	1.246444	0.438854
3	6	0	-0.259885	0.231114	-0.068586
4	6	0	0.348422	-0.942428	-0.540493
5	6	0	1.722331	-1.112255	-0.492117
6	6	0	2.500981	-0.081877	0.013687
7	1	0	2.586582	1.877104	0.869293
8	1	0	0.122123	2.150351	0.838184
9	1	0	-0.262655	-1.720595	-0.982860
10	1	0	2.197448	-2.012407	-0.858223
11	6	0	-1.721764	0.401411	-0.106283
12	6	0	-2.554106	-0.662924	0.180331
13	1	0	-2.113660	-1.615660	0.469280
14	6	0	-2.294232	1.683868	-0.449048
15	1	0	-1.574007	2.483748	-0.696076
16	1	0	-4.303574	0.253042	-0.088006
17	7	0	-3.882822	-0.639638	0.164073
18	6	0	-4.718886	-1.765075	0.530227
19	1	0	-5.373232	-2.042554	-0.298125
20	1	0	-4.086934	-2.618350	0.776693
21	1	0	-5.332742	-1.523320	1.400098
22	8	0	-3.494994	1.921380	-0.504761
23	7	0	3.963069	-0.247909	0.056657
24	8	0	4.621212	0.671781	0.494975
25	8	0	4.421551	-1.295457	-0.348378

Structure 33a ($CHCl_3$)

Energy (Hartrees): -722.077857877
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.952153	1.118230	0.438656
2	6	0	0.575930	1.267617	0.412323
3	6	0	-0.262965	0.238510	-0.051719
4	6	0	0.338070	-0.957104	-0.483485
5	6	0	1.710267	-1.130891	-0.443873
6	6	0	2.501622	-0.084721	0.013554
7	1	0	2.593199	1.910582	0.801808
8	1	0	0.145505	2.188576	0.786944
9	1	0	-0.276952	-1.753232	-0.885729
10	1	0	2.167078	-2.050676	-0.784431
11	6	0	-1.722616	0.413999	-0.089033
12	6	0	-2.559367	-0.667299	0.168256
13	1	0	-2.121164	-1.627151	0.434560
14	6	0	-2.284165	1.698502	-0.405907
15	1	0	-1.563183	2.499987	-0.638744
16	1	0	-4.314386	0.244831	-0.084109
17	7	0	-3.879690	-0.645405	0.148982
18	6	0	-4.719920	-1.785547	0.467561
19	1	0	-5.351120	-2.038418	-0.386073
20	1	0	-4.090938	-2.641235	0.711150
21	1	0	-5.356520	-1.556275	1.323897
22	8	0	-3.489468	1.949287	-0.461978
23	7	0	3.954775	-0.254328	0.044349
24	8	0	4.635166	0.688461	0.400818
25	8	0	4.412903	-1.331079	-0.287663

Structure 33a (DMSO)

Energy (Hartrees): -722.078408820
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.952832	1.121292	0.428737
2	6	0	0.576974	1.271575	0.404873
3	6	0	-0.265123	0.237854	-0.045829
4	6	0	0.334211	-0.964601	-0.463988
5	6	0	1.706354	-1.137494	-0.428548
6	6	0	2.501224	-0.086496	0.013987
7	1	0	2.592194	1.919205	0.782825
8	1	0	0.150689	2.198026	0.770504
9	1	0	-0.280941	-1.769132	-0.849061
10	1	0	2.157383	-2.063480	-0.760065
11	6	0	-1.723481	0.416838	-0.083357
12	6	0	-2.562421	-0.668088	0.166510
13	1	0	-2.125888	-1.631126	0.423393
14	6	0	-2.277822	1.703413	-0.399685
15	1	0	-1.550994	2.499994	-0.630818
16	1	0	-4.322056	0.241773	-0.078765
17	7	0	-3.880552	-0.646003	0.148672
18	6	0	-4.719075	-1.792315	0.454166
19	1	0	-5.338967	-2.043516	-0.408098
20	1	0	-4.087372	-2.644253	0.702674
21	1	0	-5.366649	-1.565163	1.302533
22	8	0	-3.481914	1.963469	-0.460013
23	7	0	3.952391	-0.255354	0.040663
24	8	0	4.635033	0.686083	0.401519
25	8	0	4.412841	-1.330138	-0.299214

Structure 33a (C_2H_5OH)

Energy (Hartrees): -722.079379046
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.952726	1.120474	0.435725
2	6	0	0.577674	1.272130	0.412074
3	6	0	-0.264122	0.243154	-0.049629
4	6	0	0.332982	-0.956256	-0.479244
5	6	0	1.704183	-1.132590	-0.442072
6	6	0	2.498798	-0.085746	0.011834
7	1	0	2.591893	1.913635	0.800690
8	1	0	0.151651	2.194581	0.787967
9	1	0	-0.283014	-1.754706	-0.875469
10	1	0	2.154021	-2.055790	-0.783254
11	6	0	-1.722720	0.422510	-0.085352
12	6	0	-2.560779	-0.667430	0.162536
13	1	0	-2.119575	-1.628376	0.419190
14	6	0	-2.274259	1.705717	-0.389898
15	1	0	-1.552835	2.506597	-0.616813
16	1	0	-4.324692	0.233479	-0.083992
17	7	0	-3.876584	-0.650900	0.144246
18	6	0	-4.710685	-1.801434	0.449711
19	1	0	-5.331530	-2.051235	-0.412110
20	1	0	-4.076338	-2.652149	0.695059
21	1	0	-5.356876	-1.576866	1.299700
22	8	0	-3.484726	1.966652	-0.444415
23	7	0	3.944852	-0.257667	0.042139
24	8	0	4.637545	0.695909	0.351428
25	8	0	4.405510	-1.349108	-0.243236

Structure 33b (vacuum)

Energy (Hartrees): -722.049771549
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.746738	-1.080483	0.665712
2	6	0	-0.375874	-1.281332	0.621547
3	6	0	0.461309	-0.421215	-0.104749
4	6	0	-0.124994	0.650234	-0.797414
5	6	0	-1.492502	0.873590	-0.753075
6	6	0	-2.281309	0.001655	-0.017536
7	1	0	-2.399781	-1.733382	1.229227
8	1	0	0.058696	-2.104579	1.176499
9	1	0	0.498156	1.291086	-1.411881
10	1	0	-1.955497	1.692358	-1.287498
11	6	0	1.914283	-0.654220	-0.150266
12	6	0	2.849246	0.327195	0.018675
13	1	0	3.891254	0.019817	-0.038513
14	6	0	2.427303	-2.011404	-0.363621
15	1	0	1.647124	-2.781893	-0.519861
16	1	0	1.695678	1.937079	0.426846
17	7	0	2.644745	1.630780	0.262470
18	6	0	3.713271	2.548858	0.616275
19	1	0	3.797934	2.675091	1.699030
20	1	0	4.655156	2.155847	0.235015
21	1	0	3.537111	3.522077	0.157420
22	8	0	3.598412	-2.321298	-0.393007
23	7	0	-3.736290	0.232388	0.038104
24	8	0	-4.406979	-0.563140	0.659878
25	8	0	-4.172557	1.205320	-0.539820

Structure 33b ($CHCl_3$)

Energy (Hartrees): -722.072783738
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.762334	-1.093774	0.635856
2	6	0	-0.392300	-1.295946	0.598559
3	6	0	0.456292	-0.412506	-0.088979
4	6	0	-0.120611	0.689654	-0.742688
5	6	0	-1.486674	0.915291	-0.704033
6	6	0	-2.287899	0.015764	-0.013002
7	1	0	-2.414409	-1.771674	1.170584
8	1	0	0.031546	-2.141938	1.127322
9	1	0	0.504945	1.358141	-1.323792
10	1	0	-1.931144	1.759633	-1.214150
11	6	0	1.906197	-0.661073	-0.139001
12	6	0	2.866357	0.312490	0.037714
13	1	0	3.903897	-0.003499	-0.043587
14	6	0	2.386446	-2.012242	-0.369139
15	1	0	1.593250	-2.762609	-0.544964
16	1	0	1.750919	1.942411	0.471163
17	7	0	2.691459	1.594972	0.331539
18	6	0	3.776699	2.539590	0.538466
19	1	0	3.716739	2.970444	1.539375
20	1	0	4.726279	2.016469	0.434527
21	1	0	3.730763	3.342439	-0.199916
22	8	0	3.556738	-2.362826	-0.401674
23	7	0	-3.735990	0.244124	0.029741
24	8	0	-4.426870	-0.573082	0.605586
25	8	0	-4.174130	1.240036	-0.512418

Structure 33b (DMSO)

Energy (Hartrees): -722.074148813
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.769876	-1.101984	0.617273
2	6	0	-0.400114	-1.303922	0.583826
3	6	0	0.454683	-0.405765	-0.079284
4	6	0	-0.118300	0.712530	-0.709964
5	6	0	-1.484321	0.936823	-0.675474
6	6	0	-2.291605	0.022242	-0.010561
7	1	0	-2.422244	-1.793950	1.133092
8	1	0	0.017663	-2.162520	1.096731
9	1	0	0.507807	1.400189	-1.267077
10	1	0	-1.920112	1.794721	-1.169923
11	6	0	1.902202	-0.661704	-0.130548
12	6	0	2.873900	0.306745	0.041322
13	1	0	3.908084	-0.016708	-0.049568
14	6	0	2.366894	-2.014412	-0.368499
15	1	0	1.563306	-2.752084	-0.550252
16	1	0	1.780210	1.950609	0.481899
17	7	0	2.714787	1.585983	0.339804
18	6	0	3.811035	2.524983	0.513915
19	1	0	3.747190	2.993998	1.496651
20	1	0	4.754509	1.987045	0.434488
21	1	0	3.773770	3.299855	-0.254011
22	8	0	3.532960	-2.383855	-0.406355
23	7	0	-3.738012	0.249886	0.026303
24	8	0	-4.434868	-0.573501	0.589107
25	8	0	-4.174917	1.251674	-0.508604

Structure 33b (C_2H_5OH)

Energy (Hartrees): -722.075656085
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.762136	-1.091158	0.638134
2	6	0	-0.392898	-1.292797	0.599351
3	6	0	0.455009	-0.407983	-0.088854
4	6	0	-0.120987	0.696250	-0.740299
5	6	0	-1.486802	0.920205	-0.702931
6	6	0	-2.287495	0.019047	-0.011693
7	1	0	-2.410235	-1.771551	1.174397
8	1	0	0.029988	-2.139658	1.127447
9	1	0	0.502090	1.371394	-1.316001
10	1	0	-1.926427	1.766325	-1.214217
11	6	0	1.904045	-0.661848	-0.141513
12	6	0	2.873364	0.312750	0.037808
13	1	0	3.910449	-0.002017	-0.048185
14	6	0	2.367726	-2.005748	-0.371585
15	1	0	1.571650	-2.750266	-0.546122
16	1	0	1.762704	1.944394	0.469004
17	7	0	2.702249	1.586327	0.339709
18	6	0	3.791137	2.530868	0.538149
19	1	0	3.715594	2.981659	1.528489
20	1	0	4.739178	2.001757	0.456209
21	1	0	3.752131	3.318069	-0.216696
22	8	0	3.542219	-2.376366	-0.409324
23	7	0	-3.730398	0.245079	0.029827
24	8	0	-4.425469	-0.557665	0.624912
25	8	0	-4.178733	1.226848	-0.533148

Structure 33c (vacuum)

Energy (Hartrees): -722.051300692
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.654712	0.980899	0.683659
2	6	0	0.294125	1.239462	0.625721
3	6	0	-0.562026	0.408496	-0.109206
4	6	0	-0.013275	-0.674266	-0.811035
5	6	0	1.345948	-0.946695	-0.761528
6	6	0	2.155713	-0.113987	-0.005457
7	1	0	2.327078	1.609168	1.252152
8	1	0	-0.114029	2.096930	1.143305
9	1	0	-0.654499	-1.288419	-1.434210
10	1	0	1.783894	-1.773999	-1.303457
11	6	0	-2.011569	0.679892	-0.160251
12	6	0	-2.964094	-0.285382	-0.015732
13	1	0	-4.008053	0.016703	-0.077032
14	6	0	-2.509594	2.043515	-0.328706
15	1	0	-3.615565	2.115134	-0.393778
16	1	0	-1.843008	-1.913682	0.401410
17	7	0	-2.784171	-1.601818	0.204980
18	6	0	-3.872229	-2.481264	0.596466
19	1	0	-4.050417	-2.462692	1.675637
20	1	0	-4.783243	-2.172385	0.083344
21	1	0	-3.643003	-3.502190	0.292949
22	8	0	-1.831426	3.042288	-0.394808
23	7	0	3.601772	-0.399497	0.060159
24	8	0	4.010102	-1.369082	-0.543701
25	8	0	4.292744	0.349371	0.716022

Structure 33c ($CHCl_3$)

Energy (Hartrees): -722.075059251
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.672135	0.967823	0.695507
2	6	0	0.312220	1.227438	0.648364
3	6	0	-0.555741	0.402062	-0.082280
4	6	0	-0.015369	-0.688400	-0.780667
5	6	0	1.342573	-0.964933	-0.741774
6	6	0	2.164641	-0.129239	0.000484
7	1	0	2.342942	1.599120	1.262917
8	1	0	-0.086594	2.079321	1.183238
9	1	0	-0.659702	-1.311411	-1.391257
10	1	0	1.761885	-1.800361	-1.286392
11	6	0	-2.000462	0.695158	-0.131997
12	6	0	-2.982541	-0.257567	0.020739
13	1	0	-4.018137	0.069002	-0.052235
14	6	0	-2.475060	2.047911	-0.331339
15	1	0	-3.578096	2.139523	-0.369558
16	1	0	-1.904063	-1.919752	0.427492
17	7	0	-2.835738	-1.556277	0.271266
18	6	0	-3.946044	-2.461701	0.517415
19	1	0	-4.042744	-2.684192	1.582749
20	1	0	-4.866932	-1.997576	0.166043
21	1	0	-3.793225	-3.393082	-0.028621
22	8	0	-1.783828	3.044529	-0.462511
23	7	0	3.604475	-0.412796	0.048262
24	8	0	4.016213	-1.384881	-0.554329
25	8	0	4.313290	0.336802	0.689617

Structure 33c (DMSO)

Energy (Hartrees): -722.077195743
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.671438	0.958846	0.709611
2	6	0	0.311895	1.218756	0.662038
3	6	0	-0.556712	0.400832	-0.077322
4	6	0	-0.016067	-0.684831	-0.783161
5	6	0	1.342363	-0.959650	-0.747877
6	6	0	2.165088	-0.130443	0.001855
7	1	0	2.338522	1.584504	1.287812
8	1	0	-0.087561	2.062468	1.209653
9	1	0	-0.659698	-1.310243	-1.392167
10	1	0	1.757349	-1.793309	-1.298701
11	6	0	-1.999945	0.698840	-0.121274
12	6	0	-2.987478	-0.252923	0.044644
13	1	0	-4.022220	0.077020	-0.025839
14	6	0	-2.470642	2.046920	-0.332551
15	1	0	-3.573675	2.140180	-0.349909
16	1	0	-1.907938	-1.919865	0.428492
17	7	0	-2.840936	-1.542075	0.315307
18	6	0	-3.945927	-2.471287	0.485053
19	1	0	-3.868248	-2.970390	1.452011
20	1	0	-4.883599	-1.918669	0.443372
21	1	0	-3.937359	-3.223668	-0.306113
22	8	0	-1.780184	3.042182	-0.502407
23	7	0	3.603810	-0.411580	0.045505
24	8	0	4.029081	-1.331937	-0.626578
25	8	0	4.303632	0.289406	0.751437

Structure 33c (C_2H_5OH)

Energy (Hartrees): -722.079017254
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.666465	0.946114	0.730780
2	6	0	0.306738	1.204539	0.686249
3	6	0	-0.556655	0.405546	-0.078993
4	6	0	-0.014200	-0.661391	-0.810902
5	6	0	1.343184	-0.939225	-0.773998
6	6	0	2.161284	-0.127066	-0.000332
7	1	0	2.329992	1.557478	1.328067
8	1	0	-0.095379	2.028875	1.261656
9	1	0	-0.655841	-1.268989	-1.439790
10	1	0	1.760940	-1.757892	-1.344943
11	6	0	-2.001602	0.701269	-0.121693
12	6	0	-2.987238	-0.256904	0.044847
13	1	0	-4.023760	0.067740	-0.021565
14	6	0	-2.475957	2.038579	-0.328963
15	1	0	-3.576009	2.138422	-0.342799
16	1	0	-1.893283	-1.914866	0.413408
17	7	0	-2.830321	-1.542400	0.312046
18	6	0	-3.929480	-2.478952	0.489539
19	1	0	-3.841115	-2.977277	1.455817
20	1	0	-4.870584	-1.932092	0.454351
21	1	0	-3.920877	-3.231087	-0.301637
22	8	0	-1.781833	3.040869	-0.501560
23	7	0	3.596066	-0.410428	0.045498
24	8	0	4.014374	-1.378438	-0.561866
25	8	0	4.311268	0.333122	0.690356

Structure 33d (vacuum)

Energy (Hartrees): -722.043792130
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.838072	0.999777	0.545664
2	6	0	0.469034	1.202748	0.487479
3	6	0	-0.376332	0.242213	-0.087802
4	6	0	0.199435	-0.914020	-0.632646
5	6	0	1.566692	-1.136183	-0.573485
6	6	0	2.364769	-0.172175	0.021052
7	1	0	2.499429	1.729103	0.993475
8	1	0	0.048104	2.113309	0.890406
9	1	0	-0.429008	-1.638369	-1.137627
10	1	0	2.018176	-2.025139	-0.992378
11	6	0	-1.841734	0.430055	-0.109307
12	6	0	-2.653020	-0.651238	0.106113
13	1	0	-2.183510	-1.591619	0.389037
14	6	0	-2.415099	1.756302	-0.318062
15	1	0	-3.520529	1.815446	-0.241856
16	1	0	-4.521302	0.072480	-0.263592
17	7	0	-3.994793	-0.744114	0.003923
18	6	0	-4.741586	-1.848236	0.580574
19	1	0	-5.642906	-2.027656	-0.004767
20	1	0	-4.126963	-2.748474	0.545532
21	1	0	-5.022962	-1.657534	1.620262
22	8	0	-1.795165	2.770474	-0.542774
23	7	0	3.820025	-0.394426	0.085925
24	8	0	4.251724	-1.430773	-0.374269
25	8	0	4.498875	0.469396	0.598929

Structure 33d ($CHCl_3$)

Energy (Hartrees): -722.068871684
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.857563	1.023711	0.493640
2	6	0	0.489088	1.227599	0.452664
3	6	0	-0.377471	0.243964	-0.056325
4	6	0	0.187478	-0.946329	-0.545342
5	6	0	1.553183	-1.171734	-0.498835
6	6	0	2.370947	-0.178352	0.021680
7	1	0	2.522073	1.778191	0.893270
8	1	0	0.084072	2.157205	0.827514
9	1	0	-0.449118	-1.699948	-0.993661
10	1	0	1.982692	-2.089164	-0.878953
11	6	0	-1.837468	0.445149	-0.070533
12	6	0	-2.664823	-0.644265	0.135881
13	1	0	-2.206645	-1.586696	0.429637
14	6	0	-2.408907	1.760858	-0.266566
15	1	0	-3.506839	1.825370	-0.148918
16	1	0	-4.509857	0.091127	-0.289266
17	7	0	-3.989375	-0.717251	0.022614
18	6	0	-4.769218	-1.862225	0.464705
19	1	0	-5.566453	-2.058558	-0.251994
20	1	0	-4.120761	-2.736755	0.518882
21	1	0	-5.209449	-1.685626	1.449162
22	8	0	-1.795611	2.782421	-0.529922
23	7	0	3.817792	-0.400620	0.063465
24	8	0	4.241604	-1.482391	-0.296658
25	8	0	4.526398	0.504932	0.458575

Structure 33d (DMSO)

Energy (Hartrees): -722.071538411
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.860046	1.031989	0.474172
2	6	0	0.492200	1.238161	0.432701
3	6	0	-0.380396	0.249568	-0.060370
4	6	0	0.183139	-0.950350	-0.531953
5	6	0	1.548107	-1.176842	-0.485707
6	6	0	2.371335	-0.178012	0.018261
7	1	0	2.523770	1.791161	0.866538
8	1	0	0.091314	2.172460	0.800123
9	1	0	-0.454240	-1.713813	-0.962090
10	1	0	1.970401	-2.103001	-0.852775
11	6	0	-1.837713	0.453332	-0.069475
12	6	0	-2.663958	-0.645077	0.132890
13	1	0	-2.199559	-1.591574	0.401689
14	6	0	-2.413116	1.765725	-0.255512
15	1	0	-3.510575	1.823933	-0.139264
16	1	0	-4.516165	0.099812	-0.230640
17	7	0	-3.984345	-0.714899	0.047793
18	6	0	-4.754345	-1.885032	0.440205
19	1	0	-5.517225	-2.088079	-0.311395
20	1	0	-4.086322	-2.742628	0.514220
21	1	0	-5.238601	-1.724938	1.406177
22	8	0	-1.805118	2.794102	-0.518584
23	7	0	3.814989	-0.402905	0.063071
24	8	0	4.239228	-1.488704	-0.288669
25	8	0	4.527253	0.504669	0.452268

Structure 33d (C_2H_5OH)

Energy (Hartrees): -722.072988548
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.861096	1.026300	0.493938
2	6	0	0.493650	1.233021	0.458701
3	6	0	-0.378765	0.252616	-0.049822
4	6	0	0.180655	-0.942051	-0.537945
5	6	0	1.544911	-1.171204	-0.496848
6	6	0	2.368627	-0.178174	0.018655
7	1	0	2.525790	1.777924	0.899207
8	1	0	0.093565	2.158482	0.849457
9	1	0	-0.459891	-1.697468	-0.977798
10	1	0	1.965430	-2.092384	-0.878381
11	6	0	-1.836276	0.458083	-0.060315
12	6	0	-2.665110	-0.641139	0.150940
13	1	0	-2.201838	-1.579732	0.447890
14	6	0	-2.407749	1.760997	-0.258813
15	1	0	-3.502566	1.830067	-0.141744
16	1	0	-4.506750	0.091285	-0.272921
17	7	0	-3.980625	-0.713665	0.044047
18	6	0	-4.759627	-1.881248	0.429551
19	1	0	-5.436650	-2.154812	-0.380097
20	1	0	-4.082765	-2.711062	0.628629
21	1	0	-5.343152	-1.671302	1.328152
22	8	0	-1.793291	2.790385	-0.535453
23	7	0	3.807947	-0.405157	0.057564
24	8	0	4.231011	-1.499210	-0.271976
25	8	0	4.530917	0.506020	0.419689

Structure 33e (vacuum)

Energy (Hartrees): -722.041527908
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.794867	1.068128	-0.442827
2	6	0	-0.412694	1.156015	-0.447895
3	6	0	0.378546	0.076806	-0.026963
4	6	0	-0.263031	-1.082256	0.429955
5	6	0	-1.646027	-1.189381	0.434694
6	6	0	-2.389681	-0.107812	-0.006795
7	1	0	-2.415150	1.890238	-0.773170
8	1	0	0.060367	2.069030	-0.781282
9	1	0	0.329598	-1.903849	0.815319
10	1	0	-2.148443	-2.079593	0.787998
11	6	0	1.858451	0.141088	-0.078350
12	6	0	2.523816	-0.975431	-0.512649
13	1	0	1.912247	-1.772595	-0.928635
14	6	0	2.530010	1.402767	0.243439
15	1	0	3.611905	1.441850	0.038026
16	1	0	4.075248	-2.157098	-0.963612
17	7	0	3.835974	-1.292240	-0.509241
18	6	0	4.905197	-0.627530	0.211399
19	1	0	5.696620	-1.352143	0.400417
20	1	0	5.328853	0.210454	-0.346877
21	1	0	4.527593	-0.262257	1.169435
22	8	0	1.974828	2.393358	0.664469
23	7	0	-3.860489	-0.206209	-0.000646
24	8	0	-4.490153	0.753500	-0.390992
25	8	0	-4.352870	-1.243015	0.392466

Structure 33e ($CHCl_3$)

Energy (Hartrees): -722.066587372
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.798978	1.074393	-0.433324
2	6	0	-0.417618	1.160915	-0.442057
3	6	0	0.380055	0.079113	-0.031676
4	6	0	-0.262569	-1.087516	0.412097
5	6	0	-1.644505	-1.194940	0.418896
6	6	0	-2.393152	-0.107010	-0.005307
7	1	0	-2.411933	1.903283	-0.761477
8	1	0	0.050884	2.073464	-0.784062
9	1	0	0.327877	-1.918649	0.780004
10	1	0	-2.135571	-2.094971	0.764274
11	6	0	1.856935	0.148351	-0.083725
12	6	0	2.528994	-0.989721	-0.490093
13	1	0	1.920446	-1.792335	-0.900005
14	6	0	2.530257	1.399555	0.217561
15	1	0	3.608114	1.433772	0.003471
16	1	0	4.060580	-2.193775	-0.889551
17	7	0	3.824728	-1.309795	-0.463659
18	6	0	4.912235	-0.615037	0.202779
19	1	0	5.705309	-1.336354	0.395051
20	1	0	5.319141	0.195131	-0.406145
21	1	0	4.562873	-0.210226	1.155477
22	8	0	1.986890	2.406134	0.644933
23	7	0	-3.855694	-0.205308	0.004148
24	8	0	-4.497682	0.770155	-0.333057
25	8	0	-4.356818	-1.259068	0.346704

Structure 33e (DMSO)

Energy (Hartrees): -722.069129458
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.799589	1.078879	-0.421394
2	6	0	-0.418465	1.164291	-0.430490
3	6	0	0.381598	0.076939	-0.035386
4	6	0	-0.262785	-1.097085	0.390003
5	6	0	-1.644526	-1.202321	0.399071
6	6	0	-2.395009	-0.107521	-0.006630
7	1	0	-2.409348	1.913933	-0.740289
8	1	0	0.048799	2.080354	-0.764405
9	1	0	0.325411	-1.938028	0.738848
10	1	0	-2.131558	-2.109590	0.731430
11	6	0	1.856103	0.149536	-0.085520
12	6	0	2.531855	-0.994710	-0.486017
13	1	0	1.927357	-1.799948	-0.896442
14	6	0	2.529860	1.398985	0.207613
15	1	0	3.605313	1.430738	-0.016579
16	1	0	4.059694	-2.201387	-0.867191
17	7	0	3.822348	-1.311518	-0.451089
18	6	0	4.910922	-0.610097	0.207120
19	1	0	5.700789	-1.332313	0.407381
20	1	0	5.318107	0.190166	-0.414374
21	1	0	4.561299	-0.190384	1.153230
22	8	0	1.993869	2.409463	0.642823
23	7	0	-3.855402	-0.203251	0.007633
24	8	0	-4.498572	0.768190	-0.344461
25	8	0	-4.359580	-1.250344	0.369433

Structure 33e (C_2H_5OH)

Energy (Hartrees): -722.070772623
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.799240	1.067651	-0.457323
2	6	0	-0.418600	1.154086	-0.469446
3	6	0	0.380868	0.080208	-0.039770
4	6	0	-0.259036	-1.083519	0.417019
5	6	0	-1.640293	-1.192046	0.427264
6	6	0	-2.390745	-0.108643	-0.008544
7	1	0	-2.410070	1.891252	-0.802949
8	1	0	0.046714	2.058205	-0.838684
9	1	0	0.332907	-1.911608	0.789832
10	1	0	-2.125890	-2.090166	0.785816
11	6	0	1.856551	0.154211	-0.086661
12	6	0	2.532909	-0.990863	-0.492686
13	1	0	1.926549	-1.790447	-0.911576
14	6	0	2.524534	1.392806	0.222513
15	1	0	3.601190	1.435219	0.015246
16	1	0	4.057503	-2.198517	-0.874367
17	7	0	3.819944	-1.310348	-0.454085
18	6	0	4.909670	-0.606166	0.200772
19	1	0	5.704845	-1.324973	0.391366
20	1	0	5.307743	0.198735	-0.420414
21	1	0	4.564830	-0.194464	1.152000
22	8	0	1.977310	2.403698	0.663001
23	7	0	-3.847312	-0.205395	0.008842
24	8	0	-4.496759	0.775917	-0.303997
25	8	0	-4.354858	-1.263287	0.334947

Structure 33f (vacuum)

Energy (Hartrees): -722.044039683
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.871643	1.176519	0.242274
2	6	0	0.487528	1.230062	0.257026
3	6	0	-0.289157	0.087385	0.002392
4	6	0	0.377981	-1.116456	-0.273723
5	6	0	1.761691	-1.193098	-0.269607
6	6	0	2.487818	-0.039468	-0.016056
7	1	0	2.475617	2.050302	0.446789
8	1	0	0.001143	2.166209	0.503465
9	1	0	-0.198597	-1.998753	-0.525994
10	1	0	2.281899	-2.117723	-0.480494
11	6	0	-1.762578	0.149833	0.032872
12	6	0	-2.444594	-0.906607	0.591194
13	1	0	-1.862790	-1.630698	1.158609
14	6	0	-2.399740	1.396327	-0.390310
15	1	0	-1.754482	2.054745	-1.002491
16	1	0	-4.045000	-1.986638	1.095590
17	7	0	-3.746898	-1.210993	0.527270
18	6	0	-4.711722	-0.704714	-0.435047
19	1	0	-5.480552	-1.464684	-0.571315
20	1	0	-5.155429	0.236165	-0.112669
21	1	0	-4.205495	-0.533306	-1.387355
22	8	0	-3.517917	1.762888	-0.090127
23	7	0	3.959166	-0.107148	-0.022150
24	8	0	4.569720	0.921288	0.178288
25	8	0	4.471271	-1.187593	-0.226420

Structure 33f ($CHCl_3$)

Energy (Hartrees): -722.066593886
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.872116	1.185102	-0.209975
2	6	0	-0.489367	1.241090	-0.232149
3	6	0	0.293349	0.092312	-0.013237
4	6	0	-0.372488	-1.122693	0.227727
5	6	0	-1.754890	-1.201144	0.230179
6	6	0	-2.486711	-0.040223	0.017281
7	1	0	-2.469239	2.069511	-0.388530
8	1	0	-0.009186	2.186004	-0.456554
9	1	0	0.202563	-2.015380	0.443837
10	1	0	-2.262383	-2.138410	0.416326
11	6	0	1.763456	0.158112	-0.045898
12	6	0	2.452551	-0.917434	-0.583405
13	1	0	1.885336	-1.643136	-1.162772
14	6	0	2.397293	1.406531	0.343620
15	1	0	1.762197	2.077598	0.950153
16	1	0	4.047574	-2.020711	-1.022489
17	7	0	3.740786	-1.226595	-0.478955
18	6	0	4.691077	-0.706829	0.488979
19	1	0	5.437637	-1.479540	0.669035
20	1	0	5.172544	0.205875	0.139443
21	1	0	4.168229	-0.485125	1.421819
22	8	0	3.517592	1.775426	0.025270
23	7	0	-3.949399	-0.109241	0.031190
24	8	0	-4.572837	0.923733	-0.119756
25	8	0	-4.470742	-1.196008	0.192655

Structure 33f (DMSO)

Energy (Hartrees): -722.067907071
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.870712	1.190134	-0.184236
2	6	0	-0.488459	1.247189	-0.211487
3	6	0	0.297054	0.093360	-0.023131
4	6	0	-0.369172	-1.128102	0.190402
5	6	0	-1.751044	-1.206203	0.197077
6	6	0	-2.485707	-0.040425	0.016536
7	1	0	-2.465222	2.080939	-0.338223
8	1	0	-0.012525	2.198954	-0.415418
9	1	0	0.204105	-2.028000	0.380137
10	1	0	-2.253053	-2.150464	0.362539
11	6	0	1.765071	0.159675	-0.057218
12	6	0	2.456200	-0.927453	-0.577986
13	1	0	1.895365	-1.659033	-1.155813
14	6	0	2.398752	1.410269	0.320351
15	1	0	1.769897	2.079704	0.934825
16	1	0	4.048297	-2.048507	-0.969214
17	7	0	3.738617	-1.237350	-0.450715
18	6	0	4.675265	-0.702835	0.521373
19	1	0	5.419076	-1.472654	0.721919
20	1	0	5.161585	0.204071	0.162787
21	1	0	4.139861	-0.465095	1.443580
22	8	0	3.513481	1.786224	-0.014041
23	7	0	-3.945742	-0.109202	0.037414
24	8	0	-4.572469	0.924602	-0.107500
25	8	0	-4.468637	-1.196789	0.198529

Structure 33f (C_2H_5OH)

Energy (Hartrees): -722.069517806
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.876628	1.192962	-0.195417
2	6	0	-0.495377	1.256133	-0.228415
3	6	0	0.295231	0.106862	-0.034398
4	6	0	-0.362897	-1.117730	0.185084
5	6	0	-1.743821	-1.203202	0.196879
6	6	0	-2.483665	-0.040596	0.014560
7	1	0	-2.475386	2.080118	-0.354595
8	1	0	-0.024395	2.208236	-0.441490
9	1	0	0.216139	-2.013386	0.377996
10	1	0	-2.240439	-2.149011	0.369962
11	6	0	1.763229	0.176346	-0.067481
12	6	0	2.455960	-0.910934	-0.597041
13	1	0	1.899816	-1.623739	-1.202323
14	6	0	2.397561	1.416288	0.309479
15	1	0	1.764691	2.108447	0.890579
16	1	0	4.043770	-2.035564	-0.983400
17	7	0	3.729990	-1.234051	-0.451425
18	6	0	4.656213	-0.728964	0.547952
19	1	0	5.354473	-1.530820	0.784420
20	1	0	5.202838	0.144601	0.193568
21	1	0	4.101537	-0.454022	1.447056
22	8	0	3.535452	1.770640	0.005248
23	7	0	-3.938827	-0.115972	0.045448
24	8	0	-4.576072	0.916169	-0.068428
25	8	0	-4.461383	-1.207769	0.184785

Structure 33g (vacuum)

Energy (Hartrees): -722.047847678
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.716025	-1.108396	-0.475418
2	6	0	0.341011	-0.938845	-0.505596
3	6	0	-0.255345	0.244769	-0.047555
4	6	0	0.573947	1.259768	0.450421
5	6	0	1.951884	1.113817	0.471257
6	6	0	2.500724	-0.073742	0.010839
7	1	0	2.185485	-2.014475	-0.834027
8	1	0	-0.277171	-1.726696	-0.919651
9	1	0	0.131347	2.163649	0.851686
10	1	0	2.600798	1.889705	0.854457
11	6	0	-1.719379	0.411652	-0.093781
12	6	0	-2.275293	1.607937	-0.437976
13	1	0	-1.658642	2.463635	-0.700130
14	6	0	-2.592599	-0.712042	0.215168
15	1	0	-2.118270	-1.650257	0.529488
16	7	0	-3.866014	-0.615033	0.157500
17	6	0	-4.678352	-1.761356	0.511149
18	1	0	-5.333884	-1.497412	1.343592
19	1	0	-5.313452	-2.029160	-0.335756
20	1	0	-4.072800	-2.629811	0.794334
21	8	0	-3.565713	1.839251	-0.515321
22	1	0	-4.029948	0.977561	-0.279843
23	7	0	3.964411	-0.242762	0.041084
24	8	0	4.628054	0.681735	0.459467
25	8	0	4.415412	-1.296430	-0.354808

Structure 33g ($CHCl_3$)

Energy (Hartrees): -722.065187833
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.712566	-1.126964	-0.431194
2	6	0	0.338229	-0.957118	-0.455932
3	6	0	-0.253445	0.244731	-0.036938
4	6	0	0.582054	1.276839	0.418594
5	6	0	1.959025	1.129800	0.434343
6	6	0	2.503692	-0.075527	0.010950
7	1	0	2.168199	-2.050010	-0.764106
8	1	0	-0.281368	-1.762020	-0.832718
9	1	0	0.147532	2.197885	0.788848
10	1	0	2.602902	1.924181	0.787729
11	6	0	-1.716745	0.412011	-0.081492
12	6	0	-2.271303	1.616327	-0.400661
13	1	0	-1.660542	2.481971	-0.643564
14	6	0	-2.593732	-0.718779	0.200627
15	1	0	-2.130978	-1.667087	0.495435
16	7	0	-3.866669	-0.607890	0.138322
17	6	0	-4.695287	-1.753068	0.461123
18	1	0	-5.360559	-1.495673	1.288479
19	1	0	-5.321294	-1.999954	-0.399433
20	1	0	-4.101038	-2.630465	0.737812
21	8	0	-3.566894	1.836944	-0.474893
22	1	0	-4.020977	0.955178	-0.254992
23	7	0	3.960258	-0.244589	0.033645
24	8	0	4.640587	0.701051	0.379747
25	8	0	4.415392	-1.322515	-0.295325

Structure 33g (DMSO)

Energy (Hartrees): -722.064529281
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.712262	-1.133844	-0.415361
2	6	0	0.337777	-0.965335	-0.438272
3	6	0	-0.252876	0.242854	-0.035019
4	6	0	0.583637	1.282199	0.403639
5	6	0	1.960301	1.134858	0.419131
6	6	0	2.504890	-0.076410	0.010981
7	1	0	2.163257	-2.063282	-0.736769
8	1	0	-0.280622	-1.778501	-0.798982
9	1	0	0.152421	2.210504	0.759388
10	1	0	2.601638	1.936506	0.760732
11	6	0	-1.715677	0.410387	-0.078204
12	6	0	-2.269865	1.616524	-0.394690
13	1	0	-1.658868	2.483075	-0.634038
14	6	0	-2.594636	-0.720197	0.198980
15	1	0	-2.137543	-1.672649	0.486663
16	7	0	-3.867783	-0.601847	0.137145
17	6	0	-4.701927	-1.746453	0.451489
18	1	0	-5.370839	-1.490374	1.276420
19	1	0	-5.324114	-1.988586	-0.413360
20	1	0	-4.109701	-2.625029	0.727173
21	8	0	-3.566067	1.832603	-0.469349
22	1	0	-4.012878	0.942296	-0.249526
23	7	0	3.959980	-0.244234	0.032608
24	8	0	4.641250	0.699585	0.386302
25	8	0	4.418386	-1.319551	-0.304703

Structure 33g (C_2H_5OH)

Energy (Hartrees): -722.064407374
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.710013	-1.127275	-0.434226
2	6	0	0.336376	-0.955591	-0.458665
3	6	0	-0.252734	0.247769	-0.038531
4	6	0	0.583499	1.280702	0.415426
5	6	0	1.959576	1.132194	0.430608
6	6	0	2.502039	-0.075616	0.008529
7	1	0	2.160278	-2.052401	-0.769271
8	1	0	-0.283126	-1.761361	-0.833908
9	1	0	0.152295	2.203506	0.785146
10	1	0	2.600661	1.927751	0.786644
11	6	0	-1.715698	0.415389	-0.078474
12	6	0	-2.267788	1.622804	-0.383963
13	1	0	-1.661019	2.493381	-0.617813
14	6	0	-2.591654	-0.720228	0.194040
15	1	0	-2.128429	-1.670262	0.479993
16	7	0	-3.864756	-0.608696	0.132470
17	6	0	-4.688760	-1.761378	0.446125
18	1	0	-5.358132	-1.512736	1.272933
19	1	0	-5.311293	-2.006147	-0.417662
20	1	0	-4.090006	-2.636350	0.718809
21	8	0	-3.569304	1.840005	-0.454304
22	1	0	-4.021530	0.951840	-0.242875
23	7	0	3.952371	-0.246273	0.034053
24	8	0	4.643211	0.712168	0.327482
25	8	0	4.410816	-1.340305	-0.239787

Structure 33h (vacuum)

Energy (Hartrees): -722.023945368
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.639411	-1.108185	-0.431558
2	6	0	0.267409	-0.911299	-0.429017
3	6	0	-0.291260	0.299591	0.003752
4	6	0	0.570315	1.307914	0.457765
5	6	0	1.945237	1.133623	0.448543
6	6	0	2.457069	-0.075919	0.002992
7	1	0	2.080417	-2.034752	-0.773584
8	1	0	-0.382815	-1.698645	-0.792295
9	1	0	0.156824	2.228908	0.851159
10	1	0	2.619540	1.903937	0.797656
11	6	0	-1.759045	0.479375	-0.023597
12	6	0	-2.262643	1.676476	-0.371868
13	1	0	-1.591966	2.482508	-0.659515
14	6	0	-2.592241	-0.684611	0.338638
15	1	0	-2.103458	-1.412340	1.005732
16	7	0	-3.776587	-0.858530	-0.068802
17	6	0	-4.475378	-2.035031	0.403572
18	1	0	-4.806876	-2.619408	-0.457803
19	1	0	-3.866878	-2.670954	1.060777
20	1	0	-5.373132	-1.721085	0.941225
21	8	0	-3.574314	1.958429	-0.391648
22	1	0	-3.710886	2.863800	-0.678845
23	7	0	3.918139	-0.272905	-0.001467
24	8	0	4.610670	0.653290	0.363185
25	8	0	4.338035	-1.348410	-0.371282

Structure 33h ($CHCl_3$)

Energy (Hartrees): -722.047099743
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.633980	-1.117636	-0.404508
2	6	0	0.263052	-0.917502	-0.401708
3	6	0	-0.292774	0.305323	0.004406
4	6	0	0.573522	1.324106	0.430412
5	6	0	1.947065	1.146573	0.420546
6	6	0	2.456083	-0.075935	0.001997
7	1	0	2.061964	-2.056895	-0.728756
8	1	0	-0.384998	-1.715827	-0.744385
9	1	0	0.167906	2.258689	0.799492
10	1	0	2.615498	1.930393	0.751112
11	6	0	-1.760582	0.484380	-0.021934
12	6	0	-2.266286	1.691588	-0.342463
13	1	0	-1.604689	2.512658	-0.605466
14	6	0	-2.590122	-0.686632	0.322435
15	1	0	-2.104663	-1.420047	0.982980
16	7	0	-3.775136	-0.866675	-0.088309
17	6	0	-4.462295	-2.055304	0.378452
18	1	0	-4.792127	-2.638115	-0.485336
19	1	0	-3.843434	-2.688695	1.026825
20	1	0	-5.361121	-1.756623	0.924252
21	8	0	-3.576566	1.967325	-0.363749
22	1	0	-3.707726	2.890992	-0.607521
23	7	0	3.909793	-0.275630	-0.002969
24	8	0	4.616515	0.660652	0.314186
25	8	0	4.335168	-1.367248	-0.325446

Structure 33h (DMSO)

Energy (Hartrees): -722.046289459
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.625134	-1.124499	-0.378558
2	6	0	0.254582	-0.920901	-0.375465
3	6	0	-0.296525	0.313002	0.003267
4	6	0	0.573633	1.339830	0.402522
5	6	0	1.946367	1.157838	0.392759
6	6	0	2.451343	-0.075756	0.001200
7	1	0	2.045563	-2.074052	-0.681843
8	1	0	-0.394583	-1.728545	-0.693752
9	1	0	0.174938	2.286080	0.748349
10	1	0	2.614321	1.950557	0.702469
11	6	0	-1.764586	0.493755	-0.020137
12	6	0	-2.269333	1.704711	-0.329375
13	1	0	-1.608717	2.527351	-0.588993
14	6	0	-2.589004	-0.680483	0.327687
15	1	0	-2.113207	-1.391246	1.018147
16	7	0	-3.757339	-0.892797	-0.116716
17	6	0	-4.436446	-2.084117	0.360704
18	1	0	-4.738724	-2.690306	-0.497219
19	1	0	-3.820494	-2.693063	1.033882
20	1	0	-5.351029	-1.789047	0.882459
21	8	0	-3.579645	1.985455	-0.339167
22	1	0	-3.702567	2.917573	-0.557173
23	7	0	3.903508	-0.279103	-0.004248
24	8	0	4.614522	0.656254	0.309999
25	8	0	4.327665	-1.373246	-0.324232

Structure 33h (C_2H_5OH)

Energy (Hartrees): -722.051634712
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.632323	-1.119507	-0.404721
2	6	0	0.261972	-0.918957	-0.402529
3	6	0	-0.293511	0.304543	0.003920
4	6	0	0.572344	1.324533	0.429972
5	6	0	1.945232	1.146868	0.421207
6	6	0	2.453919	-0.076962	0.003219
7	1	0	2.055847	-2.060106	-0.731230
8	1	0	-0.384074	-1.718905	-0.745527
9	1	0	0.168952	2.261031	0.796447
10	1	0	2.609857	1.933320	0.753605
11	6	0	-1.761050	0.485112	-0.023363
12	6	0	-2.260264	1.699258	-0.333598
13	1	0	-1.600257	2.525313	-0.582510
14	6	0	-2.589043	-0.689268	0.309440
15	1	0	-2.093417	-1.438205	0.942617
16	7	0	-3.784632	-0.862205	-0.079687
17	6	0	-4.455021	-2.067420	0.375359
18	1	0	-4.789608	-2.638971	-0.494184
19	1	0	-3.820692	-2.704655	1.003277
20	1	0	-5.349781	-1.789793	0.938648
21	8	0	-3.570109	1.978461	-0.362889
22	1	0	-3.700072	2.908146	-0.588239
23	7	0	3.902078	-0.275711	-0.002269
24	8	0	4.616258	0.662679	0.298845
25	8	0	4.333815	-1.371260	-0.310037

Structure 33i (vacuum)

Energy (Hartrees): -722.030749054
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.506187	-1.181992	-0.467329
2	6	0	0.138334	-0.956718	-0.467264
3	6	0	-0.399510	0.246583	0.010176
4	6	0	0.475653	1.228551	0.494470
5	6	0	1.845414	1.019188	0.500125
6	6	0	2.337556	-0.185279	0.018986
7	1	0	1.932016	-2.103092	-0.841464
8	1	0	-0.522225	-1.718639	-0.864473
9	1	0	0.077025	2.159672	0.873296
10	1	0	2.532367	1.765693	0.875117
11	6	0	-1.863350	0.441670	0.000881
12	6	0	-2.464090	1.616565	-0.243947
13	1	0	-3.548376	1.669151	-0.242072
14	6	0	-2.730907	-0.727837	0.267948
15	1	0	-2.242288	-1.569614	0.780131
16	7	0	-3.957471	-0.766880	-0.039794
17	6	0	-4.710989	-1.944476	0.338142
18	1	0	-5.166880	-2.378173	-0.554658
19	1	0	-4.101120	-2.707752	0.838915
20	1	0	-5.526218	-1.649614	1.003165
21	8	0	-1.786647	2.749634	-0.521608
22	1	0	-2.400097	3.463563	-0.709293
23	7	0	3.794685	-0.413239	0.023806
24	8	0	4.502521	0.484687	0.427273
25	8	0	4.196565	-1.485307	-0.375649

Structure 33i ($CHCl_3$)

Energy (Hartrees): -722.051620983
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.494302	-1.185141	-0.457837
2	6	0	0.127908	-0.954436	-0.454369
3	6	0	-0.403843	0.255161	0.017703
4	6	0	0.478506	1.236839	0.493925
5	6	0	1.847082	1.023581	0.494638
6	6	0	2.332638	-0.186691	0.017148
7	1	0	1.906045	-2.113941	-0.829700
8	1	0	-0.534981	-1.718802	-0.843006
9	1	0	0.088877	2.170181	0.877434
10	1	0	2.530438	1.775021	0.867026
11	6	0	-1.867056	0.454346	0.014063
12	6	0	-2.462076	1.636573	-0.226887
13	1	0	-3.544760	1.712685	-0.210260
14	6	0	-2.729902	-0.716430	0.283307
15	1	0	-2.252907	-1.535306	0.838781
16	7	0	-3.943700	-0.787898	-0.073995
17	6	0	-4.691063	-1.966843	0.319841
18	1	0	-5.114544	-2.436329	-0.571483
19	1	0	-4.084429	-2.703466	0.861548
20	1	0	-5.530768	-1.665987	0.951986
21	8	0	-1.780178	2.756535	-0.518993
22	1	0	-2.392478	3.483254	-0.683491
23	7	0	3.782345	-0.418936	0.017227
24	8	0	4.506446	0.488356	0.376049
25	8	0	4.186232	-1.507544	-0.340888

Structure 33i (DMSO)

Energy (Hartrees): -722.049691430
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.490395	-1.190232	-0.443467
2	6	0	0.124033	-0.958749	-0.438136
3	6	0	-0.404467	0.258102	0.019069
4	6	0	0.480104	1.244212	0.482482
5	6	0	1.848521	1.029954	0.481431
6	6	0	2.331424	-0.186613	0.016371
7	1	0	1.896122	-2.125429	-0.805812
8	1	0	-0.539742	-1.730280	-0.811208
9	1	0	0.094617	2.181564	0.860261
10	1	0	2.530243	1.786924	0.845690
11	6	0	-1.867281	0.458444	0.018875
12	6	0	-2.465036	1.641733	-0.212772
13	1	0	-3.547169	1.722138	-0.177153
14	6	0	-2.727897	-0.712720	0.293486
15	1	0	-2.262050	-1.514649	0.881306
16	7	0	-3.930565	-0.801753	-0.098301
17	6	0	-4.682818	-1.975207	0.307320
18	1	0	-5.069296	-2.477908	-0.582961
19	1	0	-4.088742	-2.685838	0.894802
20	1	0	-5.547201	-1.661195	0.898780
21	8	0	-1.787407	2.761077	-0.516587
22	1	0	-2.405189	3.492574	-0.639634
23	7	0	3.780187	-0.419922	0.013941
24	8	0	4.507908	0.492544	0.355380
25	8	0	4.183149	-1.514835	-0.328980

Structure 33i (C_2H_5OH)

Energy (Hartrees): -722.053924984
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.485162	-1.183702	-0.457635
2	6	0	0.120065	-0.948561	-0.452705
3	6	0	-0.406787	0.264457	0.017811
4	6	0	0.478966	1.243913	0.494180
5	6	0	1.846584	1.027236	0.493112
6	6	0	2.326777	-0.185997	0.015486
7	1	0	1.889587	-2.115348	-0.830712
8	1	0	-0.545501	-1.712986	-0.837308
9	1	0	0.094074	2.175899	0.885986
10	1	0	2.529392	1.777526	0.869382
11	6	0	-1.869254	0.464779	0.018884
12	6	0	-2.464776	1.649854	-0.213648
13	1	0	-3.545883	1.737822	-0.179158
14	6	0	-2.725335	-0.707590	0.295494
15	1	0	-2.258166	-1.499973	0.895128
16	7	0	-3.924708	-0.812529	-0.104252
17	6	0	-4.662847	-1.991756	0.313714
18	1	0	-5.035362	-2.514410	-0.570835
19	1	0	-4.062972	-2.684464	0.916005
20	1	0	-5.536358	-1.683382	0.894240
21	8	0	-1.784268	2.766318	-0.517866
22	1	0	-2.394261	3.503861	-0.643367
23	7	0	3.770407	-0.422683	0.014504
24	8	0	4.506218	0.488878	0.343405
25	8	0	4.174828	-1.521929	-0.315448

Structure 33j (vacuum)

Energy (Hartrees): -722.031586510
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.319057	-0.995677	-0.703592
2	6	0	-0.044018	-0.743851	-0.722598
3	6	0	-0.574605	0.363754	-0.052267
4	6	0	0.287479	1.210239	0.652579
5	6	0	1.652110	0.967173	0.687700
6	6	0	2.143143	-0.133373	0.003381
7	1	0	1.747599	-1.843632	-1.220029
8	1	0	-0.705925	-1.412886	-1.253847
9	1	0	-0.115836	2.065344	1.178881
10	1	0	2.330827	1.608528	1.232924
11	6	0	-2.029036	0.641959	-0.091965
12	6	0	-2.525240	1.874927	-0.284890
13	1	0	-3.599586	2.037304	-0.310606
14	6	0	-3.020435	-0.430325	0.082792
15	1	0	-4.071347	-0.103016	0.032652
16	7	0	-2.719369	-1.640631	0.289732
17	6	0	-3.803664	-2.583991	0.464931
18	1	0	-3.714175	-3.375650	-0.282559
19	1	0	-3.707352	-3.056836	1.444941
20	1	0	-4.798217	-2.124884	0.383577
21	8	0	-1.749209	2.964967	-0.463192
22	1	0	-2.290187	3.734353	-0.653661
23	7	0	3.594634	-0.398917	0.032015
24	8	0	4.293191	0.363491	0.665596
25	8	0	4.002091	-1.363056	-0.580021

Structure 33j ($CHCl_3$)

Energy (Hartrees): -722.054000505
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.326554	-0.965748	-0.750150
2	6	0	-0.036072	-0.713801	-0.770522
3	6	0	-0.577112	0.360432	-0.053541
4	6	0	0.277040	1.173347	0.700681
5	6	0	1.641766	0.931746	0.738265
6	6	0	2.142297	-0.135076	0.006068
7	1	0	1.753497	-1.788016	-1.308471
8	1	0	-0.687043	-1.353276	-1.351439
9	1	0	-0.132307	1.998755	1.269181
10	1	0	2.305830	1.553128	1.323952
11	6	0	-2.030721	0.639927	-0.099419
12	6	0	-2.518577	1.878385	-0.297552
13	1	0	-3.590740	2.053189	-0.331229
14	6	0	-3.022003	-0.429164	0.071616
15	1	0	-4.070262	-0.108411	-0.015804
16	7	0	-2.722188	-1.635498	0.318888
17	6	0	-3.814312	-2.575618	0.480186
18	1	0	-3.715330	-3.373420	-0.260730
19	1	0	-3.740993	-3.043974	1.465031
20	1	0	-4.804153	-2.113065	0.375505
21	8	0	-1.732290	2.952956	-0.480203
22	1	0	-2.271389	3.736092	-0.640875
23	7	0	3.588442	-0.396109	0.033518
24	8	0	4.286485	0.325632	0.717686
25	8	0	4.015300	-1.319379	-0.630703

Structure 33j (DMSO)

Energy (Hartrees): -722.053332039
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.333142	-0.934036	-0.787863
2	6	0	-0.029954	-0.684245	-0.809586
3	6	0	-0.579008	0.364017	-0.060240
4	6	0	0.267566	1.155467	0.724786
5	6	0	1.632782	0.915211	0.765114
6	6	0	2.140886	-0.127612	0.003537
7	1	0	1.763174	-1.736893	-1.371703
8	1	0	-0.674702	-1.303961	-1.419460
9	1	0	-0.147425	1.961152	1.317378
10	1	0	2.288392	1.521427	1.376042
11	6	0	-2.034124	0.635848	-0.101560
12	6	0	-2.530839	1.871751	-0.296055
13	1	0	-3.604177	2.040339	-0.322680
14	6	0	-3.016358	-0.439744	0.072867
15	1	0	-4.066272	-0.130081	-0.021199
16	7	0	-2.704459	-1.642379	0.330798
17	6	0	-3.790301	-2.592378	0.490425
18	1	0	-3.681998	-3.391503	-0.248141
19	1	0	-3.718462	-3.057364	1.477260
20	1	0	-4.782284	-2.137262	0.379399
21	8	0	-1.750342	2.948075	-0.487928
22	1	0	-2.299502	3.729234	-0.627901
23	7	0	3.586216	-0.389038	0.036705
24	8	0	4.272546	0.282595	0.782281
25	8	0	4.026322	-1.263275	-0.684361

Structure 33j (C_2H_5OH)

Energy (Hartrees): -722.057174225
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.333900	-0.940378	-0.786563
2	6	0	-0.027947	-0.686377	-0.809776
3	6	0	-0.575733	0.361053	-0.057901
4	6	0	0.272211	1.149834	0.729279
5	6	0	1.637069	0.910210	0.766447
6	6	0	2.142739	-0.133943	0.004392
7	1	0	1.762331	-1.742541	-1.372705
8	1	0	-0.673116	-1.301589	-1.423794
9	1	0	-0.141955	1.951748	1.327962
10	1	0	2.292566	1.515074	1.378824
11	6	0	-2.029611	0.637111	-0.101376
12	6	0	-2.517724	1.877122	-0.296771
13	1	0	-3.588728	2.057356	-0.329762
14	6	0	-3.018798	-0.431816	0.067457
15	1	0	-4.065108	-0.112996	-0.035805
16	7	0	-2.721755	-1.637064	0.333163
17	6	0	-3.823577	-2.570846	0.484815
18	1	0	-3.725728	-3.369424	-0.255679
19	1	0	-3.764397	-3.040927	1.469834
20	1	0	-4.808015	-2.100732	0.370985
21	8	0	-1.730247	2.948665	-0.482285
22	1	0	-2.268408	3.735429	-0.633742
23	7	0	3.583793	-0.395875	0.036224
24	8	0	4.290843	0.343142	0.694862
25	8	0	4.013292	-1.340887	-0.597809

Structure 33k (vacuum)

Energy (Hartrees): -722.031200691
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.496241	0.908273	-0.693896
2	6	0	-0.124004	0.719357	-0.709327
3	6	0	0.454901	-0.377048	-0.057738
4	6	0	-0.375055	-1.267488	0.632462
5	6	0	-1.751908	-1.095756	0.653433
6	6	0	-2.287579	-0.007349	-0.014574
7	1	0	-1.959980	1.745876	-1.196908
8	1	0	0.510133	1.425232	-1.226569
9	1	0	0.065954	-2.090051	1.183134
10	1	0	-2.404041	-1.774257	1.186321
11	6	0	1.916806	-0.610022	-0.113377
12	6	0	2.367572	-1.851535	-0.356665
13	1	0	1.681657	-2.670917	-0.551599
14	6	0	2.879749	0.484400	0.089796
15	1	0	3.936501	0.201672	0.011935
16	7	0	2.520639	1.671557	0.346928
17	6	0	3.564019	2.657206	0.540416
18	1	0	3.434574	3.461258	-0.188017
19	1	0	3.449688	3.102854	1.531198
20	1	0	4.576552	2.244260	0.444570
21	8	0	3.688206	-2.150893	-0.382385
22	1	0	3.820239	-3.055354	-0.672898
23	7	0	-3.749583	0.189846	0.007007
24	8	0	-4.418323	-0.630969	0.598672
25	8	0	-4.194663	1.159286	-0.569023

Structure 33k ($CHCl_3$)

Energy (Hartrees): -722.052752164
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.501248	0.905671	-0.706203
2	6	0	-0.129889	0.714277	-0.725861
3	6	0	0.453181	-0.376592	-0.065479
4	6	0	-0.375210	-1.263116	0.634072
5	6	0	-1.751327	-1.090851	0.658619
6	6	0	-2.290340	-0.005107	-0.014627
7	1	0	-1.958479	1.740969	-1.219609
8	1	0	0.497351	1.411153	-1.264966
9	1	0	0.065272	-2.085921	1.184895
10	1	0	-2.393050	-1.772149	1.201156
11	6	0	1.914539	-0.606724	-0.123056
12	6	0	2.365898	-1.855378	-0.346799
13	1	0	1.683475	-2.682345	-0.521681
14	6	0	2.876205	0.489237	0.061799
15	1	0	3.929706	0.221958	-0.079444
16	7	0	2.530540	1.667701	0.380187
17	6	0	3.586067	2.648054	0.546732
18	1	0	3.427786	3.469205	-0.157527
19	1	0	3.521257	3.073180	1.551578
20	1	0	4.590773	2.233770	0.395313
21	8	0	3.680045	-2.151615	-0.379850
22	1	0	3.805088	-3.072593	-0.635022
23	7	0	-3.745633	0.192432	0.011093
24	8	0	-4.423431	-0.628966	0.596464
25	8	0	-4.200462	1.166207	-0.555218

Structure 33k (DMSO)

Energy (Hartrees): -722.051728935
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.501250	0.892885	-0.722744
2	6	0	-0.130212	0.700800	-0.744307
3	6	0	0.455510	-0.383742	-0.074754
4	6	0	-0.370476	-1.267690	0.630917
5	6	0	-1.746531	-1.093643	0.658688
6	6	0	-2.287868	-0.011130	-0.018657
7	1	0	-1.956850	1.723719	-1.244777
8	1	0	0.493792	1.391098	-1.296730
9	1	0	0.069873	-2.092205	1.179543
10	1	0	-2.383562	-1.774116	1.207843
11	6	0	1.917819	-0.605149	-0.131783
12	6	0	2.377371	-1.854382	-0.339058
13	1	0	1.699680	-2.688730	-0.496541
14	6	0	2.867701	0.502652	0.038333
15	1	0	3.917970	0.265044	-0.163594
16	7	0	2.516515	1.663550	0.414076
17	6	0	3.561259	2.660581	0.558338
18	1	0	3.327624	3.520294	-0.075539
19	1	0	3.572305	3.019298	1.591071
20	1	0	4.557835	2.283495	0.298192
21	8	0	3.692309	-2.139726	-0.372116
22	1	0	3.819891	-3.067189	-0.605244
23	7	0	-3.741533	0.190666	0.014985
24	8	0	-4.417510	-0.613135	0.627903
25	8	0	-4.200220	1.151948	-0.571725

Structure 33k (C_2H_5OH)

Energy (Hartrees): -722.055500279
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.503455	0.892307	-0.727317
2	6	0	-0.133111	0.699277	-0.747488
3	6	0	0.452739	-0.381452	-0.071244
4	6	0	-0.373489	-1.261470	0.639747
5	6	0	-1.749050	-1.087573	0.666582
6	6	0	-2.289709	-0.008345	-0.017437
7	1	0	-1.958388	1.719693	-1.255717
8	1	0	0.490755	1.384969	-1.305729
9	1	0	0.067001	-2.081964	1.194232
10	1	0	-2.385794	-1.764499	1.220610
11	6	0	1.914207	-0.604602	-0.129291
12	6	0	2.371406	-1.854803	-0.340185
13	1	0	1.696293	-2.690728	-0.498901
14	6	0	2.867786	0.500226	0.036508
15	1	0	3.914497	0.260230	-0.180813
16	7	0	2.526684	1.660553	0.424499
17	6	0	3.580082	2.651082	0.554510
18	1	0	3.342333	3.513282	-0.074241
19	1	0	3.610403	3.009126	1.586929
20	1	0	4.570277	2.269264	0.277998
21	8	0	3.685730	-2.142440	-0.377644
22	1	0	3.817287	-3.068596	-0.614090
23	7	0	-3.739039	0.192488	0.013913
24	8	0	-4.422184	-0.613433	0.617772
25	8	0	-4.201373	1.157131	-0.565812

Structure 33l (vacuum)

Energy (Hartrees): -722.029841016
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.490491	0.893809	-0.715019
2	6	0	-0.118847	0.702503	-0.733883
3	6	0	0.462194	-0.382409	-0.065982
4	6	0	-0.364486	-1.261539	0.641224
5	6	0	-1.741261	-1.087615	0.666101
6	6	0	-2.279020	-0.009341	-0.015985
7	1	0	-1.956124	1.722621	-1.230712
8	1	0	0.511489	1.398150	-1.269893
9	1	0	0.078234	-2.078601	1.198640
10	1	0	-2.391178	-1.757672	1.212252
11	6	0	1.925913	-0.618459	-0.122883
12	6	0	2.360305	-1.870902	-0.368571
13	1	0	1.659487	-2.673381	-0.568717
14	6	0	2.865998	0.491064	0.077899
15	1	0	3.938721	0.266132	-0.044256
16	7	0	2.505064	1.667274	0.373787
17	6	0	3.534004	2.669389	0.549575
18	1	0	3.370204	3.478382	-0.166142
19	1	0	3.439337	3.101781	1.547961
20	1	0	4.551879	2.277026	0.420894
21	8	0	3.627268	-2.319343	-0.426541
22	1	0	4.255519	-1.629323	-0.195217
23	7	0	-3.740719	0.191520	0.011158
24	8	0	-4.406842	-0.614579	0.625006
25	8	0	-4.187155	1.149461	-0.582749

Structure 33l ($CHCl_3$)

Energy (Hartrees): -722.050877629
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.493247	0.895399	-0.719209
2	6	0	-0.122592	0.701622	-0.741506
3	6	0	0.461184	-0.383719	-0.073152
4	6	0	-0.365017	-1.263045	0.636796
5	6	0	-1.741132	-1.088315	0.664665
6	6	0	-2.280845	-0.008179	-0.016288
7	1	0	-1.951181	1.726300	-1.239029
8	1	0	0.503241	1.393335	-1.289530
9	1	0	0.076148	-2.083056	1.191217
10	1	0	-2.381638	-1.764230	1.215304
11	6	0	1.924031	-0.615811	-0.136396
12	6	0	2.360091	-1.873673	-0.356751
13	1	0	1.662199	-2.684847	-0.535053
14	6	0	2.865314	0.498863	0.031991
15	1	0	3.920938	0.299858	-0.202948
16	7	0	2.512291	1.651571	0.424254
17	6	0	3.541752	2.663445	0.553660
18	1	0	3.279703	3.523033	-0.068481
19	1	0	3.565852	3.014908	1.588253
20	1	0	4.540454	2.306915	0.270711
21	8	0	3.627810	-2.313051	-0.409548
22	1	0	4.260392	-1.620448	-0.180980
23	7	0	-3.735947	0.192626	0.013699
24	8	0	-4.412585	-0.620002	0.612164
25	8	0	-4.191195	1.160470	-0.562366

Structure 33l (DMSO)

Energy (Hartrees): -722.050281068
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.493872	0.876489	-0.743992
2	6	0	-0.123078	0.683593	-0.766153
3	6	0	0.463766	-0.388277	-0.078077
4	6	0	-0.359049	-1.257863	0.647636
5	6	0	-1.735064	-1.081485	0.678650
6	6	0	-2.277988	-0.012871	-0.018487
7	1	0	-1.951310	1.696556	-1.281231
8	1	0	0.499579	1.363264	-1.333529
9	1	0	0.083310	-2.073146	1.208340
10	1	0	-2.370299	-1.750554	1.243683
11	6	0	1.927487	-0.613955	-0.138504
12	6	0	2.366810	-1.871527	-0.354979
13	1	0	1.669401	-2.685836	-0.521445
14	6	0	2.861361	0.506217	0.033682
15	1	0	3.919282	0.319867	-0.197697
16	7	0	2.497371	1.653930	0.434056
17	6	0	3.521394	2.672718	0.569748
18	1	0	3.255515	3.532799	-0.050566
19	1	0	3.542208	3.020518	1.605881
20	1	0	4.521282	2.321809	0.286980
21	8	0	3.634945	-2.304620	-0.417164
22	1	0	4.266000	-1.600851	-0.215141
23	7	0	-3.731844	0.190127	0.015982
24	8	0	-4.402588	-0.581256	0.674417
25	8	0	-4.195389	1.119493	-0.616339

Structure 33l (C_2H_5OH)

Energy (Hartrees): -722.053386335
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.496369	0.889262	-0.732567
2	6	0	-0.126494	0.694026	-0.758380
3	6	0	0.460315	-0.386802	-0.083533
4	6	0	-0.364046	-1.265198	0.631025
5	6	0	-1.739458	-1.089899	0.662684
6	6	0	-2.281073	-0.010331	-0.019417
7	1	0	-1.952137	1.717505	-1.258878
8	1	0	0.495810	1.379542	-1.318913
9	1	0	0.077321	-2.085845	1.184497
10	1	0	-2.374700	-1.766021	1.219392
11	6	0	1.923344	-0.612639	-0.144254
12	6	0	2.361883	-1.871961	-0.352730
13	1	0	1.666168	-2.686426	-0.525621
14	6	0	2.861183	0.506595	0.014805
15	1	0	3.906172	0.322285	-0.267870
16	7	0	2.512019	1.645338	0.453860
17	6	0	3.541025	2.663350	0.559230
18	1	0	3.255032	3.526428	-0.047740
19	1	0	3.598279	3.007946	1.594889
20	1	0	4.530566	2.313957	0.240887
21	8	0	3.631815	-2.307163	-0.396795
22	1	0	4.265680	-1.616189	-0.162912
23	7	0	-3.730055	0.193136	0.019129
24	8	0	-4.411687	-0.612794	0.624513
25	8	0	-4.193103	1.159842	-0.556448

Structure 34a (vacuum)

Energy (Hartrees): -536.978895452
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.830055	0.975128	0.671377
2	6	0	-3.219463	0.977588	0.684548
3	6	0	-3.931284	-0.020250	0.025805
4	6	0	-3.235326	-1.013491	-0.655723
5	6	0	-1.845832	-1.003606	-0.684701
6	6	0	-1.113327	-0.016642	-0.012168
7	1	0	-1.290431	1.738280	1.221681
8	1	0	-3.748388	1.755095	1.224082
9	1	0	-5.014415	-0.021006	0.039725
10	1	0	-3.776469	-1.789365	-1.185441
11	1	0	-1.317139	-1.755760	-1.260171
12	6	0	0.365818	-0.017373	-0.016815
13	6	0	1.045853	-1.200173	0.114784
14	6	0	1.070052	1.241772	-0.158353
15	1	0	0.480953	-2.119704	0.254292
16	1	0	0.435569	2.129438	-0.293085
17	1	0	2.907133	-0.477639	0.020108
18	7	0	2.345779	1.362593	-0.161953
19	7	0	2.378998	-1.347449	0.097589
20	6	0	2.893079	2.691807	-0.340738
21	1	0	3.537512	2.707763	-1.223609
22	1	0	2.118026	3.460526	-0.458214
23	1	0	3.516448	2.950865	0.519198
24	6	0	3.041135	-2.596272	0.400924
25	1	0	2.344752	-3.422173	0.247601
26	1	0	3.893003	-2.741930	-0.264915
27	1	0	3.396105	-2.631340	1.435661

Structure 34a ($CHCl_3$)

Energy (Hartrees): -536.996069614
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.831439	1.005400	0.625665
2	6	0	-3.221916	1.005778	0.637756
3	6	0	-3.933201	-0.022240	0.024709
4	6	0	-3.233483	-1.044851	-0.610532
5	6	0	-1.843365	-1.034223	-0.639825
6	6	0	-1.109973	-0.015446	-0.012703
7	1	0	-1.297305	1.796604	1.141062
8	1	0	-3.751187	1.806736	1.142581
9	1	0	-5.016871	-0.024452	0.038518
10	1	0	-3.772008	-1.846219	-1.104836
11	1	0	-1.316612	-1.816500	-1.176187
12	6	0	0.369784	-0.014365	-0.016909
13	6	0	1.049987	-1.203136	0.113088
14	6	0	1.071022	1.246082	-0.155614
15	1	0	0.487584	-2.124987	0.246028
16	1	0	0.438220	2.132572	-0.299006
17	1	0	2.919876	-0.493248	0.029771
18	7	0	2.348178	1.373162	-0.148043
19	7	0	2.378370	-1.353501	0.104637
20	6	0	2.886691	2.707840	-0.327303
21	1	0	3.527454	2.731094	-1.213505
22	1	0	2.106802	3.472027	-0.438539

23	1	0	3.514140	2.969609	0.529464
24	6	0	3.038327	-2.613952	0.375942
25	1	0	2.323588	-3.428766	0.253943
26	1	0	3.860031	-2.765904	-0.325497
27	1	0	3.435845	-2.647500	1.394398

Structure 34a (DMSO)

Energy (Hartrees): -536.991996214
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.832586	1.020907	0.600279
2	6	0	-3.223701	1.020771	0.610176
3	6	0	-3.934313	-0.022759	0.022455
4	6	0	-3.232457	-1.061435	-0.584942
5	6	0	-1.841960	-1.051421	-0.612870
6	6	0	-1.108899	-0.015541	-0.011675
7	1	0	-1.302035	1.826773	1.096371
8	1	0	-3.753424	1.834228	1.094379
9	1	0	-5.018133	-0.025197	0.034774
10	1	0	-3.769452	-1.876207	-1.058792
11	1	0	-1.316867	-1.850365	-1.126022
12	6	0	0.370981	-0.012690	-0.015250
13	6	0	1.052350	-1.204165	0.111436
14	6	0	1.070544	1.248664	-0.151879
15	1	0	0.491208	-2.127438	0.238369
16	1	0	0.439411	2.135507	-0.297832
17	1	0	2.926088	-0.498287	0.032379
18	7	0	2.348488	1.376895	-0.139282
19	7	0	2.378712	-1.354662	0.105633
20	6	0	2.884784	2.713527	-0.320343
21	1	0	3.527051	2.736626	-1.205669
22	1	0	2.102985	3.475079	-0.433712
23	1	0	3.511205	2.978314	0.536387
24	6	0	3.037765	-2.620418	0.361841
25	1	0	2.320167	-3.431809	0.236379
26	1	0	3.856263	-2.764894	-0.344650
27	1	0	3.440080	-2.660593	1.377805

Structure 34a (C_2H_5OH)

Energy (Hartrees): -536.995006557
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.829931	1.012890	0.613822
2	6	0	-3.220982	1.012637	0.624730
3	6	0	-3.931937	-0.023101	0.023680
4	6	0	-3.230723	-1.053603	-0.598087
5	6	0	-1.840217	-1.043116	-0.626710
6	6	0	-1.107011	-0.015501	-0.012127
7	1	0	-1.298516	1.812007	1.120078
8	1	0	-3.750555	1.819813	1.119738
9	1	0	-5.015870	-0.025590	0.036618
10	1	0	-3.768170	-1.862063	-1.082393
11	1	0	-1.314805	-1.834640	-1.151105
12	6	0	0.373113	-0.013384	-0.016776
13	6	0	1.052103	-1.205419	0.108876

14	6	0	1.071765	1.248584	-0.151452
15	1	0	0.489213	-2.127286	0.238451
16	1	0	0.437905	2.134795	-0.288699
17	1	0	2.927966	-0.504688	0.030097
18	7	0	2.349751	1.379815	-0.146902
19	7	0	2.378912	-1.359486	0.099912
20	6	0	2.877418	2.721244	-0.322018
21	1	0	3.508550	2.756513	-1.214858
22	1	0	2.091302	3.480463	-0.418379
23	1	0	3.513113	2.981241	0.529234
24	6	0	3.033022	-2.624713	0.372334
25	1	0	2.318043	-3.436791	0.236474
26	1	0	3.863603	-2.772218	-0.319220
27	1	0	3.417861	-2.662976	1.395261

Structure 34b (vacuum)

Energy (Hartrees): -536.970529211
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.320792	-1.291246	0.748423
2	6	0	-2.687567	-1.538279	0.790718
3	6	0	-3.563985	-0.769087	0.031137
4	6	0	-3.058065	0.241889	-0.779472
5	6	0	-1.689220	0.482567	-0.828202
6	6	0	-0.795156	-0.273740	-0.058472
7	1	0	-0.648429	-1.882555	1.361184
8	1	0	-3.070816	-2.327930	1.426666
9	1	0	-4.629913	-0.959378	0.066709
10	1	0	-3.729152	0.836266	-1.389130
11	1	0	-1.298652	1.243545	-1.495899
12	6	0	0.662418	-0.025318	-0.099291
13	6	0	1.206620	1.215268	-0.036899
14	6	0	1.565478	-1.181903	-0.185093
15	1	0	1.071015	-2.143952	-0.391278
16	1	0	2.290700	1.285022	-0.076885
17	7	0	2.825813	-1.115313	-0.051723
18	7	0	0.554408	2.406192	0.064971
19	1	0	-0.427813	2.361376	0.300480
20	6	0	1.263869	3.602184	0.481564
21	1	0	2.216590	3.653194	-0.046895
22	1	0	0.681499	4.483107	0.211702
23	1	0	1.461271	3.624336	1.559008
24	6	0	3.583695	-2.337382	-0.209812
25	1	0	4.307650	-2.215406	-1.019857
26	1	0	4.155151	-2.531103	0.701896
27	1	0	2.955574	-3.212398	-0.428039

Structure 34b ($CHCl_3$)

Energy (Hartrees): -536.989413282
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.329052	-1.304276	0.720065
2	6	0	-2.697578	-1.548274	0.754045
3	6	0	-3.572714	-0.747929	0.024375

4	6	0	-3.062528	0.291570	-0.748204
5	6	0	-1.692462	0.529809	-0.788803
6	6	0	-0.798384	-0.258596	-0.049464
7	1	0	-0.660761	-1.923522	1.309970
8	1	0	-3.082051	-2.360935	1.360462
9	1	0	-4.639708	-0.936095	0.053103
10	1	0	-3.731333	0.911953	-1.334746
11	1	0	-1.306336	1.317312	-1.427742
12	6	0	0.662336	-0.021600	-0.088218
13	6	0	1.222998	1.218855	-0.024331
14	6	0	1.545280	-1.188384	-0.186753
15	1	0	1.037340	-2.132789	-0.430875
16	1	0	2.306849	1.281694	-0.079626
17	7	0	2.807910	-1.163935	-0.025939
18	7	0	0.597496	2.411149	0.096924
19	1	0	-0.386873	2.401419	0.330383
20	6	0	1.331982	3.616930	0.441955
21	1	0	2.267579	3.641275	-0.118055
22	1	0	0.743166	4.490358	0.162266
23	1	0	1.559650	3.671033	1.511623
24	6	0	3.528489	-2.405884	-0.223635
25	1	0	4.253287	-2.285665	-1.034095
26	1	0	4.098546	-2.646429	0.678320
27	1	0	2.872595	-3.253440	-0.464078

Structure 34b (DMSO)

Energy (Hartrees): -536.985840554
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.333011	-1.312863	0.705422
2	6	0	-2.702426	-1.555420	0.732924
3	6	0	-3.575655	-0.739879	0.017276
4	6	0	-3.062153	0.313975	-0.734136
5	6	0	-1.691539	0.551326	-0.768141
6	6	0	-0.799032	-0.252879	-0.043146
7	1	0	-0.667542	-1.946376	1.283457
8	1	0	-3.088732	-2.379426	1.322897
9	1	0	-4.643197	-0.926392	0.041266
10	1	0	-3.728703	0.947635	-1.309074
11	1	0	-1.307859	1.353455	-1.389995
12	6	0	0.662652	-0.021705	-0.077322
13	6	0	1.230921	1.219297	-0.009829
14	6	0	1.536369	-1.192298	-0.182946
15	1	0	1.023297	-2.129674	-0.441744
16	1	0	2.314776	1.280147	-0.070854
17	7	0	2.800012	-1.183931	-0.013236
18	7	0	0.616246	2.409844	0.120198
19	1	0	-0.372439	2.417475	0.336429
20	6	0	1.354343	3.627032	0.413966
21	1	0	2.302696	3.610831	-0.124055
22	1	0	0.779078	4.488561	0.075395
23	1	0	1.555750	3.735534	1.484292
24	6	0	3.507701	-2.431101	-0.234673
25	1	0	4.226530	-2.307098	-1.050283
26	1	0	4.083191	-2.691676	0.658434
27	1	0	2.840326	-3.267294	-0.481268

Structure 34b (C_2H_5OH)

Energy (Hartrees): -536.989251131
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.323299	-1.308346	0.712673
2	6	0	-2.691602	-1.556379	0.745168
3	6	0	-3.569444	-0.751662	0.022937
4	6	0	-3.061880	0.296780	-0.739901
5	6	0	-1.692265	0.539468	-0.778819
6	6	0	-0.795403	-0.253761	-0.047495
7	1	0	-0.653967	-1.933040	1.296089
8	1	0	-3.073403	-2.375956	1.344365
9	1	0	-4.636246	-0.942549	0.050613
10	1	0	-3.732287	0.921989	-1.319795
11	1	0	-1.312577	1.336876	-1.409302
12	6	0	0.665653	-0.016057	-0.084898
13	6	0	1.226074	1.227444	-0.017145
14	6	0	1.542019	-1.184850	-0.188224
15	1	0	1.029530	-2.122088	-0.447775
16	1	0	2.309382	1.296788	-0.075746
17	7	0	2.805506	-1.177560	-0.015477
18	7	0	0.602877	2.415767	0.109876
19	1	0	-0.385458	2.415211	0.327785
20	6	0	1.337451	3.630210	0.426414
21	1	0	2.272810	3.642815	-0.134287
22	1	0	0.746135	4.496200	0.129657
23	1	0	1.563475	3.706306	1.494770
24	6	0	3.507391	-2.429869	-0.228898
25	1	0	4.229996	-2.314811	-1.042196
26	1	0	4.078517	-2.688852	0.667270
27	1	0	2.837240	-3.264205	-0.473123

Structure 34c (vacuum)

Energy (Hartrees): -536.971709488
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.308286	-1.469955	0.880824
2	6	0	-1.293342	-2.446842	0.936333
3	6	0	-2.374212	-2.408353	0.058971
4	6	0	-2.458979	-1.387261	-0.880295
5	6	0	-1.471903	-0.407216	-0.935327
6	6	0	-0.388970	-0.429698	-0.050582
7	1	0	0.541150	-1.510366	1.550418
8	1	0	-1.215706	-3.245625	1.664878
9	1	0	-3.139917	-3.173964	0.103181
10	1	0	-3.287502	-1.356820	-1.578556
11	1	0	-1.526006	0.374707	-1.686302
12	6	0	0.646295	0.631294	-0.093105
13	6	0	0.329105	1.948647	-0.061455
14	6	0	2.066560	0.291317	-0.142958
15	1	0	1.133693	2.680508	-0.094051
16	1	0	2.748049	1.157823	-0.179517
17	7	0	2.517951	-0.893681	-0.141212
18	7	0	-0.919437	2.501764	-0.013440
19	1	0	-1.672208	1.856408	0.186763
20	6	0	3.953886	-1.063142	-0.193706
21	1	0	4.216368	-1.650615	-1.077254
22	1	0	4.505095	-0.112324	-0.223633
23	1	0	4.284130	-1.634420	0.677986

24	6	0	-1.093107	3.857355	0.476634
25	1	0	-0.367602	4.510790	-0.010908
26	1	0	-2.089995	4.211460	0.215760
27	1	0	-0.961433	3.938964	1.561790

Structure 34c ($CHCl_3$)

Energy (Hartrees): -536.991948658
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.742403	-1.298609	0.925326
2	6	0	-1.960131	-1.967276	0.961534
3	6	0	-2.957767	-1.661251	0.038498
4	6	0	-2.725959	-0.682392	-0.922564
5	6	0	-1.505082	-0.012764	-0.957645
6	6	0	-0.497729	-0.306923	-0.032475
7	1	0	0.032958	-1.544559	1.641324
8	1	0	-2.129993	-2.731538	1.711881
9	1	0	-3.905896	-2.186132	0.065941
10	1	0	-3.491960	-0.444684	-1.652408
11	1	0	-1.324454	0.737178	-1.721634
12	6	0	0.796532	0.420054	-0.056502
13	6	0	0.863496	1.779643	-0.017586
14	6	0	2.060572	-0.302202	-0.109229
15	1	0	1.843137	2.253555	-0.033001
16	1	0	2.957957	0.335965	-0.102679
17	7	0	2.169339	-1.569300	-0.165763
18	7	0	-0.170005	2.655190	0.022688
19	1	0	-1.091689	2.272006	0.188622
20	6	0	3.510164	-2.117871	-0.218586
21	1	0	3.632279	-2.695230	-1.139677
22	1	0	4.295104	-1.350310	-0.178250
23	1	0	3.656416	-2.812797	0.613243
24	6	0	0.035765	4.040520	0.409113
25	1	0	0.917770	4.430863	-0.101138
26	1	0	-0.825862	4.632016	0.100521
27	1	0	0.174158	4.156861	1.489472

Structure 34c (DMSO)

Energy (Hartrees): -536.989793943
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.768724	-1.281817	0.931581
2	6	0	-1.996985	-1.931880	0.966010
3	6	0	-2.985707	-1.614745	0.036070
4	6	0	-2.733501	-0.644053	-0.928390
5	6	0	-1.501291	0.005684	-0.962521
6	6	0	-0.502159	-0.300017	-0.031853
7	1	0	-0.004221	-1.530817	1.658983
8	1	0	-2.184236	-2.686629	1.722072
9	1	0	-3.943271	-2.122413	0.063146
10	1	0	-3.493527	-0.394105	-1.660489
11	1	0	-1.309357	0.751936	-1.727478
12	6	0	0.804310	0.404371	-0.049474
13	6	0	0.895831	1.766536	-0.000101
14	6	0	2.052990	-0.337058	-0.100021

15	1	0	1.884575	2.221471	-0.000680
16	1	0	2.961022	0.283366	-0.067993
17	7	0	2.143004	-1.607299	-0.183556
18	7	0	-0.117659	2.654194	0.040566
19	1	0	-1.057550	2.295570	0.153087
20	6	0	3.478731	-2.174099	-0.222016
21	1	0	3.612714	-2.738086	-1.150071
22	1	0	4.271089	-1.416976	-0.154089
23	1	0	3.602325	-2.883821	0.601427
24	6	0	0.094466	4.048984	0.387869
25	1	0	1.055224	4.375952	-0.011509
26	1	0	-0.691140	4.657867	-0.059312
27	1	0	0.091164	4.206988	1.470909

Structure 34c (C_2H_5OH)

Energy (Hartrees): -536.992902126
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.812583	-1.234159	0.963382
2	6	0	-2.054137	-1.858859	0.993210
3	6	0	-3.015945	-1.554615	0.031440
4	6	0	-2.724199	-0.623065	-0.960090
5	6	0	-1.479038	0.001612	-0.988901
6	6	0	-0.506884	-0.291881	-0.026682
7	1	0	-0.068021	-1.472607	1.715093
8	1	0	-2.272861	-2.583299	1.770259
9	1	0	-3.983974	-2.042508	0.054702
10	1	0	-3.463120	-0.384968	-1.717491
11	1	0	-1.254648	0.717560	-1.773774
12	6	0	0.813576	0.387260	-0.039038
13	6	0	0.927750	1.746795	0.001780
14	6	0	2.048305	-0.376817	-0.086572
15	1	0	1.923532	2.186117	0.006504
16	1	0	2.966514	0.227880	-0.047493
17	7	0	2.117578	-1.647820	-0.180138
18	7	0	-0.073520	2.651597	0.022438
19	1	0	-1.018111	2.305274	0.134561
20	6	0	3.446316	-2.231443	-0.223669
21	1	0	3.576062	-2.781430	-1.160507
22	1	0	4.248438	-1.486546	-0.141036
23	1	0	3.558853	-2.956705	0.587433
24	6	0	0.159150	4.040327	0.382373
25	1	0	1.120384	4.360527	-0.021704
26	1	0	-0.621541	4.663988	-0.052862
27	1	0	0.166219	4.189348	1.466835

Structure 34d (vacuum)

Energy (Hartrees): -536.965518265
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.675753	0.555569	0.772758
2	6	0	-3.041991	0.315537	0.819279
3	6	0	-3.602486	-0.725620	0.082999
4	6	0	-2.781533	-1.519610	-0.708178
5	6	0	-1.412740	-1.274580	-0.759508

6	6	0	-0.834559	-0.246160	-0.008495
7	1	0	-1.249389	1.369925	1.343529
8	1	0	-3.674638	0.944427	1.435381
9	1	0	-4.669998	-0.907950	0.118686
10	1	0	-3.206820	-2.320602	-1.301921
11	1	0	-0.785204	-1.873333	-1.410972
12	6	0	0.634426	-0.039887	-0.020426
13	6	0	1.445758	-1.127836	0.025596
14	6	0	1.200491	1.307205	-0.077287
15	1	0	2.287966	1.385702	0.086976
16	1	0	3.301859	-0.320993	-0.230875
17	1	0	0.988883	-2.104908	0.165913
18	7	0	0.522682	2.360420	-0.280668
19	7	0	2.804353	-1.191573	-0.131234
20	6	0	1.229157	3.622077	-0.290184
21	1	0	2.309562	3.520222	-0.112398
22	1	0	1.073420	4.112111	-1.254563
23	1	0	0.806468	4.280602	0.473068
24	6	0	3.553254	-2.285892	0.459119
25	1	0	3.034003	-3.223342	0.251551
26	1	0	4.540393	-2.340440	0.000539
27	1	0	3.670091	-2.188166	1.544361

Structure 34d ($CHCl_3$)

Energy (Hartrees): -536.986954984
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.693382	0.561730	0.765938
2	6	0	-3.061310	0.321837	0.794642
3	6	0	-3.610731	-0.729153	0.062153
4	6	0	-2.774468	-1.533756	-0.703919
5	6	0	-1.404574	-1.287047	-0.739644
6	6	0	-0.835773	-0.245279	0.004177
7	1	0	-1.278856	1.378633	1.343494
8	1	0	-3.702779	0.957054	1.395829
9	1	0	-4.678898	-0.912487	0.083499
10	1	0	-3.188868	-2.345790	-1.291411
11	1	0	-0.768235	-1.899959	-1.369655
12	6	0	0.631831	-0.028821	0.006632
13	6	0	1.452636	-1.118680	0.058395
14	6	0	1.194521	1.316444	-0.048339
15	1	0	2.270728	1.399324	0.165634
16	1	0	3.314554	-0.311294	-0.184663
17	1	0	0.999769	-2.098302	0.194790
18	7	0	0.528435	2.369111	-0.310356
19	7	0	2.801151	-1.173664	-0.077167
20	6	0	1.244744	3.628421	-0.302167
21	1	0	2.315678	3.518654	-0.083772
22	1	0	1.130444	4.116596	-1.273954
23	1	0	0.801206	4.296537	0.441820
24	6	0	3.558861	-2.318337	0.396928
25	1	0	3.003675	-3.231185	0.174066
26	1	0	4.513645	-2.361873	-0.126756
27	1	0	3.746700	-2.278196	1.474965

Structure 34d (DMSO)

Energy (Hartrees): -536.985478833
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.700475	0.563867	0.756941
2	6	0	-3.068208	0.318288	0.779610
3	6	0	-3.608645	-0.742673	0.053822
4	6	0	-2.762566	-1.551708	-0.697671
5	6	0	-1.393175	-1.298955	-0.728233
6	6	0	-0.832578	-0.245415	0.007115
7	1	0	-1.293959	1.384948	1.335033
8	1	0	-3.715700	0.954267	1.373818
9	1	0	-4.675939	-0.931912	0.071387
10	1	0	-3.168485	-2.374348	-1.276463
11	1	0	-0.750826	-1.920648	-1.343567
12	6	0	0.632888	-0.020124	0.017244
13	6	0	1.460183	-1.110600	0.073237
14	6	0	1.188353	1.325660	-0.039963
15	1	0	2.262561	1.416454	0.175158
16	1	0	3.323456	-0.299232	-0.149222
17	1	0	1.008079	-2.091934	0.201961
18	7	0	0.517163	2.375318	-0.312964
19	7	0	2.803574	-1.158620	-0.041078
20	6	0	1.231297	3.637906	-0.309227
21	1	0	2.301296	3.528987	-0.089510
22	1	0	1.118642	4.123026	-1.283123
23	1	0	0.786986	4.308805	0.432259
24	6	0	3.565358	-2.327711	0.363607
25	1	0	2.992572	-3.226563	0.130069
26	1	0	4.501620	-2.358160	-0.193152
27	1	0	3.789950	-2.321790	1.434760

Structure 34d (C_2H_5OH)

Energy (Hartrees): -536.988583101
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.693727	0.552442	0.786933
2	6	0	-3.062972	0.316177	0.809422
3	6	0	-3.614205	-0.718924	0.054882
4	6	0	-2.778234	-1.511098	-0.725253
5	6	0	-1.407165	-1.266935	-0.755490
6	6	0	-0.836452	-0.239532	0.007603
7	1	0	-1.277745	1.351514	1.389008
8	1	0	-3.703353	0.938890	1.425196
9	1	0	-4.682859	-0.901093	0.072233
10	1	0	-3.193381	-2.312801	-1.326606
11	1	0	-0.771304	-1.873872	-1.392125
12	6	0	0.631062	-0.024010	0.015115
13	6	0	1.448650	-1.120238	0.064596
14	6	0	1.197443	1.317698	-0.040530
15	1	0	2.270634	1.398112	0.183029
16	1	0	3.318668	-0.322059	-0.147159
17	1	0	0.989086	-2.098335	0.191718
18	7	0	0.539871	2.374224	-0.321022
19	7	0	2.793495	-1.180720	-0.059060
20	6	0	1.272103	3.627127	-0.309138
21	1	0	2.339788	3.502832	-0.087627
22	1	0	1.168276	4.119601	-1.280030
23	1	0	0.836016	4.300580	0.434727

24	6	0	3.539606	-2.347710	0.382430
25	1	0	2.971602	-3.247618	0.141137
26	1	0	4.491698	-2.388188	-0.146095
27	1	0	3.732661	-2.332068	1.459755

Structure 34e (vacuum)

Energy (Hartrees): -536.962557550
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.622386	0.817097	-0.662363
2	6	0	3.007594	0.859814	-0.596142
3	6	0	3.714755	-0.132361	0.080088
4	6	0	3.018934	-1.164255	0.696478
5	6	0	1.628816	-1.203242	0.633878
6	6	0	0.908025	-0.225642	-0.059037
7	1	0	1.082382	1.595759	-1.184919
8	1	0	3.540679	1.671996	-1.077248
9	1	0	4.796426	-0.093604	0.132439
10	1	0	3.554159	-1.933741	1.241066
11	1	0	1.090771	-1.990827	1.150523
12	6	0	-0.568577	-0.324827	-0.183562
13	6	0	-1.099825	-1.543020	-0.468852
14	6	0	-1.400135	0.877936	-0.085059
15	1	0	-2.427061	0.784924	-0.462046
16	1	0	-2.557012	-2.892315	-0.775008
17	1	0	-0.408506	-2.340857	-0.727205
18	7	0	-0.978531	1.994198	0.348355
19	7	0	-2.410097	-1.941749	-0.484029
20	6	0	-1.904337	3.105621	0.334633
21	1	0	-2.008162	3.499587	1.348792
22	1	0	-1.493629	3.912497	-0.278288
23	1	0	-2.900172	2.841111	-0.049362
24	6	0	-3.475561	-1.361171	0.314533
25	1	0	-3.049273	-0.865308	1.190646
26	1	0	-4.073197	-0.634834	-0.241623
27	1	0	-4.139462	-2.157236	0.654391

Structure 34e ($CHCl_3$)

Energy (Hartrees): -536.983961393
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.620549	0.782087	-0.705997
2	6	0	3.007720	0.823762	-0.662159
3	6	0	3.721996	-0.141658	0.046621
4	6	0	3.029838	-1.144509	0.715524
5	6	0	1.637733	-1.181293	0.675510
6	6	0	0.907449	-0.228991	-0.045235
7	1	0	1.077087	1.536886	-1.260957
8	1	0	3.536106	1.611991	-1.187438
9	1	0	4.804932	-0.106084	0.080899
10	1	0	3.570461	-1.895216	1.281503
11	1	0	1.107363	-1.951499	1.225890
12	6	0	-0.573924	-0.320487	-0.144422
13	6	0	-1.106929	-1.555228	-0.391904

14	6	0	-1.389282	0.888784	-0.048415
15	1	0	-2.426244	0.803437	-0.389218
16	1	0	-2.516562	-2.952240	-0.661822
17	1	0	-0.406109	-2.355033	-0.616569
18	7	0	-0.951701	2.012905	0.361226
19	7	0	-2.391846	-1.986471	-0.404976
20	6	0	-1.879058	3.126340	0.351001
21	1	0	-1.958005	3.543649	1.358848
22	1	0	-1.489588	3.921394	-0.291744
23	1	0	-2.884058	2.852383	0.001771
24	6	0	-3.549712	-1.329084	0.171151
25	1	0	-3.262631	-0.784619	1.074825
26	1	0	-4.029219	-0.634375	-0.523306
27	1	0	-4.276970	-2.094037	0.443518

Structure 34e (DMSO)

Energy (Hartrees): -536.982632561
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.619982	0.765870	-0.728036
2	6	0	3.007643	0.808933	-0.682367
3	6	0	3.720679	-0.143992	0.045432
4	6	0	3.026624	-1.136442	0.728618
5	6	0	1.633986	-1.174077	0.687207
6	6	0	0.904110	-0.232616	-0.049273
7	1	0	1.078716	1.508468	-1.302363
8	1	0	3.537350	1.586855	-1.221766
9	1	0	4.803673	-0.108245	0.080730
10	1	0	3.566014	-1.879660	1.305726
11	1	0	1.104158	-1.939841	1.244440
12	6	0	-0.577772	-0.319905	-0.144060
13	6	0	-1.112917	-1.561075	-0.375612
14	6	0	-1.385542	0.892175	-0.046495
15	1	0	-2.422564	0.817514	-0.386859
16	1	0	-2.514780	-2.965162	-0.621829
17	1	0	-0.411172	-2.363793	-0.587496
18	7	0	-0.941026	2.013644	0.370593
19	7	0	-2.390482	-1.994050	-0.380758
20	6	0	-1.863457	3.133368	0.360411
21	1	0	-1.941806	3.552064	1.368019
22	1	0	-1.471591	3.926340	-0.283907
23	1	0	-2.868646	2.861976	0.011779
24	6	0	-3.561314	-1.313146	0.139476
25	1	0	-3.301677	-0.754270	1.042812
26	1	0	-4.004591	-0.626619	-0.586010
27	1	0	-4.304660	-2.067341	0.396072

Structure 34e (C_2H_5OH)

Energy (Hartrees): -536.985780102
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.622768	0.756252	-0.747845
2	6	0	3.010260	0.802396	-0.700700
3	6	0	3.723004	-0.135228	0.046934
4	6	0	3.029482	-1.115083	0.748454

5	6	0	1.636967	-1.155465	0.705462
6	6	0	0.907860	-0.229282	-0.050342
7	1	0	1.081007	1.485545	-1.338950
8	1	0	3.540122	1.570336	-1.254182
9	1	0	4.806031	-0.097489	0.083155
10	1	0	3.569345	-1.845896	1.340931
11	1	0	1.106466	-1.910632	1.276494
12	6	0	-0.573851	-0.320057	-0.147069
13	6	0	-1.105469	-1.562179	-0.375816
14	6	0	-1.385632	0.889201	-0.050369
15	1	0	-2.418731	0.811097	-0.401152
16	1	0	-2.504187	-2.971896	-0.615966
17	1	0	-0.401731	-2.364315	-0.583257
18	7	0	-0.951957	2.010907	0.377979
19	7	0	-2.383830	-1.997729	-0.385993
20	6	0	-1.888227	3.120187	0.366477
21	1	0	-1.980077	3.532328	1.375504
22	1	0	-1.501737	3.922442	-0.269210
23	1	0	-2.887187	2.839544	0.008285
24	6	0	-3.554698	-1.317534	0.136304
25	1	0	-3.295032	-0.757587	1.039052
26	1	0	-4.001388	-0.633104	-0.589050
27	1	0	-4.297172	-2.071878	0.395509

Structure 34f (vacuum)

Energy (Hartrees): -536.961735310
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.722732	0.691749	0.988432
2	6	0	-3.103807	0.847277	1.006926
3	6	0	-3.894363	0.211258	0.054885
4	6	0	-3.288010	-0.573830	-0.919931
5	6	0	-1.904874	-0.716840	-0.944903
6	6	0	-1.098551	-0.096307	0.014741
7	1	0	-1.120012	1.169008	1.753992
8	1	0	-3.564855	1.457720	1.774940
9	1	0	-4.971081	0.330257	0.070235
10	1	0	-3.891410	-1.063831	-1.675501
11	1	0	-1.436293	-1.299199	-1.731131
12	6	0	0.383877	-0.259377	0.002125
13	6	0	0.873811	-1.526285	-0.068400
14	6	0	1.155174	0.986612	-0.030048
15	1	0	0.142717	-2.319763	-0.202673
16	1	0	0.615243	1.871052	0.340688
17	1	0	2.216466	-2.999235	0.020964
18	7	0	2.314866	1.113273	-0.534908
19	7	0	2.143598	-1.997003	0.050424
20	6	0	3.223464	-1.317428	0.744992
21	1	0	3.722852	-0.598349	0.097334
22	1	0	2.828240	-0.776654	1.610760
23	1	0	3.931718	-2.070305	1.090840
24	6	0	2.894483	2.440833	-0.535866
25	1	0	3.156039	2.718345	-1.560018
26	1	0	2.226438	3.206450	-0.118006
27	1	0	3.823847	2.434629	0.041242

Structure 34f ($CHCl_3$)

Energy (Hartrees): -536.980775719
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.721906	0.728191	0.963648
2	6	0	-3.104147	0.882719	0.983804
3	6	0	-3.900246	0.215763	0.056620
4	6	0	-3.296608	-0.600044	-0.895905
5	6	0	-1.912881	-0.743689	-0.923103
6	6	0	-1.099917	-0.091513	0.012380
7	1	0	-1.119259	1.234350	1.710716
8	1	0	-3.560861	1.518378	1.734505
9	1	0	-4.977517	0.334075	0.073761
10	1	0	-3.902674	-1.116241	-1.632360
11	1	0	-1.452664	-1.357212	-1.690636
12	6	0	0.382453	-0.259335	0.000190
13	6	0	0.876412	-1.528031	-0.074987
14	6	0	1.166293	0.979007	-0.016279
15	1	0	0.156303	-2.328289	-0.226281
16	1	0	0.676211	1.855011	0.431876
17	1	0	2.224861	-2.992505	0.032382
18	7	0	2.296679	1.106690	-0.588110
19	7	0	2.144416	-1.988642	0.062516
20	6	0	3.212124	-1.306286	0.770951
21	1	0	3.732619	-0.592502	0.132528
22	1	0	2.807526	-0.760658	1.629742
23	1	0	3.913169	-2.059384	1.130422
24	6	0	2.916574	2.417250	-0.546049
25	1	0	3.150134	2.739959	-1.564176
26	1	0	2.289121	3.179282	-0.065146
27	1	0	3.866463	2.355202	-0.005795

Structure 34f (DMSO)

Energy (Hartrees): -536.978275462
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.723356	0.772712	0.930332
2	6	0	-3.106026	0.929539	0.940360
3	6	0	-3.902667	0.219580	0.045581
4	6	0	-3.298140	-0.644020	-0.864076
5	6	0	-1.914594	-0.791611	-0.881912
6	6	0	-1.100327	-0.094435	0.021329
7	1	0	-1.123887	1.316844	1.652634
8	1	0	-3.561593	1.603267	1.658062
9	1	0	-4.979778	0.341054	0.054634
10	1	0	-3.903786	-1.196518	-1.574281
11	1	0	-1.458522	-1.448180	-1.615698
12	6	0	0.381014	-0.263948	0.014225
13	6	0	0.881373	-1.531301	-0.064660
14	6	0	1.171135	0.971625	0.003785
15	1	0	0.169464	-2.338692	-0.216106
16	1	0	0.723730	1.835885	0.513073
17	1	0	2.239634	-2.984700	0.055087
18	7	0	2.269841	1.104935	-0.627154
19	7	0	2.152789	-1.980011	0.071825
20	6	0	3.216374	-1.284190	0.773591
21	1	0	3.737526	-0.575046	0.129321
22	1	0	2.808988	-0.729780	1.625610
23	1	0	3.920037	-2.030402	1.141236

24	6	0	2.918526	2.402100	-0.562750
25	1	0	3.084301	2.776093	-1.576858
26	1	0	2.342594	3.145657	0.002747
27	1	0	3.903008	2.293741	-0.096989

Structure 34f (C_2H_5OH)

Energy (Hartrees): -536.981312625
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.719979	0.752161	0.946091
2	6	0	-3.102399	0.910147	0.957724
3	6	0	-3.898460	0.219345	0.047541
4	6	0	-3.293985	-0.625869	-0.879114
5	6	0	-1.910382	-0.774289	-0.898412
6	6	0	-1.097204	-0.096748	0.020043
7	1	0	-1.120802	1.280028	1.680770
8	1	0	-3.558627	1.569328	1.688552
9	1	0	-4.975596	0.341647	0.057908
10	1	0	-3.899436	-1.162821	-1.601445
11	1	0	-1.452847	-1.415230	-1.645139
12	6	0	0.384190	-0.268681	0.011780
13	6	0	0.881926	-1.535688	-0.067225
14	6	0	1.173309	0.967891	0.008841
15	1	0	0.168104	-2.342261	-0.214174
16	1	0	0.731729	1.822200	0.539577
17	1	0	2.234911	-2.991510	0.071721
18	7	0	2.261103	1.115796	-0.637607
19	7	0	2.155342	-1.986124	0.064359
20	6	0	3.213546	-1.285281	0.770559
21	1	0	3.731655	-0.571506	0.129199
22	1	0	2.802797	-0.736718	1.625029
23	1	0	3.922979	-2.027166	1.136130
24	6	0	2.905110	2.415030	-0.554811
25	1	0	3.053506	2.813164	-1.562281
26	1	0	2.335246	3.143220	0.035868
27	1	0	3.897242	2.301808	-0.107077

Structure 35a (vacuum)

Energy (Hartrees): -651.490690585
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.916940	-1.085126	0.761972
2	6	0	2.296251	-1.167393	0.813571
3	6	0	3.082627	-0.223966	0.148644
4	6	0	2.464947	0.792221	-0.574768
5	6	0	1.072318	0.847224	-0.632948
6	6	0	0.267108	-0.072429	0.037419
7	1	0	0.325964	-1.806874	1.315591
8	1	0	2.794320	-1.947259	1.377014
9	1	0	3.044439	1.529537	-1.114011
10	1	0	0.605568	1.616799	-1.238452
11	6	0	-1.210639	0.010197	-0.003146
12	6	0	-1.829437	1.223589	0.134776

13	6	0	-1.975189	-1.207552	-0.189136
14	1	0	-1.219906	2.106756	0.316802
15	1	0	-1.382519	-2.126091	-0.309214
16	1	0	-3.725216	0.610001	-0.039918
17	7	0	-3.254475	-1.262901	-0.239651
18	7	0	-3.152803	1.447167	0.068835
19	6	0	-3.860553	-2.562349	-0.445274
20	1	0	-4.478896	-2.541770	-1.346498
21	1	0	-3.120417	-3.367207	-0.545671
22	1	0	-4.520886	-2.796480	0.394114
23	6	0	-3.752631	2.715268	0.417688
24	1	0	-3.023872	3.514151	0.269873
25	1	0	-4.609563	2.914472	-0.227141
26	1	0	-4.086689	2.741518	1.460137
27	8	0	4.430362	-0.381858	0.263279
28	6	0	5.254209	0.555290	-0.393909
29	1	0	6.279437	0.261505	-0.178962
30	1	0	5.090246	0.537368	-1.476339
31	1	0	5.080333	1.568726	-0.017170

Structure 35a ($CHCl_3$)

Energy (Hartrees): -651.508752314
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.917832	-1.122150	0.722020
2	6	0	2.299037	-1.205095	0.765807
3	6	0	3.084096	-0.232768	0.140416
4	6	0	2.462426	0.813916	-0.536679
5	6	0	1.069352	0.870596	-0.587810
6	6	0	0.263586	-0.078682	0.044192
7	1	0	0.332347	-1.872459	1.243038
8	1	0	2.794005	-2.011861	1.294935
9	1	0	3.040310	1.575112	-1.044613
10	1	0	0.604106	1.670625	-1.154312
11	6	0	-1.215583	0.004442	0.008540
12	6	0	-1.830548	1.225436	0.144048
13	6	0	-1.979532	-1.211746	-0.181915
14	1	0	-1.219528	2.109025	0.316855
15	1	0	-1.389402	-2.128714	-0.317949
16	1	0	-3.737585	0.632494	-0.019519
17	7	0	-3.261256	-1.270237	-0.221964
18	7	0	-3.148641	1.456388	0.087840
19	6	0	-3.862054	-2.571624	-0.442386
20	1	0	-4.473123	-2.547936	-1.349304
21	1	0	-3.119379	-3.373838	-0.541155
22	1	0	-4.530485	-2.814208	0.388757
23	6	0	-3.741266	2.744840	0.381292
24	1	0	-2.989737	3.526063	0.257887
25	1	0	-4.562365	2.943165	-0.309076
26	1	0	-4.126019	2.789455	1.404630
27	8	0	4.432180	-0.390816	0.243469
28	6	0	5.255103	0.576411	-0.384534
29	1	0	6.281977	0.273781	-0.187248
30	1	0	5.085476	0.598451	-1.465332
31	1	0	5.086547	1.572858	0.035578

Structure 35a (DMSO)

Energy (Hartrees): -651.505613321
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.918570	-1.140934	0.700033
2	6	0	2.300662	-1.224515	0.739270
3	6	0	3.086291	-0.236840	0.137717
4	6	0	2.462040	0.828132	-0.510042
5	6	0	1.068801	0.885988	-0.557449
6	6	0	0.262753	-0.080725	0.049494
7	1	0	0.336038	-1.906835	1.201534
8	1	0	2.792988	-2.046410	1.247551
9	1	0	3.037892	1.604360	-0.997441
10	1	0	0.605384	1.704743	-1.098335
11	6	0	-1.216893	0.001804	0.015608
12	6	0	-1.831352	1.226333	0.146786
13	6	0	-1.979912	-1.214711	-0.173977
14	1	0	-1.219858	2.111218	0.311105
15	1	0	-1.391729	-2.132618	-0.309541
16	1	0	-3.743188	0.640172	-0.012077
17	7	0	-3.262680	-1.272701	-0.215158
18	7	0	-3.147375	1.458718	0.094535
19	6	0	-3.862155	-2.574836	-0.442103
20	1	0	-4.473971	-2.547246	-1.348589
21	1	0	-3.117984	-3.374756	-0.545521
22	1	0	-4.530511	-2.823028	0.387623
23	6	0	-3.736422	2.756083	0.361353
24	1	0	-2.978345	3.530120	0.235649
25	1	0	-4.548864	2.945906	-0.341326
26	1	0	-4.133020	2.814805	1.379037
27	8	0	4.432637	-0.396839	0.231596
28	6	0	5.250838	0.585692	-0.384716
29	1	0	6.279685	0.280339	-0.202983
30	1	0	5.070840	0.629808	-1.462922
31	1	0	5.084596	1.573182	0.055992

Structure 35a (C_2H_5OH)

Energy (Hartrees): -651.508871672
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.913063	-1.134856	0.705808
2	6	0	2.295153	-1.218075	0.750544
3	6	0	3.080014	-0.236985	0.139912
4	6	0	2.461013	0.819976	-0.523392
5	6	0	1.068103	0.877416	-0.575713
6	6	0	0.260491	-0.081922	0.041096
7	1	0	0.328484	-1.893984	1.215234
8	1	0	2.786791	-2.033656	1.270015
9	1	0	3.039756	1.589489	-1.017967
10	1	0	0.605638	1.688952	-1.128270
11	6	0	-1.218867	0.002978	0.004247
12	6	0	-1.829006	1.228663	0.135283
13	6	0	-1.982927	-1.214238	-0.177747
14	1	0	-1.214416	2.110441	0.304540
15	1	0	-1.394139	-2.133109	-0.302532
16	1	0	-3.743972	0.651802	-0.021741
17	7	0	-3.265563	-1.273083	-0.222513
18	7	0	-3.144639	1.467867	0.078522
19	6	0	-3.860435	-2.580843	-0.432110

20	1	0	-4.471114	-2.568924	-1.339588
21	1	0	-3.114187	-3.380189	-0.522627
22	1	0	-4.529264	-2.819690	0.399888
23	6	0	-3.725827	2.760796	0.384339
24	1	0	-2.972120	3.537685	0.249845
25	1	0	-4.557728	2.962673	-0.291602
26	1	0	-4.093544	2.803208	1.413779
27	8	0	4.431990	-0.395745	0.241928
28	6	0	5.255490	0.581601	-0.379504
29	1	0	6.282475	0.276362	-0.186975
30	1	0	5.080594	0.612567	-1.458628
31	1	0	5.084636	1.571774	0.052568

Structure 35b (vacuum)

Energy (Hartrees): -651.482977096
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.785361	-0.897804	-0.672621
2	6	0	2.178830	-0.880139	-0.650802
3	6	0	2.841022	0.018752	0.182110
4	6	0	2.098954	0.881750	0.992042
5	6	0	0.715989	0.843660	0.964794
6	6	0	0.023989	-0.043008	0.124451
7	1	0	0.280938	-1.589807	-1.339024
8	1	0	2.726771	-1.560397	-1.288871
9	1	0	2.633272	1.560550	1.645756
10	1	0	0.151505	1.494136	1.625119
11	6	0	-1.455862	-0.088783	0.093651
12	6	0	-2.223939	1.021450	-0.020952
13	6	0	-2.115976	-1.399175	0.171156
14	1	0	-1.442261	-2.245659	0.378132
15	1	0	-3.302469	0.887092	-0.027701
16	7	0	-3.363673	-1.582939	0.027665
17	7	0	-1.799034	2.313802	-0.116011
18	1	0	-0.814064	2.444700	-0.303839
19	6	0	-2.690614	3.343630	-0.617534
20	1	0	-3.668469	3.226999	-0.148366
21	1	0	-2.302140	4.325346	-0.346713
22	1	0	-2.819736	3.301272	-1.704947
23	6	0	-3.864742	-2.932131	0.172811
24	1	0	-4.571436	-2.971153	1.006374
25	1	0	-4.417470	-3.214135	-0.727155
26	1	0	-3.072009	-3.672641	0.349488
27	8	0	4.193106	0.126498	0.279968
28	6	0	4.977459	-0.741557	-0.509366
29	1	0	4.795302	-0.579229	-1.576593
30	1	0	6.014244	-0.505587	-0.279645
31	1	0	4.779300	-1.789381	-0.261784

Structure 35b ($CHCl_3$)

Energy (Hartrees): -651.502805176
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.793509	-0.904009	-0.651562
2	6	0	2.187391	-0.879703	-0.630904
3	6	0	2.846148	0.048166	0.173696
4	6	0	2.099058	0.935211	0.954095
5	6	0	0.715348	0.891012	0.927767
6	6	0	0.026094	-0.027393	0.118542
7	1	0	0.295893	-1.622368	-1.295380
8	1	0	2.738705	-1.577576	-1.247253
9	1	0	2.625042	1.641572	1.586270
10	1	0	0.153826	1.566141	1.565681
11	6	0	-1.454877	-0.089671	0.093394
12	6	0	-2.244043	1.012491	-0.028712
13	6	0	-2.090330	-1.407583	0.187412
14	1	0	-1.408193	-2.231108	0.447049
15	1	0	-3.320800	0.864879	-0.020994
16	7	0	-3.329222	-1.636175	0.001934
17	7	0	-1.853379	2.303578	-0.147973
18	1	0	-0.874042	2.478149	-0.333101
19	6	0	-2.782919	3.332432	-0.581900
20	1	0	-3.746464	3.174772	-0.095436
21	1	0	-2.405850	4.310391	-0.282868
22	1	0	-2.932511	3.326738	-1.666764
23	6	0	-3.791349	-2.997308	0.186844
24	1	0	-4.539704	-3.026558	0.984402
25	1	0	-4.285516	-3.344166	-0.725265
26	1	0	-2.983566	-3.696804	0.439689
27	8	0	4.197145	0.161258	0.268258
28	6	0	4.988649	-0.738071	-0.490185
29	1	0	4.813935	-0.609008	-1.562554
30	1	0	6.024593	-0.494380	-0.261668
31	1	0	4.789622	-1.776006	-0.206514

Structure 35b (DMSO)

Energy (Hartrees): -651.500146744
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.798016	-0.919847	-0.623821
2	6	0	2.191926	-0.891077	-0.603623
3	6	0	2.848895	0.068843	0.165593
4	6	0	2.096730	0.982791	0.910317
5	6	0	0.712710	0.933325	0.886145
6	6	0	0.025868	-0.017564	0.112462
7	1	0	0.305193	-1.665474	-1.239865
8	1	0	2.743629	-1.611765	-1.192891
9	1	0	2.616035	1.718216	1.514486
10	1	0	0.153303	1.632997	1.499020
11	6	0	-1.454532	-0.090632	0.090749
12	6	0	-2.256513	1.006684	-0.032372
13	6	0	-2.074490	-1.413975	0.188751
14	1	0	-1.383548	-2.228487	0.450983
15	1	0	-3.332360	0.851104	-0.018570
16	7	0	-3.310697	-1.664847	0.001477
17	7	0	-1.883224	2.296713	-0.160046

18	1	0	-0.905058	2.493825	-0.329584
19	6	0	-2.826559	3.327525	-0.559501
20	1	0	-3.788796	3.138804	-0.081861
21	1	0	-2.460859	4.299256	-0.228274
22	1	0	-2.970546	3.353849	-1.644368
23	6	0	-3.745134	-3.036169	0.192082
24	1	0	-4.490261	-3.080152	0.992295
25	1	0	-4.234339	-3.396739	-0.717581
26	1	0	-2.921066	-3.716282	0.443806
27	8	0	4.197879	0.187267	0.255514
28	6	0	4.987075	-0.746406	-0.467763
29	1	0	4.808480	-0.665063	-1.543859
30	1	0	6.024313	-0.495936	-0.253118
31	1	0	4.786338	-1.770335	-0.138868

Structure 35b (C_2H_5OH)

Energy (Hartrees): -651.503731266
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.793727	-0.905694	-0.634095
2	6	0	2.187535	-0.877529	-0.617150
3	6	0	2.843413	0.072367	0.163366
4	6	0	2.096248	0.976950	0.922295
5	6	0	0.711947	0.928668	0.900144
6	6	0	0.024309	-0.012065	0.115737
7	1	0	0.298081	-1.643043	-1.258043
8	1	0	2.739189	-1.590120	-1.216273
9	1	0	2.619181	1.702229	1.535999
10	1	0	0.153628	1.619413	1.523818
11	6	0	-1.456150	-0.087582	0.096106
12	6	0	-2.260445	1.006964	-0.026489
13	6	0	-2.069508	-1.413585	0.198008
14	1	0	-1.378700	-2.218195	0.489009
15	1	0	-3.335888	0.849651	-0.011050
16	7	0	-3.298983	-1.677314	-0.014782
17	7	0	-1.890464	2.299708	-0.154010
18	1	0	-0.913985	2.496464	-0.334228
19	6	0	-2.839963	3.320094	-0.567983
20	1	0	-3.797945	3.140324	-0.078298
21	1	0	-2.474557	4.299561	-0.260019
22	1	0	-2.993829	3.324330	-1.651921
23	6	0	-3.724174	-3.049292	0.193164
24	1	0	-4.481390	-3.085908	0.982084
25	1	0	-4.195837	-3.430247	-0.717154
26	1	0	-2.899169	-3.718131	0.469637
27	8	0	4.198124	0.189832	0.252758
28	6	0	4.989563	-0.743570	-0.471587
29	1	0	4.814952	-0.654256	-1.547334
30	1	0	6.025736	-0.494839	-0.249670
31	1	0	4.782661	-1.767005	-0.146181

Structure 35c (vacuum)

Energy (Hartrees): -651.484596569
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.618003	0.729205	-0.740176
2	6	0	-2.005864	0.621689	-0.711908
3	6	0	-2.613229	-0.248986	0.191709
4	6	0	-1.823142	-1.000366	1.063016
5	6	0	-0.444000	-0.882416	1.021330
6	6	0	0.188203	-0.023288	0.111990
7	1	0	-0.153419	1.423677	-1.428458
8	1	0	-2.595223	1.224231	-1.389789
9	1	0	-2.313910	-1.657182	1.770842
10	1	0	0.160047	-1.451518	1.720815
11	6	0	1.666277	0.077800	0.066923
12	6	0	2.460605	-1.017133	-0.016898
13	6	0	2.334568	1.376892	0.099146
14	1	0	3.540063	-0.882223	-0.031596
15	1	0	3.436527	1.329003	0.092430
16	7	0	1.732034	2.492749	0.126932
17	7	0	2.065022	-2.325710	-0.061758
18	1	0	1.078710	-2.471992	-0.232595
19	6	0	2.544589	3.689681	0.160086
20	1	0	2.299187	4.267884	1.054622
21	1	0	3.624704	3.484610	0.156225
22	1	0	2.302461	4.317745	-0.701458
23	6	0	2.961070	-3.332311	-0.601791
24	1	0	3.944524	-3.220730	-0.141730
25	1	0	2.585271	-4.323663	-0.350103
26	1	0	3.075641	-3.263112	-1.689890
27	8	0	-3.957280	-0.427284	0.302770
28	6	0	-4.790955	0.329439	-0.548070
29	1	0	-4.597164	0.099032	-1.600669
30	1	0	-5.812035	0.049057	-0.298574
31	1	0	-4.657258	1.402933	-0.380591

Structure 35c ($CHCl_3$)

Energy (Hartrees): -651.505637378
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.630917	0.690300	-0.787550
2	6	0	-2.019963	0.590765	-0.747199
3	6	0	-2.624416	-0.231789	0.203540
4	6	0	-1.829638	-0.939845	1.107861
5	6	0	-0.449348	-0.827192	1.054189
6	6	0	0.180954	-0.015980	0.099983
7	1	0	-0.172192	1.339124	-1.524554
8	1	0	-2.611602	1.157652	-1.453842
9	1	0	-2.313145	-1.563814	1.850858
10	1	0	0.154624	-1.368973	1.775528
11	6	0	1.660978	0.078517	0.038704
12	6	0	2.453788	-1.024664	-0.053459
13	6	0	2.339786	1.366829	0.071600
14	1	0	3.533131	-0.889218	-0.085610

15	1	0	3.438197	1.307225	0.021536
16	7	0	1.757220	2.495848	0.153278
17	7	0	2.059821	-2.322468	-0.089711
18	1	0	1.071315	-2.496517	-0.218710
19	6	0	2.599431	3.675804	0.172919
20	1	0	2.394921	4.256186	1.077081
21	1	0	3.672890	3.444780	0.138940
22	1	0	2.352662	4.317294	-0.678376
23	6	0	2.962243	-3.364745	-0.548314
24	1	0	3.944830	-3.216348	-0.097330
25	1	0	2.584536	-4.334880	-0.226239
26	1	0	3.073040	-3.372206	-1.638025
27	8	0	-3.967381	-0.402714	0.325585
28	6	0	-4.806964	0.322872	-0.557035
29	1	0	-4.618424	0.047885	-1.599270
30	1	0	-5.827765	0.053226	-0.292491
31	1	0	-4.672878	1.401401	-0.430579

Structure 35c (DMSO)

Energy (Hartrees): -651.504347762
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.635855	0.679081	-0.798973
2	6	0	-2.025505	0.584130	-0.752632
3	6	0	-2.628766	-0.224554	0.212155
4	6	0	-1.829940	-0.922991	1.121721
5	6	0	-0.449278	-0.814043	1.061706
6	6	0	0.179583	-0.014760	0.095986
7	1	0	-0.180403	1.310392	-1.553817
8	1	0	-2.617340	1.139244	-1.468708
9	1	0	-2.308730	-1.541506	1.872578
10	1	0	0.154744	-1.354381	1.784285
11	6	0	1.659486	0.080249	0.028071
12	6	0	2.454576	-1.025371	-0.069709
13	6	0	2.337877	1.365218	0.060933
14	1	0	3.533468	-0.887743	-0.109521
15	1	0	3.434291	1.306669	-0.010373
16	7	0	1.758352	2.497262	0.166275
17	7	0	2.061558	-2.316839	-0.106215
18	1	0	1.071780	-2.504109	-0.205532
19	6	0	2.608174	3.674334	0.176955
20	1	0	2.422284	4.254869	1.085405
21	1	0	3.678660	3.435441	0.126699
22	1	0	2.355065	4.320071	-0.669627
23	6	0	2.965810	-3.374621	-0.525666
24	1	0	3.951066	-3.200841	-0.090517
25	1	0	2.592300	-4.331456	-0.161876
26	1	0	3.064778	-3.424294	-1.614875
27	8	0	-3.969337	-0.389522	0.341093
28	6	0	-4.806659	0.308721	-0.569347
29	1	0	-4.608866	0.003753	-1.601090
30	1	0	-5.828593	0.044115	-0.304527
31	1	0	-4.676179	1.390627	-0.474884

Structure 35c (C_2H_5OH)

Energy (Hartrees): -651.507631565
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.629429	0.620957	-0.848609
2	6	0	-2.019504	0.536218	-0.796954
3	6	0	-2.623784	-0.201415	0.221126
4	6	0	-1.831152	-0.842719	1.175434
5	6	0	-0.449731	-0.744394	1.109233
6	6	0	0.181460	-0.012852	0.093335
7	1	0	-0.169505	1.193919	-1.646487
8	1	0	-2.609485	1.042763	-1.549653
9	1	0	-2.314506	-1.406008	1.966210
10	1	0	0.152012	-1.237549	1.866527
11	6	0	1.662644	0.073229	0.022715
12	6	0	2.447022	-1.039135	-0.065429
13	6	0	2.348452	1.354076	0.051642
14	1	0	3.527313	-0.913483	-0.108281
15	1	0	3.444340	1.288203	-0.019629
16	7	0	1.776212	2.489964	0.156079
17	7	0	2.039604	-2.328396	-0.085977
18	1	0	1.047211	-2.501536	-0.185987
19	6	0	2.635439	3.660238	0.164426
20	1	0	2.454682	4.243776	1.071787
21	1	0	3.704035	3.413852	0.114382
22	1	0	2.387349	4.307134	-0.682535
23	6	0	2.929636	-3.392103	-0.522538
24	1	0	3.917620	-3.239123	-0.085450
25	1	0	2.544364	-4.349362	-0.172329
26	1	0	3.027755	-3.427763	-1.612479
27	8	0	-3.970975	-0.349345	0.361987
28	6	0	-4.808166	0.300559	-0.586117
29	1	0	-4.619843	-0.073627	-1.596293
30	1	0	-5.830258	0.062653	-0.297334
31	1	0	-4.663316	1.383979	-0.558642

Structure 35d (vacuum)

Energy (Hartrees): -651.478005995
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.717396	0.919958	0.835674
2	6	0	-2.095178	0.946455	0.919991
3	6	0	-2.866114	0.033849	0.192918
4	6	0	-2.236085	-0.898768	-0.623106
5	6	0	-0.841933	-0.908717	-0.700173
6	6	0	-0.056852	-0.022153	0.031312
7	1	0	-0.133739	1.638345	1.396524
8	1	0	-2.607667	1.668572	1.543886
9	1	0	-2.803584	-1.604033	-1.215010
10	1	0	-0.362247	-1.615110	-1.369212
11	6	0	1.423270	-0.097501	-0.018487
12	6	0	2.019529	-1.315871	0.033286
13	6	0	2.225180	1.120593	-0.123913
14	1	0	3.314354	1.000516	-0.001929
15	1	0	3.979712	-0.872297	-0.311053
16	1	0	1.394270	-2.187088	0.216243

17	7	0	1.742092	2.277827	-0.318550
18	7	0	3.337495	-1.635956	-0.169412
19	6	0	2.665240	3.389478	-0.375303
20	1	0	3.716311	3.092837	-0.246596
21	1	0	2.555421	3.897431	-1.336697
22	1	0	2.406399	4.115798	0.399666
23	6	0	3.896229	-2.818963	0.459788
24	1	0	3.207720	-3.653971	0.316971
25	1	0	4.840028	-3.075147	-0.021187
26	1	0	4.067160	-2.692579	1.534986
27	8	0	-4.214995	0.142915	0.342223
28	6	0	-5.025523	-0.752015	-0.386190
29	1	0	-6.054287	-0.506624	-0.130973
30	1	0	-4.879526	-0.630236	-1.464603
31	1	0	-4.819675	-1.790911	-0.107855

Structure 35d ($CHCl_3$)

Energy (Hartrees): -651.500293594
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.721517	0.943496	0.821194
2	6	0	-2.101188	0.973217	0.903649
3	6	0	-2.872843	0.051748	0.187053
4	6	0	-2.240265	-0.890033	-0.618358
5	6	0	-0.845697	-0.900223	-0.695906
6	6	0	-0.056951	-0.006033	0.026833
7	1	0	-0.141207	1.663762	1.384845
8	1	0	-2.608141	1.704300	1.523243
9	1	0	-2.808038	-1.603978	-1.200361
10	1	0	-0.368679	-1.620263	-1.352655
11	6	0	1.424511	-0.087703	-0.010358
12	6	0	2.012237	-1.317066	0.050159
13	6	0	2.239898	1.118609	-0.106620
14	1	0	3.320603	0.988051	0.052966
15	1	0	3.987673	-0.903395	-0.263867
16	1	0	1.376911	-2.181773	0.230565
17	7	0	1.779149	2.282290	-0.339734
18	7	0	3.319497	-1.647824	-0.127003
19	6	0	2.723623	3.380194	-0.373941
20	1	0	3.764090	3.066015	-0.213703
21	1	0	2.651943	3.889235	-1.339120
22	1	0	2.456558	4.114409	0.391819
23	6	0	3.850397	-2.882521	0.425614
24	1	0	3.126049	-3.683967	0.268824
25	1	0	4.770669	-3.146371	-0.095187
26	1	0	4.058528	-2.806193	1.498213
27	8	0	-4.221215	0.157659	0.335137
28	6	0	-5.033565	-0.756212	-0.380756
29	1	0	-6.062930	-0.509739	-0.126474
30	1	0	-4.892025	-0.648689	-1.460541
31	1	0	-4.824645	-1.788770	-0.083884

Structure 35d (DMSO)

Energy (Hartrees): -651.499697786
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.722995	0.936594	0.836564
2	6	0	-2.103720	0.967217	0.913370
3	6	0	-2.874572	0.051670	0.186293
4	6	0	-2.237431	-0.885885	-0.622071
5	6	0	-0.842200	-0.895938	-0.694542
6	6	0	-0.054395	-0.005603	0.035550
7	1	0	-0.145682	1.648035	1.415388
8	1	0	-2.609712	1.692826	1.540570
9	1	0	-2.801845	-1.599374	-1.208207
10	1	0	-0.364224	-1.617565	-1.349204
11	6	0	1.427385	-0.082049	0.001008
12	6	0	2.019260	-1.313446	0.061890
13	6	0	2.236883	1.125256	-0.100168
14	1	0	3.316146	1.003248	0.068301
15	1	0	3.997757	-0.896901	-0.232446
16	1	0	1.383641	-2.179825	0.234850
17	7	0	1.771426	2.285737	-0.353169
18	7	0	3.323150	-1.637965	-0.102426
19	6	0	2.713631	3.387965	-0.385259
20	1	0	3.753342	3.074216	-0.224173
21	1	0	2.643121	3.899526	-1.349419
22	1	0	2.445123	4.119852	0.382727
23	6	0	3.848744	-2.897770	0.397532
24	1	0	3.111044	-3.684208	0.229283
25	1	0	4.757447	-3.152801	-0.147238
26	1	0	4.077076	-2.855220	1.467400
27	8	0	-4.221237	0.156445	0.328365
28	6	0	-5.027522	-0.764713	-0.390682
29	1	0	-6.059231	-0.524210	-0.140634
30	1	0	-4.882084	-0.658245	-1.469701
31	1	0	-4.812462	-1.795097	-0.092155

Structure 35d (C_2H_5OH)

Energy (Hartrees): -651.503007422
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.723789	0.928737	0.851424
2	6	0	-2.104648	0.960251	0.927569
3	6	0	-2.873140	0.056117	0.185993
4	6	0	-2.239825	-0.871131	-0.635111
5	6	0	-0.844686	-0.882047	-0.706421
6	6	0	-0.057061	-0.002962	0.037587
7	1	0	-0.145868	1.629250	1.442897
8	1	0	-2.611488	1.676278	1.565422
9	1	0	-2.806238	-1.574417	-1.231590
10	1	0	-0.366404	-1.594054	-1.371411
11	6	0	1.424437	-0.083273	0.003770
12	6	0	2.011612	-1.316260	0.059469
13	6	0	2.239513	1.120489	-0.095420
14	1	0	3.316440	0.992034	0.081942
15	1	0	3.990117	-0.903156	-0.237019
16	1	0	1.374142	-2.181174	0.232529
17	7	0	1.785080	2.283414	-0.357437

18	7	0	3.315212	-1.645193	-0.113901
19	6	0	2.742623	3.373619	-0.388544
20	1	0	3.777516	3.046945	-0.224231
21	1	0	2.682072	3.884834	-1.353331
22	1	0	2.482797	4.111182	0.376731
23	6	0	3.839313	-2.898499	0.405510
24	1	0	3.107908	-3.690362	0.234796
25	1	0	4.755778	-3.155209	-0.125283
26	1	0	4.053969	-2.845986	1.477841
27	8	0	-4.225526	0.161706	0.329049
28	6	0	-5.036135	-0.754918	-0.394327
29	1	0	-6.066049	-0.514236	-0.136919
30	1	0	-4.893682	-0.637757	-1.472288
31	1	0	-4.818132	-1.786123	-0.102107

Structure 35e (vacuum)

Energy (Hartrees): -651.474971526
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.869916	0.716497	-0.598790
2	6	0	2.258482	0.693762	-0.512924
3	6	0	2.895176	-0.360178	0.142154
4	6	0	2.129133	-1.374255	0.714421
5	6	0	0.747465	-1.331983	0.625527
6	6	0	0.085068	-0.296660	-0.048077
7	1	0	0.388472	1.543612	-1.103907
8	1	0	2.825542	1.499398	-0.959784
9	1	0	2.637793	-2.173753	1.239441
10	1	0	0.164256	-2.108013	1.109482
11	6	0	-1.392143	-0.312152	-0.196332
12	6	0	-1.988143	-1.492463	-0.510613
13	6	0	-2.162076	0.929385	-0.084348
14	1	0	-3.192284	0.889040	-0.461900
15	1	0	-3.517455	-2.752331	-0.845610
16	1	0	-1.341460	-2.322671	-0.782500
17	7	0	-1.687697	2.021635	0.356792
18	7	0	-3.320510	-1.816485	-0.537062
19	6	0	-2.561406	3.174649	0.353284
20	1	0	-2.660491	3.553904	1.373662
21	1	0	-2.106502	3.973561	-0.238568
22	1	0	-3.563485	2.964106	-0.047550
23	6	0	-4.347616	-1.205349	0.288560
24	1	0	-3.888418	-0.753373	1.171917
25	1	0	-4.913966	-0.435480	-0.241304
26	1	0	-5.047336	-1.975556	0.616407
27	8	0	4.244708	-0.476878	0.282357
28	6	0	5.048750	0.540581	-0.272384
29	1	0	6.078643	0.265668	-0.054387
30	1	0	4.912272	0.607547	-1.356704
31	1	0	4.828567	1.512319	0.181469

Structure 35e ($CHCl_3$)

Energy (Hartrees): -651.497223433
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.871833	0.683152	-0.634972
2	6	0	2.261739	0.663683	-0.559013
3	6	0	2.901622	-0.354135	0.149967
4	6	0	2.135896	-1.334788	0.780459
5	6	0	0.751767	-1.294520	0.700004
6	6	0	0.084573	-0.293744	-0.020698
7	1	0	0.391259	1.479834	-1.190083
8	1	0	2.827644	1.439976	-1.057228
9	1	0	2.641822	-2.112646	1.341265
10	1	0	0.173480	-2.049988	1.221673
11	6	0	-1.397308	-0.307443	-0.159323
12	6	0	-1.987198	-1.506227	-0.447715
13	6	0	-2.157075	0.936620	-0.052937
14	1	0	-3.192442	0.902440	-0.408302
15	1	0	-3.461494	-2.826412	-0.756486
16	1	0	-1.324675	-2.334938	-0.684097
17	7	0	-1.675159	2.035476	0.376114
18	7	0	-3.294706	-1.870209	-0.488048
19	6	0	-2.553453	3.188063	0.374741
20	1	0	-2.639976	3.580671	1.392013
21	1	0	-2.113649	3.983295	-0.234467
22	1	0	-3.560344	2.968906	-0.006258
23	6	0	-4.414572	-1.183046	0.127996
24	1	0	-4.091610	-0.687942	1.048123
25	1	0	-4.868701	-0.439981	-0.532357
26	1	0	-5.175065	-1.922622	0.379316
27	8	0	4.251358	-0.463922	0.285108
28	6	0	5.056706	0.517675	-0.344312
29	1	0	6.088044	0.253977	-0.116417
30	1	0	4.912260	0.511916	-1.428963
31	1	0	4.844470	1.516286	0.049755

Structure 35e (DMSO)

Energy (Hartrees): -651.496823554
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.863108	0.626637	-0.689305
2	6	0	2.253997	0.612371	-0.622179
3	6	0	2.898793	-0.354788	0.151998
4	6	0	2.134668	-1.290512	0.851326
5	6	0	0.749132	-1.254574	0.778583
6	6	0	0.077814	-0.302004	-0.000949
7	1	0	0.381272	1.379397	-1.302589
8	1	0	2.816383	1.350281	-1.179373
9	1	0	2.641033	-2.033042	1.457946
10	1	0	0.174718	-1.978603	1.347493
11	6	0	-1.407153	-0.308564	-0.122619
12	6	0	-2.001213	-1.520573	-0.365679
13	6	0	-2.142053	0.947030	-0.011765
14	1	0	-3.191289	0.931671	-0.317734
15	1	0	-3.451067	-2.868554	-0.656953
16	1	0	-1.330766	-2.357491	-0.543744

17	7	0	-1.624318	2.044632	0.387314
18	7	0	-3.294692	-1.902376	-0.415306
19	6	0	-2.490184	3.209185	0.407135
20	1	0	-2.510281	3.632993	1.415540
21	1	0	-2.084911	3.981099	-0.254361
22	1	0	-3.520374	2.987586	0.098546
23	6	0	-4.469575	-1.135778	-0.052145
24	1	0	-4.295023	-0.587188	0.877632
25	1	0	-4.763435	-0.428150	-0.832178
26	1	0	-5.291523	-1.833140	0.104890
27	8	0	4.247083	-0.455207	0.284299
28	6	0	5.045667	0.488611	-0.413953
29	1	0	6.079753	0.242434	-0.179656
30	1	0	4.891317	0.415190	-1.494432
31	1	0	4.832599	1.509138	-0.082157

Structure 35e (C_2H_5OH)

Energy (Hartrees): -651.500093884
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.870572	0.648491	-0.677835
2	6	0	2.260761	0.635108	-0.600252
3	6	0	2.898710	-0.349556	0.155446
4	6	0	2.133865	-1.302760	0.827536
5	6	0	0.748835	-1.267348	0.745297
6	6	0	0.082369	-0.297955	-0.017401
7	1	0	0.392065	1.413951	-1.277932
8	1	0	2.826841	1.386624	-1.135141
9	1	0	2.638116	-2.058139	1.420376
10	1	0	0.171295	-2.004301	1.294000
11	6	0	-1.400257	-0.309076	-0.152639
12	6	0	-1.990603	-1.515789	-0.420492
13	6	0	-2.149760	0.939189	-0.047819
14	1	0	-3.179583	0.920489	-0.416682
15	1	0	-3.454710	-2.849963	-0.706477
16	1	0	-1.324969	-2.348838	-0.632290
17	7	0	-1.664993	2.031428	0.402212
18	7	0	-3.290520	-1.885652	-0.462693
19	6	0	-2.539946	3.189346	0.392247
20	1	0	-2.644873	3.578403	1.409297
21	1	0	-2.087875	3.986772	-0.205186
22	1	0	-3.539551	2.975077	-0.007643
23	6	0	-4.431994	-1.157723	0.059182
24	1	0	-4.155199	-0.626634	0.974260
25	1	0	-4.836852	-0.439612	-0.658251
26	1	0	-5.214541	-1.877929	0.297108
27	8	0	4.251984	-0.452314	0.295305
28	6	0	5.057808	0.507184	-0.376096
29	1	0	6.089203	0.253302	-0.138009
30	1	0	4.910242	0.455556	-1.458409
31	1	0	4.840958	1.518654	-0.021140

Structure 35f (vacuum)

Energy (Hartrees): -651.473774810
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.856646	0.646076	1.108523
2	6	0	-2.229209	0.800917	1.176717
3	6	0	-3.052461	0.190706	0.227355
4	6	0	-2.479879	-0.566817	-0.790305
5	6	0	-1.091966	-0.698893	-0.851521
6	6	0	-0.254783	-0.111877	0.093149
7	1	0	-0.234518	1.105000	1.869953
8	1	0	-2.694371	1.379904	1.965370
9	1	0	-3.089012	-1.040965	-1.548201
10	1	0	-0.652603	-1.260999	-1.668891
11	6	0	1.227726	-0.269715	0.029411
12	6	0	1.724102	-1.533257	-0.038048
13	6	0	1.985973	0.982383	-0.050862
14	1	0	0.992736	-2.333581	-0.121216
15	1	0	1.456078	1.864155	0.341380
16	1	0	3.077096	-2.997516	0.024174
17	7	0	3.119633	1.116687	-0.609856
18	7	0	3.003612	-1.994891	0.021832
19	6	0	4.109985	-1.294912	0.651844
20	1	0	4.556680	-0.569913	-0.026942
21	1	0	3.758481	-0.757021	1.538556
22	1	0	4.850759	-2.034405	0.955946
23	6	0	3.688730	2.448522	-0.640341
24	1	0	3.911786	2.721064	-1.674842
25	1	0	3.030569	3.212119	-0.203441
26	1	0	4.638067	2.452485	-0.096511
27	8	0	-4.389774	0.395120	0.378377
28	6	0	-5.251207	-0.207467	-0.562037
29	1	0	-6.261586	0.068239	-0.267944
30	1	0	-5.053880	0.161816	-1.573772
31	1	0	-5.152995	-1.297911	-0.547781

Structure 35f ($CHCl_3$)

Energy (Hartrees): -651.493755588
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.853778	0.687987	1.081593
2	6	0	-2.227730	0.844445	1.149910
3	6	0	-3.056054	0.203579	0.224312
4	6	0	-2.486546	-0.587385	-0.770724
5	6	0	-1.098696	-0.722097	-0.832698
6	6	0	-0.255079	-0.103684	0.088897
7	1	0	-0.231992	1.175153	1.825948
8	1	0	-2.684143	1.451650	1.923502
9	1	0	-3.099091	-1.087692	-1.509321
10	1	0	-0.667666	-1.317557	-1.630968
11	6	0	1.227118	-0.270670	0.027180
12	6	0	1.724576	-1.536318	-0.044732
13	6	0	2.003204	0.971756	-0.035227
14	1	0	1.002350	-2.342741	-0.145852
15	1	0	1.535674	1.844653	0.443218
16	1	0	3.084332	-2.992028	0.042925

17	7	0	3.098256	1.105088	-0.670789
18	7	0	3.004056	-1.987780	0.036392
19	6	0	4.092890	-1.283353	0.689394
20	1	0	4.568494	-0.565426	0.021086
21	1	0	3.722704	-0.737658	1.564158
22	1	0	4.823938	-2.021978	1.017773
23	6	0	3.717654	2.416714	-0.655880
24	1	0	3.871119	2.757292	-1.683436
25	1	0	3.129155	3.169327	-0.114791
26	1	0	4.706561	2.346884	-0.192150
27	8	0	-4.392625	0.411398	0.371111
28	6	0	-5.260289	-0.227836	-0.549061
29	1	0	-6.270139	0.060573	-0.263078
30	1	0	-5.065169	0.104925	-1.573105
31	1	0	-5.164928	-1.316545	-0.491798

Structure 35f (DMSO)

Energy (Hartrees): -651.492178820
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.851601	0.759975	1.028910
2	6	0	-2.225850	0.923135	1.089880
3	6	0	-3.059808	0.224308	0.211714
4	6	0	-2.492812	-0.631909	-0.730944
5	6	0	-1.105444	-0.772674	-0.787931
6	6	0	-0.256132	-0.097015	0.088938
7	1	0	-0.230384	1.297274	1.738131
8	1	0	-2.674289	1.584083	1.823331
9	1	0	-3.107090	-1.181215	-1.432540
10	1	0	-0.682280	-1.424882	-1.545122
11	6	0	1.225009	-0.272173	0.033609
12	6	0	1.723468	-1.539124	-0.033938
13	6	0	2.012258	0.964021	-0.030356
14	1	0	1.006245	-2.349986	-0.135015
15	1	0	1.579298	1.836498	0.478431
16	1	0	3.085851	-2.989074	0.071365
17	7	0	3.088666	1.089257	-0.700004
18	7	0	3.004402	-1.983994	0.051714
19	6	0	4.085562	-1.275525	0.714300
20	1	0	4.580549	-0.568522	0.047531
21	1	0	3.703311	-0.715906	1.574982
22	1	0	4.805988	-2.014097	1.064677
23	6	0	3.735421	2.388951	-0.677462
24	1	0	3.871899	2.745523	-1.702103
25	1	0	3.173531	3.141108	-0.109172
26	1	0	4.732843	2.291029	-0.237638
27	8	0	-4.393731	0.442822	0.346635
28	6	0	-5.263195	-0.270970	-0.519262
29	1	0	-6.273623	0.032404	-0.251716
30	1	0	-5.074122	-0.018550	-1.566755
31	1	0	-5.160607	-1.351110	-0.378181

Structure 35f (C_2H_5OH)

Energy (Hartrees): -651.495442906
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.848594	0.730943	1.051330
2	6	0	-2.222902	0.893230	1.113919
3	6	0	-3.052850	0.216917	0.216137
4	6	0	-2.487692	-0.616382	-0.746127
5	6	0	-1.100312	-0.756990	-0.803598
6	6	0	-0.253070	-0.102862	0.091254
7	1	0	-0.228013	1.249047	1.775354
8	1	0	-2.673661	1.535095	1.863034
9	1	0	-3.102098	-1.146918	-1.461932
10	1	0	-0.674795	-1.389998	-1.575694
11	6	0	1.228140	-0.276909	0.033115
12	6	0	1.726160	-1.542639	-0.038077
13	6	0	2.011712	0.962132	-0.023896
14	1	0	1.008563	-2.353576	-0.135949
15	1	0	1.583718	1.824451	0.506050
16	1	0	3.086968	-2.992092	0.080554
17	7	0	3.075924	1.103175	-0.709827
18	7	0	3.009437	-1.987225	0.040509
19	6	0	4.085994	-1.272745	0.705717
20	1	0	4.573417	-0.557957	0.041965
21	1	0	3.702236	-0.722647	1.572070
22	1	0	4.815194	-2.006201	1.048780
23	6	0	3.717170	2.405885	-0.669533
24	1	0	3.841017	2.783577	-1.688016
25	1	0	3.158850	3.144419	-0.080638
26	1	0	4.719776	2.304658	-0.242652
27	8	0	-4.392572	0.434868	0.353838
28	6	0	-5.264040	-0.255992	-0.531397
29	1	0	-6.273154	0.045797	-0.256954
30	1	0	-5.069979	0.022983	-1.570851
31	1	0	-5.163298	-1.338757	-0.413658

Structure 36a (vacuum)

Energy (Hartrees): -741.472505528
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.733180	1.054393	0.544099
2	6	0	-2.117725	1.066810	0.556709
3	6	0	-2.800081	-0.006840	0.002428
4	6	0	-2.131945	-1.080141	-0.570044
5	6	0	-0.747743	-1.067871	-0.590394
6	6	0	-0.014048	-0.010667	-0.025241
7	1	0	-0.198630	1.870065	1.015925
8	1	0	-2.672864	1.880419	1.004008
9	1	0	-2.698442	-1.890038	-1.009768
10	1	0	-0.223326	-1.876858	-1.085180
11	6	0	1.456566	-0.013270	-0.024006
12	6	0	2.133434	-1.197672	0.152866
13	6	0	2.169928	1.238309	-0.198485
14	1	0	1.566536	-2.111677	0.316333
15	1	0	1.547375	2.124909	-0.381874
16	1	0	3.989118	-0.473993	0.057908
17	7	0	3.445370	1.346395	-0.186253
18	7	0	3.460430	-1.341958	0.168596
19	6	0	4.012265	2.660856	-0.411065

20	1	0	4.660988	2.634662	-1.290188
21	1	0	3.248333	3.434551	-0.560318
22	1	0	4.634463	2.940479	0.442728
23	6	0	4.127850	-2.589256	0.472905
24	1	0	3.409730	-3.408123	0.415045
25	1	0	4.922990	-2.778624	-0.249822
26	1	0	4.561222	-2.577670	1.476705
27	7	0	-4.269419	-0.005598	0.017919
28	8	0	-4.839383	-0.954433	-0.480329
29	8	0	-4.827379	0.943447	0.528832

Structure 36a ($CHCl_3$)

Energy (Hartrees): -741.492418779
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.732402	1.068861	0.517832
2	6	0	-2.115695	1.081278	0.530103
3	6	0	-2.800123	-0.007802	0.003382
4	6	0	-2.129106	-1.098114	-0.539187
5	6	0	-0.746416	-1.087381	-0.558615
6	6	0	-0.009902	-0.012359	-0.023595
7	1	0	-0.202705	1.899166	0.969250
8	1	0	-2.661481	1.911183	0.959469
9	1	0	-2.686276	-1.924795	-0.960022
10	1	0	-0.226913	-1.914498	-1.028068
11	6	0	1.457744	-0.011785	-0.024896
12	6	0	2.137047	-1.203641	0.143407
13	6	0	2.166869	1.243178	-0.191530
14	1	0	1.574970	-2.121959	0.297739
15	1	0	1.545907	2.127897	-0.383809
16	1	0	3.997926	-0.485558	0.064565
17	7	0	3.443279	1.357842	-0.166869
18	7	0	3.458467	-1.346834	0.164957
19	6	0	4.001925	2.677186	-0.391873
20	1	0	4.645844	2.658233	-1.275661
21	1	0	3.233398	3.447485	-0.532787
22	1	0	4.629993	2.957893	0.457987
23	6	0	4.126092	-2.602838	0.443302
24	1	0	3.405478	-3.417940	0.371914
25	1	0	4.920725	-2.773207	-0.284428
26	1	0	4.561012	-2.603340	1.446034
27	7	0	-4.260040	-0.005529	0.016335
28	8	0	-4.840692	-0.980002	-0.425354
29	8	0	-4.830061	0.970199	0.468714

Structure 36a (DMSO)

Energy (Hartrees): -741.489801954
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.733572	1.089333	0.475168
2	6	0	-2.116540	1.101125	0.486406
3	6	0	-2.802046	-0.007826	0.002648
4	6	0	-2.128403	-1.118322	-0.496484
5	6	0	-0.746282	-1.108787	-0.515407
6	6	0	-0.008226	-0.012336	-0.023277

7	1	0	-0.208724	1.939961	0.892581
8	1	0	-2.659134	1.949756	0.882075
9	1	0	-2.681228	-1.964194	-0.883804
10	1	0	-0.231271	-1.957699	-0.949069
11	6	0	1.458091	-0.010074	-0.024154
12	6	0	2.139576	-1.205900	0.133778
13	6	0	2.166862	1.246269	-0.181390
14	1	0	1.580059	-2.127105	0.276086
15	1	0	1.549000	2.132532	-0.372804
16	1	0	4.003351	-0.489580	0.065557
17	7	0	3.443996	1.361212	-0.149778
18	7	0	3.458614	-1.348296	0.157423
19	6	0	4.001538	2.682977	-0.369425
20	1	0	4.649827	2.667104	-1.250300
21	1	0	3.231922	3.451622	-0.511986
22	1	0	4.625968	2.963134	0.483540
23	6	0	4.125667	-2.610234	0.415857
24	1	0	3.403807	-3.422769	0.332721
25	1	0	4.920268	-2.767059	-0.314730
26	1	0	4.561040	-2.622934	1.418011
27	7	0	-4.259297	-0.005694	0.015968
28	8	0	-4.841930	-0.992497	-0.398887
29	8	0	-4.831577	0.982413	0.441951

Structure 36a (C_2H_5OH)

Energy (Hartrees): -741.491653891
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.732108	1.095193	0.460848
2	6	0	-2.113868	1.107075	0.474969
3	6	0	-2.800578	-0.007223	0.002111
4	6	0	-2.127316	-1.123186	-0.488553
5	6	0	-0.746449	-1.113934	-0.508789
6	6	0	-0.006670	-0.012188	-0.027825
7	1	0	-0.207271	1.949791	0.869940
8	1	0	-2.654907	1.959651	0.864599
9	1	0	-2.679957	-1.972992	-0.867885
10	1	0	-0.233151	-1.966949	-0.936262
11	6	0	1.457670	-0.010329	-0.029045
12	6	0	2.137778	-1.207707	0.127881
13	6	0	2.167204	1.246612	-0.181672
14	1	0	1.577344	-2.128299	0.269215
15	1	0	1.549309	2.131568	-0.377286
16	1	0	4.002201	-0.494078	0.067057
17	7	0	3.443952	1.363653	-0.143728
18	7	0	3.456008	-1.351880	0.154421
19	6	0	3.996960	2.688507	-0.360059
20	1	0	4.646909	2.677304	-1.239678
21	1	0	3.225451	3.454966	-0.502414
22	1	0	4.618989	2.969234	0.494329
23	6	0	4.119362	-2.615701	0.415368
24	1	0	3.398794	-3.427774	0.318206
25	1	0	4.923447	-2.769124	-0.305371
26	1	0	4.541449	-2.634326	1.423108
27	7	0	-4.250913	-0.005302	0.018467
28	8	0	-4.841065	-0.990799	-0.393908
29	8	0	-4.829414	0.981177	0.444773

Structure 36b (vacuum)

Energy (Hartrees): -741.462516754
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.471703	-1.091490	0.655223
2	6	0	-1.855929	-1.135725	0.685530
3	6	0	-2.567455	-0.174225	-0.018198
4	6	0	-1.935297	0.813664	-0.758698
5	6	0	-0.549604	0.839020	-0.783787
6	6	0	0.211270	-0.102866	-0.071935
7	1	0	0.094906	-1.821149	1.221834
8	1	0	-2.389210	-1.888609	1.250275
9	1	0	-2.527979	1.529124	-1.312738
10	1	0	-0.043582	1.574082	-1.399322
11	6	0	1.682726	-0.075591	-0.095137
12	6	0	2.411360	1.068001	0.014357
13	6	0	2.406689	-1.351106	-0.211970
14	1	0	1.780354	-2.226259	-0.443492
15	1	0	3.492841	0.961983	-0.017642
16	7	0	3.663370	-1.465850	-0.087920
17	7	0	1.962749	2.337087	0.167547
18	1	0	0.982950	2.459012	0.382653
19	6	0	2.854265	3.409284	0.574463
20	1	0	3.819098	3.273034	0.085721
21	1	0	2.444499	4.366988	0.253996
22	1	0	3.010729	3.433609	1.657627
23	6	0	4.244182	-2.775811	-0.289966
24	1	0	4.939811	-2.738049	-1.132412
25	1	0	4.825461	-3.054326	0.592426
26	1	0	3.495780	-3.555973	-0.485387
27	7	0	-4.039032	-0.207085	0.016227
28	8	0	-4.634715	0.666894	-0.578073
29	8	0	-4.567572	-1.104578	0.637599

Structure 36b ($CHCl_3$)

Energy (Hartrees): -741.484109236
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.486080	-1.139545	0.568506
2	6	0	-1.869107	-1.180925	0.594516
3	6	0	-2.578682	-0.151276	-0.012104
4	6	0	-1.938790	0.903669	-0.650980
5	6	0	-0.554785	0.925577	-0.674020
6	6	0	0.206134	-0.086867	-0.059919
7	1	0	0.070614	-1.926971	1.063136
8	1	0	-2.395475	-1.987121	1.088384
9	1	0	-2.518033	1.677689	-1.136894
10	1	0	-0.055724	1.718361	-1.219082
11	6	0	1.673969	-0.077542	-0.089964
12	6	0	2.435933	1.056416	0.015142
13	6	0	2.372766	-1.361698	-0.221767
14	1	0	1.742418	-2.208753	-0.527792
15	1	0	3.513252	0.927525	-0.052908
16	7	0	3.619807	-1.526218	-0.031412
17	7	0	2.039024	2.322884	0.209356
18	1	0	1.069197	2.499766	0.434582
19	6	0	2.976292	3.400549	0.480505
20	1	0	3.918955	3.189097	-0.023929

21	1	0	2.578098	4.337548	0.091030
22	1	0	3.164648	3.512934	1.552223
23	6	0	4.166040	-2.845618	-0.280419
24	1	0	4.921660	-2.786147	-1.069163
25	1	0	4.672652	-3.206299	0.619033
26	1	0	3.405188	-3.578659	-0.578824
27	7	0	-4.041276	-0.182951	0.014464
28	8	0	-4.643985	0.748838	-0.483845
29	8	0	-4.585074	-1.139015	0.533391

Structure 36b (DMSO)

Energy (Hartrees): -741.482294713
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.488024	-1.150267	0.547208
2	6	0	-1.870624	-1.190900	0.571286
3	6	0	-2.580227	-0.147147	-0.012038
4	6	0	-1.937605	0.921837	-0.625848
5	6	0	-0.554033	0.943355	-0.647944
6	6	0	0.206989	-0.084313	-0.057685
7	1	0	0.064941	-1.949825	1.026277
8	1	0	-2.393935	-2.008836	1.048975
9	1	0	-2.511426	1.710376	-1.094768
10	1	0	-0.059389	1.751271	-1.174235
11	6	0	1.673415	-0.078856	-0.086391
12	6	0	2.443395	1.055453	0.023698
13	6	0	2.366576	-1.363307	-0.218712
14	1	0	1.735187	-2.207000	-0.530271
15	1	0	3.519819	0.923682	-0.052763
16	7	0	3.613349	-1.539374	-0.022172
17	7	0	2.057551	2.314899	0.238288
18	1	0	1.083393	2.508877	0.431829
19	6	0	2.989398	3.411738	0.442063
20	1	0	3.982332	3.098417	0.121490
21	1	0	2.684681	4.276029	-0.149705
22	1	0	3.029373	3.700122	1.495421
23	6	0	4.146896	-2.864138	-0.278546
24	1	0	4.902753	-2.809944	-1.067896
25	1	0	4.650102	-3.235860	0.618661
26	1	0	3.377468	-3.586500	-0.579840
27	7	0	-4.040464	-0.179021	0.012962
28	8	0	-4.645208	0.766235	-0.460179
29	8	0	-4.586704	-1.149620	0.505271

Structure 36b (C_2H_5OH)

Energy (Hartrees): -741.484265752
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.484263	-1.157305	0.526141
2	6	0	-1.865785	-1.199398	0.556113
3	6	0	-2.578264	-0.149239	-0.014025
4	6	0	-1.939215	0.925896	-0.622693
5	6	0	-0.556659	0.948113	-0.650452

6	6	0	0.207863	-0.083876	-0.070653
7	1	0	0.071643	-1.959630	0.997220
8	1	0	-2.385783	-2.021759	1.030007
9	1	0	-2.515387	1.717356	-1.084030
10	1	0	-0.065059	1.759025	-1.174683
11	6	0	1.672624	-0.076021	-0.098563
12	6	0	2.442019	1.058773	0.015326
13	6	0	2.366484	-1.360532	-0.228155
14	1	0	1.741587	-2.197524	-0.569079
15	1	0	3.518439	0.927689	-0.058869
16	7	0	3.606553	-1.543629	0.002040
17	7	0	2.056202	2.317848	0.232667
18	1	0	1.081628	2.511229	0.424455
19	6	0	2.989022	3.412301	0.447754
20	1	0	3.981557	3.103387	0.121759
21	1	0	2.683316	4.283577	-0.133207
22	1	0	3.030700	3.688322	1.504431
23	6	0	4.139610	-2.867433	-0.262938
24	1	0	4.915641	-2.804619	-1.031546
25	1	0	4.617749	-3.257247	0.639943
26	1	0	3.375587	-3.580688	-0.596675
27	7	0	-4.032490	-0.178841	0.020838
28	8	0	-4.644113	0.775508	-0.427987
29	8	0	-4.583898	-1.156063	0.497279

Structure 36c (vacuum)

Energy (Hartrees): -741.464282981
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.286573	0.913082	0.777978
2	6	0	1.671678	0.914222	0.809115
3	6	0	2.358229	0.025249	-0.006306
4	6	0	1.706211	-0.852344	-0.857293
5	6	0	0.318786	-0.841216	-0.876094
6	6	0	-0.411540	0.027525	-0.053811
7	1	0	-0.268821	1.608740	1.391539
8	1	0	2.225213	1.587241	1.449817
9	1	0	2.282012	-1.513030	-1.491197
10	1	0	-0.209798	-1.496016	-1.560117
11	6	0	-1.889951	0.004430	-0.071018
12	6	0	-2.597945	-1.152178	0.005400
13	6	0	-2.657368	1.246664	-0.155518
14	1	0	-3.683908	-1.092359	-0.018708
15	1	0	-3.751043	1.111018	-0.185324
16	7	0	-2.139936	2.402803	-0.198070
17	7	0	-2.120784	-2.423260	0.100231
18	1	0	-1.135650	-2.518965	0.305029
19	6	0	-3.035256	3.535935	-0.295673
20	1	0	-2.801949	4.100669	-1.201583
21	1	0	-4.096616	3.251759	-0.317066
22	1	0	-2.866025	4.206544	0.550535
23	6	0	-2.980112	-3.504514	0.550290
24	1	0	-3.936844	-3.442635	0.029639
25	1	0	-2.521588	-4.459363	0.295728
26	1	0	-3.164624	-3.476545	1.629539
27	7	0	3.832343	0.018930	0.027236
28	8	0	4.406801	-0.802932	-0.655875
29	8	0	4.382256	0.833244	0.737620

Structure 36c ($CHCl_3$)

Energy (Hartrees): -741.486384992
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.304674	0.914199	0.785672
2	6	0	1.689023	0.914767	0.812068
3	6	0	2.370847	0.021957	-0.005877
4	6	0	1.711444	-0.858906	-0.850494
5	6	0	0.324737	-0.844730	-0.864383
6	6	0	-0.402681	0.029388	-0.042715
7	1	0	-0.241286	1.603915	1.415274
8	1	0	2.237577	1.588716	1.456549
9	1	0	2.274334	-1.527203	-1.488397
10	1	0	-0.201690	-1.506197	-1.543654
11	6	0	-1.879888	0.013710	-0.049752
12	6	0	-2.601547	-1.143389	0.035319
13	6	0	-2.647065	1.251304	-0.131917
14	1	0	-3.686684	-1.066294	0.026332
15	1	0	-3.738978	1.112610	-0.115075
16	7	0	-2.141538	2.414109	-0.231624
17	7	0	-2.147103	-2.408857	0.132694
18	1	0	-1.157386	-2.548771	0.288000
19	6	0	-3.058742	3.533813	-0.314880
20	1	0	-2.874925	4.087262	-1.240011
21	1	0	-4.114942	3.233475	-0.288008
22	1	0	-2.868908	4.224594	0.511593
23	6	0	-3.022666	-3.508959	0.500939
24	1	0	-3.995509	-3.367641	0.028471
25	1	0	-2.599418	-4.445295	0.138235
26	1	0	-3.162328	-3.578316	1.584307
27	7	0	3.837769	0.012567	0.021385
28	8	0	4.417082	-0.823841	-0.644173
29	8	0	4.402597	0.839528	0.709837

Structure 36c (DMSO)

Energy (Hartrees): -741.485374044
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.312802	0.913188	0.794622
2	6	0	1.696861	0.913077	0.814767
3	6	0	2.374322	0.017023	-0.004564
4	6	0	1.708797	-0.867473	-0.841282
5	6	0	0.322100	-0.850858	-0.850356
6	6	0	-0.401240	0.028731	-0.030408
7	1	0	-0.228030	1.599612	1.433129
8	1	0	2.245923	1.586434	1.459658
9	1	0	2.263623	-1.542497	-1.479334
10	1	0	-0.205430	-1.517912	-1.523449
11	6	0	-1.876974	0.021823	-0.029532
12	6	0	-2.609411	-1.134139	0.063609
13	6	0	-2.637784	1.259033	-0.113975
14	1	0	-3.693776	-1.046475	0.066691
15	1	0	-3.728495	1.127063	-0.061189
16	7	0	-2.133271	2.420955	-0.258972
17	7	0	-2.164159	-2.394258	0.161829
18	1	0	-1.170102	-2.555481	0.262726
19	6	0	-3.056815	3.538254	-0.332646
20	1	0	-2.903563	4.081061	-1.269977

21	1	0	-4.109737	3.232681	-0.272310
22	1	0	-2.849376	4.240972	0.479988
23	6	0	-3.037792	-3.518164	0.454083
24	1	0	-4.051016	-3.274060	0.134791
25	1	0	-2.700927	-4.398364	-0.094140
26	1	0	-3.049093	-3.749245	1.522965
27	7	0	3.839659	0.007451	0.014962
28	8	0	4.416773	-0.849034	-0.628303
29	8	0	4.410127	0.855810	0.674530

Structure 36c (C_2H_5OH)

Energy (Hartrees): -741.486948026
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.314655	0.888039	0.824362
2	6	0	1.698429	0.886223	0.845772
3	6	0	2.374797	0.016026	-0.002370
4	6	0	1.709525	-0.844307	-0.865048
5	6	0	0.323387	-0.829697	-0.869882
6	6	0	-0.398790	0.027755	-0.025728
7	1	0	-0.225532	1.555876	1.482819
8	1	0	2.247071	1.540551	1.510317
9	1	0	2.263722	-1.500161	-1.523403
10	1	0	-0.205704	-1.479217	-1.558482
11	6	0	-1.874880	0.021496	-0.029171
12	6	0	-2.605932	-1.134522	0.055806
13	6	0	-2.635583	1.258736	-0.117697
14	1	0	-3.690527	-1.048711	0.048461
15	1	0	-3.726306	1.123812	-0.077535
16	7	0	-2.133129	2.422537	-0.254578
17	7	0	-2.160504	-2.396421	0.156288
18	1	0	-1.169150	-2.555299	0.283731
19	6	0	-3.064818	3.533224	-0.339742
20	1	0	-2.906252	4.075389	-1.276372
21	1	0	-4.115891	3.220612	-0.289730
22	1	0	-2.871333	4.239703	0.472756
23	6	0	-3.044820	-3.508950	0.463012
24	1	0	-4.019881	-3.329556	0.009013
25	1	0	-2.631586	-4.425926	0.043568
26	1	0	-3.174183	-3.640174	1.541502
27	7	0	3.836420	0.008908	0.012511
28	8	0	4.419618	-0.764232	-0.725167
29	8	0	4.411660	0.775957	0.762408

Structure 36d (vacuum)

Energy (Hartrees): -741.459254655
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.544886	0.891084	0.672961
2	6	0	-1.927946	0.847942	0.706449
3	6	0	-2.583016	-0.165433	0.018679
4	6	0	-1.895414	-1.124191	-0.707152
5	6	0	-0.510048	-1.062329	-0.735319

6	6	0	0.191092	-0.071867	-0.033648
7	1	0	-0.022233	1.677523	1.198983
8	1	0	-2.503857	1.579232	1.257030
9	1	0	-2.442925	-1.884555	-1.247357
10	1	0	0.037893	-1.778614	-1.335905
11	6	0	1.669602	-0.068344	-0.021104
12	6	0	2.321201	-1.259470	0.075791
13	6	0	2.416637	1.186701	-0.099349
14	1	0	3.502258	1.118446	0.077479
15	1	0	4.277786	-0.726583	-0.145373
16	1	0	1.731343	-2.159716	0.232431
17	7	0	1.890512	2.315111	-0.340754
18	7	0	3.655495	-1.509464	-0.024550
19	6	0	2.759916	3.470613	-0.377336
20	1	0	3.814844	3.230156	-0.183842
21	1	0	2.676905	3.947897	-1.356740
22	1	0	2.421534	4.200876	0.362049
23	6	0	4.234539	-2.713940	0.542718
24	1	0	3.585889	-3.561846	0.316246
25	1	0	5.204942	-2.900199	0.083598
26	1	0	4.360861	-2.651767	1.628682
27	7	0	-4.054086	-0.216704	0.051821
28	8	0	-4.600472	-1.122986	-0.542360
29	8	0	-4.634372	0.648231	0.673729

Structure 36d ($CHCl_3$)

Energy (Hartrees): -741.483020791
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.559073	0.943501	0.608133
2	6	0	-1.941239	0.903766	0.636824
3	6	0	-2.595565	-0.154696	0.014766
4	6	0	-1.899670	-1.161254	-0.640503
5	6	0	-0.516064	-1.101090	-0.666923
6	6	0	0.187501	-0.064211	-0.029134
7	1	0	-0.044266	1.759724	1.095877
8	1	0	-2.510016	1.674076	1.140609
9	1	0	-2.434455	-1.960791	-1.135895
10	1	0	0.028413	-1.861825	-1.213624
11	6	0	1.660749	-0.060109	-0.003248
12	6	0	2.312286	-1.262199	0.100087
13	6	0	2.423515	1.184177	-0.056052
14	1	0	3.487304	1.108336	0.214283
15	1	0	4.270792	-0.745911	-0.157653
16	1	0	1.722180	-2.160573	0.266171
17	7	0	1.939265	2.315800	-0.377937
18	7	0	3.632863	-1.508735	0.016205
19	6	0	2.833557	3.455737	-0.357537
20	1	0	3.865739	3.194488	-0.087933
21	1	0	2.833384	3.931977	-1.341646
22	1	0	2.460564	4.197805	0.354234
23	6	0	4.215346	-2.760178	0.468230
24	1	0	3.495898	-3.564975	0.310376
25	1	0	5.110805	-2.977933	-0.113572
26	1	0	4.479430	-2.729241	1.529537
27	7	0	-4.057073	-0.205253	0.044070
28	8	0	-4.610372	-1.150542	-0.486134
29	8	0	-4.652030	0.698228	0.600511

Structure 36d (DMSO)

Energy (Hartrees): -741.482698445
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.566674	0.946441	0.608857
2	6	0	-1.948618	0.907315	0.627012
3	6	0	-2.599024	-0.161652	0.017387
4	6	0	-1.895263	-1.182400	-0.609217
5	6	0	-0.511899	-1.123898	-0.625175
6	6	0	0.188342	-0.071546	-0.005614
7	1	0	-0.058352	1.768839	1.093562
8	1	0	-2.517925	1.686914	1.115940
9	1	0	-2.421990	-1.994403	-1.093158
10	1	0	0.034260	-1.899706	-1.148833
11	6	0	1.658500	-0.055711	0.022473
12	6	0	2.323410	-1.256957	0.122898
13	6	0	2.412810	1.191558	-0.037325
14	1	0	3.472012	1.128702	0.248965
15	1	0	4.274177	-0.715886	-0.130431
16	1	0	1.742229	-2.162269	0.282539
17	7	0	1.928018	2.315783	-0.391792
18	7	0	3.640551	-1.483164	0.046946
19	6	0	2.820888	3.459027	-0.375739
20	1	0	3.849105	3.200076	-0.091679
21	1	0	2.833164	3.923200	-1.365849
22	1	0	2.440743	4.209702	0.323580
23	6	0	4.242752	-2.755711	0.404908
24	1	0	3.500540	-3.545999	0.288173
25	1	0	5.082454	-2.960880	-0.259133
26	1	0	4.598954	-2.755335	1.438686
27	7	0	-4.058266	-0.208234	0.030710
28	8	0	-4.609969	-1.161069	-0.490402
29	8	0	-4.659136	0.707013	0.564629

Structure 36d (C_2H_5OH)

Energy (Hartrees): -741.484488053
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.567901	0.953557	0.599899
2	6	0	-1.948881	0.916797	0.620668
3	6	0	-2.601768	-0.153503	0.013767
4	6	0	-1.900845	-1.175811	-0.615560
5	6	0	-0.518464	-1.119051	-0.633611
6	6	0	0.184385	-0.067903	-0.013364
7	1	0	-0.057450	1.774996	1.084180
8	1	0	-2.515401	1.697748	1.111011
9	1	0	-2.428624	-1.986574	-1.100525
10	1	0	0.026028	-1.894038	-1.160189
11	6	0	1.652745	-0.058377	0.019098
12	6	0	2.312145	-1.262679	0.116862
13	6	0	2.415345	1.185097	-0.025789
14	1	0	3.463008	1.117425	0.299209
15	1	0	4.264544	-0.725328	-0.133229
16	1	0	1.728501	-2.166612	0.274953
17	7	0	1.952130	2.309111	-0.408233
18	7	0	3.629159	-1.492532	0.038472
19	6	0	2.856802	3.443300	-0.364825
20	1	0	3.867947	3.176172	-0.032207

21	1	0	2.919712	3.896637	-1.357827
22	1	0	2.455412	4.205875	0.308987
23	6	0	4.226389	-2.762103	0.417257
24	1	0	3.488404	-3.554810	0.290353
25	1	0	5.079565	-2.970889	-0.228148
26	1	0	4.561744	-2.755128	1.458025
27	7	0	-4.054832	-0.200617	0.034855
28	8	0	-4.615144	-1.159236	-0.469666
29	8	0	-4.659644	0.718841	0.560083

Structure 36e (vacuum)

Energy (Hartrees): -741.456293393
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.538974	0.879056	-0.637636
2	6	0	1.921019	0.938867	-0.603112
3	6	0	2.621524	-0.098793	-0.001018
4	6	0	1.978703	-1.183708	0.570881
5	6	0	0.592251	-1.224749	0.530959
6	6	0	-0.152141	-0.211093	-0.087345
7	1	0	-0.017117	1.682195	-1.100059
8	1	0	2.462530	1.768294	-1.037359
9	1	0	2.557883	-1.961554	1.049676
10	1	0	0.075032	-2.045213	1.014300
11	6	0	-1.625914	-0.319016	-0.184972
12	6	0	-2.146384	-1.541078	-0.489331
13	6	0	-2.460610	0.877964	-0.041126
14	1	0	-3.494879	0.792516	-0.396691
15	1	0	-3.583946	-2.901479	-0.830706
16	1	0	-1.447341	-2.320875	-0.779902
17	7	0	-2.029974	1.980840	0.415466
18	7	0	-3.440755	-1.964964	-0.494920
19	6	0	-2.954958	3.092697	0.458675
20	1	0	-3.034474	3.452139	1.487498
21	1	0	-2.556608	3.918868	-0.135958
22	1	0	-3.958744	2.840599	0.088650
23	6	0	-4.539456	-1.384215	0.255788
24	1	0	-4.149737	-0.881487	1.144178
25	1	0	-5.119696	-0.666893	-0.329603
26	1	0	-5.208315	-2.184014	0.574972
27	7	0	4.092309	-0.039470	0.040755
28	8	0	4.678233	-0.954336	0.581647
29	8	0	4.632555	0.918895	-0.470234

Structure 36e ($CHCl_3$)

Energy (Hartrees): -741.479981810
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.538128	0.868876	-0.637796
2	6	0	1.919159	0.932499	-0.613127
3	6	0	2.626904	-0.099399	-0.004652
4	6	0	1.986671	-1.183029	0.578480
5	6	0	0.601129	-1.226781	0.548819
6	6	0	-0.152453	-0.216937	-0.070913
7	1	0	-0.017455	1.663520	-1.116464

8	1	0	2.447828	1.760829	-1.065822
9	1	0	2.561093	-1.962508	1.061302
10	1	0	0.092799	-2.049131	1.038535
11	6	0	-1.624996	-0.319193	-0.155622
12	6	0	-2.148600	-1.558946	-0.420374
13	6	0	-2.450463	0.882434	-0.028687
14	1	0	-3.481684	0.804105	-0.386995
15	1	0	-3.547051	-2.954913	-0.722144
16	1	0	-1.443836	-2.346382	-0.673800
17	7	0	-2.021765	1.988255	0.433488
18	7	0	-3.422983	-1.999317	-0.427247
19	6	0	-2.949140	3.101544	0.458170
20	1	0	-3.034108	3.479384	1.480718
21	1	0	-2.553180	3.919982	-0.150051
22	1	0	-3.950826	2.841320	0.090679
23	6	0	-4.593564	-1.351147	0.136147
24	1	0	-4.319468	-0.803611	1.041125
25	1	0	-5.071333	-0.664194	-0.566566
26	1	0	-5.313911	-2.124185	0.402622
27	7	0	4.089108	-0.036822	0.026367
28	8	0	4.692708	-0.957684	0.543860
29	8	0	4.632787	0.931613	-0.469368

Structure 36e (DMSO)

Energy (Hartrees): -741.479651528
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.538054	0.873050	-0.628511
2	6	0	1.918767	0.938893	-0.603080
3	6	0	2.629455	-0.098482	-0.005935
4	6	0	1.989528	-1.191151	0.562228
5	6	0	0.604432	-1.236771	0.533852
6	6	0	-0.153309	-0.219485	-0.071663
7	1	0	-0.016150	1.670209	-1.105265
8	1	0	2.442822	1.773347	-1.050201
9	1	0	2.561378	-1.978674	1.035162
10	1	0	0.100706	-2.069038	1.011375
11	6	0	-1.624036	-0.320296	-0.152354
12	6	0	-2.149491	-1.566284	-0.407146
13	6	0	-2.449716	0.880222	-0.033072
14	1	0	-3.476044	0.805404	-0.403964
15	1	0	-3.542744	-2.964621	-0.690107
16	1	0	-1.446470	-2.356992	-0.655366
17	7	0	-2.027632	1.986344	0.440018
18	7	0	-3.418146	-2.004283	-0.406666
19	6	0	-2.956568	3.100477	0.446757
20	1	0	-3.051830	3.489210	1.464583
21	1	0	-2.557313	3.913077	-0.167741
22	1	0	-3.953761	2.833625	0.073424
23	6	0	-4.595132	-1.342188	0.127612
24	1	0	-4.332628	-0.780731	1.027554
25	1	0	-5.056177	-0.664323	-0.594311
26	1	0	-5.320997	-2.110167	0.392359
27	7	0	4.089304	-0.032733	0.027210
28	8	0	4.697597	-0.968384	0.514539
29	8	0	4.631480	0.954191	-0.436234

Structure 36e (C_2H_5OH)

Energy (Hartrees): -741.481534809
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.540840	0.874522	-0.631571
2	6	0	1.920695	0.941915	-0.606775
3	6	0	2.632017	-0.095319	-0.008298
4	6	0	1.993282	-1.189877	0.559855
5	6	0	0.609294	-1.237086	0.530286
6	6	0	-0.149340	-0.219350	-0.074870
7	1	0	-0.014313	1.670892	-1.108558
8	1	0	2.442962	1.776738	-1.055395
9	1	0	2.565254	-1.976549	1.034392
10	1	0	0.106090	-2.069110	1.008799
11	6	0	-1.618581	-0.320632	-0.155261
12	6	0	-2.143303	-1.568189	-0.403687
13	6	0	-2.447919	0.877983	-0.039906
14	1	0	-3.468179	0.800962	-0.426141
15	1	0	-3.536766	-2.967996	-0.682793
16	1	0	-1.440175	-2.359863	-0.648260
17	7	0	-2.039335	1.982721	0.448391
18	7	0	-3.412164	-2.006627	-0.402983
19	6	0	-2.982823	3.085805	0.451909
20	1	0	-3.096216	3.464705	1.471424
21	1	0	-2.587091	3.909572	-0.149480
22	1	0	-3.971652	2.810232	0.063799
23	6	0	-4.590464	-1.339455	0.123561
24	1	0	-4.330151	-0.770420	1.019281
25	1	0	-5.051389	-0.669165	-0.605418
26	1	0	-5.316728	-2.104944	0.394689
27	7	0	4.085945	-0.027670	0.028953
28	8	0	4.699253	-0.955511	0.527969
29	8	0	4.635128	0.953521	-0.441510

Structure 36f (vacuum)

Energy (Hartrees): -741.454566128
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.666598	0.744407	0.856880
2	6	0	-2.048564	0.844336	0.859293
3	6	0	-2.776786	0.017420	0.016305
4	6	0	-2.161089	-0.893344	-0.829238
5	6	0	-0.777630	-0.969757	-0.827653
6	6	0	-0.002039	-0.165503	0.021105
7	1	0	-0.093561	1.363002	1.537312
8	1	0	-2.567039	1.536385	1.509141
9	1	0	-2.764281	-1.507277	-1.484608
10	1	0	-0.284917	-1.645364	-1.517033
11	6	0	1.479281	-0.265014	0.029772
12	6	0	2.018577	-1.517419	0.061573
13	6	0	2.208025	1.001860	-0.097062
14	1	0	1.320788	-2.347463	-0.014274
15	1	0	1.651328	1.896876	0.217010
16	1	0	3.410145	-2.928787	0.271688
17	7	0	3.355392	1.119442	-0.628613
18	7	0	3.295176	-1.930498	0.236081
19	6	0	4.368147	-1.154943	0.834587
20	1	0	4.822506	-0.481337	0.109649

21	1	0	3.976824	-0.553710	1.660613
22	1	0	5.110132	-1.851285	1.224106
23	6	0	3.905456	2.455846	-0.733771
24	1	0	4.137040	2.666649	-1.780489
25	1	0	3.230973	3.234268	-0.352464
26	1	0	4.847586	2.505989	-0.180561
27	7	0	-4.245312	0.113716	0.016689
28	8	0	-4.858905	-0.626775	-0.722991
29	8	0	-4.755468	0.927538	0.757999

Structure 36f ($CHCl_3$)

Energy (Hartrees): -741.476347648
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.665934	0.793350	0.807737
2	6	0	-2.046854	0.892881	0.810820
3	6	0	-2.780704	0.021919	0.015284
4	6	0	-2.165839	-0.933401	-0.784424
5	6	0	-0.784131	-1.011357	-0.783675
6	6	0	-0.001524	-0.162157	0.019007
7	1	0	-0.096342	1.450826	1.453530
8	1	0	-2.552924	1.621430	1.430307
9	1	0	-2.762824	-1.584908	-1.408954
10	1	0	-0.300725	-1.727871	-1.437516
11	6	0	1.476235	-0.264335	0.029621
12	6	0	2.020966	-1.520289	0.049249
13	6	0	2.219849	0.995579	-0.075759
14	1	0	1.335635	-2.357726	-0.050453
15	1	0	1.720322	1.888282	0.323992
16	1	0	3.417873	-2.921145	0.273860
17	7	0	3.333925	1.108808	-0.679665
18	7	0	3.292145	-1.921470	0.246390
19	6	0	4.357701	-1.142130	0.850405
20	1	0	4.834733	-0.480828	0.127071
21	1	0	3.959786	-0.528015	1.663822
22	1	0	5.089782	-1.838414	1.258057
23	6	0	3.928225	2.431213	-0.731759
24	1	0	4.147447	2.688416	-1.771212
25	1	0	3.289134	3.210333	-0.296360
26	1	0	4.882631	2.422859	-0.196299
27	7	0	-4.240332	0.115664	0.017246
28	8	0	-4.867212	-0.672111	-0.665689
29	8	0	-4.759366	0.975627	0.703605

Structure 36f (DMSO)

Energy (Hartrees): -741.475278691
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.664302	0.832319	0.759985
2	6	0	-2.044716	0.933861	0.760325
3	6	0	-2.784206	0.021257	0.017703
4	6	0	-2.171360	-0.981355	-0.725722
5	6	0	-0.790750	-1.063758	-0.722156
6	6	0	-0.001811	-0.170158	0.026970

7	1	0	-0.096228	1.528414	1.364465
8	1	0	-2.543985	1.700655	1.337861
9	1	0	-2.766484	-1.668642	-1.312559
10	1	0	-0.314994	-1.821740	-1.332977
11	6	0	1.472947	-0.271318	0.035834
12	6	0	2.029294	-1.524488	0.042149
13	6	0	2.226452	0.986585	-0.045381
14	1	0	1.358328	-2.371883	-0.067093
15	1	0	1.787592	1.863771	0.446457
16	1	0	3.444155	-2.906400	0.267411
17	7	0	3.297932	1.108610	-0.721920
18	7	0	3.303926	-1.907588	0.240735
19	6	0	4.360035	-1.113933	0.842129
20	1	0	4.842592	-0.458632	0.115760
21	1	0	3.953346	-0.490824	1.644375
22	1	0	5.093064	-1.801288	1.262373
23	6	0	3.934842	2.413291	-0.727089
24	1	0	4.070170	2.746944	-1.759408
25	1	0	3.367132	3.173381	-0.175858
26	1	0	4.932316	2.330802	-0.284408
27	7	0	-4.240823	0.120717	0.013025
28	8	0	-4.872245	-0.708522	-0.617168
29	8	0	-4.759356	1.027201	0.639947

Structure 36f (C_2H_5OH)

Energy (Hartrees): -741.477040319
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.663652	0.868573	0.707963
2	6	0	-2.042644	0.971525	0.706493
3	6	0	-2.787010	0.018098	0.020578
4	6	0	-2.176006	-1.028721	-0.663656
5	6	0	-0.797102	-1.113312	-0.657453
6	6	0	-0.001243	-0.178325	0.035507
7	1	0	-0.098860	1.603245	1.266904
8	1	0	-2.537551	1.773116	1.239208
9	1	0	-2.771339	-1.749138	-1.209334
10	1	0	-0.328025	-1.906119	-1.227210
11	6	0	1.470368	-0.278335	0.043891
12	6	0	2.034791	-1.528458	0.041984
13	6	0	2.232137	0.978409	-0.015214
14	1	0	1.371557	-2.381574	-0.065444
15	1	0	1.843633	1.833535	0.551110
16	1	0	3.461214	-2.901420	0.254573
17	7	0	3.265042	1.120471	-0.745042
18	7	0	3.312495	-1.903818	0.231352
19	6	0	4.376336	-1.098348	0.803001
20	1	0	4.841666	-0.448867	0.060328
21	1	0	3.984927	-0.470291	1.608826
22	1	0	5.122164	-1.777475	1.214017
23	6	0	3.926346	2.413298	-0.705144
24	1	0	4.038312	2.796355	-1.722589
25	1	0	3.389136	3.154019	-0.100099
26	1	0	4.934029	2.292728	-0.295674
27	7	0	-4.235719	0.123444	0.008563
28	8	0	-4.877715	-0.732438	-0.577001
29	8	0	-4.756974	1.064285	0.583698

Structure 37a (vacuum)

Energy (Hartrees): -1028.28229859
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.742825	0.781742	-0.746168
2	6	0	4.937705	0.065780	-0.713248
3	6	0	5.081688	-0.990823	0.183930
4	6	0	4.030469	-1.309906	1.047218
5	6	0	2.856964	-0.579886	1.011497
6	6	0	2.682858	0.475888	0.105351
7	1	0	3.633382	1.579750	-1.473040
8	1	0	5.732740	0.334037	-1.395531
9	1	0	4.168538	-2.122860	1.749295
10	1	0	2.064352	-0.813886	1.714349
11	6	0	1.416499	1.241706	0.053602
12	6	0	0.216331	0.591967	0.056544
13	6	0	1.465505	2.698550	0.030738
14	1	0	0.208287	-0.492349	0.064986
15	1	0	2.476916	3.140992	0.051196
16	8	0	0.487295	3.430047	0.010857
17	7	0	-0.995711	1.197962	0.060022
18	1	0	-0.963997	2.215737	0.093481
19	6	0	-2.235689	0.571595	0.006231
20	6	0	-3.373908	1.357496	0.240850
21	6	0	-2.387766	-0.791268	-0.281954
22	6	0	-4.635819	0.797370	0.202843
23	1	0	-3.254075	2.411943	0.461047
24	6	0	-3.651078	-1.357066	-0.312163
25	1	0	-1.533267	-1.414243	-0.507237
26	6	0	-4.758533	-0.559408	-0.067756
27	1	0	-5.522248	1.389598	0.385995
28	1	0	-3.789267	-2.406516	-0.534993
29	8	0	6.195220	-1.757496	0.295886
30	6	0	7.278542	-1.475234	-0.565820
31	1	0	8.053752	-2.198148	-0.322550
32	1	0	6.988923	-1.591544	-1.614915
33	1	0	7.660954	-0.462863	-0.401984
34	7	0	-6.096660	-1.163120	-0.105724
35	8	0	-7.045900	-0.437661	0.104728
36	8	0	-6.171359	-2.350459	-0.344014

Structure 37a ($CHCl_3$)

Energy (Hartrees): -1028.30949310
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.774195	0.821527	-0.697114
2	6	0	4.969573	0.104934	-0.661411
3	6	0	5.079067	-1.008579	0.170323
4	6	0	3.991660	-1.385595	0.964106
5	6	0	2.817313	-0.654915	0.927524
6	6	0	2.678625	0.460582	0.088171
7	1	0	3.697383	1.668514	-1.371210
8	1	0	5.793268	0.417782	-1.289405
9	1	0	4.096234	-2.243917	1.617712
10	1	0	1.996257	-0.941397	1.576297
11	6	0	1.415869	1.235699	0.044066
12	6	0	0.211203	0.588039	0.029397
13	6	0	1.480298	2.687512	0.054177

14	1	0	0.199782	-0.496034	0.009437
15	1	0	2.492766	3.121826	0.104035
16	8	0	0.507613	3.433497	0.031816
17	7	0	-0.998798	1.193457	0.048863
18	1	0	-0.982878	2.209242	0.115450
19	6	0	-2.239745	0.569509	-0.003933
20	6	0	-3.372353	1.359488	0.248316
21	6	0	-2.397143	-0.790753	-0.304759
22	6	0	-4.636011	0.804842	0.217607
23	1	0	-3.245710	2.411724	0.476729
24	6	0	-3.661875	-1.350801	-0.330532
25	1	0	-1.546120	-1.416445	-0.536582
26	6	0	-4.765798	-0.550540	-0.066435
27	1	0	-5.511947	1.407231	0.418380
28	1	0	-3.795069	-2.398765	-0.563973
29	8	0	6.191241	-1.778347	0.278536
30	6	0	7.320529	-1.420527	-0.501462
31	1	0	8.093868	-2.148348	-0.263491
32	1	0	7.093516	-1.469730	-1.570491
33	1	0	7.675073	-0.418032	-0.244458
34	7	0	-6.099205	-1.146946	-0.095640
35	8	0	-7.054237	-0.424473	0.116756
36	8	0	-6.189973	-2.337148	-0.329512

Structure 37a (DMSO)

Energy (Hartrees): -1028.30916366
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.784957	0.844647	-0.667916
2	6	0	4.978784	0.124127	-0.641060
3	6	0	5.078212	-1.014551	0.158174
4	6	0	3.980648	-1.411614	0.929079
5	6	0	2.807597	-0.677379	0.902031
6	6	0	2.680075	0.463627	0.095380
7	1	0	3.718766	1.711635	-1.317357
8	1	0	5.808579	0.453752	-1.252585
9	1	0	4.071270	-2.291060	1.556552
10	1	0	1.977743	-0.985656	1.529546
11	6	0	1.416773	1.238330	0.057088
12	6	0	0.214315	0.585085	0.032898
13	6	0	1.481360	2.689406	0.084396
14	1	0	0.208230	-0.498773	0.006169
15	1	0	2.493808	3.121759	0.146411
16	8	0	0.509455	3.437515	0.064429
17	7	0	-0.996654	1.187021	0.047778
18	1	0	-0.987611	2.203310	0.110230
19	6	0	-2.236941	0.562277	-0.002562
20	6	0	-3.370966	1.367039	0.193157
21	6	0	-2.393847	-0.809883	-0.245936
22	6	0	-4.636228	0.816843	0.160144
23	1	0	-3.244086	2.427835	0.377784
24	6	0	-3.660747	-1.364358	-0.275829
25	1	0	-1.542793	-1.452173	-0.426171
26	6	0	-4.766900	-0.549015	-0.070311
27	1	0	-5.510980	1.434145	0.315568
28	1	0	-3.789643	-2.421892	-0.464634
29	8	0	6.187206	-1.789074	0.252105
30	6	0	7.320271	-1.409025	-0.515525
31	1	0	8.090503	-2.148004	-0.303150
32	1	0	7.093740	-1.418993	-1.585460
33	1	0	7.678984	-0.417399	-0.224655
34	7	0	-6.100586	-1.140078	-0.100615
35	8	0	-7.057158	-0.410249	0.086807
36	8	0	-6.195751	-2.335746	-0.310545

Structure 37a (C_2H_5OH)

Energy (Hartrees): -1028.30975545
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.775819	0.826854	-0.691577
2	6	0	4.968017	0.104515	-0.656453
3	6	0	5.068391	-1.013422	0.169707
4	6	0	3.978164	-1.391052	0.958487
5	6	0	2.806533	-0.654580	0.922948
6	6	0	2.676663	0.466498	0.089887
7	1	0	3.705702	1.677888	-1.361474
8	1	0	5.794868	0.416861	-1.280891
9	1	0	4.073642	-2.255196	1.606489
10	1	0	1.981124	-0.944406	1.564933
11	6	0	1.415812	1.245442	0.045618
12	6	0	0.210154	0.594354	0.036904
13	6	0	1.486647	2.691436	0.045908
14	1	0	0.202753	-0.489903	0.021055
15	1	0	2.498784	3.123804	0.095115
16	8	0	0.514312	3.445854	0.014324
17	7	0	-0.998977	1.195712	0.057228
18	1	0	-0.993710	2.211481	0.128073
19	6	0	-2.238255	0.567740	0.005687
20	6	0	-3.371859	1.360788	0.244777
21	6	0	-2.390929	-0.795602	-0.284334
22	6	0	-4.634646	0.806122	0.211382
23	1	0	-3.246502	2.415289	0.463403
24	6	0	-3.654615	-1.355527	-0.315832
25	1	0	-1.538613	-1.424171	-0.503368
26	6	0	-4.760983	-0.552124	-0.065156
27	1	0	-5.509523	1.413682	0.401572
28	1	0	-3.781274	-2.405994	-0.542047
29	8	0	6.180585	-1.791067	0.274507
30	6	0	7.316724	-1.426439	-0.499403
31	1	0	8.086904	-2.158733	-0.264812
32	1	0	7.091097	-1.464510	-1.568558
33	1	0	7.669277	-0.427191	-0.229389
34	7	0	-6.088282	-1.146020	-0.101187
35	8	0	-7.047848	-0.436761	0.145624
36	8	0	-6.188740	-2.328870	-0.376165

Structure 37b (vacuum)

Energy (Hartrees): -1028.27736263
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.486865	0.899260	1.022935
2	6	0	4.473081	-0.063011	1.127683
3	6	0	4.532359	-1.111510	0.204440
4	6	0	3.594109	-1.177482	-0.824486
5	6	0	2.610813	-0.193463	-0.921065
6	6	0	2.532072	0.853700	-0.003894
7	1	0	3.443210	1.699438	1.754305
8	1	0	5.211219	-0.031575	1.919580
9	1	0	3.624953	-1.968036	-1.561920
10	1	0	1.908154	-0.230506	-1.747966
11	6	0	1.496568	1.906657	-0.107160
12	6	0	0.167403	1.659623	-0.121852
13	6	0	1.908430	3.322466	-0.164029

14	1	0	-0.502251	2.507697	-0.198309
15	1	0	3.004041	3.482690	-0.158747
16	8	0	1.151333	4.263539	-0.218102
17	8	0	5.531851	-2.007103	0.388743
18	6	0	5.646485	-3.069229	-0.536816
19	1	0	5.817525	-2.691913	-1.549766
20	1	0	6.506019	-3.654521	-0.219090
21	1	0	4.752630	-3.700649	-0.526762
22	7	0	-0.400791	0.424340	-0.017775
23	1	0	0.236098	-0.351342	0.115558
24	6	0	-1.756707	0.124146	-0.000002
25	6	0	-2.131258	-1.213146	0.202588
26	6	0	-2.750577	1.096291	-0.181707
27	6	0	-3.463178	-1.576900	0.226436
28	1	0	-1.364432	-1.966330	0.345637
29	6	0	-4.086088	0.733775	-0.153935
30	1	0	-2.496093	2.133345	-0.348490
31	6	0	-4.428794	-0.594786	0.048337
32	1	0	-3.765492	-2.603555	0.382927
33	1	0	-4.866116	1.470846	-0.290324
34	7	0	-5.846807	-0.972682	0.076599
35	8	0	-6.666758	-0.091809	-0.075445
36	8	0	-6.112148	-2.144069	0.250650

Structure 37b ($CHCl_3$)

Energy (Hartrees): -1028.30677199
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.560901	0.967301	0.939821
2	6	0	4.558772	0.015284	1.045240
3	6	0	4.561939	-1.096131	0.195495
4	6	0	3.554628	-1.236900	-0.758984
5	6	0	2.561581	-0.263173	-0.858468
6	6	0	2.537958	0.847045	-0.013449
7	1	0	3.564558	1.817950	1.613897
8	1	0	5.346973	0.109793	1.783273
9	1	0	3.538804	-2.079129	-1.437912
10	1	0	1.805046	-0.367052	-1.630615
11	6	0	1.495622	1.893598	-0.121769
12	6	0	0.160729	1.649613	-0.121274
13	6	0	1.910210	3.299096	-0.207745
14	1	0	-0.509332	2.496303	-0.209201
15	1	0	3.003675	3.457426	-0.244128
16	8	0	1.159207	4.254835	-0.247829
17	8	0	5.578048	-1.975608	0.369456
18	6	0	5.622167	-3.114303	-0.476443
19	1	0	5.723360	-2.822241	-1.525859
20	1	0	6.501070	-3.680061	-0.174072
21	1	0	4.730249	-3.734671	-0.348673
22	7	0	-0.413330	0.424966	0.005755
23	1	0	0.210442	-0.364190	0.135847
24	6	0	-1.770054	0.131722	0.019842
25	6	0	-2.141951	-1.212272	0.188263
26	6	0	-2.763807	1.110885	-0.129970
27	6	0	-3.472630	-1.577152	0.203332
28	1	0	-1.373191	-1.967573	0.308651
29	6	0	-4.098083	0.747322	-0.110309
30	1	0	-2.513175	2.154200	-0.261868
31	6	0	-4.440109	-0.588864	0.053858
32	1	0	-3.763687	-2.611197	0.331547
33	1	0	-4.871531	1.495366	-0.223840
34	7	0	-5.850732	-0.964640	0.072250
35	8	0	-6.681038	-0.080079	-0.015266
36	8	0	-6.127726	-2.144853	0.175173

Structure 37b (DMSO)

Energy (Hartrees): -1028.30745684
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.571522	0.978188	0.923255
2	6	0	4.569545	0.025740	1.029384
3	6	0	4.565521	-1.094708	0.190921
4	6	0	3.553802	-1.239682	-0.758990
5	6	0	2.560508	-0.266170	-0.858939
6	6	0	2.541985	0.850905	-0.022242
7	1	0	3.581743	1.833587	1.591491
8	1	0	5.360113	0.127374	1.764206
9	1	0	3.529588	-2.088829	-1.429277
10	1	0	1.796224	-0.380417	-1.621941
11	6	0	1.496125	1.894824	-0.125255
12	6	0	0.160016	1.648056	-0.129805
13	6	0	1.914052	3.298906	-0.196539
14	1	0	-0.513934	2.492356	-0.212942
15	1	0	3.008339	3.450538	-0.236569
16	8	0	1.170720	4.262413	-0.220740
17	8	0	5.576077	-1.978038	0.370225
18	6	0	5.586272	-3.142967	-0.443849
19	1	0	5.683965	-2.884601	-1.502118
20	1	0	6.454546	-3.720632	-0.132802
21	1	0	4.680593	-3.737114	-0.291937
22	7	0	-0.412963	0.423551	-0.013672
23	1	0	0.205713	-0.372239	0.107450
24	6	0	-1.769349	0.132837	0.001083
25	6	0	-2.140142	-1.211902	0.168933
26	6	0	-2.763300	1.112747	-0.145626
27	6	0	-3.470591	-1.575525	0.193037
28	1	0	-1.369089	-1.965921	0.283007
29	6	0	-4.097484	0.750220	-0.116184
30	1	0	-2.513144	2.155611	-0.282954
31	6	0	-4.439456	-0.586286	0.052094
32	1	0	-3.757562	-2.610439	0.323027
33	1	0	-4.867978	1.501808	-0.226991
34	7	0	-5.847889	-0.961557	0.085697
35	8	0	-6.681968	-0.076898	0.014442
36	8	0	-6.125743	-2.143243	0.185635

Structure 37b (C_2H_5OH)

Energy (Hartrees): -1028.30840849
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.560231	0.965748	0.943848
2	6	0	4.556032	0.009899	1.044253
3	6	0	4.555395	-1.096043	0.188486
4	6	0	3.552545	-1.228080	-0.771183
5	6	0	2.562036	-0.251549	-0.865269
6	6	0	2.539779	0.852988	-0.012528
7	1	0	3.565765	1.811670	1.624117
8	1	0	5.341789	0.098455	1.786294
9	1	0	3.533522	-2.067357	-1.453885
10	1	0	1.803840	-0.352362	-1.636156
11	6	0	1.495537	1.899527	-0.113611
12	6	0	0.157672	1.651342	-0.118184
13	6	0	1.910902	3.296349	-0.186094

14	1	0	-0.518945	2.493458	-0.202125
15	1	0	3.002673	3.455729	-0.218635
16	8	0	1.163010	4.264033	-0.219527
17	8	0	5.567355	-1.986856	0.362450
18	6	0	5.592524	-3.132442	-0.481565
19	1	0	5.699469	-2.843429	-1.530677
20	1	0	6.461483	-3.711694	-0.175612
21	1	0	4.688376	-3.733165	-0.350858
22	7	0	-0.410402	0.427697	0.000479
23	1	0	0.211094	-0.365182	0.129700
24	6	0	-1.767241	0.133384	0.009006
25	6	0	-2.135845	-1.207596	0.206382
26	6	0	-2.760020	1.108038	-0.173907
27	6	0	-3.465337	-1.573540	0.226321
28	1	0	-1.365023	-1.957444	0.346216
29	6	0	-4.093331	0.744598	-0.148812
30	1	0	-2.509461	2.146784	-0.339504
31	6	0	-4.433452	-0.588654	0.050966
32	1	0	-3.751109	-2.605657	0.380191
33	1	0	-4.864068	1.491355	-0.287558
34	7	0	-5.837314	-0.963992	0.078566
35	8	0	-6.675966	-0.086475	-0.030782
36	8	0	-6.120642	-2.142067	0.211176

Structure 37c (vacuum)

Energy (Hartrees): -1028.27802549
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.497688	0.881268	0.957360
2	6	0	-4.442834	-0.121531	1.041780
3	6	0	-4.405625	-1.204172	0.156689
4	6	0	-3.410156	-1.266888	-0.816196
5	6	0	-2.460221	-0.248261	-0.887473
6	6	0	-2.478445	0.829818	-0.004870
7	1	0	-3.547570	1.725845	1.633264
8	1	0	-5.234553	-0.089210	1.780038
9	1	0	-3.368664	-2.080562	-1.527342
10	1	0	-1.707941	-0.285657	-1.669553
11	6	0	-1.466638	1.905713	-0.085284
12	6	0	-0.132284	1.681081	-0.093056
13	6	0	-1.876413	3.316388	-0.106998
14	1	0	0.545956	2.524339	-0.158313
15	8	0	-5.378418	-2.133659	0.318186
16	6	0	-5.422642	-3.209507	-0.596666
17	1	0	-4.513541	-3.816427	-0.539360
18	1	0	-6.279343	-3.814494	-0.309386
19	1	0	-5.558109	-2.848945	-1.621073
20	7	0	0.457374	0.454393	0.028924
21	1	0	-0.164392	-0.318999	0.231986
22	6	0	1.818123	0.181615	0.020883
23	6	0	2.243796	-1.084440	0.452242
24	6	0	2.769270	1.114715	-0.414976
25	6	0	3.585738	-1.410143	0.462682
26	1	0	1.510264	-1.806660	0.792501
27	6	0	4.115670	0.793585	-0.395397
28	1	0	2.467894	2.083089	-0.789447
29	6	0	4.509458	-0.461563	0.043399
30	1	0	3.928534	-2.380012	0.797143
31	1	0	4.863259	1.500886	-0.728791
32	8	0	-3.013049	3.712697	-0.032360
33	1	0	-1.035010	4.034976	-0.195419
34	7	0	5.938370	-0.798431	0.057481
35	8	0	6.720386	0.055034	-0.305544
36	8	0	6.249624	-1.909819	0.431491

Structure 37c ($CHCl_3$)

Energy (Hartrees): -1028.30867136
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.425828	0.892492	0.983574
2	6	0	4.361506	-0.112603	1.141518
3	6	0	4.385304	-1.198292	0.258637
4	6	0	3.468429	-1.256665	-0.789593
5	6	0	2.530911	-0.233386	-0.935655
6	6	0	2.483829	0.845033	-0.054255
7	1	0	3.419002	1.729768	1.672018
8	1	0	5.087985	-0.079620	1.945240
9	1	0	3.477131	-2.073315	-1.499439
10	1	0	1.837120	-0.274695	-1.770211
11	6	0	1.473580	1.919672	-0.197083
12	6	0	0.133322	1.698879	-0.211313
13	6	0	1.884570	3.316494	-0.290910
14	1	0	-0.539271	2.542357	-0.322308
15	8	0	5.332948	-2.137212	0.497948
16	6	0	5.367025	-3.275224	-0.348470
17	1	0	5.584958	-2.993051	-1.382530
18	1	0	6.169203	-3.906483	0.028603
19	1	0	4.422251	-3.825341	-0.304988
20	7	0	-0.455466	0.478960	-0.093848
21	1	0	0.161814	-0.322323	-0.021230
22	6	0	-1.815737	0.206590	-0.038936
23	6	0	-2.211716	-1.139381	-0.093747
24	6	0	-2.787887	1.210183	0.080080
25	6	0	-3.547702	-1.481135	-0.042529
26	1	0	-1.457438	-1.913151	-0.184385
27	6	0	-4.128238	0.870293	0.125047
28	1	0	-2.511841	2.253036	0.155574
29	6	0	-4.494718	-0.467687	0.062052
30	1	0	-3.858669	-2.516377	-0.088215
31	1	0	-4.886500	1.636095	0.220804
32	8	0	3.031780	3.714202	-0.260106
33	1	0	1.051017	4.036841	-0.396996
34	7	0	-5.911574	-0.818643	0.109900
35	8	0	-6.724689	0.084847	0.154837
36	8	0	-6.209703	-1.997779	0.100470

Structure 37c (DMSO)

Energy (Hartrees): -1028.31077755
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.433175	0.848042	1.032801
2	6	0	-4.402419	-0.133982	1.128745
3	6	0	-4.442110	-1.178731	0.197282
4	6	0	-3.494152	-1.228172	-0.824439
5	6	0	-2.522216	-0.230494	-0.905963
6	6	0	-2.471779	0.817002	0.012293
7	1	0	-3.416788	1.653900	1.758078
8	1	0	-5.144648	-0.109166	1.918638
9	1	0	-3.502293	-2.020275	-1.561670
10	1	0	-1.800222	-0.268903	-1.716213
11	6	0	-1.450543	1.885541	-0.085840
12	6	0	-0.109817	1.660279	-0.105317
13	6	0	-1.848505	3.286342	-0.144887

14	1	0	0.562179	2.507268	-0.190214
15	8	0	-5.430779	-2.089491	0.363499
16	6	0	-5.538647	-3.124099	-0.604908
17	1	0	-4.647943	-3.758717	-0.606347
18	1	0	-6.403827	-3.718654	-0.317966
19	1	0	-5.698216	-2.710137	-1.604702
20	7	0	0.478641	0.441881	0.004399
21	1	0	-0.126832	-0.356819	0.169903
22	6	0	1.840629	0.177039	0.001242
23	6	0	2.251593	-1.127744	0.320559
24	6	0	2.801805	1.149583	-0.312438
25	6	0	3.591619	-1.455531	0.342077
26	1	0	1.505511	-1.877971	0.557005
27	6	0	4.145552	0.823781	-0.287374
28	1	0	2.515563	2.155799	-0.585877
29	6	0	4.528154	-0.471498	0.040585
30	1	0	3.910131	-2.458481	0.593186
31	1	0	4.891842	1.570118	-0.525566
32	8	0	-2.994098	3.696364	-0.135070
33	1	0	-1.005614	3.999986	-0.206744
34	7	0	5.946753	-0.808938	0.064435
35	8	0	6.751050	0.062993	-0.211374
36	8	0	6.262259	-1.947702	0.359212

Structure 37c (C_2H_5OH)

Energy (Hartrees): -1028.31228744
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.402851	0.828966	1.058572
2	6	0	-4.370603	-0.154528	1.156794
3	6	0	-4.430252	-1.178041	0.204828
4	6	0	-3.508619	-1.208603	-0.840130
5	6	0	-2.539779	-0.208705	-0.925524
6	6	0	-2.468124	0.818873	0.013557
7	1	0	-3.366435	1.618932	1.801202
8	1	0	-5.094652	-0.147838	1.963897
9	1	0	-3.536130	-1.985615	-1.592850
10	1	0	-1.838471	-0.228690	-1.754250
11	6	0	-1.448485	1.889788	-0.087340
12	6	0	-0.105657	1.665390	-0.112286
13	6	0	-1.845927	3.282976	-0.141681
14	1	0	0.566897	2.512027	-0.196654
15	8	0	-5.417772	-2.096256	0.376864
16	6	0	-5.555333	-3.109687	-0.612520
17	1	0	-4.667612	-3.747031	-0.647187
18	1	0	-6.416854	-3.704879	-0.316228
19	1	0	-5.736887	-2.670549	-1.597344
20	7	0	0.478351	0.447297	-0.008779
21	1	0	-0.130942	-0.350282	0.150124
22	6	0	1.840711	0.178164	-0.011147
23	6	0	2.245940	-1.128923	0.304328
24	6	0	2.803589	1.150142	-0.319682
25	6	0	3.584667	-1.460128	0.330122
26	1	0	1.497255	-1.878363	0.535178
27	6	0	4.146136	0.822513	-0.289454
28	1	0	2.520010	2.157341	-0.592338
29	6	0	4.523487	-0.475206	0.037209
30	1	0	3.899648	-2.464971	0.578828
31	1	0	4.895006	1.568127	-0.521882
32	8	0	-2.999938	3.688640	-0.125948
33	1	0	-1.013326	4.005153	-0.204505
34	7	0	5.937580	-0.812193	0.070748
35	8	0	6.748966	0.061491	-0.180854
36	8	0	6.255942	-1.954755	0.350731

Structure 37d (vacuum)

Energy (Hartrees): -1028.26827576
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.716144	0.841202	0.604087
2	6	0	-4.840556	0.021997	0.659447
3	6	0	-4.852971	-1.186336	-0.035382
4	6	0	-3.738207	-1.558457	-0.790143
5	6	0	-2.631360	-0.731225	-0.840503
6	6	0	-2.590151	0.477018	-0.131990
7	1	0	-3.722212	1.779043	1.144159
8	1	0	-5.692548	0.339532	1.245045
9	1	0	-3.774633	-2.488945	-1.342971
10	1	0	-1.789359	-1.015032	-1.463582
11	6	0	-1.376501	1.327694	-0.164245
12	6	0	-0.155978	0.747423	-0.042747
13	6	0	-1.506374	2.780337	-0.342593
14	1	0	-0.116957	-0.324586	0.110452
15	7	0	1.074533	1.354854	-0.047065
16	1	0	1.114055	2.361814	-0.024635
17	6	0	2.303400	0.705837	-0.009970
18	6	0	3.446726	1.468510	0.274601
19	6	0	2.438834	-0.665825	-0.263401
20	6	0	4.694771	0.879115	0.317315
21	1	0	3.345875	2.530028	0.471266
22	6	0	3.687843	-1.261169	-0.208573
23	1	0	1.583610	-1.271648	-0.528628
24	6	0	4.799690	-0.485457	0.081525
25	1	0	5.583402	1.454691	0.538888
26	1	0	3.811848	-2.318194	-0.402518
27	8	0	-5.896044	-2.054208	-0.047765
28	6	0	-7.057300	-1.695790	0.672606
29	1	0	-7.767661	-2.505469	0.522741
30	1	0	-6.843507	-1.592443	1.741032
31	1	0	-7.483785	-0.761946	0.293385
32	1	0	-0.556604	3.345560	-0.440448
33	8	0	-2.548097	3.386341	-0.400966
34	7	0	6.122411	-1.120846	0.132735
35	8	0	6.180247	-2.314927	-0.072746
36	8	0	7.075834	-0.412168	0.378466

Structure 37d ($CHCl_3$)

Energy (Hartrees): -1028.30034458
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.705088	0.824697	0.635582
2	6	0	-4.834282	0.009968	0.680394
3	6	0	-4.857825	-1.178835	-0.048816
4	6	0	-3.748793	-1.536431	-0.820133
5	6	0	-2.636970	-0.712306	-0.858673
6	6	0	-2.586395	0.479564	-0.123118
7	1	0	-3.700010	1.742888	1.210259
8	1	0	-5.679553	0.311896	1.284763
9	1	0	-3.785541	-2.454963	-1.394225
10	1	0	-1.795672	-0.991166	-1.485059
11	6	0	-1.372748	1.334745	-0.143741
12	6	0	-0.149390	0.748441	-0.026150
13	6	0	-1.508538	2.778263	-0.333336

14	1	0	-0.116891	-0.327398	0.101965
15	7	0	1.076199	1.349314	-0.013505
16	1	0	1.127700	2.358274	0.029927
17	6	0	2.303229	0.698281	0.010619
18	6	0	3.448035	1.468758	0.273023
19	6	0	2.437535	-0.676231	-0.233680
20	6	0	4.697094	0.882847	0.306072
21	1	0	3.345246	2.532675	0.456191
22	6	0	3.687594	-1.267262	-0.192573
23	1	0	1.580530	-1.288804	-0.477308
24	6	0	4.802608	-0.485517	0.079563
25	1	0	5.580922	1.471568	0.513137
26	1	0	3.801065	-2.326384	-0.382511
27	8	0	-5.906770	-2.039570	-0.075095
28	6	0	-7.058816	-1.699267	0.679171
29	1	0	-7.776093	-2.500231	0.510737
30	1	0	-6.827681	-1.639474	1.746850
31	1	0	-7.487329	-0.751806	0.339400
32	1	0	-0.571009	3.360922	-0.381601
33	8	0	-2.562929	3.367607	-0.460673
34	7	0	6.119798	-1.114699	0.119319
35	8	0	6.188019	-2.314564	-0.068241
36	8	0	7.085282	-0.408296	0.339203

Structure 37d (DMSO)

Energy (Hartrees): -1028.30272824
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.703945	0.821136	0.639032
2	6	0	-4.837321	0.011276	0.680002
3	6	0	-4.865049	-1.175188	-0.054791
4	6	0	-3.754774	-1.532707	-0.825324
5	6	0	-2.638405	-0.713093	-0.859345
6	6	0	-2.584754	0.476917	-0.120425
7	1	0	-3.695209	1.734787	1.221453
8	1	0	-5.680580	0.313494	1.287391
9	1	0	-3.789010	-2.450168	-1.401848
10	1	0	-1.794439	-0.997803	-1.479600
11	6	0	-1.370961	1.332204	-0.134627
12	6	0	-0.147123	0.741191	-0.023124
13	6	0	-1.508184	2.774658	-0.319572
14	1	0	-0.117255	-0.336822	0.088785
15	7	0	1.075788	1.339933	-0.007898
16	1	0	1.130418	2.350452	0.031208
17	6	0	2.302029	0.689233	0.017637
18	6	0	3.445185	1.466309	0.270255
19	6	0	2.439099	-0.687251	-0.217076
20	6	0	4.696255	0.885594	0.300870
21	1	0	3.336397	2.530732	0.446434
22	6	0	3.691687	-1.272426	-0.178325
23	1	0	1.584106	-1.306287	-0.451619
24	6	0	4.806288	-0.484261	0.081076
25	1	0	5.576754	1.482087	0.499387
26	1	0	3.804112	-2.332648	-0.362652
27	8	0	-5.916992	-2.030208	-0.084508
28	6	0	-7.063371	-1.687760	0.681304
29	1	0	-7.785277	-2.485246	0.516446
30	1	0	-6.823256	-1.631021	1.746886
31	1	0	-7.490876	-0.737430	0.348925
32	1	0	-0.575632	3.363939	-0.328951
33	8	0	-2.563860	3.357024	-0.485497
34	7	0	6.124627	-1.106207	0.113883
35	8	0	6.198804	-2.308979	-0.062728
36	8	0	7.091662	-0.393979	0.316541

Structure 37d (C_2H_5OH)

Energy (Hartrees): -1028.30392776
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.689512	0.808816	0.667496
2	6	0	-4.821062	-0.003510	0.708179
3	6	0	-4.853420	-1.174743	-0.048214
4	6	0	-3.754214	-1.518622	-0.838741
5	6	0	-2.640673	-0.695444	-0.874151
6	6	0	-2.581707	0.481462	-0.115526
7	1	0	-3.673254	1.709285	1.270878
8	1	0	-5.657338	0.285297	1.331427
9	1	0	-3.795243	-2.427060	-1.429305
10	1	0	-1.804337	-0.966452	-1.510577
11	6	0	-1.370530	1.341817	-0.136582
12	6	0	-0.143747	0.753234	-0.022256
13	6	0	-1.509876	2.775335	-0.337736
14	1	0	-0.114992	-0.323978	0.098042
15	7	0	1.077382	1.350289	-0.010426
16	1	0	1.134042	2.360953	0.028422
17	6	0	2.303129	0.696163	0.013994
18	6	0	3.446411	1.467857	0.279947
19	6	0	2.435234	-0.677583	-0.236991
20	6	0	4.694897	0.882462	0.313645
21	1	0	3.340738	2.531065	0.465306
22	6	0	3.684497	-1.268160	-0.198215
23	1	0	1.578812	-1.289795	-0.484119
24	6	0	4.799508	-0.485841	0.079256
25	1	0	5.576331	1.473980	0.523738
26	1	0	3.793606	-2.326665	-0.394357
27	8	0	-5.908026	-2.034554	-0.081759
28	6	0	-7.056481	-1.701986	0.688902
29	1	0	-7.776910	-2.497973	0.510755
30	1	0	-6.814851	-1.661752	1.754501
31	1	0	-7.480908	-0.747197	0.366683
32	1	0	-0.584177	3.372168	-0.357749
33	8	0	-2.572945	3.354287	-0.508929
34	7	0	6.110609	-1.112425	0.117760
35	8	0	6.192885	-2.304803	-0.120709
36	8	0	7.076564	-0.420488	0.388518

Structure 37g (vacuum)

Energy (Hartrees): -1028.27368474
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.844948	-0.437372	-0.797102
2	6	0	-4.007297	-1.205578	-0.780789
3	6	0	-5.034344	-0.876461	0.101304
4	6	0	-4.880072	0.212081	0.963600
5	6	0	-3.713296	0.954325	0.945349
6	6	0	-2.673221	0.649421	0.056976
7	1	0	-2.066535	-0.684173	-1.511784
8	1	0	-4.100168	-2.038018	-1.464821
9	1	0	-5.684979	0.442170	1.650751
10	1	0	-3.593370	1.773842	1.645685
11	6	0	-1.428188	1.452295	0.018750
12	6	0	-1.473429	2.815193	0.009155
13	6	0	-0.150685	0.782214	-0.014829

14	1	0	-2.422638	3.343885	0.020851
15	1	0	-0.161170	-0.312261	0.036224
16	8	0	-0.426511	3.612674	-0.027768
17	1	0	0.384766	3.039245	-0.071582
18	7	0	0.967515	1.421194	-0.101427
19	6	0	2.174968	0.709770	-0.038452
20	6	0	2.371839	-0.339420	0.868415
21	6	0	3.221656	1.100758	-0.881494
22	6	0	3.582692	-1.012619	0.908496
23	1	0	1.583884	-0.603721	1.563075
24	6	0	4.431739	0.429584	-0.853939
25	1	0	3.061897	1.925961	-1.564105
26	6	0	4.590443	-0.620878	0.040694
27	1	0	3.759394	-1.820714	1.605316
28	1	0	5.249648	0.704632	-1.505983
29	8	0	-6.208015	-1.549926	0.200093
30	6	0	-6.399047	-2.666639	-0.643438
31	1	0	-5.640632	-3.434437	-0.460909
32	1	0	-7.381726	-3.063798	-0.399652
33	1	0	-6.376804	-2.373850	-1.697867
34	7	0	5.879541	-1.333555	0.080118
35	8	0	6.740846	-0.979014	-0.696114
36	8	0	5.999452	-2.232771	0.884764

Structure 37g ($CHCl_3$)

Energy (Hartrees): -1028.29818551
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.832188	-0.497477	-0.733532
2	6	0	-4.007175	-1.247719	-0.722710
3	6	0	-5.069249	-0.847639	0.086581
4	6	0	-4.938002	0.294966	0.881405
5	6	0	-3.759181	1.020104	0.870460
6	6	0	-2.682358	0.642524	0.055038
7	1	0	-2.024588	-0.806891	-1.389192
8	1	0	-4.081210	-2.123846	-1.353123
9	1	0	-5.768431	0.586014	1.514346
10	1	0	-3.663964	1.885139	1.518415
11	6	0	-1.425990	1.429833	0.023246
12	6	0	-1.459471	2.793215	0.002927
13	6	0	-0.153879	0.747110	0.002168
14	1	0	-2.400691	3.336169	-0.000197
15	1	0	-0.166113	-0.345771	0.055765
16	8	0	-0.398038	3.576914	-0.029861
17	1	0	0.406783	2.986612	-0.065473
18	7	0	0.965430	1.386437	-0.082528
19	6	0	2.177779	0.685204	-0.023594
20	6	0	2.377621	-0.391327	0.851126
21	6	0	3.227999	1.119602	-0.842427
22	6	0	3.597700	-1.046437	0.882966
23	1	0	1.585926	-0.697275	1.524363
24	6	0	4.447147	0.466115	-0.824355
25	1	0	3.066006	1.965394	-1.499673
26	6	0	4.610549	-0.611003	0.039086
27	1	0	3.769063	-1.874889	1.557228
28	1	0	5.262345	0.781338	-1.461873
29	8	0	-6.255130	-1.501318	0.173610
30	6	0	-6.421803	-2.675079	-0.604915
31	1	0	-5.683520	-3.436104	-0.334764
32	1	0	-7.420275	-3.045264	-0.380318
33	1	0	-6.349531	-2.453203	-1.673848
34	7	0	5.902519	-1.305179	0.068833
35	8	0	6.761696	-0.946892	-0.712113
36	8	0	6.048416	-2.205975	0.871288

Structure 37g (DMSO)

Energy (Hartrees):
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.844948	-0.437372	-0.797102
2	6	0	-4.007297	-1.205578	-0.780789
3	6	0	-5.034344	-0.876461	0.101304
4	6	0	-4.880072	0.212081	0.963600
5	6	0	-3.713296	0.954325	0.945349
6	6	0	-2.673221	0.649421	0.056976
7	1	0	-2.066535	-0.684173	-1.511784
8	1	0	-4.100168	-2.038018	-1.464821
9	1	0	-5.684979	0.442170	1.650751
10	1	0	-3.593370	1.773842	1.645685
11	6	0	-1.428188	1.452295	0.018750
12	6	0	-1.473429	2.815193	0.009155
13	6	0	-0.150685	0.782214	-0.014829
14	1	0	-2.422638	3.343885	0.020851
15	1	0	-0.161170	-0.312261	0.036224
16	8	0	-0.426511	3.612674	-0.027768
17	1	0	0.384766	3.039245	-0.071582
18	7	0	0.967515	1.421194	-0.101427
19	6	0	2.174968	0.709770	-0.038452
20	6	0	2.371839	-0.339420	0.868415
21	6	0	3.221656	1.100758	-0.881494
22	6	0	3.582692	-1.012619	0.908496
23	1	0	1.583884	-0.603721	1.563075
24	6	0	4.431739	0.429584	-0.853939
25	1	0	3.061897	1.925961	-1.564105
26	6	0	4.590443	-0.620878	0.040694
27	1	0	3.759394	-1.820714	1.605316
28	1	0	5.249648	0.704632	-1.505983
29	8	0	-6.208015	-1.549926	0.200093
30	6	0	-6.399047	-2.666639	-0.643438
31	1	0	-5.640632	-3.434437	-0.460909
32	1	0	-7.381726	-3.063798	-0.399652
33	1	0	-6.376804	-2.373850	-1.697867
34	7	0	5.879541	-1.333555	0.080118
35	8	0	6.740846	-0.979014	-0.696114
36	8	0	5.999452	-2.232771	0.884764

Structure 37g (C_2H_5OH)

Energy (Hartrees): -1028.29684772
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.829206	-0.493792	-0.737741
2	6	0	-4.002646	-1.246815	-0.723831
3	6	0	-5.061745	-0.848370	0.089363
4	6	0	-4.932597	0.294269	0.883523
5	6	0	-3.755539	1.023423	0.868723
6	6	0	-2.680477	0.647426	0.050368
7	1	0	-2.022517	-0.804618	-1.393945
8	1	0	-4.075932	-2.124269	-1.352803
9	1	0	-5.760876	0.585601	1.519852
10	1	0	-3.662907	1.889731	1.515401
11	6	0	-1.424931	1.436409	0.016971
12	6	0	-1.462883	2.798149	0.019472

13	6	0	-0.153086	0.750628	-0.019203
14	1	0	-2.403094	3.342063	0.033675
15	1	0	-0.167801	-0.342300	0.023331
16	8	0	-0.398914	3.587076	-0.007471
17	1	0	0.409237	3.003608	-0.059667
18	7	0	0.966392	1.389555	-0.100575
19	6	0	2.175235	0.682871	-0.042234
20	6	0	2.366123	-0.396321	0.831971
21	6	0	3.231480	1.117297	-0.853731
22	6	0	3.584767	-1.052005	0.873935
23	1	0	1.567835	-0.704052	1.496827
24	6	0	4.449246	0.462676	-0.827460
25	1	0	3.078141	1.964422	-1.511491
26	6	0	4.604943	-0.614787	0.038303
27	1	0	3.745317	-1.881631	1.549645
28	1	0	5.267384	0.781498	-1.459626
29	8	0	-6.248739	-1.508283	0.179971
30	6	0	-6.412518	-2.685895	-0.600594
31	1	0	-5.667652	-3.440269	-0.332420
32	1	0	-7.408210	-3.060470	-0.370840
33	1	0	-6.344852	-2.460431	-1.668479
34	7	0	5.892814	-1.303666	0.080927
35	8	0	6.758984	-0.960794	-0.702334
36	8	0	6.045479	-2.193135	0.897467

Structure 38a (vacuum)

Energy (Hartrees): -1118.25856014
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.490931	1.197747	0.621422
2	6	0	-4.706284	0.538893	0.720384
3	6	0	-4.851537	-0.682025	0.079664
4	6	0	-3.829381	-1.253822	-0.662342
5	6	0	-2.626496	-0.573101	-0.765772
6	6	0	-2.431492	0.655087	-0.118914
7	1	0	-3.354179	2.133354	1.150712
8	1	0	-5.528534	0.944885	1.293993
9	1	0	-3.993126	-2.201465	-1.157769
10	1	0	-1.836168	-0.985641	-1.382252
11	6	0	-1.143501	1.371024	-0.206627
12	6	0	0.037245	0.683373	-0.121779
13	6	0	-1.141765	2.819429	-0.371119
14	1	0	0.012671	-0.389866	0.034705
15	1	0	-2.132634	3.292221	-0.482031
16	8	0	-0.136642	3.510942	-0.411632
17	7	0	1.261238	1.245818	-0.173544
18	1	0	1.262789	2.262819	-0.246876
19	6	0	2.485531	0.580982	-0.085558
20	6	0	3.627107	1.352080	0.168237
21	6	0	2.607152	-0.801940	-0.260175
22	6	0	4.870142	0.754462	0.259976
23	1	0	3.527654	2.423123	0.301694
24	6	0	3.849934	-1.405353	-0.160029
25	1	0	1.747370	-1.413078	-0.499166
26	6	0	4.962976	-0.621029	0.099988
27	1	0	5.762044	1.332717	0.460244
28	1	0	3.968605	-2.472150	-0.294597
29	7	0	-6.138935	-1.395058	0.186448
30	8	0	-6.235140	-2.464031	-0.376597
31	8	0	-7.018693	-0.867162	0.831297
32	7	0	6.282360	-1.265050	0.199610
33	8	0	6.331611	-2.466736	0.046273
34	8	0	7.236199	-0.553229	0.429360

Structure 38a ($CHCl_3$)

Energy (Hartrees): -1118.28825289
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.525376	1.238818	0.534194
2	6	0	-4.740339	0.579960	0.626281
3	6	0	-4.849712	-0.690069	0.077369
4	6	0	-3.786058	-1.311863	-0.563474
5	6	0	-2.584095	-0.631478	-0.662816
6	6	0	-2.427091	0.649865	-0.111604
7	1	0	-3.423549	2.213801	0.995961
8	1	0	-5.584840	1.032135	1.129001
9	1	0	-3.908099	-2.298542	-0.990567
10	1	0	-1.762518	-1.094617	-1.196479
11	6	0	-1.143452	1.373057	-0.198051
12	6	0	0.043079	0.688824	-0.107281
13	6	0	-1.155261	2.814706	-0.382990
14	1	0	0.025316	-0.385343	0.042881
15	1	0	-2.144596	3.278295	-0.526895
16	8	0	-0.154204	3.520421	-0.414296
17	7	0	1.262860	1.254786	-0.144393
18	1	0	1.279466	2.272081	-0.201924
19	6	0	2.486754	0.588449	-0.065247
20	6	0	3.624826	1.354419	0.221225
21	6	0	2.608079	-0.788894	-0.282341
22	6	0	4.867483	0.755495	0.300332
23	1	0	3.523322	2.420766	0.388875
24	6	0	3.849771	-1.393974	-0.196386
25	1	0	1.747288	-1.390439	-0.541888
26	6	0	4.962084	-0.615794	0.095092
27	1	0	5.751333	1.337223	0.525878
28	1	0	3.959693	-2.456509	-0.367796
29	7	0	-6.130686	-1.398978	0.178780
30	8	0	-6.198951	-2.523454	-0.276593
31	8	0	-7.058731	-0.826249	0.714145
32	7	0	6.275250	-1.258465	0.177988
33	8	0	6.334499	-2.460733	0.009385
34	8	0	7.240021	-0.557407	0.411174

Structure 38a (DMSO)

Energy (Hartrees): -1118.28952857
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.519215	1.207914	0.608905
2	6	0	-4.735080	0.547795	0.672478
3	6	0	-4.856931	-0.681817	0.039050
4	6	0	-3.804004	-1.261883	-0.656947
5	6	0	-2.599108	-0.582388	-0.722599
6	6	0	-2.431101	0.657929	-0.087034
7	1	0	-3.409522	2.151845	1.129938
8	1	0	-5.569910	0.971589	1.214438
9	1	0	-3.931948	-2.216704	-1.149656
10	1	0	-1.784546	-1.012488	-1.293643
11	6	0	-1.143588	1.376672	-0.139057
12	6	0	0.035062	0.673966	-0.090428
13	6	0	-1.150905	2.825227	-0.252468

14	1	0	0.001630	-0.405464	0.004493
15	1	0	-2.141395	3.296839	-0.355394
16	8	0	-0.148237	3.530063	-0.268049
17	7	0	1.260149	1.227507	-0.128886
18	1	0	1.290037	2.243684	-0.199153
19	6	0	2.481761	0.560968	-0.054172
20	6	0	3.639879	1.352836	-0.052820
21	6	0	2.589034	-0.833938	0.014537
22	6	0	4.888239	0.767037	0.015972
23	1	0	3.547071	2.431897	-0.104840
24	6	0	3.838835	-1.423423	0.083340
25	1	0	1.714038	-1.469464	0.012086
26	6	0	4.971857	-0.619274	0.083210
27	1	0	5.784198	1.373317	0.018055
28	1	0	3.933846	-2.499853	0.135192
29	7	0	-6.138578	-1.390314	0.107190
30	8	0	-6.240639	-2.448854	-0.483260
31	8	0	-7.038699	-0.885818	0.751283
32	7	0	6.288369	-1.249371	0.153617
33	8	0	6.342002	-2.464649	0.194124
34	8	0	7.269138	-0.528954	0.167558

Structure 38a (C_2H_5OH)

Energy (Hartrees): -1118.28807893
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.523960	1.240590	0.535893
2	6	0	-4.734794	0.576156	0.632112
3	6	0	-4.840020	-0.693093	0.077771
4	6	0	-3.776470	-1.307580	-0.572361
5	6	0	-2.578155	-0.622308	-0.673609
6	6	0	-2.425755	0.657613	-0.116475
7	1	0	-3.425038	2.214745	1.000448
8	1	0	-5.576056	1.026509	1.142143
9	1	0	-3.891416	-2.292808	-1.004993
10	1	0	-1.756270	-1.081716	-1.210368
11	6	0	-1.144616	1.384154	-0.201781
12	6	0	0.042328	0.695464	-0.112422
13	6	0	-1.162556	2.820674	-0.382827
14	1	0	0.020029	-0.379547	0.030204
15	1	0	-2.152126	3.282594	-0.522311
16	8	0	-0.160954	3.533901	-0.417349
17	7	0	1.261267	1.257689	-0.144109
18	1	0	1.288188	2.275220	-0.194110
19	6	0	2.482813	0.587157	-0.065969
20	6	0	3.621928	1.354912	0.212445
21	6	0	2.599704	-0.791754	-0.277595
22	6	0	4.863366	0.755713	0.294907
23	1	0	3.520688	2.422639	0.371395
24	6	0	3.840509	-1.396898	-0.192196
25	1	0	1.738144	-1.395414	-0.529756
26	6	0	4.954665	-0.617577	0.094594
27	1	0	5.746421	1.340668	0.515996
28	1	0	3.943786	-2.460856	-0.359342
29	7	0	-6.111586	-1.406057	0.183009
30	8	0	-6.187948	-2.527101	-0.284947
31	8	0	-7.041963	-0.849107	0.735670
32	7	0	6.261341	-1.259176	0.180523
33	8	0	6.333704	-2.456527	-0.028479
34	8	0	7.226232	-0.570986	0.458833

Structure 38b (vacuum)

Energy (Hartrees): -1118.25212654
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.307789	1.094243	-0.858581
2	6	0	4.346391	0.176432	-0.901350
3	6	0	4.338439	-0.871778	0.005849
4	6	0	3.340179	-1.024730	0.955922
5	6	0	2.313464	-0.092253	0.991405
6	6	0	2.276103	0.973983	0.081606
7	1	0	3.284749	1.906906	-1.575473
8	1	0	5.146930	0.254857	-1.624568
9	1	0	3.388185	-1.848777	1.655219
10	1	0	1.548403	-0.168864	1.756796
11	6	0	1.190824	1.974053	0.112154
12	6	0	-0.129490	1.668494	0.112676
13	6	0	1.532402	3.410894	0.101696
14	1	0	-0.824776	2.499753	0.127369
15	1	0	2.617246	3.630202	0.114465
16	8	0	0.725643	4.309455	0.094128
17	7	0	-0.664174	0.421715	0.052966
18	1	0	-0.018541	-0.350969	-0.049403
19	6	0	-2.020769	0.096434	0.018131
20	6	0	-2.367124	-1.244041	-0.198871
21	6	0	-3.029122	1.050935	0.199548
22	6	0	-3.693547	-1.629482	-0.242546
23	1	0	-1.587160	-1.984016	-0.340096
24	6	0	-4.358814	0.667852	0.149322
25	1	0	-2.793909	2.089099	0.387493
26	6	0	-4.675366	-0.663837	-0.070352
27	1	0	-3.977211	-2.659538	-0.411581
28	1	0	-5.152561	1.390326	0.284265
29	7	0	5.435692	-1.860460	-0.035396
30	8	0	5.389515	-2.778742	0.753777
31	8	0	6.309712	-1.689901	-0.856131
32	7	0	-6.089211	-1.064753	-0.121875
33	8	0	-6.923114	-0.197366	0.025406
34	8	0	-6.331215	-2.238159	-0.308932

Structure 38b ($CHCl_3$)

Energy (Hartrees): -1118.28414516
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.338281	1.108919	-0.835297
2	6	0	4.368841	0.181954	-0.864618
3	6	0	4.320696	-0.886142	0.020026
4	6	0	3.292125	-1.048379	0.937593
5	6	0	2.275735	-0.105960	0.961386
6	6	0	2.277283	0.979023	0.071943
7	1	0	3.347763	1.935727	-1.536796
8	1	0	5.186559	0.272944	-1.567166
9	1	0	3.300129	-1.883855	1.624956
10	1	0	1.486359	-0.195590	1.700021
11	6	0	1.197633	1.986597	0.095057
12	6	0	-0.129242	1.687755	0.085181
13	6	0	1.556021	3.409840	0.107611
14	1	0	-0.826731	2.516979	0.113337

15	1	0	2.640732	3.616498	0.146717
16	8	0	0.763615	4.330888	0.094160
17	7	0	-0.663575	0.447697	0.000611
18	1	0	-0.025047	-0.330479	-0.125032
19	6	0	-2.017436	0.119094	-0.012714
20	6	0	-2.356029	-1.221164	-0.252417
21	6	0	-3.028604	1.063310	0.209072
22	6	0	-3.678998	-1.615503	-0.281154
23	1	0	-1.571003	-1.949927	-0.420591
24	6	0	-4.355160	0.671175	0.175824
25	1	0	-2.797448	2.098377	0.418074
26	6	0	-4.665900	-0.659471	-0.070882
27	1	0	-3.947211	-2.646705	-0.467397
28	1	0	-5.144626	1.391086	0.344947
29	7	0	5.401392	-1.883559	-0.014057
30	8	0	5.290571	-2.866123	0.690651
31	8	0	6.346256	-1.673603	-0.746531
32	7	0	-6.070035	-1.068165	-0.101355
33	8	0	-6.917183	-0.221425	0.106401
34	8	0	-6.320188	-2.235133	-0.333072

Structure 38b (DMSO)

Energy (Hartrees): -1118.28635189
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.340286	1.126539	-0.809236
2	6	0	4.379086	0.210969	-0.858583
3	6	0	4.337849	-0.880643	-0.001720
4	6	0	3.303022	-1.078503	0.902005
5	6	0	2.276494	-0.147809	0.944648
6	6	0	2.274326	0.962016	0.086902
7	1	0	3.348030	1.972515	-1.487322
8	1	0	5.197652	0.333480	-1.555108
9	1	0	3.309372	-1.933019	1.565623
10	1	0	1.481542	-0.273097	1.671760
11	6	0	1.192816	1.966660	0.127105
12	6	0	-0.136955	1.672701	0.119714
13	6	0	1.561001	3.386153	0.143444
14	1	0	-0.831581	2.504311	0.153562
15	1	0	2.648246	3.581103	0.168689
16	8	0	0.780078	4.318398	0.146565
17	7	0	-0.677611	0.437494	0.035411
18	1	0	-0.045391	-0.350885	-0.062983
19	6	0	-2.031991	0.117092	0.007607
20	6	0	-2.370721	-1.235064	-0.156430
21	6	0	-3.044873	1.077291	0.140089
22	6	0	-3.693890	-1.626159	-0.194972
23	1	0	-1.583540	-1.974174	-0.257095
24	6	0	-4.371432	0.688015	0.094776
25	1	0	-2.817620	2.124856	0.281314
26	6	0	-4.682773	-0.655718	-0.071973
27	1	0	-3.957332	-2.667532	-0.323041
28	1	0	-5.158434	1.423885	0.193845
29	7	0	5.430258	-1.861569	-0.050245
30	8	0	5.351236	-2.841497	0.664640
31	8	0	6.359172	-1.645064	-0.803819
32	7	0	-6.084812	-1.059971	-0.122185
33	8	0	-6.936048	-0.191048	-0.073506
34	8	0	-6.336847	-2.247583	-0.212675

Structure 38b (C_2H_5OH)

Energy (Hartrees): -1118.28527609
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.322366	1.104619	-0.840653
2	6	0	4.360226	0.187876	-0.881804
3	6	0	4.332297	-0.878324	0.007101
4	6	0	3.314296	-1.051180	0.935176
5	6	0	2.289655	-0.118354	0.969257
6	6	0	2.273689	0.965649	0.079540
7	1	0	3.316518	1.930264	-1.543654
8	1	0	5.165704	0.288297	-1.597144
9	1	0	3.333540	-1.884626	1.625016
10	1	0	1.507567	-0.219605	1.714049
11	6	0	1.191085	1.970687	0.111410
12	6	0	-0.139252	1.670987	0.109403
13	6	0	1.553655	3.384403	0.111989
14	1	0	-0.839263	2.498150	0.138743
15	1	0	2.637691	3.589046	0.131530
16	8	0	0.766114	4.318834	0.106952
17	7	0	-0.672105	0.434429	0.032309
18	1	0	-0.036681	-0.350425	-0.076468
19	6	0	-2.027130	0.111033	0.010797
20	6	0	-2.366143	-1.232756	-0.208697
21	6	0	-3.036860	1.063925	0.203612
22	6	0	-3.689351	-1.622552	-0.248529
23	1	0	-1.580829	-1.966569	-0.352729
24	6	0	-4.363627	0.677612	0.156575
25	1	0	-2.806085	2.102160	0.398632
26	6	0	-4.675655	-0.657756	-0.069861
27	1	0	-3.954134	-2.657167	-0.421592
28	1	0	-5.149201	1.407535	0.301010
29	7	0	5.422028	-1.857435	-0.032631
30	8	0	5.337617	-2.843850	0.673324
31	8	0	6.363536	-1.639743	-0.770659
32	7	0	-6.074385	-1.058896	-0.119247
33	8	0	-6.928871	-0.198564	-0.004152
34	8	0	-6.333283	-2.239047	-0.274503

Structure 38c (vacuum)

Energy (Hartrees): -1118.25347831
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.296559	1.058751	-0.830970
2	6	0	4.288208	0.089750	-0.843728
3	6	0	4.196851	-0.965778	0.050730
4	6	0	3.162041	-1.079740	0.965222
5	6	0	2.177754	-0.101986	0.967368
6	6	0	2.223990	0.968001	0.063856
7	1	0	3.353993	1.897798	-1.511396
8	1	0	5.123249	0.139664	-1.529352
9	1	0	3.147027	-1.909704	1.658620
10	1	0	1.379217	-0.150628	1.699967
11	6	0	1.164592	1.998856	0.064872
12	6	0	-0.160459	1.714694	0.048791
13	6	0	1.517092	3.425362	0.033133

14	1	0	-0.869002	2.536135	0.056779
15	7	0	-0.709473	0.471657	-0.036299
16	1	0	-0.072853	-0.297091	-0.205307
17	6	0	-2.069434	0.164931	-0.032957
18	6	0	-2.462458	-1.104807	-0.477186
19	6	0	-3.037131	1.072115	0.415010
20	6	0	-3.797679	-1.460852	-0.490514
21	1	0	-1.713233	-1.807062	-0.825000
22	6	0	-4.376945	0.722266	0.390383
23	1	0	-2.754936	2.039808	0.806643
24	6	0	-4.740349	-0.536375	-0.062456
25	1	0	-4.119594	-2.434955	-0.833400
26	1	0	-5.140772	1.407507	0.732882
27	8	0	2.638547	3.862222	-0.035493
28	1	0	0.645883	4.110433	0.078279
29	7	0	5.247528	-2.005808	0.037245
30	8	0	5.128205	-2.929564	0.812736
31	8	0	6.157665	-1.870201	-0.749895
32	7	0	-6.164090	-0.905888	-0.079202
33	8	0	-6.962148	-0.074948	0.298031
34	8	0	-6.448834	-2.017855	-0.469159

Structure 38c ($CHCl_3$)

Energy (Hartrees): -1118.28651974
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.297022	1.049531	-0.846171
2	6	0	4.300396	0.093573	-0.849039
3	6	0	4.213486	-0.958914	0.051782
4	6	0	3.170795	-1.081747	0.958218
5	6	0	2.177295	-0.114078	0.951203
6	6	0	2.221645	0.954694	0.046110
7	1	0	3.344768	1.877776	-1.541575
8	1	0	5.132640	0.155086	-1.537504
9	1	0	3.148877	-1.906766	1.657711
10	1	0	1.371073	-0.175205	1.674553
11	6	0	1.160048	1.983709	0.040806
12	6	0	-0.170729	1.704204	0.009894
13	6	0	1.506707	3.402425	0.053922
14	1	0	-0.872594	2.531317	0.020596
15	7	0	-0.721365	0.470065	-0.088183
16	1	0	-0.097324	-0.311537	-0.258071
17	6	0	-2.081292	0.168591	-0.066670
18	6	0	-2.477494	-1.104103	-0.502931
19	6	0	-3.042912	1.078696	0.391966
20	6	0	-3.811543	-1.461127	-0.497699
21	1	0	-1.730410	-1.806137	-0.856282
22	6	0	-4.381434	0.727630	0.386670
23	1	0	-2.758537	2.048541	0.777495
24	6	0	-4.750440	-0.534530	-0.058851
25	1	0	-4.126137	-2.439579	-0.835379
26	1	0	-5.132497	1.421023	0.741132
27	8	0	2.635040	3.849172	0.048597
28	1	0	0.636915	4.086011	0.082154
29	7	0	5.270649	-1.982882	0.049311
30	8	0	5.126219	-2.951145	0.767980
31	8	0	6.230098	-1.808156	-0.673279
32	7	0	-6.166559	-0.902787	-0.053961
33	8	0	-6.973383	-0.065079	0.299500
34	8	0	-6.466118	-2.027620	-0.404081

Structure 38c (DMSO)

Energy (Hartrees): -1118.28958379
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.264938	1.058002	-0.845190
2	6	0	4.270942	0.107073	-0.895102
3	6	0	4.218619	-0.957323	-0.004421
4	6	0	3.204284	-1.097846	0.931193
5	6	0	2.208340	-0.132691	0.971921
6	6	0	2.220645	0.949239	0.082507
7	1	0	3.283534	1.890626	-1.536961
8	1	0	5.076470	0.183270	-1.613227
9	1	0	3.201299	-1.934111	1.617562
10	1	0	1.423975	-0.212725	1.717051
11	6	0	1.162664	1.980687	0.120673
12	6	0	-0.172807	1.712984	0.097987
13	6	0	1.515936	3.394939	0.166512
14	1	0	-0.861262	2.549829	0.133859
15	7	0	-0.734382	0.486518	0.002549
16	1	0	-0.114287	-0.312301	-0.088325
17	6	0	-2.093707	0.189646	-0.017513
18	6	0	-2.455666	-1.158894	-0.159603
19	6	0	-3.090224	1.168459	0.103274
20	6	0	-3.785118	-1.528773	-0.183834
21	1	0	-1.680678	-1.911787	-0.252713
22	6	0	-4.423255	0.800219	0.073205
23	1	0	-2.846182	2.214937	0.223060
24	6	0	-4.757485	-0.540671	-0.069113
25	1	0	-4.067044	-2.567456	-0.292929
26	1	0	-5.197367	1.550607	0.165148
27	8	0	2.647443	3.839709	0.189390
28	1	0	0.648599	4.080094	0.193173
29	7	0	5.280544	-1.972830	-0.051338
30	8	0	5.172264	-2.946798	0.667648
31	8	0	6.213836	-1.787795	-0.807574
32	7	0	-6.165998	-0.922872	-0.101492
33	8	0	-7.002923	-0.040030	-0.053913
34	8	0	-6.437725	-2.107209	-0.176639

Structure 38c (C_2H_5OH)

Energy (Hartrees): -1118.28891711
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.237854	1.034354	-0.877124
2	6	0	4.243543	0.083139	-0.925994
3	6	0	4.211424	-0.956597	-0.005789
4	6	0	3.219343	-1.075470	0.956711
5	6	0	2.224122	-0.109877	0.995411
6	6	0	2.217506	0.948742	0.078785
7	1	0	3.237616	1.848487	-1.591839
8	1	0	5.031564	0.140183	-1.665283
9	1	0	3.234487	-1.892464	1.666062
10	1	0	1.456768	-0.168690	1.760054
11	6	0	1.161912	1.983566	0.119494
12	6	0	-0.175412	1.717212	0.101162
13	6	0	1.517010	3.390046	0.163266
14	1	0	-0.864226	2.553647	0.137582

15	7	0	-0.733255	0.491161	0.008032
16	1	0	-0.110550	-0.306154	-0.081893
17	6	0	-2.093131	0.191348	-0.012539
18	6	0	-2.451601	-1.156973	-0.162155
19	6	0	-3.090172	1.168559	0.114753
20	6	0	-3.779978	-1.529257	-0.188642
21	1	0	-1.675932	-1.908512	-0.260225
22	6	0	-4.422238	0.799101	0.083112
23	1	0	-2.847753	2.214600	0.241738
24	6	0	-4.752954	-0.542134	-0.067879
25	1	0	-4.059551	-2.567866	-0.305216
26	1	0	-5.197834	1.547353	0.180927
27	8	0	2.657077	3.829397	0.178721
28	1	0	0.659667	4.084571	0.195245
29	7	0	5.273484	-1.967339	-0.048202
30	8	0	5.176610	-2.936325	0.679698
31	8	0	6.204183	-1.790662	-0.809903
32	7	0	-6.156941	-0.924619	-0.103324
33	8	0	-6.998962	-0.045645	-0.055195
34	8	0	-6.432737	-2.108532	-0.181837

Structure 38d (vacuum)

Energy (Hartrees): -1118.24499763
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.443413	1.147323	0.645422
2	6	0	-4.595014	0.382630	0.750071
3	6	0	-4.650638	-0.832854	0.085158
4	6	0	-3.602144	-1.302988	-0.688613
5	6	0	-2.459476	-0.523863	-0.788557
6	6	0	-2.355510	0.698268	-0.113469
7	1	0	-3.386054	2.098775	1.155778
8	1	0	-5.441944	0.709549	1.338061
9	1	0	-3.697134	-2.247643	-1.206544
10	1	0	-1.646756	-0.856702	-1.424150
11	6	0	-1.108470	1.494044	-0.197385
12	6	0	0.088671	0.858546	-0.095479
13	6	0	-1.186686	2.948020	-0.393353
14	1	0	0.085066	-0.213117	0.067669
15	7	0	1.336485	1.411168	-0.122773
16	1	0	1.418117	2.416292	-0.128532
17	6	0	2.543386	0.712879	-0.058695
18	6	0	3.705378	1.436217	0.242724
19	6	0	2.629487	-0.662651	-0.302600
20	6	0	4.930628	0.801451	0.312347
21	1	0	3.640077	2.501691	0.432541
22	6	0	3.854686	-1.304107	-0.220358
23	1	0	1.756971	-1.237554	-0.581101
24	6	0	4.987480	-0.566861	0.086549
25	1	0	5.835702	1.345313	0.546796
26	1	0	3.943826	-2.366084	-0.406342
27	1	0	-0.219208	3.472921	-0.527441
28	8	0	-2.206822	3.590092	-0.435384
29	7	0	-5.874365	-1.652170	0.196420
30	8	0	-5.899043	-2.705105	-0.403888
31	8	0	-6.775933	-1.222117	0.882034
32	7	0	6.286915	-1.251810	0.165364
33	8	0	7.258425	-0.577771	0.432161
34	8	0	6.303109	-2.446362	-0.040221

Structure 38d ($CHCl_3$)

Energy (Hartrees): -1118.27933926
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.442292	1.135577	0.670695
2	6	0	-4.594039	0.370393	0.760971
3	6	0	-4.650646	-0.831327	0.068332
4	6	0	-3.601042	-1.284551	-0.717067
5	6	0	-2.459395	-0.503056	-0.802739
6	6	0	-2.354442	0.706118	-0.102512
7	1	0	-3.382765	2.068754	1.214387
8	1	0	-5.433818	0.690805	1.363080
9	1	0	-3.685147	-2.217869	-1.257449
10	1	0	-1.644258	-0.827495	-1.439497
11	6	0	-1.108235	1.504547	-0.166937
12	6	0	0.090174	0.856173	-0.087126
13	6	0	-1.185105	2.953702	-0.342914
14	1	0	0.075211	-0.220985	0.030955
15	7	0	1.333623	1.399584	-0.093095
16	1	0	1.429557	2.406692	-0.077025
17	6	0	2.537487	0.698635	-0.040912
18	6	0	3.708661	1.441819	0.168433
19	6	0	2.616671	-0.690553	-0.204204
20	6	0	4.937053	0.814316	0.227500
21	1	0	3.645284	2.517838	0.287337
22	6	0	3.845671	-1.323293	-0.136475
23	1	0	1.736680	-1.286585	-0.402355
24	6	0	4.989227	-0.567148	0.080972
25	1	0	5.843310	1.381631	0.392899
26	1	0	3.919225	-2.395478	-0.261998
27	1	0	-0.222953	3.486528	-0.444713
28	8	0	-2.214932	3.592738	-0.413007
29	7	0	-5.867933	-1.648995	0.164905
30	8	0	-5.889204	-2.711200	-0.424490
31	8	0	-6.790683	-1.222479	0.829360
32	7	0	6.284510	-1.243057	0.150240
33	8	0	7.280012	-0.558654	0.285729
34	8	0	6.301030	-2.455989	0.070400

Structure 38d (DMSO)

Energy (Hartrees): -1118.28295575
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.442661	1.138263	0.667118
2	6	0	-4.600167	0.382336	0.754948
3	6	0	-4.657257	-0.827822	0.075372
4	6	0	-3.598078	-1.299418	-0.687042
5	6	0	-2.450085	-0.526917	-0.769784
6	6	0	-2.348161	0.694252	-0.089469
7	1	0	-3.381954	2.075625	1.203747
8	1	0	-5.441616	0.718058	1.346403
9	1	0	-3.675788	-2.240525	-1.214796
10	1	0	-1.627219	-0.870497	-1.386272
11	6	0	-1.104557	1.494190	-0.156454
12	6	0	0.095425	0.846194	-0.065059
13	6	0	-1.185620	2.937821	-0.360278
14	1	0	0.080819	-0.230778	0.057785
15	7	0	1.334306	1.392175	-0.070698

16	1	0	1.431333	2.400731	-0.065110
17	6	0	2.537976	0.693269	-0.022471
18	6	0	3.706475	1.440176	0.191906
19	6	0	2.621416	-0.694943	-0.197473
20	6	0	4.936989	0.817213	0.243159
21	1	0	3.636219	2.514459	0.321066
22	6	0	3.853140	-1.322511	-0.138595
23	1	0	1.743099	-1.292938	-0.398338
24	6	0	4.995226	-0.563181	0.081954
25	1	0	5.839545	1.389426	0.411324
26	1	0	3.926525	-2.393201	-0.276244
27	1	0	-0.226924	3.479013	-0.428126
28	8	0	-2.220210	3.564156	-0.492364
29	7	0	-5.882184	-1.631746	0.161419
30	8	0	-5.907469	-2.700909	-0.417607
31	8	0	-6.813434	-1.189543	0.806402
32	7	0	6.292597	-1.231004	0.135537
33	8	0	7.284909	-0.545558	0.301222
34	8	0	6.321527	-2.441757	0.012067

Structure 38d (C_2H_5OH)

Energy (Hartrees): -1118.28200648
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.444533	1.136843	0.679728
2	6	0	-4.596128	0.371271	0.760525
3	6	0	-4.643252	-0.831223	0.066447
4	6	0	-3.582452	-1.286921	-0.703872
5	6	0	-2.440685	-0.505426	-0.777511
6	6	0	-2.347953	0.708026	-0.082428
7	1	0	-3.389605	2.068323	1.228088
8	1	0	-5.439664	0.694009	1.356420
9	1	0	-3.652921	-2.222894	-1.241871
10	1	0	-1.615122	-0.835670	-1.397755
11	6	0	-1.107080	1.513778	-0.142833
12	6	0	0.095305	0.867472	-0.045591
13	6	0	-1.189445	2.950348	-0.350579
14	1	0	0.077766	-0.208222	0.086017
15	7	0	1.334005	1.408703	-0.056313
16	1	0	1.436663	2.416968	-0.066472
17	6	0	2.535064	0.702649	-0.012434
18	6	0	3.710300	1.445651	0.175341
19	6	0	2.606265	-0.688329	-0.168986
20	6	0	4.937478	0.815968	0.219544
21	1	0	3.648789	2.522254	0.288875
22	6	0	3.833394	-1.323521	-0.115151
23	1	0	1.722585	-1.283926	-0.352147
24	6	0	4.982854	-0.567648	0.079530
25	1	0	5.845933	1.385082	0.366464
26	1	0	3.897267	-2.396617	-0.237947
27	1	0	-0.236438	3.499188	-0.413052
28	8	0	-2.229936	3.574592	-0.491145
29	7	0	-5.856237	-1.647085	0.148935
30	8	0	-5.897724	-2.684900	-0.484659
31	8	0	-6.770889	-1.254144	0.848010
32	7	0	6.271517	-1.243526	0.128108
33	8	0	7.277098	-0.566434	0.246260
34	8	0	6.292072	-2.458960	0.050021

Structure 38g (vacuum)

Energy (Hartrees): -1118.25025153
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.531124	-0.417180	-0.832209
2	6	0	-3.708259	-1.148672	-0.863591
3	6	0	-4.760210	-0.742997	-0.056892
4	6	0	-4.668062	0.357669	0.780935
5	6	0	-3.478388	1.069226	0.811335
6	6	0	-2.397317	0.701703	0.000002
7	1	0	-1.715370	-0.702475	-1.486431
8	1	0	-3.826429	-2.009017	-1.508285
9	1	0	-5.510075	0.629260	1.403355
10	1	0	-3.377563	1.905692	1.492833
11	6	0	-1.138583	1.475402	0.010883
12	6	0	-1.163332	2.840926	0.035700
13	6	0	0.130517	0.784725	-0.027153
14	1	0	-2.103177	3.386362	0.044886
15	1	0	0.110345	-0.310229	-0.004599
16	8	0	-0.105760	3.616061	0.025168
17	1	0	0.698463	3.027251	-0.018279
18	7	0	1.252409	1.416463	-0.076236
19	6	0	2.457656	0.695968	-0.017319
20	6	0	2.636788	-0.374143	0.866795
21	6	0	3.512868	1.101521	-0.841142
22	6	0	3.844201	-1.054420	0.904508
23	1	0	1.840401	-0.649965	1.547308
24	6	0	4.719131	0.422727	-0.816416
25	1	0	3.364927	1.943052	-1.506275
26	6	0	4.862098	-0.647660	0.056265
27	1	0	4.010128	-1.878977	1.584476
28	1	0	5.545516	0.707537	-1.453460
29	7	0	-6.019788	-1.511769	-0.087460
30	8	0	-6.922834	-1.134865	0.627313
31	8	0	-6.071440	-2.471158	-0.825960
32	7	0	6.148828	-1.368075	0.093604
33	8	0	7.018497	-0.999891	-0.665835
34	8	0	6.254635	-2.284347	0.879927

Structure 38g ($CHCl_3$)

Energy (Hartrees): -1118.27723458
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.520969	-0.450988	-0.793030
2	6	0	-3.700130	-1.177942	-0.824238
3	6	0	-4.769599	-0.737770	-0.057232
4	6	0	-4.691865	0.395071	0.741194
5	6	0	-3.500259	1.101710	0.772768
6	6	0	-2.401530	0.698926	0.000429
7	1	0	-1.692018	-0.769305	-1.414742
8	1	0	-3.796642	-2.061538	-1.440843
9	1	0	-5.541050	0.700626	1.337972
10	1	0	-3.415456	1.963963	1.423679
11	6	0	-1.138930	1.465576	0.012933
12	6	0	-1.156299	2.831820	0.041603
13	6	0	0.125451	0.766055	-0.023325
14	1	0	-2.089022	3.389334	0.054807
15	1	0	0.103357	-0.327412	0.000998
16	8	0	-0.085958	3.593720	0.029963
17	1	0	0.712831	2.989957	-0.018709
18	7	0	1.248318	1.398477	-0.075448

19	6	0	2.455476	0.684372	-0.016991
20	6	0	2.632651	-0.403079	0.847550
21	6	0	3.515924	1.115613	-0.822657
22	6	0	3.844970	-1.072544	0.884886
23	1	0	1.829964	-0.705983	1.509034
24	6	0	4.727164	0.446807	-0.800083
25	1	0	3.370274	1.969927	-1.472625
26	6	0	4.869583	-0.639889	0.054547
27	1	0	4.000609	-1.909524	1.552371
28	1	0	5.551910	0.758000	-1.427226
29	7	0	-6.025015	-1.499837	-0.087576
30	8	0	-6.967586	-1.072451	0.548248
31	8	0	-6.056811	-2.518842	-0.747814
32	7	0	6.154614	-1.349020	0.090165
33	8	0	7.021450	-0.998404	-0.685180
34	8	0	6.285153	-2.252501	0.891679

Structure 38g (DMSO)

Energy (Hartrees): -1118.27690819
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.508539	-0.481262	-0.749469
2	6	0	-3.688989	-1.205554	-0.781104
3	6	0	-4.775746	-0.734427	-0.057208
4	6	0	-4.712362	0.428900	0.698661
5	6	0	-3.519949	1.133531	0.731746
6	6	0	-2.403849	0.698290	0.002153
7	1	0	-1.667509	-0.828311	-1.338382
8	1	0	-3.768943	-2.111980	-1.366082
9	1	0	-5.572056	0.763635	1.264115
10	1	0	-3.452558	2.022197	1.348220
11	6	0	-1.138909	1.459291	0.016923
12	6	0	-1.149168	2.827082	0.033456
13	6	0	0.122635	0.755736	-0.012103
14	1	0	-2.078098	3.391094	0.035791
15	1	0	0.099918	-0.336927	0.008506
16	8	0	-0.071065	3.577214	0.021546
17	1	0	0.719632	2.955214	-0.016880
18	7	0	1.246128	1.390483	-0.056661
19	6	0	2.454437	0.679129	-0.002994
20	6	0	2.625771	-0.436468	0.826800
21	6	0	3.522849	1.142504	-0.780081
22	6	0	3.840421	-1.101400	0.855523
23	1	0	1.816161	-0.768672	1.465611
24	6	0	4.736724	0.478528	-0.766035
25	1	0	3.382405	2.018707	-1.401776
26	6	0	4.873814	-0.636618	0.052719
27	1	0	3.987177	-1.961636	1.494976
28	1	0	5.564883	0.818000	-1.373895
29	7	0	-6.030875	-1.493069	-0.089407
30	8	0	-6.984073	-1.050919	0.522671
31	8	0	-6.057834	-2.527470	-0.728345
32	7	0	6.159428	-1.341721	0.078702
33	8	0	7.030857	-0.972136	-0.684635
34	8	0	6.291037	-2.263532	0.860941

Structure 38g (C_2H_5OH)

Energy (Hartrees): -1118.27527689
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-2.504910	-0.458900	-0.775464
2	6	0	-3.679783	-1.191519	-0.806553
3	6	0	-4.759293	-0.742861	-0.057173
4	6	0	-4.695199	0.404674	0.723005
5	6	0	-3.508060	1.117277	0.753970
6	6	0	-2.399295	0.705616	-0.000530
7	1	0	-1.669130	-0.786820	-1.382720
8	1	0	-3.761373	-2.085718	-1.410138
9	1	0	-5.549011	0.719756	1.308399
10	1	0	-3.437199	1.992285	1.389327
11	6	0	-1.139394	1.475302	0.012719
12	6	0	-1.163300	2.840018	0.053193
13	6	0	0.125426	0.775093	-0.032851
14	1	0	-2.095967	3.396664	0.074916
15	1	0	0.101420	-0.317850	-0.012547
16	8	0	-0.092266	3.607835	0.044326
17	1	0	0.711055	3.012776	-0.014798
18	7	0	1.248419	1.407249	-0.086060
19	6	0	2.451274	0.687356	-0.028556
20	6	0	2.621950	-0.400350	0.837995
21	6	0	3.515497	1.114605	-0.832141
22	6	0	3.831559	-1.072840	0.881301
23	1	0	1.815063	-0.701858	1.495300
24	6	0	4.724011	0.442352	-0.805379
25	1	0	3.376917	1.968578	-1.484245
26	6	0	4.860633	-0.643025	0.053321
27	1	0	3.977712	-1.909742	1.551246
28	1	0	5.549313	0.753965	-1.431788
29	7	0	-6.005360	-1.508639	-0.086865
30	8	0	-6.957887	-1.088632	0.542884
31	8	0	-6.037078	-2.533529	-0.741851
32	7	0	6.139546	-1.350162	0.096894
33	8	0	7.011669	-1.017266	-0.683603
34	8	0	6.277596	-2.243151	0.911759

Structure 39a (vacuum)

Energy (Hartrees): -1034.92201435
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.681045	-0.955719	-0.986688
2	6	0	-4.061598	-1.023478	-1.015699
3	6	0	-4.823753	-0.204234	-0.178492
4	6	0	-4.181818	0.672701	0.691461
5	6	0	-2.788440	0.716107	0.719354
6	6	0	-2.010212	-0.079970	-0.119250
7	1	0	-2.107386	-1.576882	-1.666498
8	1	0	-4.579547	-1.694535	-1.690020
9	1	0	-4.743850	1.307292	1.363316
10	1	0	-2.301262	1.372204	1.432831
11	6	0	-0.529508	-0.007967	-0.099933
12	6	0	0.084786	1.213474	-0.056159
13	6	0	0.221412	-1.243270	-0.099592
14	1	0	-0.531221	2.105922	-0.064357
15	1	0	-0.373239	-2.164539	-0.100963
16	1	0	1.976846	0.559328	0.049015
17	7	0	1.507819	-1.305780	-0.086143
18	7	0	1.418296	1.413895	0.007274
19	8	0	-6.172797	-0.337387	-0.282941
20	6	0	-6.976064	0.476009	0.544443
21	1	0	-8.007392	0.226864	0.304511
22	1	0	-6.789157	0.270265	1.603330
23	1	0	-6.802121	1.538108	0.343876
24	6	0	2.119595	-2.570563	0.008751
25	6	0	3.277211	-2.806961	-0.738867
26	6	0	1.639973	-3.575099	0.856514
27	6	0	3.915569	-4.037543	-0.672566

28	1	0	3.651078	-2.016490	-1.379054
29	6	0	2.288867	-4.802571	0.924362
30	1	0	0.778135	-3.377682	1.483853
31	6	0	3.423754	-5.042457	0.157278
32	1	0	4.804389	-4.213539	-1.267313
33	1	0	1.911670	-5.569832	1.590589
34	1	0	3.929043	-5.998856	0.215050
35	6	0	2.066104	2.654633	0.006062
36	6	0	3.404667	2.699365	0.410774
37	6	0	1.434886	3.836051	-0.392929
38	6	0	4.091397	3.903815	0.428415
39	1	0	3.894573	1.782623	0.720430
40	6	0	2.130525	5.038786	-0.358415
41	1	0	0.414762	3.823925	-0.754263
42	6	0	3.457936	5.084949	0.051759
43	1	0	5.127139	3.919634	0.746885
44	1	0	1.627663	5.946788	-0.670110
45	1	0	3.993974	6.025336	0.071016

Structure 39a ($CHCl_3$)

Energy (Hartrees): -1034.95328501
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.671652	-1.023289	-0.940245
2	6	0	-4.052790	-1.101230	-0.981241
3	6	0	-4.829788	-0.257141	-0.182136
4	6	0	-4.201734	0.652836	0.665501
5	6	0	-2.808740	0.707196	0.706111
6	6	0	-2.014880	-0.112056	-0.097960
7	1	0	-2.089718	-1.666244	-1.592462
8	1	0	-4.553712	-1.801178	-1.640260
9	1	0	-4.775881	1.307088	1.308436
10	1	0	-2.337191	1.397223	1.398419
11	6	0	-0.533195	-0.022951	-0.074101
12	6	0	0.063209	1.210627	-0.041118
13	6	0	0.230244	-1.249585	-0.074273
14	1	0	-0.567596	2.092405	-0.056243
15	1	0	-0.353493	-2.176726	-0.071079
16	1	0	1.972279	0.592385	0.051209
17	7	0	1.519216	-1.297052	-0.071686
18	7	0	1.392548	1.432109	0.012130
19	8	0	-6.176569	-0.397115	-0.298121
20	6	0	-6.997303	0.457222	0.480523
21	1	0	-8.024660	0.201107	0.228324
22	1	0	-6.835366	0.292243	1.550003
23	1	0	-6.815818	1.508642	0.237671
24	6	0	2.150219	-2.553094	0.017641
25	6	0	3.329553	-2.753538	-0.708407
26	6	0	1.672776	-3.582903	0.837809
27	6	0	3.992661	-3.972604	-0.649063
28	1	0	3.703766	-1.945357	-1.327182
29	6	0	2.345758	-4.798571	0.898075
30	1	0	0.790747	-3.417867	1.446628
31	6	0	3.503471	-5.002260	0.152725
32	1	0	4.899015	-4.118960	-1.226024
33	1	0	1.968973	-5.585447	1.542073
34	1	0	4.026933	-5.949725	0.205296
35	6	0	2.029586	2.679867	0.006855
36	6	0	3.398355	2.713446	0.298931
37	6	0	1.362848	3.873872	-0.285247
38	6	0	4.082799	3.920359	0.309752
39	1	0	3.915189	1.785691	0.521768
40	6	0	2.059244	5.077395	-0.262433
41	1	0	0.312299	3.876836	-0.546165
42	6	0	3.417855	5.113308	0.034672
43	1	0	5.142195	3.927419	0.540035
44	1	0	1.528838	5.995208	-0.489962
45	1	0	3.952425	6.055337	0.047140

Structure 39a (DMSO)

Energy (Hartrees): -1034.94674770
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.666806	-1.080878	-0.894845
2	6	0	-4.047958	-1.167637	-0.940841
3	6	0	-4.835947	-0.298540	-0.179352
4	6	0	-4.216486	0.645764	0.638238
5	6	0	-2.824034	0.709283	0.684924
6	6	0	-2.019952	-0.135141	-0.083042
7	1	0	-2.079566	-1.746452	-1.519122
8	1	0	-4.537300	-1.896341	-1.577286
9	1	0	-4.796467	1.321707	1.253104
10	1	0	-2.362238	1.430383	1.351803
11	6	0	-0.539024	-0.034371	-0.055893
12	6	0	0.046240	1.206367	-0.030800
13	6	0	0.233876	-1.254437	-0.051910
14	1	0	-0.591952	2.082882	-0.050913
15	1	0	-0.340853	-2.186706	-0.045965
16	1	0	1.964454	0.607473	0.062092
17	7	0	1.524236	-1.288086	-0.052828
18	7	0	1.373156	1.439052	0.019198
19	8	0	-6.179963	-0.446862	-0.298052
20	6	0	-7.004361	0.442741	0.440887
21	1	0	-8.031222	0.182016	0.191664
22	1	0	-6.850345	0.321095	1.517028
23	1	0	-6.815287	1.482571	0.158313
24	6	0	2.172617	-2.536078	0.025617
25	6	0	3.368149	-2.698389	-0.684348
26	6	0	1.701452	-3.592807	0.815563
27	6	0	4.055746	-3.904884	-0.639236
28	1	0	3.738178	-1.869818	-1.278704
29	6	0	2.398903	-4.795923	0.861479
30	1	0	0.804174	-3.462569	1.410592
31	6	0	3.573356	-4.961130	0.131798
32	1	0	4.974815	-4.019327	-1.203275
33	1	0	2.027046	-5.604303	1.481442
34	1	0	4.114962	-5.899025	0.173413
35	6	0	2.001333	2.691870	0.008956
36	6	0	3.374899	2.729712	0.278402
37	6	0	1.323011	3.883394	-0.267059
38	6	0	4.054541	3.939829	0.282305
39	1	0	3.898721	1.802828	0.488861
40	6	0	2.015584	5.089835	-0.252565
41	1	0	0.267191	3.884013	-0.505762
42	6	0	3.379511	5.130709	0.021365
43	1	0	5.117672	3.950556	0.494915
44	1	0	1.477616	6.006369	-0.467719
45	1	0	3.910464	6.075048	0.027483

Structure 39a (C_2H_5OH)

Energy (Hartrees): -1034.95020217
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.668237	-1.035527	-0.935907
2	6	0	-4.050420	-1.114843	-0.967784
3	6	0	-4.822168	-0.259694	-0.176353
4	6	0	-4.192129	0.663761	0.654748
5	6	0	-2.799033	0.720172	0.685936
6	6	0	-2.008704	-0.111271	-0.110283
7	1	0	-2.090035	-1.689479	-1.580774
8	1	0	-4.552772	-1.826051	-1.614254
9	1	0	-4.763364	1.327422	1.290829
10	1	0	-2.325161	1.423089	1.363806
11	6	0	-0.526912	-0.022175	-0.092202
12	6	0	0.067614	1.213183	-0.056239
13	6	0	0.233207	-1.249891	-0.089960
14	1	0	-0.564434	2.094253	-0.067744
15	1	0	-0.352931	-2.175018	-0.074299
16	1	0	1.982829	0.602439	0.036819
17	7	0	1.523146	-1.301239	-0.096862
18	7	0	1.396193	1.436893	-0.002082
19	8	0	-6.173547	-0.401801	-0.281966
20	6	0	-6.990282	0.470982	0.488148
21	1	0	-8.019240	0.213866	0.243509
22	1	0	-6.821669	0.321266	1.558210
23	1	0	-6.803086	1.516070	0.225813
24	6	0	2.146293	-2.560847	0.006373
25	6	0	3.322672	-2.779980	-0.719822
26	6	0	1.665225	-3.575113	0.844453
27	6	0	3.979900	-4.001788	-0.641781
28	1	0	3.703375	-1.985111	-1.352176
29	6	0	2.332242	-4.793406	0.923241
30	1	0	0.785386	-3.396890	1.453112
31	6	0	3.487169	-5.015777	0.178026
32	1	0	4.884142	-4.162075	-1.218792
33	1	0	1.952554	-5.567606	1.581147
34	1	0	4.006333	-5.964975	0.245280
35	6	0	2.029738	2.687610	0.003734
36	6	0	3.399659	2.719845	0.290832
37	6	0	1.358651	3.882459	-0.274759
38	6	0	4.082645	3.927998	0.309922
39	1	0	3.918790	1.790567	0.502603
40	6	0	2.054068	5.086928	-0.244014
41	1	0	0.306432	3.887368	-0.529361
42	6	0	3.414410	5.122334	0.047612
43	1	0	5.143204	3.934446	0.535870
44	1	0	1.521245	6.006195	-0.460889
45	1	0	3.947759	6.065299	0.066102

Structure 39b (vacuum)

Energy (Hartrees): -1034.91500010
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.338080	2.439586	-0.776844
2	6	0	-1.051382	3.636839	-0.746466
3	6	0	-2.085059	3.797152	0.173773
4	6	0	-2.384480	2.760505	1.062636
5	6	0	-1.660459	1.582977	1.025114
6	6	0	-0.624061	1.391760	0.096801
7	1	0	0.454158	2.318966	-1.508305
8	1	0	-0.795971	4.422193	-1.444868
9	1	0	-3.178992	2.912950	1.782879
10	1	0	-1.880915	0.798996	1.742490
11	6	0	0.157192	0.133231	0.057291
12	6	0	-0.422640	-1.091815	0.011207
13	6	0	1.615442	0.216946	0.041227
14	1	0	2.030211	1.215457	0.233610
15	1	0	0.222931	-1.962332	0.004997
16	7	0	2.380800	-0.780940	-0.182459
17	7	0	-1.760526	-1.327602	-0.084274
18	1	0	-2.356270	-0.527382	-0.251921
19	8	0	-2.847691	4.914506	0.286907
20	6	0	-2.571031	5.989713	-0.585988
21	1	0	-2.709808	5.696121	-1.631155
22	1	0	-3.280885	6.773786	-0.333234
23	1	0	-1.551642	6.361692	-0.443801
24	6	0	-2.386339	-2.577766	-0.054176
25	6	0	-3.709199	-2.671945	-0.500072
26	6	0	-1.742587	-3.723452	0.421982
27	6	0	-4.370827	-3.890415	-0.478600
28	1	0	-4.210241	-1.784428	-0.872083
29	6	0	-2.413188	-4.940706	0.424667
30	1	0	-0.733186	-3.668641	0.808174
31	6	0	-3.726135	-5.036739	-0.022610
32	1	0	-5.394940	-3.944381	-0.828392
33	1	0	-1.901392	-5.821146	0.794940
34	1	0	-4.241587	-5.988588	-0.010752
35	6	0	3.770336	-0.603876	-0.067777
36	6	0	4.359056	0.149903	0.954361
37	6	0	4.595122	-1.251616	-0.993732
38	6	0	5.741931	0.281211	1.021095
39	1	0	3.731018	0.604007	1.712426
40	6	0	5.973555	-1.107705	-0.928085
41	1	0	4.129043	-1.855066	-1.763478
42	6	0	6.554665	-0.338638	0.078191
43	1	0	6.185649	0.861415	1.821995
44	1	0	6.599848	-1.603920	-1.660379
45	1	0	7.631592	-0.236856	0.134770

Structure 39b ($CHCl_3$)

Energy (Hartrees): -1034.94811171
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.225459	2.466130	-0.783583
2	6	0	-0.872243	3.700510	-0.743084
3	6	0	-1.916908	3.898359	0.158608
4	6	0	-2.295335	2.859850	1.015329
5	6	0	-1.637114	1.643469	0.967527
6	6	0	-0.590272	1.415852	0.059390
7	1	0	0.577879	2.320821	-1.498858
8	1	0	-0.557113	4.486228	-1.416948
9	1	0	-3.096784	3.034781	1.723867
10	1	0	-1.922827	0.860768	1.663344
11	6	0	0.136378	0.123493	0.019200
12	6	0	-0.485636	-1.086350	-0.011382
13	6	0	1.593758	0.154242	0.011246
14	1	0	2.043019	1.132239	0.225000
15	1	0	0.133489	-1.975434	0.001160
16	7	0	2.334229	-0.864206	-0.227317
17	7	0	-1.824477	-1.289481	-0.093527
18	1	0	-2.412974	-0.478817	-0.245564
19	8	0	-2.616064	5.055010	0.279536
20	6	0	-2.234862	6.145673	-0.543498
21	1	0	-2.365435	5.905526	-1.602813
22	1	0	-2.895210	6.968880	-0.277555
23	1	0	-1.197542	6.437447	-0.354853
24	6	0	-2.484335	-2.523606	-0.053442
25	6	0	-3.849148	-2.550438	-0.365148
26	6	0	-1.838496	-3.714125	0.295130
27	6	0	-4.550732	-3.747215	-0.336877
28	1	0	-4.352038	-1.626483	-0.632377
29	6	0	-2.552530	-4.907336	0.309729
30	1	0	-0.790760	-3.720760	0.566669
31	6	0	-3.907432	-4.937228	-0.004543
32	1	0	-5.606944	-3.748167	-0.581658
33	1	0	-2.037078	-5.822322	0.578963
34	1	0	-4.455187	-5.871482	0.013493
35	6	0	3.726593	-0.732609	-0.078270
36	6	0	4.314444	-0.010615	0.968954
37	6	0	4.554259	-1.397525	-0.990862
38	6	0	5.699461	0.068891	1.074817
39	1	0	3.684214	0.461733	1.714662
40	6	0	5.935764	-1.306606	-0.884696
41	1	0	4.092348	-1.974397	-1.784522
42	6	0	6.516344	-0.571189	0.147631
43	1	0	6.141958	0.623980	1.894748
44	1	0	6.563366	-1.817612	-1.606328
45	1	0	7.594865	-0.510967	0.236120

Structure 39b (DMSO)

Energy (Hartrees): -1034.94246096
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.142917	2.475671	-0.745055
2	6	0	-0.756663	3.727201	-0.706374
3	6	0	-1.821829	3.942667	0.168039
4	6	0	-2.252081	2.902441	0.999450
5	6	0	-1.627036	1.668581	0.953199
6	6	0	-0.559798	1.424151	0.072876
7	1	0	0.677433	2.320432	-1.438652
8	1	0	-0.400810	4.511885	-1.361159
9	1	0	-3.071266	3.085651	1.685397
10	1	0	-1.959378	0.885367	1.627205
11	6	0	0.133912	0.114021	0.033755
12	6	0	-0.517369	-1.082250	-0.001883
13	6	0	1.589844	0.112458	0.032674
14	1	0	2.059072	1.071470	0.282986
15	1	0	0.075359	-1.989149	0.029193
16	7	0	2.311530	-0.911590	-0.246640
17	7	0	-1.857147	-1.253264	-0.107794
18	1	0	-2.427214	-0.434508	-0.290591
19	8	0	-2.490162	5.115899	0.284395
20	6	0	-2.074817	6.193106	-0.543463
21	1	0	-2.190394	5.943471	-1.601949
22	1	0	-2.725015	7.030336	-0.297513
23	1	0	-1.035963	6.468109	-0.341068
24	6	0	-2.543881	-2.472382	-0.060797
25	6	0	-3.885693	-2.485614	-0.461429
26	6	0	-1.947659	-3.657257	0.383460
27	6	0	-4.613707	-3.666765	-0.428554
28	1	0	-4.346621	-1.563711	-0.800893
29	6	0	-2.687110	-4.835629	0.400527
30	1	0	-0.921924	-3.668455	0.728882
31	6	0	-4.018949	-4.853173	-0.003000
32	1	0	-5.651291	-3.658830	-0.742628
33	1	0	-2.212695	-5.747313	0.745892
34	1	0	-4.587146	-5.775279	0.019477
35	6	0	3.706511	-0.810042	-0.090870
36	6	0	4.307368	-0.127712	0.975913
37	6	0	4.522793	-1.464470	-1.022341
38	6	0	5.694091	-0.075761	1.082603
39	1	0	3.687192	0.337822	1.734197
40	6	0	5.906336	-1.401584	-0.914502
41	1	0	4.053977	-2.010300	-1.833929
42	6	0	6.499939	-0.704844	0.137384
43	1	0	6.145741	0.450548	1.916326
44	1	0	6.524525	-1.902673	-1.651133
45	1	0	7.579342	-0.664983	0.226171

Structure 39b (C_2H_5OH)

Energy (Hartrees): -1034.94601164
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.163333	2.476261	-0.761806
2	6	0	-0.782949	3.724519	-0.712508
3	6	0	-1.835942	3.930337	0.176842
4	6	0	-2.251077	2.889130	1.012639
5	6	0	-1.620352	1.658442	0.955419
6	6	0	-0.564538	1.421966	0.060116
7	1	0	0.648013	2.325131	-1.467020
8	1	0	-0.441180	4.512500	-1.370816
9	1	0	-3.061080	3.068900	1.710745
10	1	0	-1.938613	0.871845	1.632370
11	6	0	0.135044	0.114723	0.012035
12	6	0	-0.512152	-1.083447	-0.027546
13	6	0	1.590749	0.118391	0.013246
14	1	0	2.056751	1.074825	0.279878
15	1	0	0.083136	-1.989044	0.001705
16	7	0	2.316551	-0.899281	-0.278944
17	7	0	-1.851311	-1.258997	-0.139594
18	1	0	-2.423349	-0.443496	-0.329915
19	8	0	-2.511771	5.104298	0.304955
20	6	0	-2.104472	6.193748	-0.513737
21	1	0	-2.232892	5.956006	-1.573299
22	1	0	-2.752396	7.026966	-0.248160
23	1	0	-1.063534	6.463675	-0.315993
24	6	0	-2.534146	-2.479976	-0.073142
25	6	0	-3.866079	-2.513503	-0.503573
26	6	0	-1.941955	-3.646236	0.421689
27	6	0	-4.587823	-3.697803	-0.451112
28	1	0	-4.324482	-1.605490	-0.882068
29	6	0	-2.674263	-4.828706	0.456970
30	1	0	-0.925764	-3.638591	0.794652
31	6	0	-3.995993	-4.866959	0.023154
32	1	0	-5.618222	-3.706165	-0.788793
33	1	0	-2.203610	-5.726463	0.842224
34	1	0	-4.559266	-5.791844	0.059831
35	6	0	3.709875	-0.795052	-0.107006
36	6	0	4.293228	-0.135693	0.983314
37	6	0	4.540771	-1.424630	-1.041972
38	6	0	5.677951	-0.081013	1.110631
39	1	0	3.659625	0.308052	1.743936
40	6	0	5.922405	-1.359277	-0.913538
41	1	0	4.084863	-1.953335	-1.872305
42	6	0	6.498857	-0.685245	0.162408
43	1	0	6.116708	0.425990	1.963260
44	1	0	6.552962	-1.841178	-1.652767
45	1	0	7.576977	-0.644584	0.267516

Structure 39c (vacuum)

Energy (Hartrees): -1034.91643627
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.757355	1.877408	-0.770885
2	6	0	0.730942	3.269186	-0.759327
3	6	0	-0.063224	3.936994	0.171562
4	6	0	-0.816600	3.202652	1.089942
5	6	0	-0.778903	1.819326	1.065972
6	6	0	0.000332	1.128337	0.127346
7	1	0	1.390427	1.365294	-1.484376
8	1	0	1.333972	3.813406	-1.473301
9	1	0	-1.409688	3.740313	1.819431
10	1	0	-1.346004	1.259146	1.802754
11	6	0	0.017577	-0.353927	0.099012
12	6	0	-1.122140	-1.089205	0.052677
13	6	0	1.270086	-1.092668	0.080232
14	1	0	-1.056421	-2.171610	0.048079
15	1	0	1.170679	-2.187882	0.068875
16	7	0	2.418790	-0.538247	0.091950
17	7	0	-2.385540	-0.583868	-0.043556
18	1	0	-2.463731	0.411566	-0.206271
19	8	0	-0.162775	5.288192	0.267564
20	6	0	0.600134	6.068152	-0.629117
21	1	0	0.318258	5.867225	-1.667608
22	1	0	0.379863	7.105960	-0.389066
23	1	0	1.671168	5.883380	-0.500134
24	6	0	-3.574189	-1.319184	-0.042574
25	6	0	-4.735761	-0.710850	-0.531170
26	6	0	-3.643827	-2.626367	0.447851
27	6	0	-5.938246	-1.400746	-0.538765
28	1	0	-4.684370	0.303209	-0.913214
29	6	0	-4.852738	-3.311852	0.420199
30	1	0	-2.771129	-3.102092	0.876097
31	6	0	-6.005544	-2.710297	-0.070815
32	1	0	-6.827129	-0.913430	-0.921503
33	1	0	-4.891749	-4.324816	0.803266
34	1	0	-6.943682	-3.250229	-0.082124
35	6	0	3.559635	-1.356507	0.020291
36	6	0	4.653672	-1.037708	0.831431
37	6	0	3.661343	-2.436572	-0.863861
38	6	0	5.804221	-1.812350	0.793141
39	1	0	4.573072	-0.182580	1.491792
40	6	0	4.822996	-3.200198	-0.907370
41	1	0	2.840230	-2.653953	-1.537928
42	6	0	5.895238	-2.898288	-0.075243
43	1	0	6.639481	-1.563047	1.437380
44	1	0	4.892814	-4.028499	-1.603171
45	1	0	6.799241	-3.494109	-0.111420

Structure 39c ($CHCl_3$)

Energy (Hartrees): -1034.95067007
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.640101	1.898965	-0.857645
2	6	0	0.579413	3.289993	-0.831554
3	6	0	-0.146962	3.928486	0.174255
4	6	0	-0.795795	3.165518	1.148743
5	6	0	-0.724633	1.782557	1.108037
6	6	0	-0.012369	1.121176	0.097728
7	1	0	1.210956	1.411671	-1.639996
8	1	0	1.099400	3.856086	-1.592902
9	1	0	-1.340716	3.676317	1.934448
10	1	0	-1.219061	1.202903	1.881662
11	6	0	0.039550	-0.361596	0.045633
12	6	0	-1.084705	-1.128086	0.010411
13	6	0	1.305977	-1.066336	0.023642
14	1	0	-0.986554	-2.207861	-0.004585
15	1	0	1.236982	-2.158692	-0.064559
16	7	0	2.443411	-0.488204	0.126146
17	7	0	-2.355657	-0.651271	-0.034877
18	1	0	-2.468829	0.351875	-0.122620
19	8	0	-0.274373	5.275122	0.287521
20	6	0	0.379805	6.083980	-0.676978
21	1	0	0.002723	5.880447	-1.683793
22	1	0	0.152636	7.114296	-0.409760
23	1	0	1.462664	5.931777	-0.650569
24	6	0	-3.536618	-1.401168	-0.035626
25	6	0	-4.736550	-0.728889	-0.298513
26	6	0	-3.565640	-2.773981	0.228968
27	6	0	-5.940271	-1.418046	-0.302785
28	1	0	-4.714185	0.337033	-0.501167
29	6	0	-4.779498	-3.453300	0.214155
30	1	0	-2.658436	-3.316717	0.461148
31	6	0	-5.971968	-2.787832	-0.050768
32	1	0	-6.858587	-0.879827	-0.508444
33	1	0	-4.787041	-4.517298	0.422391
34	1	0	-6.911690	-3.326340	-0.055641
35	6	0	3.602323	-1.281115	0.047997
36	6	0	4.635389	-1.042253	0.961798
37	6	0	3.778748	-2.262791	-0.935521
38	6	0	5.799362	-1.798483	0.919831
39	1	0	4.501184	-0.265676	1.706560
40	6	0	4.953935	-3.007024	-0.980582
41	1	0	3.003812	-2.419340	-1.678280
42	6	0	5.965464	-2.785792	-0.050800
43	1	0	6.584633	-1.613508	1.644403
44	1	0	5.081020	-3.758804	-1.751925
45	1	0	6.879433	-3.366907	-0.087968

Structure 39c (DMSO)

Energy (Hartrees): -1034.94664801
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.641743	1.875735	-0.860044
2	6	0	0.613123	3.268391	-0.848132
3	6	0	-0.078034	3.933850	0.166481
4	6	0	-0.727613	3.193591	1.158935
5	6	0	-0.687418	1.808672	1.132352
6	6	0	-0.004967	1.121379	0.118642
7	1	0	1.179624	1.368857	-1.653876
8	1	0	1.126720	3.814015	-1.628722
9	1	0	-1.253436	3.720663	1.947093
10	1	0	-1.186730	1.249652	1.918020
11	6	0	0.025120	-0.362799	0.088546
12	6	0	-1.111624	-1.115772	0.062539
13	6	0	1.276213	-1.087240	0.071892
14	1	0	-1.024543	-2.196590	0.059621
15	1	0	1.185927	-2.179329	0.017655
16	7	0	2.427684	-0.523333	0.138302
17	7	0	-2.372141	-0.622619	0.011516
18	1	0	-2.478312	0.382568	-0.075088
19	8	0	-0.169479	5.282188	0.268916
20	6	0	0.488517	6.063182	-0.719201
21	1	0	0.087685	5.857917	-1.716092
22	1	0	0.293893	7.102368	-0.460945
23	1	0	1.566983	5.881481	-0.711526
24	6	0	-3.562095	-1.359803	-0.016631
25	6	0	-4.747576	-0.668469	-0.295346
26	6	0	-3.611690	-2.734893	0.233134
27	6	0	-5.959870	-1.342656	-0.330410
28	1	0	-4.705658	0.398978	-0.486887
29	6	0	-4.833971	-3.398384	0.188307
30	1	0	-2.715442	-3.292132	0.473933
31	6	0	-6.013142	-2.714762	-0.092577
32	1	0	-6.867294	-0.791148	-0.549534
33	1	0	-4.858202	-4.464550	0.384288
34	1	0	-6.959085	-3.241972	-0.122309
35	6	0	3.575492	-1.332285	0.053196
36	6	0	4.680917	-0.997931	0.846159
37	6	0	3.679391	-2.415367	-0.830511
38	6	0	5.845080	-1.754017	0.788292
39	1	0	4.606728	-0.145824	1.513166
40	6	0	4.852068	-3.162209	-0.890718
41	1	0	2.849145	-2.654299	-1.486279
42	6	0	5.937278	-2.841556	-0.079210
43	1	0	6.687474	-1.489197	1.417916
44	1	0	4.920052	-3.993161	-1.584420
45	1	0	6.849857	-3.424079	-0.130227

Structure 39c (C_2H_5OH)

Energy (Hartrees): -1034.94965825
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.610508	1.878232	-0.895954
2	6	0	0.574161	3.270642	-0.904660
3	6	0	-0.096148	3.945034	0.116401
4	6	0	-0.714948	3.220153	1.137772
5	6	0	-0.665394	1.834840	1.132638
6	6	0	-0.006465	1.136701	0.111404
7	1	0	1.130385	1.361737	-1.695513
8	1	0	1.065263	3.808885	-1.704452
9	1	0	-1.222656	3.758551	1.930237
10	1	0	-1.137414	1.284635	1.941095
11	6	0	0.030153	-0.347503	0.100411
12	6	0	-1.101290	-1.107896	0.085614
13	6	0	1.284503	-1.066654	0.095624
14	1	0	-1.002745	-2.187256	0.094663
15	1	0	1.197721	-2.159110	0.047644
16	7	0	2.434852	-0.501384	0.165119
17	7	0	-2.368472	-0.628966	0.055330
18	1	0	-2.490229	0.377770	0.065277
19	8	0	-0.196242	5.299681	0.198507
20	6	0	0.443818	6.072053	-0.810171
21	1	0	0.028057	5.850021	-1.796611
22	1	0	0.247009	7.112789	-0.560410
23	1	0	1.522491	5.894026	-0.812948
24	6	0	-3.549650	-1.380188	-0.000669
25	6	0	-4.763605	-0.689190	0.098007
26	6	0	-3.562886	-2.769863	-0.156001
27	6	0	-5.967939	-1.376649	0.046864
28	1	0	-4.750754	0.389385	0.218413
29	6	0	-4.778177	-3.446235	-0.200749
30	1	0	-2.643865	-3.332928	-0.252213
31	6	0	-5.985790	-2.762253	-0.100351
32	1	0	-6.897619	-0.824253	0.125533
33	1	0	-4.773418	-4.523744	-0.322321
34	1	0	-6.926039	-3.299094	-0.139250
35	6	0	3.579881	-1.315936	0.085569
36	6	0	4.675961	-1.004317	0.899815
37	6	0	3.687221	-2.385183	-0.814194
38	6	0	5.833868	-1.770501	0.846709
39	1	0	4.599183	-0.162681	1.579697
40	6	0	4.853607	-3.142163	-0.869603
41	1	0	2.864449	-2.604136	-1.486290
42	6	0	5.929397	-2.844639	-0.037142
43	1	0	6.668865	-1.524158	1.493472
44	1	0	4.924300	-3.962064	-1.576136
45	1	0	6.837568	-3.434283	-0.085086

Structure 39d (vacuum)

Energy (Hartrees): -1034.91015853
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.203799	-0.965465	0.877518
2	6	0	-3.240099	-1.870215	0.990156
3	6	0	-3.254437	-3.030100	0.208049
4	6	0	-2.219599	-3.264543	-0.691277
5	6	0	-1.180990	-2.338280	-0.795506
6	6	0	-1.140557	-1.188447	-0.011630
7	1	0	-2.210168	-0.069998	1.485742
8	1	0	-4.058223	-1.705234	1.680414
9	1	0	-2.211051	-4.141066	-1.324983
10	1	0	-0.398412	-2.512029	-1.526314
11	6	0	0.007676	-0.256090	-0.090707
12	6	0	1.266128	-0.761094	-0.161144
13	6	0	-0.194146	1.187045	-0.070787
14	1	0	0.704367	1.801312	0.081738
15	1	0	2.339308	0.838812	-0.877679
16	1	0	1.414963	-1.829358	-0.036146
17	7	0	-1.336320	1.742274	-0.195250
18	7	0	2.415369	-0.056526	-0.421104
19	8	0	-4.318393	-3.856254	0.390689
20	6	0	-4.371116	-5.034973	-0.382967
21	1	0	-5.283682	-5.549294	-0.089789
22	1	0	-4.410610	-4.805241	-1.452568
23	1	0	-3.509434	-5.679543	-0.180838
24	6	0	-1.420260	3.140084	-0.063961
25	6	0	-2.291541	3.826722	-0.915439
26	6	0	-0.711364	3.856097	0.907683
27	6	0	-2.409976	5.206478	-0.831241
28	1	0	-2.857570	3.255406	-1.641334
29	6	0	-0.845960	5.237355	0.995741
30	1	0	-0.085297	3.323322	1.614701
31	6	0	-1.686370	5.919207	0.122807
32	1	0	-3.077758	5.729380	-1.505996
33	1	0	-0.300799	5.780140	1.759384
34	1	0	-1.791158	6.995011	0.195347
35	6	0	3.710120	-0.522890	-0.174503
36	6	0	4.786421	0.078890	-0.836018
37	6	0	3.955569	-1.563710	0.725050
38	6	0	6.080855	-0.362609	-0.609604
39	1	0	4.599152	0.887272	-1.535065
40	6	0	5.256728	-2.009648	0.927615
41	1	0	3.141780	-2.003197	1.287853
42	6	0	6.325953	-1.417046	0.266556
43	1	0	6.903108	0.115714	-1.128747
44	1	0	5.432913	-2.817837	1.627700
45	1	0	7.336965	-1.764399	0.437204

Structure 39d ($CHCl_3$)

Energy (Hartrees): -1034.94518243
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.153023	-1.024466	0.905690
2	6	0	-3.175303	-1.946878	1.021613
3	6	0	-3.187721	-3.092705	0.217098
4	6	0	-2.162387	-3.297149	-0.701768
5	6	0	-1.139418	-2.352786	-0.809155
6	6	0	-1.103970	-1.212237	-0.009034
7	1	0	-2.158937	-0.144783	1.538150
8	1	0	-3.979573	-1.802641	1.733820
9	1	0	-2.149815	-4.165868	-1.346752
10	1	0	-0.362146	-2.508553	-1.550068
11	6	0	0.022726	-0.251571	-0.096181
12	6	0	1.296254	-0.732207	-0.152460
13	6	0	-0.215269	1.182378	-0.086713
14	1	0	0.663389	1.821695	0.065808
15	1	0	2.339144	0.898269	-0.841230
16	1	0	1.463314	-1.796217	-0.010708
17	7	0	-1.373735	1.709899	-0.221607
18	7	0	2.426979	-0.010483	-0.408004
19	8	0	-4.236206	-3.937044	0.399313
20	6	0	-4.287061	-5.106923	-0.399696
21	1	0	-5.188556	-5.637862	-0.099655
22	1	0	-4.350559	-4.857503	-1.463142
23	1	0	-3.415863	-5.744528	-0.221564
24	6	0	-1.496273	3.104677	-0.080869
25	6	0	-2.389989	3.775452	-0.923651
26	6	0	-0.806484	3.832941	0.897285
27	6	0	-2.553397	5.150598	-0.821972
28	1	0	-2.940727	3.200340	-1.659562
29	6	0	-0.984353	5.208864	1.001194
30	1	0	-0.157290	3.314813	1.594919
31	6	0	-1.850094	5.875172	0.139336
32	1	0	-3.239790	5.659156	-1.489790
33	1	0	-0.451974	5.759151	1.769177
34	1	0	-1.989260	6.946523	0.225331
35	6	0	3.733040	-0.452276	-0.167907
36	6	0	4.790441	0.195371	-0.818208
37	6	0	4.007357	-1.503475	0.711585
38	6	0	6.097825	-0.214511	-0.601777
39	1	0	4.575277	1.015260	-1.495836
40	6	0	5.321905	-1.915781	0.905286
41	1	0	3.206595	-1.981190	1.262624
42	6	0	6.373613	-1.279027	0.254614
43	1	0	6.906192	0.297235	-1.111824
44	1	0	5.521971	-2.733266	1.588748
45	1	0	7.395032	-1.600345	0.418458

Structure 39d (DMSO)

Energy (Hartrees): -1034.94127955
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.077653	-1.127176	0.937886
2	6	0	-3.064318	-2.089679	1.041173
3	6	0	-3.036821	-3.222172	0.216903
4	6	0	-2.006972	-3.370459	-0.709150
5	6	0	-1.021013	-2.385173	-0.803815
6	6	0	-1.027274	-1.256353	0.014066
7	1	0	-2.110625	-0.263221	1.591788
8	1	0	-3.867284	-1.987948	1.762617
9	1	0	-1.961331	-4.228138	-1.367625
10	1	0	-0.237596	-2.503005	-1.545515
11	6	0	0.052652	-0.241256	-0.057811
12	6	0	1.350343	-0.659350	-0.109571
13	6	0	-0.266586	1.174697	-0.049963
14	1	0	0.564327	1.869103	0.121965
15	1	0	2.315422	1.064075	-0.658681
16	1	0	1.559285	-1.718648	0.001243
17	7	0	-1.453616	1.628596	-0.223139
18	7	0	2.445829	0.119358	-0.320528
19	8	0	-4.047579	-4.110091	0.388567
20	6	0	-4.038173	-5.278435	-0.418817
21	1	0	-4.910711	-5.857991	-0.123204
22	1	0	-4.114388	-5.025938	-1.480439
23	1	0	-3.134140	-5.869761	-0.246344
24	6	0	-1.668007	3.013440	-0.092649
25	6	0	-2.565094	3.628611	-0.974508
26	6	0	-1.067546	3.782082	0.913366
27	6	0	-2.819526	4.991100	-0.881615
28	1	0	-3.046660	3.025266	-1.736405
29	6	0	-1.336766	5.144198	1.007743
30	1	0	-0.412673	3.305744	1.635066
31	6	0	-2.205741	5.756857	0.108866
32	1	0	-3.506406	5.455656	-1.580510
33	1	0	-0.870659	5.725968	1.795486
34	1	0	-2.414221	6.817562	0.187176
35	6	0	3.775189	-0.278247	-0.134152
36	6	0	4.787488	0.537227	-0.654919
37	6	0	4.119826	-1.440797	0.563051
38	6	0	6.120150	0.186739	-0.492280
39	1	0	4.517776	1.442697	-1.189140
40	6	0	5.460236	-1.787210	0.704796
41	1	0	3.358099	-2.064833	1.013473
42	6	0	6.467830	-0.982771	0.182071
43	1	0	6.890790	0.830857	-0.900646
44	1	0	5.714061	-2.691230	1.247107
45	1	0	7.508737	-1.256389	0.305698

Structure 39d (C_2H_5OH)

Energy (Hartrees): -1034.94453227
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.059156	-1.154541	0.961605
2	6	0	-3.038039	-2.126096	1.057315
3	6	0	-3.004713	-3.244631	0.216262
4	6	0	-1.980530	-3.374996	-0.716952
5	6	0	-1.002651	-2.381208	-0.803281
6	6	0	-1.013700	-1.263865	0.030053
7	1	0	-2.095238	-0.298974	1.626579
8	1	0	-3.839335	-2.041167	1.783254
9	1	0	-1.933381	-4.223153	-1.387550
10	1	0	-0.222996	-2.482063	-1.551475
11	6	0	0.055839	-0.237536	-0.038000
12	6	0	1.356844	-0.642243	-0.094748
13	6	0	-0.278845	1.175049	-0.029696
14	1	0	0.542775	1.877113	0.155151
15	1	0	2.308119	1.084599	-0.664709
16	1	0	1.577419	-1.699456	0.014742
17	7	0	-1.467553	1.617762	-0.218407
18	7	0	2.445280	0.146157	-0.312177
19	8	0	-4.012659	-4.146029	0.380425
20	6	0	-4.010988	-5.293933	-0.458907
21	1	0	-4.882345	-5.879224	-0.171269
22	1	0	-4.095474	-5.009923	-1.511603
23	1	0	-3.105883	-5.888478	-0.306811
24	6	0	-1.692922	3.001760	-0.091389
25	6	0	-2.564787	3.615185	-0.999028
26	6	0	-1.127038	3.769751	0.934345
27	6	0	-2.827125	4.976408	-0.910895
28	1	0	-3.020796	3.011732	-1.776507
29	6	0	-1.404521	5.130680	1.023968
30	1	0	-0.493581	3.293171	1.674923
31	6	0	-2.247600	5.742068	0.100037
32	1	0	-3.494015	5.440198	-1.629536
33	1	0	-0.965338	5.712451	1.827172
34	1	0	-2.462642	6.801878	0.174270
35	6	0	3.777344	-0.246793	-0.131496
36	6	0	4.785062	0.548467	-0.690269
37	6	0	4.126766	-1.388087	0.597453
38	6	0	6.118572	0.198267	-0.533302
39	1	0	4.511785	1.437567	-1.249870
40	6	0	5.467497	-1.735648	0.732600
41	1	0	3.367539	-1.992847	1.077785
42	6	0	6.470710	-0.951393	0.172225
43	1	0	6.886617	0.826031	-0.971264
44	1	0	5.725518	-2.623529	1.299349
45	1	0	7.512309	-1.225125	0.290662

Structure 39e (vacuum)

Energy (Hartrees): -1034.90547117
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.619124	0.444724	-0.660448
2	6	0	3.975164	0.638491	-0.419992
3	6	0	4.703717	-0.335425	0.263069
4	6	0	4.059700	-1.490447	0.706455
5	6	0	2.708262	-1.666335	0.462517
6	6	0	1.961072	-0.711383	-0.240182
7	1	0	2.066197	1.211120	-1.188078
8	1	0	4.445927	1.547607	-0.768779
9	1	0	4.634761	-2.225547	1.255878
10	1	0	2.213361	-2.551618	0.846825
11	6	0	0.534239	-0.949038	-0.556773
12	6	0	0.136924	-2.187468	-0.935314
13	6	0	-0.440299	0.143254	-0.518472
14	1	0	-1.391163	-0.043813	-1.030783
15	1	0	-1.254601	-3.438262	-1.715164
16	1	0	0.896173	-2.936266	-1.146598
17	7	0	-0.216091	1.253066	0.066853
18	7	0	-1.161531	-2.630997	-1.118654
19	8	0	6.028938	-0.241727	0.551136
20	6	0	6.709353	0.921872	0.132390
21	1	0	7.739643	0.804008	0.460869
22	1	0	6.684355	1.024925	-0.957169
23	1	0	6.280854	1.817947	0.592374
24	6	0	-1.192130	2.263983	-0.023548
25	6	0	-1.454726	3.022658	1.120975
26	6	0	-1.864615	2.565031	-1.212504
27	6	0	-2.408124	4.030132	1.088624
28	1	0	-0.904172	2.795731	2.026129
29	6	0	-2.806448	3.587449	-1.242216
30	1	0	-1.624397	2.016193	-2.116180
31	6	0	-3.088758	4.317390	-0.092712
32	1	0	-2.615839	4.601563	1.985871
33	1	0	-3.315474	3.819343	-2.170588
34	1	0	-3.821942	5.114369	-0.120062
35	6	0	-2.293802	-2.383381	-0.316137
36	6	0	-3.544641	-2.756773	-0.815125
37	6	0	-2.207713	-1.819694	0.960039
38	6	0	-4.689475	-2.570901	-0.052699
39	1	0	-3.614589	-3.185494	-1.809485
40	6	0	-3.362681	-1.627337	1.707447
41	1	0	-1.245715	-1.534517	1.366108
42	6	0	-4.608697	-1.997786	1.211960
43	1	0	-5.650479	-2.866982	-0.456633
44	1	0	-3.280725	-1.185548	2.693671
45	1	0	-5.503006	-1.839528	1.801190

Structure 39e ($CHCl_3$)

Energy (Hartrees): -1034.93908173
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.636423	0.448170	-0.666676
2	6	0	3.993068	0.659656	-0.439693
3	6	0	4.736717	-0.300144	0.248552
4	6	0	4.106374	-1.457263	0.709097
5	6	0	2.752921	-1.648503	0.481859
6	6	0	1.988877	-0.707357	-0.223330
7	1	0	2.076029	1.200931	-1.207920
8	1	0	4.453947	1.567907	-0.805124
9	1	0	4.689449	-2.186045	1.260266
10	1	0	2.273264	-2.537500	0.877651
11	6	0	0.558835	-0.959062	-0.521138
12	6	0	0.166953	-2.210221	-0.878952
13	6	0	-0.422536	0.121814	-0.492826
14	1	0	-1.360208	-0.072383	-1.024656
15	1	0	-1.196807	-3.510577	-1.608082
16	1	0	0.928872	-2.954030	-1.097657
17	7	0	-0.230019	1.236968	0.100696
18	7	0	-1.117251	-2.679528	-1.038323
19	8	0	6.062827	-0.190136	0.521555
20	6	0	6.722885	0.997991	0.118047
21	1	0	7.754733	0.896698	0.449333
22	1	0	6.701747	1.114079	-0.969605
23	1	0	6.276007	1.877044	0.592024
24	6	0	-1.224722	2.229045	-0.011464
25	6	0	-1.525967	2.988196	1.124747
26	6	0	-1.882949	2.509494	-1.214788
27	6	0	-2.496277	3.980014	1.067351
28	1	0	-0.993739	2.779107	2.046016
29	6	0	-2.843651	3.514102	-1.268247
30	1	0	-1.619532	1.958654	-2.111149
31	6	0	-3.160684	4.247502	-0.128521
32	1	0	-2.731174	4.552431	1.957843
33	1	0	-3.341455	3.727838	-2.207578
34	1	0	-3.909161	5.030026	-0.174720
35	6	0	-2.273024	-2.390564	-0.285812
36	6	0	-3.509400	-2.770469	-0.816448
37	6	0	-2.224841	-1.789926	0.976626
38	6	0	-4.679257	-2.544387	-0.102219
39	1	0	-3.544752	-3.237692	-1.795259
40	6	0	-3.403673	-1.557928	1.675421
41	1	0	-1.274696	-1.508388	1.413276
42	6	0	-4.636751	-1.927970	1.144975
43	1	0	-5.628997	-2.845184	-0.530085
44	1	0	-3.351079	-1.087813	2.651018
45	1	0	-5.550099	-1.739230	1.695975

Structure 39e (DMSO)

Energy (Hartrees): -1034.93501546
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.637267	0.443736	-0.685885
2	6	0	3.991594	0.677123	-0.464283
3	6	0	4.743225	-0.250173	0.260996
4	6	0	4.121580	-1.396941	0.760172
5	6	0	2.770284	-1.611169	0.535407
6	6	0	1.998894	-0.701829	-0.202893
7	1	0	2.072593	1.168751	-1.260784
8	1	0	4.445200	1.574210	-0.864765
9	1	0	4.708894	-2.103617	1.335543
10	1	0	2.300369	-2.495391	0.953220
11	6	0	0.572139	-0.975192	-0.497213
12	6	0	0.196216	-2.236531	-0.845559
13	6	0	-0.418481	0.092937	-0.475105
14	1	0	-1.348877	-0.106814	-1.016935
15	1	0	-1.149812	-3.565766	-1.552599
16	1	0	0.966523	-2.972126	-1.062209
17	7	0	-0.244786	1.210658	0.124267
18	7	0	-1.076640	-2.724516	-0.994953
19	8	0	6.065375	-0.115408	0.531817
20	6	0	6.724070	1.037067	0.026083
21	1	0	7.760320	0.958917	0.349345
22	1	0	6.685821	1.065490	-1.066734
23	1	0	6.287368	1.953213	0.433834
24	6	0	-1.251036	2.190452	0.001059
25	6	0	-1.566618	2.954093	1.131044
26	6	0	-1.908165	2.454711	-1.207364
27	6	0	-2.550768	3.932614	1.064442
28	1	0	-1.038736	2.758998	2.058288
29	6	0	-2.883622	3.445054	-1.269420
30	1	0	-1.635431	1.902008	-2.099926
31	6	0	-3.214795	4.182482	-0.135670
32	1	0	-2.796268	4.507365	1.950688
33	1	0	-3.380796	3.645803	-2.212112
34	1	0	-3.974224	4.954018	-0.189977
35	6	0	-2.245456	-2.399946	-0.277510
36	6	0	-3.479479	-2.719009	-0.850451
37	6	0	-2.207509	-1.825786	0.998122
38	6	0	-4.659434	-2.455632	-0.164048
39	1	0	-3.504426	-3.169512	-1.837228
40	6	0	-3.394511	-1.556076	1.668949
41	1	0	-1.257534	-1.599341	1.467282
42	6	0	-4.626696	-1.863428	1.095273
43	1	0	-5.608428	-2.707699	-0.624080
44	1	0	-3.350994	-1.111544	2.657143
45	1	0	-5.546779	-1.648033	1.625405

Structure 39e (C_2H_5OH)

Energy (Hartrees): -1034.93873872
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.640039	0.444546	-0.697272
2	6	0	3.993729	0.680755	-0.474608
3	6	0	4.741402	-0.241413	0.258926
4	6	0	4.122425	-1.384998	0.765405
5	6	0	2.771452	-1.601398	0.540192
6	6	0	2.001769	-0.697729	-0.206321
7	1	0	2.075579	1.164433	-1.278914
8	1	0	4.448495	1.575069	-0.880043
9	1	0	4.710474	-2.086445	1.346855
10	1	0	2.300580	-2.481826	0.965005
11	6	0	0.575055	-0.973737	-0.498915
12	6	0	0.203069	-2.237116	-0.843461
13	6	0	-0.418493	0.091625	-0.474311
14	1	0	-1.348302	-0.110293	-1.016197
15	1	0	-1.138550	-3.576566	-1.541955
16	1	0	0.976073	-2.969881	-1.060417
17	7	0	-0.248601	1.208881	0.127163
18	7	0	-1.067473	-2.732403	-0.988674
19	8	0	6.068296	-0.103941	0.533691
20	6	0	6.731257	1.048312	0.029178
21	1	0	7.765233	0.967369	0.359339
22	1	0	6.697561	1.072333	-1.063560
23	1	0	6.291415	1.963398	0.435072
24	6	0	-1.259729	2.184220	0.003568
25	6	0	-1.581719	2.945582	1.133069
26	6	0	-1.914271	2.447196	-1.206260
27	6	0	-2.570439	3.919326	1.064615
28	1	0	-1.055301	2.753164	2.061757
29	6	0	-2.894657	3.432546	-1.270334
30	1	0	-1.635889	1.897451	-2.099016
31	6	0	-3.232827	4.167022	-0.136824
32	1	0	-2.820599	4.492438	1.950762
33	1	0	-3.390196	3.631587	-2.214367
34	1	0	-3.996206	4.934725	-0.192317
35	6	0	-2.238284	-2.402599	-0.275692
36	6	0	-3.471832	-2.715095	-0.852411
37	6	0	-2.200691	-1.831368	1.001133
38	6	0	-4.652479	-2.447284	-0.168554
39	1	0	-3.497176	-3.163464	-1.840245
40	6	0	-3.387936	-1.556589	1.669120
41	1	0	-1.250449	-1.610325	1.472704
42	6	0	-4.620078	-1.857071	1.091496
43	1	0	-5.601566	-2.694012	-0.631531
44	1	0	-3.345039	-1.113400	2.658024
45	1	0	-5.540541	-1.637970	1.619646

Structure 39f (vacuum)

Energy (Hartrees): -1034.90120251
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.705707	0.407871	1.077181
2	6	0	-4.032566	0.739600	1.280661
3	6	0	-4.995132	0.397574	0.328043
4	6	0	-4.606480	-0.270165	-0.830523
5	6	0	-3.261722	-0.585518	-1.023803
6	6	0	-2.290418	-0.268194	-0.078815
7	1	0	-1.975411	0.660902	1.838866
8	1	0	-4.354800	1.256030	2.176606
9	1	0	-5.325620	-0.534466	-1.594093
10	1	0	-2.964989	-1.075950	-1.944885
11	6	0	-0.856192	-0.621254	-0.280155
12	6	0	-0.553441	-1.905499	-0.610160
13	6	0	0.103660	0.473005	-0.179802
14	1	0	-1.393692	-2.570621	-0.792907
15	1	0	-0.270675	1.399778	0.275157
16	1	0	0.607120	-3.430433	-1.223927
17	7	0	1.288886	0.403803	-0.648264
18	7	0	0.654297	-2.534752	-0.763980
19	8	0	-6.273353	0.758659	0.617639
20	6	0	-7.275507	0.426551	-0.318856
21	1	0	-8.211262	0.794436	0.096185
22	1	0	-7.091976	0.909491	-1.283991
23	1	0	-7.341594	-0.657082	-0.460560
24	6	0	1.874668	-2.293622	-0.097517
25	6	0	3.061525	-2.690212	-0.711191
26	6	0	1.912888	-1.717468	1.171120
27	6	0	4.277545	-2.491187	-0.070011
28	1	0	3.026668	-3.127928	-1.703011
29	6	0	3.133140	-1.509552	1.799321
30	1	0	0.986969	-1.428230	1.653506
31	6	0	4.321539	-1.888891	1.182941
32	1	0	5.194998	-2.793210	-0.561207
33	1	0	3.154909	-1.047459	2.779454
34	1	0	5.271414	-1.717403	1.673936
35	6	0	2.169958	1.477654	-0.453765
36	6	0	3.019526	1.835546	-1.505498
37	6	0	2.275426	2.153191	0.767261
38	6	0	3.917752	2.881799	-1.354902
39	1	0	2.950042	1.282152	-2.434346
40	6	0	3.188449	3.191662	0.916196
41	1	0	1.662425	1.837988	1.604740
42	6	0	4.006558	3.566109	-0.143973
43	1	0	4.560204	3.159858	-2.182377
44	1	0	3.267773	3.702448	1.869085
45	1	0	4.719239	4.373064	-0.024145

Structure 39f ($CHCl_3$)

Energy (Hartrees): -1034.93470000
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.685476	0.483352	1.032780
2	6	0	-4.015190	0.807449	1.240366
3	6	0	-4.990106	0.393683	0.328741
4	6	0	-4.610135	-0.338217	-0.794991
5	6	0	-3.263888	-0.643406	-0.994907
6	6	0	-2.278517	-0.254210	-0.089042
7	1	0	-1.949448	0.795501	1.766516
8	1	0	-4.322803	1.373078	2.112548
9	1	0	-5.339277	-0.662740	-1.525780
10	1	0	-2.982318	-1.189349	-1.889532
11	6	0	-0.840485	-0.600073	-0.290206
12	6	0	-0.532339	-1.882257	-0.636030
13	6	0	0.110521	0.497900	-0.179465
14	1	0	-1.367019	-2.545389	-0.846822
15	1	0	-0.267729	1.415847	0.287215
16	1	0	0.612937	-3.404138	-1.263018
17	7	0	1.296671	0.450948	-0.656494
18	7	0	0.670672	-2.515249	-0.785143
19	8	0	-6.269061	0.750209	0.617421
20	6	0	-7.289401	0.318057	-0.266718
21	1	0	-8.225377	0.684696	0.150740
22	1	0	-7.151539	0.739591	-1.266943
23	1	0	-7.323070	-0.773994	-0.327090
24	6	0	1.887751	-2.315469	-0.106369
25	6	0	3.054311	-2.825626	-0.680922
26	6	0	1.951772	-1.683219	1.135857
27	6	0	4.272645	-2.685730	-0.028594
28	1	0	2.998783	-3.317257	-1.646685
29	6	0	3.176193	-1.542158	1.777977
30	1	0	1.046193	-1.308499	1.596580
31	6	0	4.343131	-2.034849	1.200465
32	1	0	5.171828	-3.079698	-0.488599
33	1	0	3.216083	-1.041879	2.739200
34	1	0	5.295678	-1.914717	1.702673
35	6	0	2.156584	1.543609	-0.457566
36	6	0	2.992178	1.929267	-1.512249
37	6	0	2.254684	2.212532	0.769029
38	6	0	3.871455	2.992478	-1.357997
39	1	0	2.930542	1.385918	-2.448496
40	6	0	3.148466	3.268291	0.920870
41	1	0	1.650878	1.882934	1.608055
42	6	0	3.953978	3.668269	-0.141115
43	1	0	4.503140	3.289616	-2.187686
44	1	0	3.222752	3.772853	1.878007
45	1	0	4.652045	4.488012	-0.018281

Structure 39f (DMSO)

Energy (Hartrees): -1034.93163485
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.689903	0.537423	1.011935
2	6	0	-4.019798	0.866847	1.215011
3	6	0	-5.000673	0.422800	0.322998
4	6	0	-4.624347	-0.342869	-0.780382
5	6	0	-3.278843	-0.653877	-0.976585
6	6	0	-2.288355	-0.236767	-0.087425
7	1	0	-1.952153	0.874836	1.732590
8	1	0	-4.319945	1.459386	2.072056
9	1	0	-5.355847	-0.693360	-1.496882
10	1	0	-3.004106	-1.231931	-1.853147
11	6	0	-0.852657	-0.596131	-0.283274
12	6	0	-0.553467	-1.887116	-0.610062
13	6	0	0.108048	0.492332	-0.180240
14	1	0	-1.389707	-2.548911	-0.817883
15	1	0	-0.242003	1.402109	0.321637
16	1	0	0.584277	-3.429064	-1.203405
17	7	0	1.279520	0.444604	-0.696860
18	7	0	0.644019	-2.531183	-0.739918
19	8	0	-6.277996	0.781680	0.607678
20	6	0	-7.299575	0.314681	-0.261318
21	1	0	-8.237525	0.684225	0.148956
22	1	0	-7.168865	0.707636	-1.273740
23	1	0	-7.322273	-0.778649	-0.290842
24	6	0	1.865975	-2.308762	-0.079730
25	6	0	3.029786	-2.825526	-0.655782
26	6	0	1.941329	-1.644020	1.145957
27	6	0	4.256311	-2.654989	-0.024952
28	1	0	2.964334	-3.350962	-1.603001
29	6	0	3.173649	-1.473236	1.766678
30	1	0	1.039915	-1.265299	1.612214
31	6	0	4.338263	-1.968542	1.184630
32	1	0	5.152302	-3.055675	-0.485682
33	1	0	3.220583	-0.948720	2.714802
34	1	0	5.296765	-1.827412	1.670342
35	6	0	2.165123	1.514201	-0.484408
36	6	0	3.000220	1.903236	-1.539153
37	6	0	2.294204	2.150337	0.757706
38	6	0	3.910081	2.938892	-1.369173
39	1	0	2.914701	1.388877	-2.490319
40	6	0	3.216908	3.179363	0.923689
41	1	0	1.688551	1.819315	1.595051
42	6	0	4.023102	3.582867	-0.137271
43	1	0	4.540680	3.239086	-2.198739
44	1	0	3.313512	3.659067	1.891674
45	1	0	4.743700	4.381197	-0.002762

Structure 39f (C_2H_5OH)

Energy (Hartrees): -1034.93485757
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.686806	0.508013	1.027093
2	6	0	-4.016064	0.841567	1.227823
3	6	0	-4.991684	0.414652	0.323508
4	6	0	-4.616972	-0.340859	-0.785862
5	6	0	-3.272060	-0.656456	-0.978992
6	6	0	-2.284279	-0.253376	-0.080506
7	1	0	-1.950381	0.832119	1.755287
8	1	0	-4.319134	1.424637	2.090619
9	1	0	-5.347535	-0.678084	-1.509666
10	1	0	-2.995030	-1.225051	-1.861068
11	6	0	-0.848357	-0.611019	-0.277479
12	6	0	-0.548329	-1.901735	-0.602840
13	6	0	0.108704	0.480728	-0.175441
14	1	0	-1.384692	-2.564935	-0.806323
15	1	0	-0.244586	1.387397	0.329898
16	1	0	0.589995	-3.445801	-1.191894
17	7	0	1.277579	0.442437	-0.698868
18	7	0	0.649438	-2.545074	-0.734325
19	8	0	-6.273145	0.783180	0.604450
20	6	0	-7.296025	0.334275	-0.275189
21	1	0	-8.231300	0.710639	0.135079
22	1	0	-7.153223	0.736915	-1.281842
23	1	0	-7.328004	-0.758228	-0.312892
24	6	0	1.874276	-2.313375	-0.080947
25	6	0	3.039880	-2.815374	-0.665381
26	6	0	1.948656	-1.653612	1.147133
27	6	0	4.267669	-2.635927	-0.039335
28	1	0	2.975771	-3.335808	-1.615530
29	6	0	3.182014	-1.473126	1.762809
30	1	0	1.045243	-1.286390	1.619091
31	6	0	4.348460	-1.954725	1.173127
32	1	0	5.165562	-3.025132	-0.506387
33	1	0	3.228632	-0.952394	2.713135
34	1	0	5.307858	-1.806634	1.655239
35	6	0	2.155549	1.518360	-0.483850
36	6	0	2.986107	1.917441	-1.538238
37	6	0	2.280694	2.152864	0.759386
38	6	0	3.886578	2.960972	-1.367016
39	1	0	2.904846	1.404304	-2.490467
40	6	0	3.193998	3.189925	0.926875
41	1	0	1.680078	1.814455	1.597448
42	6	0	3.995028	3.603505	-0.133993
43	1	0	4.513754	3.268468	-2.196644
44	1	0	3.287399	3.668130	1.896052
45	1	0	4.708550	4.408110	0.001495

Structure 40a (vacuum)

Energy (Hartrees): -1263.94462840
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.913066	3.447765	-0.956980
2	6	0	-0.952123	4.829695	-0.978779
3	6	0	-0.098633	5.570542	-0.157284
4	6	0	0.783256	4.906025	0.690214
5	6	0	0.796856	3.511871	0.712248
6	6	0	-0.033750	2.753616	-0.111343
7	1	0	-1.560413	2.890739	-1.626064
8	1	0	-1.626486	5.365040	-1.636073
9	1	0	1.445036	5.451000	1.349885
10	1	0	1.457527	3.007979	1.409723
11	6	0	0.006469	1.271999	-0.100074
12	6	0	1.216081	0.630681	-0.074896
13	6	0	-1.242107	0.545410	-0.087296
14	1	0	2.123536	1.225597	-0.090075
15	1	0	-2.151073	1.158531	-0.075342
16	1	0	0.522806	-1.246284	0.028232
17	7	0	-1.328234	-0.740333	-0.075801
18	7	0	1.388605	-0.705265	-0.023376
19	8	0	-0.205053	6.923300	-0.253366
20	6	0	0.643635	7.704093	0.559462
21	1	0	0.411666	8.741987	0.330614
22	1	0	0.457629	7.515749	1.621787
23	1	0	1.697187	7.508613	0.334673
24	6	0	-2.600852	-1.334686	0.032504
25	6	0	-2.843540	-2.520838	-0.655683
26	6	0	-3.622064	-0.814638	0.841268
27	6	0	-4.078974	-3.158787	-0.586750
28	1	0	-2.051276	-2.936329	-1.267488
29	6	0	-4.850231	-1.445272	0.923375
30	1	0	-3.436355	0.073372	1.434613
31	6	0	-5.091295	-2.617731	0.204194
32	1	0	-4.232460	-4.071457	-1.146518
33	1	0	-5.639749	-1.057378	1.555361
34	6	0	2.623913	-1.371108	-0.054749
35	6	0	2.703367	-2.666756	0.447868
36	6	0	3.777901	-0.786406	-0.589823
37	6	0	3.903728	-3.371547	0.435250
38	1	0	1.815673	-3.128171	0.866157
39	6	0	4.976943	-1.475802	-0.587166
40	1	0	3.737701	0.199721	-1.035168
41	6	0	5.052782	-2.772026	-0.074860
42	1	0	3.925234	-4.376515	0.834280
43	1	0	5.874638	-1.033007	-1.000776
44	8	0	6.276826	-3.364066	-0.126230
45	8	0	-6.329249	-3.163195	0.351635
46	6	0	6.384902	-4.683109	0.363011
47	1	0	7.425262	-4.971046	0.229499
48	1	0	6.127522	-4.734213	1.426053
49	1	0	5.743102	-5.367933	-0.200911
50	6	0	-6.602484	-4.361362	-0.341197
51	1	0	-7.628364	-4.626430	-0.094666
52	1	0	-6.513510	-4.222825	-1.423690
53	1	0	-5.931917	-5.165619	-0.021275

Structure 40a ($CHCl_3$)

Energy (Hartrees): -1263.97784391
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.926571	3.460182	-0.922451
2	6	0	-0.960814	4.843650	-0.941959
3	6	0	-0.077188	5.581349	-0.148876
4	6	0	0.830701	4.911987	0.668640
5	6	0	0.840741	3.517469	0.688365
6	6	0	-0.021231	2.761317	-0.107536
7	1	0	-1.601753	2.908966	-1.568693
8	1	0	-1.657995	5.377044	-1.578024
9	1	0	1.516857	5.454806	1.305448
10	1	0	1.528954	3.013520	1.359146
11	6	0	0.012626	1.277617	-0.099138
12	6	0	1.223360	0.631219	-0.086704
13	6	0	-1.239705	0.559521	-0.079280
14	1	0	2.133766	1.221426	-0.111360
15	1	0	-2.144745	1.176471	-0.048561
16	1	0	0.529780	-1.249642	0.023318
17	7	0	-1.333534	-0.727663	-0.085057
18	7	0	1.390914	-0.703600	-0.039309
19	8	0	-0.178784	6.934021	-0.239748
20	6	0	0.708516	7.714640	0.542936
21	1	0	0.476543	8.753661	0.316017
22	1	0	0.554536	7.534197	1.611091
23	1	0	1.751290	7.510705	0.281271
24	6	0	-2.608191	-1.318155	0.029669
25	6	0	-2.856756	-2.503744	-0.660339
26	6	0	-3.624575	-0.798177	0.845594
27	6	0	-4.092756	-3.141406	-0.586477
28	1	0	-2.069902	-2.922731	-1.277973
29	6	0	-4.853421	-1.429385	0.933354
30	1	0	-3.438214	0.091867	1.436359
31	6	0	-5.100247	-2.600803	0.212355
32	1	0	-4.251424	-4.053407	-1.146787
33	1	0	-5.636570	-1.037172	1.572022
34	6	0	2.623015	-1.379975	-0.067584
35	6	0	2.682330	-2.679057	0.431155
36	6	0	3.785393	-0.805405	-0.594874
37	6	0	3.874170	-3.398854	0.423792
38	1	0	1.785642	-3.131556	0.841356
39	6	0	4.975907	-1.512181	-0.590498
40	1	0	3.763793	0.186023	-1.030256
41	6	0	5.032960	-2.811812	-0.081880
42	1	0	3.881461	-4.405509	0.820117
43	1	0	5.878942	-1.073568	-0.999217
44	8	0	6.247535	-3.421592	-0.129786
45	8	0	-6.336580	-3.146492	0.362811
46	6	0	6.344489	-4.732936	0.399243
47	1	0	7.382512	-5.034507	0.271628
48	1	0	6.090988	-4.748083	1.463720
49	1	0	5.697119	-5.427743	-0.144297
50	6	0	-6.620775	-4.335528	-0.354276
51	1	0	-7.650534	-4.593848	-0.113647
52	1	0	-6.530722	-4.176981	-1.433219
53	1	0	-5.961211	-5.151810	-0.044501

Structure 40a (DMSO)

Energy (Hartrees): -1263.97347623
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.944501	3.362085	0.933605
2	6	0	0.979991	4.746414	0.939657
3	6	0	0.094532	5.479082	0.143108
4	6	0	-0.815195	4.801303	-0.667233
5	6	0	-0.826311	3.406709	-0.674230
6	6	0	0.036285	2.656179	0.127574
7	1	0	1.622705	2.818665	1.583532
8	1	0	1.681352	5.281265	1.570166
9	1	0	-1.504333	5.337455	-1.306672
10	1	0	-1.520294	2.899728	-1.336966
11	6	0	-0.001824	1.172506	0.138179
12	6	0	-1.215587	0.529757	0.091468
13	6	0	1.248964	0.452371	0.175238
14	1	0	-2.121761	1.125275	0.063417
15	1	0	2.157402	1.063888	0.148445
16	1	0	-0.519955	-1.353495	0.092611
17	7	0	1.335600	-0.835087	0.224738
18	7	0	-1.382507	-0.805375	0.077678
19	8	0	0.193462	6.830712	0.222409
20	6	0	-0.713540	7.600277	-0.553474
21	1	0	-0.490135	8.642705	-0.333977
22	1	0	-0.572156	7.416555	-1.622530
23	1	0	-1.750200	7.385100	-0.278043
24	6	0	2.606014	-1.441112	0.153700
25	6	0	2.811412	-2.629407	0.869741
26	6	0	3.650448	-0.954434	-0.633996
27	6	0	4.030228	-3.281773	0.830495
28	1	0	1.998939	-3.027471	1.468238
29	6	0	4.880618	-1.609783	-0.687766
30	1	0	3.501712	-0.067685	-1.240448
31	6	0	5.077192	-2.775464	0.051795
32	1	0	4.191065	-4.195449	1.391559
33	1	0	5.662458	-1.209115	-1.319711
34	6	0	-2.603503	-1.499356	0.032532
35	6	0	-2.554375	-2.881604	-0.194178
36	6	0	-3.844297	-0.892023	0.205787
37	6	0	-3.715155	-3.628809	-0.260332
38	1	0	-1.591101	-3.364208	-0.325483
39	6	0	-5.018951	-1.642126	0.130421
40	1	0	-3.924942	0.168182	0.410453
41	6	0	-4.961991	-3.013884	-0.105838
42	1	0	-3.673825	-4.697081	-0.439349
43	1	0	-5.966549	-1.137400	0.266680
44	8	0	-6.048322	-3.824201	-0.196980
45	8	0	6.231161	-3.489985	0.064870
46	6	0	-7.326203	-3.218305	-0.073545
47	1	0	-8.053505	-4.019165	-0.192617
48	1	0	-7.453026	-2.758308	0.910984
49	1	0	-7.483995	-2.467060	-0.853206
50	6	0	7.299042	-3.025655	-0.747351
51	1	0	8.113461	-3.734341	-0.609112
52	1	0	7.012026	-3.004744	-1.802773
53	1	0	7.628829	-2.029950	-0.436669

Structure 40a (C_2H_5OH)

Energy (Hartrees): -1263.97716898
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.930595	3.462867	-0.904328
2	6	0	-0.955990	4.847400	-0.927916
3	6	0	-0.049606	5.580666	-0.157733
4	6	0	0.872083	4.909915	0.642814
5	6	0	0.873228	3.515549	0.667370
6	6	0	-0.011064	2.762025	-0.107419
7	1	0	-1.624571	2.915045	-1.533568
8	1	0	-1.664654	5.381210	-1.551542
9	1	0	1.577240	5.450163	1.260895
10	1	0	1.576000	3.010771	1.322484
11	6	0	0.017808	1.278025	-0.099511
12	6	0	1.229844	0.632890	-0.092321
13	6	0	-1.237643	0.566631	-0.076406
14	1	0	2.135310	1.229266	-0.111384
15	1	0	-2.138371	1.187875	-0.023010
16	1	0	0.545147	-1.256029	-0.020458
17	7	0	-1.338671	-0.720588	-0.103997
18	7	0	1.401740	-0.701952	-0.062191
19	8	0	-0.142447	6.937597	-0.251511
20	6	0	0.789509	7.713674	0.490784
21	1	0	0.563102	8.753725	0.263045
22	1	0	0.674249	7.542437	1.564671
23	1	0	1.815868	7.488409	0.187646
24	6	0	-2.617640	-1.300898	0.024083
25	6	0	-2.889370	-2.475875	-0.676436
26	6	0	-3.614787	-0.781484	0.864022
27	6	0	-4.129686	-3.103743	-0.589011
28	1	0	-2.118685	-2.897252	-1.312985
29	6	0	-4.848127	-1.403203	0.965442
30	1	0	-3.412228	0.099842	1.462775
31	6	0	-5.117044	-2.562850	0.233862
32	1	0	-4.306406	-4.006951	-1.158380
33	1	0	-5.615392	-1.009191	1.622821
34	6	0	2.631946	-1.382559	-0.069914
35	6	0	2.632871	-2.743009	0.232724
36	6	0	3.846885	-0.759424	-0.378627
37	6	0	3.815172	-3.478186	0.245359
38	1	0	1.695406	-3.236684	0.467505
39	6	0	5.026408	-1.485516	-0.356923
40	1	0	3.886297	0.288648	-0.648140
41	6	0	5.022915	-2.845919	-0.043001
42	1	0	3.775025	-4.532578	0.485686
43	1	0	5.969094	-1.004613	-0.593124
44	8	0	6.236313	-3.468929	-0.048927
45	8	0	-6.358494	-3.101765	0.398035
46	6	0	6.267752	-4.846393	0.300706
47	1	0	7.314828	-5.141713	0.267417
48	1	0	5.876954	-5.002720	1.310167
49	1	0	5.697016	-5.446239	-0.413953
50	6	0	-6.666665	-4.277564	-0.339246
51	1	0	-7.695173	-4.529400	-0.086882
52	1	0	-6.590692	-4.096084	-1.415029
53	1	0	-6.009056	-5.103499	-0.054369

Structure 40b (vacuum)

Energy (Hartrees): -1263.93724812
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.365258	3.031955	-0.768646
2	6	0	0.067501	4.393941	-0.765302
3	6	0	-0.874365	4.888594	0.134191
4	6	0	-1.498227	4.015342	1.029560
5	6	0	-1.183778	2.668720	1.019030
6	6	0	-0.248643	2.143182	0.112109
7	1	0	1.088210	2.653279	-1.483843
8	1	0	0.567822	5.046075	-1.468390
9	1	0	-2.212749	4.423509	1.734195
10	1	0	-1.650103	2.006502	1.741490
11	6	0	0.095994	0.702315	0.102569
12	6	0	-0.841475	-0.278365	0.069038
13	6	0	1.505647	0.320853	0.098619
14	1	0	2.212727	1.135243	0.307460
15	1	0	-0.503099	-1.308787	0.087553
16	7	0	1.917474	-0.866516	-0.132240
17	7	0	-2.184309	-0.089352	-0.041958
18	1	0	-2.505136	0.847407	-0.246607
19	8	0	-1.245615	6.192445	0.219787
20	6	0	-0.621365	7.110950	-0.652259
21	1	0	-0.829570	6.867386	-1.699003
22	1	0	-1.044194	8.085263	-0.417587
23	1	0	0.461071	7.135494	-0.491751
24	6	0	-3.158470	-1.098374	0.006162
25	6	0	-4.402503	-0.875654	-0.576673
26	6	0	-2.923010	-2.322969	0.642579
27	6	0	-5.398355	-1.848098	-0.541289
28	1	0	-4.597020	0.067067	-1.076901
29	6	0	-3.903076	-3.298479	0.662251
30	1	0	-1.979680	-2.508289	1.140596
31	6	0	-5.147971	-3.072607	0.072544
32	1	0	-6.352135	-1.637380	-1.005503
33	1	0	-3.730326	-4.249443	1.151000
34	6	0	3.290063	-1.144872	-0.002266
35	6	0	4.100260	-0.594289	1.001845
36	6	0	3.866170	-2.049682	-0.891667
37	6	0	5.444863	-0.912051	1.080577
38	1	0	3.662121	0.063120	1.744319
39	6	0	5.220031	-2.365795	-0.829727
40	1	0	3.234426	-2.497802	-1.649411
41	6	0	6.017123	-1.791490	0.159548
42	1	0	6.075627	-0.501663	1.859784
43	1	0	5.632085	-3.062281	-1.547666
44	8	0	7.347137	-2.037800	0.318168
45	8	0	-6.043593	-4.093964	0.155787
46	6	0	7.955089	-2.943146	-0.576186
47	1	0	7.882960	-2.588984	-1.609701
48	1	0	9.002229	-2.998191	-0.286154
49	1	0	7.504110	-3.938089	-0.500533
50	6	0	-7.318859	-3.890795	-0.412208
51	1	0	-7.248596	-3.708073	-1.489543
52	1	0	-7.877215	-4.807758	-0.237378
53	1	0	-7.836576	-3.053089	0.066639

Structure 40b ($CHCl_3$)

Energy (Hartrees): -1263.97236584
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.465386	3.030903	-0.713488
2	6	0	0.200432	4.400044	-0.713850
3	6	0	-0.788370	4.908054	0.126867
4	6	0	-1.490877	4.039214	0.968381
5	6	0	-1.208621	2.684759	0.962855
6	6	0	-0.226942	2.145514	0.114152
7	1	0	1.226803	2.647448	-1.385243
8	1	0	0.762343	5.047657	-1.373851
9	1	0	-2.243689	4.451376	1.630452
10	1	0	-1.742715	2.031910	1.645881
11	6	0	0.090315	0.697012	0.110028
12	6	0	-0.862606	-0.275345	0.073072
13	6	0	1.491222	0.296552	0.116059
14	1	0	2.204768	1.091495	0.366522
15	1	0	-0.543019	-1.310768	0.122092
16	7	0	1.899526	-0.887039	-0.158815
17	7	0	-2.196244	-0.077638	-0.062853
18	1	0	-2.515642	0.855975	-0.291190
19	8	0	-1.133231	6.218862	0.202167
20	6	0	-0.435694	7.133881	-0.627028
21	1	0	-0.589818	6.904047	-1.685473
22	1	0	-0.851382	8.115440	-0.407951
23	1	0	0.634498	7.135025	-0.401201
24	6	0	-3.182498	-1.076009	-0.002513
25	6	0	-4.418604	-0.842659	-0.600374
26	6	0	-2.970160	-2.291004	0.659660
27	6	0	-5.431312	-1.797399	-0.554375
28	1	0	-4.592463	0.096682	-1.115182
29	6	0	-3.968912	-3.249187	0.692077
30	1	0	-2.033163	-2.485491	1.167060
31	6	0	-5.205462	-3.014466	0.086424
32	1	0	-6.378129	-1.579723	-1.030502
33	1	0	-3.810613	-4.191641	1.203269
34	6	0	3.268418	-1.182781	-0.013448
35	6	0	4.073657	-0.655683	1.008598
36	6	0	3.847126	-2.080393	-0.910701
37	6	0	5.415303	-0.988117	1.095957
38	1	0	3.636798	-0.002230	1.755572
39	6	0	5.197232	-2.413046	-0.838486
40	1	0	3.224996	-2.512530	-1.686627
41	6	0	5.989856	-1.860748	0.167917
42	1	0	6.037182	-0.590789	1.890114
43	1	0	5.611513	-3.102482	-1.562211
44	8	0	7.314249	-2.123735	0.333212
45	8	0	-6.118849	-4.018278	0.179751
46	6	0	7.925498	-3.019098	-0.579495
47	1	0	7.872479	-2.637926	-1.603704
48	1	0	8.968452	-3.092032	-0.277005
49	1	0	7.464363	-4.010027	-0.530686
50	6	0	-7.379836	-3.817675	-0.434846
51	1	0	-7.274120	-3.660227	-1.512482
52	1	0	-7.949764	-4.728036	-0.259063
53	1	0	-7.907313	-2.969134	0.011413

Structure 40b (DMSO)

Energy (Hartrees): -1263.96880145
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.494893	3.021578	-0.702985
2	6	0	0.251017	4.394458	-0.717363
3	6	0	-0.733683	4.925886	0.114878
4	6	0	-1.452855	4.074080	0.960399
5	6	0	-1.191984	2.714740	0.968026
6	6	0	-0.214216	2.153553	0.129466
7	1	0	1.253548	2.622482	-1.368958
8	1	0	0.826843	5.026331	-1.380708
9	1	0	-2.205141	4.499378	1.615094
10	1	0	-1.744166	2.078718	1.652648
11	6	0	0.084999	0.701142	0.139372
12	6	0	-0.879004	-0.263992	0.121073
13	6	0	1.480862	0.287993	0.138326
14	1	0	2.204281	1.078800	0.372015
15	1	0	-0.566911	-1.301370	0.181732
16	7	0	1.879174	-0.903092	-0.128158
17	7	0	-2.209762	-0.059706	-0.005271
18	1	0	-2.531416	0.874955	-0.230866
19	8	0	-1.056857	6.241126	0.174639
20	6	0	-0.349899	7.130530	-0.678418
21	1	0	-0.512044	6.879928	-1.730889
22	1	0	-0.751783	8.122249	-0.479574
23	1	0	0.721385	7.121820	-0.458359
24	6	0	-3.198381	-1.058140	0.037076
25	6	0	-4.437935	-0.802717	-0.545407
26	6	0	-2.984280	-2.293698	0.659282
27	6	0	-5.450151	-1.758898	-0.529667
28	1	0	-4.613267	0.155043	-1.024953
29	6	0	-3.983683	-3.252799	0.662279
30	1	0	-2.045805	-2.506983	1.156342
31	6	0	-5.222425	-2.998312	0.067946
32	1	0	-6.399031	-1.524594	-0.993825
33	1	0	-3.820541	-4.211305	1.141882
34	6	0	3.248979	-1.204641	0.004950
35	6	0	4.072140	-0.665335	1.006246
36	6	0	3.810363	-2.121361	-0.885045
37	6	0	5.413084	-1.005404	1.079706
38	1	0	3.652949	0.007521	1.746396
39	6	0	5.159347	-2.462259	-0.826879
40	1	0	3.177106	-2.563909	-1.646570
41	6	0	5.970919	-1.897281	0.158027
42	1	0	6.046571	-0.594837	1.858128
43	1	0	5.557621	-3.166851	-1.545374
44	8	0	7.294167	-2.163880	0.306277
45	8	0	-6.135904	-4.002361	0.127716
46	6	0	7.887466	-3.069198	-0.612926
47	1	0	7.806631	-2.699760	-1.639360
48	1	0	8.938192	-3.134491	-0.336521
49	1	0	7.431376	-4.060895	-0.540846
50	6	0	-7.398581	-3.775187	-0.480129
51	1	0	-7.291987	-3.574468	-1.550367
52	1	0	-7.969170	-4.691597	-0.340777
53	1	0	-7.924314	-2.944069	-0.000738

Structure 40b (C_2H_5OH)

Energy (Hartrees): -1263.97270505
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.463863	3.013159	-0.724160
2	6	0	0.208905	4.384112	-0.734899
3	6	0	-0.758753	4.906674	0.120984
4	6	0	-1.449885	4.054002	0.986940
5	6	0	-1.178169	2.696611	0.990333
6	6	0	-0.217926	2.142448	0.127739
7	1	0	1.208540	2.617425	-1.407924
8	1	0	0.762128	5.019950	-1.413508
9	1	0	-2.187570	4.476263	1.660378
10	1	0	-1.705949	2.056256	1.690086
11	6	0	0.089025	0.691354	0.132223
12	6	0	-0.873056	-0.274967	0.113171
13	6	0	1.486401	0.285286	0.126990
14	1	0	2.205700	1.079573	0.361549
15	1	0	-0.561274	-1.312694	0.167704
16	7	0	1.891337	-0.902881	-0.143196
17	7	0	-2.204589	-0.069705	-0.009966
18	1	0	-2.525784	0.866789	-0.228077
19	8	0	-1.092618	6.224725	0.186437
20	6	0	-0.405241	7.124086	-0.674783
21	1	0	-0.585468	6.876229	-1.724594
22	1	0	-0.811051	8.111399	-0.462039
23	1	0	0.668722	7.119107	-0.470027
24	6	0	-3.193772	-1.067615	0.032509
25	6	0	-4.433084	-0.810792	-0.550087
26	6	0	-2.980686	-2.302037	0.656669
27	6	0	-5.447006	-1.764784	-0.531905
28	1	0	-4.607016	0.146134	-1.031893
29	6	0	-3.982074	-3.259300	0.662584
30	1	0	-2.042418	-2.515501	1.154142
31	6	0	-5.219156	-3.001334	0.069008
32	1	0	-6.395964	-1.530569	-0.995952
33	1	0	-3.822293	-4.217612	1.144292
34	6	0	3.263308	-1.194310	-0.007439
35	6	0	4.074125	-0.659704	1.005777
36	6	0	3.837726	-2.096912	-0.903472
37	6	0	5.417203	-0.990568	1.086109
38	1	0	3.643625	0.000671	1.750685
39	6	0	5.188517	-2.428855	-0.838220
40	1	0	3.214014	-2.536179	-1.674699
41	6	0	5.985505	-1.868539	0.159496
42	1	0	6.042826	-0.584931	1.873752
43	1	0	5.598110	-3.123294	-1.560249
44	8	0	7.314817	-2.129612	0.317051
45	8	0	-6.139020	-4.006771	0.133774
46	6	0	7.920593	-3.037390	-0.594070
47	1	0	7.853179	-2.666691	-1.620600
48	1	0	8.966970	-3.101801	-0.301190
49	1	0	7.460795	-4.027235	-0.524530
50	6	0	-7.405176	-3.778867	-0.470861
51	1	0	-7.299126	-3.583965	-1.541819
52	1	0	-7.975983	-4.694078	-0.324204
53	1	0	-7.924505	-2.944424	0.008933

Structure 40c (vacuum)

Energy (Hartrees): -1263.93862770
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.756656	2.436935	-0.775180
2	6	0	0.735976	3.829057	-0.756932
3	6	0	-0.051841	4.495889	0.179709
4	6	0	-0.805312	3.760380	1.096834
5	6	0	-0.772775	2.377025	1.066556
6	6	0	0.000478	1.686219	0.122561
7	1	0	1.385945	1.925467	-1.492303
8	1	0	1.338891	4.373995	-1.470529
9	1	0	-1.393668	4.296911	1.831038
10	1	0	-1.339350	1.816021	1.803045
11	6	0	0.014883	0.203970	0.093538
12	6	0	-1.128054	-0.528844	0.066841
13	6	0	1.264014	-0.538941	0.052680
14	1	0	-1.064918	-1.612376	0.065747
15	1	0	1.155974	-1.633452	0.052366
16	7	0	2.416247	0.008800	0.033216
17	7	0	-2.394277	-0.031044	-0.011695
18	1	0	-2.488607	0.959733	-0.190422
19	8	0	-0.144982	5.847924	0.282952
20	6	0	0.622891	6.628034	-0.608684
21	1	0	0.340266	6.435347	-1.648602
22	1	0	0.409440	7.665956	-0.362693
23	1	0	1.692796	6.435543	-0.480933
24	6	0	-3.570920	-0.794442	0.031738
25	6	0	-4.725417	-0.315380	-0.580012
26	6	0	-3.624642	-2.023905	0.698958
27	6	0	-5.913457	-1.040809	-0.541983
28	1	0	-4.697308	0.633634	-1.104419
29	6	0	-4.797010	-2.757920	0.719929
30	1	0	-2.755793	-2.397039	1.226938
31	6	0	-5.951089	-2.275631	0.100775
32	1	0	-6.789860	-0.633300	-1.027047
33	1	0	-4.848097	-3.709751	1.234144
34	6	0	3.553297	-0.815334	-0.057525
35	6	0	4.694413	-0.450537	0.653299
36	6	0	3.614242	-1.958279	-0.868858
37	6	0	5.853161	-1.220587	0.608167
38	1	0	4.658377	0.447448	1.258644
39	6	0	4.766075	-2.722645	-0.932327
40	1	0	2.760439	-2.228398	-1.480340
41	6	0	5.890711	-2.365828	-0.186166
42	1	0	6.713622	-0.912306	1.186937
43	1	0	4.824884	-3.598657	-1.566976
44	8	0	-7.052130	-3.070349	0.185943
45	8	0	6.973875	-3.182248	-0.311414
46	6	0	-8.231926	-2.619664	-0.443222
47	1	0	-8.080524	-2.488765	-1.519738
48	1	0	-8.979199	-3.391916	-0.275298
49	1	0	-8.579795	-1.677416	-0.007093
50	6	0	8.140838	-2.830276	0.398059
51	1	0	7.960605	-2.818046	1.477915
52	1	0	8.879461	-3.594407	0.165215
53	1	0	8.517370	-1.852065	0.081379

Structure 40c ($CHCl_3$)

Energy (Hartrees): -1263.97496700
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.653121	2.450716	-0.847299
2	6	0	0.614203	3.842766	-0.814808
3	6	0	-0.099475	4.488317	0.195233
4	6	0	-0.759905	3.731200	1.166448
5	6	0	-0.709378	2.347636	1.120018
6	6	0	-0.007465	1.678306	0.107035
7	1	0	1.215795	1.958181	-1.632086
8	1	0	1.141859	4.404128	-1.574404
9	1	0	-1.296424	4.246777	1.954881
10	1	0	-1.212209	1.772720	1.891699
11	6	0	0.025920	0.194997	0.058472
12	6	0	-1.111673	-0.554955	0.046310
13	6	0	1.278828	-0.530776	0.011496
14	1	0	-1.030711	-1.637287	0.036551
15	1	0	1.182004	-1.623423	-0.040623
16	7	0	2.431212	0.027092	0.050875
17	7	0	-2.378195	-0.071717	0.010585
18	1	0	-2.496499	0.925489	-0.122773
19	8	0	-0.204083	5.836876	0.316012
20	6	0	0.465126	6.639672	-0.642761
21	1	0	0.083217	6.452028	-1.650902
22	1	0	0.258637	7.672281	-0.367478
23	1	0	1.544867	6.465991	-0.618813
24	6	0	-3.552033	-0.843523	0.045438
25	6	0	-4.728679	-0.307718	-0.472497
26	6	0	-3.583028	-2.126626	0.603932
27	6	0	-5.918384	-1.030800	-0.451820
28	1	0	-4.715386	0.687325	-0.904862
29	6	0	-4.760555	-2.855786	0.609267
30	1	0	-2.696052	-2.553789	1.055685
31	6	0	-5.936617	-2.318208	0.081640
32	1	0	-6.812119	-0.581075	-0.863198
33	1	0	-4.790747	-3.849798	1.040276
34	6	0	3.576581	-0.786857	-0.048735
35	6	0	4.705739	-0.437626	0.691817
36	6	0	3.659604	-1.903610	-0.895273
37	6	0	5.872834	-1.195818	0.639654
38	1	0	4.658853	0.439032	1.328331
39	6	0	4.819657	-2.657085	-0.964258
40	1	0	2.816111	-2.166123	-1.524457
41	6	0	5.931823	-2.315091	-0.190587
42	1	0	6.723035	-0.899787	1.240193
43	1	0	4.889552	-3.512460	-1.626703
44	8	0	-7.039603	-3.112190	0.139320
45	8	0	7.023788	-3.116611	-0.323338
46	6	0	-8.249987	-2.589584	-0.380968
47	1	0	-8.154283	-2.357374	-1.446155
48	1	0	-8.997487	-3.369622	-0.248831
49	1	0	-8.561457	-1.693982	0.165495
50	6	0	8.177591	-2.783843	0.428927
51	1	0	7.972570	-2.814844	1.503367
52	1	0	8.925125	-3.536212	0.183905
53	1	0	8.556715	-1.794637	0.154638

Structure 40c (DMSO)

Energy (Hartrees): -1263.97276969
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.637905	2.452786	-0.863280
2	6	0	0.614143	3.845567	-0.834261
3	6	0	-0.071300	4.500988	0.190463
4	6	0	-0.722135	3.750595	1.174410
5	6	0	-0.686253	2.366050	1.131000
6	6	0	-0.007453	1.687771	0.108167
7	1	0	1.172499	1.954174	-1.664423
8	1	0	1.127449	4.399003	-1.609604
9	1	0	-1.244387	4.269942	1.970121
10	1	0	-1.185802	1.799630	1.911144
11	6	0	0.021620	0.204127	0.065064
12	6	0	-1.117265	-0.548663	0.062656
13	6	0	1.269206	-0.524699	0.017413
14	1	0	-1.029396	-1.630282	0.051992
15	1	0	1.167320	-1.616015	-0.034434
16	7	0	2.427378	0.028479	0.058184
17	7	0	-2.381338	-0.069090	0.041690
18	1	0	-2.508815	0.930173	-0.075052
19	8	0	-0.156531	5.848620	0.310833
20	6	0	0.507395	6.639223	-0.665329
21	1	0	0.103045	6.454458	-1.664803
22	1	0	0.323114	7.675886	-0.389832
23	1	0	1.584167	6.447472	-0.662253
24	6	0	-3.554295	-0.845046	0.061053
25	6	0	-4.738353	-0.284296	-0.412432
26	6	0	-3.576972	-2.153532	0.557552
27	6	0	-5.928759	-1.006986	-0.408771
28	1	0	-4.730698	0.731348	-0.794254
29	6	0	-4.756547	-2.880238	0.548499
30	1	0	-2.683772	-2.606755	0.970033
31	6	0	-5.941283	-2.318166	0.066019
32	1	0	-6.827373	-0.536508	-0.785350
33	1	0	-4.776806	-3.893714	0.932474
34	6	0	3.567529	-0.794136	-0.042333
35	6	0	4.707962	-0.441286	0.680045
36	6	0	3.635853	-1.924498	-0.873172
37	6	0	5.872085	-1.204699	0.624882
38	1	0	4.677049	0.443496	1.306977
39	6	0	4.791841	-2.684486	-0.943600
40	1	0	2.784546	-2.195624	-1.488210
41	6	0	5.916541	-2.337749	-0.188440
42	1	0	6.729849	-0.902680	1.211786
43	1	0	4.844573	-3.550970	-1.593447
44	8	0	-7.043823	-3.111029	0.104774
45	8	0	7.001489	-3.144984	-0.319779
46	6	0	-8.261826	-2.556618	-0.369195
47	1	0	-8.186029	-2.280490	-1.425113
48	1	0	-9.014333	-3.334477	-0.253890
49	1	0	-8.553310	-1.681168	0.218480
50	6	0	8.165703	-2.800092	0.415667
51	1	0	7.971041	-2.808812	1.492064
52	1	0	8.908903	-3.558995	0.178427
53	1	0	8.543751	-1.817171	0.118975

Structure 40c (C_2H_5OH)

Energy (Hartrees): -1263.97643639
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.608528	2.456722	-0.877360
2	6	0	0.573988	3.849210	-0.844670
3	6	0	-0.096793	4.493595	0.195009
4	6	0	-0.721162	3.738631	1.190908
5	6	0	-0.674377	2.354360	1.143841
6	6	0	-0.011000	1.685060	0.105502
7	1	0	1.130466	1.963804	-1.690384
8	1	0	1.067592	4.409955	-1.627614
9	1	0	-1.231053	4.253419	1.997862
10	1	0	-1.152988	1.781755	1.932560
11	6	0	0.027215	0.201456	0.057727
12	6	0	-1.108242	-0.555283	0.051250
13	6	0	1.279028	-0.519792	0.010905
14	1	0	-1.018157	-1.636721	0.037154
15	1	0	1.183938	-1.611470	-0.045400
16	7	0	2.433932	0.039340	0.059289
17	7	0	-2.373952	-0.077800	0.027711
18	1	0	-2.501978	0.921727	-0.085374
19	8	0	-0.192745	5.845689	0.320239
20	6	0	0.449517	6.647757	-0.663210
21	1	0	0.028553	6.463579	-1.655536
22	1	0	0.260588	7.680817	-0.377249
23	1	0	1.527045	6.462748	-0.675734
24	6	0	-3.545504	-0.855062	0.053350
25	6	0	-4.731678	-0.297081	-0.418608
26	6	0	-3.564613	-2.161054	0.555882
27	6	0	-5.921228	-1.020732	-0.407809
28	1	0	-4.726439	0.716922	-0.804904
29	6	0	-4.743512	-2.889218	0.553680
30	1	0	-2.669792	-2.611006	0.968515
31	6	0	-5.928270	-2.328594	0.072815
32	1	0	-6.822295	-0.554007	-0.783278
33	1	0	-4.762974	-3.901548	0.941451
34	6	0	3.576553	-0.779860	-0.041892
35	6	0	4.708559	-0.438990	0.699271
36	6	0	3.653761	-1.893718	-0.892972
37	6	0	5.873126	-1.201303	0.643074
38	1	0	4.670402	0.434317	1.341606
39	6	0	4.810836	-2.652360	-0.965124
40	1	0	2.808784	-2.152088	-1.522172
41	6	0	5.924449	-2.317650	-0.190763
42	1	0	6.725158	-0.910888	1.244069
43	1	0	4.872995	-3.506442	-1.630703
44	8	0	-7.034805	-3.125238	0.119825
45	8	0	7.015448	-3.126264	-0.324591
46	6	0	-8.255095	-2.580728	-0.364681
47	1	0	-8.173085	-2.315083	-1.422530
48	1	0	-9.002154	-3.363203	-0.244715
49	1	0	-8.551275	-1.702347	0.215726
50	6	0	8.176904	-2.791781	0.423472
51	1	0	7.974213	-2.821235	1.497684
52	1	0	8.921599	-3.545653	0.174798
53	1	0	8.551873	-1.803159	0.143799

Structure 40d (vacuum)

Energy (Hartrees): -1263.93265609
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.357099	2.706466	0.871332
2	6	0	1.675692	4.045929	0.967888
3	6	0	1.006535	4.990427	0.182796
4	6	0	0.020898	4.571014	-0.704154
5	6	0	-0.286089	3.212333	-0.792857
6	6	0	0.354166	2.260296	-0.004192
7	1	0	1.887875	1.987859	1.482327
8	1	0	2.443562	4.394664	1.647627
9	1	0	-0.500456	5.273051	-1.340619
10	1	0	-1.029592	2.891534	-1.514566
11	6	0	-0.040556	0.834076	-0.061837
12	6	0	-1.358771	0.515223	-0.140647
13	6	0	0.959020	-0.225550	-0.015801
14	1	0	0.581375	-1.238093	0.186432
15	1	0	-1.303032	-1.422453	-0.822398
16	1	0	-2.101747	1.300190	-0.032929
17	7	0	2.209472	-0.024743	-0.175054
18	7	0	-1.885725	-0.726993	-0.384164
19	8	0	1.392962	6.283803	0.350447
20	6	0	0.750694	7.263960	-0.434817
21	1	0	1.194288	8.216501	-0.152956
22	1	0	0.916734	7.086718	-1.502352
23	1	0	-0.325303	7.290231	-0.233940
24	6	0	3.092806	-1.108342	-0.016873
25	6	0	4.200530	-1.180885	-0.858389
26	6	0	2.941781	-2.091560	0.972531
27	6	0	5.110444	-2.229387	-0.766545
28	1	0	4.333897	-0.403686	-1.601471
29	6	0	3.851472	-3.128509	1.083560
30	1	0	2.125387	-2.018899	1.682411
31	6	0	4.935607	-3.211943	0.207906
32	1	0	5.949748	-2.259078	-1.448095
33	1	0	3.751854	-3.883292	1.854228
34	6	0	-3.230321	-1.068782	-0.175183
35	6	0	-3.800413	-2.114260	-0.895707
36	6	0	-4.019317	-0.384600	0.756747
37	6	0	-5.131553	-2.474593	-0.707052
38	1	0	-3.202383	-2.652361	-1.623446
39	6	0	-5.349475	-0.723973	0.929304
40	1	0	-3.584003	0.396979	1.367250
41	6	0	-5.918143	-1.770298	0.202119
42	1	0	-5.537692	-3.294058	-1.284248
43	1	0	-5.967965	-0.200120	1.647532
44	8	0	-7.229003	-2.032258	0.455546
45	8	0	5.771684	-4.269389	0.393721
46	6	0	-7.831049	-3.093081	-0.253532
47	1	0	-7.331502	-4.044329	-0.042920
48	1	0	-8.861084	-3.142339	0.092356
49	1	0	-7.818866	-2.906050	-1.332302
50	6	0	6.888584	-4.377628	-0.461467
51	1	0	7.419945	-5.275542	-0.153704
52	1	0	6.578894	-4.479043	-1.506749
53	1	0	7.550832	-3.511471	-0.361449

Structure 40d ($CHCl_3$)

Energy (Hartrees): -1263.96975910
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.350598	2.709277	0.894544
2	6	0	1.675966	4.049287	0.985542
3	6	0	1.023192	4.991627	0.182448
4	6	0	0.046970	4.569366	-0.715184
5	6	0	-0.264860	3.210891	-0.799122
6	6	0	0.360644	2.259627	0.004845
7	1	0	1.864023	1.995325	1.527034
8	1	0	2.435205	4.395225	1.677805
9	1	0	-0.463108	5.270543	-1.362499
10	1	0	-1.004875	2.890447	-1.525208
11	6	0	-0.035968	0.831981	-0.048512
12	6	0	-1.361018	0.519092	-0.127973
13	6	0	0.959852	-0.225759	0.000095
14	1	0	0.581864	-1.238821	0.188268
15	1	0	-1.309435	-1.445505	-0.724252
16	1	0	-2.094009	1.314381	-0.029047
17	7	0	2.215260	-0.026579	-0.154066
18	7	0	-1.898011	-0.713260	-0.352586
19	8	0	1.411613	6.284161	0.343957
20	6	0	0.768824	7.267647	-0.448817
21	1	0	1.208756	8.221067	-0.161904
22	1	0	0.945697	7.092659	-1.514294
23	1	0	-0.307303	7.291653	-0.252410
24	6	0	3.096079	-1.116041	-0.006432
25	6	0	4.221153	-1.168180	-0.828862
26	6	0	2.925300	-2.127856	0.951537
27	6	0	5.129980	-2.219680	-0.748918
28	1	0	4.373183	-0.375255	-1.552588
29	6	0	3.831490	-3.170479	1.048584
30	1	0	2.095063	-2.078489	1.647624
31	6	0	4.933821	-3.231247	0.191884
32	1	0	5.983243	-2.230509	-1.414178
33	1	0	3.710517	-3.945169	1.797269
34	6	0	-3.249905	-1.042994	-0.160758
35	6	0	-3.778304	-2.158355	-0.807252
36	6	0	-4.082606	-0.290652	0.675877
37	6	0	-5.112059	-2.520641	-0.641209
38	1	0	-3.141757	-2.752590	-1.454761
39	6	0	-5.415542	-0.635614	0.826006
40	1	0	-3.687635	0.551886	1.230415
41	6	0	-5.942878	-1.750508	0.172002
42	1	0	-5.485220	-3.395777	-1.156617
43	1	0	-6.064138	-0.056095	1.472733
44	8	0	-7.259035	-2.010817	0.395743
45	8	0	5.762463	-4.296352	0.358501
46	6	0	-7.817995	-3.153461	-0.229079
47	1	0	-7.314058	-4.068539	0.097111
48	1	0	-8.861001	-3.186149	0.080291
49	1	0	-7.767261	-3.073893	-1.319387
50	6	0	6.919438	-4.365485	-0.457723
51	1	0	7.444504	-5.271146	-0.159819
52	1	0	6.654393	-4.432966	-1.517207
53	1	0	7.569238	-3.500400	-0.294565

Structure 40d (DMSO)

Energy (Hartrees): -1263.96796176
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.325400	2.705884	0.887596
2	6	0	1.634452	4.050355	0.980807
3	6	0	0.967881	4.987574	0.181562
4	6	0	-0.005304	4.552886	-0.714983
5	6	0	-0.299228	3.190359	-0.801881
6	6	0	0.340979	2.243668	-0.002710
7	1	0	1.844158	1.998953	1.524471
8	1	0	2.387638	4.401306	1.677505
9	1	0	-0.530020	5.248283	-1.357030
10	1	0	-1.042570	2.864446	-1.522319
11	6	0	-0.039129	0.810933	-0.056038
12	6	0	-1.365235	0.486977	-0.119608
13	6	0	0.966769	-0.233960	-0.020291
14	1	0	0.605003	-1.252379	0.166021
15	1	0	-1.301897	-1.490521	-0.667750
16	1	0	-2.100388	1.279785	-0.016553
17	7	0	2.220846	-0.018130	-0.185149
18	7	0	-1.896131	-0.745466	-0.327813
19	8	0	1.336152	6.283234	0.345764
20	6	0	0.652307	7.260450	-0.425112
21	1	0	1.069373	8.222188	-0.132269
22	1	0	0.816851	7.103906	-1.495084
23	1	0	-0.420745	7.250385	-0.212791
24	6	0	3.116833	-1.095371	-0.033475
25	6	0	4.251814	-1.131011	-0.844145
26	6	0	2.953744	-2.108881	0.924702
27	6	0	5.181435	-2.163800	-0.750134
28	1	0	4.399963	-0.340712	-1.572149
29	6	0	3.878869	-3.133731	1.034449
30	1	0	2.112662	-2.077835	1.608738
31	6	0	4.994903	-3.175935	0.192921
32	1	0	6.041274	-2.159614	-1.407254
33	1	0	3.759340	-3.908685	1.783420
34	6	0	-3.250291	-1.073694	-0.143165
35	6	0	-3.763350	-2.211145	-0.763286
36	6	0	-4.098251	-0.300071	0.657955
37	6	0	-5.098492	-2.574149	-0.607791
38	1	0	-3.111898	-2.822153	-1.379823
39	6	0	-5.432068	-0.647376	0.798498
40	1	0	-3.718271	0.563351	1.190561
41	6	0	-5.945901	-1.783836	0.169785
42	1	0	-5.459063	-3.466438	-1.102661
43	1	0	-6.089760	-0.048104	1.417776
44	8	0	-7.262586	-2.044251	0.380180
45	8	0	5.843415	-4.219739	0.374580
46	6	0	-7.807141	-3.201551	-0.235524
47	1	0	-7.307314	-4.109201	0.115727
48	1	0	-8.856085	-3.231532	0.053378
49	1	0	-7.733400	-3.141671	-1.325532
50	6	0	7.015605	-4.259627	-0.426055
51	1	0	7.561833	-5.148992	-0.117342
52	1	0	6.767347	-4.337954	-1.488548
53	1	0	7.637504	-3.375296	-0.258411

Structure 40d (C_2H_5OH)

Energy (Hartrees): -1263.97162997
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.314575	2.718083	0.925775
2	6	0	1.630678	4.061931	1.005192
3	6	0	0.986713	4.987831	0.176599
4	6	0	0.028784	4.549102	-0.732488
5	6	0	-0.272839	3.187424	-0.804253
6	6	0	0.345889	2.250012	0.022010
7	1	0	1.815197	2.016684	1.583345
8	1	0	2.372097	4.420773	1.710846
9	1	0	-0.476163	5.239098	-1.395943
10	1	0	-1.002191	2.853925	-1.535574
11	6	0	-0.036792	0.817783	-0.022485
12	6	0	-1.362195	0.495178	-0.090958
13	6	0	0.968997	-0.227297	0.013989
14	1	0	0.607531	-1.244437	0.207583
15	1	0	-1.296783	-1.481125	-0.643734
16	1	0	-2.097808	1.288373	0.006332
17	7	0	2.221974	-0.014716	-0.162386
18	7	0	-1.892140	-0.738605	-0.300596
19	8	0	1.364085	6.288529	0.327353
20	6	0	0.718334	7.259614	-0.486089
21	1	0	1.146498	8.219733	-0.204016
22	1	0	0.909649	7.071622	-1.546146
23	1	0	-0.359060	7.271847	-0.299541
24	6	0	3.112392	-1.098002	-0.017852
25	6	0	4.225780	-1.156491	-0.856229
26	6	0	2.962302	-2.095117	0.958669
27	6	0	5.144843	-2.199303	-0.772512
28	1	0	4.364510	-0.377315	-1.597993
29	6	0	3.877877	-3.129993	1.058669
30	1	0	2.140234	-2.042765	1.664395
31	6	0	4.968394	-3.195497	0.187777
32	1	0	5.987312	-2.214939	-1.451446
33	1	0	3.769344	-3.893794	1.820996
34	6	0	-3.248126	-1.065106	-0.127604
35	6	0	-3.760404	-2.194987	-0.762283
36	6	0	-4.097574	-0.296964	0.676758
37	6	0	-5.097604	-2.554565	-0.619322
38	1	0	-3.107724	-2.802245	-1.381218
39	6	0	-5.433910	-0.640344	0.804703
40	1	0	-3.716616	0.558144	1.222103
41	6	0	-5.944871	-1.767450	0.159545
42	1	0	-5.459262	-3.440224	-1.125255
43	1	0	-6.095055	-0.046910	1.426385
44	8	0	-7.270038	-2.025102	0.356449
45	8	0	5.811415	-4.253377	0.359320
46	6	0	-7.814879	-3.178025	-0.271321
47	1	0	-7.320277	-4.087531	0.081538
48	1	0	-8.866359	-3.203892	0.008725
49	1	0	-7.730169	-3.109460	-1.359662
50	6	0	6.963118	-4.318584	-0.472166
51	1	0	7.504340	-5.211808	-0.165858
52	1	0	6.683046	-4.406397	-1.525666
53	1	0	7.598289	-3.439907	-0.329041

Structure 41a (vacuum)

Energy (Hartrees): -1443.90494329
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.036590	3.520538	1.010964
2	6	0	1.147745	4.897004	1.059587
3	6	0	0.381787	5.695062	0.204188
4	6	0	-0.485906	5.092283	-0.703490
5	6	0	-0.575616	3.701925	-0.748456
6	6	0	0.167372	2.891778	0.106932
7	1	0	1.616195	2.919562	1.703886
8	1	0	1.811980	5.384937	1.762232
9	1	0	-1.079494	5.682745	-1.388023
10	1	0	-1.225666	3.243663	-1.486309
11	6	0	0.043398	1.413850	0.073777
12	6	0	-1.196433	0.844014	0.028976
13	6	0	1.254266	0.623526	0.083990
14	1	0	-2.064321	1.492516	0.043542
15	1	0	2.193372	1.188714	0.100791
16	1	0	-0.604173	-1.072115	-0.071458
17	7	0	1.274999	-0.664950	0.076302
18	7	0	-1.441066	-0.487560	-0.038320
19	8	0	0.554330	7.034148	0.330440
20	6	0	-0.202275	7.878249	-0.512864
21	1	0	0.076403	8.895837	-0.249473
22	1	0	0.032725	7.697271	-1.566381
23	1	0	-1.275558	7.740369	-0.348275
24	6	0	2.515071	-1.317401	0.014469
25	6	0	2.700796	-2.458233	0.805099
26	6	0	3.544065	-0.892522	-0.836522
27	6	0	3.905740	-3.138134	0.786002
28	1	0	1.890853	-2.785289	1.445212
29	6	0	4.751662	-1.572460	-0.869354
30	1	0	3.382560	-0.045833	-1.492643
31	6	0	4.914833	-2.679582	-0.050968
32	1	0	4.077304	-4.011103	1.401144
33	1	0	5.558666	-1.265809	-1.521102
34	6	0	-2.687269	-1.101363	-0.024929
35	6	0	-2.739990	-2.479759	-0.284630
36	6	0	-3.875183	-0.407430	0.244461
37	6	0	-3.947381	-3.150310	-0.287645
38	1	0	-1.821399	-3.015755	-0.493688
39	6	0	-5.087460	-1.075627	0.233906
40	1	0	-3.865155	0.647137	0.482163
41	6	0	-5.111308	-2.436375	-0.032680
42	1	0	-4.002631	-4.211504	-0.489320
43	1	0	-6.013794	-0.556769	0.440703
44	7	0	6.198253	-3.402891	-0.081506
45	8	0	6.315675	-4.367181	0.644096
46	8	0	7.058939	-2.987919	-0.828071
47	7	0	-6.399403	-3.141321	-0.039213
48	8	0	-7.398521	-2.488797	0.179903
49	8	0	-6.385968	-4.333469	-0.263709

Structure 41a ($CHCl_3$)

Energy (Hartrees): -1443.94192725
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.981876	3.579812	0.973914
2	6	0	1.047321	4.961392	1.004617
3	6	0	0.216005	5.724242	0.178033
4	6	0	-0.670370	5.081996	-0.684441
5	6	0	-0.714482	3.688843	-0.712375
6	6	0	0.094154	2.911351	0.116812
7	1	0	1.614960	3.008169	1.644736
8	1	0	1.727964	5.474323	1.674363
9	1	0	-1.314325	5.645504	-1.346671
10	1	0	-1.386901	3.205023	-1.413478
11	6	0	0.016886	1.428229	0.102214
12	6	0	-1.209159	0.823087	0.065049
13	6	0	1.251704	0.678097	0.115962
14	1	0	-2.096333	1.445554	0.073275
15	1	0	2.172392	1.270621	0.124685
16	1	0	-0.567550	-1.083743	-0.031422
17	7	0	1.308607	-0.611138	0.119991
18	7	0	-1.415202	-0.514548	0.009783
19	8	0	0.344398	7.070909	0.283453
20	6	0	-0.493145	7.880278	-0.526241
21	1	0	-0.244829	8.910944	-0.280331
22	1	0	-0.301854	7.705111	-1.589044
23	1	0	-1.549182	7.698904	-0.305173
24	6	0	2.559013	-1.236618	0.047680
25	6	0	2.744386	-2.418524	0.778853
26	6	0	3.598884	-0.755903	-0.762081
27	6	0	3.953681	-3.088313	0.739265
28	1	0	1.929314	-2.790110	1.388262
29	6	0	4.812193	-1.421632	-0.812356
30	1	0	3.444474	0.126598	-1.371157
31	6	0	4.971966	-2.575669	-0.056838
32	1	0	4.112476	-3.994574	1.308473
33	1	0	5.620649	-1.063879	-1.436018
34	6	0	-2.641573	-1.163617	0.011026
35	6	0	-2.645162	-2.544054	-0.249499
36	6	0	-3.854023	-0.505519	0.267301
37	6	0	-3.829806	-3.251499	-0.272960
38	1	0	-1.706542	-3.050823	-0.443071
39	6	0	-5.043603	-1.210737	0.236569
40	1	0	-3.880337	0.548545	0.507099
41	6	0	-5.020656	-2.573001	-0.034465
42	1	0	-3.838526	-4.313228	-0.480271
43	1	0	-5.984176	-0.712441	0.430910
44	7	0	6.253462	-3.285538	-0.112971
45	8	0	6.367701	-4.310929	0.529548
46	8	0	7.139463	-2.813016	-0.797968
47	7	0	-6.279829	-3.311443	-0.070016
48	8	0	-7.312652	-2.692929	0.105526
49	8	0	-6.236093	-4.509694	-0.275424

Structure 41a (DMSO)

Energy (Hartrees): -1443.93880738
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.992411	3.606752	0.948090
2	6	0	1.050394	4.989742	0.965395
3	6	0	0.183462	5.742852	0.166453
4	6	0	-0.732073	5.087733	-0.656277
5	6	0	-0.768790	3.694127	-0.671881
6	6	0	0.076397	2.926484	0.130647
7	1	0	1.657529	3.045678	1.596544
8	1	0	1.756139	5.507994	1.604602
9	1	0	-1.405664	5.640885	-1.297625
10	1	0	-1.467132	3.202342	-1.341450
11	6	0	0.009644	1.442990	0.124870
12	6	0	-1.213951	0.829198	0.094951
13	6	0	1.249954	0.703270	0.131908
14	1	0	-2.106394	1.443993	0.104381
15	1	0	2.166547	1.301275	0.128012
16	1	0	-0.557047	-1.076128	0.021746
17	7	0	1.313033	-0.586504	0.143651
18	7	0	-1.407930	-0.509658	0.049227
19	8	0	0.305622	7.090435	0.255672
20	6	0	-0.578498	7.882824	-0.524883
21	1	0	-0.338582	8.919142	-0.294668
22	1	0	-0.427555	7.703993	-1.593356
23	1	0	-1.621773	7.684522	-0.262571
24	6	0	2.562557	-1.209957	0.060307
25	6	0	2.739546	-2.411862	0.761584
26	6	0	3.609035	-0.713770	-0.732597
27	6	0	3.945146	-3.087117	0.710117
28	1	0	1.919516	-2.798359	1.355151
29	6	0	4.818417	-1.384806	-0.794576
30	1	0	3.465797	0.185398	-1.319662
31	6	0	4.970253	-2.559123	-0.067711
32	1	0	4.091421	-4.009193	1.256859
33	1	0	5.629157	-1.011382	-1.405918
34	6	0	-2.626827	-1.170533	0.034655
35	6	0	-2.601881	-2.562423	-0.157981
36	6	0	-3.856708	-0.516846	0.205084
37	6	0	-3.775035	-3.287387	-0.197113
38	1	0	-1.648658	-3.063194	-0.285607
39	6	0	-5.033997	-1.241396	0.163243
40	1	0	-3.909446	0.548616	0.380762
41	6	0	-4.983830	-2.615489	-0.040359
42	1	0	-3.757767	-4.357840	-0.352015
43	1	0	-5.985836	-0.743780	0.293370
44	7	0	6.247324	-3.272160	-0.135490
45	8	0	6.363933	-4.302562	0.501127
46	8	0	7.132859	-2.799677	-0.823470
47	7	0	-6.229847	-3.371582	-0.089213
48	8	0	-7.277060	-2.766437	0.054943
49	8	0	-6.166862	-4.573785	-0.274438

Structure 41a (C_2H_5OH)

Energy (Hartrees): -1443.93962684
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.687213	3.322234	-0.748875
2	6	0	-2.075082	4.660845	-0.722065
3	6	0	-1.392657	5.555904	0.099356
4	6	0	-0.335301	5.098776	0.890901
5	6	0	0.029889	3.763602	0.861375
6	6	0	-0.633704	2.846175	0.033216
7	1	0	-2.213785	2.645089	-1.413974
8	1	0	-2.894034	4.986962	-1.349594
9	1	0	0.177804	5.802224	1.537243
10	1	0	0.832598	3.423485	1.507616
11	6	0	-0.235507	1.416704	-0.015060
12	6	0	1.092317	1.089784	-0.007199
13	6	0	-1.284419	0.422636	-0.048807
14	1	0	1.824449	1.888302	0.013784
15	1	0	-2.307901	0.802591	0.033766
16	1	0	0.878792	-0.914955	-0.083834
17	7	0	-1.071221	-0.844880	-0.167696
18	7	0	1.580402	-0.174472	-0.032624
19	8	0	-1.687326	6.881255	0.198786
20	6	0	-2.757786	7.380483	-0.593872
21	1	0	-2.824529	8.443638	-0.370791
22	1	0	-2.552453	7.243449	-1.659169
23	1	0	-3.700062	6.891925	-0.330873
24	6	0	-2.159556	-1.719327	-0.080516
25	6	0	-2.187532	-2.831396	-0.934846
26	6	0	-3.182411	-1.547690	0.865078
27	6	0	-3.232733	-3.734436	-0.878288
28	1	0	-1.386346	-2.967094	-1.651536
29	6	0	-4.231749	-2.447792	0.932971
30	1	0	-3.138036	-0.722481	1.565926
31	6	0	-4.243319	-3.525223	0.055377
32	1	0	-3.267979	-4.586353	-1.544357
33	1	0	-5.020357	-2.325520	1.663799
34	6	0	2.912639	-0.553914	-0.019997
35	6	0	3.187538	-1.932893	-0.056501
36	6	0	3.975164	0.362683	0.030200
37	6	0	4.487645	-2.391043	-0.041963
38	1	0	2.363879	-2.637344	-0.094844
39	6	0	5.279407	-0.094033	0.043352
40	1	0	3.801633	1.429280	0.059259
41	6	0	5.524612	-1.462588	0.007636
42	1	0	4.698987	-3.451804	-0.069546
43	1	0	6.102643	0.607136	0.082937
44	7	0	-5.346664	-4.477845	0.124843
45	8	0	-5.302575	-5.469102	-0.580619
46	8	0	-6.268434	-4.241405	0.884508
47	7	0	6.897619	-1.934462	0.021623
48	8	0	7.796287	-1.110535	0.038379
49	8	0	7.099834	-3.136947	0.015488

Structure 41b (vacuum)

Energy (Hartrees): -1443.89916485
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.407378	3.169581	-0.821601
2	6	0	0.159118	4.540157	-0.789612
3	6	0	-0.710134	5.058933	0.169049
4	6	0	-1.313138	4.199072	1.092561
5	6	0	-1.050027	2.842424	1.051631
6	6	0	-0.188502	2.296859	0.086616
7	1	0	1.074599	2.774077	-1.580534
8	1	0	0.640541	5.182054	-1.514757
9	1	0	-1.970586	4.625314	1.840352
10	1	0	-1.497801	2.189027	1.793851
11	6	0	0.097131	0.842641	0.043940
12	6	0	-0.876858	-0.098006	0.011638
13	6	0	1.488966	0.402525	0.013828
14	1	0	2.236460	1.191129	0.169799
15	1	0	-0.585670	-1.141528	-0.000686
16	7	0	1.841745	-0.809333	-0.189422
17	7	0	-2.214199	0.167825	-0.065639
18	1	0	-2.476462	1.133377	-0.220660
19	8	0	-1.026803	6.370090	0.287641
20	6	0	-0.417198	7.280854	-0.605821
21	1	0	-0.688890	7.058365	-1.642248
22	1	0	-0.793913	8.264383	-0.335688
23	1	0	0.671896	7.265872	-0.500514
24	6	0	-3.245327	-0.760885	-0.032903
25	6	0	-4.530333	-0.340554	-0.409521
26	6	0	-3.046172	-2.087001	0.375688
27	6	0	-5.592035	-1.223610	-0.393204
28	1	0	-4.685422	0.684391	-0.727006
29	6	0	-4.107507	-2.975509	0.383378
30	1	0	-2.074505	-2.425909	0.707331
31	6	0	-5.365751	-2.536774	-0.001648
32	1	0	-6.586650	-0.914884	-0.685085
33	1	0	-3.974021	-4.002191	0.696838
34	6	0	3.197212	-1.142555	-0.099080
35	6	0	4.031941	-0.647856	0.912893
36	6	0	3.714988	-2.048502	-1.034968
37	6	0	5.366449	-1.018900	0.966709
38	1	0	3.622621	0.005450	1.674013
39	6	0	5.047849	-2.415583	-0.996694
40	1	0	3.050680	-2.444346	-1.792749
41	6	0	5.854995	-1.890362	0.004982
42	1	0	6.026810	-0.653018	1.741350
43	1	0	5.469647	-3.102198	-1.718221
44	7	0	-6.488508	-3.482504	0.012598
45	8	0	-6.260202	-4.620954	0.363949
46	8	0	-7.576447	-3.067763	-0.329051
47	7	0	7.272429	-2.285127	0.057979
48	8	0	7.950304	-1.830145	0.955318
49	8	0	7.678413	-3.039614	-0.800502

Structure 41b ($CHCl_3$)

Energy (Hartrees): -1443.93767487
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.432810	3.158672	-0.803054
2	6	0	0.188961	4.530403	-0.771025
3	6	0	-0.692747	5.049075	0.177244
4	6	0	-1.311719	4.188511	1.090032
5	6	0	-1.055077	2.829613	1.047566
6	6	0	-0.181395	2.284470	0.093396
7	1	0	1.112235	2.765466	-1.552822
8	1	0	0.682676	5.173472	-1.487364
9	1	0	-1.982283	4.609295	1.830354
10	1	0	-1.524101	2.177253	1.777669
11	6	0	0.097511	0.827815	0.047978
12	6	0	-0.882699	-0.111381	0.018471
13	6	0	1.485544	0.388838	0.018590
14	1	0	2.230918	1.172021	0.200730
15	1	0	-0.602735	-1.158391	0.019363
16	7	0	1.847635	-0.818362	-0.219317
17	7	0	-2.214944	0.160845	-0.062483
18	1	0	-2.480936	1.124819	-0.234437
19	8	0	-1.006113	6.362102	0.291643
20	6	0	-0.398890	7.270157	-0.614736
21	1	0	-0.669794	7.035784	-1.648297
22	1	0	-0.782325	8.254750	-0.354630
23	1	0	0.689522	7.265233	-0.506444
24	6	0	-3.250027	-0.760386	-0.026493
25	6	0	-4.524396	-0.335656	-0.438645
26	6	0	-3.069134	-2.079328	0.416883
27	6	0	-5.592673	-1.208766	-0.425912
28	1	0	-4.661576	0.684447	-0.779714
29	6	0	-4.137319	-2.957768	0.422949
30	1	0	-2.107910	-2.420347	0.777163
31	6	0	-5.385223	-2.517172	-0.000580
32	1	0	-6.574381	-0.888810	-0.748450
33	1	0	-4.009516	-3.976008	0.765467
34	6	0	3.201873	-1.147390	-0.119078
35	6	0	4.027670	-0.660016	0.905801
36	6	0	3.730929	-2.044855	-1.059269
37	6	0	5.361217	-1.029077	0.968313
38	1	0	3.613798	-0.010403	1.667682
39	6	0	5.062714	-2.412145	-1.011586
40	1	0	3.078824	-2.435923	-1.830828
41	6	0	5.860906	-1.893582	0.002951
42	1	0	6.005818	-0.662708	1.756251
43	1	0	5.482525	-3.092888	-1.740188
44	7	0	-6.508694	-3.448879	0.007703
45	8	0	-6.306113	-4.589640	0.378833
46	8	0	-7.594892	-3.040016	-0.357759
47	7	0	7.271405	-2.283871	0.064985
48	8	0	7.956199	-1.818964	0.955666
49	8	0	7.690719	-3.051655	-0.779194

Structure 41b (DMSO)

Energy (Hartrees): -1443.93521558
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.497655	3.187022	-0.779690
2	6	0	0.281014	4.563191	-0.738932
3	6	0	-0.635824	5.087678	0.173154
4	6	0	-1.316761	4.225943	1.040035
5	6	0	-1.085681	2.862369	0.990531
6	6	0	-0.176624	2.312309	0.072655
7	1	0	1.205599	2.791610	-1.501537
8	1	0	0.824432	5.204223	-1.420447
9	1	0	-2.016014	4.645859	1.754181
10	1	0	-1.604062	2.213550	1.689586
11	6	0	0.085763	0.853483	0.023485
12	6	0	-0.899050	-0.083723	-0.002782
13	6	0	1.469471	0.404233	-0.002950
14	1	0	2.220498	1.177540	0.194245
15	1	0	-0.621442	-1.131334	0.007775
16	7	0	1.823680	-0.804217	-0.255837
17	7	0	-2.229749	0.184355	-0.086645
18	1	0	-2.505529	1.145728	-0.263062
19	8	0	-0.924564	6.405270	0.292312
20	6	0	-0.232533	7.310638	-0.557267
21	1	0	-0.447889	7.106628	-1.609873
22	1	0	-0.597168	8.302950	-0.299350
23	1	0	0.846604	7.264800	-0.385394
24	6	0	-3.259232	-0.741387	-0.038015
25	6	0	-4.540313	-0.321579	-0.435732
26	6	0	-3.067026	-2.060264	0.402796
27	6	0	-5.603207	-1.200688	-0.414302
28	1	0	-4.685795	0.698917	-0.772350
29	6	0	-4.129836	-2.944430	0.416861
30	1	0	-2.101156	-2.398293	0.753638
31	6	0	-5.384849	-2.509735	0.006367
32	1	0	-6.588454	-0.881646	-0.727331
33	1	0	-3.988896	-3.961574	0.757607
34	6	0	3.172416	-1.149453	-0.143288
35	6	0	4.001010	-0.663347	0.880784
36	6	0	3.692580	-2.067332	-1.069531
37	6	0	5.326003	-1.058396	0.958629
38	1	0	3.596622	0.006319	1.630420
39	6	0	5.016013	-2.460885	-1.006505
40	1	0	3.041341	-2.456971	-1.842847
41	6	0	5.816058	-1.947196	0.009499
42	1	0	5.968951	-0.691308	1.747752
43	1	0	5.424333	-3.158829	-1.725445
44	7	0	-6.501776	-3.445890	0.026052
45	8	0	-6.287093	-4.592513	0.376776
46	8	0	-7.599693	-3.039180	-0.310184
47	7	0	7.214022	-2.371175	0.092555
48	8	0	7.895073	-1.933296	1.001176
49	8	0	7.631589	-3.141578	-0.751986

Structure 41b (C_2H_5OH)

Energy (Hartrees): -1443.93607795
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.491995	3.152556	-0.795357
2	6	0	0.280697	4.529511	-0.756074
3	6	0	-0.611824	5.058641	0.175575
4	6	0	-1.276813	4.205905	1.061867
5	6	0	-1.052237	2.841000	1.012562
6	6	0	-0.165854	2.285090	0.076901
7	1	0	1.182283	2.750847	-1.530817
8	1	0	0.808714	5.166660	-1.453121
9	1	0	-1.957609	4.633150	1.789695
10	1	0	-1.557034	2.195830	1.724834
11	6	0	0.090344	0.824629	0.029506
12	6	0	-0.900995	-0.104703	0.002824
13	6	0	1.472447	0.371719	0.003639
14	1	0	2.224156	1.144515	0.199616
15	1	0	-0.635345	-1.155321	0.013026
16	7	0	1.826504	-0.836970	-0.249515
17	7	0	-2.229341	0.178898	-0.085800
18	1	0	-2.491418	1.143602	-0.265666
19	8	0	-0.892833	6.383056	0.296815
20	6	0	-0.208550	7.286760	-0.563483
21	1	0	-0.442016	7.082345	-1.611767
22	1	0	-0.565736	8.279852	-0.297982
23	1	0	0.872043	7.233412	-0.404787
24	6	0	-3.269338	-0.733260	-0.039278
25	6	0	-4.541177	-0.301649	-0.455187
26	6	0	-3.097717	-2.049500	0.418982
27	6	0	-5.614556	-1.166315	-0.435785
28	1	0	-4.670297	0.716571	-0.804965
29	6	0	-4.171073	-2.919618	0.433225
30	1	0	-2.139686	-2.394345	0.784597
31	6	0	-5.416695	-2.473422	0.003668
32	1	0	-6.592026	-0.837733	-0.763061
33	1	0	-4.046133	-3.933792	0.788835
34	6	0	3.176497	-1.176154	-0.137434
35	6	0	3.997091	-0.695598	0.895906
36	6	0	3.706850	-2.078587	-1.073262
37	6	0	5.325850	-1.075734	0.971322
38	1	0	3.583112	-0.040891	1.653495
39	6	0	5.034056	-2.457702	-1.013504
40	1	0	3.061508	-2.465494	-1.852836
41	6	0	5.826798	-1.945714	0.009830
42	1	0	5.962897	-0.711658	1.766725
43	1	0	5.451219	-3.142205	-1.740428
44	7	0	-6.541500	-3.391134	0.022453
45	8	0	-6.357601	-4.531368	0.413684
46	8	0	-7.628501	-2.986632	-0.354320
47	7	0	7.226850	-2.346535	0.084027
48	8	0	7.909043	-1.909842	0.993554
49	8	0	7.659768	-3.100500	-0.768761

Structure 41c (vacuum)

Energy (Hartrees): -1443.90018400
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.664834	2.576886	-0.817813
2	6	0	0.592705	3.966538	-0.831225
3	6	0	-0.171657	4.627269	0.130372
4	6	0	-0.849652	3.887354	1.102879
5	6	0	-0.768258	2.506147	1.102450
6	6	0	-0.017867	1.824109	0.134467
7	1	0	1.270967	2.071147	-1.559453
8	1	0	1.135921	4.515076	-1.588465
9	1	0	-1.418725	4.420729	1.854212
10	1	0	-1.276194	1.943012	1.879347
11	6	0	0.040479	0.342547	0.126698
12	6	0	-1.077543	-0.423248	0.093169
13	6	0	1.313214	-0.358579	0.120919
14	1	0	-0.989251	-1.502987	0.102426
15	1	0	1.253727	-1.456276	0.107410
16	7	0	2.440603	0.238975	0.148642
17	7	0	-2.350326	0.068457	0.000840
18	1	0	-2.431038	1.069267	-0.131149
19	8	0	-0.310955	5.972551	0.206886
20	6	0	0.374786	6.763696	-0.743431
21	1	0	0.039812	6.537900	-1.760540
22	1	0	0.134126	7.796835	-0.504232
23	1	0	1.456521	6.615039	-0.672194
24	6	0	-3.532081	-0.656715	-0.000461
25	6	0	-4.718982	0.020864	-0.322957
26	6	0	-3.586085	-2.020787	0.319752
27	6	0	-5.928999	-0.643196	-0.335795
28	1	0	-4.680174	1.075795	-0.570290
29	6	0	-4.797949	-2.690151	0.298640
30	1	0	-2.695747	-2.563349	0.605620
31	6	0	-5.953875	-1.998110	-0.029607
32	1	0	-6.849451	-0.132120	-0.583635
33	1	0	-4.858361	-3.741976	0.544309
34	6	0	3.609542	-0.525240	0.079049
35	6	0	4.668911	-0.195697	0.935036
36	6	0	3.773435	-1.560602	-0.852025
37	6	0	5.850976	-0.913038	0.897694
38	1	0	4.536618	0.623058	1.630835
39	6	0	4.959541	-2.275976	-0.906280
40	1	0	2.977530	-1.779700	-1.553783
41	6	0	5.977068	-1.945138	-0.024624
42	1	0	6.675396	-0.684754	1.559590
43	1	0	5.109443	-3.072852	-1.622114
44	7	0	-7.235957	-2.712544	-0.045481
45	8	0	-7.223438	-3.896379	0.219697
46	8	0	-8.229889	-2.075180	-0.324212
47	7	0	7.238871	-2.701099	-0.079199
48	8	0	7.327221	-3.590791	-0.899299
49	8	0	8.114723	-2.390693	0.700310

Structure 41c ($CHCl_3$)

Energy (Hartrees): -1443.94031593
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.638153	2.561852	-0.857135
2	6	0	0.588434	3.952998	-0.872857
3	6	0	-0.122779	4.627861	0.120582
4	6	0	-0.771668	3.900321	1.122577
5	6	0	-0.712539	2.516709	1.123674
6	6	0	-0.012430	1.820951	0.128300
7	1	0	1.196606	2.046487	-1.630403
8	1	0	1.105739	4.491736	-1.655474
9	1	0	-1.305704	4.439083	1.896782
10	1	0	-1.205028	1.964901	1.918643
11	6	0	0.033094	0.337240	0.127172
12	6	0	-1.089874	-0.428640	0.108378
13	6	0	1.296354	-0.370687	0.126958
14	1	0	-1.000699	-1.508588	0.131773
15	1	0	1.230687	-1.465367	0.096536
16	7	0	2.431648	0.221317	0.181701
17	7	0	-2.357633	0.065273	0.028272
18	1	0	-2.450705	1.068653	-0.089242
19	8	0	-0.235586	5.976272	0.196382
20	6	0	0.423643	6.753875	-0.791393
21	1	0	0.039905	6.529166	-1.790985
22	1	0	0.208584	7.792647	-0.548354
23	1	0	1.504741	6.590137	-0.764786
24	6	0	-3.540338	-0.655405	0.018068
25	6	0	-4.728480	0.049761	-0.239544
26	6	0	-3.595629	-2.036143	0.261582
27	6	0	-5.942919	-0.603563	-0.262284
28	1	0	-4.683807	1.117130	-0.425048
29	6	0	-4.812224	-2.693873	0.233587
30	1	0	-2.702566	-2.601827	0.488530
31	6	0	-5.971579	-1.975434	-0.030408
32	1	0	-6.859180	-0.064155	-0.462138
33	1	0	-4.864619	-3.757857	0.422635
34	6	0	3.596183	-0.545003	0.104252
35	6	0	4.681475	-0.181897	0.916484
36	6	0	3.738127	-1.613025	-0.795736
37	6	0	5.865836	-0.893384	0.868515
38	1	0	4.570876	0.659218	1.589970
39	6	0	4.924335	-2.324751	-0.860090
40	1	0	2.922719	-1.864434	-1.463276
41	6	0	5.968788	-1.958193	-0.021188
42	1	0	6.703845	-0.629999	1.500059
43	1	0	5.047220	-3.144613	-1.555209
44	7	0	-7.251792	-2.675368	-0.056710
45	8	0	-7.252429	-3.878495	0.125407
46	8	0	-8.257848	-2.022248	-0.260156
47	7	0	7.224765	-2.707848	-0.087135
48	8	0	7.315269	-3.604213	-0.904098
49	8	0	8.116681	-2.400734	0.679981

Structure 41c (DMSO)

Energy (Hartrees): -1443.93960096
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.645601	2.582954	-0.858316
2	6	0	0.607800	3.974859	-0.872357
3	6	0	-0.101337	4.654243	0.120626
4	6	0	-0.760967	3.928506	1.117564
5	6	0	-0.712830	2.543936	1.117078
6	6	0	-0.011941	1.844419	0.125037
7	1	0	1.197308	2.064810	-1.635139
8	1	0	1.128643	4.509560	-1.655608
9	1	0	-1.299776	4.466505	1.889192
10	1	0	-1.218846	1.995956	1.906150
11	6	0	0.029766	0.360820	0.121400
12	6	0	-1.093213	-0.408544	0.097065
13	6	0	1.286824	-0.351609	0.126183
14	1	0	-0.996143	-1.487823	0.115627
15	1	0	1.213621	-1.444507	0.082294
16	7	0	2.429012	0.232065	0.202338
17	7	0	-2.359850	0.079412	0.019878
18	1	0	-2.466163	1.083538	-0.088606
19	8	0	-0.201401	6.002649	0.197321
20	6	0	0.467088	6.770620	-0.794604
21	1	0	0.081643	6.545927	-1.793265
22	1	0	0.263614	7.812789	-0.556198
23	1	0	1.546122	6.594411	-0.768315
24	6	0	-3.537198	-0.650115	0.010170
25	6	0	-4.729645	0.050354	-0.240409
26	6	0	-3.581979	-2.032440	0.248235
27	6	0	-5.940437	-0.609499	-0.259806
28	1	0	-4.689468	1.118319	-0.423039
29	6	0	-4.794913	-2.696366	0.223067
30	1	0	-2.684645	-2.594487	0.467584
31	6	0	-5.960363	-1.982783	-0.031306
32	1	0	-6.858855	-0.071701	-0.454360
33	1	0	-4.836380	-3.761357	0.409286
34	6	0	3.584380	-0.546789	0.120477
35	6	0	4.676161	-0.201140	0.932845
36	6	0	3.713395	-1.612699	-0.785292
37	6	0	5.853233	-0.924099	0.877991
38	1	0	4.579338	0.635481	1.614426
39	6	0	4.891675	-2.335878	-0.856004
40	1	0	2.893570	-1.856463	-1.450469
41	6	0	5.943614	-1.984946	-0.018492
42	1	0	6.692807	-0.669080	1.511173
43	1	0	4.999261	-3.154024	-1.555676
44	7	0	-7.235512	-2.688084	-0.050075
45	8	0	-7.229731	-3.895075	0.115073
46	8	0	-8.249978	-2.038084	-0.229240
47	7	0	7.190441	-2.745557	-0.093614
48	8	0	7.272619	-3.635455	-0.920240
49	8	0	8.088169	-2.455978	0.675628

Structure 41c (C_2H_5OH)

Energy (Hartrees): -1443.94018740
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.602060	2.596349	-0.886400
2	6	0	0.553776	3.987989	-0.892148
3	6	0	-0.127329	4.654161	0.127542
4	6	0	-0.747366	3.921638	1.143215
5	6	0	-0.688703	2.537343	1.134661
6	6	0	-0.016162	1.849290	0.115651
7	1	0	1.130575	2.085598	-1.684217
8	1	0	1.045235	4.531522	-1.688234
9	1	0	-1.263799	4.453898	1.934303
10	1	0	-1.163811	1.981025	1.937047
11	6	0	0.035034	0.365808	0.102814
12	6	0	-1.083389	-0.408525	0.081548
13	6	0	1.296366	-0.339227	0.101661
14	1	0	-0.982342	-1.487478	0.093124
15	1	0	1.229664	-1.432063	0.048719
16	7	0	2.435286	0.248894	0.188207
17	7	0	-2.353450	0.075964	0.015403
18	1	0	-2.462580	1.080754	-0.083843
19	8	0	-0.237277	6.006381	0.214109
20	6	0	0.400945	6.788709	-0.788641
21	1	0	-0.009922	6.568284	-1.777722
22	1	0	0.194858	7.826710	-0.534554
23	1	0	1.480897	6.618454	-0.787868
24	6	0	-3.526808	-0.657426	0.011853
25	6	0	-4.725518	0.039528	-0.221387
26	6	0	-3.562370	-2.042349	0.239678
27	6	0	-5.932235	-0.626128	-0.238171
28	1	0	-4.692769	1.109374	-0.394321
29	6	0	-4.770701	-2.712648	0.217801
30	1	0	-2.660644	-2.601463	0.447886
31	6	0	-5.942120	-2.002554	-0.022990
32	1	0	-6.854883	-0.090989	-0.420149
33	1	0	-4.804389	-3.779420	0.395457
34	6	0	3.591603	-0.527983	0.107728
35	6	0	4.665427	-0.210984	0.954742
36	6	0	3.736748	-1.566180	-0.827592
37	6	0	5.839320	-0.938069	0.906248
38	1	0	4.555995	0.604792	1.659205
39	6	0	4.912003	-2.293923	-0.892408
40	1	0	2.931190	-1.783742	-1.518985
41	6	0	5.944705	-1.973833	-0.018482
42	1	0	6.664452	-0.706595	1.566757
43	1	0	5.031269	-3.091629	-1.613752
44	7	0	-7.207489	-2.713470	-0.044742
45	8	0	-7.199985	-3.922018	0.118633
46	8	0	-8.230367	-2.075081	-0.226746
47	7	0	7.183631	-2.738976	-0.081965
48	8	0	7.277159	-3.625514	-0.912332
49	8	0	8.077151	-2.463747	0.698994

Structure 41d (vacuum)

Energy (Hartrees): -1443.89284103
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.277997	2.965815	0.878346
2	6	0	1.538759	4.312907	1.022714
3	6	0	0.842088	5.254262	0.256562
4	6	0	-0.112022	4.823790	-0.660863
5	6	0	-0.362629	3.458577	-0.796314
6	6	0	0.307414	2.510712	-0.027818
7	1	0	1.827699	2.251325	1.477676
8	1	0	2.279944	4.671681	1.726242
9	1	0	-0.651908	5.524660	-1.282695
10	1	0	-1.082342	3.130645	-1.538756
11	6	0	-0.028155	1.072867	-0.138552
12	6	0	-1.328308	0.697635	-0.226406
13	6	0	1.014977	0.054249	-0.127869
14	1	0	0.685029	-0.981587	0.032403
15	1	0	-1.172316	-1.190887	-1.027546
16	1	0	-2.106423	1.442592	-0.094910
17	7	0	2.256800	0.314520	-0.268602
18	7	0	-1.786494	-0.567033	-0.527180
19	8	0	1.169407	6.551972	0.473336
20	6	0	0.495219	7.535792	-0.283581
21	1	0	0.895371	8.493236	0.041871
22	1	0	0.682715	7.406758	-1.354091
23	1	0	-0.582666	7.508902	-0.095054
24	6	0	3.173745	-0.734862	-0.133777
25	6	0	4.234008	-0.810391	-1.046152
26	6	0	3.089548	-1.670672	0.906319
27	6	0	5.162012	-1.832760	-0.957997
28	1	0	4.303976	-0.060748	-1.824232
29	6	0	4.023160	-2.690154	1.010869
30	1	0	2.308051	-1.575736	1.650846
31	6	0	5.038819	-2.759761	0.070035
32	1	0	5.978809	-1.920344	-1.661583
33	1	0	3.979782	-3.419805	1.808207
34	6	0	-3.081414	-1.019026	-0.316756
35	6	0	-3.506419	-2.180217	-0.980807
36	6	0	-3.963762	-0.355094	0.546177
37	6	0	-4.789245	-2.659403	-0.804984
38	1	0	-2.823973	-2.697509	-1.645861
39	6	0	-5.255720	-0.826521	0.712106
40	1	0	-3.637571	0.507805	1.111249
41	6	0	-5.654014	-1.968771	0.034910
42	1	0	-5.132648	-3.550939	-1.312136
43	1	0	-5.952060	-0.330296	1.374828
44	7	0	-7.021972	-2.470297	0.220461
45	8	0	-7.752708	-1.848306	0.962408
46	8	0	-7.336844	-3.475312	-0.381458
47	7	0	6.030169	-3.844232	0.172840
48	8	0	6.911946	-3.879904	-0.658704
49	8	0	5.902533	-4.637737	1.081161

Structure 41d ($CHCl_3$)

Energy (Hartrees): -1443.93393649
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.264827	2.963323	0.881256
2	6	0	1.518425	4.314015	1.022877
3	6	0	0.814464	5.250216	0.256161
4	6	0	-0.141326	4.812085	-0.657142
5	6	0	-0.382662	3.444451	-0.790981
6	6	0	0.297800	2.499507	-0.025336
7	1	0	1.815337	2.254829	1.488153
8	1	0	2.258675	4.673793	1.728241
9	1	0	-0.690585	5.510086	-1.274977
10	1	0	-1.109299	3.111999	-1.525075
11	6	0	-0.025728	1.056987	-0.138001
12	6	0	-1.329510	0.676127	-0.211836
13	6	0	1.022024	0.049797	-0.137919
14	1	0	0.700406	-0.989424	-0.000256
15	1	0	-1.170548	-1.232556	-0.966876
16	1	0	-2.105473	1.421312	-0.069187
17	7	0	2.266951	0.320926	-0.269334
18	7	0	-1.790376	-0.583151	-0.500225
19	8	0	1.132656	6.551610	0.467766
20	6	0	0.435601	7.531325	-0.284651
21	1	0	0.826438	8.494090	0.039027
22	1	0	0.617283	7.407165	-1.356314
23	1	0	-0.639313	7.491322	-0.084326
24	6	0	3.188735	-0.723078	-0.137903
25	6	0	4.287198	-0.753199	-1.009213
26	6	0	3.075126	-1.699469	0.863867
27	6	0	5.225251	-1.765496	-0.919803
28	1	0	4.382620	0.020990	-1.760959
29	6	0	4.015622	-2.710801	0.968919
30	1	0	2.262111	-1.645902	1.578333
31	6	0	5.072082	-2.732923	0.068442
32	1	0	6.068187	-1.809049	-1.596660
33	1	0	3.939088	-3.466220	1.739750
34	6	0	-3.087676	-1.026908	-0.299983
35	6	0	-3.490432	-2.214408	-0.934204
36	6	0	-3.992907	-0.338605	0.521763
37	6	0	-4.772974	-2.695354	-0.770872
38	1	0	-2.788110	-2.747904	-1.565011
39	6	0	-5.283007	-0.814479	0.678363
40	1	0	-3.690751	0.548970	1.061741
41	6	0	-5.660660	-1.983417	0.030603
42	1	0	-5.090604	-3.605797	-1.261346
43	1	0	-5.988237	-0.293786	1.312510
44	7	0	-7.020445	-2.485859	0.205241
45	8	0	-7.778900	-1.854552	0.916578
46	8	0	-7.330059	-3.511630	-0.370834
47	7	0	6.066199	-3.804961	0.169280
48	8	0	6.966202	-3.829613	-0.647264
49	8	0	5.940705	-4.619663	1.062760

Structure 41d (DMSO)

Energy (Hartrees): -1443.93380009
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.278869	2.958373	0.898354
2	6	0	1.547100	4.309262	1.017549
3	6	0	0.848957	5.240995	0.238892
4	6	0	-0.116787	4.796278	-0.661801
5	6	0	-0.371916	3.428691	-0.773337
6	6	0	0.304680	2.488345	0.002147
7	1	0	1.821691	2.254791	1.518728
8	1	0	2.292594	4.669445	1.717592
9	1	0	-0.665962	5.488852	-1.286035
10	1	0	-1.110400	3.093439	-1.494372
11	6	0	-0.025478	1.045552	-0.088754
12	6	0	-1.333612	0.668152	-0.142345
13	6	0	1.020165	0.039855	-0.097900
14	1	0	0.706559	-0.997231	0.063948
15	1	0	-1.167433	-1.262033	-0.828029
16	1	0	-2.104339	1.419424	-0.004211
17	7	0	2.262654	0.311065	-0.271797
18	7	0	-1.797014	-0.590841	-0.404224
19	8	0	1.179792	6.541710	0.426204
20	6	0	0.475482	7.514114	-0.333276
21	1	0	0.871093	8.480506	-0.026637
22	1	0	0.645461	7.374774	-1.404675
23	1	0	-0.597254	7.477924	-0.122656
24	6	0	3.187204	-0.730523	-0.144956
25	6	0	4.261299	-0.781433	-1.045923
26	6	0	3.101993	-1.684886	0.881043
27	6	0	5.201997	-1.791484	-0.961337
28	1	0	4.336623	-0.027368	-1.820358
29	6	0	4.045027	-2.693841	0.980973
30	1	0	2.306208	-1.619685	1.613645
31	6	0	5.077072	-2.736749	0.052288
32	1	0	6.023412	-1.847322	-1.663353
33	1	0	3.985423	-3.431890	1.770057
34	6	0	-3.102764	-1.021613	-0.237464
35	6	0	-3.482395	-2.228137	-0.851057
36	6	0	-4.037370	-0.306906	0.527674
37	6	0	-4.771648	-2.701360	-0.725521
38	1	0	-2.754489	-2.781588	-1.433920
39	6	0	-5.333258	-0.776614	0.647217
40	1	0	-3.756164	0.596987	1.051649
41	6	0	-5.688864	-1.964086	0.019082
42	1	0	-5.068261	-3.626128	-1.202111
43	1	0	-6.059356	-0.233447	1.237503
44	7	0	-7.054213	-2.457397	0.153567
45	8	0	-7.836908	-1.812328	0.828077
46	8	0	-7.350412	-3.492454	-0.416229
47	7	0	6.074266	-3.803808	0.150139
48	8	0	6.959385	-3.840876	-0.684095
49	8	0	5.970671	-4.605366	1.059812

Structure 41d (C_2H_5OH)

Energy (Hartrees): -1443.93433898
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.274054	2.959723	0.909481
2	6	0	1.544403	4.310412	1.027343
3	6	0	0.853904	5.238896	0.239956
4	6	0	-0.104998	4.796913	-0.667689
5	6	0	-0.362481	3.429803	-0.777562
6	6	0	0.305945	2.490857	0.006676
7	1	0	1.810507	2.256104	1.535574
8	1	0	2.285173	4.672339	1.731820
9	1	0	-0.645984	5.490200	-1.298291
10	1	0	-1.094494	3.093496	-1.504770
11	6	0	-0.025679	1.048508	-0.083919
12	6	0	-1.333083	0.672926	-0.143029
13	6	0	1.019452	0.041511	-0.090206
14	1	0	0.706227	-0.992847	0.089131
15	1	0	-1.167639	-1.252860	-0.846069
16	1	0	-2.104395	1.423970	-0.007319
17	7	0	2.259850	0.308481	-0.283114
18	7	0	-1.796026	-0.586442	-0.412881
19	8	0	1.187443	6.544622	0.427073
20	6	0	0.492576	7.519490	-0.341132
21	1	0	0.890734	8.484056	-0.031983
22	1	0	0.672697	7.375002	-1.409888
23	1	0	-0.581131	7.486021	-0.136904
24	6	0	3.182466	-0.733876	-0.153344
25	6	0	4.235440	-0.812352	-1.077180
26	6	0	3.115464	-1.661748	0.897976
27	6	0	5.173519	-1.823725	-0.988258
28	1	0	4.296213	-0.078548	-1.872041
29	6	0	4.055300	-2.672394	1.002505
30	1	0	2.336959	-1.573185	1.646641
31	6	0	5.066470	-2.742716	0.051965
32	1	0	5.977606	-1.900692	-1.708190
33	1	0	4.010476	-3.389247	1.811835
34	6	0	-3.099647	-1.018412	-0.243232
35	6	0	-3.483288	-2.220281	-0.864626
36	6	0	-4.029863	-0.308899	0.533006
37	6	0	-4.771441	-2.693371	-0.736824
38	1	0	-2.759099	-2.769646	-1.456000
39	6	0	-5.324498	-0.778329	0.656453
40	1	0	-3.745068	0.590289	1.063176
41	6	0	-5.684088	-1.961067	0.019829
42	1	0	-5.070720	-3.613997	-1.219999
43	1	0	-6.046692	-0.238866	1.255009
44	7	0	-7.043537	-2.452786	0.157899
45	8	0	-7.823689	-1.822695	0.851473
46	8	0	-7.353418	-3.477027	-0.426602
47	7	0	6.057410	-3.808676	0.156017
48	8	0	6.951640	-3.852783	-0.669298
49	8	0	5.948672	-4.614222	1.062815

Structure 42a (vacuum)

Energy (Hartrees): -1353.92511389
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.368987	0.408364	-0.721154
2	6	0	4.739266	0.206257	-0.732959
3	6	0	5.261807	-0.857443	-0.011766
4	6	0	4.453488	-1.712437	0.723361
5	6	0	3.087099	-1.486875	0.737027
6	6	0	2.512926	-0.432321	0.008735
7	1	0	2.951856	1.212270	-1.315776
8	1	0	5.401866	0.843852	-1.302690
9	1	0	4.902179	-2.519714	1.286539
10	1	0	2.456110	-2.119253	1.350592
11	6	0	1.056143	-0.210362	0.004022
12	6	0	0.210585	-1.294475	0.005263
13	6	0	0.551667	1.145262	0.002718
14	1	0	0.631666	-2.295060	-0.006603
15	1	0	1.302978	1.942130	0.047552
16	1	0	-1.509518	-0.278647	0.051795
17	7	0	-0.700938	1.438625	-0.026004
18	7	0	-1.128075	-1.228290	0.011901
19	6	0	-1.091968	2.790141	0.063808
20	6	0	-2.194161	3.208784	-0.676605
21	6	0	-0.453111	3.721235	0.894834
22	6	0	-2.633899	4.528570	-0.636418
23	1	0	-2.700406	2.486385	-1.306169
24	6	0	-0.889409	5.032626	0.950493
25	1	0	0.368973	3.405174	1.526931
26	6	0	-1.976741	5.448970	0.178715
27	1	0	-3.484859	4.819182	-1.237509
28	1	0	-0.412487	5.756716	1.599706
29	6	0	-1.998504	-2.333404	-0.054130
30	6	0	-3.264375	-2.227215	0.511619
31	6	0	-1.637008	-3.527079	-0.687321
32	6	0	-4.160415	-3.291213	0.466866
33	1	0	-3.550188	-1.305471	1.005926
34	6	0	-2.516572	-4.593634	-0.718356
35	1	0	-0.677388	-3.616518	-1.182081
36	6	0	-3.784021	-4.487324	-0.140905
37	1	0	-5.136321	-3.172729	0.917728
38	1	0	-2.250039	-5.522005	-1.207967
39	8	0	-4.573098	-5.588724	-0.230217
40	8	0	-2.327440	6.756288	0.301567
41	6	0	-5.861409	-5.519776	0.344184
42	1	0	-6.320021	-6.491308	0.175137
43	1	0	-5.803876	-5.326981	1.420166
44	1	0	-6.466374	-4.743252	-0.134746
45	6	0	-3.431550	7.212313	-0.450491
46	1	0	-3.543201	8.268050	-0.214097
47	1	0	-3.253399	7.097057	-1.524502
48	1	0	-4.346448	6.678602	-0.173692
49	7	0	6.715350	-1.083340	-0.023619
50	8	0	7.147130	-2.005479	0.636453
51	8	0	7.396107	-0.334738	-0.692982

Structure 42a ($CHCl_3$)

Energy (Hartrees): -1353.95968815
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.366491	0.136471	-0.678779
2	6	0	4.712434	-0.185425	-0.707176
3	6	0	5.143780	-1.313907	-0.021357
4	6	0	4.264131	-2.117070	0.693819
5	6	0	2.924166	-1.772729	0.723899
6	6	0	2.440611	-0.647601	0.032485
7	1	0	3.026761	0.995424	-1.244714
8	1	0	5.418086	0.415840	-1.264906
9	1	0	4.630626	-2.981453	1.231724
10	1	0	2.245298	-2.371858	1.318919
11	6	0	1.010016	-0.297894	0.045450
12	6	0	0.073230	-1.309108	0.054377
13	6	0	0.630935	1.096823	0.036329
14	1	0	0.407122	-2.341940	0.032837
15	1	0	1.451724	1.821160	0.058274
16	1	0	-1.569814	-0.162759	0.131315
17	7	0	-0.590838	1.505905	0.021399
18	7	0	-1.252782	-1.133214	0.072488
19	6	0	-0.843587	2.892307	0.093371
20	6	0	-1.915320	3.408473	-0.632286
21	6	0	-0.093252	3.769644	0.890652
22	6	0	-2.215244	4.768331	-0.613822
23	1	0	-2.511937	2.733042	-1.235666
24	6	0	-0.389827	5.121416	0.923971
25	1	0	0.708950	3.385060	1.510993
26	6	0	-1.445246	5.633271	0.164068
27	1	0	-3.045443	5.134060	-1.203533
28	1	0	0.180949	5.800923	1.546558
29	6	0	-2.209656	-2.165787	-0.021923
30	6	0	-3.457730	-1.981785	0.564876
31	6	0	-1.945901	-3.356740	-0.706124
32	6	0	-4.434217	-2.971526	0.491761
33	1	0	-3.667245	-1.057709	1.092890
34	6	0	-2.907095	-4.350439	-0.766837
35	1	0	-0.998911	-3.501047	-1.213119
36	6	0	-4.156343	-4.168920	-0.166881
37	1	0	-5.394143	-2.798565	0.960129
38	1	0	-2.713242	-5.275989	-1.296197
39	8	0	-5.030329	-5.201055	-0.284341
40	8	0	-1.653789	6.972833	0.257565
41	6	0	-6.308956	-5.052566	0.311157
42	1	0	-6.843074	-5.980045	0.114002
43	1	0	-6.226132	-4.905184	1.392173
44	1	0	-6.856828	-4.217020	-0.134962
45	6	0	-2.710362	7.528836	-0.506844
46	1	0	-2.701680	8.597478	-0.300470
47	1	0	-2.551243	7.364668	-1.576935
48	1	0	-3.676394	7.110631	-0.208244
49	7	0	6.563693	-1.665932	-0.051443
50	8	0	6.921986	-2.655728	0.558141
51	8	0	7.318097	-0.953111	-0.685526

Structure 42a (DMSO)

Energy (Hartrees): -1353.95597772
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.383234	0.580293	-0.647765
2	6	0	4.758912	0.428828	-0.670163
3	6	0	5.321311	-0.666747	-0.026281
4	6	0	4.541312	-1.600394	0.646245
5	6	0	3.169211	-1.426319	0.672721
6	6	0	2.555307	-0.342461	0.017483
7	1	0	2.944550	1.414276	-1.182388
8	1	0	5.386177	1.137678	-1.194352
9	1	0	5.005212	-2.435444	1.154290
10	1	0	2.568536	-2.132327	1.233725
11	6	0	1.092499	-0.176703	0.018986
12	6	0	0.292476	-1.302254	0.015034
13	6	0	0.538284	1.158307	0.021331
14	1	0	0.757855	-2.281853	-0.003502
15	1	0	1.254746	1.982820	0.091718
16	1	0	-1.479126	-0.367604	0.056599
17	7	0	-0.727068	1.401016	-0.033888
18	7	0	-1.043926	-1.292973	0.016275
19	6	0	-1.178664	2.733508	0.061655
20	6	0	-2.318928	3.093456	-0.655739
21	6	0	-0.569868	3.701405	0.875082
22	6	0	-2.825973	4.389790	-0.612187
23	1	0	-2.808326	2.345239	-1.270089
24	6	0	-1.073091	4.990278	0.934360
25	1	0	0.286530	3.436348	1.485359
26	6	0	-2.198385	5.348479	0.184474
27	1	0	-3.704806	4.632516	-1.195152
28	1	0	-0.611282	5.735985	1.571861
29	6	0	-1.884522	-2.422661	-0.030750
30	6	0	-3.215442	-2.264935	0.346125
31	6	0	-1.442113	-3.679379	-0.457433
32	6	0	-4.102446	-3.337233	0.315464
33	1	0	-3.563988	-1.290955	0.673736
34	6	0	-2.318580	-4.751228	-0.477761
35	1	0	-0.422928	-3.828272	-0.792464
36	6	0	-3.653053	-4.593283	-0.092116
37	1	0	-5.129451	-3.176812	0.615765
38	1	0	-1.981992	-5.726458	-0.810304
39	8	0	-4.431469	-5.702711	-0.153113
40	8	0	-2.614003	6.634655	0.304803
41	6	0	-5.801089	-5.558476	0.194246
42	1	0	-6.250702	-6.541568	0.068325
43	1	0	-5.913712	-5.239017	1.234239
44	1	0	-6.300825	-4.843716	-0.466172
45	6	0	-3.746782	7.031005	-0.454707
46	1	0	-3.905148	8.084937	-0.234114
47	1	0	-3.564662	6.908147	-1.526394
48	1	0	-4.635840	6.463316	-0.164724
49	7	0	6.771745	-0.842254	-0.056428
50	8	0	7.245331	-1.817002	0.498882
51	8	0	7.440422	-0.007117	-0.637758

Structure 42a (C_2H_5OH)

Energy (Hartrees): -1353.95809644
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.377829	0.517012	-0.650165
2	6	0	4.749561	0.340819	-0.677795
3	6	0	5.294642	-0.760356	-0.027100
4	6	0	4.501222	-1.676319	0.655754
5	6	0	3.133128	-1.478155	0.684710
6	6	0	2.536375	-0.387209	0.024512
7	1	0	2.951272	1.354332	-1.189470
8	1	0	5.386699	1.033914	-1.211203
9	1	0	4.951798	-2.515579	1.169219
10	1	0	2.521383	-2.168957	1.252805
11	6	0	1.077959	-0.194851	0.028247
12	6	0	0.258058	-1.305711	0.024734
13	6	0	0.549358	1.150551	0.027546
14	1	0	0.705565	-2.293604	0.010107
15	1	0	1.281723	1.960906	0.099484
16	1	0	-1.499435	-0.342722	0.056988
17	7	0	-0.710409	1.418870	-0.031326
18	7	0	-1.077962	-1.274207	0.020151
19	6	0	-1.130568	2.762216	0.062565
20	6	0	-2.245541	3.155950	-0.676504
21	6	0	-0.514751	3.707385	0.896310
22	6	0	-2.720797	4.464082	-0.632751
23	1	0	-2.739954	2.425637	-1.308133
24	6	0	-0.986460	5.008463	0.955371
25	1	0	0.320659	3.415636	1.523300
26	6	0	-2.085507	5.398045	0.184948
27	1	0	-3.580657	4.734298	-1.231737
28	1	0	-0.520422	5.738241	1.608368
29	6	0	-1.933023	-2.393359	-0.031322
30	6	0	-3.258614	-2.225395	0.359204
31	6	0	-1.507006	-3.649094	-0.476203
32	6	0	-4.156662	-3.288277	0.325610
33	1	0	-3.594423	-1.251584	0.700370
34	6	0	-2.394191	-4.712071	-0.499264
35	1	0	-0.492783	-3.803689	-0.823894
36	6	0	-3.721731	-4.542754	-0.098615
37	1	0	-5.179389	-3.121909	0.637256
38	1	0	-2.071452	-5.687664	-0.844822
39	8	0	-4.514334	-5.648727	-0.162314
40	8	0	-2.473257	6.698893	0.307499
41	6	0	-5.881046	-5.497702	0.200772
42	1	0	-6.336905	-6.477378	0.070350
43	1	0	-5.977555	-5.187173	1.244754
44	1	0	-6.379875	-4.773859	-0.449790
45	6	0	-3.587782	7.129035	-0.464008
46	1	0	-3.723865	8.184001	-0.233426
47	1	0	-3.391472	7.012246	-1.533541
48	1	0	-4.490892	6.576948	-0.188997
49	7	0	6.736469	-0.959771	-0.060557
50	8	0	7.202078	-1.933331	0.505822
51	8	0	7.422582	-0.146847	-0.655407

Structure 42b (vacuum)

Energy (Hartrees): -1353.91565026
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.345761	2.908427	-0.779779
2	6	0	-0.034750	4.240879	-0.816555
3	6	0	-1.096514	4.650216	-0.023530
4	6	0	-1.773492	3.773913	0.812301
5	6	0	-1.376024	2.446805	0.842037
6	6	0	-0.318565	1.984762	0.041105
7	1	0	1.158924	2.570258	-1.411640
8	1	0	0.465635	4.958255	-1.453022
9	1	0	-2.579962	4.140486	1.432975
10	1	0	-1.866709	1.760938	1.523527
11	6	0	0.109141	0.574245	0.072168
12	6	0	-0.762997	-0.471140	0.064400
13	6	0	1.541839	0.278495	0.073038
14	1	0	2.201770	1.131963	0.278218
15	1	0	-0.344834	-1.471395	0.116298
16	7	0	2.016870	-0.886827	-0.138506
17	7	0	-2.109615	-0.399056	-0.066070
18	1	0	-2.512552	0.494056	-0.315162
19	6	0	-2.994317	-1.492192	0.001185
20	6	0	-4.221460	-1.416512	-0.648034
21	6	0	-2.680041	-2.647660	0.724747
22	6	0	-5.127794	-2.471755	-0.592785
23	1	0	-4.474394	-0.527694	-1.216320
24	6	0	-3.568745	-3.706119	0.764446
25	1	0	-1.749664	-2.713212	1.275143
26	6	0	-4.799135	-3.629979	0.107999
27	1	0	-6.073335	-2.375996	-1.108650
28	1	0	-3.336148	-4.605673	1.320719
29	6	0	3.402301	-1.092727	0.003020
30	6	0	4.179858	-0.470572	0.990876
31	6	0	4.024668	-1.991875	-0.859412
32	6	0	5.538834	-0.714225	1.078434
33	1	0	3.707248	0.182755	1.715585
34	6	0	5.393259	-2.233570	-0.788944
35	1	0	3.419222	-2.494930	-1.603939
36	6	0	6.157897	-1.588528	0.182598
37	1	0	6.145599	-0.248745	1.845549
38	1	0	5.842223	-2.927412	-1.486801
39	8	0	7.497080	-1.759214	0.347374
40	8	0	-5.601992	-4.720217	0.217076
41	6	0	8.155335	-2.651869	-0.525152
42	1	0	8.069750	-2.323455	-1.566031
43	1	0	9.202281	-2.646751	-0.229842
44	1	0	7.755348	-3.666416	-0.429221
45	6	0	-6.855732	-4.676682	-0.430940
46	1	0	-6.737364	-4.549907	-1.511900
47	1	0	-7.333474	-5.632741	-0.229717
48	1	0	-7.478278	-3.868172	-0.034260
49	7	0	-1.515596	6.062349	-0.064904
50	8	0	-2.462004	6.387031	0.620640
51	8	0	-0.890442	6.812965	-0.783151

Structure 42b ($CHCl_3$)

Energy (Hartrees): -1353.95230340
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.442061	2.905638	-0.764587
2	6	0	0.119460	4.252615	-0.791462
3	6	0	-0.950647	4.694426	-0.024806
4	6	0	-1.693177	3.832191	0.772004
5	6	0	-1.353520	2.489931	0.791440
6	6	0	-0.286493	1.996781	0.020526
7	1	0	1.261744	2.548245	-1.377383
8	1	0	0.677292	4.949243	-1.403020
9	1	0	-2.505831	4.212604	1.376435
10	1	0	-1.902751	1.820257	1.443589
11	6	0	0.096320	0.574155	0.053188
12	6	0	-0.802545	-0.455873	0.061321
13	6	0	1.517834	0.243034	0.058567
14	1	0	2.196165	1.074482	0.286925
15	1	0	-0.406807	-1.463230	0.142371
16	7	0	1.974360	-0.929449	-0.177345
17	7	0	-2.140745	-0.366392	-0.074027
18	1	0	-2.540854	0.525235	-0.341015
19	6	0	-3.041949	-1.447262	0.004093
20	6	0	-4.274656	-1.343857	-0.633073
21	6	0	-2.739799	-2.611527	0.718483
22	6	0	-5.197096	-2.385236	-0.579909
23	1	0	-4.517007	-0.443854	-1.188516
24	6	0	-3.646552	-3.656414	0.757059
25	1	0	-1.804848	-2.700035	1.258621
26	6	0	-4.880497	-3.555066	0.109274
27	1	0	-6.146386	-2.270714	-1.086185
28	1	0	-3.419220	-4.562225	1.306851
29	6	0	3.354345	-1.164656	-0.016849
30	6	0	4.125222	-0.584221	1.001975
31	6	0	3.977792	-2.053099	-0.892221
32	6	0	5.478904	-0.856698	1.106962
33	1	0	3.653646	0.062710	1.733595
34	6	0	5.340299	-2.324886	-0.802811
35	1	0	3.382261	-2.526833	-1.664809
36	6	0	6.099031	-1.719745	0.199547
37	1	0	6.075767	-0.418150	1.898592
38	1	0	5.790168	-3.009366	-1.509994
39	8	0	7.431257	-1.920646	0.380650
40	8	0	-5.701334	-4.632695	0.211810
41	6	0	8.091058	-2.803204	-0.511025
42	1	0	8.027713	-2.443716	-1.542468
43	1	0	9.134103	-2.820510	-0.200351
44	1	0	7.677373	-3.814076	-0.445414
45	6	0	-6.972326	-4.551147	-0.411350
46	1	0	-6.874374	-4.409728	-1.491918
47	1	0	-7.466042	-5.501326	-0.216917
48	1	0	-7.568499	-3.738480	0.014939
49	7	0	-1.304448	6.117402	-0.050824
50	8	0	-2.265192	6.479096	0.600210
51	8	0	-0.620502	6.864652	-0.722249

Structure 42b (DMSO)

Energy (Hartrees): -1353.94945012
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.511916	2.884464	-0.747967
2	6	0	0.225457	4.239191	-0.773176
3	6	0	-0.849498	4.704375	-0.026862
4	6	0	-1.634721	3.855404	0.743568
5	6	0	-1.333210	2.504082	0.759017
6	6	0	-0.258695	1.989107	0.013016
7	1	0	1.338434	2.512633	-1.342592
8	1	0	0.818090	4.921934	-1.367579
9	1	0	-2.454825	4.248071	1.329974
10	1	0	-1.922256	1.847271	1.388949
11	6	0	0.094552	0.559222	0.046466
12	6	0	-0.822511	-0.457876	0.058852
13	6	0	1.508568	0.205890	0.055679
14	1	0	2.197917	1.025428	0.290877
15	1	0	-0.443415	-1.470208	0.154961
16	7	0	1.952950	-0.972236	-0.187654
17	7	0	-2.155514	-0.349969	-0.082277
18	1	0	-2.546847	0.545874	-0.352535
19	6	0	-3.074749	-1.414628	0.000158
20	6	0	-4.321096	-1.269155	-0.602948
21	6	0	-2.781654	-2.600432	0.682007
22	6	0	-5.266388	-2.289891	-0.549505
23	1	0	-4.555746	-0.348734	-1.127690
24	6	0	-3.713301	-3.624115	0.722222
25	1	0	-1.836427	-2.725228	1.196333
26	6	0	-4.960629	-3.481840	0.107496
27	1	0	-6.225010	-2.141025	-1.029010
28	1	0	-3.491250	-4.545066	1.248906
29	6	0	3.330742	-1.219795	-0.020792
30	6	0	4.103263	-0.641523	0.998619
31	6	0	3.951309	-2.116751	-0.890479
32	6	0	5.454503	-0.925116	1.109294
33	1	0	3.636359	0.015622	1.724202
34	6	0	5.311601	-2.400181	-0.795233
35	1	0	3.358241	-2.589117	-1.666271
36	6	0	6.072606	-1.796930	0.207504
37	1	0	6.049216	-0.485394	1.902164
38	1	0	5.757694	-3.090751	-1.499135
39	8	0	7.400841	-2.007360	0.391998
40	8	0	-5.804275	-4.540396	0.207411
41	6	0	8.053788	-2.895754	-0.502841
42	1	0	7.987541	-2.537035	-1.534078
43	1	0	9.097912	-2.918398	-0.196314
44	1	0	7.634190	-3.903732	-0.435184
45	6	0	-7.084808	-4.412403	-0.393174
46	1	0	-7.000517	-4.246691	-1.471280
47	1	0	-7.599786	-5.354069	-0.212837
48	1	0	-7.652326	-3.594655	0.060875
49	7	0	-1.159523	6.136014	-0.046074
50	8	0	-2.077206	6.533722	0.646759
51	8	0	-0.483715	6.859602	-0.753195

Structure 42b (C_2H_5OH)

Energy (Hartrees): -1353.95162125
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.513064	2.891099	-0.720230
2	6	0	0.220671	4.243486	-0.756672
3	6	0	-0.867715	4.706499	-0.027430
4	6	0	-1.656513	3.858817	0.741792
5	6	0	-1.345731	2.510501	0.771707
6	6	0	-0.262039	1.995966	0.037651
7	1	0	1.345931	2.519527	-1.306175
8	1	0	0.815707	4.924958	-1.350260
9	1	0	-2.483981	4.250831	1.318352
10	1	0	-1.934610	1.855355	1.403590
11	6	0	0.093222	0.568008	0.075945
12	6	0	-0.822028	-0.451040	0.086177
13	6	0	1.507799	0.215771	0.079911
14	1	0	2.197357	1.034244	0.317578
15	1	0	-0.440284	-1.462497	0.180648
16	7	0	1.951608	-0.960619	-0.171764
17	7	0	-2.155010	-0.348264	-0.059241
18	1	0	-2.549898	0.546099	-0.328949
19	6	0	-3.067831	-1.419649	0.014142
20	6	0	-4.307340	-1.284787	-0.605138
21	6	0	-2.773553	-2.600566	0.703311
22	6	0	-5.244778	-2.312995	-0.561783
23	1	0	-4.542602	-0.368073	-1.136024
24	6	0	-3.697146	-3.631982	0.733749
25	1	0	-1.834447	-2.715195	1.231207
26	6	0	-4.935487	-3.499305	0.101349
27	1	0	-6.198400	-2.174257	-1.054053
28	1	0	-3.476102	-4.550720	1.265222
29	6	0	3.330988	-1.207013	-0.014082
30	6	0	4.106418	-0.639071	1.008190
31	6	0	3.948070	-2.093568	-0.896795
32	6	0	5.458825	-0.922049	1.109710
33	1	0	3.641373	0.008427	1.743644
34	6	0	5.308750	-2.376758	-0.810613
35	1	0	3.351823	-2.558406	-1.674698
36	6	0	6.070861	-1.783257	0.195419
37	1	0	6.057808	-0.490776	1.904344
38	1	0	5.753210	-3.059389	-1.523209
39	8	0	7.405673	-1.995895	0.372336
40	8	0	-5.773868	-4.569774	0.191056
41	6	0	8.055829	-2.884324	-0.527242
42	1	0	7.989132	-2.519235	-1.555834
43	1	0	9.099677	-2.910557	-0.219961
44	1	0	7.630977	-3.889841	-0.460529
45	6	0	-7.050680	-4.455934	-0.424387
46	1	0	-6.953241	-4.291190	-1.501121
47	1	0	-7.556009	-5.403510	-0.247574
48	1	0	-7.629321	-3.643496	0.024307
49	7	0	-1.189932	6.129698	-0.067223
50	8	0	-2.167836	6.520172	0.544464
51	8	0	-0.468058	6.868607	-0.711730

Structure 42c (vacuum)

Energy (Hartrees): -1353.91729647
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.800598	2.240807	0.879437
2	6	0	-0.772187	3.626288	0.903110
3	6	0	0.038728	4.291470	-0.005155
4	6	0	0.811394	3.619361	-0.939019
5	6	0	0.773861	2.232514	-0.947557
6	6	0	-0.020234	1.523727	-0.036086
7	1	0	-1.438316	1.702785	1.567381
8	1	0	-1.363474	4.194682	1.608146
9	1	0	1.412482	4.179313	-1.642497
10	1	0	1.347592	1.688689	-1.689974
11	6	0	-0.033244	0.043761	-0.049851
12	6	0	1.110598	-0.691380	-0.053935
13	6	0	-1.288094	-0.693269	-0.022174
14	1	0	1.035997	-1.774298	-0.076380
15	1	0	-1.185657	-1.787458	-0.049810
16	7	0	-2.434038	-0.135625	0.005835
17	7	0	2.381442	-0.216617	0.022414
18	1	0	2.503781	0.765921	0.225985
19	6	0	3.543183	-1.009652	-0.034352
20	6	0	4.694735	-0.591615	0.623179
21	6	0	3.574772	-2.205206	-0.760085
22	6	0	5.862858	-1.347917	0.573318
23	1	0	4.681650	0.330932	1.193452
24	6	0	4.725617	-2.971361	-0.792865
25	1	0	2.707017	-2.524746	-1.324452
26	6	0	5.879287	-2.551680	-0.127547
27	1	0	6.739848	-0.990316	1.095219
28	1	0	4.761470	-3.897829	-1.352412
29	6	0	-3.581672	-0.949497	0.071026
30	6	0	-4.718740	-0.544880	-0.623363
31	6	0	-3.651827	-2.120989	0.838998
32	6	0	-5.884820	-1.304839	-0.606336
33	1	0	-4.674671	0.375278	-1.193728
34	6	0	-4.810820	-2.875640	0.874724
35	1	0	-2.801285	-2.421580	1.440744
36	6	0	-5.932337	-2.479767	0.142958
37	1	0	-6.742868	-0.965935	-1.170991
38	1	0	-4.878326	-3.774038	1.476200
39	8	0	6.957706	-3.370942	-0.229310
40	8	0	-7.021316	-3.289658	0.237065
41	6	0	8.145192	-2.974910	0.424190
42	1	0	7.991474	-2.888340	1.504618
43	1	0	8.874716	-3.756544	0.225493
44	1	0	8.515809	-2.023273	0.029892
45	6	0	-8.185272	-2.903451	-0.461104
46	1	0	-8.001848	-2.851756	-1.539144
47	1	0	-8.928640	-3.671455	-0.258931
48	1	0	-8.556495	-1.936025	-0.107846
49	7	0	0.075797	5.766144	0.017514
50	8	0	0.782370	6.322672	-0.796400
51	8	0	-0.599377	6.332605	0.849850

Structure 42c ($CHCl_3$)

Energy (Hartrees): -1353.95464051
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.782078	2.246634	0.924012
2	6	0	-0.759487	3.631632	0.925947
3	6	0	0.035676	4.283782	-0.007583
4	6	0	0.800073	3.597995	-0.940311
5	6	0	0.767520	2.211453	-0.925640
6	6	0	-0.014359	1.515683	0.006884
7	1	0	-1.400897	1.721943	1.640112
8	1	0	-1.343907	4.201422	1.635843
9	1	0	1.394024	4.138959	-1.664726
10	1	0	1.338857	1.660894	-1.665026
11	6	0	-0.033880	0.035805	0.016608
12	6	0	1.106084	-0.715415	0.014180
13	6	0	-1.289511	-0.690859	0.040356
14	1	0	1.012043	-1.796842	-0.003342
15	1	0	-1.192640	-1.783644	0.076526
16	7	0	-2.437841	-0.128924	-0.010841
17	7	0	2.375393	-0.255224	0.074405
18	1	0	2.518310	0.732861	0.245156
19	6	0	3.537935	-1.046887	0.000715
20	6	0	4.723584	-0.555569	0.539857
21	6	0	3.543187	-2.299261	-0.622576
22	6	0	5.901167	-1.296098	0.476425
23	1	0	4.728415	0.415738	1.023351
24	6	0	4.707895	-3.046245	-0.671007
25	1	0	2.647432	-2.687509	-1.091910
26	6	0	5.895284	-2.553881	-0.124267
27	1	0	6.804462	-0.882482	0.904819
28	1	0	4.720373	-4.016418	-1.153760
29	6	0	-3.589210	-0.938682	0.057325
30	6	0	-4.703897	-0.572148	-0.695977
31	6	0	-3.688626	-2.068402	0.883888
32	6	0	-5.874123	-1.327087	-0.675342
33	1	0	-4.644194	0.314719	-1.317075
34	6	0	-4.852134	-2.818372	0.921916
35	1	0	-2.856189	-2.343935	1.522096
36	6	0	-5.950201	-2.459620	0.135516
37	1	0	-6.713317	-1.018106	-1.284664
38	1	0	-4.935741	-3.683988	1.569180
39	8	0	6.983714	-3.360075	-0.232078
40	8	0	-7.045846	-3.258963	0.237096
41	6	0	8.211129	-2.879707	0.290105
42	1	0	8.137538	-2.693762	1.365929
43	1	0	8.942750	-3.665111	0.110514
44	1	0	8.527505	-1.966067	-0.222490
45	6	0	-8.186329	-2.911203	-0.529332
46	1	0	-7.962839	-2.925975	-1.600338
47	1	0	-8.939556	-3.665441	-0.309024
48	1	0	-8.567366	-1.925522	-0.245523
49	7	0	0.064674	5.752633	-0.011210
50	8	0	0.747818	6.308551	-0.848544
51	8	0	-0.593792	6.338935	0.824484

Structure 42c (DMSO)

Energy (Hartrees): -1353.95273629
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.737442	2.252577	0.936640
2	6	0	-0.708263	3.637111	0.959838
3	6	0	0.055296	4.300007	0.006646
4	6	0	0.783522	3.624758	-0.962178
5	6	0	0.744016	2.238213	-0.968577
6	6	0	-0.009352	1.532252	-0.020953
7	1	0	-1.324481	1.719575	1.673937
8	1	0	-1.261048	4.194566	1.704219
9	1	0	1.358515	4.169923	-1.698683
10	1	0	1.291063	1.698577	-1.733916
11	6	0	-0.038594	0.052849	-0.030803
12	6	0	1.097259	-0.709341	-0.055214
13	6	0	-1.293209	-0.668171	0.001910
14	1	0	0.989019	-1.789217	-0.074443
15	1	0	-1.196933	-1.760445	0.030154
16	7	0	-2.445704	-0.105942	-0.034450
17	7	0	2.367145	-0.259805	-0.016803
18	1	0	2.523971	0.730263	0.136279
19	6	0	3.523548	-1.063456	-0.056199
20	6	0	4.714741	-0.545853	0.445911
21	6	0	3.518674	-2.352013	-0.600778
22	6	0	5.888205	-1.295419	0.424864
23	1	0	4.726426	0.455673	0.863304
24	6	0	4.680721	-3.106010	-0.608804
25	1	0	2.618525	-2.768623	-1.036241
26	6	0	5.873792	-2.588794	-0.096654
27	1	0	6.794712	-0.860088	0.824204
28	1	0	4.681087	-4.105329	-1.028540
29	6	0	-3.591419	-0.923713	0.045827
30	6	0	-4.722786	-0.559336	-0.684383
31	6	0	-3.669654	-2.062391	0.863651
32	6	0	-5.888624	-1.321493	-0.649928
33	1	0	-4.683449	0.332012	-1.301426
34	6	0	-4.827679	-2.820680	0.914001
35	1	0	-2.824620	-2.341253	1.483866
36	6	0	-5.943434	-2.463344	0.150526
37	1	0	-6.739558	-1.011863	-1.242723
38	1	0	-4.888903	-3.694075	1.553714
39	8	0	6.957776	-3.404206	-0.155265
40	8	0	-7.030699	-3.269829	0.261384
41	6	0	8.183143	-2.896455	0.351417
42	1	0	8.101364	-2.658236	1.416064
43	1	0	8.918345	-3.687179	0.214756
44	1	0	8.500801	-2.007017	-0.200544
45	6	0	-8.184617	-2.918882	-0.487482
46	1	0	-7.974594	-2.918912	-1.561019
47	1	0	-8.930907	-3.679778	-0.266897
48	1	0	-8.566970	-1.938505	-0.188042
49	7	0	0.091457	5.767745	0.024032
50	8	0	0.748731	6.334765	-0.827521
51	8	0	-0.537023	6.345704	0.889759

Structure 42c (C_2H_5OH)

Energy (Hartrees): -1353.95466899
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.739940	2.256218	0.923453
2	6	0	-0.704441	3.640038	0.949262
3	6	0	0.074217	4.299730	0.005610
4	6	0	0.806452	3.623234	-0.960017
5	6	0	0.754907	2.237650	-0.972429
6	6	0	-0.008453	1.533978	-0.030479
7	1	0	-1.333692	1.724861	1.656447
8	1	0	-1.258961	4.198754	1.691582
9	1	0	1.388666	4.166453	-1.692598
10	1	0	1.299704	1.696571	-1.738431
11	6	0	-0.043115	0.055203	-0.040911
12	6	0	1.090393	-0.710200	-0.061189
13	6	0	-1.300270	-0.661823	-0.007460
14	1	0	0.979466	-1.789875	-0.078991
15	1	0	-1.207700	-1.754275	0.024365
16	7	0	-2.450771	-0.096430	-0.048055
17	7	0	2.361916	-0.264446	-0.016169
18	1	0	2.520781	0.725237	0.136650
19	6	0	3.516077	-1.071288	-0.054992
20	6	0	4.707180	-0.557836	0.451742
21	6	0	3.508493	-2.357462	-0.604317
22	6	0	5.878590	-1.310243	0.431264
23	1	0	4.720511	0.442125	0.872883
24	6	0	4.668596	-3.114734	-0.611601
25	1	0	2.608604	-2.769658	-1.044532
26	6	0	5.859579	-2.600659	-0.094420
27	1	0	6.785891	-0.879581	0.833923
28	1	0	4.669209	-4.113069	-1.034339
29	6	0	-3.597484	-0.912463	0.037052
30	6	0	-4.725161	-0.558198	-0.703800
31	6	0	-3.679041	-2.037343	0.872489
32	6	0	-5.891029	-1.319551	-0.662848
33	1	0	-4.683036	0.323877	-1.333748
34	6	0	-4.837581	-2.794740	0.929771
35	1	0	-2.836621	-2.305167	1.501193
36	6	0	-5.947384	-2.447242	0.155456
37	1	0	-6.740096	-1.019568	-1.263275
38	1	0	-4.903834	-3.657816	1.583164
39	8	0	6.945976	-3.422143	-0.152642
40	8	0	-7.039734	-3.255505	0.274086
41	6	0	8.173671	-2.921320	0.360477
42	1	0	8.086429	-2.687752	1.425376
43	1	0	8.903787	-3.716506	0.222469
44	1	0	8.494683	-2.032146	-0.189324
45	6	0	-8.196746	-2.912388	-0.477265
46	1	0	-7.987106	-2.929383	-1.550378
47	1	0	-8.942622	-3.669370	-0.242083
48	1	0	-8.573723	-1.927234	-0.188339
49	7	0	0.123893	5.762335	0.030787
50	8	0	0.885858	6.327693	-0.730944
51	8	0	-0.597182	6.351445	0.813619

Structure 42d (vacuum)

Energy (Hartrees): -1353.91301870
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.475376	2.391116	0.750671
2	6	0	1.890792	3.710700	0.791056
3	6	0	1.229313	4.644119	0.003761
4	6	0	0.174444	4.294394	-0.822622
5	6	0	-0.225743	2.966464	-0.855451
6	6	0	0.401797	1.997000	-0.061840
7	1	0	1.984684	1.653505	1.354902
8	1	0	2.711905	4.026706	1.419982
9	1	0	-0.301244	5.048237	-1.435038
10	1	0	-1.019640	2.671573	-1.531317
11	6	0	-0.079678	0.599414	-0.068732
12	6	0	-1.420243	0.369693	-0.133036
13	6	0	0.855310	-0.516695	0.002385
14	1	0	0.421414	-1.502040	0.224131
15	1	0	-1.502805	-1.607681	-0.670295
16	1	0	-2.106806	1.207533	-0.053372
17	7	0	2.112122	-0.386965	-0.171448
18	7	0	-2.037302	-0.833106	-0.309034
19	6	0	2.948065	-1.507961	-0.013811
20	6	0	4.055950	-1.612397	-0.851202
21	6	0	2.754165	-2.494072	0.965121
22	6	0	4.926619	-2.693665	-0.766193
23	1	0	4.220510	-0.832902	-1.585492
24	6	0	3.625172	-3.564046	1.069541
25	1	0	1.939177	-2.398474	1.673968
26	6	0	4.710576	-3.678327	0.197935
27	1	0	5.768018	-2.747267	-1.443546
28	1	0	3.496302	-4.321668	1.833013
29	6	0	-3.416163	-1.045251	-0.117317
30	6	0	-4.075787	-2.023586	-0.852943
31	6	0	-4.141114	-0.289971	0.810132
32	6	0	-5.438696	-2.249503	-0.682055
33	1	0	-3.525092	-2.611671	-1.579217
34	6	0	-5.500202	-0.493922	0.965416
35	1	0	-3.635484	0.441272	1.429268
36	6	0	-6.161229	-1.474174	0.223020
37	1	0	-5.919382	-3.019891	-1.269435
38	1	0	-6.072648	0.084908	1.679497
39	8	0	-7.492292	-1.603419	0.457882
40	8	0	5.505395	-4.765799	0.378497
41	6	0	-8.194480	-2.587646	-0.271860
42	1	0	-7.798946	-3.587987	-0.068341
43	1	0	-9.227442	-2.532422	0.063496
44	1	0	-8.149941	-2.388715	-1.347449
45	6	0	6.632487	-4.900934	-0.460753
46	1	0	7.128098	-5.819622	-0.155032
47	1	0	6.336448	-4.979901	-1.511714
48	1	0	7.320560	-4.058374	-0.338376
49	7	0	1.671596	6.049000	0.036932
50	8	0	1.073334	6.844516	-0.657193
51	8	0	2.606938	6.328187	0.756799

Structure 42d ($CHCl_3$)

Energy (Hartrees): -1353.95124508
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.480555	2.392804	0.747142
2	6	0	1.894874	3.712209	0.779349
3	6	0	1.219406	4.644386	-0.000537
4	6	0	0.148748	4.290703	-0.808400
5	6	0	-0.249627	2.963038	-0.832726
6	6	0	0.394695	1.992797	-0.049884
7	1	0	1.997043	1.662214	1.354810
8	1	0	2.724461	4.022113	1.400733
9	1	0	-0.346060	5.036076	-1.416769
10	1	0	-1.059238	2.669478	-1.490406
11	6	0	-0.080407	0.594656	-0.049733
12	6	0	-1.427947	0.364523	-0.103641
13	6	0	0.854508	-0.517564	0.017781
14	1	0	0.424903	-1.500734	0.247295
15	1	0	-1.512303	-1.624444	-0.589140
16	1	0	-2.109304	1.206450	-0.023370
17	7	0	2.112081	-0.389088	-0.177632
18	7	0	-2.044977	-0.831118	-0.258972
19	6	0	2.953213	-1.508245	-0.022755
20	6	0	4.071959	-1.597894	-0.849992
21	6	0	2.757580	-2.506985	0.944260
22	6	0	4.953008	-2.671978	-0.766041
23	1	0	4.241517	-0.813620	-1.579193
24	6	0	3.635931	-3.572535	1.044857
25	1	0	1.933216	-2.430282	1.644818
26	6	0	4.733647	-3.669263	0.184926
27	1	0	5.803481	-2.710478	-1.433739
28	1	0	3.499058	-4.337804	1.800439
29	6	0	-3.427938	-1.039311	-0.083400
30	6	0	-4.057796	-2.062249	-0.786173
31	6	0	-4.181247	-0.247589	0.789562
32	6	0	-5.422844	-2.293260	-0.641510
33	1	0	-3.477224	-2.681454	-1.462240
34	6	0	-5.543061	-0.460521	0.920309
35	1	0	-3.702289	0.522167	1.383619
36	6	0	-6.175532	-1.481706	0.207285
37	1	0	-5.882155	-3.096311	-1.202546
38	1	0	-6.136115	0.148824	1.592320
39	8	0	-7.511627	-1.614872	0.411821
40	8	0	5.534355	-4.752666	0.360590
41	6	0	-8.190848	-2.629848	-0.309071
42	1	0	-7.797545	-3.620489	-0.062092
43	1	0	-9.233472	-2.570991	-0.002902
44	1	0	-8.119535	-2.461206	-1.387963
45	6	0	6.694615	-4.855888	-0.447953
46	1	0	7.195452	-5.771305	-0.138339
47	1	0	6.434639	-4.926186	-1.508385
48	1	0	7.363342	-4.004973	-0.287147
49	7	0	1.658755	6.042317	0.024670
50	8	0	1.048306	6.847811	-0.651652
51	8	0	2.611986	6.330539	0.721967

Structure 42d (DMSO)

Energy (Hartrees): -1353.94951946
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.525555	2.377156	0.775902
2	6	0	1.976060	3.685003	0.788279
3	6	0	1.322280	4.624417	-0.002232
4	6	0	0.235418	4.288280	-0.796866
5	6	0	-0.199234	2.971925	-0.801587
6	6	0	0.426575	1.993723	-0.012760
7	1	0	2.021490	1.643203	1.397111
8	1	0	2.815465	3.977737	1.404980
9	1	0	-0.247069	5.036193	-1.411990
10	1	0	-1.024859	2.695112	-1.446668
11	6	0	-0.074922	0.605655	0.002816
12	6	0	-1.430916	0.404198	-0.039630
13	6	0	0.841016	-0.519950	0.059088
14	1	0	0.401984	-1.498712	0.284808
15	1	0	-1.549099	-1.604410	-0.408028
16	1	0	-2.086448	1.267442	0.019726
17	7	0	2.100371	-0.411020	-0.152978
18	7	0	-2.074212	-0.775903	-0.156791
19	6	0	2.921348	-1.547990	-0.015091
20	6	0	4.036910	-1.649388	-0.846149
21	6	0	2.710330	-2.555203	0.940428
22	6	0	4.900921	-2.739116	-0.776615
23	1	0	4.221073	-0.862864	-1.569965
24	6	0	3.570388	-3.637265	1.025634
25	1	0	1.886373	-2.476042	1.641256
26	6	0	4.665711	-3.744605	0.162508
27	1	0	5.747599	-2.784367	-1.448983
28	1	0	3.416879	-4.408574	1.772126
29	6	0	-3.466259	-0.955343	-0.032750
30	6	0	-4.049289	-2.079031	-0.612564
31	6	0	-4.275991	-0.051136	0.662260
32	6	0	-5.420237	-2.302723	-0.522695
33	1	0	-3.425251	-2.787828	-1.147065
34	6	0	-5.643041	-0.261896	0.738932
35	1	0	-3.845271	0.808891	1.160824
36	6	0	-6.228559	-1.384624	0.148057
37	1	0	-5.837920	-3.186865	-0.985694
38	1	0	-6.274283	0.436255	1.276426
39	8	0	-7.574026	-1.503458	0.284999
40	8	0	5.446051	-4.843277	0.321176
41	6	0	-8.194352	-2.632032	-0.313748
42	1	0	-7.819433	-3.564634	0.117948
43	1	0	-9.258129	-2.539604	-0.103179
44	1	0	-8.038228	-2.638685	-1.396540
45	6	0	6.610518	-4.945631	-0.485565
46	1	0	7.099812	-5.871972	-0.190427
47	1	0	6.354552	-4.992697	-1.547876
48	1	0	7.287406	-4.104917	-0.306939
49	7	0	1.801022	6.007953	-0.002844
50	8	0	1.208235	6.821462	-0.687096
51	8	0	2.769952	6.280719	0.681239

Structure 42d (C_2H_5OH)

Energy (Hartrees): -1353.95162430
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.521910	2.401167	0.803835
2	6	0	1.973639	3.707784	0.797758
3	6	0	1.326507	4.633242	-0.015527
4	6	0	0.244627	4.285199	-0.812987
5	6	0	-0.191626	2.970009	-0.796870
6	6	0	0.429099	2.005253	0.012586
7	1	0	2.011165	1.677653	1.442577
8	1	0	2.808425	4.009618	1.416491
9	1	0	-0.231234	5.021595	-1.447170
10	1	0	-1.011854	2.681791	-1.443922
11	6	0	-0.067841	0.616685	0.045847
12	6	0	-1.421885	0.407743	0.001520
13	6	0	0.854356	-0.504230	0.108491
14	1	0	0.426193	-1.479086	0.370342
15	1	0	-1.526180	-1.604525	-0.353147
16	1	0	-2.083328	1.267246	0.049083
17	7	0	2.106197	-0.398205	-0.143473
18	7	0	-2.057358	-0.778058	-0.108276
19	6	0	2.926830	-1.535363	-0.001398
20	6	0	3.973918	-1.703644	-0.907222
21	6	0	2.775838	-2.478255	1.026773
22	6	0	4.826541	-2.801723	-0.836375
23	1	0	4.111548	-0.965646	-1.690089
24	6	0	3.629539	-3.565829	1.116069
25	1	0	2.004820	-2.343024	1.777870
26	6	0	4.653515	-3.740062	0.181228
27	1	0	5.616798	-2.905372	-1.568335
28	1	0	3.523323	-4.289585	1.916696
29	6	0	-3.450995	-0.959736	-0.002757
30	6	0	-4.027562	-2.074420	-0.605873
31	6	0	-4.266636	-0.064490	0.696178
32	6	0	-5.399679	-2.297024	-0.536354
33	1	0	-3.397980	-2.775461	-1.144125
34	6	0	-5.635112	-0.273471	0.752568
35	1	0	-3.838899	0.786632	1.212733
36	6	0	-6.212023	-1.385962	0.136890
37	1	0	-5.814396	-3.173133	-1.017044
38	1	0	-6.274035	0.416459	1.292193
39	8	0	-7.564953	-1.503352	0.254106
40	8	0	5.440059	-4.839981	0.352157
41	6	0	-8.184773	-2.620451	-0.370660
42	1	0	-7.818802	-3.559742	0.053176
43	1	0	-9.250126	-2.523398	-0.170313
44	1	0	-8.014145	-2.608684	-1.450859
45	6	0	6.477580	-5.063229	-0.594220
46	1	0	6.971581	-5.982180	-0.284101
47	1	0	6.067850	-5.190340	-1.600131
48	1	0	7.199403	-4.241750	-0.587757
49	7	0	1.807731	6.010429	-0.039598
50	8	0	1.227266	6.816614	-0.744520
51	8	0	2.771286	6.300045	0.646789

Structure 43a (vacuum)

Energy (Hartrees): -1533.88114121
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.919075	2.949419	-0.864768
2	6	0	-2.411655	4.245116	-0.857294
3	6	0	-1.805603	5.179333	-0.031345
4	6	0	-0.734878	4.856622	0.787836
5	6	0	-0.264306	3.552815	0.779201
6	6	0	-0.839038	2.580760	-0.050644
7	1	0	-2.361381	2.221340	-1.534910
8	1	0	-3.240760	4.542197	-1.485338
9	1	0	-0.303819	5.613319	1.429387
10	1	0	0.539558	3.276755	1.451660
11	6	0	-0.326203	1.193590	-0.067203
12	6	0	1.025119	0.976027	-0.029939
13	6	0	-1.281252	0.107466	-0.101774
14	1	0	1.689765	1.831676	-0.009745
15	1	0	-2.338635	0.393764	-0.070636
16	1	0	0.954062	-1.024091	-0.041295
17	7	0	-0.949792	-1.135501	-0.148706
18	7	0	1.609741	-0.239051	-0.026036
19	6	0	-1.960852	-2.106456	-0.065542
20	6	0	-1.866052	-3.236352	-0.886733
21	6	0	-3.021467	-1.998184	0.842964
22	6	0	-2.835273	-4.223028	-0.835580
23	1	0	-1.032234	-3.315093	-1.573266
24	6	0	-3.992499	-2.985297	0.907146
25	1	0	-3.064184	-1.154539	1.521118
26	6	0	-3.885388	-4.078128	0.061280
27	1	0	-2.792781	-5.097672	-1.470648
28	1	0	-4.817322	-2.926366	1.604451
29	6	0	2.976976	-0.510051	-0.019722
30	6	0	3.368564	-1.845303	0.149291
31	6	0	3.952927	0.481205	-0.180503
32	6	0	4.706801	-2.188817	0.167350
33	1	0	2.610783	-2.610042	0.275800
34	6	0	5.295249	0.140901	-0.156473
35	1	0	3.682596	1.515627	-0.341228
36	6	0	5.655385	-1.186270	0.017748
37	1	0	5.026000	-3.213726	0.299825
38	1	0	6.065166	0.890697	-0.280291
39	7	0	-4.915274	-5.131854	0.126425
40	8	0	-4.795382	-6.078499	-0.620977
41	8	0	-5.817620	-4.984014	0.921998
42	7	0	7.082380	-1.541922	0.041055
43	8	0	7.885640	-0.643684	-0.092791
44	8	0	7.364922	-2.711005	0.193587
45	7	0	-2.321981	6.561530	-0.017887
46	8	0	-1.769630	7.357576	0.710142
47	8	0	-3.265083	6.813568	-0.735786

Structure 43a ($CHCl_3$)

Energy (Hartrees): -1533.92114983
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.768089	3.033663	-0.825071
2	6	0	-2.177096	4.357094	-0.824606
3	6	0	-1.486138	5.264434	-0.033485
4	6	0	-0.409621	4.885560	0.757175
5	6	0	-0.021826	3.555816	0.754117
6	6	0	-0.684926	2.608818	-0.040627
7	1	0	-2.281975	2.326509	-1.465619
8	1	0	-3.006966	4.686363	-1.435596
9	1	0	0.097187	5.615487	1.374406
10	1	0	0.790204	3.244151	1.400564
11	6	0	-0.259906	1.192996	-0.057716
12	6	0	1.078179	0.896950	-0.012130
13	6	0	-1.281628	0.170548	-0.105880
14	1	0	1.793109	1.710836	0.023406
15	1	0	-2.318811	0.519404	-0.063731
16	1	0	0.908013	-1.105523	-0.043246
17	7	0	-1.027083	-1.090968	-0.173618
18	7	0	1.594046	-0.347893	-0.019236
19	6	0	-2.094093	-1.995511	-0.085043
20	6	0	-2.091663	-3.117355	-0.925230
21	6	0	-3.125420	-1.833539	0.850991
22	6	0	-3.119070	-4.041654	-0.861447
23	1	0	-1.284174	-3.242981	-1.636466
24	6	0	-4.155225	-2.756767	0.926969
25	1	0	-3.102370	-0.996778	1.538962
26	6	0	-4.137467	-3.844572	0.064608
27	1	0	-3.137068	-4.904888	-1.513460
28	1	0	-4.952732	-2.644744	1.649456
29	6	0	2.944558	-0.686883	-0.014715
30	6	0	3.268825	-2.044555	0.126732
31	6	0	3.967559	0.260910	-0.153884
32	6	0	4.588112	-2.452182	0.140918
33	1	0	2.474541	-2.775059	0.230691
34	6	0	5.290450	-0.143370	-0.131581
35	1	0	3.748036	1.309855	-0.296798
36	6	0	5.586031	-1.491944	0.016950
37	1	0	4.845391	-3.497087	0.251742
38	1	0	6.088371	0.579425	-0.238450
39	7	0	-5.223667	-4.827118	0.141760
40	8	0	-5.160373	-5.806911	-0.573971
41	8	0	-6.134038	-4.611679	0.917332
42	7	0	6.986290	-1.913753	0.039268
43	8	0	7.843664	-1.053280	-0.013256
44	8	0	7.223396	-3.103929	0.111252
45	7	0	-1.911846	6.669246	-0.028465
46	8	0	-1.290852	7.451325	0.663449
47	8	0	-2.863573	6.979184	-0.716816

Structure 43a (DMSO)

Energy (Hartrees): -1533.91962498
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.104377	2.879810	-0.761351
2	6	0	-2.627386	4.162049	-0.784682
3	6	0	-1.985205	5.155345	-0.056876
4	6	0	-0.843530	4.900128	0.691870
5	6	0	-0.341292	3.610162	0.715162
6	6	0	-0.954592	2.578662	-0.013545
7	1	0	-2.584120	2.110010	-1.354168
8	1	0	-3.508761	4.393284	-1.368097
9	1	0	-0.370431	5.691029	1.258482
10	1	0	0.525868	3.396229	1.328829
11	6	0	-0.404403	1.207775	0.002383
12	6	0	0.959237	1.039908	0.030911
13	6	0	-1.324070	0.093546	-0.021067
14	1	0	1.596548	1.916249	0.022026
15	1	0	-2.390357	0.338468	-0.018558
16	1	0	0.965728	-0.969768	0.043756
17	7	0	-0.937531	-1.136774	-0.039862
18	7	0	1.583367	-0.152642	0.045492
19	6	0	-1.889783	-2.160958	0.010996
20	6	0	-1.610632	-3.335028	-0.703324
21	6	0	-3.064785	-2.078613	0.773609
22	6	0	-2.502097	-4.391752	-0.698728
23	1	0	-0.690031	-3.396923	-1.271466
24	6	0	-3.961874	-3.133544	0.788626
25	1	0	-3.265104	-1.197913	1.371899
26	6	0	-3.669896	-4.271705	0.046998
27	1	0	-2.297657	-5.294696	-1.258468
28	1	0	-4.869756	-3.082222	1.375061
29	6	0	2.955543	-0.379919	0.025852
30	6	0	3.377720	-1.716901	0.088655
31	6	0	3.906045	0.647271	-0.055718
32	6	0	4.721909	-2.029487	0.074560
33	1	0	2.636786	-2.505907	0.153101
34	6	0	5.254376	0.336683	-0.067770
35	1	0	3.611979	1.686551	-0.114348
36	6	0	5.647814	-0.994254	-0.001805
37	1	0	5.050966	-3.058830	0.123751
38	1	0	5.994539	1.123194	-0.132925
39	7	0	-4.617446	-5.388270	0.063817
40	8	0	-4.346169	-6.379954	-0.586665
41	8	0	-5.632049	-5.271005	0.724935
42	7	0	7.072252	-1.315084	-0.013469
43	8	0	7.868799	-0.395386	-0.054186
44	8	0	7.396967	-2.487884	0.020173
45	7	0	-2.531359	6.514986	-0.077016
46	8	0	-1.952035	7.375148	0.558905
47	8	0	-3.538451	6.719165	-0.728180

Structure 43a (C_2H_5OH)

Energy (Hartrees): -1533.91833091
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.055145	2.900201	-0.763820
2	6	0	-2.564491	4.187083	-0.795766
3	6	0	-1.917624	5.174831	-0.063755
4	6	0	-0.786231	4.910714	0.698123
5	6	0	-0.301079	3.614880	0.732753
6	6	0	-0.918456	2.588519	-0.000153
7	1	0	-2.533601	2.134479	-1.362857
8	1	0	-3.435911	4.426473	-1.391038
9	1	0	-0.311513	5.697843	1.268991
10	1	0	0.554367	3.391285	1.359332
11	6	0	-0.386360	1.211226	0.026621
12	6	0	0.974484	1.026700	0.065514
13	6	0	-1.320939	0.109131	-0.004965
14	1	0	1.623047	1.894620	0.055403
15	1	0	-2.383936	0.368313	-0.014389
16	1	0	0.955362	-0.982489	0.087342
17	7	0	-0.950859	-1.126184	-0.020293
18	7	0	1.583692	-0.173974	0.089128
19	6	0	-1.918656	-2.136071	0.018032
20	6	0	-1.654658	-3.308458	-0.704860
21	6	0	-3.093539	-2.041494	0.779426
22	6	0	-2.561144	-4.351488	-0.710284
23	1	0	-0.733298	-3.380395	-1.270635
24	6	0	-4.005056	-3.083565	0.787341
25	1	0	-3.281692	-1.161723	1.383172
26	6	0	-3.727448	-4.220001	0.036827
27	1	0	-2.367611	-5.253538	-1.275508
28	1	0	-4.913081	-3.022648	1.372848
29	6	0	2.952091	-0.418045	0.060848
30	6	0	3.359086	-1.760109	0.122756
31	6	0	3.913462	0.598459	-0.030777
32	6	0	4.698500	-2.088735	0.092907
33	1	0	2.609803	-2.540525	0.196088
34	6	0	5.257005	0.272555	-0.062467
35	1	0	3.631605	1.641442	-0.084055
36	6	0	5.635083	-1.063620	-0.001130
37	1	0	5.015378	-3.122216	0.139321
38	1	0	6.005182	1.050589	-0.137495
39	7	0	-4.686369	-5.321155	0.044629
40	8	0	-4.457176	-6.291278	-0.654225
41	8	0	-5.676081	-5.224244	0.746828
42	7	0	7.050280	-1.400020	-0.041363
43	8	0	7.858842	-0.497283	-0.166754
44	8	0	7.370113	-2.571964	0.051530
45	7	0	-2.447412	6.536009	-0.093964
46	8	0	-1.818474	7.414345	0.466957
47	8	0	-3.496318	6.735359	-0.678400

Structure 43b (vacuum)

Energy (Hartrees): -1533.87328099
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.408241	3.017060	-0.891807
2	6	0	0.114216	4.372442	-0.904049
3	6	0	-0.824789	4.852934	-0.004187
4	6	0	-1.465927	4.031671	0.910238
5	6	0	-1.155273	2.679760	0.913844
6	6	0	-0.222681	2.150587	0.009923
7	1	0	1.124280	2.619731	-1.602383
8	1	0	0.587842	5.052850	-1.599042
9	1	0	-2.176699	4.456320	1.606597
10	1	0	-1.614982	2.027819	1.648648
11	6	0	0.109506	0.709470	0.012933
12	6	0	-0.829971	-0.269462	0.007782
13	6	0	1.518202	0.318133	-0.013379
14	1	0	2.241960	1.131994	0.123876
15	1	0	-0.485563	-1.297018	0.018214
16	7	0	1.905376	-0.886248	-0.183852
17	7	0	-2.175449	-0.081278	-0.075419
18	1	0	-2.501255	0.858833	-0.260409
19	6	0	-3.151117	-1.075904	-0.034500
20	6	0	-4.449928	-0.744506	-0.444188
21	6	0	-2.875635	-2.373127	0.414521
22	6	0	-5.455876	-1.691740	-0.421500
23	1	0	-4.662644	0.259925	-0.792680
24	6	0	-3.879716	-3.326712	0.427152
25	1	0	-1.891604	-2.641757	0.773184
26	6	0	-5.154227	-2.976390	0.008809
27	1	0	-6.462743	-1.454160	-0.737309
28	1	0	-3.689278	-4.334883	0.769984
29	6	0	3.271929	-1.178315	-0.087259
30	6	0	4.087054	-0.645543	0.920095
31	6	0	3.817076	-2.078397	-1.012094
32	6	0	5.432552	-0.974847	0.980451
33	1	0	3.656114	0.003430	1.673019
34	6	0	5.160973	-2.403178	-0.967591
35	1	0	3.166922	-2.503153	-1.766465
36	6	0	5.948639	-1.841566	0.029349
37	1	0	6.080182	-0.580248	1.751756
38	1	0	5.605569	-3.084630	-1.680303
39	7	0	-6.217995	-3.991453	0.029654
40	8	0	-5.923771	-5.103437	0.412905
41	8	0	-7.322197	-3.652012	-0.338838
42	7	0	7.378685	-2.192264	0.089823
43	8	0	8.040317	-1.699837	0.978765
44	8	0	7.806598	-2.949687	-0.754545
45	7	0	-1.150552	6.294317	-0.016626
46	8	0	-2.000949	6.680426	0.754952
47	8	0	-0.547252	6.995699	-0.798113

Structure 43b ($CHCl_3$)

Energy (Hartrees): -1533.91479474
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.442097	3.014084	-0.885179
2	6	0	0.165697	4.372410	-0.902684
3	6	0	-0.780313	4.865574	-0.014831
4	6	0	-1.445793	4.052102	0.891251
5	6	0	-1.154030	2.696949	0.898340
6	6	0	-0.214666	2.155977	0.007659
7	1	0	1.165269	2.610605	-1.585194
8	1	0	0.663189	5.037555	-1.595964
9	1	0	-2.161336	4.475713	1.583358
10	1	0	-1.637546	2.055533	1.626928
11	6	0	0.103779	0.711368	0.016228
12	6	0	-0.841889	-0.266931	0.031953
13	6	0	1.506783	0.314922	-0.016910
14	1	0	2.233829	1.120961	0.137216
15	1	0	-0.505262	-1.296654	0.055843
16	7	0	1.895603	-0.889180	-0.215793
17	7	0	-2.183216	-0.078012	-0.034963
18	1	0	-2.520402	0.861609	-0.212341
19	6	0	-3.158661	-1.069427	-0.000039
20	6	0	-4.467405	-0.709929	-0.357176
21	6	0	-2.879827	-2.387659	0.386446
22	6	0	-5.478397	-1.650004	-0.351627
23	1	0	-4.681611	0.313109	-0.646385
24	6	0	-3.890173	-3.332810	0.385351
25	1	0	-1.888284	-2.682450	0.702485
26	6	0	-5.174305	-2.956897	0.013061
27	1	0	-6.488427	-1.381172	-0.630969
28	1	0	-3.687320	-4.354322	0.678863
29	6	0	3.257718	-1.186550	-0.109696
30	6	0	4.066933	-0.668697	0.912421
31	6	0	3.808466	-2.083368	-1.037243
32	6	0	5.407879	-1.009141	0.985510
33	1	0	3.635689	-0.019164	1.664763
34	6	0	5.147692	-2.421496	-0.979232
35	1	0	3.168542	-2.497762	-1.806844
36	6	0	5.929377	-1.874497	0.032951
37	1	0	6.041018	-0.620117	1.771885
38	1	0	5.585204	-3.101714	-1.697824
39	7	0	-6.235930	-3.962014	0.008538
40	8	0	-5.950400	-5.097757	0.335171
41	8	0	-7.352273	-3.612845	-0.323925
42	7	0	7.348155	-2.235129	0.106717
43	8	0	8.020073	-1.738175	0.989416
44	8	0	7.784435	-3.011617	-0.720235
45	7	0	-1.084007	6.304893	-0.029912
46	8	0	-1.942836	6.712791	0.725312
47	8	0	-0.460567	7.009909	-0.796646

Structure 43b (DMSO)

Energy (Hartrees): -1533.91377862
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.559556	3.016676	-0.745860
2	6	0	-0.326603	4.382502	-0.726154
3	6	0	0.661904	4.872535	0.116644
4	6	0	1.412199	4.045247	0.941113
5	6	0	1.162541	2.682365	0.912393
6	6	0	0.180554	2.145550	0.066711
7	1	0	-1.315790	2.620293	-1.413961
8	1	0	-0.893785	5.053170	-1.357828
9	1	0	2.162917	4.459552	1.600721
10	1	0	1.719238	2.032664	1.578514
11	6	0	-0.100300	0.694199	0.045540
12	6	0	0.869376	-0.262195	0.007874
13	6	0	-1.493602	0.267641	0.056000
14	1	0	-2.233079	1.066030	0.181663
15	1	0	0.559200	-1.300359	0.035387
16	7	0	-1.860599	-0.957616	-0.032302
17	7	0	2.200417	-0.044024	-0.109806
18	1	0	2.517907	0.903529	-0.289418
19	6	0	3.194771	-1.015353	-0.090940
20	6	0	4.488823	-0.633750	-0.479548
21	6	0	2.949576	-2.336138	0.311815
22	6	0	5.516984	-1.554702	-0.485378
23	1	0	4.675514	0.390270	-0.783612
24	6	0	3.976791	-3.261962	0.298531
25	1	0	1.971369	-2.647534	0.652602
26	6	0	5.246845	-2.864434	-0.101450
27	1	0	6.514249	-1.265410	-0.789001
28	1	0	3.795240	-4.282650	0.608033
29	6	0	-3.225751	-1.254702	-0.030138
30	6	0	-4.166676	-0.492992	-0.741449
31	6	0	-3.649541	-2.397000	0.665618
32	6	0	-5.506176	-0.842764	-0.726450
33	1	0	-3.841902	0.361009	-1.324369
34	6	0	-4.985751	-2.750715	0.692490
35	1	0	-2.914293	-2.992723	1.193298
36	6	0	-5.897393	-1.963687	-0.003987
37	1	0	-6.236894	-0.262782	-1.274558
38	1	0	-5.319222	-3.622538	1.239686
39	7	0	6.327631	-3.845277	-0.110809
40	8	0	6.067436	-4.991453	0.206927
41	8	0	7.439558	-3.471791	-0.437444
42	7	0	-7.312423	-2.336527	0.013275
43	8	0	-8.103635	-1.618810	-0.569825
44	8	0	-7.632439	-3.346224	0.612502
45	7	0	0.917593	6.318756	0.141944
46	8	0	1.778519	6.734519	0.892701
47	8	0	0.255174	7.029055	-0.589051

Structure 43b (C_2H_5OH)

Energy (Hartrees): -1533.91246890
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.447350	2.965452	-0.847797
2	6	0	-0.186013	4.326161	-0.846954
3	6	0	0.716556	4.824152	0.084031
4	6	0	1.356863	4.013088	1.010703
5	6	0	1.082405	2.654651	0.995623
6	6	0	0.184895	2.110698	0.065623
7	1	0	-1.139634	2.559501	-1.576997
8	1	0	-0.663765	4.986574	-1.558534
9	1	0	2.042304	4.435628	1.733400
10	1	0	1.550057	2.012469	1.734067
11	6	0	-0.113925	0.661359	0.058965
12	6	0	0.848599	-0.301183	0.049713
13	6	0	-1.512390	0.253997	0.043248
14	1	0	-2.243646	1.069907	0.023450
15	1	0	0.528799	-1.335849	0.051631
16	7	0	-1.897402	-0.967426	0.099714
17	7	0	2.185330	-0.084215	-0.004145
18	1	0	2.509035	0.875704	-0.073010
19	6	0	3.182409	-1.050506	-0.034159
20	6	0	4.506484	-0.608589	-0.192571
21	6	0	2.917929	-2.422588	0.091647
22	6	0	5.547039	-1.512682	-0.233027
23	1	0	4.707957	0.452748	-0.286726
24	6	0	3.958724	-3.331103	0.045868
25	1	0	1.912131	-2.794426	0.228977
26	6	0	5.260264	-2.869763	-0.117115
27	1	0	6.566928	-1.173208	-0.355548
28	1	0	3.761251	-4.390810	0.139998
29	6	0	-3.265771	-1.242884	0.050235
30	6	0	-4.126133	-0.620775	-0.868070
31	6	0	-3.773869	-2.219779	0.920258
32	6	0	-5.472305	-0.942589	-0.894331
33	1	0	-3.731321	0.098659	-1.576051
34	6	0	-5.118475	-2.538065	0.912572
35	1	0	-3.098712	-2.710719	1.610986
36	6	0	-5.949609	-1.891472	0.002504
37	1	0	-6.141886	-0.470949	-1.601645
38	1	0	-5.519767	-3.276286	1.594265
39	7	0	6.350811	-3.829647	-0.164766
40	8	0	6.085302	-5.016407	-0.084736
41	8	0	7.488860	-3.409705	-0.283604
42	7	0	-7.368832	-2.228292	-0.018463
43	8	0	-8.079338	-1.696053	-0.852166
44	8	0	-7.787560	-3.026428	0.800437
45	7	0	1.001706	6.262075	0.090052
46	8	0	1.791705	6.689743	0.909534
47	8	0	0.436159	6.964864	-0.725316

Structure 43c (vacuum)

Energy (Hartrees): -1533.87483041
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.753310	2.427325	0.896754
2	6	0	-0.694940	3.812052	0.930790
3	6	0	0.114788	4.464352	0.013217
4	6	0	0.857013	3.785448	-0.939346
5	6	0	0.789691	2.399081	-0.958672
6	6	0	-0.004547	1.704739	-0.038445
7	1	0	-1.388035	1.898069	1.594924
8	1	0	-1.261193	4.388001	1.650141
9	1	0	1.458669	4.339067	-1.647421
10	1	0	1.339174	1.848226	-1.714366
11	6	0	-0.048366	0.223428	-0.057573
12	6	0	1.073849	-0.537822	-0.031930
13	6	0	-1.320363	-0.482288	-0.069843
14	1	0	0.978966	-1.617582	-0.056399
15	1	0	-1.254582	-1.579251	-0.075252
16	7	0	-2.448027	0.112091	-0.098157
17	7	0	2.350092	-0.069205	0.082416
18	1	0	2.460225	0.917047	0.281032
19	6	0	3.513646	-0.833541	0.045290
20	6	0	4.699348	-0.262879	0.529037
21	6	0	3.533722	-2.133032	-0.476173
22	6	0	5.881518	-0.978116	0.507120
23	1	0	4.683880	0.743013	0.932986
24	6	0	4.714755	-2.856594	-0.486598
25	1	0	2.643510	-2.575476	-0.901914
26	6	0	5.871468	-2.272473	0.005274
27	1	0	6.804815	-0.555110	0.879672
28	1	0	4.752937	-3.861167	-0.886000
29	6	0	-3.615810	-0.660343	-0.053813
30	6	0	-4.667634	-0.322063	-0.914172
31	6	0	-3.779003	-1.712821	0.856685
32	6	0	-5.843977	-1.050592	-0.902418
33	1	0	-4.536309	0.510930	-1.593047
34	6	0	-4.959598	-2.439053	0.885641
35	1	0	-2.989152	-1.937716	1.563476
36	6	0	-5.969684	-2.100462	-0.001037
37	1	0	-6.663860	-0.817019	-1.568134
38	1	0	-5.110527	-3.249732	1.585516
39	7	0	7.124976	-3.041468	-0.014680
40	8	0	7.079980	-4.174653	-0.443555
41	8	0	8.123640	-2.493522	0.400257
42	7	0	-7.225875	-2.869898	0.025466
43	8	0	-7.314062	-3.773436	0.829660
44	8	0	-8.093827	-2.554621	-0.760020
45	7	0	0.186546	5.940693	0.048527
46	8	0	0.900071	6.484114	-0.766280
47	8	0	-0.469288	6.511760	0.891320

Structure 43c ($CHCl_3$)

Energy (Hartrees): -1533.91741099
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.748768	2.405553	0.921070
2	6	0	-0.724841	3.790307	0.966146
3	6	0	0.040815	4.469075	0.027798
4	6	0	0.774764	3.815485	-0.950322
5	6	0	0.740812	2.428524	-0.979534
6	6	0	-0.012633	1.708573	-0.044593
7	1	0	-1.341565	1.857067	1.642043
8	1	0	-1.284847	4.337579	1.712501
9	1	0	1.346710	4.379615	-1.674758
10	1	0	1.288678	1.899456	-1.751643
11	6	0	-0.033870	0.226868	-0.081125
12	6	0	1.098270	-0.527988	-0.076572
13	6	0	-1.291343	-0.493591	-0.097018
14	1	0	1.007609	-1.607530	-0.125833
15	1	0	-1.210644	-1.587340	-0.088760
16	7	0	-2.431828	0.086501	-0.145553
17	7	0	2.366153	-0.052600	0.038151
18	1	0	2.482799	0.932912	0.246597
19	6	0	3.531508	-0.811168	0.011968
20	6	0	4.707033	-0.225601	0.505737
21	6	0	3.565224	-2.115684	-0.499506
22	6	0	5.893925	-0.930630	0.504944
23	1	0	4.675610	0.783596	0.900484
24	6	0	4.751603	-2.828228	-0.491496
25	1	0	2.682145	-2.572744	-0.925559
26	6	0	5.899368	-2.230827	0.012225
27	1	0	6.803866	-0.489512	0.889307
28	1	0	4.791696	-3.835280	-0.884985
29	6	0	-3.587955	-0.697130	-0.087350
30	6	0	-4.674649	-0.335061	-0.896923
31	6	0	-3.715677	-1.782374	0.792923
32	6	0	-5.848465	-1.065555	-0.865503
33	1	0	-4.575530	0.519809	-1.554712
34	6	0	-4.891393	-2.512795	0.841278
35	1	0	-2.898147	-2.033495	1.457889
36	6	0	-5.938003	-2.146493	0.005513
37	1	0	-6.688448	-0.803713	-1.495055
38	1	0	-5.003931	-3.346511	1.521516
39	7	0	7.152179	-2.984913	0.012979
40	8	0	7.133219	-4.127006	-0.403605
41	8	0	8.151093	-2.432228	0.431304
42	7	0	-7.184241	-2.915315	0.055169
43	8	0	-7.266575	-3.820860	0.862369
44	8	0	-8.074742	-2.612671	-0.714804
45	7	0	0.071546	5.940371	0.070279
46	8	0	0.739313	6.519766	-0.761977
47	8	0	-0.570683	6.498029	0.936190

Structure 43c (DMSO)

Energy (Hartrees): -1533.91774205
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.623238	2.467692	-0.977487
2	6	0	-0.569594	3.851972	-0.952537
3	6	0	0.112610	4.467931	0.089105
4	6	0	0.736488	3.751960	1.099575
5	6	0	0.672331	2.366072	1.058770
6	6	0	-0.000870	1.710055	0.021857
7	1	0	-1.145886	1.966816	-1.783061
8	1	0	-1.042019	4.442567	-1.726081
9	1	0	1.250677	4.264076	1.901984
10	1	0	1.139341	1.789518	1.849992
11	6	0	-0.054750	0.229208	-0.017000
12	6	0	1.059525	-0.554156	-0.012421
13	6	0	-1.322187	-0.465174	-0.060736
14	1	0	0.933662	-1.629838	-0.026955
15	1	0	-1.257088	-1.559066	-0.076540
16	7	0	-2.458042	0.131816	-0.090510
17	7	0	2.338271	-0.102882	-0.013900
18	1	0	2.485261	0.901199	-0.042620
19	6	0	3.494845	-0.871827	-0.038835
20	6	0	4.719366	-0.186995	-0.103534
21	6	0	3.485850	-2.274305	-0.000983
22	6	0	5.911585	-0.880490	-0.131890
23	1	0	4.721099	0.896713	-0.135922
24	6	0	4.680548	-2.971028	-0.030831
25	1	0	2.562176	-2.834054	0.051136
26	6	0	5.879150	-2.271090	-0.095095
27	1	0	6.854867	-0.353375	-0.183677
28	1	0	4.680292	-4.052527	-0.004007
29	6	0	-3.616730	-0.649493	-0.042153
30	6	0	-4.706105	-0.276421	-0.843843
31	6	0	-3.742762	-1.748675	0.821965
32	6	0	-5.880200	-1.007042	-0.820608
33	1	0	-4.611593	0.586751	-1.491932
34	6	0	-4.918071	-2.479275	0.862124
35	1	0	-2.922345	-2.014712	1.477775
36	6	0	-5.968034	-2.101298	0.034467
37	1	0	-6.719003	-0.733010	-1.446832
38	1	0	-5.023011	-3.324820	1.528849
39	7	0	7.135097	-3.012180	-0.129766
40	8	0	7.088132	-4.228374	-0.090114
41	8	0	8.173453	-2.379691	-0.198518
42	7	0	-7.211176	-2.872429	0.073600
43	8	0	-7.297967	-3.781921	0.877741
44	8	0	-8.099686	-2.570593	-0.701180
45	7	0	0.176367	5.937161	0.120782
46	8	0	0.822259	6.462360	1.006082
47	8	0	-0.419764	6.552924	-0.740635

Structure 43c (C_2H_5OH)

Energy (Hartrees): -1533.91672400
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.729777	2.437764	0.940510
2	6	0	-0.693667	3.821969	0.972226
3	6	0	0.078232	4.483235	0.025198
4	6	0	0.803391	3.813397	-0.949285
5	6	0	0.751449	2.427214	-0.968210
6	6	0	-0.005722	1.724498	-0.023339
7	1	0	-1.317184	1.902131	1.676046
8	1	0	-1.242759	4.378066	1.720441
9	1	0	1.381783	4.360526	-1.681901
10	1	0	1.292215	1.886917	-1.737548
11	6	0	-0.042752	0.243559	-0.041186
12	6	0	1.079897	-0.527992	-0.028933
13	6	0	-1.303714	-0.464515	-0.056909
14	1	0	0.969591	-1.606348	-0.061159
15	1	0	-1.231508	-1.557239	-0.016365
16	7	0	-2.442297	0.120292	-0.150610
17	7	0	2.352175	-0.066402	0.069074
18	1	0	2.486497	0.924416	0.244729
19	6	0	3.508498	-0.834169	0.031893
20	6	0	4.708373	-0.230616	0.442045
21	6	0	3.513362	-2.163880	-0.414141
22	6	0	5.889451	-0.943059	0.427876
23	1	0	4.700375	0.799242	0.780942
24	6	0	4.694288	-2.882783	-0.421455
25	1	0	2.610462	-2.637375	-0.775324
26	6	0	5.867235	-2.267883	0.001259
27	1	0	6.815309	-0.484323	0.748920
28	1	0	4.707013	-3.909002	-0.764414
29	6	0	-3.595851	-0.664375	-0.090795
30	6	0	-4.654708	-0.360183	-0.959994
31	6	0	-3.748309	-1.699682	0.845649
32	6	0	-5.822220	-1.099067	-0.931528
33	1	0	-4.539427	0.453618	-1.665769
34	6	0	-4.917555	-2.438826	0.890488
35	1	0	-2.953975	-1.906106	1.553289
36	6	0	-5.935499	-2.131944	-0.004748
37	1	0	-6.636222	-0.878984	-1.609493
38	1	0	-5.042593	-3.235230	1.612217
39	7	0	7.107199	-3.027369	-0.008445
40	8	0	7.075681	-4.187947	-0.378519
41	8	0	8.129604	-2.473136	0.355786
42	7	0	-7.168819	-2.909037	0.037857
43	8	0	-7.268802	-3.794377	0.868440
44	8	0	-8.050233	-2.643488	-0.759601
45	7	0	0.129252	5.948655	0.057392
46	8	0	0.891930	6.515010	-0.701375
47	8	0	-0.591750	6.532782	0.842616

Structure 43d (vacuum)

Energy (Hartrees): -1533.86921125
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.354660	2.688999	0.749305
2	6	0	1.676782	4.032013	0.849591
3	6	0	0.985120	4.942800	0.063604
4	6	0	-0.006756	4.554399	-0.820549
5	6	0	-0.313963	3.204192	-0.912841
6	6	0	0.346023	2.256836	-0.121685
7	1	0	1.884684	1.968069	1.356352
8	1	0	2.445349	4.383314	1.524622
9	1	0	-0.507549	5.296702	-1.427112
10	1	0	-1.058673	2.878262	-1.629535
11	6	0	-0.046704	0.830589	-0.185089
12	6	0	-1.365873	0.516718	-0.256463
13	6	0	0.957414	-0.225363	-0.143513
14	1	0	0.590037	-1.245741	0.032349
15	1	0	-1.311679	-1.430019	-0.907895
16	1	0	-2.103486	1.306461	-0.157284
17	7	0	2.206190	-0.008346	-0.286417
18	7	0	-1.895223	-0.728642	-0.477790
19	6	0	3.095739	-1.081811	-0.142233
20	6	0	4.159837	-1.177951	-1.047115
21	6	0	2.982039	-2.016134	0.895564
22	6	0	5.065772	-2.219614	-0.953646
23	1	0	4.251899	-0.428394	-1.822944
24	6	0	3.894055	-3.054910	1.005700
25	1	0	2.198442	-1.905765	1.635856
26	6	0	4.915034	-3.144024	0.072574
27	1	0	5.886174	-2.322917	-1.650812
28	1	0	3.830470	-3.784128	1.802134
29	6	0	-3.229186	-1.075963	-0.274974
30	6	0	-3.727561	-2.227421	-0.899778
31	6	0	-4.069259	-0.311670	0.543813
32	6	0	-5.046565	-2.600970	-0.728053
33	1	0	-3.076748	-2.821825	-1.531348
34	6	0	-5.396535	-0.675270	0.704130
35	1	0	-3.686008	0.545559	1.081108
36	6	0	-5.868087	-1.811421	0.065999
37	1	0	-5.450835	-3.484332	-1.203759
38	1	0	-6.063069	-0.099435	1.332283
39	7	0	-7.274955	-2.201602	0.246238
40	8	0	-7.967244	-1.493198	0.944949
41	8	0	-7.652569	-3.206738	-0.316851
42	7	0	5.884372	-4.248925	0.183809
43	8	0	6.768700	-4.303827	-0.643132
44	8	0	5.735205	-5.036117	1.093822
45	7	0	1.323576	6.376470	0.167512
46	8	0	0.691556	7.151540	-0.517158
47	8	0	2.210771	6.688010	0.931677

Structure 43d ($CHCl_3$)

Energy (Hartrees): -1533.91285956
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.357369	2.671886	0.729402
2	6	0	1.681761	4.013164	0.840051
3	6	0	0.977619	4.933507	0.073621
4	6	0	-0.031574	4.553812	-0.797592
5	6	0	-0.339026	3.205385	-0.901072
6	6	0	0.337079	2.247132	-0.134363
7	1	0	1.891981	1.947353	1.328797
8	1	0	2.460700	4.347109	1.512375
9	1	0	-0.550002	5.295249	-1.390704
10	1	0	-1.101286	2.890286	-1.604007
11	6	0	-0.050337	0.821029	-0.215234
12	6	0	-1.375126	0.511010	-0.289927
13	6	0	0.951754	-0.231971	-0.173821
14	1	0	0.586702	-1.254257	-0.018305
15	1	0	-1.323867	-1.446989	-0.914018
16	1	0	-2.107706	1.304339	-0.181588
17	7	0	2.205278	-0.010693	-0.303881
18	7	0	-1.908039	-0.724926	-0.512109
19	6	0	3.096132	-1.079687	-0.154371
20	6	0	4.193332	-1.145968	-1.024173
21	6	0	2.956566	-2.039939	0.858800
22	6	0	5.107804	-2.178226	-0.921756
23	1	0	4.307071	-0.382663	-1.784333
24	6	0	3.874387	-3.071217	0.977056
25	1	0	2.144642	-1.959357	1.572088
26	6	0	4.931156	-3.128415	0.078808
27	1	0	5.950181	-2.248630	-1.596839
28	1	0	3.780532	-3.815405	1.756835
29	6	0	-3.238268	-1.068428	-0.298523
30	6	0	-3.722380	-2.253353	-0.873273
31	6	0	-4.088157	-0.275786	0.484904
32	6	0	-5.037397	-2.631142	-0.689485
33	1	0	-3.059923	-2.868179	-1.472195
34	6	0	-5.410092	-0.645845	0.660028
35	1	0	-3.716355	0.610057	0.982066
36	6	0	-5.869877	-1.815245	0.069828
37	1	0	-5.422070	-3.540697	-1.131191
38	1	0	-6.075194	-0.043736	1.264785
39	7	0	-7.264863	-2.208473	0.264557
40	8	0	-7.974914	-1.483966	0.934582
41	8	0	-7.645954	-3.240033	-0.254169
42	7	0	5.902641	-4.220391	0.197400
43	8	0	6.803933	-4.274038	-0.615838
44	8	0	5.757452	-5.019620	1.101435
45	7	0	1.315726	6.358834	0.187478
46	8	0	0.656886	7.154380	-0.451939
47	8	0	2.235477	6.670132	0.917010

Structure 43d (DMSO)

Energy (Hartrees): -1533.91397261
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.363253	2.666940	0.758503
2	6	0	1.692692	4.008110	0.850655
3	6	0	0.992499	4.920434	0.069959
4	6	0	-0.019446	4.530808	-0.794796
5	6	0	-0.331817	3.182313	-0.879791
6	6	0	0.341977	2.232236	-0.100473
7	1	0	1.890337	1.950319	1.374622
8	1	0	2.470408	4.345571	1.522822
9	1	0	-0.540100	5.262428	-1.398076
10	1	0	-1.099962	2.862152	-1.574123
11	6	0	-0.046565	0.805641	-0.155486
12	6	0	-1.376332	0.500012	-0.204178
13	6	0	0.958106	-0.241123	-0.125570
14	1	0	0.607664	-1.265062	0.042832
15	1	0	-1.320204	-1.505566	-0.630944
16	1	0	-2.096320	1.307192	-0.129236
17	7	0	2.208580	-0.013231	-0.295713
18	7	0	-1.919345	-0.736323	-0.354606
19	6	0	3.106023	-1.077326	-0.160811
20	6	0	4.185712	-1.146561	-1.053246
21	6	0	2.992134	-2.032085	0.861442
22	6	0	5.107097	-2.173530	-0.962852
23	1	0	4.281820	-0.391483	-1.824306
24	6	0	3.916176	-3.058411	0.967167
25	1	0	2.191760	-1.953878	1.587822
26	6	0	4.955975	-3.117641	0.048103
27	1	0	5.933676	-2.242180	-1.657455
28	1	0	3.836140	-3.797082	1.753923
29	6	0	-3.262588	-1.057644	-0.200738
30	6	0	-3.679862	-2.331774	-0.618618
31	6	0	-4.192407	-0.171608	0.362804
32	6	0	-5.000474	-2.711841	-0.494632
33	1	0	-2.955761	-3.016745	-1.045312
34	6	0	-5.519086	-0.546737	0.477247
35	1	0	-3.892171	0.798387	0.735317
36	6	0	-5.910243	-1.808691	0.047203
37	1	0	-5.325040	-3.691991	-0.817709
38	1	0	-6.241769	0.131603	0.911233
39	7	0	-7.309011	-2.202548	0.180534
40	8	0	-8.090155	-1.399469	0.657379
41	8	0	-7.630813	-3.316330	-0.191629
42	7	0	5.934952	-4.201151	0.154511
43	8	0	6.825930	-4.252718	-0.672512
44	8	0	5.811297	-4.999922	1.063859
45	7	0	1.336581	6.343796	0.163200
46	8	0	0.678884	7.136205	-0.483694
47	8	0	2.262390	6.662658	0.884315

Structure 43d (C_2H_5OH)

Energy (Hartrees): -1533.91276409
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.346609	2.674619	0.765210
2	6	0	1.667746	4.017178	0.857919
3	6	0	0.970382	4.922926	0.066344
4	6	0	-0.028634	4.526612	-0.810937
5	6	0	-0.332813	3.176502	-0.894901
6	6	0	0.336580	2.233300	-0.103544
7	1	0	1.869475	1.962194	1.389898
8	1	0	2.434842	4.360934	1.539113
9	1	0	-0.544836	5.253522	-1.423925
10	1	0	-1.089781	2.848820	-1.598105
11	6	0	-0.046249	0.805306	-0.154116
12	6	0	-1.374131	0.495079	-0.202010
13	6	0	0.963193	-0.237221	-0.121832
14	1	0	0.618447	-1.260871	0.059624
15	1	0	-1.309213	-1.510543	-0.629657
16	1	0	-2.097713	1.299496	-0.131346
17	7	0	2.210945	-0.006808	-0.306895
18	7	0	-1.911662	-0.745409	-0.349230
19	6	0	3.110984	-1.068095	-0.170041
20	6	0	4.170434	-1.158829	-1.084737
21	6	0	3.018888	-1.998055	0.876874
22	6	0	5.093687	-2.183073	-0.990097
23	1	0	4.249366	-0.422601	-1.875692
24	6	0	3.944410	-3.021762	0.987252
25	1	0	2.234719	-1.901187	1.618661
26	6	0	4.964289	-3.102400	0.047032
27	1	0	5.903845	-2.268240	-1.702107
28	1	0	3.881995	-3.740526	1.793718
29	6	0	-3.252586	-1.071694	-0.194337
30	6	0	-3.668074	-2.344669	-0.618873
31	6	0	-4.182514	-0.190588	0.377722
32	6	0	-4.987322	-2.727196	-0.496116
33	1	0	-2.943980	-3.026054	-1.051429
34	6	0	-5.508116	-0.566968	0.490462
35	1	0	-3.881761	0.776122	0.758445
36	6	0	-5.897684	-1.827041	0.051344
37	1	0	-5.311260	-3.705395	-0.826030
38	1	0	-6.231187	0.107349	0.930273
39	7	0	-7.292004	-2.219569	0.177371
40	8	0	-8.083512	-1.414001	0.635321
41	8	0	-7.615221	-3.338474	-0.181577
42	7	0	5.942682	-4.179851	0.159993
43	8	0	6.840771	-4.235953	-0.660066
44	8	0	5.819885	-4.981000	1.068585
45	7	0	1.301384	6.344943	0.164131
46	8	0	0.654590	7.136579	-0.495839
47	8	0	2.208882	6.676632	0.903485

4. Computational data: cartesian coordinates for all optimized structures at B3LYP/6311++G(d,p) level:

Structure 32a (vacuum)

Energy (Hartrees): -632.352282811
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.139830	1.197425	0.708252
2	6	0	0.758351	1.281206	0.629954
3	6	0	-0.005400	0.292261	-0.018023
4	6	0	0.690998	-0.782156	-0.581852
5	6	0	2.080579	-0.892245	-0.494834
6	6	0	2.813839	0.105417	0.149616
7	1	0	2.718792	1.962185	1.212295
8	1	0	0.257598	2.120961	1.099114
9	1	0	0.143988	-1.545717	-1.124961
10	1	0	2.571703	-1.742198	-0.949639
11	6	0	-1.483185	0.393754	-0.099456
12	6	0	-2.276958	-0.705614	0.178156
13	1	0	-1.806857	-1.632286	0.499676
14	6	0	-2.102945	1.639277	-0.477774
15	1	0	-1.410190	2.472231	-0.697115
16	1	0	-4.042450	0.145796	-0.179344
17	7	0	-3.611930	-0.739993	0.093167
18	6	0	-4.428921	-1.869391	0.491759
19	1	0	-5.156319	-2.108923	-0.288085
20	1	0	-3.794753	-2.743589	0.650270
21	1	0	-4.971979	-1.663754	1.420337
22	8	0	-3.321785	1.829900	-0.584453
23	8	0	4.174274	0.109101	0.284105
24	6	0	4.912026	-0.971841	-0.266818
25	1	0	4.780207	-1.034858	-1.352734
26	1	0	5.957311	-0.764210	-0.043202
27	1	0	4.627264	-1.926249	0.190117

Structure 32a ($CHCl_3$)

Energy (Hartrees): -632.370670406
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.143094	1.207792	0.694675
2	6	0	0.759948	1.292835	0.618971
3	6	0	-0.007567	0.294124	-0.010502
4	6	0	0.686374	-0.795167	-0.552471
5	6	0	2.076311	-0.905519	-0.468346
6	6	0	2.814162	0.104569	0.153170
7	1	0	2.720391	1.984127	1.184335
8	1	0	0.263395	2.143789	1.072934
9	1	0	0.137661	-1.573978	-1.071967
10	1	0	2.566167	-1.766329	-0.904282
11	6	0	-1.486874	0.401920	-0.097282
12	6	0	-2.284140	-0.703602	0.184856
13	1	0	-1.813080	-1.631609	0.498801
14	6	0	-2.091369	1.643047	-0.479455
15	1	0	-1.393836	2.466242	-0.714214
16	1	0	-4.059183	0.136527	-0.159491
17	7	0	-3.612574	-0.737946	0.116397
18	6	0	-4.429537	-1.889251	0.459499
19	1	0	-5.072822	-2.163099	-0.380930
20	1	0	-3.787528	-2.737389	0.700744
21	1	0	-5.062354	-1.670065	1.324492
22	8	0	-3.315591	1.853480	-0.581114
23	8	0	4.174802	0.105640	0.280292
24	6	0	4.911734	-0.977697	-0.285035
25	1	0	4.766214	-1.035219	-1.368712
26	1	0	5.959488	-0.766296	-0.073866
27	1	0	4.636998	-1.932343	0.175467

Structure 32a (DMSO)

Energy (Hartrees): -632.369929614
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.152285	1.243271	0.629353
2	6	0	0.767584	1.326511	0.568687
3	6	0	-0.009521	0.303735	-0.009430
4	6	0	0.678430	-0.809184	-0.512241
5	6	0	2.069228	-0.917843	-0.440280
6	6	0	2.817429	0.117640	0.126657
7	1	0	2.733247	2.039778	1.081271
8	1	0	0.279891	2.196370	0.995314
9	1	0	0.124320	-1.612130	-0.987215
10	1	0	2.551332	-1.798843	-0.843617
11	6	0	-1.489328	0.409303	-0.083648
12	6	0	-2.281188	-0.708356	0.177684
13	1	0	-1.805185	-1.641686	0.466435
14	6	0	-2.097421	1.654338	-0.441892
15	1	0	-1.400734	2.480920	-0.667298
16	1	0	-4.065588	0.125472	-0.140940
17	7	0	-3.607405	-0.748402	0.114871
18	6	0	-4.414554	-1.917575	0.424010
19	1	0	-5.043661	-2.179908	-0.430582
20	1	0	-3.763495	-2.760889	0.656157
21	1	0	-5.060616	-1.720333	1.283974
22	8	0	-3.322514	1.868627	-0.534200
23	8	0	4.178153	0.122997	0.232351
24	6	0	4.898575	-1.020814	-0.233284
25	1	0	4.748621	-1.178481	-1.305954
26	1	0	5.950114	-0.807179	-0.044905
27	1	0	4.609362	-1.923422	0.314372

Structure 32a (C_2H_5OH)

Energy (Hartrees): -632.372936422
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.148270	1.232639	0.652032
2	6	0	0.763847	1.318094	0.588389
3	6	0	-0.010431	0.304737	-0.008216
4	6	0	0.676385	-0.801750	-0.525681
5	6	0	2.066833	-0.912626	-0.451642
6	6	0	2.810902	0.113922	0.133685
7	1	0	2.729629	2.021313	1.117332
8	1	0	0.274703	2.181582	1.026357
9	1	0	0.122413	-1.596399	-1.014718
10	1	0	2.550758	-1.787112	-0.866695
11	6	0	-1.490632	0.413839	-0.088023
12	6	0	-2.283778	-0.704110	0.182271
13	1	0	-1.804274	-1.631971	0.482304
14	6	0	-2.089030	1.653303	-0.454500
15	1	0	-1.393369	2.476809	-0.685552
16	1	0	-4.073199	0.114739	-0.151140
17	7	0	-3.607202	-0.750550	0.117157
18	6	0	-4.410032	-1.921946	0.433348
19	1	0	-5.037746	-2.189715	-0.420323
20	1	0	-3.756534	-2.761730	0.670487
21	1	0	-5.056863	-1.720517	1.291562
22	8	0	-3.320357	1.873679	-0.549119
23	8	0	4.177019	0.115921	0.245392
24	6	0	4.903912	-1.013249	-0.250481
25	1	0	4.754955	-1.138457	-1.327189
26	1	0	5.953555	-0.798738	-0.052827
27	1	0	4.615626	-1.929870	0.273035

Structure 32b (vacuum)

Energy (Hartrees): -632.345481740
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.881130	-1.067195	1.002489
2	6	0	-0.506087	-1.205865	0.893027
3	6	0	0.239668	-0.452679	-0.032945
4	6	0	-0.466346	0.444619	-0.842732
5	6	0	-1.850146	0.604907	-0.737909
6	6	0	-2.565534	-0.156532	0.188784
7	1	0	-2.447669	-1.651105	1.718136
8	1	0	0.006267	-1.905449	1.544549
9	1	0	0.067097	1.014867	-1.596344
10	1	0	-2.351525	1.305920	-1.392105
11	6	0	1.708683	-0.627934	-0.154520
12	6	0	2.604257	0.400109	-0.044771
13	1	0	3.656874	0.150526	-0.148054
14	6	0	2.261187	-1.963547	-0.380396
15	1	0	1.495522	-2.762638	-0.464224
16	1	0	1.373230	1.952158	0.364932
17	7	0	2.334894	1.704817	0.175177
18	6	0	3.355352	2.684355	0.512521
19	1	0	3.515455	2.763495	1.594349
20	1	0	4.298232	2.398315	0.044480
21	1	0	3.070031	3.666150	0.129256
22	8	0	3.445756	-2.247761	-0.482247
23	8	0	-3.916409	-0.088008	0.373721
24	6	0	-4.669313	0.799144	-0.441653
25	1	0	-4.360557	1.839839	-0.292915
26	1	0	-4.579718	0.540488	-1.502374
27	1	0	-5.705802	0.683569	-0.129086

Structure 32b ($CHCl_3$)

Energy (Hartrees): -632.366413590
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.893113	-1.109851	0.959574
2	6	0	-0.515847	-1.244956	0.855822
3	6	0	0.237612	-0.458567	-0.036088
4	6	0	-0.463072	0.469927	-0.816835
5	6	0	-1.847432	0.627731	-0.716314
6	6	0	-2.571148	-0.167651	0.176069
7	1	0	-2.461016	-1.721932	1.651275
8	1	0	-0.010805	-1.969285	1.486142
9	1	0	0.073797	1.075414	-1.540153
10	1	0	-2.343211	1.355852	-1.344893
11	6	0	1.709959	-0.632029	-0.150870
12	6	0	2.612351	0.401868	-0.014207
13	1	0	3.665874	0.160226	-0.122234
14	6	0	2.251399	-1.952928	-0.391758
15	1	0	1.485033	-2.743796	-0.512479
16	1	0	1.387369	1.957799	0.402336
17	7	0	2.350074	1.685422	0.249645
18	6	0	3.366919	2.703554	0.466564
19	1	0	3.402355	3.007327	1.517402
20	1	0	4.341487	2.305373	0.184212
21	1	0	3.158889	3.584543	-0.145818
22	8	0	3.443225	-2.262151	-0.477793
23	8	0	-3.922768	-0.101725	0.352713
24	6	0	-4.667472	0.841972	-0.417465
25	1	0	-4.346513	1.867907	-0.209836
26	1	0	-4.582671	0.637329	-1.489525
27	1	0	-5.705693	0.721880	-0.110262

Structure 32b (DMSO)

Energy (Hartrees): -632.366632581
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.908293	-1.160959	0.900108
2	6	0	-0.529668	-1.292072	0.802769
3	6	0	0.235140	-0.455214	-0.032527
4	6	0	-0.456864	0.523343	-0.759240
5	6	0	-1.841756	0.677975	-0.662763
6	6	0	-2.578127	-0.171101	0.168927
7	1	0	-2.480674	-1.815154	1.548547
8	1	0	-0.033548	-2.054819	1.393696
9	1	0	0.085594	1.175619	-1.436131
10	1	0	-2.328267	1.448231	-1.246641
11	6	0	1.706413	-0.632121	-0.145675
12	6	0	2.617301	0.398830	-0.004822
13	1	0	3.669284	0.150817	-0.111788
14	6	0	2.237638	-1.953431	-0.392864
15	1	0	1.463085	-2.734349	-0.527746
16	1	0	1.407927	1.972716	0.397116
17	7	0	2.368097	1.679416	0.264483
18	6	0	3.394043	2.695253	0.449461
19	1	0	3.373131	3.082028	1.472206
20	1	0	4.373554	2.257395	0.258076
21	1	0	3.236625	3.526984	-0.242221
22	8	0	3.427011	-2.279429	-0.474631
23	8	0	-3.930783	-0.114073	0.330666
24	6	0	-4.661028	0.874282	-0.401480
25	1	0	-4.351309	1.886251	-0.122607
26	1	0	-4.543854	0.736835	-1.480773
27	1	0	-5.706850	0.730851	-0.132771

Structure 32b (C_2H_5OH)

Energy (Hartrees): -632.370471028
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.891591	-1.116050	0.955577
2	6	0	-0.513525	-1.249897	0.852192
3	6	0	0.238460	-0.459015	-0.036303
4	6	0	-0.461072	0.474601	-0.812164
5	6	0	-1.845383	0.631183	-0.711793
6	6	0	-2.567691	-0.170091	0.175768
7	1	0	-2.457769	-1.732495	1.645350
8	1	0	-0.008626	-1.977252	1.479362
9	1	0	0.074851	1.088303	-1.529156
10	1	0	-2.340994	1.364585	-1.334283
11	6	0	1.711599	-0.634354	-0.151806
12	6	0	2.617581	0.405060	-0.005462
13	1	0	3.672849	0.170779	-0.109167
14	6	0	2.241160	-1.945610	-0.394903
15	1	0	1.476196	-2.733210	-0.521903
16	1	0	1.386114	1.958180	0.391969
17	7	0	2.351873	1.677407	0.269398
18	6	0	3.362144	2.710162	0.454299
19	1	0	3.317860	3.109050	1.471296
20	1	0	4.350669	2.284321	0.284077
21	1	0	3.202009	3.530019	-0.250648
22	8	0	3.440738	-2.271179	-0.481419
23	8	0	-3.923337	-0.104251	0.351080
24	6	0	-4.666876	0.847163	-0.418984
25	1	0	-4.340182	1.869360	-0.206503
26	1	0	-4.578972	0.642881	-1.490152
27	1	0	-5.705164	0.728174	-0.111844

Structure 32c (vacuum)

Energy (Hartrees): -632.346504613
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.796401	1.012927	0.954594
2	6	0	0.431442	1.209621	0.828848
3	6	0	-0.340539	0.428780	-0.050746
4	6	0	0.325877	-0.538369	-0.809902
5	6	0	1.702735	-0.748472	-0.694023
6	6	0	2.444274	0.029394	0.196458
7	1	0	2.387401	1.617176	1.632525
8	1	0	-0.048918	1.986798	1.409104
9	1	0	-0.227612	-1.125221	-1.535774
10	1	0	2.176106	-1.501368	-1.310199
11	6	0	-1.802778	0.641751	-0.178571
12	6	0	-2.721844	-0.367631	-0.089255
13	1	0	-3.773692	-0.114496	-0.200648
14	6	0	-2.357129	1.976840	-0.369150
15	1	0	-3.466309	1.989321	-0.471017
16	1	0	-1.533477	-1.944610	0.336995
17	7	0	-2.485579	-1.684946	0.116888
18	6	0	-3.532704	-2.623014	0.489847
19	1	0	-3.741751	-2.614711	1.566617
20	1	0	-4.452036	-2.372895	-0.042818
21	1	0	-3.240462	-3.633553	0.199449
22	8	0	-1.733318	3.022349	-0.414293
23	8	0	3.790450	-0.086234	0.393724
24	6	0	4.508473	-1.043255	-0.371611
25	1	0	4.154489	-2.061402	-0.174524
26	1	0	4.435476	-0.833749	-1.444444
27	1	0	5.547536	-0.957018	-0.057867

Structure 32c ($CHCl_3$)

Energy (Hartrees): -632.368716106
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.777901	0.882805	1.088714
2	6	0	0.412244	1.089786	0.964576
3	6	0	-0.341302	0.431748	-0.023663
4	6	0	0.341066	-0.432972	-0.885985
5	6	0	1.716455	-0.655175	-0.773481
6	6	0	2.441773	0.005872	0.220385
7	1	0	2.350721	1.395164	1.853521
8	1	0	-0.081729	1.774256	1.644482
9	1	0	-0.200959	-0.936512	-1.680050
10	1	0	2.202901	-1.327075	-1.468270
11	6	0	-1.805849	0.660965	-0.150372
12	6	0	-2.735943	-0.351238	-0.042421
13	1	0	-3.787378	-0.097941	-0.154223
14	6	0	-2.343709	1.979305	-0.374603
15	1	0	-3.451658	2.008939	-0.444754
16	1	0	-1.544883	-1.940066	0.346326
17	7	0	-2.501602	-1.647615	0.193554
18	6	0	-3.539873	-2.648016	0.388204
19	1	0	-3.595748	-2.962537	1.435101
20	1	0	-4.503604	-2.229494	0.097493
21	1	0	-3.341632	-3.526396	-0.230936
22	8	0	-1.708439	3.027602	-0.490738
23	8	0	3.784307	-0.133641	0.422416
24	6	0	4.521618	-0.990447	-0.449287
25	1	0	4.167451	-2.024587	-0.387214
26	1	0	4.470023	-0.643344	-1.486180
27	1	0	5.554473	-0.944585	-0.106012

Structure 32c (DMSO)

Energy (Hartrees): -632.370008220
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.777463	0.869895	1.104889
2	6	0	0.410399	1.074274	0.983280
3	6	0	-0.340497	0.434925	-0.019316
4	6	0	0.345820	-0.412833	-0.895667
5	6	0	1.721990	-0.632981	-0.786353
6	6	0	2.445936	0.011879	0.220072
7	1	0	2.344704	1.366099	1.884716
8	1	0	-0.086797	1.738278	1.681451
9	1	0	-0.194851	-0.911185	-1.693889
10	1	0	2.209229	-1.295583	-1.489472
11	6	0	-1.805942	0.662590	-0.140217
12	6	0	-2.736302	-0.354238	-0.029089
13	1	0	-3.788386	-0.100661	-0.132281
14	6	0	-2.346215	1.975393	-0.368329
15	1	0	-3.454660	2.001866	-0.420677
16	1	0	-1.542640	-1.949891	0.329874
17	7	0	-2.500318	-1.646347	0.202602
18	6	0	-3.537082	-2.654137	0.369679
19	1	0	-3.538813	-3.043148	1.391997
20	1	0	-4.509608	-2.208312	0.161495
21	1	0	-3.375128	-3.485693	-0.320877
22	8	0	-1.715608	3.027056	-0.510599
23	8	0	3.787049	-0.128248	0.418645
24	6	0	4.515327	-0.997411	-0.453146
25	1	0	4.145183	-2.025372	-0.390679
26	1	0	4.468778	-0.650763	-1.490068
27	1	0	5.548311	-0.965809	-0.108980

Structure 32c (C_2H_5OH)

Energy (Hartrees):
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.759488	0.771182	1.174103
2	6	0	0.394414	0.986550	1.047416
3	6	0	-0.340309	0.420594	-0.008948
4	6	0	0.354126	-0.370492	-0.930294
5	6	0	1.727777	-0.601409	-0.815909
6	6	0	2.436150	-0.024452	0.240375
7	1	0	2.317568	1.214126	1.991745
8	1	0	-0.112540	1.603937	1.781159
9	1	0	-0.177390	-0.811895	-1.767234
10	1	0	2.225070	-1.216728	-1.553914
11	6	0	-1.801976	0.674182	-0.142901
12	6	0	-2.752862	-0.328169	-0.035488
13	1	0	-3.800236	-0.059319	-0.146259
14	6	0	-2.310919	1.988076	-0.373340
15	1	0	-3.413459	2.051180	-0.439986
16	1	0	-1.578230	-1.934916	0.319744
17	7	0	-2.533776	-1.617334	0.207275
18	6	0	-3.580331	-2.622436	0.331406
19	1	0	-3.509667	-3.125607	1.298909
20	1	0	-4.555003	-2.141376	0.253515
21	1	0	-3.492229	-3.372254	-0.459781
22	8	0	-1.645085	3.031435	-0.505120
23	8	0	3.780626	-0.175530	0.444402
24	6	0	4.533888	-0.947066	-0.498331
25	1	0	4.192511	-1.986178	-0.521510
26	1	0	4.473854	-0.513017	-1.500714
27	1	0	5.565169	-0.913219	-0.149388

Structure 32d (vacuum)

Energy (Hartrees): -632.338543040
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.034593	1.094496	0.744057
2	6	0	0.661377	1.241448	0.645023
3	6	0	-0.129060	0.288767	-0.025185
4	6	0	0.531775	-0.794983	-0.611463
5	6	0	1.915659	-0.960899	-0.513810
6	6	0	2.674567	-0.011263	0.170204
7	1	0	2.637369	1.829400	1.264309
8	1	0	0.190072	2.108110	1.088902
9	1	0	-0.036246	-1.522285	-1.182127
10	1	0	2.380050	-1.814151	-0.989767
11	6	0	-1.606420	0.415074	-0.098486
12	6	0	-2.381337	-0.703793	0.087846
13	1	0	-1.884491	-1.617853	0.404341
14	6	0	-2.232538	1.707445	-0.340407
15	1	0	-3.345855	1.706523	-0.305274
16	1	0	-4.257875	-0.067910	-0.393157
17	7	0	-3.715981	-0.869232	-0.107757
18	6	0	-4.454593	-1.966310	0.498891
19	1	0	-5.357222	-2.164687	-0.081209
20	1	0	-3.838095	-2.867526	0.485019
21	1	0	-4.741594	-1.760260	1.537321
22	8	0	-1.662718	2.765549	-0.545678
23	8	0	4.031792	-0.063679	0.324720
24	6	0	4.736196	-1.155325	-0.247322
25	1	0	4.619206	-1.181282	-1.336491
26	1	0	5.785095	-0.995254	-0.002249
27	1	0	4.407555	-2.111120	0.176248

Structure 32d ($CHCl_3$)

Energy (Hartrees): -632.361282855
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.037744	1.069697	0.789574
2	6	0	0.662506	1.218460	0.697064
3	6	0	-0.131671	0.288024	-0.000230
4	6	0	0.528243	-0.785119	-0.609685
5	6	0	1.912910	-0.954401	-0.519174
6	6	0	2.676132	-0.020546	0.183074
7	1	0	2.637828	1.791980	1.331788
8	1	0	0.193353	2.068853	1.175828
9	1	0	-0.042278	-1.504774	-1.187696
10	1	0	2.376597	-1.798180	-1.012794
11	6	0	-1.609278	0.431635	-0.079843
12	6	0	-2.400831	-0.685796	0.128546
13	1	0	-1.910972	-1.597696	0.461285
14	6	0	-2.215649	1.709531	-0.361335
15	1	0	-3.324166	1.725255	-0.328720
16	1	0	-4.269799	-0.045011	-0.366098
17	7	0	-3.724049	-0.832724	-0.045663
18	6	0	-4.471515	-1.984372	0.438955
19	1	0	-5.281574	-2.214016	-0.255522
20	1	0	-3.807475	-2.847959	0.497723
21	1	0	-4.899189	-1.803559	1.431202
22	8	0	-1.631412	2.763708	-0.613707
23	8	0	4.033783	-0.078853	0.327705
24	6	0	4.738049	-1.150182	-0.298247
25	1	0	4.601031	-1.136210	-1.384493
26	1	0	5.790587	-0.989039	-0.067492
27	1	0	4.425598	-2.121001	0.100440

Structure 32d (DMSO)

Energy (Hartrees): -632.362888714
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.042547	1.077627	0.782547
2	6	0	0.666273	1.229286	0.694346
3	6	0	-0.134399	0.298691	0.004070
4	6	0	0.521886	-0.781792	-0.598391
5	6	0	1.906530	-0.955019	-0.511458
6	6	0	2.677160	-0.018236	0.180464
7	1	0	2.644041	1.801359	1.321797
8	1	0	0.201231	2.080841	1.175505
9	1	0	-0.052378	-1.509006	-1.163101
10	1	0	2.363682	-1.807109	-0.996932
11	6	0	-1.612267	0.445241	-0.071167
12	6	0	-2.399647	-0.680520	0.140070
13	1	0	-1.899859	-1.591319	0.459565
14	6	0	-2.220526	1.716779	-0.359942
15	1	0	-3.328102	1.727917	-0.330868
16	1	0	-4.278470	-0.047586	-0.322112
17	7	0	-3.719036	-0.829983	-0.009410
18	6	0	-4.448735	-2.019161	0.407436
19	1	0	-5.185517	-2.284879	-0.353118
20	1	0	-3.749895	-2.847485	0.527741
21	1	0	-4.967784	-1.855219	1.357353
22	8	0	-1.639255	2.774143	-0.622803
23	8	0	4.033459	-0.080549	0.319015
24	6	0	4.727491	-1.164448	-0.303673
25	1	0	4.581964	-1.159146	-1.388492
26	1	0	5.782656	-1.008975	-0.081872
27	1	0	4.410163	-2.128958	0.104896

Structure 32d (C_2H_5OH)

Energy (Hartrees): -632.366841950
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.036178	1.053064	0.824648
2	6	0	0.660117	1.207626	0.736068
3	6	0	-0.134743	0.304610	0.005065
4	6	0	0.522616	-0.751542	-0.636991
5	6	0	1.906437	-0.928030	-0.550023
6	6	0	2.670350	-0.018703	0.182683
7	1	0	2.635634	1.753345	1.396317
8	1	0	0.192257	2.035690	1.255215
9	1	0	-0.050192	-1.454988	-1.232526
10	1	0	2.367536	-1.760136	-1.065419
11	6	0	-1.613909	0.451133	-0.071192
12	6	0	-2.400816	-0.677433	0.150518
13	1	0	-1.897428	-1.582049	0.481452
14	6	0	-2.220134	1.710251	-0.370908
15	1	0	-3.324738	1.731344	-0.344925
16	1	0	-4.277679	-0.054969	-0.324429
17	7	0	-3.715909	-0.831168	0.000533
18	6	0	-4.442283	-2.025406	0.411897
19	1	0	-5.155046	-2.309784	-0.364593
20	1	0	-3.737081	-2.843003	0.562084
21	1	0	-4.988340	-1.853369	1.344602
22	8	0	-1.632410	2.771394	-0.647162
23	8	0	4.031080	-0.088256	0.327607
24	6	0	4.729275	-1.163554	-0.309648
25	1	0	4.595058	-1.133992	-1.395046
26	1	0	5.781801	-1.014549	-0.071569
27	1	0	4.401701	-2.132553	0.078834

Structure 32e (vacuum)

Energy (Hartrees): -632.334758056
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.990257	1.173519	-0.664625
2	6	0	-0.606639	1.198979	-0.626013
3	6	0	0.128645	0.138541	-0.064637
4	6	0	-0.594528	-0.927860	0.475881
5	6	0	-1.991302	-0.971331	0.441036
6	6	0	-2.695751	0.086034	-0.133835
7	1	0	-2.551183	1.991263	-1.101380
8	1	0	-0.083431	2.054334	-1.032259
9	1	0	-0.063975	-1.741290	0.960007
10	1	0	-2.505210	-1.816950	0.878399
11	6	0	1.619073	0.140787	-0.054971
12	6	0	2.251539	-1.011672	-0.458686
13	1	0	1.607845	-1.783230	-0.872035
14	6	0	2.323891	1.359376	0.334555
15	1	0	3.424113	1.330986	0.252806
16	1	0	3.726834	-2.303641	-0.875180
17	7	0	3.548075	-1.419041	-0.431275
18	6	0	4.695116	-0.770141	0.177795
19	1	0	5.501016	-1.500812	0.260084
20	1	0	5.058703	0.077915	-0.411315
21	1	0	4.445506	-0.415709	1.181566
22	8	0	1.792092	2.395903	0.701007
23	8	0	-4.058267	0.158959	-0.218902
24	6	0	-4.828105	-0.900574	0.328417
25	1	0	-4.612687	-1.852821	-0.169519
26	1	0	-4.655188	-1.006663	1.405215
27	1	0	-5.869560	-0.632930	0.156198

Structure 32e ($CHCl_3$)

Energy (Hartrees): -632.358014972
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.991942	1.162301	-0.698839
2	6	0	-0.606571	1.187890	-0.659781
3	6	0	0.130606	0.145695	-0.066711
4	6	0	-0.594694	-0.907781	0.499344
5	6	0	-1.991880	-0.953021	0.464037
6	6	0	-2.697996	0.088680	-0.138737
7	1	0	-2.548374	1.968919	-1.163156
8	1	0	-0.085104	2.028087	-1.101082
9	1	0	-0.065279	-1.713862	0.996867
10	1	0	-2.506413	-1.788881	0.919344
11	6	0	1.622930	0.149360	-0.056523
12	6	0	2.255708	-1.013711	-0.463434
13	1	0	1.610027	-1.781798	-0.879704
14	6	0	2.328029	1.348921	0.340750
15	1	0	3.423923	1.325512	0.243579
16	1	0	3.710402	-2.320141	-0.854600
17	7	0	3.538305	-1.419515	-0.434725
18	6	0	4.693723	-0.771423	0.163625
19	1	0	5.497460	-1.505156	0.229239
20	1	0	5.047223	0.075154	-0.432467
21	1	0	4.457508	-0.419763	1.171751
22	8	0	1.802544	2.388588	0.744222
23	8	0	-4.059824	0.155140	-0.226953
24	6	0	-4.831608	-0.902591	0.339876
25	1	0	-4.610739	-1.861154	-0.141315
26	1	0	-4.664910	-0.983856	1.418893
27	1	0	-5.873455	-0.642208	0.155929

Structure 32e (DMSO)

Energy (Hartrees): -632.359726987
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.990869	1.140920	-0.744321
2	6	0	-0.604579	1.166350	-0.703280
3	6	0	0.131875	0.142354	-0.078563
4	6	0	-0.595296	-0.897555	0.510618
5	6	0	-1.992915	-0.942482	0.475738
6	6	0	-2.699477	0.084012	-0.153971
7	1	0	-2.543843	1.933706	-1.236330
8	1	0	-0.082062	1.990735	-1.173377
9	1	0	-0.067086	-1.695172	1.022894
10	1	0	-2.507194	-1.768126	0.949540
11	6	0	1.624488	0.152145	-0.058625
12	6	0	2.262851	-1.010728	-0.469021
13	1	0	1.621235	-1.779899	-0.889526
14	6	0	2.319349	1.345792	0.362572
15	1	0	3.415106	1.329154	0.269321
16	1	0	3.716447	-2.314839	-0.851056
17	7	0	3.542335	-1.409863	-0.438847
18	6	0	4.696180	-0.758278	0.159379
19	1	0	5.503850	-1.488104	0.213196
20	1	0	5.038526	0.095447	-0.432661
21	1	0	4.462078	-0.415541	1.171221
22	8	0	1.787857	2.376738	0.788917
23	8	0	-4.059514	0.147136	-0.243058
24	6	0	-4.826926	-0.887065	0.378221
25	1	0	-4.603529	-1.866867	-0.055374
26	1	0	-4.654288	-0.915040	1.458684
27	1	0	-5.870418	-0.640188	0.186057

Structure 32e (C_2H_5OH)

Energy (Hartrees): -632.363914761
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.985736	1.116021	-0.786961
2	6	0	-0.599397	1.142841	-0.741366
3	6	0	0.132215	0.141785	-0.076753
4	6	0	-0.595205	-0.878551	0.544709
5	6	0	-1.992121	-0.925214	0.504756
6	6	0	-2.693105	0.079213	-0.163584
7	1	0	-2.537949	1.891130	-1.307390
8	1	0	-0.074566	1.948684	-1.241551
9	1	0	-0.067829	-1.657742	1.085564
10	1	0	-2.509628	-1.734535	1.002456
11	6	0	1.626035	0.153087	-0.047728
12	6	0	2.266652	-1.008965	-0.467315
13	1	0	1.623220	-1.773832	-0.892554
14	6	0	2.313750	1.333721	0.389158
15	1	0	3.408974	1.323532	0.324380
16	1	0	3.716764	-2.310366	-0.857968
17	7	0	3.543360	-1.405759	-0.443757
18	6	0	4.702293	-0.744419	0.135826
19	1	0	5.520646	-1.463488	0.161289
20	1	0	5.017564	0.119724	-0.455834
21	1	0	4.488265	-0.418467	1.157427
22	8	0	1.769875	2.370088	0.813281
23	8	0	-4.057968	0.137811	-0.262862
24	6	0	-4.832182	-0.874136	0.389999
25	1	0	-4.609640	-1.866267	-0.014021
26	1	0	-4.660323	-0.866305	1.470439
27	1	0	-5.873466	-0.627246	0.186261

Structure 32f (vacuum)

Energy (Hartrees): -632.337409049
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.076347	1.337995	-0.407203
2	6	0	-0.690845	1.325436	-0.403493
3	6	0	0.037085	0.175942	-0.038407
4	6	0	-0.702594	-0.955142	0.324916
5	6	0	-2.099223	-0.965873	0.308636
6	6	0	-2.794112	0.188562	-0.055154
7	1	0	-2.626913	2.225733	-0.695084
8	1	0	-0.159901	2.218643	-0.713513
9	1	0	-0.181061	-1.847776	0.653469
10	1	0	-2.623525	-1.866318	0.599924
11	6	0	1.524234	0.170091	-0.044034
12	6	0	2.160961	-0.909496	-0.617644
13	1	0	1.541335	-1.587494	-1.200410
14	6	0	2.196031	1.360651	0.464633
15	1	0	1.538279	2.021476	1.064192
16	1	0	3.673368	-2.114394	-1.121272
17	7	0	3.449077	-1.310021	-0.559498
18	6	0	4.458860	-0.908006	0.410949
19	1	0	5.288500	-1.612913	0.347606
20	1	0	4.805937	0.109143	0.229481
21	1	0	4.039238	-0.943679	1.421465
22	8	0	3.352240	1.705341	0.249182
23	8	0	-4.155350	0.298343	-0.095619
24	6	0	-4.937415	-0.837559	0.243517
25	1	0	-4.739161	-1.676970	-0.432324
26	1	0	-4.758886	-1.153070	1.277497
27	1	0	-5.975672	-0.527320	0.136661

Structure 32f ($CHCl_3$)

Energy (Hartrees): -632.357393150
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.077571	1.353534	-0.367137
2	6	0	-0.690711	1.342695	-0.375026
3	6	0	0.042034	0.181962	-0.054561
4	6	0	-0.696072	-0.964227	0.269749
5	6	0	-2.092906	-0.976067	0.263635
6	6	0	-2.792614	0.191233	-0.050562
7	1	0	-2.626885	2.253915	-0.618606
8	1	0	-0.164701	2.248581	-0.656179
9	1	0	-0.173556	-1.870858	0.555984
10	1	0	-2.614307	-1.888021	0.523056
11	6	0	1.529736	0.177633	-0.062220
12	6	0	2.172249	-0.907213	-0.638521
13	1	0	1.570666	-1.571507	-1.254238
14	6	0	2.199251	1.360028	0.439409
15	1	0	1.552738	2.019834	1.049815
16	1	0	3.690203	-2.118093	-1.095943
17	7	0	3.444704	-1.318115	-0.531845
18	6	0	4.422433	-0.924822	0.471386
19	1	0	5.203393	-1.685117	0.495123
20	1	0	4.856331	0.052761	0.257180
21	1	0	3.945155	-0.872054	1.454481
22	8	0	3.357759	1.716435	0.208762
23	8	0	-4.153955	0.299306	-0.073913
24	6	0	-4.935211	-0.848320	0.256803
25	1	0	-4.758589	-1.669229	-0.445958
26	1	0	-4.732757	-1.187166	1.277921
27	1	0	-5.974764	-0.530788	0.183762

Structure 32f (DMSO)

Energy (Hartrees): -632.357452572
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.076855	1.364421	-0.340129
2	6	0	-0.689121	1.353648	-0.348855
3	6	0	0.044484	0.188495	-0.045460
4	6	0	-0.695019	-0.961771	0.264590
5	6	0	-2.091885	-0.973600	0.257750
6	6	0	-2.793353	0.197438	-0.041925
7	1	0	-2.622549	2.270266	-0.580684
8	1	0	-0.165308	2.264403	-0.618594
9	1	0	-0.174183	-1.874095	0.535331
10	1	0	-2.612213	-1.889758	0.504229
11	6	0	1.532103	0.180631	-0.061504
12	6	0	2.164494	-0.922192	-0.621673
13	1	0	1.555047	-1.595436	-1.219226
14	6	0	2.205252	1.368450	0.416962
15	1	0	1.563545	2.032366	1.028356
16	1	0	3.660731	-2.165070	-1.050873
17	7	0	3.431165	-1.340390	-0.514454
18	6	0	4.420347	-0.929594	0.469463
19	1	0	5.207133	-1.683507	0.487269
20	1	0	4.841488	0.049403	0.236940
21	1	0	3.958291	-0.869675	1.459800
22	8	0	3.360056	1.730702	0.170112
23	8	0	-4.153244	0.301498	-0.068580
24	6	0	-4.928305	-0.861651	0.232110
25	1	0	-4.730167	-1.669326	-0.479410
26	1	0	-4.737186	-1.215147	1.250130
27	1	0	-5.970131	-0.554938	0.147677

Structure 32f (C_2H_5OH)

Energy (Hartrees): -632.361084755
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.081131	1.362591	-0.353821
2	6	0	-0.693385	1.358942	-0.366932
3	6	0	0.044774	0.197530	-0.063154
4	6	0	-0.686218	-0.958050	0.245823
5	6	0	-2.082863	-0.976590	0.244889
6	6	0	-2.787710	0.192334	-0.049667
7	1	0	-2.633965	2.264704	-0.592669
8	1	0	-0.173613	2.271554	-0.638111
9	1	0	-0.158877	-1.867706	0.513395
10	1	0	-2.599044	-1.894822	0.492287
11	6	0	1.532711	0.195753	-0.071865
12	6	0	2.172527	-0.892365	-0.660351
13	1	0	1.576763	-1.533747	-1.304977
14	6	0	2.201273	1.365823	0.429249
15	1	0	1.557983	2.038208	1.025207
16	1	0	3.676735	-2.119837	-1.100184
17	7	0	3.429308	-1.323274	-0.529352
18	6	0	4.390317	-0.960397	0.501684
19	1	0	5.113778	-1.771612	0.583941
20	1	0	4.908308	-0.028087	0.271943
21	1	0	3.877300	-0.838312	1.459137
22	8	0	3.374298	1.715921	0.211674
23	8	0	-4.153702	0.291975	-0.065559
24	6	0	-4.925773	-0.865902	0.271410
25	1	0	-4.749500	-1.680933	-0.436918
26	1	0	-4.705239	-1.203939	1.288220
27	1	0	-5.967679	-0.553732	0.211687

Structure 32g (vacuum)

Energy (Hartrees): -632.341942983
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.071978	-0.897109	-0.470031
2	6	0	0.681993	-0.791039	-0.544085
3	6	0	-0.005776	0.306004	-0.014440
4	6	0	0.762051	1.308386	0.605109
5	6	0	2.144198	1.226303	0.672820
6	6	0	2.812227	0.119653	0.136602
7	1	0	2.558152	-1.762936	-0.899350
8	1	0	0.130633	-1.577014	-1.049241
9	1	0	0.262749	2.157189	1.059219
10	1	0	2.727785	2.001831	1.154499
11	6	0	-1.482803	0.408098	-0.105542
12	6	0	-2.087774	1.580385	-0.464878
13	1	0	-1.509740	2.464208	-0.717832
14	6	0	-2.310025	-0.746691	0.196136
15	1	0	-1.794543	-1.662087	0.513839
16	7	0	-3.594789	-0.715898	0.121889
17	6	0	-4.357245	-1.900902	0.463729
18	1	0	-5.041830	-1.674683	1.286941
19	1	0	-4.969486	-2.204747	-0.390909
20	1	0	-3.718551	-2.744749	0.758692
21	8	0	-3.397705	1.758652	-0.556044
22	1	0	-3.822999	0.872943	-0.322756
23	8	0	4.172739	0.124643	0.259900
24	6	0	4.904924	-0.975632	-0.260801
25	1	0	4.621601	-1.913523	0.229575
26	1	0	4.765020	-1.073714	-1.342940
27	1	0	5.951972	-0.762520	-0.051505

Structure 32g ($CHCl_3$)

Energy (Hartrees): -632.356845918
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.072694	-0.911622	-0.440179
2	6	0	0.681929	-0.808563	-0.509776
3	6	0	-0.004291	0.307102	-0.014030
4	6	0	0.766083	1.328936	0.571171
5	6	0	2.149667	1.248926	0.633636
6	6	0	2.816164	0.126081	0.127460
7	1	0	2.558412	-1.791561	-0.841061
8	1	0	0.129441	-1.614337	-0.981472
9	1	0	0.271384	2.194002	0.999309
10	1	0	2.731125	2.042706	1.089042
11	6	0	-1.482455	0.408266	-0.104584
12	6	0	-2.088890	1.583856	-0.446905
13	1	0	-1.520085	2.475515	-0.692798
14	6	0	-2.309362	-0.752722	0.186827
15	1	0	-1.799098	-1.673064	0.491928
16	7	0	-3.594493	-0.713510	0.116376
17	6	0	-4.366740	-1.897813	0.444721
18	1	0	-5.041256	-1.677372	1.278202
19	1	0	-4.990893	-2.177804	-0.409667
20	1	0	-3.734446	-2.752463	0.717595
21	8	0	-3.405865	1.751809	-0.529161
22	1	0	-3.819417	0.851866	-0.300914
23	8	0	4.176905	0.135302	0.237024
24	6	0	4.908427	-0.993375	-0.241356
25	1	0	4.633960	-1.904671	0.300055
26	1	0	4.756927	-1.141935	-1.315386
27	1	0	5.957705	-0.767659	-0.054277

Structure 32g (DMSO)

Energy (Hartrees): -632.355061608
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.068839	-0.920051	-0.416610
2	6	0	0.677648	-0.816454	-0.479753
3	6	0	-0.004154	0.314780	-0.012386
4	6	0	0.772367	1.352849	0.535818
5	6	0	2.156576	1.271445	0.591794
6	6	0	2.819273	0.132149	0.115945
7	1	0	2.548930	-1.813636	-0.793433
8	1	0	0.121962	-1.637102	-0.920662
9	1	0	0.283964	2.233118	0.939417
10	1	0	2.739605	2.078909	1.020737
11	6	0	-1.482593	0.413239	-0.095599
12	6	0	-2.094917	1.590685	-0.422565
13	1	0	-1.531059	2.488888	-0.656108
14	6	0	-2.304749	-0.755611	0.180794
15	1	0	-1.793907	-1.679641	0.470580
16	7	0	-3.590413	-0.717326	0.111157
17	6	0	-4.359365	-1.909661	0.422464
18	1	0	-5.037251	-1.702020	1.256489
19	1	0	-4.979694	-2.181418	-0.437452
20	1	0	-3.722679	-2.763295	0.685864
21	8	0	-3.413298	1.749789	-0.501770
22	1	0	-3.815772	0.839379	-0.284115
23	8	0	4.178747	0.139308	0.218099
24	6	0	4.898924	-1.015842	-0.221414
25	1	0	4.614055	-1.903724	0.351724
26	1	0	4.743151	-1.200649	-1.288740
27	1	0	5.950894	-0.795475	-0.043957

Structure 32g (C_2H_5OH)

Energy (Hartrees): -632.356713333
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.067219	-0.915055	-0.428484
2	6	0	0.676245	-0.810651	-0.492739
3	6	0	-0.005269	0.315688	-0.013366
4	6	0	0.768980	1.347503	0.548566
5	6	0	2.153168	1.265280	0.606123
6	6	0	2.813720	0.131355	0.117881
7	1	0	2.549303	-1.803551	-0.814677
8	1	0	0.120746	-1.625566	-0.944580
9	1	0	0.279301	2.222473	0.962079
10	1	0	2.736647	2.067049	1.045486
11	6	0	-1.483888	0.415521	-0.098108
12	6	0	-2.091066	1.591389	-0.429960
13	1	0	-1.529744	2.489113	-0.669151
14	6	0	-2.305635	-0.753779	0.183544
15	1	0	-1.791135	-1.673949	0.479057
16	7	0	-3.590671	-0.720008	0.112765
17	6	0	-4.351824	-1.916376	0.430227
18	1	0	-5.028135	-1.710187	1.265842
19	1	0	-4.974065	-2.193264	-0.426551
20	1	0	-3.710515	-2.766394	0.693603
21	8	0	-3.415771	1.752594	-0.509009
22	1	0	-3.824710	0.846633	-0.287861
23	8	0	4.178838	0.137409	0.223064
24	6	0	4.904608	-1.012926	-0.225268
25	1	0	4.617633	-1.905175	0.339227
26	1	0	4.752676	-1.184914	-1.294922
27	1	0	5.954617	-0.789928	-0.039834

Structure 32h (vacuum)

Energy (Hartrees): -632.317223084
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.836062	-1.220466	-0.748686
2	6	0	0.476027	-0.956281	-0.724492
3	6	0	-0.041675	0.181597	-0.078799
4	6	0	0.871754	1.030482	0.552953
5	6	0	2.246652	0.784999	0.529499
6	6	0	2.735155	-0.347318	-0.124197
7	1	0	2.228047	-2.094892	-1.254388
8	1	0	-0.199964	-1.634504	-1.233753
9	1	0	0.506380	1.893319	1.099054
10	1	0	2.913434	1.469126	1.037217
11	6	0	-1.505543	0.453493	-0.075588
12	6	0	-1.925301	1.701931	-0.372449
13	1	0	-1.198327	2.461060	-0.648176
14	6	0	-2.393408	-0.667299	0.274724
15	1	0	-1.874816	-1.524162	0.735539
16	7	0	-3.651560	-0.695075	0.088422
17	6	0	-4.367691	-1.875057	0.526765
18	1	0	-4.908531	-2.305901	-0.322013
19	1	0	-3.720148	-2.649792	0.968060
20	1	0	-5.122250	-1.584932	1.265209
21	8	0	-3.217997	2.104228	-0.349578
22	1	0	-3.266010	3.031069	-0.601780
23	8	0	4.054568	-0.692267	-0.202699
24	6	0	5.014122	0.153278	0.415335
25	1	0	4.850929	0.220707	1.496635
26	1	0	5.982661	-0.306727	0.225758
27	1	0	5.000022	1.159321	-0.018476

Structure 32h ($CHCl_3$)

Energy (Hartrees): -632.337988449
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.819394	-1.267477	-0.672115
2	6	0	0.460026	-0.992189	-0.653673
3	6	0	-0.045587	0.183770	-0.068302
4	6	0	0.880833	1.061075	0.507555
5	6	0	2.253681	0.805726	0.485963
6	6	0	2.730321	-0.366765	-0.105352
7	1	0	2.196642	-2.174197	-1.131448
8	1	0	-0.221337	-1.695391	-1.120281
9	1	0	0.530320	1.958677	1.005340
10	1	0	2.929326	1.513443	0.947792
11	6	0	-1.508767	0.465713	-0.068685
12	6	0	-1.919453	1.722452	-0.352518
13	1	0	-1.193880	2.484706	-0.620035
14	6	0	-2.399985	-0.653910	0.275445
15	1	0	-1.893705	-1.494533	0.773258
16	7	0	-3.652436	-0.708195	0.042422
17	6	0	-4.362546	-1.893928	0.485288
18	1	0	-4.870831	-2.353092	-0.369197
19	1	0	-3.714335	-2.645990	0.959786
20	1	0	-5.143767	-1.604602	1.196451
21	8	0	-3.206635	2.135225	-0.320585
22	1	0	-3.242143	3.073086	-0.548251
23	8	0	4.046185	-0.723918	-0.170896
24	6	0	5.024909	0.175007	0.351022
25	1	0	4.883826	0.340930	1.423801
26	1	0	5.988103	-0.306892	0.186790
27	1	0	5.005461	1.133913	-0.176879

Structure 32h (DMSO)

Energy (Hartrees): -632.336251463
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.814455	-1.286721	-0.644751
2	6	0	0.454782	-1.009118	-0.627526
3	6	0	-0.046661	0.182398	-0.070730
4	6	0	0.884211	1.073841	0.477307
5	6	0	2.256250	0.815717	0.456923
6	6	0	2.730249	-0.373140	-0.105483
7	1	0	2.184237	-2.207170	-1.082699
8	1	0	-0.228185	-1.725706	-1.070959
9	1	0	0.538808	1.987399	0.948948
10	1	0	2.934055	1.535619	0.896020
11	6	0	-1.509420	0.467613	-0.071215
12	6	0	-1.914942	1.729556	-0.342379
13	1	0	-1.186659	2.492516	-0.599090
14	6	0	-2.401883	-0.651192	0.271154
15	1	0	-1.901012	-1.486631	0.781252
16	7	0	-3.652578	-0.712579	0.025200
17	6	0	-4.361168	-1.898523	0.476003
18	1	0	-4.859976	-2.370876	-0.377073
19	1	0	-3.711788	-2.640063	0.963746
20	1	0	-5.149708	-1.606142	1.178135
21	8	0	-3.199722	2.148751	-0.303420
22	1	0	-3.222396	3.094238	-0.503511
23	8	0	4.044241	-0.730200	-0.166273
24	6	0	5.020243	0.179301	0.350400
25	1	0	4.870451	0.359792	1.419234
26	1	0	5.985416	-0.302499	0.198887
27	1	0	5.001950	1.130767	-0.189972

Structure 32h (C_2H_5OH)

Energy (Hartrees): -632.343172379
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.820114	-1.267635	-0.679254
2	6	0	0.459752	-0.993247	-0.662069
3	6	0	-0.046409	0.178688	-0.069778
4	6	0	0.877928	1.053324	0.514400
5	6	0	2.250932	0.798615	0.494667
6	6	0	2.727790	-0.369445	-0.104390
7	1	0	2.196991	-2.171514	-1.145304
8	1	0	-0.219288	-1.694891	-1.134649
9	1	0	0.526593	1.950032	1.013393
10	1	0	2.925463	1.504505	0.960864
11	6	0	-1.509801	0.463541	-0.073172
12	6	0	-1.912459	1.725310	-0.350776
13	1	0	-1.186262	2.491435	-0.602188
14	6	0	-2.401569	-0.656833	0.260452
15	1	0	-1.891813	-1.515370	0.719556
16	7	0	-3.662856	-0.696803	0.063078
17	6	0	-4.362630	-1.896760	0.491863
18	1	0	-4.890404	-2.335238	-0.361560
19	1	0	-3.701439	-2.658022	0.929644
20	1	0	-5.126742	-1.629198	1.229468
21	8	0	-3.199825	2.143216	-0.332749
22	1	0	-3.226848	3.089016	-0.530493
23	8	0	4.048474	-0.724086	-0.169972
24	6	0	5.025702	0.182056	0.354619
25	1	0	4.881032	0.343443	1.426810
26	1	0	5.990667	-0.295324	0.188274
27	1	0	4.996748	1.140025	-0.172963

Structure 32i (vacuum)

Energy (Hartrees): -632.323211947
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.855249	-1.007992	-0.426390
2	6	0	0.469404	-0.846413	-0.468557
3	6	0	-0.159944	0.297511	0.034860
4	6	0	0.663340	1.293490	0.592681
5	6	0	2.039504	1.147182	0.642855
6	6	0	2.649139	-0.005636	0.132927
7	1	0	2.294014	-1.907874	-0.836101
8	1	0	-0.126241	-1.630184	-0.923750
9	1	0	0.214822	2.192601	0.994060
10	1	0	2.666901	1.915827	1.078356
11	6	0	-1.635754	0.424530	-0.016042
12	6	0	-2.299995	1.571245	-0.258539
13	1	0	-3.384548	1.571136	-0.265416
14	6	0	-2.447485	-0.786496	0.229968
15	1	0	-1.912596	-1.606678	0.733061
16	7	0	-3.674877	-0.904097	-0.083382
17	6	0	-4.358385	-2.127588	0.285341
18	1	0	-4.799512	-2.581643	-0.607654
19	1	0	-3.705037	-2.866418	0.774965
20	1	0	-5.186970	-1.892836	0.961868
21	8	0	-1.683858	2.755836	-0.520643
22	1	0	-2.346962	3.432453	-0.684805
23	8	0	4.010792	-0.054642	0.229181
24	6	0	4.684914	-1.200651	-0.270602
25	1	0	4.516696	-1.327343	-1.345761
26	1	0	5.744404	-1.025343	-0.090488
27	1	0	4.373776	-2.109660	0.256029

Structure 32i ($CHCl_3$)

Energy (Hartrees): -632.342068112
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.842613	-1.015437	-0.403631
2	6	0	0.456674	-0.849648	-0.435331
3	6	0	-0.165456	0.306479	0.053428
4	6	0	0.666927	1.307395	0.590256
5	6	0	2.044343	1.157663	0.628531
6	6	0	2.646257	-0.004915	0.128850
7	1	0	2.275368	-1.924300	-0.800066
8	1	0	-0.144948	-1.641396	-0.868998
9	1	0	0.228160	2.213056	0.988846
10	1	0	2.674363	1.934040	1.047904
11	6	0	-1.642545	0.438248	0.005337
12	6	0	-2.303002	1.587777	-0.246874
13	1	0	-3.387156	1.608822	-0.238988
14	6	0	-2.451622	-0.769434	0.266345
15	1	0	-1.947701	-1.547812	0.856930
16	7	0	-3.649203	-0.936357	-0.136673
17	6	0	-4.336810	-2.150493	0.265363
18	1	0	-4.697331	-2.676821	-0.624486
19	1	0	-3.709156	-2.834733	0.854879
20	1	0	-5.220882	-1.891021	0.857927
21	8	0	-1.683825	2.759765	-0.533554
22	1	0	-2.347207	3.442738	-0.694100
23	8	0	4.007483	-0.056151	0.207335
24	6	0	4.678752	-1.215958	-0.285434
25	1	0	4.497399	-1.357711	-1.355682
26	1	0	5.740419	-1.034932	-0.121470
27	1	0	4.377055	-2.114407	0.262721

Structure 32i (DMSO)

Energy (Hartrees): -632.339679055
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.839413	-1.022440	-0.380813
2	6	0	0.453276	-0.856937	-0.406467
3	6	0	-0.166036	0.313839	0.052408
4	6	0	0.671172	1.329530	0.554071
5	6	0	2.049193	1.180661	0.585013
6	6	0	2.648659	0.003468	0.114740
7	1	0	2.267528	-1.944258	-0.751784
8	1	0	-0.150304	-1.663569	-0.808680
9	1	0	0.237567	2.246071	0.932593
10	1	0	2.679754	1.969897	0.979214
11	6	0	-1.643337	0.442643	0.015276
12	6	0	-2.313102	1.590886	-0.221888
13	1	0	-3.397081	1.610295	-0.190568
14	6	0	-2.446122	-0.769170	0.279270
15	1	0	-1.954906	-1.529420	0.901832
16	7	0	-3.627787	-0.957664	-0.161086
17	6	0	-4.318816	-2.169671	0.247632
18	1	0	-4.646926	-2.718369	-0.641290
19	1	0	-3.703571	-2.833520	0.871291
20	1	0	-5.222660	-1.903166	0.806438
21	8	0	-1.704928	2.765600	-0.519644
22	1	0	-2.376082	3.453010	-0.625233
23	8	0	4.007752	-0.046603	0.182425
24	6	0	4.669427	-1.234920	-0.262403
25	1	0	4.478372	-1.424049	-1.323146
26	1	0	5.733342	-1.054236	-0.114483
27	1	0	4.364522	-2.104350	0.328133

Structure 32i (C_2H_5OH)

Energy (Hartrees): -632.345320089
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.835976	-1.009319	-0.410877
2	6	0	0.450177	-0.840992	-0.440186
3	6	0	-0.169647	0.316599	0.049913
4	6	0	0.664578	1.315719	0.587254
5	6	0	2.042578	1.164390	0.621393
6	6	0	2.640540	0.000675	0.120406
7	1	0	2.266477	-1.919848	-0.806065
8	1	0	-0.153370	-1.633913	-0.869386
9	1	0	0.229680	2.218924	0.996155
10	1	0	2.672968	1.939698	1.043064
11	6	0	-1.647654	0.446497	0.010679
12	6	0	-2.310693	1.596762	-0.235100
13	1	0	-3.393892	1.629637	-0.207105
14	6	0	-2.447934	-0.763834	0.280795
15	1	0	-1.953825	-1.517369	0.909308
16	7	0	-3.629085	-0.962900	-0.158201
17	6	0	-4.307976	-2.177267	0.265987
18	1	0	-4.637214	-2.737765	-0.614893
19	1	0	-3.684129	-2.830409	0.891963
20	1	0	-5.210649	-1.914193	0.827958
21	8	0	-1.692914	2.765574	-0.539295
22	1	0	-2.354272	3.460655	-0.653536
23	8	0	4.005115	-0.054078	0.197949
24	6	0	4.672971	-1.231101	-0.271604
25	1	0	4.496939	-1.386281	-1.340129
26	1	0	5.734137	-1.054507	-0.100632
27	1	0	4.355649	-2.115070	0.289502

Structure 32j (vacuum)

Energy (Hartrees): -632.323707519
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.675666	-0.845418	-0.580212
2	6	0	0.294049	-0.668667	-0.651668
3	6	0	-0.342251	0.396781	-0.008242
4	6	0	0.459001	1.284313	0.730464
5	6	0	1.831492	1.115423	0.818285
6	6	0	2.452355	0.048654	0.159393
7	1	0	2.125476	-1.682401	-1.097273
8	1	0	-0.295608	-1.382334	-1.210002
9	1	0	-0.001142	2.116943	1.247036
10	1	0	2.443651	1.798588	1.394897
11	6	0	-1.811553	0.584917	-0.098549
12	6	0	-2.397524	1.785620	-0.295896
13	1	0	-3.479805	1.870064	-0.339753
14	6	0	-2.750369	-0.537427	0.031783
15	1	0	-3.814699	-0.254768	-0.045544
16	7	0	-2.416823	-1.748761	0.223647
17	6	0	-3.473093	-2.732729	0.345224
18	1	0	-3.342899	-3.505284	-0.419656
19	1	0	-3.391882	-3.233159	1.315445
20	1	0	-4.485772	-2.309005	0.250000
21	8	0	-1.705859	2.945853	-0.454069
22	1	0	-2.315477	3.665988	-0.638456
23	8	0	3.809063	-0.034185	0.301636
24	6	0	4.492960	-1.102320	-0.337281
25	1	0	5.545399	-0.973442	-0.088937
26	1	0	4.150077	-2.075226	0.031696
27	1	0	4.370405	-1.062861	-1.425335

Structure 32j ($CHCl_3$)

Energy (Hartrees): -632.344157269
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.696462	-0.753940	-0.693469
2	6	0	0.315917	-0.568535	-0.781472
3	6	0	-0.347426	0.388915	-0.008510
4	6	0	0.424182	1.161089	0.875636
5	6	0	1.796390	0.984773	0.980265
6	6	0	2.444553	0.024928	0.193498
7	1	0	2.168779	-1.503958	-1.314114
8	1	0	-0.248316	-1.185983	-1.469436
9	1	0	-0.058125	1.907496	1.495809
10	1	0	2.382825	1.581106	1.670203
11	6	0	-1.817343	0.587671	-0.115803
12	6	0	-2.379002	1.798801	-0.326857
13	1	0	-3.457824	1.912440	-0.383694
14	6	0	-2.760281	-0.525709	0.016877
15	1	0	-3.820391	-0.246641	-0.087615
16	7	0	-2.428990	-1.735465	0.243797
17	6	0	-3.493690	-2.714841	0.362208
18	1	0	-3.357965	-3.498584	-0.391018
19	1	0	-3.430911	-3.205115	1.339487
20	1	0	-4.501121	-2.287095	0.246311
21	8	0	-1.657270	2.933180	-0.488680
22	1	0	-2.250644	3.675365	-0.660033
23	8	0	3.795343	-0.076693	0.363696
24	6	0	4.509332	-1.047466	-0.401414
25	1	0	5.550699	-0.960997	-0.093173
26	1	0	4.153970	-2.061135	-0.190570
27	1	0	4.432812	-0.844643	-1.474620

Structure 32j (DMSO)

Energy (Hartrees): -632.343360336
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.717276	-0.648904	-0.783373
2	6	0	0.338231	-0.454701	-0.884506
3	6	0	-0.352038	0.387659	-0.008042
4	6	0	0.388629	1.036156	0.993256
5	6	0	1.759495	0.850335	1.111670
6	6	0	2.436266	0.005520	0.222029
7	1	0	2.211646	-1.305488	-1.487079
8	1	0	-0.201630	-0.970305	-1.670574
9	1	0	-0.116020	1.689976	1.695821
10	1	0	2.320900	1.351542	1.892322
11	6	0	-1.822261	0.590169	-0.126300
12	6	0	-2.378188	1.804143	-0.332496
13	1	0	-3.456202	1.923893	-0.393823
14	6	0	-2.759893	-0.525892	-0.000192
15	1	0	-3.820159	-0.256739	-0.112865
16	7	0	-2.416803	-1.733153	0.233953
17	6	0	-3.475230	-2.722628	0.350374
18	1	0	-3.328546	-3.509271	-0.397945
19	1	0	-3.415267	-3.207182	1.330924
20	1	0	-4.483717	-2.302492	0.225549
21	8	0	-1.647277	2.932506	-0.485239
22	1	0	-2.240614	3.681000	-0.633552
23	8	0	3.779884	-0.115711	0.413831
24	6	0	4.516686	-0.976294	-0.459818
25	1	0	5.549802	-0.932642	-0.117380
26	1	0	4.158530	-2.008340	-0.396984
27	1	0	4.464203	-0.629619	-1.496435

Structure 32j (C_2H_5OH)

Energy (Hartrees): -632.348815618
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.720552	-0.644155	-0.794559
2	6	0	0.342990	-0.441766	-0.899227
3	6	0	-0.349482	0.376241	-0.001880
4	6	0	0.385389	0.990939	1.024276
5	6	0	1.755107	0.797174	1.145828
6	6	0	2.432411	-0.021418	0.234098
7	1	0	2.218336	-1.281113	-1.513685
8	1	0	-0.193654	-0.930587	-1.704621
9	1	0	-0.122928	1.625321	1.742249
10	1	0	2.313944	1.273738	1.943773
11	6	0	-1.816982	0.595920	-0.129304
12	6	0	-2.348384	1.820075	-0.339841
13	1	0	-3.421737	1.966593	-0.415209
14	6	0	-2.771920	-0.504634	-0.011963
15	1	0	-3.825509	-0.218567	-0.143810
16	7	0	-2.454087	-1.716540	0.236563
17	6	0	-3.536100	-2.682601	0.336329
18	1	0	-3.398430	-3.470162	-0.412573
19	1	0	-3.500701	-3.172282	1.315216
20	1	0	-4.533346	-2.240228	0.200130
21	8	0	-1.591883	2.934581	-0.479017
22	1	0	-2.161188	3.697990	-0.643602
23	8	0	3.780677	-0.151066	0.430182
24	6	0	4.531448	-0.957920	-0.484355
25	1	0	5.563772	-0.910347	-0.139985
26	1	0	4.190783	-1.997301	-0.466992
27	1	0	4.468746	-0.562512	-1.502557

Structure 32k (vacuum)

Energy (Hartrees): -632.323282313
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.850883	0.708436	-0.609836
2	6	0	-0.463004	0.597247	-0.677458
3	6	0	0.223451	-0.423069	-0.011806
4	6	0	-0.536326	-1.323486	0.753145
5	6	0	-1.918724	-1.228148	0.828056
6	6	0	-2.587975	-0.210211	0.142384
7	1	0	-2.339680	1.512160	-1.144043
8	1	0	0.093291	1.322707	-1.255453
9	1	0	-0.032112	-2.098421	1.320278
10	1	0	-2.497241	-1.921880	1.426384
11	6	0	1.698357	-0.572474	-0.121343
12	6	0	2.211529	-1.796422	-0.365774
13	1	0	1.566749	-2.652779	-0.535003
14	6	0	2.610145	0.567168	0.038519
15	1	0	3.676246	0.331726	-0.076580
16	7	0	2.219786	1.752083	0.294590
17	6	0	3.232802	2.778982	0.433859
18	1	0	3.042782	3.577454	-0.290972
19	1	0	3.151772	3.231654	1.427383
20	1	0	4.260850	2.410201	0.294365
21	8	0	3.555342	-2.044058	-0.410024
22	1	0	3.709045	-2.948227	-0.696594
23	8	0	-3.948194	-0.191217	0.276248
24	6	0	-4.679972	0.833007	-0.381680
25	1	0	-4.385911	1.826965	-0.027055
26	1	0	-4.551998	0.782293	-1.468656
27	1	0	-5.725884	0.657578	-0.134368

Structure 32k ($CHCl_3$)

Energy (Hartrees): -632.342926527
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.865191	0.661876	-0.670396
2	6	0	-0.477701	0.544923	-0.750809
3	6	0	0.223213	-0.421975	-0.021248
4	6	0	-0.523276	-1.269163	0.814685
5	6	0	-1.905809	-1.169045	0.903192
6	6	0	-2.588634	-0.201165	0.158848
7	1	0	-2.365098	1.422937	-1.254971
8	1	0	0.063822	1.221595	-1.400286
9	1	0	-0.010591	-2.009244	1.419759
10	1	0	-2.470250	-1.825080	1.556285
11	6	0	1.699998	-0.569606	-0.136706
12	6	0	2.213977	-1.798229	-0.368948
13	1	0	1.572969	-2.660442	-0.521556
14	6	0	2.606862	0.571654	0.014826
15	1	0	3.668638	0.352027	-0.151304
16	7	0	2.225784	1.748887	0.326984
17	6	0	3.246108	2.773917	0.451161
18	1	0	3.015588	3.602586	-0.226959
19	1	0	3.224710	3.184605	1.466284
20	1	0	4.263096	2.413700	0.236413
21	8	0	3.551132	-2.043644	-0.425793
22	1	0	3.698854	-2.965724	-0.669725
23	8	0	-3.945430	-0.172930	0.310183
24	6	0	-4.692278	0.809717	-0.407136
25	1	0	-4.404292	1.823630	-0.111180
26	1	0	-4.571616	0.692109	-1.488810
27	1	0	-5.735541	0.640252	-0.142776

Structure 32k (DMSO)

Energy (Hartrees): -632.341402284
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.870299	0.644994	-0.689192
2	6	0	-0.483092	0.524532	-0.775639
3	6	0	0.223657	-0.420242	-0.022135
4	6	0	-0.516457	-1.244175	0.842113
5	6	0	-1.898812	-1.140420	0.937303
6	6	0	-2.588661	-0.193366	0.171102
7	1	0	-2.374161	1.386282	-1.295436
8	1	0	0.051946	1.177530	-1.455132
9	1	0	-0.000330	-1.972388	1.458673
10	1	0	-2.455725	-1.782069	1.611007
11	6	0	1.700099	-0.569071	-0.144652
12	6	0	2.211408	-1.801055	-0.368645
13	1	0	1.567385	-2.664118	-0.503942
14	6	0	2.604755	0.573666	-0.001058
15	1	0	3.663181	0.364848	-0.196109
16	7	0	2.227545	1.745253	0.340899
17	6	0	3.249708	2.771803	0.456508
18	1	0	3.002301	3.610296	-0.203548
19	1	0	3.253600	3.166533	1.478279
20	1	0	4.260141	2.415221	0.210647
21	8	0	3.545600	-2.046848	-0.434444
22	1	0	3.688672	-2.974471	-0.663517
23	8	0	-3.941854	-0.158887	0.330581
24	6	0	-4.693158	0.791223	-0.430825
25	1	0	-4.404960	1.817670	-0.183946
26	1	0	-4.574255	0.622544	-1.505488
27	1	0	-5.735466	0.633893	-0.156163

Structure 32k (C_2H_5OH)

Energy (Hartrees): -632.346693103
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.871590	0.635572	-0.700946
2	6	0	-0.484514	0.514129	-0.785472
3	6	0	0.222701	-0.417159	-0.015821
4	6	0	-0.515931	-1.226455	0.862937
5	6	0	-1.898738	-1.121881	0.956433
6	6	0	-2.586420	-0.189078	0.173238
7	1	0	-2.376773	1.365778	-1.319450
8	1	0	0.049486	1.154460	-1.477744
9	1	0	0.000869	-1.943373	1.492124
10	1	0	-2.456929	-1.751266	1.640926
11	6	0	1.698890	-0.568876	-0.141039
12	6	0	2.205745	-1.801714	-0.370724
13	1	0	1.562567	-2.664786	-0.506977
14	6	0	2.605738	0.572163	-0.003793
15	1	0	3.659768	0.365317	-0.223183
16	7	0	2.236821	1.741323	0.356528
17	6	0	3.263576	2.766104	0.449863
18	1	0	2.999862	3.607603	-0.199754
19	1	0	3.296444	3.157515	1.472222
20	1	0	4.266725	2.410354	0.175307
21	8	0	3.539930	-2.053438	-0.443184
22	1	0	3.682499	-2.980231	-0.675194
23	8	0	-3.945812	-0.154220	0.331038
24	6	0	-4.699940	0.787303	-0.441001
25	1	0	-4.412261	1.815415	-0.202107
26	1	0	-4.578607	0.605722	-1.512948
27	1	0	-5.741441	0.628850	-0.163811

Structure 32l (vacuum)

Energy (Hartrees): -632.322700994
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.848420	0.693238	-0.632573
2	6	0	-0.461504	0.575495	-0.706893
3	6	0	0.226377	-0.426410	-0.016452
4	6	0	-0.529062	-1.303853	0.777930
5	6	0	-1.910573	-1.202426	0.859602
6	6	0	-2.582139	-0.201779	0.151056
7	1	0	-2.339223	1.482057	-1.186763
8	1	0	0.091233	1.281653	-1.312417
9	1	0	-0.022772	-2.067912	1.357723
10	1	0	-2.486772	-1.879619	1.478665
11	6	0	1.702346	-0.583149	-0.130389
12	6	0	2.200520	-1.818236	-0.379492
13	1	0	1.542759	-2.661391	-0.549802
14	6	0	2.597828	0.562418	0.031475
15	1	0	3.677921	0.366230	-0.107208
16	7	0	2.218659	1.744441	0.309789
17	6	0	3.227108	2.774310	0.442666
18	1	0	3.021248	3.579417	-0.269955
19	1	0	3.162552	3.215009	1.442468
20	1	0	4.255126	2.412118	0.280313
21	8	0	3.497083	-2.209065	-0.462727
22	1	0	4.091706	-1.472649	-0.279256
23	8	0	-3.940784	-0.175331	0.293874
24	6	0	-4.675949	0.826719	-0.394022
25	1	0	-4.380541	1.831782	-0.073457
26	1	0	-4.552846	0.740124	-1.479216
27	1	0	-5.720578	0.659304	-0.136254

Structure 32l ($CHCl_3$)

Energy (Hartrees): -632.341472716
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.861153	0.641717	-0.694007
2	6	0	-0.474524	0.519731	-0.779441
3	6	0	0.228908	-0.423483	-0.022732
4	6	0	-0.511930	-1.241959	0.845233
5	6	0	-1.893747	-1.136380	0.939715
6	6	0	-2.580045	-0.192470	0.168371
7	1	0	-2.364009	1.382981	-1.301058
8	1	0	0.063280	1.172932	-1.456035
9	1	0	0.004021	-1.965476	1.467351
10	1	0	-2.454995	-1.771142	1.616089
11	6	0	1.706329	-0.579469	-0.144762
12	6	0	2.198747	-1.819141	-0.383952
13	1	0	1.536949	-2.662594	-0.541415
14	6	0	2.601124	0.568441	0.005127
15	1	0	3.669781	0.390828	-0.197043
16	7	0	2.220053	1.737008	0.344833
17	6	0	3.227017	2.775482	0.453252
18	1	0	2.964362	3.608156	-0.207727
19	1	0	3.228167	3.173040	1.473569
20	1	0	4.243185	2.434396	0.204310
21	8	0	3.491861	-2.214091	-0.470587
22	1	0	4.099866	-1.486655	-0.279858
23	8	0	-3.935550	-0.157741	0.326918
24	6	0	-4.687460	0.795549	-0.424187
25	1	0	-4.399478	1.820698	-0.169917
26	1	0	-4.572585	0.634810	-1.500920
27	1	0	-5.728998	0.635524	-0.147528

Structure 32l (DMSO)

Energy (Hartrees): -632.340323618
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.865053	0.624877	-0.708483
2	6	0	-0.478647	0.500030	-0.798338
3	6	0	0.229218	-0.429866	-0.028082
4	6	0	-0.507752	-1.235892	0.854798
5	6	0	-1.889601	-1.127671	0.953720
6	6	0	-2.580948	-0.194056	0.172511
7	1	0	-2.370266	1.354522	-1.327613
8	1	0	0.054728	1.138676	-1.492836
9	1	0	0.010019	-1.953428	1.482448
10	1	0	-2.444792	-1.754939	1.642199
11	6	0	1.707168	-0.579331	-0.150822
12	6	0	2.208438	-1.818197	-0.376880
13	1	0	1.551859	-2.669252	-0.515797
14	6	0	2.594748	0.574333	-0.006077
15	1	0	3.660662	0.408839	-0.222525
16	7	0	2.209597	1.737093	0.353073
17	6	0	3.215979	2.779105	0.461208
18	1	0	2.944076	3.617637	-0.188810
19	1	0	3.228023	3.165703	1.485822
20	1	0	4.228275	2.441231	0.197284
21	8	0	3.502990	-2.201622	-0.467448
22	1	0	4.105827	-1.460002	-0.311113
23	8	0	-3.932939	-0.152223	0.338439
24	6	0	-4.684652	0.791648	-0.430331
25	1	0	-4.382853	1.819224	-0.205624
26	1	0	-4.581863	0.602671	-1.503267
27	1	0	-5.724676	0.650362	-0.138947

Structure 32l (C_2H_5OH)

Energy (Hartrees): -632.344937003
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.865981	0.608209	-0.727419
2	6	0	-0.479528	0.482093	-0.813940
3	6	0	0.229817	-0.419627	-0.012473
4	6	0	-0.503909	-1.193768	0.900443
5	6	0	-1.886215	-1.083540	0.997389
6	6	0	-2.576932	-0.181229	0.181886
7	1	0	-2.373800	1.313723	-1.371855
8	1	0	0.051855	1.094583	-1.533175
9	1	0	0.015708	-1.888552	1.551887
10	1	0	-2.441475	-1.685878	1.708049
11	6	0	1.707433	-0.578911	-0.140850
12	6	0	2.189950	-1.822423	-0.379155
13	1	0	1.519673	-2.663851	-0.511188
14	6	0	2.602957	0.568539	0.001049
15	1	0	3.667452	0.391284	-0.208870
16	7	0	2.223348	1.736255	0.352709
17	6	0	3.238161	2.771959	0.448726
18	1	0	2.970172	3.606527	-0.207828
19	1	0	3.257998	3.168912	1.469097
20	1	0	4.247279	2.425732	0.183953
21	8	0	3.479297	-2.227091	-0.493098
22	1	0	4.104459	-1.501017	-0.356936
23	8	0	-3.935496	-0.139475	0.343841
24	6	0	-4.692583	0.771378	-0.461403
25	1	0	-4.402254	1.807711	-0.265116
26	1	0	-4.577186	0.547592	-1.526005
27	1	0	-5.732747	0.625897	-0.172437

Structure 33a (vacuum)

Energy (Hartrees): -722.362481898
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.950915	1.109030	0.459639
2	6	0	0.572013	1.254369	0.423425
3	6	0	-0.262916	0.231381	-0.068780
4	6	0	0.352682	-0.950795	-0.525642
5	6	0	1.728474	-1.118087	-0.478775
6	6	0	2.517571	-0.081552	0.012594
7	1	0	2.589513	1.892167	0.844644
8	1	0	0.133795	2.165847	0.811055
9	1	0	-0.253607	-1.739821	-0.955028
10	1	0	2.199236	-2.024217	-0.834804
11	6	0	-1.726793	0.399462	-0.104534
12	6	0	-2.561714	-0.675035	0.176060
13	1	0	-2.125350	-1.628947	0.462111
14	6	0	-2.306792	1.679862	-0.438247
15	1	0	-1.593656	2.488046	-0.678362
16	1	0	-4.292273	0.266041	-0.096025
17	7	0	-3.892495	-0.642783	0.150353
18	6	0	-4.751358	-1.750257	0.529307
19	1	0	-5.466743	-1.968035	-0.267544
20	1	0	-4.146277	-2.640932	0.705540
21	1	0	-5.307293	-1.520550	1.443074
22	8	0	-3.518298	1.915173	-0.496856
23	7	0	3.977863	-0.246448	0.056444
24	8	0	4.646411	0.686655	0.489238
25	8	0	4.445960	-1.308736	-0.341446

Structure 33a ($CHCl_3$)

Energy (Hartrees): -722.383730141
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.958718	1.127412	0.416376
2	6	0	0.581975	1.277312	0.389649
3	6	0	-0.266704	0.237812	-0.050658
4	6	0	0.341933	-0.969761	-0.457136
5	6	0	1.715232	-1.140233	-0.420470
6	6	0	2.519040	-0.085127	0.012954
7	1	0	2.595802	1.929113	0.764193
8	1	0	0.157135	2.207426	0.745882
9	1	0	-0.268345	-1.779466	-0.837912
10	1	0	2.167608	-2.067724	-0.743998
11	6	0	-1.727116	0.412540	-0.086898
12	6	0	-2.567714	-0.677167	0.164391
13	1	0	-2.134214	-1.638754	0.424122
14	6	0	-2.294183	1.697211	-0.394569
15	1	0	-1.578888	2.504362	-0.623676
16	1	0	-4.307296	0.257536	-0.084420
17	7	0	-3.890080	-0.646335	0.142515
18	6	0	-4.750321	-1.776170	0.456057
19	1	0	-5.407240	-1.995016	-0.389400
20	1	0	-4.140508	-2.654773	0.668458
21	1	0	-5.367886	-1.552052	1.329772
22	8	0	-3.509384	1.948544	-0.450766
23	7	0	3.965989	-0.252782	0.042720
24	8	0	4.658692	0.698905	0.405560
25	8	0	4.436606	-1.339925	-0.295776

Structure 33a (DMSO)

Energy (Hartrees): -722.384317921
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.959062	1.129894	0.407316
2	6	0	0.583180	1.281244	0.382539
3	6	0	-0.269058	0.237723	-0.044713
4	6	0	0.337604	-0.976157	-0.439157
5	6	0	1.710531	-1.146073	-0.406953
6	6	0	2.518595	-0.087233	0.013093
7	1	0	2.595037	1.936014	0.746851
8	1	0	0.162091	2.216417	0.729483
9	1	0	-0.273235	-1.792471	-0.804483
10	1	0	2.157182	-2.079009	-0.722731
11	6	0	-1.727582	0.415828	-0.080861
12	6	0	-2.569768	-0.677655	0.163489
13	1	0	-2.136595	-1.641020	0.415936
14	6	0	-2.287468	1.703066	-0.386715
15	1	0	-1.565954	2.505839	-0.611060
16	1	0	-4.314996	0.252081	-0.080815
17	7	0	-3.889856	-0.647966	0.142637
18	6	0	-4.748116	-1.784397	0.441813
19	1	0	-5.384490	-2.009555	-0.417546
20	1	0	-4.135048	-2.655762	0.671771
21	1	0	-5.386213	-1.557623	1.299560
22	8	0	-3.501242	1.963712	-0.449165
23	7	0	3.961849	-0.254126	0.039085
24	8	0	4.657936	0.697458	0.403598
25	8	0	4.435354	-1.340884	-0.304199

Structure 33a (C_2H_5OH)

Energy (Hartrees): -722.385520289
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.958948	1.131846	0.407702
2	6	0	0.584290	1.284235	0.382806
3	6	0	-0.268481	0.242220	-0.048051
4	6	0	0.336202	-0.971641	-0.446599
5	6	0	1.707814	-1.144039	-0.413434
6	6	0	2.516967	-0.086453	0.011040
7	1	0	2.593946	1.936433	0.752580
8	1	0	0.164048	2.217873	0.734753
9	1	0	-0.275252	-1.785046	-0.817169
10	1	0	2.152523	-2.076513	-0.733400
11	6	0	-1.726547	0.420933	-0.082590
12	6	0	-2.568510	-0.676823	0.159971
13	1	0	-2.131580	-1.638136	0.413404
14	6	0	-2.282710	1.706081	-0.378579
15	1	0	-1.566249	2.511705	-0.601241
16	1	0	-4.318964	0.243126	-0.087306
17	7	0	-3.886482	-0.652600	0.138441
18	6	0	-4.740505	-1.793205	0.437796
19	1	0	-5.376639	-2.018146	-0.421608
20	1	0	-4.124997	-2.662985	0.666545
21	1	0	-5.378442	-1.568044	1.295934
22	8	0	-3.502195	1.968234	-0.434384
23	7	0	3.952907	-0.256280	0.040500
24	8	0	4.659703	0.701348	0.373236
25	8	0	4.428969	-1.354211	-0.268284

Structure 33b (vacuum)

Energy (Hartrees): -722.353863520
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.756731	-1.075428	0.668351
2	6	0	-0.384447	-1.278085	0.624134
3	6	0	0.461751	-0.417840	-0.102189
4	6	0	-0.132389	0.656433	-0.794380
5	6	0	-1.502017	0.878034	-0.751532
6	6	0	-2.301011	0.008032	-0.015490
7	1	0	-2.405704	-1.730965	1.232831
8	1	0	0.043196	-2.103581	1.180319
9	1	0	0.482792	1.300678	-1.412296
10	1	0	-1.959860	1.696332	-1.290367
11	6	0	1.915680	-0.656351	-0.148258
12	6	0	2.866894	0.319528	0.022591
13	1	0	3.901947	-0.006874	-0.036801
14	6	0	2.420188	-2.016393	-0.366243
15	1	0	1.631498	-2.780680	-0.517986
16	1	0	1.745925	1.959674	0.418475
17	7	0	2.689294	1.627041	0.274245
18	6	0	3.772426	2.540864	0.609807
19	1	0	3.839289	2.711416	1.689386
20	1	0	4.716577	2.118568	0.265787
21	1	0	3.623482	3.500679	0.110676
22	8	0	3.594978	-2.343046	-0.407487
23	7	0	-3.754601	0.238782	0.038282
24	8	0	-4.436232	-0.558207	0.673065
25	8	0	-4.199251	1.216407	-0.554134

Structure 33b ($CHCl_3$)

Energy (Hartrees): -722.377614472
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.771599	-1.094510	0.631627
2	6	0	-0.401024	-1.298793	0.593714
3	6	0	0.457747	-0.410627	-0.087069
4	6	0	-0.125755	0.699982	-0.732358
5	6	0	-1.493229	0.923583	-0.695492
6	6	0	-2.307028	0.021266	-0.011103
7	1	0	-2.420176	-1.777278	1.163380
8	1	0	0.015513	-2.149410	1.119576
9	1	0	0.493978	1.376484	-1.308980
10	1	0	-1.931973	1.770907	-1.204528
11	6	0	1.907928	-0.662949	-0.136616
12	6	0	2.881145	0.308097	0.038005
13	1	0	3.912515	-0.023552	-0.042351
14	6	0	2.381803	-2.017081	-0.367564
15	1	0	1.582499	-2.762525	-0.539533
16	1	0	1.793009	1.962717	0.457166
17	7	0	2.727808	1.595609	0.331658
18	6	0	3.826402	2.531113	0.534842
19	1	0	3.758670	2.983884	1.527079
20	1	0	4.773090	1.997777	0.454139
21	1	0	3.800618	3.323692	-0.217988
22	8	0	3.556249	-2.382828	-0.409812
23	7	0	-3.749666	0.249138	0.029810
24	8	0	-4.455247	-0.577912	0.605915
25	8	0	-4.196386	1.258688	-0.514372

Structure 33b (DMSO)

Energy (Hartrees): -722.379276549
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.778835	-1.104389	0.609691
2	6	0	-0.408895	-1.308891	0.574727
3	6	0	0.455951	-0.405359	-0.080037
4	6	0	-0.123481	0.721937	-0.700990
5	6	0	-1.490504	0.944623	-0.667713
6	6	0	-2.310869	0.026852	-0.010377
7	1	0	-2.427761	-1.800466	1.123401
8	1	0	0.002198	-2.172190	1.083882
9	1	0	0.497848	1.417939	-1.251626
10	1	0	-1.921211	1.806562	-1.158643
11	6	0	1.903928	-0.663392	-0.129410
12	6	0	2.887689	0.303630	0.040259
13	1	0	3.916038	-0.034113	-0.051251
14	6	0	2.364618	-2.018770	-0.365189
15	1	0	1.556879	-2.753044	-0.544238
16	1	0	1.820176	1.967841	0.475902
17	7	0	2.748738	1.587002	0.340048
18	6	0	3.856125	2.518858	0.510040
19	1	0	3.794523	2.996286	1.490634
20	1	0	4.798565	1.977512	0.434146
21	1	0	3.824301	3.292991	-0.261335
22	8	0	3.535484	-2.401827	-0.408298
23	7	0	-3.750038	0.254400	0.027290
24	8	0	-4.462141	-0.581367	0.587519
25	8	0	-4.196695	1.273228	-0.504002

Structure 33b (C_2H_5OH)

Energy (Hartrees): -722.381015333
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.771971	-1.094563	0.628903
2	6	0	-0.402908	-1.299044	0.588638
3	6	0	0.456026	-0.406100	-0.087217
4	6	0	-0.125632	0.710510	-0.724649
5	6	0	-1.492257	0.932350	-0.689583
6	6	0	-2.307532	0.025179	-0.010192
7	1	0	-2.416733	-1.781472	1.159856
8	1	0	0.012579	-2.153073	1.109806
9	1	0	0.493226	1.396354	-1.290718
10	1	0	-1.925877	1.784415	-1.195065
11	6	0	1.904982	-0.663502	-0.139228
12	6	0	2.887659	0.308154	0.036030
13	1	0	3.918373	-0.021977	-0.053849
14	6	0	2.362095	-2.011312	-0.370180
15	1	0	1.561179	-2.750477	-0.544757
16	1	0	1.806547	1.961410	0.469053
17	7	0	2.739053	1.586237	0.341401
18	6	0	3.841191	2.522278	0.531741
19	1	0	3.766518	2.988512	1.516671
20	1	0	4.786856	1.986461	0.459615
21	1	0	3.812011	3.303907	-0.231814
22	8	0	3.540798	-2.397190	-0.413325
23	7	0	-3.741698	0.250033	0.029712
24	8	0	-4.452933	-0.562386	0.626495
25	8	0	-4.201126	1.245620	-0.535942

Structure 33c (vacuum)

Energy (Hartrees): -722.355147894
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.664440	0.977080	0.688247
2	6	0	0.302141	1.236620	0.630765
3	6	0	-0.562062	0.408990	-0.107961
4	6	0	-0.004621	-0.672764	-0.814854
5	6	0	1.356794	-0.943972	-0.766213
6	6	0	2.175421	-0.116788	-0.004929
7	1	0	2.332507	1.605919	1.260564
8	1	0	-0.099889	2.092695	1.154103
9	1	0	-0.637580	-1.286323	-1.445945
10	1	0	1.790314	-1.768613	-1.315099
11	6	0	-2.013451	0.683177	-0.156733
12	6	0	-2.978379	-0.280506	-0.008309
13	1	0	-4.016782	0.037202	-0.068264
14	6	0	-2.515836	2.044233	-0.329367
15	1	0	-3.625432	2.104286	-0.390241
16	1	0	-1.881085	-1.935500	0.384492
17	7	0	-2.819508	-1.599828	0.217532
18	6	0	-3.914770	-2.485315	0.587722
19	1	0	-4.058117	-2.534113	1.672913
20	1	0	-4.838835	-2.129953	0.129774
21	1	0	-3.717371	-3.491554	0.214575
22	8	0	-1.847917	3.058432	-0.406389
23	7	0	3.620478	-0.402927	0.060858
24	8	0	4.036269	-1.382527	-0.549080
25	8	0	4.322575	0.351683	0.723495

Structure 33c ($CHCl_3$)

Energy (Hartrees): -722.379549702
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.680869	0.970570	0.694013
2	6	0	0.320006	1.232106	0.646383
3	6	0	-0.556707	0.406091	-0.082908
4	6	0	-0.008869	-0.687569	-0.781322
5	6	0	1.350431	-0.962665	-0.743732
6	6	0	2.183477	-0.129301	-0.000436
7	1	0	2.347878	1.603675	1.262944
8	1	0	-0.072663	2.084709	1.183232
9	1	0	-0.647648	-1.313694	-1.393225
10	1	0	1.764873	-1.797556	-1.291862
11	6	0	-2.003627	0.697874	-0.127535
12	6	0	-2.992879	-0.257174	0.035488
13	1	0	-4.024443	0.078524	-0.035809
14	6	0	-2.489283	2.046197	-0.328693
15	1	0	-3.595614	2.122219	-0.358422
16	1	0	-1.928201	-1.936140	0.418921
17	7	0	-2.858573	-1.554518	0.307363
18	6	0	-3.969724	-2.478459	0.491976
19	1	0	-3.897557	-2.967634	1.466389
20	1	0	-4.909068	-1.927937	0.444503
21	1	0	-3.969374	-3.244914	-0.288118
22	8	0	-1.813337	3.061439	-0.474999
23	7	0	3.618451	-0.413520	0.047928
24	8	0	4.037928	-1.400889	-0.554583
25	8	0	4.341722	0.345575	0.690209

Structure 33c (DMSO)

Energy (Hartrees): -722.381820441
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.685919	0.967012	0.696956
2	6	0	0.325441	1.227940	0.652218
3	6	0	-0.554888	0.402335	-0.074876
4	6	0	-0.009353	-0.695435	-0.769427
5	6	0	1.349541	-0.970895	-0.734029
6	6	0	2.187128	-0.134653	0.002378
7	1	0	2.351492	1.600453	1.267343
8	1	0	-0.065612	2.077123	1.195653
9	1	0	-0.649179	-1.328953	-1.372226
10	1	0	1.757137	-1.811290	-1.278931
11	6	0	-1.999104	0.701216	-0.117055
12	6	0	-2.998017	-0.250613	0.043924
13	1	0	-4.026455	0.093976	-0.027819
14	6	0	-2.478383	2.047647	-0.325686
15	1	0	-3.584151	2.126716	-0.343455
16	1	0	-1.948692	-1.941264	0.419250
17	7	0	-2.874162	-1.544871	0.312291
18	6	0	-3.992709	-2.464645	0.474247
19	1	0	-3.925847	-2.968829	1.441064
20	1	0	-4.928263	-1.907985	0.427051
21	1	0	-3.985287	-3.218795	-0.317388
22	8	0	-1.801637	3.062136	-0.497167
23	7	0	3.619669	-0.416278	0.044324
24	8	0	4.038116	-1.413141	-0.546302
25	8	0	4.350127	0.354437	0.668627

Structure 33c (C_2H_5OH)

Energy (Hartrees): -722.383786909
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.676948	0.948427	0.728220
2	6	0	0.316849	1.209221	0.683197
3	6	0	-0.555999	0.406471	-0.076893
4	6	0	-0.007250	-0.668322	-0.803251
5	6	0	1.351076	-0.944248	-0.768387
6	6	0	2.182034	-0.130716	0.001207
7	1	0	2.337295	1.563144	1.324447
8	1	0	-0.078414	2.037108	1.256714
9	1	0	-0.644625	-1.281080	-1.429705
10	1	0	1.762772	-1.764803	-1.339769
11	6	0	-2.002168	0.702623	-0.119352
12	6	0	-2.997290	-0.256187	0.045015
13	1	0	-4.028380	0.080479	-0.023336
14	6	0	-2.484471	2.038229	-0.328806
15	1	0	-3.586746	2.125034	-0.342785
16	1	0	-1.928456	-1.934116	0.410016
17	7	0	-2.859247	-1.546246	0.314255
18	6	0	-3.969546	-2.475986	0.486460
19	1	0	-3.886035	-2.982604	1.450504
20	1	0	-4.909629	-1.926331	0.452973
21	1	0	-3.965497	-3.227424	-0.307563
22	8	0	-1.802501	3.057952	-0.507382
23	7	0	3.609861	-0.412038	0.044931
24	8	0	4.038153	-1.394488	-0.564125
25	8	0	4.340889	0.341724	0.690225

Structure 33d (vacuum)

Energy (Hartrees): -722.348730156
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.849751	1.012687	0.520733
2	6	0	0.478784	1.216823	0.466350
3	6	0	-0.379602	0.244056	-0.080386
4	6	0	0.199544	-0.928467	-0.601198
5	6	0	1.568497	-1.149258	-0.546141
6	6	0	2.381364	-0.173318	0.020895
7	1	0	2.509803	1.754597	0.948602
8	1	0	0.066074	2.139265	0.848057
9	1	0	-0.426980	-1.668228	-1.085803
10	1	0	2.012926	-2.048916	-0.948927
11	6	0	-1.846415	0.436307	-0.102235
12	6	0	-2.663172	-0.652956	0.111566
13	1	0	-2.195349	-1.591663	0.396781
14	6	0	-2.427488	1.756854	-0.312668
15	1	0	-3.538205	1.796544	-0.254702
16	1	0	-4.529833	0.073834	-0.255861
17	7	0	-4.005852	-0.747427	0.005645
18	6	0	-4.766940	-1.860515	0.555560
19	1	0	-5.659095	-2.029938	-0.049174
20	1	0	-4.157057	-2.764935	0.524441
21	1	0	-5.071638	-1.682175	1.592783
22	8	0	-1.823543	2.792902	-0.524766
23	7	0	3.835298	-0.395552	0.080584
24	8	0	4.271896	-1.450239	-0.370067
25	8	0	4.528808	0.483485	0.580500

Structure 33d ($CHCl_3$)

Energy (Hartrees): -722.374236952
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.867076	1.036486	0.465751
2	6	0	0.497809	1.242050	0.426424
3	6	0	-0.381224	0.246504	-0.051920
4	6	0	0.188122	-0.959880	-0.513151
5	6	0	1.554716	-1.183322	-0.470800
6	6	0	2.387979	-0.179119	0.020484
7	1	0	2.529588	1.802791	0.844402
8	1	0	0.099696	2.183220	0.776193
9	1	0	-0.445932	-1.727975	-0.939011
10	1	0	1.977657	-2.110760	-0.832138
11	6	0	-1.841492	0.450536	-0.067648
12	6	0	-2.672319	-0.648587	0.136665
13	1	0	-2.214040	-1.586742	0.436927
14	6	0	-2.422946	1.761398	-0.260669
15	1	0	-3.525648	1.805407	-0.161970
16	1	0	-4.517146	0.082441	-0.294664
17	7	0	-3.997582	-0.727418	0.016446
18	6	0	-4.788233	-1.873095	0.448517
19	1	0	-5.547124	-2.100753	-0.302185
20	1	0	-4.137131	-2.739608	0.566463
21	1	0	-5.284367	-1.672507	1.403054
22	8	0	-1.825698	2.807044	-0.505917
23	7	0	3.828847	-0.400794	0.059250
24	8	0	4.262746	-1.494646	-0.305084
25	8	0	4.551536	0.513120	0.457393

Structure 33d (DMSO)

Energy (Hartrees): -722.377051276
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.869960	1.042619	0.448000
2	6	0	0.501635	1.249712	0.411201
3	6	0	-0.384417	0.248534	-0.047318
4	6	0	0.182711	-0.969125	-0.486971
5	6	0	1.548506	-1.192655	-0.448569
6	6	0	2.388820	-0.181288	0.019598
7	1	0	2.532719	1.814246	0.815551
8	1	0	0.107316	2.195496	0.752510
9	1	0	-0.452959	-1.748077	-0.889767
10	1	0	1.963889	-2.129098	-0.795212
11	6	0	-1.840694	0.458297	-0.060825
12	6	0	-2.674315	-0.646964	0.138515
13	1	0	-2.213242	-1.589170	0.419345
14	6	0	-2.421936	1.767540	-0.248808
15	1	0	-3.523274	1.810048	-0.149610
16	1	0	-4.522296	0.095149	-0.249842
17	7	0	-3.995273	-0.718731	0.040895
18	6	0	-4.780703	-1.890052	0.410128
19	1	0	-5.464309	-2.147007	-0.401584
20	1	0	-4.112072	-2.730308	0.595815
21	1	0	-5.364185	-1.692487	1.313669
22	8	0	-1.826212	2.816441	-0.499170
23	7	0	3.825258	-0.402627	0.054141
24	8	0	4.260158	-1.503768	-0.294115
25	8	0	4.553694	0.518702	0.432556

Structure 33d (C_2H_5OH)

Energy (Hartrees): -722.378724649
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.868393	1.037448	0.469786
2	6	0	0.500944	1.245211	0.434526
3	6	0	-0.383025	0.253187	-0.046518
4	6	0	0.182094	-0.956650	-0.508475
5	6	0	1.546796	-1.182498	-0.471699
6	6	0	2.386109	-0.179424	0.018026
7	1	0	2.529521	1.800352	0.857820
8	1	0	0.106893	2.181001	0.803303
9	1	0	-0.455061	-1.725705	-0.927707
10	1	0	1.961621	-2.112125	-0.836846
11	6	0	-1.839634	0.461865	-0.058648
12	6	0	-2.672789	-0.646015	0.147759
13	1	0	-2.209824	-1.582293	0.444875
14	6	0	-2.419591	1.762562	-0.252728
15	1	0	-3.517423	1.815352	-0.146498
16	1	0	-4.516660	0.086569	-0.269309
17	7	0	-3.990231	-0.721968	0.038335
18	6	0	-4.777677	-1.889392	0.419338
19	1	0	-5.460649	-2.152637	-0.390614
20	1	0	-4.110952	-2.728840	0.614490
21	1	0	-5.361604	-1.680330	1.319853
22	8	0	-1.818937	2.812742	-0.519060
23	7	0	3.816005	-0.404129	0.054358
24	8	0	4.252957	-1.508011	-0.287407
25	8	0	4.553979	0.513216	0.428165

Structure 33e (vacuum)

Energy (Hartrees): -722.344809443
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.797120	1.050064	-0.487705
2	6	0	-0.412689	1.138150	-0.477839
3	6	0	0.379036	0.075654	-0.005189
4	6	0	-0.275749	-1.067201	0.487394
5	6	0	-1.660406	-1.172610	0.479047
6	6	0	-2.407352	-0.108500	-0.013546
7	1	0	-2.408018	1.860779	-0.860068
8	1	0	0.061760	2.039224	-0.838580
9	1	0	0.306462	-1.877230	0.911426
10	1	0	-2.163716	-2.049959	0.861173
11	6	0	1.863903	0.145712	-0.029643
12	6	0	2.535508	-0.986717	-0.436787
13	1	0	1.914170	-1.795845	-0.809751
14	6	0	2.523109	1.400640	0.332077
15	1	0	3.622129	1.411717	0.248287
16	1	0	4.042259	-2.214360	-0.902208
17	7	0	3.845197	-1.325453	-0.473613
18	6	0	4.997465	-0.600999	0.037633
19	1	0	5.848959	-1.281813	0.054946
20	1	0	5.256781	0.258974	-0.587158
21	1	0	4.811933	-0.253606	1.057083
22	8	0	1.952601	2.417366	0.690853
23	7	0	-3.877065	-0.207419	-0.024777
24	8	0	-4.511467	0.747287	-0.459706
25	8	0	-4.384119	-1.241270	0.398969

Structure 33e ($CHCl_3$)

Energy (Hartrees): -722.370307612
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.809607	1.077335	-0.427492
2	6	0	-0.427178	1.168543	-0.436852
3	6	0	0.381556	0.084753	-0.036693
4	6	0	-0.265736	-1.090028	0.397384
5	6	0	-1.648046	-1.199328	0.406909
6	6	0	-2.411220	-0.109490	-0.006771
7	1	0	-2.420922	1.908825	-0.750570
8	1	0	0.034563	2.086978	-0.769232
9	1	0	0.321483	-1.925663	0.759101
10	1	0	-2.131724	-2.104411	0.747859
11	6	0	1.859965	0.161620	-0.079792
12	6	0	2.540322	-0.986720	-0.471194
13	1	0	1.932438	-1.789673	-0.877659
14	6	0	2.536399	1.407296	0.230338
15	1	0	3.622106	1.419296	0.054289
16	1	0	4.053110	-2.213894	-0.865061
17	7	0	3.835227	-1.323084	-0.442907
18	6	0	4.958064	-0.633410	0.177477
19	1	0	5.757707	-1.358900	0.328087
20	1	0	5.340238	0.177876	-0.447764
21	1	0	4.663269	-0.227921	1.147956
22	8	0	1.999563	2.437861	0.634123
23	7	0	-3.868292	-0.210484	0.005285
24	8	0	-4.524889	0.770620	-0.342189
25	8	0	-4.378166	-1.273601	0.360124

Structure 33e (DMSO)

Energy (Hartrees): -722.372936410
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.809993	1.082800	-0.411421
2	6	0	-0.428202	1.172593	-0.420450
3	6	0	0.382859	0.081970	-0.038524
4	6	0	-0.266932	-1.100702	0.374823
5	6	0	-1.648714	-1.207237	0.386426
6	6	0	-2.413962	-0.109954	-0.007447
7	1	0	-2.417962	1.921100	-0.723306
8	1	0	0.033076	2.094929	-0.742028
9	1	0	0.317775	-1.946239	0.716579
10	1	0	-2.128866	-2.119566	0.713027
11	6	0	1.858080	0.161451	-0.080858
12	6	0	2.542607	-0.994135	-0.461584
13	1	0	1.938726	-1.802032	-0.863438
14	6	0	2.536398	1.406577	0.214893
15	1	0	3.619797	1.413957	0.028636
16	1	0	4.051503	-2.224097	-0.834212
17	7	0	3.832830	-1.325413	-0.426284
18	6	0	4.957927	-0.627189	0.180946
19	1	0	5.753018	-1.354214	0.345315
20	1	0	5.341657	0.168376	-0.463187
21	1	0	4.663867	-0.198778	1.141604
22	8	0	2.008086	2.443329	0.622449
23	7	0	-3.867210	-0.207971	0.007987
24	8	0	-4.525796	0.774708	-0.340030
25	8	0	-4.381332	-1.270136	0.366115

Structure 33e (C_2H_5OH)

Energy (Hartrees): -722.374861905
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.809226	1.071357	-0.450451
2	6	0	-0.428141	1.162244	-0.461551
3	6	0	0.382199	0.084212	-0.045631
4	6	0	-0.263185	-1.089760	0.396182
5	6	0	-1.644237	-1.199083	0.409490
6	6	0	-2.409918	-0.111623	-0.012028
7	1	0	-2.417686	1.898934	-0.788899
8	1	0	0.030861	2.073368	-0.818367
9	1	0	0.325247	-1.923889	0.759306
10	1	0	-2.122671	-2.103481	0.759873
11	6	0	1.858401	0.165630	-0.082304
12	6	0	2.543991	-0.988207	-0.474238
13	1	0	1.939360	-1.789086	-0.889011
14	6	0	2.530172	1.399154	0.237549
15	1	0	3.613188	1.420836	0.063094
16	1	0	4.052244	-2.214961	-0.852870
17	7	0	3.831556	-1.320579	-0.436075
18	6	0	4.955537	-0.621069	0.173296
19	1	0	5.756387	-1.344150	0.325756
20	1	0	5.330121	0.183158	-0.465037
21	1	0	4.663664	-0.206093	1.140413
22	8	0	1.990344	2.431415	0.662578
23	7	0	-3.857911	-0.209029	0.010150
24	8	0	-4.523179	0.770900	-0.336467
25	8	0	-4.377139	-1.267878	0.374555

Structure 33f (vacuum)

Energy (Hartrees): -722.346877316
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.883033	1.174826	-0.256749
2	6	0	-0.497378	1.234744	-0.273616
3	6	0	0.291871	0.096633	-0.009978
4	6	0	-0.377891	-1.109354	0.277056
5	6	0	-1.762938	-1.190203	0.277512
6	6	0	-2.503599	-0.041918	0.013843
7	1	0	-2.486839	2.046654	-0.468104
8	1	0	-0.020399	2.173180	-0.528193
9	1	0	0.197224	-1.990661	0.535494
10	1	0	-2.274780	-2.116495	0.499770
11	6	0	1.768220	0.167684	-0.037419
12	6	0	2.454994	-0.903943	-0.578944
13	1	0	1.868224	-1.630825	-1.135728
14	6	0	2.393453	1.413594	0.401719
15	1	0	1.729064	2.065735	1.001899
16	1	0	4.022492	-2.029545	-1.078129
17	7	0	3.756420	-1.232060	-0.523426
18	6	0	4.771283	-0.727169	0.394836
19	1	0	5.615980	-1.415963	0.372911
20	1	0	5.089746	0.279766	0.126862
21	1	0	4.366181	-0.694582	1.409931
22	8	0	3.524109	1.795800	0.134836
23	7	0	-3.973361	-0.115468	0.023750
24	8	0	-4.598931	0.914804	-0.202660
25	8	0	-4.489954	-1.203595	0.256758

Structure 33f ($CHCl_3$)

Energy (Hartrees): -722.369711796
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.882529	1.185464	-0.215329
2	6	0	-0.499188	1.247417	-0.241679
3	6	0	0.296752	0.100604	-0.023967
4	6	0	-0.372195	-1.118901	0.219296
5	6	0	-1.755084	-1.201011	0.228224
6	6	0	-2.502878	-0.042794	0.016137
7	1	0	-2.479844	2.069141	-0.393770
8	1	0	-0.028412	2.195637	-0.469102
9	1	0	0.201994	-2.012290	0.432890
10	1	0	-2.254330	-2.141104	0.419289
11	6	0	1.768274	0.174602	-0.054824
12	6	0	2.463621	-0.916701	-0.571656
13	1	0	1.894623	-1.644489	-1.144281
14	6	0	2.391704	1.425406	0.342642
15	1	0	1.740185	2.093588	0.935820
16	1	0	4.033975	-2.055985	-1.001019
17	7	0	3.749952	-1.248341	-0.464679
18	6	0	4.741602	-0.728752	0.467781
19	1	0	5.545743	-1.460984	0.539753
20	1	0	5.136907	0.234268	0.143901
21	1	0	4.288238	-0.597441	1.453308
22	8	0	3.523999	1.808267	0.050921
23	7	0	-3.959679	-0.116793	0.035272
24	8	0	-4.599915	0.922961	-0.122594
25	8	0	-4.488018	-1.215780	0.207837

Structure 33f (DMSO)

Energy (Hartrees): -722.371131491
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.881374	1.192025	-0.184065
2	6	0	-0.499053	1.256256	-0.215482
3	6	0	0.300830	0.104045	-0.033539
4	6	0	-0.367945	-1.123446	0.177500
5	6	0	-1.749828	-1.206278	0.190747
6	6	0	-2.501857	-0.042880	0.016314
7	1	0	-2.477086	2.081835	-0.335207
8	1	0	-0.033068	2.212102	-0.419250
9	1	0	0.205250	-2.024027	0.361149
10	1	0	-2.243238	-2.154239	0.357115
11	6	0	1.769347	0.178290	-0.067457
12	6	0	2.465983	-0.924744	-0.568303
13	1	0	1.904297	-1.655109	-1.144221
14	6	0	2.395953	1.431454	0.311489
15	1	0	1.752409	2.103843	0.908126
16	1	0	4.033945	-2.080084	-0.948177
17	7	0	3.745087	-1.258302	-0.434200
18	6	0	4.718534	-0.730515	0.511337
19	1	0	5.512492	-1.469246	0.617387
20	1	0	5.132608	0.221203	0.176587
21	1	0	4.241055	-0.572253	1.481611
22	8	0	3.524906	1.815301	0.002410
23	7	0	-3.954069	-0.117558	0.042206
24	8	0	-4.599159	0.924578	-0.099672
25	8	0	-4.484413	-1.219660	0.204461

Structure 33f (C_2H_5OH)

Energy (Hartrees): -722.372927941
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.886202	1.198069	-0.176783
2	6	0	-0.505391	1.268220	-0.212790
3	6	0	0.299797	0.117736	-0.040010
4	6	0	-0.362463	-1.114805	0.164996
5	6	0	-1.742831	-1.204426	0.181629
6	6	0	-2.500694	-0.042157	0.017183
7	1	0	-2.484910	2.086865	-0.322141
8	1	0	-0.045268	2.227215	-0.414140
9	1	0	0.215117	-2.013755	0.343017
10	1	0	-2.230635	-2.155780	0.344982
11	6	0	1.767219	0.193231	-0.076944
12	6	0	2.463877	-0.913736	-0.580898
13	1	0	1.907145	-1.628330	-1.180928
14	6	0	2.398930	1.438506	0.290848
15	1	0	1.759951	2.134962	0.859895
16	1	0	4.028499	-2.074045	-0.949998
17	7	0	3.733585	-1.260807	-0.424804
18	6	0	4.697604	-0.751896	0.542152
19	1	0	5.424933	-1.541633	0.730385
20	1	0	5.208478	0.139341	0.176112
21	1	0	4.187671	-0.502041	1.474240
22	8	0	3.546150	1.799638	-0.003920
23	7	0	-3.945399	-0.123618	0.047438
24	8	0	-4.602468	0.916359	-0.067325
25	8	0	-4.477102	-1.230281	0.186725

Structure 33g (vacuum)

Energy (Hartrees): -722.350994599
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.724135	-1.119031	-0.456383
2	6	0	0.346781	-0.954369	-0.487454
3	6	0	-0.259592	0.238221	-0.049874
4	6	0	0.577120	1.264118	0.428855
5	6	0	1.956555	1.120326	0.451503
6	6	0	2.517137	-0.075148	0.010671
7	1	0	2.191108	-2.031469	-0.800922
8	1	0	-0.264360	-1.755043	-0.886373
9	1	0	0.138775	2.176574	0.814684
10	1	0	2.599489	1.906655	0.822428
11	6	0	-1.725148	0.404769	-0.094777
12	6	0	-2.285310	1.611289	-0.429280
13	1	0	-1.674737	2.471421	-0.687726
14	6	0	-2.602038	-0.715584	0.206081
15	1	0	-2.133992	-1.660286	0.507767
16	7	0	-3.882340	-0.611172	0.155810
17	6	0	-4.710921	-1.750875	0.500374
18	1	0	-5.365100	-1.489203	1.337123
19	1	0	-5.354534	-2.004657	-0.346873
20	1	0	-4.120341	-2.634554	0.775402
21	8	0	-3.580709	1.840354	-0.499791
22	1	0	-4.041081	0.966071	-0.264390
23	7	0	3.979772	-0.239674	0.042088
24	8	0	4.651411	0.699915	0.454206
25	8	0	4.443102	-1.306754	-0.346252

Structure 33g ($CHCl_3$)

Energy (Hartrees): -722.368275643
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.720038	-1.142613	-0.395796
2	6	0	0.344268	-0.977837	-0.421108
3	6	0	-0.258064	0.238006	-0.038975
4	6	0	0.586755	1.285779	0.381965
5	6	0	1.964154	1.140685	0.399707
6	6	0	2.521984	-0.077518	0.011244
7	1	0	2.172423	-2.076103	-0.701358
8	1	0	-0.267929	-1.799901	-0.770296
9	1	0	0.158189	2.219465	0.724866
10	1	0	2.602609	1.949131	0.728784
11	6	0	-1.721429	0.404572	-0.081200
12	6	0	-2.281386	1.621387	-0.382182
13	1	0	-1.676888	2.492797	-0.615426
14	6	0	-2.603226	-0.723437	0.186393
15	1	0	-2.148989	-1.679890	0.463187
16	7	0	-3.882671	-0.603766	0.132747
17	6	0	-4.729026	-1.742407	0.439750
18	1	0	-5.392080	-1.490996	1.273097
19	1	0	-5.363758	-1.968378	-0.422422
20	1	0	-4.150943	-2.636970	0.701972
21	8	0	-3.580835	1.839549	-0.448109
22	1	0	-4.031937	0.942109	-0.234333
23	7	0	3.973096	-0.241488	0.033598
24	8	0	4.663434	0.716946	0.378690
25	8	0	4.442642	-1.330768	-0.294492

Structure 33g (DMSO)

Energy (Hartrees): -722.367582613
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.719259	-1.146277	-0.387203
2	6	0	0.343615	-0.982262	-0.410382
3	6	0	-0.257523	0.237790	-0.038009
4	6	0	0.588302	1.290322	0.370627
5	6	0	1.965144	1.144139	0.388944
6	6	0	2.522966	-0.077996	0.010282
7	1	0	2.167008	-2.084052	-0.686310
8	1	0	-0.268235	-1.809255	-0.748121
9	1	0	0.162232	2.229247	0.701866
10	1	0	2.601424	1.957342	0.710240
11	6	0	-1.720109	0.403856	-0.078312
12	6	0	-2.281040	1.621285	-0.378686
13	1	0	-1.677458	2.493995	-0.609351
14	6	0	-2.602207	-0.724535	0.186683
15	1	0	-2.152114	-1.682786	0.460563
16	7	0	-3.881930	-0.599286	0.132701
17	6	0	-4.733186	-1.736567	0.435273
18	1	0	-5.399670	-1.483727	1.265524
19	1	0	-5.364270	-1.960556	-0.430228
20	1	0	-4.156930	-2.631102	0.699258
21	8	0	-3.581377	1.832911	-0.446261
22	1	0	-4.024088	0.925383	-0.231430
23	7	0	3.971367	-0.241475	0.033465
24	8	0	4.663418	0.714283	0.389370
25	8	0	4.444798	-1.328154	-0.304419

Structure 33g (C_2H_5OH)

Energy (Hartrees): -722.367546364
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.717044	-1.145530	-0.391165
2	6	0	0.342590	-0.979496	-0.415442
3	6	0	-0.257490	0.240864	-0.040210
4	6	0	0.589432	1.292774	0.369736
5	6	0	1.965219	1.146183	0.387362
6	6	0	2.521939	-0.077523	0.008304
7	1	0	2.163170	-2.083419	-0.692498
8	1	0	-0.269702	-1.804544	-0.757035
9	1	0	0.164498	2.230740	0.704912
10	1	0	2.600549	1.958772	0.712028
11	6	0	-1.719367	0.407015	-0.077078
12	6	0	-2.278187	1.626786	-0.365278
13	1	0	-1.678575	2.503171	-0.590407
14	6	0	-2.600731	-0.725053	0.180971
15	1	0	-2.147873	-1.682680	0.452239
16	7	0	-3.880138	-0.603558	0.125967
17	6	0	-4.725352	-1.746914	0.424380
18	1	0	-5.393246	-1.500820	1.255462
19	1	0	-5.355572	-1.970316	-0.441818
20	1	0	-4.145459	-2.639956	0.685060
21	8	0	-3.582623	1.839502	-0.427767
22	1	0	-4.030476	0.932782	-0.221861
23	7	0	3.963358	-0.243026	0.034111
24	8	0	4.665744	0.722687	0.345712
25	8	0	4.439325	-1.343723	-0.257456

Structure 33h (vacuum)

Energy (Hartrees): -722.325993773
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.658862	-1.093692	-0.486935
2	6	0	0.283663	-0.907242	-0.495645
3	6	0	-0.297425	0.282112	-0.018374
4	6	0	0.559041	1.276347	0.489104
5	6	0	1.936721	1.110270	0.493827
6	6	0	2.472577	-0.077147	0.004393
7	1	0	2.107654	-2.002441	-0.863855
8	1	0	-0.349185	-1.685948	-0.903959
9	1	0	0.138016	2.179331	0.914600
10	1	0	2.596194	1.871756	0.886899
11	6	0	-1.768665	0.460033	-0.053011
12	6	0	-2.258779	1.673978	-0.393942
13	1	0	-1.576503	2.474401	-0.666533
14	6	0	-2.600741	-0.706076	0.296175
15	1	0	-2.069507	-1.492632	0.856348
16	7	0	-3.831517	-0.830653	0.006934
17	6	0	-4.513407	-2.024422	0.463068
18	1	0	-4.952533	-2.538205	-0.397647
19	1	0	-3.863260	-2.726926	1.007738
20	1	0	-5.344461	-1.734947	1.113860
21	8	0	-3.569812	1.980333	-0.430146
22	1	0	-3.681197	2.894150	-0.710515
23	7	0	3.933953	-0.264333	0.013784
24	8	0	4.624024	0.652108	0.447002
25	8	0	4.376620	-1.324767	-0.413596

Structure 33h ($CHCl_3$)

Energy (Hartrees): -722.348848591
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.653782	-1.107123	-0.459973
2	6	0	0.279977	-0.919276	-0.467306
3	6	0	-0.299399	0.281823	-0.013070
4	6	0	0.561969	1.288096	0.467235
5	6	0	1.937798	1.120918	0.469916
6	6	0	2.472716	-0.079560	0.004514
7	1	0	2.090660	-2.027631	-0.822269
8	1	0	-0.350669	-1.708383	-0.857837
9	1	0	0.148354	2.204260	0.870682
10	1	0	2.590842	1.896751	0.845327
11	6	0	-1.769864	0.461583	-0.048547
12	6	0	-2.252834	1.689581	-0.361584
13	1	0	-1.571406	2.499880	-0.601590
14	6	0	-2.602789	-0.711230	0.269499
15	1	0	-2.068892	-1.522045	0.786154
16	7	0	-3.843645	-0.824987	0.006089
17	6	0	-4.508526	-2.041551	0.434852
18	1	0	-4.976569	-2.521591	-0.430770
19	1	0	-3.837112	-2.762887	0.923575
20	1	0	-5.317435	-1.786355	1.127542
21	8	0	-3.558468	1.999147	-0.410942
22	1	0	-3.657637	2.928582	-0.657860
23	7	0	3.923289	-0.266630	0.011105
24	8	0	4.629563	0.667364	0.388142
25	8	0	4.373326	-1.348865	-0.361766

Structure 33h (DMSO)

Energy (Hartrees): -722.347957109
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.647962	-1.104776	-0.464337
2	6	0	0.274699	-0.914369	-0.474597
3	6	0	-0.302904	0.288654	-0.022824
4	6	0	0.558495	1.295113	0.457250
5	6	0	1.933613	1.124312	0.464332
6	6	0	2.467955	-0.078632	0.002757
7	1	0	2.080261	-2.027964	-0.825101
8	1	0	-0.355670	-1.704953	-0.862710
9	1	0	0.147672	2.214843	0.854972
10	1	0	2.584142	1.901803	0.840665
11	6	0	-1.774055	0.468065	-0.055823
12	6	0	-2.254179	1.700468	-0.357840
13	1	0	-1.570777	2.510819	-0.590892
14	6	0	-2.598257	-0.709879	0.264774
15	1	0	-2.056502	-1.512353	0.784305
16	7	0	-3.838615	-0.843292	0.002442
17	6	0	-4.480908	-2.070021	0.443691
18	1	0	-4.942916	-2.566492	-0.416167
19	1	0	-3.793662	-2.773455	0.935036
20	1	0	-5.291818	-1.825058	1.138155
21	8	0	-3.558970	2.017154	-0.401709
22	1	0	-3.647187	2.953669	-0.628920
23	7	0	3.916069	-0.268910	0.015143
24	8	0	4.624413	0.658527	0.409010
25	8	0	4.368277	-1.348063	-0.369395

Structure 33h (C_2H_5OH)

Energy (Hartrees): -722.353363094
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.653852	-1.104138	-0.474472
2	6	0	0.281111	-0.917118	-0.484668
3	6	0	-0.300401	0.279994	-0.020268
4	6	0	0.557988	1.283831	0.472509
5	6	0	1.932666	1.117324	0.479817
6	6	0	2.470979	-0.079925	0.005327
7	1	0	2.088556	-2.021316	-0.847715
8	1	0	-0.346461	-1.703687	-0.885256
9	1	0	0.143803	2.197164	0.881329
10	1	0	2.579458	1.891930	0.868329
11	6	0	-1.770042	0.460155	-0.056129
12	6	0	-2.246356	1.695529	-0.357953
13	1	0	-1.565531	2.509840	-0.582914
14	6	0	-2.600630	-0.715949	0.248812
15	1	0	-2.056409	-1.545162	0.720314
16	7	0	-3.853315	-0.818689	0.028724
17	6	0	-4.499231	-2.051875	0.447067
18	1	0	-5.003266	-2.506955	-0.411759
19	1	0	-3.805634	-2.784822	0.882301
20	1	0	-5.277582	-1.822380	1.182435
21	8	0	-3.550348	2.009043	-0.417189
22	1	0	-3.647845	2.943842	-0.646857
23	7	0	3.912905	-0.265370	0.015738
24	8	0	4.627013	0.667389	0.391231
25	8	0	4.372606	-1.348558	-0.353004

Structure 33i (vacuum)

Energy (Hartrees): -722.332217672
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.516820	-1.184125	-0.462288
2	6	0	0.146578	-0.963400	-0.465848
3	6	0	-0.403755	0.244461	0.002097
4	6	0	0.478163	1.232145	0.478357
5	6	0	1.849621	1.024753	0.489431
6	6	0	2.355193	-0.183790	0.018499
7	1	0	1.941248	-2.107823	-0.830768
8	1	0	-0.504526	-1.734315	-0.859816
9	1	0	0.084127	2.168336	0.847591
10	1	0	2.529398	1.779073	0.860972
11	6	0	-1.869138	0.437648	-0.007844
12	6	0	-2.483858	1.616349	-0.240795
13	1	0	-3.567915	1.657407	-0.234065
14	6	0	-2.735358	-0.734694	0.252592
15	1	0	-2.236435	-1.585887	0.739514
16	7	0	-3.973898	-0.774939	-0.028096
17	6	0	-4.724638	-1.956697	0.347370
18	1	0	-5.212654	-2.372044	-0.539515
19	1	0	-4.108720	-2.738776	0.816376
20	1	0	-5.521090	-1.673792	1.043073
21	8	0	-1.825615	2.767399	-0.516206
22	1	0	-2.457980	3.473893	-0.679646
23	7	0	3.811508	-0.407990	0.027577
24	8	0	4.525704	0.493876	0.451926
25	8	0	4.226599	-1.483959	-0.389408

Structure 33i ($CHCl_3$)

Energy (Hartrees): -722.352849739
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.502824	-1.193691	-0.436556
2	6	0	0.134805	-0.967434	-0.433760
3	6	0	-0.407872	0.252746	0.015664
4	6	0	0.483391	1.245037	0.469940
5	6	0	1.853038	1.033556	0.473169
6	6	0	2.351390	-0.186240	0.017225
7	1	0	1.911327	-2.129129	-0.793486
8	1	0	-0.520381	-1.744661	-0.807429
9	1	0	0.099423	2.187271	0.834541
10	1	0	2.530578	1.796611	0.830833
11	6	0	-1.871362	0.450665	0.010455
12	6	0	-2.480961	1.637038	-0.217471
13	1	0	-3.563528	1.699935	-0.196117
14	6	0	-2.735062	-0.721510	0.270774
15	1	0	-2.254365	-1.544850	0.816424
16	7	0	-3.956934	-0.797693	-0.077643
17	6	0	-4.705535	-1.977575	0.316854
18	1	0	-5.145530	-2.441589	-0.571594
19	1	0	-4.098731	-2.725625	0.847238
20	1	0	-5.538443	-1.680467	0.963008
21	8	0	-1.819864	2.775897	-0.504592
22	1	0	-2.451006	3.493456	-0.649437
23	7	0	3.796894	-0.413825	0.016786
24	8	0	4.531221	0.502799	0.381894
25	8	0	4.214018	-1.511933	-0.348020

Structure 33i (DMSO)

Energy (Hartrees): -722.350819965
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.497817	-1.201719	-0.412027
2	6	0	0.130201	-0.974060	-0.406044
3	6	0	-0.408185	0.256692	0.020128
4	6	0	0.486871	1.256495	0.450954
5	6	0	1.856029	1.043428	0.450780
6	6	0	2.350747	-0.186155	0.016128
7	1	0	1.899280	-2.146423	-0.752007
8	1	0	-0.527093	-1.760552	-0.756058
9	1	0	0.108383	2.205547	0.803033
10	1	0	2.533282	1.814342	0.791734
11	6	0	-1.870868	0.455331	0.019283
12	6	0	-2.485458	1.641701	-0.198279
13	1	0	-3.567402	1.706292	-0.155952
14	6	0	-2.732655	-0.717235	0.284611
15	1	0	-2.267933	-1.518971	0.873151
16	7	0	-3.939440	-0.814792	-0.110491
17	6	0	-4.696106	-1.987154	0.296241
18	1	0	-5.087163	-2.492215	-0.592915
19	1	0	-4.107954	-2.704005	0.886110
20	1	0	-5.562287	-1.672304	0.888106
21	8	0	-1.831886	2.781741	-0.497431
22	1	0	-2.470244	3.501464	-0.600645
23	7	0	3.794265	-0.414918	0.011453
24	8	0	4.533676	0.508603	0.353266
25	8	0	4.210084	-1.521487	-0.333578

Structure 33i (C_2H_5OH)

Energy (Hartrees): -722.355131766
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.492022	-1.203566	-0.407197
2	6	0	0.126030	-0.973005	-0.400549
3	6	0	-0.410496	0.260716	0.022489
4	6	0	0.487371	1.260145	0.451352
5	6	0	1.855279	1.044909	0.450899
6	6	0	2.347734	-0.187331	0.017600
7	1	0	1.890558	-2.149798	-0.746586
8	1	0	-0.533023	-1.758485	-0.749645
9	1	0	0.110374	2.209147	0.805192
10	1	0	2.533540	1.814789	0.792479
11	6	0	-1.871616	0.460411	0.020331
12	6	0	-2.483586	1.649936	-0.196574
13	1	0	-3.564794	1.720963	-0.156946
14	6	0	-2.731854	-0.712122	0.283801
15	1	0	-2.269798	-1.505829	0.885151
16	7	0	-3.934433	-0.822524	-0.122565
17	6	0	-4.680687	-1.999288	0.294189
18	1	0	-5.058656	-2.521749	-0.590333
19	1	0	-4.089019	-2.700855	0.898235
20	1	0	-5.555598	-1.688432	0.874828
21	8	0	-1.827874	2.787446	-0.491833
22	1	0	-2.457949	3.514220	-0.593545
23	7	0	3.783993	-0.416899	0.009444
24	8	0	4.532511	0.506418	0.337351
25	8	0	4.203647	-1.526718	-0.326146

Structure 33j (vacuum)

Energy (Hartrees): -722.333091536
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.330515	-0.987919	-0.710854
2	6	0	-0.034931	-0.738470	-0.729268
3	6	0	-0.576030	0.365843	-0.051838
4	6	0	0.292391	1.208184	0.660371
5	6	0	1.658874	0.965609	0.695382
6	6	0	2.161969	-0.131203	0.003600
7	1	0	1.755671	-1.832162	-1.235609
8	1	0	-0.690645	-1.409429	-1.264800
9	1	0	-0.105713	2.059755	1.195560
10	1	0	2.332169	1.606719	1.247169
11	6	0	-2.034348	0.637568	-0.087482
12	6	0	-2.548293	1.871108	-0.282992
13	1	0	-3.624464	2.018941	-0.303501
14	6	0	-3.023868	-0.434450	0.090212
15	1	0	-4.074402	-0.099906	0.051323
16	7	0	-2.734470	-1.655008	0.287079
17	6	0	-3.822432	-2.595600	0.465064
18	1	0	-3.751625	-3.381236	-0.293622
19	1	0	-3.718357	-3.086156	1.437675
20	1	0	-4.820082	-2.133436	0.405243
21	8	0	-1.791439	2.978699	-0.475977
22	1	0	-2.354421	3.738778	-0.650590
23	7	0	3.613119	-0.394186	0.031611
24	8	0	4.321189	0.374862	0.672635
25	8	0	4.030030	-1.366253	-0.588264

Structure 33j ($CHCl_3$)

Energy (Hartrees): -722.354951784
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.339324	-0.950107	-0.767233
2	6	0	-0.025080	-0.700446	-0.788434
3	6	0	-0.578282	0.363195	-0.055684
4	6	0	0.280059	1.166089	0.713631
5	6	0	1.646265	0.925706	0.751250
6	6	0	2.161302	-0.131800	0.005100
7	1	0	1.764512	-1.763086	-1.339356
8	1	0	-0.667888	-1.334746	-1.382676
9	1	0	-0.126455	1.982378	1.296242
10	1	0	2.303576	1.541405	1.349528
11	6	0	-2.036046	0.634700	-0.096812
12	6	0	-2.542571	1.873746	-0.294517
13	1	0	-3.616494	2.033727	-0.323216
14	6	0	-3.023582	-0.435636	0.075783
15	1	0	-4.071881	-0.111322	-0.007493
16	7	0	-2.733589	-1.650948	0.320809
17	6	0	-3.829731	-2.588717	0.481902
18	1	0	-3.739466	-3.387598	-0.261801
19	1	0	-3.758550	-3.064855	1.465244
20	1	0	-4.822678	-2.125671	0.382985
21	8	0	-1.776172	2.967127	-0.486473
22	1	0	-2.336021	3.739138	-0.642218
23	7	0	3.604013	-0.390920	0.034019
24	8	0	4.315763	0.351415	0.707821
25	8	0	4.038961	-1.338125	-0.617716

Structure 33j (DMSO)

Energy (Hartrees): -722.354100105
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.352104	-0.877944	-0.848156
2	6	0	-0.013041	-0.631888	-0.871164
3	6	0	-0.582264	0.367459	-0.064252
4	6	0	0.258539	1.112654	0.778005
5	6	0	1.625384	0.874473	0.819162
6	6	0	2.156973	-0.120749	0.001861
7	1	0	1.787758	-1.641666	-1.477541
8	1	0	-0.643224	-1.215302	-1.529309
9	1	0	-0.161512	1.878040	1.417974
10	1	0	2.267496	1.445206	1.475724
11	6	0	-2.042555	0.629177	-0.100640
12	6	0	-2.556739	1.865132	-0.295301
13	1	0	-3.631330	2.021189	-0.316937
14	6	0	-3.016212	-0.450466	0.077827
15	1	0	-4.067526	-0.142233	-0.009835
16	7	0	-2.707005	-1.660599	0.334405
17	6	0	-3.792037	-2.613488	0.497717
18	1	0	-3.686616	-3.417785	-0.238442
19	1	0	-3.721243	-3.079643	1.486191
20	1	0	-4.789492	-2.164377	0.388233
21	8	0	-1.793305	2.958214	-0.497794
22	1	0	-2.361365	3.729447	-0.631552
23	7	0	3.598758	-0.379696	0.038273
24	8	0	4.292093	0.284437	0.807803
25	8	0	4.054196	-1.249772	-0.702959

Structure 33j (C_2H_5OH)

Energy (Hartrees): -722.357970198
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.360092	-0.843264	-0.887536
2	6	0	-0.004885	-0.599273	-0.910301
3	6	0	-0.581668	0.365997	-0.068066
4	6	0	0.250828	1.080641	0.808537
5	6	0	1.616966	0.842602	0.852693
6	6	0	2.156168	-0.119362	0.000192
7	1	0	1.801508	-1.580672	-1.543769
8	1	0	-0.629228	-1.156355	-1.596661
9	1	0	-0.177085	1.821053	1.472808
10	1	0	2.252010	1.388659	1.536518
11	6	0	-2.042263	0.626201	-0.103546
12	6	0	-2.551679	1.864846	-0.295252
13	1	0	-3.624526	2.030281	-0.319977
14	6	0	-3.014633	-0.452758	0.073903
15	1	0	-4.065385	-0.143457	-0.016216
16	7	0	-2.708338	-1.663152	0.336350
17	6	0	-3.800430	-2.608865	0.500457
18	1	0	-3.702968	-3.413858	-0.235852
19	1	0	-3.732515	-3.076606	1.488171
20	1	0	-4.794912	-2.153291	0.392529
21	8	0	-1.782517	2.954682	-0.491677
22	1	0	-2.340156	3.731365	-0.635288
23	7	0	3.592230	-0.378551	0.040873
24	8	0	4.276989	0.226660	0.866454
25	8	0	4.067408	-1.193317	-0.750941

Structure 33k (vacuum)

Energy (Hartrees): -722.332623865
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.503756	0.910120	-0.694725
2	6	0	-0.129332	0.722995	-0.711072
3	6	0	0.458949	-0.374184	-0.059390
4	6	0	-0.377527	-1.263893	0.634771
5	6	0	-1.755884	-1.091463	0.657841
6	6	0	-2.303163	-0.003674	-0.012639
7	1	0	-1.963447	1.747421	-1.201311
8	1	0	0.498645	1.432896	-1.229566
9	1	0	0.058850	-2.087001	1.188164
10	1	0	-2.402456	-1.771637	1.194819
11	6	0	1.923524	-0.606393	-0.115284
12	6	0	2.370476	-1.857347	-0.359626
13	1	0	1.682990	-2.673818	-0.555800
14	6	0	2.889956	0.482168	0.085300
15	1	0	3.944583	0.192199	-0.001978
16	7	0	2.548181	1.678441	0.352157
17	6	0	3.600293	2.657099	0.542614
18	1	0	3.466418	3.475581	-0.171728
19	1	0	3.505428	3.093784	1.541629
20	1	0	4.614170	2.245279	0.427599
21	8	0	3.693669	-2.171746	-0.386299
22	1	0	3.811271	-3.083132	-0.668981
23	7	0	-3.764330	0.191561	0.007996
24	8	0	-4.442378	-0.631018	0.614397
25	8	0	-4.219368	1.163493	-0.584432

Structure 33k ($CHCl_3$)

Energy (Hartrees): -722.353952278
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.508693	0.908102	-0.706901
2	6	0	-0.135705	0.718733	-0.726482
3	6	0	0.456407	-0.373340	-0.066071
4	6	0	-0.379251	-1.259815	0.636224
5	6	0	-1.756167	-1.086646	0.662532
6	6	0	-2.307272	-0.000691	-0.012809
7	1	0	-1.961704	1.742424	-1.224565
8	1	0	0.485521	1.419135	-1.266899
9	1	0	0.056668	-2.083053	1.189299
10	1	0	-2.392932	-1.769359	1.208204
11	6	0	1.919552	-0.602783	-0.124554
12	6	0	2.366696	-1.861248	-0.348529
13	1	0	1.682165	-2.685090	-0.522309
14	6	0	2.885914	0.486898	0.053327
15	1	0	3.935089	0.212738	-0.107728
16	7	0	2.561201	1.672443	0.390639
17	6	0	3.627517	2.644515	0.548596
18	1	0	3.449282	3.491640	-0.122076
19	1	0	3.603882	3.041564	1.568781
20	1	0	4.629019	2.236788	0.348641
21	8	0	3.682734	-2.172299	-0.384534
22	1	0	3.793963	-3.098284	-0.636069
23	7	0	-3.758432	0.195079	0.011895
24	8	0	-4.447499	-0.627169	0.613408
25	8	0	-4.224524	1.171528	-0.572000

Structure 33k (DMSO)

Energy (Hartrees): -722.352798771
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.509870	0.897268	-0.722268
2	6	0	-0.137198	0.707468	-0.743833
3	6	0	0.457449	-0.378593	-0.074791
4	6	0	-0.376176	-1.263407	0.632244
5	6	0	-1.752740	-1.088793	0.661713
6	6	0	-2.306317	-0.005160	-0.016521
7	1	0	-1.961450	1.727186	-1.248127
8	1	0	0.480606	1.400755	-1.297958
9	1	0	0.059732	-2.088711	1.182222
10	1	0	-2.384937	-1.771469	1.212677
11	6	0	1.921316	-0.600886	-0.130321
12	6	0	2.373849	-1.860154	-0.343447
13	1	0	1.691917	-2.688199	-0.506348
14	6	0	2.879566	0.495528	0.042845
15	1	0	3.927868	0.238227	-0.145840
16	7	0	2.552250	1.672623	0.410069
17	6	0	3.615091	2.652027	0.558348
18	1	0	3.415694	3.507225	-0.096223
19	1	0	3.613220	3.033941	1.584747
20	1	0	4.613504	2.254229	0.328477
21	8	0	3.689719	-2.164555	-0.379549
22	1	0	3.800234	-3.096130	-0.614004
23	7	0	-3.755016	0.194855	0.016482
24	8	0	-4.442929	-0.612103	0.642035
25	8	0	-4.225145	1.161509	-0.583647

Structure 33k (C_2H_5OH)

Energy (Hartrees): -722.356677823
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.511621	0.904284	-0.717313
2	6	0	-0.140003	0.713641	-0.737483
3	6	0	0.453886	-0.375135	-0.070825
4	6	0	-0.381491	-1.261680	0.633547
5	6	0	-1.757030	-1.086973	0.662292
6	6	0	-2.309830	-0.000583	-0.014427
7	1	0	-1.961468	1.735251	-1.243185
8	1	0	0.478315	1.407223	-1.290517
9	1	0	0.053536	-2.087548	1.183316
10	1	0	-2.389443	-1.770606	1.211912
11	6	0	1.916016	-0.600051	-0.128368
12	6	0	2.365293	-1.861377	-0.343024
13	1	0	1.685065	-2.690667	-0.505476
14	6	0	2.879975	0.492043	0.037450
15	1	0	3.923427	0.230705	-0.171532
16	7	0	2.566485	1.668454	0.420219
17	6	0	3.641835	2.637413	0.551994
18	1	0	3.437138	3.498668	-0.092681
19	1	0	3.666650	3.013665	1.580020
20	1	0	4.631334	2.232584	0.298075
21	8	0	3.679569	-2.168784	-0.383336
22	1	0	3.794109	-3.099586	-0.617841
23	7	0	-3.751813	0.197650	0.015275
24	8	0	-4.448708	-0.614162	0.627478
25	8	0	-4.226304	1.170207	-0.574593

Structure 33l (vacuum)

Energy (Hartrees): -722.331642165
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.500989	0.896139	-0.715849
2	6	0	-0.127089	0.705871	-0.735002
3	6	0	0.461994	-0.379863	-0.066212
4	6	0	-0.371798	-1.257879	0.644569
5	6	0	-1.749940	-1.082273	0.670934
6	6	0	-2.298182	-0.004287	-0.013986
7	1	0	-1.961858	1.724630	-1.235668
8	1	0	0.498007	1.405088	-1.271812
9	1	0	0.065509	-2.075804	1.204783
10	1	0	-2.395187	-1.753556	1.220549
11	6	0	1.928281	-0.615563	-0.122500
12	6	0	2.363373	-1.875625	-0.370833
13	1	0	1.665477	-2.679658	-0.569186
14	6	0	2.876196	0.482088	0.080032
15	1	0	3.947681	0.233163	-0.029682
16	7	0	2.542207	1.673655	0.369964
17	6	0	3.588149	2.657991	0.553419
18	1	0	3.436016	3.483180	-0.149047
19	1	0	3.508533	3.081781	1.559011
20	1	0	4.603774	2.255410	0.415087
21	8	0	3.633110	-2.331004	-0.434430
22	1	0	4.267292	-1.633525	-0.230068
23	7	0	-3.759321	0.195776	0.011991
24	8	0	-4.435310	-0.611773	0.639796
25	8	0	-4.214726	1.156987	-0.597251

Structure 33l ($CHCl_3$)

Energy (Hartrees): -722.352281898
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.504365	0.902811	-0.715673
2	6	0	-0.131877	0.710825	-0.739063
3	6	0	0.460382	-0.378238	-0.074596
4	6	0	-0.373428	-1.260487	0.634084
5	6	0	-1.750216	-1.084980	0.664116
6	6	0	-2.301630	-0.001371	-0.014112
7	1	0	-1.957949	1.735014	-1.236181
8	1	0	0.487973	1.407823	-1.285852
9	1	0	0.062866	-2.083446	1.187238
10	1	0	-2.386045	-1.764926	1.214273
11	6	0	1.924885	-0.611440	-0.136586
12	6	0	2.357349	-1.878285	-0.361432
13	1	0	1.659041	-2.686105	-0.545509
14	6	0	2.877358	0.488203	0.036228
15	1	0	3.932704	0.262094	-0.181917
16	7	0	2.553890	1.659454	0.417949
17	6	0	3.606797	2.647807	0.554697
18	1	0	3.382717	3.507769	-0.084783
19	1	0	3.620593	3.017567	1.585025
20	1	0	4.606227	2.265918	0.299251
21	8	0	3.625015	-2.332258	-0.414573
22	1	0	4.267026	-1.641665	-0.195474
23	7	0	-3.752687	0.197971	0.016101
24	8	0	-4.440559	-0.618599	0.626102
25	8	0	-4.218843	1.171972	-0.571578

Structure 33l (DMSO)

Energy (Hartrees): -722.351528484
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.504764	0.879197	-0.746548
2	6	0	-0.132271	0.687499	-0.768390
3	6	0	0.462680	-0.382336	-0.075056
4	6	0	-0.367875	-1.249010	0.656091
5	6	0	-1.744439	-1.071906	0.687128
6	6	0	-2.298958	-0.004989	-0.015693
7	1	0	-1.957718	1.695860	-1.291594
8	1	0	0.484320	1.366137	-1.341980
9	1	0	0.069932	-2.062495	1.221997
10	1	0	-2.375261	-1.740534	1.256559
11	6	0	1.928046	-0.610557	-0.132458
12	6	0	2.361446	-1.876918	-0.358983
13	1	0	1.661407	-2.686514	-0.528803
14	6	0	2.874710	0.491841	0.049498
15	1	0	3.935576	0.268822	-0.137309
16	7	0	2.539595	1.665628	0.417340
17	6	0	3.590695	2.656450	0.568371
18	1	0	3.384133	3.507370	-0.089329
19	1	0	3.579108	3.040263	1.593779
20	1	0	4.594409	2.269226	0.343685
21	8	0	3.628484	-2.325939	-0.432428
22	1	0	4.271563	-1.623624	-0.251747
23	7	0	-3.748232	0.196306	0.016598
24	8	0	-4.433277	-0.589482	0.671159
25	8	0	-4.220535	1.142462	-0.613306

Structure 33l (C_2H_5OH)

Energy (Hartrees): -722.354742381
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.505895	0.893516	-0.732242
2	6	0	-0.134545	0.700529	-0.755046
3	6	0	0.459680	-0.379384	-0.075312
4	6	0	-0.373460	-1.255377	0.643540
5	6	0	-1.749058	-1.079024	0.674372
6	6	0	-2.302282	-0.001274	-0.014783
7	1	0	-1.956704	1.717811	-1.267684
8	1	0	0.482496	1.385730	-1.320122
9	1	0	0.062715	-2.074949	1.201764
10	1	0	-2.380278	-1.755019	1.234683
11	6	0	1.923515	-0.609148	-0.135248
12	6	0	2.353424	-1.878213	-0.356115
13	1	0	1.652583	-2.686825	-0.527307
14	6	0	2.875482	0.491317	0.032344
15	1	0	3.925959	0.267855	-0.200588
16	7	0	2.553953	1.658183	0.434709
17	6	0	3.613116	2.644988	0.558854
18	1	0	3.381091	3.508083	-0.073815
19	1	0	3.647063	3.011352	1.590017
20	1	0	4.605701	2.261553	0.284254
21	8	0	3.620630	-2.331374	-0.421559
22	1	0	4.269985	-1.640118	-0.224976
23	7	0	-3.744800	0.199175	0.017304
24	8	0	-4.440850	-0.607129	0.637211
25	8	0	-4.219098	1.167931	-0.578465