Electronic Supplementary Information (ESI)

Amphipathic 1,3-oxazolidines from *N*-alkyl glucamines and benzaldehydes: Stereochemical and mechanistic studies.

Esther Matamoros,* Pedro Cintas and Juan C. Palacios*

Departamento de Química Orgánica e Inorgánica, Facultad de Ciencias, and IACYS-Unidad de Química Verde y Desarrollo Sostenible, Universidad de Extremadura, E-06006 Badajoz, Spain

E-mail: esthermc@unex.es; palacios@unex.es

ORCID
Esther Matamoros: 0000-0003-4460-2065
Pedro Cintas: 0000-0002-2608-3604
Juan Carlos Palacios: 0000-0002-5004-4744

Summary

Pages	**Supporting Data**
2	Tables S1-S9
9	Figures S1-S27
19	IR Spectra. (Fig. S28-S50)
27	NMR Spectra (Fig. S51-S140)
72	Cartesian Coordinates and Calculated Energies at the M06-2X/6-311G(d,p) Level in Gas Phase, Benzene and DMSO (SMD Model).

Table S1 ^{1}H NMR chemical shifts (δ, ppm) of the heterocyclic atoms of various oxazolidines[a]

Compound	H-2	H-5	H-4a	H-4b	$\Delta\delta_{H-4}$[b]	Configuration
21a	4.90	4.28	3.41	2.34	1.07	*R*
21b	5.17	4.20	2.88	2.81	0.07	*S*
22a	5.18	4.28	3.42	2.31	1.11	*R*
22b	5.28	4.19	3.09	2.73	0.36	*S*
23a	4.90	4.22	3.42	2.27	1.15	*R*
23b	5.06	4.17	3.08	2.68	0.40	*S*
24a	4.74	4.22	3.40	2.27	1.13	*R*
24b	4.98	4.18	2.97	2.71	0.26	*S*
25a	4.66	4.24	3.40	2.24	1.16	*R*
26a	4.63	4.24	3.40	2.23	1.17	*R*
27a[c]	4.68	4.25	3.40	2.25	1.15	*R*
28a	4.64	4.23	3.39	2.24	1.15	*R*
29a	4.64	4.23	3.40	2.24	1.16	*R*
30a	4.63	4.25	3.39	2.25	1.14	*R*
31a	4.61	4.25	3.41	2.23	1.18	*R*
32b	4.99	4.16	3.10	2.64	0.46	*S*
34b	5.13	4.19	2.89	2.78	0.11	*S*
35a	4.90	4.34	3.41	2.32	1.09	*R*
35b	5.12	4.20	2.95	2.77	0.18	*S*
36a	4.73	4.25	3.39	2.26	1.13	*R*
36b	4.93	4.17	2.98	2.68	0.30	*S*
37a	4.63	4.22	3.40	2.23	1.17	*R*
37b	4.76	4.17	3.12	2.60	0.52	*S*
38a	4.67	4.25	3.40	2.25	1.15	*R*
38b	4.83	4.18	3.09	2.63	0.46	*S*
39a	4.65	4.23	3.38	2.24	1.14	*R*
40a	4.62	4.19	3.39	2.23	1.16	*R*
41a	4.60	4.23	3.39	2.21	1.18	*R*

[a]At 500 MHz in DMSO-d_6; [b]$\Delta\delta_{H-4} = \delta_{H-4a} - \delta_{H-4b}$; [c]recorded at 400 MHz.

Table S2. ^{13}C NMR Chemical shifts (δ, ppm) of several oxazolidines.[a]

Product	C-2	C-4	C-5	N-CH_2	C-1'[c]	C-2'[c]	C-3'[c]	C-4'
21a	94.7	53.6	79.5	45.3	71.1	71.1	71.0	63.3
21b	95.2	52.5	79.5	46.6	71.3	71.1	70.9	63.4
22a	91.8	53.6	79.2	45.0	71.1	71.0	71.0	63.3
22b	92.9	52.0	78.0	46.0	71.1	70.9	70.9	63.4
23a	94.1	53.6	78.2	44.9	71.0	70.9	70.9	63.2
23b	94.6	52.3	77.6	45.1	71.2	71.1	71.0	63.7
24a	94.6	53.1	78.6	44.7	70.6	70.5	70.8	62.8
24b	95.1	51.9	77.2	45.6	70.7	70.3	70.3	62.9
25a	96.0	53.7	78.9	45.1	71.1	71.0	71.0	63.3
26a	96.1	53.7	78.8	44.9	71.1	71.0	71.0	63.3
27a[b]	96.2	53.7	78.9	45.0	71.1	71.0	71.0	63.3
28a	96.6	54.2	79.3	45.5	71.7	71.6	71.6	63.9
29a	96.0	53.7	78.7	45.0	71.1	71.0	71.0	63.3
30a	96.8	54.2	79.4	45.5	71.7	71.6	71.6	63.9
31a	96.5	54.2	79.1	45.4	71.7	71.6	71.6	63.9
32b	94.2	52.0	77.2	45.6	70.8	70.7	70.7	63.3
34b	96.1	53.4	78.6	52.8	71.9	71.6	71.4	63.9
35a	95.3	54.5	80.1	51.3	71.7	71.6	71.5	63.9
35b	95.9	53.4	78.6	52.5	71.9	71.6	71.4	64.0
36a	95.5	54.2	79.3	50.9	71.2	71.1	71.0	63.5
36b	96.4	53.3	78.2	52.2	71.7	71.6	71.4	64.0
37a	96.2	54.1	78.8	50.7	71.1	71.0	71.0	63.3
37b	96.5	54.5	77.1	50.7	71.1	70.3	70.3	63.2
38a	96.9	54.6	79.5	51.3	71.7	71.6	71.6	63.9
38b	97.5	53.4	78.1	51.9	71.6	71.4	71.4	64.1
39a	96.7	54.6	79.5	51.3	71.7	71.6	71.6	63.9
40a	96.9	56.6	79.5	51.2	71.7	71.5	71.5	63.9
41a	96.8	54.6	79.4	51.1	71.7	71.5	71.5	63.9

[a] At 125 MHz in DMSO-d_6; [b] at 100 MHz; [c] the chemical shifts of these carbons can be interchanged.

Table S3. ^{13}C NMR chemical shifts (δ, ppm) of **43**-**45**.

	C-2	C-4	C-5	C-1'[c]/C-6[d]	C-4'[c]/C-3'[d]	N-CH_3

Table S3 ^{1}H NMR chemical shifts (δ, ppm) at the heterocyclic moiety of **43**-**45**

		H-2	H-4[a]	H-4b	$\Delta\delta_{H-4}$[c]	H-5	H-1'[d]/H-6[e]	N-CH_3
	a[a]	4.75	3.29	2.74	0.55	4.51	3.55	2.14
43	**b**[a]	4.90	3.18	2.74	0.44	4.35	3.55	2.24
	c[b]	4.73	3.11	2.63	0.48	3.78	3.60	1.92
	a[a]	4.58	3.25	2.66	0.59	4.46	3.50	2.09
44	**b**[a]	4.61	3.26	2.70	0.56	4.33	3.50	2.14
	c[a]	4.49	3.08	2.63	0.45	3.76	3.55	1.88
	a[b]	4.52	3.24	2.66	0.58	4.43	3.50	2.07
45	**b**[a]	4.53	3.27	2.69	0.58	4.31	3.50	2.10
	c[a]	4.39	3.07	2.57	0.50	3.75	3.53	1.86

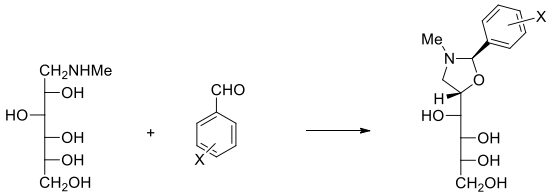
[a]At 500 MHz in DMSO-d_6; [b]recorded at 400 MHz in DMSO-d_6; [c]$\Delta\delta_{H-4} = \delta_{H-4a} - \delta_{H-4b}$; [d]oxazolidine; [e]oxazine.

Table S4. ^{13}C NMR chemical shifts (δ, ppm) of **43**-**45**.

		C-2	C-4	C-5	C-1'[c]/C-6[d]	C-4'[c]/C-3'[d]	N-CH_3
	a[a]	96.7	56.7	77.5	70.4	63.4	37.8
43	**b**[a]	96.7	56.1	77.3	71.6	63.4	38.3
	c[b]	94.4	60.7	63.1	78.9	63.2	39.5
	a[a]	98.2	56.8	76.8	70.6	63.4	37.7
44	**b**[a]	98.0	56.7	76.6	72.1	63.6	38.3
	c[a]	96.2	61.0	63.2	78.9	63.3	40.0
	a[b]	98.0	56.7	76.5	70.6	63.4	37.6
45	**b**[a]	97.2	54.3	75.7	71.7	63.0	37.4
	c[a]	95.5	60.5	62.6	78.2	63.8	37.0

[a] At 125MHz in DMSO-d_6; [b] 100MHz in DMSO-d_6; [c] oxazolidine; [d] oxazine.

Table S5. Chemical shift (δ, ppm) of heterocyclic protons, optical rotations (º) and configuration at C-2 of oxazolidines **2S**-**12S**.[a,b]



1 **2S-12S**

Comp.	X	H-4a	H-4b	$\Delta\delta_{H-4}$[c]	Configuration[d]	$[\alpha]_D$[e]
2S	4-NO_2	3.35	2.42	0.93	*R*	+11.0
3S	3-MeO	3.32	2.34	0.98	*R*	+12.0
4S	3-Br	3.31	2.35	0.96	*R*	+7.0
5S	4-Cl	3.32	2.35	0.97	*R*	+6.0
6S	H	3.33	2.37	0.96	*R*	+12.0
7S	2-Me	3.31	2.41	1.00	*R*	+22.0
8S	3-Me	3.32	2.34	0.98	*R*	+14.0
9S	4-Me	3.34	2.34	1.00	*R*	+11.0
10S	4-Et	3.32	2.34	0.98	*R*	+8.0
11S	4-MeO	3.30	2.31	0.99	*R*	+11.0
12S	2,4-$(Me)_2$	3.33	2.37	0.96	*R*	+14.0

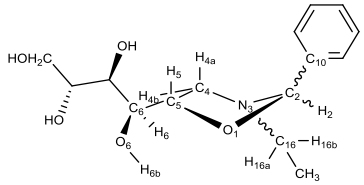
[a] At 400 MHz, in DMSO-d_6; [b] Reference 6; [c] $\Delta\delta_{H-4} = \delta_{H-4a} - \delta_{H-4b}$; [d] At C-2; [e]In C_5D_5N.

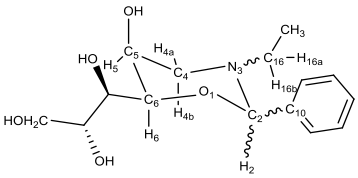
Table S6. Geometry (Å and °) and energy (kcal mol^{-1}) data for intramolecular hydrogen bonds in compounds **21**, **27** and **31**.[a]

					Gas phase				Benzene				DMSO			
	Et	**Arom**	**H Bond**	***D*-H···*A***	***d*(*D*-H)**	***d*(H···*A*)**	***d*(*D*···*A*)**	**Đ(*DHA*)**	***d*(*D*-H)**	***d*(H···*A*)**	***d*(*D*···*A*)**	**Đ(*DHA*)**	***d*(*D*-H)**	***d*(H···*A*)**	***d*(*D*···*A*)**	**Đ(*DHA*)**
21a	ec	ax	O	O6-H···O1	0.963	2.029	2.600	116.04	0.964	2.030	2.599	115.83	0.9647	2.0251	2.5948	115.82
	ec	ax	N	O6-H···N2	0.970	2.065	2.863	138.39	0.971	2.022	2.843	141.05	0.9742	1.9590	2.8063	144.01
	ax	ax	O	O6-H···O1	0.963	2.046	2.591	113.97	0.964	2.037	2.594	114.83	0.9647	2.0426	2.5942	114.38
	ec	ec	O	O6-H···O1	0.963	2.054	2.606	114.59	0.964	2.057	2.605	114.20	0.9642	2.0769	2.6144	113.42
21b	ec	ec	O	O6-H···O1	0.965	1.965	2.591	120.41	0.965	1.965	2.589	120.21	0.9654	1.9846	2.5912	118.76
	ec	ec	N	O6-H···N2	0.971	1.976	2.831	145.71	0.973	1.960	2.822	146.32	0.9748	1.9322	2.8013	147.11
	ax	ec	O	O6-H···O1	0.963	2.013	2.599	117.23	0.963	2.017	2.598	116.83	0.9643	2.0552	2.6031	114.16
21c	ec	ec	O	O7-H···O1	0.963	2.069	2.608	113.62	0.963	2.067	2.612	114.06	0.9642	2.0517	2.6136	115.32
	ax	ec	O	O7-H···O1	0.963	2.065	2.627	115.46	0.963	2.056	2.622	115.73	0.9642	2.0609	2.6265	115.67
21d	ec	ax	O	O7-H···O1	0.962	2.064	2.576	111.39	0.963	2.052	2.578	112.44	0.9642	2.0332	2.5841	114.31
	ax	ax	O	O7-H···O1	0.963	2.068	2.591	112.27	0.964	2.057	2.590	112.97	0.9645	2.0588	2.5997	113.60
27a	ec	ax	O	O6-H···O1	0.964	2.011	2.596	117.06	0.964	2.008	2.593	117.08	0.9648	2.0204	2.5929	116.02
	ec	ax	N	O6-H···N2	0.971	2.036	2.842	139.18	0.973	2.002	2.825	141.03	0.9761	1.9074	2.7819	147.73
	ax	ax	O	O6-H···O1	0.964	2.025	2.589	115.37	0.964	2.025	2.586	115.13	0.9645	2.0423	2.5900	114.07
	ec	ec	O	O6-H···O1	0.964	2.034	2.603	115.84	0.964	2.034	2.603	115.81	0.9645	2.0559	2.6113	114.77
27b	ec	ec	O	O6-H···O1	0.966	1.963	2.585	120.03	0.966	1.971	2.587	119.53	0.9659	1.9819	2.5891	118.76
	ec	ec	N	O6-H···N2	0.972	1.969	2.821	145.04	0.974	1.952	2.810	145.61	0.9754	1.9248	2.7923	146.76
	ax	ec	O	O6-H···O1	0.964	1.986	2.587	118.42	0.964	1.991	2.586	117.90	0.9648	2.0225	2.5912	115.71
27c	ec	ec	O	O7-H···O1	0.963	2.044	2.599	114.76	0.964	2.037	2.597	115.12	0.9642	2.0492	2.6138	115.53
	ax	ec	O	O7-H···O1	0.963	2.045	2.617	116.21	0.964	2.046	2.619	116.25	0.9645	2.0437	2.6181	116.31
27d	ec	ax	O	O7-H···O1	0.963	2.039	2.579	113.49	0.964	2.038	2.585	114.04	0.9643	2.0315	2.5912	115.02
	ax	ax	O	O7-H···O1	0.963	2.037	2.588	114.36	0.964	2.043	2.595	114.49	0.9646	2.0435	2.5992	114.73
31a	ec	ax	O	O6-H···O1	0.964	2.001	2.591	117.52	0.964	1.997	2.589	117.64	0.9649	2.0156	2.5916	116.29
	ec	ax	N	O6-H···N2	0.972	2.001	2.822	140.78	0.974	1.962	2.800	142.76	0.9755	1.9343	2.7876	144.63
	ax	ax	O	O6-H···O1	0.964	2.017	2.587	115.88	0.964	2.019	2.586	115.60	0.9647	2.0474	2.5945	114.03
	ec	ec	O	O6-H···O1	0.964	2.028	2.600	116.09	0.964	2.026	2.601	116.25	0.9646	2.0530	2.6099	114.88
31b	ec	ec	O	O6-H···O1	0.966	1.969	2.586	119.59	0.966	1.969	2.586	119.64	0.9658	1.9795	2.5881	118.88
	ec	ec	N	O6-H···N2	0.972	1.973	2.824	144.95	0.973	1.957	2.815	145.64	0.9759	1.9267	2.7957	146.95
	ax	ec	O	O6-H···O1	0.964	1.988	2.588	118.34	0.964	1.987	2.586	118.12	0.9648	2.0266	2.5932	115.55
31c	ec	ec	O	O7-H···O1	0.963	2.044	2.600	114.82	0.964	2.040	2.601	115.18	0.9643	2.0271	2.6017	116.27
	ax	ec	O	O7-H···O1	0.963	2.040	2.615	116.41	0.964	2.045	2.618	116.22	0.9645	2.0439	2.6185	116.33
31d	ec	ax	O	O7-H···O1	0.966	2.042	2.581	113.46	0.963	2.030	2.584	114.64	0.9644	2.0435	2.6040	115.16
	ax	ax	O	O7-H···O1	0.963	2.039	2.590	114.40	0.964	2.031	2.589	114.88	0.9647	2.0314	2.5934	115.20

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

Table S7. NBO data of **27.**[a,b]





		27a				27b			27c		27d	
Donor	Aceptor	ec-ax (N)	ec-ax (O)	ax-ax	ec-ec	ec (O)	ec-ec (N)	ax-ec	ec-ec	ax-ec	ec-ax	ax-ax
LP(1) N3	BD*(1) O1 - C2	1.18	1.13	11.31	1.4	0.91	1.14	12.24	3.61	18.15	7.42	16.84
LP(1) N3	BD*(1) C2 - C10	7.81	8.64	2.41	1.94	2.1	1.53	--	0.68	0.65	10.9	3.04
LP(1) N3	BD*(1) C2 - H2	3.87	4.45	--	9.45	8.97	7.71	3.44	8.88	2.61	1.61	--
LP(1) N3	BD*(1) C4 - H4a	2.81	3.02	--	8.39	2.77	2.65	--	--	0.89	0.82	0.76
LP(1) N3	BD*(1) C4 - H4b	8.07	9.18	4.26	3.69	8.78	7.63	4.21	8.71	3.4	9.9	3.71
LP(1) N3	BD*(1) C4 - C5	--	--	6.2	--	--	--	6.65	0.99	8.47	2.78	8.24
LP(1) N3	BD*(1) O6 - H6b	6.4	--	--	--	--	9.04	--	--	--	--	--
LP(1) N3	BD*(1) C16 - H16a	8.34	9.17	7.71	8.89	8.7	7.9	6.84	8.31	5.19	6.58	7.12
LP(1) N3	BD*(1) O5 - H5a	--	--	--	--	--	--	--	0.98	--	1.21	--
LP(1) O1	BD*(2) C2 - N3	3.35	3.33	2.73	1.43	3.07	2.79	2.51	0.78	0.76	0.76	1.23
LP(1) O1	BD*(1) C4 - C5	3.35	3.09	3.21	2.92	2.98	3.44	3.16	--	--	--	--
LP(2) O1	BD*(1) C2 - C10	7.62	7.17	7.84	1.25	3.18	2.77	0.98	--	0.88	5.67	5.82
LP(2) O1	BD*(2) C2 - N3	0.78	--	3.18	4.25	0.84	2.12	3.79	10.23	9.91	8.77	8.66
LP(2) O1	BD*(1) C2 - H2	5.24	5.45	2.01	9.45	8.8	10.14	8.81	6.57	5.33	3.74	3.31
LP(2) O1	BD*(1) C5 - H5	4.72	4.32	7.56	3.88	4.24	5.39	7.44	0.6	0.65	0.54	0.66
LP(2) O1	BD*(1) C5 - C6	6.41	5.78	3.47	5.75	6.29	6.14	3.8	5.88	5.97	6.25	5.94
LP(2) O1	BD*(1) C6 - H6	0.62	--	--	--	--	0.66	--	6.51	6.14	6.02	5.99
LP(1) O1	BD*(1) O6 - H6b	--	1.04	1.61	1.05	1.66	--	2.15	1.35	1.21	1.39	1.43
LP(2) O1	BD*(1) O6 - H6b	--	2.16	0.73	1.73	2.67	--	0.76	0.65	1.04	0.62	0.72
LP(2) O2	BD*(1) O5 - H5b	--	--	--	--	--	--	--	--	0.56	--	0.71

[a]At the M06-2X/6-311G(d,p) level in gas phase. [b]In kcal mol^{-1}

Table S8. Relative electronic and Gibbs energies for isomers and conformers of **34**, **38** and **39**[a]

			Gas phase		Benzene		DMSO	
	Octyl[b]	**Aryl[c]**	**ΔE**	**ΔG**	**ΔE**	**ΔG**	**ΔE**	**ΔG**
34a	eq	ax	2.78	2.98	2.82	2.77	2.60	2.45
34b	eq	eq	0.00	0.00	0.00	0.00	0.00	0.00
34c	eq	eq	1.96	0.64	1.70	0.72	1.21	2.63
34d	ax	ax	0.77	1.95	1.07	2.10	1.25	2.73
38a	eq	ax	2.70	3.57	2.80	2.70	2.93	0.99
38b	eq	eq	0.00	0.00	0.00	0.00	0.00	0.00
38c	eq	eq	1.72	0.93	1.54	0.81	1.52	0.60
38d	ax	ax	1.06	1.98	1.33	1.66	1.63	2.09
39a	eq	ax	2.31	1.84	2.38	1.36	2.48	0.50
39b	eq	eq	0.00	0.00	0.00	0.00	0.00	0.00
39c	eq	eq	1.35	2.28	1.58	0.95	1.26	0.85
39d	ax	ax	0.70	3.19	1.02	1.57	1.38	1.88

[a]In kcal mol^{-1}; [b]arrangement of the octyl group with respect to the ring; [c]arrangement of the aromatic ring with respect to either oxazolidine or oxazine rings.

Table S9. Relative electronic and Gibbs energies for isomers/conformers of compounds **43**-**45**[a]

				Gas phase		Benzene		DMSO	
	Methyl[b]	**Aryl**[c]	**H-bond**[d]	**ΔE**	**ΔG**	**ΔE**	**ΔG**	**ΔE**	**ΔG**
43a	eq	ax	O	3.66	2.57	4.18	3.17	4.21	4.01
	eq	ax	N	2.53	2.28	2.32	2.04	1.98	2.02
	eq	eq	O	2.33	0.49	2.62	1.29	3.03	2.18
	ax	ax	O	1.79	1.40	2.44	1.91	3.27	3.01
43b	eq	eq	O	1.70	0.32	2.17	1.16	2.37	1.90
	eq	eq	N	0.00	0.00	0.00	0.00	0.00	0.00
	ax	eq	O	3.84	2.97	4.48	3.27	4.81	4.76
43c	eq	eq	O	2.65	1.59	1.66	1.47	-0.42	0.10
	ax	eq	O	3.44	2.87	3.31	2.49	2.71	2.96
43d	eq	ax	O	6.63	5.23	5.81	4.85	4.07	2.84
	ax	ax	O	3.72	3.79	3.71	3.70	3.19	3.88
44a	eq	ax	O	3.84	3.31	4.40	3.84	4.53	3.78
	eq	ax	N	2.30	1.95	2.21	2.17	2.07	2.00
	eq	eq	O	2.61	1.06	2.84	1.65	3.09	1.83
	ax	ax	O	2.47	1.23	3.10	1.63	3.63	2.94
44b	eq	eq	O	1.59	0.81	2.08	1.48	2.34	1.48
	eq	eq	N	0.00	0.00	0.00	0.00	0.00	0.00
	ax	eq	O	4.01	3.31	4.63	3.76	4.85	4.15
44c	eq	eq	O	2.28	1.51	1.54	0.78	-0.40	-0.63
	ax	eq	O	4.27	4.10	3.94	4.23	3.08	3.06
44d	eq	ax	O	5.96	4.81	5.29	5.64	4.11	3.78
	ax	ax	O	4.34	4.34	4.21	3.72	3.61	3.16
45a	eq	ax	O	4.12	3.82	4.68	4.13	4.81	4.58
	eq	ax	N	2.57	2.52	2.50	2.57	2.37	2.62
	eq	eq	O	2.62	1.28	2.90	1.85	3.15	1.80
	ax	ax	O	2.64	2.20	3.28	2.28	3.97	4.09
45b	eq	eq	O	1.57	1.01	2.08	1.25	2.35	1.94
	eq	eq	N	0.00	0.00	0.00	0.00	0.00	0.00
	ax	eq	O	4.39	3.76	4.98	4.90	5.23	4.82
45c	eq	eq	O	2.35	2.42	1.63	1.53	-0.23	-0.84
	ax	eq	O	4.71	4.88	4.46	4.50	3.57	3.87
45d	eq	ax	O	5.93	6.11	5.42	5.31	4.25	5.21
	ax	ax	O	4.44	5.29	4.37	4.82	3.88	4.32

[a]In kcal mol^{-1}; [b]disposition of ethyl with respect to the ring; [c]arrangement of the aromatic group relative to either oxazolidine or oxazine rings; [d]H-bonded heteroatom to the first OH giving rise to a pseudo-cycle.

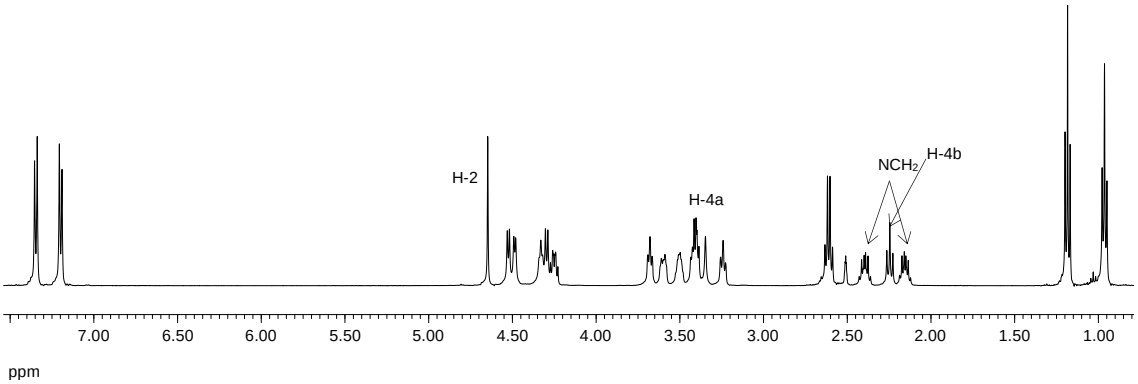


Figure S1. ^{1}H NMR spectrum of **28a**, recorded in DMSO-d_6.

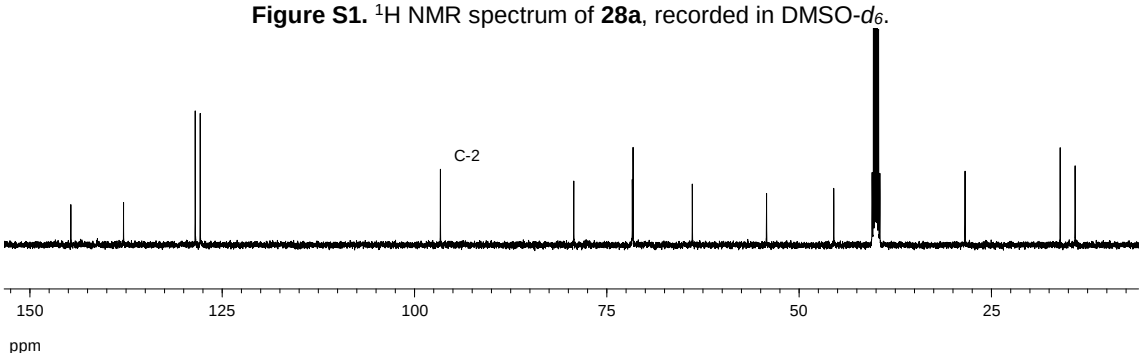


Figure S2. ^{13}C NMR spectrum of **28a**, recorded in DMSO-d_6.

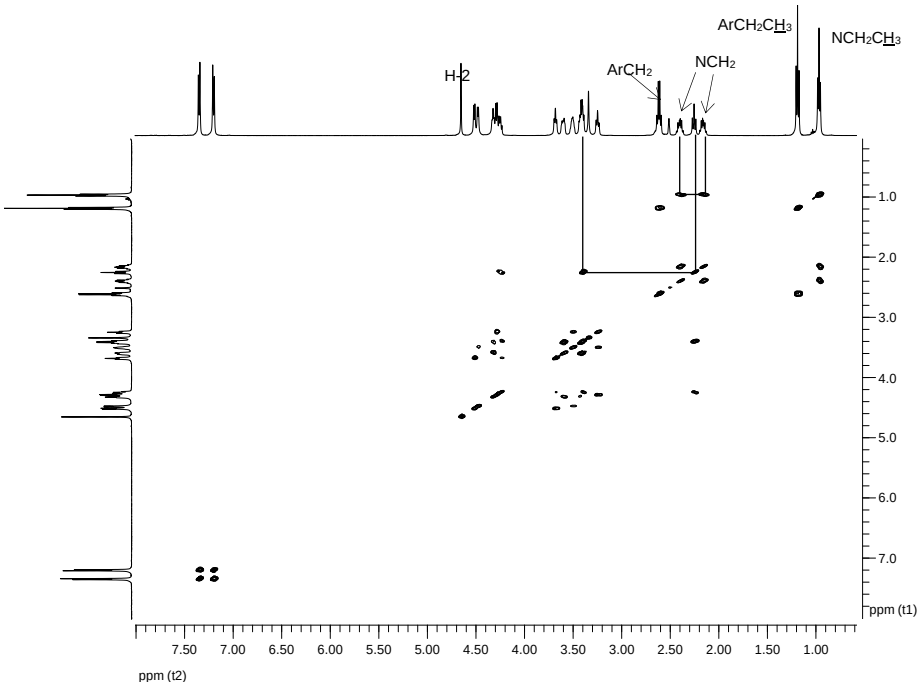


Figure S3. ^{1}H-^{1}H COSY spectrum of **28a**, recorded in DMSO-d_6.

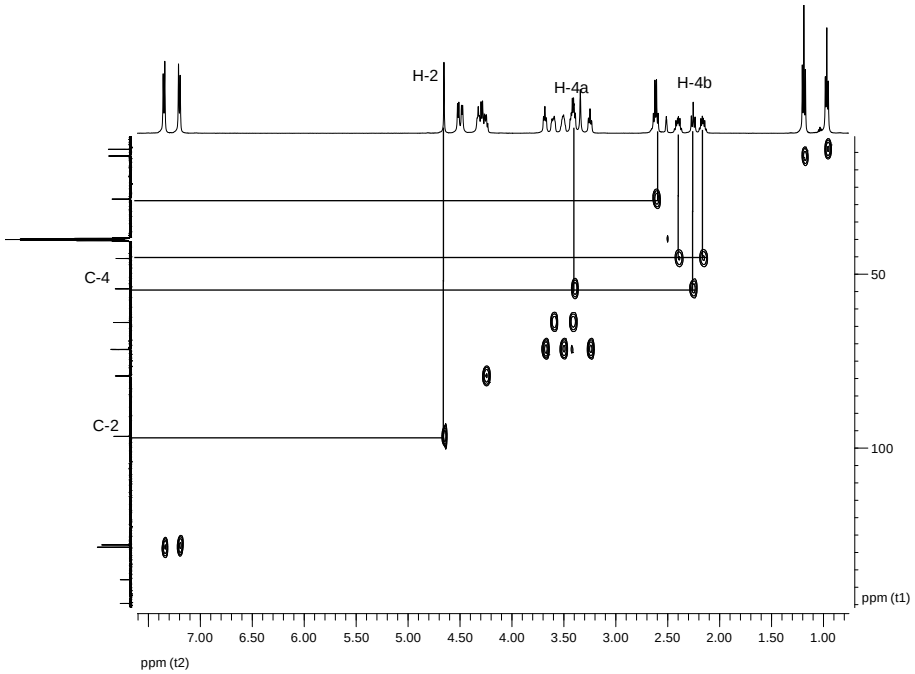


Figure 4S. HMQC spectrum of **28a**, recorded in DMSO-d_6.

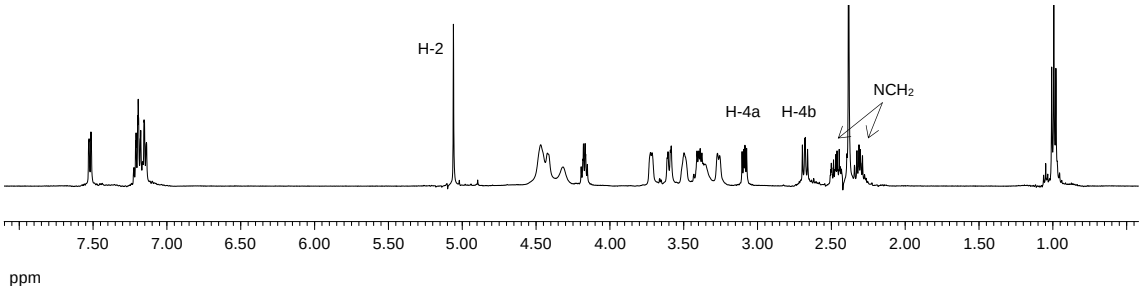


Figure S5. ^{1}H NMR spectrum of **23b**, recorded in DMSO-d_6.

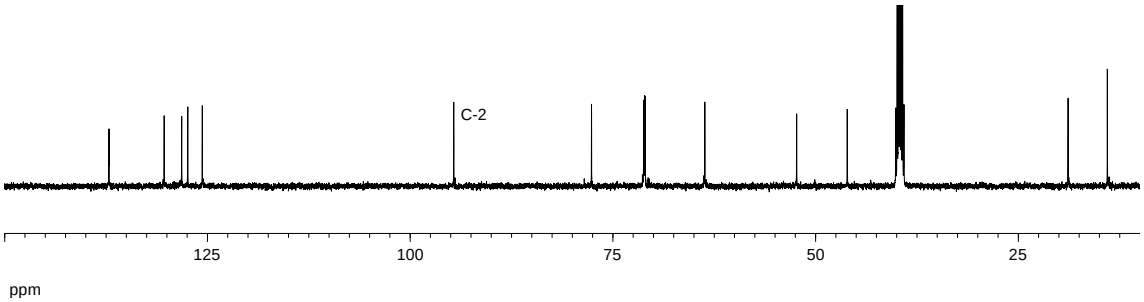


Figure S6. ^{13}C NMR spectrum of **23b**, recorded in DMSO-d_6.

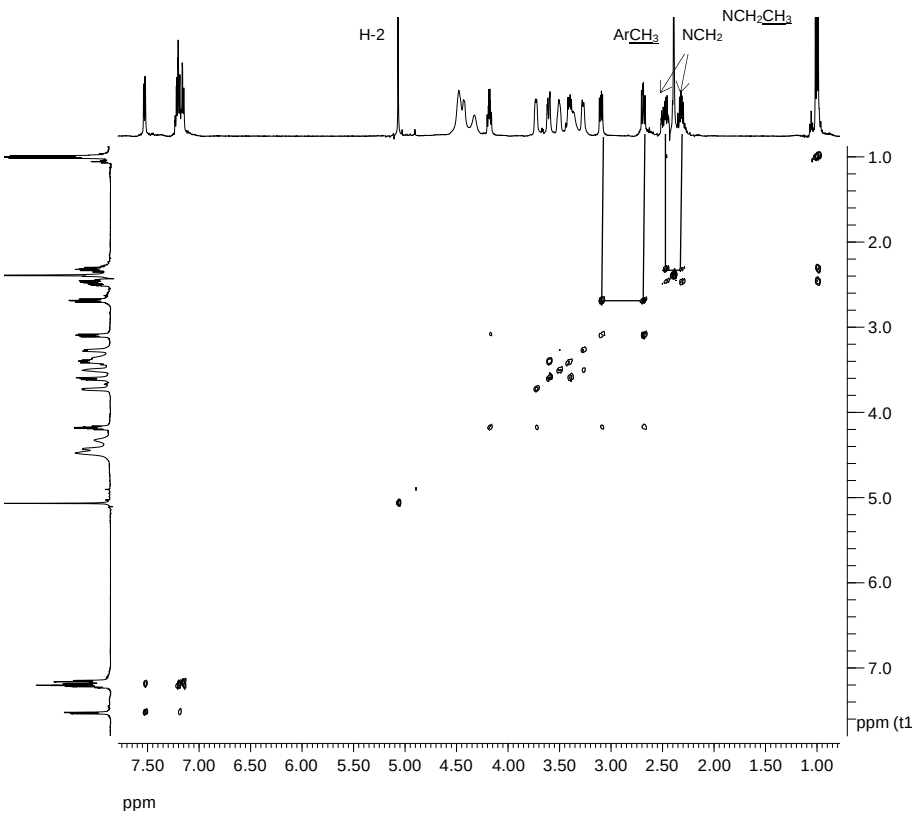


Figure S7. ^{1}H-^{1}H COSY spectrum of **23b**, recorded in DMSO-*d*$_6$.

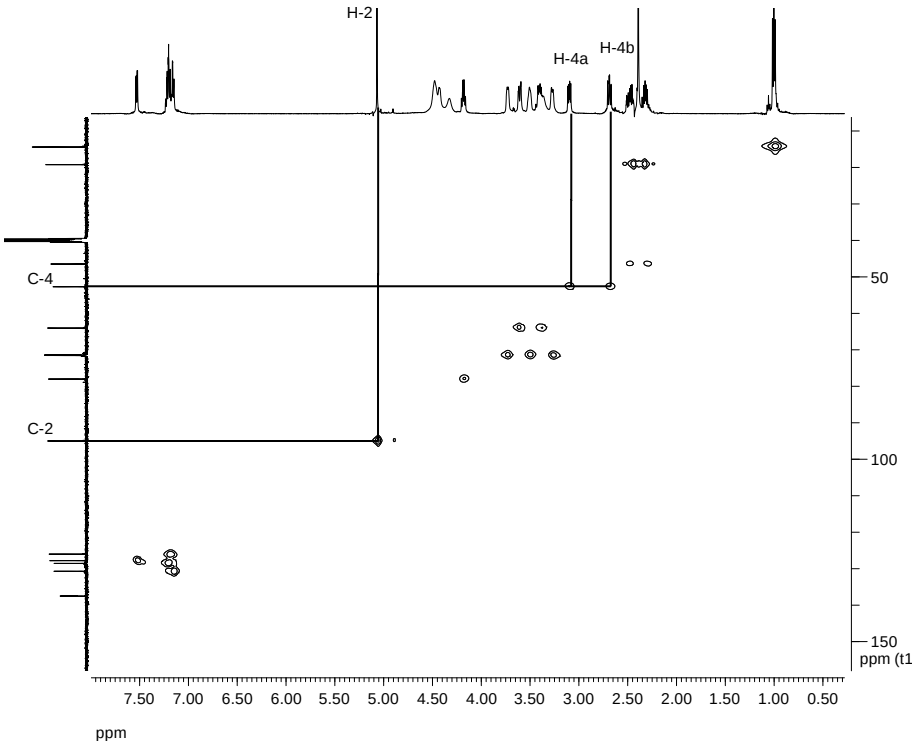


Figure S8. HMQC spectrum of **23b**, recorded in DMSO-*d*$_6$.

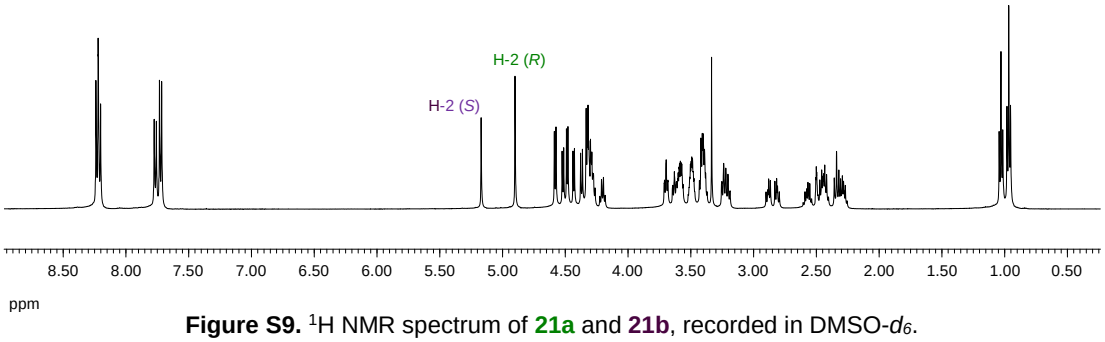


Figure S9. ^{1}H NMR spectrum of **21a** and **21b**, recorded in DMSO-d_6.

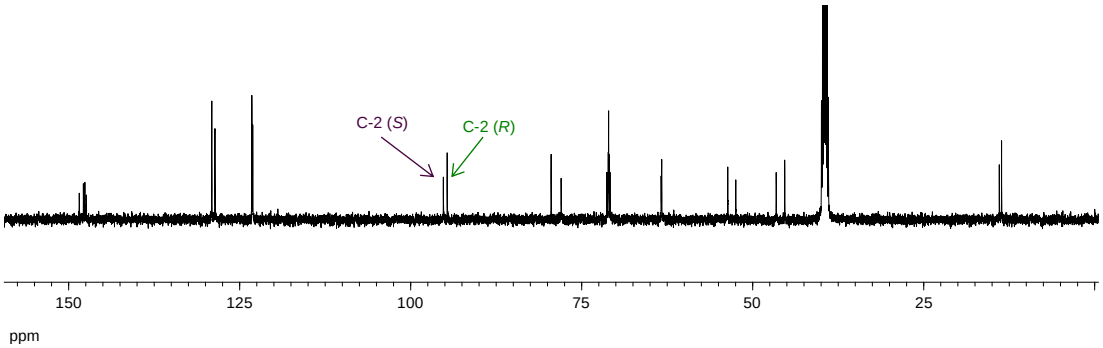


Figure S10. ^{13}C NMR spectrum of **21a** and **21b**, recorded in DMSO-d_6.

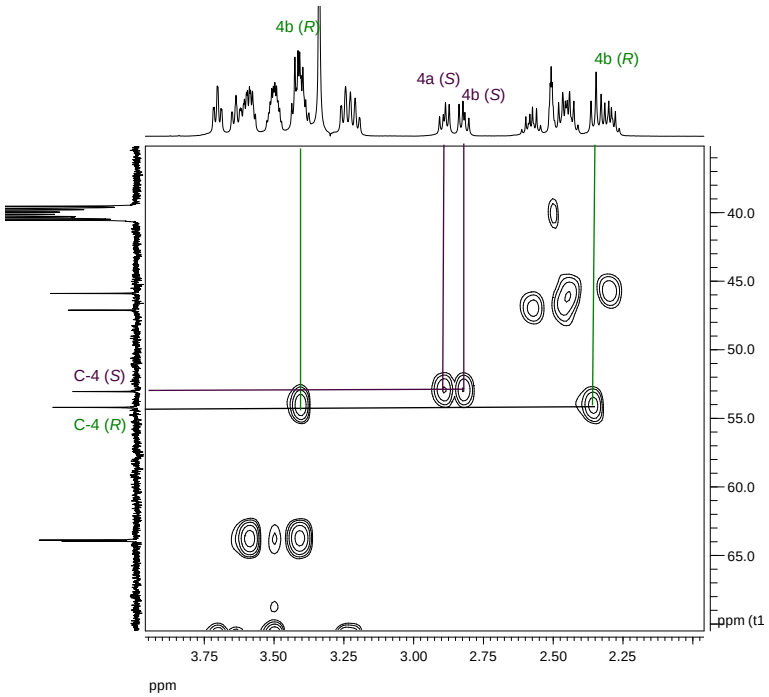


Figure S11. HMQC spectrum of **21a** and **21b**, recorded in DMSO-d_6.

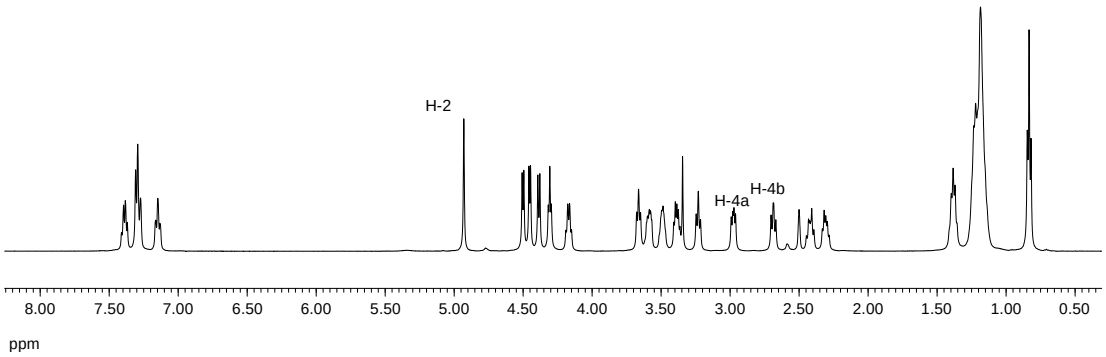


Figure S12. ^{1}H NMR spectrum of **36b**, recorded in DMSO-d_6.

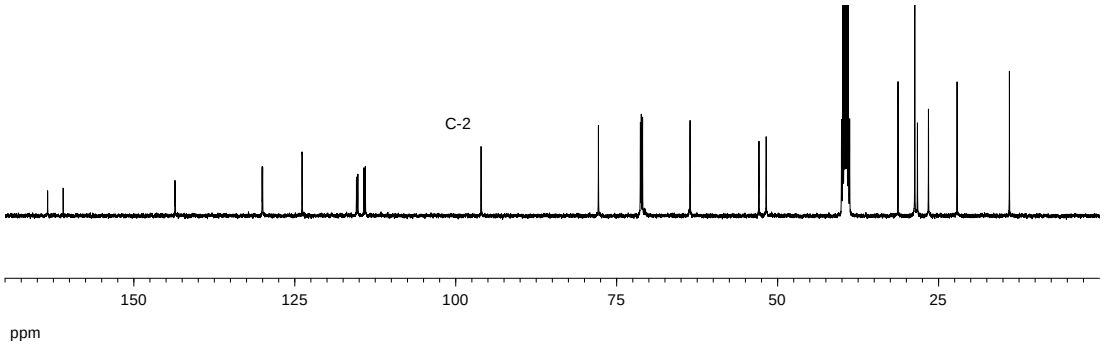


Figure S13. ^{13}C NMR spectrum of **36b**, recorded in DMSO-d_6.

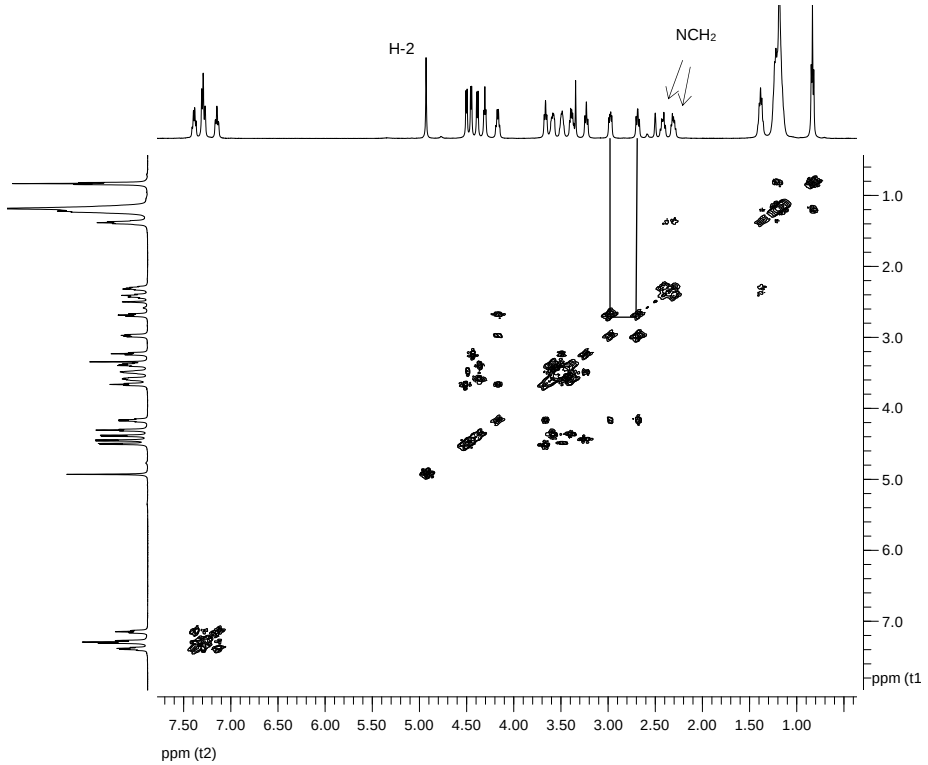


Figure S14. ^{1}H-^{1}H COSY spectrum of **36b**, recorded in DMSO-d_6.

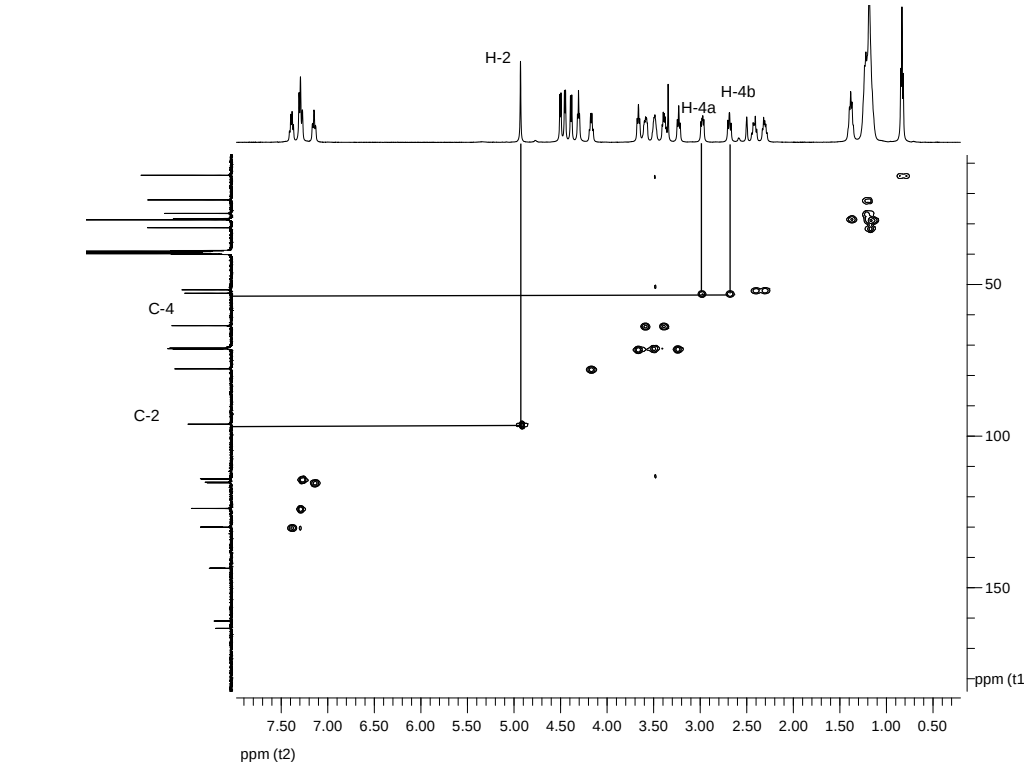


Figure S15. HMQC spectrum of **36b**, recorded in DMSO-d_6.

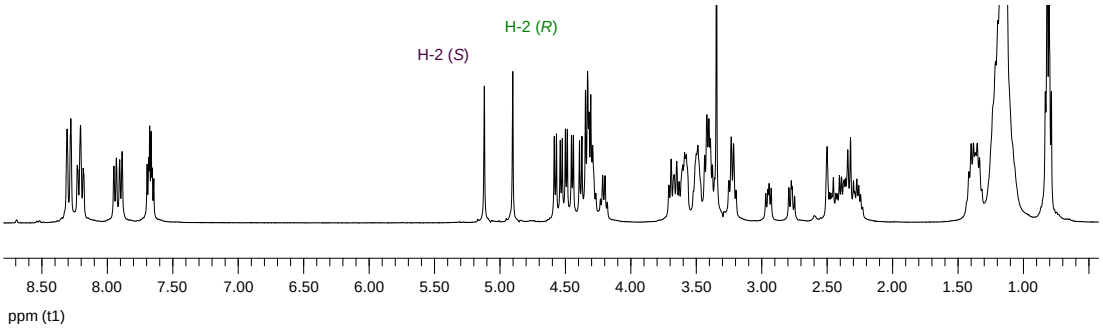


Figure S16. ^{1}H NMR spectrum of **35a** and **35b**, recorded in DMSO-d_6.

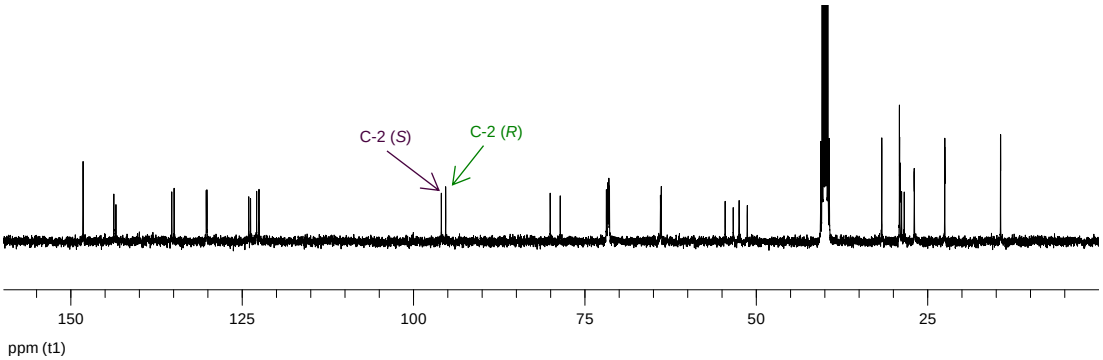


Figure S17. ^{13}C NMR spectrum of **35a** and **35b**, recorded in DMSO-d_6.

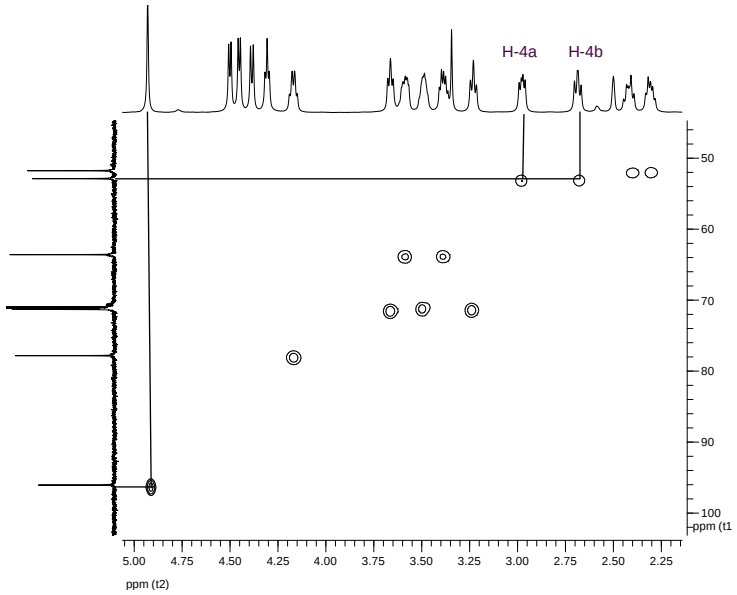


Figure S18. ^{1}H-^{1}H COSY spectrum of **35b**, recorded in DMSO-*d*$_6$.

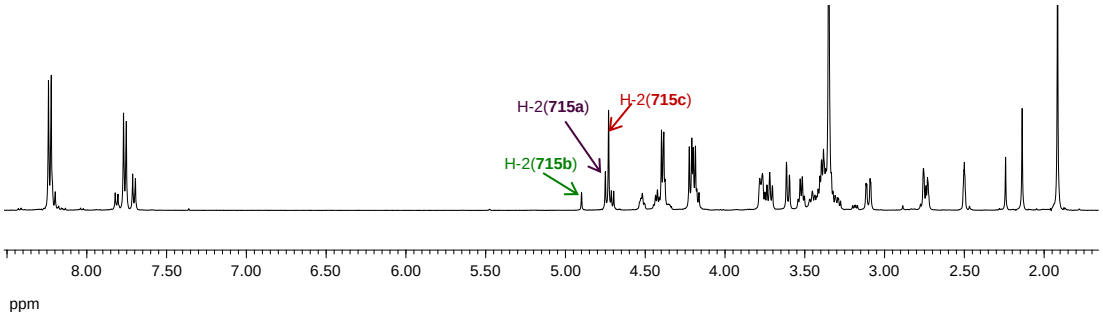


Figure S19. ^{1}H NMR spectrum of **43** (**43a**, **43b** and **43c**), recorded in DMSO-*d*$_6$.

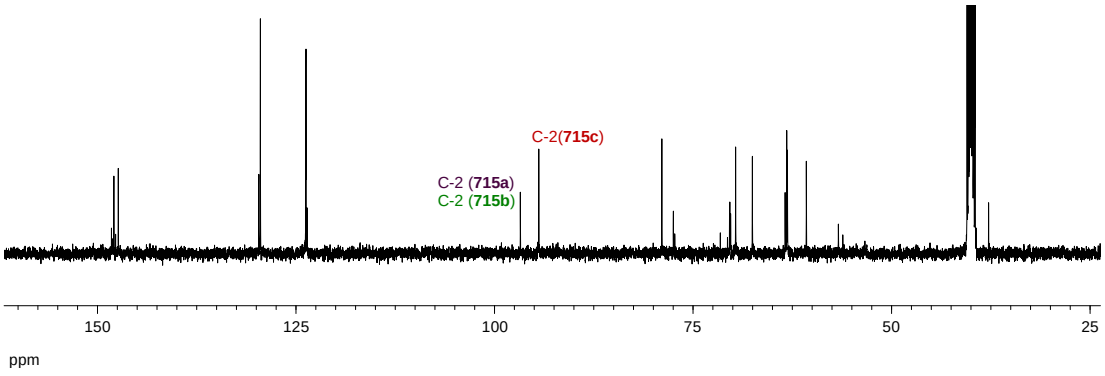


Figure S20. ^{13}C NMR spectrum of **43** (**43a**, **43b** and **43c**), recorded in DMSO-*d*$_6$.

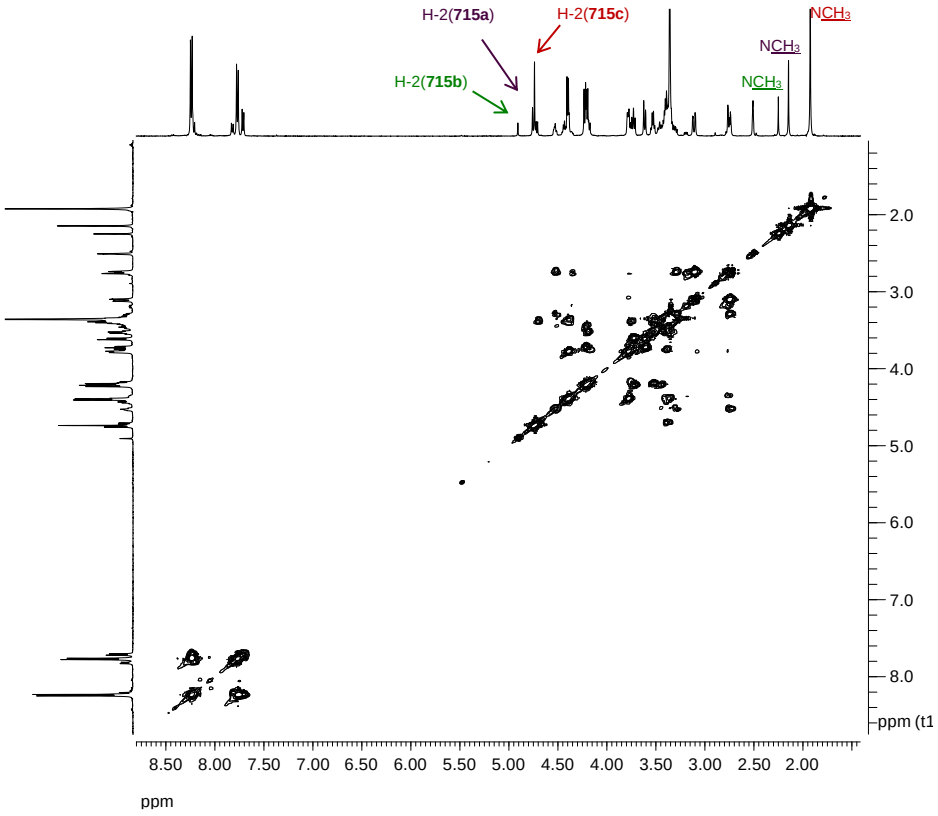


Figure S21. ^{1}H-^{1}H COSY spectrum of **43** (**43a**, **43b** and **43c**), recorded in DMSO-d_6.

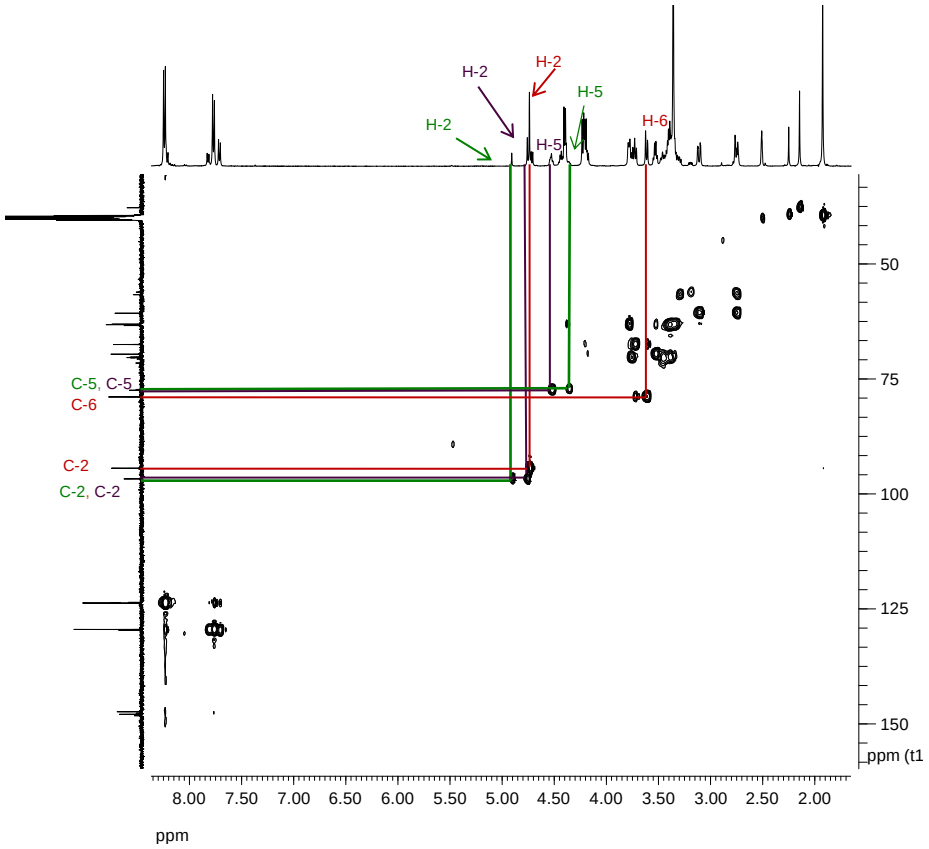


Figure S22. HMQC spectrum of **43** (**43a**, **43b** and **43c**), recorded in DMSO-d_6.

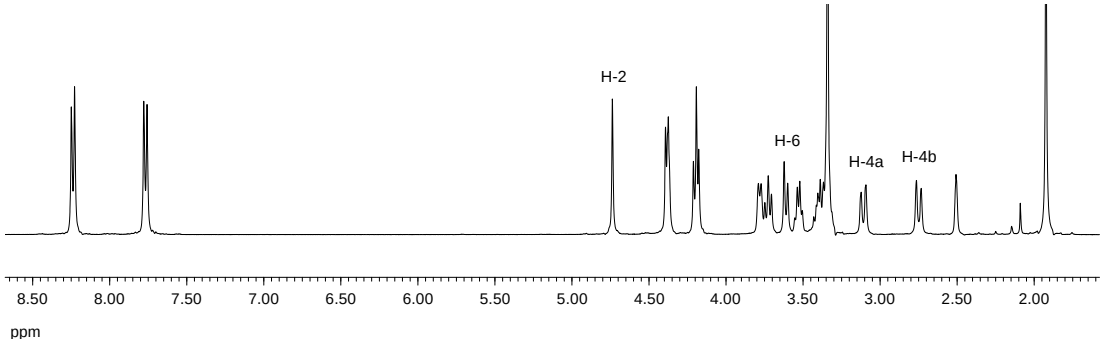


Figure S23. ^{1}H NMR spectrum of **43c**, recorded in DMSO-d_6.

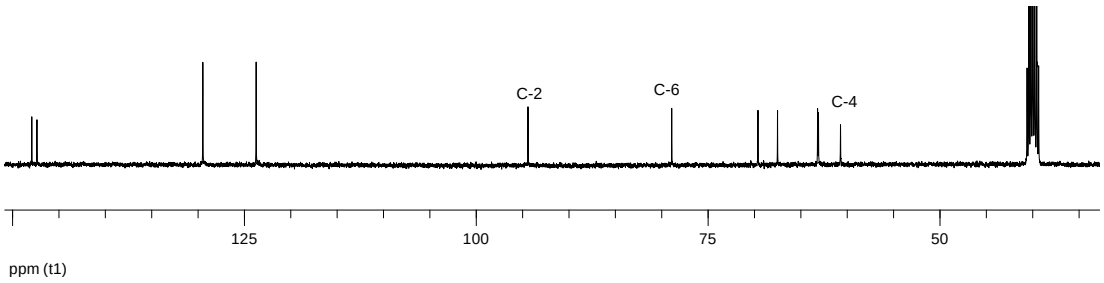


Figure S24. ^{13}C NMR spectrum of **43c**, recorded in DMSO-d_6.

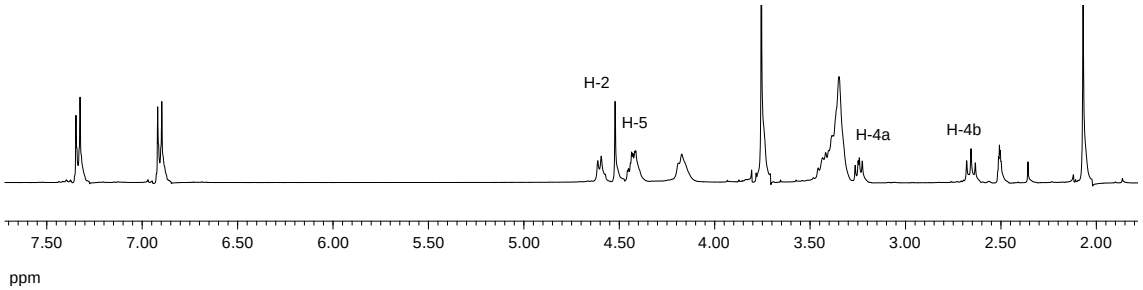


Figure S25. ^{1}H NMR spectrum of **45a**, recorded in DMSO-d_6.

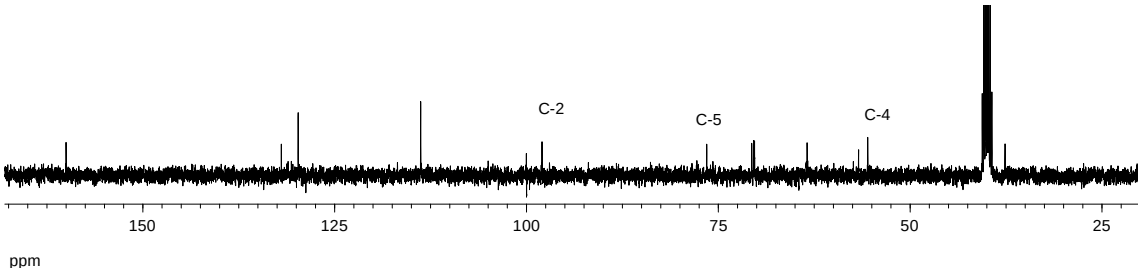


Figure S26. ^{13}C NMR spectrum of **45a**, recorded in DMSO-d_6.

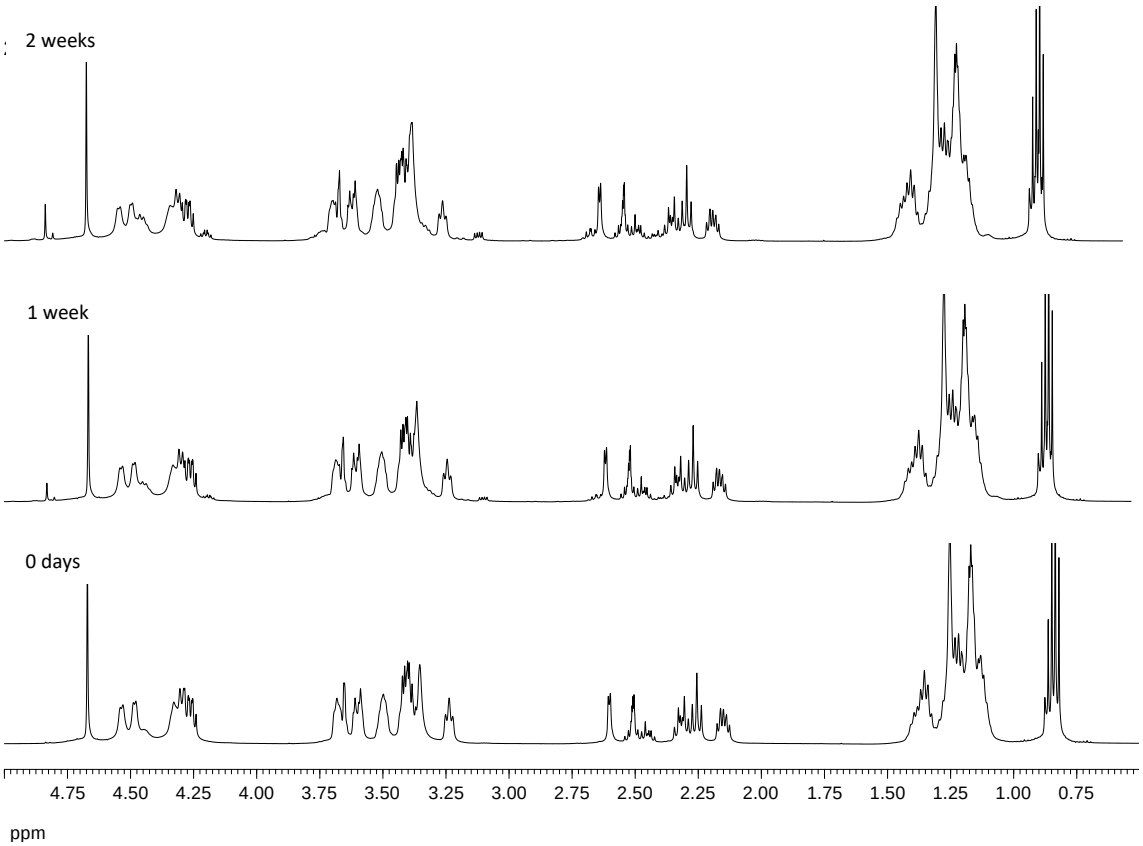


Figure S27. Isomerization of **38a** (*R*-configured oxazolidine) as monitored in solution for two weeks (DMSO-d_6).

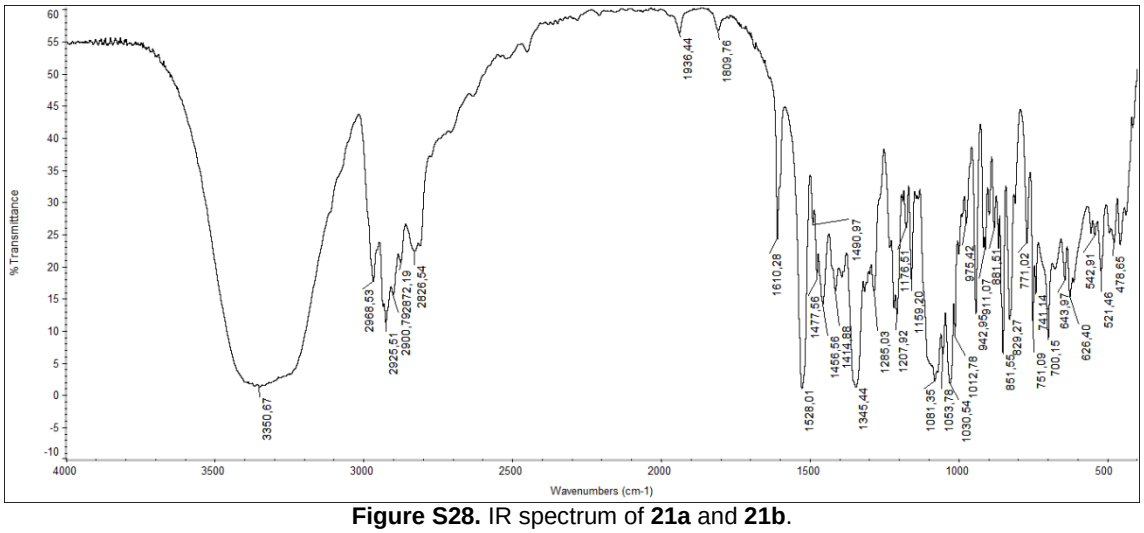


Figure S28. IR spectrum of **21a** and **21b**.

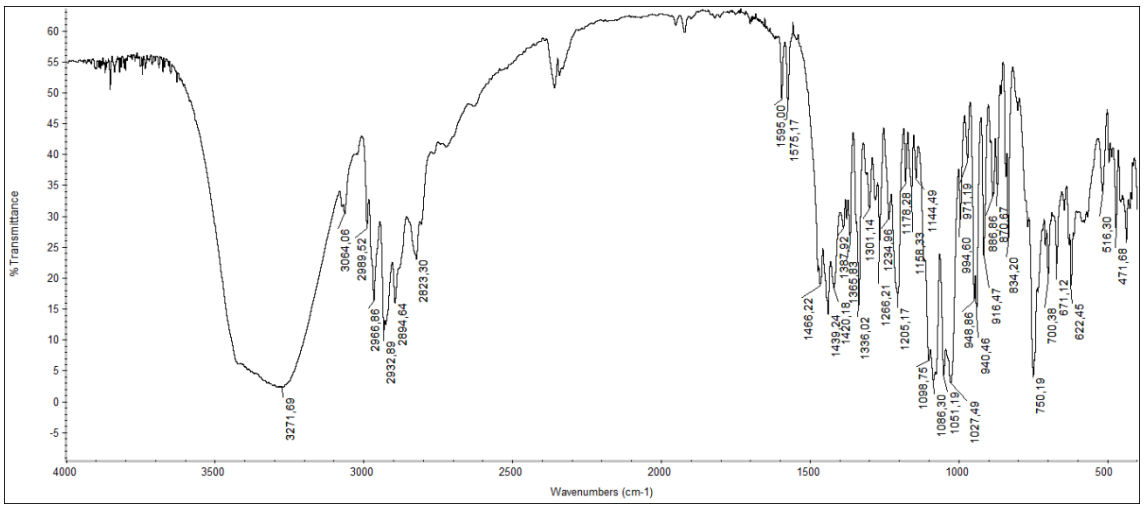


Figure S29. IR spectrum of **22a** and **22b**.

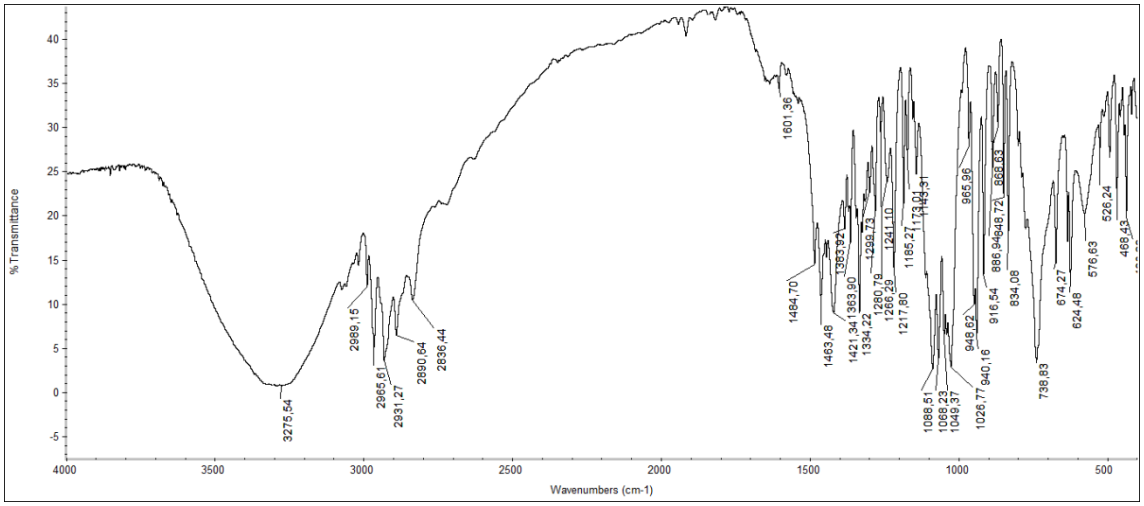


Figure S30. IR spectrum of **23a** and **23b**.

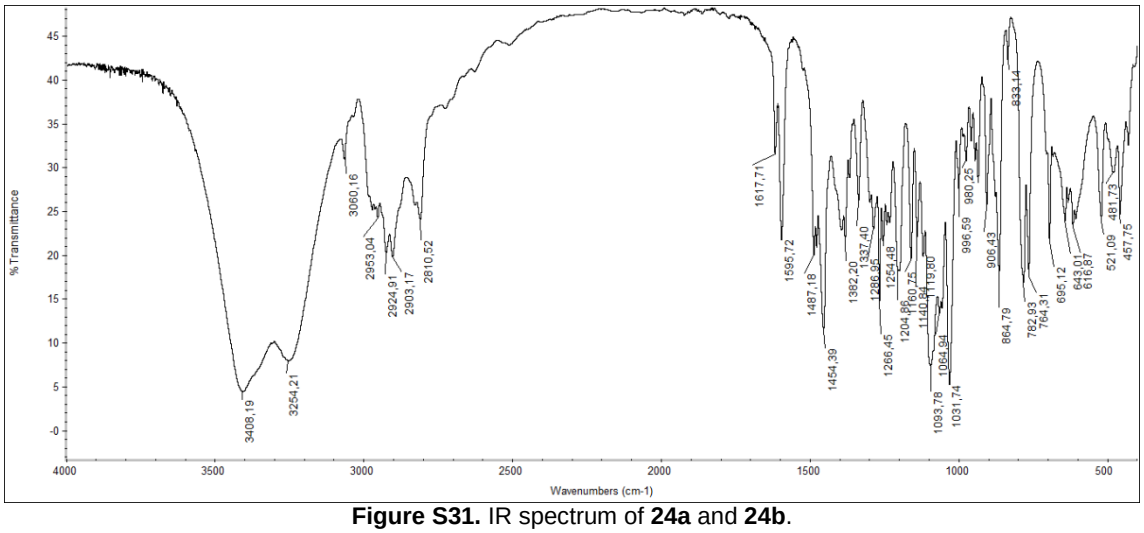


Figure S31. IR spectrum of **24a** and **24b**.

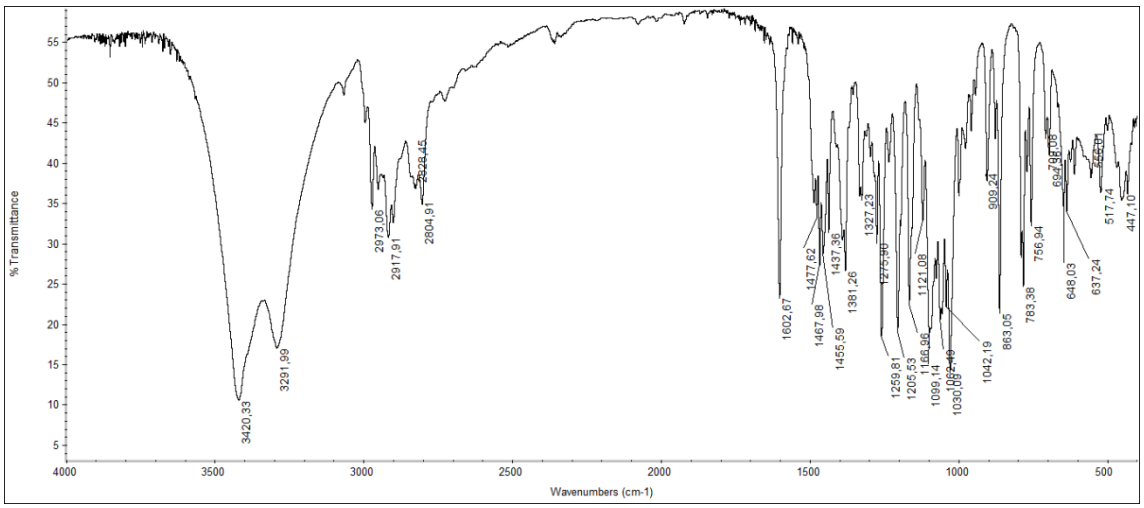


Figure S32. IR spectrum of **25a**.

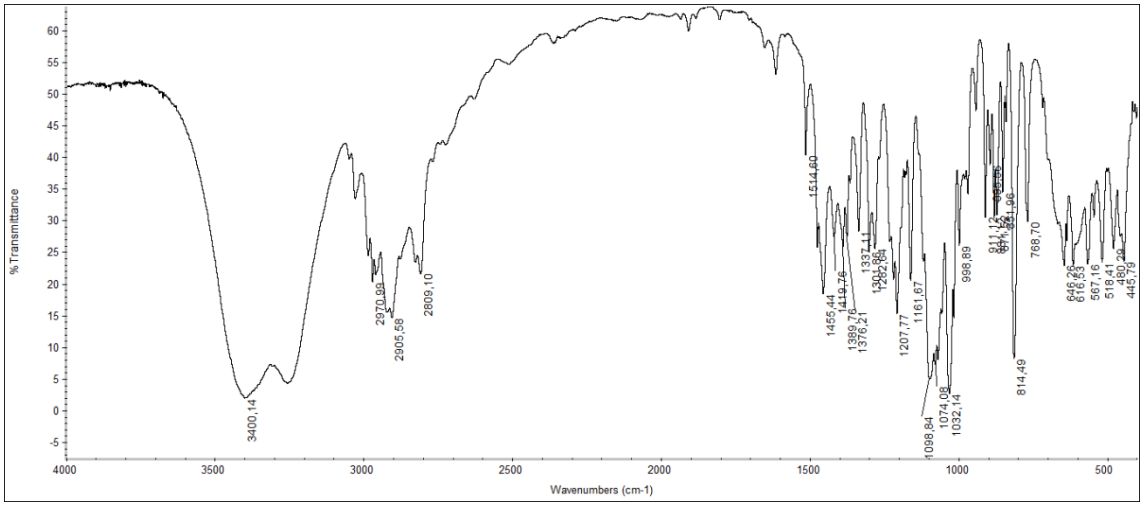


Figure S33. IR spectrum of **26a**.

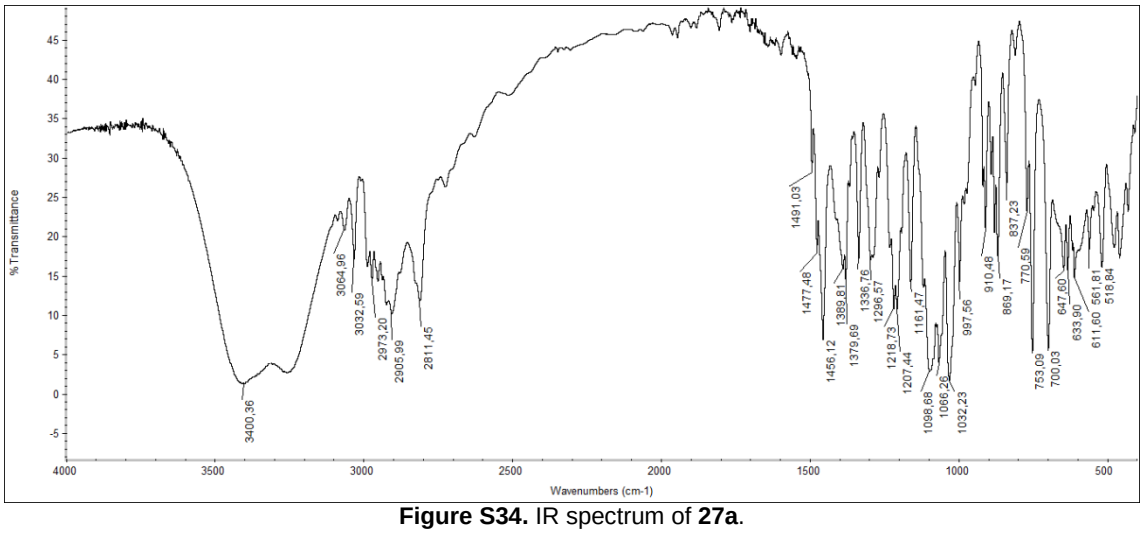


Figure S34. IR spectrum of **27a**.

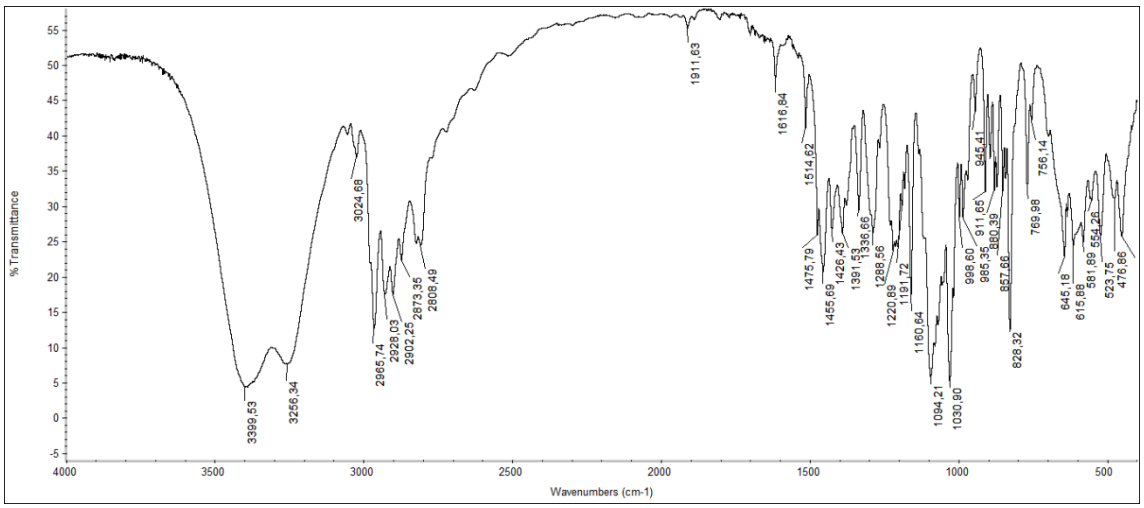


Figure S35. IR spectrum of **28a**.

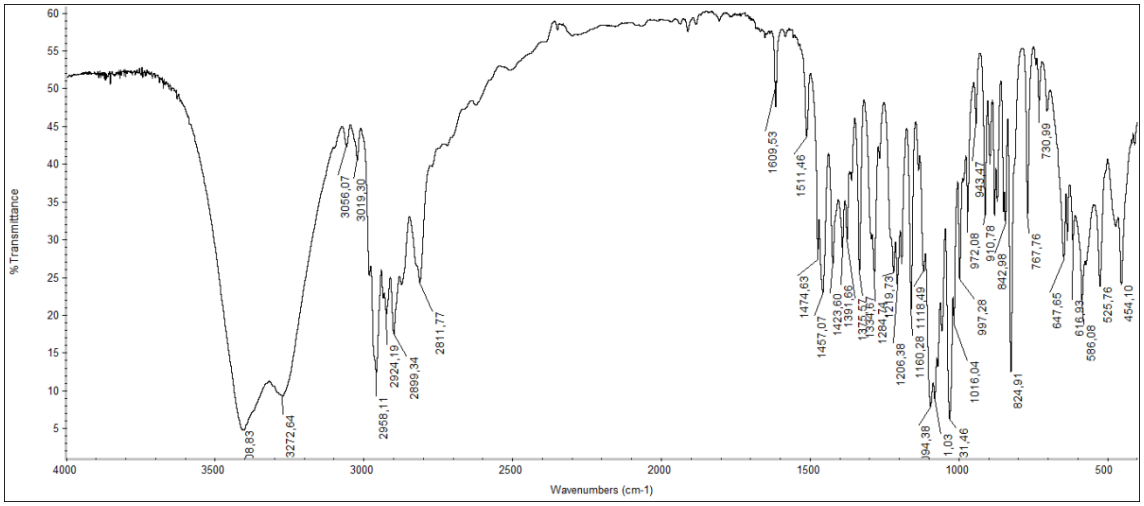


Figure S36. IR spectrum of **29a**.

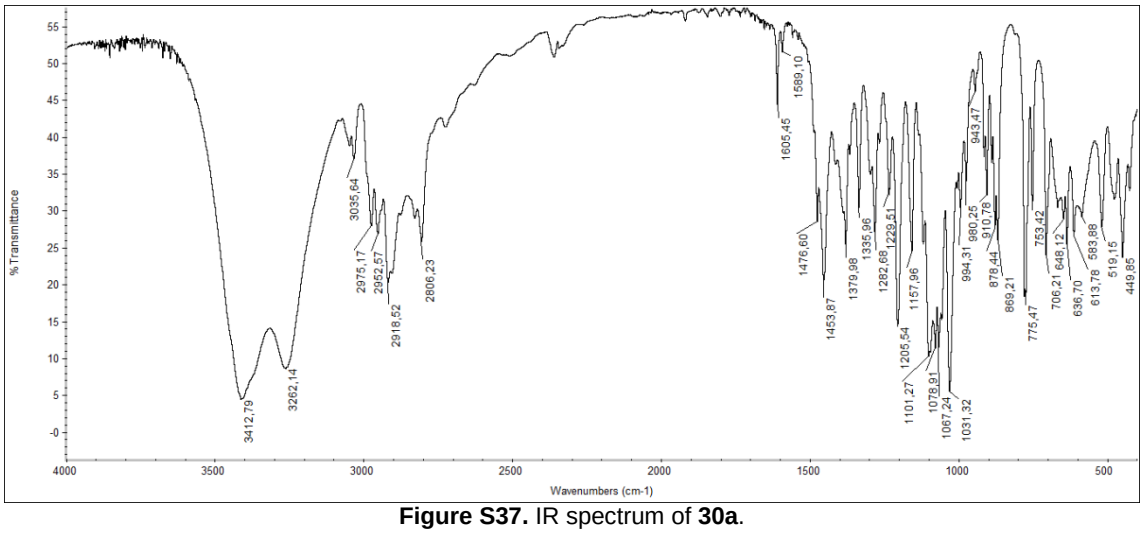


Figure S37. IR spectrum of **30a**.

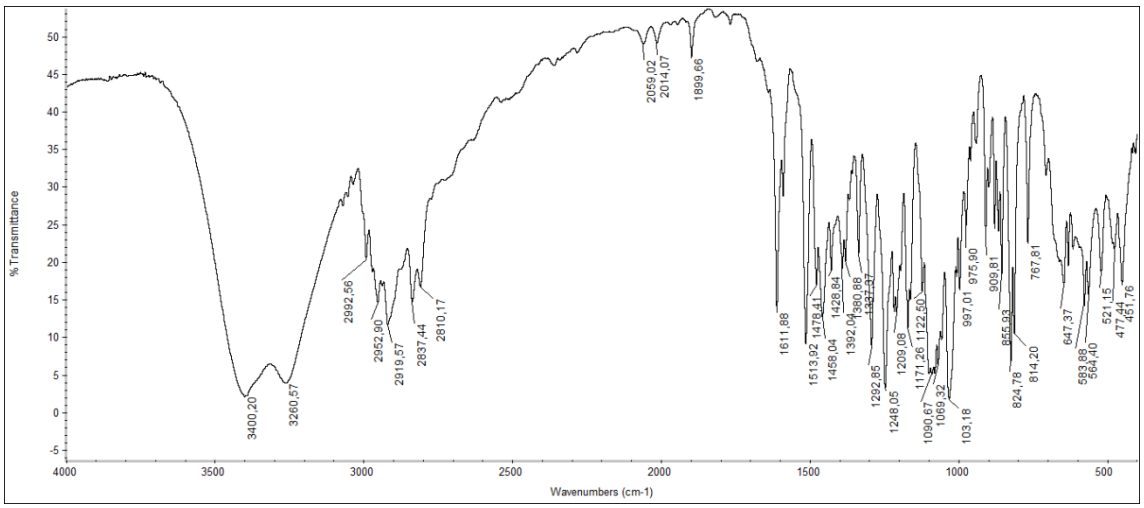


Figure S38. IR spectrum of **31a**.

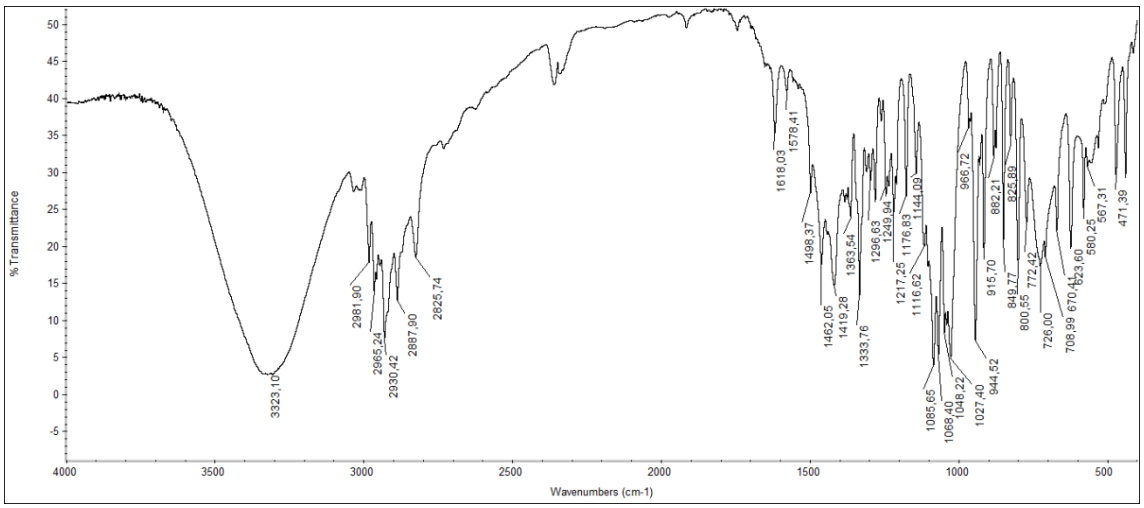


Figure S39. IR spectrum of **32b**.

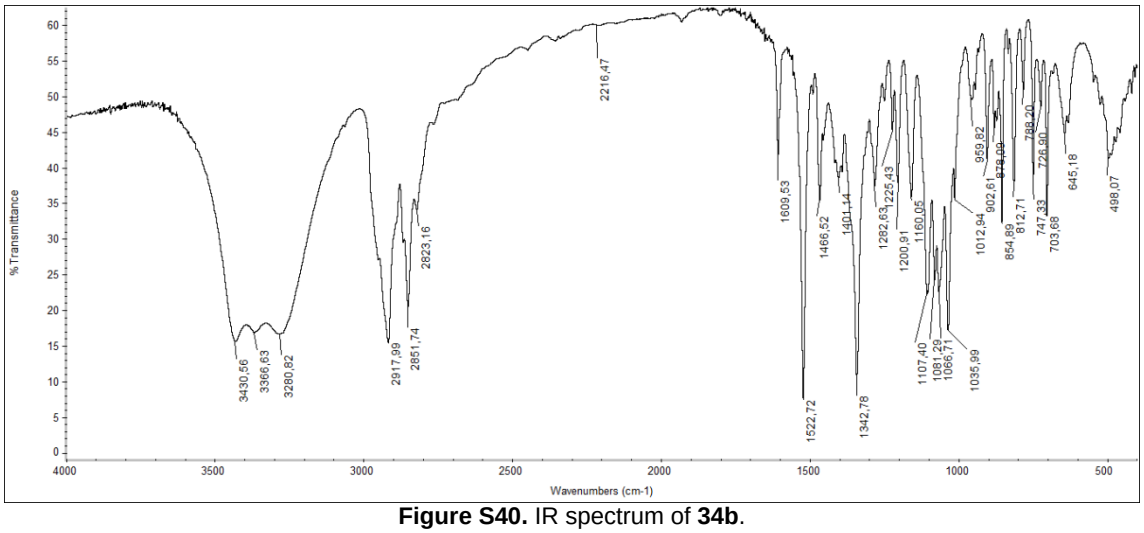


Figure S40. IR spectrum of **34b**.

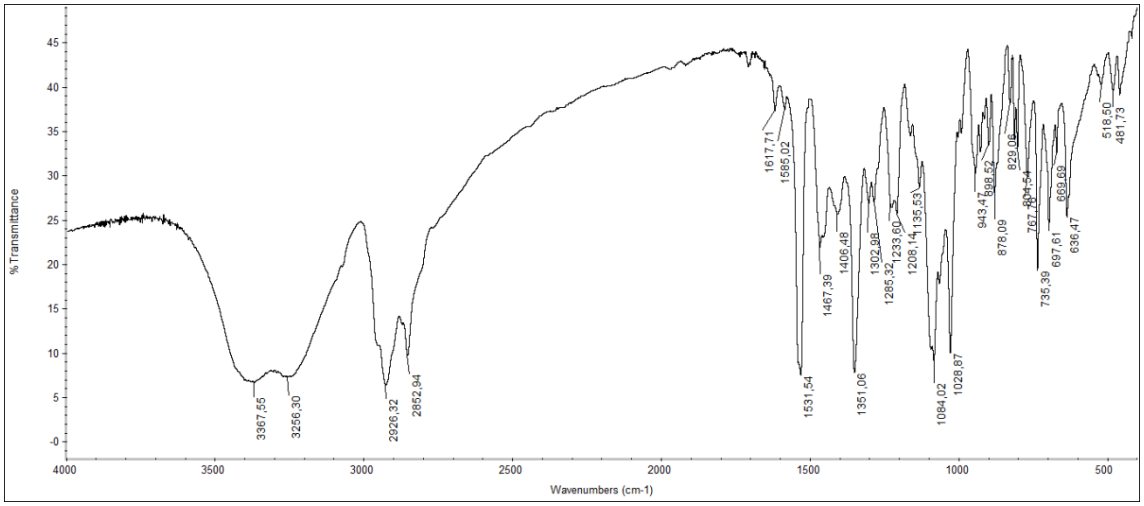


Figure S41. IR spectrum of **35a** and **35b**.

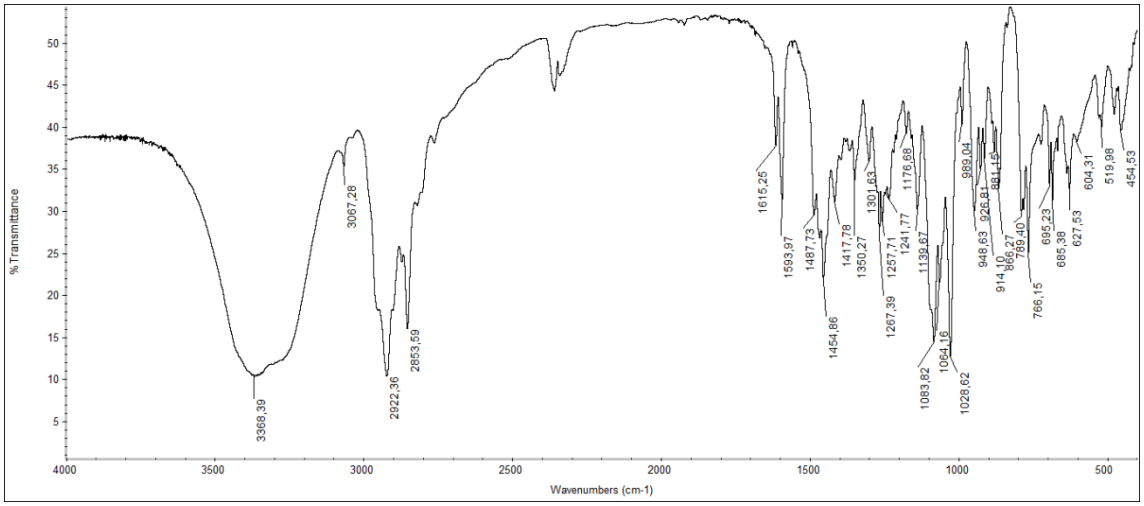


Figure S42. IR spectrum of **36a** and **36b**.

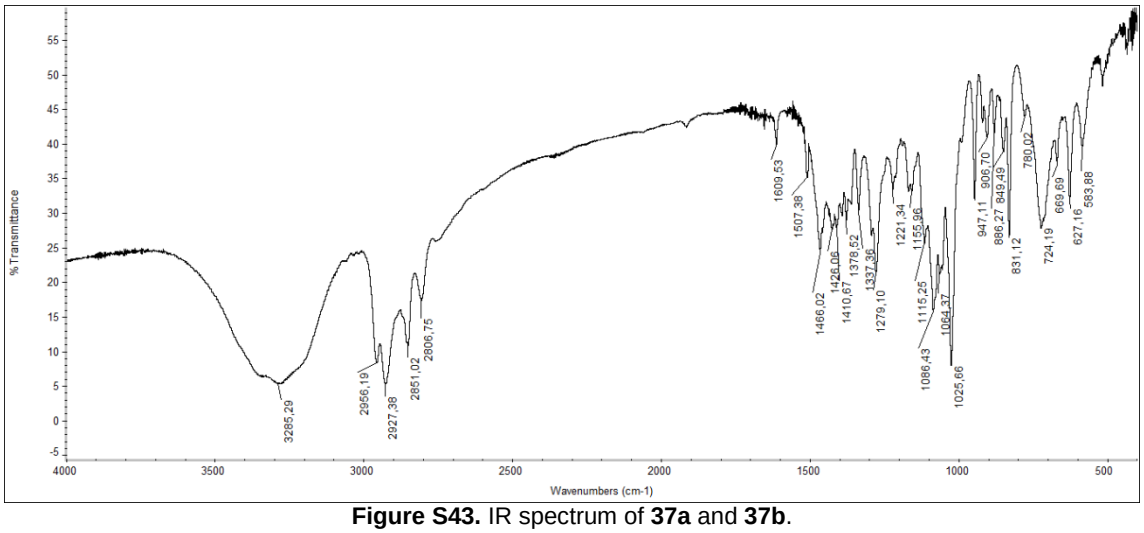


Figure S43. IR spectrum of **37a** and **37b**.

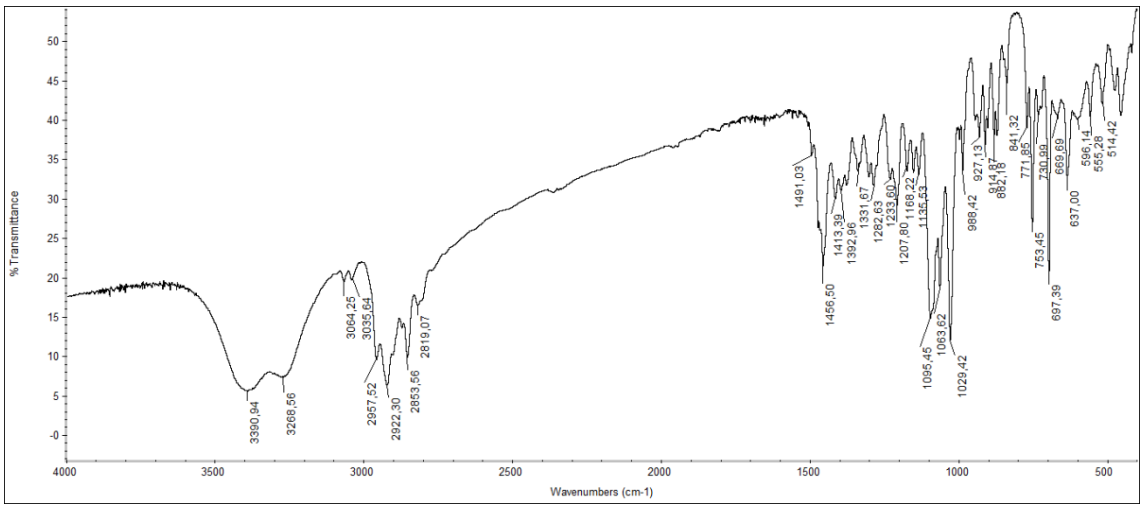


Figure S44. IR spectrum of **38a** and **38b**.

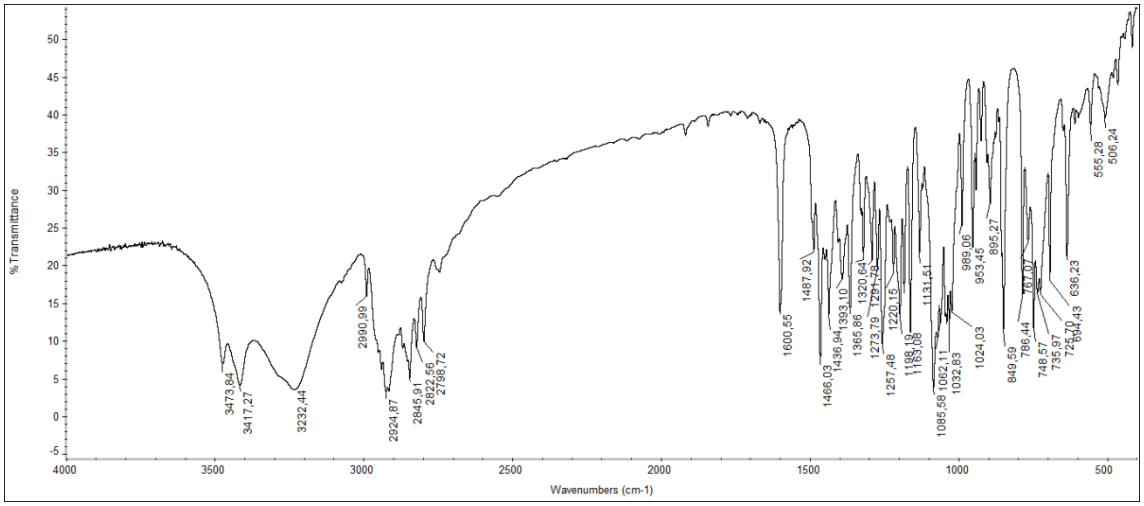


Figure S45. IR spectrum of **39a**.

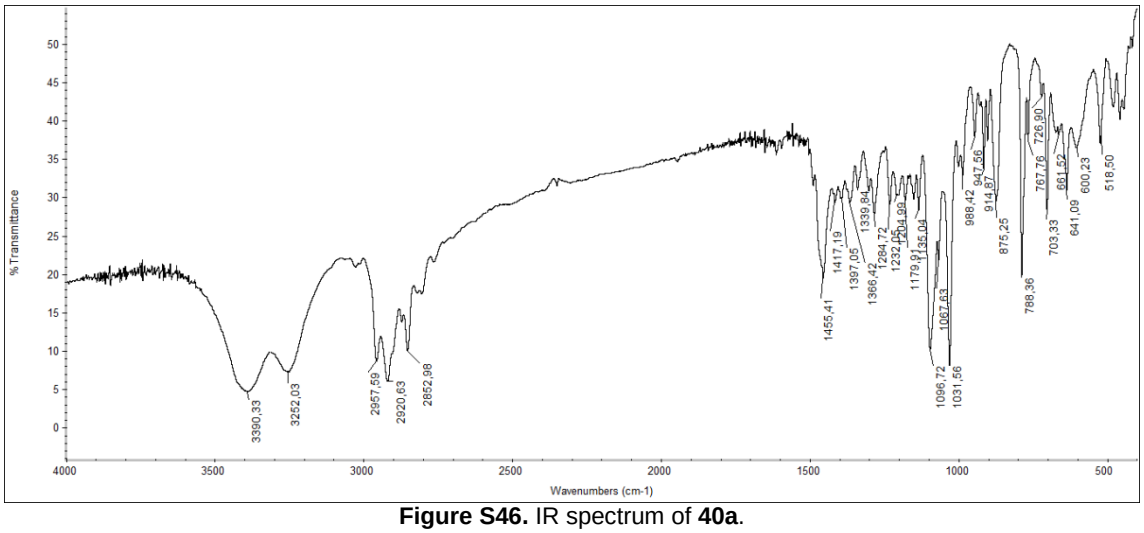


Figure S46. IR spectrum of **40a**.

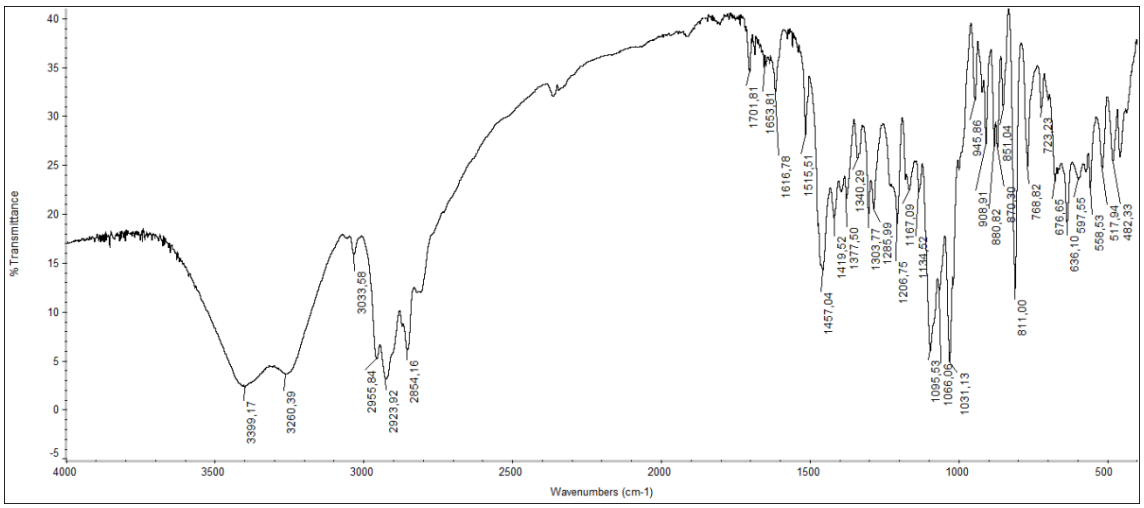


Figure S47. IR spectrum of **41a**.

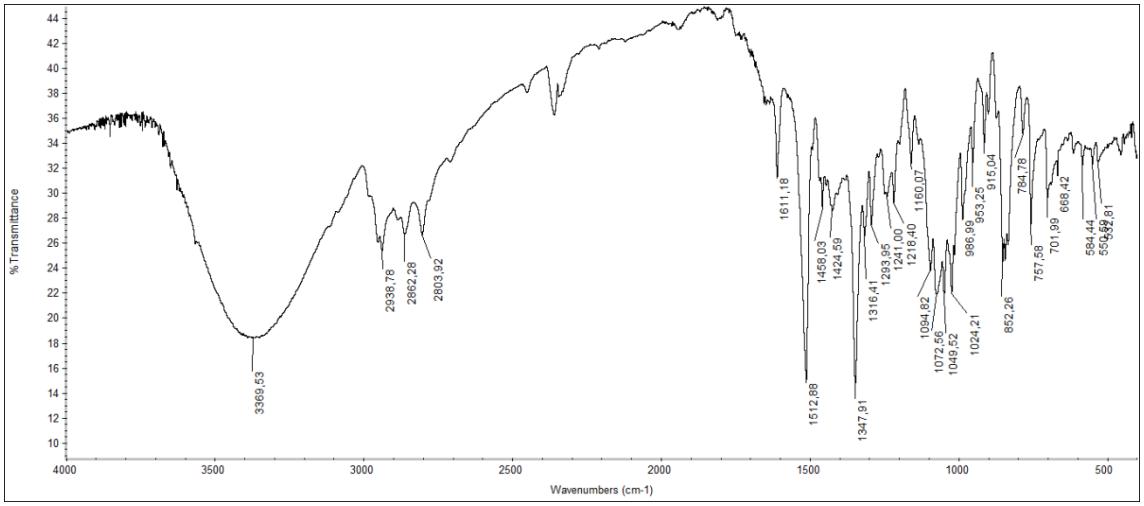


Figure S48. IR spectrum of **43a**, **43b** and **43c**.

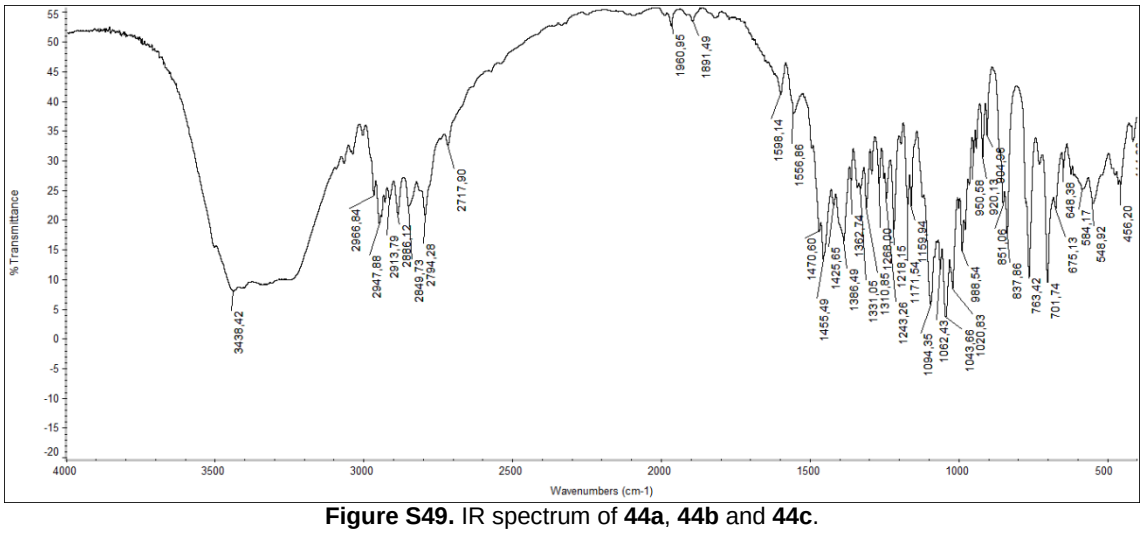


Figure S49. IR spectrum of **44a**, **44b** and **44c**.

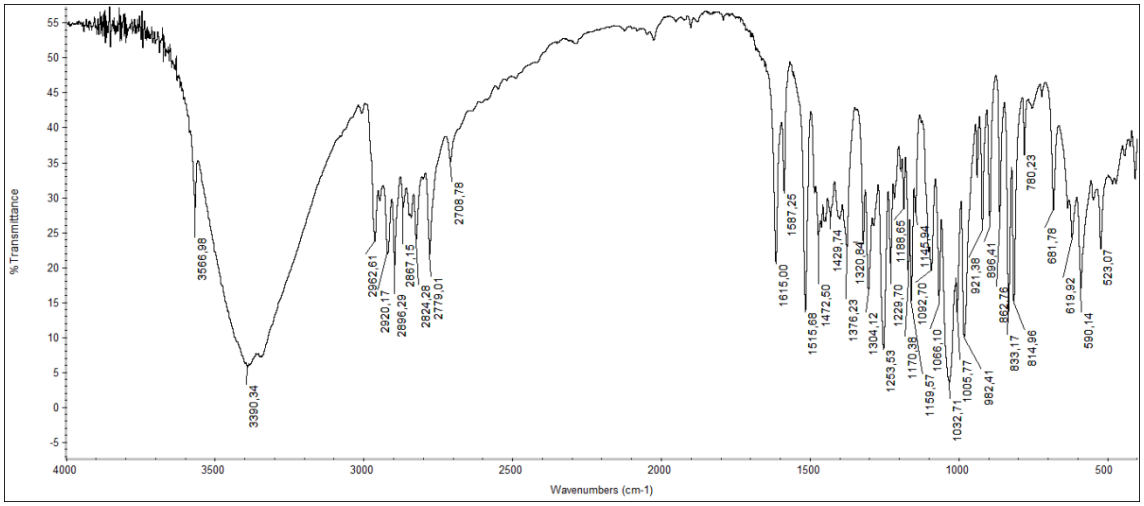


Figure S50. IR spectrum of **45a**, **45b** and **45c**.

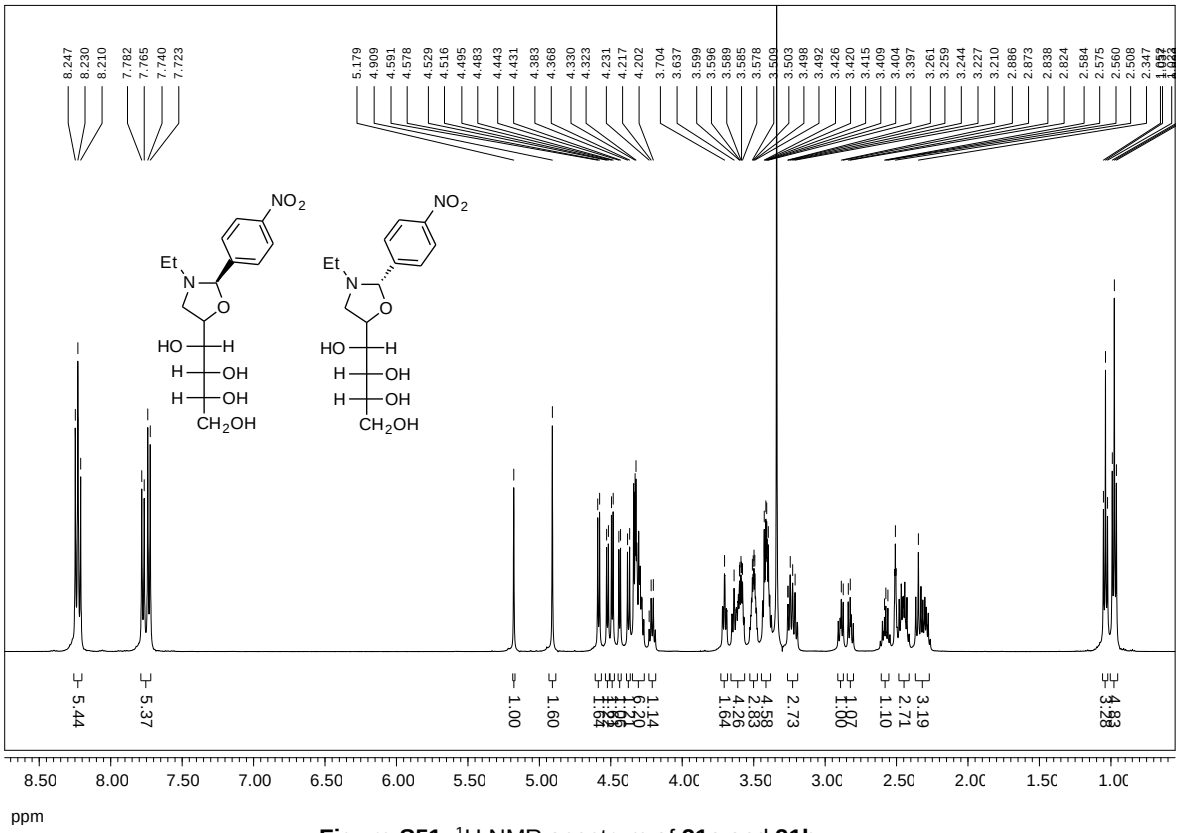


Figure S51. ^{1}H NMR spectrum of **21a** and **21b**.

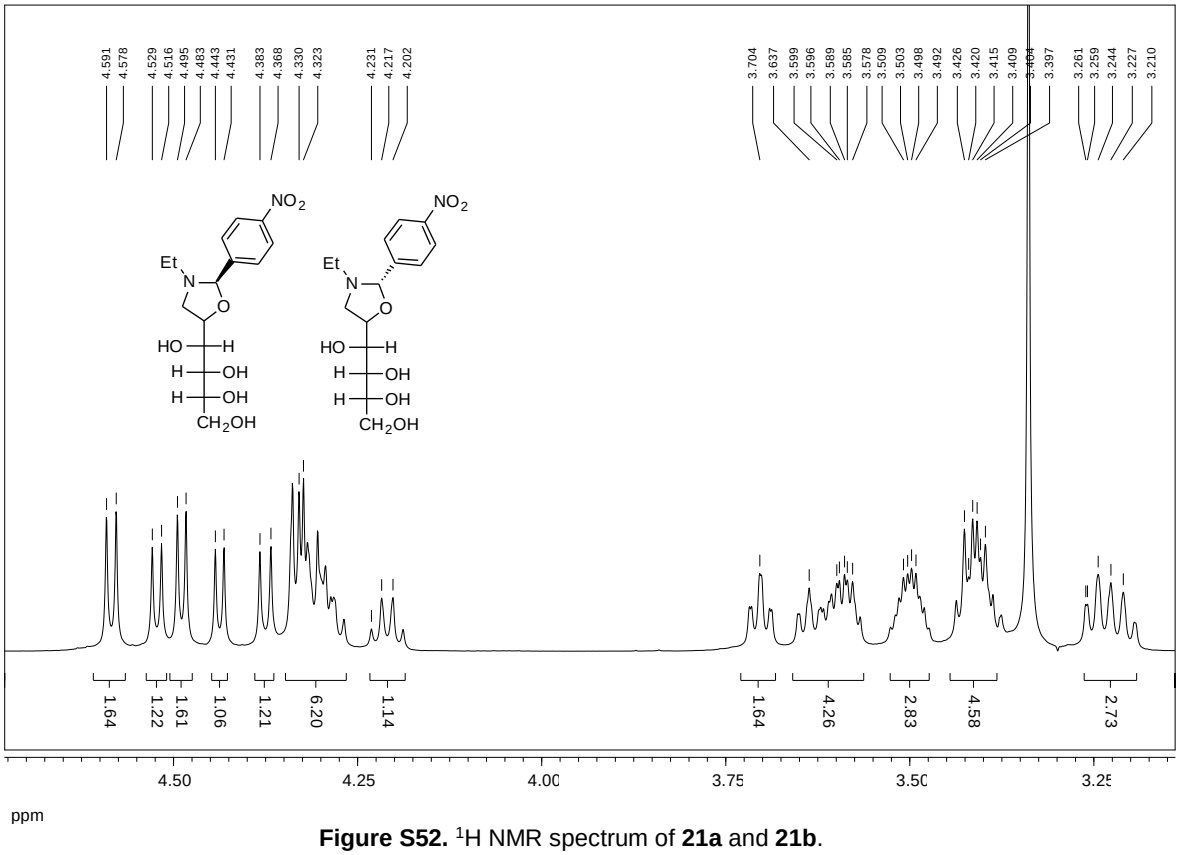


Figure S52. ^{1}H NMR spectrum of **21a** and **21b**.

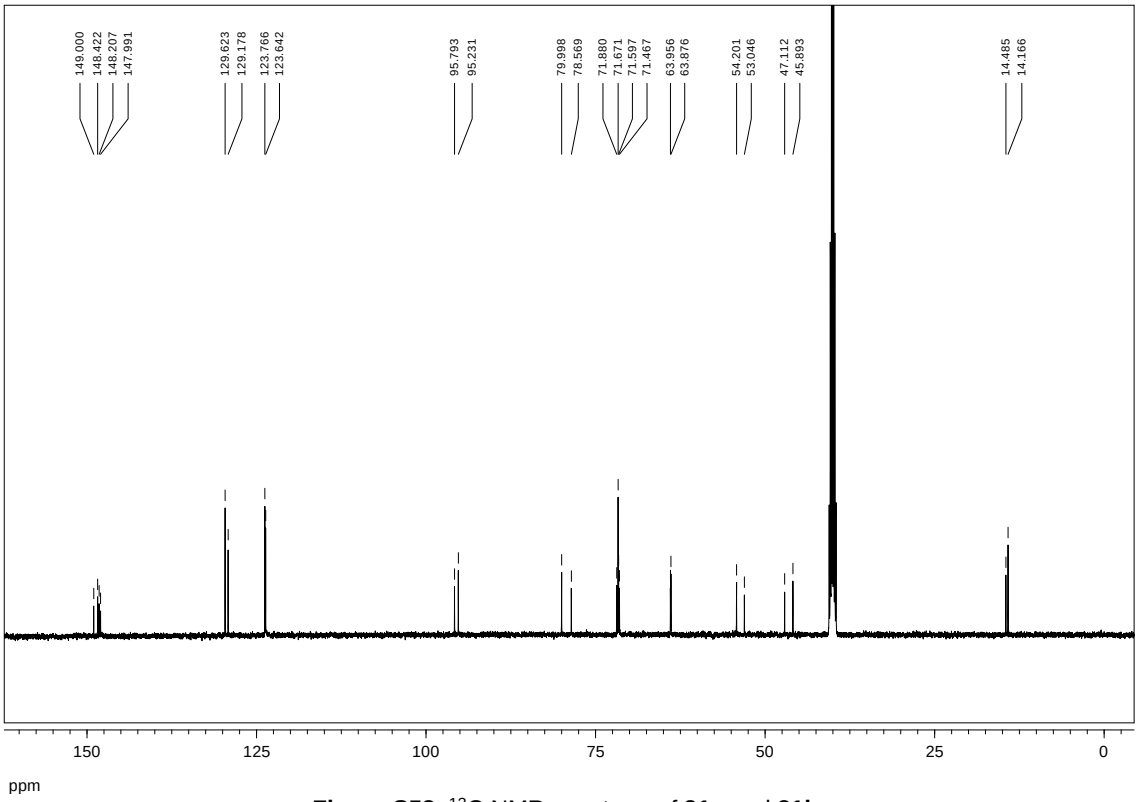


Figure S53. ^{13}C NMR spectrum of **21a** and **21b**.

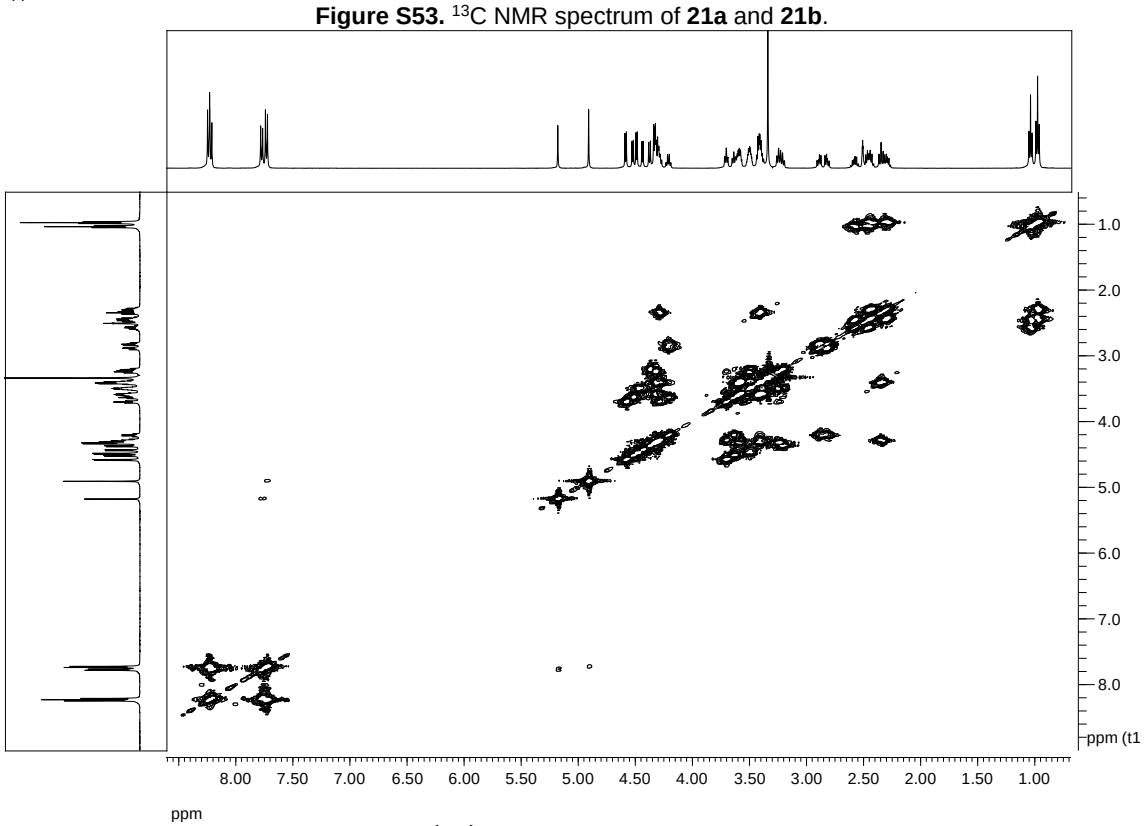


Figure S54. ^{1}H-^{1}H COSY spectrum of **21a** and **21b**.

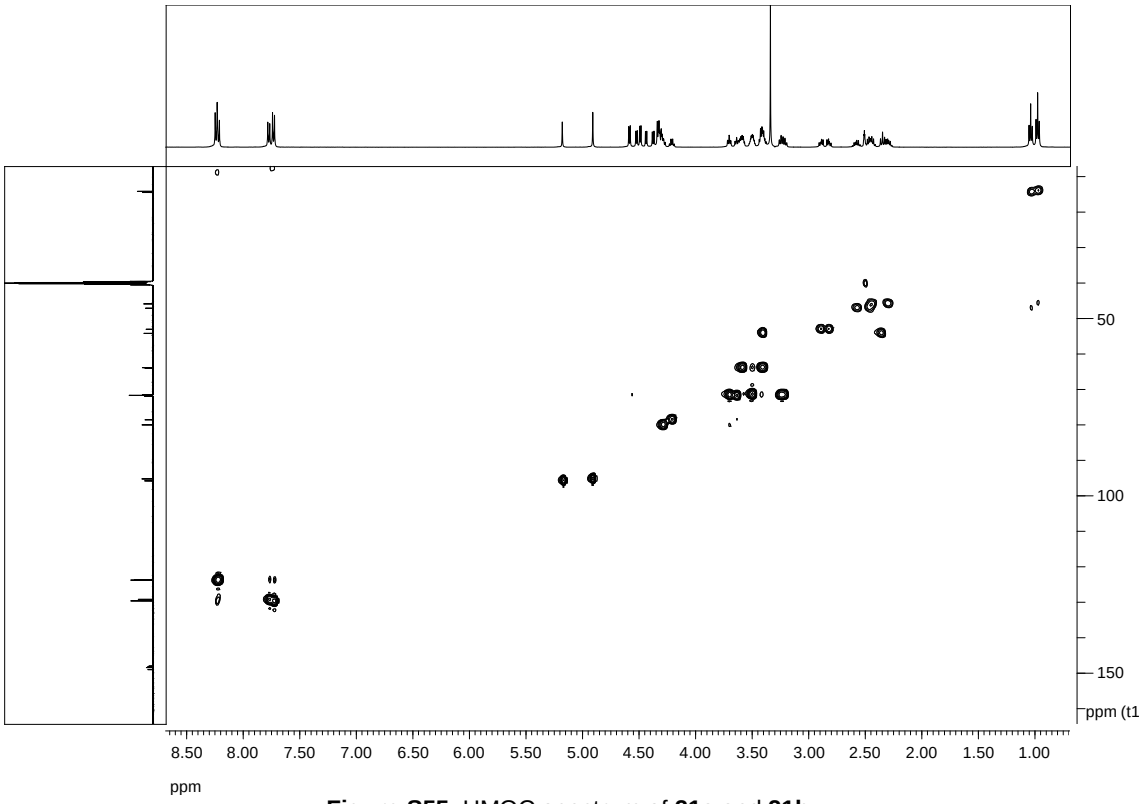


Figure S55. HMQC spectrum of **21a** and **21b**.

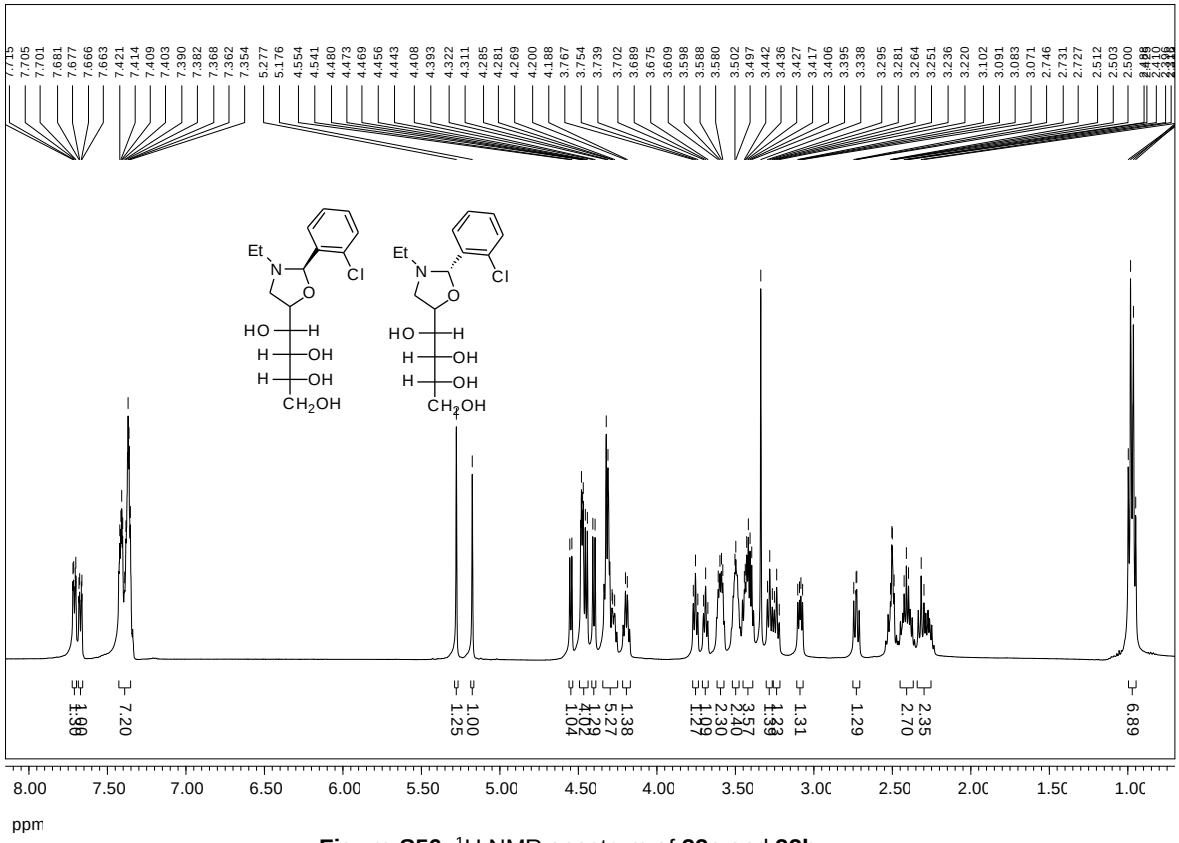


Figure S56. ^{1}H NMR spectrum of **22a** and **22b**.

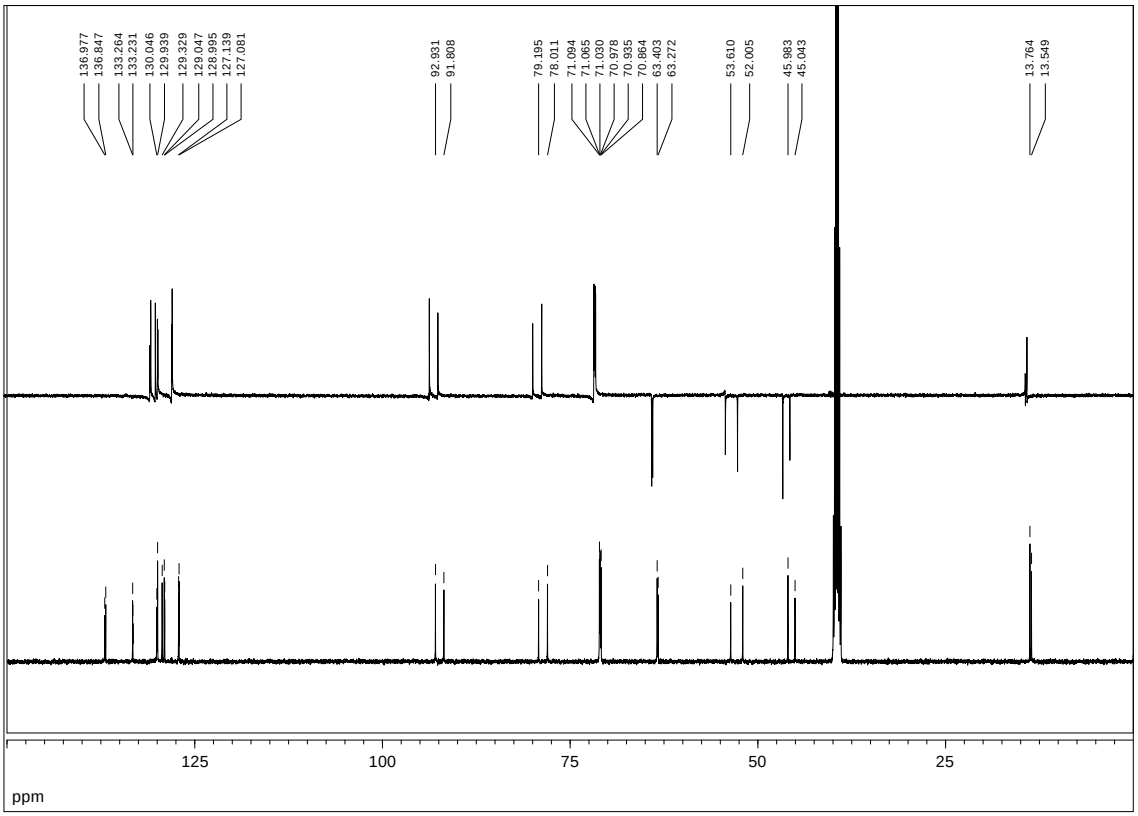


Figure S57. ^{13}C NMR and DEPT spectra of **22a** and **22b**.

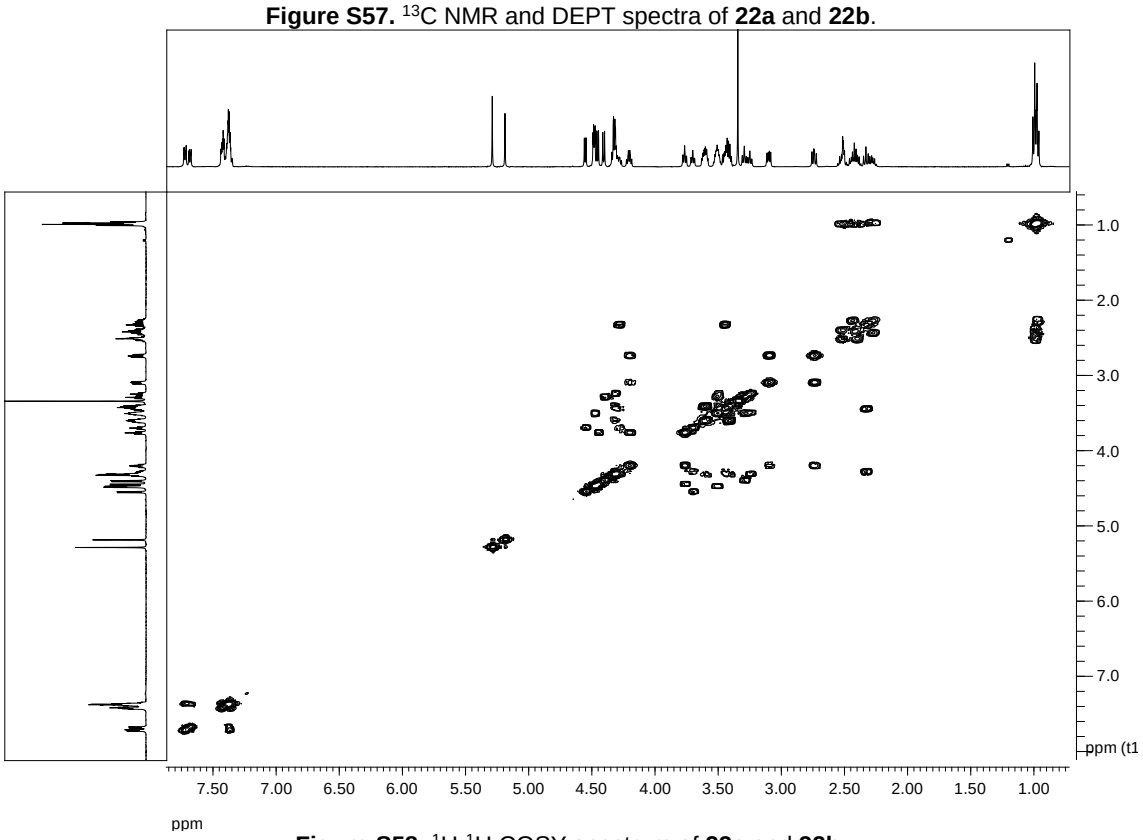


Figure S58. ^{1}H-^{1}H COSY spectrum of **22a** and **22b**.

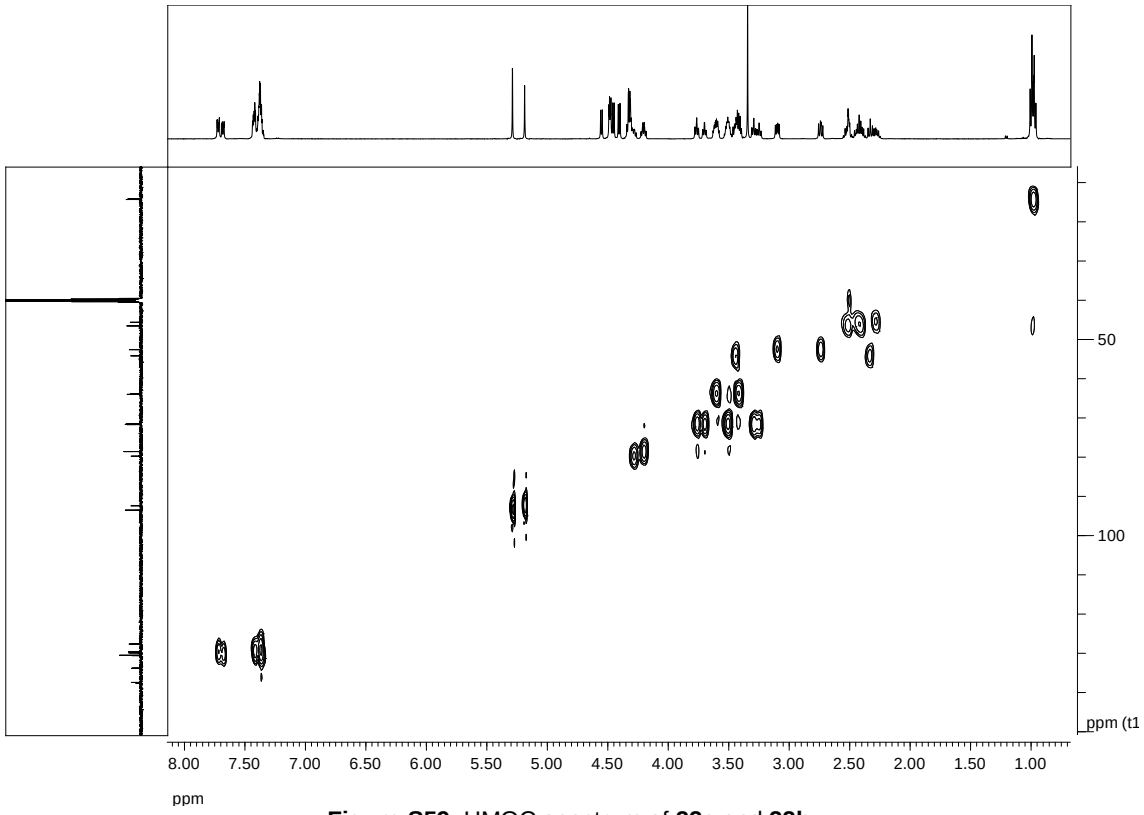


Figure S59. HMQC spectrum of **22a** and **22b**.

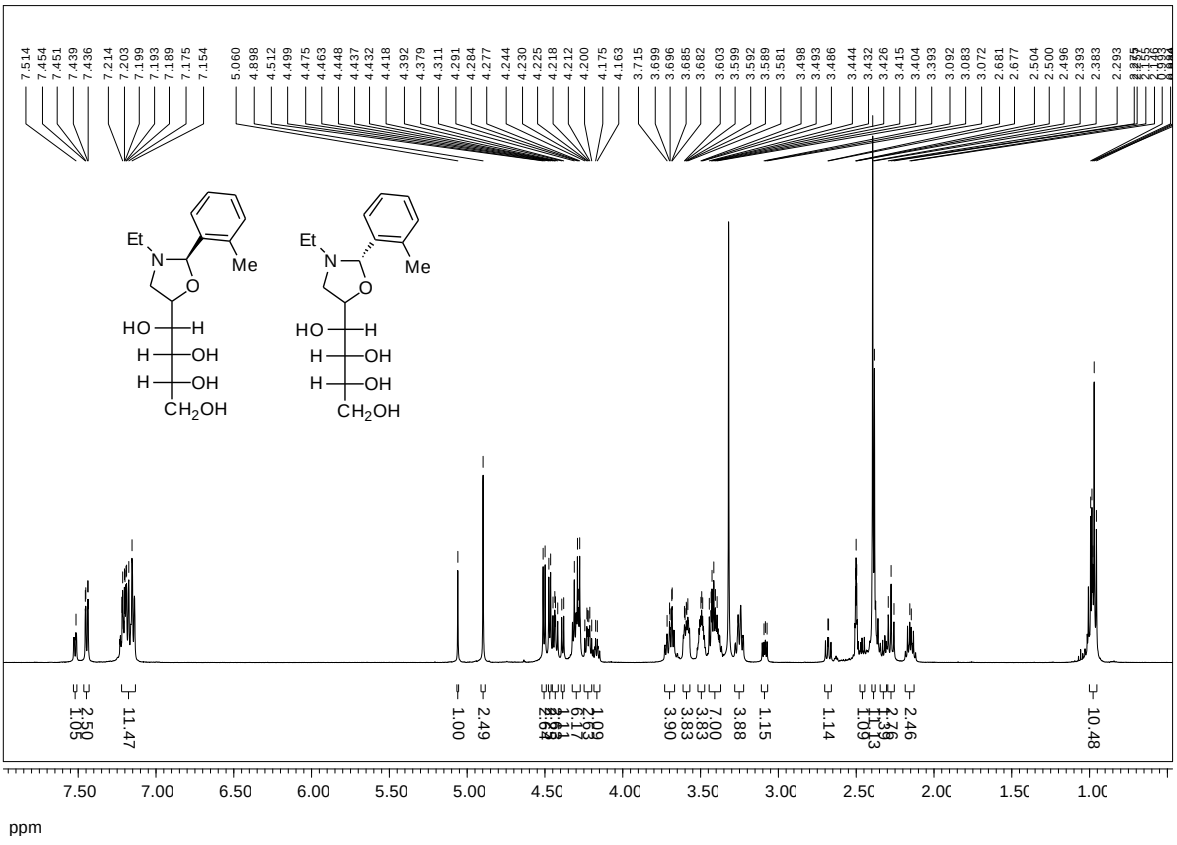


Figure S60. ^{1}H NMR spectrum of **23a** and **23b**.

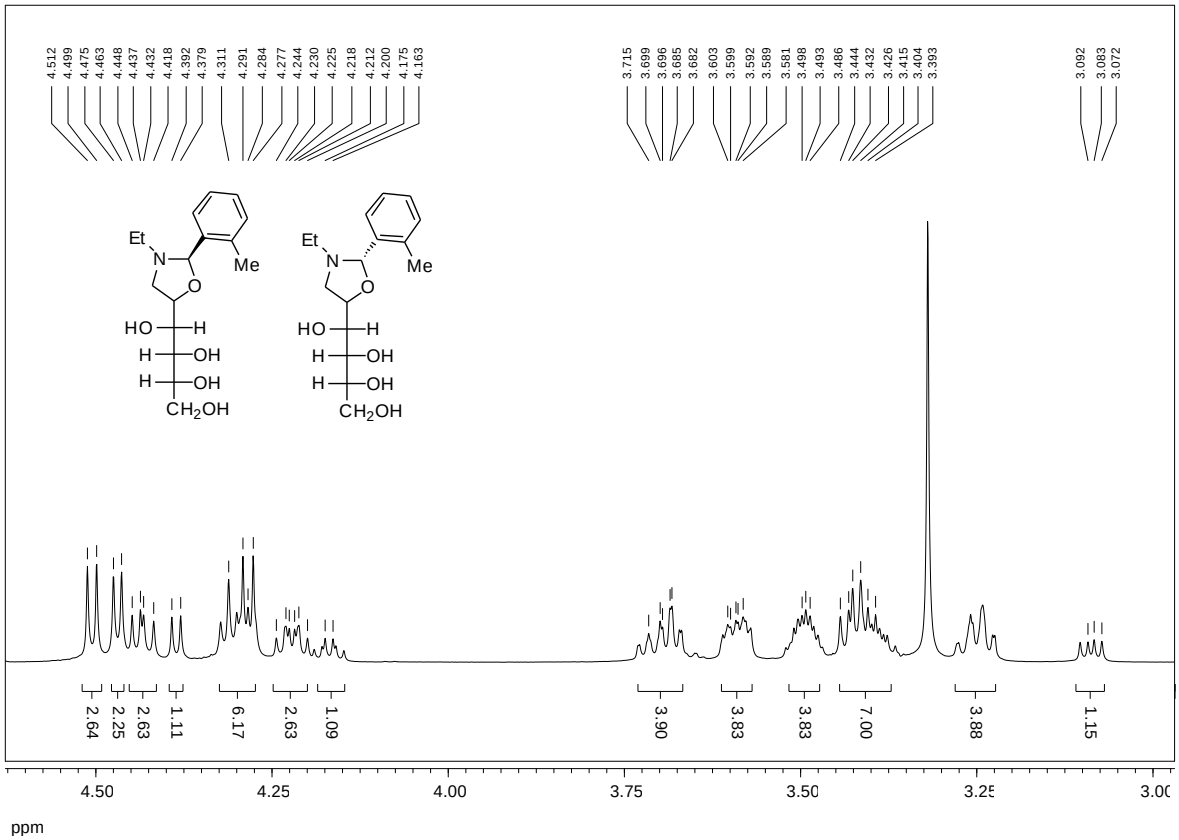


Figure S61. ^{1}H NMR spectrum of **23a** and **23b**.

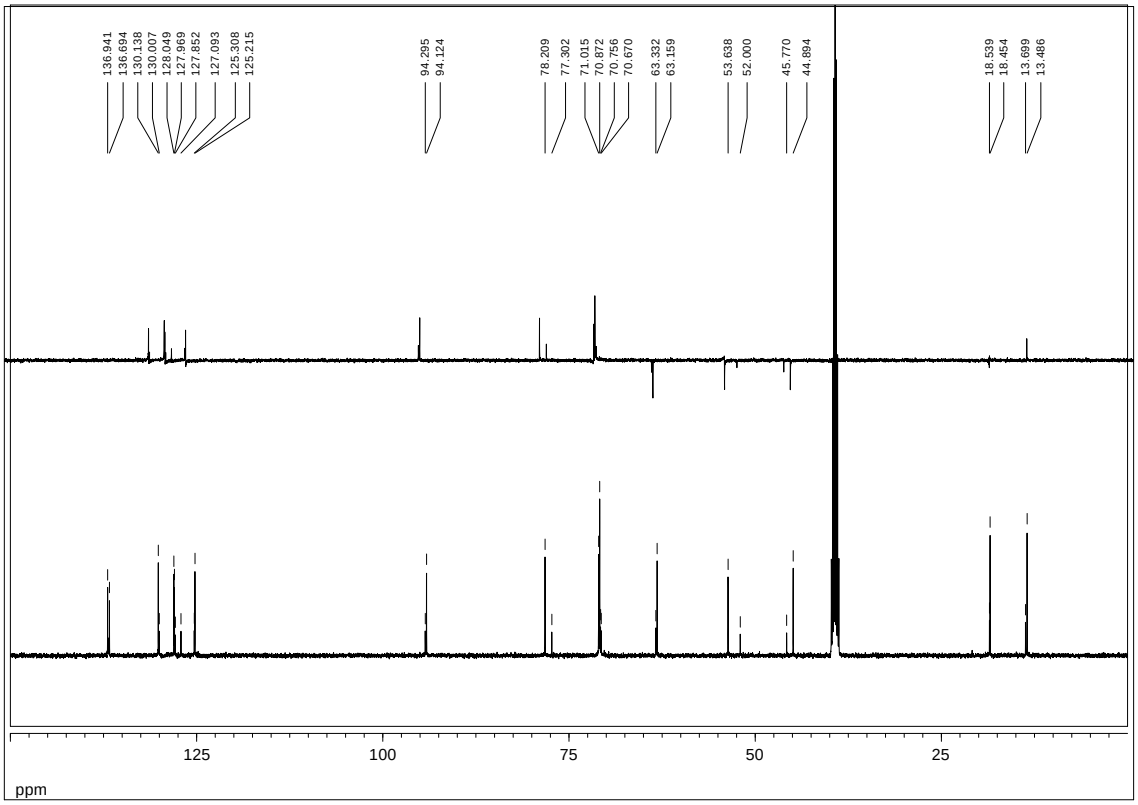


Figure S62. ^{13}C NMR and DEPT spectra of **23a** and **23b**.

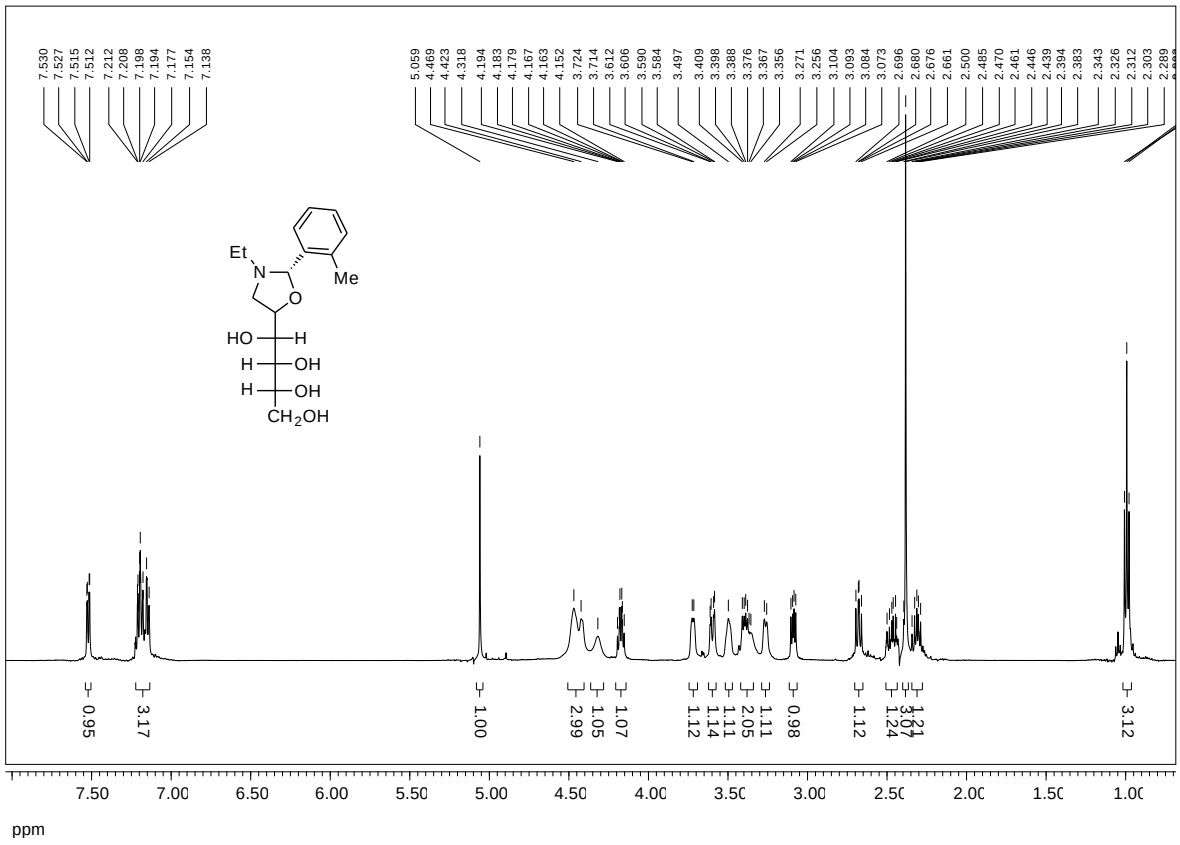


Figure S63. ^{1}H NMR spectrum of **23b**.

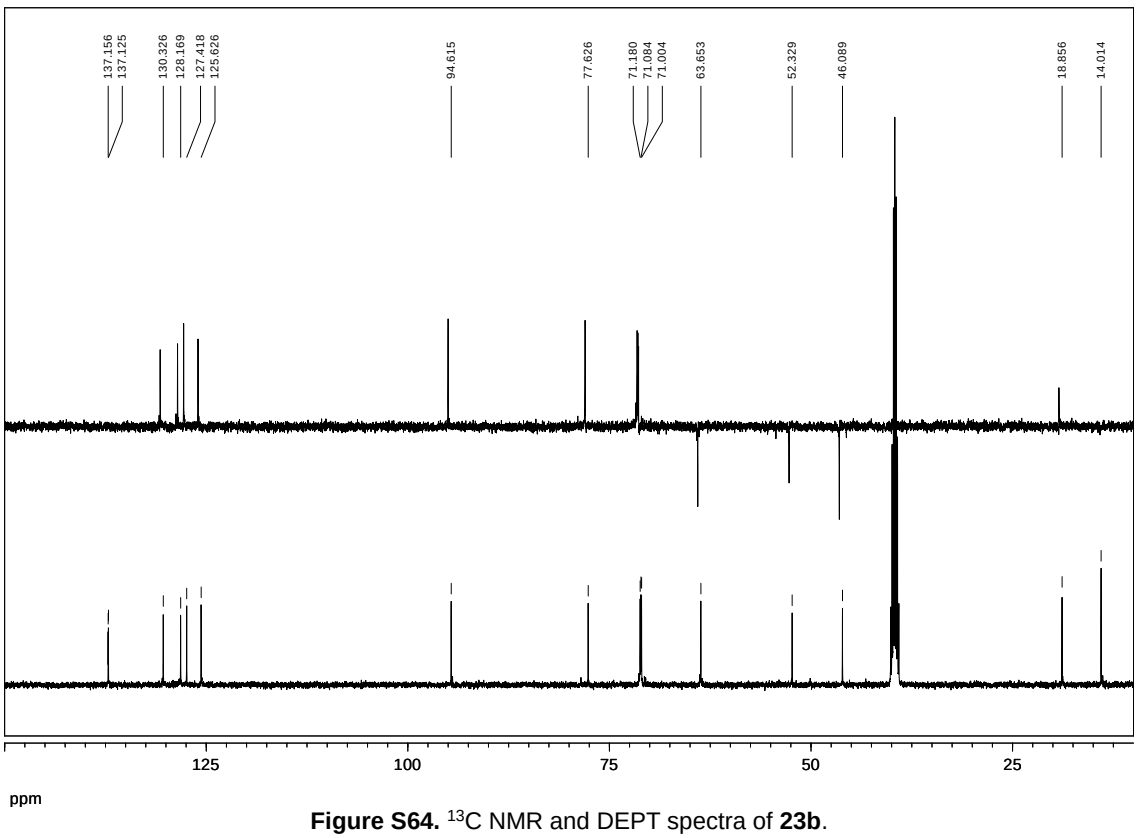


Figure S64. ^{13}C NMR and DEPT spectra of **23b**.

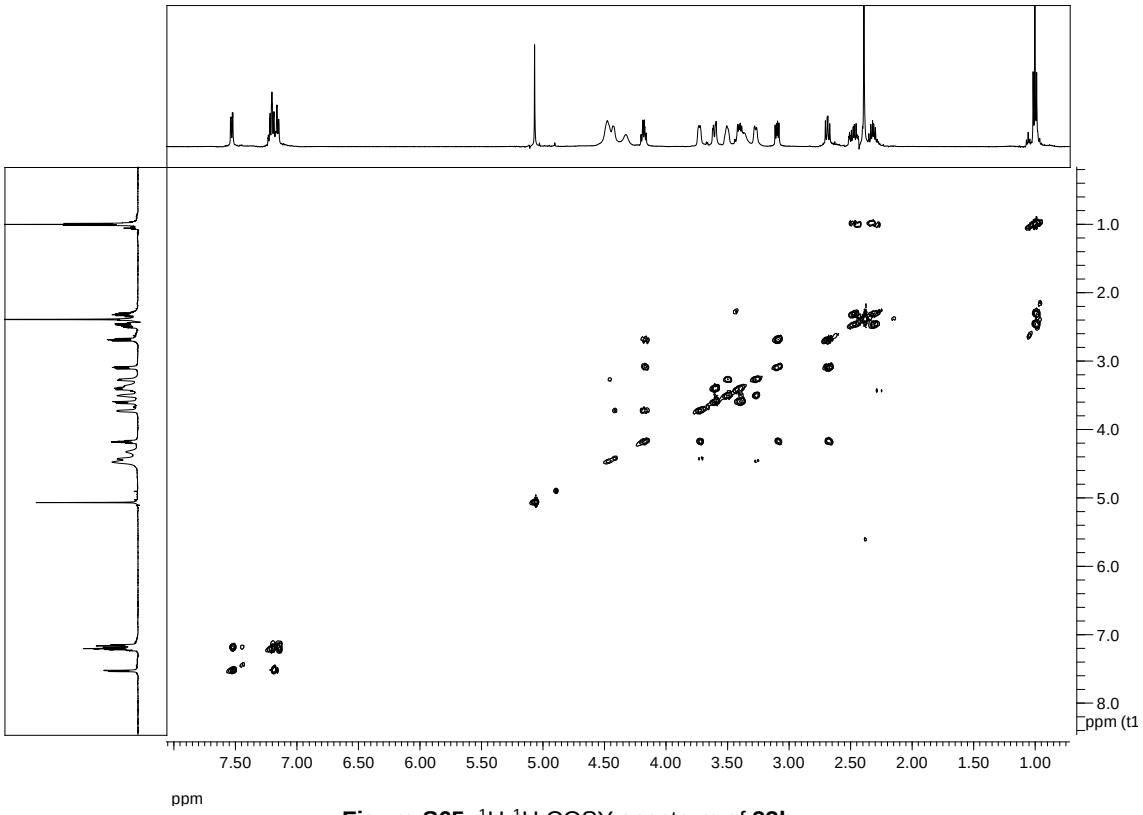


Figure S65. ^{1}H-^{1}H COSY spectrum of **23b**.

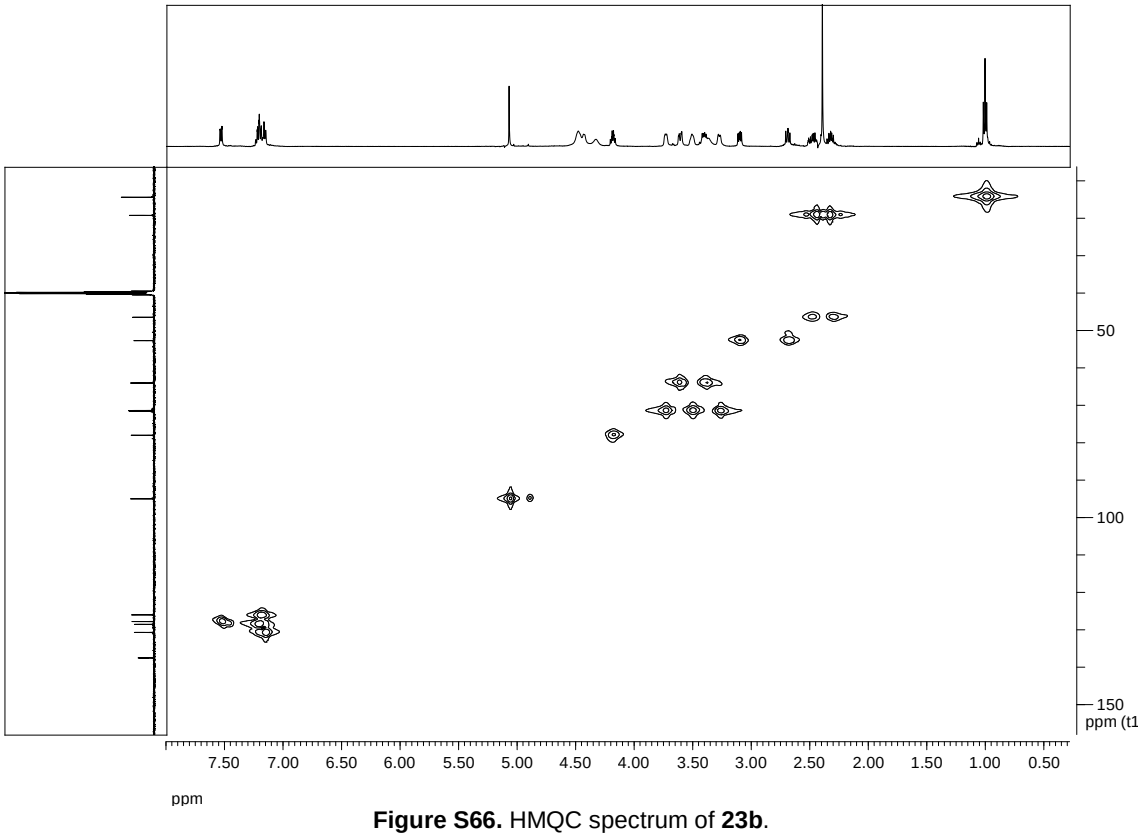


Figure S66. HMQC spectrum of **23b**.

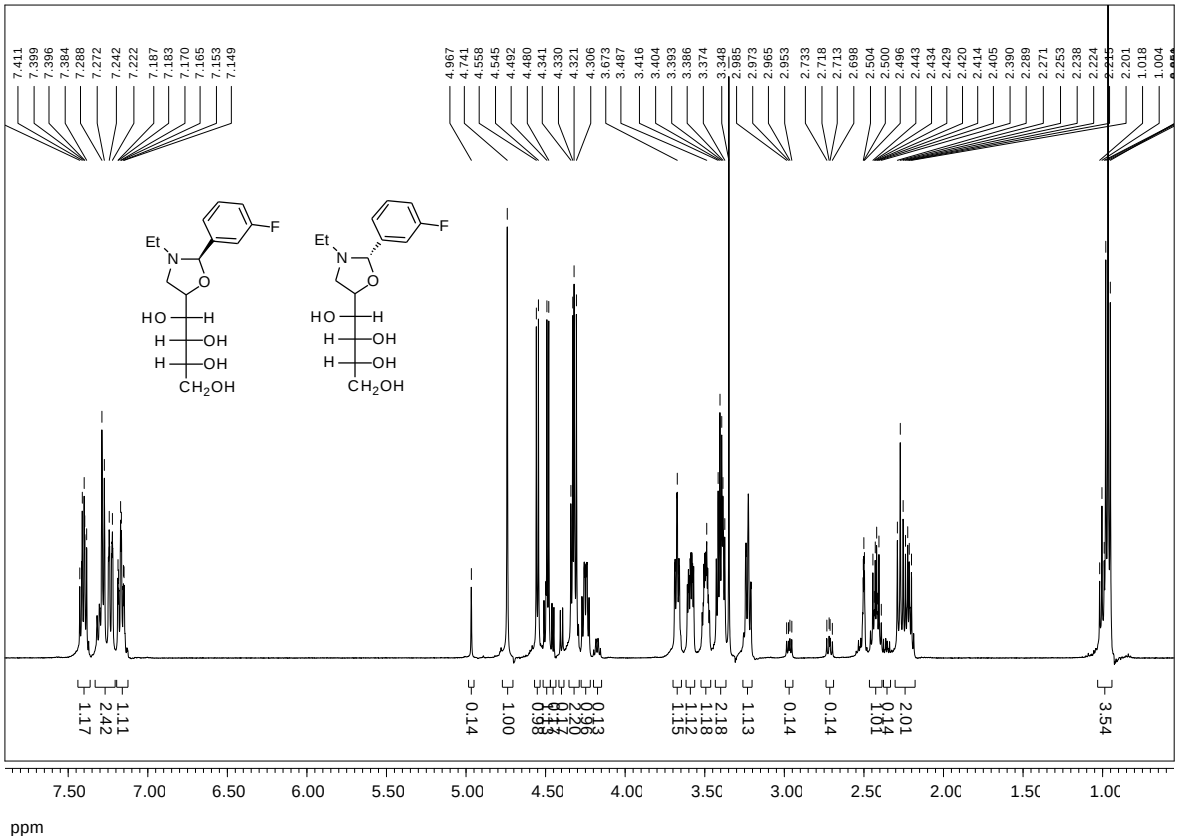


Figure S67. ^{1}H NMR spectrum of **24a** and **24b**.

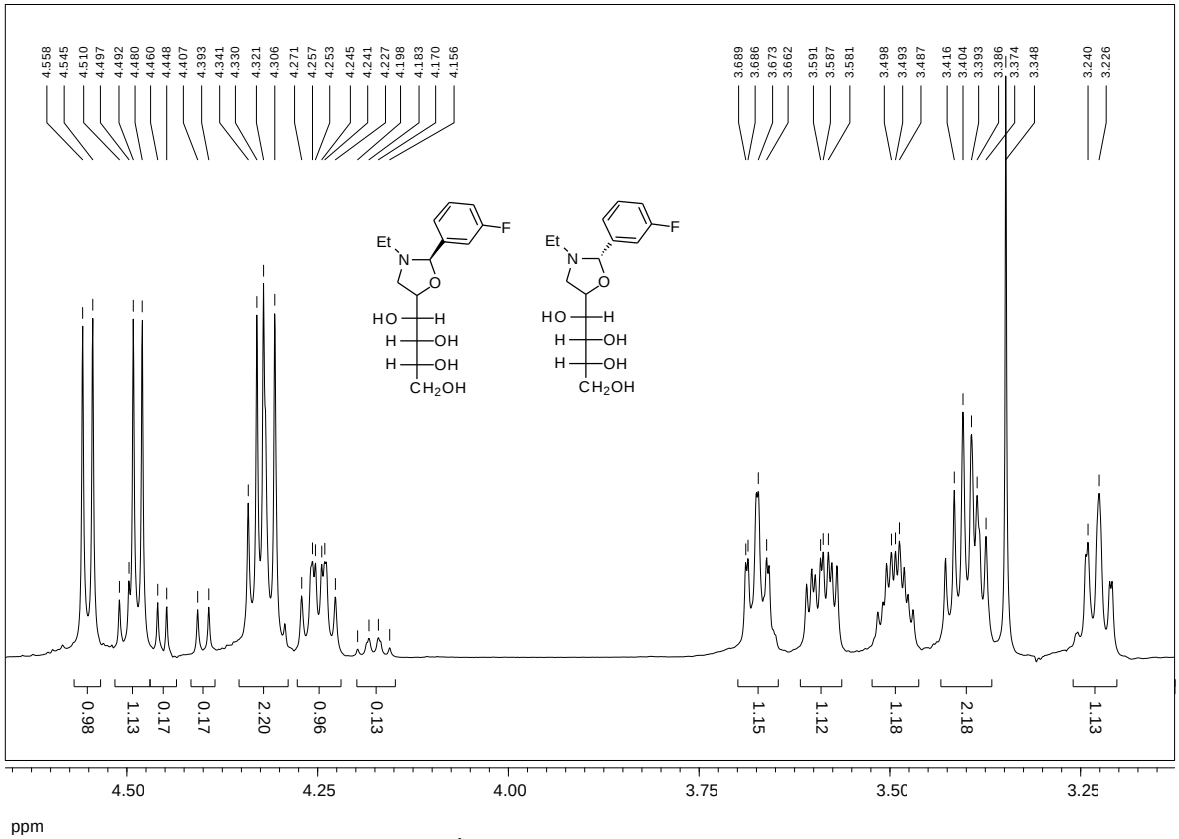


Figure S68. ^{1}H NMR spectrum of **24a** and **24b**.

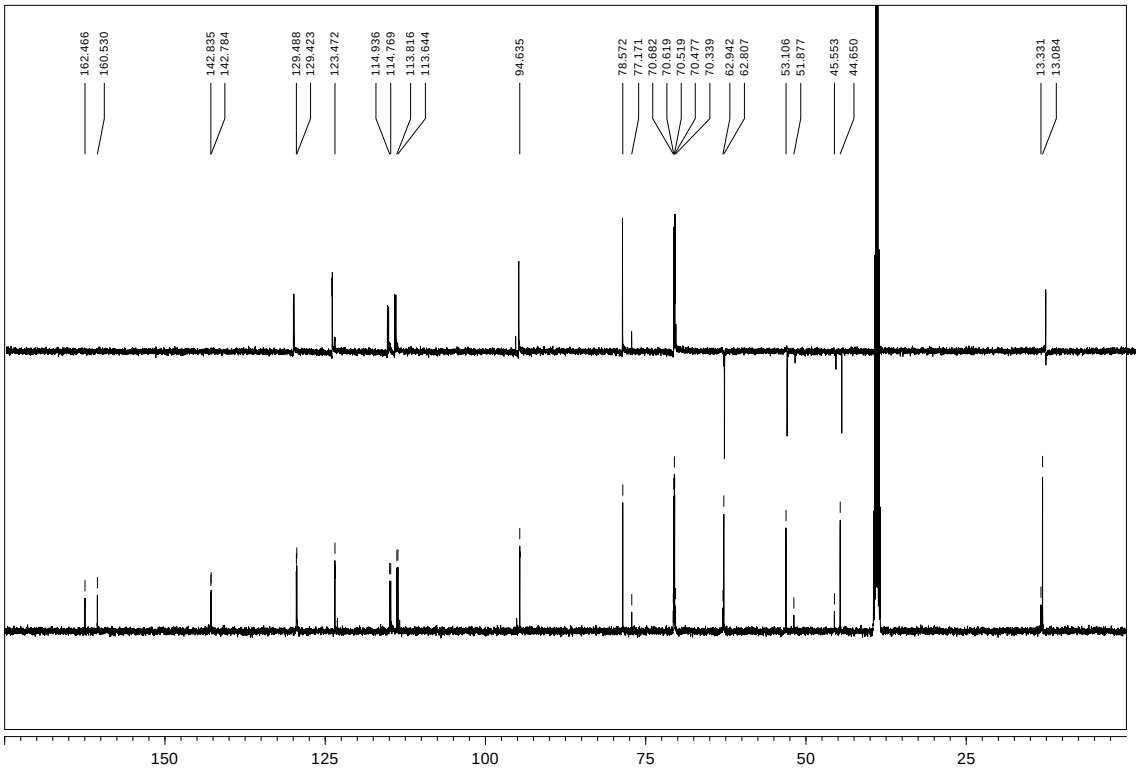


Figure S69. ^{13}C NMR and DEPT spectra of **24a** and **24b**.

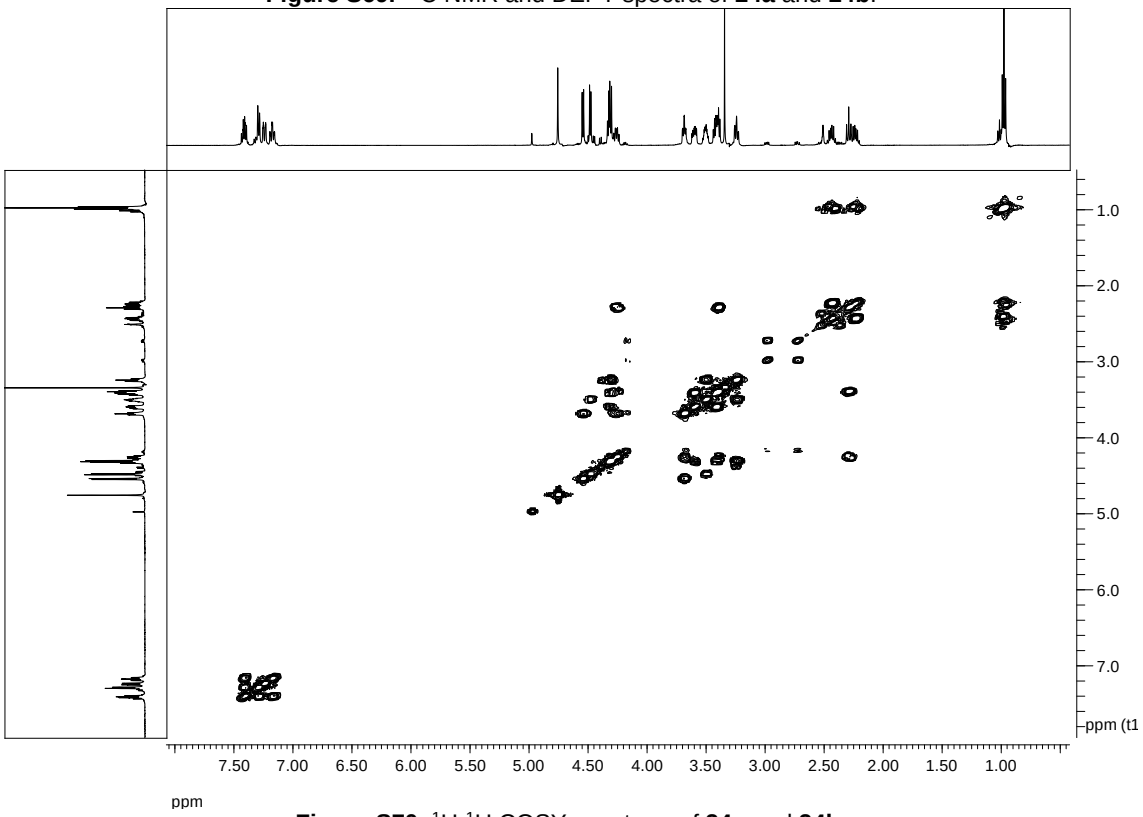


Figure S70. ^{1}H-^{1}H COSY spectrum of **24a** and **24b**.

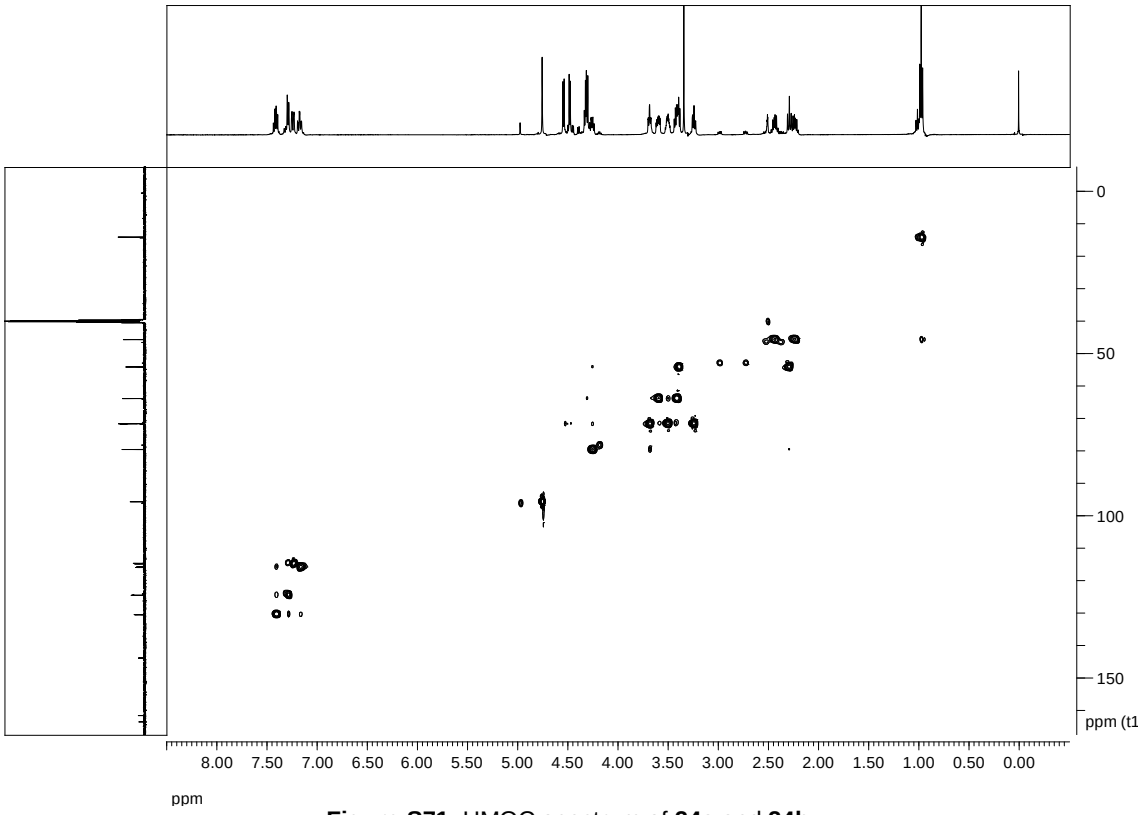


Figure S71. HMQC spectrum of **24a** and **24b**.

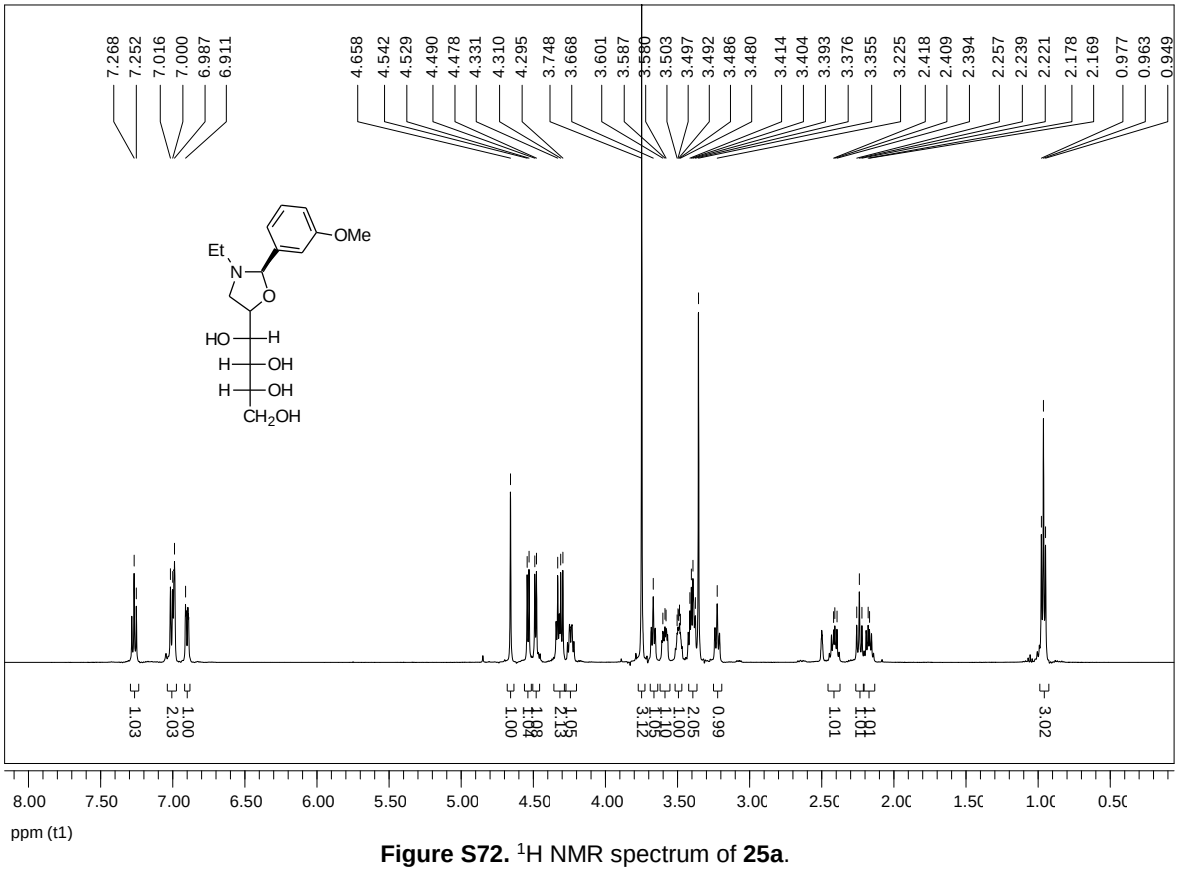


Figure S72. ^{1}H NMR spectrum of **25a**.

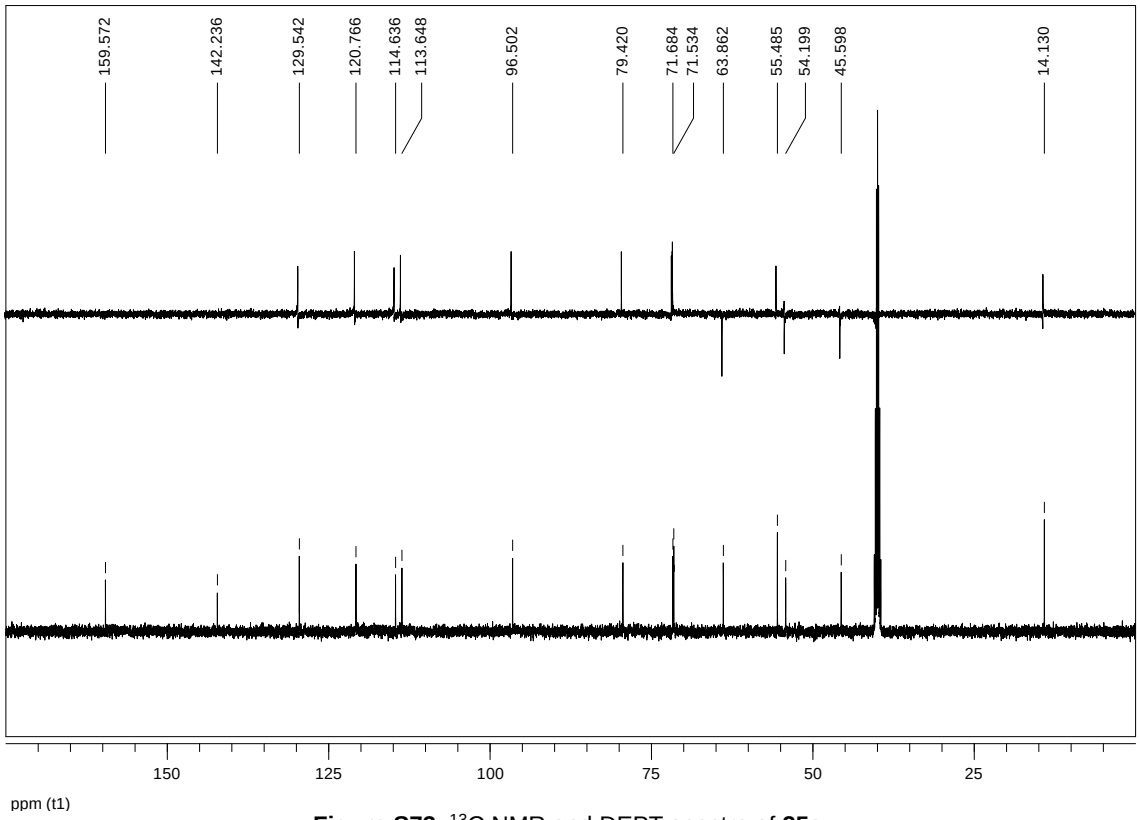


Figure S73. ^{13}C NMR and DEPT spectra of **25a**.

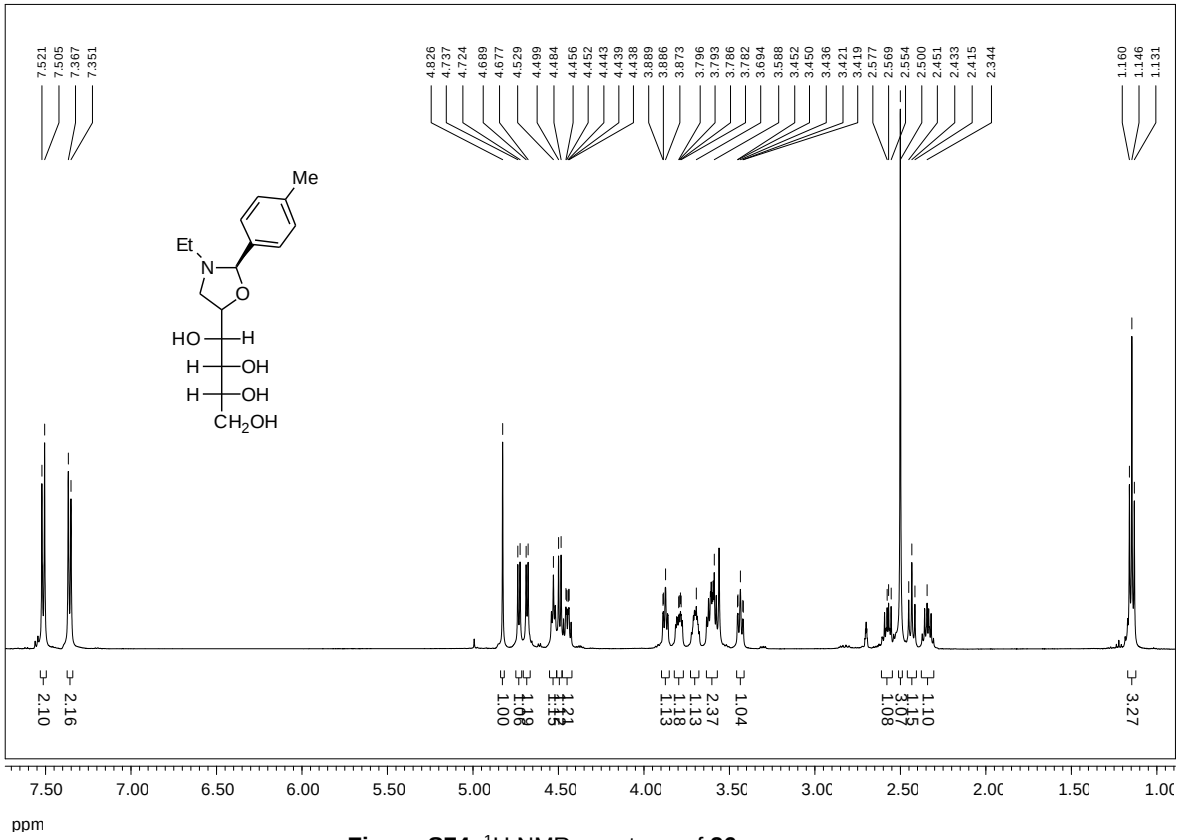


Figure S74. ^{1}H NMR spectrum of **26a**.

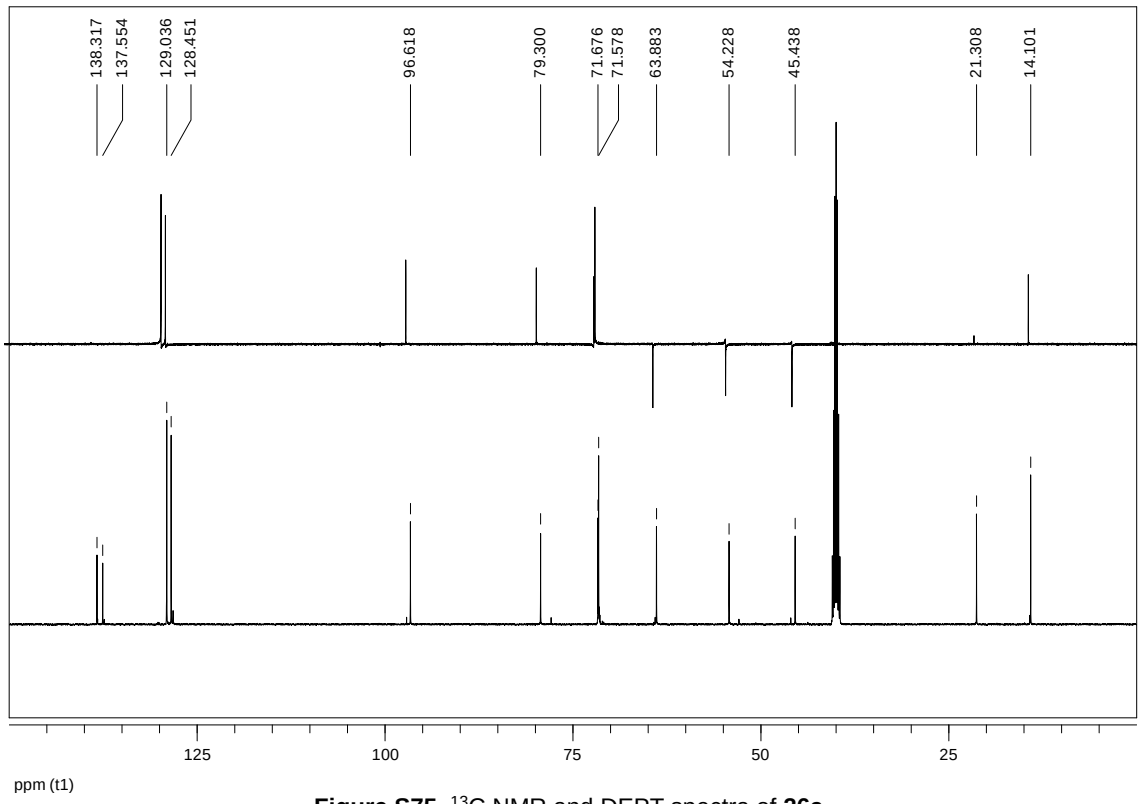


Figure S75. ^{13}C NMR and DEPT spectra of **26a**.

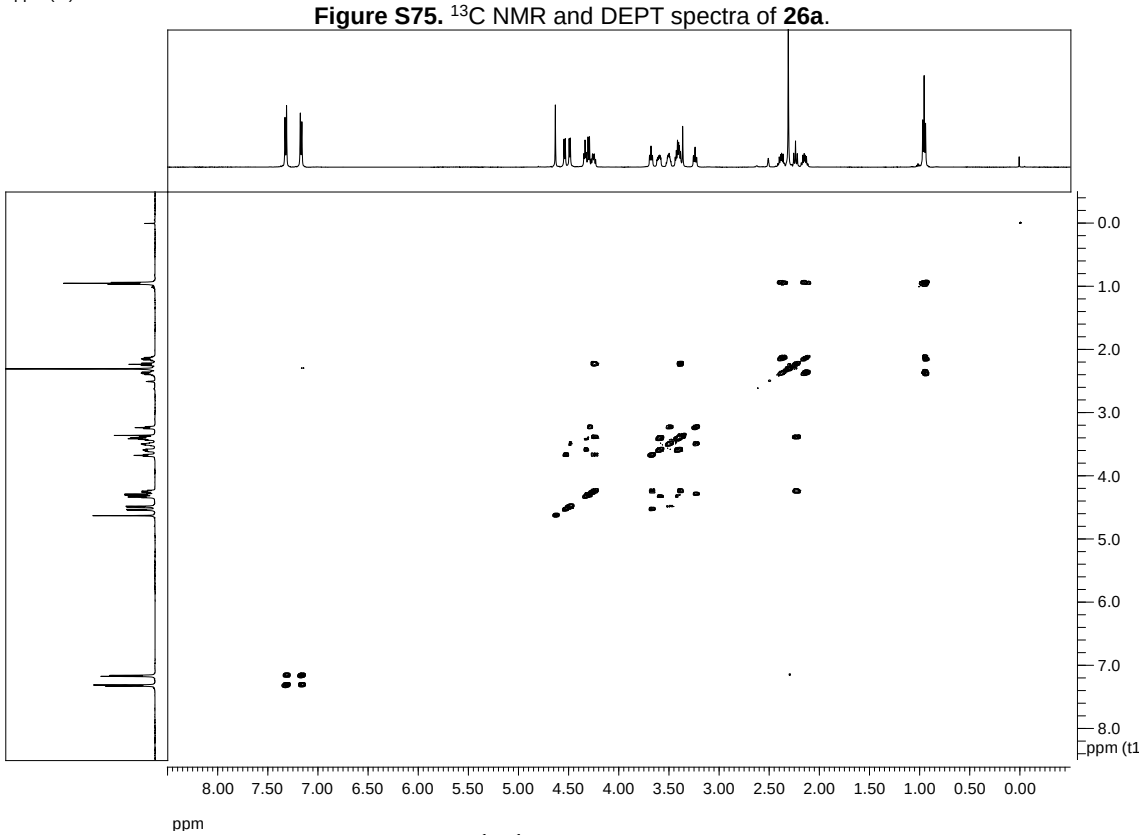


Figure S76. ^{1}H-^{1}H COSY spectrum of **26a**.

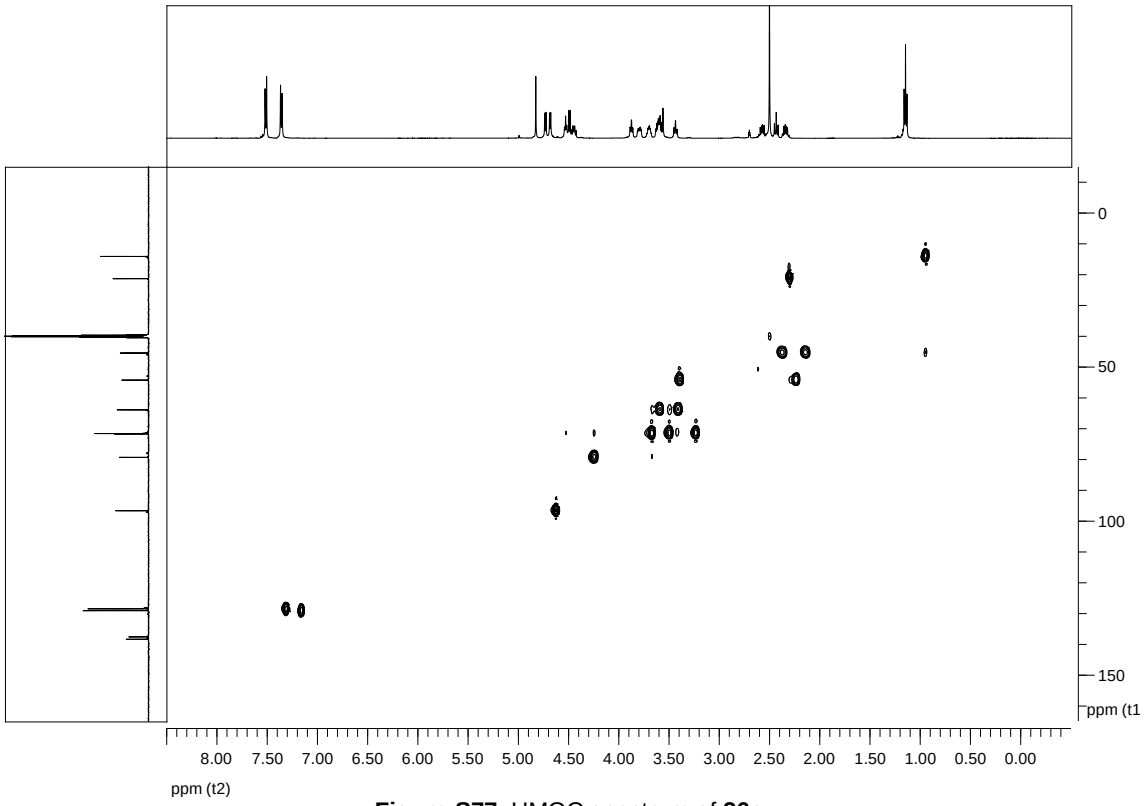


Figure S77. HMQC spectrum of **26a**.

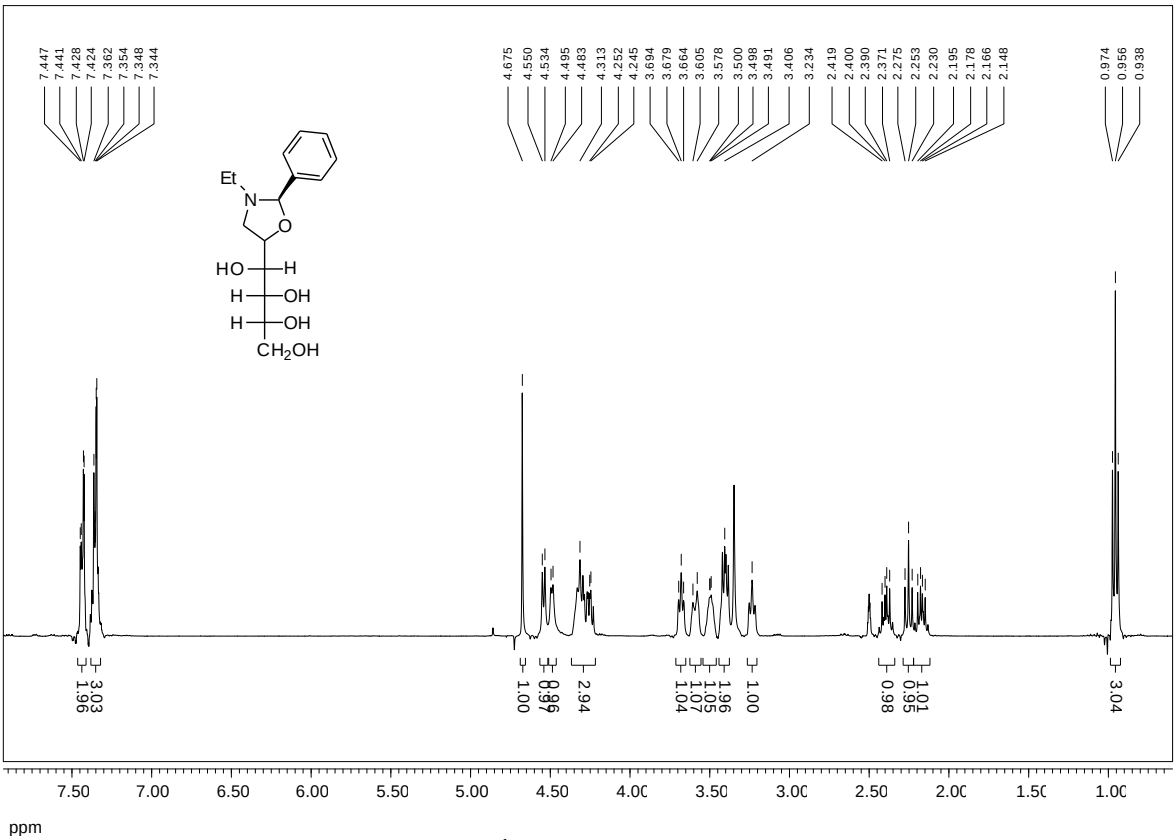


Figure S78. ^{1}H NMR spectrum of **27a**.

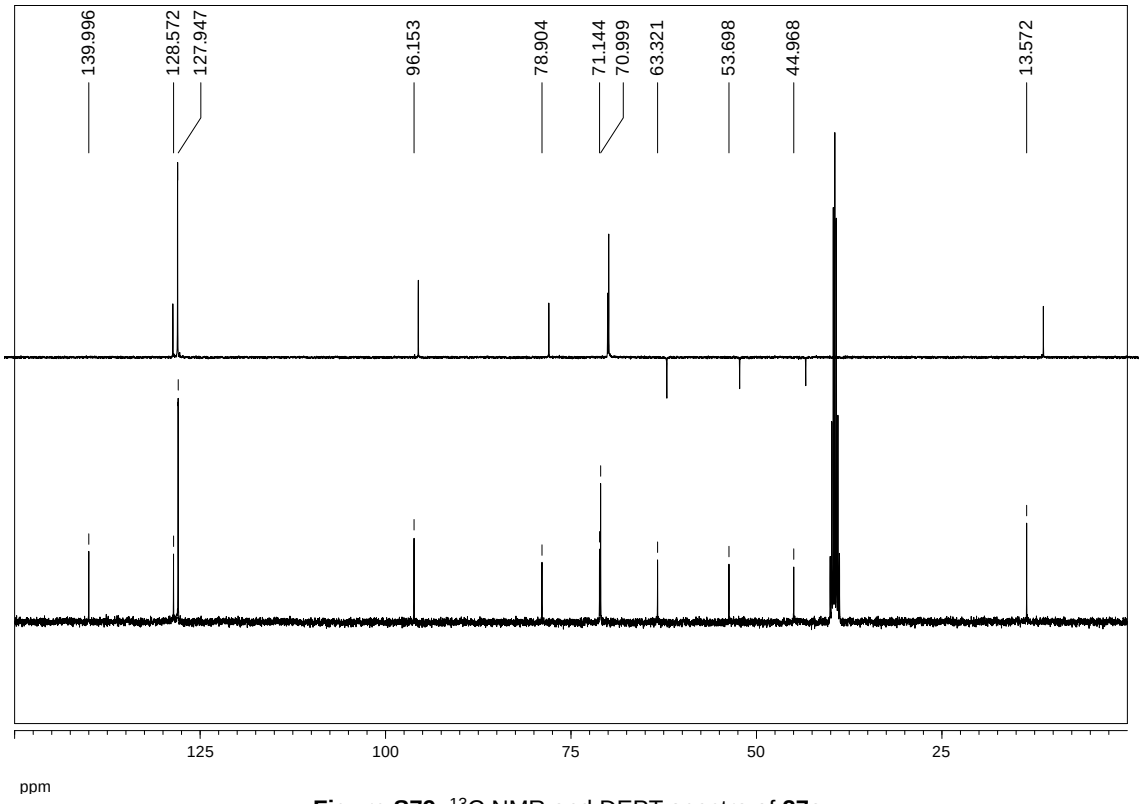


Figure S79. ^{13}C NMR and DEPT spectra of **27a**.

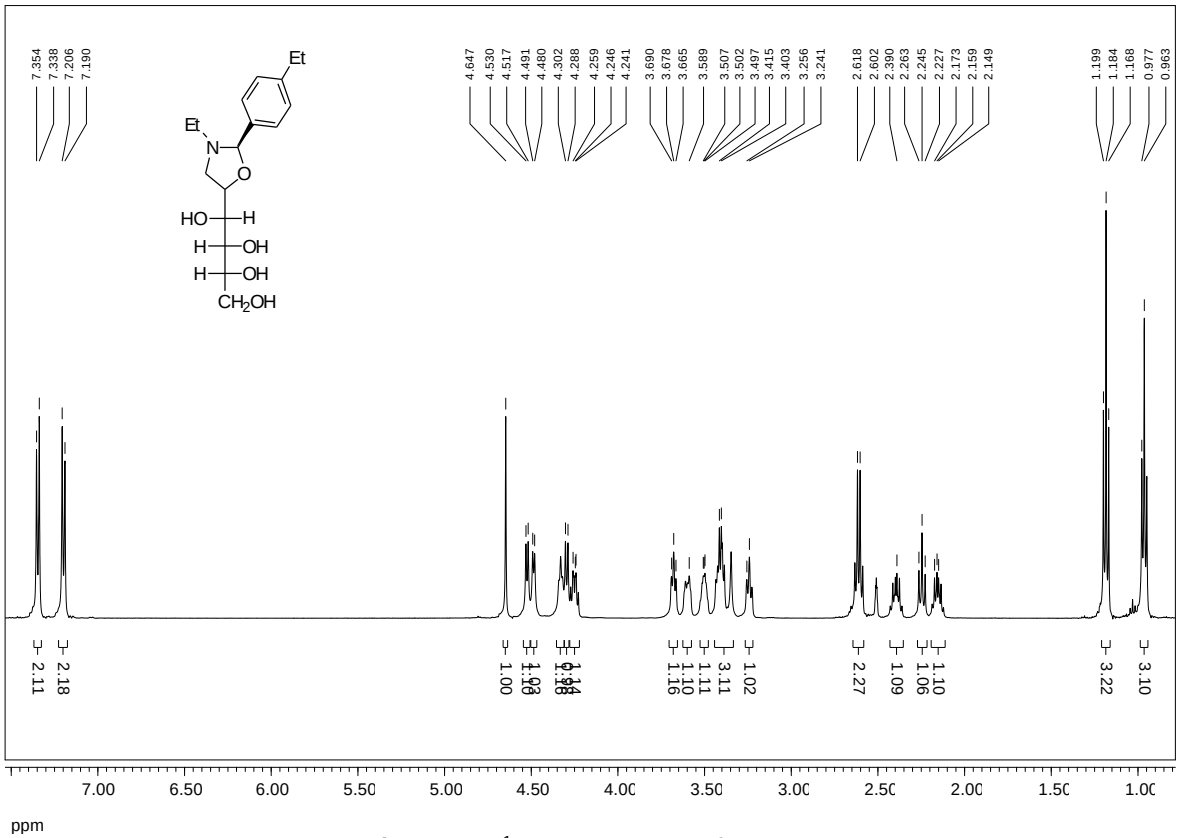


Figure S80. ^{1}H NMR spectrum of **28a**.

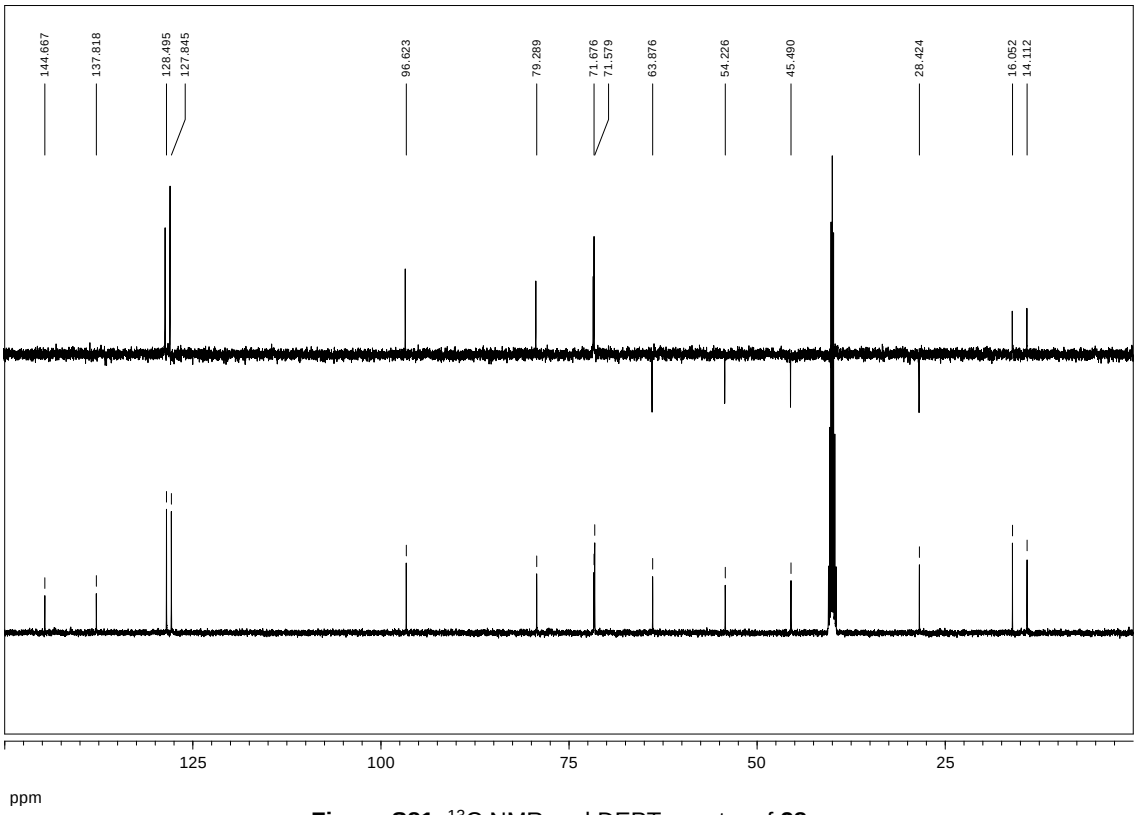


Figure S81. ^{13}C NMR and DEPT spectra of **28a**.

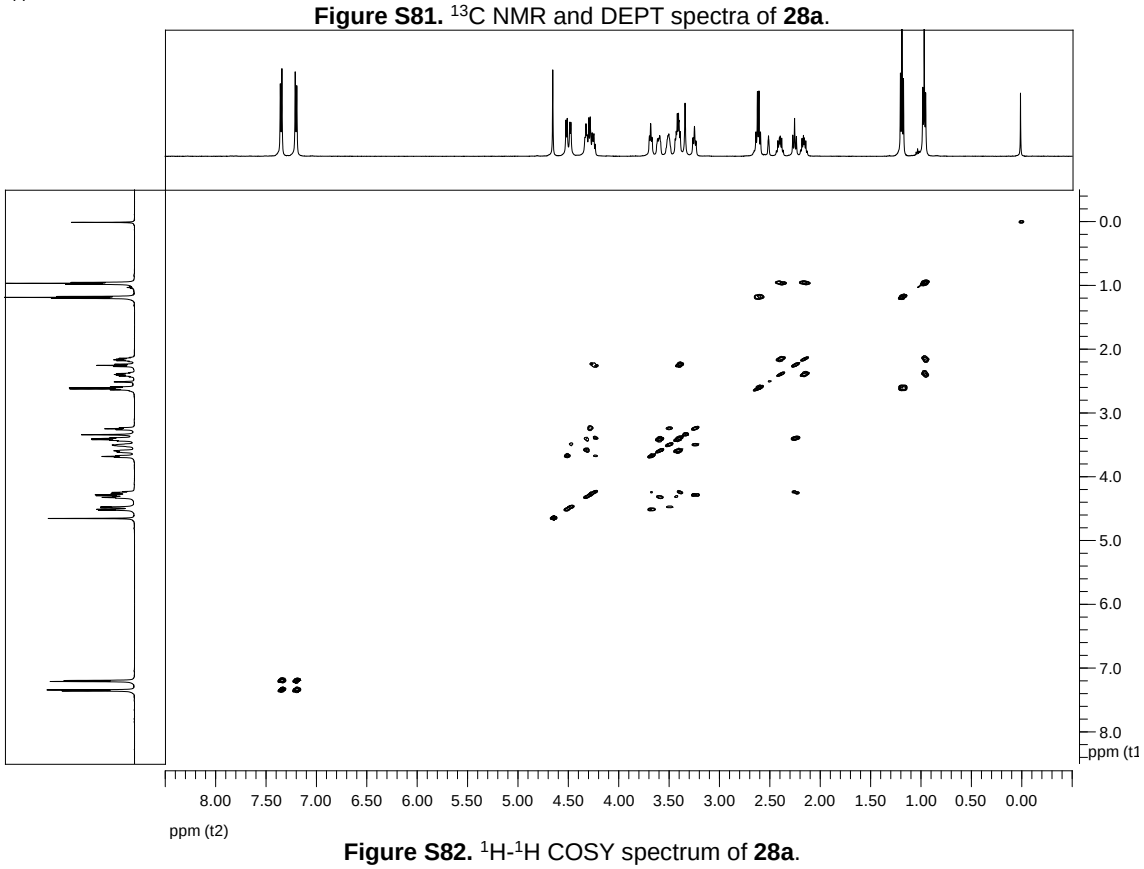


Figure S82. ^{1}H-^{1}H COSY spectrum of **28a**.

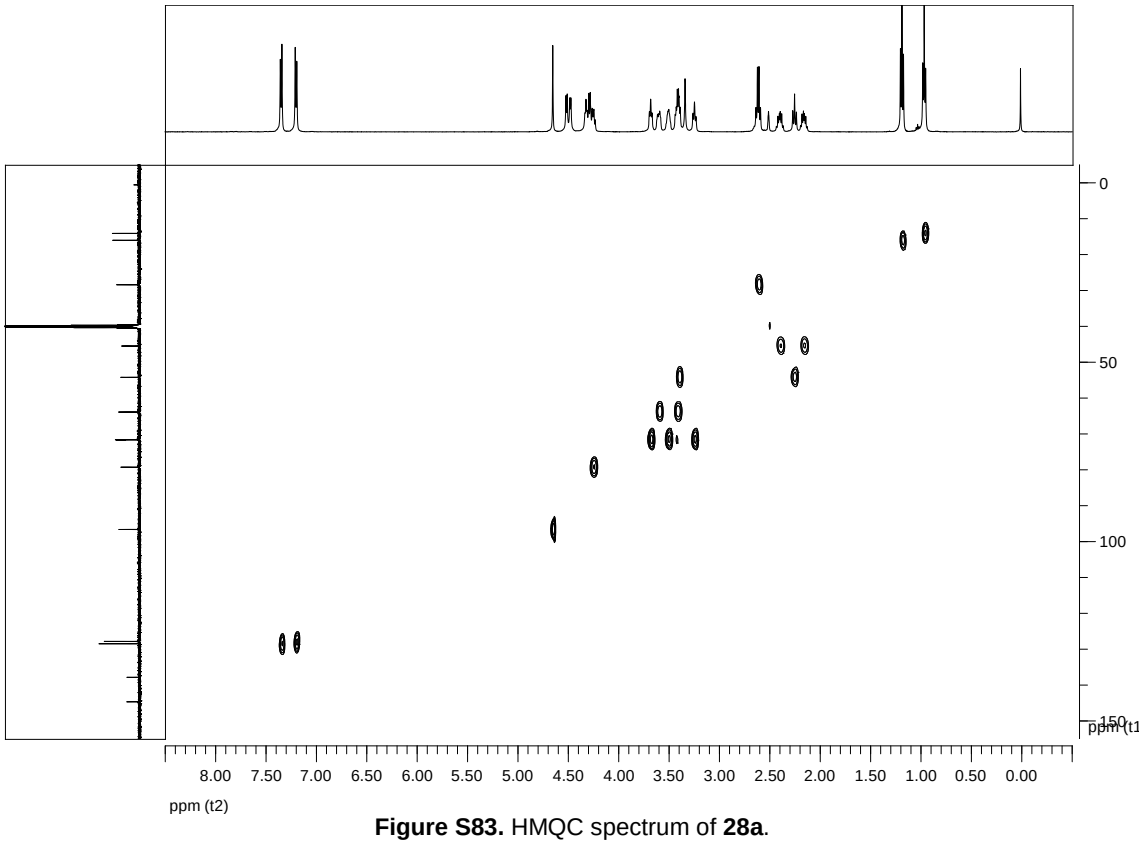


Figure S83. HMQC spectrum of **28a**.

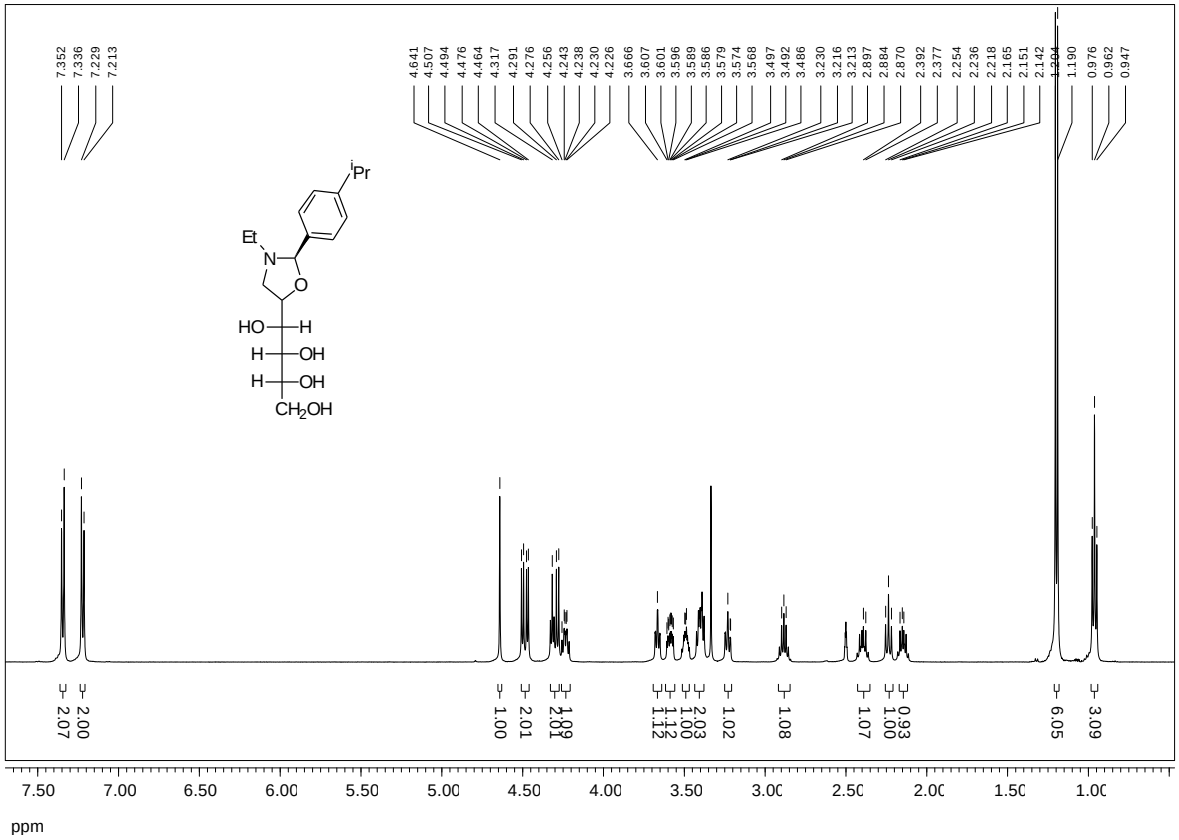


Figure S84. ^{1}H NMR spectrum of **29a**.

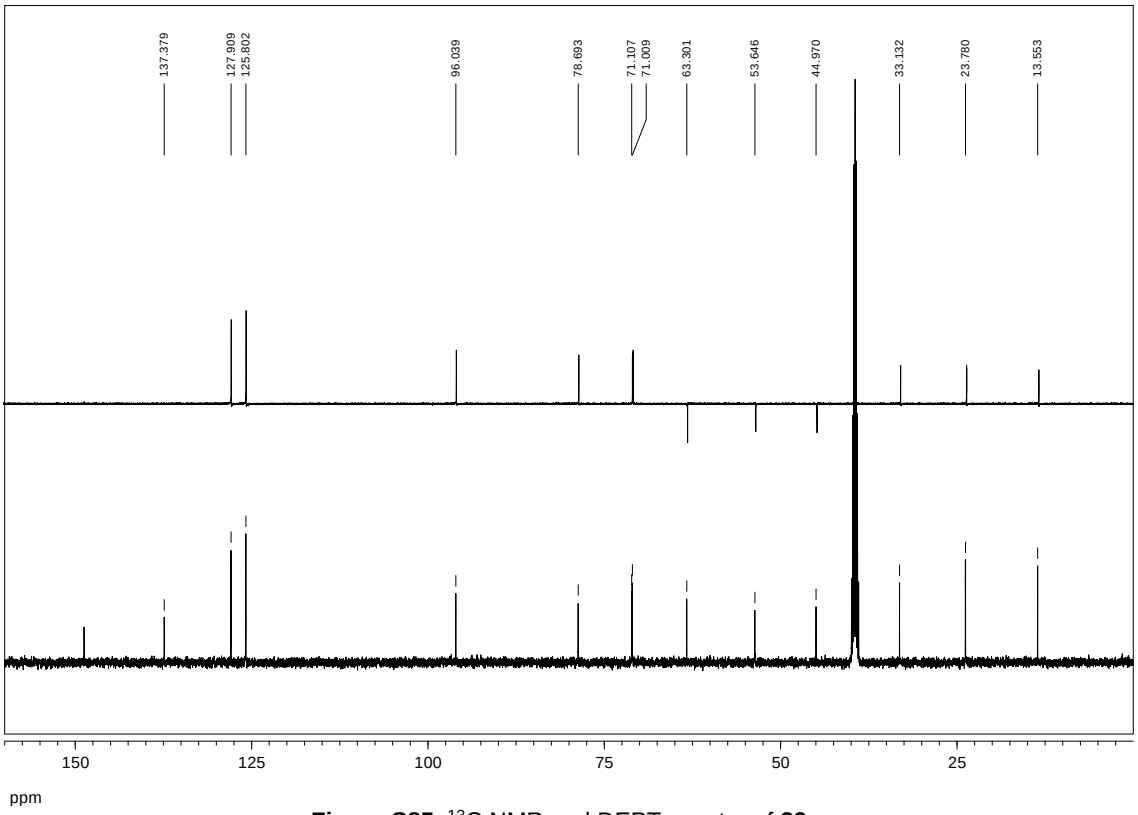


Figure S85. ^{13}C NMR and DEPT spectra of **29a**.

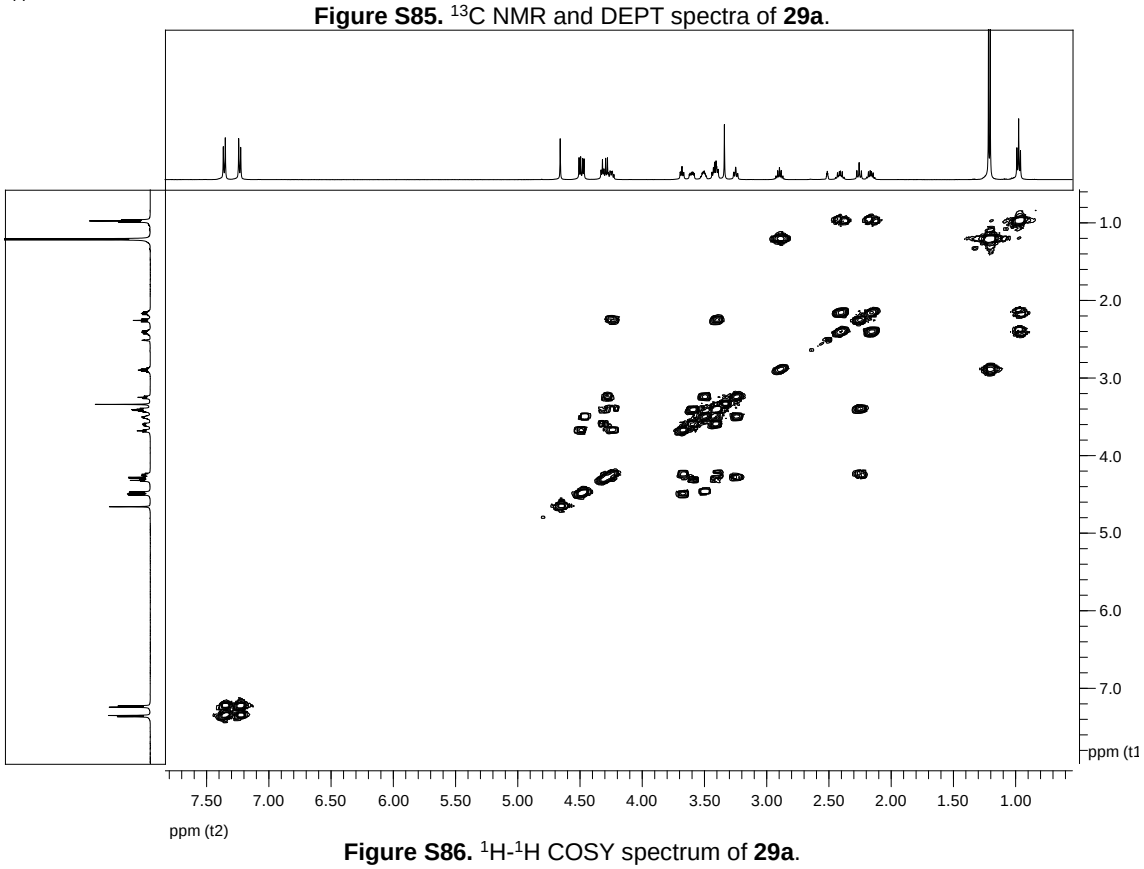


Figure S86. ^{1}H-^{1}H COSY spectrum of **29a**.

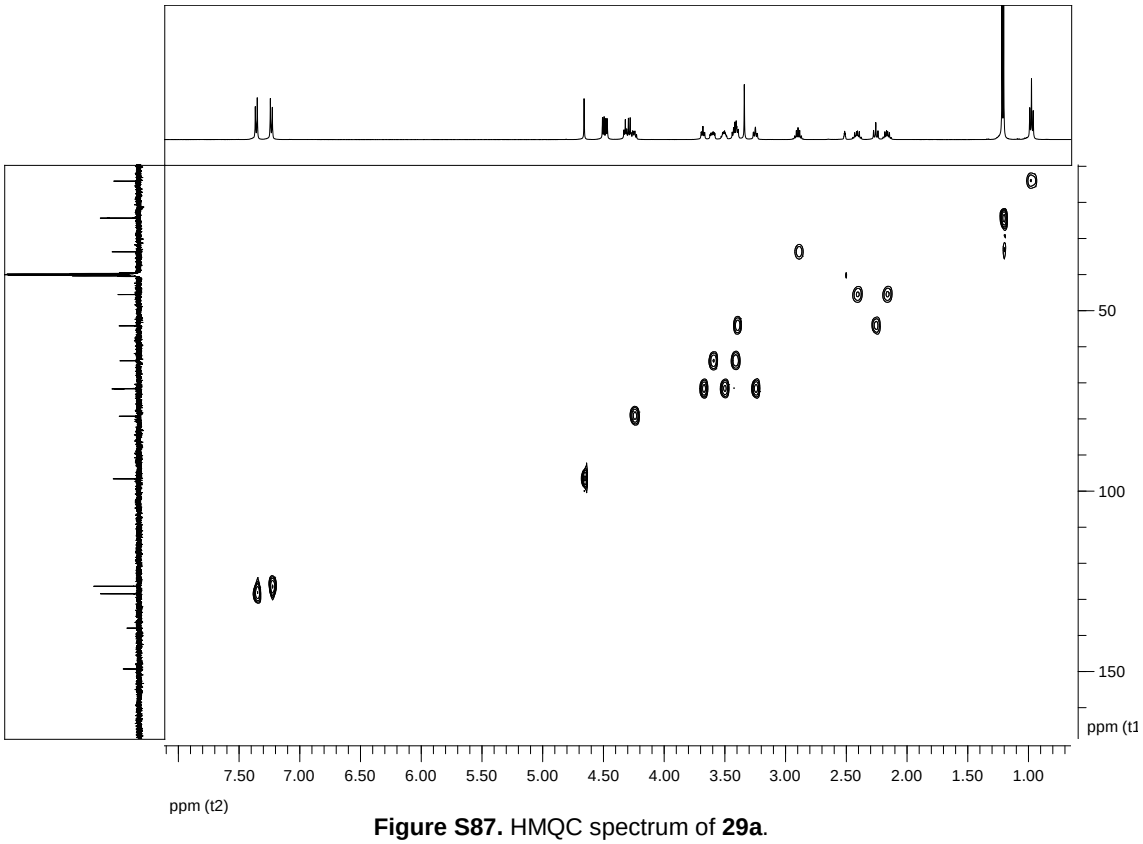


Figure S87. HMQC spectrum of **29a**.

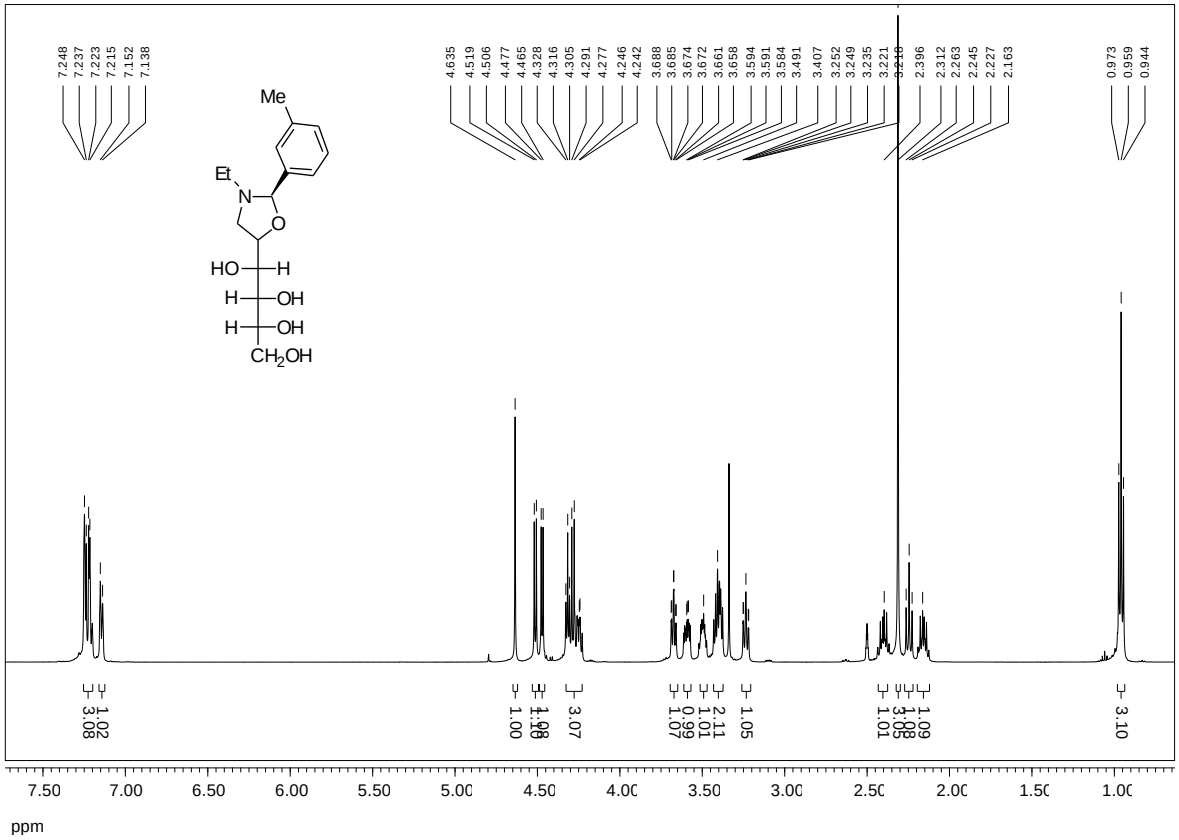


Figure S88. ^{1}H NMR spectrum of **30a**.

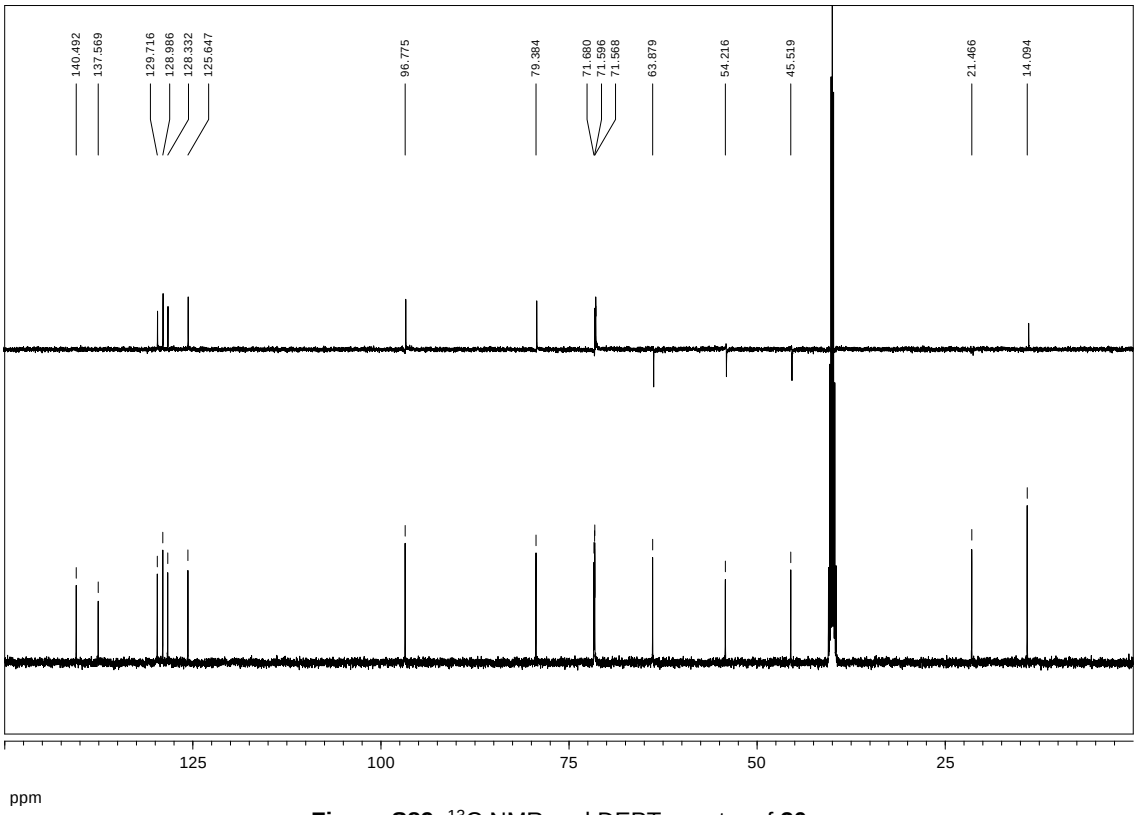


Figure S89. ^{13}C NMR and DEPT spectra of **30a**.

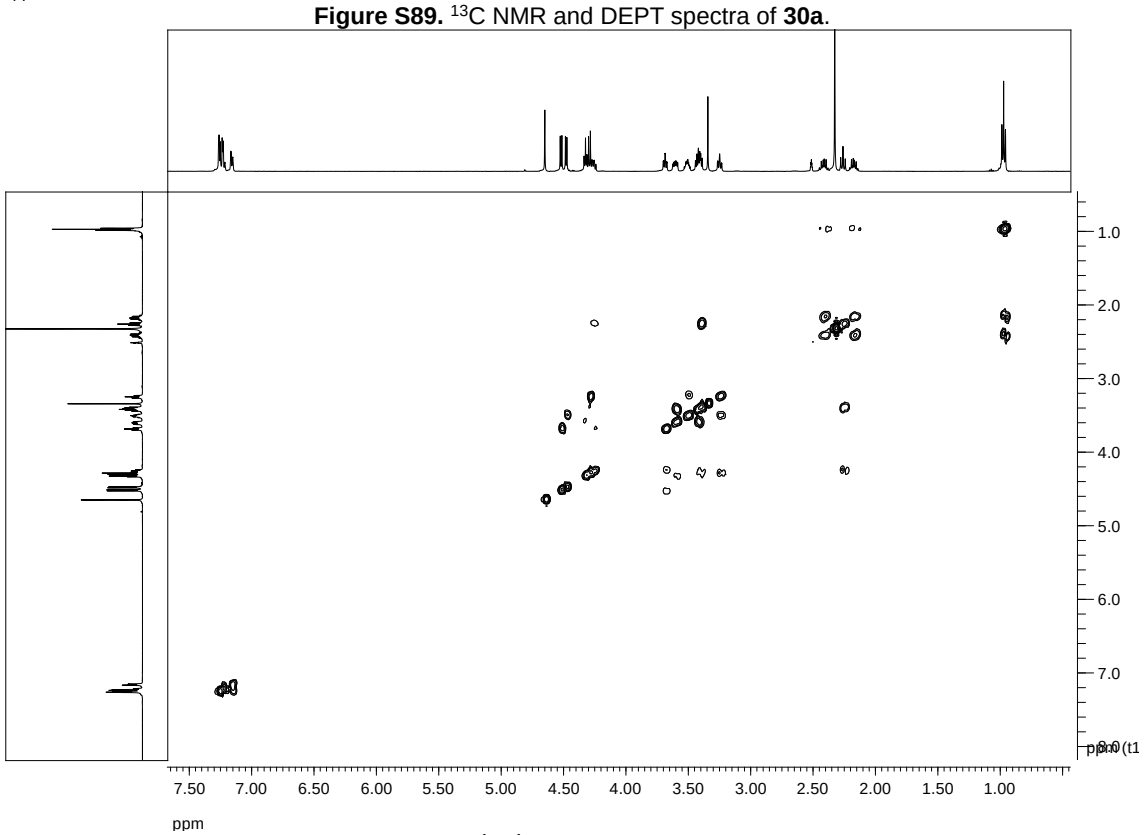


Figure S90. ^{1}H-^{1}H COSY spectrum of **30a**.

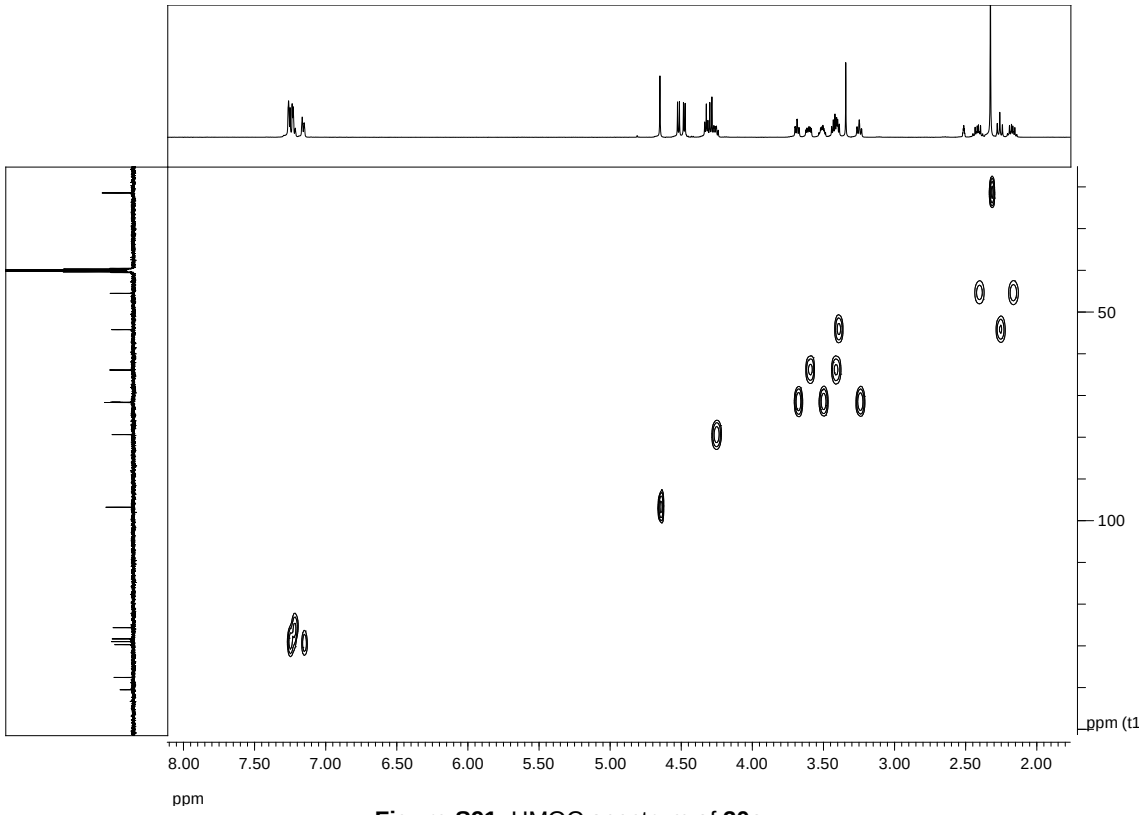


Figure S91. HMQC spectrum of **30a**.

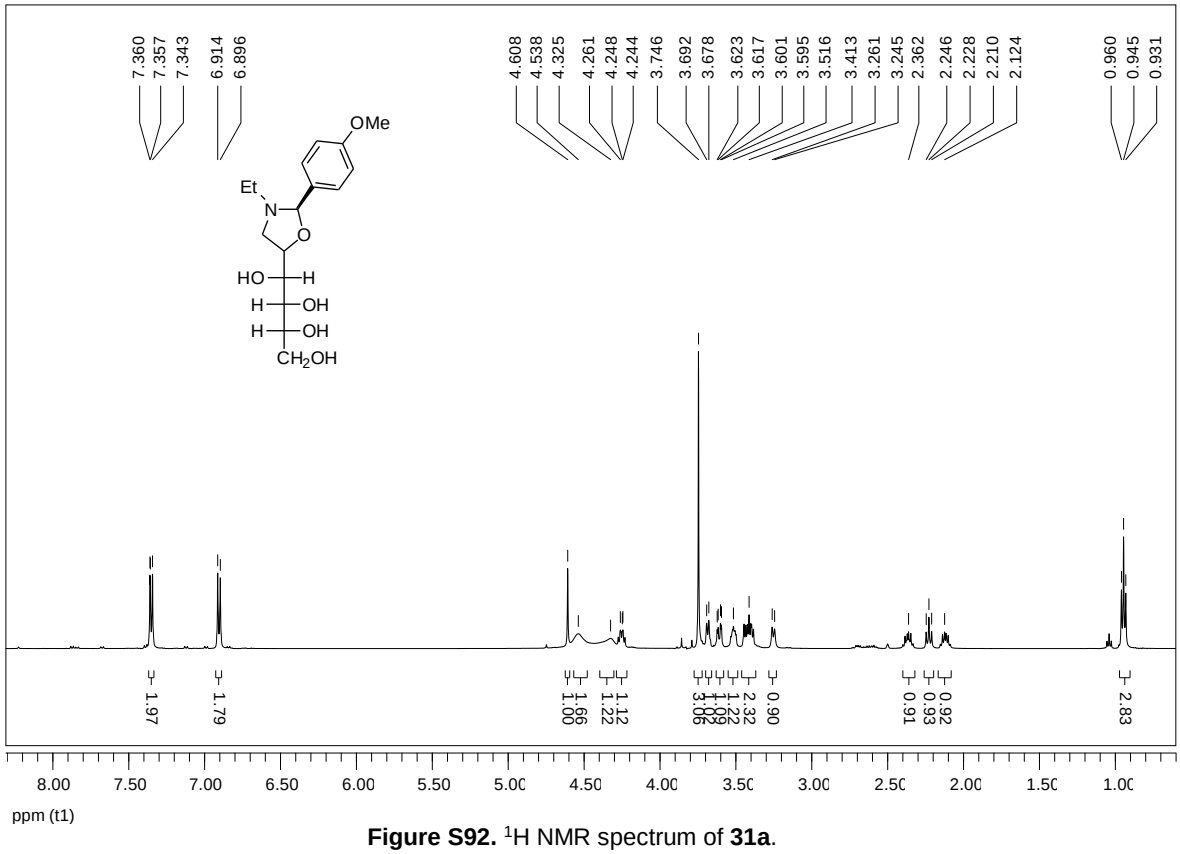


Figure S92. ^{1}H NMR spectrum of **31a**.

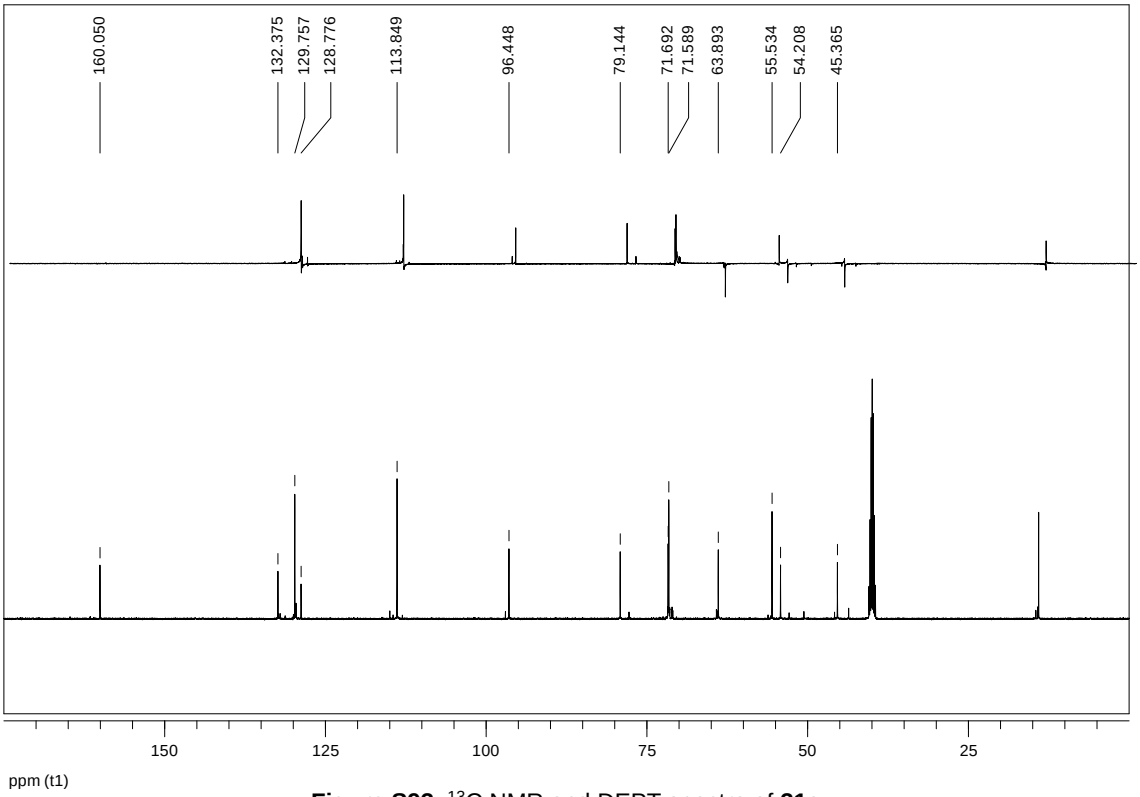


Figure S93. ^{13}C NMR and DEPT spectra of **31a**.

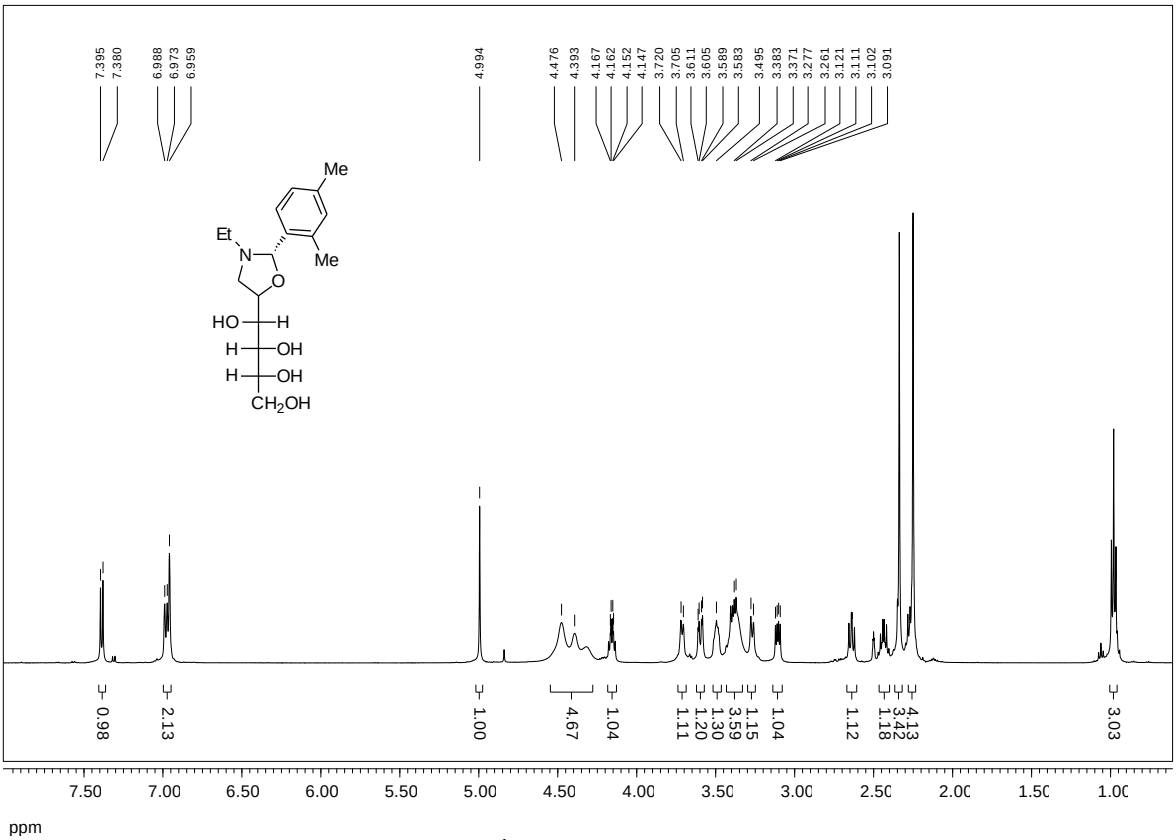


Figure S94. ^{1}H NMR spectrum of **32b**.

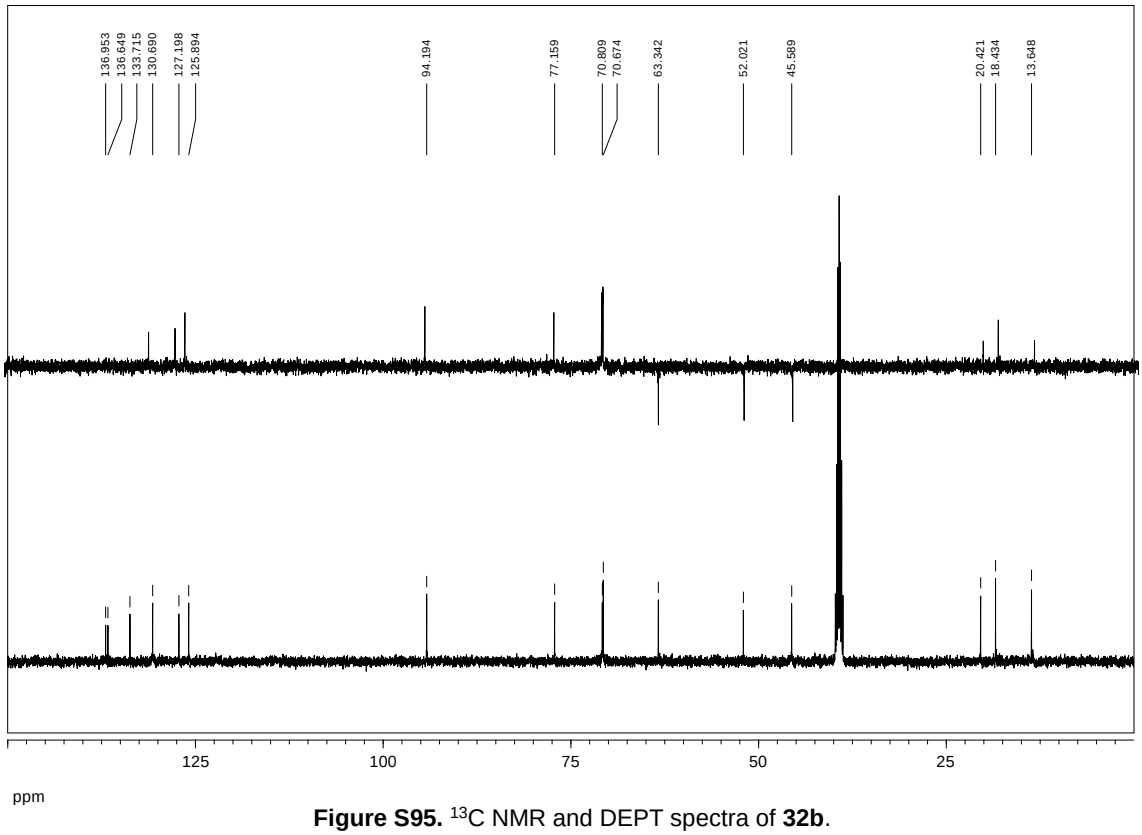


Figure S95. ^{13}C NMR and DEPT spectra of **32b**.

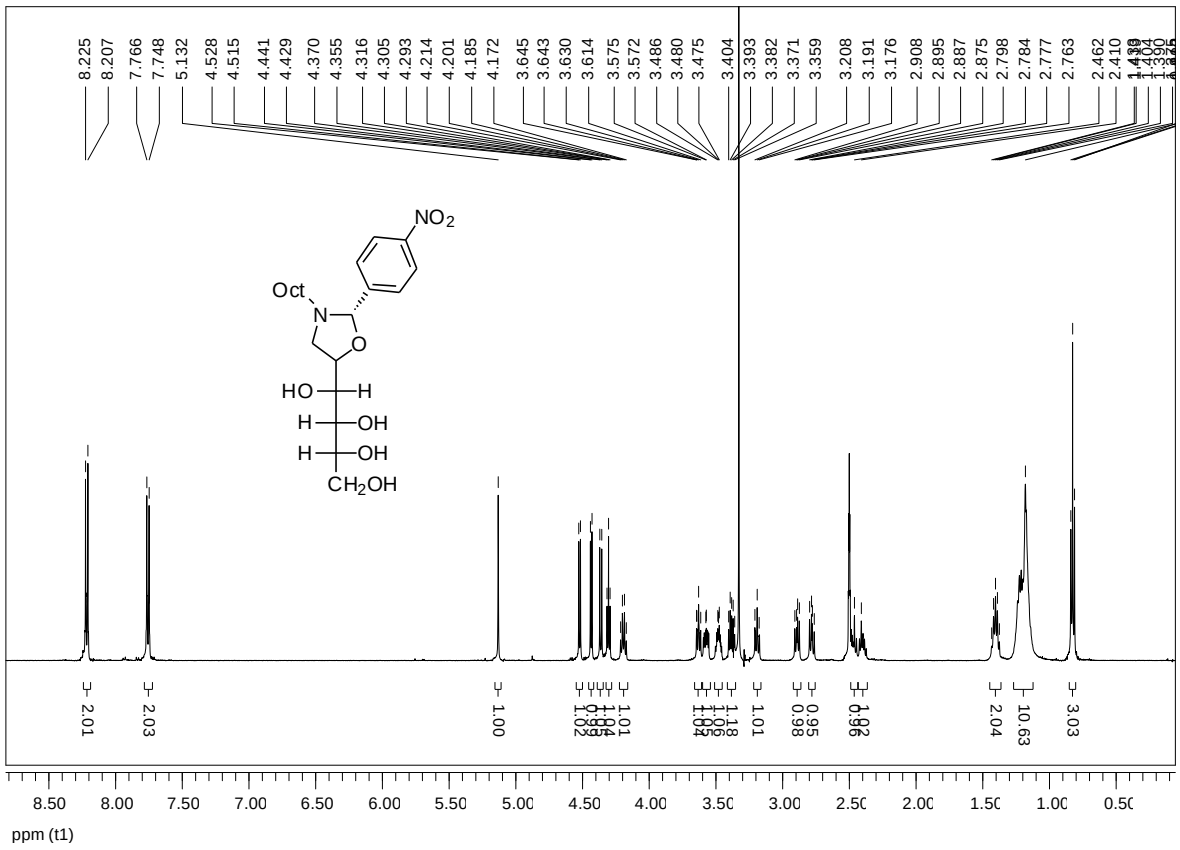


Figure S96. ^{1}H NMR spectrum of **34b**.

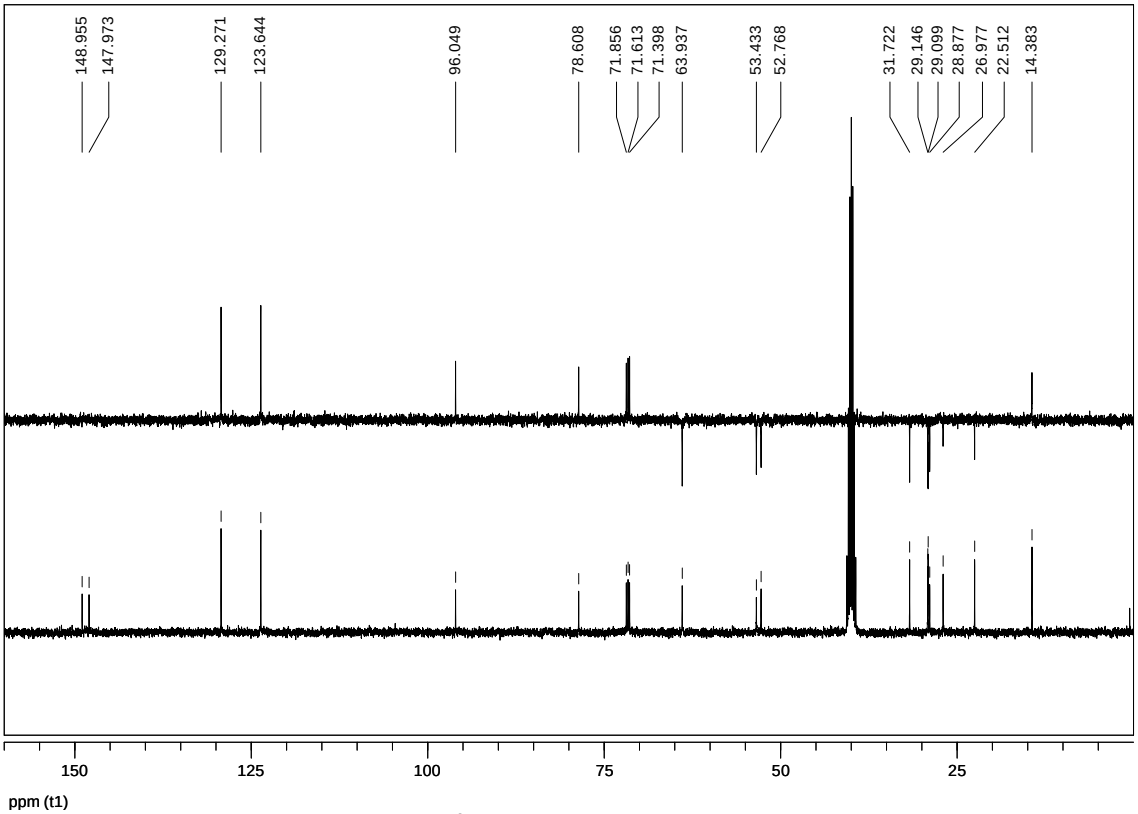


Figure S97. ^{13}C NMR and DEPT spectra of **34b**.

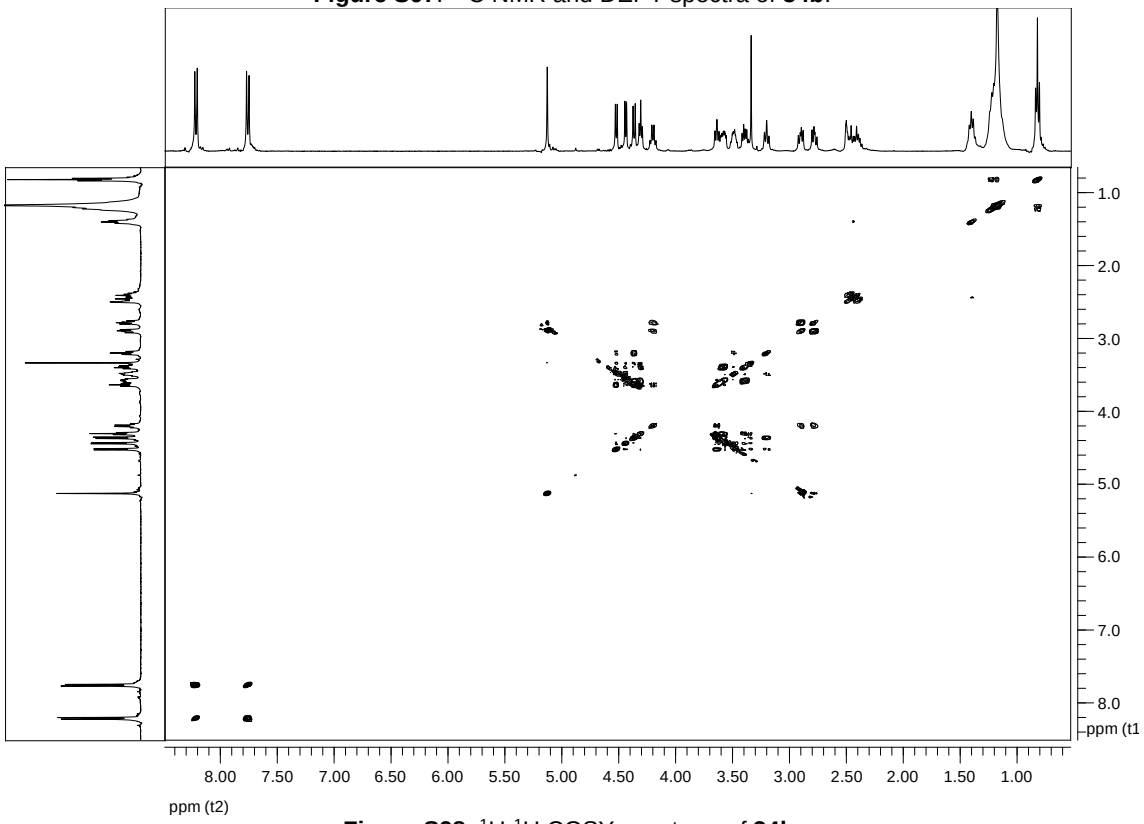


Figure S98. ^{1}H-^{1}H COSY spectrum of **34b**.

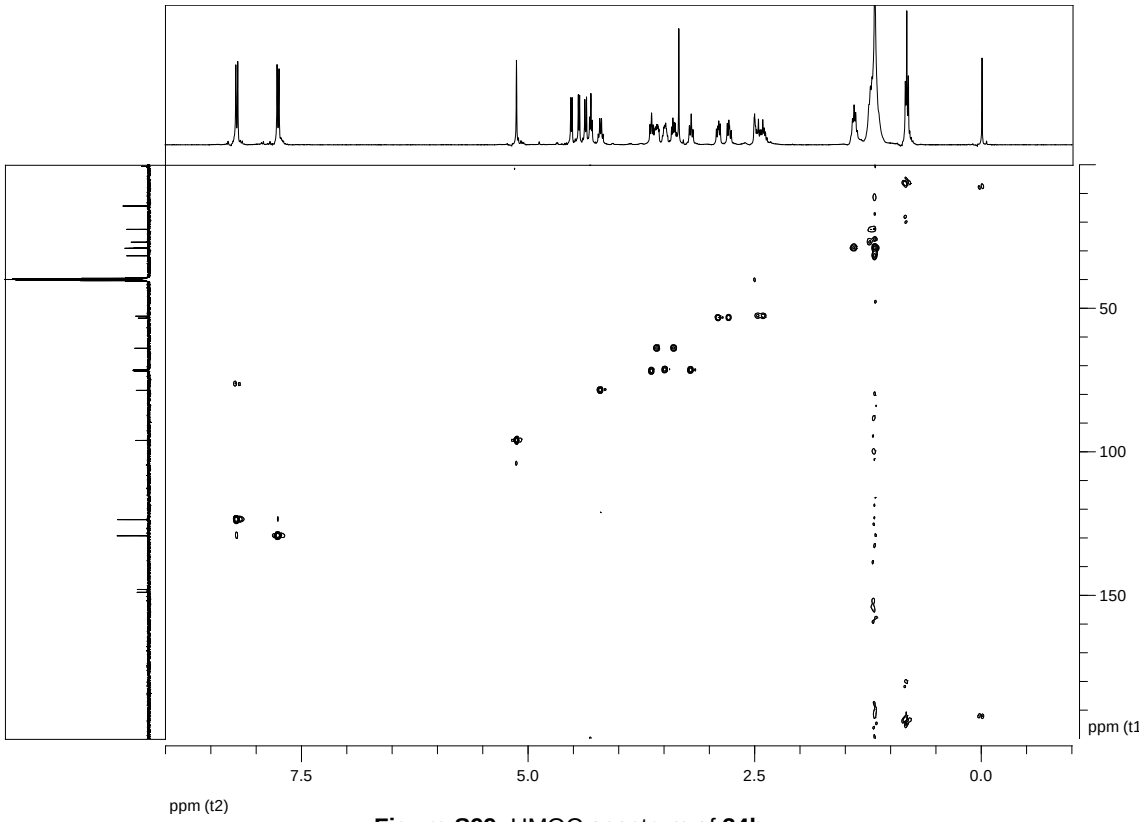


Figure S99. HMQC spectrum of **34b**.

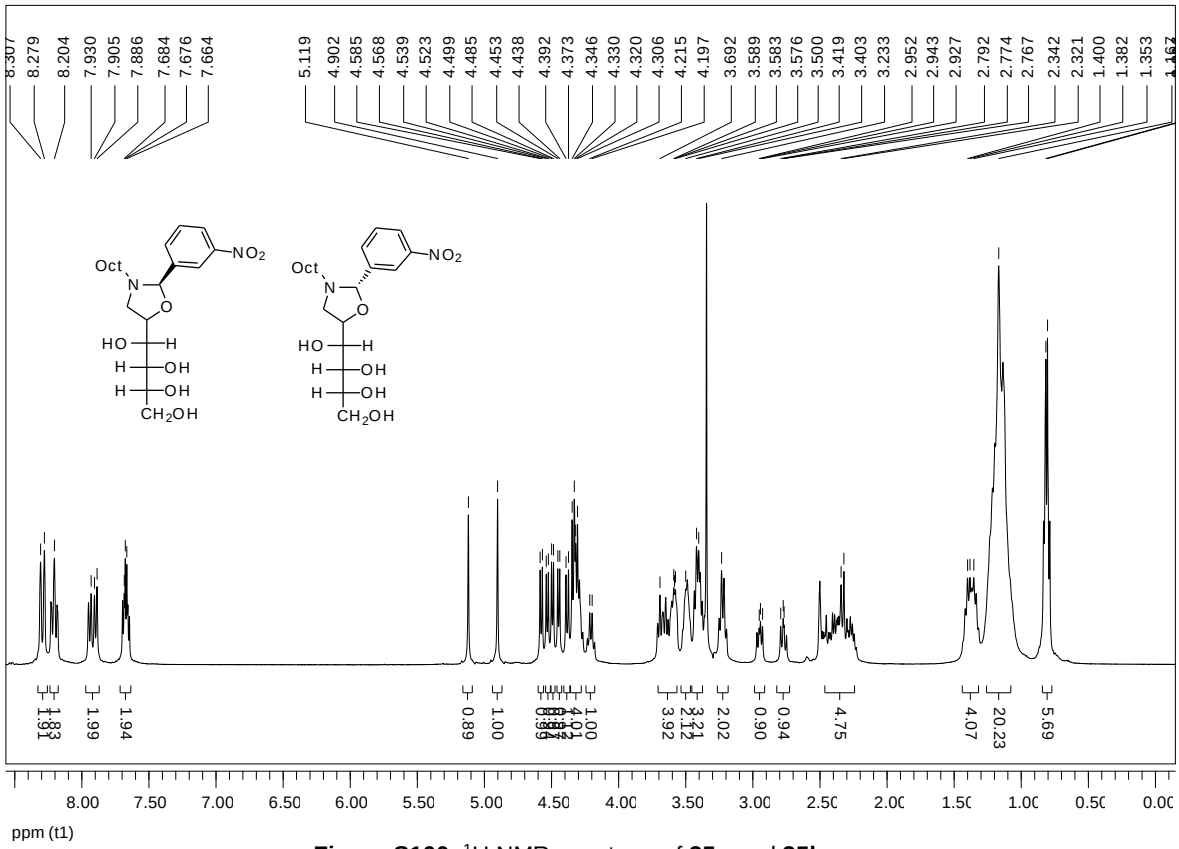


Figure S100. ^{1}H NMR spectrum of **35a** and **35b.**

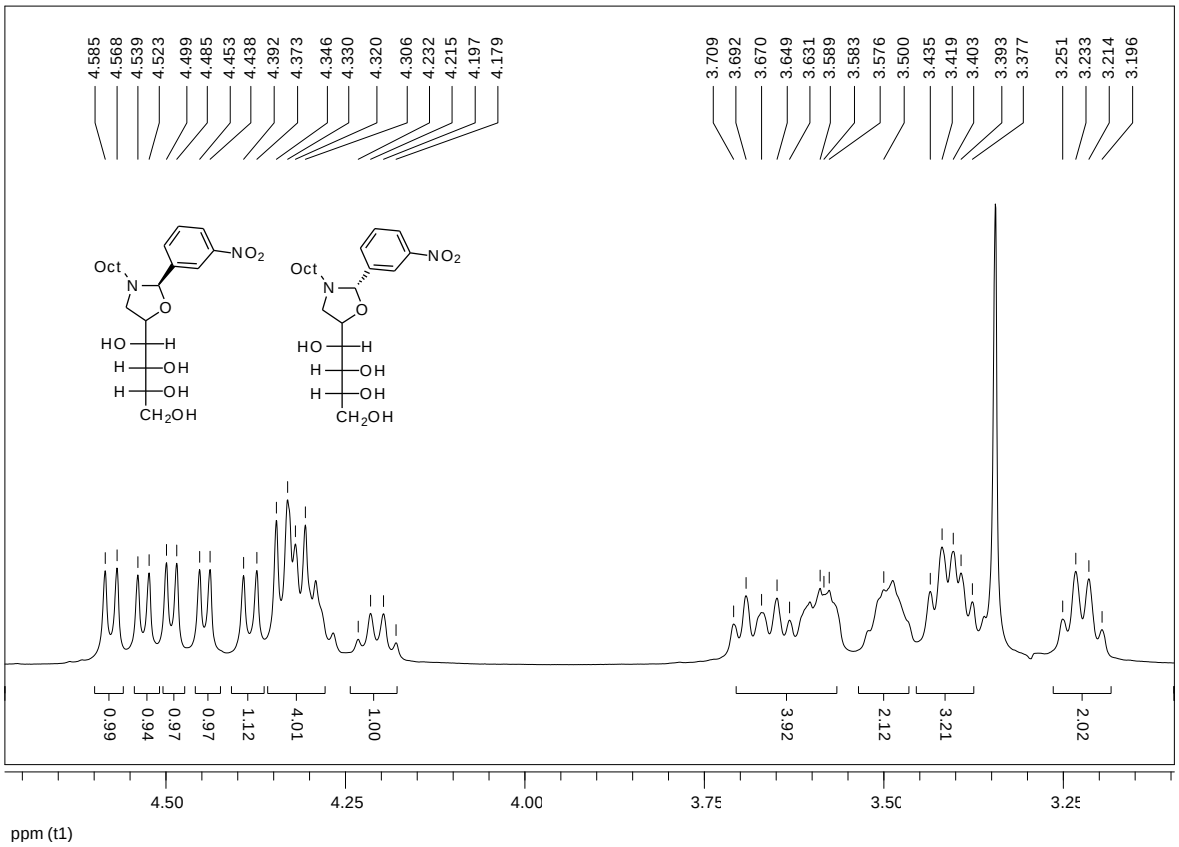


Figure S101. ^{1}H NMR spectrum of **35a** and **35b**

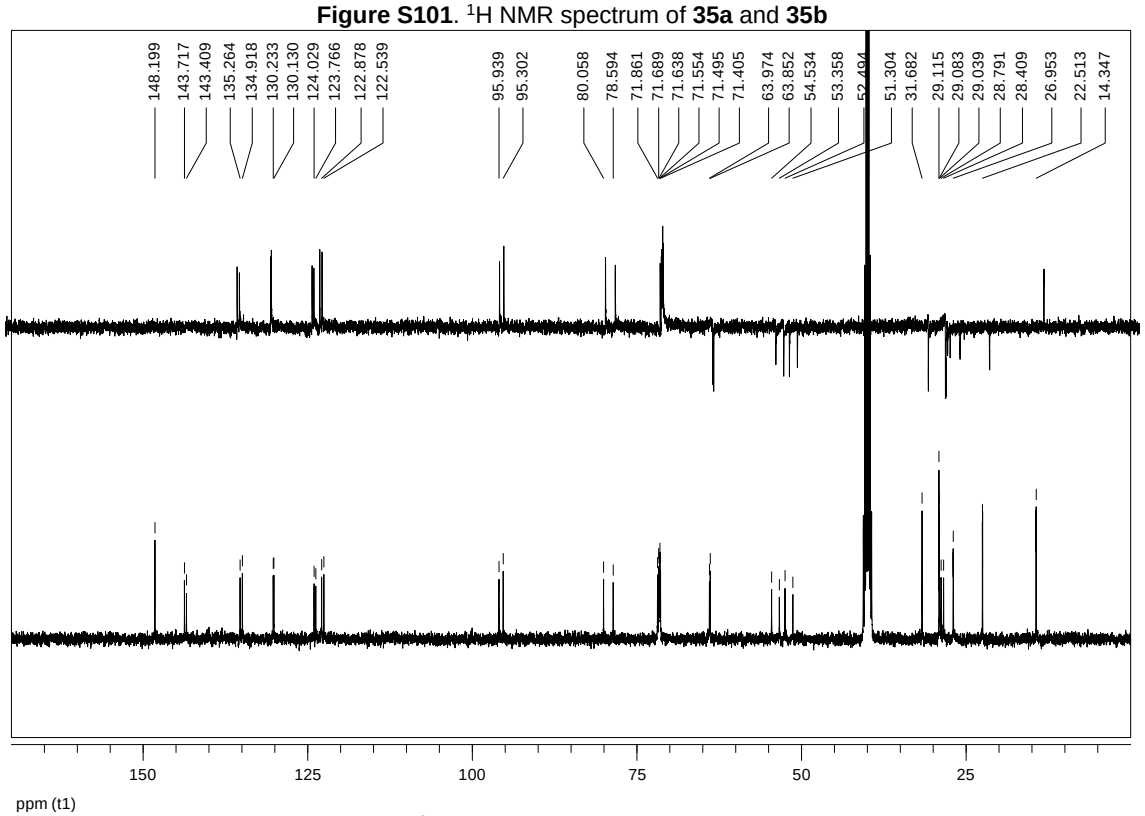


Figure S102. ^{13}C NMR and DEPT spectra of **35a** and **35b**.

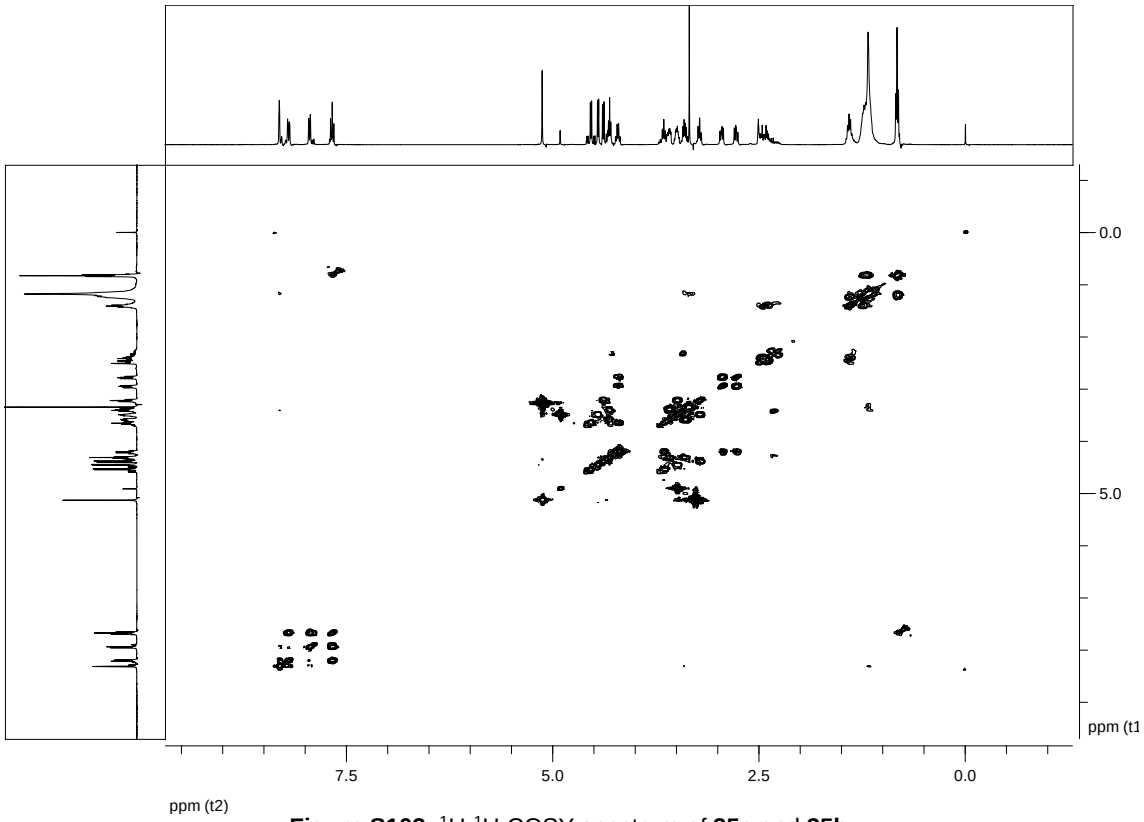


Figure S103. ^{1}H-^{1}H COSY spectrum of **35a** and **35b**.

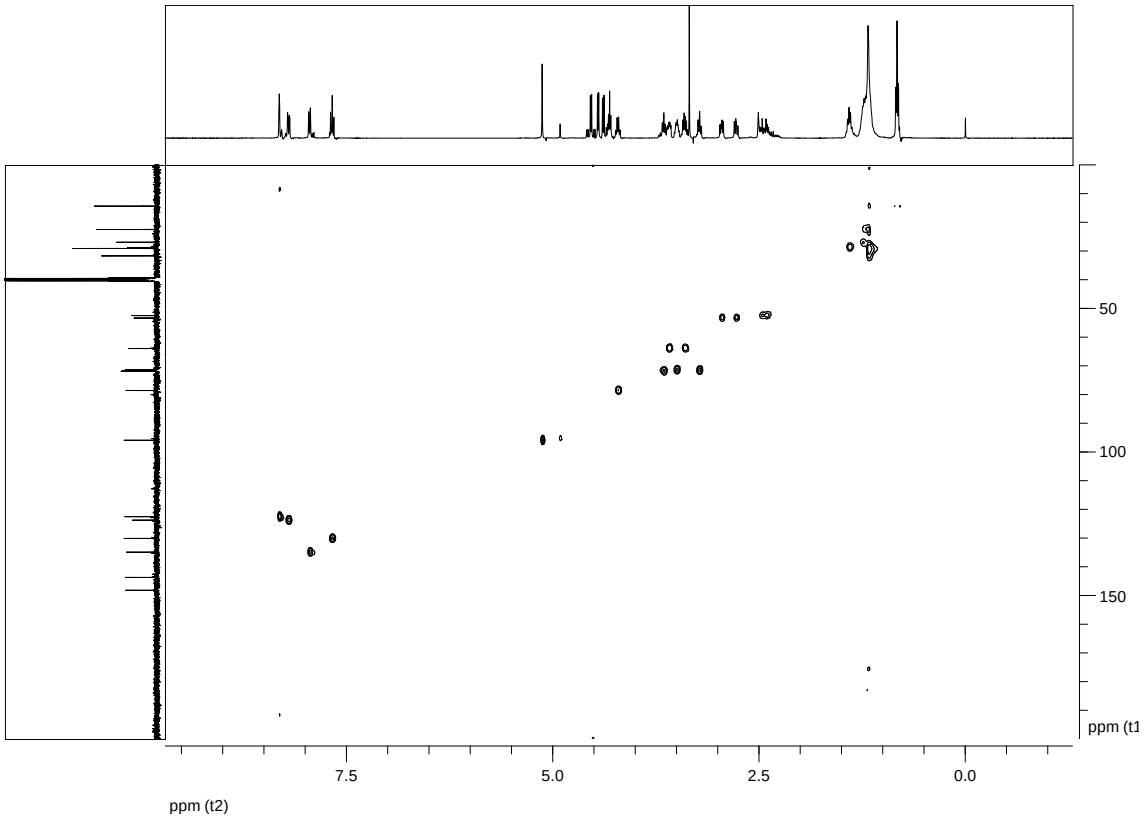


Figure S104. HMQC spectrum of **35a** and **35b**.

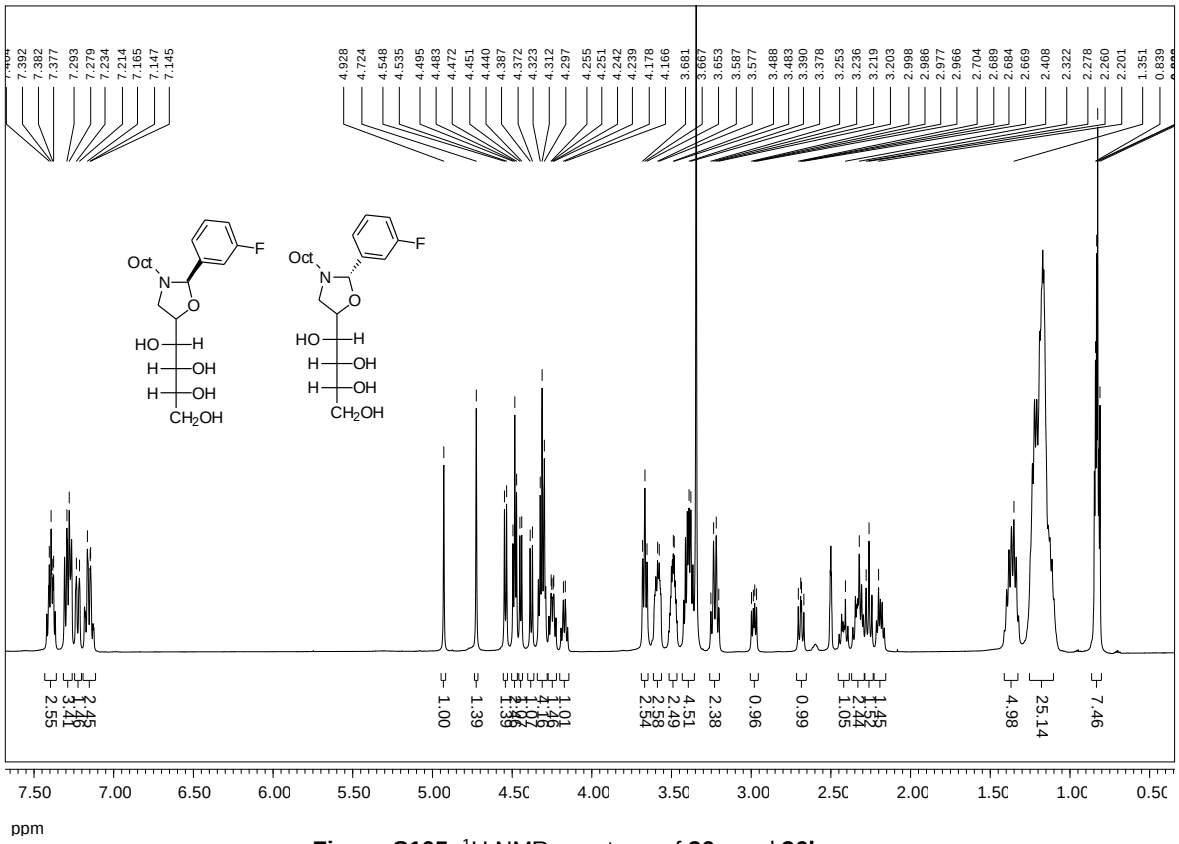


Figure S105. ^{1}H NMR spectrum of **36a** and **36b**.

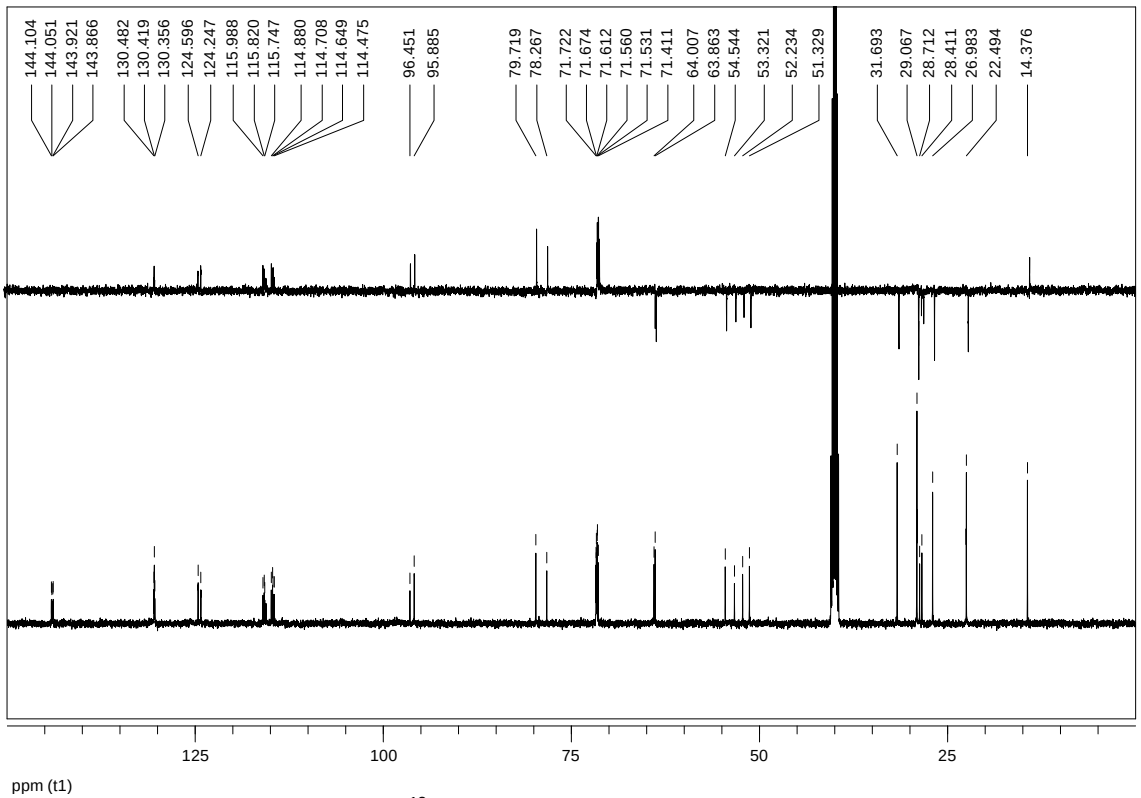


Figure S106. ^{13}C NMR and DEPT spectra of **36a** and **36b**.

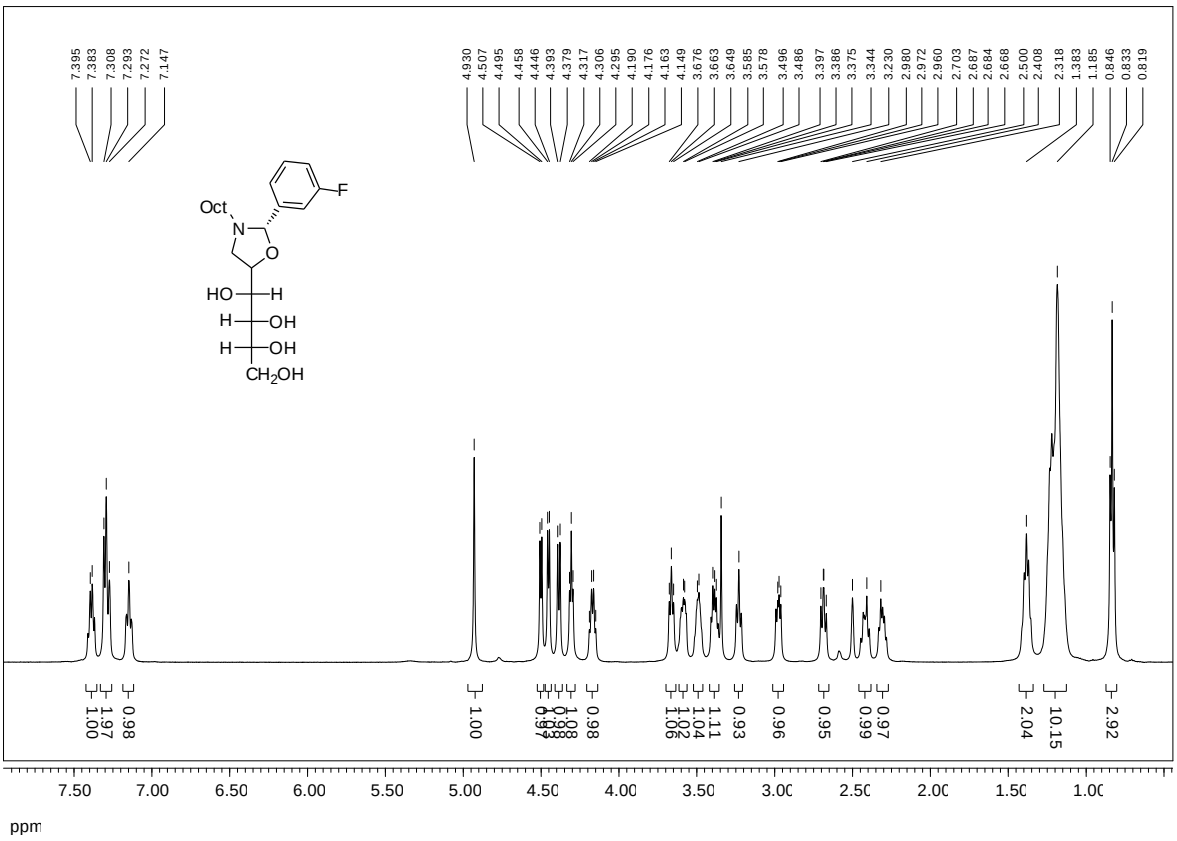


Figure S107. ^{1}H NMR spectrum of **36b**.

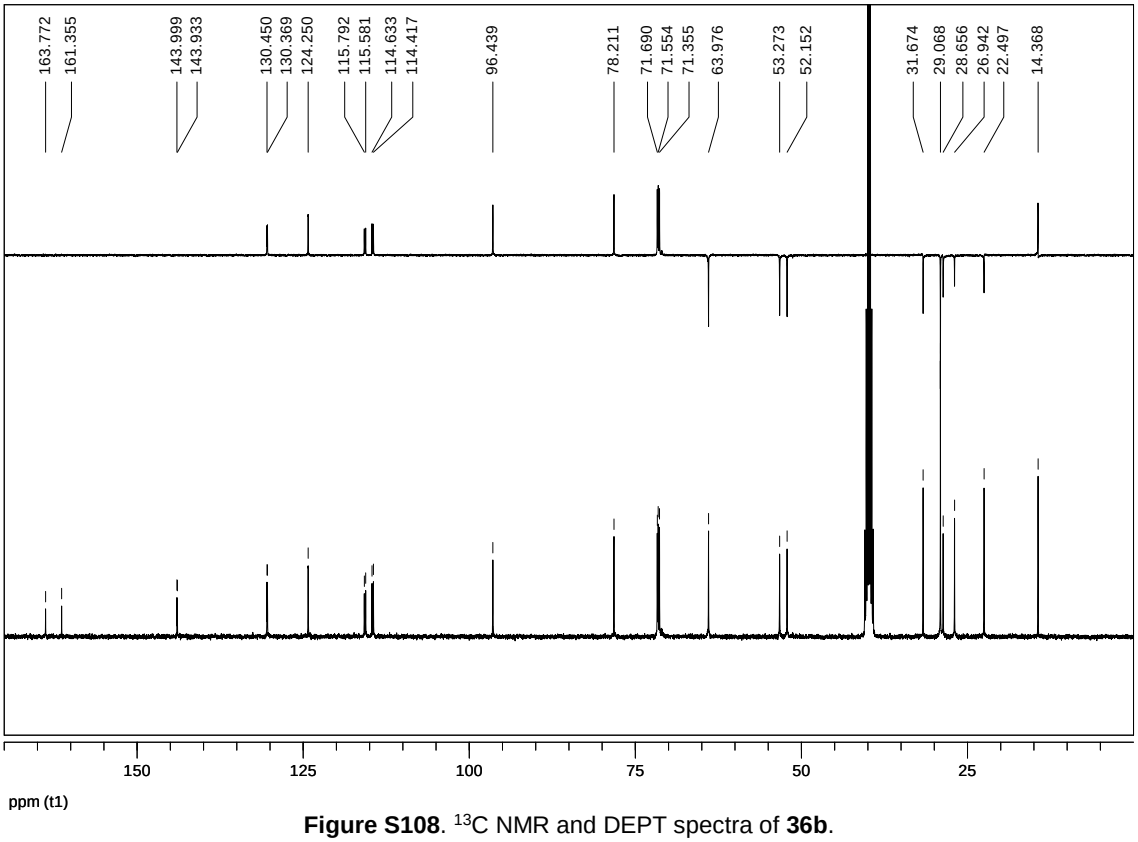


Figure S108. ^{13}C NMR and DEPT spectra of **36b**.

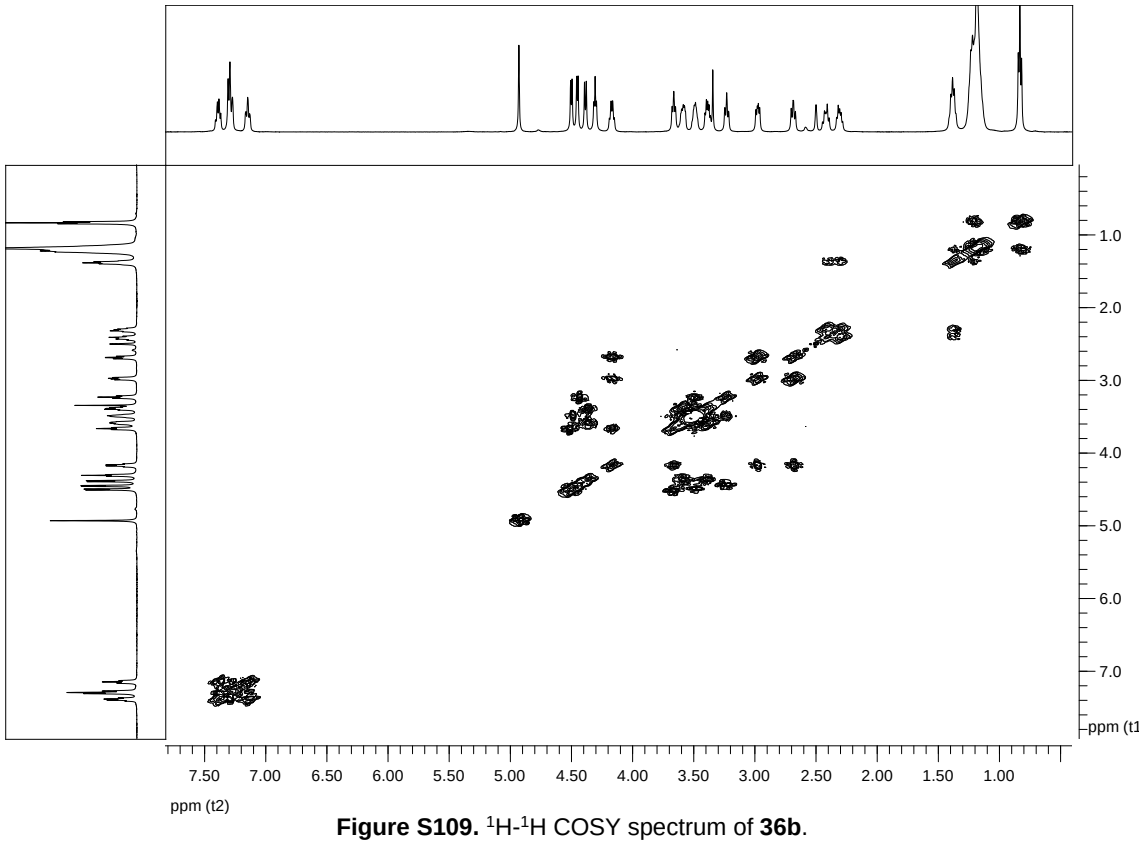


Figure S109. ^{1}H-^{1}H COSY spectrum of **36b**.

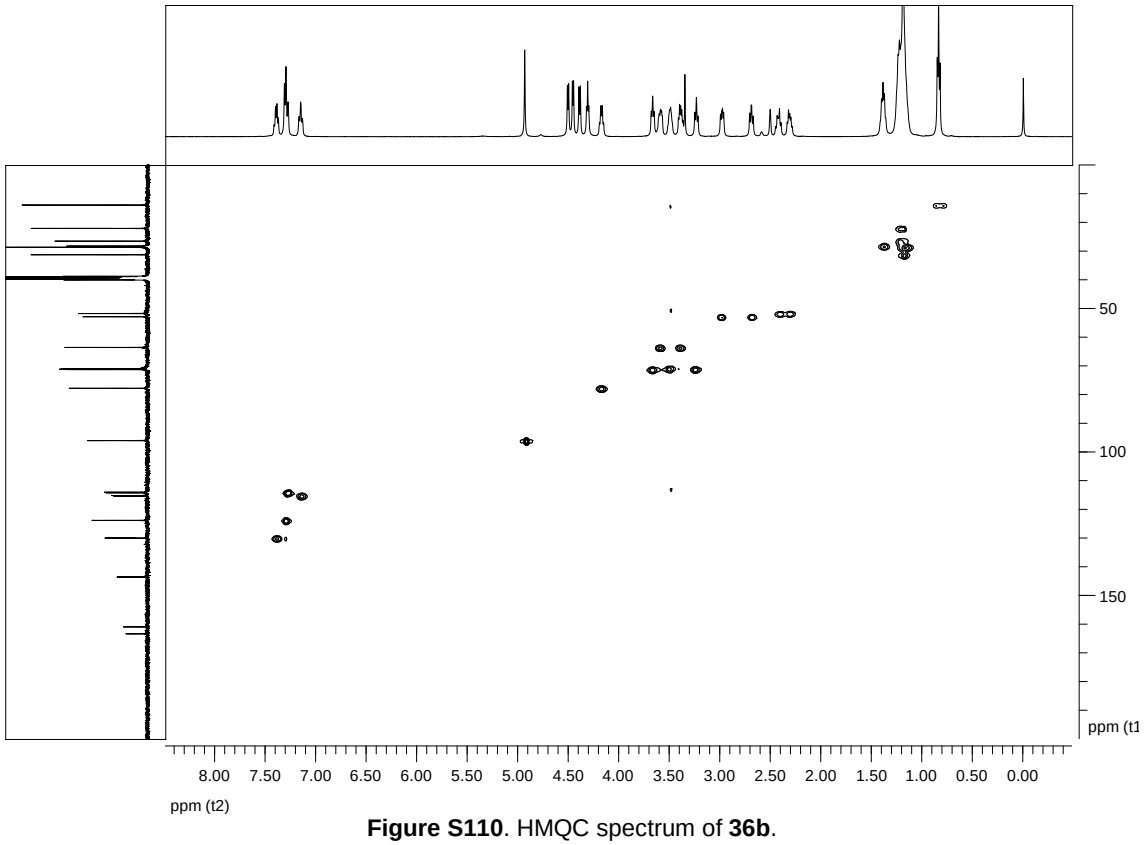


Figure S110. HMQC spectrum of **36b**.

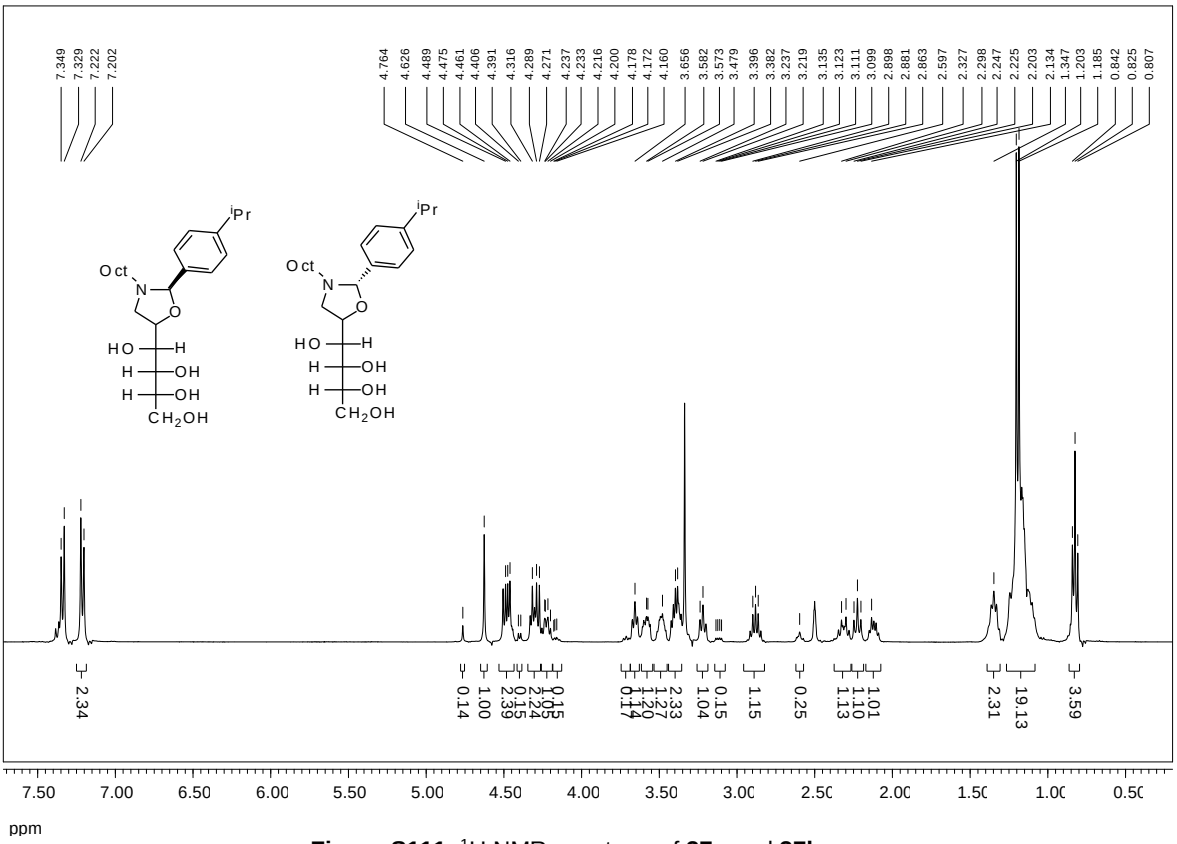


Figure S111. ^{1}H NMR spectrum of **37a** and **37b**.

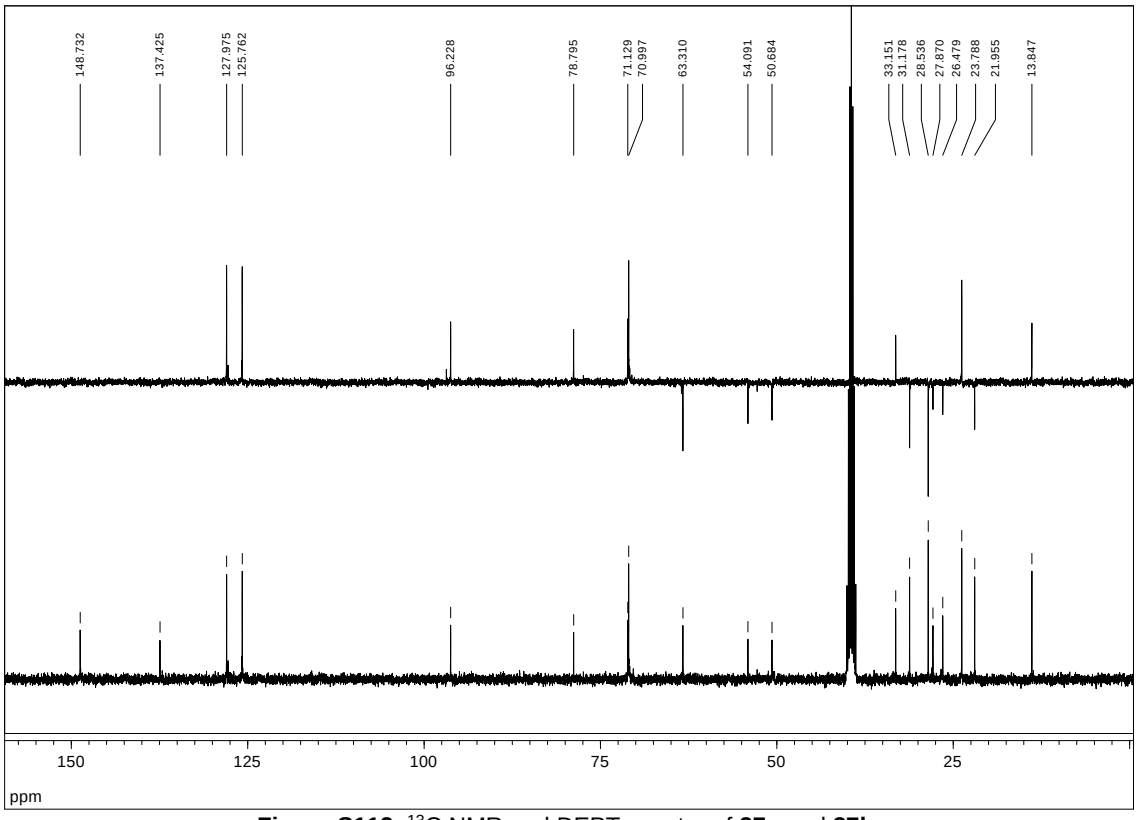


Figure S112. ^{13}C NMR and DEPT spectra of **37a** and **37b**.

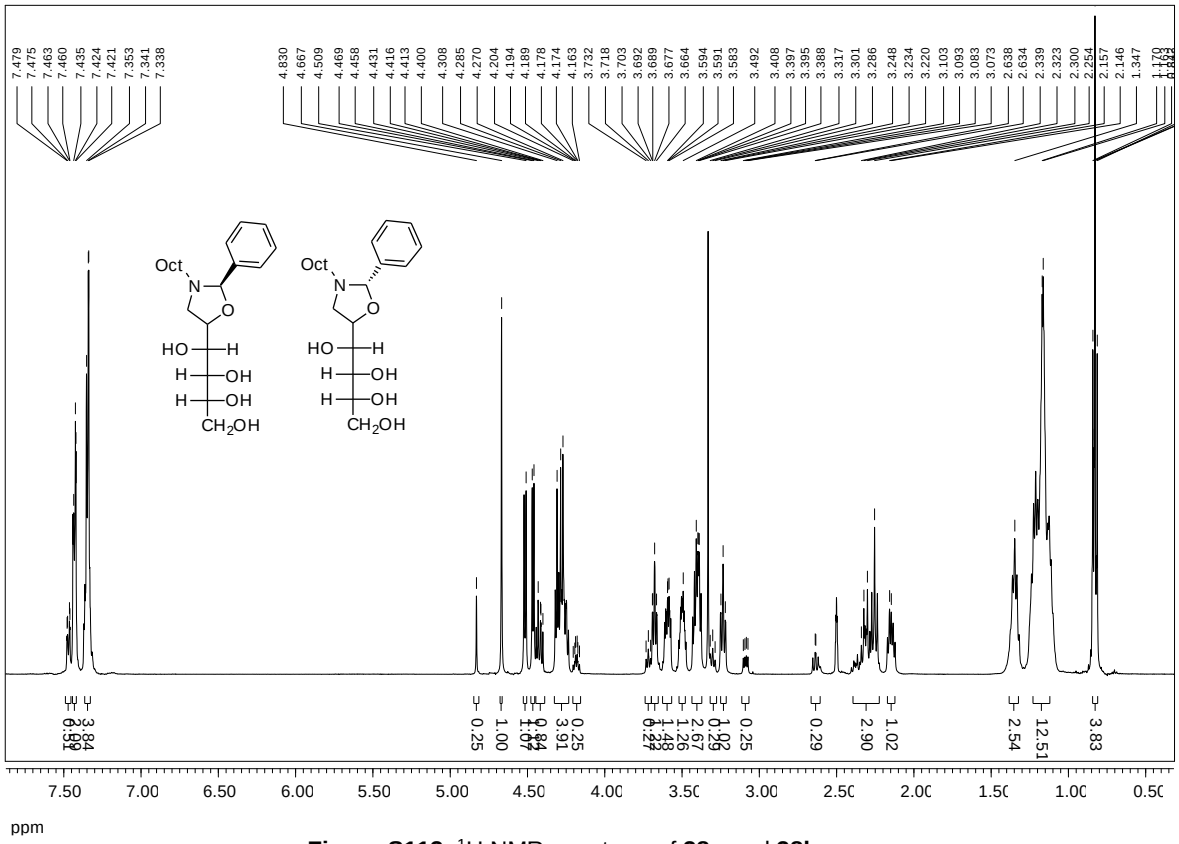


Figure S113. ^{1}H NMR spectrum of **38a** and **38b**.

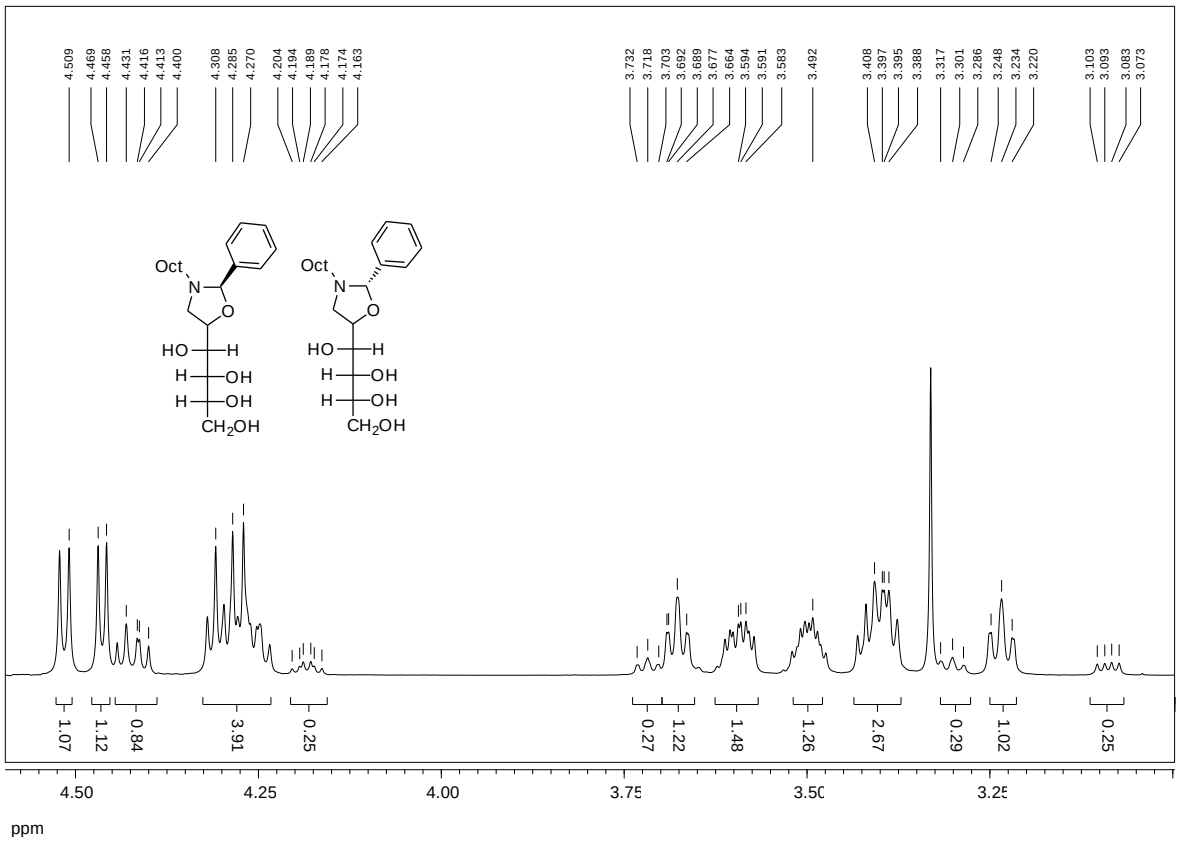


Figure S114. ^{1}H NMR spectrum of **38a** and **38b**

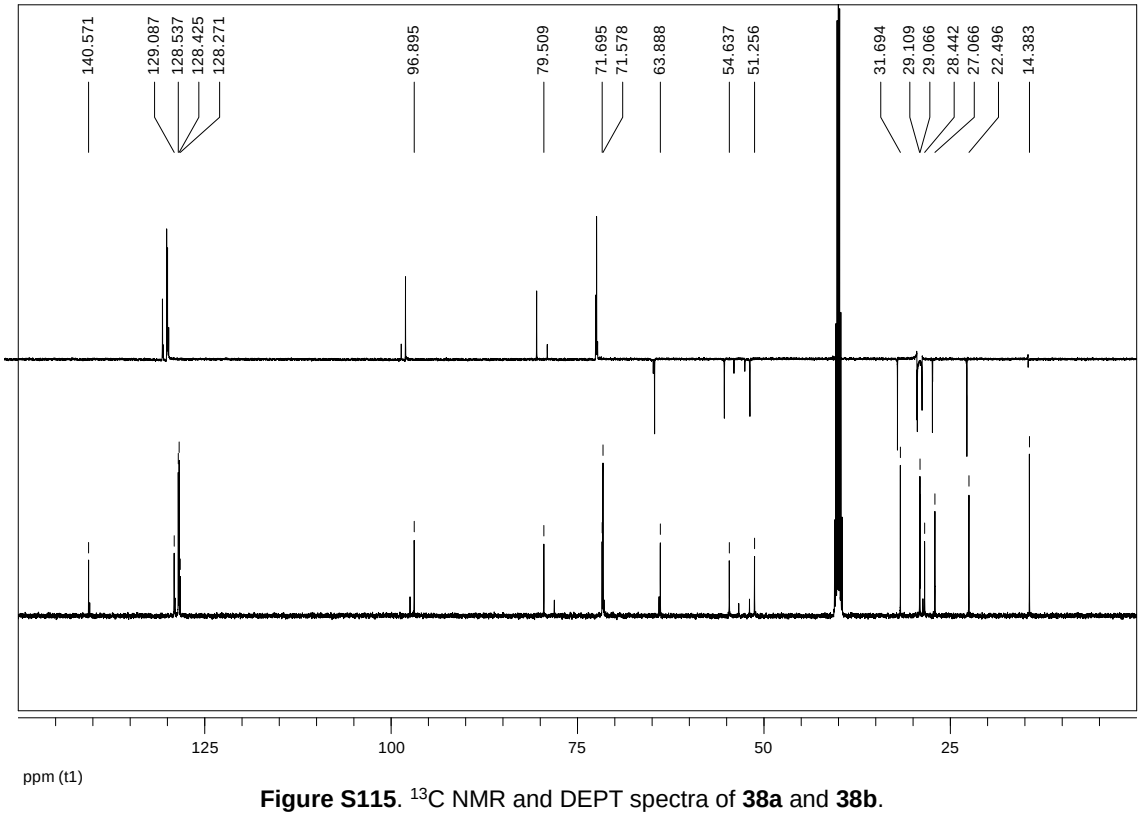


Figure S115. ^{13}C NMR and DEPT spectra of **38a** and **38b**.

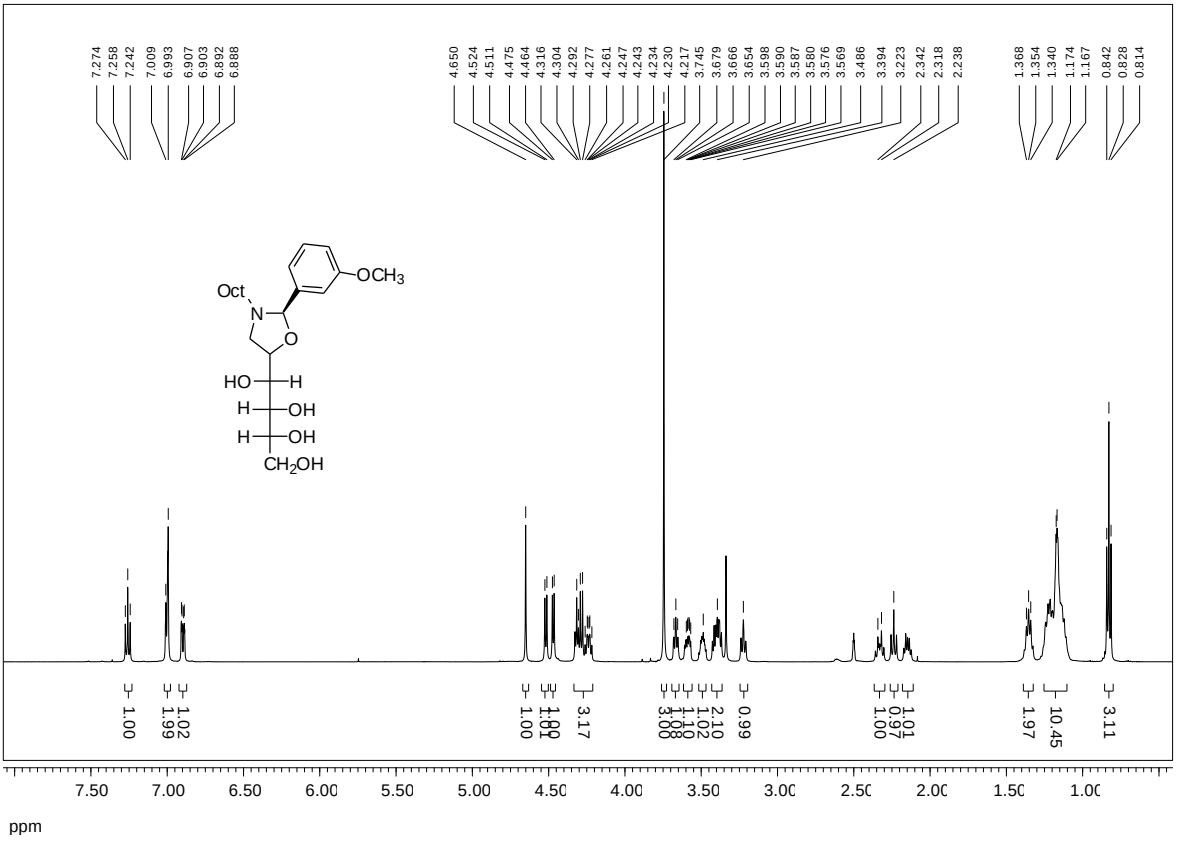


Figure S116. ^{1}H NMR spectrum of **39a**.

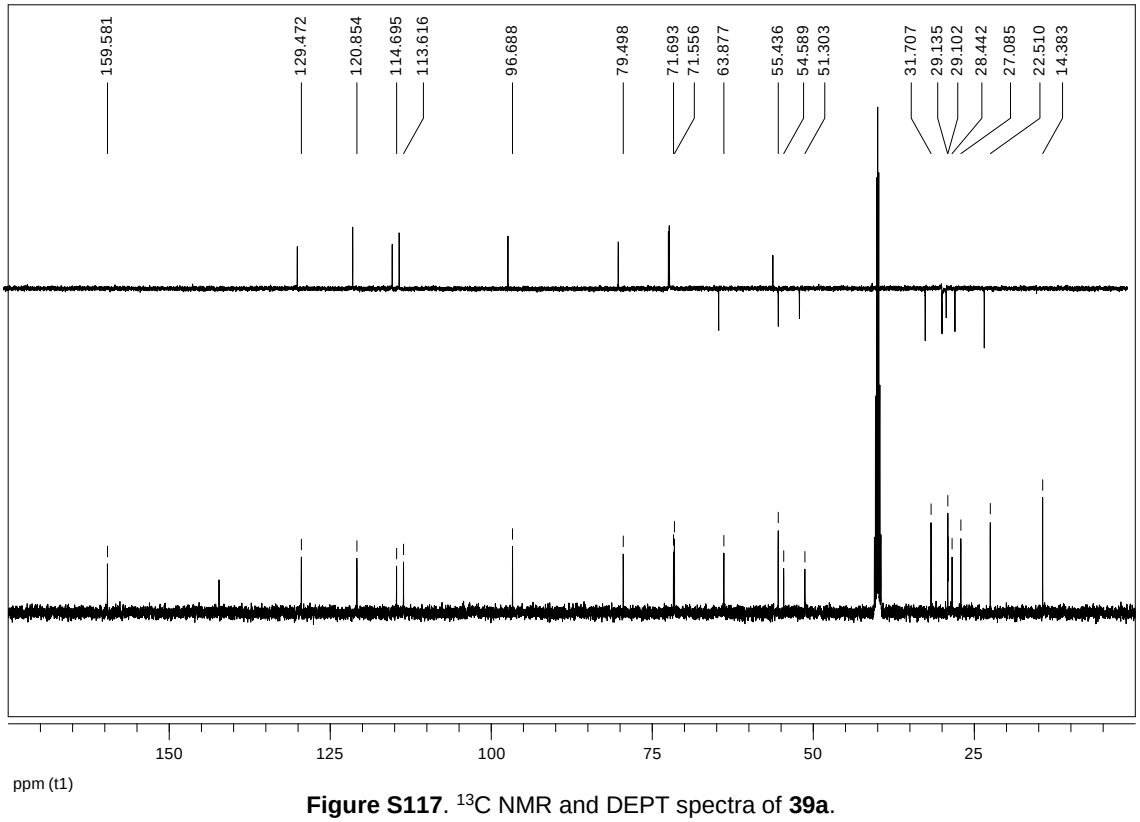


Figure S117. ^{13}C NMR and DEPT spectra of **39a**.

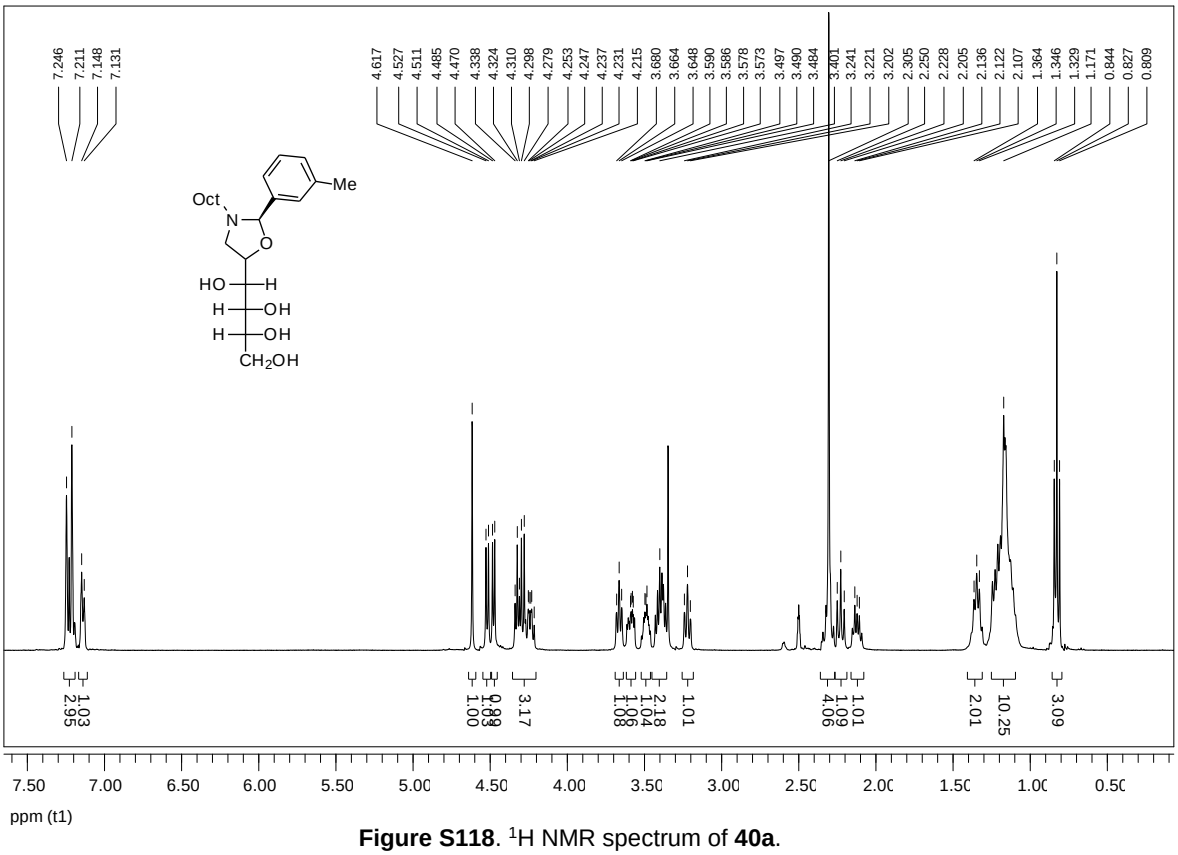


Figure S118. ^{1}H NMR spectrum of **40a**.

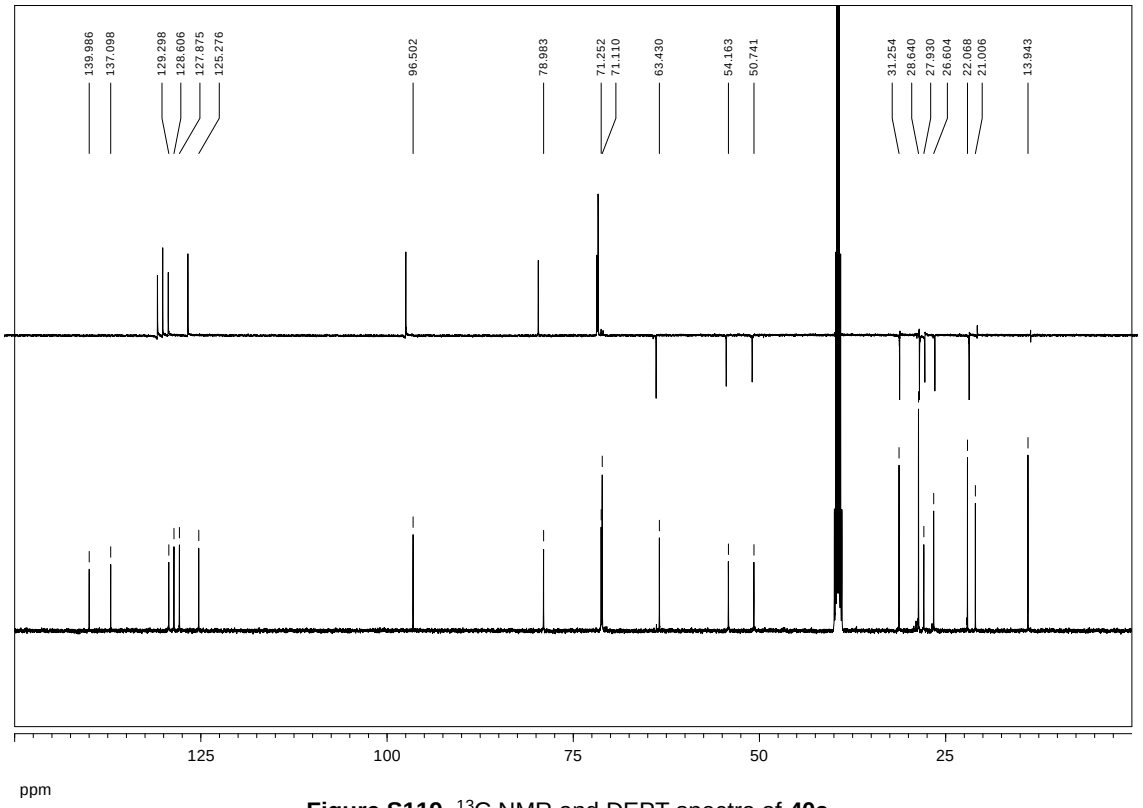


Figure S119. ^{13}C NMR and DEPT spectra of **40a**.

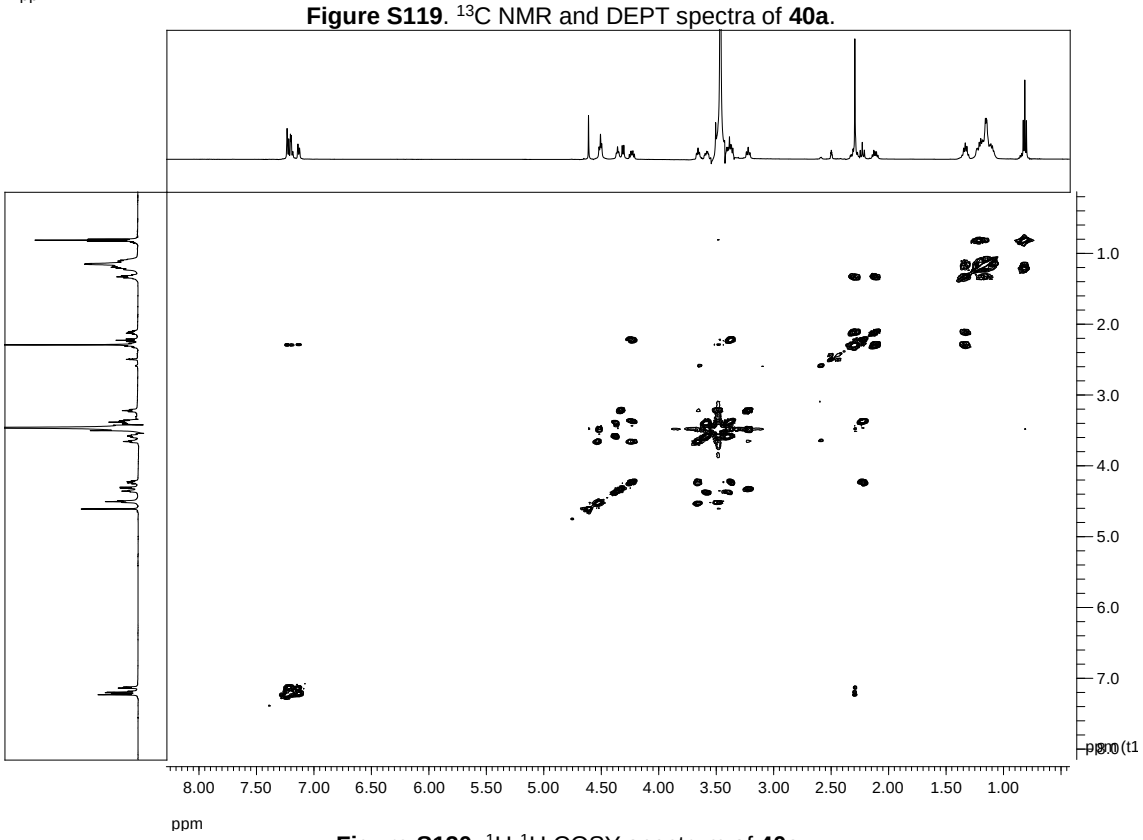


Figure S120. ^{1}H-^{1}H COSY spectrum of **40a**.

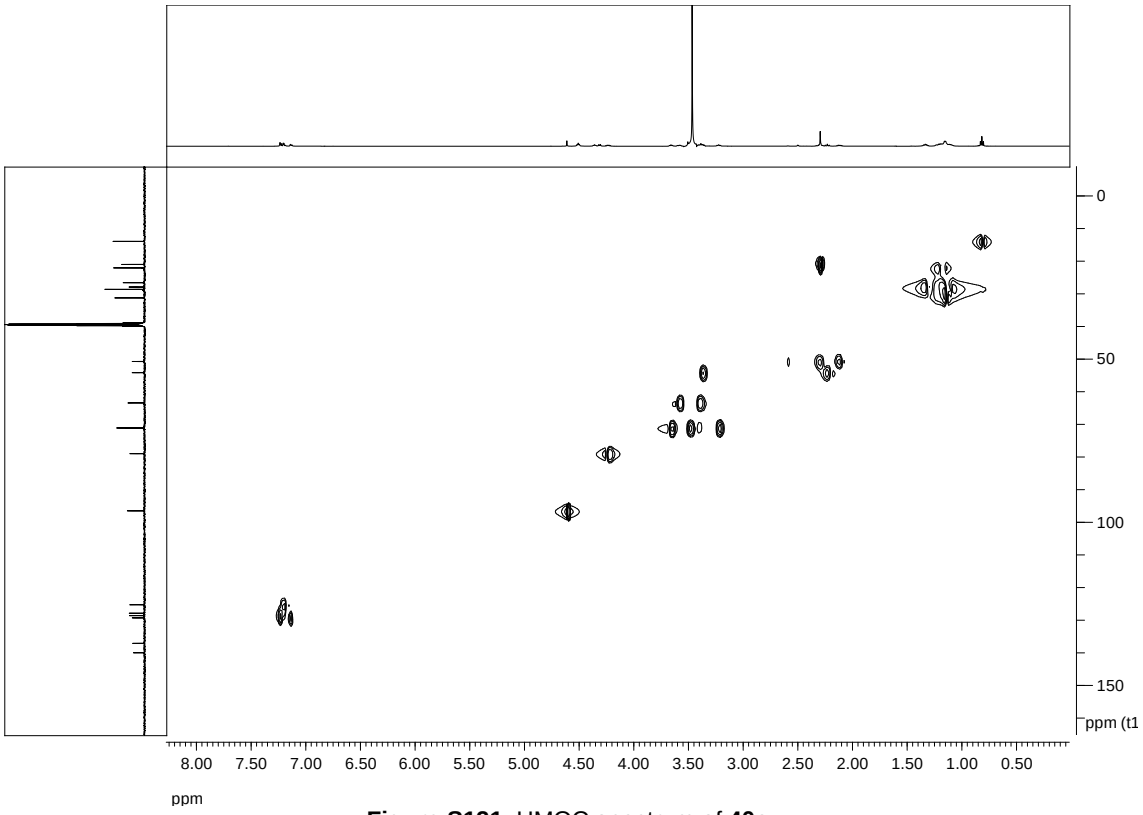


Figure S121. HMQC spectrum of **40a**.

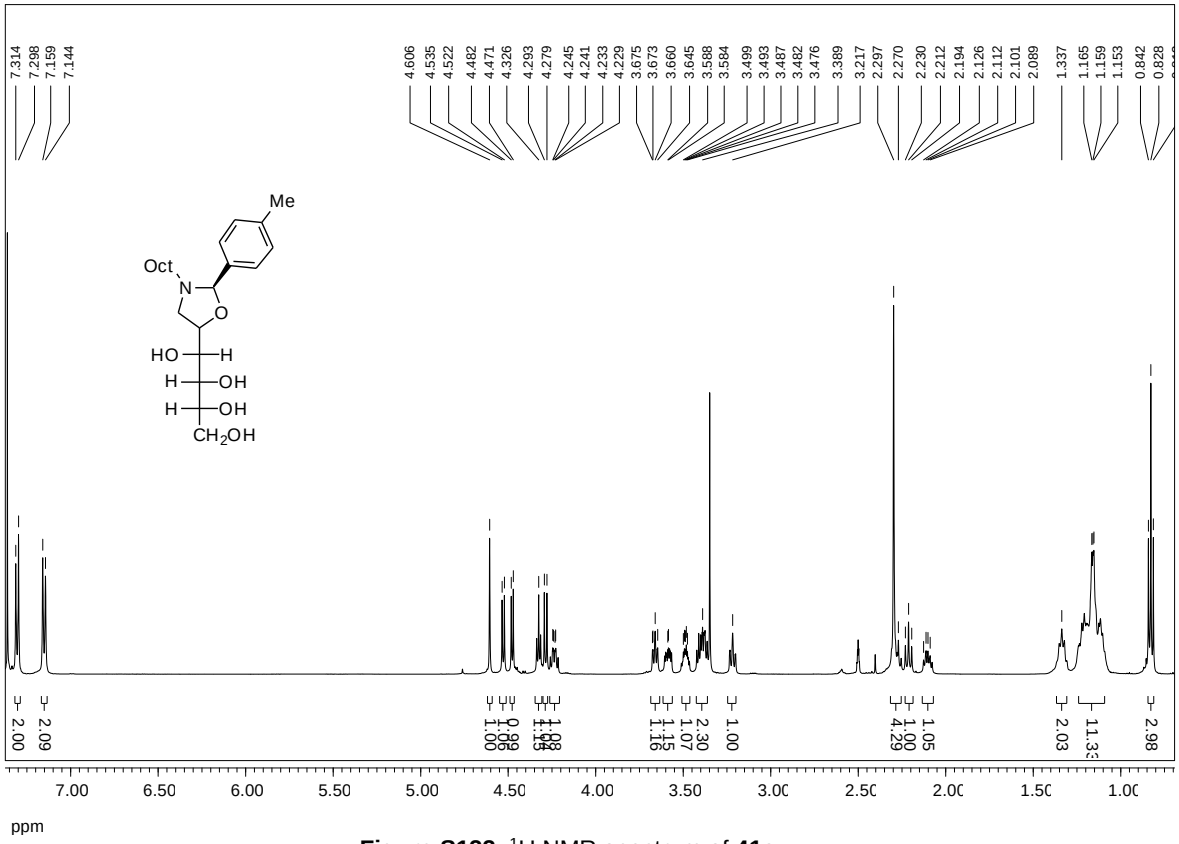


Figure S122. ^{1}H NMR spectrum of **41a**.

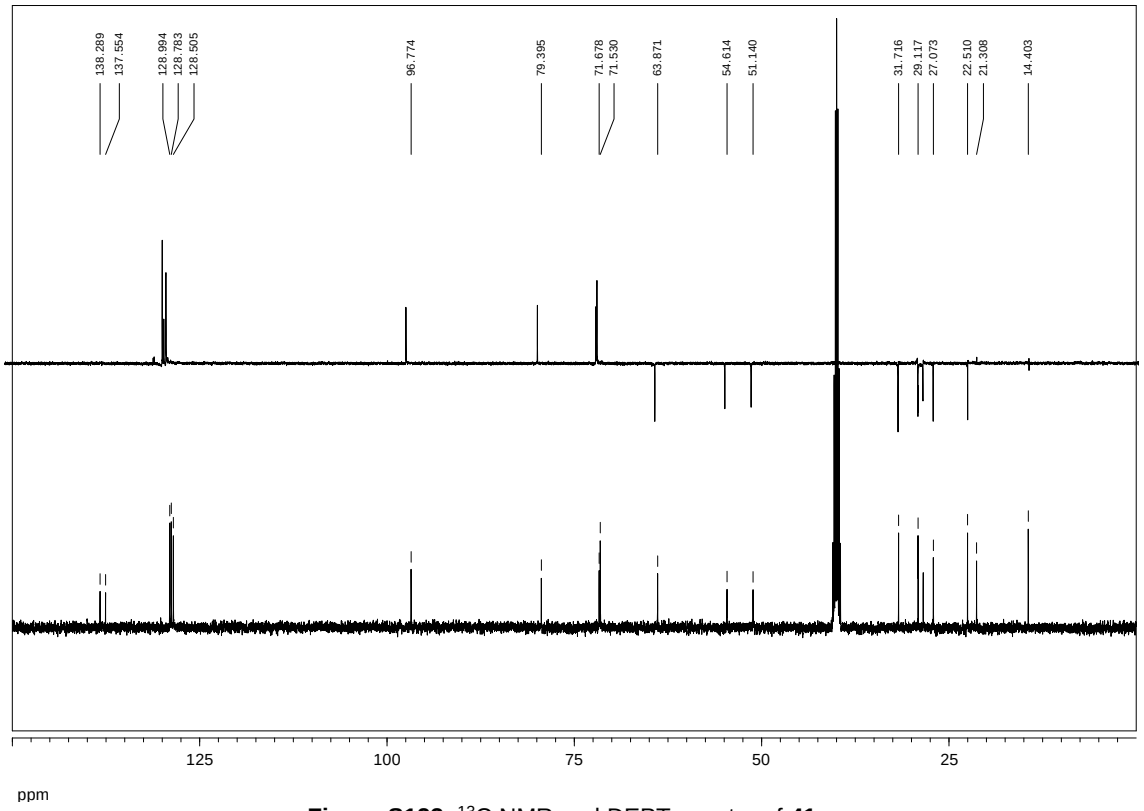


Figure S123. ^{13}C NMR and DEPT spectra of **41a**.

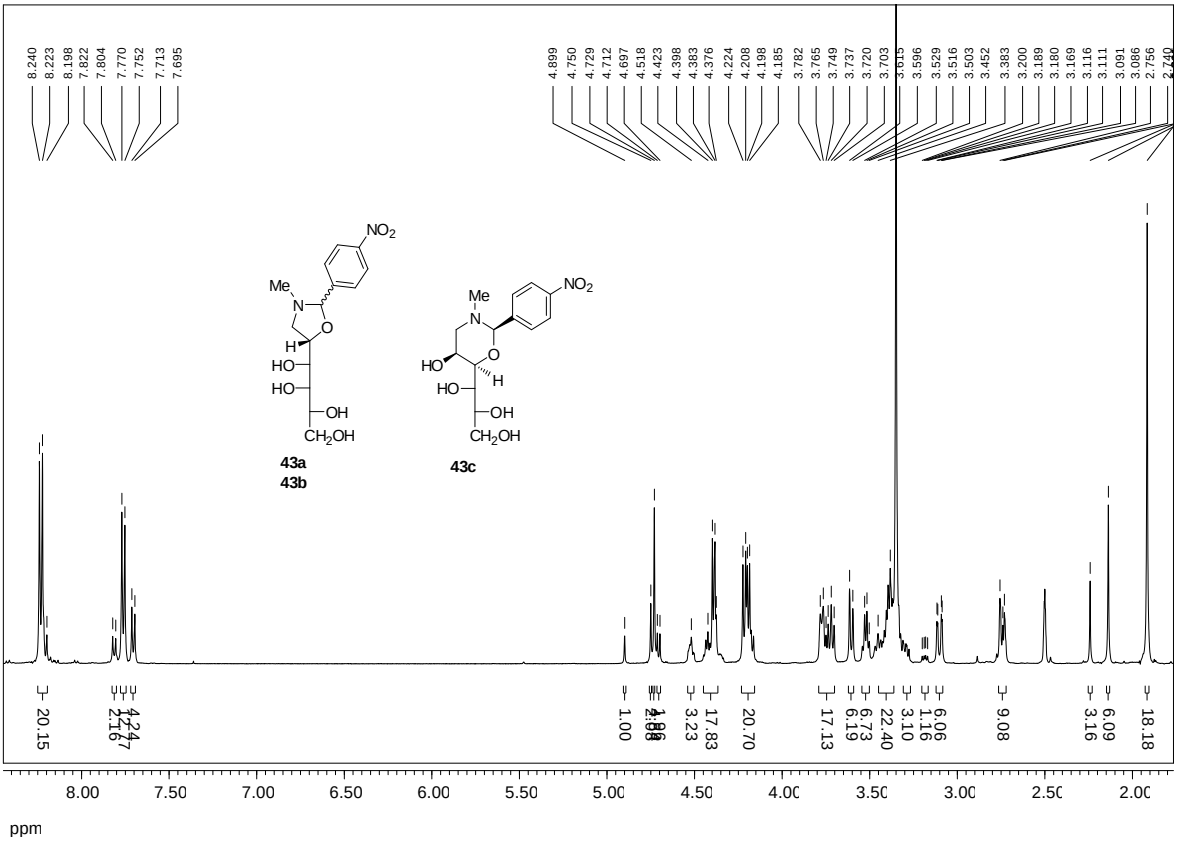


Figure S124. ^{1}H NMR spectrum of **43a**, **43b** and **43c**.

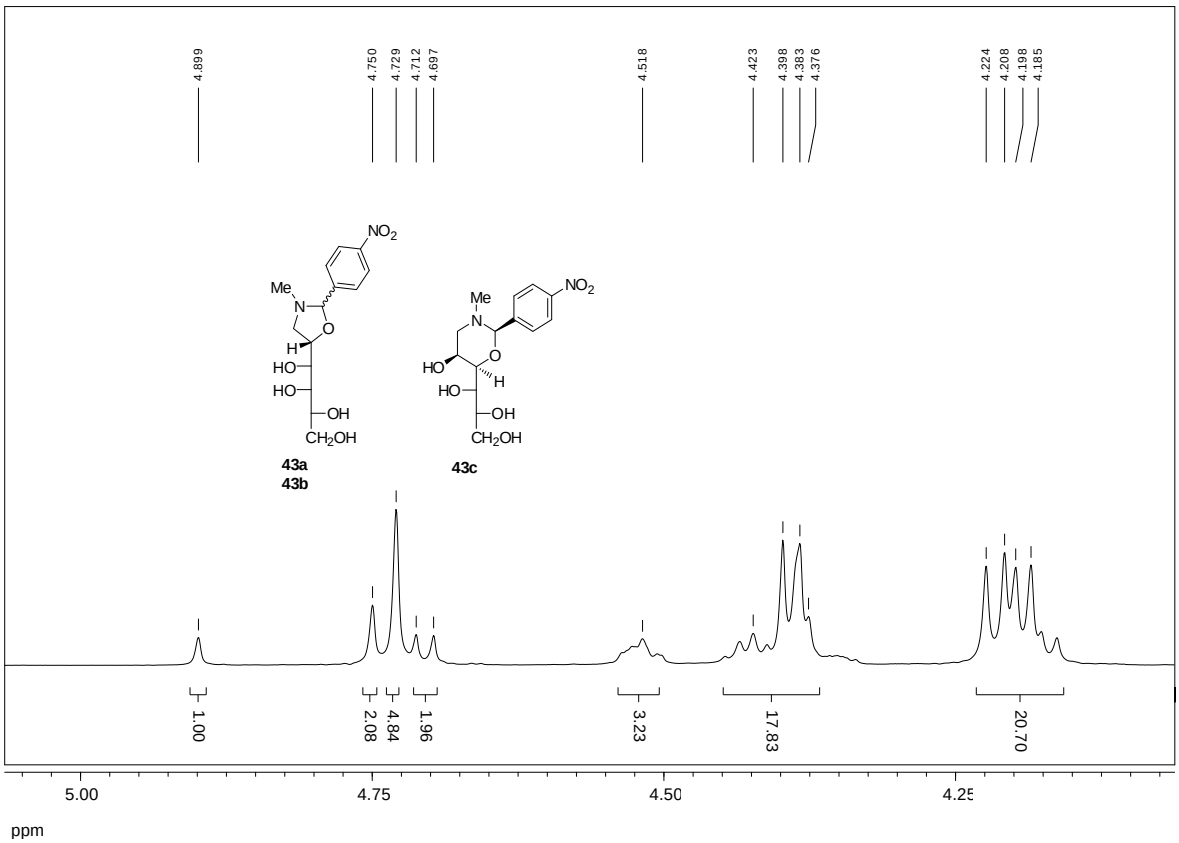


Figure S125. ^{1}H NMR spectrum of **43a**, **43b** and **43c**.

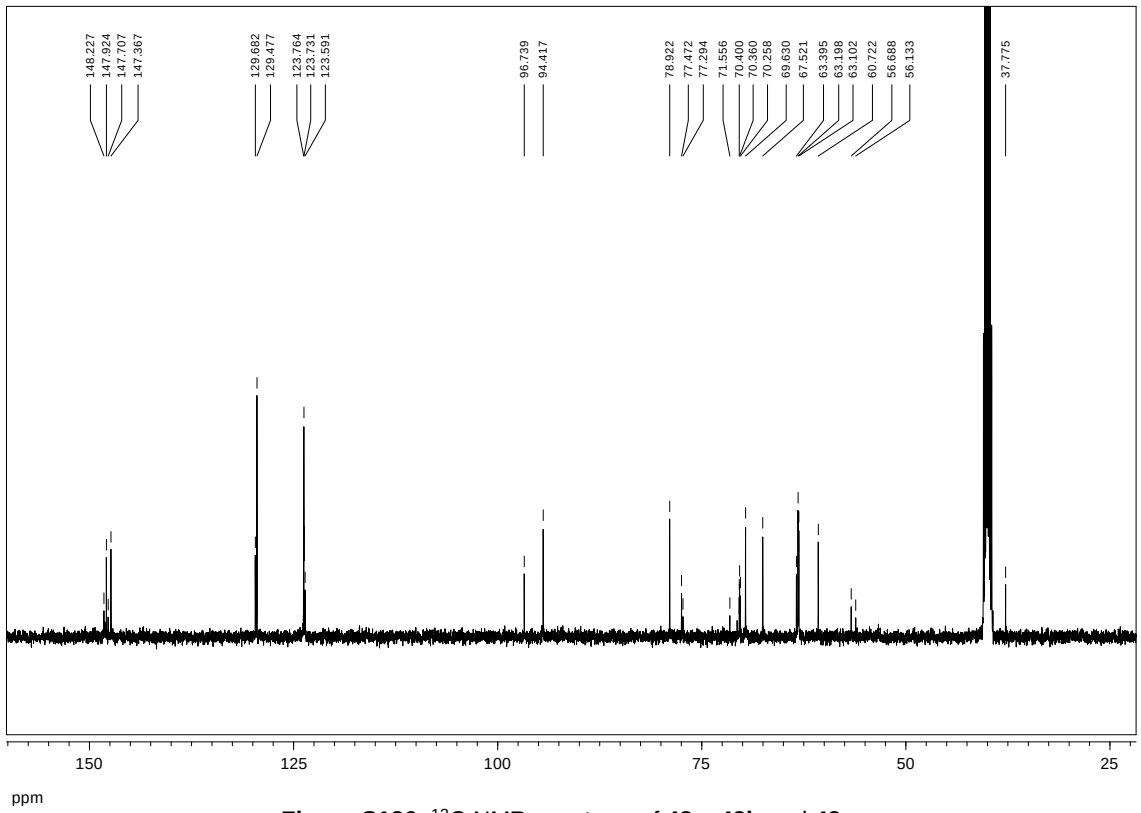


Figure S126. ^{13}C NMR spectrum of **43a**, **43b** and **43c**.

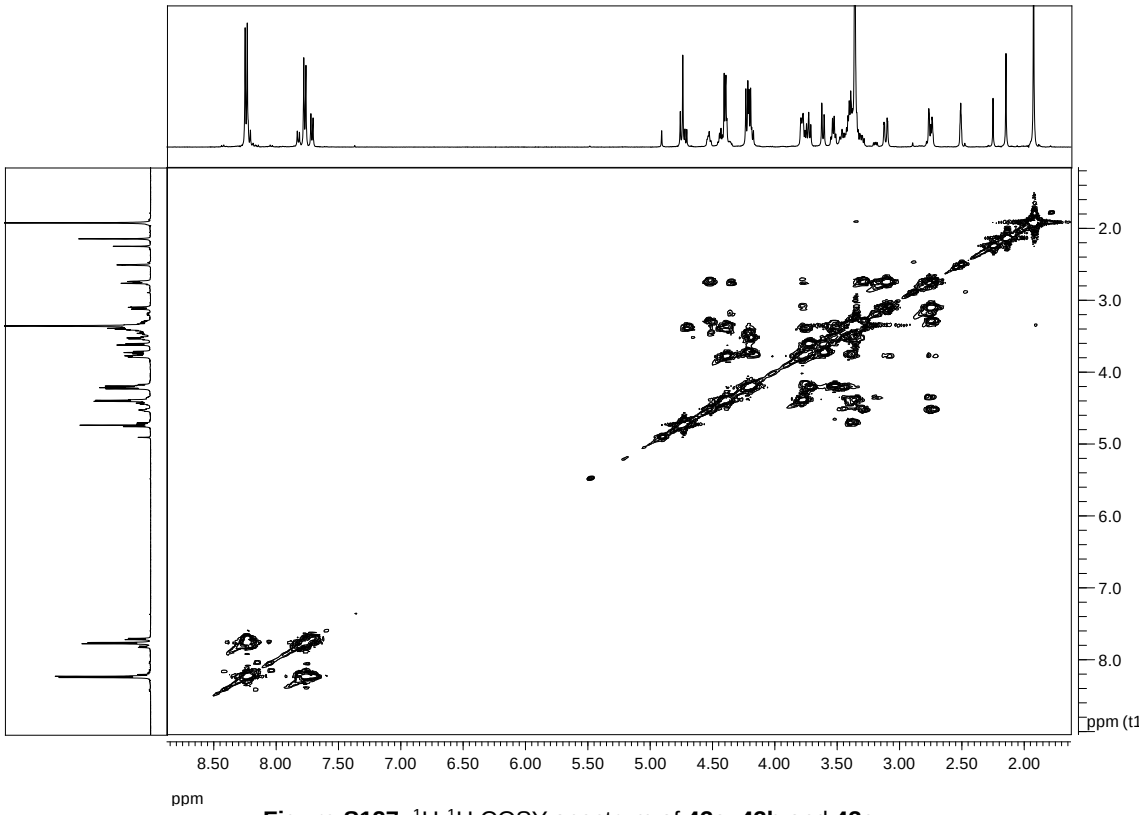


Figure S127. ^{1}H-^{1}H COSY spectrum of **43a**, **43b** and **43c**.

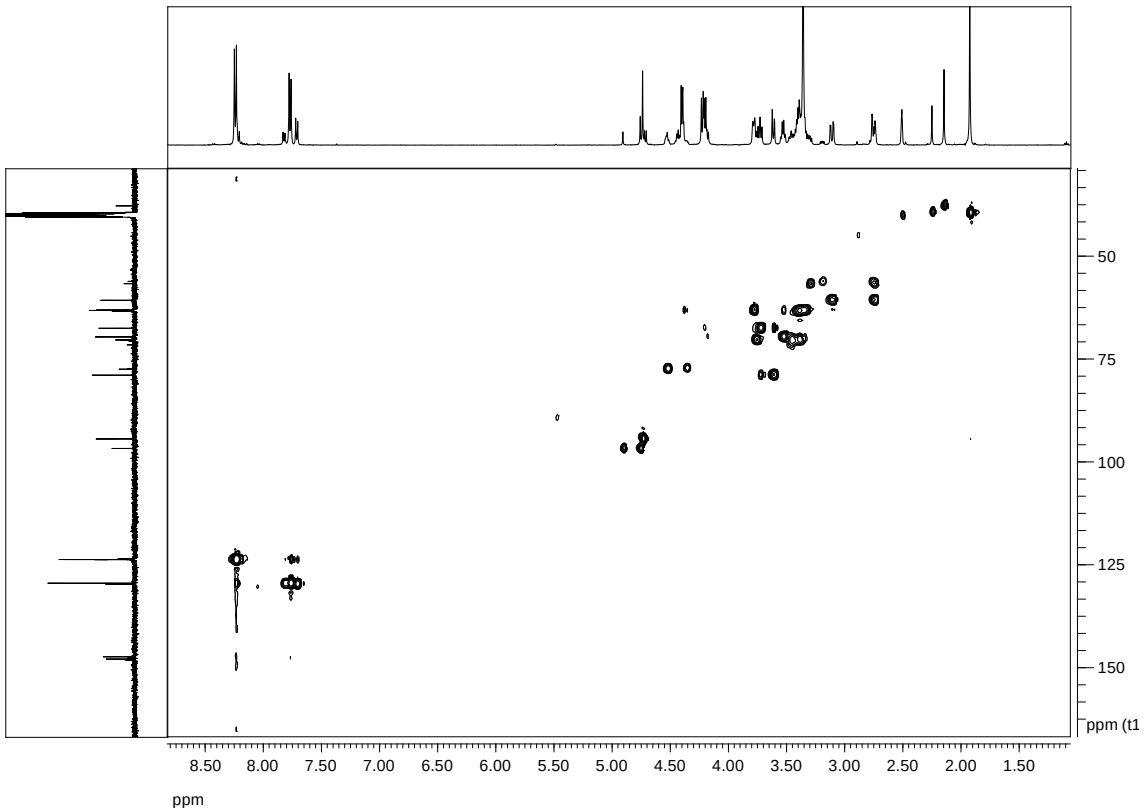


Figure S128. HMQC spectrum of **43a**, **43b** and **43c**.

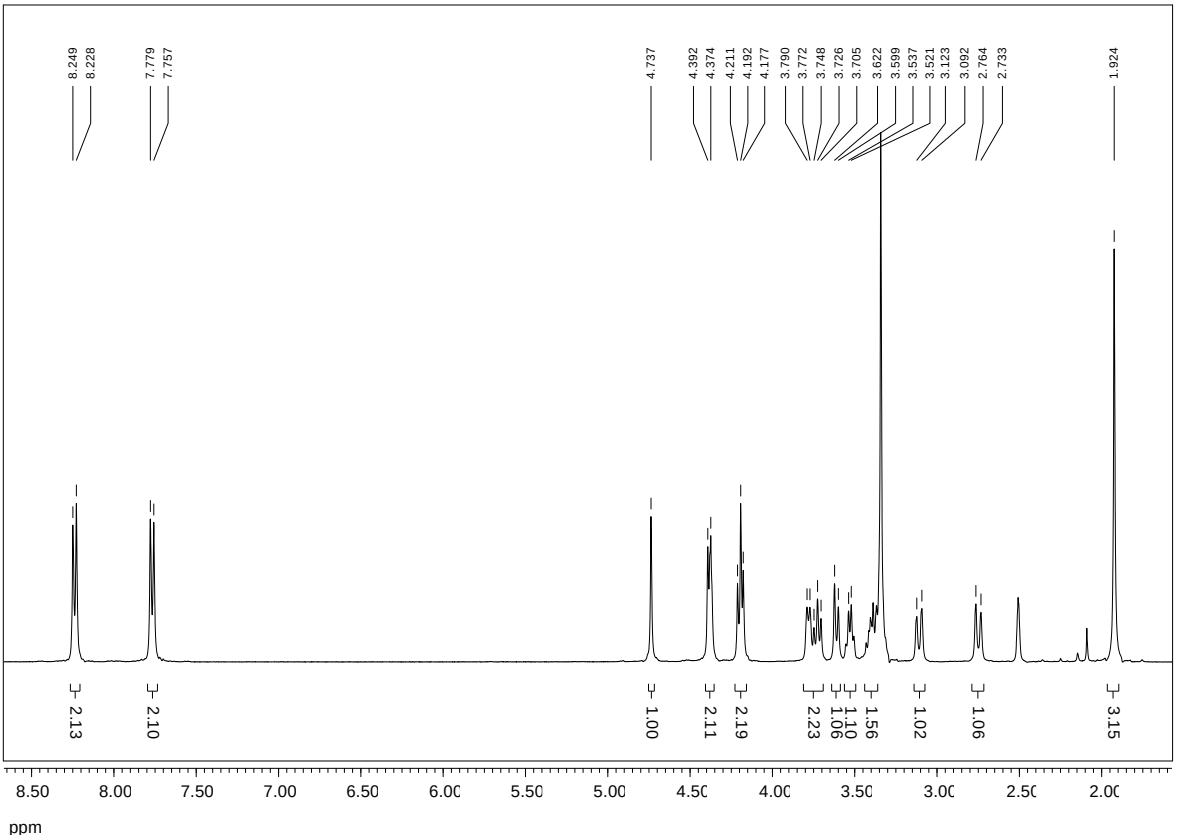


Figure S129. ^{1}H NMR spectrum of **43c**.

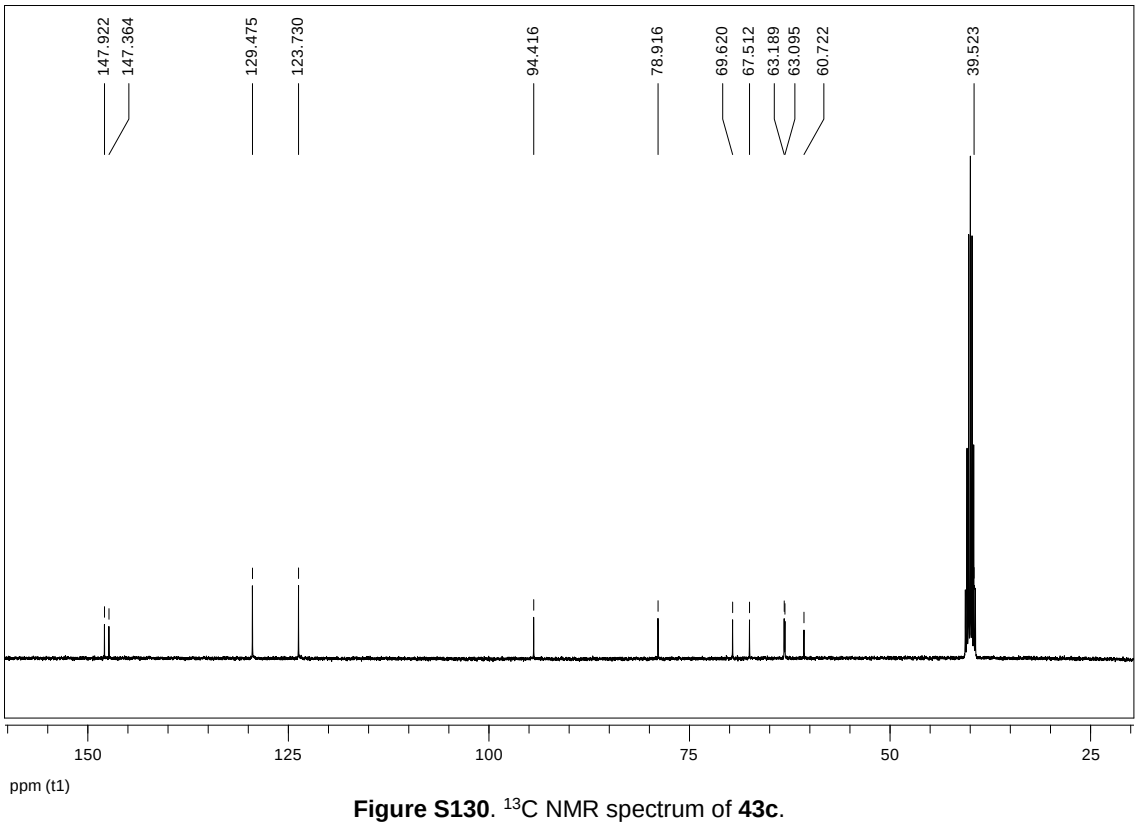


Figure S130. ^{13}C NMR spectrum of **43c**.

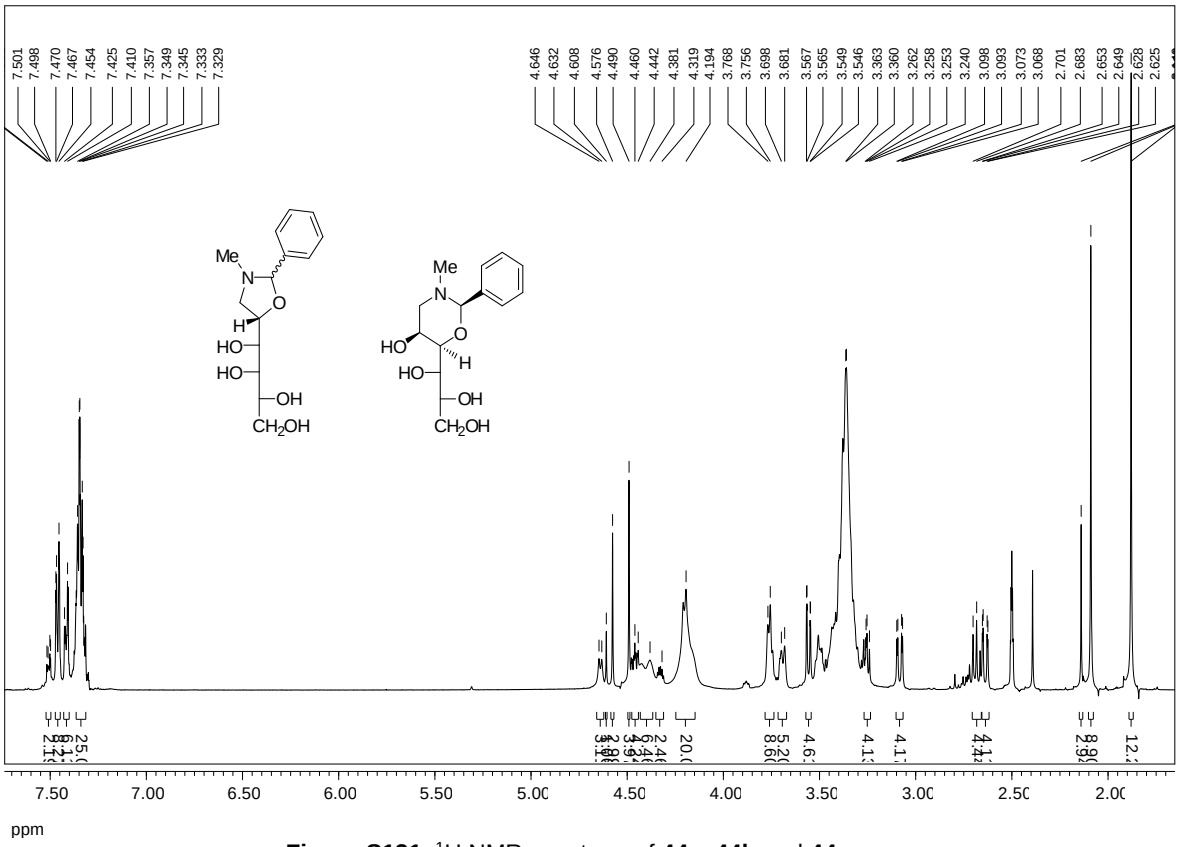


Figure S131. ^{1}H NMR spectrum of **44a**, **44b** and **44c**.

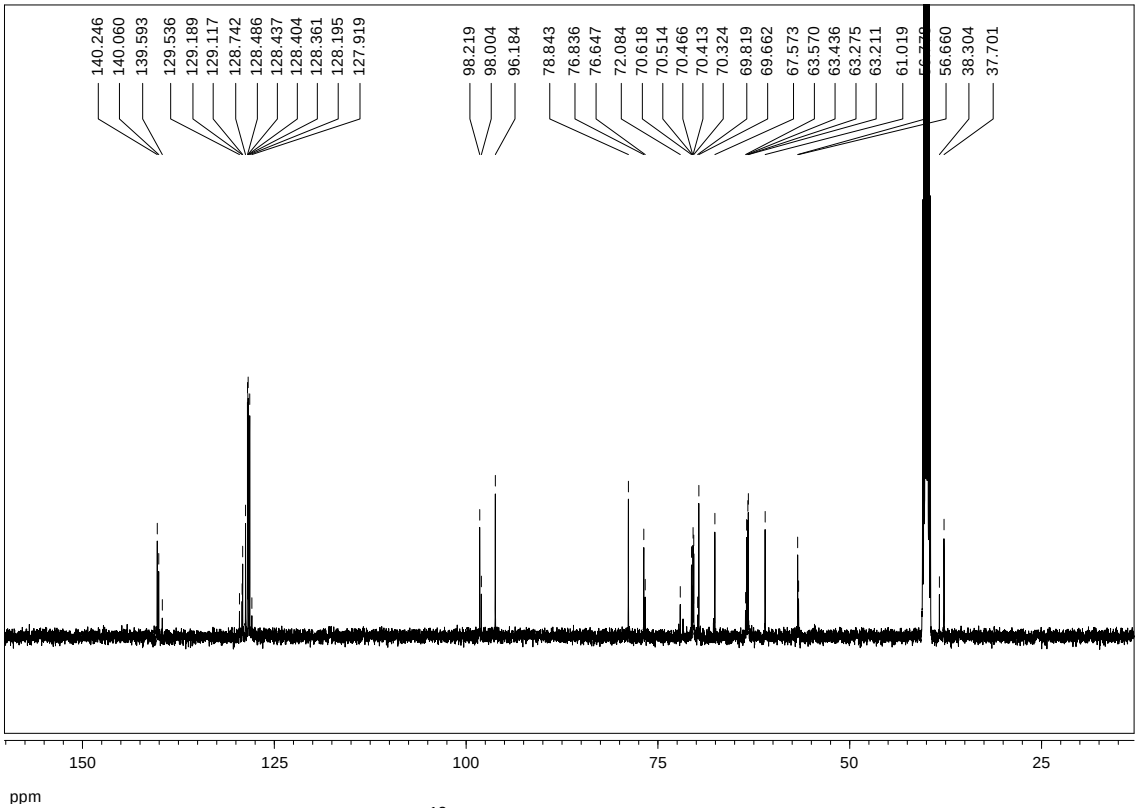


Figure S132. ^{13}C NMR spectrum of **44a**, **44b** and **44c**.

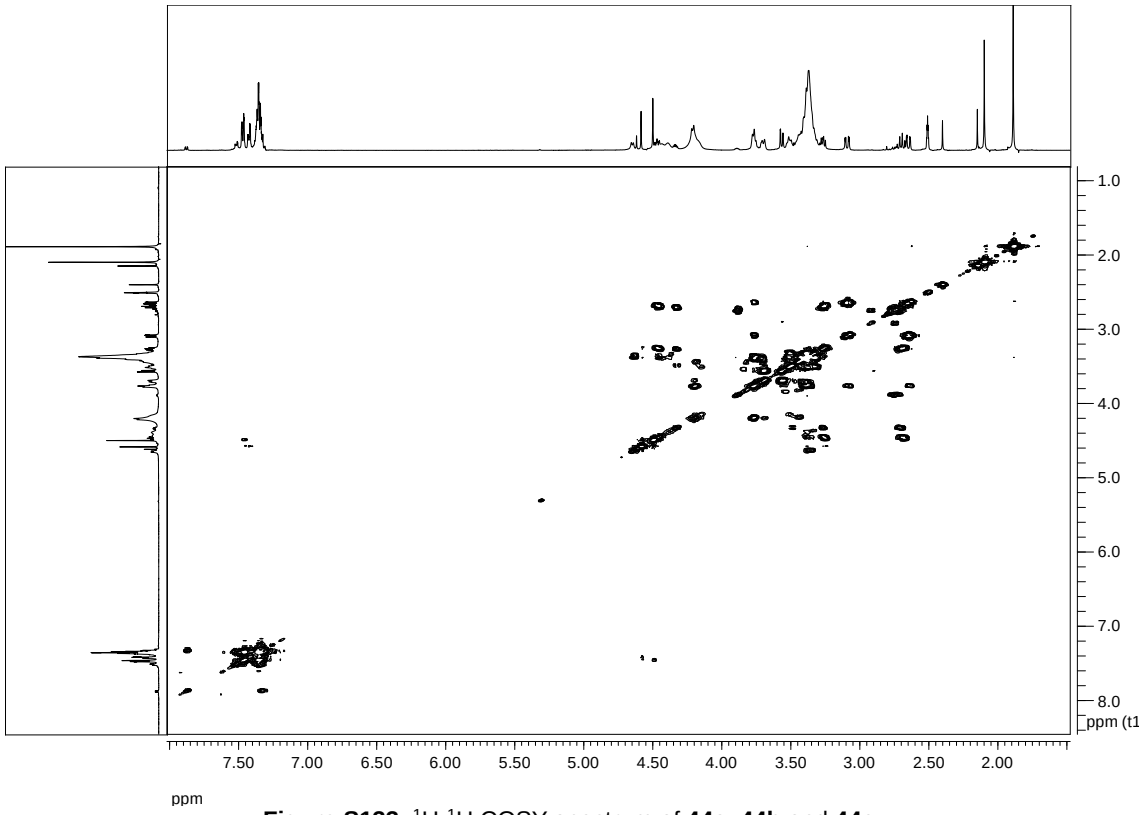


Figure S133. ^{1}H-^{1}H COSY spectrum of **44a**, **44b** and **44c**.

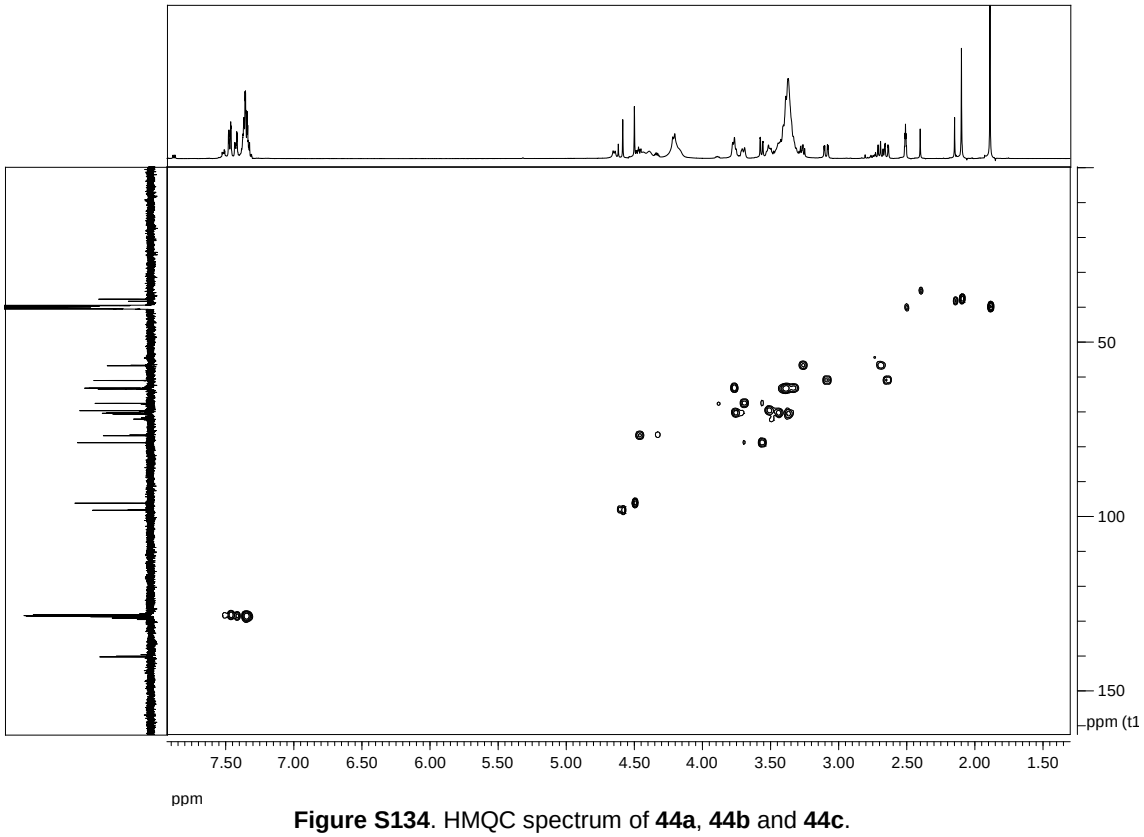


Figure S134. HMQC spectrum of **44a**, **44b** and **44c**.

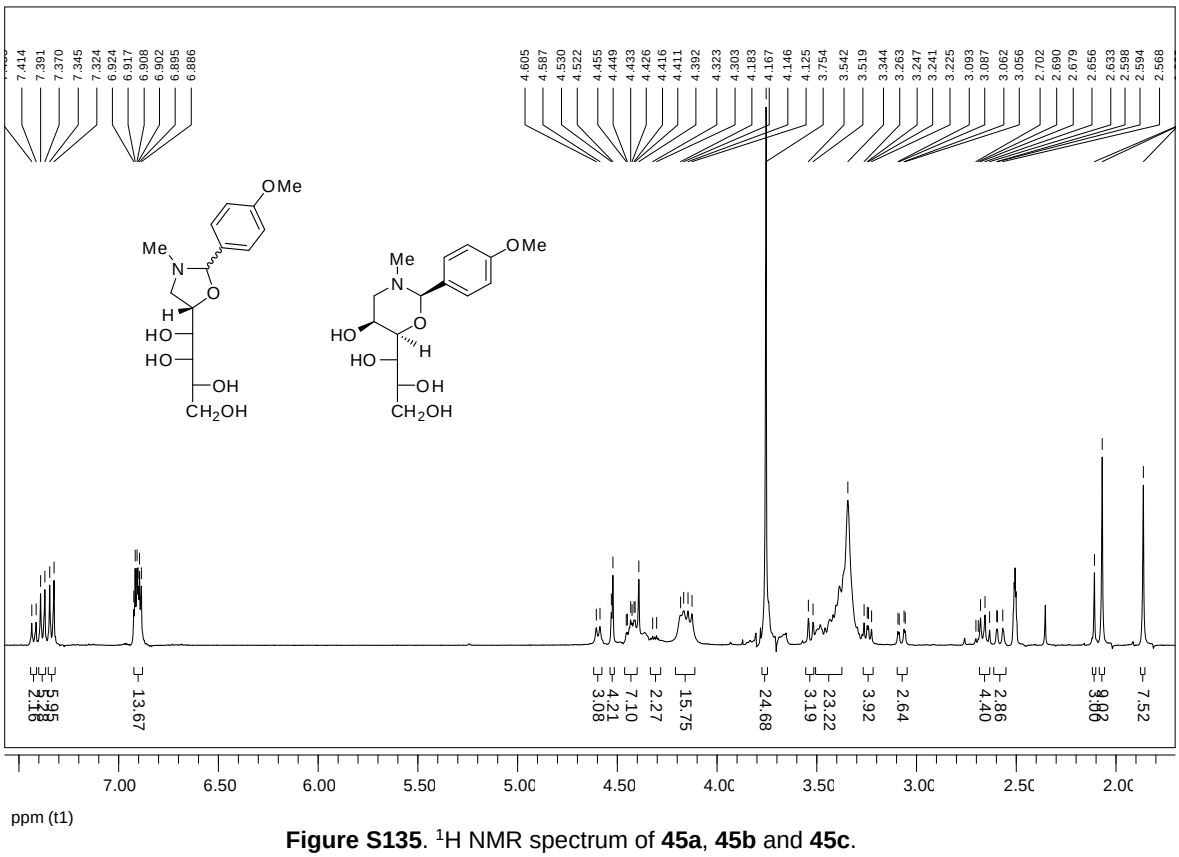


Figure S135. ^{1}H NMR spectrum of **45a**, **45b** and **45c**.

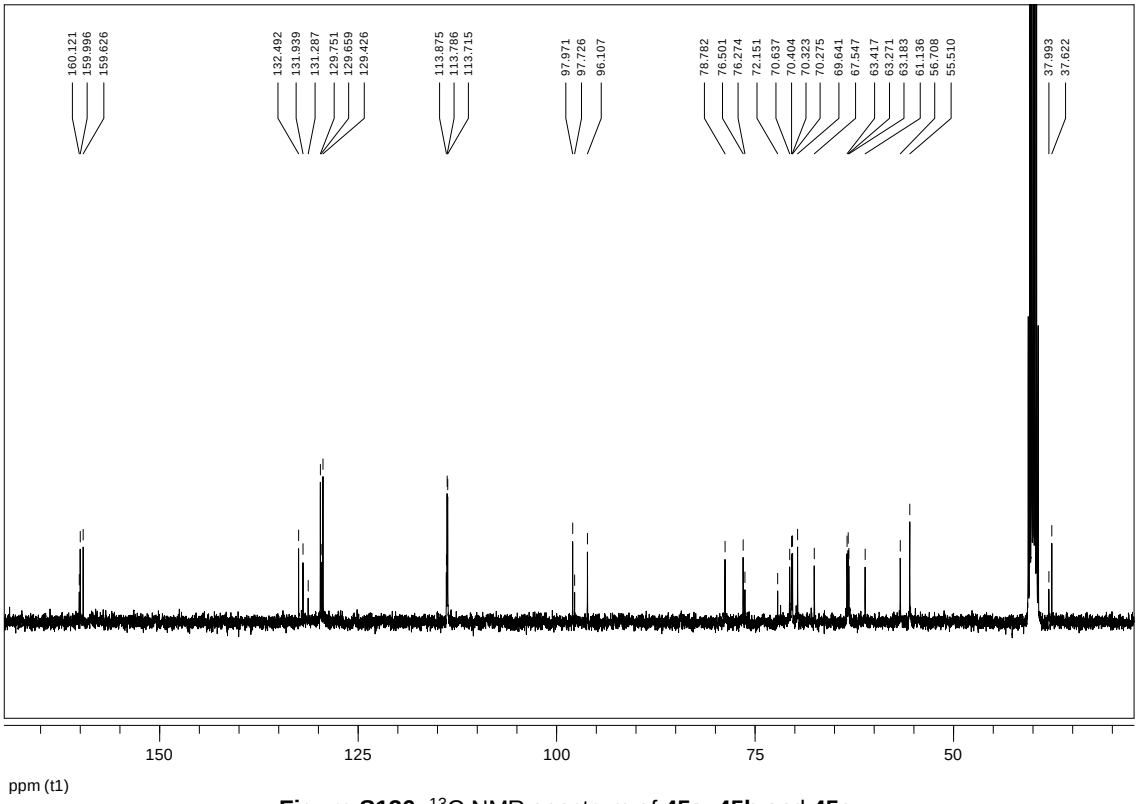


Figure S136. ^{13}C NMR spectrum of **45a**, **45b** and **45c**.

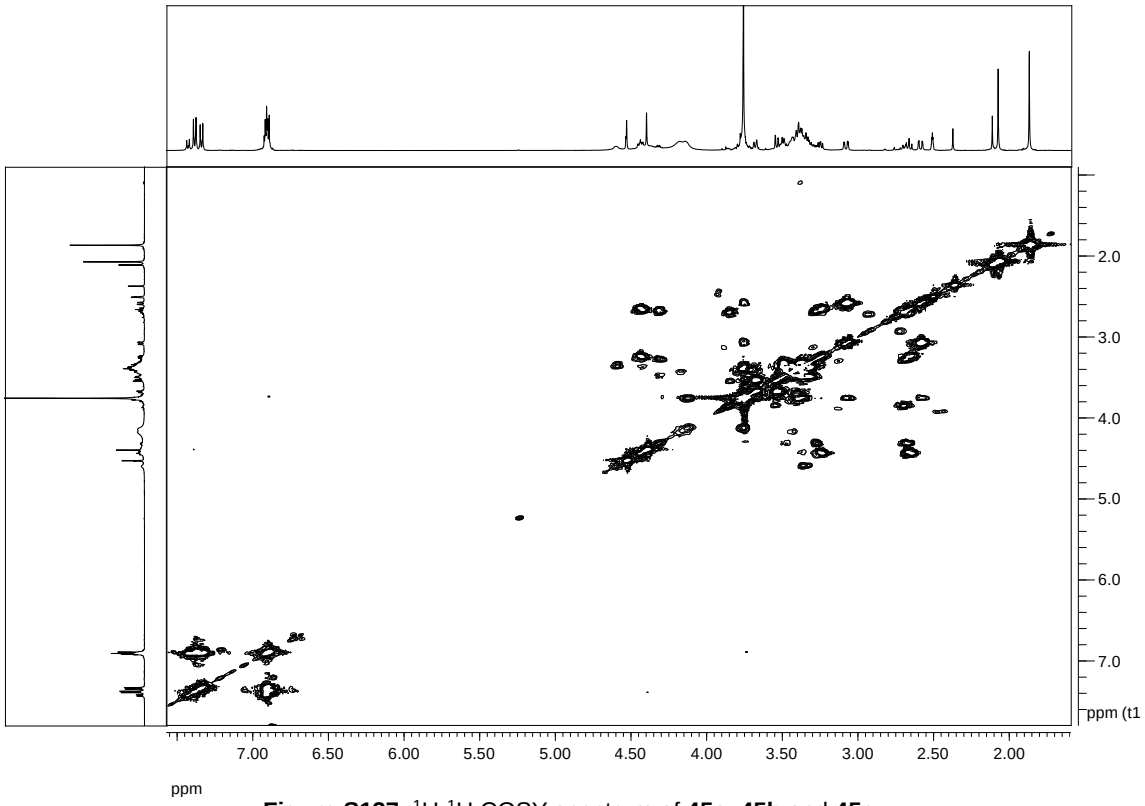


Figure S137. ^{1}H-^{1}H COSY spectrum of **45a**, **45b** and **45c**.

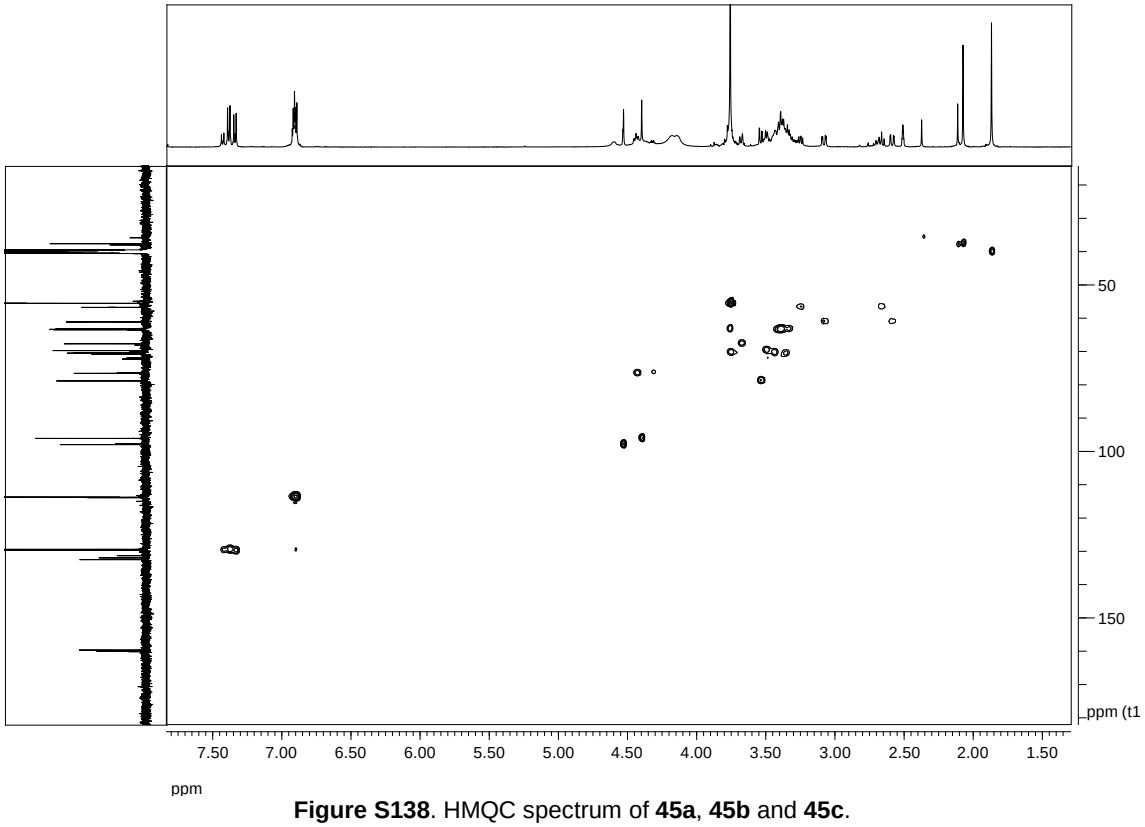


Figure S138. HMQC spectrum of **45a**, **45b** and **45c**.

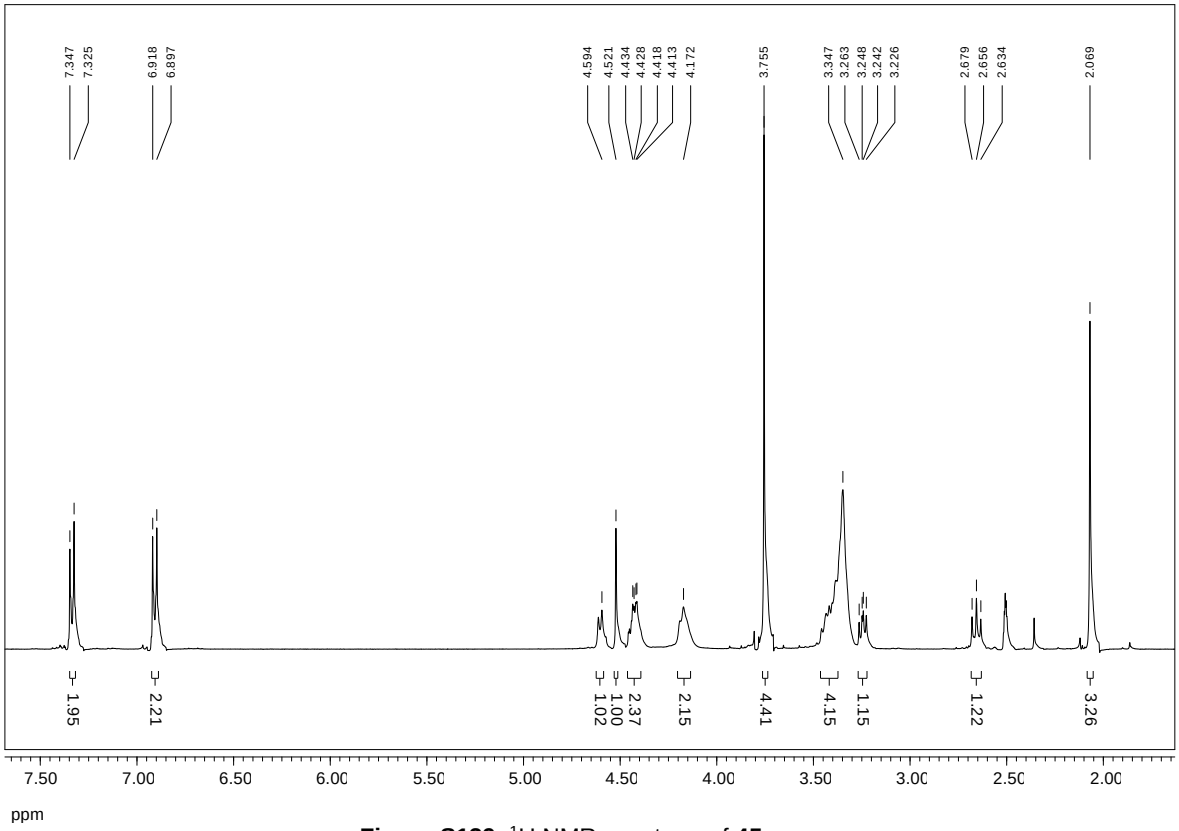


Figure S139. ^{1}H NMR spectrum of **45a**.

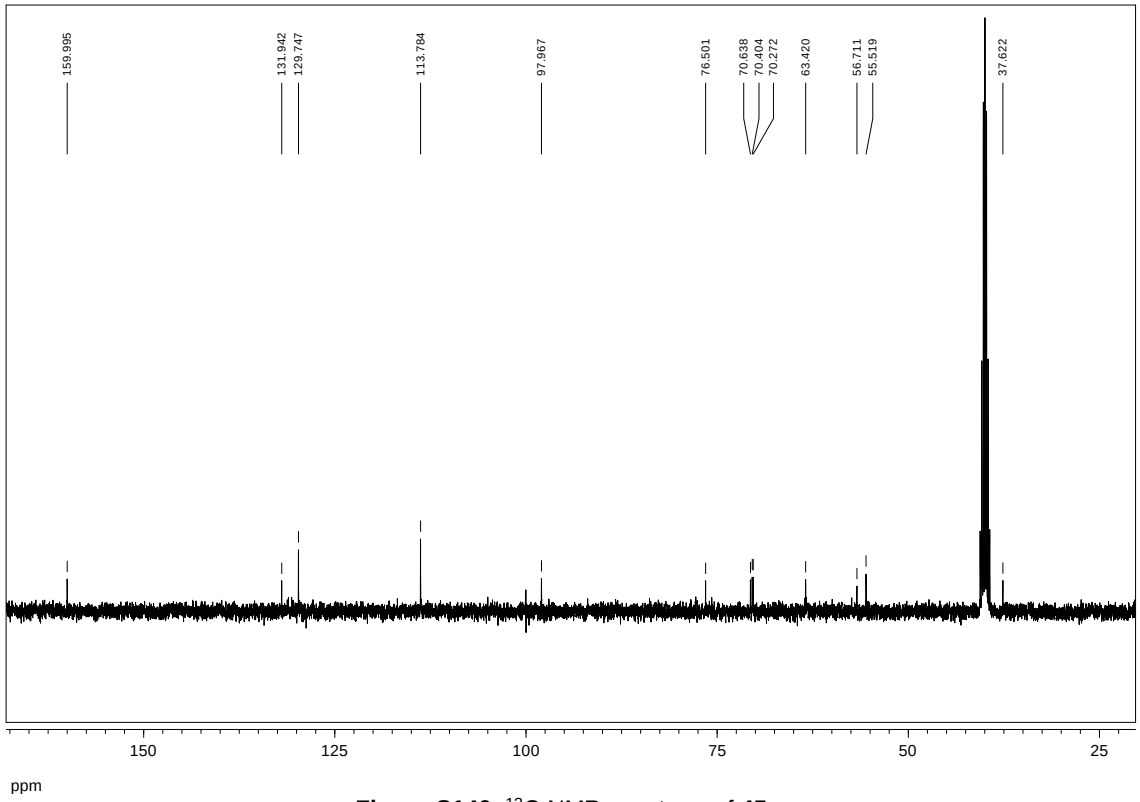


Figure S140. ^{13}C NMR spectrum of **45a**.

Structure 21a (^{2}E ec-ax H-bond O) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1220.6352544
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.990879	0.532992	0.681353
2	6	0	-2.062913	-0.842614	0.462777
3	6	0	-3.272682	-1.444555	0.145860
4	6	0	-4.404543	-0.649173	0.063115
5	6	0	-4.373383	0.716548	0.296897
6	6	0	-3.154376	1.299397	0.609643
7	1	0	-1.170343	-1.446938	0.564555
8	1	0	-3.355391	-2.508374	-0.029092
9	1	0	-5.288339	1.289600	0.238016
10	1	0	-3.108471	2.365127	0.807317
11	6	0	-0.657381	1.218831	0.951141
12	1	0	-0.825884	2.075105	1.613370
13	7	0	0.052044	1.665826	-0.244014
14	8	0	0.239868	0.320478	1.567309
15	6	0	1.241162	-0.106663	0.618243
16	6	0	0.776629	0.490941	-0.707800
17	1	0	1.611033	0.776032	-1.345190
18	1	0	0.143780	-0.214163	-1.269113
19	1	0	1.252693	-1.198011	0.613713
20	6	0	2.591084	0.441783	1.093925
21	1	0	2.688381	1.481068	0.744937
22	6	0	3.817965	-0.349626	0.645130
23	1	0	3.718673	-1.375458	1.027701
24	6	0	4.012780	-0.416584	-0.867205
25	1	0	3.955179	0.594557	-1.283333
26	6	0	5.359727	-1.019501	-1.228143
27	1	0	5.504464	-0.938157	-2.311272
28	1	0	6.155482	-0.493321	-0.697582
29	8	0	2.661924	0.401375	2.509273
30	1	0	1.788901	0.643738	2.836880
31	8	0	4.965894	0.271656	1.189489
32	1	0	4.761183	0.446079	2.114771
33	8	0	2.979969	-1.187362	-1.460679
34	1	0	3.259207	-2.106340	-1.365073
35	8	0	5.276690	-2.386059	-0.836723
36	1	0	6.105721	-2.822715	-1.037128
37	6	0	-0.732560	2.370781	-1.245638
38	1	0	-1.475482	1.708496	-1.718922
39	1	0	-1.288068	3.162030	-0.732089
40	6	0	0.162227	2.992266	-2.309580
41	1	0	-0.428926	3.611875	-2.985683
42	1	0	0.926937	3.613943	-1.840491
43	1	0	0.658049	2.226351	-2.908765
44	7	0	-5.696536	-1.282596	-0.273307
45	8	0	-6.670807	-0.565827	-0.331321
46	8	0	-5.697847	-2.477017	-0.471673

Structure 21a (^{2}E ec-ax H-bond N) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1220.6376728
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.556364	0.130660	-0.565912
2	6	0	1.763097	-0.784569	0.465758
3	6	0	3.035537	-1.271616	0.732350
4	6	0	4.087674	-0.836053	-0.056715
5	6	0	3.913619	0.052062	-1.106661
6	6	0	2.635453	0.528752	-1.356146
7	1	0	0.916615	-1.138101	1.041797
8	1	0	3.221890	-1.983061	1.525024
9	1	0	4.765399	0.345196	-1.704679
10	1	0	2.475063	1.214195	-2.181604
11	6	0	0.173274	0.713351	-0.826894
12	1	0	0.033860	0.839706	-1.905822
13	7	0	-0.087157	1.995559	-0.159749
14	8	0	-0.827531	-0.134191	-0.321503
15	6	0	-1.358995	0.407001	0.905556
16	6	0	-0.460781	1.609455	1.200559

17	1	0	-1.010573	2.412607	1.691181
18	1	0	0.411878	1.334031	1.810958
19	1	0	-1.301670	-0.370020	1.665489
20	6	0	-2.820111	0.811027	0.705317
21	1	0	-3.280633	0.935040	1.693694
22	6	0	-3.652689	-0.198988	-0.089906
23	1	0	-3.165511	-0.359848	-1.059272
24	6	0	-3.839099	-1.549719	0.599774
25	1	0	-4.346004	-1.384872	1.555186
26	6	0	-4.684218	-2.475787	-0.260066
27	1	0	-4.880275	-3.395257	0.302157
28	1	0	-5.624506	-1.982962	-0.520627
29	8	0	-2.941896	2.068501	0.045237
30	1	0	-2.118924	2.233042	-0.440231
31	8	0	-4.949624	0.340395	-0.266952
32	1	0	-4.815189	1.256990	-0.532745
33	8	0	-2.599534	-2.169660	0.885192
34	1	0	-2.226967	-2.422291	0.031384
35	8	0	-3.897523	-2.750742	-1.414006
36	1	0	-4.358262	-3.388400	-1.960744
37	6	0	0.933338	3.029182	-0.278704
38	1	0	1.857540	2.742183	0.245702
39	1	0	1.179485	3.125528	-1.340643
40	6	0	0.425171	4.364995	0.247659
41	1	0	1.152794	5.151752	0.043338
42	1	0	-0.519659	4.628038	-0.231708
43	1	0	0.266001	4.334528	1.326912
44	7	0	5.445881	-1.349402	0.220119
45	8	0	6.346924	-0.948646	-0.482667
46	8	0	5.570533	-2.134363	1.133055

Structure 21a (^{2}E ax-ax) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1220.6382662
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.902580	0.802265	0.327153
2	6	0	-2.191533	-0.161383	1.291632
3	6	0	-3.316465	-0.964675	1.167555
4	6	0	-4.138065	-0.780535	0.067490
5	6	0	-3.876552	0.169608	-0.908184
6	6	0	-2.747268	0.963474	-0.770813
7	1	0	-1.521321	-0.281583	2.133347
8	1	0	-3.562780	-1.723476	1.897270
9	1	0	-4.548100	0.266634	-1.750055
10	1	0	-2.496433	1.701824	-1.522511
11	6	0	-0.683202	1.698218	0.491080
12	1	0	-0.974400	2.628955	0.983579
13	7	0	-0.032412	1.954331	-0.772019
14	8	0	0.291827	1.071198	1.322937
15	6	0	1.093978	0.234375	0.470637
16	6	0	0.747575	0.721456	-0.961749
17	1	0	1.628163	0.913645	-1.571573
18	1	0	0.144183	-0.025053	-1.476841
19	1	0	0.798068	-0.807926	0.620131
20	6	0	2.546326	0.440939	0.902687
21	1	0	2.930743	1.367730	0.447886
22	6	0	3.504928	-0.698232	0.562963
23	1	0	3.125158	-1.613552	1.038894
24	6	0	3.670813	-0.964836	-0.930092
25	1	0	3.937403	-0.030357	-1.434722
26	6	0	4.761013	-1.992162	-1.188902
27	1	0	4.932041	-2.061311	-2.268824
28	1	0	5.678599	-1.697270	-0.675907
29	8	0	2.625268	0.538153	2.316082
30	1	0	1.889944	1.091529	2.600383
31	8	0	4.782460	-0.368593	1.071188
32	1	0	4.640735	-0.060772	1.973036
33	8	0	2.451580	-1.424281	-1.486688
34	1	0	2.423512	-2.370894	-1.299065
35	8	0	4.245171	-3.219863	-0.684545
36	1	0	4.873553	-3.922369	-0.857723
37	6	0	0.786466	3.175976	-0.724175
38	1	0	1.344764	3.249367	0.221242
39	1	0	1.521340	3.105450	-1.528569
40	6	0	-0.068665	4.416873	-0.936308
41	1	0	0.551309	5.315486	-0.931806
42	1	0	-0.587181	4.351351	-1.894059
43	1	0	-0.820101	4.530178	-0.151378
44	7	0	-5.335958	-1.634182	-0.076496
45	8	0	-6.033402	-1.459235	-1.050961

46	8	0	-5.544308	-2.454479	0.789616

Structure 21a (E_2 ec-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1220.6356596
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.108162	-0.070577	-0.396683
2	6	0	2.528493	-0.068457	0.933460
3	6	0	3.867606	-0.235371	1.242208
4	6	0	4.768259	-0.401543	0.197531
5	6	0	4.381422	-0.408718	-1.130717
6	6	0	3.031468	-0.242213	-1.421241
7	1	0	1.790089	0.074057	1.712606
8	1	0	4.228175	-0.237672	2.261385
9	1	0	5.125606	-0.543069	-1.903365
10	1	0	2.697646	-0.244934	-2.453032
11	6	0	0.643428	0.135308	-0.690227
12	1	0	0.468061	0.075999	-1.783698
13	7	0	0.142895	1.380021	-0.141539
14	8	0	-0.118559	-0.855392	-0.032552
15	6	0	-1.415010	-0.307297	0.288845
16	6	0	-1.301093	1.175852	-0.084233
17	1	0	-1.772844	1.365031	-1.066671
18	1	0	-1.771127	1.822705	0.648807
19	1	0	-1.566982	-0.450683	1.361030
20	6	0	-2.439713	-1.125517	-0.501350
21	1	0	-2.407779	-0.812033	-1.556847
22	6	0	-3.893965	-1.080648	-0.032964
23	1	0	-3.928375	-1.420227	1.011650
24	6	0	-4.554453	0.293342	-0.113289
25	1	0	-4.363661	0.735532	-1.096281
26	6	0	-6.055979	0.196366	0.102745
27	1	0	-6.500272	1.184045	-0.063759
28	1	0	-6.484883	-0.535112	-0.584242
29	8	0	-2.104113	-2.501699	-0.405159
30	1	0	-1.149228	-2.564212	-0.516954
31	8	0	-4.639153	-1.952001	-0.861042
32	1	0	-4.126679	-2.765684	-0.923051
33	8	0	-3.999757	1.159158	0.861522
34	1	0	-4.449938	0.938888	1.686552
35	8	0	-6.212046	-0.198617	1.461731
36	1	0	-7.144779	-0.291643	1.660259
37	6	0	0.561192	2.554984	-0.891552
38	1	0	1.654051	2.546574	-0.937208
39	1	0	0.187346	2.505048	-1.930813
40	6	0	0.086148	3.840198	-0.229825
41	1	0	0.496623	4.708503	-0.747223
42	1	0	-1.002371	3.920994	-0.250492
43	1	0	0.413847	3.865449	0.810928
44	7	0	6.201830	-0.575653	0.516989
45	8	0	6.966405	-0.726301	-0.409921
46	8	0	6.519546	-0.555447	1.684921

Structure 21a (^{2}E ec-ax H-bond O) (M06-2X, Benzene)

Energy (Hartrees): = - 1220.6575388
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.993919	0.528246	0.675570
2	6	0	-2.066166	-0.846598	0.450668
3	6	0	-3.276115	-1.447499	0.132927
4	6	0	-4.408402	-0.651229	0.055022
5	6	0	-4.376175	0.714747	0.291713
6	6	0	-3.157069	1.296200	0.605415
7	1	0	-1.175011	-1.454253	0.546083
8	1	0	-3.352454	-2.511298	-0.045599
9	1	0	-5.287390	1.294153	0.235350
10	1	0	-3.111429	2.361217	0.806777
11	6	0	-0.662226	1.213376	0.959402
12	1	0	-0.836207	2.059698	1.632194
13	7	0	0.054760	1.674950	-0.225320
14	8	0	0.233342	0.306775	1.568829
15	6	0	1.234795	-0.114518	0.615895
16	6	0	0.777653	0.504079	-0.703188

17	1	0	1.615466	0.799026	-1.331722
18	1	0	0.144534	-0.189752	-1.277246
19	1	0	1.239950	-1.205727	0.597591
20	6	0	2.585661	0.421606	1.103559
21	1	0	2.686029	1.467328	0.775570
22	6	0	3.814060	-0.362706	0.644925
23	1	0	3.716078	-1.392821	1.016092
24	6	0	4.010968	-0.412463	-0.868686
25	1	0	3.945966	0.601550	-1.276013
26	6	0	5.359382	-1.002689	-1.242524
27	1	0	5.492272	-0.915319	-2.326641
28	1	0	6.160631	-0.471066	-0.725146
29	8	0	2.651034	0.355960	2.520389
30	1	0	1.780527	0.610839	2.846684
31	8	0	4.960965	0.253784	1.201640
32	1	0	4.752982	0.412903	2.129152
33	8	0	2.982187	-1.186115	-1.468285
34	1	0	3.264344	-2.104247	-1.369116
35	8	0	5.299723	-2.371840	-0.854852
36	1	0	6.105679	-2.809677	-1.137530
37	6	0	-0.718105	2.403882	-1.220207
38	1	0	-1.464142	1.756979	-1.709016
39	1	0	-1.266685	3.193749	-0.697622
40	6	0	0.188681	3.030543	-2.269918
41	1	0	-0.391344	3.677146	-2.931137
42	1	0	0.965814	3.628771	-1.789195
43	1	0	0.669741	2.270569	-2.889226
44	7	0	-5.698192	-1.281695	-0.284036
45	8	0	-6.673687	-0.565542	-0.353401
46	8	0	-5.707248	-2.478323	-0.476597

Structure 21a (^{2}E ec-ax H-bond N) (M06-2X, Benzene)

Energy (Hartrees): = - 1220.6606267
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.569811	0.138539	0.549999
2	6	0	-1.783926	-0.765951	-0.489966
3	6	0	-3.056165	-1.256899	-0.747507
4	6	0	-4.101011	-0.838251	0.061404
5	6	0	-3.920098	0.043335	1.116611
6	6	0	-2.642288	0.526669	1.354742
7	1	0	-0.945370	-1.107112	-1.084521
8	1	0	-3.242224	-1.959543	-1.548250
9	1	0	-4.762231	0.328874	1.731831
10	1	0	-2.476520	1.207186	2.183238
11	6	0	-0.184692	0.718822	0.806720
12	1	0	-0.044510	0.847358	1.884897
13	7	0	0.080855	1.998435	0.136528
14	8	0	0.811761	-0.137275	0.301282
15	6	0	1.367694	0.412407	-0.910538
16	6	0	0.470057	1.610925	-1.219114
17	1	0	1.020169	2.415140	-1.707821
18	1	0	-0.394025	1.331307	-1.838881
19	1	0	1.330311	-0.358390	-1.677863
20	6	0	2.822039	0.821348	-0.674211
21	1	0	3.298048	0.970862	-1.651885
22	6	0	3.647887	-0.200510	0.114734
23	1	0	3.135992	-0.395018	1.064997
24	6	0	3.875331	-1.528907	-0.605666
25	1	0	4.390062	-1.331574	-1.550702
26	6	0	4.727323	-2.464030	0.236148
27	1	0	4.945482	-3.363300	-0.350221
28	1	0	5.661315	-1.969818	0.517054
29	8	0	2.921404	2.061140	0.024816
30	1	0	2.064379	2.236832	0.446697
31	8	0	4.930263	0.356991	0.348463
32	1	0	4.765668	1.262373	0.636585
33	8	0	2.650239	-2.165944	-0.922829
34	1	0	2.261998	-2.427261	-0.078469
35	8	0	3.942160	-2.787577	1.378594
36	1	0	4.405699	-3.452915	1.891637
37	6	0	-0.943147	3.031190	0.245099
38	1	0	-1.854958	2.746767	-0.301421
39	1	0	-1.210854	3.117731	1.302225
40	6	0	-0.429924	4.371668	-0.260514
41	1	0	-1.169846	5.151612	-0.070857
42	1	0	0.498505	4.643863	0.246353
43	1	0	-0.242066	4.351281	-1.335889
44	7	0	-5.454671	-1.363974	-0.199262
45	8	0	-6.339572	-1.044400	0.565063

46	8	0	-5.602996	-2.084137	-1.162546

Structure 21a (^{2}E ax-ax) (M06-2X, Benzene)

Energy (Hartrees): = - 1220.6603437
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.944810	0.705847	0.348053
2	6	0	-2.235684	-0.327789	1.236156
3	6	0	-3.398057	-1.073045	1.089093
4	6	0	-4.255933	-0.757997	0.047421
5	6	0	-3.992651	0.264850	-0.852884
6	6	0	-2.824942	0.994844	-0.695839
7	1	0	-1.545439	-0.546809	2.040973
8	1	0	-3.643279	-1.882346	1.763070
9	1	0	-4.689819	0.470145	-1.653549
10	1	0	-2.577665	1.788296	-1.390609
11	6	0	-0.697520	1.558648	0.528161
12	1	0	-0.967992	2.488356	1.034923
13	7	0	-0.046480	1.826226	-0.731854
14	8	0	0.263227	0.893212	1.348984
15	6	0	1.125320	0.128058	0.485288
16	6	0	0.737073	0.600162	-0.937275
17	1	0	1.596797	0.796947	-1.574119
18	1	0	0.119594	-0.153268	-1.427150
19	1	0	0.915704	-0.934322	0.632449
20	6	0	2.563466	0.449809	0.901147
21	1	0	2.871826	1.398380	0.435169
22	6	0	3.605385	-0.612048	0.556165
23	1	0	3.311950	-1.548776	1.050696
24	6	0	3.761212	-0.882045	-0.938678
25	1	0	3.905521	0.067509	-1.464456
26	6	0	4.948636	-1.784351	-1.224662
27	1	0	5.074791	-1.865122	-2.310088
28	1	0	5.854159	-1.371483	-0.774824
29	8	0	2.648948	0.568252	2.314037
30	1	0	1.864678	1.051259	2.598214
31	8	0	4.860949	-0.170656	1.039076
32	1	0	4.707523	0.135521	1.939867
33	8	0	2.582821	-1.483442	-1.450641
34	1	0	2.657498	-2.420931	-1.231431
35	8	0	4.612147	-3.049164	-0.663621
36	1	0	5.298212	-3.681250	-0.889144
37	6	0	0.749903	3.063727	-0.688866
38	1	0	1.277669	3.171712	0.270269
39	1	0	1.509033	2.991412	-1.470259
40	6	0	-0.126740	4.279027	-0.949138
41	1	0	0.468652	5.194730	-0.930783
42	1	0	-0.605898	4.193483	-1.926474
43	1	0	-0.911077	4.378870	-0.194023
44	7	0	-5.496148	-1.540940	-0.111659
45	8	0	-6.247874	-1.229389	-1.010297
46	8	0	-5.692967	-2.449502	0.666340

Structure 21a (E_2 ec-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 1220.6580232
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.113942	-0.052468	-0.404013
2	6	0	2.529773	-0.055694	0.928020
3	6	0	3.866697	-0.229180	1.241787
4	6	0	4.770951	-0.397776	0.199889
5	6	0	4.388880	-0.397060	-1.130509
6	6	0	3.041388	-0.221485	-1.425952
7	1	0	1.792625	0.085394	1.708885
8	1	0	4.217112	-0.234966	2.264625
9	1	0	5.130180	-0.533267	-1.905798
10	1	0	2.713099	-0.217841	-2.459493
11	6	0	0.649284	0.153410	-0.704287
12	1	0	0.480046	0.102531	-1.797842
13	7	0	0.141824	1.391679	-0.145328
14	8	0	-0.110718	-0.847732	-0.056993
15	6	0	-1.406681	-0.306047	0.281324
16	6	0	-1.301750	1.178350	-0.085763

17	1	0	-1.776502	1.369558	-1.065456
18	1	0	-1.770480	1.819189	0.653515
19	1	0	-1.546237	-0.455347	1.354472
20	6	0	-2.434568	-1.125789	-0.503148
21	1	0	-2.406868	-0.813269	-1.558408
22	6	0	-3.888298	-1.088504	-0.030404
23	1	0	-3.918440	-1.430698	1.013345
24	6	0	-4.557345	0.282047	-0.106945
25	1	0	-4.369246	0.728918	-1.088199
26	6	0	-6.058284	0.184506	0.108967
27	1	0	-6.499220	1.175589	-0.046409
28	1	0	-6.496385	-0.531794	-0.588642
29	8	0	-2.091818	-2.502815	-0.407802
30	1	0	-1.139715	-2.561088	-0.545283
31	8	0	-4.629539	-1.966127	-0.858753
32	1	0	-4.109729	-2.775430	-0.920704
33	8	0	-4.004940	1.146621	0.871773
34	1	0	-4.447242	0.913033	1.697830
35	8	0	-6.223004	-0.229090	1.461661
36	1	0	-7.159436	-0.242462	1.671542
37	6	0	0.547736	2.576183	-0.889931
38	1	0	1.640722	2.584288	-0.931908
39	1	0	0.177207	2.526306	-1.929682
40	6	0	0.054742	3.851494	-0.223965
41	1	0	0.465401	4.726883	-0.730348
42	1	0	-1.034251	3.927354	-0.256701
43	1	0	0.370010	3.874330	0.821378
44	7	0	6.198458	-0.588202	0.524600
45	8	0	6.963636	-0.786639	-0.394319
46	8	0	6.522205	-0.535900	1.691178

Structure 21a (^{2}E ec-ax H-bond O) (M06-2X, DMSO)

Energy (Hartrees): = - 1220.6617601
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.986723	0.551956	0.675765
2	6	0	-2.042840	-0.827296	0.469914
3	6	0	-3.246712	-1.445417	0.161648
4	6	0	-4.387353	-0.660971	0.073168
5	6	0	-4.370253	0.709315	0.290973
6	6	0	-3.157391	1.308246	0.596338
7	1	0	-1.145757	-1.427274	0.563403
8	1	0	-3.304313	-2.512740	-0.003150
9	1	0	-5.283924	1.284412	0.227741
10	1	0	-3.120334	2.376799	0.779445
11	6	0	-0.663883	1.259222	0.941031
12	1	0	-0.848941	2.123920	1.585038
13	7	0	0.047870	1.688927	-0.260879
14	8	0	0.243785	0.382229	1.578489
15	6	0	1.231021	-0.080331	0.628043
16	6	0	0.768784	0.501649	-0.706063
17	1	0	1.604378	0.779192	-1.346263
18	1	0	0.128706	-0.205456	-1.254887
19	1	0	1.225651	-1.171341	0.643959
20	6	0	2.590100	0.462627	1.083299
21	1	0	2.696698	1.493473	0.714041
22	6	0	3.808502	-0.344879	0.642069
23	1	0	3.708787	-1.358711	1.055069
24	6	0	3.985988	-0.455930	-0.871229
25	1	0	3.904317	0.538819	-1.320090
26	6	0	5.331333	-1.051742	-1.244309
27	1	0	5.433340	-1.027569	-2.334116
28	1	0	6.142216	-0.479762	-0.788212
29	8	0	2.667145	0.453129	2.503359
30	1	0	1.802255	0.738360	2.821589
31	8	0	4.965088	0.287837	1.167174
32	1	0	4.755615	0.498619	2.084504
33	8	0	2.952720	-1.262114	-1.420928
34	1	0	3.231801	-2.173101	-1.260699
35	8	0	5.311163	-2.396780	-0.772988
36	1	0	6.065978	-2.859929	-1.147619
37	6	0	-0.747118	2.365447	-1.278385
38	1	0	-1.467164	1.676802	-1.748076
39	1	0	-1.324661	3.148568	-0.778261
40	6	0	0.140082	2.987345	-2.346684
41	1	0	-0.463587	3.581497	-3.035738
42	1	0	0.887616	3.639610	-1.888775
43	1	0	0.658984	2.223391	-2.929942
44	7	0	-5.667641	-1.308788	-0.256049
45	8	0	-6.652170	-0.605424	-0.352188

46	8	0	-5.671543	-2.511878	-0.417160

Structure 21a (^{2}E ec-ax H-bond N) (M06-2X, DMSO)

Energy (Hartrees): = - 1220.6648769
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.579054	0.109242	0.541868
2	6	0	-1.819554	-0.748920	-0.531905
3	6	0	-3.098816	-1.226409	-0.779565
4	6	0	-4.123361	-0.838143	0.070895
5	6	0	-3.915702	-0.001214	1.157935
6	6	0	-2.630886	0.468299	1.386618
7	1	0	-1.001245	-1.059920	-1.170086
8	1	0	-3.300522	-1.891637	-1.608084
9	1	0	-4.738787	0.267622	1.805797
10	1	0	-2.441987	1.116873	2.235487
11	6	0	-0.191742	0.684089	0.791546
12	1	0	-0.048282	0.814852	1.868284
13	7	0	0.066810	1.962090	0.116212
14	8	0	0.802218	-0.176295	0.277961
15	6	0	1.368884	0.390148	-0.922594
16	6	0	0.453399	1.570413	-1.240315
17	1	0	0.986272	2.378388	-1.741701
18	1	0	-0.407829	1.271571	-1.853222
19	1	0	1.358657	-0.375798	-1.694592
20	6	0	2.810266	0.832051	-0.663119
21	1	0	3.290893	1.000599	-1.635480
22	6	0	3.650346	-0.176267	0.128332
23	1	0	3.116659	-0.409100	1.057767
24	6	0	3.947462	-1.480103	-0.609705
25	1	0	4.473462	-1.246724	-1.540081
26	6	0	4.814862	-2.401838	0.230006
27	1	0	5.059755	-3.288590	-0.363490
28	1	0	5.738317	-1.892917	0.520005
29	8	0	2.870580	2.065038	0.056544
30	1	0	1.982419	2.242363	0.415496
31	8	0	4.903258	0.425319	0.420528
32	1	0	4.686489	1.321174	0.705971
33	8	0	2.751313	-2.155329	-0.964532
34	1	0	2.341897	-2.418075	-0.130484
35	8	0	4.038484	-2.758722	1.370088
36	1	0	4.464939	-3.503975	1.802576
37	6	0	-0.966005	2.987790	0.225538
38	1	0	-1.865335	2.704313	-0.341080
39	1	0	-1.249370	3.056508	1.279475
40	6	0	-0.450959	4.335235	-0.257015
41	1	0	-1.204715	5.106261	-0.084581
42	1	0	0.458468	4.614325	0.280770
43	1	0	-0.230237	4.320267	-1.326580
44	7	0	-5.482005	-1.345882	-0.182000
45	8	0	-6.357013	-1.044735	0.603396
46	8	0	-5.656138	-2.038784	-1.163082

Structure 21a (^{2}E ax-ax) (M06-2X, DMSO)

Energy (Hartrees): = - 1220.6637192
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.960280	0.686536	0.379823
2	6	0	-2.148819	-0.494965	1.092386
3	6	0	-3.314436	-1.234274	0.930264
4	6	0	-4.279261	-0.760426	0.055842
5	6	0	-4.123183	0.418803	-0.662247
6	6	0	-2.951378	1.137221	-0.495140
7	1	0	-1.382333	-0.837532	1.776088
8	1	0	-3.474333	-2.157696	1.470409
9	1	0	-4.900987	0.755925	-1.333508
10	1	0	-2.796763	2.055546	-1.050049
11	6	0	-0.703653	1.526459	0.543464
12	1	0	-0.963146	2.465464	1.037851
13	7	0	-0.068933	1.772304	-0.732623
14	8	0	0.261046	0.860306	1.358050
15	6	0	1.136191	0.109153	0.494549
16	6	0	0.712954	0.542852	-0.927549
17	1	0	1.557093	0.728686	-1.588162

18	1	0	0.081612	-0.223591	-1.379840
19	1	0	0.965067	-0.956311	0.666260
20	6	0	2.571877	0.485825	0.873285
21	1	0	2.846014	1.424247	0.369394
22	6	0	3.632732	-0.560864	0.544200
23	1	0	3.370606	-1.487187	1.075104
24	6	0	3.767053	-0.876414	-0.944565
25	1	0	3.858740	0.058377	-1.506227
26	6	0	4.978964	-1.744173	-1.231933
27	1	0	5.070100	-1.868984	-2.315839
28	1	0	5.885428	-1.276990	-0.840851
29	8	0	2.676396	0.655802	2.282100
30	1	0	1.891483	1.145896	2.554843
31	8	0	4.886513	-0.073778	0.995043
32	1	0	4.728737	0.279373	1.878290
33	8	0	2.600427	-1.541825	-1.406919
34	1	0	2.708236	-2.461096	-1.130185
35	8	0	4.722439	-2.996953	-0.602096
36	1	0	5.364260	-3.636208	-0.925024
37	6	0	0.731809	3.010760	-0.715753
38	1	0	1.257487	3.137384	0.241376
39	1	0	1.491682	2.919400	-1.494294
40	6	0	-0.144767	4.220766	-0.997081
41	1	0	0.454291	5.134592	-0.999983
42	1	0	-0.628063	4.118456	-1.971520
43	1	0	-0.923835	4.335462	-0.238415
44	7	0	-5.518549	-1.535129	-0.118622
45	8	0	-6.353816	-1.104375	-0.886994
46	8	0	-5.640982	-2.563800	0.514033

Structure 21a (E_2 ec-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 1220.661623
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.103307	-0.072823	-0.354751
2	6	0	2.558245	-0.074123	0.965010
3	6	0	3.905934	-0.233036	1.239796
4	6	0	4.780339	-0.387647	0.170126
5	6	0	4.359352	-0.387606	-1.149403
6	6	0	3.001788	-0.228077	-1.404748
7	1	0	1.847215	0.053565	1.772242
8	1	0	4.279444	-0.237642	2.254607
9	1	0	5.074267	-0.509538	-1.951493
10	1	0	2.643044	-0.224117	-2.427885
11	6	0	0.630656	0.120506	-0.618308
12	1	0	0.427475	0.032105	-1.701189
13	7	0	0.138176	1.379585	-0.086365
14	8	0	-0.106553	-0.855519	0.093095
15	6	0	-1.416983	-0.317502	0.376122
16	6	0	-1.307856	1.168069	0.004746
17	1	0	-1.798766	1.360618	-0.964659
18	1	0	-1.756619	1.813216	0.753188
19	1	0	-1.599039	-0.468927	1.442255
20	6	0	-2.413419	-1.134178	-0.450889
21	1	0	-2.341252	-0.819573	-1.502669
22	6	0	-3.882991	-1.086197	-0.035829
23	1	0	-3.956146	-1.438438	1.002829
24	6	0	-4.526713	0.296833	-0.122750
25	1	0	-4.264029	0.764831	-1.076167
26	6	0	-6.039495	0.230395	-0.008985
27	1	0	-6.442641	1.237530	-0.156594
28	1	0	-6.453463	-0.442591	-0.762567
29	8	0	-2.079135	-2.514825	-0.343456
30	1	0	-1.125565	-2.574217	-0.473594
31	8	0	-4.600739	-1.952950	-0.899922
32	1	0	-4.072682	-2.757373	-0.962582
33	8	0	-4.023817	1.124876	0.915053
34	1	0	-4.514287	0.862849	1.705446
35	8	0	-6.313969	-0.230733	1.311431
36	1	0	-7.246991	-0.088740	1.495482
37	6	0	0.517622	2.531347	-0.898587
38	1	0	1.607989	2.533418	-0.987159
39	1	0	0.103269	2.435813	-1.916729
40	6	0	0.054116	3.835267	-0.268764
41	1	0	0.429142	4.685642	-0.841616
42	1	0	-1.035887	3.903085	-0.244726
43	1	0	0.427192	3.916234	0.755103
44	7	0	6.216998	-0.556059	0.451646
45	8	0	6.961896	-0.745263	-0.487496
46	8	0	6.579654	-0.496814	1.608144

Structure 21b (^{2}E ec-ec H-bond O) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1220.6390864
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.962593	0.569213	-0.648108
2	6	0	-1.988332	-0.532628	0.208989
3	6	0	-3.194612	-1.111348	0.565858
4	6	0	-4.365097	-0.563561	0.056301
5	6	0	-4.371942	0.528310	-0.793209
6	6	0	-3.150751	1.091624	-1.146005
7	1	0	-1.055843	-0.931607	0.592616
8	1	0	-3.248737	-1.967326	1.224142
9	1	0	-5.312476	0.913280	-1.162213
10	1	0	-3.124854	1.944902	-1.814644
11	6	0	-0.633758	1.186127	-1.012725
12	1	0	-0.789174	1.990604	-1.756411
13	7	0	0.080298	1.671450	0.154841
14	8	0	0.223457	0.211703	-1.581668
15	6	0	1.546986	0.357032	-1.031992
16	6	0	1.474890	1.675703	-0.271580
17	1	0	2.153969	1.705616	0.577877
18	1	0	1.705067	2.525052	-0.935797
19	1	0	2.251597	0.382870	-1.862626
20	6	0	1.816911	-0.846089	-0.112763
21	1	0	1.456784	-0.603826	0.898427
22	6	0	3.281307	-1.271110	-0.022950
23	1	0	3.637475	-1.493625	-1.039176
24	6	0	4.199935	-0.219266	0.593710
25	1	0	3.781431	0.102230	1.553104
26	6	0	5.597492	-0.769075	0.824900
27	1	0	6.183286	-0.025299	1.376519
28	1	0	5.540792	-1.702403	1.388539
29	8	0	1.135619	-1.998479	-0.584526
30	1	0	0.381504	-1.686545	-1.099333
31	8	0	3.362002	-2.422377	0.793221
32	1	0	2.668262	-3.017203	0.487799
33	8	0	4.278698	0.921615	-0.245699
34	1	0	4.944004	0.704908	-0.910635
35	8	0	6.141569	-0.968812	-0.476063
36	1	0	7.035322	-1.305377	-0.396864
37	6	0	-0.425591	2.945561	0.644504
38	1	0	-0.307571	3.729981	-0.124382
39	1	0	-1.497806	2.826363	0.825997
40	6	0	0.264983	3.368999	1.932475
41	1	0	-0.196711	4.273331	2.331458
42	1	0	0.182170	2.576006	2.677777
43	1	0	1.323222	3.580319	1.767299
44	7	0	-5.658155	-1.172250	0.436842
45	8	0	-6.664802	-0.669906	-0.011052
46	8	0	-5.627253	-2.132944	1.172576

Structure 21b (^{2}E ec-ec H-bond N) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1220.6414382
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.416184	0.509402	-0.707919
2	6	0	-1.326809	-0.405768	0.341838
3	6	0	-2.424172	-1.177024	0.688435
4	6	0	-3.600802	-1.013472	-0.029988
5	6	0	-3.718527	-0.117156	-1.077775
6	6	0	-2.605864	0.644636	-1.415709
7	1	0	-0.392316	-0.508991	0.880953
8	1	0	-2.386509	-1.896207	1.494719
9	1	0	-4.657026	-0.033088	-1.607758
10	1	0	-2.665663	1.346564	-2.240377
11	6	0	-0.218743	1.359364	-1.055109
12	1	0	-0.379803	1.843313	-2.036604
13	7	0	0.056811	2.372364	-0.033189
14	8	0	0.950669	0.577599	-1.102541
15	6	0	2.043381	1.313775	-0.528247
16	6	0	1.458016	2.708272	-0.297778

17	1	0	1.911808	3.213638	0.555759
18	1	0	1.558279	3.339371	-1.194754
19	1	0	2.868790	1.310111	-1.236273
20	6	0	2.488179	0.648114	0.773583
21	1	0	3.434591	1.111933	1.086372
22	6	0	2.706841	-0.864757	0.669332
23	1	0	1.798866	-1.319240	0.252278
24	6	0	3.899277	-1.269598	-0.195209
25	1	0	4.801702	-0.807974	0.216891
26	6	0	4.070237	-2.780126	-0.198688
27	1	0	4.993376	-3.028748	-0.733609
28	1	0	4.115174	-3.150170	0.828395
29	8	0	1.544307	0.840735	1.826502
30	1	0	0.781991	1.335946	1.484319
31	8	0	2.969027	-1.367086	1.967060
32	1	0	2.328132	-0.944058	2.549147
33	8	0	3.758621	-0.807930	-1.525058
34	1	0	3.078623	-1.362638	-1.927120
35	8	0	2.936431	-3.288789	-0.893038
36	1	0	3.005167	-4.242766	-0.950285
37	6	0	-0.869750	3.498952	-0.067844
38	1	0	-0.817575	4.002105	-1.048580
39	1	0	-1.880042	3.095864	0.041278
40	6	0	-0.590386	4.494123	1.048504
41	1	0	-1.359917	5.267005	1.065927
42	1	0	-0.586900	3.986299	2.014859
43	1	0	0.373704	4.988235	0.913938
44	7	0	-4.776666	-1.832453	0.336500
45	8	0	-5.796801	-1.657272	-0.292046
46	8	0	-4.643957	-2.624543	1.241971

Structure 21b (^{2}E ax-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1220.6330062
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.004556	-0.379202	-0.669667
2	6	0	2.311170	0.885024	-0.175223
3	6	0	3.630353	1.234865	0.081664
4	6	0	4.622219	0.302254	-0.173222
5	6	0	4.349010	-0.959196	-0.681216
6	6	0	3.027122	-1.290831	-0.931740
7	1	0	1.514175	1.593330	0.008980
8	1	0	3.900536	2.207505	0.468865
9	1	0	5.161165	-1.647688	-0.868731
10	1	0	2.779193	-2.273361	-1.317471
11	6	0	0.582629	-0.809219	-0.909475
12	1	0	0.545047	-1.402909	-1.832991
13	7	0	-0.018360	-1.613969	0.139553
14	8	0	-0.266286	0.325838	-1.077942
15	6	0	-1.612887	-0.117754	-0.844386
16	6	0	-1.429523	-1.545422	-0.263458
17	1	0	-2.089682	-1.761188	0.572448
18	1	0	-1.623684	-2.288191	-1.038612
19	1	0	-2.145417	-0.134012	-1.798890
20	6	0	-2.258670	0.895534	0.102621
21	1	0	-1.962312	0.668601	1.138177
22	6	0	-3.782659	0.968808	0.044643
23	1	0	-4.071029	1.222258	-0.985200
24	6	0	-4.495085	-0.321571	0.440545
25	1	0	-4.112028	-0.663986	1.407682
26	6	0	-5.996035	-0.112324	0.553593
27	1	0	-6.450829	-1.025245	0.953969
28	1	0	-6.204004	0.735639	1.208915
29	8	0	-1.838765	2.211921	-0.226729
30	1	0	-0.929101	2.148012	-0.535818
31	8	0	-4.211125	1.974431	0.941611
32	1	0	-3.653235	2.741529	0.772865
33	8	0	-4.233848	-1.339534	-0.511134
34	1	0	-4.858994	-1.185777	-1.230448
35	8	0	-6.442321	0.126326	-0.777331
36	1	0	-7.387942	0.281347	-0.771272
37	6	0	0.220321	-1.115972	1.509537
38	1	0	0.298771	-0.020252	1.540433
39	1	0	-0.662238	-1.378946	2.096380
40	6	0	1.438371	-1.757340	2.164528
41	1	0	1.472151	-1.494217	3.224253
42	1	0	1.373429	-2.843025	2.075396
43	1	0	2.373549	-1.430864	1.709520
44	7	0	6.028416	0.668906	0.099416
45	8	0	6.877099	-0.160747	-0.139300

46	8	0	6.239837	1.774385	0.545361

Structure 21b (^{2}E ec-ec H-bond O) (M06-2X, Benzene)

Energy (Hartrees): = - 1220.6613835
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.972033	0.561522	-0.646814
2	6	0	-2.003534	-0.529300	0.224081
3	6	0	-3.211237	-1.104789	0.580200
4	6	0	-4.378835	-0.561197	0.058185
5	6	0	-4.380311	0.522135	-0.803308
6	6	0	-3.157180	1.080116	-1.156838
7	1	0	-1.074809	-0.924093	0.620738
8	1	0	-3.262932	-1.953875	1.247692
9	1	0	-5.315544	0.909226	-1.183557
10	1	0	-3.128289	1.925379	-1.835421
11	6	0	-0.639918	1.172911	-1.011984
12	1	0	-0.790044	1.969102	-1.764079
13	7	0	0.072667	1.666264	0.153138
14	8	0	0.216011	0.186520	-1.566142
15	6	0	1.543943	0.345134	-1.027002
16	6	0	1.468295	1.667478	-0.273219
17	1	0	2.144069	1.702475	0.578776
18	1	0	1.697180	2.513692	-0.941021
19	1	0	2.241197	0.370792	-1.864017
20	6	0	1.829395	-0.852979	-0.105855
21	1	0	1.470426	-0.613631	0.906343
22	6	0	3.298117	-1.265875	-0.021351
23	1	0	3.651065	-1.485782	-1.039058
24	6	0	4.213514	-0.208687	0.593179
25	1	0	3.795794	0.115502	1.551955
26	6	0	5.614435	-0.747554	0.824775
27	1	0	6.198279	0.007170	1.363452
28	1	0	5.572486	-1.671101	1.405971
29	8	0	1.157258	-2.012992	-0.577233
30	1	0	0.380002	-1.704987	-1.059339
31	8	0	3.389043	-2.421025	0.791860
32	1	0	2.698255	-3.018791	0.484764
33	8	0	4.287426	0.930127	-0.251428
34	1	0	4.943763	0.707038	-0.923674
35	8	0	6.157755	-0.966574	-0.473777
36	1	0	7.069495	-1.252852	-0.385203
37	6	0	-0.429770	2.947879	0.631238
38	1	0	-0.312510	3.723758	-0.145505
39	1	0	-1.501267	2.834034	0.819174
40	6	0	0.267042	3.382511	1.910962
41	1	0	-0.200083	4.285181	2.309130
42	1	0	0.197443	2.593921	2.663425
43	1	0	1.322363	3.603803	1.737814
44	7	0	-5.671748	-1.165450	0.436021
45	8	0	-6.682302	-0.625623	0.040300
46	8	0	-5.646981	-2.165117	1.120175

Structure 21b (^{2}E ec-ec H-bond N) (M06-2X, Benzene)

Energy (Hartrees): = - 1220.6642615
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.409699	0.523901	-0.700514
2	6	0	-1.338359	-0.358722	0.378358
3	6	0	-2.438255	-1.125249	0.726551
4	6	0	-3.601144	-0.989754	-0.020387
5	6	0	-3.701637	-0.124667	-1.096645
6	6	0	-2.586351	0.632822	-1.434475
7	1	0	-0.415703	-0.445341	0.940541
8	1	0	-2.406943	-1.818763	1.555386
9	1	0	-4.626974	-0.056744	-1.651723
10	1	0	-2.633652	1.310753	-2.279677
11	6	0	-0.208140	1.365794	-1.056059
12	1	0	-0.372037	1.846541	-2.037594
13	7	0	0.085934	2.378045	-0.039771
14	8	0	0.955531	0.571146	-1.108955
15	6	0	2.059219	1.303592	-0.548021
16	6	0	1.486626	2.703650	-0.325184

17	1	0	1.953723	3.217314	0.515852
18	1	0	1.578970	3.322444	-1.230600
19	1	0	2.878954	1.290910	-1.262280
20	6	0	2.510418	0.645192	0.755827
21	1	0	3.468573	1.096407	1.049347
22	6	0	2.696451	-0.873831	0.669939
23	1	0	1.774175	-1.312621	0.268714
24	6	0	3.871508	-1.321108	-0.197900
25	1	0	4.790871	-0.882316	0.201681
26	6	0	4.002438	-2.835067	-0.192507
27	1	0	4.910315	-3.111441	-0.739738
28	1	0	4.060388	-3.203960	0.834692
29	8	0	1.582841	0.872069	1.818572
30	1	0	0.820208	1.364073	1.468629
31	8	0	2.954949	-1.365254	1.974888
32	1	0	2.321669	-0.921617	2.550493
33	8	0	3.732887	-0.868341	-1.532689
34	1	0	3.026639	-1.401861	-1.918312
35	8	0	2.844947	-3.326351	-0.860912
36	1	0	2.936385	-4.273829	-0.982170
37	6	0	-0.832000	3.513802	-0.068825
38	1	0	-0.779266	4.016177	-1.049034
39	1	0	-1.845511	3.120844	0.046545
40	6	0	-0.540103	4.505520	1.045954
41	1	0	-1.305341	5.283580	1.064180
42	1	0	-0.539480	4.000205	2.014294
43	1	0	0.426563	4.995179	0.910297
44	7	0	-4.776135	-1.806789	0.341790
45	8	0	-5.786165	-1.661560	-0.312428
46	8	0	-4.662109	-2.575457	1.271483

Structure 21b (^{2}E ax-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 1220.6548393
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.009160	-0.373731	-0.660307
2	6	0	2.324331	0.899074	-0.193765
3	6	0	3.645961	1.245364	0.055612
4	6	0	4.631341	0.298748	-0.174048
5	6	0	4.348699	-0.974257	-0.649200
6	6	0	3.025183	-1.301675	-0.893756
7	1	0	1.535601	1.620977	-0.026657
8	1	0	3.917007	2.227190	0.418442
9	1	0	5.151209	-1.678672	-0.818988
10	1	0	2.771241	-2.291912	-1.255357
11	6	0	0.585975	-0.798715	-0.905513
12	1	0	0.550800	-1.385416	-1.833322
13	7	0	-0.019186	-1.610698	0.136170
14	8	0	-0.263330	0.338074	-1.066869
15	6	0	-1.611470	-0.110036	-0.843393
16	6	0	-1.428152	-1.543454	-0.278563
17	1	0	-2.092718	-1.770078	0.550794
18	1	0	-1.609374	-2.276949	-1.065605
19	1	0	-2.139170	-0.114319	-1.800529
20	6	0	-2.261898	0.888798	0.116885
21	1	0	-1.970367	0.645550	1.149467
22	6	0	-3.785907	0.967298	0.056485
23	1	0	-4.070958	1.247035	-0.967279
24	6	0	-4.504260	-0.329770	0.421212
25	1	0	-4.126422	-0.695427	1.381652
26	6	0	-6.005697	-0.126119	0.531959
27	1	0	-6.460074	-1.053109	0.899116
28	1	0	-6.226144	0.694347	1.217993
29	8	0	-1.836659	2.210711	-0.190609
30	1	0	-0.915352	2.149405	-0.465336
31	8	0	-4.211892	1.956403	0.976067
32	1	0	-3.649830	2.724108	0.823638
33	8	0	-4.240072	-1.326285	-0.553657
34	1	0	-4.855708	-1.146400	-1.275639
35	8	0	-6.451144	0.160080	-0.790306
36	1	0	-7.409727	0.207849	-0.792277
37	6	0	0.205847	-1.115505	1.510546
38	1	0	0.288241	-0.020311	1.542573
39	1	0	-0.682960	-1.377390	2.088104
40	6	0	1.414483	-1.759859	2.177842
41	1	0	1.424773	-1.514376	3.242849
42	1	0	1.360797	-2.845494	2.072912
43	1	0	2.358417	-1.420239	1.750313
44	7	0	6.037869	0.662038	0.086453

45	8	0	6.887207	-0.167060	-0.157801
46	8	0	6.260685	1.767737	0.529775

Structure 21b (^{2}E ec-ec H-bond O) (M06-2X, DMSO)

Energy (Hartrees): = - 1220.6648592
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.982565	0.553980	-0.635284
2	6	0	-2.023039	-0.536553	0.236261
3	6	0	-3.234645	-1.104228	0.592016
4	6	0	-4.397297	-0.552447	0.066345
5	6	0	-4.390552	0.532562	-0.794218
6	6	0	-3.163307	1.082657	-1.146301
7	1	0	-1.100236	-0.939497	0.639132
8	1	0	-3.286715	-1.951608	1.261913
9	1	0	-5.319259	0.930520	-1.179814
10	1	0	-3.127340	1.928927	-1.823217
11	6	0	-0.646489	1.153789	-1.004204
12	1	0	-0.789519	1.946109	-1.759068
13	7	0	0.070731	1.648948	0.159119
14	8	0	0.199638	0.151063	-1.548562
15	6	0	1.536324	0.320548	-1.031751
16	6	0	1.465708	1.642669	-0.276660
17	1	0	2.143557	1.676087	0.574056
18	1	0	1.688575	2.488187	-0.946078
19	1	0	2.220869	0.349622	-1.879276
20	6	0	1.841500	-0.876610	-0.119185
21	1	0	1.469087	-0.654934	0.892027
22	6	0	3.315980	-1.261502	-0.024280
23	1	0	3.673977	-1.486236	-1.039091
24	6	0	4.212760	-0.180035	0.576254
25	1	0	3.775446	0.174161	1.515048
26	6	0	5.614793	-0.692180	0.852261
27	1	0	6.181891	0.100295	1.351670
28	1	0	5.581397	-1.576195	1.492637
29	8	0	1.199677	-2.047867	-0.611150
30	1	0	0.376850	-1.754058	-1.021683
31	8	0	3.421176	-2.411279	0.800095
32	1	0	2.729153	-3.013299	0.503244
33	8	0	4.292129	0.930964	-0.305771
34	1	0	4.941981	0.677548	-0.974211
35	8	0	6.182430	-0.988220	-0.421364
36	1	0	7.125708	-1.135812	-0.306637
37	6	0	-0.418047	2.948082	0.611571
38	1	0	-0.295712	3.702057	-0.183982
39	1	0	-1.490108	2.850357	0.806006
40	6	0	0.291643	3.404111	1.876255
41	1	0	-0.163348	4.322007	2.253602
42	1	0	0.218179	2.636818	2.650915
43	1	0	1.348609	3.607587	1.690530
44	7	0	-5.692010	-1.149049	0.438838
45	8	0	-6.702600	-0.600153	0.051578
46	8	0	-5.678783	-2.157882	1.112934

Structure 21b (^{2}E ec-ec H-bond N) (M06-2X, DMSO)

Energy (Hartrees): = - 1220.6683257
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.417877	0.528031	-0.706053
2	6	0	-1.315920	-0.408920	0.324325
3	6	0	-2.407143	-1.189101	0.670045
4	6	0	-3.592743	-1.011860	-0.032363
5	6	0	-3.724421	-0.091705	-1.059629
6	6	0	-2.617817	0.679641	-1.394631
7	1	0	-0.377763	-0.528354	0.853926
8	1	0	-2.346368	-1.921136	1.463660
9	1	0	-4.664680	0.014093	-1.583006
10	1	0	-2.690820	1.403181	-2.199124
11	6	0	-0.225578	1.384400	-1.058474
12	1	0	-0.398538	1.878392	-2.029457
13	7	0	0.067382	2.380799	-0.025927
14	8	0	0.944831	0.594054	-1.129280
15	6	0	2.043374	1.321079	-0.548309

16	6	0	1.467196	2.715995	-0.315885
17	1	0	1.936118	3.229203	0.523951
18	1	0	1.549302	3.337370	-1.219175
19	1	0	2.870287	1.320576	-1.253815
20	6	0	2.485780	0.651235	0.753090
21	1	0	3.439419	1.104473	1.056484
22	6	0	2.677908	-0.866725	0.652506
23	1	0	1.775307	-1.301873	0.205472
24	6	0	3.892453	-1.295261	-0.168935
25	1	0	4.788709	-0.842393	0.265474
26	6	0	4.051210	-2.805582	-0.167548
27	1	0	4.974364	-3.061990	-0.697471
28	1	0	4.102329	-3.181711	0.857383
29	8	0	1.545970	0.866848	1.809478
30	1	0	0.786733	1.360622	1.448936
31	8	0	2.873565	-1.379993	1.962348
32	1	0	2.225353	-0.923192	2.511633
33	8	0	3.796464	-0.838382	-1.508501
34	1	0	3.117399	-1.387725	-1.920534
35	8	0	2.916598	-3.324893	-0.856957
36	1	0	3.083221	-4.249857	-1.059692
37	6	0	-0.850087	3.519775	-0.048528
38	1	0	-0.789187	4.028536	-1.023382
39	1	0	-1.865685	3.129523	0.058240
40	6	0	-0.557002	4.497478	1.077683
41	1	0	-1.314392	5.283475	1.094574
42	1	0	-0.571413	3.983826	2.042165
43	1	0	0.417291	4.975137	0.953372
44	7	0	-4.757208	-1.839733	0.327539
45	8	0	-5.779454	-1.690560	-0.309228
46	8	0	-4.632251	-2.628139	1.241559

Structure 21b (^{2}E ax-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 1220.6594914
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.008931	-0.402543	-0.671596
2	6	0	2.310212	0.876021	-0.208964
3	6	0	3.626722	1.230665	0.054314
4	6	0	4.620466	0.288234	-0.161686
5	6	0	4.351998	-0.988450	-0.636127
6	6	0	3.032843	-1.324684	-0.893231
7	1	0	1.518677	1.597423	-0.050124
8	1	0	3.880650	2.217377	0.416786
9	1	0	5.156127	-1.693025	-0.798400
10	1	0	2.791451	-2.316432	-1.259678
11	6	0	0.590832	-0.843783	-0.915600
12	1	0	0.568240	-1.475197	-1.812758
13	7	0	-0.020989	-1.607470	0.162513
14	8	0	-0.258373	0.282995	-1.136765
15	6	0	-1.607562	-0.147937	-0.884605
16	6	0	-1.428813	-1.557559	-0.265460
17	1	0	-2.096277	-1.749865	0.570461
18	1	0	-1.598527	-2.318358	-1.028984
19	1	0	-2.145105	-0.184641	-1.835223
20	6	0	-2.243240	0.887510	0.045079
21	1	0	-1.934231	0.686638	1.080612
22	6	0	-3.767122	0.958150	0.009868
23	1	0	-4.072906	1.203306	-1.016986
24	6	0	-4.466382	-0.335721	0.424159
25	1	0	-4.028563	-0.706357	1.356565
26	6	0	-5.956370	-0.137214	0.631893
27	1	0	-6.384751	-1.078748	0.991496
28	1	0	-6.138662	0.650528	1.366018
29	8	0	-1.825529	2.197320	-0.327206
30	1	0	-0.881889	2.140809	-0.517410
31	8	0	-4.180183	1.980051	0.902949
32	1	0	-3.602353	2.731933	0.728793
33	8	0	-4.264656	-1.331263	-0.569463
34	1	0	-4.897569	-1.121770	-1.268680
35	8	0	-6.491501	0.201993	-0.644436
36	1	0	-7.450371	0.148729	-0.594188
37	6	0	0.189600	-1.034705	1.511497
38	1	0	0.273694	0.059535	1.482019
39	1	0	-0.705539	-1.262335	2.093421
40	6	0	1.392683	-1.638137	2.224913
41	1	0	1.410999	-1.300996	3.264583
42	1	0	1.324761	-2.728679	2.218350
43	1	0	2.339573	-1.351187	1.764743
44	7	0	6.018736	0.660183	0.113887

45	8	0	6.882914	-0.153178	-0.139408
46	8	0	6.232273	1.759988	0.580212

Structure 21c ($^5C_2$ ec-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1220.6385534
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.219797	1.499066	0.306715
2	6	0	-1.225608	2.501555	-0.271874
3	6	0	-1.983801	0.150298	-0.371682
4	1	0	-1.350602	3.446965	0.254146
5	1	0	-1.420387	2.667101	-1.346700
6	1	0	-3.244183	1.823360	0.133278
7	1	0	-2.156422	0.235621	-1.455839
8	8	0	-0.614925	-0.209383	-0.154889
9	7	0	0.140733	2.013124	-0.049972
10	6	0	-2.800166	-1.015262	0.183322
11	1	0	-2.803042	-0.934531	1.277636
12	6	0	-4.232404	-1.017418	-0.327118
13	1	0	-4.209876	-1.114590	-1.422480
14	6	0	-5.008111	-2.194377	0.236929
15	1	0	-4.955465	-2.158807	1.332272
16	1	0	-4.579632	-3.132203	-0.123578
17	8	0	-2.243487	-2.244762	-0.240568
18	1	0	-1.289762	-2.164866	-0.136662
19	8	0	-4.858088	0.190667	0.052649
20	1	0	-5.804143	0.036227	-0.049872
21	8	0	-6.347039	-2.012491	-0.211666
22	1	0	-6.912891	-2.647790	0.229551
23	8	0	-2.037650	1.401369	1.703001
24	1	0	-1.087302	1.305838	1.835985
25	6	0	1.145057	2.975218	-0.515735
26	1	0	1.038809	3.149285	-1.601541
27	1	0	2.129650	2.532242	-0.357778
28	6	0	1.675135	0.130477	-0.455451
29	6	0	2.084112	-0.100997	0.858238
30	6	0	2.513655	-0.199574	-1.514228
31	6	0	3.327668	-0.652966	1.116970
32	1	0	1.417476	0.157542	1.671378
33	6	0	3.765876	-0.753485	-1.273920
34	1	0	2.190037	-0.024329	-2.533967
35	6	0	4.145178	-0.967127	0.039547
36	1	0	3.675113	-0.844855	2.122709
37	1	0	4.440741	-1.019759	-2.075455
38	6	0	0.302563	0.712554	-0.696935
39	1	0	0.117458	0.799819	-1.787012
40	6	0	1.082424	4.301168	0.231748
41	1	0	1.970916	4.891904	0.003997
42	1	0	0.212573	4.897932	-0.044066
43	1	0	1.053148	4.120602	1.308145
44	7	0	5.475738	-1.556020	0.306060
45	8	0	5.786305	-1.729001	1.463091
46	8	0	6.167610	-1.826053	-0.649855

Structure 21c ($^5C_2$ ax-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1220.6363429
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.267144	1.631603	0.052255
2	6	0	1.184754	2.486841	0.728569
3	6	0	2.017911	0.167187	0.421297
4	1	0	1.286847	3.526522	0.416006
5	1	0	1.325110	2.447900	1.815122
6	1	0	3.259073	1.929865	0.388880
7	1	0	2.091753	0.037645	1.511621
8	8	0	0.678494	-0.161119	0.019104
9	7	0	-0.178894	2.028769	0.426870
10	6	0	2.921016	-0.863079	-0.254687
11	1	0	3.009090	-0.611664	-1.319725
12	6	0	4.313250	-0.908957	0.356965
13	1	0	4.215959	-1.164083	1.422567
14	6	0	5.163074	-1.977597	-0.307987
15	1	0	5.193092	-1.783443	-1.387566

16	1	0	4.735481	-2.965520	-0.122554
17	8	0	2.381445	-2.158994	-0.078906
18	1	0	1.427560	-2.075697	-0.177893
19	8	0	4.925802	0.352999	0.199736
20	1	0	5.866019	0.207693	0.355987
21	8	0	6.456860	-1.838846	0.267754
22	1	0	7.074486	-2.393254	-0.211587
23	8	0	2.246542	1.797711	-1.354464
24	1	0	1.487129	1.308769	-1.687844
25	6	0	-0.677276	2.414518	-0.909259
26	1	0	-0.682644	1.551300	-1.589386
27	1	0	0.026096	3.131139	-1.335438
28	6	0	-1.655171	0.063255	0.495561
29	6	0	-1.920103	-0.791871	-0.569327
30	6	0	-2.682979	0.435963	1.362219
31	6	0	-3.209191	-1.265069	-0.783188
32	1	0	-1.115301	-1.084833	-1.230782
33	6	0	-3.972201	-0.031727	1.167811
34	1	0	-2.467731	1.113708	2.180670
35	6	0	-4.208952	-0.873745	0.090301
36	1	0	-3.448278	-1.925458	-1.605233
37	1	0	-4.788563	0.240535	1.822166
38	6	0	-0.274797	0.624123	0.739010
39	1	0	-0.039983	0.518129	1.808137
40	6	0	-2.066685	3.040286	-0.859185
41	1	0	-2.350999	3.405762	-1.848687
42	1	0	-2.820998	2.323943	-0.532209
43	1	0	-2.069433	3.881251	-0.163496
44	7	0	-5.582085	-1.375766	-0.129560
45	8	0	-6.438330	-1.013610	0.645871
46	8	0	-5.761524	-2.115842	-1.070604

Structure 21c ($^5C_2$ ec-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 1220.6617263
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.216907	1.505371	0.290627
2	6	0	-1.222495	2.504378	-0.293152
3	6	0	-1.982804	0.155231	-0.383895
4	1	0	-1.345947	3.453525	0.226848
5	1	0	-1.419816	2.663133	-1.367853
6	1	0	-3.240002	1.833310	0.116509
7	1	0	-2.152768	0.241790	-1.468123
8	8	0	-0.614715	-0.205779	-0.162563
9	7	0	0.143903	2.016312	-0.069670
10	6	0	-2.796901	-1.014669	0.164278
11	1	0	-2.771701	-0.965425	1.260085
12	6	0	-4.243846	-0.996501	-0.303915
13	1	0	-4.257822	-1.014878	-1.403800
14	6	0	-4.996738	-2.215005	0.201179
15	1	0	-4.904079	-2.264986	1.293133
16	1	0	-4.586691	-3.125287	-0.242241
17	8	0	-2.252738	-2.235840	-0.304604
18	1	0	-1.296469	-2.156341	-0.219252
19	8	0	-4.867206	0.177064	0.179518
20	1	0	-5.814877	0.012895	0.106126
21	8	0	-6.353194	-2.008179	-0.181991
22	1	0	-6.902248	-2.656286	0.264929
23	8	0	-2.034017	1.411135	1.688717
24	1	0	-1.083221	1.308404	1.818208
25	6	0	1.147755	2.978364	-0.540002
26	1	0	1.034202	3.156859	-1.623653
27	1	0	2.132802	2.533733	-0.389321
28	6	0	1.676801	0.128268	-0.459536
29	6	0	2.093276	-0.066909	0.858016
30	6	0	2.505191	-0.239054	-1.514469
31	6	0	3.334366	-0.619799	1.124975
32	1	0	1.438033	0.222518	1.670367
33	6	0	3.754708	-0.794996	-1.266116
34	1	0	2.177143	-0.090842	-2.537085
35	6	0	4.141777	-0.972941	0.051133
36	1	0	3.681861	-0.780108	2.136295
37	1	0	4.418023	-1.086614	-2.068706
38	6	0	0.306332	0.712962	-0.710599
39	1	0	0.124120	0.791990	-1.800427
40	6	0	1.093553	4.300698	0.212644
41	1	0	1.982685	4.889992	-0.019821
42	1	0	0.224095	4.902911	-0.054106
43	1	0	1.073632	4.119033	1.289716
44	7	0	5.469425	-1.558565	0.325501

45	8	0	5.788976	-1.708730	1.484621
46	8	0	6.161810	-1.852914	-0.624406

Structure 21c ($^5C_2$ ax-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 1220.6589075
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.269292	1.636659	0.070326
2	6	0	1.182040	2.493118	0.736766
3	6	0	2.016178	0.171268	0.432646
4	1	0	1.288566	3.533147	0.426353
5	1	0	1.314876	2.451360	1.823846
6	1	0	3.256430	1.935821	0.420100
7	1	0	2.086637	0.037927	1.522277
8	8	0	0.677537	-0.152495	0.023522
9	7	0	-0.180472	2.037059	0.424250
10	6	0	2.916042	-0.860127	-0.247751
11	1	0	3.000313	-0.610081	-1.313193
12	6	0	4.311326	-0.916016	0.356904
13	1	0	4.218715	-1.167567	1.423619
14	6	0	5.152320	-1.989009	-0.312186
15	1	0	5.180801	-1.796994	-1.392078
16	1	0	4.724585	-2.977226	-0.127255
17	8	0	2.367511	-2.154420	-0.073892
18	1	0	1.414179	-2.061524	-0.175153
19	8	0	4.934444	0.342015	0.195013
20	1	0	5.874836	0.184665	0.341578
21	8	0	6.450848	-1.861670	0.257817
22	1	0	7.066244	-2.393194	-0.252390
23	8	0	2.266763	1.806463	-1.338029
24	1	0	1.503922	1.328183	-1.680468
25	6	0	-0.666110	2.418686	-0.918326
26	1	0	-0.658205	1.556442	-1.599849
27	1	0	0.035358	3.142903	-1.334572
28	6	0	-1.657745	0.069713	0.495845
29	6	0	-1.915623	-0.805550	-0.554718
30	6	0	-2.692768	0.461898	1.346088
31	6	0	-3.202945	-1.282699	-0.768647
32	1	0	-1.109310	-1.113302	-1.207517
33	6	0	-3.980467	-0.009403	1.151789
34	1	0	-2.486123	1.155716	2.153320
35	6	0	-4.209582	-0.874156	0.089892
36	1	0	-3.429454	-1.959265	-1.581142
37	1	0	-4.797076	0.280421	1.798418
38	6	0	-0.278077	0.632609	0.741071
39	1	0	-0.045705	0.530905	1.810448
40	6	0	-2.058319	3.037649	-0.887018
41	1	0	-2.325531	3.411812	-1.878676
42	1	0	-2.819277	2.317815	-0.582867
43	1	0	-2.079311	3.873700	-0.184756
44	7	0	-5.577885	-1.381407	-0.128837
45	8	0	-6.433648	-1.049725	0.662753
46	8	0	-5.765996	-2.100052	-1.086438

Structure 21c ($^5C_2$ ec-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 1220.6663214
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.206856	1.505927	0.303387
2	6	0	-1.217413	2.506968	-0.282940
3	6	0	-1.982846	0.164540	-0.388826
4	1	0	-1.336868	3.457529	0.235733
5	1	0	-1.420715	2.662200	-1.355764
6	1	0	-3.229944	1.841016	0.143825
7	1	0	-2.157845	0.270564	-1.469573
8	8	0	-0.615240	-0.204801	-0.176586
9	7	0	0.150505	2.017206	-0.066759
10	6	0	-2.796447	-1.012168	0.143052
11	1	0	-2.751121	-0.999474	1.239293
12	6	0	-4.253320	-0.970713	-0.291627
13	1	0	-4.293383	-0.911016	-1.389131
14	6	0	-4.993392	-2.221722	0.149722

15	1	0	-4.876467	-2.345448	1.233133
16	1	0	-4.595415	-3.101291	-0.361194
17	8	0	-2.264180	-2.223323	-0.370583
18	1	0	-1.305447	-2.131071	-0.326733
19	8	0	-4.870885	0.165922	0.286158
20	1	0	-5.818966	-0.003857	0.223388
21	8	0	-6.359867	-1.998475	-0.188984
22	1	0	-6.896793	-2.652506	0.267880
23	8	0	-2.006963	1.394470	1.701821
24	1	0	-1.055318	1.269719	1.812818
25	6	0	1.147835	2.981436	-0.551559
26	1	0	1.011169	3.164840	-1.630454
27	1	0	2.135631	2.535368	-0.422804
28	6	0	1.676609	0.129763	-0.463517
29	6	0	2.077390	-0.088217	0.855880
30	6	0	2.518043	-0.214330	-1.516319
31	6	0	3.316003	-0.644681	1.127475
32	1	0	1.414527	0.183188	1.669022
33	6	0	3.765674	-0.772555	-1.263416
34	1	0	2.202265	-0.044122	-2.539403
35	6	0	4.136683	-0.975393	0.055762
36	1	0	3.645969	-0.821018	2.142175
37	1	0	4.434730	-1.044173	-2.068429
38	6	0	0.309183	0.718398	-0.720156
39	1	0	0.130543	0.805693	-1.807656
40	6	0	1.109226	4.298229	0.211006
41	1	0	1.991773	4.890170	-0.040209
42	1	0	0.231155	4.898681	-0.030950
43	1	0	1.116621	4.111235	1.287919
44	7	0	5.457584	-1.566234	0.334974
45	8	0	5.761054	-1.754479	1.494705
46	8	0	6.172211	-1.832555	-0.608774

Structure 21c ($^5C_2$ ax-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 1220.6637384
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.262001	1.637971	0.089412
2	6	0	1.170124	2.480027	0.764776
3	6	0	2.016844	0.169587	0.437274
4	1	0	1.268013	3.524574	0.465964
5	1	0	1.308654	2.421307	1.849890
6	1	0	3.243930	1.940331	0.451942
7	1	0	2.089340	0.033854	1.525769
8	8	0	0.680479	-0.160680	0.027058
9	7	0	-0.192216	2.018498	0.452610
10	6	0	2.922428	-0.853026	-0.246139
11	1	0	2.986267	-0.621954	-1.317131
12	6	0	4.330155	-0.873242	0.332312
13	1	0	4.262432	-1.026767	1.419363
14	6	0	5.151064	-2.005170	-0.261177
15	1	0	5.147097	-1.918664	-1.354537
16	1	0	4.733991	-2.972056	0.028606
17	8	0	2.390987	-2.152595	-0.043943
18	1	0	1.436299	-2.069732	-0.150338
19	8	0	4.961063	0.361791	0.046057
20	1	0	5.904084	0.197347	0.170639
21	8	0	6.468674	-1.832327	0.253795
22	1	0	7.069336	-2.381805	-0.258423
23	8	0	2.268576	1.826273	-1.318934
24	1	0	1.508618	1.349731	-1.672942
25	6	0	-0.673963	2.396699	-0.892908
26	1	0	-0.624202	1.546203	-1.586908
27	1	0	0.003406	3.154658	-1.288126
28	6	0	-1.653591	0.042933	0.510431
29	6	0	-1.931518	-0.750011	-0.599510
30	6	0	-2.669228	0.364513	1.411960
31	6	0	-3.223566	-1.208565	-0.824576
32	1	0	-1.140708	-1.008661	-1.291745
33	6	0	-3.962026	-0.087258	1.205812
34	1	0	-2.443752	0.981703	2.274740
35	6	0	-4.213334	-0.863268	0.081637
36	1	0	-3.461029	-1.820221	-1.684405
37	1	0	-4.760835	0.152749	1.893873
38	6	0	-0.276643	0.607436	0.760027
39	1	0	-0.041255	0.498747	1.827057
40	6	0	-2.088977	2.962883	-0.874795
41	1	0	-2.358272	3.326795	-1.869947
42	1	0	-2.826989	2.215168	-0.579111
43	1	0	-2.149908	3.799540	-0.174605

44	7	0	-5.585078	-1.345508	-0.151654
45	8	0	-6.439829	-1.038440	0.653434
46	8	0	-5.788962	-2.024377	-1.136658

Structure 21d ($^5C_2$ ec-ax) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1220.6359682
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.834210	1.257363	-0.877743
2	6	0	-0.567846	2.046378	-1.222260
3	6	0	-1.445538	0.141323	0.098526
4	1	0	-0.842760	2.898944	-1.845448
5	1	0	0.144481	1.419012	-1.781545
6	1	0	-2.286270	0.818917	-1.765258
7	1	0	-0.719981	-0.530854	-0.380939
8	8	0	-0.842532	0.740438	1.257253
9	7	0	-0.018787	2.539934	0.032934
10	6	0	-2.617071	-0.681468	0.639355
11	1	0	-3.460957	-0.001642	0.812249
12	6	0	-3.035771	-1.783942	-0.318892
13	1	0	-2.192765	-2.481784	-0.428196
14	6	0	-4.225050	-2.557654	0.220230
15	1	0	-5.045565	-1.854718	0.411477
16	1	0	-3.950247	-3.066038	1.147614
17	8	0	-2.242147	-1.343647	1.835043
18	1	0	-1.820865	-0.680478	2.390783
19	8	0	-3.366643	-1.206075	-1.564491
20	1	0	-3.847788	-1.887107	-2.048323
21	8	0	-4.574629	-3.476605	-0.808643
22	1	0	-5.406727	-3.895520	-0.583803
23	8	0	-2.784708	2.123198	-0.297437
24	1	0	-2.311075	2.582577	0.407555
25	6	0	0.762782	3.768101	0.000434
26	1	0	1.395148	3.811547	-0.897850
27	1	0	1.440909	3.769916	0.859246
28	6	0	1.464785	0.550911	0.561135
29	6	0	2.501817	0.991866	-0.258918
30	6	0	1.504982	-0.746952	1.076785
31	6	0	3.573035	0.160454	-0.559481
32	1	0	2.475772	1.989631	-0.676560
33	6	0	2.565595	-1.591737	0.785791
34	1	0	0.681449	-1.101376	1.685647
35	6	0	3.583983	-1.116827	-0.026127
36	1	0	4.386940	0.480559	-1.195086
37	1	0	2.615157	-2.601517	1.169183
38	6	0	0.319424	1.492108	0.963803
39	1	0	0.600342	1.968241	1.908267
40	6	0	-0.138223	4.998352	0.048799
41	1	0	0.447503	5.917378	-0.022789
42	1	0	-0.853359	4.984423	-0.776537
43	1	0	-0.702868	5.013216	0.982577
44	7	0	4.719072	-2.009493	-0.341763
45	8	0	5.589158	-1.571858	-1.061464
46	8	0	4.705922	-3.119960	0.139853

Structure 21d ($^5C_2$ ax-ax) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1220.6399453
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.845524	1.221889	-1.044859
2	6	0	-0.565548	1.954735	-1.464133
3	6	0	-1.453793	0.193434	0.015213
4	1	0	-0.804972	2.744665	-2.176619
5	1	0	0.106711	1.244896	-1.960457
6	1	0	-2.300517	0.717140	-1.896011
7	1	0	-0.722163	-0.506054	-0.409433
8	8	0	-0.851313	0.913373	1.104145
9	7	0	0.145976	2.549303	-0.327199
10	6	0	-2.597387	-0.609997	0.638142
11	1	0	-3.459303	0.053751	0.787007
12	6	0	-3.014903	-1.778898	-0.238615
13	1	0	-2.151095	-2.450292	-0.352570

14	6	0	-4.147268	-2.568215	0.394161
15	1	0	-4.983799	-1.887505	0.596652
16	1	0	-3.808862	-3.024753	1.327469
17	8	0	-2.175011	-1.180089	1.864354
18	1	0	-1.735749	-0.476694	2.353768
19	8	0	-3.423902	-1.276612	-1.493000
20	1	0	-3.901350	-1.997515	-1.919580
21	8	0	-4.510717	-3.543410	-0.575709
22	1	0	-5.313753	-3.982984	-0.291972
23	8	0	-2.807913	2.127766	-0.534858
24	1	0	-2.530424	2.357636	0.357815
25	6	0	-0.357894	3.841726	0.155400
26	1	0	-1.058237	3.715561	0.994481
27	1	0	-0.925803	4.308389	-0.650507
28	6	0	1.469614	0.602867	0.418096
29	6	0	2.544791	0.996802	-0.376985
30	6	0	1.461406	-0.669851	0.991705
31	6	0	3.606429	0.131489	-0.604073
32	1	0	2.532733	1.985767	-0.818508
33	6	0	2.513675	-1.546547	0.772008
34	1	0	0.612611	-0.982665	1.589031
35	6	0	3.568506	-1.125039	-0.022624
36	1	0	4.451877	0.409192	-1.218359
37	1	0	2.529025	-2.540248	1.197583
38	6	0	0.351893	1.593928	0.728075
39	1	0	0.638191	2.140411	1.630746
40	6	0	0.791439	4.746576	0.581792
41	1	0	0.416373	5.698260	0.964300
42	1	0	1.388885	4.280514	1.369717
43	1	0	1.448801	4.942217	-0.266849
44	7	0	4.693539	-2.053343	-0.262990
45	8	0	5.595759	-1.665490	-0.971401
46	8	0	4.640795	-3.141887	0.264443

Structure 21d ($^5C_2$ ec-ax) (M06-2X, Benzene)

Energy (Hartrees): = - 1220.6586157
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.818399	1.255960	-0.882154
2	6	0	-0.546996	2.038157	-1.221381
3	6	0	-1.441048	0.136603	0.094390
4	1	0	-0.812419	2.890604	-1.848692
5	1	0	0.163277	1.405175	-1.776197
6	1	0	-2.268965	0.822524	-1.772893
7	1	0	-0.721419	-0.541468	-0.385835
8	8	0	-0.833846	0.728528	1.254561
9	7	0	-0.004336	2.530761	0.036581
10	6	0	-2.619285	-0.676353	0.637078
11	1	0	-3.450103	0.012948	0.833609
12	6	0	-3.075371	-1.758781	-0.328075
13	1	0	-2.239618	-2.456024	-0.486009
14	6	0	-4.247440	-2.541768	0.236171
15	1	0	-5.059637	-1.844737	0.478125
16	1	0	-3.944805	-3.078900	1.138476
17	8	0	-2.236695	-1.358930	1.820411
18	1	0	-1.780502	-0.711469	2.368239
19	8	0	-3.452990	-1.155018	-1.549666
20	1	0	-3.963427	-1.823952	-2.021199
21	8	0	-4.640473	-3.435009	-0.801069
22	1	0	-5.482688	-3.830313	-0.565302
23	8	0	-2.766593	2.128662	-0.303855
24	1	0	-2.283253	2.597815	0.389086
25	6	0	0.778723	3.760162	0.008734
26	1	0	1.410944	3.804211	-0.888945
27	1	0	1.454328	3.760655	0.869403
28	6	0	1.478042	0.541718	0.565967
29	6	0	2.520404	0.987781	-0.245397
30	6	0	1.515501	-0.760037	1.071965
31	6	0	3.590610	0.156794	-0.549024
32	1	0	2.500923	1.988820	-0.655470
33	6	0	2.573842	-1.605920	0.776725
34	1	0	0.693707	-1.119027	1.680095
35	6	0	3.595969	-1.126823	-0.028976
36	1	0	4.405065	0.487169	-1.178768
37	1	0	2.613441	-2.618241	1.154799
38	6	0	0.330785	1.482266	0.966942
39	1	0	0.609115	1.955564	1.913234
40	6	0	-0.121029	4.989899	0.059764
41	1	0	0.467159	5.908330	-0.010459
42	1	0	-0.837264	4.983305	-0.765417

43	1	0	-0.684146	5.007752	0.995233
44	7	0	4.726036	-2.018412	-0.351735
45	8	0	5.617723	-1.569869	-1.039687
46	8	0	4.696941	-3.146504	0.089876

Structure 21d ($^5C_2$ ax-ax) (M06-2X, Benece)

Energy (Hartrees): = - 1220.662224
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.840570	1.222115	-1.049810
2	6	0	-0.560386	1.956736	-1.464293
3	6	0	-1.452622	0.191438	0.009667
4	1	0	-0.796479	2.747512	-2.176863
5	1	0	0.109130	1.245103	-1.961586
6	1	0	-2.289440	0.719460	-1.905648
7	1	0	-0.724479	-0.510148	-0.417442
8	8	0	-0.846298	0.906656	1.099260
9	7	0	0.151217	2.547696	-0.325848
10	6	0	-2.598442	-0.608192	0.635346
11	1	0	-3.452600	0.061018	0.801571
12	6	0	-3.039077	-1.765727	-0.246261
13	1	0	-2.176937	-2.430378	-0.404365
14	6	0	-4.146071	-2.574495	0.406695
15	1	0	-4.983375	-1.908477	0.650515
16	1	0	-3.778973	-3.049999	1.319531
17	8	0	-2.167098	-1.189532	1.854743
18	1	0	-1.706716	-0.493731	2.336867
19	8	0	-3.494392	-1.243849	-1.478517
20	1	0	-3.987106	-1.960178	-1.896302
21	8	0	-4.533324	-3.536912	-0.568608
22	1	0	-5.340176	-3.966385	-0.275551
23	8	0	-2.810539	2.124687	-0.543723
24	1	0	-2.528272	2.370736	0.343710
25	6	0	-0.350252	3.840802	0.160602
26	1	0	-1.062187	3.713817	0.989481
27	1	0	-0.900169	4.319976	-0.650639
28	6	0	1.477594	0.600737	0.415913
29	6	0	2.552459	0.994698	-0.380443
30	6	0	1.472771	-0.671554	0.990799
31	6	0	3.614043	0.130000	-0.608511
32	1	0	2.544140	1.982693	-0.824196
33	6	0	2.525299	-1.547718	0.772421
34	1	0	0.627141	-0.986451	1.591168
35	6	0	3.578845	-1.126541	-0.025272
36	1	0	4.455654	0.413465	-1.225564
37	1	0	2.536185	-2.539011	1.203903
38	6	0	0.357406	1.589889	0.726704
39	1	0	0.642701	2.132508	1.631745
40	6	0	0.796836	4.735158	0.610924
41	1	0	0.418355	5.684772	0.996914
42	1	0	1.381360	4.261303	1.404292
43	1	0	1.467335	4.940699	-0.225866
44	7	0	4.701041	-2.052792	-0.268296
45	8	0	5.588192	-1.681808	-1.006275
46	8	0	4.669974	-3.131331	0.283927

Structure 21d ($^5C_2$ ec-ax) (M06-2X, DMSO)

Energy (Hartrees): = - 1220.6628257
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.808694	1.262596	-0.875535
2	6	0	-0.536628	2.044799	-1.207124
3	6	0	-1.436647	0.141328	0.099540
4	1	0	-0.794612	2.898217	-1.836403
5	1	0	0.175006	1.409662	-1.756671
6	1	0	-2.252828	0.833446	-1.771449
7	1	0	-0.715434	-0.533744	-0.382367
8	8	0	-0.833549	0.727442	1.264031
9	7	0	-0.003828	2.536144	0.055961
10	6	0	-2.611532	-0.679692	0.634391
11	1	0	-3.438223	0.003873	0.865198
12	6	0	-3.092897	-1.730330	-0.354298

13	1	0	-2.245761	-2.384781	-0.606680
14	6	0	-4.198472	-2.583763	0.241088
15	1	0	-5.016003	-1.933118	0.574426
16	1	0	-3.822181	-3.156474	1.091786
17	8	0	-2.210523	-1.393969	1.794382
18	1	0	-1.703646	-0.770932	2.327855
19	8	0	-3.576584	-1.081489	-1.517167
20	1	0	-4.104229	-1.746253	-1.976824
21	8	0	-4.631525	-3.439927	-0.812597
22	1	0	-5.470434	-3.834650	-0.557327
23	8	0	-2.760757	2.137481	-0.298250
24	1	0	-2.265405	2.623681	0.375653
25	6	0	0.801310	3.753683	0.025035
26	1	0	1.438354	3.781770	-0.868681
27	1	0	1.468558	3.747263	0.891520
28	6	0	1.477809	0.542035	0.571495
29	6	0	2.494429	0.971739	-0.280332
30	6	0	1.538087	-0.745294	1.112451
31	6	0	3.560631	0.137964	-0.591190
32	1	0	2.460412	1.960055	-0.718781
33	6	0	2.592218	-1.593998	0.812071
34	1	0	0.740476	-1.093708	1.757398
35	6	0	3.588208	-1.131285	-0.036352
36	1	0	4.351288	0.462518	-1.253641
37	1	0	2.644273	-2.593682	1.221572
38	6	0	0.334503	1.482941	0.979833
39	1	0	0.617924	1.949245	1.927465
40	6	0	-0.080952	4.995601	0.060122
41	1	0	0.524687	5.903560	-0.001443
42	1	0	-0.780563	4.998184	-0.779837
43	1	0	-0.658993	5.024597	0.986738
44	7	0	4.709887	-2.025305	-0.366961
45	8	0	5.581733	-1.597883	-1.095312
46	8	0	4.703290	-3.143474	0.104954

Structure 21d ($^5C_2$ ax-ax) (M06-2X, DMSO)

Energy (Hartrees): = - 1220.665877
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.825415	1.214046	-1.052698
2	6	0	-0.543442	1.947494	-1.461276
3	6	0	-1.444476	0.181960	0.006545
4	1	0	-0.775531	2.740331	-2.173221
5	1	0	0.122098	1.231332	-1.957537
6	1	0	-2.263760	0.711116	-1.913964
7	1	0	-0.725504	-0.526058	-0.425693
8	8	0	-0.830266	0.887280	1.097387
9	7	0	0.169151	2.533851	-0.321179
10	6	0	-2.591753	-0.609262	0.636550
11	1	0	-3.422011	0.072987	0.859619
12	6	0	-3.101330	-1.720202	-0.268218
13	1	0	-2.255478	-2.368968	-0.539147
14	6	0	-4.151214	-2.566228	0.431107
15	1	0	-4.954960	-1.915756	0.796770
16	1	0	-3.708332	-3.103681	1.272653
17	8	0	-2.132212	-1.243365	1.820982
18	1	0	-1.631162	-0.575804	2.304195
19	8	0	-3.665193	-1.135848	-1.428354
20	1	0	-4.209092	-1.829282	-1.821884
21	8	0	-4.639973	-3.465019	-0.560660
22	1	0	-5.445084	-3.873433	-0.229059
23	8	0	-2.804839	2.115589	-0.557695
24	1	0	-2.522455	2.380904	0.325259
25	6	0	-0.333585	3.825758	0.169936
26	1	0	-1.063384	3.697415	0.982273
27	1	0	-0.856367	4.318439	-0.651339
28	6	0	1.494479	0.584872	0.410926
29	6	0	2.574690	0.989633	-0.373450
30	6	0	1.489268	-0.694503	0.970219
31	6	0	3.640821	0.131707	-0.603957
32	1	0	2.573029	1.982381	-0.806184
33	6	0	2.543079	-1.567562	0.745455
34	1	0	0.646242	-1.019250	1.568432
35	6	0	3.602029	-1.133937	-0.039131
36	1	0	4.484282	0.432881	-1.210260
37	1	0	2.546601	-2.563536	1.166657
38	6	0	0.374173	1.571433	0.728161
39	1	0	0.663193	2.108042	1.635228
40	6	0	0.809944	4.705318	0.655811
41	1	0	0.427234	5.653227	1.042387

42	1	0	1.370108	4.218056	1.458644
43	1	0	1.501006	4.916948	-0.163341
44	7	0	4.726851	-2.051808	-0.282165
45	8	0	5.672711	-1.635418	-0.918724
46	8	0	4.650235	-3.176436	0.167942

Structure 27a (^{2}E ec-ax H-bond O) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1016.1511189
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.866366	-0.398571	-0.357824
2	6	0	2.707346	-1.429450	0.566848
3	6	0	3.797922	-1.900122	1.289743
4	6	0	5.060264	-1.351985	1.089034
5	6	0	5.230278	-0.336972	0.153576
6	6	0	4.138066	0.132230	-0.566500
7	1	0	1.730503	-1.879745	0.699779
8	1	0	3.663639	-2.702358	2.005739
9	1	0	5.909947	-1.721748	1.650460
10	1	0	6.213865	0.083770	-0.019307
11	1	0	4.275461	0.916254	-1.305293
12	6	0	1.676796	0.186218	-1.103864
13	1	0	2.005401	0.525636	-2.092184
14	7	0	0.997503	1.289318	-0.424302
15	8	0	0.662125	-0.787225	-1.261013
16	6	0	-0.430157	-0.512421	-0.361794
17	6	0	0.076746	0.642379	0.499214
18	1	0	-0.723204	1.318916	0.794473
19	1	0	0.569182	0.274975	1.413167
20	1	0	-0.626188	-1.419247	0.213906
21	6	0	-1.650680	-0.145856	-1.214676
22	1	0	-1.590814	0.922806	-1.470268
23	6	0	-3.008275	-0.428982	-0.575039
24	1	0	-3.055846	-1.501331	-0.337300
25	6	0	-3.284793	0.360019	0.701897
26	1	0	-3.082755	1.420627	0.520235
27	6	0	-4.728991	0.204707	1.148033
28	1	0	-4.913729	0.878472	1.992215
29	1	0	-5.399009	0.440435	0.319093
30	8	0	-1.665383	-0.921822	-2.402009
31	1	0	-0.746545	-1.015224	-2.678024
32	8	0	-4.015124	-0.085311	-1.507734
33	1	0	-3.731361	-0.454712	-2.351364
34	8	0	-2.423417	-0.070881	1.743081
35	1	0	-2.837668	-0.862724	2.107471
36	8	0	-4.853011	-1.153813	1.557434
37	1	0	-5.753314	-1.316691	1.841802
38	6	0	1.849399	2.321119	0.144746
39	1	0	2.454589	1.933536	0.980228
40	1	0	2.548410	2.638863	-0.635473
41	6	0	1.030677	3.520087	0.605958
42	1	0	1.689694	4.333364	0.914389
43	1	0	0.392260	3.873309	-0.205947
44	1	0	0.397654	3.265586	1.458132

Structure 27a (^{2}E ec-ax H-bond N) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1016.1542038
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.254952	-0.741039	-0.393912
2	6	0	2.265519	-1.520305	0.761796
3	6	0	3.386051	-2.276363	1.088745
4	6	0	4.501331	-2.270303	0.258121
5	6	0	4.488675	-1.513602	-0.908815
6	6	0	3.368385	-0.756926	-1.232260
7	1	0	1.381326	-1.555741	1.387974
8	1	0	3.383548	-2.881125	1.987951
9	1	0	5.371542	-2.863848	0.512021
10	1	0	5.347036	-1.519782	-1.570018
11	1	0	3.355853	-0.178291	-2.151192
12	6	0	1.064742	0.140583	-0.735690
13	1	0	0.956520	0.197571	-1.824194

14	7	0	1.133591	1.511192	-0.200523
15	8	0	-0.120979	-0.374843	-0.175174
16	6	0	-0.529809	0.428209	0.947415
17	6	0	0.648603	1.375134	1.172430
18	1	0	0.321770	2.338973	1.563165
19	1	0	1.405595	0.941867	1.842264
20	1	0	-0.712550	-0.242770	1.784775
21	6	0	-1.821350	1.181920	0.615944
22	1	0	-2.279649	1.509370	1.558012
23	6	0	-2.851804	0.357890	-0.161829
24	1	0	-2.375555	-0.008181	-1.079729
25	6	0	-3.424281	-0.832642	0.604694
26	1	0	-3.934881	-0.456328	1.496250
27	6	0	-4.422217	-1.589686	-0.256404
28	1	0	-4.882053	-2.378117	0.349748
29	1	0	-5.186630	-0.899138	-0.623354
30	8	0	-1.577008	2.364397	-0.142582
31	1	0	-0.719347	2.261361	-0.585801
32	8	0	-3.948869	1.198378	-0.472065
33	1	0	-3.558941	2.024916	-0.778868
34	8	0	-2.409119	-1.712301	1.047325
35	1	0	-1.994926	-2.070373	0.252319
36	8	0	-3.667155	-2.152077	-1.323016
37	1	0	-4.255086	-2.656625	-1.886514
38	6	0	2.400754	2.212183	-0.363823
39	1	0	3.200157	1.731166	0.219792
40	1	0	2.683266	2.136464	-1.418301
41	6	0	2.272585	3.679204	0.024637
42	1	0	3.186501	4.218224	-0.229590
43	1	0	1.435665	4.141637	-0.502610
44	1	0	2.107933	3.796450	1.097372

Structure 27a (^{2}E ax-ax) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1016.1537698
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.764826	-0.282531	0.258796
2	6	0	-2.817589	-1.336539	1.167113
3	6	0	-3.722669	-2.376566	0.978543
4	6	0	-4.580549	-2.367326	-0.115344
5	6	0	-4.527453	-1.315935	-1.025227
6	6	0	-3.622445	-0.278195	-0.840004
7	1	0	-2.143619	-1.336139	2.015489
8	1	0	-3.756489	-3.195878	1.687064
9	1	0	-5.285138	-3.177519	-0.260925
10	1	0	-5.188261	-1.307955	-1.884113
11	1	0	-3.556350	0.536131	-1.552003
12	6	0	-1.818527	0.886661	0.476363
13	1	0	-2.342503	1.700252	0.983533
14	7	0	-1.233247	1.343035	-0.763942
15	8	0	-0.723015	0.513811	1.318068
16	6	0	0.314830	-0.005330	0.470630
17	6	0	-0.150740	0.369416	-0.959810
18	1	0	0.643646	0.789753	-1.573396
19	1	0	-0.537995	-0.511733	-1.470956
20	1	0	0.372440	-1.088599	0.605988
21	6	0	1.618843	0.658793	0.919641
22	1	0	1.692176	1.658325	0.462673
23	6	0	2.898716	-0.107397	0.595994
24	1	0	2.829573	-1.099576	1.063904
25	6	0	3.163224	-0.292668	-0.895883
26	1	0	3.095025	0.679560	-1.395434
27	6	0	4.544094	-0.876259	-1.143934
28	1	0	4.735995	-0.883115	-2.222709
29	1	0	5.297815	-0.278932	-0.626993
30	8	0	1.642912	0.783774	2.333086
31	1	0	0.752717	1.036869	2.601903
32	8	0	3.992786	0.615729	1.126575
33	1	0	3.733167	0.874245	2.017795
34	8	0	2.184370	-1.140263	-1.471092
35	1	0	2.470438	-2.039510	-1.268653
36	8	0	4.486658	-2.206265	-0.638383
37	1	0	5.336846	-2.629481	-0.766127
38	6	0	-0.783848	2.739761	-0.678471
39	1	0	-0.308003	2.954827	0.290446
40	1	0	-0.024978	2.888354	-1.449718
41	6	0	-1.941873	3.697130	-0.923935
42	1	0	-1.601715	4.733834	-0.881641
43	1	0	-2.378722	3.508592	-1.905981
44	1	0	-2.728135	3.574061	-0.175408

Structure 27a (E_2 ec-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1016.1516741
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.001890	-0.371023	-0.105425
2	6	0	3.429587	-0.199140	1.210164
3	6	0	4.752775	-0.442079	1.547104
4	6	0	5.657534	-0.856225	0.570587
5	6	0	5.234532	-1.026438	-0.740793
6	6	0	3.904092	-0.785031	-1.077048
7	1	0	2.711102	0.133729	1.949870
8	1	0	5.084859	-0.309547	2.569958
9	1	0	6.691516	-1.044846	0.834641
10	1	0	5.935403	-1.348790	-1.501566
11	1	0	3.566445	-0.918315	-2.099826
12	6	0	1.561134	-0.094472	-0.444260
13	1	0	1.394098	-0.256366	-1.529281
14	7	0	1.129698	1.230510	-0.041050
15	8	0	0.715675	-0.954410	0.296418
16	6	0	-0.563834	-0.311715	0.450853
17	6	0	-0.325926	1.133991	-0.011821
18	1	0	-0.762639	1.295407	-1.014702
19	1	0	-0.764057	1.860201	0.665189
20	1	0	-0.824858	-0.369268	1.509926
21	6	0	-1.563387	-1.125519	-0.377612
22	1	0	-1.416762	-0.892443	-1.444167
23	6	0	-3.047546	-0.966820	-0.050642
24	1	0	-3.191895	-1.211154	1.011173
25	6	0	-3.619293	0.425382	-0.306727
26	1	0	-3.330055	0.759501	-1.308098
27	6	0	-5.135938	0.426383	-0.203177
28	1	0	-5.507854	1.414510	-0.496553
29	1	0	-5.554358	-0.345773	-0.851252
30	8	0	-1.322412	-2.507831	-0.158451
31	1	0	-0.365142	-2.620202	-0.142407
32	8	0	-3.769316	-1.868799	-0.867514
33	1	0	-3.295487	-2.706554	-0.821235
34	8	0	-3.088888	1.352476	0.623692
35	1	0	-3.604708	1.230250	1.430234
36	8	0	-5.418299	0.173852	1.169573
37	1	0	-6.367501	0.154619	1.298694
38	6	0	1.648520	2.290849	-0.889818
39	1	0	2.737385	2.191656	-0.912604
40	1	0	1.284225	2.170969	-1.927167
41	6	0	1.268092	3.667218	-0.363618
42	1	0	1.741850	4.448062	-0.960746
43	1	0	0.188232	3.824601	-0.401550
44	1	0	1.594836	3.771713	0.672483

Structure 27a (^{2}E ec-ax H-bond O) (M06-2X, Benzene)

Energy (Hartrees): = - 1016.1713248
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.870117	-0.401115	0.358861
2	6	0	-2.713141	-1.426746	-0.572986
3	6	0	-3.806895	-1.896847	-1.292218
4	6	0	-5.070170	-1.354370	-1.079738
5	6	0	-5.237976	-0.345343	-0.136767
6	6	0	-4.142734	0.123987	0.579458
7	1	0	-1.735746	-1.872553	-0.718877
8	1	0	-3.674426	-2.694011	-2.014595
9	1	0	-5.922174	-1.723563	-1.638601
10	1	0	-6.222170	0.071047	0.044844
11	1	0	-4.277293	0.904114	1.322944
12	6	0	-1.678354	0.188341	1.098641
13	1	0	-2.004584	0.530358	2.086482
14	7	0	-1.001189	1.289700	0.413564
15	8	0	-0.661247	-0.784441	1.255652
16	6	0	0.431798	-0.509233	0.356228
17	6	0	-0.077073	0.642690	-0.507364
18	1	0	0.720782	1.322916	-0.800711
19	1	0	-0.567181	0.272436	-1.421029

20	1	0	0.629811	-1.417381	-0.216450
21	6	0	1.650682	-0.137022	1.210372
22	1	0	1.590746	0.932665	1.460808
23	6	0	3.011134	-0.423154	0.577478
24	1	0	3.060441	-1.497085	0.348192
25	6	0	3.293940	0.356292	-0.704696
26	1	0	3.089444	1.418171	-0.535027
27	6	0	4.738489	0.199039	-1.146872
28	1	0	4.919690	0.855790	-2.005160
29	1	0	5.412485	0.460674	-0.328617
30	8	0	1.660165	-0.906232	2.404424
31	1	0	0.739635	-0.991104	2.678971
32	8	0	4.014182	-0.073812	1.514937
33	1	0	3.727295	-0.442143	2.358170
34	8	0	2.436937	-0.086905	-1.746198
35	1	0	2.850034	-0.887875	-2.092707
36	8	0	4.875758	-1.167538	-1.524849
37	1	0	5.765329	-1.311642	-1.854762
38	6	0	-1.854801	2.320809	-0.156899
39	1	0	-2.457528	1.932582	-0.993493
40	1	0	-2.554394	2.638300	0.622796
41	6	0	-1.038516	3.519770	-0.619965
42	1	0	-1.700231	4.334753	-0.920015
43	1	0	-0.394029	3.873607	0.187819
44	1	0	-0.411565	3.270883	-1.478865

Structure 27a (^{2}E ec-ax H-bond N) (M06-2X, Benzene)

Energy (Hartrees): = - 1016.1748878
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.257195	-0.740945	-0.386890
2	6	0	2.288809	-1.513560	0.773541
3	6	0	3.416787	-2.265036	1.087138
4	6	0	4.518650	-2.261005	0.238303
5	6	0	4.485400	-1.510213	-0.932568
6	6	0	3.357878	-0.757959	-1.242900
7	1	0	1.417539	-1.545095	1.418038
8	1	0	3.430092	-2.863768	1.990590
9	1	0	5.394524	-2.851156	0.481636
10	1	0	5.333244	-1.517816	-1.607601
11	1	0	3.329459	-0.183914	-2.164380
12	6	0	1.058477	0.134686	-0.716498
13	1	0	0.936479	0.188008	-1.803469
14	7	0	1.124399	1.507302	-0.185860
15	8	0	-0.118073	-0.388658	-0.138028
16	6	0	-0.536228	0.432160	0.968213
17	6	0	0.642394	1.378242	1.189110
18	1	0	0.320190	2.344347	1.578276
19	1	0	1.398287	0.946688	1.860455
20	1	0	-0.725489	-0.224199	1.815106
21	6	0	-1.824612	1.183197	0.614832
22	1	0	-2.291288	1.520577	1.549217
23	6	0	-2.847658	0.353676	-0.168702
24	1	0	-2.357905	-0.024562	-1.074523
25	6	0	-3.443196	-0.824992	0.598814
26	1	0	-3.974568	-0.437738	1.473403
27	6	0	-4.420289	-1.595100	-0.273898
28	1	0	-4.889310	-2.378527	0.331462
29	1	0	-5.186356	-0.917636	-0.662312
30	8	0	-1.570298	2.356119	-0.158069
31	1	0	-0.693711	2.254694	-0.566804
32	8	0	-3.933628	1.199080	-0.511775
33	1	0	-3.527719	2.015648	-0.825589
34	8	0	-2.439124	-1.701222	1.076945
35	1	0	-1.996713	-2.055446	0.295380
36	8	0	-3.647411	-2.165507	-1.324005
37	1	0	-4.205666	-2.763660	-1.824938
38	6	0	2.387665	2.214803	-0.359725
39	1	0	3.188085	1.749449	0.234733
40	1	0	2.671771	2.124060	-1.412315
41	6	0	2.251887	3.686021	0.005447
42	1	0	3.168643	4.222129	-0.247592
43	1	0	1.422040	4.143477	-0.538401
44	1	0	2.076891	3.820978	1.074805

Structure 27a (^{2}E ax-ax) (M06-2X, Benzene)

Energy (Hartrees): = - 1016.1739095
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.772786	-0.285452	0.257807
2	6	0	-2.817504	-1.355602	1.148242
3	6	0	-3.731654	-2.387925	0.956885
4	6	0	-4.606057	-2.356646	-0.123712
5	6	0	-4.561094	-1.289842	-1.016585
6	6	0	-3.646699	-0.260338	-0.828542
7	1	0	-2.132408	-1.375440	1.987600
8	1	0	-3.758941	-3.218607	1.652798
9	1	0	-5.318140	-3.160151	-0.271859
10	1	0	-5.235387	-1.263301	-1.864882
11	1	0	-3.590407	0.565327	-1.528676
12	6	0	-1.817190	0.876836	0.479634
13	1	0	-2.335772	1.688613	0.994798
14	7	0	-1.233357	1.340958	-0.758592
15	8	0	-0.721178	0.490506	1.314864
16	6	0	0.319777	-0.014880	0.462163
17	6	0	-0.147068	0.372862	-0.963752
18	1	0	0.645832	0.805218	-1.571063
19	1	0	-0.530001	-0.504928	-1.484369
20	1	0	0.382794	-1.098993	0.587609
21	6	0	1.620827	0.651309	0.918327
22	1	0	1.690491	1.654504	0.470411
23	6	0	2.905125	-0.107726	0.593854
24	1	0	2.838124	-1.102218	1.057002
25	6	0	3.177496	-0.285083	-0.898324
26	1	0	3.106020	0.687485	-1.396563
27	6	0	4.559626	-0.863722	-1.147637
28	1	0	4.744519	-0.881243	-2.227554
29	1	0	5.319215	-0.257399	-0.649459
30	8	0	1.639205	0.765647	2.334854
31	1	0	0.749522	1.026519	2.599203
32	8	0	3.994138	0.617362	1.136644
33	1	0	3.727386	0.866961	2.028521
34	8	0	2.203211	-1.136758	-1.478784
35	1	0	2.487406	-2.034355	-1.264769
36	8	0	4.519409	-2.188321	-0.625430
37	1	0	5.348825	-2.626786	-0.827138
38	6	0	-0.788039	2.740117	-0.667901
39	1	0	-0.310358	2.951366	0.300531
40	1	0	-0.032698	2.894385	-1.441295
41	6	0	-1.947310	3.696743	-0.903839
42	1	0	-1.605585	4.733319	-0.855678
43	1	0	-2.386953	3.519566	-1.887549
44	1	0	-2.732959	3.572049	-0.154366

Structure 27a (E_2 ec-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 1016.1721308
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.003690	-0.372551	-0.100047
2	6	0	3.424816	-0.184286	1.216140
3	6	0	4.745146	-0.427328	1.565536
4	6	0	5.654758	-0.858150	0.600416
5	6	0	5.238891	-1.044434	-0.711478
6	6	0	3.911419	-0.802499	-1.060543
7	1	0	2.705318	0.161739	1.949342
8	1	0	5.070204	-0.281557	2.589212
9	1	0	6.686574	-1.047137	0.873717
10	1	0	5.943610	-1.379984	-1.463420
11	1	0	3.581505	-0.947958	-2.084417
12	6	0	1.564710	-0.095836	-0.451582
13	1	0	1.404068	-0.264868	-1.535196
14	7	0	1.132566	1.232455	-0.056987
15	8	0	0.715067	-0.952139	0.291354
16	6	0	-0.565265	-0.307982	0.439833
17	6	0	-0.324159	1.137265	-0.022141
18	1	0	-0.763107	1.299887	-1.023016
19	1	0	-0.756035	1.863767	0.658891
20	1	0	-0.831103	-0.365872	1.497491
21	6	0	-1.564086	-1.114552	-0.397968
22	1	0	-1.420263	-0.866560	-1.461062
23	6	0	-3.048156	-0.963886	-0.065838
24	1	0	-3.190773	-1.241478	0.987910
25	6	0	-3.619273	0.437054	-0.276002

26	1	0	-3.330846	0.806568	-1.264969
27	6	0	-5.134783	0.443447	-0.170683
28	1	0	-5.498359	1.448637	-0.411563
29	1	0	-5.565753	-0.284171	-0.861315
30	8	0	-1.318571	-2.501053	-0.199645
31	1	0	-0.360468	-2.609712	-0.192319
32	8	0	-3.770788	-1.843994	-0.908442
33	1	0	-3.300906	-2.684891	-0.878142
34	8	0	-3.083715	1.328758	0.687537
35	1	0	-3.589217	1.167534	1.494310
36	8	0	-5.424646	0.118365	1.185094
37	1	0	-6.372030	0.180965	1.324752
38	6	0	1.646780	2.287855	-0.917174
39	1	0	2.736126	2.194143	-0.941346
40	1	0	1.280390	2.157851	-1.951868
41	6	0	1.264086	3.667456	-0.404004
42	1	0	1.736214	4.442816	-1.010531
43	1	0	0.183994	3.826071	-0.441966
44	1	0	1.592680	3.788076	0.630436

Structure 27a (^{2}E ec-ax H-bond O) (M06-2X, DMSO)

Energy (Hartrees): = - 1016.1747009
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.852258	-0.390872	0.363943
2	6	0	-2.651322	-1.434151	-0.540931
3	6	0	-3.722105	-1.956396	-1.260995
4	6	0	-5.004610	-1.446373	-1.079030
5	6	0	-5.214410	-0.415835	-0.166860
6	6	0	-4.142784	0.104876	0.551510
7	1	0	-1.659437	-1.852826	-0.671350
8	1	0	-3.555871	-2.767203	-1.961276
9	1	0	-5.837755	-1.857049	-1.637918
10	1	0	-6.212435	-0.021954	-0.011068
11	1	0	-4.308231	0.902110	1.270167
12	6	0	-1.693190	0.246125	1.116648
13	1	0	-2.056122	0.613023	2.081257
14	7	0	-1.015195	1.336258	0.412840
15	8	0	-0.661781	-0.699462	1.338269
16	6	0	0.421390	-0.473313	0.410507
17	6	0	-0.073487	0.667508	-0.477848
18	1	0	0.729516	1.342970	-0.769056
19	1	0	-0.552932	0.283245	-1.390791
20	1	0	0.590119	-1.399376	-0.142571
21	6	0	1.659856	-0.109094	1.236008
22	1	0	1.622682	0.964255	1.474671
23	6	0	3.003403	-0.420201	0.580345
24	1	0	3.033946	-1.498314	0.368214
25	6	0	3.263670	0.334981	-0.721449
26	1	0	3.051102	1.398134	-0.572308
27	6	0	4.700155	0.185504	-1.189225
28	1	0	4.846579	0.816276	-2.072255
29	1	0	5.392485	0.492180	-0.402218
30	8	0	1.679393	-0.865937	2.440303
31	1	0	0.767140	-0.894725	2.753179
32	8	0	4.029650	-0.070150	1.495450
33	1	0	3.747702	-0.415268	2.350503
34	8	0	2.393662	-0.141279	-1.739014
35	1	0	2.805144	-0.954210	-2.060572
36	8	0	4.863738	-1.190674	-1.523330
37	1	0	5.689630	-1.290055	-2.005517
38	6	0	-1.881525	2.321244	-0.221902
39	1	0	-2.431360	1.881576	-1.069452
40	1	0	-2.623853	2.635234	0.518083
41	6	0	-1.092310	3.532558	-0.697055
42	1	0	-1.773204	4.295407	-1.080653
43	1	0	-0.517681	3.963059	0.126575
44	1	0	-0.400926	3.270371	-1.500952

Structure 27a (^{2}E ec-ax H-bond N) (M06-2X, DMSO)

Energy (Hartrees): = - 1016.177963
No imaginary frequencies

Standard orientation:

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

1	6	0	2.364175	-0.741496	-0.444539
2	6	0	2.329796	-1.585123	0.666300
3	6	0	3.424598	-2.388051	0.973008
4	6	0	4.559592	-2.362178	0.167209
5	6	0	4.593823	-1.534468	-0.951648
6	6	0	3.499466	-0.730359	-1.255205
7	1	0	1.438596	-1.626976	1.282856
8	1	0	3.389090	-3.040090	1.838493
9	1	0	5.409990	-2.990897	0.405411
10	1	0	5.469425	-1.520390	-1.590807
11	1	0	3.522138	-0.092243	-2.133818
12	6	0	1.205062	0.185971	-0.768535
13	1	0	1.174499	0.357681	-1.849160
14	7	0	1.246902	1.491506	-0.089615
15	8	0	-0.022080	-0.375685	-0.345645
16	6	0	-0.523757	0.336084	0.799615
17	6	0	0.640610	1.233557	1.217795
18	1	0	0.297739	2.162219	1.676136
19	1	0	1.328937	0.724964	1.906834
20	1	0	-0.799228	-0.388606	1.563035
21	6	0	-1.755974	1.152478	0.407894
22	1	0	-2.179916	1.580830	1.327277
23	6	0	-2.847005	0.341355	-0.305267
24	1	0	-2.372343	-0.281692	-1.073434
25	6	0	-3.669327	-0.544475	0.630214
26	1	0	-4.144702	0.096258	1.378735
27	6	0	-4.746012	-1.302631	-0.126009
28	1	0	-5.374172	-1.836862	0.594284
29	1	0	-5.362144	-0.609757	-0.704819
30	8	0	-1.409440	2.227834	-0.464433
31	1	0	-0.445743	2.195718	-0.615960
32	8	0	-3.764597	1.245545	-0.903073
33	1	0	-3.215185	1.951716	-1.265024
34	8	0	-2.851597	-1.471814	1.327281
35	1	0	-2.644727	-2.163877	0.685944
36	8	0	-4.062454	-2.223576	-0.973361
37	1	0	-4.703115	-2.855391	-1.312510
38	6	0	2.537320	2.173332	-0.075059
39	1	0	3.264581	1.620608	0.537978
40	1	0	2.914645	2.181836	-1.101593
41	6	0	2.399943	3.598341	0.439025
42	1	0	3.354059	4.121347	0.348018
43	1	0	1.648858	4.144926	-0.136871
44	1	0	2.107877	3.615692	1.491347

Structure 27a (^{2}E ax-ax) (M06-2X, DMSO)

Energy (Hartrees): = - 1016.1766646
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.778572	-0.287278	0.278954
2	6	0	-2.701945	-1.446107	1.047378
3	6	0	-3.612266	-2.482646	0.846422
4	6	0	-4.607035	-2.363805	-0.117826
5	6	0	-4.690340	-1.202372	-0.883878
6	6	0	-3.779304	-0.171367	-0.687461
7	1	0	-1.928182	-1.535760	1.800972
8	1	0	-3.542049	-3.383836	1.445290
9	1	0	-5.314881	-3.170007	-0.272976
10	1	0	-5.463673	-1.102870	-1.637361
11	1	0	-3.832063	0.729406	-1.289790
12	6	0	-1.816651	0.872677	0.486861
13	1	0	-2.332942	1.694145	0.987852
14	7	0	-1.238337	1.313871	-0.765268
15	8	0	-0.719168	0.492455	1.320849
16	6	0	0.325380	-0.013385	0.471093
17	6	0	-0.153753	0.339759	-0.957541
18	1	0	0.633992	0.760754	-1.579376
19	1	0	-0.543519	-0.550988	-1.451913
20	1	0	0.406327	-1.093386	0.619599
21	6	0	1.622413	0.680381	0.897142
22	1	0	1.681177	1.667987	0.416945
23	6	0	2.906802	-0.082007	0.584159
24	1	0	2.848158	-1.061751	1.079255
25	6	0	3.159414	-0.305695	-0.905845
26	1	0	3.053661	0.645457	-1.436925
27	6	0	4.546922	-0.863506	-1.167485
28	1	0	4.697334	-0.930168	-2.250008
29	1	0	5.309817	-0.214055	-0.732763
30	8	0	1.648747	0.838566	2.311369

31	1	0	0.766769	1.134382	2.566226
32	8	0	3.998955	0.663990	1.097331
33	1	0	3.729205	0.952739	1.976849
34	8	0	2.192594	-1.202031	-1.434276
35	1	0	2.497171	-2.081896	-1.176502
36	8	0	4.566006	-2.161334	-0.577543
37	1	0	5.344557	-2.627210	-0.895712
38	6	0	-0.783074	2.714047	-0.694210
39	1	0	-0.297541	2.931517	0.268013
40	1	0	-0.032165	2.853810	-1.474432
41	6	0	-1.939969	3.673253	-0.927906
42	1	0	-1.591453	4.707908	-0.885548
43	1	0	-2.386024	3.498111	-1.909871
44	1	0	-2.720518	3.553761	-0.171927

Structure 27a (E_2 ec-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 1016.1751918
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.998193	-0.366340	-0.096258
2	6	0	3.448543	-0.229108	1.217553
3	6	0	4.780434	-0.470554	1.526797
4	6	0	5.673174	-0.847168	0.522766
5	6	0	5.228272	-0.981778	-0.787084
6	6	0	3.889181	-0.743343	-1.095286
7	1	0	2.745942	0.070338	1.987332
8	1	0	5.127966	-0.365569	2.548302
9	1	0	6.713474	-1.034215	0.764064
10	1	0	5.919069	-1.273210	-1.569932
11	1	0	3.535893	-0.848280	-2.116320
12	6	0	1.549858	-0.092479	-0.410011
13	1	0	1.360461	-0.263120	-1.486431
14	7	0	1.125240	1.238556	-0.007163
15	8	0	0.723077	-0.946966	0.362159
16	6	0	-0.567069	-0.316376	0.496624
17	6	0	-0.334206	1.135744	0.049419
18	1	0	-0.784381	1.308476	-0.942793
19	1	0	-0.755926	1.852747	0.747058
20	1	0	-0.849950	-0.389604	1.548697
21	6	0	-1.544452	-1.119019	-0.368152
22	1	0	-1.374644	-0.864691	-1.424980
23	6	0	-3.035006	-0.968815	-0.071830
24	1	0	-3.205265	-1.263468	0.973238
25	6	0	-3.591111	0.440532	-0.269429
26	1	0	-3.250074	0.838790	-1.229657
27	6	0	-5.109260	0.460337	-0.238335
28	1	0	-5.448593	1.479020	-0.452682
29	1	0	-5.518500	-0.225738	-0.982725
30	8	0	-1.300926	-2.508748	-0.169849
31	1	0	-0.342764	-2.618190	-0.183645
32	8	0	-3.737888	-1.836658	-0.947376
33	1	0	-3.255819	-2.671514	-0.932759
34	8	0	-3.097618	1.296515	0.750030
35	1	0	-3.642232	1.105038	1.524923
36	8	0	-5.479069	0.077396	1.084313
37	1	0	-6.409090	0.285365	1.211732
38	6	0	1.607402	2.286267	-0.899753
39	1	0	2.696325	2.199207	-0.959445
40	1	0	1.207329	2.138421	-1.917712
41	6	0	1.233582	3.670115	-0.392631
42	1	0	1.673335	4.437956	-1.032421
43	1	0	0.151073	3.817547	-0.389495
44	1	0	1.603863	3.814418	0.625237

Structure 27b (^{2}E ec-ec H-bond O) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1016.155372
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.850356	-0.146371	-0.413220
2	6	0	-2.674732	-1.069893	0.617936
3	6	0	-3.766391	-1.754107	1.131681
4	6	0	-5.042885	-1.515594	0.624623

5	6	0	-5.221469	-0.594830	-0.399162
6	6	0	-4.123010	0.085977	-0.919009
7	1	0	-1.678105	-1.242540	1.010946
8	1	0	-3.626541	-2.474512	1.928894
9	1	0	-5.894826	-2.049227	1.029036
10	1	0	-6.211951	-0.408750	-0.797021
11	1	0	-4.256368	0.802477	-1.723142
12	6	0	-1.653869	0.592297	-0.956058
13	1	0	-1.965000	1.235283	-1.801745
14	7	0	-0.965160	1.364225	0.065544
15	8	0	-0.673765	-0.319888	-1.429634
16	6	0	0.631741	0.123070	-1.021915
17	6	0	0.380498	1.521910	-0.470418
18	1	0	1.094124	1.800185	0.302708
19	1	0	0.424424	2.274693	-1.275582
20	1	0	1.276703	0.119559	-1.900346
21	6	0	1.151444	-0.851356	0.049076
22	1	0	0.813557	-0.500959	1.035933
23	6	0	2.668294	-1.024871	0.079801
24	1	0	2.997178	-1.351222	-0.917384
25	6	0	3.436988	0.239961	0.455458
26	1	0	3.023971	0.644293	1.385357
27	6	0	4.915054	-0.048696	0.658397
28	1	0	5.401392	0.852640	1.048171
29	1	0	5.037403	-0.879207	1.356309
30	8	0	0.646753	-2.157658	-0.179500
31	1	0	-0.196406	-2.051817	-0.638005
32	8	0	2.985727	-2.004379	1.049695
33	1	0	2.372337	-2.732655	0.901979
34	8	0	3.287741	1.231429	-0.547527
35	1	0	3.935986	1.009322	-1.227149
36	8	0	5.418529	-0.366553	-0.635652
37	1	0	6.352747	-0.568815	-0.569365
38	6	0	-1.649399	2.601014	0.407859
39	1	0	-1.697742	3.272691	-0.468457
40	1	0	-2.677556	2.342878	0.677261
41	6	0	-0.977795	3.311649	1.574043
42	1	0	-1.563728	4.180284	1.878833
43	1	0	-0.891888	2.631016	2.422946
44	1	0	0.021871	3.660242	1.307420

Structure 27b (^{2}E ec-ec H-bond N) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1016.1580489
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.949579	-0.940343	-0.456715
2	6	0	-1.402698	-1.511013	0.692326
3	6	0	-1.965588	-2.657983	1.233015
4	6	0	-3.078470	-3.242576	0.632093
5	6	0	-3.623769	-2.678441	-0.513637
6	6	0	-3.054651	-1.530383	-1.059230
7	1	0	-0.536504	-1.051561	1.155268
8	1	0	-1.535629	-3.100545	2.123549
9	1	0	-3.515311	-4.138852	1.056212
10	1	0	-4.485360	-3.133223	-0.987514
11	1	0	-3.470893	-1.092877	-1.961332
12	6	0	-1.352727	0.323782	-1.019039
13	1	0	-1.768670	0.514341	-2.026444
14	7	0	-1.585574	1.485521	-0.154814
15	8	0	0.053056	0.231965	-1.104167
16	6	0	0.640488	1.487901	-0.731782
17	6	0	-0.560386	2.426543	-0.607033
18	1	0	-0.396329	3.216871	0.126796
19	1	0	-0.822681	2.874103	-1.578923
20	1	0	1.335750	1.786573	-1.512840
21	6	0	1.398168	1.338071	0.588373
22	1	0	2.013412	2.237617	0.732469
23	6	0	2.316964	0.112724	0.652638
24	1	0	1.728490	-0.777449	0.397167
25	6	0	3.526322	0.186036	-0.277659
26	1	0	4.109189	1.075495	-0.020167
27	6	0	4.403445	-1.045062	-0.117845
28	1	0	5.314353	-0.908641	-0.711566
29	1	0	4.655696	-1.183334	0.936565
30	8	0	0.519060	1.241836	1.707947
31	1	0	-0.395704	1.182238	1.384090
32	8	0	2.831721	0.011618	1.968642
33	1	0	2.083946	0.180756	2.552792
34	8	0	3.137057	0.317329	-1.631497
35	1	0	2.755195	-0.532821	-1.882600

36	8	0	3.634829	-2.131279	-0.622336
37	1	0	4.141764	-2.939702	-0.538228
38	6	0	-2.955524	1.980733	-0.204970
39	1	0	-3.209803	2.292616	-1.232809
40	1	0	-3.612199	1.146844	0.056146
41	6	0	-3.174317	3.134287	0.762779
42	1	0	-4.227692	3.418026	0.780451
43	1	0	-2.876371	2.842087	1.771580
44	1	0	-2.597500	4.015380	0.474434

Structure 27b (^{2}E ax-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1016.149514
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.903031	0.010924	-0.609792
2	6	0	3.070492	1.218868	0.060138
3	6	0	4.345331	1.654098	0.406117
4	6	0	5.458773	0.888363	0.077742
5	6	0	5.295650	-0.311252	-0.608650
6	6	0	4.021957	-0.744079	-0.954470
7	1	0	2.200096	1.812407	0.312070
8	1	0	4.469190	2.594387	0.929990
9	1	0	6.450985	1.228782	0.348656
10	1	0	6.160579	-0.907100	-0.875058
11	1	0	3.886867	-1.684547	-1.478481
12	6	0	1.536945	-0.528225	-0.936289
13	1	0	1.576306	-1.045744	-1.904292
14	7	0	0.975582	-1.464928	0.023675
15	8	0	0.589409	0.539758	-1.047868
16	6	0	-0.717240	-0.019348	-0.859555
17	6	0	-0.428471	-1.472367	-0.401635
18	1	0	-1.082961	-1.812725	0.396743
19	1	0	-0.550994	-2.155772	-1.243835
20	1	0	-1.251768	0.007934	-1.812997
21	6	0	-1.433669	0.858223	0.171070
22	1	0	-1.134074	0.551394	1.184784
23	6	0	-2.958640	0.844909	0.096846
24	1	0	-3.253350	1.162858	-0.913249
25	6	0	-3.593388	-0.513966	0.379088
26	1	0	-3.198523	-0.906428	1.322096
27	6	0	-5.105453	-0.406199	0.486890
28	1	0	-5.507481	-1.372468	0.811532
29	1	0	-5.370373	0.375518	1.201466
30	8	0	-1.087331	2.222504	-0.023381
31	1	0	-0.183154	2.233304	-0.356857
32	8	0	-3.456723	1.748269	1.065226
33	1	0	-2.935982	2.553473	0.971145
34	8	0	-3.260235	-1.436844	-0.643948
35	1	0	-3.880708	-1.261212	-1.362006
36	8	0	-5.555260	-0.094656	-0.827940
37	1	0	-6.506285	0.021660	-0.817488
38	6	0	1.159315	-1.091084	1.439279
39	1	0	1.161153	-0.001848	1.581213
40	1	0	0.290940	-1.473894	1.980296
41	6	0	2.414774	-1.705920	2.047471
42	1	0	2.425545	-1.539332	3.127240
43	1	0	2.424154	-2.780682	1.858223
44	1	0	3.325445	-1.275382	1.630864

Structure 27b (^{2}E ec-ec H-bond O) (M06-2X, Benzene)

Energy (Hartrees): = - 1016.175563
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.861018	-0.150576	-0.414099
2	6	0	-2.693607	-1.087703	0.606611
3	6	0	-3.792982	-1.755943	1.125843
4	6	0	-5.069908	-1.487053	0.634740
5	6	0	-5.240753	-0.552624	-0.378605
6	6	0	-4.134516	0.111221	-0.904846
7	1	0	-1.697542	-1.283798	0.990368
8	1	0	-3.659019	-2.486794	1.914879
9	1	0	-5.928309	-2.006999	1.043960
10	1	0	-6.231844	-0.341943	-0.763232

11	1	0	-4.262331	0.838766	-1.700165
12	6	0	-1.657036	0.578603	-0.955163
13	1	0	-1.960185	1.219690	-1.804001
14	7	0	-0.966183	1.350123	0.066067
15	8	0	-0.680224	-0.344340	-1.418110
16	6	0	0.629729	0.104489	-1.025481
17	6	0	0.380277	1.503059	-0.472080
18	1	0	1.092371	1.778678	0.303708
19	1	0	0.424957	2.256836	-1.275669
20	1	0	1.265541	0.102045	-1.910567
21	6	0	1.161217	-0.869166	0.038721
22	1	0	0.811768	-0.534091	1.026645
23	6	0	2.679990	-1.021060	0.080551
24	1	0	3.018123	-1.357156	-0.909925
25	6	0	3.432243	0.258857	0.441045
26	1	0	3.001110	0.684775	1.352808
27	6	0	4.909536	-0.005030	0.674578
28	1	0	5.380312	0.917717	1.032284
29	1	0	5.038082	-0.799186	1.412823
30	8	0	0.678663	-2.182735	-0.207493
31	1	0	-0.183197	-2.081292	-0.631346
32	8	0	3.001808	-1.987811	1.064615
33	1	0	2.402108	-2.727282	0.915580
34	8	0	3.289660	1.222289	-0.591858
35	1	0	3.942182	0.978785	-1.260505
36	8	0	5.438249	-0.375218	-0.595294
37	1	0	6.385126	-0.507132	-0.511406
38	6	0	-1.642574	2.594218	0.404583
39	1	0	-1.689926	3.260848	-0.474854
40	1	0	-2.670806	2.345297	0.681451
41	6	0	-0.961149	3.306926	1.562781
42	1	0	-1.546335	4.175187	1.871768
43	1	0	-0.866368	2.630329	2.414894
44	1	0	0.035526	3.659074	1.288092

Structure 27b (^{2}E ec-ec H-bond N) (M06-2X, Benzene)

Energy (Hartrees): = - 1016.178868
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.948024	-0.943579	-0.455697
2	6	0	-1.399060	-1.512251	0.693781
3	6	0	-1.955220	-2.662842	1.234811
4	6	0	-3.065438	-3.253068	0.633980
5	6	0	-3.613745	-2.691026	-0.511844
6	6	0	-3.051051	-1.539587	-1.057772
7	1	0	-0.535218	-1.049764	1.158433
8	1	0	-1.522362	-3.103068	2.125509
9	1	0	-3.497764	-4.151792	1.058378
10	1	0	-4.474065	-3.149707	-0.985052
11	1	0	-3.471544	-1.103778	-1.958850
12	6	0	-1.358157	0.323942	-1.020408
13	1	0	-1.778740	0.512991	-2.025010
14	7	0	-1.584590	1.486621	-0.156244
15	8	0	0.050121	0.232812	-1.113597
16	6	0	0.636702	1.491812	-0.746945
17	6	0	-0.565337	2.428082	-0.624645
18	1	0	-0.400337	3.228218	0.097907
19	1	0	-0.834645	2.862733	-1.599781
20	1	0	1.328623	1.791429	-1.530496
21	6	0	1.398149	1.351041	0.572560
22	1	0	2.014206	2.251311	0.706096
23	6	0	2.313295	0.122793	0.649082
24	1	0	1.722379	-0.766331	0.396611
25	6	0	3.530363	0.181585	-0.272373
26	1	0	4.120629	1.066698	-0.016496
27	6	0	4.396403	-1.055867	-0.106804
28	1	0	5.306337	-0.932352	-0.704822
29	1	0	4.659716	-1.191146	0.945593
30	8	0	0.518232	1.267234	1.694414
31	1	0	-0.395928	1.201852	1.365682
32	8	0	2.816439	0.026230	1.971951
33	1	0	2.060238	0.197600	2.545222
34	8	0	3.149300	0.309758	-1.630685
35	1	0	2.757175	-0.537564	-1.876399
36	8	0	3.618905	-2.143272	-0.596064
37	1	0	4.150294	-2.941684	-0.566244
38	6	0	-2.956037	1.983349	-0.194918
39	1	0	-3.216832	2.298228	-1.219471
40	1	0	-3.613120	1.151180	0.069729
41	6	0	-3.167581	3.133057	0.777559

42	1	0	-4.221144	3.418070	0.798848
43	1	0	-2.869921	2.838038	1.786318
44	1	0	-2.591396	4.015744	0.491629

Structure 27b (^{2}E ax-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 1016.1693149
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.909596	0.017147	-0.606009
2	6	0	3.087873	1.221481	0.068504
3	6	0	4.367920	1.650202	0.405475
4	6	0	5.475577	0.880589	0.065381
5	6	0	5.301259	-0.317348	-0.621875
6	6	0	4.022767	-0.743754	-0.959125
7	1	0	2.223755	1.819917	0.331008
8	1	0	4.500213	2.588387	0.931654
9	1	0	6.471831	1.215749	0.329096
10	1	0	6.161529	-0.917076	-0.895723
11	1	0	3.880150	-1.681714	-1.486010
12	6	0	1.539398	-0.514544	-0.930971
13	1	0	1.573977	-1.022735	-1.903878
14	7	0	0.977465	-1.459638	0.021802
15	8	0	0.592781	0.555986	-1.026835
16	6	0	-0.715300	-0.008242	-0.854592
17	6	0	-0.427122	-1.464190	-0.405497
18	1	0	-1.080362	-1.807171	0.392863
19	1	0	-0.547561	-2.142501	-1.252064
20	1	0	-1.240747	0.026680	-1.812881
21	6	0	-1.440621	0.859303	0.178221
22	1	0	-1.141507	0.548150	1.190352
23	6	0	-2.965792	0.842491	0.101066
24	1	0	-3.258880	1.171728	-0.905651
25	6	0	-3.599962	-0.520617	0.367455
26	1	0	-3.205587	-0.925221	1.305353
27	6	0	-5.112150	-0.423067	0.474668
28	1	0	-5.507701	-1.401911	0.767971
29	1	0	-5.391212	0.328343	1.216488
30	8	0	-1.098208	2.227462	-0.009015
31	1	0	-0.180679	2.242397	-0.305025
32	8	0	-3.466169	1.737465	1.078373
33	1	0	-2.948515	2.545421	0.988804
34	8	0	-3.264300	-1.429102	-0.669184
35	1	0	-3.881416	-1.237478	-1.386593
36	8	0	-5.566783	-0.069756	-0.828257
37	1	0	-6.526446	-0.070147	-0.833329
38	6	0	1.159863	-1.097665	1.441373
39	1	0	1.172092	-0.009746	1.591064
40	1	0	0.287742	-1.477248	1.978450
41	6	0	2.407644	-1.727995	2.046895
42	1	0	2.421296	-1.563076	3.127500
43	1	0	2.406559	-2.803833	1.859219
44	1	0	3.324949	-1.308632	1.632244

Structure 27b (^{2}E ec-ec H-bond O) (M06-2X, DMSO)

Energy (Hartrees): = - 1016.1784942
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.873936	-0.157256	-0.406200
2	6	0	-2.723452	-1.141432	0.573061
3	6	0	-3.837621	-1.793613	1.084379
4	6	0	-5.112943	-1.460749	0.627101
5	6	0	-5.266885	-0.478306	-0.344215
6	6	0	-4.146436	0.169445	-0.862505
7	1	0	-1.730494	-1.393757	0.932215
8	1	0	-3.715787	-2.559825	1.841647
9	1	0	-5.982408	-1.967790	1.029626
10	1	0	-6.256207	-0.216008	-0.701113
11	1	0	-4.261572	0.934333	-1.624310
12	6	0	-1.658162	0.558045	-0.939310
13	1	0	-1.947582	1.199793	-1.790285
14	7	0	-0.969864	1.329435	0.086645
15	8	0	-0.686927	-0.378994	-1.386853
16	6	0	0.627706	0.078264	-1.013023

17	6	0	0.380526	1.474489	-0.452137
18	1	0	1.090412	1.743952	0.327983
19	1	0	0.422836	2.231078	-1.251866
20	1	0	1.251033	0.081259	-1.907091
21	6	0	1.179655	-0.897085	0.036683
22	1	0	0.826885	-0.582742	1.029976
23	6	0	2.700376	-1.020535	0.076528
24	1	0	3.041198	-1.353067	-0.914155
25	6	0	3.429368	0.275858	0.428098
26	1	0	2.978027	0.713537	1.323999
27	6	0	4.907380	0.047044	0.687577
28	1	0	5.353797	0.992971	1.011771
29	1	0	5.048038	-0.707998	1.463906
30	8	0	0.720577	-2.217886	-0.228975
31	1	0	-0.164958	-2.122761	-0.602715
32	8	0	3.039250	-1.983823	1.061790
33	1	0	2.446976	-2.730253	0.915697
34	8	0	3.286103	1.216342	-0.627418
35	1	0	3.940095	0.954925	-1.288764
36	8	0	5.466052	-0.369676	-0.556042
37	1	0	6.424241	-0.326354	-0.487168
38	6	0	-1.637687	2.591868	0.386196
39	1	0	-1.678051	3.226890	-0.515116
40	1	0	-2.668973	2.363045	0.669884
41	6	0	-0.949605	3.337297	1.518615
42	1	0	-1.526850	4.222545	1.793108
43	1	0	-0.863259	2.695392	2.398857
44	1	0	0.051507	3.667084	1.232293

Structure 27b (^{2}E ec-ec H-bond N) (M06-2X, DMSO)

Energy (Hartrees): = - 1016.18208
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.944277	-0.946153	-0.458014
2	6	0	-1.379039	-1.528007	0.678239
3	6	0	-1.924098	-2.689081	1.211471
4	6	0	-3.038728	-3.277465	0.614791
5	6	0	-3.603502	-2.701404	-0.517216
6	6	0	-3.052738	-1.539167	-1.054585
7	1	0	-0.512709	-1.068137	1.141917
8	1	0	-1.480423	-3.138713	2.092478
9	1	0	-3.462319	-4.183825	1.032276
10	1	0	-4.468185	-3.156642	-0.986279
11	1	0	-3.487408	-1.090553	-1.942446
12	6	0	-1.367759	0.329654	-1.018684
13	1	0	-1.798994	0.524405	-2.015791
14	7	0	-1.590996	1.483810	-0.142449
15	8	0	0.042746	0.241923	-1.125611
16	6	0	0.627537	1.499093	-0.743086
17	6	0	-0.575666	2.430558	-0.617117
18	1	0	-0.411413	3.234569	0.100847
19	1	0	-0.852725	2.858417	-1.591690
20	1	0	1.320568	1.810307	-1.520510
21	6	0	1.385547	1.348178	0.577504
22	1	0	1.999541	2.248210	0.717655
23	6	0	2.299492	0.118225	0.645843
24	1	0	1.713875	-0.763450	0.357602
25	6	0	3.539749	0.200247	-0.241974
26	1	0	4.123507	1.078279	0.049728
27	6	0	4.402374	-1.041200	-0.093480
28	1	0	5.319836	-0.904941	-0.675294
29	1	0	4.656991	-1.205367	0.956820
30	8	0	0.498509	1.253573	1.695425
31	1	0	-0.414004	1.203293	1.354472
32	8	0	2.766039	-0.017419	1.980852
33	1	0	1.993289	0.153204	2.532904
34	8	0	3.190583	0.361978	-1.607483
35	1	0	2.829414	-0.490098	-1.883889
36	8	0	3.633811	-2.122435	-0.615815
37	1	0	4.216343	-2.877344	-0.737801
38	6	0	-2.964332	1.982149	-0.188075
39	1	0	-3.215954	2.293935	-1.214364
40	1	0	-3.625009	1.151421	0.073638
41	6	0	-3.178308	3.134176	0.780376
42	1	0	-4.231536	3.421728	0.790699
43	1	0	-2.891391	2.842020	1.793735
44	1	0	-2.595329	4.012835	0.495538

Structure 27b (^{2}E ax-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 1016.1730778
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.911210	-0.004026	-0.612404
2	6	0	3.090335	1.210414	0.045551
3	6	0	4.370891	1.635161	0.388923
4	6	0	5.477306	0.852316	0.071488
5	6	0	5.301957	-0.353443	-0.603472
6	6	0	4.022958	-0.776019	-0.947547
7	1	0	2.229705	1.819918	0.295399
8	1	0	4.504519	2.579870	0.903623
9	1	0	6.473245	1.184250	0.341606
10	1	0	6.161214	-0.961323	-0.863173
11	1	0	3.879772	-1.717840	-1.468126
12	6	0	1.541727	-0.540935	-0.930821
13	1	0	1.580640	-1.081097	-1.885445
14	7	0	0.975398	-1.455839	0.051710
15	8	0	0.598231	0.528101	-1.062735
16	6	0	-0.712401	-0.028400	-0.871566
17	6	0	-0.427853	-1.472478	-0.388291
18	1	0	-1.084905	-1.794969	0.415647
19	1	0	-0.534615	-2.166897	-1.223515
20	1	0	-1.242035	-0.015324	-1.827661
21	6	0	-1.433041	0.860066	0.146298
22	1	0	-1.132574	0.569406	1.163080
23	6	0	-2.957353	0.839132	0.074846
24	1	0	-3.254731	1.154598	-0.935204
25	6	0	-3.582814	-0.525247	0.358337
26	1	0	-3.157666	-0.935563	1.279817
27	6	0	-5.090227	-0.436783	0.514190
28	1	0	-5.469921	-1.424452	0.795654
29	1	0	-5.352751	0.288469	1.287550
30	8	0	-1.091090	2.225476	-0.073012
31	1	0	-0.149580	2.238094	-0.283543
32	8	0	-3.455454	1.750325	1.041692
33	1	0	-2.923441	2.549072	0.949126
34	8	0	-3.277312	-1.426966	-0.695837
35	1	0	-3.906127	-1.215433	-1.398064
36	8	0	-5.598168	-0.049350	-0.760299
37	1	0	-6.548667	-0.194983	-0.763612
38	6	0	1.136268	-1.028643	1.458039
39	1	0	1.129612	0.064415	1.557804
40	1	0	0.262828	-1.395759	2.000814
41	6	0	2.385798	-1.611459	2.106501
42	1	0	2.379434	-1.399866	3.179051
43	1	0	2.405427	-2.695553	1.970223
44	1	0	3.304602	-1.196788	1.688079

Structure 27c ($^5C_2$ ec-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1016.1554255
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.083353	1.593149	0.194756
2	6	0	0.147720	2.270818	-0.399897
3	6	0	-1.159421	0.172077	-0.363274
4	1	0	0.236974	3.262071	0.042850
5	1	0	0.041532	2.380771	-1.494519
6	1	0	-1.990530	2.137847	-0.058963
7	1	0	-1.270449	0.200330	-1.458644
8	8	0	0.068450	-0.485557	-0.043812
9	7	0	1.339361	1.487404	-0.057301
10	6	0	-2.257666	-0.703521	0.239164
11	1	0	-2.293700	-0.503567	1.317634
12	6	0	-3.621672	-0.430259	-0.375034
13	1	0	-3.571670	-0.677770	-1.445413
14	6	0	-4.688557	-1.300433	0.263500
15	1	0	-4.689442	-1.117554	1.345261
16	1	0	-4.477868	-2.354090	0.066309
17	8	0	-1.992977	-2.068964	-0.019864
18	1	0	-1.046581	-2.192256	0.110247
19	8	0	-3.948639	0.932576	-0.194675
20	1	0	-4.894985	0.997206	-0.365528
21	8	0	-5.918491	-0.883537	-0.321043
22	1	0	-6.643829	-1.284225	0.160429
23	8	0	-0.978698	1.575798	1.602926

24	1	0	-0.087381	1.257964	1.790609
25	6	0	2.570825	2.140022	-0.510723
26	1	0	2.568933	2.251278	-1.610214
27	1	0	3.405350	1.485929	-0.256325
28	6	0	2.390131	-0.735704	-0.267169
29	6	0	2.676052	-1.009410	1.069827
30	6	0	3.189104	-1.276244	-1.266970
31	6	0	3.757717	-1.813937	1.399374
32	1	0	2.042031	-0.586236	1.840048
33	6	0	4.276461	-2.081496	-0.937643
34	1	0	2.962587	-1.066389	-2.307255
35	6	0	4.561374	-2.349647	0.395187
36	1	0	3.976758	-2.025995	2.439259
37	1	0	4.896860	-2.499489	-1.721246
38	1	0	5.406573	-2.976267	0.654194
39	6	0	1.206080	0.135966	-0.602971
40	1	0	1.075689	0.182266	-1.703637
41	6	0	2.794198	3.496160	0.147631
42	1	0	3.814037	3.833483	-0.043626
43	1	0	2.118500	4.264012	-0.230422
44	1	0	2.653957	3.411083	1.227265

Structure 27c ($^5C_2$ ax-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1016.1528944
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.156150	1.669723	0.158138
2	6	0	-0.074398	2.255221	0.866869
3	6	0	1.182016	0.163126	0.424796
4	1	0	-0.167015	3.316053	0.631224
5	1	0	0.062629	2.163960	1.951054
6	1	0	2.071749	2.124953	0.533985
7	1	0	1.268838	-0.023379	1.506240
8	8	0	-0.063826	-0.382006	-0.028180
9	7	0	-1.323202	1.572892	0.505499
10	6	0	2.269411	-0.632420	-0.295915
11	1	0	2.324730	-0.290163	-1.337580
12	6	0	3.638495	-0.467135	0.346076
13	1	0	3.574387	-0.791438	1.395314
14	6	0	4.672606	-1.332532	-0.352812
15	1	0	4.676777	-1.083562	-1.421435
16	1	0	4.428275	-2.388846	-0.220874
17	8	0	1.972078	-2.013975	-0.226823
18	1	0	1.016807	-2.092228	-0.323863
19	8	0	4.020581	0.889501	0.265418
20	1	0	4.969720	0.903087	0.433193
21	8	0	5.917002	-0.994114	0.250601
22	1	0	6.627176	-1.393318	-0.254120
23	8	0	1.115436	1.925017	-1.235035
24	1	0	0.456879	1.331925	-1.611860
25	6	0	-1.881156	1.955559	-0.805931
26	1	0	-1.703767	1.170316	-1.553984
27	1	0	-1.339750	2.836372	-1.154458
28	6	0	-2.405085	-0.638721	0.397527
29	6	0	-2.514966	-1.383555	-0.771552
30	6	0	-3.477570	-0.589765	1.285764
31	6	0	-3.697030	-2.059935	-1.059489
32	1	0	-1.673554	-1.430253	-1.452043
33	6	0	-4.654405	-1.269642	1.002442
34	1	0	-3.389964	0.001957	2.191121
35	6	0	-4.767794	-2.003040	-0.175973
36	1	0	-3.778107	-2.634136	-1.974779
37	1	0	-5.484295	-1.226690	1.697649
38	1	0	-5.686325	-2.532014	-0.400092
39	6	0	-1.162434	0.153714	0.720169
40	1	0	-0.921957	0.019650	1.784688
41	6	0	-3.371892	2.270298	-0.739439
42	1	0	-3.719467	2.652720	-1.702409
43	1	0	-3.958233	1.385014	-0.491224
44	1	0	-3.554976	3.029017	0.023874

Structure 27c ($^5C_2$ ec-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 1016.1763356
No imaginary frequencies

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-1.079903	1.601133	0.185624
2	6	0	0.147849	2.274077	-0.420277
3	6	0	-1.158138	0.176475	-0.362111
4	1	0	0.239780	3.270073	0.011574
5	1	0	0.033800	2.373258	-1.514403
6	1	0	-1.986494	2.146678	-0.068072
7	1	0	-1.269015	0.198887	-1.457309
8	8	0	0.070671	-0.476790	-0.036425
9	7	0	1.343094	1.495115	-0.077847
10	6	0	-2.254617	-0.699807	0.244026
11	1	0	-2.288334	-0.503637	1.323160
12	6	0	-3.623136	-0.431310	-0.363551
13	1	0	-3.576816	-0.670923	-1.435940
14	6	0	-4.685117	-1.307936	0.274284
15	1	0	-4.686043	-1.134340	1.357519
16	1	0	-4.476598	-2.361056	0.071065
17	8	0	-1.983670	-2.065740	-0.015628
18	1	0	-1.035370	-2.181025	0.111889
19	8	0	-3.956927	0.930213	-0.174516
20	1	0	-4.906364	0.987283	-0.333655
21	8	0	-5.919807	-0.894436	-0.304173
22	1	0	-6.640209	-1.286978	0.193978
23	8	0	-0.969215	1.593467	1.595542
24	1	0	-0.077146	1.273653	1.779515
25	6	0	2.568757	2.148325	-0.549621
26	1	0	2.548437	2.264065	-1.647733
27	1	0	3.407237	1.493488	-0.310710
28	6	0	2.390777	-0.735190	-0.261366
29	6	0	2.733064	-0.925978	1.077244
30	6	0	3.126775	-1.366953	-1.256917
31	6	0	3.806938	-1.739066	1.412321
32	1	0	2.155092	-0.428306	1.847640
33	6	0	4.205101	-2.182616	-0.921772
34	1	0	2.857661	-1.221246	-2.297983
35	6	0	4.545798	-2.368599	0.412090
36	1	0	4.070356	-1.884767	2.453464
37	1	0	4.774973	-2.672128	-1.702885
38	1	0	5.385029	-3.001933	0.675231
39	6	0	1.209502	0.137769	-0.607523
40	1	0	1.076883	0.167811	-1.707242
41	6	0	2.804680	3.500867	0.110155
42	1	0	3.822698	3.836324	-0.096700
43	1	0	2.126147	4.273320	-0.254277
44	1	0	2.684240	3.414850	1.192781

Structure 27c ($^5C_2$ ax-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 1016.173418
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.156292	1.668766	0.173083
2	6	0	-0.075491	2.249572	0.882796
3	6	0	1.179888	0.160273	0.425804
4	1	0	-0.166676	3.312919	0.657631
5	1	0	0.060663	2.146096	1.965720
6	1	0	2.069141	2.120585	0.559808
7	1	0	1.262545	-0.032699	1.506003
8	8	0	-0.065394	-0.380066	-0.035553
9	7	0	-1.324194	1.570974	0.512038
10	6	0	2.268109	-0.634580	-0.294928
11	1	0	2.318396	-0.304182	-1.340556
12	6	0	3.640714	-0.460119	0.338302
13	1	0	3.578996	-0.748711	1.398192
14	6	0	4.670647	-1.350199	-0.335241
15	1	0	4.676385	-1.139389	-1.411927
16	1	0	4.429375	-2.402407	-0.168681
17	8	0	1.970750	-2.017214	-0.213859
18	1	0	1.015385	-2.093983	-0.316288
19	8	0	4.031885	0.892353	0.213357
20	1	0	4.982866	0.901289	0.374059
21	8	0	5.918547	-0.997637	0.254756
22	1	0	6.625661	-1.397673	-0.256304
23	8	0	1.124931	1.938924	-1.219320
24	1	0	0.460722	1.357006	-1.604848
25	6	0	-1.879500	1.966057	-0.797069
26	1	0	-1.704281	1.187733	-1.552381
27	1	0	-1.337903	2.849986	-1.137194
28	6	0	-2.407426	-0.642082	0.391293
29	6	0	-2.525420	-1.368330	-0.789406

30	6	0	-3.474460	-0.608446	1.287664
31	6	0	-3.707635	-2.045215	-1.077552
32	1	0	-1.690931	-1.403449	-1.479424
33	6	0	-4.651559	-1.288505	1.003526
34	1	0	-3.381690	-0.033775	2.203720
35	6	0	-4.772123	-2.004798	-0.184897
36	1	0	-3.794400	-2.605407	-2.001339
37	1	0	-5.475725	-1.259147	1.706722
38	1	0	-5.690358	-2.534823	-0.409317
39	6	0	-1.164537	0.149338	0.717922
40	1	0	-0.923361	0.009773	1.780944
41	6	0	-3.368190	2.285586	-0.727745
42	1	0	-3.716738	2.670076	-1.690174
43	1	0	-3.959768	1.402922	-0.480449
44	1	0	-3.550557	3.045652	0.035448

Structure 27c ($^5C_2$ ec-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 1016.1797947
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.075808	1.597557	0.170875
2	6	0	0.153602	2.271362	-0.427850
3	6	0	-1.150100	0.176858	-0.381323
4	1	0	0.242906	3.269769	-0.000717
5	1	0	0.043781	2.363830	-1.521791
6	1	0	-1.978370	2.146876	-0.089658
7	1	0	-1.247024	0.208309	-1.476835
8	8	0	0.075147	-0.480448	-0.043932
9	7	0	1.350225	1.495088	-0.077752
10	6	0	-2.249576	-0.710025	0.197077
11	1	0	-2.253649	-0.591208	1.287849
12	6	0	-3.632401	-0.373786	-0.340654
13	1	0	-3.607572	-0.426221	-1.439044
14	6	0	-4.669907	-1.361237	0.164531
15	1	0	-4.636751	-1.386960	1.260615
16	1	0	-4.468356	-2.360051	-0.228700
17	8	0	-2.003489	-2.060545	-0.163432
18	1	0	-1.053304	-2.190817	-0.064112
19	8	0	-3.984048	0.931698	0.082519
20	1	0	-4.940645	0.986023	-0.033961
21	8	0	-5.926267	-0.866633	-0.291681
22	1	0	-6.623992	-1.332007	0.179132
23	8	0	-0.975902	1.586023	1.584811
24	1	0	-0.087205	1.256349	1.771637
25	6	0	2.570058	2.145559	-0.574309
26	1	0	2.536112	2.237034	-1.673389
27	1	0	3.415328	1.500548	-0.330405
28	6	0	2.397272	-0.734405	-0.244268
29	6	0	2.714740	-0.933004	1.100216
30	6	0	3.154056	-1.357547	-1.230611
31	6	0	3.782866	-1.748953	1.450748
32	1	0	2.122403	-0.443430	1.865704
33	6	0	4.226937	-2.175433	-0.879909
34	1	0	2.906102	-1.201289	-2.275585
35	6	0	4.541694	-2.371633	0.460000
36	1	0	4.026284	-1.901821	2.496081
37	1	0	4.813493	-2.657682	-1.653510
38	1	0	5.376264	-3.006552	0.734930
39	6	0	1.219624	0.136391	-0.608090
40	1	0	1.098064	0.165276	-1.707173
41	6	0	2.806746	3.512663	0.052885
42	1	0	3.816455	3.851804	-0.187222
43	1	0	2.110498	4.269009	-0.312266
44	1	0	2.715263	3.450613	1.140509

Structure 27c ($^5C_2$ ax-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 1016.177145
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.157164	1.666716	0.197866
2	6	0	-0.075606	2.240789	0.909488
3	6	0	1.178530	0.156506	0.433144
4	1	0	-0.166511	3.306843	0.696280

5	1	0	0.062189	2.120625	1.989891
6	1	0	2.065404	2.112857	0.601800
7	1	0	1.262087	-0.043447	1.511254
8	8	0	-0.067780	-0.379247	-0.032744
9	7	0	-1.327144	1.567132	0.531050
10	6	0	2.264383	-0.633369	-0.295867
11	1	0	2.306345	-0.309073	-1.343472
12	6	0	3.641455	-0.453592	0.326142
13	1	0	3.580821	-0.704629	1.395385
14	6	0	4.663704	-1.369820	-0.323710
15	1	0	4.669099	-1.193918	-1.406256
16	1	0	4.420532	-2.415927	-0.125325
17	8	0	1.966349	-2.017850	-0.211366
18	1	0	1.011238	-2.090143	-0.324827
19	8	0	4.047000	0.892924	0.157875
20	1	0	4.999963	0.890359	0.311407
21	8	0	5.917046	-1.009750	0.251865
22	1	0	6.618111	-1.403241	-0.275814
23	8	0	1.141063	1.960066	-1.192470
24	1	0	0.477584	1.387950	-1.595771
25	6	0	-1.862771	1.963030	-0.787418
26	1	0	-1.652464	1.199657	-1.548990
27	1	0	-1.336848	2.865075	-1.102903
28	6	0	-2.408409	-0.643879	0.393492
29	6	0	-2.542318	-1.330936	-0.809827
30	6	0	-3.463860	-0.638041	1.304840
31	6	0	-3.732341	-1.991436	-1.107330
32	1	0	-1.717866	-1.346131	-1.512917
33	6	0	-4.649285	-1.300939	1.010742
34	1	0	-3.354807	-0.102389	2.242892
35	6	0	-4.787448	-1.975442	-0.200993
36	1	0	-3.833211	-2.520244	-2.048352
37	1	0	-5.464955	-1.292911	1.724760
38	1	0	-5.711690	-2.492190	-0.432966
39	6	0	-1.164258	0.141307	0.728314
40	1	0	-0.924173	-0.005058	1.789835
41	6	0	-3.359159	2.251971	-0.749314
42	1	0	-3.693022	2.632761	-1.718432
43	1	0	-3.941914	1.358414	-0.517235
44	1	0	-3.574030	3.008490	0.009722

Structure 27d ($^5C_2$ ec-ax) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1016.1522064
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.432806	1.513196	0.770268
2	6	0	-1.045507	1.486189	1.171289
3	6	0	0.710070	0.277751	-0.094932
4	1	0	-1.279948	2.405847	1.710592
5	1	0	-1.257965	0.628279	1.828448
6	1	0	1.083923	1.501723	1.642171
7	1	0	0.509579	-0.633337	0.485655
8	8	0	-0.166747	0.316098	-1.231195
9	7	0	-1.820915	1.454569	-0.060307
10	6	0	2.120286	0.205769	-0.683714
11	1	0	2.417121	1.218150	-0.985771
12	6	0	3.133372	-0.345947	0.306310
13	1	0	2.836747	-1.372280	0.567238
14	6	0	4.522705	-0.393416	-0.303168
15	1	0	4.792302	0.614094	-0.643754
16	1	0	4.536916	-1.085334	-1.148557
17	8	0	2.145003	-0.683293	-1.787510
18	1	0	1.369788	-0.470236	-2.317592
19	8	0	3.145967	0.474838	1.456027
20	1	0	3.953204	0.244818	1.929833
21	8	0	5.383977	-0.818875	0.748183
22	1	0	6.293897	-0.717326	0.465187
23	8	0	0.702398	2.697871	0.051727
24	1	0	0.031245	2.726675	-0.641948
25	6	0	-3.163576	2.014959	-0.033452
26	1	0	-3.654763	1.817208	0.929853
27	1	0	-3.766408	1.513852	-0.796946
28	6	0	-1.930142	-1.068295	-0.314901
29	6	0	-2.985171	-1.206962	0.583612
30	6	0	-1.259523	-2.212890	-0.749486
31	6	0	-3.369867	-2.465914	1.035828
32	1	0	-3.509301	-0.329862	0.942540
33	6	0	-1.640828	-3.469580	-0.296809
34	1	0	-0.415726	-2.108831	-1.422322
35	6	0	-2.700639	-3.600500	0.595071

36	1	0	-4.190121	-2.557299	1.737970
37	1	0	-1.105184	-4.348114	-0.636638
38	1	0	-2.997576	-4.580300	0.949297
39	6	0	-1.541321	0.301670	-0.884700
40	1	0	-2.071999	0.440714	-1.831279
41	6	0	-3.138888	3.518400	-0.294296
42	1	0	-4.139333	3.950049	-0.215656
43	1	0	-2.491042	4.021209	0.427436
44	1	0	-2.746399	3.718623	-1.292991

Structure 27d ($^5C_2$ ax-ax) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1016.1559038
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.480594	1.470164	-0.959270
2	6	0	0.978872	1.402803	-1.422268
3	6	0	-0.702311	0.315589	0.016636
4	1	0	1.202608	2.247987	-2.074241
5	1	0	1.130156	0.481648	-1.996948
6	1	0	-1.161169	1.373170	-1.803951
7	1	0	-0.502944	-0.636073	-0.492336
8	8	0	0.229648	0.483213	1.097629
9	7	0	1.927588	1.410036	-0.304652
10	6	0	-2.081879	0.248480	0.675967
11	1	0	-2.410959	1.268564	0.914957
12	6	0	-3.116728	-0.408777	-0.222549
13	1	0	-2.792054	-1.440031	-0.424604
14	6	0	-4.475768	-0.461822	0.451615
15	1	0	-4.769757	0.557379	0.732472
16	1	0	-4.427748	-1.091153	1.343436
17	8	0	-2.021966	-0.551496	1.843861
18	1	0	-1.217023	-0.291605	2.304767
19	8	0	-3.209432	0.328638	-1.423461
20	1	0	-4.023518	0.034613	-1.847330
21	8	0	-5.362107	-0.992503	-0.527786
22	1	0	-6.262738	-0.912175	-0.209994
23	8	0	-0.761075	2.714331	-0.340352
24	1	0	-0.382783	2.676002	0.544171
25	6	0	2.231713	2.718311	0.285153
26	1	0	1.608758	2.919253	1.169978
27	1	0	1.983465	3.489156	-0.445925
28	6	0	1.964835	-1.003169	0.227605
29	6	0	3.049482	-1.205404	-0.622250
30	6	0	1.272690	-2.106311	0.727301
31	6	0	3.436834	-2.494991	-0.971331
32	1	0	3.577021	-0.340533	-1.007223
33	6	0	1.659496	-3.394074	0.375749
34	1	0	0.414544	-1.951670	1.372292
35	6	0	2.743734	-3.591947	-0.473030
36	1	0	4.279467	-2.641991	-1.636625
37	1	0	1.110467	-4.243970	0.763435
38	1	0	3.043575	-4.596353	-0.747354
39	6	0	1.601154	0.407433	0.675970
40	1	0	2.162933	0.629653	1.586899
41	6	0	3.703933	2.811481	0.667833
42	1	0	3.927155	3.776221	1.128828
43	1	0	3.976081	2.027250	1.378982
44	1	0	4.328036	2.690341	-0.219035

Structure 27d ($^5C_2$ ec-ax) (M06-2X, Benzene)

Energy (Hartrees): = - 1016.1726849
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.453432	-1.509809	-0.759129
2	6	0	-1.024450	-1.506695	-1.161328
3	6	0	0.715651	-0.260160	0.090109
4	1	0	-1.248872	-2.433887	-1.692254
5	1	0	-1.242740	-0.658555	-1.828520
6	1	0	1.103050	-1.502637	-1.632019
7	1	0	0.504340	0.640346	-0.503114
8	8	0	-0.160884	-0.293531	1.226300
9	7	0	-1.800299	-1.471358	0.069676

10	6	0	2.123061	-0.157667	0.680791
11	1	0	2.424090	-1.152447	1.032320
12	6	0	3.145896	0.347865	-0.324887
13	1	0	2.828389	1.340384	-0.676236
14	6	0	4.518777	0.481935	0.309559
15	1	0	4.804986	-0.482185	0.747959
16	1	0	4.502040	1.248047	1.088451
17	8	0	2.132689	0.780033	1.745734
18	1	0	1.349782	0.587335	2.273298
19	8	0	3.212058	-0.561841	-1.405797
20	1	0	4.032894	-0.353460	-1.867251
21	8	0	5.399018	0.833569	-0.754238
22	1	0	6.303792	0.748092	-0.445564
23	8	0	0.737658	-2.682900	-0.024091
24	1	0	0.052681	-2.718080	0.656674
25	6	0	-3.139211	-2.045881	0.050552
26	1	0	-3.632960	-1.863671	-0.913934
27	1	0	-3.745079	-1.542549	0.809991
28	6	0	-1.950734	1.052997	0.299667
29	6	0	-2.987937	1.164533	-0.623697
30	6	0	-1.326752	2.216002	0.755313
31	6	0	-3.400137	2.414158	-1.079196
32	1	0	-3.475519	0.273960	-1.000632
33	6	0	-1.735897	3.463600	0.300751
34	1	0	-0.498297	2.135783	1.450074
35	6	0	-2.778539	3.566927	-0.615347
36	1	0	-4.205930	2.484421	-1.800756
37	1	0	-1.237509	4.356460	0.660157
38	1	0	-3.098439	4.539476	-0.970539
39	6	0	-1.537860	-0.305743	0.880702
40	1	0	-2.064925	-0.442344	1.829252
41	6	0	-3.101297	-3.544773	0.328660
42	1	0	-4.100317	-3.982788	0.260338
43	1	0	-2.457371	-4.054786	-0.392241
44	1	0	-2.704328	-3.733786	1.328420

Structure 27d ($^5C_2$ ax-ax) (M06-2X, Benece)

Energy (Hartrees): = - 1016.1761347
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.501491	-1.463426	-0.951597
2	6	0	-0.959099	-1.429247	-1.413132
3	6	0	0.706478	-0.294429	0.010550
4	1	0	-1.169098	-2.288227	-2.051632
5	1	0	-1.122652	-0.520404	-2.003772
6	1	0	1.175933	-1.364669	-1.800990
7	1	0	0.495131	0.648641	-0.509956
8	8	0	-0.223019	-0.460839	1.093443
9	7	0	-1.907202	-1.434513	-0.295432
10	6	0	2.083142	-0.199268	0.672182
11	1	0	2.409676	-1.206303	0.962693
12	6	0	3.131571	0.408801	-0.246270
13	1	0	2.788389	1.405991	-0.558496
14	6	0	4.464142	0.565712	0.464924
15	1	0	4.774651	-0.407753	0.864580
16	1	0	4.374161	1.285422	1.281983
17	8	0	2.010481	0.652437	1.804192
18	1	0	1.204417	0.404358	2.270754
19	8	0	3.291176	-0.434363	-1.370119
20	1	0	4.120534	-0.162745	-1.780330
21	8	0	5.375836	1.015426	-0.533083
22	1	0	6.268123	0.958104	-0.183936
23	8	0	0.809265	-2.696268	-0.319876
24	1	0	0.418050	-2.662088	0.559720
25	6	0	-2.203484	-2.740102	0.305774
26	1	0	-1.565958	-2.942237	1.179775
27	1	0	-1.975911	-3.512336	-0.430698
28	6	0	-1.989539	0.984174	0.212634
29	6	0	-3.057613	1.159322	-0.664668
30	6	0	-1.343544	2.106327	0.732270
31	6	0	-3.472452	2.438773	-1.021442
32	1	0	-3.553066	0.282778	-1.065651
33	6	0	-1.759239	3.384222	0.376289
34	1	0	-0.498268	1.976598	1.398960
35	6	0	-2.826268	3.554062	-0.500496
36	1	0	-4.300823	2.562890	-1.709329
37	1	0	-1.246760	4.248307	0.782994
38	1	0	-3.148227	4.550600	-0.779325
39	6	0	-1.597405	-0.416036	0.673443
40	1	0	-2.152488	-0.637693	1.588163

41	6	0	-3.667406	-2.830827	0.715996
42	1	0	-3.882648	-3.798962	1.174945
43	1	0	-3.926509	-2.052952	1.439391
44	1	0	-4.310798	-2.705223	-0.157026

Structure 27d ($^5C_2$ ec-ax) (M06-2X, DMSO)

Energy (Hartrees): = - 1016.1757923
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.458063	-1.495603	-0.753485
2	6	0	-1.020728	-1.504644	-1.148018
3	6	0	0.714755	-0.243652	0.092768
4	1	0	-1.243916	-2.430074	-1.682327
5	1	0	-1.248659	-0.655614	-1.810007
6	1	0	1.101561	-1.484375	-1.630882
7	1	0	0.496969	0.651356	-0.506389
8	8	0	-0.156886	-0.275492	1.232453
9	7	0	-1.786327	-1.480974	0.089864
10	6	0	2.120952	-0.122088	0.679786
11	1	0	2.420290	-1.100738	1.075544
12	6	0	3.153157	0.337433	-0.338967
13	1	0	2.824281	1.298152	-0.761343
14	6	0	4.512830	0.534246	0.308072
15	1	0	4.806229	-0.392618	0.815838
16	1	0	4.475277	1.349105	1.034410
17	8	0	2.124114	0.858125	1.707898
18	1	0	1.324453	0.699851	2.223062
19	8	0	3.258381	-0.639131	-1.359768
20	1	0	4.091756	-0.447531	-1.807490
21	8	0	5.409441	0.829384	-0.759706
22	1	0	6.309430	0.750315	-0.429842
23	8	0	0.753121	-2.668941	-0.016887
24	1	0	0.044021	-2.723297	0.639017
25	6	0	-3.123903	-2.063940	0.073361
26	1	0	-3.625335	-1.872108	-0.884296
27	1	0	-3.722921	-1.575627	0.847260
28	6	0	-1.966043	1.043102	0.301190
29	6	0	-2.995809	1.134688	-0.633741
30	6	0	-1.362589	2.218454	0.755262
31	6	0	-3.416936	2.376435	-1.105046
32	1	0	-3.472237	0.236983	-1.008065
33	6	0	-1.780479	3.458528	0.285234
34	1	0	-0.545719	2.157456	1.465940
35	6	0	-2.812072	3.541427	-0.646697
36	1	0	-4.216791	2.430593	-1.835001
37	1	0	-1.298426	4.360802	0.644389
38	1	0	-3.138923	4.507133	-1.015002
39	6	0	-1.537490	-0.306629	0.892234
40	1	0	-2.061319	-0.441332	1.842245
41	6	0	-3.070323	-3.565856	0.328932
42	1	0	-4.067492	-4.008936	0.263889
43	1	0	-2.431970	-4.058611	-0.409416
44	1	0	-2.661948	-3.767037	1.322190

Structure 27d ($^5C_2$ ax-ax) (M06-2X, DMSO)

Energy (Hartrees): = - 1016.1788941
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.506236	-1.459497	-0.952195
2	6	0	-0.954143	-1.434964	-1.412975
3	6	0	0.703533	-0.289537	0.008845
4	1	0	-1.160534	-2.294538	-2.052028
5	1	0	-1.116203	-0.526399	-2.004616
6	1	0	1.174254	-1.351381	-1.805642
7	1	0	0.489665	0.649467	-0.517952
8	8	0	-0.226479	-0.456484	1.090377
9	7	0	-1.905637	-1.442212	-0.297665
10	6	0	2.077245	-0.181304	0.673015
11	1	0	2.401741	-1.179426	0.994053
12	6	0	3.133235	0.401797	-0.253591
13	1	0	2.778558	1.375574	-0.621578
14	6	0	4.451338	0.612465	0.470883

15	1	0	4.770597	-0.335075	0.921464
16	1	0	4.342140	1.367592	1.252548
17	8	0	1.996164	0.698228	1.784874
18	1	0	1.183716	0.463124	2.248713
19	8	0	3.331761	-0.490239	-1.335897
20	1	0	4.173897	-0.228289	-1.727781
21	8	0	5.374929	1.030674	-0.531045
22	1	0	6.264791	0.956821	-0.173610
23	8	0	0.830532	-2.692853	-0.325762
24	1	0	0.430900	-2.673493	0.551563
25	6	0	-2.185902	-2.750252	0.310359
26	1	0	-1.534837	-2.947042	1.174769
27	1	0	-1.969833	-3.520585	-0.431659
28	6	0	-2.000590	0.977030	0.207699
29	6	0	-3.073101	1.149469	-0.665969
30	6	0	-1.355989	2.103394	0.721775
31	6	0	-3.492398	2.427872	-1.025002
32	1	0	-3.572987	0.274390	-1.064904
33	6	0	-1.773717	3.380493	0.362286
34	1	0	-0.511666	1.980135	1.390832
35	6	0	-2.844616	3.546983	-0.511824
36	1	0	-4.324633	2.547929	-1.709376
37	1	0	-1.261146	4.246690	0.765158
38	1	0	-3.168949	4.542296	-0.793182
39	6	0	-1.601198	-0.420785	0.670847
40	1	0	-2.156194	-0.642995	1.585159
41	6	0	-3.642259	-2.847543	0.743176
42	1	0	-3.841404	-3.816468	1.208008
43	1	0	-3.892344	-2.069317	1.469602
44	1	0	-4.301379	-2.731861	-0.120243

Structure 31a (^{2}E ec-ax H-bond O) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1130.6614413
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.207223	0.187512	0.664005
2	6	0	-2.225059	-1.104987	0.131561
3	6	0	-3.408351	-1.680200	-0.292779
4	6	0	-4.611554	-0.976262	-0.186078
5	6	0	-4.614477	0.304931	0.360509
6	6	0	-3.411144	0.868215	0.781290
7	1	0	-1.302749	-1.671483	0.077887
8	1	0	-3.439149	-2.682801	-0.700850
9	1	0	-5.532823	0.864689	0.472389
10	1	0	-3.422991	1.863060	1.216793
11	6	0	-0.909477	0.862919	1.069040
12	1	0	-1.112827	1.572036	1.879196
13	7	0	-0.200825	1.565495	-0.002646
14	8	0	0.027985	-0.098767	1.518875
15	6	0	1.070487	-0.273505	0.539894
16	6	0	0.594322	0.539762	-0.660899
17	1	0	1.423822	0.978814	-1.212447
18	1	0	0.008993	-0.079346	-1.359144
19	1	0	1.152007	-1.341241	0.326777
20	6	0	2.374384	0.252825	1.153446
21	1	0	2.418777	1.341508	0.999588
22	6	0	3.657089	-0.379592	0.618029
23	1	0	3.597108	-1.464689	0.784586
24	6	0	3.915606	-0.134348	-0.865922
25	1	0	3.821987	0.936381	-1.075119
26	6	0	5.306419	-0.593584	-1.270539
27	1	0	5.493360	-0.287935	-2.306154
28	1	0	6.049448	-0.153135	-0.603114
29	8	0	2.407698	-0.035322	2.542043
30	1	0	1.503097	0.062696	2.860609
31	8	0	4.749948	0.168680	1.330428
32	1	0	4.489624	0.162638	2.258379
33	8	0	2.950238	-0.812839	-1.652793
34	1	0	3.266762	-1.722021	-1.719878
35	8	0	5.280060	-2.013979	-1.167238
36	1	0	6.142170	-2.362752	-1.397423
37	6	0	-1.021941	2.386470	-0.877559
38	1	0	-1.695782	1.770064	-1.494518
39	1	0	-1.657114	3.012724	-0.242894
40	6	0	-0.165489	3.277508	-1.767650
41	1	0	-0.796722	3.955021	-2.345392
42	1	0	0.520530	3.869036	-1.158565
43	1	0	0.421519	2.688760	-2.475264
44	8	0	-5.717751	-1.627539	-0.626759
45	6	0	-6.955825	-0.956784	-0.528201

46	1	0	-6.955085	-0.033585	-1.116853
47	1	0	-7.700873	-1.640150	-0.928943
48	1	0	-7.199330	-0.723913	0.513534

Structure 31a (^{2}E ec-ax H-bond N) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1130.6646128
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.745534	-0.105560	-0.417822
2	6	0	1.950610	-0.861450	0.739903
3	6	0	3.202367	-1.363422	1.044531
4	6	0	4.282859	-1.128404	0.189087
5	6	0	4.089256	-0.398799	-0.982253
6	6	0	2.820867	0.099695	-1.271720
7	1	0	1.109976	-1.079146	1.388660
8	1	0	3.376689	-1.954805	1.934814
9	1	0	4.900836	-0.222059	-1.674467
10	1	0	2.674217	0.655064	-2.193351
11	6	0	0.396049	0.512322	-0.730483
12	1	0	0.262174	0.561651	-1.816863
13	7	0	0.184029	1.863109	-0.177270
14	8	0	-0.648772	-0.247712	-0.163702
15	6	0	-1.230319	0.455710	0.948634
16	6	0	-0.267011	1.616043	1.191559
17	1	0	-0.778987	2.490869	1.593267
18	1	0	0.560397	1.333818	1.859168
19	1	0	-1.289938	-0.239718	1.783453
20	6	0	-2.640752	0.939211	0.596003
21	1	0	-3.166501	1.175878	1.530223
22	6	0	-3.476744	-0.080451	-0.184113
23	1	0	-2.915223	-0.369236	-1.080739
24	6	0	-3.836564	-1.339639	0.601591
25	1	0	-4.431366	-1.045174	1.471431
26	6	0	-4.653670	-2.290717	-0.257679
27	1	0	-4.973903	-3.135054	0.362714
28	1	0	-5.523479	-1.766185	-0.662511
29	8	0	-2.624099	2.139047	-0.173704
30	1	0	-1.743944	2.221455	-0.576814
31	8	0	-4.704387	0.529752	-0.540360
32	1	0	-4.470118	1.410319	-0.854929
33	8	0	-2.687988	-2.005713	1.089204
34	1	0	-2.212736	-2.326297	0.312637
35	8	0	-3.778458	-2.730523	-1.290081
36	1	0	-4.234549	-3.378357	-1.828509
37	6	0	1.285500	2.805222	-0.325525
38	1	0	2.161195	2.487842	0.260226
39	1	0	1.584258	2.796895	-1.378307
40	6	0	0.862288	4.212573	0.074282
41	1	0	1.656464	4.925338	-0.153166
42	1	0	-0.039099	4.507338	-0.466768
43	1	0	0.656011	4.277313	1.144190
44	8	0	5.468821	-1.660958	0.576057
45	6	0	6.585207	-1.457929	-0.264003
46	1	0	6.806283	-0.391800	-0.379016
47	1	0	7.422804	-1.949858	0.224804
48	1	0	6.426528	-1.905421	-1.250522

Structure 31a (^{2}E ax-ax) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1130.6641488
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.126645	0.573269	0.404948
2	6	0	-2.331690	-0.383130	1.401166
3	6	0	-3.414533	-1.242836	1.342014
4	6	0	-4.321966	-1.157744	0.283797
5	6	0	-4.128438	-0.205170	-0.715871
6	6	0	-3.030770	0.649194	-0.646263
7	1	0	-1.626086	-0.451123	2.220646
8	1	0	-3.583752	-1.995044	2.102573
9	1	0	-4.811539	-0.121691	-1.550048
10	1	0	-2.861006	1.376781	-1.431674
11	6	0	-0.960142	1.541972	0.480386
12	1	0	-1.275373	2.486857	0.929444

13	7	0	-0.359971	1.761923	-0.817394
14	8	0	0.082313	1.020875	1.311682
15	6	0	0.923519	0.206565	0.479881
16	6	0	0.482880	0.566923	-0.962993
17	1	0	1.321009	0.764680	-1.628527
18	1	0	-0.100940	-0.246713	-1.391660
19	1	0	0.732968	-0.846101	0.706181
20	6	0	2.369148	0.574248	0.824531
21	1	0	2.652707	1.483637	0.271327
22	6	0	3.409971	-0.505361	0.539338
23	1	0	3.128961	-1.405740	1.103713
24	6	0	3.546210	-0.880901	-0.933643
25	1	0	3.701722	0.028800	-1.523026
26	6	0	4.721652	-1.817598	-1.156945
27	1	0	4.852644	-1.969819	-2.234210
28	1	0	5.626110	-1.388505	-0.720993
29	8	0	2.496278	0.812088	2.217872
30	1	0	1.697916	1.277934	2.490748
31	8	0	4.671814	-0.028206	0.965604
32	1	0	4.528914	0.354277	1.838517
33	8	0	2.359050	-1.497402	-1.400328
34	1	0	2.413531	-2.416487	-1.110875
35	8	0	4.356344	-3.038440	-0.521362
36	1	0	5.069702	-3.670647	-0.619048
37	6	0	0.383139	3.029483	-0.867291
38	1	0	0.944382	3.207283	0.062558
39	1	0	1.114685	2.949913	-1.674394
40	6	0	-0.551694	4.196275	-1.153988
41	1	0	0.006363	5.133176	-1.210170
42	1	0	-1.066703	4.034581	-2.102243
43	1	0	-1.307931	4.306146	-0.373151
44	8	0	-5.351345	-2.043392	0.312958
45	6	0	-6.290814	-1.988746	-0.738511
46	1	0	-5.816677	-2.183284	-1.706089
47	1	0	-7.021073	-2.767808	-0.531798
48	1	0	-6.795349	-1.017397	-0.770778

Structure 31a (E_2 ec-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1130.6624364
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.324288	-0.082094	-0.192409
2	6	0	2.773547	0.099004	1.119582
3	6	0	4.105978	-0.068914	1.432595
4	6	0	5.023572	-0.421819	0.434091
5	6	0	4.589504	-0.601183	-0.875658
6	6	0	3.235870	-0.430336	-1.173747
7	1	0	2.054943	0.378865	1.880816
8	1	0	4.477913	0.063373	2.440987
9	1	0	5.277909	-0.871846	-1.664151
10	1	0	2.896028	-0.573618	-2.194537
11	6	0	0.865652	0.103529	-0.499397
12	1	0	0.688911	-0.050843	-1.584133
13	7	0	0.349591	1.388379	-0.064473
14	8	0	0.090913	-0.824826	0.239297
15	6	0	-1.225279	-0.273599	0.427360
16	6	0	-1.095050	1.191251	-0.018295
17	1	0	-1.554775	1.334620	-1.013810
18	1	0	-1.574646	1.876764	0.672979
19	1	0	-1.460709	-0.363095	1.490342
20	6	0	-2.183363	-1.143534	-0.393696
21	1	0	-2.075357	-0.886122	-1.459464
22	6	0	-3.668030	-1.092833	-0.035521
23	1	0	-3.774205	-1.351959	1.027451
24	6	0	-4.339836	0.257444	-0.273173
25	1	0	-4.093696	0.613908	-1.278249
26	6	0	-5.850530	0.153299	-0.140752
27	1	0	-6.296199	1.113960	-0.422708
28	1	0	-6.226813	-0.644320	-0.783739
29	8	0	-1.840884	-2.508424	-0.200760
30	1	0	-0.877684	-2.550890	-0.200724
31	8	0	-4.340608	-2.039574	-0.844053
32	1	0	-3.803176	-2.839198	-0.817838
33	8	0	-3.857246	1.216098	0.651006
34	1	0	-4.347214	1.055755	1.466964
35	8	0	-6.087472	-0.121517	1.236314
36	1	0	-7.028817	-0.225323	1.381275
37	6	0	0.782922	2.496940	-0.898821
38	1	0	1.875461	2.470836	-0.938115
39	1	0	0.412137	2.372681	-1.933484

40	6	0	0.319382	3.834876	-0.340731
41	1	0	0.728759	4.656374	-0.930961
42	1	0	-0.769172	3.919187	-0.358406
43	1	0	0.656296	3.943409	0.691681
44	8	0	6.309430	-0.563025	0.843280
45	6	0	7.270354	-0.920696	-0.126576
46	1	0	7.342131	-0.162449	-0.913263
47	1	0	8.219910	-0.985363	0.399595
48	1	0	7.037986	-1.891211	-0.576981

Structure 31a (^{2}E ec-ax H-bond O) (M06-2X, Benzene)

Energy (Hartrees): = - 1130.6822235
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.214360	0.166271	0.645489
2	6	0	-2.240486	-1.090317	0.031814
3	6	0	-3.432263	-1.643824	-0.398855
4	6	0	-4.636547	-0.956227	-0.215265
5	6	0	-4.630115	0.288624	0.410804
6	6	0	-3.418280	0.832005	0.834455
7	1	0	-1.319097	-1.648952	-0.086444
8	1	0	-3.465886	-2.618748	-0.870111
9	1	0	-5.548039	0.834333	0.582866
10	1	0	-3.422313	1.797870	1.331208
11	6	0	-0.911455	0.826446	1.059573
12	1	0	-1.111401	1.517493	1.885669
13	7	0	-0.199955	1.550647	0.003362
14	8	0	0.023070	-0.150893	1.486971
15	6	0	1.078010	-0.293165	0.515686
16	6	0	0.607513	0.543836	-0.670375
17	1	0	1.440009	1.002307	-1.201977
18	1	0	0.031831	-0.060478	-1.388477
19	1	0	1.171765	-1.355141	0.281591
20	6	0	2.371187	0.234770	1.152632
21	1	0	2.410898	1.325394	1.013447
22	6	0	3.665365	-0.382369	0.626269
23	1	0	3.610041	-1.469544	0.779344
24	6	0	3.942713	-0.117704	-0.851631
25	1	0	3.842385	0.953926	-1.051979
26	6	0	5.340085	-0.561707	-1.247884
27	1	0	5.529473	-0.252080	-2.281907
28	1	0	6.080154	-0.112614	-0.582511
29	8	0	2.387293	-0.069248	2.539987
30	1	0	1.476852	0.020923	2.845195
31	8	0	4.744859	0.163856	1.363822
32	1	0	4.470857	0.139349	2.287677
33	8	0	2.991554	-0.796989	-1.657351
34	1	0	3.313466	-1.704904	-1.721998
35	8	0	5.334399	-1.982628	-1.145123
36	1	0	6.189821	-2.317856	-1.422369
37	6	0	-1.020756	2.384404	-0.861862
38	1	0	-1.685435	1.774870	-1.494942
39	1	0	-1.662882	2.996394	-0.220478
40	6	0	-0.165628	3.294084	-1.732669
41	1	0	-0.800287	3.974868	-2.303805
42	1	0	0.512343	3.885779	-1.113668
43	1	0	0.429798	2.722246	-2.447697
44	8	0	-5.750246	-1.584831	-0.663523
45	6	0	-6.994763	-0.943275	-0.461839
46	1	0	-7.040899	0.014927	-0.989520
47	1	0	-7.747896	-1.613298	-0.871985
48	1	0	-7.194647	-0.786828	0.603016

Structure 31a (^{2}E ec-ax H-bond N) (M06-2X, Benzene)

Energy (Hartrees): = - 1130.6859297
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.753009	-0.110889	0.391958
2	6	0	-1.989629	-0.811706	-0.794676
3	6	0	-3.248825	-1.302749	-1.088017
4	6	0	-4.305394	-1.114678	-0.190890
5	6	0	-4.079909	-0.439302	1.007592
6	6	0	-2.805135	0.050977	1.284270
7	1	0	-1.170519	-0.994620	-1.480667

8	1	0	-3.443003	-1.851170	-2.001976
9	1	0	-4.872922	-0.299339	1.729685
10	1	0	-2.634836	0.566445	2.224914
11	6	0	-0.397952	0.497911	0.697733
12	1	0	-0.254553	0.532673	1.783214
13	7	0	-0.181589	1.854476	0.160976
14	8	0	0.637595	-0.264181	0.110284
15	6	0	1.243920	0.467043	-0.969897
16	6	0	0.281922	1.628736	-1.207598
17	1	0	0.794217	2.510944	-1.592658
18	1	0	-0.536661	1.355755	-1.888778
19	1	0	1.323995	-0.206703	-1.820202
20	6	0	2.644606	0.947411	-0.574067
21	1	0	3.187679	1.210799	-1.491040
22	6	0	3.470420	-0.086355	0.199688
23	1	0	2.890256	-0.399209	1.076031
24	6	0	3.860143	-1.325934	-0.603181
25	1	0	4.459879	-1.011354	-1.462692
26	6	0	4.680987	-2.283982	0.243434
27	1	0	5.001522	-3.120522	-0.387484
28	1	0	5.556752	-1.768307	0.647643
29	8	0	2.604565	2.124695	0.231755
30	1	0	1.701219	2.211172	0.584153
31	8	0	4.682941	0.528137	0.604480
32	1	0	4.426436	1.396351	0.936845
33	8	0	2.723502	-1.997762	-1.115234
34	1	0	2.227839	-2.312352	-0.348943
35	8	0	3.817839	-2.739498	1.279164
36	1	0	4.278806	-3.409098	1.788782
37	6	0	-1.281751	2.797659	0.320384
38	1	0	-2.152467	2.495549	-0.280170
39	1	0	-1.588095	2.768595	1.370401
40	6	0	-0.854679	4.211211	-0.048187
41	1	0	-1.653366	4.917703	0.185787
42	1	0	0.039355	4.501217	0.508691
43	1	0	-0.638353	4.300371	-1.114861
44	8	0	-5.499505	-1.632143	-0.566600
45	6	0	-6.590492	-1.484748	0.322055
46	1	0	-6.818178	-0.429473	0.503692
47	1	0	-7.441451	-1.955441	-0.166395
48	1	0	-6.399260	-1.988933	1.274788

Structure 31a (^{2}E ax-ax) (M06-2X, Benzene)

Energy (Hartrees): = - 1130.684812
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.136059	0.552129	0.402778
2	6	0	-2.323603	-0.440350	1.366822
3	6	0	-3.410887	-1.295107	1.300554
4	6	0	-4.343215	-1.167668	0.268010
5	6	0	-4.169903	-0.175499	-0.697514
6	6	0	-3.066937	0.671529	-0.622070
7	1	0	-1.602294	-0.541416	2.169087
8	1	0	-3.562426	-2.073634	2.038561
9	1	0	-4.874531	-0.056489	-1.509426
10	1	0	-2.918593	1.429398	-1.383337
11	6	0	-0.963998	1.515166	0.486503
12	1	0	-1.278518	2.457682	0.940538
13	7	0	-0.360243	1.744989	-0.807946
14	8	0	0.074739	0.983512	1.316338
15	6	0	0.929575	0.186701	0.480058
16	6	0	0.492494	0.557698	-0.960367
17	1	0	1.332244	0.770929	-1.619005
18	1	0	-0.082537	-0.257085	-1.399442
19	1	0	0.750623	-0.870295	0.695176
20	6	0	2.369361	0.566624	0.836886
21	1	0	2.643435	1.488081	0.300058
22	6	0	3.427321	-0.494675	0.542713
23	1	0	3.159475	-1.404788	1.097993
24	6	0	3.573418	-0.853058	-0.934366
25	1	0	3.708943	0.064623	-1.515916
26	6	0	4.765095	-1.763782	-1.173724
27	1	0	4.886031	-1.907634	-2.253209
28	1	0	5.670892	-1.320626	-0.753991
29	8	0	2.483845	0.785951	2.236482
30	1	0	1.684455	1.253250	2.505209
31	8	0	4.680587	-0.000939	0.981065
32	1	0	4.527341	0.364410	1.859746
33	8	0	2.397209	-1.489853	-1.405220
34	1	0	2.468974	-2.408306	-1.116215

35	8	0	4.440511	-2.996573	-0.538443
36	1	0	5.126171	-3.637626	-0.738194
37	6	0	0.372030	3.020580	-0.852057
38	1	0	0.927430	3.201329	0.080582
39	1	0	1.106682	2.949868	-1.657013
40	6	0	-0.572009	4.178950	-1.137013
41	1	0	-0.021124	5.121100	-1.187661
42	1	0	-1.083010	4.020641	-2.088930
43	1	0	-1.331705	4.280303	-0.357678
44	8	0	-5.372295	-2.050980	0.283520
45	6	0	-6.356616	-1.931475	-0.725344
46	1	0	-5.928954	-2.082793	-1.721736
47	1	0	-7.086428	-2.714261	-0.527907
48	1	0	-6.854059	-0.957106	-0.682807

Structure 31a (E_2 ec-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 1130.6833593
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.324062	-0.055002	-0.187733
2	6	0	2.791521	0.205301	1.104732
3	6	0	4.124502	0.034233	1.416350
4	6	0	5.025645	-0.403784	0.435975
5	6	0	4.573607	-0.660648	-0.855543
6	6	0	3.220647	-0.483146	-1.152739
7	1	0	2.088884	0.549885	1.854679
8	1	0	4.505239	0.228139	2.411961
9	1	0	5.249353	-0.996300	-1.630434
10	1	0	2.869898	-0.687661	-2.159599
11	6	0	0.861934	0.121154	-0.489918
12	1	0	0.677754	-0.060505	-1.567890
13	7	0	0.341403	1.412770	-0.078640
14	8	0	0.099335	-0.795442	0.278570
15	6	0	-1.225164	-0.257089	0.444710
16	6	0	-1.103014	1.209663	-0.000435
17	1	0	-1.584145	1.355547	-0.984108
18	1	0	-1.565481	1.893730	0.704343
19	1	0	-1.476558	-0.350470	1.503392
20	6	0	-2.164998	-1.130162	-0.396439
21	1	0	-2.052061	-0.857849	-1.457574
22	6	0	-3.653000	-1.103834	-0.048677
23	1	0	-3.762321	-1.396766	1.005078
24	6	0	-4.338869	0.245595	-0.248471
25	1	0	-4.098970	0.633719	-1.243100
26	6	0	-5.847961	0.129438	-0.116770
27	1	0	-6.295628	1.101056	-0.353921
28	1	0	-6.230656	-0.633463	-0.797824
29	8	0	-1.805627	-2.494873	-0.219868
30	1	0	-0.841614	-2.522239	-0.210461
31	8	0	-4.309850	-2.036354	-0.888983
32	1	0	-3.768615	-2.833839	-0.871804
33	8	0	-3.861000	1.180798	0.703606
34	1	0	-4.338388	0.982457	1.519242
35	8	0	-6.087721	-0.212784	1.244708
36	1	0	-7.034668	-0.227872	1.399629
37	6	0	0.748570	2.504420	-0.950205
38	1	0	1.840177	2.487616	-1.013471
39	1	0	0.355315	2.352376	-1.972105
40	6	0	0.287774	3.852479	-0.417067
41	1	0	0.678109	4.660194	-1.039332
42	1	0	-0.801755	3.931752	-0.412738
43	1	0	0.647024	3.996250	0.604118
44	8	0	6.310567	-0.544834	0.840697
45	6	0	7.250494	-1.017098	-0.105276
46	1	0	7.350341	-0.326043	-0.948477
47	1	0	8.201368	-1.079422	0.420320
48	1	0	6.977447	-2.010888	-0.474246

Structure 31a (^{2}E ec-ax H-bond O) (M06-2X, DMSO)

Energy (Hartrees): = - 1130.6869354
No imaginary frequencies

Standard orientation:

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

1	6	0	-2.188991	0.282372	0.667291
2	6	0	-2.166441	-1.067336	0.299666
3	6	0	-3.328927	-1.720080	-0.074653
4	6	0	-4.550482	-1.037675	-0.086159
5	6	0	-4.592531	0.303918	0.295195
6	6	0	-3.411732	0.944070	0.669347
7	1	0	-1.233967	-1.620444	0.321929
8	1	0	-3.318469	-2.766433	-0.357770
9	1	0	-5.524052	0.853840	0.312312
10	1	0	-3.453502	1.986464	0.971919
11	6	0	-0.918568	1.039937	1.013842
12	1	0	-1.158132	1.828670	1.733517
13	7	0	-0.207974	1.630919	-0.122091
14	8	0	0.042573	0.166801	1.585106
15	6	0	1.052680	-0.158795	0.606045
16	6	0	0.579162	0.532692	-0.670478
17	1	0	1.409230	0.910936	-1.264811
18	1	0	-0.017353	-0.145769	-1.298853
19	1	0	1.094748	-1.245298	0.511304
20	6	0	2.386020	0.389997	1.125949
21	1	0	2.456629	1.454224	0.855431
22	6	0	3.637189	-0.327621	0.625778
23	1	0	3.569298	-1.380494	0.934533
24	6	0	3.837797	-0.282170	-0.888302
25	1	0	3.732035	0.748973	-1.238690
26	6	0	5.206474	-0.798283	-1.294904
27	1	0	5.324004	-0.662604	-2.375114
28	1	0	5.993412	-0.251972	-0.770630
29	8	0	2.450275	0.252621	2.540096
30	1	0	1.568168	0.465687	2.867993
31	8	0	4.765531	0.287731	1.227837
32	1	0	4.535323	0.405233	2.156677
33	8	0	2.839677	-1.061075	-1.533594
34	1	0	3.144738	-1.974584	-1.456728
35	8	0	5.219031	-2.183797	-0.959779
36	1	0	5.989874	-2.588406	-1.367995
37	6	0	-1.030249	2.353992	-1.082838
38	1	0	-1.695278	1.671011	-1.635636
39	1	0	-1.668662	3.041626	-0.519720
40	6	0	-0.171076	3.142405	-2.060764
41	1	0	-0.801822	3.760729	-2.703079
42	1	0	0.518150	3.794943	-1.519110
43	1	0	0.414567	2.481979	-2.704310
44	8	0	-5.630287	-1.758913	-0.469093
45	6	0	-6.884975	-1.094748	-0.504681
46	1	0	-6.865533	-0.249114	-1.198493
47	1	0	-7.604723	-1.831200	-0.856711
48	1	0	-7.179365	-0.747425	0.490082

Structure 31a (^{2}E ec-ax H-bond N) (M06-2X, DMSO)

Energy (Hartrees): = - 1130.6903405
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.759802	-0.124095	0.409731
2	6	0	-1.981776	-0.848982	-0.765522
3	6	0	-3.238026	-1.349857	-1.062257
4	6	0	-4.307201	-1.140578	-0.183424
5	6	0	-4.095654	-0.439913	1.004556
6	6	0	-2.823839	0.056373	1.286287
7	1	0	-1.159361	-1.036572	-1.446913
8	1	0	-3.417963	-1.913019	-1.970815
9	1	0	-4.898337	-0.280942	1.712229
10	1	0	-2.664154	0.595513	2.215440
11	6	0	-0.412474	0.500244	0.719783
12	1	0	-0.283887	0.558668	1.805284
13	7	0	-0.202503	1.845176	0.154873
14	8	0	0.638044	-0.265830	0.157750
15	6	0	1.226365	0.441878	-0.950412
16	6	0	0.251796	1.587045	-1.212092
17	1	0	0.748397	2.462909	-1.630223
18	1	0	-0.568780	1.285121	-1.877328
19	1	0	1.305327	-0.249427	-1.785872
20	6	0	2.623183	0.947863	-0.577459
21	1	0	3.146119	1.213353	-1.505343
22	6	0	3.476912	-0.065162	0.192848
23	1	0	2.905197	-0.391323	1.069944
24	6	0	3.896013	-1.294982	-0.609749
25	1	0	4.478597	-0.968225	-1.476238
26	6	0	4.745985	-2.234034	0.228478
27	1	0	5.067284	-3.068979	-0.402681

28	1	0	5.625543	-1.708515	0.611158
29	8	0	2.569816	2.127080	0.228045
30	1	0	1.653421	2.221602	0.548911
31	8	0	4.673700	0.581710	0.602162
32	1	0	4.388510	1.445467	0.924326
33	8	0	2.769715	-1.998291	-1.108584
34	1	0	2.292361	-2.317644	-0.332473
35	8	0	3.914560	-2.697202	1.288644
36	1	0	4.338429	-3.460062	1.691548
37	6	0	-1.308722	2.785327	0.297973
38	1	0	-2.172427	2.472105	-0.306982
39	1	0	-1.620843	2.766629	1.346220
40	6	0	-0.886813	4.194569	-0.089961
41	1	0	-1.694798	4.897656	0.122084
42	1	0	-0.002968	4.501339	0.475114
43	1	0	-0.656606	4.263618	-1.155442
44	8	0	-5.497769	-1.660903	-0.562678
45	6	0	-6.608807	-1.457336	0.298635
46	1	0	-6.811194	-0.391497	0.439225
47	1	0	-7.459284	-1.924597	-0.193686
48	1	0	-6.448420	-1.932073	1.271206

Structure 31a (^{2}E ax-ax) (M06-2X, DMSO)

Energy (Hartrees): = - 1130.6887685
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.136018	0.552427	0.403563
2	6	0	-2.295269	-0.477398	1.332915
3	6	0	-3.383360	-1.333238	1.263620
4	6	0	-4.344889	-1.171822	0.261640
5	6	0	-4.200161	-0.141677	-0.670189
6	6	0	-3.097497	0.706026	-0.589936
7	1	0	-1.555282	-0.609291	2.113709
8	1	0	-3.509838	-2.137362	1.979199
9	1	0	-4.927089	0.007634	-1.457596
10	1	0	-2.981442	1.496995	-1.323249
11	6	0	-0.964156	1.516725	0.485393
12	1	0	-1.283211	2.463245	0.926915
13	7	0	-0.355781	1.733511	-0.810745
14	8	0	0.070543	0.991494	1.323371
15	6	0	0.927508	0.185664	0.496803
16	6	0	0.498201	0.543905	-0.947889
17	1	0	1.342256	0.755519	-1.601586
18	1	0	-0.074625	-0.275723	-1.381968
19	1	0	0.747796	-0.869162	0.722592
20	6	0	2.366772	0.566201	0.849376
21	1	0	2.637107	1.489215	0.315144
22	6	0	3.421790	-0.493844	0.544539
23	1	0	3.160123	-1.403152	1.104264
24	6	0	3.544949	-0.854835	-0.934917
25	1	0	3.634653	0.062632	-1.524734
26	6	0	4.752799	-1.733498	-1.206661
27	1	0	4.835695	-1.886703	-2.287553
28	1	0	5.663764	-1.259666	-0.834620
29	8	0	2.483653	0.778620	2.252252
30	1	0	1.709742	1.292429	2.512578
31	8	0	4.680632	0.001115	0.972670
32	1	0	4.528333	0.384563	1.844254
33	8	0	2.374275	-1.531335	-1.369148
34	1	0	2.483345	-2.442450	-1.067109
35	8	0	4.497475	-2.969345	-0.543434
36	1	0	5.125584	-3.622236	-0.866034
37	6	0	0.386203	3.006619	-0.855459
38	1	0	0.933577	3.185647	0.081197
39	1	0	1.127821	2.925562	-1.652691
40	6	0	-0.547990	4.169683	-1.150117
41	1	0	0.012456	5.106655	-1.194435
42	1	0	-1.049296	4.019134	-2.109157
43	1	0	-1.313944	4.275890	-0.377288
44	8	0	-5.372121	-2.054738	0.272294
45	6	0	-6.377753	-1.903375	-0.718856
46	1	0	-5.964127	-2.021692	-1.724694
47	1	0	-7.102932	-2.693099	-0.533223
48	1	0	-6.872414	-0.931052	-0.635699

Structure 31a (E_2 ec-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 1130.6877561
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.319560	-0.122912	-0.167934
2	6	0	2.765226	-0.046674	1.156174
3	6	0	4.103754	-0.202850	1.458293
4	6	0	5.034537	-0.434321	0.434288
5	6	0	4.603365	-0.507376	-0.888938
6	6	0	3.244738	-0.352317	-1.174603
7	1	0	2.046011	0.137387	1.946637
8	1	0	4.462182	-0.148987	2.479776
9	1	0	5.300810	-0.681568	-1.697261
10	1	0	2.910742	-0.410180	-2.206013
11	6	0	0.859881	0.072866	-0.471019
12	1	0	0.678021	-0.075457	-1.552206
13	7	0	0.358155	1.365930	-0.028698
14	8	0	0.082317	-0.850699	0.274539
15	6	0	-1.236186	-0.294993	0.448786
16	6	0	-1.092073	1.176455	0.028679
17	1	0	-1.553861	1.340998	-0.959930
18	1	0	-1.554317	1.854060	0.739800
19	1	0	-1.492486	-0.404012	1.504849
20	6	0	-2.188378	-1.131571	-0.412908
21	1	0	-2.062390	-0.839369	-1.466211
22	6	0	-3.676270	-1.073889	-0.073767
23	1	0	-3.801342	-1.403461	0.967497
24	6	0	-4.312506	0.307387	-0.221885
25	1	0	-4.015008	0.748161	-1.178034
26	6	0	-5.828364	0.245263	-0.159153
27	1	0	-6.224357	1.249488	-0.341829
28	1	0	-6.218070	-0.443561	-0.911418
29	8	0	-1.859952	-2.509511	-0.261414
30	1	0	-0.897467	-2.560940	-0.299729
31	8	0	-4.354272	-1.957586	-0.952848
32	1	0	-3.825968	-2.764021	-0.973763
33	8	0	-3.844129	1.162999	0.809530
34	1	0	-4.358521	0.919825	1.590673
35	8	0	-6.148662	-0.186726	1.161069
36	1	0	-7.085355	-0.031501	1.312669
37	6	0	0.773679	2.461806	-0.896400
38	1	0	1.864516	2.432476	-0.971075
39	1	0	0.368857	2.320716	-1.913623
40	6	0	0.336048	3.811210	-0.348846
41	1	0	0.726087	4.616551	-0.974585
42	1	0	-0.752578	3.901508	-0.328101
43	1	0	0.712878	3.949841	0.667374
44	8	0	6.321895	-0.571953	0.827424
45	6	0	7.294588	-0.803354	-0.181573
46	1	0	7.339345	0.032123	-0.886265
47	1	0	8.248511	-0.891360	0.334376
48	1	0	7.089500	-1.730798	-0.724278

Structure 31b (^{2}E ec-ec H-bond O) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1130.6661191
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.181664	0.356383	-0.564337
2	6	0	-2.157422	-0.625714	0.432391
3	6	0	-3.326880	-1.216326	0.863179
4	6	0	-4.554895	-0.831732	0.308531
5	6	0	-4.592644	0.144520	-0.682243
6	6	0	-3.398095	0.726635	-1.110757
7	1	0	-1.206251	-0.916796	0.865852
8	1	0	-3.331509	-1.979855	1.631104
9	1	0	-5.527027	0.457148	-1.127506
10	1	0	-3.427727	1.483301	-1.888355
11	6	0	-0.892989	0.986670	-1.016758
12	1	0	-1.098023	1.722685	-1.817777
13	7	0	-0.151884	1.594980	0.076560
14	8	0	-0.007489	0.002396	-1.537202
15	6	0	1.324037	0.250302	-1.056881
16	6	0	1.221182	1.625892	-0.407925
17	1	0	1.934032	1.759669	0.403243
18	1	0	1.383632	2.423361	-1.152593
19	1	0	1.998979	0.230214	-1.912657
20	6	0	1.677824	-0.855781	-0.048475
21	1	0	1.334456	-0.543048	0.949378
22	6	0	3.160623	-1.211363	0.032246

23	1	0	3.503231	-1.494000	-0.973599
24	6	0	4.048831	-0.082347	0.549687
25	1	0	3.630867	0.298283	1.487375
26	6	0	5.467437	-0.563517	0.804221
27	1	0	6.031691	0.240841	1.289449
28	1	0	5.448746	-1.451656	1.438810
29	8	0	1.039436	-2.072001	-0.403301
30	1	0	0.223552	-1.831752	-0.860545
31	8	0	3.308753	-2.297021	0.927159
32	1	0	2.615210	-2.925369	0.697618
33	8	0	4.078185	0.993279	-0.374429
34	1	0	4.733379	0.744585	-1.037807
35	8	0	6.007441	-0.845420	-0.483468
36	1	0	6.907023	-1.160339	-0.385433
37	6	0	-0.696956	2.878871	0.487314
38	1	0	-0.635238	3.609155	-0.340201
39	1	0	-1.757267	2.727591	0.708718
40	6	0	0.011030	3.425884	1.718191
41	1	0	-0.477157	4.338533	2.063802
42	1	0	-0.017187	2.687819	2.521798
43	1	0	1.054773	3.666024	1.505586
44	8	0	-5.645844	-1.468255	0.803009
45	6	0	-6.906239	-1.115547	0.274048
46	1	0	-7.635166	-1.729348	0.797895
47	1	0	-7.127881	-0.057987	0.450442
48	1	0	-6.958895	-1.324721	-0.799255

Structure 31b (^{2}E ec-ec H-bond N) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1130.6684178
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.598542	0.249828	-0.606714
2	6	0	-1.442960	-0.523311	0.549064
3	6	0	-2.464093	-1.341288	0.985554
4	6	0	-3.669637	-1.404954	0.274404
5	6	0	-3.834614	-0.644798	-0.879513
6	6	0	-2.789326	0.174279	-1.309441
7	1	0	-0.508988	-0.477405	1.098400
8	1	0	-2.365078	-1.950699	1.875131
9	1	0	-4.751582	-0.681164	-1.451096
10	1	0	-2.915301	0.760318	-2.214475
11	6	0	-0.490317	1.159540	-1.057286
12	1	0	-0.727807	1.566647	-2.058601
13	7	0	-0.242424	2.260554	-0.120146
14	8	0	0.744262	0.474663	-1.113333
15	6	0	1.794211	1.339225	-0.655566
16	6	0	1.104277	2.694589	-0.491860
17	1	0	1.558609	3.299919	0.293794
18	1	0	1.100494	3.260129	-1.437276
19	1	0	2.582299	1.349969	-1.405371
20	6	0	2.360201	0.815886	0.665504
21	1	0	3.297281	1.352099	0.871192
22	6	0	2.655895	-0.687352	0.675690
23	1	0	1.743965	-1.221323	0.379782
24	6	0	3.796595	-1.110660	-0.247331
25	1	0	4.701083	-0.569050	0.045903
26	6	0	4.053916	-2.604150	-0.133044
27	1	0	4.936123	-2.855132	-0.732459
28	1	0	4.218872	-2.870400	0.914142
29	8	0	1.483630	1.059403	1.764903
30	1	0	0.643686	1.409563	1.423076
31	8	0	3.046891	-1.053446	1.987472
32	1	0	2.426082	-0.609540	2.575980
33	8	0	3.529361	-0.776512	-1.595544
34	1	0	2.803138	-1.347930	-1.874296
35	8	0	2.893166	-3.235954	-0.660242
36	1	0	3.013434	-4.185868	-0.629585
37	6	0	-1.266478	3.296614	-0.154639
38	1	0	-1.321015	3.745858	-1.161672
39	1	0	-2.226276	2.810475	0.038579
40	6	0	-1.012252	4.375714	0.887610
41	1	0	-1.850110	5.073572	0.921144
42	1	0	-0.895222	3.925634	1.875429
43	1	0	-0.111094	4.948838	0.660608
44	8	0	-4.610140	-2.235557	0.788671
45	6	0	-5.840128	-2.337445	0.103620
46	1	0	-5.698324	-2.726972	-0.909701
47	1	0	-6.447438	-3.033918	0.677017
48	1	0	-6.347716	-1.368582	0.053638

Structure 31b (^{2}E ax-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1130.6600729
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.214545	-0.204907	-0.668117
2	6	0	2.440505	1.015939	-0.030601
3	6	0	3.724341	1.414012	0.294242
4	6	0	4.814942	0.597558	-0.019762
5	6	0	4.603490	-0.616181	-0.673059
6	6	0	3.304028	-0.999645	-0.994583
7	1	0	1.599199	1.653060	0.213900
8	1	0	3.917906	2.357169	0.789621
9	1	0	5.429184	-1.262074	-0.937763
10	1	0	3.138931	-1.949999	-1.491688
11	6	0	0.827630	-0.704581	-0.958149
12	1	0	0.835623	-1.270689	-1.899273
13	7	0	0.233248	-1.569132	0.049160
14	8	0	-0.076357	0.396853	-1.116717
15	6	0	-1.403070	-0.091344	-0.881862
16	6	0	-1.173547	-1.534222	-0.363842
17	1	0	-1.834785	-1.812221	0.452874
18	1	0	-1.332932	-2.246472	-1.175539
19	1	0	-1.953957	-0.081283	-1.826292
20	6	0	-2.059460	0.862656	0.120482
21	1	0	-1.755094	0.587385	1.141759
22	6	0	-3.584388	0.916605	0.074272
23	1	0	-3.885074	1.204872	-0.942900
24	6	0	-4.274665	-0.398165	0.427274
25	1	0	-3.873117	-0.773066	1.374663
26	6	0	-5.776243	-0.213814	0.570320
27	1	0	-6.213504	-1.148005	0.940298
28	1	0	-5.983889	0.604388	1.262582
29	8	0	-1.655640	2.199752	-0.140169
30	1	0	-0.757114	2.154463	-0.486095
31	8	0	-4.021139	1.882543	1.011422
32	1	0	-3.463298	2.656332	0.875952
33	8	0	-4.014319	-1.375433	-0.566060
34	1	0	-4.642759	-1.194899	-1.275946
35	8	0	-6.247474	0.072320	-0.742736
36	1	0	-7.192497	0.227377	-0.712299
37	6	0	0.449209	-1.142513	1.444476
38	1	0	0.489971	-0.048917	1.541406
39	1	0	-0.424351	-1.471785	2.011981
40	6	0	1.691368	-1.773958	2.063370
41	1	0	1.717650	-1.569862	3.136469
42	1	0	1.665983	-2.854521	1.912173
43	1	0	2.610422	-1.385911	1.623720
44	8	0	6.032275	1.074174	0.340795
45	6	0	7.159450	0.269422	0.066152
46	1	0	8.019663	0.816760	0.444470
47	1	0	7.089600	-0.697115	0.575738
48	1	0	7.277931	0.106075	-1.009887

Structure 31b (^{2}E ec-ec H-bond O) (M06-2X, Benzene)

Energy (Hartrees): = - 1130.6869115
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.188272	0.334010	-0.575416
2	6	0	-2.162746	-0.706960	0.359610
3	6	0	-3.335101	-1.291623	0.791982
4	6	0	-4.569047	-0.840342	0.302687
5	6	0	-4.608596	0.198259	-0.623542
6	6	0	-3.411108	0.771092	-1.057177
7	1	0	-1.209668	-1.053664	0.746251
8	1	0	-3.333717	-2.101954	1.510963
9	1	0	-5.547609	0.564362	-1.016634
10	1	0	-3.443446	1.575786	-1.785312
11	6	0	-0.897865	0.966978	-1.021956
12	1	0	-1.100558	1.702795	-1.822417
13	7	0	-0.161936	1.577601	0.075105
14	8	0	-0.007175	-0.016801	-1.537370
15	6	0	1.325672	0.241440	-1.061270

16	6	0	1.213377	1.613154	-0.405978
17	1	0	1.920000	1.745615	0.410936
18	1	0	1.375028	2.414456	-1.146081
19	1	0	1.996979	0.230983	-1.920146
20	6	0	1.691420	-0.867387	-0.061537
21	1	0	1.330107	-0.573755	0.935434
22	6	0	3.179070	-1.200192	0.034024
23	1	0	3.533437	-1.481733	-0.967769
24	6	0	4.049882	-0.057793	0.554077
25	1	0	3.617151	0.331843	1.481221
26	6	0	5.470658	-0.515777	0.833571
27	1	0	6.020674	0.308836	1.301167
28	1	0	5.463842	-1.381752	1.498783
29	8	0	1.077876	-2.092278	-0.439801
30	1	0	0.256534	-1.857522	-0.890245
31	8	0	3.330921	-2.285581	0.931691
32	1	0	2.651641	-2.925081	0.689976
33	8	0	4.080155	1.006432	-0.385338
34	1	0	4.739399	0.749785	-1.042258
35	8	0	6.029643	-0.831687	-0.437976
36	1	0	6.944088	-1.096781	-0.318129
37	6	0	-0.706980	2.865912	0.478097
38	1	0	-0.651136	3.588041	-0.356406
39	1	0	-1.765287	2.717589	0.709591
40	6	0	0.008396	3.426027	1.697756
41	1	0	-0.490798	4.332268	2.046104
42	1	0	0.001524	2.691996	2.506369
43	1	0	1.045794	3.683643	1.472991
44	8	0	-5.660626	-1.477408	0.789293
45	6	0	-6.929361	-1.058885	0.324293
46	1	0	-7.658962	-1.686540	0.832117
47	1	0	-7.120120	-0.010631	0.575456
48	1	0	-7.024088	-1.200682	-0.757016

Structure 31b (^{2}E ec-ec H-bond N) (M06-2X, Benzene)

Energy (Hartrees): = - 1130.6897073
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.609826	0.244372	-0.604462
2	6	0	-1.443316	-0.553765	0.532625
3	6	0	-2.461821	-1.378033	0.965617
4	6	0	-3.677829	-1.421969	0.270210
5	6	0	-3.855101	-0.634037	-0.863936
6	6	0	-2.812378	0.189924	-1.290902
7	1	0	-0.502861	-0.523908	1.072066
8	1	0	-2.349133	-2.006735	1.840551
9	1	0	-4.780883	-0.653724	-1.422402
10	1	0	-2.950331	0.797241	-2.180298
11	6	0	-0.505666	1.162462	-1.051147
12	1	0	-0.746818	1.574162	-2.048590
13	7	0	-0.256114	2.258467	-0.108725
14	8	0	0.732641	0.479887	-1.115275
15	6	0	1.781175	1.347152	-0.657538
16	6	0	1.087063	2.699242	-0.489204
17	1	0	1.543514	3.308939	0.291791
18	1	0	1.074855	3.262908	-1.434981
19	1	0	2.567719	1.366120	-1.408985
20	6	0	2.352476	0.822226	0.660573
21	1	0	3.282551	1.369222	0.869077
22	6	0	2.664105	-0.678541	0.665367
23	1	0	1.760597	-1.219584	0.357282
24	6	0	3.819904	-1.087676	-0.245849
25	1	0	4.713647	-0.528523	0.047355
26	6	0	4.106952	-2.574666	-0.126837
27	1	0	4.991992	-2.810899	-0.728216
28	1	0	4.288288	-2.837518	0.918730
29	8	0	1.468734	1.049685	1.759156
30	1	0	0.631433	1.406427	1.413745
31	8	0	3.039113	-1.047972	1.982856
32	1	0	2.401619	-0.612904	2.560750
33	8	0	3.552896	-0.765086	-1.598952
34	1	0	2.838276	-1.351806	-1.876255
35	8	0	2.958551	-3.237592	-0.643626
36	1	0	3.121153	-4.183188	-0.641419
37	6	0	-1.283606	3.293678	-0.135745
38	1	0	-1.354789	3.732541	-1.145571
39	1	0	-2.239505	2.809340	0.079574
40	6	0	-1.016080	4.383690	0.889982
41	1	0	-1.857076	5.078633	0.927319
42	1	0	-0.884502	3.947974	1.883111

43	1	0	-0.121643	4.960120	0.643695
44	8	0	-4.613799	-2.259582	0.776291
45	6	0	-5.848484	-2.356913	0.092429
46	1	0	-5.709830	-2.729098	-0.927863
47	1	0	-6.448849	-3.069486	0.654722
48	1	0	-6.367143	-1.393123	0.065180

Structure 31b (^{2}E ax-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 1130.6804868
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.219162	-0.202479	-0.649732
2	6	0	2.452101	1.012290	-0.002607
3	6	0	3.740345	1.409936	0.307788
4	6	0	4.828651	0.598323	-0.028580
5	6	0	4.609161	-0.612474	-0.686041
6	6	0	3.306046	-0.995109	-0.993480
7	1	0	1.615054	1.648773	0.258768
8	1	0	3.935628	2.350495	0.808394
9	1	0	5.432679	-1.255776	-0.964592
10	1	0	3.136832	-1.940995	-1.498105
11	6	0	0.829566	-0.698281	-0.936955
12	1	0	0.833776	-1.257503	-1.881974
13	7	0	0.232903	-1.569226	0.064510
14	8	0	-0.073481	0.406358	-1.083785
15	6	0	-1.401914	-0.086469	-0.863366
16	6	0	-1.173831	-1.532038	-0.352611
17	1	0	-1.835363	-1.811691	0.463487
18	1	0	-1.329654	-2.239889	-1.168787
19	1	0	-1.943562	-0.070638	-1.813031
20	6	0	-2.068397	0.857540	0.142477
21	1	0	-1.775385	0.569755	1.163262
22	6	0	-3.592932	0.917457	0.080915
23	1	0	-3.880813	1.225037	-0.934143
24	6	0	-4.293065	-0.400390	0.404387
25	1	0	-3.908966	-0.789858	1.352842
26	6	0	-5.796970	-0.221115	0.522201
27	1	0	-6.238486	-1.166140	0.857823
28	1	0	-6.027755	0.572470	1.235987
29	8	0	-1.656628	2.197683	-0.098985
30	1	0	-0.745539	2.151437	-0.411532
31	8	0	-4.035084	1.872364	1.029474
32	1	0	-3.474012	2.646441	0.908342
33	8	0	-4.016245	-1.363453	-0.599961
34	1	0	-4.628735	-1.165004	-1.319524
35	8	0	-6.248319	0.104031	-0.789201
36	1	0	-7.207374	0.138762	-0.787956
37	6	0	0.446287	-1.152734	1.463859
38	1	0	0.494168	-0.060231	1.567581
39	1	0	-0.429845	-1.480929	2.027797
40	6	0	1.682588	-1.795607	2.080241
41	1	0	1.711170	-1.594279	3.154398
42	1	0	1.650734	-2.876833	1.929709
43	1	0	2.606696	-1.415393	1.643168
44	8	0	6.049609	1.073631	0.313719
45	6	0	7.176101	0.273739	0.007284
46	1	0	8.043586	0.824552	0.365460
47	1	0	7.127037	-0.693341	0.517851
48	1	0	7.271602	0.114890	-1.071561

Structure 31b (^{2}E ec-ec H-bond O) (M06-2X, DMSO)

Energy (Hartrees): = - 1130.6910847
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.193136	0.330415	-0.569085
2	6	0	-2.171520	-0.701456	0.376545
3	6	0	-3.346048	-1.283592	0.810652
4	6	0	-4.579512	-0.838995	0.311028
5	6	0	-4.614688	0.188594	-0.629676
6	6	0	-3.415622	0.760577	-1.061514
7	1	0	-1.221483	-1.046320	0.773492
8	1	0	-3.341983	-2.085215	1.540107
9	1	0	-5.552201	0.550584	-1.030794

10	1	0	-3.445682	1.560082	-1.795557
11	6	0	-0.901607	0.960914	-1.016669
12	1	0	-1.101914	1.697607	-1.814631
13	7	0	-0.162080	1.568194	0.081440
14	8	0	-0.016863	-0.031262	-1.531283
15	6	0	1.321585	0.227946	-1.066277
16	6	0	1.213960	1.597096	-0.405658
17	1	0	1.921081	1.725516	0.411653
18	1	0	1.370940	2.399720	-1.143997
19	1	0	1.985567	0.220904	-1.930978
20	6	0	1.696524	-0.885809	-0.077647
21	1	0	1.327396	-0.609247	0.921094
22	6	0	3.186790	-1.200553	0.024928
23	1	0	3.546978	-1.479628	-0.975513
24	6	0	4.040647	-0.042532	0.540112
25	1	0	3.584454	0.370097	1.445442
26	6	0	5.458447	-0.477824	0.863738
27	1	0	5.991213	0.370957	1.305222
28	1	0	5.451189	-1.310596	1.570315
29	8	0	1.099024	-2.114639	-0.476551
30	1	0	0.252753	-1.880642	-0.878902
31	8	0	3.345314	-2.286818	0.924277
32	1	0	2.668224	-2.928989	0.682193
33	8	0	4.084443	0.995570	-0.429382
34	1	0	4.751607	0.715048	-1.069235
35	8	0	6.050305	-0.849566	-0.378621
36	1	0	6.997940	-0.944911	-0.246265
37	6	0	-0.695122	2.871594	0.462419
38	1	0	-0.623946	3.576966	-0.383208
39	1	0	-1.757418	2.741868	0.688473
40	6	0	0.019638	3.441678	1.677448
41	1	0	-0.466029	4.364961	1.999638
42	1	0	-0.009466	2.728078	2.504410
43	1	0	1.064317	3.672687	1.457141
44	8	0	-5.672865	-1.467143	0.800759
45	6	0	-6.943354	-1.036889	0.333902
46	1	0	-7.677780	-1.648416	0.853911
47	1	0	-7.115941	0.016878	0.571426
48	1	0	-7.042015	-1.191460	-0.744585

Structure 31b (^{2}E ec-ec H-bond N) (M06-2X, DMSO)

Energy (Hartrees): = - 1130.6968331
No imaginary frequencies
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.649929	0.237151	-0.608984
2	6	0	-1.419259	-0.673046	0.429125
3	6	0	-2.410111	-1.549703	0.827848
4	6	0	-3.662723	-1.534323	0.197670
5	6	0	-3.903141	-0.634413	-0.839510
6	6	0	-2.888348	0.239184	-1.234043
7	1	0	-0.453307	-0.688364	0.922954
8	1	0	-2.243852	-2.261540	1.628109
9	1	0	-4.857937	-0.604861	-1.346855
10	1	0	-3.076554	0.935271	-2.045818
11	6	0	-0.579066	1.211308	-1.019072
12	1	0	-0.850668	1.678274	-1.981631
13	7	0	-0.334176	2.252940	-0.015039
14	8	0	0.674327	0.559432	-1.151043
15	6	0	1.710337	1.415321	-0.643084
16	6	0	0.995122	2.741814	-0.396497
17	1	0	1.453906	3.321902	0.405002
18	1	0	0.952154	3.349681	-1.312041
19	1	0	2.498163	1.491441	-1.391072
20	6	0	2.289250	0.827662	0.644110
21	1	0	3.184176	1.407149	0.906712
22	6	0	2.683449	-0.641075	0.507483
23	1	0	1.810126	-1.189014	0.127834
24	6	0	3.852460	-0.894445	-0.446005
25	1	0	4.627337	-0.133421	-0.308456
26	6	0	4.463107	-2.267374	-0.192718
27	1	0	5.124469	-2.508955	-1.026894
28	1	0	5.052562	-2.254091	0.727976
29	8	0	1.376325	0.904669	1.737808
30	1	0	0.553235	1.320476	1.418489
31	8	0	3.040220	-1.149210	1.788242
32	1	0	2.368883	-0.807667	2.392710
33	8	0	3.410477	-0.771630	-1.790445
34	1	0	2.673264	-1.384382	-1.899637
35	8	0	3.463628	-3.276570	-0.146641
36	1	0	3.011942	-3.155813	0.696733
37	6	0	-1.377417	3.276004	0.014537

38	1	0	-1.466878	3.748878	-0.976763
39	1	0	-2.325089	2.773645	0.225676
40	6	0	-1.105037	4.330020	1.075010
41	1	0	-1.952159	5.015317	1.143311
42	1	0	-0.959461	3.863177	2.052530
43	1	0	-0.217339	4.919926	0.836392
44	8	0	-4.567246	-2.426776	0.661470
45	6	0	-5.858949	-2.420941	0.070516
46	1	0	-5.808940	-2.657792	-0.996304
47	1	0	-6.427233	-3.193840	0.584033
48	1	0	-6.351875	-1.454173	0.208828

Structure 31b (^{2}E ax-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 1130.685572
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.222164	-0.201964	-0.663906
2	6	0	2.458063	1.020692	-0.031989
3	6	0	3.747354	1.408978	0.291170
4	6	0	4.832751	0.579785	-0.015661
5	6	0	4.609677	-0.637299	-0.662882
6	6	0	3.306441	-1.009592	-0.984015
7	1	0	1.626268	1.671215	0.212569
8	1	0	3.940889	2.355999	0.781514
9	1	0	5.430471	-1.292121	-0.923076
10	1	0	3.135671	-1.958963	-1.482418
11	6	0	0.833030	-0.698818	-0.950803
12	1	0	0.841646	-1.278678	-1.882634
13	7	0	0.234458	-1.550466	0.069554
14	8	0	-0.068534	0.402604	-1.121149
15	6	0	-1.398833	-0.087933	-0.894043
16	6	0	-1.171761	-1.523618	-0.358889
17	1	0	-1.834917	-1.788051	0.460984
18	1	0	-1.315887	-2.242915	-1.167093
19	1	0	-1.939879	-0.087889	-1.843889
20	6	0	-2.066617	0.869417	0.096440
21	1	0	-1.758753	0.610287	1.119578
22	6	0	-3.591487	0.905882	0.055340
23	1	0	-3.898685	1.198755	-0.958564
24	6	0	-4.261594	-0.423818	0.397062
25	1	0	-3.823684	-0.827404	1.315594
26	6	0	-5.758515	-0.272859	0.597133
27	1	0	-6.165786	-1.239712	0.910618
28	1	0	-5.968564	0.476910	1.362990
29	8	0	-1.676162	2.209920	-0.186446
30	1	0	-0.737034	2.176776	-0.405157
31	8	0	-4.032458	1.868818	0.999781
32	1	0	-3.468570	2.640272	0.871685
33	8	0	-4.025498	-1.364443	-0.641151
34	1	0	-4.663098	-1.141644	-1.331977
35	8	0	-6.290774	0.108736	-0.668846
36	1	0	-7.244961	-0.007525	-0.642821
37	6	0	0.428000	-1.082665	1.458011
38	1	0	0.464004	0.012639	1.522004
39	1	0	-0.451765	-1.397992	2.022865
40	6	0	1.662774	-1.690071	2.112276
41	1	0	1.676736	-1.443712	3.177410
42	1	0	1.641216	-2.778131	2.012142
43	1	0	2.590985	-1.323612	1.670063
44	8	0	6.052898	1.042938	0.340464
45	6	0	7.177261	0.224438	0.050486
46	1	0	8.046821	0.767501	0.415042
47	1	0	7.108011	-0.738072	0.565863
48	1	0	7.279637	0.057419	-1.025791

Structure 31c ($^5C_2$ ec-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1130.6661793
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.988884	1.538262	0.216174
2	6	0	-0.926067	2.453742	-0.384206
3	6	0	-1.787250	0.137041	-0.360505
4	1	0	-1.030234	3.437896	0.071122

5	1	0	-1.069742	2.553455	-1.475616
6	1	0	-2.989809	1.894521	-0.019354
7	1	0	-1.913042	0.156499	-1.454598
8	8	0	-0.450066	-0.266474	-0.060580
9	7	0	0.403174	1.920453	-0.069387
10	6	0	-2.682882	-0.948293	0.235447
11	1	0	-2.745270	-0.777303	1.317667
12	6	0	-4.081777	-0.940169	-0.360646
13	1	0	-3.997616	-1.135556	-1.439758
14	6	0	-4.940030	-2.031705	0.252060
15	1	0	-4.961508	-1.893495	1.340255
16	1	0	-4.523654	-3.012794	0.012288
17	8	0	-2.155161	-2.229066	-0.052369
18	1	0	-1.201849	-2.162859	0.069186
19	8	0	-4.676840	0.319986	-0.128351
20	1	0	-5.618581	0.196366	-0.292137
21	8	0	-6.237922	-1.851718	-0.306167
22	1	0	-6.856639	-2.419863	0.155034
23	8	0	-1.862400	1.526376	1.622425
24	1	0	-0.923202	1.386687	1.793464
25	6	0	1.469369	2.809396	-0.538553
26	1	0	1.418008	2.930487	-1.635970
27	1	0	2.422906	2.330469	-0.314474
28	6	0	1.872227	-0.044227	-0.312079
29	6	0	2.246983	-0.227269	1.022855
30	6	0	2.742028	-0.441818	-1.312801
31	6	0	3.466664	-0.789108	1.339385
32	1	0	1.566474	0.082234	1.807476
33	6	0	3.981016	-1.009259	-1.010996
34	1	0	2.461380	-0.308590	-2.352431
35	6	0	4.344671	-1.182462	0.321380
36	1	0	3.776361	-0.939498	2.366022
37	1	0	4.637786	-1.308122	-1.816084
38	6	0	0.535998	0.572337	-0.626631
39	1	0	0.384105	0.599650	-1.725325
40	6	0	1.437529	4.175319	0.136382
41	1	0	2.362266	4.712914	-0.079131
42	1	0	0.609629	4.796582	-0.206843
43	1	0	1.352979	4.052021	1.218186
44	8	0	5.519187	-1.719484	0.734409
45	6	0	6.447508	-2.107286	-0.256307
46	1	0	7.313170	-2.493266	0.276803
47	1	0	6.037183	-2.892293	-0.899628
48	1	0	6.749669	-1.253293	-0.871132

Structure 31c ($^5C_2$ ax-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1130.6633565
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.009853	1.647880	0.143797
2	6	0	0.876427	2.403650	0.853083
3	6	0	1.823433	0.153988	0.417881
4	1	0	0.933709	3.465835	0.611950
5	1	0	1.003567	2.298605	1.937370
6	1	0	2.982077	1.971569	0.513474
7	1	0	1.884104	-0.037289	1.500150
8	8	0	0.512797	-0.211054	-0.032313
9	7	0	-0.456956	1.902696	0.498577
10	6	0	2.789083	-0.788784	-0.299032
11	1	0	2.901487	-0.456153	-1.339335
12	6	0	4.161377	-0.825943	0.355849
13	1	0	4.040068	-1.156658	1.398009
14	6	0	5.071927	-1.815362	-0.349361
15	1	0	5.128712	-1.547117	-1.411856
16	1	0	4.675121	-2.827651	-0.244730
17	8	0	2.295614	-2.113424	-0.237826
18	1	0	1.339195	-2.051627	-0.335983
19	8	0	4.730625	0.465420	0.305230
20	1	0	5.669334	0.343716	0.487157
21	8	0	6.342156	-1.672474	0.277520
22	1	0	6.992825	-2.170634	-0.219484
23	8	0	1.998033	1.900090	-1.250831
24	1	0	1.264927	1.397511	-1.621367
25	6	0	-0.960815	2.357274	-0.811196
26	1	0	-0.886180	1.559209	-1.563393
27	1	0	-0.309715	3.161691	-1.157008
28	6	0	-1.838472	-0.137731	0.401609
29	6	0	-2.066524	-0.865003	-0.765984
30	6	0	-2.892377	0.062132	1.282840
31	6	0	-3.326906	-1.362057	-1.050147

32	1	0	-1.248255	-1.038461	-1.454144
33	6	0	-4.164684	-0.432681	1.014173
34	1	0	-2.724145	0.635024	2.188944
35	6	0	-4.385003	-1.146596	-0.164062
36	1	0	-3.524465	-1.926116	-1.953105
37	1	0	-4.963025	-0.258396	1.722232
38	6	0	-0.498790	0.474947	0.718023
39	1	0	-0.272750	0.313084	1.781897
40	6	0	-2.398270	2.862842	-0.745821
41	1	0	-2.685114	3.305548	-1.702967
42	1	0	-3.097349	2.057494	-0.519140
43	1	0	-2.487300	3.624127	0.031529
44	8	0	-5.580078	-1.673256	-0.530434
45	6	0	-6.680497	-1.467242	0.330047
46	1	0	-6.891659	-0.400271	0.455114
47	1	0	-7.529742	-1.950324	-0.147380
48	1	0	-6.508493	-1.921900	1.311060

Structure 31c ($^5C_2$ ec-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 1130.6876936
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.991015	1.543262	0.208350
2	6	0	-0.930266	2.457505	-0.396747
3	6	0	-1.784665	0.139875	-0.359824
4	1	0	-1.036673	3.445491	0.049928
5	1	0	-1.075737	2.547549	-1.487996
6	1	0	-2.991445	1.897645	-0.032200
7	1	0	-1.905833	0.156470	-1.454238
8	8	0	-0.447194	-0.257687	-0.052162
9	7	0	0.401625	1.931289	-0.078446
10	6	0	-2.677756	-0.950476	0.231267
11	1	0	-2.732177	-0.797526	1.316454
12	6	0	-4.083628	-0.935187	-0.349553
13	1	0	-4.012595	-1.074881	-1.438417
14	6	0	-4.923672	-2.064605	0.219001
15	1	0	-4.930374	-1.989494	1.313592
16	1	0	-4.510030	-3.030612	-0.079897
17	8	0	-2.146524	-2.226811	-0.077439
18	1	0	-1.192411	-2.154954	0.038731
19	8	0	-4.692511	0.305209	-0.047865
20	1	0	-5.636596	0.170066	-0.191665
21	8	0	-6.232768	-1.867699	-0.308365
22	1	0	-6.841238	-2.448527	0.153768
23	8	0	-1.867886	1.540277	1.616786
24	1	0	-0.927785	1.403844	1.788775
25	6	0	1.461696	2.823175	-0.560014
26	1	0	1.399046	2.940957	-1.656659
27	1	0	2.419379	2.349133	-0.343381
28	6	0	1.876139	-0.034921	-0.306045
29	6	0	2.260316	-0.195912	1.029375
30	6	0	2.738282	-0.453119	-1.306284
31	6	0	3.479892	-0.759088	1.346721
32	1	0	1.590100	0.131466	1.816153
33	6	0	3.975997	-1.022848	-1.003635
34	1	0	2.452236	-0.334442	-2.346432
35	6	0	4.348187	-1.177046	0.329420
36	1	0	3.793706	-0.891774	2.375033
37	1	0	4.626446	-1.337619	-1.808206
38	6	0	0.539361	0.579493	-0.625986
39	1	0	0.387284	0.596471	-1.723714
40	6	0	1.433623	4.189765	0.111870
41	1	0	2.353572	4.730525	-0.119286
42	1	0	0.599013	4.809059	-0.219888
43	1	0	1.368439	4.071177	1.196152
44	8	0	5.520257	-1.715419	0.741371
45	6	0	6.427115	-2.156718	-0.251457
46	1	0	7.290578	-2.548378	0.282659
47	1	0	5.990757	-2.952456	-0.863316
48	1	0	6.746355	-1.330114	-0.894199

Structure 31c ($^5C_2$ ax-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 1130.6843437
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.014323	1.645797	0.168558
2	6	0	0.880599	2.402663	0.876050
3	6	0	1.820192	0.151629	0.432465
4	1	0	0.943839	3.466346	0.642446
5	1	0	1.004416	2.289013	1.959652
6	1	0	2.983938	1.965781	0.548588
7	1	0	1.874796	-0.044171	1.513874
8	8	0	0.509643	-0.203955	-0.026517
9	7	0	-0.454149	1.909931	0.513116
10	6	0	2.779297	-0.798200	-0.284072
11	1	0	2.872221	-0.486898	-1.332689
12	6	0	4.164999	-0.823271	0.343672
13	1	0	4.065786	-1.107772	1.401726
14	6	0	5.054981	-1.846464	-0.339766
15	1	0	5.092315	-1.625991	-1.413945
16	1	0	4.660363	-2.853520	-0.186391
17	8	0	2.283960	-2.122257	-0.191572
18	1	0	1.327953	-2.058925	-0.297375
19	8	0	4.744667	0.460874	0.227064
20	1	0	5.686867	0.334158	0.389430
21	8	0	6.340147	-1.688420	0.253591
22	1	0	6.979752	-2.188602	-0.258336
23	8	0	2.015306	1.907010	-1.226235
24	1	0	1.278416	1.414453	-1.604123
25	6	0	-0.952861	2.376013	-0.794779
26	1	0	-0.873380	1.587205	-1.555933
27	1	0	-0.304828	3.188063	-1.128643
28	6	0	-1.842333	-0.129062	0.397793
29	6	0	-2.078731	-0.802832	-0.800730
30	6	0	-2.888986	0.021104	1.298289
31	6	0	-3.338566	-1.296160	-1.094848
32	1	0	-1.268714	-0.939647	-1.507087
33	6	0	-4.160406	-0.472082	1.020558
34	1	0	-2.717126	0.549194	2.230870
35	6	0	-4.388854	-1.132912	-0.187233
36	1	0	-3.537006	-1.820004	-2.022090
37	1	0	-4.952351	-0.339235	1.745140
38	6	0	-0.503263	0.479881	0.725196
39	1	0	-0.282877	0.311707	1.788573
40	6	0	-2.390450	2.878913	-0.730016
41	1	0	-2.681190	3.312279	-1.690901
42	1	0	-3.090382	2.076089	-0.494699
43	1	0	-2.481665	3.649334	0.038868
44	8	0	-5.582548	-1.652143	-0.561702
45	6	0	-6.669647	-1.517529	0.334018
46	1	0	-6.901159	-0.465020	0.526229
47	1	0	-7.520919	-1.987885	-0.154169
48	1	0	-6.471183	-2.029271	1.281214

Structure 31c ($^5C_2$ ec-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 1130.6922954
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.985904	1.546052	0.210328
2	6	0	-0.925010	2.456433	-0.397358
3	6	0	-1.785886	0.143882	-0.360206
4	1	0	-1.029637	3.448922	0.039929
5	1	0	-1.069714	2.535963	-1.488174
6	1	0	-2.984353	1.906622	-0.028770
7	1	0	-1.904561	0.167394	-1.453869
8	8	0	-0.449315	-0.259196	-0.049884
9	7	0	0.407511	1.929251	-0.075514
10	6	0	-2.683158	-0.946266	0.223836
11	1	0	-2.731018	-0.810692	1.311553
12	6	0	-4.093520	-0.917671	-0.345571
13	1	0	-4.030063	-1.015405	-1.439256
14	6	0	-4.926274	-2.067522	0.192238
15	1	0	-4.924855	-2.030500	1.288488
16	1	0	-4.515096	-3.023493	-0.139905
17	8	0	-2.155545	-2.222664	-0.101183
18	1	0	-1.198802	-2.142221	-0.011066
19	8	0	-4.707909	0.309774	0.005040
20	1	0	-5.652822	0.167717	-0.131737
21	8	0	-6.241101	-1.861287	-0.317502
22	1	0	-6.845750	-2.434698	0.162592
23	8	0	-1.859532	1.540275	1.622256
24	1	0	-0.920127	1.386736	1.788206

25	6	0	1.462855	2.819611	-0.575636
26	1	0	1.375367	2.942403	-1.668711
27	1	0	2.423929	2.341691	-0.382014
28	6	0	1.874696	-0.040757	-0.302515
29	6	0	2.253198	-0.210371	1.033685
30	6	0	2.742908	-0.449984	-1.302666
31	6	0	3.473376	-0.774872	1.352900
32	1	0	1.580977	0.109230	1.822877
33	6	0	3.980781	-1.019697	-0.998590
34	1	0	2.462003	-0.321475	-2.343200
35	6	0	4.348580	-1.182595	0.335983
36	1	0	3.779052	-0.911832	2.383664
37	1	0	4.636284	-1.325475	-1.802886
38	6	0	0.540775	0.577274	-0.626490
39	1	0	0.389542	0.595594	-1.722163
40	6	0	1.455220	4.181730	0.105389
41	1	0	2.364192	4.726446	-0.158303
42	1	0	0.605442	4.798429	-0.190981
43	1	0	1.432275	4.058405	1.191354
44	8	0	5.520482	-1.720059	0.746343
45	6	0	6.434344	-2.146171	-0.254371
46	1	0	7.298823	-2.539529	0.276674
47	1	0	6.000710	-2.934751	-0.876112
48	1	0	6.747107	-1.309435	-0.885893

Structure 31c ($^5C_2$ ax-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 1130.689393
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.007215	1.645414	0.185087
2	6	0	0.868494	2.392703	0.892784
3	6	0	1.822103	0.150412	0.442859
4	1	0	0.924750	3.458184	0.664734
5	1	0	0.995632	2.269601	1.974321
6	1	0	2.970119	1.969853	0.578327
7	1	0	1.882045	-0.044355	1.523394
8	8	0	0.511912	-0.213224	-0.013320
9	7	0	-0.466099	1.894107	0.529485
10	6	0	2.783243	-0.792734	-0.278991
11	1	0	2.858550	-0.494772	-1.332583
12	6	0	4.177773	-0.797631	0.329533
13	1	0	4.093095	-1.040085	1.399066
14	6	0	5.061030	-1.841481	-0.330503
15	1	0	5.087859	-1.656834	-1.411349
16	1	0	4.671833	-2.844695	-0.142918
17	8	0	2.298070	-2.121660	-0.168354
18	1	0	1.341631	-2.062355	-0.277653
19	8	0	4.759247	0.482544	0.158136
20	1	0	5.703572	0.353587	0.310460
21	8	0	6.353561	-1.668025	0.243900
22	1	0	6.989681	-2.155708	-0.287501
23	8	0	2.021066	1.916750	-1.210076
24	1	0	1.286075	1.428523	-1.599588
25	6	0	-0.952767	2.346892	-0.788907
26	1	0	-0.837918	1.562866	-1.549766
27	1	0	-0.323102	3.179198	-1.107044
28	6	0	-1.838523	-0.152474	0.413316
29	6	0	-2.079817	-0.797496	-0.800514
30	6	0	-2.883452	-0.019600	1.319893
31	6	0	-3.344507	-1.274865	-1.105187
32	1	0	-1.273732	-0.922359	-1.513984
33	6	0	-4.160116	-0.494368	1.030882
34	1	0	-2.707191	0.477984	2.268751
35	6	0	-4.395943	-1.120251	-0.195377
36	1	0	-3.542350	-1.774961	-2.046253
37	1	0	-4.950539	-0.372976	1.759647
38	6	0	-0.502394	0.460385	0.743434
39	1	0	-0.280344	0.295908	1.806276
40	6	0	-2.403496	2.815403	-0.754191
41	1	0	-2.685604	3.231368	-1.725353
42	1	0	-3.091504	2.000416	-0.522279
43	1	0	-2.528640	3.594701	0.001784
44	8	0	-5.595586	-1.612671	-0.582645
45	6	0	-6.686810	-1.465225	0.314463
46	1	0	-6.889872	-0.410287	0.521178
47	1	0	-7.547162	-1.906833	-0.184383
48	1	0	-6.502544	-1.994924	1.253718

Structure 31d ($^5C_2$ ec-ax) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1130.6626018
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.495975	1.358392	-0.900204
2	6	0	-0.127044	1.954426	-1.240149
3	6	0	-1.278193	0.215680	0.098056
4	1	0	-0.272600	2.828205	-1.878372
5	1	0	0.494513	1.222864	-1.780141
6	1	0	-1.996959	0.975939	-1.787270
7	1	0	-0.644814	-0.557628	-0.358276
8	8	0	-0.614930	0.746907	1.255125
9	7	0	0.472174	2.386525	0.013822
10	6	0	-2.560134	-0.427046	0.630592
11	1	0	-3.301198	0.366426	0.790275
12	6	0	-3.125237	-1.464815	-0.325885
13	1	0	-2.378323	-2.262623	-0.448169
14	6	0	-4.396231	-2.084802	0.225482
15	1	0	-5.119260	-1.285080	0.428872
16	1	0	-4.177166	-2.628904	1.147176
17	8	0	-2.293605	-1.125705	1.834918
18	1	0	-1.745898	-0.538842	2.366819
19	8	0	-3.397974	-0.845920	-1.566660
20	1	0	-3.964239	-1.462101	-2.044563
21	8	0	-4.872816	-2.947629	-0.802460
22	1	0	-5.747818	-3.259314	-0.566776
23	8	0	-2.318735	2.360776	-0.342826
24	1	0	-1.788768	2.752766	0.362895
25	6	0	1.433510	3.477337	-0.033638
26	1	0	2.044042	3.426683	-0.946428
27	1	0	2.125553	3.370462	0.807271
28	6	0	1.649948	0.215780	0.590774
29	6	0	2.732874	0.461868	-0.240997
30	6	0	1.521409	-1.063080	1.147190
31	6	0	3.680484	-0.524187	-0.517596
32	1	0	2.855229	1.436577	-0.697809
33	6	0	2.448537	-2.051877	0.881615
34	1	0	0.662482	-1.286697	1.770312
35	6	0	3.541026	-1.787709	0.049777
36	1	0	4.508322	-0.291788	-1.173392
37	1	0	2.351561	-3.045996	1.300144
38	6	0	0.652916	1.315059	0.967154
39	1	0	0.975455	1.769923	1.908510
40	6	0	0.735250	4.832443	0.037360
41	1	0	1.451288	5.651546	-0.061700
42	1	0	-0.004367	4.924841	-0.761343
43	1	0	0.213467	4.935088	0.990581
44	8	0	4.397417	-2.820883	-0.148440
45	6	0	5.510977	-2.596773	-0.986507
46	1	0	6.061347	-3.534303	-1.013384
47	1	0	5.197056	-2.330354	-2.000949
48	1	0	6.156331	-1.807918	-0.586433

Structure 31d ($^5C_2$ ax-ax) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1130.666403
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.505020	1.288957	-1.079595
2	6	0	-0.133149	1.843950	-1.478206
3	6	0	-1.275790	0.242752	0.010816
4	1	0	-0.254758	2.644932	-2.208468
5	1	0	0.453178	1.044903	-1.946169
6	1	0	-2.001069	0.828302	-1.933084
7	1	0	-0.636819	-0.559519	-0.379730
8	8	0	-0.606395	0.898691	1.098729
9	7	0	0.623241	2.362792	-0.333828
10	6	0	-2.534843	-0.375146	0.622651
11	1	0	-3.292997	0.410075	0.742537
12	6	0	-3.109652	-1.487641	-0.238655
13	1	0	-2.349898	-2.276554	-0.338011
14	6	0	-4.344190	-2.095297	0.401963
15	1	0	-5.077420	-1.298981	0.580867
16	1	0	-4.078134	-2.571989	1.348358
17	8	0	-2.222422	-0.973298	1.868544

18	1	0	-1.650882	-0.348646	2.327909
19	8	0	-3.442063	-0.954534	-1.503635
20	1	0	-4.010090	-1.611355	-1.921707
21	8	0	-4.838514	-3.033972	-0.547474
22	1	0	-5.702442	-3.337893	-0.265044
23	8	0	-2.354801	2.323501	-0.612685
24	1	0	-2.066790	2.535588	0.281195
25	6	0	0.271310	3.711999	0.122578
26	1	0	-0.442405	3.681919	0.959833
27	1	0	-0.234727	4.229415	-0.693825
28	6	0	1.664867	0.267865	0.457634
29	6	0	2.781384	0.479925	-0.337980
30	6	0	1.504017	-0.981839	1.066191
31	6	0	3.730237	-0.522237	-0.537566
32	1	0	2.907092	1.446698	-0.811791
33	6	0	2.434368	-1.986066	0.874892
34	1	0	0.624651	-1.174311	1.671465
35	6	0	3.557846	-1.761873	0.073638
36	1	0	4.586644	-0.320811	-1.166504
37	1	0	2.317070	-2.961033	1.331591
38	6	0	0.691272	1.403006	0.738728
39	1	0	1.019460	1.927462	1.639879
40	6	0	1.516606	4.483479	0.542924
41	1	0	1.256079	5.483101	0.897755
42	1	0	2.045778	3.967157	1.348183
43	1	0	2.200697	4.575044	-0.302171
44	8	0	4.412753	-2.808345	-0.050643
45	6	0	5.559321	-2.625160	-0.853110
46	1	0	6.102496	-3.566802	-0.821690
47	1	0	5.287077	-2.397104	-1.888722
48	1	0	6.195555	-1.825528	-0.459960

Structure 31d ($^5C_2$ ec-ax) (M06-2X, Benzene)

Energy (Hartrees): = - 1130.683688
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.501092	1.361904	-0.898850
2	6	0	-0.136652	1.961851	-1.245345
3	6	0	-1.276467	0.217987	0.096938
4	1	0	-0.286196	2.838067	-1.879737
5	1	0	0.476861	1.231324	-1.795153
6	1	0	-2.003074	0.981541	-1.786100
7	1	0	-0.639405	-0.551368	-0.361294
8	8	0	-0.614428	0.752290	1.252618
9	7	0	0.471247	2.391638	0.004970
10	6	0	-2.555058	-0.432783	0.629827
11	1	0	-3.298242	0.356399	0.799629
12	6	0	-3.124193	-1.465845	-0.330708
13	1	0	-2.371496	-2.254563	-0.473642
14	6	0	-4.383905	-2.102827	0.227716
15	1	0	-5.110305	-1.313808	0.458855
16	1	0	-4.152916	-2.665899	1.135175
17	8	0	-2.281069	-1.135963	1.830888
18	1	0	-1.707990	-0.559898	2.348624
19	8	0	-3.420970	-0.836023	-1.562146
20	1	0	-4.001113	-1.447770	-2.030202
21	8	0	-4.873079	-2.951202	-0.807313
22	1	0	-5.754974	-3.247486	-0.571517
23	8	0	-2.325671	2.362110	-0.334790
24	1	0	-1.785015	2.763669	0.358324
25	6	0	1.447235	3.471708	-0.050279
26	1	0	2.031471	3.424364	-0.979373
27	1	0	2.159690	3.342929	0.770000
28	6	0	1.654754	0.227130	0.596084
29	6	0	2.684422	0.434651	-0.311180
30	6	0	1.582106	-1.015372	1.238250
31	6	0	3.631208	-0.554827	-0.580526
32	1	0	2.764526	1.380317	-0.833837
33	6	0	2.511279	-2.005900	0.985142
34	1	0	0.767050	-1.210914	1.926139
35	6	0	3.548088	-1.781668	0.072758
36	1	0	4.414993	-0.355856	-1.298862
37	1	0	2.454399	-2.970924	1.474208
38	6	0	0.653559	1.325724	0.962931
39	1	0	0.972462	1.785258	1.903027
40	6	0	0.770682	4.833877	0.058563
41	1	0	1.498930	5.643866	-0.033174
42	1	0	0.023212	4.957078	-0.729298
43	1	0	0.263903	4.927948	1.021565

44	8	0	4.409302	-2.810892	-0.111767
45	6	0	5.441563	-2.640105	-1.064281
46	1	0	6.010220	-3.567838	-1.061652
47	1	0	5.032739	-2.471555	-2.065848
48	1	0	6.103698	-1.811934	-0.792795

Structure 31d ($^5C_2$ ax-ax) (M06-2X, Benece)

Energy (Hartrees): = - 1130.6872775
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.509781	1.294047	-1.076272
2	6	0	-0.138325	1.847507	-1.475747
3	6	0	-1.281401	0.240658	0.007212
4	1	0	-0.258989	2.651030	-2.203434
5	1	0	0.440466	1.046908	-1.950404
6	1	0	-2.006566	0.840678	-1.933203
7	1	0	-0.648726	-0.561877	-0.392643
8	8	0	-0.604445	0.886256	1.096173
9	7	0	0.623521	2.357553	-0.331669
10	6	0	-2.540346	-0.376248	0.621833
11	1	0	-3.293730	0.410681	0.757502
12	6	0	-3.130653	-1.476865	-0.245354
13	1	0	-2.371214	-2.261208	-0.376916
14	6	0	-4.351354	-2.097468	0.409735
15	1	0	-5.078659	-1.306103	0.630011
16	1	0	-4.067382	-2.602320	1.336228
17	8	0	-2.220349	-0.986221	1.861395
18	1	0	-1.632229	-0.372104	2.315311
19	8	0	-3.493123	-0.922749	-1.494601
20	1	0	-4.078317	-1.570504	-1.904493
21	8	0	-4.874394	-3.011845	-0.548956
22	1	0	-5.742787	-3.299816	-0.258783
23	8	0	-2.358694	2.328250	-0.602216
24	1	0	-2.057056	2.547601	0.285992
25	6	0	0.290148	3.711166	0.128540
26	1	0	-0.425385	3.691009	0.964645
27	1	0	-0.202542	4.239815	-0.688971
28	6	0	1.670011	0.261372	0.453843
29	6	0	2.793632	0.479463	-0.331459
30	6	0	1.509245	-0.992165	1.054756
31	6	0	3.746376	-0.519588	-0.529792
32	1	0	2.924609	1.447906	-0.800711
33	6	0	2.443479	-1.994092	0.865170
34	1	0	0.628021	-1.190767	1.655320
35	6	0	3.572217	-1.764225	0.071991
36	1	0	4.607659	-0.312277	-1.150515
37	1	0	2.322556	-2.970790	1.318329
38	6	0	0.692876	1.394315	0.737153
39	1	0	1.020664	1.915430	1.639941
40	6	0	1.545152	4.463293	0.551533
41	1	0	1.297169	5.466811	0.905981
42	1	0	2.067690	3.941745	1.358390
43	1	0	2.231899	4.549080	-0.293004
44	8	0	4.427454	-2.807262	-0.056652
45	6	0	5.574258	-2.622468	-0.864418
46	1	0	6.114625	-3.566808	-0.839785
47	1	0	5.301237	-2.390275	-1.898776
48	1	0	6.217553	-1.830359	-0.467816

Structure 31d ($^5C_2$ ec-ax) (M06-2X, DMSO)

Energy (Hartrees): = - 1130.6880513
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.505480	1.339775	-0.877922
2	6	0	-0.148545	1.957702	-1.217899
3	6	0	-1.266988	0.184113	0.098271
4	1	0	-0.303395	2.840817	-1.841306
5	1	0	0.469491	1.240059	-1.778269
6	1	0	-2.004506	0.970079	-1.771530
7	1	0	-0.627921	-0.572059	-0.379623
8	8	0	-0.602820	0.699614	1.261124
9	7	0	0.454796	2.377276	0.038507

10	6	0	-2.524380	-0.495927	0.636362
11	1	0	-3.239713	0.280430	0.935759
12	6	0	-3.190094	-1.412182	-0.379482
13	1	0	-2.450205	-2.142442	-0.738707
14	6	0	-4.351706	-2.169795	0.240750
15	1	0	-5.047106	-1.453078	0.693845
16	1	0	-3.993062	-2.862176	1.005482
17	8	0	-2.179269	-1.316077	1.743567
18	1	0	-1.562406	-0.795333	2.271093
19	8	0	-3.670368	-0.627698	-1.457105
20	1	0	-4.316532	-1.185990	-1.906775
21	8	0	-4.975130	-2.864706	-0.836892
22	1	0	-5.839554	-3.167141	-0.543339
23	8	0	-2.339485	2.325692	-0.295369
24	1	0	-1.784403	2.739991	0.379881
25	6	0	1.435827	3.456194	-0.012444
26	1	0	2.021715	3.408526	-0.939389
27	1	0	2.142379	3.324275	0.812013
28	6	0	1.674073	0.220398	0.592564
29	6	0	2.671345	0.435258	-0.350216
30	6	0	1.653467	-1.010615	1.260402
31	6	0	3.632670	-0.537530	-0.632604
32	1	0	2.715103	1.371941	-0.892943
33	6	0	2.596445	-1.986059	0.994141
34	1	0	0.878116	-1.209150	1.992185
35	6	0	3.598706	-1.755483	0.043621
36	1	0	4.390067	-0.332023	-1.377479
37	1	0	2.578490	-2.939231	1.509714
38	6	0	0.657259	1.298626	0.977442
39	1	0	0.973278	1.746370	1.923648
40	6	0	0.760500	4.818278	0.095510
41	1	0	1.493808	5.625185	0.015770
42	1	0	0.025047	4.947438	-0.703258
43	1	0	0.243438	4.909996	1.053714
44	8	0	4.479459	-2.765126	-0.150491
45	6	0	5.488661	-2.571906	-1.130704
46	1	0	6.079934	-3.485286	-1.138392
47	1	0	5.051715	-2.415278	-2.121548
48	1	0	6.132993	-1.725529	-0.875508

Structure 31d ($^5C_2$ ax-ax) (M06-2X, DMSO)

Energy (Hartrees): = - 1130.6911981
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.507665	1.282041	-1.079118
2	6	0	-0.140720	1.847826	-1.475037
3	6	0	-1.274840	0.233656	0.007233
4	1	0	-0.265334	2.651337	-2.202212
5	1	0	0.439463	1.048884	-1.951004
6	1	0	-1.988835	0.819577	-1.939878
7	1	0	-0.640251	-0.566454	-0.394867
8	8	0	-0.600161	0.882036	1.095412
9	7	0	0.620060	2.361863	-0.331560
10	6	0	-2.528073	-0.390600	0.624708
11	1	0	-3.277171	0.394482	0.789734
12	6	0	-3.136634	-1.473635	-0.252464
13	1	0	-2.375631	-2.248213	-0.427129
14	6	0	-4.335776	-2.117903	0.419462
15	1	0	-5.064064	-1.338854	0.675636
16	1	0	-4.027494	-2.641622	1.327327
17	8	0	-2.189843	-1.022961	1.850145
18	1	0	-1.590593	-0.417294	2.302577
19	8	0	-3.540999	-0.893853	-1.479886
20	1	0	-4.143477	-1.534957	-1.876993
21	8	0	-4.876896	-3.018229	-0.543598
22	1	0	-5.753385	-3.284951	-0.251320
23	8	0	-2.378041	2.306496	-0.618074
24	1	0	-2.077134	2.551122	0.264872
25	6	0	0.267120	3.711360	0.132522
26	1	0	-0.459906	3.680315	0.957377
27	1	0	-0.213158	4.239776	-0.692585
28	6	0	1.676279	0.268919	0.452181
29	6	0	2.794070	0.482949	-0.344147
30	6	0	1.525477	-0.981785	1.061918
31	6	0	3.748692	-0.514593	-0.544941
32	1	0	2.925792	1.447456	-0.821344
33	6	0	2.461425	-1.983401	0.871431
34	1	0	0.652142	-1.180317	1.673910
35	6	0	3.583906	-1.756966	0.066590
36	1	0	4.604525	-0.308490	-1.173981

37	1	0	2.342846	-2.955810	1.335643
38	6	0	0.694399	1.398256	0.737290
39	1	0	1.021343	1.919086	1.640172
40	6	0	1.507203	4.472039	0.581429
41	1	0	1.239471	5.469017	0.940331
42	1	0	2.020087	3.949159	1.393723
43	1	0	2.206993	4.577370	-0.250780
44	8	0	4.443481	-2.795022	-0.060445
45	6	0	5.590136	-2.603120	-0.876386
46	1	0	6.138247	-3.542710	-0.849135
47	1	0	5.309799	-2.376022	-1.909083
48	1	0	6.224967	-1.802925	-0.484521

Structure 34a (M06-2X, Gas Phase)

Energy (Hartrees): = - 1456.4568924
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.474891	1.436715	0.260376
2	6	0	-1.429725	2.350944	-0.184682
3	6	0	-1.131534	3.704922	-0.259782
4	6	0	0.129072	4.126542	0.129634
5	6	0	1.093427	3.250120	0.601895
6	6	0	0.778103	1.901060	0.665991
7	1	0	-2.421454	2.002081	-0.444584
8	1	0	-1.855149	4.431791	-0.602473
9	1	0	2.056016	3.631069	0.913658
10	1	0	1.516451	1.203497	1.046009
11	6	0	-0.785006	-0.055944	0.298613
12	1	0	-0.368762	-0.489595	1.212034
13	7	0	-0.312477	-0.814371	-0.870313
14	8	0	-2.174098	-0.275082	0.283587
15	6	0	-2.601044	-0.628364	-1.048531
16	6	0	-1.324618	-0.530768	-1.887020
17	1	0	-1.287382	-1.287928	-2.671477
18	1	0	-1.204057	0.466377	-2.333891
19	1	0	-3.372301	0.075125	-1.357606
20	6	0	-3.182299	-2.039914	-1.035471
21	1	0	-3.724569	-2.197841	-1.976777
22	6	0	-4.145005	-2.317601	0.123083
23	1	0	-3.624762	-2.105723	1.065220
24	6	0	-5.434217	-1.499596	0.075729
25	1	0	-5.942770	-1.702997	-0.871638
26	6	0	-6.353766	-1.878764	1.225267
27	1	0	-7.306243	-1.351766	1.101997
28	1	0	-6.515772	-2.959492	1.227829
29	8	0	-2.162045	-3.032923	-0.987817
30	1	0	-1.359594	-2.622178	-0.632372
31	8	0	-4.528840	-3.678873	0.058672
32	1	0	-3.715782	-4.169436	-0.106992
33	8	0	-5.171873	-0.109100	0.120508
34	1	0	-4.866228	0.072436	1.017800
35	8	0	-5.688344	-1.443950	2.406083
36	1	0	-6.252371	-1.610685	3.162346
37	6	0	1.067401	-0.641808	-1.303594
38	1	0	1.156266	-1.136546	-2.275247
39	1	0	1.312110	0.419371	-1.468311
40	6	0	2.065500	-1.279432	-0.342478
41	1	0	1.919170	-0.898704	0.674238
42	1	0	1.868081	-2.354982	-0.296629
43	7	0	0.453564	5.566545	0.055234
44	8	0	1.559700	5.908062	0.410758
45	8	0	-0.406161	6.311341	-0.358601
46	6	0	3.508104	-1.024909	-0.771844
47	1	0	3.656932	-1.410776	-1.787526
48	1	0	3.687372	0.056105	-0.824385
49	6	0	4.532841	-1.660172	0.164603
50	1	0	4.399979	-1.255568	1.175444
51	1	0	4.341241	-2.737281	0.236128
52	6	0	5.973465	-1.431311	-0.286076
53	1	0	6.110191	-1.855170	-1.288276
54	1	0	6.158318	-0.354320	-0.379601
55	6	0	7.003107	-2.038912	0.663086
56	1	0	6.812491	-3.114065	0.766766
57	1	0	6.874860	-1.606204	1.662869
58	6	0	8.443394	-1.825016	0.202883
59	1	0	8.571298	-2.263781	-0.792618
60	1	0	8.630030	-0.751313	0.092816
61	6	0	9.462524	-2.428690	1.165849
62	1	0	10.485461	-2.270120	0.819679

63	1	0	9.370726	-1.981519	2.159075
64	1	0	9.306860	-3.505498	1.271327

Structure 34a (M06-2X, Benzene)

Energy (Hartrees): = - 1456.4860408
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.514424	1.493322	0.235970
2	6	0	-1.451992	2.406064	-0.248780
3	6	0	-1.158454	3.761741	-0.301369
4	6	0	0.081697	4.186811	0.148606
5	6	0	1.030141	3.310713	0.654260
6	6	0	0.718460	1.960047	0.697004
7	1	0	-2.428250	2.056720	-0.561542
8	1	0	-1.874247	4.482539	-0.672319
9	1	0	1.978964	3.687752	1.010440
10	1	0	1.442728	1.263724	1.104927
11	6	0	-0.817089	-0.001126	0.258161
12	1	0	-0.401752	-0.439739	1.169539
13	7	0	-0.334699	-0.745168	-0.914658
14	8	0	-2.208600	-0.222881	0.232111
15	6	0	-2.619080	-0.618398	-1.093937
16	6	0	-1.348918	-0.470060	-1.932128
17	1	0	-1.288376	-1.210465	-2.730866
18	1	0	-1.256075	0.536664	-2.362220
19	1	0	-3.422682	0.043876	-1.409933
20	6	0	-3.131903	-2.058829	-1.067118
21	1	0	-3.688975	-2.240724	-1.995275
22	6	0	-4.045901	-2.387093	0.118112
23	1	0	-3.503871	-2.155479	1.042991
24	6	0	-5.376932	-1.637519	0.124371
25	1	0	-5.920968	-1.880417	-0.793530
26	6	0	-6.220999	-2.042849	1.321105
27	1	0	-7.195275	-1.547482	1.245548
28	1	0	-6.356524	-3.127754	1.333461
29	8	0	-2.064621	-3.004941	-1.040629
30	1	0	-1.267859	-2.544370	-0.730595
31	8	0	-4.360667	-3.768488	0.062276
32	1	0	-3.525110	-4.212185	-0.124228
33	8	0	-5.184585	-0.233910	0.136177
34	1	0	-4.786232	-0.027411	0.990939
35	8	0	-5.515330	-1.589608	2.471255
36	1	0	-6.065315	-1.730431	3.244640
37	6	0	1.050192	-0.571031	-1.334912
38	1	0	1.144399	-1.052258	-2.312721
39	1	0	1.300234	0.491252	-1.479855
40	6	0	2.033953	-1.227933	-0.371625
41	1	0	1.889946	-0.844162	0.644298
42	1	0	1.816817	-2.300187	-0.329366
43	7	0	0.398313	5.627313	0.105371
44	8	0	1.489493	5.976329	0.501504
45	8	0	-0.450480	6.377246	-0.325305
46	6	0	3.482841	-1.002467	-0.796770
47	1	0	3.630281	-1.406182	-1.805771
48	1	0	3.680158	0.074545	-0.862882
49	6	0	4.492467	-1.640133	0.155091
50	1	0	4.367427	-1.210071	1.156494
51	1	0	4.277339	-2.711135	0.249051
52	6	0	5.938591	-1.453695	-0.298664
53	1	0	6.068700	-1.913204	-1.286078
54	1	0	6.143489	-0.383767	-0.426420
55	6	0	6.956102	-2.048490	0.672226
56	1	0	6.740006	-3.113885	0.818711
57	1	0	6.841815	-1.572574	1.654087
58	6	0	8.400173	-1.889923	0.200670
59	1	0	8.516058	-2.379946	-0.772365
60	1	0	8.611596	-0.827226	0.038832
61	6	0	9.408656	-2.468255	1.189128
62	1	0	10.433871	-2.354252	0.830116
63	1	0	9.336356	-1.967621	2.158703
64	1	0	9.228876	-3.534511	1.352672

Structure 34a (M06-2X, DMSO)

Energy (Hartrees): = - 1456.4871681
No imaginary frequencies

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.459692	1.503537	0.284631
2	6	0	-1.358721	2.416827	-0.268802
3	6	0	-1.043388	3.766602	-0.336418
4	6	0	0.180617	4.183394	0.164758
5	6	0	1.092142	3.306117	0.734268
6	6	0	0.758194	1.961066	0.792942
7	1	0	-2.319711	2.076678	-0.634800
8	1	0	-1.732808	4.483868	-0.760618
9	1	0	2.032089	3.671418	1.125305
10	1	0	1.452235	1.261836	1.246431
11	6	0	-0.783686	0.015502	0.326458
12	1	0	-0.368911	-0.416492	1.240519
13	7	0	-0.313172	-0.746972	-0.839732
14	8	0	-2.181360	-0.187297	0.307663
15	6	0	-2.598449	-0.613171	-1.006973
16	6	0	-1.333813	-0.483495	-1.855272
17	1	0	-1.279157	-1.233596	-2.645730
18	1	0	-1.240168	0.515448	-2.301395
19	1	0	-3.403576	0.037003	-1.341461
20	6	0	-3.101464	-2.053920	-0.939629
21	1	0	-3.570447	-2.292734	-1.903983
22	6	0	-4.119949	-2.318286	0.176374
23	1	0	-3.709716	-1.933211	1.117707
24	6	0	-5.493695	-1.693807	-0.063916
25	1	0	-5.889591	-2.075763	-1.009423
26	6	0	-6.462148	-2.039628	1.054079
27	1	0	-7.452005	-1.650453	0.794524
28	1	0	-6.519469	-3.122957	1.187194
29	8	0	-2.027627	-2.973586	-0.740781
30	1	0	-1.219100	-2.457389	-0.570841
31	8	0	-4.324251	-3.721056	0.266405
32	1	0	-3.442023	-4.104956	0.191167
33	8	0	-5.408731	-0.282207	-0.182387
34	1	0	-5.246664	0.041082	0.713190
35	8	0	-5.962764	-1.397246	2.225073
36	1	0	-6.655531	-1.403366	2.891516
37	6	0	1.068883	-0.570601	-1.273425
38	1	0	1.154315	-1.049847	-2.252745
39	1	0	1.312992	0.492807	-1.417726
40	6	0	2.060896	-1.224334	-0.317971
41	1	0	1.910151	-0.854568	0.701739
42	1	0	1.863453	-2.301565	-0.294966
43	7	0	0.519428	5.615075	0.103046
44	8	0	1.605421	5.960892	0.520210
45	8	0	-0.304668	6.374273	-0.363163
46	6	0	3.504555	-0.968219	-0.741668
47	1	0	3.640576	-1.296926	-1.779385
48	1	0	3.700364	0.111002	-0.727856
49	6	0	4.521609	-1.678011	0.148322
50	1	0	4.392538	-1.343084	1.184838
51	1	0	4.317703	-2.755645	0.140802
52	6	0	5.965269	-1.436041	-0.285483
53	1	0	6.089508	-1.767770	-1.323727
54	1	0	6.171298	-0.358642	-0.276062
55	6	0	6.985324	-2.152317	0.595964
56	1	0	6.773845	-3.228869	0.593495
57	1	0	6.869540	-1.814899	1.633462
58	6	0	8.428301	-1.924308	0.151658
59	1	0	8.542668	-2.264595	-0.883565
60	1	0	8.639406	-0.849090	0.151448
61	6	0	9.437357	-2.644505	1.041038
62	1	0	10.462398	-2.480915	0.699713
63	1	0	9.368776	-2.292200	2.074339
64	1	0	9.254234	-3.722917	1.043928

Structure 34b (M06-2X, Gas Phase)

Energy (Hartrees): = - 1456.461326
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.156914	1.380958	-0.931026
2	6	0	-1.675892	1.529717	0.356014
3	6	0	-1.879002	2.794898	0.882544
4	6	0	-1.554596	3.895890	0.101170
5	6	0	-1.042262	3.779807	-1.179132
6	6	0	-0.849041	2.502962	-1.693145
7	1	0	-1.920875	0.648085	0.937049
8	1	0	-2.282204	2.945164	1.874440
9	1	0	-0.810324	4.670531	-1.746188

10	1	0	-0.456979	2.381213	-2.697008
11	6	0	-0.917204	-0.003660	-1.479532
12	1	0	-0.712880	0.058266	-2.565008
13	7	0	0.183869	-0.687373	-0.797640
14	8	0	-2.035467	-0.829142	-1.257190
15	6	0	-1.592095	-2.151527	-0.909293
16	6	0	-0.077494	-2.092036	-1.119392
17	1	0	0.463812	-2.758618	-0.446535
18	1	0	0.192709	-2.324025	-2.161524
19	1	0	-2.086174	-2.863205	-1.566758
20	6	0	-1.964188	-2.456898	0.540644
21	1	0	-1.788262	-3.527493	0.717532
22	6	0	-3.419984	-2.145380	0.903012
23	1	0	-3.631287	-1.101972	0.635318
24	6	0	-4.444918	-3.045127	0.215005
25	1	0	-4.225767	-4.085502	0.473737
26	6	0	-5.852717	-2.703068	0.675252
27	1	0	-6.550376	-3.432439	0.249222
28	1	0	-5.900655	-2.725296	1.766624
29	8	0	-1.160666	-1.728877	1.468283
30	1	0	-0.554828	-1.148671	0.978409
31	8	0	-3.583471	-2.347426	2.295128
32	1	0	-2.814892	-1.943000	2.712524
33	8	0	-4.369211	-2.937221	-1.193613
34	1	0	-4.735669	-2.071745	-1.413165
35	8	0	-6.113880	-1.401197	0.162367
36	1	0	-6.995035	-1.130708	0.423837
37	6	0	1.502721	-0.195043	-1.176607
38	1	0	1.664476	-0.327035	-2.261488
39	1	0	1.525946	0.879732	-0.970045
40	6	0	2.619353	-0.881029	-0.400038
41	1	0	2.383444	-0.833784	0.668523
42	1	0	2.664733	-1.941549	-0.670629
43	7	0	-1.766699	5.249680	0.658014
44	8	0	-1.477286	6.193268	-0.043601
45	8	0	-2.214181	5.327441	1.779964
46	6	0	3.979459	-0.238778	-0.662828
47	1	0	3.945569	0.816518	-0.367464
48	1	0	4.190575	-0.253204	-1.738905
49	6	0	5.115632	-0.934370	0.083238
50	1	0	5.160803	-1.986274	-0.223499
51	1	0	4.895185	-0.935328	1.157290
52	6	0	6.474754	-0.280069	-0.152535
53	1	0	6.429706	0.770779	0.157993
54	1	0	6.694132	-0.275014	-1.227096
55	6	0	7.611081	-0.977173	0.591510
56	1	0	7.389199	-0.987169	1.665589
57	1	0	7.660417	-2.027180	0.278030
58	6	0	8.970807	-0.319685	0.365277
59	1	0	9.190750	-0.308413	-0.707688
60	1	0	8.920197	0.727900	0.681165
61	6	0	10.095978	-1.029459	1.114147
62	1	0	10.179842	-2.070836	0.792673
63	1	0	11.060215	-0.547232	0.943348
64	1	0	9.906745	-1.028993	2.190672

Structure 34b (M06-2X, Benzene)

Energy (Hartrees): = - 1456.4905281
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.149375	1.383955	-0.941199
2	6	0	-1.653542	1.535195	0.351544
3	6	0	-1.839827	2.800326	0.884055
4	6	0	-1.511089	3.900553	0.102471
5	6	0	-1.012129	3.782157	-1.183623
6	6	0	-0.835903	2.505296	-1.702656
7	1	0	-1.903147	0.656508	0.935045
8	1	0	-2.232864	2.944899	1.880938
9	1	0	-0.775171	4.668311	-1.755903
10	1	0	-0.453076	2.383572	-2.709913
11	6	0	-0.926255	-0.000498	-1.498625
12	1	0	-0.731373	0.065814	-2.584522
13	7	0	0.171174	-0.700058	-0.827902
14	8	0	-2.053026	-0.816692	-1.270048
15	6	0	-1.618043	-2.146148	-0.934002
16	6	0	-0.106497	-2.099445	-1.163389
17	1	0	0.438503	-2.779300	-0.507393
18	1	0	0.145819	-2.320883	-2.211672
19	1	0	-2.124650	-2.850651	-1.589525
20	6	0	-1.975136	-2.456754	0.519091

21	1	0	-1.810598	-3.530577	0.685591
22	6	0	-3.421419	-2.126231	0.905659
23	1	0	-3.626081	-1.082815	0.633678
24	6	0	-4.469407	-3.021778	0.247080
25	1	0	-4.253105	-4.062939	0.505510
26	6	0	-5.866506	-2.670065	0.730479
27	1	0	-6.575571	-3.394366	0.314646
28	1	0	-5.905306	-2.697476	1.822402
29	8	0	-1.145309	-1.745087	1.438113
30	1	0	-0.548753	-1.163191	0.936089
31	8	0	-3.558976	-2.310723	2.304836
32	1	0	-2.775363	-1.909797	2.697899
33	8	0	-4.422767	-2.920676	-1.164955
34	1	0	-4.786612	-2.052116	-1.377752
35	8	0	-6.131784	-1.363856	0.229254
36	1	0	-7.043352	-1.136199	0.424511
37	6	0	1.494962	-0.217255	-1.207688
38	1	0	1.653145	-0.347039	-2.292515
39	1	0	1.527956	0.856261	-0.996429
40	6	0	2.607347	-0.913931	-0.433753
41	1	0	2.367370	-0.878041	0.634588
42	1	0	2.654862	-1.971103	-0.716826
43	7	0	-1.708449	5.252834	0.661564
44	8	0	-1.416788	6.198997	-0.037720
45	8	0	-2.149655	5.337937	1.786796
46	6	0	3.967901	-0.265821	-0.681116
47	1	0	3.928345	0.786088	-0.374287
48	1	0	4.186008	-0.268944	-1.755949
49	6	0	5.101090	-0.965558	0.065990
50	1	0	5.153398	-2.013608	-0.252857
51	1	0	4.871503	-0.978980	1.138185
52	6	0	6.459705	-0.302675	-0.149756
53	1	0	6.405646	0.745243	0.169511
54	1	0	6.690607	-0.288281	-1.221951
55	6	0	7.591761	-0.999886	0.601236
56	1	0	7.358054	-1.018445	1.672836
57	1	0	7.649859	-2.047209	0.279985
58	6	0	8.951351	-0.334869	0.396217
59	1	0	9.186785	-0.317971	-0.673667
60	1	0	8.892656	0.710859	0.717656
61	6	0	10.069774	-1.042085	1.155981
62	1	0	10.165762	-2.081961	0.831357
63	1	0	11.034318	-0.553627	0.999915
64	1	0	9.869212	-1.047556	2.230988

Structure 34b (M06-2X, DMSO)

Energy (Hartrees): = - 1456.4913047
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.173408	1.375158	-0.936915
2	6	0	-1.730647	1.503281	0.337082
3	6	0	-1.976802	2.758481	0.868821
4	6	0	-1.655802	3.872543	0.102959
5	6	0	-1.100420	3.777745	-1.162683
6	6	0	-0.863153	2.510166	-1.680405
7	1	0	-1.974646	0.616523	0.910784
8	1	0	-2.409949	2.879651	1.852340
9	1	0	-0.864737	4.670319	-1.725919
10	1	0	-0.434979	2.404519	-2.671157
11	6	0	-0.896399	0.001594	-1.497620
12	1	0	-0.681341	0.078727	-2.576785
13	7	0	0.205639	-0.670470	-0.806366
14	8	0	-2.008860	-0.847695	-1.294442
15	6	0	-1.540852	-2.163164	-0.942486
16	6	0	-0.031125	-2.076040	-1.157686
17	1	0	0.526561	-2.748555	-0.505316
18	1	0	0.234911	-2.276041	-2.205708
19	1	0	-2.017172	-2.887424	-1.598507
20	6	0	-1.902621	-2.477453	0.509049
21	1	0	-1.721343	-3.548037	0.674855
22	6	0	-3.356571	-2.167969	0.885373
23	1	0	-3.580174	-1.134144	0.593089
24	6	0	-4.385976	-3.095812	0.242673
25	1	0	-4.145661	-4.128788	0.511459
26	6	0	-5.790734	-2.771604	0.720839
27	1	0	-6.484707	-3.506329	0.299614
28	1	0	-5.838556	-2.808689	1.812117
29	8	0	-1.087457	-1.751078	1.432464
30	1	0	-0.509489	-1.151398	0.925824
31	8	0	-3.493715	-2.319929	2.290890

32	1	0	-2.710725	-1.900528	2.667086
33	8	0	-4.343202	-3.010229	-1.172645
34	1	0	-4.713212	-2.145516	-1.391285
35	8	0	-6.084076	-1.465820	0.230346
36	1	0	-7.022717	-1.299059	0.354629
37	6	0	1.523104	-0.158307	-1.178947
38	1	0	1.683825	-0.281575	-2.262756
39	1	0	1.537074	0.914689	-0.962479
40	6	0	2.641849	-0.842913	-0.404947
41	1	0	2.403568	-0.810741	0.664362
42	1	0	2.699234	-1.898732	-0.690622
43	7	0	-1.918717	5.211540	0.659137
44	8	0	-1.682071	6.173654	-0.041508
45	8	0	-2.358522	5.281290	1.787992
46	6	0	3.995055	-0.180705	-0.652649
47	1	0	3.950411	0.865984	-0.328857
48	1	0	4.203756	-0.167992	-1.729225
49	6	0	5.137253	-0.886296	0.074279
50	1	0	5.200107	-1.924429	-0.273968
51	1	0	4.910213	-0.929461	1.146560
52	6	0	6.488168	-0.203494	-0.125728
53	1	0	6.427705	0.830058	0.236676
54	1	0	6.710022	-0.146058	-1.198536
55	6	0	7.631402	-0.921179	0.587524
56	1	0	7.403581	-0.990704	1.658550
57	1	0	7.700075	-1.951289	0.216373
58	6	0	8.982145	-0.232052	0.407233
59	1	0	9.209525	-0.160256	-0.662256
60	1	0	8.914282	0.795321	0.781989
61	6	0	10.112703	-0.964953	1.123289
62	1	0	10.211843	-1.988108	0.749262
63	1	0	11.072708	-0.462907	0.980352
64	1	0	9.921779	-1.020233	2.198941

Structure 34c (M06-2X, Gas Phase)

Energy (Hartrees): = - 1456.4582016
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.143463	-2.155090	-0.123741
2	6	0	-0.810293	-2.045006	0.607442
3	6	0	-3.046412	-1.030889	0.386062
4	1	0	-0.131566	-2.806786	0.223777
5	1	0	-0.950775	-2.215223	1.689390
6	1	0	-2.615875	-3.117784	0.063228
7	1	0	-3.217700	-1.143204	1.467944
8	8	0	-2.368116	0.209475	0.157356
9	7	0	-0.225484	-0.723007	0.355813
10	6	0	-4.388810	-0.895665	-0.331560
11	1	0	-4.213733	-1.043646	-1.404801
12	6	0	-5.411738	-1.906545	0.161745
13	1	0	-5.594251	-1.717730	1.229707
14	6	0	-6.729257	-1.755808	-0.576881
15	1	0	-6.543895	-1.858507	-1.653403
16	1	0	-7.165323	-0.775960	-0.368894
17	8	0	-4.956937	0.373657	-0.073438
18	1	0	-4.241320	1.013933	-0.142021
19	8	0	-4.903618	-3.210232	-0.032892
20	1	0	-5.661975	-3.799497	0.050243
21	8	0	-7.549795	-2.817549	-0.101131
22	1	0	-8.344008	-2.863201	-0.635809
23	8	0	-1.938136	-2.046947	-1.515681
24	1	0	-1.356035	-1.287357	-1.633729
25	6	0	1.118543	-0.621910	0.933513
26	1	0	1.140570	-1.070751	1.941666
27	1	0	1.371225	0.434013	1.053516
28	6	0	-0.612396	1.700973	0.524575
29	6	0	-0.292647	2.022301	-0.795138
30	6	0	-0.481028	2.657457	1.525393
31	6	0	0.162311	3.290638	-1.115953
32	1	0	-0.402380	1.266031	-1.562345
33	6	0	-0.022486	3.934356	1.222896
34	1	0	-0.735399	2.406002	2.548887
35	6	0	0.289955	4.221908	-0.094244
36	1	0	0.417560	3.571358	-2.128464
37	1	0	0.095507	4.698094	1.979099
38	6	0	-1.133782	0.316307	0.831650
39	1	0	-1.314250	0.212947	1.920903
40	6	0	2.182434	-1.264068	0.049939
41	1	0	1.937968	-2.312182	-0.148364

42	1	0	2.179136	-0.751294	-0.917445
43	7	0	0.781338	5.576905	-0.426351
44	8	0	1.022986	5.812234	-1.588853
45	8	0	0.911053	6.362137	0.485882
46	6	0	3.569409	-1.182572	0.683200
47	1	0	3.804349	-0.136321	0.914153
48	1	0	3.564728	-1.716734	1.640984
49	6	0	4.667544	-1.757436	-0.208152
50	1	0	4.682439	-1.213353	-1.159924
51	1	0	4.429779	-2.799894	-0.451971
52	6	0	6.051079	-1.691150	0.433882
53	1	0	6.282559	-0.649721	0.688643
54	1	0	6.037981	-2.244564	1.380678
55	6	0	7.155856	-2.247916	-0.460453
56	1	0	7.171693	-1.692548	-1.406114
57	1	0	6.925004	-3.288783	-0.718601
58	6	0	8.538956	-2.183668	0.183607
59	1	0	8.766562	-1.143808	0.442249
60	1	0	8.522349	-2.740062	1.126960
61	6	0	9.634481	-2.739812	-0.722503
62	1	0	9.682349	-2.181813	-1.661194
63	1	0	10.616034	-2.682482	-0.248274
64	1	0	9.440686	-3.787107	-0.968521

Structure 34c (M06-2X, Benzene)

Energy (Hartrees): = - 1456.4878174
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.172146	-2.151758	0.078671
2	6	0	0.848487	-2.051782	-0.670543
3	6	0	3.067907	-1.010124	-0.405196
4	1	0	0.175361	-2.829845	-0.309750
5	1	0	1.008162	-2.202902	-1.751923
6	1	0	2.658289	-3.106753	-0.111545
7	1	0	3.257950	-1.111529	-1.484660
8	8	0	2.368350	0.218229	-0.174804
9	7	0	0.242066	-0.742513	-0.404611
10	6	0	4.395123	-0.857783	0.339010
11	1	0	4.202486	-1.013920	1.407880
12	6	0	5.451521	-1.842960	-0.136900
13	1	0	5.663612	-1.634937	-1.195690
14	6	0	6.740979	-1.682929	0.647154
15	1	0	6.525613	-1.811143	1.715210
16	1	0	7.168173	-0.691707	0.476187
17	8	0	4.941608	0.427295	0.103284
18	1	0	4.207698	1.048591	0.159471
19	8	0	4.962149	-3.160335	0.021160
20	1	0	5.736255	-3.732335	-0.040877
21	8	0	7.602614	-2.715981	0.178783
22	1	0	8.362694	-2.771583	0.762488
23	8	0	1.942674	-2.059961	1.470301
24	1	0	1.340431	-1.314065	1.581437
25	6	0	-1.103967	-0.656251	-0.983189
26	1	0	-1.121720	-1.111821	-1.987530
27	1	0	-1.366522	0.396382	-1.109330
28	6	0	0.595168	1.689914	-0.541703
29	6	0	0.285110	2.000332	0.783323
30	6	0	0.430515	2.646036	-1.538645
31	6	0	-0.188401	3.259170	1.114387
32	1	0	0.415690	1.246540	1.550076
33	6	0	-0.048151	3.912676	-1.226073
34	1	0	0.674397	2.403801	-2.566867
35	6	0	-0.346278	4.191368	0.097055
36	1	0	-0.433907	3.526003	2.133174
37	1	0	-0.189035	4.671796	-1.983158
38	6	0	1.137972	0.315837	-0.862002
39	1	0	1.330963	0.228617	-1.949049
40	6	0	-2.159661	-1.302239	-0.092092
41	1	0	-1.911664	-2.350788	0.100673
42	1	0	-2.148285	-0.790846	0.876359
43	7	0	-0.854730	5.534471	0.439430
44	8	0	-1.050189	5.780201	1.609775
45	8	0	-1.047932	6.311418	-0.470295
46	6	0	-3.553532	-1.219190	-0.710625
47	1	0	-3.788257	-0.172255	-0.938913
48	1	0	-3.560663	-1.754664	-1.667713
49	6	0	-4.643048	-1.790295	0.194284
50	1	0	-4.640333	-1.248657	1.147734
51	1	0	-4.408800	-2.835318	0.430875
52	6	0	-6.036358	-1.711930	-0.426131

53	1	0	-6.263178	-0.667753	-0.674218
54	1	0	-6.042547	-2.263627	-1.374101
55	6	0	-7.131707	-2.261416	0.484857
56	1	0	-7.124637	-1.710157	1.433156
57	1	0	-6.907654	-3.306176	0.733560
58	6	0	-8.526618	-2.179440	-0.132049
59	1	0	-8.748752	-1.136185	-0.382610
60	1	0	-8.536464	-2.734097	-1.076720
61	6	0	-9.610157	-2.725323	0.793262
62	1	0	-9.637322	-2.168587	1.734218
63	1	0	-10.600477	-2.656295	0.337437
64	1	0	-9.425397	-3.775904	1.034208

Structure 34c (M06-2X, DMSO)

Energy (Hartrees): = - 1456.4893731
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.167122	-2.140158	0.102418
2	6	0	0.837772	-2.048655	-0.635861
3	6	0	3.059427	-1.014802	-0.417280
4	1	0	0.163407	-2.820018	-0.262578
5	1	0	0.992559	-2.211191	-1.715093
6	1	0	2.642969	-3.102837	-0.074975
7	1	0	3.221264	-1.137941	-1.498272
8	8	0	2.373244	0.222451	-0.189976
9	7	0	0.236595	-0.733627	-0.381550
10	6	0	4.406911	-0.850815	0.281590
11	1	0	4.244427	-0.913490	1.365057
12	6	0	5.423735	-1.905032	-0.128709
13	1	0	5.538039	-1.878592	-1.222296
14	6	0	6.778019	-1.633688	0.503931
15	1	0	6.656567	-1.557209	1.591289
16	1	0	7.199771	-0.702677	0.118999
17	8	0	4.974361	0.400775	-0.072572
18	1	0	4.248036	1.034493	-0.060272
19	8	0	4.960232	-3.177190	0.287586
20	1	0	5.738633	-3.747827	0.268229
21	8	0	7.592211	-2.753306	0.164647
22	1	0	8.376452	-2.738278	0.721280
23	8	0	1.955274	-2.017269	1.497956
24	1	0	1.367545	-1.256948	1.597291
25	6	0	-1.106344	-0.652233	-0.972292
26	1	0	-1.115142	-1.124608	-1.967927
27	1	0	-1.365188	0.398747	-1.119235
28	6	0	0.593929	1.692315	-0.535082
29	6	0	0.295421	2.000649	0.793654
30	6	0	0.420441	2.648376	-1.530899
31	6	0	-0.177006	3.258566	1.130286
32	1	0	0.431616	1.248655	1.561899
33	6	0	-0.056808	3.914241	-1.212909
34	1	0	0.653256	2.404701	-2.561351
35	6	0	-0.344768	4.190924	0.113793
36	1	0	-0.414293	3.517368	2.153302
37	1	0	-0.202822	4.669225	-1.973334
38	6	0	1.130483	0.317644	-0.862400
39	1	0	1.304894	0.223829	-1.949832
40	6	0	-2.169442	-1.282294	-0.079504
41	1	0	-1.921764	-2.327511	0.132501
42	1	0	-2.172329	-0.752243	0.879538
43	7	0	-0.853543	5.529384	0.460810
44	8	0	-1.047389	5.776469	1.632987
45	8	0	-1.053339	6.313204	-0.443745
46	6	0	-3.556463	-1.212340	-0.713608
47	1	0	-3.792791	-0.168499	-0.954471
48	1	0	-3.549495	-1.758980	-1.664314
49	6	0	-4.650765	-1.780327	0.186982
50	1	0	-4.656195	-1.232090	1.136959
51	1	0	-4.415350	-2.823842	0.429945
52	6	0	-6.040220	-1.709692	-0.442031
53	1	0	-6.271107	-0.666540	-0.691377
54	1	0	-6.037763	-2.263734	-1.388798
55	6	0	-7.136322	-2.264619	0.464363
56	1	0	-7.135398	-1.712824	1.412644
57	1	0	-6.908598	-3.309032	0.711944
58	6	0	-8.529475	-2.188690	-0.156335
59	1	0	-8.756911	-1.145561	-0.403262
60	1	0	-8.533756	-2.741757	-1.102184
61	6	0	-9.610409	-2.744332	0.766072
62	1	0	-9.639173	-2.191306	1.709515
63	1	0	-10.601634	-2.677682	0.310988

64	1	0	-9.419281	-3.795385	1.001222

Structure 34d (M06-2X, Gas Phase)

Energy (Hartrees): = - 1456.460099
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.432111	-1.942932	-1.271247
2	6	0	0.515092	-0.858944	-1.847810
3	6	0	2.134535	-1.342524	-0.054081
4	1	0	-0.053667	-1.257843	-2.688202
5	1	0	1.129189	-0.030070	-2.219696
6	1	0	2.172853	-2.256931	-2.005339
7	1	0	2.712649	-0.462387	-0.364559
8	8	0	1.112450	-0.939633	0.874219
9	7	0	-0.425089	-0.331100	-0.854186
10	6	0	3.050618	-2.280737	0.733284
11	1	0	2.576613	-3.268936	0.798235
12	6	0	4.417022	-2.428542	0.083767
13	1	0	4.892712	-1.437413	0.047968
14	6	0	5.312027	-3.354397	0.888041
15	1	0	4.807266	-4.321721	1.004723
16	1	0	5.510658	-2.920973	1.871193
17	8	0	3.292462	-1.745774	2.022747
18	1	0	2.434757	-1.480740	2.370827
19	8	0	4.242981	-2.943890	-1.219017
20	1	0	5.114095	-3.248380	-1.497918
21	8	0	6.498277	-3.492316	0.114994
22	1	0	7.048155	-4.174246	0.503871
23	8	0	0.692870	-3.095115	-0.906990
24	1	0	0.243102	-2.890715	-0.080556
25	6	0	-1.634972	-1.125184	-0.608835
26	1	0	-1.536469	-1.741173	0.299291
27	1	0	-1.768011	-1.824195	-1.437160
28	6	0	0.978412	1.403056	0.201704
29	6	0	0.468975	2.375363	-0.657799
30	6	0	2.099089	1.688253	0.983970
31	6	0	1.066144	3.625544	-0.740626
32	1	0	-0.397655	2.134483	-1.261385
33	6	0	2.708713	2.932239	0.910133
34	1	0	2.507963	0.924053	1.634992
35	6	0	2.175813	3.878933	0.048938
36	1	0	0.691878	4.396775	-1.399471
37	1	0	3.580593	3.178319	1.500461
38	6	0	0.245409	0.073602	0.351680
39	1	0	-0.509768	0.203357	1.131798
40	6	0	-2.863669	-0.230806	-0.483462
41	1	0	-2.692537	0.520374	0.297776
42	1	0	-2.982015	0.321217	-1.421734
43	7	0	2.817721	5.207835	-0.031014
44	8	0	2.342584	6.011610	-0.802030
45	8	0	3.776782	5.408512	0.680420
46	6	0	-4.134924	-1.015273	-0.170527
47	1	0	-4.280510	-1.791209	-0.931868
48	1	0	-4.016097	-1.539874	0.785287
49	6	0	-5.377940	-0.130481	-0.110251
50	1	0	-5.499199	0.386530	-1.069619
51	1	0	-5.230988	0.651168	0.644742
52	6	0	-6.653265	-0.907126	0.208240
53	1	0	-6.795212	-1.694374	-0.541946
54	1	0	-6.536389	-1.416875	1.172273
55	6	0	-7.896555	-0.022191	0.252302
56	1	0	-8.015366	0.484934	-0.713029
57	1	0	-7.753805	0.768001	0.999453
58	6	0	-9.174128	-0.794399	0.574765
59	1	0	-9.314304	-1.584282	-0.170984
60	1	0	-9.055123	-1.298140	1.540128
61	6	0	-10.407668	0.104409	0.611520
62	1	0	-10.561552	0.592313	-0.354458
63	1	0	-11.310670	-0.460806	0.849516
64	1	0	-10.293845	0.888295	1.364804

Structure 34d (M06-2X, Benzene)

Energy (Hartrees): = - 1456.488815
No imaginary frequencies

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-1.428190	-1.947254	1.258750
2	6	0	-0.498153	-0.870343	1.826116
3	6	0	-2.142581	-1.341920	0.050918
4	1	0	0.079232	-1.273069	2.658908
5	1	0	-1.106592	-0.042109	2.208296
6	1	0	-2.160449	-2.255734	2.003716
7	1	0	-2.713546	-0.460847	0.371677
8	8	0	-1.130592	-0.940586	-0.888699
9	7	0	0.431371	-0.344018	0.822208
10	6	0	-3.073387	-2.275041	-0.727085
11	1	0	-2.605430	-3.264909	-0.804616
12	6	0	-4.431617	-2.420026	-0.058546
13	1	0	-4.890664	-1.423304	0.015880
14	6	0	-5.358735	-3.308754	-0.867689
15	1	0	-4.880161	-4.284525	-1.017888
16	1	0	-5.569791	-2.851513	-1.837453
17	8	0	-3.327839	-1.734392	-2.012947
18	1	0	-2.473296	-1.459567	-2.363130
19	8	0	-4.243010	-2.975604	1.227477
20	1	0	-5.115339	-3.273955	1.510868
21	8	0	-6.536845	-3.439879	-0.078844
22	1	0	-7.089612	-4.125661	-0.460228
23	8	0	-0.702577	-3.107077	0.884602
24	1	0	-0.247548	-2.900031	0.060984
25	6	0	1.640329	-1.138487	0.566612
26	1	0	1.538025	-1.746606	-0.345913
27	1	0	1.775334	-1.841621	1.390917
28	6	0	-0.972844	1.401226	-0.217298
29	6	0	-0.457772	2.367915	0.645658
30	6	0	-2.095962	1.695691	-0.993127
31	6	0	-1.051052	3.618942	0.738253
32	1	0	0.410705	2.126097	1.246085
33	6	0	-2.702865	2.940111	-0.910240
34	1	0	-2.510837	0.938599	-1.648320
35	6	0	-2.164757	3.880447	-0.044043
36	1	0	-0.666635	4.380573	1.402544
37	1	0	-3.577104	3.184722	-1.498128
38	6	0	-0.249087	0.066656	-0.375486
39	1	0	0.497507	0.192985	-1.164071
40	6	0	2.870117	-0.244871	0.445871
41	1	0	2.702534	0.503234	-0.339014
42	1	0	2.983640	0.307943	1.384604
43	7	0	-2.804057	5.206642	0.051433
44	8	0	-2.326039	6.007689	0.825478
45	8	0	-3.769734	5.418749	-0.649661
46	6	0	4.144046	-1.030109	0.144503
47	1	0	4.284183	-1.801824	0.911205
48	1	0	4.032268	-1.558606	-0.809996
49	6	0	5.386433	-0.143464	0.089983
50	1	0	5.495258	0.382080	1.046336
51	1	0	5.245980	0.630828	-0.673905
52	6	0	6.668813	-0.918082	-0.206229
53	1	0	6.805635	-1.696461	0.554215
54	1	0	6.565449	-1.437918	-1.166480
55	6	0	7.908299	-0.026843	-0.244562
56	1	0	8.010773	0.492232	0.716380
57	1	0	7.770867	0.753278	-1.003331
58	6	0	9.196386	-0.792822	-0.539800
59	1	0	9.333180	-1.572625	0.217384
60	1	0	9.097018	-1.307870	-1.501603
61	6	0	10.423455	0.113971	-0.568482
62	1	0	10.561268	0.615694	0.393418
63	1	0	11.334510	-0.448773	-0.784333
64	1	0	10.320272	0.888022	-1.334202

Structure 34d (M06-2X, DMSO)

Energy (Hartrees): = - 1456.4893176
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.467524	-1.935488	1.283759
2	6	0	-0.533754	-0.869192	1.862798
3	6	0	-2.149802	-1.329157	0.059012
4	1	0	0.023382	-1.275885	2.707620
5	1	0	-1.144120	-0.035747	2.230639
6	1	0	-2.218438	-2.220271	2.019619
7	1	0	-2.721551	-0.444831	0.369367
8	8	0	-1.117860	-0.936870	-0.861228
9	7	0	0.419180	-0.352290	0.876302

10	6	0	-3.071273	-2.256520	-0.736076
11	1	0	-2.600880	-3.243925	-0.825518
12	6	0	-4.435597	-2.415876	-0.082796
13	1	0	-4.884473	-1.418701	0.033648
14	6	0	-5.364908	-3.263029	-0.932829
15	1	0	-4.896318	-4.237212	-1.118008
16	1	0	-5.566449	-2.769576	-1.886352
17	8	0	-3.313315	-1.700327	-2.019531
18	1	0	-2.456665	-1.401168	-2.346488
19	8	0	-4.265732	-3.030260	1.182084
20	1	0	-5.143894	-3.344037	1.431057
21	8	0	-6.553730	-3.413066	-0.161361
22	1	0	-7.082495	-4.115550	-0.550864
23	8	0	-0.756757	-3.115646	0.937727
24	1	0	-0.266514	-2.922546	0.129795
25	6	0	1.624127	-1.159887	0.638253
26	1	0	1.519320	-1.789960	-0.258344
27	1	0	1.758723	-1.836694	1.484622
28	6	0	-0.948774	1.404855	-0.189814
29	6	0	-0.438900	2.369149	0.679577
30	6	0	-2.053632	1.710954	-0.987405
31	6	0	-1.019326	3.626896	0.759458
32	1	0	0.416932	2.126176	1.297172
33	6	0	-2.649449	2.961312	-0.917709
34	1	0	-2.463197	0.961597	-1.654298
35	6	0	-2.116616	3.898215	-0.043598
36	1	0	-0.632510	4.381342	1.430757
37	1	0	-3.509347	3.208244	-1.525644
38	6	0	-0.235845	0.063271	-0.334311
39	1	0	0.524263	0.184254	-1.110129
40	6	0	2.854987	-0.271902	0.492097
41	1	0	2.677345	0.469444	-0.296731
42	1	0	2.988754	0.285765	1.425812
43	7	0	-2.741191	5.228778	0.035493
44	8	0	-2.244408	6.046208	0.782732
45	8	0	-3.719673	5.439678	-0.651045
46	6	0	4.120819	-1.062115	0.172871
47	1	0	4.267397	-1.837967	0.934401
48	1	0	3.993821	-1.582901	-0.783964
49	6	0	5.363672	-0.177284	0.108371
50	1	0	5.490369	0.334077	1.070475
51	1	0	5.210454	0.606978	-0.643101
52	6	0	6.639671	-0.947862	-0.221845
53	1	0	6.788788	-1.738226	0.524080
54	1	0	6.519730	-1.450206	-1.189666
55	6	0	7.877981	-0.055646	-0.265826
56	1	0	7.997788	0.444638	0.703294
57	1	0	7.726992	0.737516	-1.008623
58	6	0	9.160118	-0.815468	-0.598353
59	1	0	9.309965	-1.609444	0.141726
60	1	0	9.043470	-1.310756	-1.568814
61	6	0	10.386257	0.092110	-0.630729
62	1	0	10.541072	0.572627	0.339746
63	1	0	11.293016	-0.466206	-0.876047
64	1	0	10.267763	0.881976	-1.378246

Structure 38a (M06-2X, Gas Phase)

Energy (Hartrees): = - 1251.9733112
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.514659	2.108180	0.292776
2	6	0	-1.464488	3.010617	-0.183337
3	6	0	-1.187512	4.373219	-0.215439
4	6	0	0.037568	4.849824	0.237226
5	6	0	0.982354	3.958328	0.734540
6	6	0	0.703761	2.596981	0.764877
7	1	0	-2.433964	2.643814	-0.499821
8	1	0	-1.935179	5.065081	-0.585090
9	1	0	1.932227	4.323867	1.106657
10	1	0	1.439295	1.908604	1.169049
11	6	0	-0.785124	0.610335	0.285506
12	1	0	-0.366307	0.157440	1.188705
13	7	0	-0.279183	-0.106658	-0.899961
14	8	0	-2.170572	0.349831	0.247306
15	6	0	-2.565704	-0.024209	-1.086845
16	6	0	-1.295007	0.166451	-1.915811
17	1	0	-1.216958	-0.559094	-2.726872
18	1	0	-1.220225	1.184437	-2.322940
19	1	0	-3.383177	0.626864	-1.391446
20	6	0	-3.048879	-1.475424	-1.093476

21	1	0	-3.605499	-1.649302	-2.023669
22	6	0	-3.953751	-1.845155	0.085752
23	1	0	-3.416485	-1.619148	1.014786
24	6	0	-5.298443	-1.121183	0.104127
25	1	0	-5.838928	-1.369594	-0.814289
26	6	0	-6.127225	-1.559653	1.300723
27	1	0	-7.116779	-1.094623	1.229343
28	1	0	-6.220077	-2.649002	1.305573
29	8	0	-1.964667	-2.399981	-1.092829
30	1	0	-1.180953	-1.937097	-0.755698
31	8	0	-4.245270	-3.228847	0.003333
32	1	0	-3.405294	-3.654722	-0.202185
33	8	0	-5.139372	0.284664	0.126382
34	1	0	-4.734251	0.495433	0.976739
35	8	0	-5.431156	-1.086024	2.447757
36	1	0	-5.941752	-1.295842	3.230806
37	6	0	1.097282	0.127843	-1.314096
38	1	0	1.211537	-0.325202	-2.303581
39	1	0	1.308839	1.202058	-1.428867
40	6	0	2.101837	-0.518660	-0.365737
41	1	0	1.946504	-0.160680	0.657521
42	1	0	1.916903	-1.597459	-0.345093
43	6	0	3.543921	-0.240557	-0.781199
44	1	0	3.703995	-0.606062	-1.802798
45	1	0	3.712491	0.842868	-0.810832
46	6	0	4.566076	-0.885448	0.151723
47	1	0	4.427949	-0.492669	1.166457
48	1	0	4.374282	-1.963391	0.210139
49	6	0	6.009457	-0.653371	-0.288088
50	1	0	6.152217	-1.069330	-1.292779
51	1	0	6.195966	0.424187	-0.371528
52	6	0	7.031731	-1.270401	0.663118
53	1	0	6.834937	-2.345015	0.760839
54	1	0	6.900297	-0.841920	1.664324
55	6	0	8.475772	-1.062624	0.212112
56	1	0	8.607244	-1.499397	-0.783800
57	1	0	8.668730	0.010402	0.106092
58	6	0	9.485882	-1.674529	1.179492
59	1	0	10.511916	-1.521538	0.839879
60	1	0	9.390792	-1.229236	2.173285
61	1	0	9.322932	-2.750579	1.281658
62	1	0	0.250259	5.911911	0.215911

Structure 38a (M06-2X, Benzene)

Energy (Hartrees): = - 1252.0002689
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.514261	2.122087	0.289979
2	6	0	-1.446624	3.041545	-0.189689
3	6	0	-1.155652	4.401981	-0.197998
4	6	0	0.067137	4.859481	0.280990
5	6	0	0.995647	3.950683	0.778735
6	6	0	0.702671	2.591588	0.786352
7	1	0	-2.413763	2.690949	-0.531353
8	1	0	-1.890469	5.106477	-0.570376
9	1	0	1.944493	4.301182	1.168310
10	1	0	1.426117	1.890091	1.190099
11	6	0	-0.798103	0.626407	0.262414
12	1	0	-0.381620	0.159369	1.159157
13	7	0	-0.302294	-0.081303	-0.931920
14	8	0	-2.189243	0.381201	0.222502
15	6	0	-2.585158	0.001662	-1.110241
16	6	0	-1.319650	0.207874	-1.941987
17	1	0	-1.242816	-0.501771	-2.766897
18	1	0	-1.249487	1.231996	-2.332842
19	1	0	-3.409178	0.644525	-1.413273
20	6	0	-3.052896	-1.456073	-1.118009
21	1	0	-3.623564	-1.628946	-2.039630
22	6	0	-3.928754	-1.847637	0.076566
23	1	0	-3.372350	-1.624116	0.994730
24	6	0	-5.282956	-1.144041	0.138461
25	1	0	-5.848218	-1.393382	-0.764754
26	6	0	-6.072281	-1.597230	1.355116
27	1	0	-7.061718	-1.127326	1.323581
28	1	0	-6.179102	-2.685761	1.346655
29	8	0	-1.957118	-2.369468	-1.139507
30	1	0	-1.171713	-1.890678	-0.824315
31	8	0	-4.199573	-3.237155	-0.010510
32	1	0	-3.354139	-3.644012	-0.233301
33	8	0	-5.139888	0.265094	0.163073

34	1	0	-4.665205	0.473441	0.977578
35	8	0	-5.339813	-1.151826	2.490699
36	1	0	-5.851819	-1.340778	3.279813
37	6	0	1.078245	0.138391	-1.343657
38	1	0	1.187072	-0.307584	-2.336789
39	1	0	1.303066	1.210513	-1.448028
40	6	0	2.071734	-0.527990	-0.397095
41	1	0	1.905643	-0.185890	0.629949
42	1	0	1.884201	-1.606793	-0.397518
43	6	0	3.518453	-0.246829	-0.795142
44	1	0	3.687393	-0.599202	-1.820015
45	1	0	3.688111	0.836750	-0.808624
46	6	0	4.532816	-0.903190	0.138858
47	1	0	4.389931	-0.517760	1.155812
48	1	0	4.337813	-1.981127	0.186523
49	6	0	5.979628	-0.671526	-0.291415
50	1	0	6.129106	-1.091743	-1.293452
51	1	0	6.165192	0.406114	-0.377300
52	6	0	6.997650	-1.282586	0.668884
53	1	0	6.796885	-2.355518	0.777393
54	1	0	6.866222	-0.841782	1.664863
55	6	0	8.443773	-1.086178	0.218402
56	1	0	8.577595	-1.542703	-0.768532
57	1	0	8.640150	-0.015587	0.093591
58	6	0	9.450669	-1.680852	1.198814
59	1	0	10.478053	-1.537336	0.856858
60	1	0	9.358119	-1.215457	2.184183
61	1	0	9.287393	-2.755022	1.323452
62	1	0	0.291218	5.919819	0.277802

Structure 38a (M06-2X, DMSO)

Energy (Hartrees): = - 1252.0003521
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.469570	2.144594	0.327690
2	6	0	-1.343226	3.062012	-0.258108
3	6	0	-1.034240	4.419120	-0.272961
4	6	0	0.146799	4.874584	0.305932
5	6	0	1.014762	3.967720	0.907425
6	6	0	0.704861	2.611009	0.920069
7	1	0	-2.278021	2.716450	-0.685314
8	1	0	-1.722207	5.123074	-0.727598
9	1	0	1.929406	4.317252	1.372812
10	1	0	1.377826	1.908616	1.402256
11	6	0	-0.765758	0.652720	0.310395
12	1	0	-0.350635	0.191545	1.210497
13	7	0	-0.270133	-0.065447	-0.877296
14	8	0	-2.161538	0.418689	0.271495
15	6	0	-2.554425	-0.004294	-1.048938
16	6	0	-1.294268	0.194555	-1.889837
17	1	0	-1.212436	-0.529804	-2.701871
18	1	0	-1.233625	1.209062	-2.304965
19	1	0	-3.388222	0.615050	-1.372230
20	6	0	-2.992724	-1.468938	-1.012964
21	1	0	-3.479966	-1.699214	-1.970179
22	6	0	-3.962244	-1.814416	0.122796
23	1	0	-3.522636	-1.467950	1.065941
24	6	0	-5.355554	-1.207083	-0.028902
25	1	0	-5.776983	-1.528881	-0.985862
26	6	0	-6.280185	-1.650690	1.091283
27	1	0	-7.278699	-1.243930	0.900636
28	1	0	-6.332701	-2.741945	1.130710
29	8	0	-1.877349	-2.349916	-0.875426
30	1	0	-1.092407	-1.804282	-0.681590
31	8	0	-4.129357	-3.224818	0.147720
32	1	0	-3.240440	-3.579422	0.022964
33	8	0	-5.298442	0.210843	-0.053081
34	1	0	-5.038390	0.476471	0.838156
35	8	0	-5.740342	-1.111438	2.294588
36	1	0	-6.403407	-1.192659	2.986000
37	6	0	1.106995	0.168372	-1.296874
38	1	0	1.217101	-0.284023	-2.286703
39	1	0	1.315121	1.243124	-1.410046
40	6	0	2.110314	-0.474998	-0.346363
41	1	0	1.953563	-0.110014	0.673916
42	1	0	1.926691	-1.554917	-0.327531
43	6	0	3.552155	-0.200655	-0.764332
44	1	0	3.698834	-0.532014	-1.799728
45	1	0	3.734585	0.880889	-0.752948

46	6	0	4.570419	-0.895458	0.136421
47	1	0	4.432012	-0.553814	1.169551
48	1	0	4.374259	-1.974592	0.136000
49	6	0	6.015758	-0.647768	-0.288240
50	1	0	6.151253	-0.989253	-1.321883
51	1	0	6.215065	0.430904	-0.287565
52	6	0	7.031591	-1.349277	0.610036
53	1	0	6.825246	-2.426807	0.617223
54	1	0	6.904208	-1.001299	1.642679
55	6	0	8.477809	-1.119338	0.177543
56	1	0	8.604427	-1.470859	-0.852478
57	1	0	8.684066	-0.043260	0.167460
58	6	0	9.480678	-1.824921	1.085582
59	1	0	10.508754	-1.658407	0.754965
60	1	0	9.397816	-1.462993	2.114517
61	1	0	9.303832	-2.904311	1.096787
62	1	0	0.384183	5.932356	0.298226

Structure 38b (M06-2X, Gas Phase)

Energy (Hartrees): = - 1251.9776092
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.215700	2.186082	-0.416984
2	6	0	-1.744696	2.135805	0.872155
3	6	0	-1.861758	3.298860	1.619741
4	6	0	-1.449269	4.518663	1.087222
5	6	0	-0.922601	4.571766	-0.196606
6	6	0	-0.811747	3.405125	-0.948818
7	1	0	-2.066626	1.182999	1.277771
8	1	0	-2.277627	3.256768	2.619319
9	1	0	-0.604487	5.518689	-0.616235
10	1	0	-0.412611	3.443945	-1.957607
11	6	0	-1.068885	0.916508	-1.214265
12	1	0	-0.853508	1.164258	-2.270851
13	7	0	-0.020956	0.037080	-0.686102
14	8	0	-2.241721	0.135251	-1.147563
15	6	0	-1.888707	-1.253711	-1.062830
16	6	0	-0.373286	-1.256873	-1.271654
17	1	0	0.117740	-2.077015	-0.745991
18	1	0	-0.115362	-1.299222	-2.341966
19	1	0	-2.426291	-1.793597	-1.838893
20	6	0	-2.286131	-1.806121	0.306797
21	1	0	-2.202405	-2.901563	0.269900
22	6	0	-3.711017	-1.448502	0.743853
23	1	0	-3.836266	-0.360968	0.668119
24	6	0	-4.806053	-2.127453	-0.075827
25	1	0	-4.670948	-3.211213	-0.007929
26	6	0	-6.181605	-1.764515	0.459233
27	1	0	-6.934933	-2.347662	-0.082115
28	1	0	-6.230288	-1.981822	1.529194
29	8	0	-1.419936	-1.348549	1.343925
30	1	0	-0.806035	-0.691401	0.974723
31	8	0	-3.886626	-1.880503	2.081707
32	1	0	-3.078737	-1.627520	2.542644
33	8	0	-4.722844	-1.779699	-1.444523
34	1	0	-4.992970	-0.854731	-1.500913
35	8	0	-6.340252	-0.374858	0.196541
36	1	0	-7.208532	-0.097634	0.491474
37	6	0	1.327295	0.507624	-0.973986
38	1	0	1.477652	0.597384	-2.065269
39	1	0	1.422761	1.511200	-0.547821
40	6	0	2.398973	-0.398715	-0.382453
41	1	0	2.175642	-0.564904	0.676860
42	1	0	2.371200	-1.378103	-0.872534
43	6	0	3.796453	0.197366	-0.534959
44	1	0	3.838649	1.159577	-0.011267
45	1	0	3.989482	0.411908	-1.593147
46	6	0	4.895540	-0.717005	0.000541
47	1	0	4.866930	-1.672273	-0.537166
48	1	0	4.692738	-0.948790	1.052931
49	6	0	6.290325	-0.108693	-0.123764
50	1	0	6.319675	0.842738	0.420802
51	1	0	6.489104	0.131715	-1.175343
52	6	0	7.393688	-1.023976	0.400959
53	1	0	7.192644	-1.269844	1.450870
54	1	0	7.369751	-1.973576	-0.147432
55	6	0	8.787765	-0.411299	0.285425
56	1	0	8.986262	-0.164609	-0.763262
57	1	0	8.810156	0.535830	0.835055
58	6	0	9.881268	-1.337626	0.811504

59	1	0	9.890797	-2.280338	0.258313
60	1	0	10.870420	-0.885092	0.719209
61	1	0	9.716501	-1.573317	1.866056
62	1	0	-1.541868	5.425629	1.672820

Structure 38b (M06-2X, Benzene)

Energy (Hartrees): = - 1252.0047379
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.205741	2.215648	-0.421961
2	6	0	-1.786837	2.187047	0.845505
3	6	0	-1.908410	3.358247	1.580638
4	6	0	-1.446299	4.564654	1.057936
5	6	0	-0.865331	4.596086	-0.203593
6	6	0	-0.751312	3.422142	-0.944090
7	1	0	-2.144767	1.244559	1.245203
8	1	0	-2.366603	3.332892	2.562430
9	1	0	-0.507386	5.532587	-0.615376
10	1	0	-0.309721	3.444877	-1.935704
11	6	0	-1.054058	0.938032	-1.207243
12	1	0	-0.829160	1.176297	-2.262951
13	7	0	-0.015244	0.056503	-0.664156
14	8	0	-2.233117	0.161912	-1.143808
15	6	0	-1.886349	-1.228372	-1.047773
16	6	0	-0.370554	-1.238321	-1.248783
17	1	0	0.115828	-2.059698	-0.721235
18	1	0	-0.109271	-1.283069	-2.317719
19	1	0	-2.418695	-1.773801	-1.823480
20	6	0	-2.292858	-1.771239	0.322867
21	1	0	-2.185625	-2.864987	0.299109
22	6	0	-3.730687	-1.434585	0.738630
23	1	0	-3.884435	-0.354736	0.618713
24	6	0	-4.804180	-2.178952	-0.053821
25	1	0	-4.641093	-3.254554	0.063361
26	6	0	-6.194249	-1.831152	0.452330
27	1	0	-6.926503	-2.463538	-0.062211
28	1	0	-6.252292	-1.997673	1.530993
29	8	0	-1.448214	-1.278138	1.362970
30	1	0	-0.821312	-0.639528	0.979857
31	8	0	-3.901557	-1.813649	2.095133
32	1	0	-3.098720	-1.523870	2.543906
33	8	0	-4.723334	-1.889997	-1.438269
34	1	0	-5.045004	-0.985066	-1.537159
35	8	0	-6.395203	-0.461301	0.120609
36	1	0	-7.284619	-0.207345	0.375544
37	6	0	1.339442	0.515769	-0.948720
38	1	0	1.491749	0.601979	-2.039344
39	1	0	1.443892	1.518552	-0.523491
40	6	0	2.403115	-0.398288	-0.353999
41	1	0	2.181092	-0.556711	0.706969
42	1	0	2.365731	-1.379233	-0.840361
43	6	0	3.804913	0.187054	-0.513257
44	1	0	3.854774	1.151327	0.006150
45	1	0	3.994883	0.394717	-1.573447
46	6	0	4.901571	-0.731237	0.021841
47	1	0	4.861595	-1.690767	-0.507808
48	1	0	4.705854	-0.951692	1.078064
49	6	0	6.300213	-0.134118	-0.120103
50	1	0	6.340929	0.822061	0.415637
51	1	0	6.490774	0.094692	-1.175859
52	6	0	7.403400	-1.051628	0.402595
53	1	0	7.213197	-1.283368	1.457784
54	1	0	7.366105	-2.007265	-0.134770
55	6	0	8.801481	-0.451959	0.263746
56	1	0	8.990759	-0.218561	-0.789870
57	1	0	8.840275	0.500343	0.803921
58	6	0	9.893910	-1.380542	0.785845
59	1	0	9.895163	-2.328551	0.240607
60	1	0	10.885355	-0.934306	0.679257
61	1	0	9.741688	-1.606653	1.844866
62	1	0	-1.543409	5.478232	1.632881

Structure 38b (M06-2X, DMSO)

Energy (Hartrees): = - 1252.0050186
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.219532	2.194131	-0.425675
2	6	0	-1.771414	2.144593	0.855541
3	6	0	-1.901515	3.308059	1.603530
4	6	0	-1.479046	4.528948	1.078321
5	6	0	-0.928236	4.581347	-0.197024
6	6	0	-0.803427	3.414620	-0.948971
7	1	0	-2.100569	1.192942	1.259775
8	1	0	-2.333147	3.265472	2.597067
9	1	0	-0.599213	5.528237	-0.609724
10	1	0	-0.382089	3.452163	-1.948849
11	6	0	-1.059188	0.927209	-1.227133
12	1	0	-0.833221	1.178916	-2.277649
13	7	0	-0.019294	0.044071	-0.690464
14	8	0	-2.239481	0.145575	-1.173919
15	6	0	-1.884472	-1.244854	-1.077383
16	6	0	-0.372354	-1.245614	-1.293627
17	1	0	0.124212	-2.073217	-0.786164
18	1	0	-0.122073	-1.268177	-2.364484
19	1	0	-2.418790	-1.794665	-1.847945
20	6	0	-2.274137	-1.791928	0.297432
21	1	0	-2.184859	-2.886239	0.260763
22	6	0	-3.697170	-1.431128	0.742919
23	1	0	-3.835560	-0.350379	0.615077
24	6	0	-4.800579	-2.166580	-0.015622
25	1	0	-4.655061	-3.243163	0.113102
26	6	0	-6.174964	-1.784948	0.507177
27	1	0	-6.927224	-2.398801	0.001326
28	1	0	-6.232378	-1.952646	1.585729
29	8	0	-1.398127	-1.320488	1.324649
30	1	0	-0.783043	-0.676033	0.927910
31	8	0	-3.841982	-1.787181	2.110722
32	1	0	-3.018643	-1.508290	2.529279
33	8	0	-4.741626	-1.896891	-1.406980
34	1	0	-5.057551	-0.989746	-1.507120
35	8	0	-6.351818	-0.407765	0.183544
36	1	0	-7.279080	-0.183961	0.303037
37	6	0	1.334282	0.509686	-0.981132
38	1	0	1.475940	0.605149	-2.070866
39	1	0	1.441360	1.508946	-0.547357
40	6	0	2.400981	-0.409092	-0.400549
41	1	0	2.176088	-0.593370	0.656251
42	1	0	2.374506	-1.378209	-0.910248
43	6	0	3.797286	0.193795	-0.536051
44	1	0	3.831556	1.147361	0.004175
45	1	0	3.993477	0.423404	-1.590523
46	6	0	4.896565	-0.724660	-0.008228
47	1	0	4.873942	-1.671675	-0.560989
48	1	0	4.689839	-0.969633	1.040865
49	6	0	6.290060	-0.109979	-0.117411
50	1	0	6.311493	0.836150	0.437236
51	1	0	6.494914	0.138236	-1.166243
52	6	0	7.392677	-1.026116	0.407605
53	1	0	7.187789	-1.275474	1.456295
54	1	0	7.372870	-1.972458	-0.147105
55	6	0	8.787331	-0.413074	0.301372
56	1	0	8.993784	-0.167144	-0.746330
57	1	0	8.808319	0.532556	0.854424
58	6	0	9.875463	-1.340718	0.833499
59	1	0	9.887842	-2.284364	0.280257
60	1	0	10.867158	-0.890238	0.745198
61	1	0	9.706298	-1.574478	1.888575
62	1	0	-1.581218	5.436141	1.662843

Structure 38c (M06-2X, Gas Phase)

Energy (Hartrees): = - 1251.9748609
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.010780	-1.623317	-0.025942
2	6	0	0.703572	-1.398360	-0.777858
3	6	0	2.947698	-0.464514	-0.372142
4	1	0	-0.003678	-2.183694	-0.507311
5	1	0	0.876377	-1.445631	-1.867859
6	1	0	2.470909	-2.568071	-0.310497
7	1	0	3.145506	-0.448800	-1.455553
8	8	0	2.286842	0.750134	-0.009158
9	7	0	0.139080	-0.102820	-0.389737
10	6	0	4.273125	-0.450849	0.387998

11	1	0	4.069055	-0.739626	1.426944
12	6	0	5.293422	-1.403972	-0.213829
13	1	0	5.499287	-1.081740	-1.245122
14	6	0	6.597875	-1.368163	0.561393
15	1	0	6.390286	-1.603305	1.612724
16	1	0	7.049101	-0.376134	0.486193
17	8	0	4.864074	0.832681	0.319266
18	1	0	4.147425	1.467043	0.428959
19	8	0	4.766968	-2.715322	-0.199321
20	1	0	5.520815	-3.298532	-0.342649
21	8	0	7.416234	-2.372564	-0.030060
22	1	0	8.200459	-2.492175	0.507440
23	8	0	1.763021	-1.672477	1.362712
24	1	0	1.211828	-0.903320	1.550950
25	6	0	-1.196250	0.088545	-0.961957
26	1	0	-1.240563	-0.318121	-1.986439
27	1	0	-1.398949	1.158963	-1.038658
28	6	0	0.568025	2.320242	-0.263120
29	6	0	0.117209	2.485610	1.046188
30	6	0	0.577991	3.406763	-1.129305
31	6	0	-0.326417	3.727427	1.478655
32	1	0	0.113001	1.630377	1.711909
33	6	0	0.133206	4.653512	-0.696552
34	1	0	0.934222	3.278949	-2.146050
35	6	0	-0.320025	4.813830	0.606546
36	1	0	-0.677469	3.851687	2.496150
37	1	0	0.141523	5.496677	-1.376756
38	6	0	1.076712	0.970500	-0.706991
39	1	0	1.300333	0.989134	-1.792991
40	6	0	-2.281475	-0.543847	-0.097216
41	1	0	-2.063997	-1.603794	0.070851
42	1	0	-2.257711	-0.059193	0.884463
43	6	0	-3.668306	-0.400513	-0.718672
44	1	0	-3.866120	0.658114	-0.926940
45	1	0	-3.690414	-0.915029	-1.686976
46	6	0	-4.780067	-0.951849	0.170794
47	1	0	-4.765518	-0.426899	1.133343
48	1	0	-4.579098	-2.006991	0.391985
49	6	0	-6.166713	-0.821170	-0.454552
50	1	0	-6.360723	0.232672	-0.688740
51	1	0	-6.185090	-1.357773	-1.410869
52	6	0	-7.282472	-1.350761	0.442782
53	1	0	-7.268090	-0.810048	1.396973
54	1	0	-7.087176	-2.403143	0.682761
55	6	0	-8.669166	-1.226244	-0.184668
56	1	0	-8.861028	-0.175258	-0.426726
57	1	0	-8.683214	-1.769655	-1.135554
58	6	0	-9.774840	-1.753994	0.726187
59	1	0	-9.792708	-1.206483	1.672108
60	1	0	-10.758746	-1.655487	0.263547
61	1	0	-9.616353	-2.810509	0.957421
62	1	0	-0.667462	5.782654	0.945177

Structure 38c (M06-2X, Benzene)

Energy (Hartrees): = - 1252.0022785
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.023969	-1.621392	-0.049817
2	6	0	0.718541	-1.397398	-0.804290
3	6	0	2.955365	-0.455384	-0.384254
4	1	0	0.017334	-2.193643	-0.551623
5	1	0	0.898294	-1.423367	-1.893088
6	1	0	2.488165	-2.562095	-0.340968
7	1	0	3.155924	-0.434511	-1.466714
8	8	0	2.286683	0.753811	-0.017296
9	7	0	0.142891	-0.112544	-0.394176
10	6	0	4.280002	-0.431314	0.377542
11	1	0	4.077498	-0.702484	1.421296
12	6	0	5.305072	-1.392152	-0.204770
13	1	0	5.490081	-1.110627	-1.252008
14	6	0	6.622224	-1.313816	0.545676
15	1	0	6.439268	-1.509549	1.609426
16	1	0	7.068338	-0.323670	0.426265
17	8	0	4.864438	0.856074	0.290357
18	1	0	4.140684	1.485576	0.385069
19	8	0	4.796665	-2.710014	-0.129357
20	1	0	5.559000	-3.286899	-0.256053
21	8	0	7.442606	-2.331800	-0.021240
22	1	0	8.219296	-2.444877	0.530945
23	8	0	1.768829	-1.682073	1.339126

24	1	0	1.185731	-0.934186	1.520766
25	6	0	-1.197747	0.073445	-0.958713
26	1	0	-1.235470	-0.296958	-1.996884
27	1	0	-1.419315	1.141903	-0.996290
28	6	0	0.557699	2.316492	-0.260967
29	6	0	0.215664	2.504994	1.078215
30	6	0	0.442708	3.373978	-1.155802
31	6	0	-0.242346	3.741457	1.512756
32	1	0	0.310924	1.676167	1.770464
33	6	0	-0.018209	4.614552	-0.721141
34	1	0	0.712407	3.227366	-2.196668
35	6	0	-0.361665	4.798322	0.612451
36	1	0	-0.506561	3.884280	2.554121
37	1	0	-0.106976	5.434123	-1.424509
38	6	0	1.071824	0.970824	-0.711544
39	1	0	1.289616	0.993990	-1.797460
40	6	0	-2.273714	-0.604848	-0.116903
41	1	0	-2.057606	-1.672531	-0.006072
42	1	0	-2.241988	-0.169779	0.887719
43	6	0	-3.665981	-0.428228	-0.719027
44	1	0	-3.854525	0.638896	-0.889082
45	1	0	-3.702759	-0.910462	-1.703528
46	6	0	-4.775827	-0.995869	0.163369
47	1	0	-4.747750	-0.498027	1.140141
48	1	0	-4.583816	-2.058999	0.352079
49	6	0	-6.166706	-0.832488	-0.446224
50	1	0	-6.345790	0.228640	-0.658702
51	1	0	-6.202239	-1.351408	-1.411974
52	6	0	-7.283851	-1.359915	0.451604
53	1	0	-7.253287	-0.834421	1.414049
54	1	0	-7.103431	-2.419132	0.672614
55	6	0	-8.674396	-1.203664	-0.161093
56	1	0	-8.851256	-0.146639	-0.388607
57	1	0	-8.709017	-1.736632	-1.117626
58	6	0	-9.781012	-1.721608	0.752961
59	1	0	-9.787547	-1.181490	1.703885
60	1	0	-10.766866	-1.604274	0.297021
61	1	0	-9.640201	-2.783107	0.974946
62	1	0	-0.719859	5.762723	0.953380

Structure 38c (M06-2X, DMSO)

Energy (Hartrees): = - 1252.0025953
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.996741	-1.613748	-0.075345
2	6	0	0.696463	-1.366346	-0.829263
3	6	0	2.943734	-0.459058	-0.400055
4	1	0	-0.018175	-2.155995	-0.592034
5	1	0	0.882045	-1.378580	-1.916024
6	1	0	2.445200	-2.558372	-0.377121
7	1	0	3.141323	-0.434825	-1.482187
8	8	0	2.291581	0.757700	-0.021907
9	7	0	0.136053	-0.078628	-0.404417
10	6	0	4.269511	-0.454246	0.358159
11	1	0	4.066959	-0.692894	1.409640
12	6	0	5.272379	-1.453808	-0.197516
13	1	0	5.443505	-1.223284	-1.259189
14	6	0	6.600376	-1.366542	0.532914
15	1	0	6.429516	-1.517942	1.605609
16	1	0	7.062825	-0.389844	0.373008
17	8	0	4.881180	0.820838	0.240335
18	1	0	4.164630	1.462623	0.308521
19	8	0	4.748480	-2.762638	-0.055679
20	1	0	5.506566	-3.350253	-0.162856
21	8	0	7.401604	-2.416431	-0.003541
22	1	0	8.155461	-2.550912	0.578066
23	8	0	1.740372	-1.683299	1.316649
24	1	0	1.176820	-0.920390	1.502582
25	6	0	-1.202383	0.121568	-0.974116
26	1	0	-1.248123	-0.281334	-1.998397
27	1	0	-1.403977	1.192406	-1.047421
28	6	0	0.578626	2.341371	-0.252080
29	6	0	0.223906	2.517819	1.086371
30	6	0	0.491581	3.412625	-1.134864
31	6	0	-0.217782	3.757321	1.532644
32	1	0	0.294962	1.679680	1.771261
33	6	0	0.047292	4.655963	-0.688343
34	1	0	0.767358	3.272897	-2.175205
35	6	0	-0.307749	4.828760	0.644752
36	1	0	-0.492594	3.891059	2.572759

37	1	0	-0.021043	5.485862	-1.382300
38	6	0	1.077107	0.994923	-0.717587
39	1	0	1.294455	1.024366	-1.801405
40	6	0	-2.283596	-0.514591	-0.107380
41	1	0	-2.052598	-1.570966	0.067828
42	1	0	-2.273420	-0.019865	0.870506
43	6	0	-3.670252	-0.394609	-0.733872
44	1	0	-3.876711	0.658832	-0.960262
45	1	0	-3.683766	-0.928934	-1.691490
46	6	0	-4.776439	-0.940817	0.165868
47	1	0	-4.766370	-0.397300	1.118511
48	1	0	-4.564923	-1.990747	0.403260
49	6	0	-6.165944	-0.834810	-0.458084
50	1	0	-6.372328	0.213983	-0.705220
51	1	0	-6.180692	-1.387733	-1.405355
52	6	0	-7.271626	-1.363796	0.452267
53	1	0	-7.255692	-0.810794	1.399706
54	1	0	-7.066034	-2.412596	0.700642
55	6	0	-8.664722	-1.258254	-0.164243
56	1	0	-8.870700	-0.210731	-0.411334
57	1	0	-8.683852	-1.812104	-1.109431
58	6	0	-9.754618	-1.789408	0.761968
59	1	0	-9.768727	-1.234910	1.704870
60	1	0	-10.745529	-1.701801	0.309647
61	1	0	-9.585733	-2.844131	0.997540
62	1	0	-0.654366	5.794653	0.994179

Structure 38d (M06-2X, Gas Phase)

Energy (Hartrees): = - 1251.9759227
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.916489	-1.106299	1.326834
2	6	0	-0.911194	-0.116965	1.927532
3	6	0	-2.487220	-0.464300	0.062976
4	1	0	-0.428222	-0.560948	2.798846
5	1	0	-1.446498	0.780934	2.257681
6	1	0	-2.722201	-1.315217	2.029531
7	1	0	-2.982741	0.479132	0.325116
8	8	0	-1.383443	-0.195075	-0.815944
9	7	0	0.124953	0.287815	0.971974
10	6	0	-3.455314	-1.327033	-0.749508
11	1	0	-3.093189	-2.363738	-0.749274
12	6	0	-4.865853	-1.296352	-0.184000
13	1	0	-5.226238	-0.257599	-0.210984
14	6	0	-5.808318	-2.148203	-1.015083
15	1	0	-5.407949	-3.168345	-1.068746
16	1	0	-5.897481	-1.733288	-2.021830
17	8	0	-3.558462	-0.825997	-2.070844
18	1	0	-2.660194	-0.617011	-2.349004
19	8	0	-4.832312	-1.777629	1.143272
20	1	0	-5.747924	-1.971558	1.373900
21	8	0	-7.049933	-2.127951	-0.318854
22	1	0	-7.641640	-2.766794	-0.719270
23	8	0	-1.294647	-2.344294	1.026202
24	1	0	-0.793665	-2.214613	0.214247
25	6	0	1.236495	-0.649299	0.780543
26	1	0	1.079569	-1.290364	-0.102168
27	1	0	1.278361	-1.320002	1.641509
28	6	0	-1.055404	2.138778	-0.165139
29	6	0	-0.519752	3.068631	0.723106
30	6	0	-2.092717	2.523995	-1.014622
31	6	0	-1.017292	4.366887	0.764941
32	1	0	0.284515	2.758475	1.380052
33	6	0	-2.590920	3.820611	-0.969079
34	1	0	-2.526053	1.797491	-1.693631
35	6	0	-2.053326	4.746327	-0.080445
36	1	0	-0.596036	5.082135	1.461772
37	1	0	-3.403047	4.106882	-1.626711
38	6	0	-0.445992	0.745535	-0.268455
39	1	0	0.351599	0.779792	-1.015258
40	6	0	2.562355	0.089670	0.630423
41	1	0	2.474317	0.834753	-0.169826
42	1	0	2.753760	0.648827	1.552020
43	6	0	3.727129	-0.848621	0.327595
44	1	0	3.811558	-1.597142	1.124912
45	1	0	3.516933	-1.404436	-0.594395
46	6	0	5.058682	-0.116432	0.179317
47	1	0	5.277535	0.429985	1.104426
48	1	0	4.967876	0.639551	-0.610124

49	6	0	6.223360	-1.048024	-0.146290
50	1	0	6.320974	-1.799627	0.646490
51	1	0	5.998648	-1.599872	-1.067101
52	6	0	7.550911	-0.312715	-0.311351
53	1	0	7.779571	0.236927	0.609892
54	1	0	7.450972	0.441495	-1.101631
55	6	0	8.716159	-1.240883	-0.646460
56	1	0	8.819994	-1.989596	0.146401
57	1	0	8.482678	-1.793371	-1.563012
58	6	0	10.033425	-0.489271	-0.819872
59	1	0	10.295413	0.051456	0.093242
60	1	0	10.855938	-1.167043	-1.055798
61	1	0	9.959198	0.242694	-1.628350
62	1	0	-2.442988	5.756675	-0.045173

Structure 38d (M06-2X, Benzene)

Energy (Hartrees): = - 1252.0026257
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.911387	-1.097753	1.314274
2	6	0	-0.895625	-0.116295	1.909410
3	6	0	-2.497907	-0.447247	0.062136
4	1	0	-0.401352	-0.568065	2.770465
5	1	0	-1.428447	0.776740	2.256175
6	1	0	-2.706925	-1.306250	2.028440
7	1	0	-2.996312	0.490415	0.339485
8	8	0	-1.406498	-0.164540	-0.827980
9	7	0	0.127628	0.297181	0.944020
10	6	0	-3.470140	-1.304859	-0.750691
11	1	0	-3.084451	-2.331491	-0.800720
12	6	0	-4.865963	-1.334768	-0.148357
13	1	0	-5.244933	-0.303726	-0.090606
14	6	0	-5.818077	-2.146149	-1.009295
15	1	0	-5.400484	-3.150196	-1.154524
16	1	0	-5.956124	-1.664068	-1.979968
17	8	0	-3.617680	-0.758719	-2.051446
18	1	0	-2.729073	-0.529009	-2.345505
19	8	0	-4.790053	-1.908362	1.141625
20	1	0	-5.695509	-2.149144	1.370829
21	8	0	-7.036753	-2.207417	-0.274406
22	1	0	-7.610056	-2.860266	-0.682181
23	8	0	-1.301175	-2.339664	0.999189
24	1	0	-0.794434	-2.203869	0.191189
25	6	0	1.238035	-0.638900	0.731276
26	1	0	1.073317	-1.267774	-0.158446
27	1	0	1.286574	-1.318028	1.585239
28	6	0	-1.061508	2.163664	-0.162353
29	6	0	-0.516965	3.086829	0.728409
30	6	0	-2.106056	2.559015	-0.998869
31	6	0	-1.011583	4.386148	0.784525
32	1	0	0.293020	2.773796	1.377128
33	6	0	-2.601471	3.856510	-0.939873
34	1	0	-2.547749	1.839912	-1.680148
35	6	0	-2.054377	4.774829	-0.048946
36	1	0	-0.582630	5.095079	1.483529
37	1	0	-3.418995	4.149013	-1.588491
38	6	0	-0.457919	0.768256	-0.284088
39	1	0	0.329509	0.807035	-1.041099
40	6	0	2.564855	0.098846	0.582780
41	1	0	2.478775	0.846475	-0.215402
42	1	0	2.757218	0.652608	1.507872
43	6	0	3.727414	-0.842627	0.279070
44	1	0	3.801198	-1.598511	1.070682
45	1	0	3.521010	-1.388065	-0.650077
46	6	0	5.065159	-0.117175	0.149698
47	1	0	5.275333	0.423331	1.080482
48	1	0	4.988618	0.642380	-0.637986
49	6	0	6.229005	-1.054655	-0.164150
50	1	0	6.307856	-1.812521	0.624979
51	1	0	6.016256	-1.597417	-1.093361
52	6	0	7.565460	-0.328490	-0.300067
53	1	0	7.781169	0.213081	0.629239
54	1	0	7.486085	0.431042	-1.087790
55	6	0	8.730233	-1.263471	-0.619182
56	1	0	8.813075	-2.019555	0.169531
57	1	0	8.512462	-1.805673	-1.545934
58	6	0	10.056667	-0.522342	-0.758142
59	1	0	10.310012	0.002989	0.167006
60	1	0	10.877544	-1.204997	-0.988944
61	1	0	10.006731	0.221919	-1.557923

62	1	0	-2.441512	5.785964	-0.002545

Structure 38d (M06-2X, DMSO)

Energy (Hartrees): = - 1252.0024187
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.922444	-1.072903	1.331131
2	6	0	-0.913836	-0.087341	1.929039
3	6	0	-2.491619	-0.436382	0.065020
4	1	0	-0.430793	-0.529776	2.801344
5	1	0	-1.456298	0.806073	2.259857
6	1	0	-2.726546	-1.265723	2.040054
7	1	0	-2.999331	0.499527	0.331244
8	8	0	-1.390885	-0.154037	-0.812894
9	7	0	0.122322	0.321020	0.974834
10	6	0	-3.448997	-1.300759	-0.757051
11	1	0	-3.043872	-2.318246	-0.829430
12	6	0	-4.843261	-1.369992	-0.153614
13	1	0	-5.231101	-0.346336	-0.046713
14	6	0	-5.792005	-2.153271	-1.043366
15	1	0	-5.370763	-3.148949	-1.227958
16	1	0	-5.938138	-1.638277	-1.995474
17	8	0	-3.606456	-0.733699	-2.049400
18	1	0	-2.720810	-0.482412	-2.337303
19	8	0	-4.762287	-2.000909	1.111863
20	1	0	-5.666421	-2.267506	1.319932
21	8	0	-7.010875	-2.248714	-0.310650
22	1	0	-7.560282	-2.922988	-0.720931
23	8	0	-1.315320	-2.324815	1.043341
24	1	0	-0.783539	-2.202751	0.248199
25	6	0	1.230238	-0.623999	0.777849
26	1	0	1.058917	-1.276032	-0.093041
27	1	0	1.285900	-1.274891	1.653164
28	6	0	-1.054341	2.178697	-0.157248
29	6	0	-0.521985	3.108039	0.735700
30	6	0	-2.088369	2.571275	-1.008911
31	6	0	-1.018390	4.408051	0.780808
32	1	0	0.281198	2.804200	1.397131
33	6	0	-2.586395	3.869279	-0.961998
34	1	0	-2.519356	1.851967	-1.696761
35	6	0	-2.051946	4.792669	-0.067259
36	1	0	-0.597940	5.120090	1.482216
37	1	0	-3.395144	4.158616	-1.623386
38	6	0	-0.448796	0.782450	-0.264667
39	1	0	0.347703	0.818502	-1.011960
40	6	0	2.555715	0.108138	0.599038
41	1	0	2.461538	0.838520	-0.213890
42	1	0	2.764938	0.676658	1.511998
43	6	0	3.711129	-0.842320	0.298050
44	1	0	3.786136	-1.589381	1.098000
45	1	0	3.495052	-1.394694	-0.624612
46	6	0	5.049962	-0.122733	0.153270
47	1	0	5.271026	0.420093	1.080381
48	1	0	4.968901	0.632999	-0.637846
49	6	0	6.207169	-1.065504	-0.167509
50	1	0	6.288286	-1.822405	0.622546
51	1	0	5.985763	-1.607100	-1.095469
52	6	0	7.544911	-0.344233	-0.312716
53	1	0	7.770218	0.194007	0.616391
54	1	0	7.462221	0.416207	-1.099414
55	6	0	8.702891	-1.283150	-0.642821
56	1	0	8.789070	-2.040575	0.144445
57	1	0	8.475230	-1.822259	-1.569141
58	6	0	10.030758	-0.546593	-0.791090
59	1	0	10.292924	-0.024009	0.133469
60	1	0	10.847480	-1.232294	-1.029238
61	1	0	9.976482	0.199062	-1.589677
62	1	0	-2.440646	5.803836	-0.029971

Structure 39a (M06-2X, Gas Phase)

Energy (Hartrees): = - 1366.4837692
No imaginary frequencies

Standard orientation:

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

1	6	0	-0.398047	1.567326	0.443819
2	6	0	-1.324695	2.488322	-0.017563
3	6	0	-1.053359	3.858538	0.040253
4	6	0	0.152035	4.309278	0.574671
5	6	0	1.070354	3.377090	1.055292
6	6	0	0.805240	2.018811	0.996802
7	1	0	-2.287756	2.171882	-0.399354
8	1	0	2.000286	3.727935	1.486964
9	1	0	1.524217	1.309311	1.391087
10	6	0	-0.668652	0.074217	0.326424
11	1	0	-0.240705	-0.441625	1.190477
12	7	0	-0.164515	-0.548799	-0.913255
13	8	0	-2.052858	-0.187438	0.281174
14	6	0	-2.456409	-0.505411	-1.064147
15	6	0	-1.202422	-0.237622	-1.896383
16	1	0	-1.121288	-0.911198	-2.750658
17	1	0	-1.155704	0.804167	-2.242053
18	1	0	-3.293396	0.139926	-1.323468
19	6	0	-2.902529	-1.967530	-1.141405
20	1	0	-3.479445	-2.103267	-2.065225
21	6	0	-3.764934	-2.427379	0.038225
22	1	0	-3.208749	-2.236949	0.963861
23	6	0	-5.128102	-1.744981	0.131822
24	1	0	-5.689120	-1.966395	-0.780962
25	6	0	-5.905723	-2.266034	1.329646
26	1	0	-6.908822	-1.825917	1.313563
27	1	0	-5.969352	-3.356364	1.280429
28	8	0	-1.795867	-2.862200	-1.220944
29	1	0	-1.014495	-2.399118	-0.877874
30	8	0	-4.020903	-3.812352	-0.112723
31	1	0	-3.175388	-4.202613	-0.362186
32	8	0	-5.008763	-0.338275	0.215697
33	1	0	-4.565809	-0.153819	1.053330
34	8	0	-5.185989	-1.833422	2.478196
35	1	0	-5.665306	-2.100402	3.263486
36	6	0	1.195798	-0.232382	-1.329433
37	1	0	1.311722	-0.608152	-2.350235
38	1	0	1.361854	0.854940	-1.367502
39	6	0	2.240039	-0.900695	-0.440485
40	1	0	2.034168	-0.686442	0.613151
41	1	0	2.155898	-1.986123	-0.554723
42	6	0	3.655680	-0.440574	-0.777108
43	1	0	3.853598	-0.617460	-1.841305
44	1	0	3.727226	0.643566	-0.626253
45	6	0	4.724768	-1.140619	0.058278
46	1	0	4.525754	-0.965194	1.122519
47	1	0	4.651570	-2.223935	-0.093716
48	6	0	6.141754	-0.678612	-0.273095
49	1	0	6.340447	-0.855095	-1.337052
50	1	0	6.214726	0.405165	-0.122035
51	6	0	7.211188	-1.377971	0.562402
52	1	0	7.137627	-2.461960	0.412649
53	1	0	7.014204	-1.200968	1.626774
54	6	0	8.629539	-0.919364	0.230165
55	1	0	8.824782	-1.097442	-0.832746
56	1	0	8.701444	0.163282	0.379807
57	6	0	9.687397	-1.626964	1.073348
58	1	0	10.694315	-1.287928	0.823073
59	1	0	9.525062	-1.439528	2.137893
60	1	0	9.648961	-2.708150	0.917622
61	1	0	0.380124	5.364378	0.635537
62	8	0	-2.028927	4.668383	-0.441127
63	6	0	-1.813493	6.062388	-0.382645
64	1	0	-0.938698	6.353911	-0.972716
65	1	0	-2.703540	6.522107	-0.805315
66	1	0	-1.684916	6.400511	0.650473

Structure 39a (M06-2X, Benzene)

Energy (Hartrees): = - 1366.5114647
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.449404	1.623338	0.452943
2	6	0	-1.408693	2.509393	-0.013243
3	6	0	-1.191565	3.889474	0.049179
4	6	0	-0.005610	4.384641	0.589034
5	6	0	0.946214	3.487456	1.071684
6	6	0	0.733360	2.119486	1.011871
7	1	0	-2.355677	2.154226	-0.402763
8	1	0	1.861228	3.874188	1.505522

9	1	0	1.475548	1.435811	1.408976
10	6	0	-0.661135	0.120253	0.338553
11	1	0	-0.218374	-0.374301	1.207694
12	7	0	-0.127908	-0.490942	-0.893185
13	8	0	-2.037051	-0.192651	0.285474
14	6	0	-2.415710	-0.543833	-1.058851
15	6	0	-1.169664	-0.229122	-1.885782
16	1	0	-1.054178	-0.902477	-2.736516
17	1	0	-1.166564	0.810812	-2.239141
18	1	0	-3.277102	0.059593	-1.336811
19	6	0	-2.794546	-2.024917	-1.119796
20	1	0	-3.331861	-2.203112	-2.060546
21	6	0	-3.675459	-2.502768	0.039708
22	1	0	-3.166052	-2.259254	0.979759
23	6	0	-5.078382	-1.900392	0.067154
24	1	0	-5.588807	-2.157202	-0.866227
25	6	0	-5.880963	-2.448507	1.234966
26	1	0	-6.901557	-2.054194	1.173822
27	1	0	-5.901783	-3.541112	1.194504
28	8	0	-1.644220	-2.868945	-1.136499
29	1	0	-0.885862	-2.342128	-0.831353
30	8	0	-3.841854	-3.906378	-0.082570
31	1	0	-2.963262	-4.246586	-0.288232
32	8	0	-5.038452	-0.486426	0.142186
33	1	0	-4.651958	-0.273670	1.000847
34	8	0	-5.232573	-1.981259	2.412707
35	1	0	-5.756520	-2.238601	3.174225
36	6	0	1.228309	-0.144649	-1.302227
37	1	0	1.358949	-0.526186	-2.319056
38	1	0	1.369471	0.945763	-1.347687
39	6	0	2.278200	-0.785254	-0.400530
40	1	0	2.083585	-0.531106	0.646478
41	1	0	2.185106	-1.873802	-0.477210
42	6	0	3.695571	-0.353319	-0.767406
43	1	0	3.879915	-0.570378	-1.826680
44	1	0	3.785264	0.734116	-0.653652
45	6	0	4.761941	-1.042293	0.081109
46	1	0	4.579666	-0.822641	1.140223
47	1	0	4.664151	-2.128963	-0.030094
48	6	0	6.185110	-0.625641	-0.283270
49	1	0	6.364695	-0.840833	-1.343649
50	1	0	6.287427	0.460218	-0.166099
51	6	0	7.247461	-1.327633	0.559480
52	1	0	7.142093	-2.413436	0.443382
53	1	0	7.069998	-1.112285	1.620367
54	6	0	8.673987	-0.920808	0.195725
55	1	0	8.848205	-1.130183	-0.865408
56	1	0	8.782709	0.162321	0.320134
57	6	0	9.722218	-1.641325	1.038564
58	1	0	10.735566	-1.336041	0.768201
59	1	0	9.582041	-1.429210	2.102146
60	1	0	9.654006	-2.724646	0.905016
61	1	0	0.182261	5.447811	0.650451
62	8	0	-2.194019	4.663070	-0.432800
63	6	0	-2.041717	6.067247	-0.348536
64	1	0	-1.183508	6.411531	-0.934558
65	1	0	-2.952522	6.493760	-0.764176
66	1	0	-1.932733	6.394539	0.690452

Structure 39a (M06-2X, DMSO)

Energy (Hartrees): = -1366.5129216
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.372458	1.621771	0.505856
2	6	0	-1.276186	2.538881	-0.012906
3	6	0	-1.012006	3.911467	0.049436
4	6	0	0.164774	4.368245	0.643872
5	6	0	1.060232	3.440161	1.175155
6	6	0	0.801511	2.078573	1.114244
7	1	0	-2.209874	2.213846	-0.457707
8	1	0	1.968377	3.797491	1.647511
9	1	0	1.500821	1.369494	1.543944
10	6	0	-0.630015	0.126323	0.393872
11	1	0	-0.188982	-0.379169	1.256970
12	7	0	-0.128040	-0.497242	-0.844624
13	8	0	-2.017672	-0.146085	0.358184
14	6	0	-2.418718	-0.501523	-0.978879
15	6	0	-1.178259	-0.215220	-1.824274
16	1	0	-1.087502	-0.889279	-2.677756
17	1	0	-1.157725	0.822538	-2.181570

18	1	0	-3.274341	0.110443	-1.255142
19	6	0	-2.813200	-1.977473	-1.023231
20	1	0	-3.283343	-2.171124	-1.997184
21	6	0	-3.784938	-2.408982	0.081256
22	1	0	-3.378414	-2.080286	1.045574
23	6	0	-5.201512	-1.859095	-0.077172
24	1	0	-5.585096	-2.155536	-1.057979
25	6	0	-6.129267	-2.397016	0.998323
26	1	0	-7.144061	-2.038089	0.797246
27	1	0	-6.121176	-3.489971	0.995137
28	8	0	-1.671869	-2.828771	-0.914822
29	1	0	-0.897788	-2.266288	-0.726163
30	8	0	-3.891327	-3.825216	0.048446
31	1	0	-2.987143	-4.137170	-0.079519
32	8	0	-5.211251	-0.440665	-0.033213
33	1	0	-5.038940	-0.209837	0.888610
34	8	0	-5.649304	-1.876137	2.235121
35	1	0	-6.314660	-2.039064	2.909817
36	6	0	1.229484	-0.173081	-1.270551
37	1	0	1.340504	-0.552111	-2.290391
38	1	0	1.385397	0.915356	-1.313573
39	6	0	2.278993	-0.830756	-0.381569
40	1	0	2.090044	-0.589615	0.669545
41	1	0	2.182990	-1.918084	-0.476869
42	6	0	3.695431	-0.398437	-0.750640
43	1	0	3.864211	-0.577984	-1.819589
44	1	0	3.795823	0.682840	-0.594679
45	6	0	4.764160	-1.128987	0.058668
46	1	0	4.588616	-0.956636	1.127705
47	1	0	4.662057	-2.208868	-0.104173
48	6	0	6.186511	-0.700273	-0.294121
49	1	0	6.357782	-0.862729	-1.365420
50	1	0	6.294820	0.377336	-0.120073
51	6	0	7.249918	-1.450259	0.504521
52	1	0	7.137969	-2.527937	0.331895
53	1	0	7.080213	-1.287412	1.576163
54	6	0	8.676546	-1.033146	0.153806
55	1	0	8.845314	-1.194352	-0.916761
56	1	0	8.791363	0.042189	0.329969
57	6	0	9.723362	-1.798430	0.958050
58	1	0	10.738301	-1.493110	0.692213
59	1	0	9.592601	-1.627143	2.030471
60	1	0	9.641301	-2.874653	0.780129
61	1	0	0.387575	5.424856	0.708194
62	8	0	-1.959614	4.717710	-0.485577
63	6	0	-1.741160	6.119718	-0.423212
64	1	0	-0.837010	6.405190	-0.968889
65	1	0	-2.606068	6.580448	-0.896241
66	1	0	-1.668618	6.463661	0.612811

Structure 39b (M06-2X, Gas Phase)

Energy (Hartrees): = - 1366.4874576
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.211008	1.750550	-0.080892
2	6	0	-1.661819	1.512668	1.211183
3	6	0	-1.757045	2.576067	2.103742
4	6	0	-1.406929	3.859531	1.715981
5	6	0	-0.957081	4.097250	0.416688
6	6	0	-0.861922	3.037939	-0.486325
7	1	0	-1.936930	0.508051	1.509420
8	1	0	-2.111292	2.403443	3.113013
9	1	0	-0.524700	3.195427	-1.503442
10	6	0	-1.070354	0.603313	-1.049588
11	1	0	-0.873309	0.997205	-2.065086
12	7	0	-0.009183	-0.330286	-0.662884
13	8	0	-2.236311	-0.190053	-1.077881
14	6	0	-1.870971	-1.574598	-1.186803
15	6	0	-0.359073	-1.535320	-1.414946
16	1	0	0.143861	-2.415046	-1.011330
17	1	0	-0.116258	-1.429477	-2.484315
18	1	0	-2.416265	-2.008993	-2.021516
19	6	0	-2.243841	-2.312397	0.099964
20	1	0	-2.175968	-3.392016	-0.094040
21	6	0	-3.653068	-2.007634	0.618643
22	1	0	-3.755440	-0.920592	0.729332
23	6	0	-4.778208	-2.517007	-0.279564
24	1	0	-4.671217	-3.600160	-0.393625
25	6	0	-6.134869	-2.214444	0.335242
26	1	0	-6.911812	-2.676898	-0.283940

27	1	0	-6.175314	-2.611321	1.352856
28	8	0	-1.347364	-2.019883	1.170723
29	1	0	-0.756726	-1.298217	0.896741
30	8	0	-3.814375	-2.654887	1.868671
31	1	0	-2.999518	-2.485836	2.354882
32	8	0	-4.707528	-1.951742	-1.574512
33	1	0	-4.914933	-1.014985	-1.469476
34	8	0	-6.257255	-0.797060	0.317168
35	1	0	-7.102412	-0.551345	0.695229
36	6	0	1.331651	0.187866	-0.897236
37	1	0	1.479477	0.397832	-1.972385
38	1	0	1.413058	1.140167	-0.363948
39	6	0	2.415854	-0.761450	-0.403982
40	1	0	2.201255	-1.027556	0.636593
41	1	0	2.392495	-1.690833	-0.983326
42	6	0	3.807493	-0.142045	-0.508881
43	1	0	3.838187	0.781092	0.081782
44	1	0	4.001868	0.148242	-1.548701
45	6	0	4.913835	-1.080661	-0.033644
46	1	0	4.890374	-2.001569	-0.628531
47	1	0	4.714849	-1.377556	1.003031
48	6	0	6.304438	-0.456951	-0.122872
49	1	0	6.325492	0.465754	0.469503
50	1	0	6.504093	-0.161982	-1.160364
51	6	0	7.412826	-1.390003	0.358047
52	1	0	7.213591	-1.685348	1.395502
53	1	0	7.393613	-2.313376	-0.233676
54	6	0	8.803708	-0.765646	0.270672
55	1	0	9.001784	-0.473022	-0.766259
56	1	0	8.820586	0.157114	0.860557
57	6	0	9.901460	-1.708232	0.757443
58	1	0	9.914335	-2.627383	0.165880
59	1	0	10.888692	-1.248286	0.683204
60	1	0	9.738599	-1.988033	1.801463
61	1	0	-1.475237	4.699977	2.395340
62	8	0	-0.640237	5.384505	0.123242
63	6	0	-0.196753	5.668725	-1.186030
64	1	0	-0.964055	5.422704	-1.927432
65	1	0	0.000002	6.737929	-1.211867
66	1	0	0.724075	5.124713	-1.421223

Structure 39b (M06-2X, Benzene)

Energy (Hartrees): = - 1366.5152619
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.194123	1.763312	-0.077488
2	6	0	-1.624919	1.521693	1.221548
3	6	0	-1.710339	2.582788	2.117996
4	6	0	-1.370541	3.868664	1.727314
5	6	0	-0.941991	4.110971	0.421032
6	6	0	-0.855925	3.052962	-0.485544
7	1	0	-1.893628	0.516132	1.522946
8	1	0	-2.048062	2.406956	3.132715
9	1	0	-0.534319	3.214551	-1.507282
10	6	0	-1.063201	0.618509	-1.052020
11	1	0	-0.868321	1.015873	-2.065550
12	7	0	-0.009622	-0.326715	-0.673445
13	8	0	-2.237967	-0.166455	-1.078690
14	6	0	-1.882845	-1.553862	-1.192720
15	6	0	-0.373562	-1.523412	-1.434231
16	1	0	0.127619	-2.410527	-1.045470
17	1	0	-0.141175	-1.408953	-2.504402
18	1	0	-2.435507	-1.985446	-2.023834
19	6	0	-2.249155	-2.292688	0.095714
20	1	0	-2.174785	-3.371560	-0.099166
21	6	0	-3.658660	-1.991782	0.619648
22	1	0	-3.775836	-0.903481	0.695617
23	6	0	-4.786104	-2.551561	-0.246051
24	1	0	-4.665299	-3.636688	-0.319908
25	6	0	-6.142669	-2.245062	0.365739
26	1	0	-6.917918	-2.750169	-0.221424
27	1	0	-6.173661	-2.595557	1.400735
28	8	0	-1.348659	-1.989994	1.162061
29	1	0	-0.747117	-1.282988	0.868828
30	8	0	-3.796711	-2.596242	1.895785
31	1	0	-2.973968	-2.403288	2.360108
32	8	0	-4.737037	-2.033303	-1.563572
33	1	0	-4.993809	-1.105473	-1.490285
34	8	0	-6.294724	-0.831868	0.285829
35	1	0	-7.169074	-0.596752	0.603029

36	6	0	1.336923	0.180983	-0.908675
37	1	0	1.488629	0.376591	-1.985086
38	1	0	1.422085	1.138747	-0.386228
39	6	0	2.414899	-0.766131	-0.396998
40	1	0	2.205193	-1.001522	0.652100
41	1	0	2.379161	-1.710349	-0.951123
42	6	0	3.811209	-0.160704	-0.526909
43	1	0	3.848610	0.783675	0.028873
44	1	0	4.005087	0.088275	-1.577429
45	6	0	4.913716	-1.087080	-0.018217
46	1	0	4.879847	-2.032069	-0.573647
47	1	0	4.718631	-1.337337	1.031442
48	6	0	6.309063	-0.478344	-0.141954
49	1	0	6.340362	0.468774	0.410220
50	1	0	6.504578	-0.230589	-1.192529
51	6	0	7.414626	-1.397727	0.372445
52	1	0	7.221383	-1.643974	1.423793
53	1	0	7.383580	-2.346463	-0.177333
54	6	0	8.810668	-0.790482	0.246989
55	1	0	9.004522	-0.545755	-0.803239
56	1	0	8.842444	0.156438	0.796950
57	6	0	9.904247	-1.719670	0.765603
58	1	0	9.910790	-2.663156	0.212584
59	1	0	10.894608	-1.269330	0.666526
60	1	0	9.748622	-1.955060	1.822090
61	1	0	-1.432681	4.705638	2.412339
62	8	0	-0.634667	5.397421	0.123863
63	6	0	-0.243638	5.691421	-1.203291
64	1	0	-1.038031	5.445744	-1.915365
65	1	0	-0.056350	6.763017	-1.231210
66	1	0	0.673176	5.159816	-1.478047

Structure 39b (M06-2X, DMSO)

Energy (Hartrees): = - 1366.5168808
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.213407	1.749681	-0.087452
2	6	0	-1.649980	1.493368	1.208743
3	6	0	-1.756136	2.547596	2.112108
4	6	0	-1.432656	3.841697	1.730687
5	6	0	-0.998363	4.098245	0.427575
6	6	0	-0.890941	3.046239	-0.486087
7	1	0	-1.904086	0.482221	1.505661
8	1	0	-2.096165	2.361332	3.124611
9	1	0	-0.559067	3.217017	-1.503279
10	6	0	-1.060565	0.614110	-1.070346
11	1	0	-0.861225	1.019348	-2.077399
12	7	0	-0.002494	-0.323302	-0.686028
13	8	0	-2.232190	-0.181767	-1.109980
14	6	0	-1.861041	-1.567879	-1.210760
15	6	0	-0.354833	-1.520180	-1.456743
16	1	0	0.158656	-2.404960	-1.079461
17	1	0	-0.128662	-1.390201	-2.525101
18	1	0	-2.407627	-2.014512	-2.037233
19	6	0	-2.215868	-2.302575	0.083840
20	1	0	-2.143536	-3.381017	-0.110630
21	6	0	-3.619488	-1.995991	0.620683
22	1	0	-3.737710	-0.906689	0.674819
23	6	0	-4.757917	-2.576727	-0.216113
24	1	0	-4.637114	-3.662825	-0.267878
25	6	0	-6.108580	-2.256966	0.400096
26	1	0	-6.889295	-2.762281	-0.178149
27	1	0	-6.142707	-2.601926	1.436828
28	8	0	-1.302979	-1.995241	1.141181
29	1	0	-0.708057	-1.286955	0.831926
30	8	0	-3.737086	-2.567449	1.916042
31	1	0	-2.902479	-2.364042	2.355129
32	8	0	-4.724195	-2.087050	-1.547269
33	1	0	-4.981003	-1.158029	-1.488408
34	8	0	-6.258981	-0.842267	0.316058
35	1	0	-7.162017	-0.619150	0.559362
36	6	0	1.341400	0.195035	-0.927954
37	1	0	1.483829	0.391486	-2.003844
38	1	0	1.425883	1.152781	-0.404731
39	6	0	2.423350	-0.749501	-0.422091
40	1	0	2.215072	-0.994681	0.625745
41	1	0	2.393825	-1.688177	-0.985668
42	6	0	3.815499	-0.134000	-0.542384
43	1	0	3.844889	0.805372	0.022558
44	1	0	4.010773	0.123566	-1.590471

45	6	0	4.918775	-1.060153	-0.036618
46	1	0	4.894231	-1.997929	-0.604878
47	1	0	4.716876	-1.322825	1.009119
48	6	0	6.311797	-0.443624	-0.140889
49	1	0	6.333046	0.497636	0.422025
50	1	0	6.516838	-0.186356	-1.187477
51	6	0	7.414047	-1.364390	0.376843
52	1	0	7.209442	-1.620452	1.423980
53	1	0	7.392692	-2.307084	-0.184010
54	6	0	8.809538	-0.752712	0.274137
55	1	0	9.017011	-0.502144	-0.772260
56	1	0	8.831563	0.190236	0.831719
57	6	0	9.895926	-1.684551	0.802540
58	1	0	9.906795	-2.625849	0.245264
59	1	0	10.888463	-1.235505	0.716540
60	1	0	9.725937	-1.922598	1.856530
61	1	0	-1.512225	4.670585	2.424406
62	8	0	-0.706919	5.388166	0.138670
63	6	0	-0.316044	5.692789	-1.192440
64	1	0	-1.103884	5.429982	-1.904536
65	1	0	-0.150098	6.767804	-1.217352
66	1	0	0.610313	5.177738	-1.463116

Structure 39c (M06-2X, Gas Phase)

Energy (Hartrees): = - 1366.4853011
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.944410	-1.776177	-0.287589
2	6	0	1.637174	-1.914586	-1.060824
3	6	0	3.375778	-0.310975	-0.362930
4	1	0	1.285862	-2.944570	-0.981157
5	1	0	1.791442	-1.675680	-2.127936
6	1	0	3.721623	-2.411839	-0.707966
7	1	0	3.539325	-0.017765	-1.411988
8	8	0	2.316429	0.484032	0.174523
9	7	0	0.634348	-1.039154	-0.444619
10	6	0	4.608685	0.047510	0.465390
11	1	0	4.531797	-0.476677	1.426457
12	6	0	5.906792	-0.342554	-0.223649
13	1	0	5.972512	0.207776	-1.173566
14	6	0	7.106920	0.034902	0.626040
15	1	0	7.004542	-0.439441	1.610070
16	1	0	7.155688	1.120006	0.742173
17	8	0	4.684045	1.448413	0.649756
18	1	0	3.786018	1.749970	0.823085
19	8	0	5.908011	-1.736187	-0.455758
20	1	0	6.824387	-1.967457	-0.645308
21	8	0	8.239257	-0.478983	-0.068117
22	1	0	9.013344	-0.388955	0.489568
23	8	0	2.744482	-2.171428	1.052368
24	1	0	1.916932	-1.752559	1.320482
25	6	0	-0.698407	-1.233916	-1.032614
26	1	0	-0.706410	-2.216310	-1.513896
27	1	0	-0.878655	-0.503803	-1.838089
28	6	0	0.110527	1.300692	0.127778
29	6	0	0.052358	1.382408	1.512274
30	6	0	-0.778896	2.024517	-0.665218
31	6	0	-0.924723	2.175634	2.107709
32	1	0	0.758083	0.817792	2.107805
33	6	0	-1.762048	2.807238	-0.060689
34	1	0	-0.699722	1.960155	-1.743152
35	6	0	-1.835154	2.875044	1.332820
36	1	0	-0.982858	2.242841	3.187647
37	6	0	1.094618	0.353639	-0.513959
38	1	0	1.254414	0.638212	-1.574391
39	6	0	-1.843329	-1.188939	-0.023904
40	1	0	-1.698679	-1.998004	0.699655
41	1	0	-1.819739	-0.255480	0.540954
42	6	0	-3.202200	-1.324629	-0.705509
43	1	0	-3.312340	-0.527166	-1.452038
44	1	0	-3.254271	-2.272762	-1.255393
45	6	0	-4.364264	-1.243669	0.281225
46	1	0	-4.310262	-0.287814	0.816417
47	1	0	-4.251364	-2.028376	1.038803
48	6	0	-5.731418	-1.376442	-0.384614
49	1	0	-5.842466	-0.594357	-1.145687
50	1	0	-5.785374	-2.334064	-0.916841
51	6	0	-6.890176	-1.284149	0.605064
52	1	0	-6.839261	-0.324413	1.133683
53	1	0	-6.776202	-2.062027	1.369942

54	6	0	-8.260287	-1.424223	-0.054408
55	1	0	-8.373711	-0.647026	-0.817968
56	1	0	-8.309366	-2.383425	-0.581188
57	6	0	-9.406236	-1.330578	0.949939
58	1	0	-9.393336	-0.366928	1.465767
59	1	0	-10.378038	-1.438428	0.464408
60	1	0	-9.321185	-2.113149	1.708472
61	1	0	-2.606586	3.493180	1.774633
62	8	0	-2.683647	3.536501	-0.738108
63	6	0	-2.659554	3.479654	-2.148500
64	1	0	-3.477296	4.110603	-2.488634
65	1	0	-1.714717	3.864161	-2.545828
66	1	0	-2.816605	2.456638	-2.506972

Structure 39c (M06-2X, Benzene)

Energy (Hartrees): = - 1366.5127377
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.902977	-1.779229	-0.343322
2	6	0	1.592802	-1.878358	-1.117533
3	6	0	3.364932	-0.323128	-0.395872
4	1	0	1.221349	-2.902689	-1.059202
5	1	0	1.752439	-1.620813	-2.178825
6	1	0	3.663974	-2.425731	-0.776600
7	1	0	3.537867	-0.021526	-1.440710
8	8	0	2.321339	0.487259	0.150292
9	7	0	0.608224	-0.995730	-0.481852
10	6	0	4.599935	0.009277	0.440019
11	1	0	4.491993	-0.482830	1.414676
12	6	0	5.898144	-0.445723	-0.208801
13	1	0	5.986829	0.034964	-1.194225
14	6	0	7.097988	-0.036707	0.627912
15	1	0	6.975367	-0.432436	1.643781
16	1	0	7.180563	1.051856	0.665965
17	8	0	4.714270	1.413751	0.588001
18	1	0	3.823961	1.739592	0.760180
19	8	0	5.877107	-1.853257	-0.343962
20	1	0	6.794945	-2.111608	-0.488655
21	8	0	8.226439	-0.627359	-0.011072
22	1	0	8.985445	-0.549699	0.571259
23	8	0	2.695012	-2.194000	0.991510
24	1	0	1.872336	-1.765880	1.262406
25	6	0	-0.731499	-1.160095	-1.066206
26	1	0	-0.755229	-2.132323	-1.566769
27	1	0	-0.905887	-0.410207	-1.853965
28	6	0	0.131759	1.345444	0.130623
29	6	0	0.079965	1.400035	1.517397
30	6	0	-0.739865	2.110036	-0.644247
31	6	0	-0.869490	2.211348	2.132730
32	1	0	0.769468	0.803925	2.101651
33	6	0	-1.696317	2.911250	-0.019788
34	1	0	-0.667805	2.064711	-1.723688
35	6	0	-1.760325	2.955002	1.375604
36	1	0	-0.921544	2.258841	3.214301
37	6	0	1.092149	0.389381	-0.534671
38	1	0	1.250226	0.687044	-1.590449
39	6	0	-1.867760	-1.123196	-0.047439
40	1	0	-1.706034	-1.926933	0.678854
41	1	0	-1.851249	-0.185463	0.511603
42	6	0	-3.230473	-1.283390	-0.716726
43	1	0	-3.360635	-0.490231	-1.464507
44	1	0	-3.267189	-2.234230	-1.263153
45	6	0	-4.388446	-1.224964	0.277033
46	1	0	-4.359705	-0.263195	0.803614
47	1	0	-4.249882	-2.000139	1.040242
48	6	0	-5.754185	-1.404151	-0.381981
49	1	0	-5.891795	-0.629850	-1.146749
50	1	0	-5.778064	-2.366057	-0.908871
51	6	0	-6.914995	-1.345531	0.608423
52	1	0	-6.898392	-0.381516	1.131511
53	1	0	-6.775553	-2.115607	1.377061
54	6	0	-8.278619	-1.537151	-0.052570
55	1	0	-8.420982	-0.762873	-0.814460
56	1	0	-8.290039	-2.496860	-0.580981
57	6	0	-9.430147	-1.490262	0.946957
58	1	0	-9.455248	-0.530960	1.471407
59	1	0	-10.396043	-1.625827	0.454988
60	1	0	-9.326684	-2.276073	1.700588
61	1	0	-2.509279	3.587615	1.836255
62	8	0	-2.596373	3.679606	-0.679492

63	6	0	-2.581030	3.646529	-2.093673
64	1	0	-3.383637	4.305418	-2.418971
65	1	0	-1.630124	4.015221	-2.491284
66	1	0	-2.770688	2.635988	-2.470768

Structure 39c (M06-2X, DMSO)

Energy (Hartrees): = - 1366.5148779
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.912994	-1.782957	-0.289352
2	6	0	1.591590	-1.907015	-1.037871
3	6	0	3.365398	-0.327534	-0.382651
4	1	0	1.225114	-2.931480	-0.955080
5	1	0	1.734068	-1.668048	-2.104508
6	1	0	3.667063	-2.436660	-0.723537
7	1	0	3.508713	-0.050045	-1.437638
8	8	0	2.327978	0.486987	0.172602
9	7	0	0.608864	-1.015144	-0.406977
10	6	0	4.619502	0.032831	0.410193
11	1	0	4.537898	-0.414383	1.408750
12	6	0	5.901009	-0.457144	-0.246764
13	1	0	5.940663	-0.071958	-1.276222
14	6	0	7.126179	0.040305	0.501244
15	1	0	7.048123	-0.254639	1.554824
16	1	0	7.199963	1.127921	0.433483
17	8	0	4.734040	1.444646	0.496867
18	1	0	3.842226	1.772063	0.661109
19	8	0	5.900710	-1.873909	-0.251036
20	1	0	6.819645	-2.126504	-0.403560
21	8	0	8.240001	-0.596257	-0.120149
22	1	0	9.004107	-0.500866	0.455826
23	8	0	2.732970	-2.168990	1.062191
24	1	0	1.922192	-1.722151	1.340533
25	6	0	-0.727801	-1.188009	-1.003381
26	1	0	-0.748885	-2.169156	-1.485597
27	1	0	-0.890039	-0.450204	-1.803556
28	6	0	0.130634	1.335222	0.153888
29	6	0	0.085670	1.418631	1.540790
30	6	0	-0.751525	2.073674	-0.634139
31	6	0	-0.867880	2.235597	2.143706
32	1	0	0.780380	0.839912	2.137338
33	6	0	-1.713216	2.879903	-0.021732
34	1	0	-0.687764	1.997288	-1.712596
35	6	0	-1.769600	2.954992	1.374018
36	1	0	-0.915513	2.306952	3.224532
37	6	0	1.090082	0.370756	-0.500005
38	1	0	1.235239	0.642559	-1.562137
39	6	0	-1.875787	-1.132818	0.001409
40	1	0	-1.738510	-1.937138	0.732867
41	1	0	-1.857354	-0.191700	0.556362
42	6	0	-3.229752	-1.278602	-0.688392
43	1	0	-3.342762	-0.478611	-1.431463
44	1	0	-3.261816	-2.225024	-1.242344
45	6	0	-4.401999	-1.223357	0.287920
46	1	0	-4.372578	-0.270471	0.831357
47	1	0	-4.285317	-2.013927	1.039265
48	6	0	-5.758156	-1.374322	-0.396873
49	1	0	-5.876088	-0.581151	-1.145524
50	1	0	-5.781988	-2.324451	-0.944773
51	6	0	-6.933113	-1.327408	0.576581
52	1	0	-6.915310	-0.376061	1.122757
53	1	0	-6.813728	-2.118334	1.327494
54	6	0	-8.287715	-1.488240	-0.109843
55	1	0	-8.411046	-0.693840	-0.854318
56	1	0	-8.300645	-2.435275	-0.660759
57	6	0	-9.451906	-1.453083	0.875169
58	1	0	-9.475003	-0.504340	1.419211
59	1	0	-10.412944	-1.570315	0.368530
60	1	0	-9.363637	-2.255928	1.613029
61	1	0	-2.520706	3.589802	1.829402
62	8	0	-2.623138	3.622093	-0.694978
63	6	0	-2.615497	3.544119	-2.113185
64	1	0	-3.425984	4.185191	-2.453807
65	1	0	-1.669163	3.907084	-2.524728
66	1	0	-2.795808	2.520094	-2.454041

Structure 39d (M06-2X, Gas Phase)

Energy (Hartrees): = - 1366.486348

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.845618	-1.415967	-1.365732
2	6	0	0.834703	-0.355019	-1.815989
3	6	0	2.451584	-0.936634	-0.046451
4	1	0	0.328484	-0.685434	-2.723736
5	1	0	1.367553	0.574962	-2.044705
6	1	0	2.632192	-1.545799	-2.108004
7	1	0	2.945004	0.031359	-0.200506
8	8	0	1.370028	-0.776769	0.884852
9	7	0	-0.175712	-0.069369	-0.793115
10	6	0	3.433322	-1.896181	0.629625
11	1	0	3.064993	-2.923392	0.507092
12	6	0	4.830589	-1.796998	0.040058
13	1	0	5.197276	-0.771241	0.191482
14	6	0	5.787765	-2.750631	0.731556
15	1	0	5.385454	-3.768793	0.657596
16	1	0	5.898770	-2.472677	1.782412
17	8	0	3.568439	-1.565737	2.000725
18	1	0	2.678066	-1.385819	2.321290
19	8	0	4.762848	-2.103318	-1.336977
20	1	0	5.671965	-2.263124	-1.614087
21	8	0	7.014630	-2.638251	0.018130
22	1	0	7.611345	-3.327466	0.313732
23	8	0	1.217302	-2.676154	-1.200468
24	1	0	0.725329	-2.632545	-0.373916
25	6	0	-1.305527	-0.998401	-0.707975
26	1	0	-1.148415	-1.767387	0.065929
27	1	0	-1.386236	-1.532616	-1.657395
28	6	0	1.036289	1.620551	0.541598
29	6	0	0.487663	2.638974	-0.219872
30	6	0	2.089474	1.897070	1.419683
31	6	0	0.981033	3.942629	-0.118838
32	1	0	-0.324891	2.434419	-0.906195
33	6	0	2.575184	3.190752	1.513004
34	1	0	2.536558	1.096968	1.997414
35	6	0	2.030555	4.224854	0.752314
36	1	0	3.396501	3.408583	2.185513
37	6	0	0.423475	0.225499	0.481257
38	1	0	-0.355943	0.166357	1.245295
39	6	0	-2.608269	-0.258170	-0.421411
40	1	0	-2.510255	0.308907	0.512398
41	1	0	-2.765319	0.479612	-1.214790
42	6	0	-3.809433	-1.194912	-0.326830
43	1	0	-3.913237	-1.747548	-1.268561
44	1	0	-3.632090	-1.945947	0.452664
45	6	0	-5.113103	-0.457963	-0.028667
46	1	0	-5.276965	0.309999	-0.794052
47	1	0	-5.017020	0.074330	0.925358
48	6	0	-6.327793	-1.381028	0.027645
49	1	0	-6.429624	-1.904357	-0.930802
50	1	0	-6.161849	-2.155936	0.785863
51	6	0	-7.626251	-0.640454	0.338218
52	1	0	-7.786197	0.141627	-0.414056
53	1	0	-7.528104	-0.124797	1.301399
54	6	0	-8.848162	-1.555502	0.379440
55	1	0	-8.946182	-2.067397	-0.583988
56	1	0	-8.687536	-2.337261	1.129698
57	6	0	-10.135948	-0.797455	0.692459
58	1	0	-10.324371	-0.027176	-0.059961
59	1	0	-11.000773	-1.463172	0.714900
60	1	0	-10.067935	-0.301738	1.664381
61	1	0	2.431390	5.224702	0.846014
62	8	0	0.373803	4.861114	-0.913495
63	6	0	0.848941	6.188961	-0.860705
64	1	0	1.901279	6.246048	-1.157744
65	1	0	0.243575	6.753966	-1.565760
66	1	0	0.730542	6.614421	0.141152

Structure 39d (M06-2X, Benzene)

Energy (Hartrees): = - 1366.5136424
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.858075	-1.421381	-1.352498
2	6	0	0.833693	-0.374192	-1.803466

3	6	0	2.475770	-0.922634	-0.045965
4	1	0	0.321036	-0.716915	-2.703024
5	1	0	1.360560	0.554909	-2.048762
6	1	0	2.636139	-1.550457	-2.103704
7	1	0	2.963364	0.044638	-0.220611
8	8	0	1.405110	-0.754856	0.895963
9	7	0	-0.167764	-0.085320	-0.773260
10	6	0	3.470646	-1.865803	0.635431
11	1	0	3.100812	-2.895977	0.549886
12	6	0	4.858234	-1.786947	0.018976
13	1	0	5.221175	-0.752647	0.111473
14	6	0	5.834402	-2.701303	0.737307
15	1	0	5.437169	-3.723947	0.732315
16	1	0	5.974973	-2.368037	1.768528
17	8	0	3.627063	-1.498365	1.996277
18	1	0	2.740696	-1.308770	2.323916
19	8	0	4.769279	-2.161590	-1.341298
20	1	0	5.674432	-2.343865	-1.619561
21	8	0	7.045597	-2.627312	-0.008933
22	1	0	7.635519	-3.321884	0.292333
23	8	0	1.244484	-2.688062	-1.167988
24	1	0	0.746083	-2.635578	-0.345117
25	6	0	-1.294705	-1.018234	-0.671731
26	1	0	-1.131349	-1.778326	0.109378
27	1	0	-1.377642	-1.559998	-1.616618
28	6	0	1.032876	1.636522	0.532677
29	6	0	0.448550	2.643717	-0.218633
30	6	0	2.100077	1.936605	1.386068
31	6	0	0.918886	3.957511	-0.132018
32	1	0	-0.375715	2.422810	-0.885953
33	6	0	2.565172	3.239632	1.463589
34	1	0	2.573612	1.148377	1.959020
35	6	0	1.984605	4.261304	0.712890
36	1	0	3.398645	3.475068	2.115482
37	6	0	0.440226	0.230496	0.491657
38	1	0	-0.330080	0.168650	1.264612
39	6	0	-2.600634	-0.280976	-0.389796
40	1	0	-2.506536	0.289520	0.542410
41	1	0	-2.759020	0.451725	-1.187958
42	6	0	-3.799486	-1.221545	-0.296289
43	1	0	-3.894058	-1.780532	-1.235338
44	1	0	-3.624850	-1.965767	0.490262
45	6	0	-5.108750	-0.487275	-0.013779
46	1	0	-5.268794	0.274251	-0.786461
47	1	0	-5.022445	0.051707	0.937463
48	6	0	-6.321278	-1.414266	0.038789
49	1	0	-6.411524	-1.946066	-0.916228
50	1	0	-6.160147	-2.181480	0.805898
51	6	0	-7.626447	-0.676389	0.329571
52	1	0	-7.783209	0.096521	-0.432878
53	1	0	-7.539590	-0.150308	1.288252
54	6	0	-8.845327	-1.596057	0.370012
55	1	0	-8.933944	-2.119135	-0.588558
56	1	0	-8.689985	-2.368292	1.131474
57	6	0	-10.139050	-0.841542	0.662317
58	1	0	-10.330478	-0.083618	-0.102509
59	1	0	-11.000132	-1.513093	0.688849
60	1	0	-10.083990	-0.330801	1.627763
61	1	0	2.369642	5.268728	0.792617
62	8	0	0.276009	4.862792	-0.910253
63	6	0	0.721345	6.204483	-0.862009
64	1	0	1.761072	6.291348	-1.193606
65	1	0	0.081433	6.759673	-1.545188
66	1	0	0.619864	6.623614	0.144214

Structure 39d (M06-2X, DMSO)

Energy (Hartrees): = - 1366.5146845
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.858117	-1.390975	-1.370286
2	6	0	0.850717	-0.331936	-1.829681
3	6	0	2.457979	-0.909788	-0.050802
4	1	0	0.347965	-0.664236	-2.738902
5	1	0	1.396904	0.589201	-2.063001
6	1	0	2.647079	-1.510454	-2.111668
7	1	0	2.966757	0.048319	-0.217259
8	8	0	1.376710	-0.725074	0.875575
9	7	0	-0.164237	-0.031890	-0.814860
10	6	0	3.423322	-1.864470	0.651875
11	1	0	3.006027	-2.879341	0.629876

12	6	0	4.801197	-1.890095	0.008920
13	1	0	5.193067	-0.862988	-0.028085
14	6	0	5.768411	-2.744871	0.809469
15	1	0	5.344763	-3.748779	0.933580
16	1	0	5.944843	-2.301744	1.792176
17	8	0	3.616858	-1.433535	1.991365
18	1	0	2.740181	-1.208231	2.324699
19	8	0	4.681274	-2.418415	-1.299980
20	1	0	5.577909	-2.669485	-1.554360
21	8	0	6.965358	-2.792889	0.037098
22	1	0	7.522576	-3.495715	0.383724
23	8	0	1.238541	-2.660352	-1.216395
24	1	0	0.717376	-2.618785	-0.406091
25	6	0	-1.290937	-0.969773	-0.724517
26	1	0	-1.122554	-1.743781	0.040623
27	1	0	-1.381138	-1.487660	-1.682148
28	6	0	1.039661	1.671111	0.515062
29	6	0	0.475883	2.692391	-0.234804
30	6	0	2.100917	1.954703	1.381793
31	6	0	0.959548	4.001595	-0.134097
32	1	0	-0.345009	2.486946	-0.911673
33	6	0	2.580276	3.252912	1.474008
34	1	0	2.560390	1.159717	1.956876
35	6	0	2.020564	4.287749	0.724775
36	1	0	3.408309	3.474480	2.138036
37	6	0	0.430252	0.272365	0.460725
38	1	0	-0.351970	0.220212	1.222004
39	6	0	-2.595719	-0.242164	-0.417535
40	1	0	-2.496105	0.307904	0.526149
41	1	0	-2.768668	0.502612	-1.202149
42	6	0	-3.786508	-1.193259	-0.331547
43	1	0	-3.889307	-1.729453	-1.283003
44	1	0	-3.594925	-1.953176	0.435837
45	6	0	-5.096314	-0.475945	-0.013195
46	1	0	-5.272208	0.303509	-0.764661
47	1	0	-5.000727	0.037247	0.951556
48	6	0	-6.300606	-1.413605	0.030535
49	1	0	-6.401266	-1.918080	-0.938385
50	1	0	-6.122511	-2.199935	0.774464
51	6	0	-7.606098	-0.694163	0.361166
52	1	0	-7.779274	0.098329	-0.377549
53	1	0	-7.508629	-0.196419	1.334063
54	6	0	-8.817341	-1.623663	0.392199
55	1	0	-8.915594	-2.119757	-0.579894
56	1	0	-8.646735	-2.414893	1.130823
57	6	0	-10.111392	-0.885972	0.722994
58	1	0	-10.317198	-0.108886	-0.018914
59	1	0	-10.968094	-1.563828	0.743502
60	1	0	-10.043922	-0.401830	1.701622
61	1	0	2.415770	5.290500	0.816537
62	8	0	0.335966	4.920135	-0.910165
63	6	0	0.808560	6.258027	-0.848924
64	1	0	1.852877	6.322758	-1.168364
65	1	0	0.185968	6.829552	-1.534336
66	1	0	0.706128	6.669415	0.159531

Structure 43a (^{2}E ec-ax H-bond O) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1181.3341946
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.096912	0.358069	0.640612
2	6	0	-2.355216	-0.861976	0.016441
3	6	0	-3.648329	-1.206566	-0.352320
4	6	0	-4.673256	-0.316326	-0.074906
5	6	0	-4.455548	0.895333	0.561766
6	6	0	-3.155729	1.223220	0.918088
7	1	0	-1.542764	-1.556467	-0.155956
8	1	0	-3.875016	-2.146267	-0.836776
9	1	0	-5.292542	1.547282	0.770052
10	1	0	-2.963023	2.162687	1.425589
11	6	0	-0.675925	0.784257	0.983295
12	1	0	-0.692235	1.375180	1.905157
13	7	0	0.003387	1.542529	-0.063044
14	8	0	0.146322	-0.350978	1.168749
15	6	0	1.033713	-0.498916	0.041730
16	6	0	0.540067	0.533813	-0.965014
17	1	0	1.355160	0.939753	-1.563639
18	1	0	-0.227937	0.107245	-1.630359
19	1	0	0.944961	-1.530731	-0.312168
20	6	0	2.454016	-0.252194	0.539986

21	1	0	2.578477	0.822751	0.723358
22	6	0	3.522403	-0.686229	-0.467311
23	1	0	3.242505	-1.665717	-0.882170
24	6	0	4.876132	-0.877502	0.239980
25	1	0	4.856103	-1.858448	0.724971
26	6	0	6.051375	-0.813507	-0.727752
27	1	0	6.950937	-1.197674	-0.237512
28	1	0	5.853296	-1.404457	-1.623378
29	8	0	2.659789	-0.991767	1.737269
30	1	0	1.850076	-0.898814	2.252964
31	8	0	3.545139	0.246674	-1.530803
32	1	0	4.422219	0.653364	-1.571841
33	8	0	5.135971	0.138148	1.197755
34	1	0	4.514932	-0.002439	1.921316
35	8	0	6.254493	0.529201	-1.150692
36	1	0	6.330514	1.047169	-0.340087
37	6	0	-0.738448	2.611080	-0.700251
38	1	0	-1.102006	3.310188	0.056604
39	1	0	-0.063323	3.154780	-1.362599
40	1	0	-1.597574	2.255582	-1.289086
41	7	0	-6.053806	-0.680326	-0.457281
42	8	0	-6.932499	0.109763	-0.193123
43	8	0	-6.216700	-1.744256	-1.011433

Structure 43a (^{2}E ec-ax H-bond N) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1181.3360066
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.930089	0.277576	-0.458919
2	6	0	2.251065	-0.822836	0.335123
3	6	0	3.571917	-1.224283	0.480873
4	6	0	4.555255	-0.513754	-0.188642
5	6	0	4.268302	0.567825	-1.006462
6	6	0	2.942950	0.955137	-1.137810
7	1	0	1.457513	-1.381879	0.814992
8	1	0	3.849279	-2.074576	1.088704
9	1	0	5.071628	1.075756	-1.522054
10	1	0	2.692511	1.791320	-1.782329
11	6	0	0.495249	0.768200	-0.566458
12	1	0	0.330647	1.196081	-1.561803
13	7	0	0.123725	1.778425	0.444269
14	8	0	-0.400873	-0.294646	-0.350805
15	6	0	-1.158955	-0.072233	0.846149
16	6	0	-0.350017	0.991891	1.581830
17	1	0	-0.963471	1.608911	2.242151
18	1	0	0.475283	0.555769	2.164377
19	1	0	-1.235492	-1.018327	1.384600
20	6	0	-2.569332	0.389018	0.494657
21	1	0	-3.105820	0.567079	1.437613
22	6	0	-3.325964	-0.715055	-0.243641
23	1	0	-2.686756	-1.089365	-1.051527
24	6	0	-4.609177	-0.154377	-0.887226
25	1	0	-4.339347	0.243830	-1.870479
26	6	0	-5.689140	-1.217764	-1.045026
27	1	0	-6.471615	-0.850018	-1.715836
28	1	0	-5.272468	-2.140264	-1.451174
29	8	0	-2.573418	1.563614	-0.303979
30	1	0	-1.737020	2.034941	-0.156161
31	8	0	-3.530055	-1.779971	0.667073
32	1	0	-4.470750	-1.825244	0.886168
33	8	0	-5.217842	0.864876	-0.102551
34	1	0	-4.613328	1.616663	-0.107856
35	8	0	-6.238140	-1.531925	0.228844
36	1	0	-6.493420	-0.684569	0.613035
37	6	0	1.113430	2.793777	0.760858
38	1	0	1.410153	3.316152	-0.150689
39	1	0	0.662128	3.521963	1.436225
40	1	0	2.012650	2.378870	1.236129
41	7	0	5.964629	-0.934520	-0.038009
42	8	0	6.803142	-0.295949	-0.633844
43	8	0	6.189082	-1.887144	0.674047

Structure 43a (^{2}E ec-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1181.3363164
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.166096	0.249565	0.349086
2	6	0	-2.687359	0.100210	-0.936522
3	6	0	-4.026204	-0.204334	-1.114891
4	6	0	-4.823276	-0.354666	0.012764
5	6	0	-4.335118	-0.212438	1.299579
6	6	0	-2.987655	0.092046	1.458680
7	1	0	-2.029059	0.239668	-1.785086
8	1	0	-4.464151	-0.325550	-2.096082
9	1	0	-5.001467	-0.339487	2.141216
10	1	0	-2.575295	0.208102	2.454812
11	6	0	-0.703874	0.582597	0.508017
12	1	0	-0.465245	0.712223	1.582417
13	7	0	-0.314673	1.749765	-0.261097
14	8	0	0.092773	-0.462182	-0.021358
15	6	0	1.266174	0.112228	-0.624697
16	6	0	1.132856	1.609741	-0.363248
17	1	0	1.643243	1.885206	0.573711
18	1	0	1.544595	2.219383	-1.166743
19	1	0	1.229192	-0.118492	-1.694523
20	6	0	2.476922	-0.560481	-0.005126
21	1	0	2.548852	-0.258772	1.048784
22	6	0	3.778670	-0.160412	-0.694595
23	1	0	3.643289	-0.250117	-1.781259
24	6	0	4.915190	-1.125196	-0.301781
25	1	0	4.854939	-1.993949	-0.965016
26	6	0	6.290285	-0.481739	-0.429097
27	1	0	7.062880	-1.254454	-0.374579
28	1	0	6.385732	0.054242	-1.374418
29	8	0	2.340903	-1.971924	-0.103852
30	1	0	1.429718	-2.178362	0.135224
31	8	0	4.027191	1.202522	-0.407133
32	1	0	4.820449	1.265671	0.143825
33	8	0	4.832059	-1.540991	1.054310
34	1	0	4.047883	-2.097758	1.123957
35	8	0	6.469909	0.471007	0.611645
36	1	0	6.287139	-0.003403	1.431697
37	6	0	-0.751914	3.000811	0.328620
38	1	0	-0.336495	3.152123	1.338948
39	1	0	-0.433247	3.829524	-0.304290
40	1	0	-1.841849	3.017654	0.389967
41	7	0	-6.255570	-0.676052	-0.168991
42	8	0	-6.931144	-0.798580	0.828324
43	8	0	-6.660566	-0.795733	-1.303522

Structure 43a (E_2 ax-ax) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1181.3371761
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.119108	0.806531	0.477370
2	6	0	-2.459962	-0.364827	1.151674
3	6	0	-3.643618	-1.027083	0.857089
4	6	0	-4.470205	-0.494075	-0.118829
5	6	0	-4.157479	0.667817	-0.807383
6	6	0	-2.970163	1.317969	-0.501747
7	1	0	-1.785783	-0.758278	1.902003
8	1	0	-3.931505	-1.938629	1.362059
9	1	0	-4.835377	1.037955	-1.564113
10	1	0	-2.679853	2.216819	-1.031333
11	6	0	-0.833838	1.540528	0.833979
12	1	0	-1.030603	2.284918	1.609147
13	7	0	-0.227603	2.149304	-0.324537
14	8	0	0.131954	0.626833	1.358988
15	6	0	0.808014	0.057991	0.227753
16	6	0	0.458666	1.007844	-0.951225
17	1	0	1.343576	1.328523	-1.497260
18	1	0	-0.221216	0.510131	-1.644508
19	1	0	0.416538	-0.952134	0.058174
20	6	0	2.279346	-0.037996	0.598909
21	1	0	2.709407	0.971367	0.643127
22	6	0	3.098308	-0.833002	-0.420592
23	1	0	2.538579	-1.737078	-0.701550
24	6	0	4.417474	-1.308170	0.212495
25	1	0	4.186404	-2.187757	0.821357
26	6	0	5.466196	-1.676238	-0.828482
27	1	0	6.283932	-2.219983	-0.346296
28	1	0	5.036879	-2.301987	-1.612792
29	8	0	2.404444	-0.682155	1.861340

30	1	0	1.722053	-0.305716	2.428661
31	8	0	3.252430	-0.027208	-1.573008
32	1	0	4.195152	0.058173	-1.773923
33	8	0	5.026553	-0.303512	1.010408
34	1	0	4.470293	-0.199744	1.790629
35	8	0	5.958263	-0.498874	-1.456854
36	1	0	6.245178	0.078735	-0.738982
37	6	0	0.694928	3.223337	0.049195
38	1	0	1.191875	3.590571	-0.848434
39	1	0	0.127150	4.048056	0.483192
40	1	0	1.458429	2.903043	0.770483
41	7	0	-5.731354	-1.193385	-0.442347
42	8	0	-6.434557	-0.708906	-1.300791
43	8	0	-5.981558	-2.206448	0.172081

Structure 43a (^{2}E ec-ax H-bond O) (M06-2X, Benzene)

Energy (Hartrees): = - 1181.3551202
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.100761	0.376710	0.651537
2	6	0	-2.348026	-0.869007	0.074734
3	6	0	-3.634644	-1.231596	-0.299464
4	6	0	-4.664386	-0.330484	-0.078562
5	6	0	-4.457908	0.907113	0.512376
6	6	0	-3.164834	1.251685	0.876314
7	1	0	-1.533732	-1.569445	-0.061856
8	1	0	-3.845609	-2.192545	-0.748499
9	1	0	-5.294669	1.570505	0.682260
10	1	0	-2.982948	2.211585	1.348290
11	6	0	-0.684746	0.822063	0.993567
12	1	0	-0.710341	1.430921	1.902718
13	7	0	-0.007804	1.562055	-0.067932
14	8	0	0.148178	-0.302040	1.204626
15	6	0	1.024308	-0.478075	0.071574
16	6	0	0.524788	0.535079	-0.951806
17	1	0	1.334590	0.931897	-1.563210
18	1	0	-0.246512	0.095653	-1.604009
19	1	0	0.928399	-1.516058	-0.261338
20	6	0	2.450550	-0.227489	0.552112
21	1	0	2.580136	0.848889	0.723860
22	6	0	3.508934	-0.676492	-0.460869
23	1	0	3.213876	-1.650665	-0.876562
24	6	0	4.864787	-0.886586	0.235454
25	1	0	4.831483	-1.862069	0.729937
26	6	0	6.033788	-0.862510	-0.740146
27	1	0	6.929222	-1.254128	-0.248049
28	1	0	5.822045	-1.469866	-1.621776
29	8	0	2.665716	-0.953555	1.757361
30	1	0	1.870261	-0.830621	2.289355
31	8	0	3.541675	0.261407	-1.522907
32	1	0	4.431800	0.636961	-1.575285
33	8	0	5.152803	0.135506	1.180169
34	1	0	4.528880	0.018941	1.906122
35	8	0	6.264541	0.468493	-1.193502
36	1	0	6.368913	1.000970	-0.395142
37	6	0	-0.747770	2.619594	-0.725758
38	1	0	-1.114379	3.332845	0.016399
39	1	0	-0.070502	3.152213	-1.395830
40	1	0	-1.603189	2.254921	-1.314257
41	7	0	-6.035593	-0.710432	-0.467261
42	8	0	-6.927186	0.074266	-0.225355
43	8	0	-6.190530	-1.784363	-1.007037

Structure 43a (^{2}E ec-ax H-bond N) (M06-2X, Benzene)

Energy (Hartrees): = - 1181.3580938
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.932819	0.281333	-0.455076
2	6	0	2.250197	-0.822746	0.335717
3	6	0	3.569558	-1.228463	0.481387
4	6	0	4.555843	-0.517484	-0.184621
5	6	0	4.272651	0.572052	-0.994532
6	6	0	2.948781	0.962966	-1.126334

7	1	0	1.457553	-1.380794	0.818386
8	1	0	3.837744	-2.082853	1.087771
9	1	0	5.073987	1.086290	-1.507130
10	1	0	2.701469	1.804562	-1.764777
11	6	0	0.498143	0.772541	-0.573471
12	1	0	0.342133	1.192478	-1.573048
13	7	0	0.117493	1.786033	0.426850
14	8	0	-0.401553	-0.289428	-0.356221
15	6	0	-1.145592	-0.070300	0.852016
16	6	0	-0.339390	1.004837	1.575097
17	1	0	-0.952966	1.621575	2.235276
18	1	0	0.492910	0.579177	2.154260
19	1	0	-1.203148	-1.013874	1.397051
20	6	0	-2.563578	0.380332	0.514653
21	1	0	-3.091873	0.548668	1.463669
22	6	0	-3.322846	-0.718849	-0.230165
23	1	0	-2.684808	-1.096011	-1.037414
24	6	0	-4.600804	-0.152884	-0.878508
25	1	0	-4.323120	0.256386	-1.854737
26	6	0	-5.678658	-1.212177	-1.065623
27	1	0	-6.454675	-0.831358	-1.736853
28	1	0	-5.260861	-2.125965	-1.490233
29	8	0	-2.578486	1.564940	-0.271240
30	1	0	-1.728359	2.021504	-0.143799
31	8	0	-3.540736	-1.787446	0.677260
32	1	0	-4.485618	-1.830001	0.877283
33	8	0	-5.217978	0.856829	-0.086072
34	1	0	-4.608252	1.604722	-0.069946
35	8	0	-6.244304	-1.554121	0.196655
36	1	0	-6.510837	-0.715654	0.593465
37	6	0	1.085954	2.827555	0.721480
38	1	0	1.364614	3.343271	-0.199842
39	1	0	0.622617	3.556196	1.388767
40	1	0	1.996866	2.442504	1.199553
41	7	0	5.960978	-0.943729	-0.037335
42	8	0	6.806446	-0.306056	-0.626828
43	8	0	6.187467	-1.903371	0.666892

Structure 43a (^{2}E ec-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 1181.3576021
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.171572	0.245631	0.345079
2	6	0	-2.671896	-0.030854	-0.927966
3	6	0	-4.010683	-0.337960	-1.100180
4	6	0	-4.831204	-0.358811	0.021629
5	6	0	-4.363906	-0.089860	1.296227
6	6	0	-3.015413	0.212595	1.449561
7	1	0	-2.001578	0.007493	-1.777909
8	1	0	-4.426206	-0.554948	-2.074608
9	1	0	-5.042261	-0.117369	2.137574
10	1	0	-2.620999	0.425596	2.436962
11	6	0	-0.711668	0.595939	0.495733
12	1	0	-0.480014	0.780710	1.562131
13	7	0	-0.329250	1.727781	-0.329771
14	8	0	0.095250	-0.467267	0.019461
15	6	0	1.263778	0.085954	-0.614930
16	6	0	1.119991	1.592907	-0.423728
17	1	0	1.626441	1.916890	0.499350
18	1	0	1.523923	2.166701	-1.257451
19	1	0	1.225711	-0.193577	-1.673048
20	6	0	2.480657	-0.550250	0.031913
21	1	0	2.547755	-0.206192	1.072785
22	6	0	3.782230	-0.170011	-0.671452
23	1	0	3.645488	-0.283178	-1.755530
24	6	0	4.918245	-1.125748	-0.260232
25	1	0	4.840731	-2.019839	-0.886632
26	6	0	6.296714	-0.505964	-0.442738
27	1	0	7.061406	-1.285158	-0.369284
28	1	0	6.382494	-0.018278	-1.415064
29	8	0	2.354513	-1.966879	-0.009899
30	1	0	1.452095	-2.170978	0.262873
31	8	0	4.037784	1.199088	-0.410135
32	1	0	4.850862	1.266452	0.110115
33	8	0	4.855976	-1.484242	1.114676
34	1	0	4.066667	-2.028320	1.219357
35	8	0	6.515517	0.493209	0.549234
36	1	0	6.353661	0.059050	1.396035
37	6	0	-0.773601	3.004573	0.196711
38	1	0	-0.372103	3.203033	1.204247

39	1	0	-0.445756	3.803847	-0.469361
40	1	0	-1.864456	3.027971	0.242493
41	7	0	-6.262211	-0.675606	-0.154630
42	8	0	-6.970243	-0.651125	0.828668
43	8	0	-6.645506	-0.942032	-1.273004

Structure 43a (E_2 ax-ax) (M06-2X, Benzene)

Energy (Hartrees): = - 1181.3579028
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.122871	0.796015	0.482199
2	6	0	-2.461543	-0.388448	1.135083
3	6	0	-3.648544	-1.042740	0.837254
4	6	0	-4.483306	-0.487269	-0.119899
5	6	0	-4.174481	0.689510	-0.785743
6	6	0	-2.982964	1.330169	-0.477472
7	1	0	-1.784102	-0.800802	1.872227
8	1	0	-3.927585	-1.964529	1.328546
9	1	0	-4.855224	1.082178	-1.528611
10	1	0	-2.700626	2.240294	-0.992027
11	6	0	-0.830987	1.518485	0.842051
12	1	0	-1.022437	2.254375	1.626203
13	7	0	-0.224546	2.139275	-0.310010
14	8	0	0.130942	0.592258	1.351687
15	6	0	0.811917	0.040705	0.213954
16	6	0	0.464431	1.007466	-0.950765
17	1	0	1.350221	1.340915	-1.487572
18	1	0	-0.210166	0.518242	-1.655429
19	1	0	0.424263	-0.967642	0.027493
20	6	0	2.282906	-0.054150	0.590280
21	1	0	2.706563	0.957515	0.642243
22	6	0	3.110615	-0.849037	-0.422554
23	1	0	2.562317	-1.762347	-0.691739
24	6	0	4.439905	-1.298880	0.210699
25	1	0	4.230161	-2.188409	0.812376
26	6	0	5.498952	-1.639012	-0.828219
27	1	0	6.327477	-2.167569	-0.347148
28	1	0	5.087411	-2.272991	-1.615386
29	8	0	2.403765	-0.703291	1.851974
30	1	0	1.726731	-0.319929	2.421817
31	8	0	3.254469	-0.061010	-1.591289
32	1	0	4.197738	0.075991	-1.757989
33	8	0	5.026184	-0.285265	1.017418
34	1	0	4.457613	-0.190090	1.790185
35	8	0	5.970780	-0.447776	-1.452107
36	1	0	6.254827	0.129351	-0.732244
37	6	0	0.693122	3.214247	0.073056
38	1	0	1.183885	3.596846	-0.822192
39	1	0	0.123133	4.030923	0.520023
40	1	0	1.463434	2.892196	0.786548
41	7	0	-5.746642	-1.175476	-0.446152
42	8	0	-6.470925	-0.662738	-1.271756
43	8	0	-5.987743	-2.213862	0.131109

Structure 43a (^{2}E ec-ax H-bond O) (M06-2X, DMSO)

Energy (Hartrees): = - 1181.3590239
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.104719	0.398092	0.621136
2	6	0	-2.336315	-0.832452	0.004419
3	6	0	-3.623684	-1.211657	-0.349708
4	6	0	-4.667996	-0.343418	-0.067143
5	6	0	-4.474849	0.880079	0.558002
6	6	0	-3.180588	1.242208	0.900522
7	1	0	-1.512021	-1.508818	-0.186568
8	1	0	-3.817832	-2.162006	-0.828349
9	1	0	-5.317399	1.522924	0.773605
10	1	0	-3.004371	2.190677	1.396930
11	6	0	-0.694328	0.862419	0.956077
12	1	0	-0.731382	1.492088	1.849518
13	7	0	-0.019792	1.585134	-0.122008
14	8	0	0.146365	-0.250695	1.197323

15	6	0	1.025387	-0.452009	0.070342
16	6	0	0.530717	0.539427	-0.976104
17	1	0	1.342935	0.930602	-1.588342
18	1	0	-0.229354	0.082854	-1.628222
19	1	0	0.930213	-1.494769	-0.245591
20	6	0	2.448857	-0.194055	0.554731
21	1	0	2.579276	0.884088	0.715683
22	6	0	3.514838	-0.652907	-0.446402
23	1	0	3.210674	-1.615602	-0.879954
24	6	0	4.855016	-0.892873	0.265540
25	1	0	4.786048	-1.858491	0.774626
26	6	0	6.034183	-0.932927	-0.694746
27	1	0	6.909975	-1.338127	-0.179565
28	1	0	5.812829	-1.561548	-1.558677
29	8	0	2.655096	-0.901290	1.773819
30	1	0	1.864797	-0.746208	2.306292
31	8	0	3.583783	0.307785	-1.491436
32	1	0	4.500337	0.609074	-1.562305
33	8	0	5.164826	0.138880	1.195740
34	1	0	4.520620	0.059674	1.909628
35	8	0	6.318056	0.377811	-1.186621
36	1	0	6.440078	0.928953	-0.402838
37	6	0	-0.795161	2.595383	-0.818805
38	1	0	-1.191711	3.317070	-0.100772
39	1	0	-0.136179	3.126941	-1.508052
40	1	0	-1.633595	2.176235	-1.395063
41	7	0	-6.037401	-0.742603	-0.431750
42	8	0	-6.939165	0.032770	-0.189099
43	8	0	-6.192929	-1.825910	-0.956329

Structure 43a (^{2}E ec-ax H-bond N) (M06-2X, DMSO)

Energy (Hartrees): = - 1181.362582
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.933026	0.275164	-0.456036
2	6	0	2.258337	-0.805392	0.364469
3	6	0	3.579435	-1.205133	0.509860
4	6	0	4.558688	-0.510656	-0.185055
5	6	0	4.267376	0.557378	-1.021548
6	6	0	2.941675	0.942811	-1.152468
7	1	0	1.475421	-1.348793	0.879344
8	1	0	3.847864	-2.041342	1.141048
9	1	0	5.058907	1.065230	-1.555628
10	1	0	2.686514	1.770119	-1.806108
11	6	0	0.499269	0.764695	-0.579494
12	1	0	0.350057	1.185307	-1.578870
13	7	0	0.116285	1.774243	0.421643
14	8	0	-0.403887	-0.300192	-0.366623
15	6	0	-1.136209	-0.087859	0.852154
16	6	0	-0.329542	0.987941	1.572129
17	1	0	-0.940528	1.600925	2.237772
18	1	0	0.508266	0.563683	2.142749
19	1	0	-1.181523	-1.031276	1.398113
20	6	0	-2.557483	0.364970	0.531078
21	1	0	-3.074435	0.522483	1.487778
22	6	0	-3.329948	-0.715870	-0.226859
23	1	0	-2.701568	-1.089821	-1.042832
24	6	0	-4.602313	-0.129458	-0.865830
25	1	0	-4.318204	0.300942	-1.830549
26	6	0	-5.683586	-1.176178	-1.090811
27	1	0	-6.453800	-0.770321	-1.753492
28	1	0	-5.267646	-2.076486	-1.544754
29	8	0	-2.573996	1.563659	-0.235905
30	1	0	-1.711055	2.003119	-0.116519
31	8	0	-3.564424	-1.797673	0.665628
32	1	0	-4.512980	-1.830683	0.849020
33	8	0	-5.218242	0.864578	-0.050659
34	1	0	-4.594567	1.599903	-0.000983
35	8	0	-6.261149	-1.557743	0.158540
36	1	0	-6.531761	-0.731479	0.578993
37	6	0	1.089320	2.813233	0.716503
38	1	0	1.385648	3.311853	-0.208613
39	1	0	0.622858	3.550914	1.371482
40	1	0	1.988205	2.422427	1.212512
41	7	0	5.962117	-0.932093	-0.039113
42	8	0	6.806819	-0.318705	-0.658067
43	8	0	6.200782	-1.869629	0.693746

Structure 43a (^{2}E ec-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 1181.3609027
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.174476	0.244584	0.331875
2	6	0	-2.648684	-0.234634	-0.890556
3	6	0	-3.989386	-0.542155	-1.047369
4	6	0	-4.837486	-0.356572	0.038479
5	6	0	-4.396771	0.118175	1.262906
6	6	0	-3.046056	0.417537	1.401742
7	1	0	-1.958854	-0.359963	-1.716584
8	1	0	-4.378226	-0.915025	-1.985173
9	1	0	-5.091437	0.248337	2.081362
10	1	0	-2.671175	0.790243	2.348623
11	6	0	-0.715675	0.604828	0.460308
12	1	0	-0.482193	0.854644	1.510519
13	7	0	-0.344518	1.691942	-0.433352
14	8	0	0.093915	-0.479964	0.039171
15	6	0	1.265108	0.046088	-0.615273
16	6	0	1.108243	1.559891	-0.510452
17	1	0	1.598693	1.938276	0.399648
18	1	0	1.511278	2.089209	-1.373687
19	1	0	1.240416	-0.292664	-1.656031
20	6	0	2.484241	-0.539827	0.073165
21	1	0	2.542901	-0.139753	1.094021
22	6	0	3.784791	-0.189059	-0.649140
23	1	0	3.646836	-0.344047	-1.727106
24	6	0	4.924415	-1.123318	-0.204424
25	1	0	4.843151	-2.044887	-0.788387
26	6	0	6.300724	-0.517139	-0.434533
27	1	0	7.064239	-1.294056	-0.335750
28	1	0	6.372770	-0.079827	-1.431337
29	8	0	2.368901	-1.959281	0.110700
30	1	0	1.477342	-2.152359	0.425468
31	8	0	4.046302	1.191586	-0.442063
32	1	0	4.858409	1.267328	0.078067
33	8	0	4.876161	-1.417192	1.188016
34	1	0	4.075897	-1.937915	1.326856
35	8	0	6.540848	0.529901	0.506623
36	1	0	6.400458	0.134774	1.376864
37	6	0	-0.785250	2.993814	0.040036
38	1	0	-0.388012	3.224683	1.041229
39	1	0	-0.445590	3.762854	-0.655533
40	1	0	-1.876428	3.026249	0.078688
41	7	0	-6.267670	-0.673377	-0.122476
42	8	0	-6.995336	-0.521831	0.836764
43	8	0	-6.642989	-1.068137	-1.206906

Structure 43a (E_2 ax-ax) (M06-2X, DMSO)

Energy (Hartrees): = - 1181.3605229
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.123565	0.805754	0.471684
2	6	0	-2.425388	-0.404112	1.095676
3	6	0	-3.608069	-1.070778	0.806771
4	6	0	-4.476463	-0.501739	-0.112331
5	6	0	-4.206481	0.702119	-0.747969
6	6	0	-3.019475	1.353829	-0.447873
7	1	0	-1.727391	-0.828903	1.806177
8	1	0	-3.852350	-2.011702	1.280584
9	1	0	-4.908980	1.112068	-1.461014
10	1	0	-2.776846	2.288776	-0.937450
11	6	0	-0.838343	1.545614	0.819517
12	1	0	-1.041476	2.297397	1.584969
13	7	0	-0.235821	2.147800	-0.346982
14	8	0	0.131285	0.640099	1.347857
15	6	0	0.811144	0.064437	0.220990
16	6	0	0.463328	1.006964	-0.962215
17	1	0	1.349322	1.340634	-1.498505
18	1	0	-0.203358	0.497856	-1.660770
19	1	0	0.422181	-0.946327	0.052429
20	6	0	2.282619	-0.026835	0.595127
21	1	0	2.707251	0.984758	0.635118
22	6	0	3.103998	-0.840471	-0.408656
23	1	0	2.547112	-1.748894	-0.673584

24	6	0	4.427685	-1.300215	0.226471
25	1	0	4.208633	-2.179733	0.838431
26	6	0	5.476827	-1.675585	-0.808713
27	1	0	6.296790	-2.211031	-0.321570
28	1	0	5.049860	-2.316506	-1.581593
29	8	0	2.403516	-0.660070	1.866552
30	1	0	1.747224	-0.246010	2.440148
31	8	0	3.265324	-0.062870	-1.586543
32	1	0	4.212873	0.057501	-1.740668
33	8	0	5.031778	-0.283015	1.018498
34	1	0	4.453476	-0.155050	1.779907
35	8	0	5.972537	-0.502768	-1.456494
36	1	0	6.273233	0.079488	-0.746737
37	6	0	0.682110	3.230090	0.022544
38	1	0	1.164718	3.607869	-0.879529
39	1	0	0.111852	4.044596	0.472742
40	1	0	1.459354	2.912112	0.729481
41	7	0	-5.731449	-1.202822	-0.429431
42	8	0	-6.485113	-0.686519	-1.228516
43	8	0	-5.947096	-2.260880	0.124918

Structure 43b (^{2}E ec-ec H-bond O) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1181.3373272
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.960867	0.942758	-0.292682
2	6	0	-1.761696	-0.396405	0.045634
3	6	0	-2.844162	-1.239538	0.229735
4	6	0	-4.121417	-0.715251	0.074781
5	6	0	-4.351135	0.607838	-0.257099
6	6	0	-3.250955	1.437293	-0.444280
7	1	0	-0.749880	-0.766013	0.167244
8	1	0	-2.724689	-2.281876	0.490770
9	1	0	-5.365952	0.964046	-0.366489
10	1	0	-3.400914	2.477296	-0.711942
11	6	0	-0.762884	1.842176	-0.470560
12	1	0	-1.093028	2.833890	-0.835463
13	7	0	0.018708	1.958979	0.746757
14	8	0	0.135829	1.289361	-1.417203
15	6	0	1.484193	1.464508	-0.944058
16	6	0	1.329630	2.378687	0.264772
17	1	0	2.105425	2.212083	1.011375
18	1	0	1.329662	3.436734	-0.046525
19	1	0	2.064748	1.909234	-1.756111
20	6	0	2.035138	0.083277	-0.592558
21	1	0	1.621642	-0.219368	0.378808
22	6	0	3.559705	0.067012	-0.469943
23	1	0	3.990113	0.604224	-1.326983
24	6	0	4.087058	-1.379145	-0.543758
25	1	0	4.153371	-1.649887	-1.602169
26	6	0	5.456319	-1.531500	0.107005
27	1	0	5.891952	-2.493902	-0.177584
28	1	0	6.128196	-0.729627	-0.202840
29	8	0	1.664755	-0.850115	-1.598908
30	1	0	0.783132	-0.594448	-1.897831
31	8	0	3.922659	0.767687	0.704710
32	1	0	4.356732	0.153516	1.313938
33	8	0	3.251591	-2.299758	0.143834
34	1	0	2.431983	-2.356591	-0.360683
35	8	0	5.328435	-1.445060	1.520985
36	1	0	4.657482	-2.095516	1.761299
37	6	0	-0.572731	2.838927	1.735344
38	1	0	-1.549548	2.453263	2.033975
39	1	0	0.065925	2.868838	2.618441
40	1	0	-0.698178	3.867060	1.356239
41	7	0	-5.283143	-1.609242	0.271964
42	8	0	-6.386318	-1.127027	0.145317
43	8	0	-5.054989	-2.765704	0.547202

Structure 43b (^{2}E ec-ec H-bond N) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1181.340031
No imaginary frequencies

Standard orientation:

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

1	6	0	-1.771523	0.857393	-0.460112
2	6	0	-1.501801	-0.423700	0.021824
3	6	0	-2.536090	-1.327480	0.206956
4	6	0	-3.829524	-0.925609	-0.095901
5	6	0	-4.126844	0.337090	-0.578333
6	6	0	-3.077812	1.229145	-0.764236
7	1	0	-0.478888	-0.700959	0.247415
8	1	0	-2.363121	-2.328891	0.576073
9	1	0	-5.151710	0.595855	-0.805695
10	1	0	-3.278112	2.220516	-1.156569
11	6	0	-0.645878	1.846185	-0.633099
12	1	0	-0.975154	2.664078	-1.301843
13	7	0	-0.187427	2.402642	0.643289
14	8	0	0.496517	1.228125	-1.174933
15	6	0	1.671252	1.772426	-0.554956
16	6	0	1.130007	2.930071	0.284911
17	1	0	1.728464	3.129124	1.176265
18	1	0	1.047225	3.853767	-0.308861
19	1	0	2.369569	2.088013	-1.331233
20	6	0	2.347748	0.700985	0.289717
21	1	0	3.243521	1.149290	0.740984
22	6	0	2.829893	-0.461342	-0.579745
23	1	0	2.005949	-0.772479	-1.233498
24	6	0	3.209699	-1.668324	0.300532
25	1	0	2.297761	-2.245659	0.485209
26	6	0	4.250142	-2.563576	-0.360788
27	1	0	4.306623	-3.517290	0.172813
28	1	0	3.996657	-2.751616	-1.404913
29	8	0	1.494892	0.195575	1.310716
30	1	0	0.770308	0.826108	1.457131
31	8	0	3.870467	0.027051	-1.404930
32	1	0	4.704550	-0.373655	-1.124498
33	8	0	3.797009	-1.281449	1.536935
34	1	0	3.105988	-0.847508	2.051394
35	8	0	5.515702	-1.915101	-0.348482
36	1	0	5.668782	-1.666326	0.571000
37	6	0	-1.095121	3.383592	1.213744
38	1	0	-2.052529	2.910811	1.438496
39	1	0	-0.675348	3.767134	2.144058
40	1	0	-1.266108	4.228860	0.528643
41	7	0	-4.936447	-1.887266	0.099563
42	8	0	-6.057733	-1.505853	-0.152103
43	8	0	-4.649627	-2.993090	0.499621

Structure 43b (^{2}E ax-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1181.3339075
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.159838	0.680360	-0.496494
2	6	0	-2.329234	-0.698830	-0.554845
3	6	0	-3.561661	-1.264836	-0.253125
4	6	0	-4.603545	-0.426419	0.103738
5	6	0	-4.464333	0.952839	0.168652
6	6	0	-3.230011	1.501980	-0.138044
7	1	0	-1.493053	-1.324256	-0.836094
8	1	0	-3.725702	-2.332828	-0.289017
9	1	0	-5.311059	1.562199	0.452864
10	1	0	-3.081970	2.574894	-0.086903
11	6	0	-0.833212	1.326028	-0.790804
12	1	0	-0.968848	2.093231	-1.566244
13	7	0	-0.215115	1.966156	0.353009
14	8	0	0.110896	0.369940	-1.278270
15	6	0	1.411966	0.932643	-1.067585
16	6	0	1.158617	2.144945	-0.129786
17	1	0	1.870701	2.193929	0.690919
18	1	0	1.215787	3.071648	-0.704906
19	1	0	1.814067	1.252375	-2.036644
20	6	0	2.295449	-0.180435	-0.528380
21	1	0	1.951322	-0.473951	0.471022
22	6	0	3.763610	0.232321	-0.393178
23	1	0	4.055920	0.817438	-1.277507
24	6	0	4.668291	-1.012337	-0.367485
25	1	0	4.786052	-1.352417	-1.401089
26	6	0	6.039723	-0.722378	0.229656
27	1	0	6.717694	-1.551973	0.008245
28	1	0	6.458450	0.198405	-0.179852
29	8	0	2.229285	-1.291874	-1.417331
30	1	0	1.307997	-1.379773	-1.685041
31	8	0	3.877744	1.062544	0.746868

32	1	0	4.529611	0.678226	1.350521
33	8	0	4.131798	-2.054222	0.434729
34	1	0	3.357145	-2.387962	-0.031767
35	8	0	5.925596	-0.538800	1.635471
36	1	0	5.468995	-1.322818	1.963988
37	6	0	-0.280700	1.162528	1.578381
38	1	0	0.361225	1.627356	2.326082
39	1	0	-1.301567	1.159797	1.961060
40	1	0	0.039577	0.121536	1.439319
41	7	0	-5.916373	-1.023336	0.428412
42	8	0	-6.811749	-0.268251	0.735218
43	8	0	-6.011402	-2.228744	0.367927

Structure 43b (^{2}E ec-ec H-bond O) (M06-2X, Benzene)

Energy (Hartrees): = - 1181.3583325
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.978090	0.927589	-0.297052
2	6	0	-1.787200	-0.401804	0.082443
3	6	0	-2.873663	-1.239129	0.268197
4	6	0	-4.147167	-0.717678	0.073573
5	6	0	-4.368657	0.596528	-0.300100
6	6	0	-3.264276	1.419647	-0.487992
7	1	0	-0.779600	-0.770768	0.236349
8	1	0	-2.754661	-2.273177	0.560830
9	1	0	-5.378451	0.956772	-0.440200
10	1	0	-3.407544	2.451972	-0.787053
11	6	0	-0.776099	1.822295	-0.475648
12	1	0	-1.100586	2.808785	-0.855944
13	7	0	-0.003948	1.954653	0.746740
14	8	0	0.129909	1.251273	-1.406093
15	6	0	1.476702	1.450424	-0.934537
16	6	0	1.309068	2.372502	0.266629
17	1	0	2.078547	2.216204	1.021791
18	1	0	1.307525	3.427548	-0.052643
19	1	0	2.051158	1.899416	-1.748715
20	6	0	2.048855	0.078598	-0.580263
21	1	0	1.633304	-0.236677	0.386161
22	6	0	3.574098	0.083932	-0.449304
23	1	0	4.002006	0.647265	-1.290243
24	6	0	4.126641	-1.350399	-0.550882
25	1	0	4.189530	-1.603456	-1.613723
26	6	0	5.505872	-1.491172	0.078908
27	1	0	5.951316	-2.442957	-0.225847
28	1	0	6.164120	-0.678156	-0.231637
29	8	0	1.700373	-0.856355	-1.594549
30	1	0	0.802552	-0.633781	-1.871675
31	8	0	3.920731	0.760133	0.746966
32	1	0	4.373143	0.136894	1.332754
33	8	0	3.312832	-2.296320	0.131196
34	1	0	2.487100	-2.352199	-0.363942
35	8	0	5.401749	-1.428050	1.498564
36	1	0	4.753056	-2.100189	1.741914
37	6	0	-0.601586	2.854084	1.714903
38	1	0	-1.580087	2.475495	2.018337
39	1	0	0.031705	2.902655	2.601647
40	1	0	-0.725803	3.874493	1.315847
41	7	0	-5.311682	-1.602845	0.275751
42	8	0	-6.415483	-1.123018	0.134769
43	8	0	-5.094600	-2.757826	0.571060

Structure 43b (^{2}E ec-ec H-bond N) (M06-2X, Benzene)

Energy (Hartrees): = - 1181.3617887
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.773602	0.858557	-0.467070
2	6	0	-1.502389	-0.424131	0.009880
3	6	0	-2.534197	-1.330341	0.195029
4	6	0	-3.829125	-0.928015	-0.102753
5	6	0	-4.128305	0.336297	-0.582041
6	6	0	-3.081214	1.230227	-0.767539
7	1	0	-0.479728	-0.701974	0.235183
8	1	0	-2.353434	-2.330892	0.562937

9	1	0	-5.152129	0.601516	-0.807113
10	1	0	-3.284413	2.223125	-1.154048
11	6	0	-0.649478	1.850969	-0.634103
12	1	0	-0.979734	2.672203	-1.295982
13	7	0	-0.187999	2.395269	0.645269
14	8	0	0.494472	1.235042	-1.182250
15	6	0	1.669428	1.780824	-0.560414
16	6	0	1.125597	2.932634	0.284344
17	1	0	1.724897	3.133074	1.174458
18	1	0	1.034669	3.856226	-0.307312
19	1	0	2.364316	2.106059	-1.335721
20	6	0	2.350938	0.709843	0.281563
21	1	0	3.245326	1.163478	0.730065
22	6	0	2.833548	-0.458212	-0.580952
23	1	0	2.013488	-0.772590	-1.237485
24	6	0	3.208121	-1.663431	0.304186
25	1	0	2.294636	-2.237514	0.489474
26	6	0	4.241341	-2.570250	-0.349955
27	1	0	4.294165	-3.518231	0.194617
28	1	0	3.982498	-2.773664	-1.389984
29	8	0	1.500067	0.208254	1.307178
30	1	0	0.771338	0.838600	1.442938
31	8	0	3.882732	0.020575	-1.405740
32	1	0	4.710266	-0.386239	-1.115255
33	8	0	3.796293	-1.273259	1.540734
34	1	0	3.107416	-0.824785	2.046294
35	8	0	5.515283	-1.932334	-0.350866
36	1	0	5.679031	-1.681179	0.566544
37	6	0	-1.092793	3.368534	1.234076
38	1	0	-2.044140	2.891589	1.476149
39	1	0	-0.658905	3.749850	2.159187
40	1	0	-1.280167	4.216395	0.556986
41	7	0	-4.933799	-1.886232	0.102716
42	8	0	-6.057658	-1.514115	-0.157160
43	8	0	-4.651693	-2.987829	0.521437

Structure 43b (^{2}E ax-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 1181.3546491
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.165596	0.679401	-0.496804
2	6	0	-2.331670	-0.701233	-0.541071
3	6	0	-3.565104	-1.266643	-0.243885
4	6	0	-4.612570	-0.426392	0.094627
5	6	0	-4.477355	0.954589	0.141942
6	6	0	-3.241600	1.502747	-0.159448
7	1	0	-1.493964	-1.331906	-0.806347
8	1	0	-3.719716	-2.336393	-0.268664
9	1	0	-5.324698	1.570876	0.409216
10	1	0	-3.099618	2.576989	-0.121373
11	6	0	-0.835973	1.325459	-0.778877
12	1	0	-0.965527	2.095876	-1.551719
13	7	0	-0.225402	1.960476	0.373806
14	8	0	0.111633	0.370109	-1.259058
15	6	0	1.411001	0.938276	-1.047200
16	6	0	1.152186	2.142003	-0.100316
17	1	0	1.856175	2.182060	0.727804
18	1	0	1.216084	3.073656	-0.666449
19	1	0	1.808404	1.269237	-2.014067
20	6	0	2.300307	-0.174963	-0.515155
21	1	0	1.967628	-0.463498	0.489695
22	6	0	3.772926	0.232050	-0.406482
23	1	0	4.054394	0.806216	-1.300412
24	6	0	4.675356	-1.014964	-0.378718
25	1	0	4.789067	-1.361905	-1.410310
26	6	0	6.052311	-0.726863	0.203957
27	1	0	6.724242	-1.561646	-0.016705
28	1	0	6.474866	0.186445	-0.218335
29	8	0	2.218344	-1.291195	-1.398113
30	1	0	1.289474	-1.389642	-1.636133
31	8	0	3.913337	1.076625	0.722912
32	1	0	4.553002	0.676839	1.329289
33	8	0	4.141385	-2.052403	0.433803
34	1	0	3.355466	-2.376894	-0.020980
35	8	0	5.955770	-0.531635	1.612283
36	1	0	5.507558	-1.315183	1.954119
37	6	0	-0.295186	1.147716	1.592892
38	1	0	0.340186	1.609306	2.348891
39	1	0	-1.317403	1.139425	1.973231
40	1	0	0.030427	0.108886	1.450688

41	7	0	-5.923132	-1.021345	0.419214
42	8	0	-6.831393	-0.266786	0.692486
43	8	0	-6.014139	-2.229686	0.396270

Structure 43b (^{2}E ec-ec H-bond O) (M06-2X, DMSO)

Energy (Hartrees): = - 1181.3619661
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.983319	0.910721	-0.323803
2	6	0	-1.789162	-0.438033	-0.020140
3	6	0	-2.875117	-1.273312	0.180565
4	6	0	-4.150755	-0.730349	0.077007
5	6	0	-4.375495	0.603468	-0.221196
6	6	0	-3.272354	1.424131	-0.425145
7	1	0	-0.782448	-0.832615	0.061451
8	1	0	-2.745081	-2.320991	0.415008
9	1	0	-5.384116	0.986425	-0.294750
10	1	0	-3.418459	2.471847	-0.663300
11	6	0	-0.786987	1.812211	-0.506870
12	1	0	-1.116216	2.792159	-0.894174
13	7	0	-0.026090	1.962605	0.724507
14	8	0	0.130040	1.238524	-1.426282
15	6	0	1.472795	1.448459	-0.944574
16	6	0	1.289021	2.381407	0.244609
17	1	0	2.051993	2.241677	1.009458
18	1	0	1.280591	3.431201	-0.087782
19	1	0	2.055120	1.893969	-1.754855
20	6	0	2.047500	0.081129	-0.582660
21	1	0	1.593672	-0.258382	0.357779
22	6	0	3.565968	0.099672	-0.385328
23	1	0	4.024890	0.707962	-1.176750
24	6	0	4.141800	-1.318630	-0.529404
25	1	0	4.200293	-1.539525	-1.599116
26	6	0	5.532804	-1.454656	0.071231
27	1	0	5.981352	-2.396338	-0.258225
28	1	0	6.174807	-0.630514	-0.243654
29	8	0	1.751711	-0.840890	-1.627217
30	1	0	0.842768	-0.656360	-1.897020
31	8	0	3.842317	0.710288	0.867547
32	1	0	4.377774	0.095577	1.388458
33	8	0	3.348050	-2.295372	0.136068
34	1	0	2.516642	-2.345359	-0.350690
35	8	0	5.464328	-1.415798	1.497720
36	1	0	4.839562	-2.108340	1.748307
37	6	0	-0.634396	2.896839	1.657114
38	1	0	-1.615129	2.528318	1.966355
39	1	0	-0.006210	2.979525	2.545307
40	1	0	-0.757745	3.899089	1.217038
41	7	0	-5.311518	-1.611702	0.294141
42	8	0	-6.419385	-1.123584	0.212595
43	8	0	-5.097637	-2.779915	0.543591

Structure 43b (^{2}E ec-ec H-bond N) (M06-2X, DMSO)

Energy (Hartrees): = - 1181.3657379
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.755107	0.866696	-0.477627
2	6	0	-1.464929	-0.427229	-0.042402
3	6	0	-2.486838	-1.343741	0.148957
4	6	0	-3.791890	-0.937865	-0.098078
5	6	0	-4.110667	0.339063	-0.531725
6	6	0	-3.072902	1.241663	-0.726862
7	1	0	-0.436503	-0.709835	0.149045
8	1	0	-2.284179	-2.352344	0.482570
9	1	0	-5.140175	0.612828	-0.717673
10	1	0	-3.290803	2.245442	-1.075415
11	6	0	-0.643896	1.872567	-0.650495
12	1	0	-0.986247	2.691647	-1.305597
13	7	0	-0.182722	2.413182	0.630513
14	8	0	0.505052	1.267125	-1.209501
15	6	0	1.677277	1.804482	-0.571535
16	6	0	1.130843	2.955453	0.269231
17	1	0	1.728057	3.159786	1.159502

18	1	0	1.033914	3.874861	-0.325860
19	1	0	2.379525	2.133332	-1.338165
20	6	0	2.346648	0.730656	0.276665
21	1	0	3.250238	1.178162	0.711799
22	6	0	2.797182	-0.462798	-0.567906
23	1	0	1.965745	-0.774761	-1.210077
24	6	0	3.154029	-1.661498	0.332886
25	1	0	2.230861	-2.214738	0.530499
26	6	0	4.158812	-2.602902	-0.313671
27	1	0	4.198199	-3.539389	0.250783
28	1	0	3.879674	-2.824214	-1.344571
29	8	0	1.496290	0.261546	1.319610
30	1	0	0.760819	0.893389	1.422294
31	8	0	3.852230	-0.027631	-1.415534
32	1	0	4.669880	-0.443200	-1.110225
33	8	0	3.758742	-1.264899	1.561090
34	1	0	3.087797	-0.772427	2.050431
35	8	0	5.450785	-1.995174	-0.345949
36	1	0	5.635047	-1.731145	0.564602
37	6	0	-1.088100	3.394801	1.210016
38	1	0	-2.042326	2.923181	1.452283
39	1	0	-0.652562	3.781657	2.132017
40	1	0	-1.269021	4.233801	0.522175
41	7	0	-4.883385	-1.905891	0.107870
42	8	0	-6.023160	-1.518044	-0.044890
43	8	0	-4.584683	-3.039569	0.420948

Structure 43b (^{2}E ax-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 1181.358069
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.162130	0.717399	-0.476296
2	6	0	-2.293906	-0.668317	-0.508192
3	6	0	-3.518728	-1.259631	-0.226973
4	6	0	-4.591705	-0.439355	0.083779
5	6	0	-4.490783	0.945253	0.118796
6	6	0	-3.262896	1.519004	-0.168008
7	1	0	-1.438688	-1.285865	-0.750398
8	1	0	-3.641161	-2.333911	-0.245497
9	1	0	-5.353360	1.550007	0.363410
10	1	0	-3.152139	2.597525	-0.146394
11	6	0	-0.840358	1.390538	-0.731571
12	1	0	-0.981804	2.204470	-1.454788
13	7	0	-0.226031	1.959597	0.456484
14	8	0	0.107353	0.468905	-1.273167
15	6	0	1.411065	1.007700	-1.012399
16	6	0	1.151654	2.164460	-0.012738
17	1	0	1.854462	2.167324	0.817468
18	1	0	1.211912	3.119395	-0.538795
19	1	0	1.830040	1.381134	-1.953277
20	6	0	2.278284	-0.138934	-0.513532
21	1	0	1.938610	-0.453197	0.480956
22	6	0	3.757981	0.238331	-0.393112
23	1	0	4.050032	0.841017	-1.263709
24	6	0	4.639376	-1.021294	-0.413062
25	1	0	4.727979	-1.342329	-1.454964
26	6	0	6.035049	-0.770267	0.138149
27	1	0	6.684106	-1.613701	-0.114157
28	1	0	6.462694	0.140812	-0.283215
29	8	0	2.175502	-1.227212	-1.429433
30	1	0	1.237519	-1.326488	-1.633019
31	8	0	3.914491	1.032958	0.774443
32	1	0	4.578987	0.611310	1.337096
33	8	0	4.103994	-2.071365	0.385417
34	1	0	3.295509	-2.359199	-0.055303
35	8	0	5.985140	-0.596576	1.555505
36	1	0	5.539556	-1.381461	1.899239
37	6	0	-0.293615	1.075247	1.626783
38	1	0	0.354185	1.484481	2.402612
39	1	0	-1.313342	1.054811	2.014862
40	1	0	0.019685	0.043962	1.420070
41	7	0	-5.891738	-1.060766	0.387187
42	8	0	-6.830375	-0.328103	0.621827
43	8	0	-5.955622	-2.272699	0.388202

Structure 43c ($^5C_2$ ec-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1181.3358108
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.239226	1.336221	0.659238
2	6	0	-1.309742	2.498221	0.336458
3	6	0	-1.949234	0.193741	-0.317625
4	1	0	-1.469349	3.301236	1.058744
5	1	0	-1.511261	2.890674	-0.675443
6	1	0	-3.282464	1.649730	0.581704
7	1	0	-2.203172	0.532034	-1.334804
8	8	0	-0.568780	-0.128670	-0.261552
9	7	0	0.063533	2.013271	0.471918
10	6	0	-2.707324	-1.101991	-0.032730
11	1	0	-2.444744	-1.821005	-0.815024
12	6	0	-4.225838	-0.930408	-0.030361
13	1	0	-4.515125	-0.236464	0.773610
14	6	0	-4.813572	-0.447940	-1.345040
15	1	0	-4.426368	-1.081661	-2.156546
16	1	0	-4.525531	0.587192	-1.546246
17	8	0	-2.324669	-1.706381	1.189191
18	1	0	-2.298851	-0.999843	1.848798
19	8	0	-4.816210	-2.195378	0.209643
20	1	0	-4.309878	-2.600047	0.923510
21	8	0	-6.219384	-0.477619	-1.298271
22	1	0	-6.452088	-1.337351	-0.931050
23	8	0	-2.016741	0.923317	2.000190
24	1	0	-1.057958	0.979472	2.123621
25	6	0	1.021343	3.106405	0.356857
26	1	0	1.033838	3.546432	-0.653972
27	1	0	0.746339	3.887184	1.066572
28	1	0	2.025092	2.760146	0.599874
29	6	0	1.702253	0.407137	-0.413366
30	6	0	2.019038	-0.450529	0.639292
31	6	0	2.671677	0.754755	-1.348271
32	6	0	3.305291	-0.951085	0.767353
33	1	0	1.241245	-0.740030	1.334543
34	6	0	3.966189	0.264024	-1.233775
35	1	0	2.417125	1.410998	-2.173215
36	6	0	4.254305	-0.577987	-0.173025
37	1	0	3.583198	-1.621290	1.568848
38	1	0	4.741816	0.513435	-1.944377
39	6	0	0.296425	0.949323	-0.509879
40	1	0	0.114025	1.341678	-1.531839
41	7	0	5.629508	-1.108547	-0.045158
42	8	0	5.859047	-1.841371	0.890076
43	8	0	6.435899	-0.773261	-0.883698

Structure 43c ($^5C_2$ ax-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1181.3345548
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.183259	1.629741	0.013110
2	6	0	-1.114490	2.589381	-0.525473
3	6	0	-1.860706	0.216980	-0.489633
4	1	0	-1.263187	3.578478	-0.090380
5	1	0	-1.227267	2.678278	-1.612983
6	1	0	-3.172754	1.927263	-0.338415
7	1	0	-1.921607	0.221388	-1.589676
8	8	0	-0.525928	-0.106330	-0.107112
9	7	0	0.254497	2.144237	-0.248652
10	6	0	-2.756500	-0.915327	0.018913
11	1	0	-2.289011	-1.845051	-0.322779
12	6	0	-4.169717	-0.838528	-0.558958
13	1	0	-4.125596	-0.683504	-1.646653
14	6	0	-4.936083	-2.120876	-0.279554
15	1	0	-4.857338	-2.347108	0.788268
16	1	0	-4.510792	-2.946363	-0.861766
17	8	0	-2.808781	-0.993248	1.424479
18	1	0	-3.317597	-0.222197	1.711388
19	8	0	-4.826637	0.247512	0.065674
20	1	0	-5.771241	0.085450	-0.042732
21	8	0	-6.281577	-1.861380	-0.658242
22	1	0	-6.849061	-2.534992	-0.279718
23	8	0	-2.222987	1.673860	1.431981
24	1	0	-1.549947	1.061617	1.751594
25	6	0	0.719266	2.362348	1.124303
26	1	0	0.473176	1.539627	1.807355

27	1	0	1.804033	2.484382	1.131581
28	1	0	0.265814	3.273065	1.512570
29	6	0	1.806778	0.261625	-0.469202
30	6	0	2.031370	-0.930068	0.212188
31	6	0	2.883920	1.003092	-0.958310
32	6	0	3.329847	-1.386425	0.407660
33	1	0	1.187167	-1.491474	0.589155
34	6	0	4.182762	0.559950	-0.772750
35	1	0	2.690434	1.939735	-1.468893
36	6	0	4.378507	-0.632682	-0.089987
37	1	0	3.538405	-2.306803	0.935363
38	1	0	5.037186	1.112811	-1.137599
39	6	0	0.409516	0.785117	-0.706115
40	1	0	0.215587	0.788445	-1.790628
41	7	0	5.760747	-1.113406	0.115261
42	8	0	6.660316	-0.426413	-0.315818
43	8	0	5.906797	-2.163355	0.700479

Structure 43c ($^5C_2$ ec-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 1181.3591466
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.232493	1.364026	0.657625
2	6	0	-1.306746	2.517001	0.294837
3	6	0	-1.952014	0.199175	-0.295354
4	1	0	-1.460434	3.341468	0.993610
5	1	0	-1.517904	2.876905	-0.726285
6	1	0	-3.276192	1.677276	0.586427
7	1	0	-2.206941	0.518053	-1.317902
8	8	0	-0.570684	-0.126587	-0.234473
9	7	0	0.068817	2.036147	0.432213
10	6	0	-2.710563	-1.089600	0.014347
11	1	0	-2.427210	-1.830531	-0.740078
12	6	0	-4.230565	-0.930478	-0.022655
13	1	0	-4.545285	-0.208121	0.745145
14	6	0	-4.791548	-0.510308	-1.368980
15	1	0	-4.376561	-1.167406	-2.147038
16	1	0	-4.516331	0.520660	-1.604354
17	8	0	-2.352886	-1.652190	1.265766
18	1	0	-2.293223	-0.915045	1.889663
19	8	0	-4.815530	-2.192794	0.256534
20	1	0	-4.329120	-2.554637	1.006736
21	8	0	-6.200550	-0.563386	-1.356956
22	1	0	-6.427566	-1.411386	-0.959342
23	8	0	-1.991391	0.981852	2.007574
24	1	0	-1.031855	1.056174	2.120638
25	6	0	1.024740	3.125707	0.273921
26	1	0	1.025199	3.537707	-0.748267
27	1	0	0.760147	3.927076	0.964866
28	1	0	2.032713	2.788979	0.515511
29	6	0	1.699206	0.404224	-0.416852
30	6	0	2.040722	-0.363579	0.696496
31	6	0	2.644078	0.663675	-1.404249
32	6	0	3.324603	-0.867531	0.829151
33	1	0	1.285969	-0.579003	1.442532
34	6	0	3.937089	0.169753	-1.285940
35	1	0	2.372154	1.252433	-2.273359
36	6	0	4.248771	-0.585926	-0.167590
37	1	0	3.614019	-1.471369	1.678134
38	1	0	4.689736	0.353862	-2.040084
39	6	0	0.293500	0.945930	-0.520901
40	1	0	0.104024	1.306178	-1.551786
41	7	0	5.617973	-1.123062	-0.037376
42	8	0	5.859395	-1.821050	0.922944
43	8	0	6.419701	-0.833756	-0.899108

Structure 43c ($^5C_2$ ax-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 1181.3565148
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.183780	1.622458	0.008964
2	6	0	-1.115274	2.586925	-0.520711

3	6	0	-1.860501	0.214460	-0.503593
4	1	0	-1.263546	3.574102	-0.080852
5	1	0	-1.228578	2.679710	-1.607443
6	1	0	-3.171764	1.924421	-0.343488
7	1	0	-1.919750	0.226972	-1.602869
8	8	0	-0.524987	-0.111139	-0.120075
9	7	0	0.254594	2.140242	-0.245311
10	6	0	-2.758390	-0.920021	-0.005505
11	1	0	-2.316594	-1.846461	-0.387071
12	6	0	-4.186240	-0.806046	-0.542863
13	1	0	-4.167142	-0.578748	-1.618111
14	6	0	-4.946277	-2.104176	-0.330198
15	1	0	-4.843932	-2.405255	0.717223
16	1	0	-4.537507	-2.888704	-0.976928
17	8	0	-2.775171	-1.036678	1.399636
18	1	0	-3.289947	-0.280935	1.714785
19	8	0	-4.829379	0.237131	0.167872
20	1	0	-5.775761	0.066956	0.086188
21	8	0	-6.302655	-1.824821	-0.655567
22	1	0	-6.857444	-2.518788	-0.291742
23	8	0	-2.229848	1.653918	1.429582
24	1	0	-1.539333	1.058623	1.744399
25	6	0	0.719388	2.353899	1.127467
26	1	0	0.469706	1.535137	1.814564
27	1	0	1.805144	2.471501	1.137861
28	1	0	0.275104	3.270037	1.515150
29	6	0	1.808106	0.258777	-0.479046
30	6	0	2.034055	-0.931007	0.206220
31	6	0	2.885769	1.000552	-0.967685
32	6	0	3.332304	-1.384432	0.407563
33	1	0	1.192459	-1.495847	0.584216
34	6	0	4.184833	0.561482	-0.775820
35	1	0	2.695497	1.934733	-1.484203
36	6	0	4.381469	-0.628428	-0.087359
37	1	0	3.533829	-2.303952	0.939780
38	1	0	5.035624	1.119233	-1.142171
39	6	0	0.410306	0.783707	-0.713893
40	1	0	0.217528	0.796360	-1.798030
41	7	0	5.761866	-1.104562	0.122552
42	8	0	6.665125	-0.420100	-0.308285
43	8	0	5.913988	-2.153031	0.711437

Structure 43c ($^5C_2$ ec-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 1181.3664062
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.227753	1.371110	0.645739
2	6	0	-1.304490	2.515334	0.256616
3	6	0	-1.952094	0.188916	-0.285325
4	1	0	-1.453744	3.357258	0.935264
5	1	0	-1.517937	2.846614	-0.772126
6	1	0	-3.271028	1.682128	0.572095
7	1	0	-2.200702	0.493240	-1.312087
8	8	0	-0.569609	-0.143491	-0.211573
9	7	0	0.074004	2.038443	0.399819
10	6	0	-2.720324	-1.087571	0.044073
11	1	0	-2.437166	-1.846602	-0.692294
12	6	0	-4.238443	-0.918754	-0.011760
13	1	0	-4.555548	-0.164131	0.721916
14	6	0	-4.777116	-0.548020	-1.379824
15	1	0	-4.355684	-1.234653	-2.127289
16	1	0	-4.493210	0.472153	-1.645313
17	8	0	-2.379761	-1.622024	1.316542
18	1	0	-2.281350	-0.860305	1.906508
19	8	0	-4.837128	-2.167431	0.314521
20	1	0	-4.367450	-2.489441	1.093440
21	8	0	-6.192193	-0.599665	-1.385769
22	1	0	-6.422362	-1.432446	-0.958395
23	8	0	-1.976870	1.011024	2.005375
24	1	0	-1.015157	1.085198	2.105536
25	6	0	1.022465	3.127241	0.184813
26	1	0	1.009953	3.489122	-0.855106
27	1	0	0.755922	3.956789	0.841024
28	1	0	2.035573	2.808403	0.432315
29	6	0	1.698544	0.393318	-0.418890
30	6	0	2.069832	-0.283028	0.743960
31	6	0	2.616056	0.572167	-1.449268
32	6	0	3.355339	-0.781056	0.881724
33	1	0	1.341282	-0.426001	1.533011
34	6	0	3.910169	0.080778	-1.328492

35	1	0	2.322640	1.099029	-2.350246
36	6	0	4.250532	-0.586476	-0.162585
37	1	0	3.663233	-1.311694	1.772313
38	1	0	4.638362	0.208242	-2.117763
39	6	0	0.291222	0.927783	-0.530675
40	1	0	0.094813	1.262092	-1.566535
41	7	0	5.618786	-1.115504	-0.026557
42	8	0	5.917340	-1.655603	1.018413
43	8	0	6.375271	-0.983563	-0.966226

Structure 43c ($^5C_2$ ax-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 1181.3614204
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.181155	1.617308	0.030323
2	6	0	-1.115634	2.583583	-0.499661
3	6	0	-1.861510	0.214140	-0.492234
4	1	0	-1.257495	3.569317	-0.053747
5	1	0	-1.241653	2.676841	-1.584372
6	1	0	-3.167389	1.923848	-0.322729
7	1	0	-1.921135	0.237024	-1.589895
8	8	0	-0.524206	-0.115356	-0.110044
9	7	0	0.259336	2.135447	-0.241680
10	6	0	-2.764051	-0.920279	-0.009422
11	1	0	-2.339243	-1.843822	-0.414847
12	6	0	-4.193858	-0.779005	-0.534405
13	1	0	-4.173032	-0.485418	-1.592400
14	6	0	-4.947293	-2.089873	-0.401266
15	1	0	-4.849420	-2.455303	0.625988
16	1	0	-4.531142	-2.830947	-1.091770
17	8	0	-2.771411	-1.065694	1.397001
18	1	0	-3.288848	-0.317435	1.724141
19	8	0	-4.846273	0.218755	0.238038
20	1	0	-5.789709	0.029460	0.157353
21	8	0	-6.306841	-1.801621	-0.712436
22	1	0	-6.854531	-2.514748	-0.371214
23	8	0	-2.228858	1.641374	1.454266
24	1	0	-1.532685	1.049165	1.763695
25	6	0	0.735555	2.339680	1.128609
26	1	0	0.452585	1.540997	1.826702
27	1	0	1.826057	2.408879	1.134150
28	1	0	0.335493	3.280527	1.506503
29	6	0	1.805679	0.253365	-0.484633
30	6	0	2.045414	-0.859952	0.315433
31	6	0	2.872189	0.923359	-1.088439
32	6	0	3.344919	-1.308682	0.517586
33	1	0	1.215831	-1.372817	0.783323
34	6	0	4.173360	0.490081	-0.896935
35	1	0	2.676345	1.794051	-1.704284
36	6	0	4.382861	-0.623435	-0.092762
37	1	0	3.551251	-2.169833	1.138585
38	1	0	5.010031	0.997089	-1.357933
39	6	0	0.407108	0.776473	-0.714530
40	1	0	0.208200	0.789160	-1.796113
41	7	0	5.762128	-1.091099	0.121084
42	8	0	6.664004	-0.440660	-0.365700
43	8	0	5.925928	-2.101429	0.773507

Structure 43d ($^5C_2$ ec-ax) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1181.3294613
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.989981	1.145305	0.890104
2	6	0	0.841593	2.021014	1.390559
3	6	0	1.464658	0.208035	-0.203291
4	1	0	1.238168	2.767807	2.081708
5	1	0	0.103874	1.406068	1.927619
6	1	0	2.415458	0.573130	1.716601
7	1	0	0.691991	-0.443517	0.232459
8	8	0	0.897445	0.994143	-1.248079
9	7	0	0.304056	2.707278	0.225538
10	6	0	2.528421	-0.680588	-0.845354

11	1	0	2.026663	-1.339731	-1.561510
12	6	0	3.273123	-1.556200	0.161694
13	1	0	3.827557	-0.914245	0.862571
14	6	0	2.397101	-2.516376	0.947570
15	1	0	1.767745	-3.077529	0.241154
16	1	0	1.744111	-1.975587	1.637618
17	8	0	3.485082	0.044323	-1.595351
18	1	0	3.736867	0.807914	-1.058794
19	8	0	4.189470	-2.371081	-0.548097
20	1	0	4.625384	-1.795638	-1.187064
21	8	0	3.188660	-3.380105	1.726598
22	1	0	3.886720	-3.695943	1.142466
23	8	0	3.022775	1.970201	0.372034
24	1	0	2.564741	2.608731	-0.193033
25	6	0	-0.400713	3.957999	0.429471
26	1	0	-1.345564	3.878161	0.982256
27	1	0	0.250143	4.643647	0.976479
28	1	0	-0.617383	4.407007	-0.542375
29	6	0	-1.391025	0.944119	-0.500864
30	6	0	-2.239391	1.176362	0.579416
31	6	0	-1.678979	-0.103238	-1.381743
32	6	0	-3.362383	0.382847	0.784080
33	1	0	-2.029596	1.973026	1.279084
34	6	0	-2.793736	-0.904031	-1.194477
35	1	0	-1.009715	-0.288350	-2.213653
36	6	0	-3.617450	-0.641181	-0.109901
37	1	0	-4.033489	0.542785	1.616652
38	1	0	-3.035715	-1.718869	-1.862966
39	6	0	-0.167232	1.817825	-0.812992
40	1	0	-0.417582	2.437884	-1.678854
41	7	0	-4.811395	-1.488189	0.100134
42	8	0	-5.515937	-1.231364	1.050393
43	8	0	-5.005345	-2.381333	-0.692967

Structure 43d ($^5C_2$ ax-ax) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1181.3341041
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.767504	1.243359	0.951073
2	6	0	0.552641	2.092061	1.338710
3	6	0	1.318487	0.240409	-0.115615
4	1	0	0.862515	2.877716	2.029016
5	1	0	-0.175948	1.454932	1.854936
6	1	0	2.147261	0.707714	1.823152
7	1	0	0.544005	-0.404241	0.324737
8	8	0	0.767901	0.970119	-1.213960
9	7	0	-0.106284	2.712943	0.186564
10	6	0	2.398764	-0.672393	-0.702195
11	1	0	1.932516	-1.184860	-1.550854
12	6	0	2.875918	-1.720715	0.302883
13	1	0	2.014500	-2.199240	0.789858
14	6	0	3.706260	-2.791144	-0.385969
15	1	0	4.477679	-2.300082	-0.987364
16	1	0	3.067827	-3.401281	-1.034921
17	8	0	3.501742	0.032444	-1.224564
18	1	0	3.987833	0.362434	-0.456348
19	8	0	3.673748	-1.051677	1.261009
20	1	0	4.222073	-1.730038	1.672766
21	8	0	4.277744	-3.571095	0.656155
22	1	0	4.993187	-4.098667	0.297412
23	8	0	2.820612	2.067175	0.473186
24	1	0	2.704940	2.143359	-0.481496
25	6	0	0.516885	3.935983	-0.314042
26	1	0	1.405616	3.766781	-0.933071
27	1	0	-0.214865	4.490063	-0.906952
28	1	0	0.810512	4.557190	0.531846
29	6	0	-1.564463	0.857177	-0.517426
30	6	0	-2.554412	1.297004	0.359236
31	6	0	-1.704527	-0.378475	-1.152344
32	6	0	-3.669755	0.511027	0.615872
33	1	0	-2.434069	2.260994	0.837721
34	6	0	-2.812021	-1.176246	-0.907380
35	1	0	-0.934439	-0.709655	-1.839183
36	6	0	-3.774353	-0.713847	-0.022409
37	1	0	-4.449603	0.827415	1.294697
38	1	0	-2.944360	-2.138125	-1.383437
39	6	0	-0.372631	1.752294	-0.851166
40	1	0	-0.617001	2.302308	-1.763941
41	7	0	-4.954977	-1.560346	0.248714
42	8	0	-5.778313	-1.136498	1.028744

43	8	0	-5.023075	-2.624453	-0.325680

Structure 43d ($^5C_2$ ec-ax) (M06-2X, Benzene)

Energy (Hartrees): = - 1181.352537
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.986078	1.173475	0.919957
2	6	0	0.824162	2.047755	1.390752
3	6	0	1.486403	0.229114	-0.180934
4	1	0	1.201498	2.798576	2.088184
5	1	0	0.076298	1.433044	1.912733
6	1	0	2.396672	0.606741	1.757243
7	1	0	0.707841	-0.420229	0.245027
8	8	0	0.935209	1.006271	-1.242366
9	7	0	0.314485	2.727254	0.209554
10	6	0	2.557631	-0.664392	-0.801519
11	1	0	2.075123	-1.271249	-1.575154
12	6	0	3.213637	-1.614962	0.201472
13	1	0	3.718380	-1.035542	0.988244
14	6	0	2.263771	-2.610459	0.843000
15	1	0	1.680864	-3.105155	0.052402
16	1	0	1.569627	-2.109065	1.521664
17	8	0	3.580527	0.063286	-1.459952
18	1	0	3.776517	0.829904	-0.903342
19	8	0	4.175863	-2.396286	-0.489986
20	1	0	4.661851	-1.783752	-1.054920
21	8	0	2.978988	-3.552066	1.611405
22	1	0	3.711584	-3.841140	1.055903
23	8	0	3.025566	2.006939	0.420705
24	1	0	2.571463	2.647177	-0.147263
25	6	0	-0.373217	3.991881	0.383698
26	1	0	-1.326506	3.935626	0.924977
27	1	0	0.280304	4.675999	0.930125
28	1	0	-0.569025	4.430248	-0.597666
29	6	0	-1.366881	0.960066	-0.526529
30	6	0	-2.235565	1.222755	0.531036
31	6	0	-1.635919	-0.115813	-1.378810
32	6	0	-3.357705	0.431066	0.742881
33	1	0	-2.040617	2.040946	1.209868
34	6	0	-2.749140	-0.917072	-1.183358
35	1	0	-0.956891	-0.326306	-2.196655
36	6	0	-3.592403	-0.624529	-0.120705
37	1	0	-4.038966	0.619662	1.561123
38	1	0	-2.969340	-1.753733	-1.832477
39	6	0	-0.139506	1.833375	-0.830633
40	1	0	-0.378903	2.446198	-1.704314
41	7	0	-4.781021	-1.471206	0.099896
42	8	0	-5.513300	-1.182615	1.021466
43	8	0	-4.954117	-2.403510	-0.654237

Structure 43d ($^5C_2$ ax-ax) (M06-2X, Benece)

Energy (Hartrees): = - 1181.3558766
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.759803	1.235976	0.955793
2	6	0	0.542978	2.083165	1.338589
3	6	0	1.319274	0.231243	-0.112646
4	1	0	0.848234	2.870559	2.029056
5	1	0	-0.183448	1.444042	1.854945
6	1	0	2.134233	0.700945	1.830356
7	1	0	0.552505	-0.421226	0.328362
8	8	0	0.761715	0.955648	-1.212112
9	7	0	-0.114517	2.700028	0.183494
10	6	0	2.406896	-0.672424	-0.700079
11	1	0	1.940275	-1.205984	-1.535063
12	6	0	2.914397	-1.700322	0.311565
13	1	0	2.066553	-2.171671	0.827707
14	6	0	3.731070	-2.779677	-0.378202
15	1	0	4.490260	-2.300993	-1.004861
16	1	0	3.081145	-3.401598	-1.004004
17	8	0	3.492754	0.045307	-1.244702
18	1	0	3.990401	0.374110	-0.483451

19	8	0	3.735211	-1.011745	1.239076
20	1	0	4.303637	-1.681926	1.638082
21	8	0	4.329355	-3.544508	0.661285
22	1	0	5.048943	-4.061264	0.291322
23	8	0	2.817921	2.061125	0.485980
24	1	0	2.690527	2.161876	-0.465071
25	6	0	0.502387	3.924679	-0.319484
26	1	0	1.391702	3.761897	-0.940573
27	1	0	-0.231347	4.473922	-0.915040
28	1	0	0.791088	4.552131	0.524156
29	6	0	-1.575467	0.845386	-0.520358
30	6	0	-2.573262	1.297085	0.342342
31	6	0	-1.713926	-0.396940	-1.143142
32	6	0	-3.691321	0.516328	0.600466
33	1	0	-2.459229	2.265786	0.812854
34	6	0	-2.824643	-1.190008	-0.897628
35	1	0	-0.942543	-0.740956	-1.821933
36	6	0	-3.792757	-0.716820	-0.023844
37	1	0	-4.471717	0.847348	1.271814
38	1	0	-2.949369	-2.156093	-1.367718
39	6	0	-0.380311	1.737711	-0.852776
40	1	0	-0.624435	2.286671	-1.766218
41	7	0	-4.970648	-1.559835	0.254474
42	8	0	-5.784315	-1.144734	1.051141
43	8	0	-5.055387	-2.619996	-0.327425

Structure 43d ($^5C_2$ ec-ax) (M06-2X, DMSO)

Energy (Hartrees): = - 1181.3592506
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.991416	1.176177	0.911186
2	6	0	0.830926	2.048438	1.382069
3	6	0	1.486714	0.227752	-0.182402
4	1	0	1.202939	2.802096	2.079375
5	1	0	0.083010	1.433032	1.901882
6	1	0	2.407323	0.612474	1.747308
7	1	0	0.713076	-0.419581	0.253532
8	8	0	0.929715	0.999100	-1.247372
9	7	0	0.318421	2.726335	0.199735
10	6	0	2.555342	-0.666191	-0.803501
11	1	0	2.070336	-1.284809	-1.565965
12	6	0	3.227135	-1.601615	0.201897
13	1	0	3.736060	-1.011100	0.976401
14	6	0	2.286544	-2.591322	0.862080
15	1	0	1.690556	-3.090731	0.085201
16	1	0	1.606895	-2.081228	1.547535
17	8	0	3.571615	0.066941	-1.474027
18	1	0	3.739174	0.850208	-0.929876
19	8	0	4.190206	-2.385610	-0.493210
20	1	0	4.679434	-1.767494	-1.049803
21	8	0	3.016144	-3.535091	1.624970
22	1	0	3.741970	-3.819991	1.058130
23	8	0	3.026476	2.014672	0.397510
24	1	0	2.554996	2.669549	-0.140621
25	6	0	-0.398698	3.973109	0.402374
26	1	0	-1.267994	3.897967	1.066735
27	1	0	0.285521	4.709465	0.831736
28	1	0	-0.739739	4.350301	-0.564108
29	6	0	-1.368520	0.950268	-0.518862
30	6	0	-2.240836	1.218135	0.534806
31	6	0	-1.635259	-0.129091	-1.368252
32	6	0	-3.365060	0.428400	0.743541
33	1	0	-2.051677	2.037297	1.213960
34	6	0	-2.750159	-0.928334	-1.176753
35	1	0	-0.956189	-0.345515	-2.184247
36	6	0	-3.598172	-0.629825	-0.118581
37	1	0	-4.044832	0.626467	1.560893
38	1	0	-2.963507	-1.764109	-1.829457
39	6	0	-0.145820	1.826695	-0.830871
40	1	0	-0.397660	2.434696	-1.704081
41	7	0	-4.787116	-1.470956	0.096988
42	8	0	-5.532121	-1.178786	1.009544
43	8	0	-4.959804	-2.411503	-0.650412

Structure 43d ($^5C_2$ ax-ax) (M06-2X, DMSO)

Energy (Hartrees): = - 1181.3606539
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.767401	1.227970	0.951907
2	6	0	0.560080	2.084691	1.342635
3	6	0	1.312343	0.231908	-0.115676
4	1	0	0.871587	2.869818	2.033261
5	1	0	-0.164735	1.445107	1.860301
6	1	0	2.135815	0.686344	1.825222
7	1	0	0.541371	-0.411586	0.328810
8	8	0	0.759984	0.966639	-1.212558
9	7	0	-0.103802	2.707544	0.192609
10	6	0	2.382965	-0.688793	-0.700100
11	1	0	1.895821	-1.257573	-1.498677
12	6	0	2.919998	-1.676611	0.337700
13	1	0	2.090569	-2.074117	0.937393
14	6	0	3.638961	-2.828097	-0.342059
15	1	0	4.360211	-2.424518	-1.059981
16	1	0	2.915948	-3.458290	-0.870647
17	8	0	3.454443	0.012774	-1.299894
18	1	0	3.985764	0.335652	-0.559391
19	8	0	3.833886	-0.975829	1.169583
20	1	0	4.422422	-1.650502	1.531736
21	8	0	4.300199	-3.554231	0.688993
22	1	0	4.978915	-4.103743	0.285907
23	8	0	2.838478	2.040559	0.481682
24	1	0	2.690491	2.168462	-0.463397
25	6	0	0.525897	3.924209	-0.317023
26	1	0	1.414910	3.749410	-0.935885
27	1	0	-0.200246	4.473767	-0.921345
28	1	0	0.815802	4.554681	0.524476
29	6	0	-1.572187	0.853796	-0.508294
30	6	0	-2.573564	1.304931	0.350853
31	6	0	-1.704384	-0.392322	-1.125698
32	6	0	-3.691754	0.523424	0.605774
33	1	0	-2.469231	2.273252	0.823857
34	6	0	-2.814881	-1.186744	-0.884358
35	1	0	-0.928723	-0.743819	-1.795703
36	6	0	-3.789136	-0.711058	-0.017869
37	1	0	-4.472390	0.860939	1.273787
38	1	0	-2.927440	-2.154563	-1.354219
39	6	0	-0.379973	1.747618	-0.844730
40	1	0	-0.634104	2.299833	-1.753415
41	7	0	-4.969146	-1.548873	0.250272
42	8	0	-5.788350	-1.137917	1.046133
43	8	0	-5.061479	-2.606842	-0.337767

Structure 44a (^{2}E ec-ax H-bond O) (M06-2X, Gas Phase)

Energy (Hartrees): = - 976.8505209
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.058359	-0.180968	0.356184
2	6	0	-3.230090	-0.899043	-0.825494
3	6	0	-4.495492	-1.038281	-1.385748
4	6	0	-5.602348	-0.469074	-0.765503
5	6	0	-5.441100	0.233033	0.424176
6	6	0	-4.175145	0.371502	0.980876
7	1	0	-2.373120	-1.372095	-1.290287
8	1	0	-4.618762	-1.599780	-2.304288
9	1	0	-6.587985	-0.582277	-1.201116
10	1	0	-6.301125	0.665865	0.921179
11	1	0	-4.052838	0.909270	1.916435
12	6	0	-1.679103	0.053285	0.950758
13	1	0	-1.761159	0.092969	2.042367
14	7	0	-0.996201	1.259502	0.481381
15	8	0	-0.796086	-0.995157	0.587783
16	6	0	0.158611	-0.517769	-0.378243
17	6	0	-0.357223	0.862676	-0.764572
18	1	0	0.454191	1.542346	-1.023922
19	1	0	-1.067844	0.800474	-1.604182
20	1	0	0.168834	-1.229366	-1.209710
21	6	0	1.525411	-0.499066	0.300651
22	1	0	1.555708	0.352382	0.992693
23	6	0	2.688685	-0.355826	-0.683439
24	1	0	2.522145	-1.038963	-1.527927
25	6	0	4.009979	-0.788488	-0.014473

26	1	0	4.078888	-1.877734	-0.096869
27	6	0	5.228462	-0.149700	-0.669568
28	1	0	6.134918	-0.666036	-0.339190
29	1	0	5.161715	-0.204058	-1.757126
30	8	0	1.709512	-1.721615	1.005925
31	1	0	0.855268	-1.930779	1.403123
32	8	0	2.699456	0.961505	-1.200670
33	1	0	3.488999	1.416790	-0.876345
34	8	0	4.085146	-0.397673	1.349291
35	1	0	3.413914	-0.909865	1.816180
36	8	0	5.290843	1.228287	-0.322923
37	1	0	5.232261	1.253658	0.640047
38	6	0	-1.786967	2.470935	0.405250
39	1	0	-2.227728	2.684694	1.381930
40	1	0	-1.128161	3.300410	0.143522
41	1	0	-2.597598	2.413517	-0.336573

Structure 44a (^{2}E ec-ax H-bond N) (M06-2X, Gas Phase)

Energy (Hartrees): = - 976.8529803
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.844343	-0.227856	-0.450372
2	6	0	3.049463	-1.282372	0.436996
3	6	0	4.323511	-1.810881	0.614686
4	6	0	5.400254	-1.297185	-0.099736
5	6	0	5.198150	-0.258495	-1.002505
6	6	0	3.924227	0.269132	-1.177477
7	1	0	2.201684	-1.707221	0.961230
8	1	0	4.473651	-2.632973	1.304309
9	1	0	6.391049	-1.714427	0.035346
10	1	0	6.029658	0.132974	-1.576329
11	1	0	3.765093	1.069530	-1.894006
12	6	0	1.475014	0.407979	-0.607257
13	1	0	1.355586	0.772731	-1.633701
14	7	0	1.212109	1.533396	0.315531
15	8	0	0.456512	-0.522021	-0.315792
16	6	0	-0.252862	-0.133042	0.866592
17	6	0	0.671767	0.893843	1.513704
18	1	0	0.133753	1.621747	2.125351
19	1	0	1.453910	0.419443	2.124573
20	1	0	-0.420308	-1.022760	1.476359
21	6	0	-1.611917	0.448876	0.493534
22	1	0	-2.123209	0.725796	1.426606
23	6	0	-2.482901	-0.606880	-0.188192
24	1	0	-1.888071	-1.095310	-0.968515
25	6	0	-3.693598	0.053931	-0.873413
26	1	0	-3.372390	0.376375	-1.868777
27	6	0	-4.877538	-0.896429	-1.000655
28	1	0	-5.607699	-0.483208	-1.703364
29	1	0	-4.554267	-1.876321	-1.354199
30	8	0	-1.501813	1.581256	-0.357477
31	1	0	-0.598621	1.934202	-0.279056
32	8	0	-2.807477	-1.590472	0.778423
33	1	0	-3.748908	-1.522142	0.985830
34	8	0	-4.199578	1.167075	-0.145438
35	1	0	-3.516056	1.847395	-0.173601
36	8	0	-5.475811	-1.088618	0.275636
37	1	0	-5.644047	-0.201062	0.614603
38	6	0	2.307658	2.457502	0.553292
39	1	0	2.661675	2.861405	-0.397253
40	1	0	1.939458	3.287173	1.158930
41	1	0	3.155214	1.986389	1.068933

Structure 44a (^{2}E ec-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 976.8524799
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.135013	-0.128470	0.242357
2	6	0	-3.649812	-0.242935	-1.048418
3	6	0	-4.967763	-0.631227	-1.237499
4	6	0	-5.780238	-0.906339	-0.138405
5	6	0	-5.270286	-0.792324	1.148036
6	6	0	-3.945841	-0.404233	1.335996

7	1	0	-3.004865	-0.011671	-1.888132
8	1	0	-5.367913	-0.719737	-2.240655
9	1	0	-6.809980	-1.208316	-0.288726
10	1	0	-5.899192	-1.006404	2.003925
11	1	0	-3.540806	-0.314422	2.338843
12	6	0	-1.705109	0.303100	0.429449
13	1	0	-1.477641	0.378373	1.512055
14	7	0	-1.396740	1.548867	-0.251101
15	8	0	-0.816813	-0.633514	-0.162783
16	6	0	0.322573	0.075385	-0.674066
17	6	0	0.058045	1.535631	-0.314744
18	1	0	0.518113	1.782049	0.656446
19	1	0	0.442115	2.233042	-1.058760
20	1	0	0.344055	-0.077949	-1.758277
21	6	0	1.564224	-0.540313	-0.055580
22	1	0	1.576623	-0.310147	1.018466
23	6	0	2.851652	0.007442	-0.666349
24	1	0	2.753258	-0.003486	-1.760539
25	6	0	4.046590	-0.900601	-0.314632
26	1	0	4.068147	-1.714483	-1.046508
27	6	0	5.371830	-0.150124	-0.345952
28	1	0	6.199837	-0.865332	-0.336703
29	1	0	5.446400	0.472954	-1.238310
30	8	0	1.544504	-1.948599	-0.254014
31	1	0	0.640149	-2.235265	-0.078900
32	8	0	2.992396	1.358127	-0.268483
33	1	0	3.749957	1.429427	0.328866
34	8	0	3.960259	-1.432629	1.000199
35	1	0	3.212387	-2.041672	1.000511
36	8	0	5.456189	0.717725	0.777817
37	1	0	5.284615	0.161008	1.546983
38	6	0	-1.951931	2.715715	0.405606
39	1	0	-1.575847	2.831409	1.436453
40	1	0	-1.687873	3.609530	-0.161012
41	1	0	-3.040157	2.635892	0.434991

Structure 44a (E_2 ax-ax) (M06-2X, Gas Phase)

Energy (Hartrees): = - 976.8527004
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.078101	0.062927	0.263931
2	6	0	-3.271391	-1.297752	0.489153
3	6	0	-4.342469	-1.959832	-0.102327
4	6	0	-5.227179	-1.265973	-0.919899
5	6	0	-5.035329	0.093265	-1.147205
6	6	0	-3.964314	0.755488	-0.558929
7	1	0	-2.574459	-1.832076	1.123682
8	1	0	-4.484493	-3.019559	0.074471
9	1	0	-6.060171	-1.782178	-1.382342
10	1	0	-5.718210	0.638015	-1.788501
11	1	0	-3.790702	1.808842	-0.744220
12	6	0	-1.932230	0.802573	0.937894
13	1	0	-2.267588	1.251621	1.875865
14	7	0	-1.355602	1.800670	0.068559
15	8	0	-0.867789	-0.100026	1.263613
16	6	0	-0.053918	-0.210342	0.088780
17	6	0	-0.487011	0.989554	-0.797912
18	1	0	0.364606	1.564020	-1.156643
19	1	0	-1.061673	0.633222	-1.653944
20	1	0	-0.268366	-1.168500	-0.399584
21	6	0	1.393758	-0.205252	0.556478
22	1	0	1.656870	0.798829	0.914813
23	6	0	2.381678	-0.559428	-0.556938
24	1	0	1.988298	-1.415116	-1.124480
25	6	0	3.726085	-1.008011	0.043751
26	1	0	3.614691	-2.053131	0.349098
27	6	0	4.875563	-0.888505	-0.949100
28	1	0	5.742995	-1.440478	-0.574714
29	1	0	4.592809	-1.287557	-1.924583
30	8	0	1.551519	-1.156582	1.603686
31	1	0	0.777205	-1.063185	2.170747
32	8	0	2.470620	0.546760	-1.435435
33	1	0	3.388013	0.852978	-1.463334
34	8	0	4.116579	-0.212759	1.154056
35	1	0	3.497942	-0.416995	1.864539
36	8	0	5.206936	0.481785	-1.138876
37	1	0	5.347652	0.838013	-0.253075
38	6	0	-0.615433	2.814233	0.820741
39	1	0	-0.114718	3.480929	0.118615
40	1	0	-1.318426	3.408234	1.407327

41	1	0	0.135759	2.388293	1.499491

Structure 44a (^{2}E ec-ax H-bond O) (M06-2X, Benzene)

Energy (Hartrees): = - 976.8692297
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.061802	-0.181209	-0.355267
2	6	0	3.225064	-0.903467	0.825721
3	6	0	4.487665	-1.050594	1.391402
4	6	0	5.600092	-0.483340	0.778493
5	6	0	5.447011	0.224212	-0.409414
6	6	0	4.184118	0.370374	-0.972198
7	1	0	2.364351	-1.371815	1.289038
8	1	0	4.604040	-1.615301	2.309224
9	1	0	6.583345	-0.601712	1.218853
10	1	0	6.311179	0.656740	-0.900117
11	1	0	4.069073	0.912523	-1.906150
12	6	0	1.686302	0.062043	-0.956440
13	1	0	1.774696	0.107358	-2.046905
14	7	0	1.003954	1.266989	-0.482525
15	8	0	0.796467	-0.985680	-0.604286
16	6	0	-0.156473	-0.513656	0.367597
17	6	0	0.362008	0.864274	0.760374
18	1	0	-0.447206	1.545836	1.021349
19	1	0	1.069910	0.798121	1.601149
20	1	0	-0.165368	-1.228846	1.195562
21	6	0	-1.525312	-0.486952	-0.309905
22	1	0	-1.559548	0.378263	-0.984671
23	6	0	-2.690581	-0.372062	0.676433
24	1	0	-2.523970	-1.075514	1.503495
25	6	0	-4.011408	-0.789142	-0.003343
26	1	0	-4.080697	-1.879902	0.051744
27	6	0	-5.233254	-0.176792	0.667973
28	1	0	-6.136720	-0.684140	0.315816
29	1	0	-5.174735	-0.272767	1.753231
30	8	0	-1.705866	-1.694551	-1.042563
31	1	0	-0.854164	-1.884484	-1.455389
32	8	0	-2.706722	0.934444	1.226035
33	1	0	-3.499845	1.389682	0.910705
34	8	0	-4.086871	-0.362629	-1.357921
35	1	0	-3.409346	-0.856787	-1.835782
36	8	0	-5.303652	1.215037	0.371122
37	1	0	-5.257009	1.276882	-0.591155
38	6	0	1.793756	2.478829	-0.401407
39	1	0	2.240547	2.694777	-1.375053
40	1	0	1.133612	3.309186	-0.143582
41	1	0	2.598598	2.424887	0.347099

Structure 44a (^{2}E ec-ax H-bond N) (M06-2X, Benzene)

Energy (Hartrees): = - 976.8727179
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.844955	-0.234899	-0.444579
2	6	0	3.079966	-1.261163	0.469085
3	6	0	4.362444	-1.774600	0.632748
4	6	0	5.418104	-1.274724	-0.122546
5	6	0	5.186414	-0.263735	-1.049870
6	6	0	3.904270	0.249607	-1.210453
7	1	0	2.250515	-1.675519	1.030239
8	1	0	4.534751	-2.574686	1.343319
9	1	0	6.415334	-1.680649	0.001275
10	1	0	6.001411	0.117540	-1.654023
11	1	0	3.723311	1.029953	-1.943892
12	6	0	1.468078	0.387612	-0.591191
13	1	0	1.334768	0.736702	-1.621188
14	7	0	1.203578	1.521594	0.317938
15	8	0	0.460009	-0.549861	-0.275041
16	6	0	-0.254626	-0.137235	0.897244
17	6	0	0.668421	0.900660	1.528329
18	1	0	0.130854	1.638163	2.128736
19	1	0	1.450993	0.436974	2.145974
20	1	0	-0.422321	-1.014150	1.524830
21	6	0	-1.611563	0.442390	0.508754

22	1	0	-2.125805	0.730184	1.436692
23	6	0	-2.485619	-0.611898	-0.172733
24	1	0	-1.889343	-1.115546	-0.941973
25	6	0	-3.682480	0.051701	-0.879351
26	1	0	-3.345313	0.365992	-1.871860
27	6	0	-4.870345	-0.889174	-1.025473
28	1	0	-5.588707	-0.468178	-1.735802
29	1	0	-4.552143	-1.869259	-1.383747
30	8	0	-1.490428	1.568994	-0.350526
31	1	0	-0.581473	1.911885	-0.268936
32	8	0	-2.835533	-1.583960	0.800300
33	1	0	-3.780528	-1.503054	0.985452
34	8	0	-4.192170	1.172892	-0.163710
35	1	0	-3.497954	1.843130	-0.178095
36	8	0	-5.491585	-1.085519	0.242050
37	1	0	-5.671694	-0.199344	0.579355
38	6	0	2.288210	2.463381	0.531024
39	1	0	2.627943	2.858927	-0.428411
40	1	0	1.914173	3.297670	1.127214
41	1	0	3.146455	2.014194	1.048775

Structure 44a (^{2}E ec-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 976.8717092
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.141434	-0.123722	0.238783
2	6	0	-3.669011	-0.178161	-1.051336
3	6	0	-4.983030	-0.577891	-1.248021
4	6	0	-5.778894	-0.926521	-0.157172
5	6	0	-5.255999	-0.873892	1.128503
6	6	0	-3.936401	-0.472635	1.324337
7	1	0	-3.039513	0.106281	-1.886897
8	1	0	-5.392227	-0.618205	-2.250847
9	1	0	-6.805590	-1.236947	-0.313162
10	1	0	-5.871665	-1.143566	1.978689
11	1	0	-3.523060	-0.429682	2.326947
12	6	0	-1.712789	0.310626	0.437457
13	1	0	-1.489995	0.370223	1.520936
14	7	0	-1.401358	1.565954	-0.224479
15	8	0	-0.822850	-0.619451	-0.166285
16	6	0	0.318568	0.095453	-0.667766
17	6	0	0.054465	1.550470	-0.288482
18	1	0	0.512143	1.783224	0.686673
19	1	0	0.435899	2.257998	-1.024528
20	1	0	0.341049	-0.042916	-1.753791
21	6	0	1.559755	-0.530332	-0.056732
22	1	0	1.570336	-0.317655	1.020745
23	6	0	2.850994	0.022305	-0.657733
24	1	0	2.751333	0.041425	-1.751401
25	6	0	4.040480	-0.901860	-0.332432
26	1	0	4.047970	-1.703878	-1.077182
27	6	0	5.374542	-0.169591	-0.369845
28	1	0	6.191937	-0.896994	-0.374195
29	1	0	5.453179	0.456579	-1.259773
30	8	0	1.536804	-1.936476	-0.276882
31	1	0	0.636864	-2.227528	-0.085483
32	8	0	3.006213	1.361793	-0.221601
33	1	0	3.776898	1.407177	0.361387
34	8	0	3.962214	-1.452417	0.976837
35	1	0	3.204410	-2.049423	0.976553
36	8	0	5.486671	0.689806	0.761116
37	1	0	5.326848	0.128292	1.529748
38	6	0	-1.950264	2.725737	0.450672
39	1	0	-1.580941	2.820251	1.485774
40	1	0	-1.674694	3.627917	-0.097791
41	1	0	-3.039973	2.659784	0.472087

Structure 44a (E_2 ax-ax) (M06-2X, Benzene)

Energy (Hartrees): = - 976.8712986
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.086656	0.062414	0.263422
2	6	0	-3.280370	-1.301805	0.468222

3	6	0	-4.364680	-1.951112	-0.114628
4	6	0	-5.263182	-1.241266	-0.903326
5	6	0	-5.072030	0.121828	-1.109814
6	6	0	-3.987743	0.770700	-0.530451
7	1	0	-2.574966	-1.850467	1.080961
8	1	0	-4.505870	-3.013730	0.046713
9	1	0	-6.106331	-1.747255	-1.359096
10	1	0	-5.765431	0.680000	-1.728365
11	1	0	-3.818757	1.827469	-0.701448
12	6	0	-1.926762	0.789814	0.928559
13	1	0	-2.252851	1.241385	1.868442
14	7	0	-1.346952	1.784405	0.057169
15	8	0	-0.868890	-0.123420	1.246087
16	6	0	-0.046075	-0.227281	0.075538
17	6	0	-0.481807	0.970920	-0.810415
18	1	0	0.367620	1.547183	-1.171219
19	1	0	-1.057068	0.613450	-1.665754
20	1	0	-0.249752	-1.185846	-0.415950
21	6	0	1.400485	-0.207442	0.550974
22	1	0	1.656491	0.805462	0.888564
23	6	0	2.396879	-0.587276	-0.546388
24	1	0	2.019134	-1.469810	-1.081105
25	6	0	3.747634	-0.988691	0.073467
26	1	0	3.656956	-2.024610	0.413770
27	6	0	4.900637	-0.886588	-0.915406
28	1	0	5.776517	-1.403164	-0.511247
29	1	0	4.637157	-1.336157	-1.874189
30	8	0	1.558881	-1.134623	1.620279
31	1	0	0.787563	-1.024316	2.188884
32	8	0	2.473215	0.486126	-1.469047
33	1	0	3.384963	0.808763	-1.493403
34	8	0	4.118088	-0.146940	1.158272
35	1	0	3.497224	-0.335222	1.871481
36	8	0	5.208800	0.482506	-1.163990
37	1	0	5.349851	0.878260	-0.294739
38	6	0	-0.606920	2.800212	0.806987
39	1	0	-0.103462	3.464806	0.104017
40	1	0	-1.310181	3.398246	1.389741
41	1	0	0.142634	2.378959	1.490502

Structure 44a (^{2}E ec-ax H-bond O) (M06-2X, DMSO)

Energy (Hartrees): = - 976.8719895
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.073780	-0.177726	-0.348822
2	6	0	3.191771	-0.921366	0.825535
3	6	0	4.438878	-1.113202	1.414472
4	6	0	5.579702	-0.568506	0.831982
5	6	0	5.470374	0.163980	-0.346974
6	6	0	4.223306	0.354580	-0.933677
7	1	0	2.309525	-1.366961	1.271449
8	1	0	4.519312	-1.694293	2.326262
9	1	0	6.550580	-0.721043	1.289758
10	1	0	6.356316	0.580976	-0.812244
11	1	0	4.139968	0.917328	-1.858814
12	6	0	1.719440	0.103701	-0.981687
13	1	0	1.841162	0.172782	-2.066912
14	7	0	1.044658	1.310336	-0.496715
15	8	0	0.803142	-0.936564	-0.678397
16	6	0	-0.143884	-0.481280	0.308586
17	6	0	0.376944	0.888082	0.728075
18	1	0	-0.428801	1.575376	0.986315
19	1	0	1.070459	0.804066	1.578537
20	1	0	-0.152227	-1.208017	1.126221
21	6	0	-1.514691	-0.452631	-0.359742
22	1	0	-1.545021	0.382321	-1.071581
23	6	0	-2.667783	-0.264322	0.632344
24	1	0	-2.465260	-0.853992	1.537193
25	6	0	-3.980505	-0.799938	0.039669
26	1	0	-3.956548	-1.889947	0.128004
27	6	0	-5.211507	-0.282427	0.767528
28	1	0	-6.086443	-0.866517	0.467800
29	1	0	-5.087574	-0.366755	1.848336
30	8	0	-1.715921	-1.686995	-1.042754
31	1	0	-0.886680	-1.871983	-1.501710
32	8	0	-2.720482	1.109405	0.994070
33	1	0	-3.618097	1.429089	0.826898
34	8	0	-4.155037	-0.415361	-1.319606
35	1	0	-3.471704	-0.880162	-1.818445
36	8	0	-5.420527	1.099765	0.472489

37	1	0	-5.455801	1.159413	-0.490949
38	6	0	1.863578	2.499860	-0.360227
39	1	0	2.355183	2.720951	-1.310570
40	1	0	1.217947	3.342972	-0.106120
41	1	0	2.635284	2.407210	0.418784

Structure 44a (^{2}E ec-ax H-bond N) (M06-2X, DMSO)

Energy (Hartrees): = - 976.8759144
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.850174	-0.227775	-0.442936
2	6	0	3.069325	-1.264804	0.463874
3	6	0	4.346891	-1.792024	0.631740
4	6	0	5.413789	-1.292090	-0.109429
5	6	0	5.198292	-0.265757	-1.025312
6	6	0	3.921028	0.260116	-1.191841
7	1	0	2.235675	-1.673097	1.024072
8	1	0	4.507435	-2.599141	1.337510
9	1	0	6.407075	-1.707185	0.018647
10	1	0	6.022537	0.119372	-1.614842
11	1	0	3.751530	1.054131	-1.913080
12	6	0	1.478292	0.403008	-0.606218
13	1	0	1.366216	0.760319	-1.635156
14	7	0	1.202617	1.526629	0.308146
15	8	0	0.459507	-0.535236	-0.314174
16	6	0	-0.243478	-0.146432	0.876353
17	6	0	0.675982	0.889393	1.514672
18	1	0	0.136599	1.616080	2.125765
19	1	0	1.463186	0.422599	2.122958
20	1	0	-0.392975	-1.031987	1.496048
21	6	0	-1.606603	0.432371	0.510214
22	1	0	-2.108472	0.706570	1.448490
23	6	0	-2.489084	-0.607098	-0.182234
24	1	0	-1.905193	-1.098486	-0.968396
25	6	0	-3.692570	0.068760	-0.864992
26	1	0	-3.364822	0.401292	-1.854274
27	6	0	-4.878430	-0.869852	-1.027430
28	1	0	-5.604155	-0.430921	-1.718542
29	1	0	-4.558880	-1.836083	-1.420171
30	8	0	-1.492640	1.574425	-0.331599
31	1	0	-0.578418	1.908750	-0.252506
32	8	0	-2.835838	-1.598917	0.776321
33	1	0	-3.781263	-1.517217	0.959675
34	8	0	-4.196974	1.175408	-0.121381
35	1	0	-3.494760	1.837970	-0.114718
36	8	0	-5.491073	-1.109685	0.240249
37	1	0	-5.682461	-0.235687	0.603798
38	6	0	2.282231	2.473813	0.528769
39	1	0	2.629724	2.865530	-0.429440
40	1	0	1.899542	3.306130	1.122025
41	1	0	3.134682	2.026935	1.058399

Structure 44a (^{2}E ec-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 976.8742948
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.150568	-0.121778	0.241537
2	6	0	-3.606433	-0.478081	-1.028546
3	6	0	-4.923530	-0.878627	-1.209115
4	6	0	-5.796831	-0.919913	-0.121574
5	6	0	-5.347019	-0.560382	1.143494
6	6	0	-4.022444	-0.163969	1.324006
7	1	0	-2.920681	-0.436896	-1.867836
8	1	0	-5.273856	-1.159295	-2.195898
9	1	0	-6.825213	-1.231877	-0.264208
10	1	0	-6.022903	-0.589184	1.990474
11	1	0	-3.665369	0.115743	2.310176
12	6	0	-1.724405	0.330035	0.418471
13	1	0	-1.513875	0.489600	1.492100
14	7	0	-1.416675	1.528029	-0.350722
15	8	0	-0.826291	-0.644086	-0.095779
16	6	0	0.316052	0.032590	-0.651718
17	6	0	0.042309	1.511907	-0.396022

18	1	0	0.480243	1.824988	0.564618
19	1	0	0.426790	2.158290	-1.184950
20	1	0	0.344885	-0.194050	-1.722734
21	6	0	1.559185	-0.531141	0.012329
22	1	0	1.561360	-0.236777	1.070094
23	6	0	2.849452	-0.014503	-0.624029
24	1	0	2.750893	-0.057332	-1.717053
25	6	0	4.037635	-0.915402	-0.248212
26	1	0	4.013918	-1.785237	-0.911045
27	6	0	5.379593	-0.217508	-0.408824
28	1	0	6.183006	-0.958322	-0.361290
29	1	0	5.436829	0.302311	-1.366283
30	8	0	1.548606	-1.951454	-0.098624
31	1	0	0.663816	-2.236117	0.161799
32	8	0	3.007643	1.346841	-0.250886
33	1	0	3.835269	1.427409	0.243241
34	8	0	3.993896	-1.330729	1.112806
35	1	0	3.235673	-1.921981	1.191287
36	8	0	5.553513	0.762368	0.615643
37	1	0	5.432282	0.292013	1.450391
38	6	0	-1.964665	2.737127	0.239517
39	1	0	-1.599417	2.898058	1.266768
40	1	0	-1.680628	3.597655	-0.368578
41	1	0	-3.055226	2.679140	0.260823

Structure 44a (E_2 ax-ax) (M06-2X, DMSO)

Energy (Hartrees): = - 976.8734343
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.095740	0.065098	0.262936
2	6	0	-3.211051	-1.314154	0.420164
3	6	0	-4.295692	-1.995723	-0.128225
4	6	0	-5.274171	-1.302107	-0.832103
5	6	0	-5.164403	0.078241	-0.987624
6	6	0	-4.079840	0.757563	-0.444761
7	1	0	-2.446772	-1.851759	0.969118
8	1	0	-4.373241	-3.070263	-0.005745
9	1	0	-6.117233	-1.831921	-1.260689
10	1	0	-5.923854	0.624401	-1.535824
11	1	0	-3.984713	1.829880	-0.574755
12	6	0	-1.933347	0.833269	0.876186
13	1	0	-2.259227	1.353577	1.779655
14	7	0	-1.358641	1.765748	-0.068612
15	8	0	-0.875401	-0.054523	1.252195
16	6	0	-0.040898	-0.228893	0.096977
17	6	0	-0.489576	0.893363	-0.874029
18	1	0	0.352369	1.450378	-1.279336
19	1	0	-1.063172	0.464455	-1.697899
20	1	0	-0.224090	-1.223386	-0.325608
21	6	0	1.403906	-0.151137	0.572694
22	1	0	1.643771	0.887286	0.833653
23	6	0	2.407490	-0.601118	-0.491547
24	1	0	2.038595	-1.520604	-0.966102
25	6	0	3.755896	-0.950091	0.158692
26	1	0	3.658337	-1.949083	0.593102
27	6	0	4.906215	-0.965724	-0.835455
28	1	0	5.780131	-1.434910	-0.374398
29	1	0	4.639124	-1.528070	-1.731504
30	8	0	1.572902	-0.992685	1.709954
31	1	0	0.815218	-0.824762	2.283550
32	8	0	2.484487	0.415817	-1.480971
33	1	0	3.410762	0.680289	-1.569745
34	8	0	4.134815	-0.009966	1.158413
35	1	0	3.508664	-0.120918	1.884122
36	8	0	5.224515	0.363940	-1.249445
37	1	0	5.389415	0.858674	-0.436390
38	6	0	-0.616300	2.831464	0.611684
39	1	0	-0.111944	3.445436	-0.135461
40	1	0	-1.320221	3.464348	1.155317
41	1	0	0.133105	2.455752	1.320535

Structure 44b (^{2}E ec-ec H-bond O) (M06-2X, Gas Phase)

Energy (Hartrees): = - 976.8541021
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.838389	0.007100	0.142177
2	6	0	2.315018	-1.160656	-0.413254
3	6	0	3.156785	-2.211035	-0.747059
4	6	0	4.529985	-2.100109	-0.532997
5	6	0	5.054927	-0.937873	0.015685
6	6	0	4.206670	0.113943	0.355405
7	1	0	1.246148	-1.227638	-0.586298
8	1	0	2.747617	-3.117685	-1.176833
9	1	0	5.186471	-2.920989	-0.795986
10	1	0	6.121579	-0.848669	0.183291
11	1	0	4.611496	1.022157	0.790094
12	6	0	1.905111	1.134969	0.500154
13	1	0	2.479237	1.967292	0.950991
14	7	0	1.118713	1.590000	-0.633112
15	8	0	0.936144	0.701472	1.447134
16	6	0	-0.352093	1.218864	1.078031
17	6	0	-0.036467	2.229256	-0.017240
18	1	0	-0.858916	2.343724	-0.722783
19	1	0	0.220663	3.209097	0.419867
20	1	0	-0.799526	1.664803	1.969810
21	6	0	-1.200725	0.045273	0.583428
22	1	0	-0.912422	-0.173752	-0.453408
23	6	0	-2.699874	0.344207	0.597396
24	1	0	-2.959652	0.796662	1.564435
25	6	0	-3.507901	-0.965055	0.486789
26	1	0	-3.597302	-1.382296	1.494748
27	6	0	-4.897387	-0.741919	-0.096980
28	1	0	-5.511139	-1.632767	0.067778
29	1	0	-5.382997	0.118061	0.366400
30	8	0	-0.974674	-1.090932	1.407162
31	1	0	-0.041763	-1.059259	1.657482
32	8	0	-2.983874	1.300291	-0.407261
33	1	0	-3.519871	0.879580	-1.094185
34	8	0	-2.898899	-1.913191	-0.378841
35	1	0	-2.079275	-2.186717	0.049900
36	8	0	-4.792983	-0.463822	-1.488210
37	1	0	-4.264132	-1.182686	-1.855144
38	6	0	1.860207	2.425324	-1.555177
39	1	0	2.711465	1.866461	-1.949026
40	1	0	1.216565	2.703319	-2.390469
41	1	0	2.233180	3.347022	-1.076896

Structure 44b (^{2}E ec-ec H-bond N) (M06-2X, Gas Phase)

Energy (Hartrees): = - 976.8566424
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.579478	-0.288404	-0.394675
2	6	0	-1.941152	-1.387563	0.178586
3	6	0	-2.662493	-2.542203	0.448778
4	6	0	-4.022013	-2.607302	0.151125
5	6	0	-4.658850	-1.514576	-0.423043
6	6	0	-3.934563	-0.358423	-0.699743
7	1	0	-0.882276	-1.325969	0.402967
8	1	0	-2.165092	-3.396799	0.891918
9	1	0	-4.580591	-3.511146	0.363572
10	1	0	-5.714244	-1.562662	-0.663091
11	1	0	-4.424733	0.492925	-1.162002
12	6	0	-1.809912	0.979260	-0.656547
13	1	0	-2.378180	1.616803	-1.360657
14	7	0	-1.524809	1.735774	0.567838
15	8	0	-0.534865	0.710290	-1.196031
16	6	0	0.415643	1.636827	-0.655451
17	6	0	-0.448721	2.624440	0.130046
18	1	0	0.071417	3.064075	0.983665
19	1	0	-0.828935	3.430569	-0.517335
20	1	0	0.970466	2.099076	-1.473331
21	6	0	1.405701	0.893611	0.233676
22	1	0	2.128430	1.628311	0.614567
23	6	0	2.202755	-0.130771	-0.575925
24	1	0	1.501312	-0.714622	-1.183456
25	6	0	2.935533	-1.111808	0.360837
26	1	0	2.241618	-1.924741	0.599044
27	6	0	4.193271	-1.689988	-0.276195
28	1	0	4.534191	-2.553799	0.302992
29	1	0	4.001613	-1.999659	-1.304358
30	8	0	0.769350	0.237573	1.323929
31	1	0	-0.128976	0.596348	1.426648

32	8	0	3.042670	0.581635	-1.466005
33	1	0	3.957744	0.489426	-1.168886
34	8	0	3.388424	-0.494891	1.560254
35	1	0	2.600816	-0.239930	2.056080
36	8	0	5.207445	-0.694169	-0.320877
37	1	0	5.270562	-0.353292	0.579571
38	6	0	-2.684187	2.416567	1.116479
39	1	0	-3.442147	1.681853	1.392082
40	1	0	-2.392231	2.965649	2.012336
41	1	0	-3.120488	3.125651	0.394947

Structure 44b (^{2}E ax-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 976.8502451
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.123527	-0.074738	-0.283754
2	6	0	3.102762	1.290715	-0.023827
3	6	0	4.239709	1.922882	0.471381
4	6	0	5.397465	1.193500	0.710522
5	6	0	5.419642	-0.174557	0.451093
6	6	0	4.287732	-0.804808	-0.047644
7	1	0	2.195680	1.850442	-0.211587
8	1	0	4.219243	2.987819	0.670268
9	1	0	6.281302	1.686759	1.096902
10	1	0	6.320365	-0.747421	0.636742
11	1	0	4.293053	-1.871804	-0.244763
12	6	0	1.909130	-0.805354	-0.788671
13	1	0	2.176462	-1.390390	-1.679785
14	7	0	1.313074	-1.718963	0.166690
15	8	0	0.873503	0.111260	-1.164929
16	6	0	-0.355156	-0.619767	-1.150789
17	6	0	-0.001824	-1.953587	-0.437547
18	1	0	-0.743556	-2.237226	0.306043
19	1	0	0.082493	-2.753207	-1.176982
20	1	0	-0.674686	-0.789114	-2.186708
21	6	0	-1.389589	0.262458	-0.469756
22	1	0	-1.141133	0.369516	0.593439
23	6	0	-2.808215	-0.308768	-0.542775
24	1	0	-2.977881	-0.721313	-1.548159
25	6	0	-3.846155	0.809456	-0.342851
26	1	0	-3.941875	1.338819	-1.296079
27	6	0	-5.208385	0.272310	0.077485
28	1	0	-5.962144	1.057407	-0.034614
29	1	0	-5.495626	-0.586186	-0.531889
30	8	0	-1.393024	1.539374	-1.103062
31	1	0	-0.471248	1.759288	-1.280316
32	8	0	-2.900814	-1.368578	0.390789
33	1	0	-3.616965	-1.177263	1.012556
34	8	0	-3.475774	1.715517	0.686419
35	1	0	-2.707015	2.197455	0.359865
36	8	0	-5.156014	-0.173362	1.427090
37	1	0	-4.795822	0.567547	1.929745
38	6	0	1.223897	-1.170941	1.523156
39	1	0	0.621522	-1.849476	2.127070
40	1	0	2.221358	-1.115572	1.959502
41	1	0	0.774707	-0.169821	1.565338

Structure 44b (^{2}E ec-ec H-bond O) (M06-2X, Benzene)

Energy (Hartrees): = - 976.8729161
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.841187	0.002979	-0.146920
2	6	0	-2.314202	-1.164224	0.407291
3	6	0	-3.153039	-2.216005	0.745776
4	6	0	-4.527520	-2.106839	0.537423
5	6	0	-5.056228	-0.945233	-0.010136
6	6	0	-4.211058	0.108119	-0.354470
7	1	0	-1.244879	-1.231612	0.578406
8	1	0	-2.740344	-3.121530	1.175212
9	1	0	-5.182099	-2.928317	0.804444
10	1	0	-6.124039	-0.857486	-0.173019
11	1	0	-4.619416	1.015908	-0.787054
12	6	0	-1.910920	1.135087	-0.503280

13	1	0	-2.486014	1.964180	-0.956544
14	7	0	-1.128337	1.593419	0.631994
15	8	0	-0.936285	0.702053	-1.447358
16	6	0	0.351329	1.221989	-1.074915
17	6	0	0.028882	2.232278	0.017939
18	1	0	0.846179	2.349664	0.728822
19	1	0	-0.226806	3.210760	-0.421454
20	1	0	0.800327	1.669640	-1.965063
21	6	0	1.201776	0.048563	-0.581026
22	1	0	0.913270	-0.175326	0.454593
23	6	0	2.701844	0.346190	-0.595432
24	1	0	2.962119	0.802645	-1.559901
25	6	0	3.511755	-0.962498	-0.487792
26	1	0	3.605239	-1.376809	-1.496346
27	6	0	4.901540	-0.742983	0.093926
28	1	0	5.511506	-1.636722	-0.069582
29	1	0	5.393552	0.110846	-0.374285
30	8	0	0.975966	-1.086303	-1.408685
31	1	0	0.037928	-1.063865	-1.641087
32	8	0	2.988724	1.298550	0.415035
33	1	0	3.518298	0.867564	1.100453
34	8	0	2.902848	-1.914634	0.375857
35	1	0	2.079352	-2.181060	-0.050301
36	8	0	4.804281	-0.461430	1.487603
37	1	0	4.283244	-1.183135	1.861060
38	6	0	-1.870034	2.434724	1.549320
39	1	0	-2.724044	1.882193	1.946919
40	1	0	-1.227337	2.713403	2.385842
41	1	0	-2.239566	3.356361	1.069082

Structure 44b (^{2}E ec-ec H-bond N) (M06-2X, Benzene)

Energy (Hartrees): = - 976.8762374
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.584788	-0.286719	-0.391366
2	6	0	-1.953749	-1.383164	0.196037
3	6	0	-2.677200	-2.537510	0.463833
4	6	0	-4.033197	-2.604876	0.149319
5	6	0	-4.663540	-1.514418	-0.437304
6	6	0	-3.936921	-0.358481	-0.710641
7	1	0	-0.897872	-1.320718	0.434824
8	1	0	-2.184721	-3.389374	0.918375
9	1	0	-4.594013	-3.508264	0.359480
10	1	0	-5.716600	-1.563578	-0.688808
11	1	0	-4.422415	0.492070	-1.179198
12	6	0	-1.813694	0.980904	-0.653020
13	1	0	-2.383394	1.619250	-1.353828
14	7	0	-1.518261	1.733707	0.569376
15	8	0	-0.539290	0.708185	-1.200254
16	6	0	0.413820	1.637926	-0.665605
17	6	0	-0.447146	2.625347	0.122836
18	1	0	0.075928	3.068833	0.972462
19	1	0	-0.833852	3.427506	-0.524491
20	1	0	0.960518	2.103253	-1.487140
21	6	0	1.409671	0.898979	0.221269
22	1	0	2.130840	1.638515	0.595489
23	6	0	2.207008	-0.132902	-0.579611
24	1	0	1.509525	-0.720134	-1.187750
25	6	0	2.935632	-1.112679	0.362404
26	1	0	2.241200	-1.924937	0.599615
27	6	0	4.192618	-1.698115	-0.267068
28	1	0	4.531339	-2.557866	0.319401
29	1	0	4.002488	-2.020694	-1.291658
30	8	0	0.774766	0.251746	1.318855
31	1	0	-0.125325	0.611723	1.414137
32	8	0	3.056416	0.571223	-1.471775
33	1	0	3.967317	0.477202	-1.162494
34	8	0	3.385990	-0.492482	1.562611
35	1	0	2.595952	-0.223874	2.047885
36	8	0	5.213128	-0.705326	-0.319722
37	1	0	5.282076	-0.360971	0.579421
38	6	0	-2.670443	2.415067	1.132974
39	1	0	-3.423534	1.683494	1.430174
40	1	0	-2.363274	2.970221	2.020353
41	1	0	-3.120859	3.119490	0.416071

Structure 44b (^{2}E ax-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 976.8688655

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.126856	-0.076603	-0.288270
2	6	0	3.096600	1.287197	-0.016884
3	6	0	4.231724	1.924929	0.476077
4	6	0	5.397458	1.203352	0.702296
5	6	0	5.429716	-0.162346	0.430401
6	6	0	4.299757	-0.798117	-0.067081
7	1	0	2.184125	1.843097	-0.191463
8	1	0	4.203369	2.988227	0.684425
9	1	0	6.279391	1.700907	1.088432
10	1	0	6.336820	-0.729155	0.605040
11	1	0	4.315582	-1.863281	-0.274965
12	6	0	1.912297	-0.816483	-0.781194
13	1	0	2.179626	-1.415639	-1.662531
14	7	0	1.317913	-1.716204	0.190577
15	8	0	0.874704	0.092906	-1.168124
16	6	0	-0.354668	-0.639089	-1.141446
17	6	0	0.002252	-1.961259	-0.409607
18	1	0	-0.735042	-2.235801	0.341498
19	1	0	0.086048	-2.770695	-1.138098
20	1	0	-0.674870	-0.825497	-2.173805
21	6	0	-1.389193	0.252748	-0.471294
22	1	0	-1.141360	0.372521	0.590668
23	6	0	-2.810737	-0.313445	-0.542394
24	1	0	-2.980486	-0.735374	-1.543222
25	6	0	-3.846423	0.808792	-0.352309
26	1	0	-3.942855	1.331114	-1.309161
27	6	0	-5.211973	0.281613	0.066528
28	1	0	-5.960586	1.071418	-0.048064
29	1	0	-5.506680	-0.573904	-0.543559
30	8	0	-1.388373	1.523217	-1.119239
31	1	0	-0.464187	1.750073	-1.275569
32	8	0	-2.912318	-1.364783	0.403306
33	1	0	-3.627698	-1.156837	1.020548
34	8	0	-3.474338	1.722116	0.672157
35	1	0	-2.699503	2.194218	0.345015
36	8	0	-5.169548	-0.163054	1.419734
37	1	0	-4.817111	0.579727	1.925708
38	6	0	1.228115	-1.148345	1.538730
39	1	0	0.622817	-1.815871	2.152938
40	1	0	2.224102	-1.090959	1.979478
41	1	0	0.781408	-0.145740	1.568677

Structure 44b (^{2}E ec-ec H-bond O) (M06-2X, DMSO)

Energy (Hartrees): = - 976.8754891
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.870607	-0.037211	-0.175141
2	6	0	-2.361905	-1.250954	0.290227
3	6	0	-3.225539	-2.265507	0.681159
4	6	0	-4.605694	-2.071889	0.617323
5	6	0	-5.115901	-0.863046	0.158529
6	6	0	-4.247060	0.151551	-0.240949
7	1	0	-1.287508	-1.396083	0.342549
8	1	0	-2.827084	-3.207987	1.039535
9	1	0	-5.278310	-2.864090	0.925690
10	1	0	-6.187521	-0.707894	0.108460
11	1	0	-4.639765	1.095885	-0.605300
12	6	0	-1.925449	1.070161	-0.567868
13	1	0	-2.487168	1.879659	-1.067138
14	7	0	-1.172680	1.584919	0.569127
15	8	0	-0.929831	0.590047	-1.463583
16	6	0	0.344431	1.155901	-1.104434
17	6	0	-0.006925	2.202757	-0.056756
18	1	0	0.793168	2.361683	0.665605
19	1	0	-0.267231	3.157119	-0.541405
20	1	0	0.790405	1.582922	-2.006138
21	6	0	1.218059	0.017249	-0.583127
22	1	0	0.868221	-0.266926	0.417857
23	6	0	2.698131	0.394259	-0.468610
24	1	0	2.990099	0.983974	-1.348243
25	6	0	3.578885	-0.865976	-0.471663
26	1	0	3.666959	-1.200939	-1.509297
27	6	0	4.974744	-0.609364	0.076464

28	1	0	5.623612	-1.455744	-0.166629
29	1	0	5.402819	0.296859	-0.354862
30	8	0	1.108355	-1.092389	-1.470290
31	1	0	0.172693	-1.151765	-1.704118
32	8	0	2.858424	1.206923	0.686184
33	1	0	3.518065	0.789038	1.257068
34	8	0	3.043000	-1.905322	0.340477
35	1	0	2.228255	-2.189987	-0.090890
36	8	0	4.924385	-0.420281	1.491779
37	1	0	4.472891	-1.198726	1.842410
38	6	0	-1.945195	2.499015	1.392312
39	1	0	-2.817313	1.984118	1.801419
40	1	0	-1.330669	2.843983	2.225496
41	1	0	-2.290363	3.376967	0.822723

Structure 44b (^{2}E ec-ec H-bond N) (M06-2X, DMSO)

Energy (Hartrees): = - 976.8792163
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.565982	-0.298471	-0.394745
2	6	0	-1.903240	-1.394327	0.159837
3	6	0	-2.602379	-2.563606	0.433713
4	6	0	-3.967006	-2.645389	0.158869
5	6	0	-4.629362	-1.554919	-0.394047
6	6	0	-3.926987	-0.384726	-0.674490
7	1	0	-0.841960	-1.321163	0.371594
8	1	0	-2.085123	-3.414386	0.862797
9	1	0	-4.509914	-3.558662	0.374460
10	1	0	-5.689442	-1.614494	-0.612466
11	1	0	-4.436895	0.466530	-1.115164
12	6	0	-1.821925	0.985050	-0.660887
13	1	0	-2.409697	1.616187	-1.350081
14	7	0	-1.526117	1.733889	0.563342
15	8	0	-0.546598	0.732759	-1.225524
16	6	0	0.402383	1.662323	-0.677107
17	6	0	-0.466204	2.639712	0.111724
18	1	0	0.053388	3.091253	0.958649
19	1	0	-0.867452	3.432439	-0.536497
20	1	0	0.947900	2.139382	-1.492243
21	6	0	1.397879	0.925339	0.212329
22	1	0	2.120530	1.668365	0.575427
23	6	0	2.187488	-0.125309	-0.571189
24	1	0	1.488301	-0.721752	-1.167805
25	6	0	2.910557	-1.093871	0.385228
26	1	0	2.208241	-1.892606	0.642066
27	6	0	4.152744	-1.713571	-0.237640
28	1	0	4.484990	-2.560298	0.370370
29	1	0	3.947304	-2.065647	-1.249340
30	8	0	0.762426	0.297164	1.322234
31	1	0	-0.142123	0.655200	1.397641
32	8	0	3.045969	0.555551	-1.477621
33	1	0	3.954556	0.442212	-1.167845
34	8	0	3.376033	-0.452833	1.570331
35	1	0	2.590495	-0.155369	2.046440
36	8	0	5.190441	-0.736892	-0.329740
37	1	0	5.278166	-0.371272	0.560042
38	6	0	-2.683185	2.411990	1.126439
39	1	0	-3.432813	1.678466	1.428733
40	1	0	-2.374677	2.972992	2.009612
41	1	0	-3.135805	3.108070	0.404568

Structure 44b (^{2}E ax-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 976.8714809
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.130082	-0.088715	-0.285505
2	6	0	3.075375	1.269699	0.014938
3	6	0	4.210004	1.925548	0.486749
4	6	0	5.399799	1.227353	0.663987
5	6	0	5.456094	-0.132303	0.363853
6	6	0	4.325915	-0.785989	-0.112928
7	1	0	2.146311	1.810011	-0.121260
8	1	0	4.162863	2.984002	0.716634

9	1	0	6.281593	1.739117	1.032267
10	1	0	6.381738	-0.680251	0.497866
11	1	0	4.364903	-1.844959	-0.348911
12	6	0	1.917268	-0.846075	-0.757017
13	1	0	2.186762	-1.472621	-1.617595
14	7	0	1.322136	-1.717560	0.244164
15	8	0	0.882228	0.052404	-1.169151
16	6	0	-0.351716	-0.672337	-1.115550
17	6	0	0.002883	-1.973850	-0.349800
18	1	0	-0.731405	-2.223326	0.412870
19	1	0	0.082557	-2.801648	-1.057508
20	1	0	-0.678733	-0.888463	-2.139037
21	6	0	-1.379799	0.239071	-0.460686
22	1	0	-1.133419	0.373607	0.599683
23	6	0	-2.804967	-0.318332	-0.530282
24	1	0	-2.972223	-0.761682	-1.521392
25	6	0	-3.834993	0.811154	-0.371838
26	1	0	-3.905991	1.326456	-1.334153
27	6	0	-5.216527	0.299910	0.006913
28	1	0	-5.951412	1.098996	-0.126079
29	1	0	-5.503279	-0.547486	-0.617794
30	8	0	-1.366568	1.500967	-1.125832
31	1	0	-0.438220	1.740742	-1.234893
32	8	0	-2.920267	-1.345329	0.445951
33	1	0	-3.669701	-1.132255	1.019590
34	8	0	-3.479160	1.728867	0.657100
35	1	0	-2.688386	2.185919	0.346181
36	8	0	-5.223880	-0.152402	1.361936
37	1	0	-4.888817	0.587192	1.885038
38	6	0	1.227457	-1.100739	1.572410
39	1	0	0.614504	-1.743306	2.205820
40	1	0	2.221177	-1.032916	2.018283
41	1	0	0.784146	-0.096634	1.563738

Structure 44c ($^5C_2$ ec-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 976.8530072
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.156791	1.401103	0.594021
2	6	0	-0.046447	2.360963	0.188627
3	6	0	-1.066396	0.152003	-0.287530
4	1	0	-0.064140	3.234883	0.843179
5	1	0	-0.186706	2.700558	-0.852806
6	1	0	-2.133413	1.878043	0.486689
7	1	0	-1.250009	0.451373	-1.332099
8	8	0	0.235567	-0.397182	-0.181347
9	7	0	1.224408	1.661983	0.369192
10	6	0	-2.046504	-0.962043	0.074401
11	1	0	-1.899379	-1.778587	-0.639449
12	6	0	-3.510426	-0.527958	0.007803
13	1	0	-3.689689	0.272709	0.741074
14	6	0	-3.973714	-0.065832	-1.362794
15	1	0	-3.681102	-0.822008	-2.106384
16	1	0	-3.504932	0.884005	-1.632228
17	8	0	-1.805933	-1.518341	1.354145
18	1	0	-1.625259	-0.776306	1.947234
19	8	0	-4.320908	-1.644699	0.329433
20	1	0	-3.909848	-2.062184	1.095427
21	8	0	-5.364883	0.147536	-1.369425
22	1	0	-5.749255	-0.623244	-0.937822
23	8	0	-0.995707	1.060969	1.964512
24	1	0	-0.040010	0.951256	2.079889
25	6	0	2.352664	2.563437	0.173950
26	1	0	2.423725	2.925109	-0.865405
27	1	0	2.226796	3.426329	0.829097
28	1	0	3.284853	2.063714	0.432939
29	6	0	2.570655	-0.247643	-0.409833
30	6	0	2.814346	-1.026672	0.719145
31	6	0	3.536666	-0.150086	-1.404700
32	6	0	4.025551	-1.692042	0.853567
33	1	0	2.038965	-1.120895	1.470181
34	6	0	4.751786	-0.814603	-1.269176
35	1	0	3.338779	0.447830	-2.288635
36	6	0	4.997433	-1.583410	-0.138303
37	1	0	4.212834	-2.300962	1.729963
38	1	0	5.501531	-0.734656	-2.047149
39	1	0	5.941754	-2.103697	-0.031025
40	6	0	1.266057	0.497974	-0.524777
41	1	0	1.119282	0.835430	-1.571972

Structure 44c ($^5C_2$ ax-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 976.8498376
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.052036	1.635453	-0.104720
2	6	0	0.159522	2.369055	-0.692867
3	6	0	-0.946799	0.154015	-0.487834
4	1	0	0.161517	3.402711	-0.344075
5	1	0	0.072755	2.381876	-1.786443
6	1	0	-1.980354	2.052172	-0.499661
7	1	0	-0.992337	0.080974	-1.586544
8	8	0	0.312446	-0.340418	-0.046261
9	7	0	1.437060	1.743027	-0.348052
10	6	0	-2.016844	-0.781786	0.080359
11	1	0	-1.691517	-1.796414	-0.173319
12	6	0	-3.391455	-0.539058	-0.543609
13	1	0	-3.303968	-0.476898	-1.637965
14	6	0	-4.348237	-1.666281	-0.193021
15	1	0	-4.322835	-1.818570	0.890326
16	1	0	-4.043330	-2.588267	-0.701025
17	8	0	-2.108263	-0.736758	1.485741
18	1	0	-2.485769	0.128320	1.695885
19	8	0	-3.888340	0.677891	-0.020615
20	1	0	-4.843330	0.653428	-0.152346
21	8	0	-5.633540	-1.239748	-0.627945
22	1	0	-6.302244	-1.784931	-0.210365
23	8	0	-1.097157	1.798537	1.305711
24	1	0	-0.524890	1.119908	1.682881
25	6	0	1.918537	2.004481	1.010593
26	1	0	1.537942	1.294672	1.756044
27	1	0	3.008270	1.948262	1.031444
28	1	0	1.613138	3.006650	1.308751
29	6	0	2.683281	-0.372265	-0.372039
30	6	0	2.711161	-1.522177	0.408658
31	6	0	3.872409	0.140163	-0.891534
32	6	0	3.923763	-2.156325	0.668324
33	1	0	1.783743	-1.910935	0.808768
34	6	0	5.079078	-0.494764	-0.633124
35	1	0	3.839568	1.048193	-1.484613
36	6	0	5.106901	-1.647410	0.148644
37	1	0	3.940320	-3.050717	1.280162
38	1	0	5.999484	-0.091639	-1.039081
39	1	0	6.048721	-2.143332	0.351423
40	6	0	1.390098	0.340676	-0.689825
41	1	0	1.208255	0.284654	-1.774959

Structure 44c ($^5C_2$ ec-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 976.8737769
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.154248	1.424496	0.564330
2	6	0	-0.046316	2.372967	0.129374
3	6	0	-1.066569	0.153646	-0.285301
4	1	0	-0.061014	3.265662	0.757995
5	1	0	-0.192757	2.680809	-0.920264
6	1	0	-2.130262	1.900329	0.449289
7	1	0	-1.253947	0.425433	-1.335851
8	8	0	0.237516	-0.392737	-0.167264
9	7	0	1.227754	1.681235	0.323496
10	6	0	-2.043118	-0.953287	0.106170
11	1	0	-1.889133	-1.790812	-0.581656
12	6	0	-3.509506	-0.529131	0.020704
13	1	0	-3.694472	0.299723	0.719724
14	6	0	-3.971060	-0.128122	-1.368451
15	1	0	-3.675097	-0.911309	-2.081586
16	1	0	-3.507017	0.811612	-1.677378
17	8	0	-1.805992	-1.467235	1.406346
18	1	0	-1.609980	-0.704612	1.968762
19	8	0	-4.316421	-1.636920	0.389333
20	1	0	-3.903269	-2.017748	1.173596
21	8	0	-5.366541	0.076376	-1.388291
22	1	0	-5.746950	-0.681558	-0.930583
23	8	0	-0.986801	1.116952	1.944733

24	1	0	-0.029451	1.017136	2.059422
25	6	0	2.350152	2.582460	0.094531
26	1	0	2.411273	2.918444	-0.953701
27	1	0	2.226069	3.462025	0.728133
28	1	0	3.288870	2.097675	0.360242
29	6	0	2.571429	-0.251078	-0.404495
30	6	0	2.850181	-0.927457	0.782179
31	6	0	3.497679	-0.263198	-1.440978
32	6	0	4.054343	-1.602770	0.930420
33	1	0	2.110233	-0.930656	1.574163
34	6	0	4.706429	-0.938119	-1.291977
35	1	0	3.275625	0.257576	-2.366864
36	6	0	4.985085	-1.607165	-0.106330
37	1	0	4.267232	-2.132169	1.851818
38	1	0	5.425464	-0.944888	-2.102762
39	1	0	5.924262	-2.135293	0.010514
40	6	0	1.268256	0.495234	-0.538883
41	1	0	1.119525	0.801628	-1.594108

Structure 44c ($^5C_2$ ax-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 976.8699568
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.055867	1.626465	-0.108504
2	6	0	0.153873	2.366233	-0.691731
3	6	0	-0.946473	0.147472	-0.496495
4	1	0	0.153468	3.399413	-0.340921
5	1	0	0.067635	2.380206	-1.785003
6	1	0	-1.983399	2.042723	-0.506133
7	1	0	-0.989344	0.078492	-1.594729
8	8	0	0.314589	-0.345288	-0.052645
9	7	0	1.433710	1.742503	-0.345972
10	6	0	-2.017194	-0.791789	0.063798
11	1	0	-1.710052	-1.804179	-0.219218
12	6	0	-3.398535	-0.517294	-0.533005
13	1	0	-3.320022	-0.392593	-1.622227
14	6	0	-4.352322	-1.661841	-0.238163
15	1	0	-4.325066	-1.875705	0.835074
16	1	0	-4.051409	-2.555718	-0.795793
17	8	0	-2.088208	-0.777245	1.472755
18	1	0	-2.496996	0.068904	1.700633
19	8	0	-3.892962	0.669526	0.062767
20	1	0	-4.850814	0.640917	-0.050816
21	8	0	-5.641952	-1.214586	-0.640969
22	1	0	-6.306138	-1.771529	-0.228406
23	8	0	-1.106682	1.784392	1.303781
24	1	0	-0.533426	1.105136	1.678758
25	6	0	1.911179	2.004679	1.013149
26	1	0	1.522670	1.305424	1.764787
27	1	0	3.001017	1.942418	1.041181
28	1	0	1.617256	3.012844	1.304326
29	6	0	2.686341	-0.371047	-0.378063
30	6	0	2.723600	-1.498712	0.434998
31	6	0	3.871419	0.127336	-0.921481
32	6	0	3.938874	-2.125817	0.701190
33	1	0	1.801130	-1.879164	0.854602
34	6	0	5.081104	-0.500159	-0.656653
35	1	0	3.836162	1.018603	-1.539701
36	6	0	5.117355	-1.630146	0.157805
37	1	0	3.961024	-3.003434	1.337140
38	1	0	5.997655	-0.107060	-1.081417
39	1	0	6.061510	-2.120168	0.365508
40	6	0	1.390575	0.340192	-0.693937
41	1	0	1.209323	0.289137	-1.778805

Structure 44c ($^5C_2$ ec-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 976.8798482
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.152752	1.417460	0.572665
2	6	0	-0.049452	2.368166	0.136577
3	6	0	-1.068859	0.153455	-0.284852

4	1	0	-0.060068	3.261038	0.764841
5	1	0	-0.202557	2.672406	-0.911597
6	1	0	-2.128786	1.892984	0.463321
7	1	0	-1.254588	0.434037	-1.331762
8	8	0	0.237174	-0.397886	-0.167635
9	7	0	1.230856	1.680010	0.321211
10	6	0	-2.045848	-0.953467	0.101099
11	1	0	-1.899341	-1.786225	-0.594122
12	6	0	-3.511169	-0.526425	0.024676
13	1	0	-3.691958	0.300907	0.725525
14	6	0	-3.970132	-0.120769	-1.362474
15	1	0	-3.670290	-0.897418	-2.080190
16	1	0	-3.507896	0.822388	-1.660160
17	8	0	-1.803873	-1.475077	1.401417
18	1	0	-1.586169	-0.711545	1.956026
19	8	0	-4.319434	-1.636474	0.396323
20	1	0	-3.910843	-2.004081	1.189667
21	8	0	-5.372108	0.075687	-1.385235
22	1	0	-5.747195	-0.691064	-0.937543
23	8	0	-0.976755	1.098089	1.954088
24	1	0	-0.017912	0.998877	2.060168
25	6	0	2.340847	2.588570	0.051044
26	1	0	2.378097	2.894569	-1.006601
27	1	0	2.215560	3.483497	0.662477
28	1	0	3.290853	2.122450	0.313248
29	6	0	2.570434	-0.249318	-0.404270
30	6	0	2.873221	-0.877667	0.804104
31	6	0	3.477490	-0.303374	-1.457027
32	6	0	4.078265	-1.552754	0.955159
33	1	0	2.156600	-0.836868	1.617241
34	6	0	4.687996	-0.977045	-1.305092
35	1	0	3.239235	0.186250	-2.395860
36	6	0	4.989218	-1.601205	-0.099587
37	1	0	4.309766	-2.042606	1.894211
38	1	0	5.392263	-1.015013	-2.128317
39	1	0	5.930007	-2.126353	0.020217
40	6	0	1.266235	0.495466	-0.542818
41	1	0	1.116248	0.800422	-1.596155

Structure 44c ($^5C_2$ ax-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 976.874314
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.059051	1.617931	-0.109806
2	6	0	0.147722	2.358058	-0.695643
3	6	0	-0.947145	0.139318	-0.492348
4	1	0	0.148613	3.393198	-0.350106
5	1	0	0.055805	2.361874	-1.787849
6	1	0	-1.984065	2.030668	-0.516380
7	1	0	-0.986573	0.068820	-1.589108
8	8	0	0.316925	-0.350570	-0.042892
9	7	0	1.432553	1.737606	-0.351865
10	6	0	-2.020087	-0.796983	0.063164
11	1	0	-1.728185	-1.808951	-0.234725
12	6	0	-3.401210	-0.502073	-0.523332
13	1	0	-3.316548	-0.330530	-1.604727
14	6	0	-4.350466	-1.660507	-0.278877
15	1	0	-4.332946	-1.917443	0.785164
16	1	0	-4.039637	-2.530124	-0.867284
17	8	0	-2.083727	-0.795983	1.476508
18	1	0	-2.514512	0.038410	1.706776
19	8	0	-3.905298	0.659963	0.120273
20	1	0	-4.864642	0.613933	0.019602
21	8	0	-5.642500	-1.206963	-0.671362
22	1	0	-6.301902	-1.777931	-0.266139
23	8	0	-1.118430	1.785059	1.303907
24	1	0	-0.546721	1.107286	1.684671
25	6	0	1.904504	1.998326	1.009990
26	1	0	1.498761	1.311640	1.764355
27	1	0	2.993708	1.918353	1.045746
28	1	0	1.628988	3.014566	1.292174
29	6	0	2.687754	-0.370956	-0.378757
30	6	0	2.746309	-1.455680	0.490550
31	6	0	3.859607	0.095213	-0.977719
32	6	0	3.968475	-2.070549	0.759378
33	1	0	1.836441	-1.816260	0.953432
34	6	0	5.076519	-0.518926	-0.710607
35	1	0	3.811383	0.948127	-1.647223
36	6	0	5.133784	-1.605544	0.161138
37	1	0	4.006259	-2.914747	1.438657

38	1	0	5.981695	-0.151042	-1.180321
39	1	0	6.083100	-2.085517	0.369929
40	6	0	1.387373	0.331496	-0.694993
41	1	0	1.202818	0.275645	-1.777896

Structure 44d ($^5C_2$ ec-ax) (M06-2X, Gas Phase)

Energy (Hartrees): = - 976.8471481
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.692316	1.437833	0.867396
2	6	0	-0.726728	1.687378	1.377876
3	6	0	0.652657	0.329930	-0.193401
4	1	0	-0.717972	2.555659	2.040769
5	1	0	-1.081692	0.815528	1.946797
6	1	0	1.348701	1.160444	1.694357
7	1	0	0.270771	-0.590157	0.273028
8	8	0	-0.224481	0.734809	-1.238575
9	7	0	-1.538436	2.004814	0.212587
10	6	0	1.996286	0.011986	-0.842707
11	1	0	1.830518	-0.791307	-1.568470
12	6	0	3.056871	-0.461786	0.151191
13	1	0	3.260521	0.335423	0.881859
14	6	0	2.707662	-1.741544	0.890548
15	1	0	2.385632	-2.495619	0.157144
16	1	0	1.889266	-1.574233	1.595174
17	8	0	2.533634	1.095093	-1.580202
18	1	0	2.374774	1.892388	-1.056673
19	8	0	4.243456	-0.746166	-0.569974
20	1	0	4.356536	-0.019021	-1.193493
21	8	0	3.809265	-2.194809	1.641101
22	1	0	4.569550	-2.132383	1.052648
23	8	0	1.206629	2.637322	0.304319
24	1	0	0.493041	2.961802	-0.263975
25	6	0	-2.753744	2.768048	0.416876
26	1	0	-3.532640	2.259807	0.999574
27	1	0	-2.503484	3.699567	0.929826
28	1	0	-3.178729	3.025344	-0.556036
29	6	0	-2.204346	-0.376593	-0.424696
30	6	0	-3.037931	-0.547505	0.676877
31	6	0	-1.973921	-1.466157	-1.268806
32	6	0	-3.632879	-1.781406	0.931159
33	1	0	-3.223842	0.274688	1.354614
34	6	0	-2.564075	-2.696528	-1.015916
35	1	0	-1.315382	-1.338581	-2.120783
36	6	0	-3.398364	-2.857782	0.086687
37	1	0	-4.276776	-1.897946	1.794779
38	1	0	-2.372580	-3.531786	-1.679067
39	1	0	-3.859329	-3.817767	0.285730
40	6	0	-1.551059	0.960577	-0.793650
41	1	0	-2.072317	1.365754	-1.665877

Structure 44d ($^5C_2$ ax-ax) (M06-2X, Gas Phase)

Energy (Hartrees): = - 976.8497284
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.554079	1.382764	-0.877353
2	6	0	0.881436	1.700098	-1.307271
3	6	0	-0.499594	0.211965	0.109069
4	1	0	0.884975	2.593936	-1.932937
5	1	0	1.264487	0.864675	-1.905430
6	1	0	-1.158919	1.110834	-1.744375
7	1	0	-0.064404	-0.654691	-0.408789
8	8	0	0.341321	0.589362	1.198853
9	7	0	1.788319	1.914372	-0.176831
10	6	0	-1.830091	-0.235235	0.717513
11	1	0	-1.576035	-0.956207	1.502398
12	6	0	-2.730493	-0.925529	-0.308247
13	1	0	-2.153389	-1.664780	-0.881734
14	6	0	-3.886502	-1.631431	0.380732
15	1	0	-4.365578	-0.924407	1.065103
16	1	0	-3.515171	-2.494612	0.945000
17	8	0	-2.535988	0.806010	1.354219

18	1	0	-2.855302	1.378776	0.643712
19	8	0	-3.238890	0.075955	-1.169463
20	1	0	-4.030027	-0.297631	-1.575053
21	8	0	-4.773994	-2.035925	-0.654393
22	1	0	-5.622146	-2.261736	-0.269329
23	8	0	-1.163105	2.521630	-0.284245
24	1	0	-0.955269	2.484082	0.657172
25	6	0	1.733927	3.239617	0.433766
26	1	0	0.904121	3.374909	1.138352
27	1	0	2.668604	3.423417	0.969640
28	1	0	1.635192	3.991810	-0.348629
29	6	0	2.381730	-0.428795	0.334436
30	6	0	3.399573	-0.395295	-0.614576
31	6	0	2.045257	-1.644669	0.930015
32	6	0	4.064425	-1.564142	-0.973127
33	1	0	3.660188	0.555767	-1.063669
34	6	0	2.709504	-2.811434	0.572584
35	1	0	1.256373	-1.665730	1.674020
36	6	0	3.720900	-2.774287	-0.382560
37	1	0	4.853655	-1.526893	-1.714900
38	1	0	2.439438	-3.750543	1.041168
39	1	0	4.239489	-3.683644	-0.661973
40	6	0	1.690554	0.852045	0.791496
41	1	0	2.177460	1.191763	1.709434

Structure 44d ($^5C_2$ ec-ax) (M06-2X, Benzene)

Energy (Hartrees): = - 976.8678135
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.679276	-1.438720	0.878119
2	6	0	0.746709	-1.674962	1.373044
3	6	0	-0.659251	-0.332324	-0.185464
4	1	0	0.754334	-2.536526	2.044616
5	1	0	1.107791	-0.796161	1.927199
6	1	0	-1.331540	-1.167687	1.710090
7	1	0	-0.287596	0.592074	0.279071
8	8	0	0.216465	-0.724956	-1.238069
9	7	0	1.543210	-1.995863	0.198965
10	6	0	-2.009702	-0.030398	-0.828779
11	1	0	-1.853452	0.759688	-1.570869
12	6	0	-3.064989	0.458205	0.164638
13	1	0	-3.245294	-0.315407	0.925159
14	6	0	-2.726096	1.767876	0.852763
15	1	0	-2.434124	2.504917	0.090497
16	1	0	-1.892274	1.640620	1.547036
17	8	0	-2.549059	-1.133116	-1.539589
18	1	0	-2.349872	-1.921489	-1.014783
19	8	0	-4.268415	0.698793	-0.548808
20	1	0	-4.379369	-0.054429	-1.141464
21	8	0	-3.824482	2.228069	1.609726
22	1	0	-4.592293	2.140446	1.034032
23	8	0	-1.183212	-2.648163	0.319083
24	1	0	-0.457858	-2.975539	-0.234170
25	6	0	2.749623	-2.774985	0.400494
26	1	0	3.474769	-2.333552	1.096004
27	1	0	2.478155	-3.761374	0.786257
28	1	0	3.248767	-2.917113	-0.560487
29	6	0	2.203035	0.388605	-0.432312
30	6	0	3.104724	0.527163	0.619962
31	6	0	1.914791	1.505964	-1.221197
32	6	0	3.711043	1.754953	0.877846
33	1	0	3.337819	-0.317807	1.254002
34	6	0	2.515323	2.731159	-0.963487
35	1	0	1.207907	1.405534	-2.037206
36	6	0	3.418081	2.859472	0.088647
37	1	0	4.409964	1.845480	1.701254
38	1	0	2.277893	3.588023	-1.583516
39	1	0	3.888276	3.814750	0.290476
40	6	0	1.549185	-0.948652	-0.803323
41	1	0	2.065963	-1.348569	-1.680406

Structure 44d ($^5C_2$ ax-ax) (M06-2X, Benece)

Energy (Hartrees): = - 976.869529
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.571866	1.375646	0.875152
2	6	0	-0.860423	1.701608	1.308478
3	6	0	0.510222	0.199002	-0.103373
4	1	0	-0.860305	2.597558	1.931219
5	1	0	-1.242576	0.869714	1.911940
6	1	0	1.177350	1.107039	1.742831
7	1	0	0.078036	-0.662967	0.423656
8	8	0	-0.335583	0.570078	-1.192573
9	7	0	-1.768864	1.914131	0.179165
10	6	0	1.836820	-0.256237	-0.714441
11	1	0	1.581050	-1.001915	-1.474955
12	6	0	2.753830	-0.911733	0.320031
13	1	0	2.178911	-1.612736	0.940915
14	6	0	3.881919	-1.667747	-0.359841
15	1	0	4.365071	-1.002960	-1.083071
16	1	0	3.484407	-2.546322	-0.880627
17	8	0	2.527178	0.773925	-1.388140
18	1	0	2.871193	1.351376	-0.693171
19	8	0	3.298919	0.121532	1.123034
20	1	0	4.099180	-0.245263	1.518062
21	8	0	4.783755	-2.047266	0.673300
22	1	0	5.624208	-2.288841	0.277430
23	8	0	1.185790	2.509017	0.272948
24	1	0	0.957030	2.476510	-0.663986
25	6	0	-1.722301	3.238093	-0.433459
26	1	0	-0.889523	3.385605	-1.132881
27	1	0	-2.654210	3.411758	-0.978222
28	1	0	-1.641853	3.994219	0.348205
29	6	0	-2.391214	-0.423592	-0.324323
30	6	0	-3.437127	-0.364271	0.593706
31	6	0	-2.054805	-1.652805	-0.892531
32	6	0	-4.131306	-1.518357	0.945398
33	1	0	-3.699500	0.594702	1.025061
34	6	0	-2.747603	-2.805598	-0.540957
35	1	0	-1.246460	-1.698147	-1.614370
36	6	0	-3.788713	-2.741399	0.380486
37	1	0	-4.942124	-1.459565	1.662513
38	1	0	-2.476829	-3.754728	-0.989189
39	1	0	-4.330567	-3.639377	0.653788
40	6	0	-1.681798	0.847197	-0.785068
41	1	0	-2.167113	1.188285	-1.703408

Structure 44d ($^5C_2$ ec-ax) (M06-2X, DMSO)

Energy (Hartrees): = - 976.8726608
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.711085	-1.463247	0.858050
2	6	0	0.702350	-1.712850	1.374186
3	6	0	-0.663646	-0.338126	-0.183467
4	1	0	0.699948	-2.586317	2.030186
5	1	0	1.043857	-0.844583	1.953758
6	1	0	-1.375425	-1.202917	1.682972
7	1	0	-0.284287	0.570631	0.304029
8	8	0	0.217959	-0.726454	-1.234533
9	7	0	1.523778	-2.017676	0.209835
10	6	0	-2.002051	-0.004688	-0.833619
11	1	0	-1.828964	0.795600	-1.560833
12	6	0	-3.058419	0.483010	0.158512
13	1	0	-3.253081	-0.296266	0.908533
14	6	0	-2.702406	1.778262	0.862357
15	1	0	-2.391630	2.519220	0.112231
16	1	0	-1.878232	1.624350	1.561409
17	8	0	-2.550999	-1.094238	-1.564060
18	1	0	-2.339967	-1.891090	-1.055310
19	8	0	-4.256884	0.746198	-0.561546
20	1	0	-4.380622	-0.010967	-1.147084
21	8	0	-3.803564	2.252635	1.616115
22	1	0	-4.566127	2.185037	1.030285
23	8	0	-1.212068	-2.661283	0.263175
24	1	0	-0.467325	-2.993758	-0.261529
25	6	0	2.761369	-2.740942	0.441713
26	1	0	3.492699	-2.214663	1.067432
27	1	0	2.528149	-3.692170	0.926333
28	1	0	3.232297	-2.956625	-0.520420
29	6	0	2.209209	0.366439	-0.416154
30	6	0	2.979803	0.557717	0.728633
31	6	0	2.055571	1.432595	-1.308420

32	6	0	3.585012	1.789581	0.977409
33	1	0	3.112004	-0.242838	1.443953
34	6	0	2.657308	2.660045	-1.062492
35	1	0	1.452327	1.292546	-2.198937
36	6	0	3.426309	2.842698	0.085197
37	1	0	4.177192	1.922239	1.875808
38	1	0	2.527195	3.474673	-1.765985
39	1	0	3.896878	3.799667	0.280077
40	6	0	1.546031	-0.966424	-0.786777
41	1	0	2.068981	-1.367325	-1.659740

Structure 44d ($^5C_2$ ax-ax) (M06-2X, DMSO)

Energy (Hartrees): = - 976.8734632
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.567754	1.369928	0.876015
2	6	0	-0.861671	1.701520	1.312929
3	6	0	0.499550	0.205917	-0.114837
4	1	0	-0.858897	2.593906	1.941100
5	1	0	-1.240156	0.865950	1.913172
6	1	0	1.164545	1.084315	1.743893
7	1	0	0.064188	-0.657646	0.405124
8	8	0	-0.346518	0.593939	-1.200303
9	7	0	-1.777035	1.922033	0.188672
10	6	0	1.822921	-0.256985	-0.722731
11	1	0	1.570278	-1.022337	-1.463780
12	6	0	2.741823	-0.889570	0.324017
13	1	0	2.157000	-1.550171	0.977859
14	6	0	3.840637	-1.698767	-0.339075
15	1	0	4.339057	-1.076455	-1.089267
16	1	0	3.412362	-2.581304	-0.826218
17	8	0	2.509164	0.765204	-1.419207
18	1	0	2.864454	1.343412	-0.730803
19	8	0	3.324492	0.160295	1.083544
20	1	0	4.132983	-0.210485	1.459463
21	8	0	4.744942	-2.069252	0.697057
22	1	0	5.578163	-2.330703	0.294097
23	8	0	1.201008	2.505105	0.291964
24	1	0	0.944509	2.507805	-0.638725
25	6	0	-1.716724	3.248491	-0.420984
26	1	0	-0.873134	3.394734	-1.107856
27	1	0	-2.637738	3.424268	-0.982915
28	1	0	-1.648655	4.001974	0.364849
29	6	0	-2.389256	-0.418068	-0.327734
30	6	0	-3.414010	-0.382454	0.615750
31	6	0	-2.054296	-1.637488	-0.919639
32	6	0	-4.086524	-1.549326	0.971622
33	1	0	-3.678427	0.564822	1.071058
34	6	0	-2.725712	-2.802776	-0.565719
35	1	0	-1.257817	-1.670561	-1.655325
36	6	0	-3.744087	-2.762442	0.383588
37	1	0	-4.879207	-1.507845	1.710348
38	1	0	-2.453185	-3.743325	-1.031154
39	1	0	-4.267388	-3.670333	0.661092
40	6	0	-1.692189	0.861417	-0.784181
41	1	0	-2.187684	1.207021	-1.695261

Structure 45a (^{2}E ec-ax H-bond O) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1091.3608722
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.323908	-0.031133	0.587357
2	6	0	-2.545276	-0.900583	-0.484634
3	6	0	-3.819711	-1.105371	-0.980349
4	6	0	-4.912032	-0.447024	-0.408609
5	6	0	-4.711931	0.407435	0.673762
6	6	0	-3.420093	0.600820	1.159071
7	1	0	-1.709750	-1.439075	-0.916348
8	1	0	-4.006496	-1.779348	-1.807112
9	1	0	-5.540220	0.915232	1.148708
10	1	0	-3.273181	1.262011	2.008194
11	6	0	-0.925344	0.270353	1.094866

12	1	0	-0.966806	0.469988	2.171119
13	7	0	-0.243287	1.384548	0.434396
14	8	0	-0.063739	-0.832559	0.859808
15	6	0	0.845945	-0.519732	-0.210741
16	6	0	0.332352	0.802586	-0.768658
17	1	0	1.140244	1.422475	-1.157299
18	1	0	-0.417596	0.636008	-1.558491
19	1	0	0.803715	-1.343735	-0.930134
20	6	0	2.246854	-0.433968	0.388294
21	1	0	2.325959	0.505681	0.950102
22	6	0	3.355274	-0.451534	-0.667211
23	1	0	3.126058	-1.229446	-1.409553
24	6	0	4.700447	-0.838896	-0.023033
25	1	0	4.721966	-1.930118	0.058381
26	6	0	5.894734	-0.365906	-0.842557
27	1	0	6.800852	-0.871527	-0.495131
28	1	0	5.750801	-0.578523	-1.902934
29	8	0	2.452215	-1.549061	1.248169
30	1	0	1.618305	-1.679363	1.716063
31	8	0	3.367208	0.792526	-1.341863
32	1	0	4.204705	1.240132	-1.157827
33	8	0	4.881940	-0.250857	1.257163
34	1	0	4.233246	-0.663456	1.839293
35	8	0	6.037007	1.043576	-0.715079
36	1	0	6.049065	1.216053	0.234351
37	6	0	-1.020061	2.587777	0.221028
38	1	0	-1.420091	2.941426	1.174439
39	1	0	-0.360618	3.361530	-0.175523
40	1	0	-1.859053	2.444641	-0.476402
41	8	0	-6.120084	-0.711904	-0.966511
42	6	0	-7.247580	-0.051285	-0.432550
43	1	0	-7.146052	1.035779	-0.515794
44	1	0	-8.098385	-0.380473	-1.024495
45	1	0	-7.408049	-0.322740	0.615909

Structure 45a (^{2}E ec-ax H-bond N) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1091.3633548
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.152773	0.091966	-0.405762
2	6	0	2.422182	-0.935678	0.502821
3	6	0	3.717211	-1.369711	0.716085
4	6	0	4.778844	-0.790073	0.014945
5	6	0	4.524018	0.219721	-0.911403
6	6	0	3.212317	0.644493	-1.112129
7	1	0	1.599853	-1.416348	1.019826
8	1	0	3.940965	-2.170032	1.410358
9	1	0	5.322955	0.671470	-1.483088
10	1	0	3.020619	1.422642	-1.845216
11	6	0	0.747700	0.627095	-0.594904
12	1	0	0.622380	0.979058	-1.625057
13	7	0	0.378920	1.734447	0.315384
14	8	0	-0.207961	-0.373496	-0.319540
15	6	0	-0.951853	-0.043346	0.859406
16	6	0	-0.119556	1.058059	1.510889
17	1	0	-0.721877	1.740880	2.114648
18	1	0	0.692577	0.650956	2.131275
19	1	0	-1.048005	-0.942710	1.470526
20	6	0	-2.351766	0.425929	0.478645
21	1	0	-2.888379	0.662101	1.408593
22	6	0	-3.131657	-0.695500	-0.208209
23	1	0	-2.494602	-1.132911	-0.985252
24	6	0	-4.389449	-0.132151	-0.898022
25	1	0	-4.094590	0.205469	-1.896527
26	6	0	-5.499884	-1.168305	-1.016746
27	1	0	-6.260603	-0.812531	-1.718633
28	1	0	-5.106538	-2.123343	-1.367227
29	8	0	-2.327515	1.563196	-0.372970
30	1	0	-1.453613	1.984147	-0.294330
31	8	0	-3.380750	-1.703932	0.755417
32	1	0	-4.324559	-1.707409	0.963706
33	8	0	-4.976324	0.945871	-0.177196
34	1	0	-4.342755	1.673481	-0.206439
35	8	0	-6.078515	-1.396931	0.262533
36	1	0	-6.301658	-0.520916	0.599907
37	6	0	1.397445	2.740592	0.560495
38	1	0	1.729258	3.166584	-0.388588
39	1	0	0.960648	3.542099	1.158536
40	1	0	2.273166	2.336476	1.085908
41	8	0	6.010135	-1.284831	0.293382

42	6	0	7.108029	-0.751540	-0.416617
43	1	0	7.224327	0.319484	-0.221548
44	1	0	7.986255	-1.281494	-0.055480
45	1	0	7.001049	-0.916599	-1.493562

Structure 45a (^{2}E ec-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1091.3632652
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.402084	0.157767	0.194682
2	6	0	-2.920786	0.081770	-1.102190
3	6	0	-4.251386	-0.217175	-1.306775
4	6	0	-5.097776	-0.445228	-0.213384
5	6	0	-4.593356	-0.372231	1.081713
6	6	0	-3.243072	-0.071611	1.269639
7	1	0	-2.259609	0.271781	-1.939624
8	1	0	-4.676251	-0.281735	-2.300811
9	1	0	-5.225442	-0.546307	1.941436
10	1	0	-2.848645	-0.016634	2.279222
11	6	0	-0.952473	0.493255	0.395684
12	1	0	-0.724975	0.523804	1.480681
13	7	0	-0.559742	1.735965	-0.247760
14	8	0	-0.118763	-0.478959	-0.220991
15	6	0	1.070173	0.170683	-0.694888
16	6	0	0.891919	1.634888	-0.299543
17	1	0	1.356903	1.828458	0.681271
18	1	0	1.324283	2.326053	-1.022689
19	1	0	1.100645	0.045432	-1.782549
20	6	0	2.260092	-0.539518	-0.076071
21	1	0	2.267732	-0.343885	1.004973
22	6	0	3.591018	-0.057389	-0.648229
23	1	0	3.509975	-0.021159	-1.743158
24	6	0	4.718023	-1.055479	-0.314307
25	1	0	4.702468	-1.837774	-1.080048
26	6	0	6.089103	-0.391937	-0.288518
27	1	0	6.868684	-1.159917	-0.296441
28	1	0	6.223102	0.263552	-1.150115
29	8	0	2.153507	-1.937207	-0.319169
30	1	0	1.229020	-2.168869	-0.168998
31	8	0	3.816363	1.265782	-0.199735
32	1	0	4.557365	1.260536	0.421994
33	8	0	4.570780	-1.635360	0.974715
34	1	0	3.780420	-2.187357	0.936922
35	8	0	6.205650	0.418441	0.874498
36	1	0	5.979504	-0.158594	1.614074
37	6	0	-1.048584	2.916684	0.435365
38	1	0	-0.674657	2.983360	1.471625
39	1	0	-0.727390	3.807613	-0.105926
40	1	0	-2.139720	2.901146	0.455987
41	8	0	-6.388706	-0.725829	-0.520715
42	6	0	-7.282679	-0.949246	0.548715
43	1	0	-8.253039	-1.138586	0.095647
44	1	0	-6.981971	-1.818518	1.142441
45	1	0	-7.349648	-0.070487	1.198233

Structure 45a (E_2 ax-ax) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1091.3632357
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.346886	0.632529	0.486047
2	6	0	-2.664542	-0.489573	1.255423
3	6	0	-3.827385	-1.200613	1.019996
4	6	0	-4.701954	-0.801410	0.005971
5	6	0	-4.394326	0.314513	-0.770421
6	6	0	-3.219129	1.020375	-0.521947
7	1	0	-1.983416	-0.805590	2.036781
8	1	0	-4.087258	-2.074742	1.604253
9	1	0	-5.049241	0.640264	-1.566935
10	1	0	-2.962683	1.879002	-1.131407
11	6	0	-1.090677	1.437842	0.769672
12	1	0	-1.290533	2.228418	1.496940
13	7	0	-0.522480	1.987541	-0.439660
14	8	0	-0.072589	0.602206	1.337517

15	6	0	0.610113	-0.012178	0.237479
16	6	0	0.196086	0.832312	-0.998086
17	1	0	1.055034	1.145893	-1.587966
18	1	0	-0.479018	0.257072	-1.632864
19	1	0	0.269715	-1.050667	0.147314
20	6	0	2.091836	-0.001025	0.583960
21	1	0	2.470446	1.028044	0.522960
22	6	0	2.937473	-0.848852	-0.368043
23	1	0	2.428060	-1.807813	-0.538852
24	6	0	4.296854	-1.177570	0.276102
25	1	0	4.141227	-2.022614	0.953947
26	6	0	5.357222	-1.542221	-0.754941
27	1	0	6.214782	-1.999829	-0.252606
28	1	0	4.961293	-2.242093	-1.492493
29	8	0	2.270770	-0.511740	1.900515
30	1	0	1.559524	-0.136231	2.432684
31	8	0	3.021572	-0.172651	-1.608270
32	1	0	3.950341	0.021824	-1.796814
33	8	0	4.842367	-0.075199	0.987794
34	1	0	4.274611	0.060107	1.755390
35	8	0	5.763452	-0.376171	-1.461127
36	1	0	6.007186	0.264901	-0.782313
37	6	0	0.359486	3.120765	-0.159886
38	1	0	0.844716	3.429470	-1.086057
39	1	0	-0.239064	3.958576	0.202133
40	1	0	1.134372	2.894956	0.585433
41	8	0	-5.815670	-1.562557	-0.147255
42	6	0	-6.725092	-1.195591	-1.162293
43	1	0	-6.256152	-1.241317	-2.150664
44	1	0	-7.536921	-1.917743	-1.113946
45	1	0	-7.123360	-0.189594	-0.994903

Structure 45a (^{2}E ec-ax H-bond O) (M06-2X, Benzene)

Energy (Hartrees): = - 1091.3801918
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.327849	-0.040008	0.572986
2	6	0	-2.553318	-0.861559	-0.535805
3	6	0	-3.831549	-1.053119	-1.028698
4	6	0	-4.923995	-0.429244	-0.417873
5	6	0	-4.718992	0.376975	0.700707
6	6	0	-3.423629	0.559174	1.181558
7	1	0	-1.719724	-1.374313	-1.002049
8	1	0	-4.018833	-1.690480	-1.884552
9	1	0	-5.546343	0.857951	1.204954
10	1	0	-3.273754	1.182055	2.058805
11	6	0	-0.927230	0.250069	1.081584
12	1	0	-0.966120	0.427451	2.161509
13	7	0	-0.244952	1.377226	0.442580
14	8	0	-0.067025	-0.849865	0.820846
15	6	0	0.849812	-0.513986	-0.237547
16	6	0	0.338040	0.819652	-0.768853
17	1	0	1.145832	1.450277	-1.139729
18	1	0	-0.406232	0.670404	-1.566905
19	1	0	0.811453	-1.320951	-0.975776
20	6	0	2.247246	-0.442267	0.373499
21	1	0	2.321937	0.482176	0.960788
22	6	0	3.366459	-0.434208	-0.671491
23	1	0	3.143072	-1.187898	-1.439696
24	6	0	4.705843	-0.842424	-0.028016
25	1	0	4.725748	-1.935359	0.024424
26	6	0	5.908894	-0.359090	-0.826307
27	1	0	6.809658	-0.874134	-0.478525
28	1	0	5.778230	-0.556511	-1.891406
29	8	0	2.445219	-1.578755	1.208512
30	1	0	1.612349	-1.709052	1.678817
31	8	0	3.391113	0.832183	-1.308033
32	1	0	4.231510	1.263910	-1.101482
33	8	0	4.880296	-0.286560	1.268925
34	1	0	4.220199	-0.705672	1.833701
35	8	0	6.059787	1.049747	-0.675740
36	1	0	6.078480	1.207887	0.276362
37	6	0	-1.022018	2.583785	0.248756
38	1	0	-1.429164	2.919097	1.205904
39	1	0	-0.361169	3.367350	-0.127097
40	1	0	-1.854528	2.457149	-0.459630
41	8	0	-6.134143	-0.675472	-0.975252
42	6	0	-7.266341	-0.069699	-0.381298
43	1	0	-7.189753	1.022187	-0.400260
44	1	0	-8.122132	-0.377629	-0.978867

45	1	0	-7.406260	-0.411011	0.649381

Structure 45a (^{2}E ec-ax H-bond N) (M06-2X, Benzene)

Energy (Hartrees): = - 1091.3836678
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.155978	0.084370	-0.407690
2	6	0	2.428813	-0.948105	0.494441
3	6	0	3.725745	-1.380240	0.704580
4	6	0	4.786541	-0.791149	0.009243
5	6	0	4.528066	0.224626	-0.910657
6	6	0	3.215018	0.646362	-1.109320
7	1	0	1.610099	-1.432587	1.014164
8	1	0	3.948487	-2.184387	1.395423
9	1	0	5.326389	0.683917	-1.477941
10	1	0	3.021461	1.430409	-1.835633
11	6	0	0.750165	0.620217	-0.595039
12	1	0	0.626865	0.974745	-1.624199
13	7	0	0.376215	1.720977	0.318032
14	8	0	-0.207278	-0.383759	-0.324032
15	6	0	-0.945900	-0.059878	0.861532
16	6	0	-0.113062	1.039696	1.514712
17	1	0	-0.713345	1.718714	2.124474
18	1	0	0.701963	0.631283	2.129512
19	1	0	-1.035399	-0.960785	1.471017
20	6	0	-2.347483	0.413491	0.488884
21	1	0	-2.877603	0.646121	1.423131
22	6	0	-3.138618	-0.696392	-0.205163
23	1	0	-2.507737	-1.139102	-0.984060
24	6	0	-4.390456	-0.119107	-0.894385
25	1	0	-4.091564	0.221874	-1.890343
26	6	0	-5.509036	-1.142759	-1.029663
27	1	0	-6.266084	-0.768674	-1.726041
28	1	0	-5.126652	-2.094745	-1.400513
29	8	0	-2.319669	1.559162	-0.353323
30	1	0	-1.437821	1.967802	-0.275014
31	8	0	-3.403851	-1.708614	0.754106
32	1	0	-4.350032	-1.701628	0.951146
33	8	0	-4.971244	0.959202	-0.166483
34	1	0	-4.326659	1.677876	-0.182201
35	8	0	-6.094783	-1.391326	0.245357
36	1	0	-6.324171	-0.521347	0.594728
37	6	0	1.378555	2.744192	0.555730
38	1	0	1.697932	3.176049	-0.395240
39	1	0	0.930737	3.539689	1.154310
40	1	0	2.263282	2.359749	1.080791
41	8	0	6.018600	-1.281040	0.284939
42	6	0	7.119853	-0.722554	-0.406444
43	1	0	7.222805	0.346872	-0.196251
44	1	0	8.001656	-1.244672	-0.040250
45	1	0	7.032595	-0.879629	-1.486317

Structure 45a (^{2}E ec-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 1091.3830329
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.397878	0.159821	0.174339
2	6	0	-2.950389	0.164586	-1.110905
3	6	0	-4.284859	-0.130620	-1.300367
4	6	0	-5.102134	-0.436678	-0.202956
5	6	0	-4.563300	-0.444505	1.080922
6	6	0	-3.210619	-0.146025	1.253358
7	1	0	-2.316370	0.413313	-1.954526
8	1	0	-4.731672	-0.130870	-2.287220
9	1	0	-5.170970	-0.679739	1.944225
10	1	0	-2.791219	-0.154056	2.254376
11	6	0	-0.944593	0.488217	0.365745
12	1	0	-0.700973	0.469061	1.446540
13	7	0	-0.557766	1.758962	-0.225569
14	8	0	-0.122810	-0.455466	-0.309920
15	6	0	1.077152	0.208151	-0.738787
16	6	0	0.894957	1.658965	-0.294663
17	1	0	1.365431	1.823628	0.687967

18	1	0	1.316083	2.374832	-1.000497
19	1	0	1.127509	0.118904	-1.828800
20	6	0	2.253654	-0.526905	-0.120182
21	1	0	2.240010	-0.366054	0.966471
22	6	0	3.601572	-0.040823	-0.649652
23	1	0	3.546198	0.030011	-1.744082
24	6	0	4.713326	-1.058138	-0.319883
25	1	0	4.711042	-1.817614	-1.108276
26	6	0	6.090798	-0.413911	-0.247411
27	1	0	6.859952	-1.192630	-0.250348
28	1	0	6.258843	0.252864	-1.094380
29	8	0	2.142335	-1.916509	-0.409304
30	1	0	1.216640	-2.149429	-0.266573
31	8	0	3.831569	1.266388	-0.152959
32	1	0	4.563916	1.229342	0.477885
33	8	0	4.531775	-1.672807	0.949970
34	1	0	3.733561	-2.210379	0.879962
35	8	0	6.194034	0.374672	0.935072
36	1	0	5.954982	-0.214829	1.661075
37	6	0	-1.029824	2.907959	0.521801
38	1	0	-0.660159	2.910519	1.561433
39	1	0	-0.690019	3.822635	0.033237
40	1	0	-2.121388	2.915255	0.538802
41	8	0	-6.397301	-0.705087	-0.493458
42	6	0	-7.267214	-0.999345	0.583028
43	1	0	-8.247950	-1.164109	0.141034
44	1	0	-6.954009	-1.904645	1.112688
45	1	0	-7.325791	-0.162775	1.286468

Structure 45a (E_2 ax-ax) (M06-2X, Benzene)

Energy (Hartrees): = - 1091.3824218
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.355469	0.631198	0.491306
2	6	0	-2.683298	-0.485481	1.265237
3	6	0	-3.849524	-1.191541	1.029082
4	6	0	-4.718793	-0.794047	0.008985
5	6	0	-4.402871	0.318116	-0.770380
6	6	0	-3.224531	1.019068	-0.520225
7	1	0	-2.008604	-0.804243	2.051374
8	1	0	-4.112683	-2.062132	1.618061
9	1	0	-5.054372	0.644794	-1.569772
10	1	0	-2.965630	1.875421	-1.132313
11	6	0	-1.092451	1.427428	0.775810
12	1	0	-1.286386	2.211874	1.510874
13	7	0	-0.524010	1.987514	-0.428816
14	8	0	-0.077559	0.580455	1.332352
15	6	0	0.611617	-0.018081	0.226744
16	6	0	0.200263	0.841354	-0.998482
17	1	0	1.060440	1.168964	-1.579139
18	1	0	-0.467096	0.271209	-1.646219
19	1	0	0.275893	-1.056438	0.120626
20	6	0	2.092231	-0.005880	0.580713
21	1	0	2.464053	1.026452	0.541545
22	6	0	2.949355	-0.834550	-0.378997
23	1	0	2.443361	-1.789909	-0.576450
24	6	0	4.302173	-1.175473	0.271335
25	1	0	4.138008	-2.024782	0.941122
26	6	0	5.368277	-1.545339	-0.750220
27	1	0	6.220845	-2.003920	-0.240149
28	1	0	4.978788	-2.250244	-1.486652
29	8	0	2.264843	-0.538455	1.890597
30	1	0	1.560722	-0.158058	2.429274
31	8	0	3.050655	-0.128067	-1.603677
32	1	0	3.985585	0.039866	-1.786811
33	8	0	4.848678	-0.079256	0.994482
34	1	0	4.274024	0.054687	1.757306
35	8	0	5.787340	-0.383356	-1.460965
36	1	0	6.040293	0.257359	-0.784677
37	6	0	0.351971	3.123310	-0.139786
38	1	0	0.834952	3.444599	-1.063358
39	1	0	-0.250185	3.955217	0.230730
40	1	0	1.130160	2.896591	0.601893
41	8	0	-5.832902	-1.550408	-0.146044
42	6	0	-6.720815	-1.209765	-1.193279
43	1	0	-6.227397	-1.271383	-2.168554
44	1	0	-7.526368	-1.940772	-1.152923
45	1	0	-7.137588	-0.206958	-1.055094

Structure 45a (^{2}E ec-ax H-bond O) (M06-2X, DMSO)

Energy (Hartrees): = - 1091.3841915
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.331445	-0.042158	0.575174
2	6	0	-2.543044	-0.843712	-0.551420
3	6	0	-3.818761	-1.036928	-1.054548
4	6	0	-4.920722	-0.434146	-0.437034
5	6	0	-4.727633	0.354137	0.697915
6	6	0	-3.435924	0.537723	1.189237
7	1	0	-1.703839	-1.336545	-1.030149
8	1	0	-3.990990	-1.659120	-1.925293
9	1	0	-5.561431	0.821223	1.205101
10	1	0	-3.294025	1.148072	2.076591
11	6	0	-0.937795	0.253412	1.099154
12	1	0	-0.990891	0.429509	2.177887
13	7	0	-0.257495	1.387356	0.465463
14	8	0	-0.068147	-0.841498	0.845515
15	6	0	0.845740	-0.504471	-0.216995
16	6	0	0.331700	0.829268	-0.744871
17	1	0	1.136063	1.464930	-1.114532
18	1	0	-0.410313	0.678961	-1.543947
19	1	0	0.806235	-1.307069	-0.959280
20	6	0	2.244455	-0.437496	0.390173
21	1	0	2.318329	0.469961	1.003473
22	6	0	3.359116	-0.387520	-0.659298
23	1	0	3.123951	-1.092255	-1.468485
24	6	0	4.695425	-0.844853	-0.050179
25	1	0	4.683223	-1.938110	-0.016644
26	6	0	5.898204	-0.397310	-0.867186
27	1	0	6.788435	-0.939211	-0.534989
28	1	0	5.742424	-0.594724	-1.928929
29	8	0	2.451387	-1.593737	1.196621
30	1	0	1.632361	-1.717146	1.693015
31	8	0	3.397700	0.922578	-1.209261
32	1	0	4.285870	1.279948	-1.070884
33	8	0	4.909061	-0.310637	1.251898
34	1	0	4.247450	-0.721050	1.821553
35	8	0	6.099091	1.009722	-0.723524
36	1	0	6.153213	1.169368	0.227620
37	6	0	-1.055517	2.579980	0.255435
38	1	0	-1.496320	2.900817	1.202426
39	1	0	-0.404325	3.379082	-0.104884
40	1	0	-1.865482	2.436224	-0.475430
41	8	0	-6.126352	-0.678550	-1.002507
42	6	0	-7.267287	-0.091992	-0.393294
43	1	0	-7.198304	0.999789	-0.391020
44	1	0	-8.120861	-0.396707	-0.995506
45	1	0	-7.399291	-0.454059	0.630555

Structure 45a (^{2}E ec-ax H-bond N) (M06-2X, DMSO)

Energy (Hartrees): = - 1091.3880806
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.158812	0.083085	-0.404863
2	6	0	2.433777	-0.939698	0.508266
3	6	0	3.732226	-1.373172	0.716367
4	6	0	4.791925	-0.793230	0.009707
5	6	0	4.531020	0.217639	-0.916656
6	6	0	3.217374	0.639691	-1.113809
7	1	0	1.620343	-1.413315	1.046720
8	1	0	3.952095	-2.169063	1.418493
9	1	0	5.328453	0.673984	-1.488050
10	1	0	3.021679	1.422001	-1.841365
11	6	0	0.754003	0.619576	-0.599490
12	1	0	0.640898	0.977321	-1.628007
13	7	0	0.373683	1.714137	0.314899
14	8	0	-0.206715	-0.388717	-0.338486
15	6	0	-0.940228	-0.073161	0.855451
16	6	0	-0.108950	1.025306	1.510845
17	1	0	-0.708113	1.699010	2.126884
18	1	0	0.709222	0.615269	2.119252
19	1	0	-1.019980	-0.975175	1.464160
20	6	0	-2.343886	0.402454	0.493322

21	1	0	-2.864657	0.629854	1.433716
22	6	0	-3.145994	-0.693198	-0.209872
23	1	0	-2.526060	-1.130666	-1.000117
24	6	0	-4.398178	-0.101654	-0.885747
25	1	0	-4.102336	0.250105	-1.878475
26	6	0	-5.520260	-1.116954	-1.039026
27	1	0	-6.279487	-0.722667	-1.721118
28	1	0	-5.142498	-2.058420	-1.439722
29	8	0	-2.315515	1.557559	-0.338150
30	1	0	-1.427895	1.957529	-0.256672
31	8	0	-3.417103	-1.718844	0.737663
32	1	0	-4.364715	-1.704419	0.928111
33	8	0	-4.971684	0.969615	-0.139578
34	1	0	-4.314864	1.677699	-0.134576
35	8	0	-6.102601	-1.400452	0.233681
36	1	0	-6.340230	-0.541137	0.604792
37	6	0	1.374789	2.739375	0.555004
38	1	0	1.706368	3.159459	-0.396979
39	1	0	0.921738	3.538672	1.144246
40	1	0	2.250882	2.355827	1.095344
41	8	0	6.024629	-1.281613	0.281359
42	6	0	7.125419	-0.706609	-0.407841
43	1	0	7.211603	0.363038	-0.195261
44	1	0	8.011918	-1.219341	-0.040015
45	1	0	7.040671	-0.861605	-1.487508

Structure 45a (^{2}E ec-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 1091.3868453
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.413227	0.142355	0.180267
2	6	0	-2.920475	-0.006238	-1.115612
3	6	0	-4.254289	-0.301835	-1.317954
4	6	0	-5.117040	-0.452330	-0.221782
5	6	0	-4.623071	-0.307291	1.073273
6	6	0	-3.270682	-0.011536	1.258362
7	1	0	-2.254417	0.119663	-1.962345
8	1	0	-4.661721	-0.419328	-2.315538
9	1	0	-5.267649	-0.418728	1.934742
10	1	0	-2.886713	0.101571	2.267436
11	6	0	-0.963730	0.484854	0.380772
12	1	0	-0.739088	0.533544	1.462649
13	7	0	-0.575607	1.723738	-0.280853
14	8	0	-0.131112	-0.494824	-0.227970
15	6	0	1.068497	0.148196	-0.693443
16	6	0	0.879628	1.619804	-0.331091
17	1	0	1.333499	1.835799	0.648713
18	1	0	1.305391	2.298139	-1.070460
19	1	0	1.121670	-0.001287	-1.776721
20	6	0	2.253798	-0.537525	-0.035006
21	1	0	2.246996	-0.302953	1.037770
22	6	0	3.591541	-0.077347	-0.612054
23	1	0	3.522127	-0.068742	-1.708317
24	6	0	4.709215	-1.068631	-0.247465
25	1	0	4.640608	-1.909154	-0.944208
26	6	0	6.096619	-0.455736	-0.359751
27	1	0	6.851233	-1.246748	-0.320847
28	1	0	6.205351	0.087732	-1.299558
29	8	0	2.153529	-1.944798	-0.226564
30	1	0	1.241679	-2.180370	-0.014831
31	8	0	3.821591	1.253514	-0.172209
32	1	0	4.655492	1.267571	0.317536
33	8	0	4.609775	-1.530587	1.095721
34	1	0	3.809922	-2.068291	1.139592
35	8	0	6.312021	0.480110	0.697819
36	1	0	6.137815	-0.003976	1.515124
37	6	0	-1.042313	2.907265	0.420305
38	1	0	-0.668418	2.948291	1.456418
39	1	0	-0.700961	3.799724	-0.107037
40	1	0	-2.134272	2.919899	0.442386
41	8	0	-6.405966	-0.733333	-0.521516
42	6	0	-7.314223	-0.886276	0.559893
43	1	0	-8.285463	-1.083084	0.110363
44	1	0	-7.032310	-1.728835	1.198217
45	1	0	-7.371722	0.026361	1.160347

Structure 45a (E_2 ax-ax) (M06-2X, DMSO)

Energy (Hartrees): = - 1091.3855272

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.354670	0.597546	0.485243
2	6	0	-2.602490	-0.621035	1.122209
3	6	0	-3.764299	-1.331603	0.867463
4	6	0	-4.712626	-0.833755	-0.031818
5	6	0	-4.477666	0.383366	-0.674072
6	6	0	-3.302635	1.083979	-0.408724
7	1	0	-1.873598	-1.016076	1.820613
8	1	0	-3.959386	-2.279374	1.355999
9	1	0	-5.190977	0.791832	-1.377923
10	1	0	-3.119755	2.024302	-0.916497
11	6	0	-1.102285	1.402512	0.795502
12	1	0	-1.314412	2.170962	1.541857
13	7	0	-0.535714	1.997116	-0.396076
14	8	0	-0.081187	0.558513	1.338008
15	6	0	0.619780	-0.011225	0.223822
16	6	0	0.209724	0.872117	-0.984118
17	1	0	1.071210	1.229260	-1.545081
18	1	0	-0.440733	0.306525	-1.653598
19	1	0	0.291391	-1.048572	0.089177
20	6	0	2.097955	-0.004681	0.586411
21	1	0	2.464964	1.029661	0.590716
22	6	0	2.961600	-0.798081	-0.397618
23	1	0	2.455177	-1.742012	-0.640041
24	6	0	4.306841	-1.170299	0.247856
25	1	0	4.131231	-2.035403	0.893455
26	6	0	5.371058	-1.534514	-0.776119
27	1	0	6.215686	-2.012559	-0.271665
28	1	0	4.974052	-2.223670	-1.523051
29	8	0	2.262929	-0.586604	1.877428
30	1	0	1.580619	-0.195858	2.437020
31	8	0	3.082960	-0.038707	-1.592411
32	1	0	4.024237	0.105726	-1.762544
33	8	0	4.863111	-0.096163	0.999065
34	1	0	4.281734	0.031305	1.758205
35	8	0	5.810682	-0.365091	-1.468864
36	1	0	6.082763	0.257093	-0.781889
37	6	0	0.335256	3.130187	-0.069472
38	1	0	0.798370	3.497615	-0.986266
39	1	0	-0.268674	3.935021	0.353696
40	1	0	1.128823	2.874311	0.644922
41	8	0	-5.817021	-1.595665	-0.215948
42	6	0	-6.807715	-1.110764	-1.110672
43	1	0	-6.410518	-1.010841	-2.125138
44	1	0	-7.603731	-1.852899	-1.107151
45	1	0	-7.207224	-0.148904	-0.775858

Structure 45b (^{2}E ec-ec H-bond O) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1091.3649362
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.151431	0.732373	-0.233311
2	6	0	-1.875586	-0.553967	0.243179
3	6	0	-2.895694	-1.455559	0.462356
4	6	0	-4.224582	-1.087300	0.211855
5	6	0	-4.512744	0.190246	-0.258394
6	6	0	-3.466146	1.087724	-0.479188
7	1	0	-0.846294	-0.830175	0.446396
8	1	0	-2.705736	-2.456004	0.830749
9	1	0	-5.529269	0.498518	-0.459860
10	1	0	-3.691057	2.081500	-0.852963
11	6	0	-1.019495	1.692649	-0.471716
12	1	0	-1.417021	2.650133	-0.860472
13	7	0	-0.202199	1.906183	0.711267
14	8	0	-0.109131	1.168659	-1.433675
15	6	0	1.236360	1.415423	-0.997312
16	6	0	1.067735	2.374511	0.173766
17	1	0	1.873332	2.284297	0.901870
18	1	0	1.002195	3.415992	-0.184712
19	1	0	1.786827	1.845078	-1.838274
20	6	0	1.846169	0.071596	-0.592263
21	1	0	1.479639	-0.185486	0.410639
22	6	0	3.373742	0.098230	-0.536461
23	1	0	3.751441	0.580989	-1.447958

24	6	0	3.935982	-1.339001	-0.526718
25	1	0	4.010955	-1.670182	-1.567352
26	6	0	5.306130	-1.420717	0.134360
27	1	0	5.768139	-2.385449	-0.096481
28	1	0	5.958010	-0.618596	-0.214393
29	8	0	1.461692	-0.927769	-1.527663
30	1	0	0.557142	-0.713618	-1.791795
31	8	0	3.779126	0.897539	0.559624
32	1	0	4.172241	0.326015	1.234090
33	8	0	3.124176	-2.241848	0.211550
34	1	0	2.292729	-2.318389	-0.271847
35	8	0	5.167224	-1.264442	1.541380
36	1	0	4.498752	-1.908215	1.805807
37	6	0	-0.813203	2.789541	1.682700
38	1	0	-1.761426	2.364409	2.017413
39	1	0	-0.155741	2.886509	2.547489
40	1	0	-1.002296	3.795488	1.270242
41	8	0	-5.153942	-2.042968	0.459311
42	6	0	-6.506698	-1.719037	0.216840
43	1	0	-6.672139	-1.473846	-0.837228
44	1	0	-7.080159	-2.605708	0.476406
45	1	0	-6.831261	-0.880192	0.840992

Structure 45b (^{2}E ec-ec H-bond N) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1091.3674438
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.966364	0.596317	-0.420409
2	6	0	-1.636754	-0.616457	0.194995
3	6	0	-2.609760	-1.565912	0.430347
4	6	0	-3.937718	-1.325772	0.054913
5	6	0	-4.276335	-0.124915	-0.562211
6	6	0	-3.279802	0.823339	-0.797163
7	1	0	-0.607254	-0.804906	0.479178
8	1	0	-2.378146	-2.512919	0.901657
9	1	0	-5.291788	0.082596	-0.870082
10	1	0	-3.542844	1.754175	-1.289931
11	6	0	-0.912146	1.642375	-0.647454
12	1	0	-1.301774	2.414636	-1.338407
13	7	0	-0.457641	2.283009	0.592555
14	8	0	0.265715	1.083724	-1.190023
15	6	0	1.407871	1.745361	-0.631682
16	6	0	0.801094	2.897331	0.171962
17	1	0	1.407551	3.184738	1.033621
18	1	0	0.626560	3.782329	-0.460369
19	1	0	2.062775	2.073723	-1.440204
20	6	0	2.184261	0.771126	0.245910
21	1	0	3.070030	1.297570	0.627120
22	6	0	2.696074	-0.413484	-0.576438
23	1	0	1.870643	-0.791337	-1.191265
24	6	0	3.149667	-1.558404	0.348266
25	1	0	2.267066	-2.160196	0.588383
26	6	0	4.205400	-2.444213	-0.302081
27	1	0	4.308233	-3.373193	0.267458
28	1	0	3.933681	-2.682719	-1.331184
29	8	0	1.409082	0.289950	1.338144
30	1	0	0.618098	0.849219	1.431662
31	8	0	3.694136	0.073258	-1.455632
32	1	0	4.552175	-0.267401	-1.169547
33	8	0	3.757468	-1.091076	1.546878
34	1	0	3.066028	-0.648931	2.054145
35	8	0	5.447810	-1.753427	-0.347052
36	1	0	5.604387	-1.451336	0.555734
37	6	0	-1.424078	3.207226	1.157773
38	1	0	-2.337655	2.667023	1.410443
39	1	0	-1.017101	3.645646	2.069717
40	1	0	-1.672343	4.019352	0.455843
41	8	0	-4.815060	-2.322109	0.329808
42	6	0	-6.162087	-2.133100	-0.048600
43	1	0	-6.689105	-3.035302	0.252656
44	1	0	-6.600066	-1.268904	0.461333
45	1	0	-6.254805	-2.002397	-1.131612

Structure 45b (^{2}E ax-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1091.3604517
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.399713	0.423807	-0.496827
2	6	0	-2.533578	-0.961683	-0.425737
3	6	0	-3.748906	-1.534161	-0.091138
4	6	0	-4.855309	-0.728245	0.183573
5	6	0	-4.731518	0.660028	0.118349
6	6	0	-3.505261	1.220193	-0.225217
7	1	0	-1.677608	-1.588981	-0.638668
8	1	0	-3.873720	-2.608408	-0.035949
9	1	0	-5.570934	1.308524	0.328502
10	1	0	-3.403602	2.299805	-0.268078
11	6	0	-1.095689	1.088816	-0.836451
12	1	0	-1.239688	1.776910	-1.681853
13	7	0	-0.502911	1.856773	0.242639
14	8	0	-0.106645	0.126783	-1.224401
15	6	0	1.162106	0.771645	-1.091811
16	6	0	0.862015	2.048650	-0.257686
17	1	0	1.573949	2.190109	0.552287
18	1	0	0.886574	2.926992	-0.906329
19	1	0	1.534180	1.022424	-2.093165
20	6	0	2.113297	-0.234176	-0.462418
21	1	0	1.824180	-0.409038	0.581708
22	6	0	3.567121	0.246177	-0.453560
23	1	0	3.792547	0.719447	-1.420579
24	6	0	4.526203	-0.948306	-0.312710
25	1	0	4.616974	-1.411760	-1.300174
26	6	0	5.906663	-0.531842	0.178920
27	1	0	6.613611	-1.352970	0.027146
28	1	0	6.263429	0.348441	-0.358516
29	8	0	2.055877	-1.452676	-1.198291
30	1	0	1.128589	-1.593553	-1.420816
31	8	0	3.698404	1.226415	0.559141
32	1	0	4.382840	0.944959	1.182282
33	8	0	4.069832	-1.901468	0.636010
34	1	0	3.283036	-2.308853	0.255346
35	8	0	5.844085	-0.182740	1.556285
36	1	0	5.428016	-0.935241	1.994526
37	6	0	-0.535797	1.161212	1.532678
38	1	0	0.069181	1.726432	2.241635
39	1	0	-1.560231	1.129522	1.903671
40	1	0	-0.155737	0.132056	1.485214
41	8	0	-6.000911	-1.382220	0.502218
42	6	0	-7.149650	-0.603662	0.761708
43	1	0	-7.424517	0.000393	-0.109003
44	1	0	-7.948398	-1.309170	0.978331
45	1	0	-6.999341	0.051079	1.626275

Structure 45b (^{2}E ec-ec H-bond O) (M06-2X, Benzene)

Energy (Hartrees): = - 1091.384339
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.155704	0.729809	-0.234106
2	6	0	-1.876392	-0.560112	0.230917
3	6	0	-2.894511	-1.465540	0.447418
4	6	0	-4.225893	-1.097084	0.208072
5	6	0	-4.517350	0.184719	-0.250593
6	6	0	-3.473181	1.085734	-0.468930
7	1	0	-0.846335	-0.840885	0.425695
8	1	0	-2.697172	-2.468496	0.806282
9	1	0	-5.535618	0.493639	-0.443993
10	1	0	-3.702490	2.082555	-0.832513
11	6	0	-1.025869	1.693493	-0.474517
12	1	0	-1.424890	2.646185	-0.870768
13	7	0	-0.209890	1.920528	0.707877
14	8	0	-0.112287	1.162051	-1.431537
15	6	0	1.233858	1.414061	-0.996743
16	6	0	1.061367	2.382531	0.165438
17	1	0	1.863699	2.300855	0.898052
18	1	0	0.996148	3.420231	-0.202405
19	1	0	1.783378	1.839671	-1.840413
20	6	0	1.846500	0.072620	-0.585630
21	1	0	1.479785	-0.184430	0.417139
22	6	0	3.375024	0.097582	-0.531460
23	1	0	3.754005	0.581874	-1.441208
24	6	0	3.937266	-1.339576	-0.522756
25	1	0	4.007101	-1.673371	-1.562778
26	6	0	5.312767	-1.425219	0.124159

27	1	0	5.765001	-2.395088	-0.104806
28	1	0	5.969843	-0.634178	-0.240166
29	8	0	1.462139	-0.929992	-1.519596
30	1	0	0.550986	-0.725780	-1.769415
31	8	0	3.782787	0.892667	0.569445
32	1	0	4.179941	0.314635	1.235888
33	8	0	3.128850	-2.240339	0.224549
34	1	0	2.291720	-2.311747	-0.250051
35	8	0	5.195190	-1.259275	1.534537
36	1	0	4.534473	-1.904845	1.815031
37	6	0	-0.818783	2.825182	1.661863
38	1	0	-1.765543	2.409686	2.013156
39	1	0	-0.158535	2.943226	2.522403
40	1	0	-1.010139	3.821598	1.228479
41	8	0	-5.152575	-2.053202	0.453526
42	6	0	-6.511265	-1.724102	0.233980
43	1	0	-6.695941	-1.477130	-0.816433
44	1	0	-7.083104	-2.611384	0.498370
45	1	0	-6.826930	-0.890374	0.869254

Structure 45b (^{2}E ec-ec H-bond N) (M06-2X, Benzene)

Energy (Hartrees): = - 1091.3876483
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.971073	0.600172	-0.408206
2	6	0	-1.660440	-0.581828	0.273955
3	6	0	-2.634411	-1.530952	0.508931
4	6	0	-3.947596	-1.320814	0.067240
5	6	0	-4.268166	-0.150281	-0.615682
6	6	0	-3.270463	0.797749	-0.848157
7	1	0	-0.643606	-0.751279	0.610761
8	1	0	-2.411160	-2.452424	1.032925
9	1	0	-5.272076	0.034087	-0.973358
10	1	0	-3.521508	1.704903	-1.389167
11	6	0	-0.914486	1.643475	-0.641295
12	1	0	-1.304392	2.412776	-1.333636
13	7	0	-0.446533	2.285662	0.591143
14	8	0	0.260363	1.075600	-1.189952
15	6	0	1.407494	1.745661	-0.648735
16	6	0	0.806586	2.901748	0.152579
17	1	0	1.420857	3.198011	1.005365
18	1	0	0.622413	3.780427	-0.484617
19	1	0	2.050913	2.073797	-1.466517
20	6	0	2.196874	0.782031	0.229724
21	1	0	3.089118	1.314155	0.586489
22	6	0	2.693017	-0.421535	-0.575771
23	1	0	1.861644	-0.808389	-1.176416
24	6	0	3.150365	-1.553420	0.362730
25	1	0	2.266289	-2.141800	0.628071
26	6	0	4.180826	-2.468654	-0.284938
27	1	0	4.286745	-3.381864	0.309466
28	1	0	3.881816	-2.739102	-1.298712
29	8	0	1.438168	0.326913	1.345542
30	1	0	0.644649	0.886483	1.428671
31	8	0	3.689755	0.042620	-1.473153
32	1	0	4.542094	-0.318318	-1.195133
33	8	0	3.784113	-1.068193	1.542124
34	1	0	3.106522	-0.602008	2.047003
35	8	0	5.434169	-1.797406	-0.381227
36	1	0	5.623955	-1.478697	0.509747
37	6	0	-1.404271	3.212546	1.167869
38	1	0	-2.314416	2.676249	1.441500
39	1	0	-0.981914	3.654822	2.071321
40	1	0	-1.664731	4.022253	0.468233
41	8	0	-4.827848	-2.310107	0.348187
42	6	0	-6.168509	-2.138570	-0.070577
43	1	0	-6.700970	-3.031119	0.252055
44	1	0	-6.622426	-1.259164	0.397416
45	1	0	-6.238320	-2.052812	-1.159616

Structure 45b (^{2}E ax-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 1091.3797188
No imaginary frequencies
Standard orientation:

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

1	6	0	-2.406124	0.413943	-0.502756
2	6	0	-2.546353	-0.970705	-0.422630
3	6	0	-3.765980	-1.536357	-0.089251
4	6	0	-4.870477	-0.724657	0.178604
5	6	0	-4.739952	0.663325	0.104657
6	6	0	-3.510515	1.216229	-0.239145
7	1	0	-1.693788	-1.605859	-0.627216
8	1	0	-3.891857	-2.610636	-0.028349
9	1	0	-5.577304	1.316738	0.308999
10	1	0	-3.407603	2.295647	-0.290189
11	6	0	-1.097639	1.072623	-0.841020
12	1	0	-1.234903	1.751650	-1.694524
13	7	0	-0.508431	1.853430	0.232419
14	8	0	-0.107806	0.104856	-1.210317
15	6	0	1.160953	0.753981	-1.087376
16	6	0	0.858482	2.039514	-0.267768
17	1	0	1.565305	2.188896	0.545110
18	1	0	0.886333	2.910814	-0.925552
19	1	0	1.530117	0.995906	-2.091579
20	6	0	2.116889	-0.241657	-0.447360
21	1	0	1.834121	-0.399715	0.601158
22	6	0	3.571826	0.237558	-0.460838
23	1	0	3.788441	0.694193	-1.437284
24	6	0	4.533960	-0.952642	-0.305681
25	1	0	4.618314	-1.435798	-1.284001
26	6	0	5.920134	-0.527737	0.159511
27	1	0	6.623487	-1.354053	0.019198
28	1	0	6.275112	0.336293	-0.404926
29	8	0	2.054374	-1.473124	-1.162426
30	1	0	1.122291	-1.631541	-1.352499
31	8	0	3.715741	1.235723	0.535863
32	1	0	4.405106	0.957584	1.155044
33	8	0	4.087365	-1.887023	0.668276
34	1	0	3.293828	-2.298054	0.305517
35	8	0	5.878982	-0.144549	1.531268
36	1	0	5.478405	-0.889433	1.996879
37	6	0	-0.541801	1.174110	1.530819
38	1	0	0.061704	1.749097	2.233941
39	1	0	-1.565583	1.146974	1.905279
40	1	0	-0.159637	0.145187	1.499389
41	8	0	-6.018427	-1.369454	0.499449
42	6	0	-7.161227	-0.581057	0.773271
43	1	0	-7.450179	0.018145	-0.096196
44	1	0	-7.961511	-1.280897	1.005599
45	1	0	-6.996072	0.074592	1.634133

Structure 45b (^{2}E ec-ec H-bond O) (M06-2X, DMSO)

Energy (Hartrees): = - 1091.3881133
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.173409	0.690034	-0.283949
2	6	0	-1.895123	-0.622145	0.115412
3	6	0	-2.919029	-1.518010	0.352829
4	6	0	-4.255014	-1.117418	0.201138
5	6	0	-4.544999	0.186671	-0.195131
6	6	0	-3.495815	1.076793	-0.435987
7	1	0	-0.863559	-0.936358	0.240007
8	1	0	-2.716623	-2.537633	0.659734
9	1	0	-5.565986	0.521192	-0.320374
10	1	0	-3.724056	2.092006	-0.745919
11	6	0	-1.045475	1.658026	-0.516188
12	1	0	-1.443980	2.604919	-0.922181
13	7	0	-0.256314	1.900342	0.685171
14	8	0	-0.109157	1.125520	-1.450466
15	6	0	1.227310	1.406347	-0.996869
16	6	0	1.019314	2.375315	0.157994
17	1	0	1.808018	2.310782	0.906949
18	1	0	0.942523	3.408535	-0.216751
19	1	0	1.783017	1.842307	-1.831043
20	6	0	1.859668	0.076825	-0.586913
21	1	0	1.439106	-0.233160	0.378679
22	6	0	3.380205	0.149309	-0.425449
23	1	0	3.804899	0.730815	-1.254738
24	6	0	3.995417	-1.257766	-0.510726
25	1	0	4.063505	-1.520564	-1.570473
26	6	0	5.387172	-1.331021	0.099291
27	1	0	5.867356	-2.268018	-0.197446
28	1	0	6.004898	-0.497620	-0.238736
29	8	0	1.567288	-0.901736	-1.580556
30	1	0	0.647969	-0.749161	-1.836299

31	8	0	3.667609	0.833203	0.787171
32	1	0	4.187302	0.241901	1.349548
33	8	0	3.227746	-2.229790	0.191646
34	1	0	2.394005	-2.311096	-0.287268
35	8	0	5.308504	-1.249036	1.523292
36	1	0	4.696911	-1.947082	1.790702
37	6	0	-0.893568	2.829944	1.600668
38	1	0	-1.845216	2.419548	1.945784
39	1	0	-0.250864	2.980126	2.469724
40	1	0	-1.082866	3.808802	1.130987
41	8	0	-5.187062	-2.063082	0.460218
42	6	0	-6.551740	-1.691837	0.325681
43	1	0	-6.782162	-1.399995	-0.703152
44	1	0	-7.131109	-2.574706	0.588053
45	1	0	-6.807795	-0.874978	1.006767

Structure 45b (^{2}E ec-ec H-bond N) (M06-2X, DMSO)

Energy (Hartrees): = - 1091.3918612
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.963994	0.599313	-0.421079
2	6	0	-1.622336	-0.618103	0.178818
3	6	0	-2.587138	-1.578893	0.414431
4	6	0	-3.922491	-1.342704	0.056902
5	6	0	-4.274505	-0.133281	-0.540423
6	6	0	-3.286084	0.823930	-0.776421
7	1	0	-0.590036	-0.805505	0.455673
8	1	0	-2.335547	-2.527499	0.874491
9	1	0	-5.296525	0.074394	-0.828541
10	1	0	-3.561350	1.762350	-1.248232
11	6	0	-0.918211	1.654809	-0.652063
12	1	0	-1.314888	2.425333	-1.336453
13	7	0	-0.453618	2.289589	0.585278
14	8	0	0.260085	1.094286	-1.208610
15	6	0	1.405436	1.758677	-0.651586
16	6	0	0.800421	2.910614	0.149391
17	1	0	1.411186	3.208285	1.003731
18	1	0	0.611975	3.786588	-0.488320
19	1	0	2.053623	2.095802	-1.461525
20	6	0	2.187258	0.791653	0.229501
21	1	0	3.078698	1.325180	0.585458
22	6	0	2.676448	-0.424582	-0.559385
23	1	0	1.840249	-0.826627	-1.142751
24	6	0	3.143496	-1.539389	0.394683
25	1	0	2.261692	-2.119460	0.682886
26	6	0	4.154722	-2.477591	-0.246730
27	1	0	4.271170	-3.370761	0.374473
28	1	0	3.827663	-2.782191	-1.241759
29	8	0	1.423022	0.345860	1.346585
30	1	0	0.627309	0.907081	1.412569
31	8	0	3.668290	0.019001	-1.477071
32	1	0	4.516181	-0.354688	-1.201915
33	8	0	3.796405	-1.031518	1.555439
34	1	0	3.127919	-0.546169	2.054717
35	8	0	5.412440	-1.817637	-0.397158
36	1	0	5.635232	-1.483079	0.480944
37	6	0	-1.413223	3.226178	1.149307
38	1	0	-2.325115	2.696186	1.430821
39	1	0	-0.988694	3.680954	2.045394
40	1	0	-1.669874	4.022926	0.435261
41	8	0	-4.791287	-2.344032	0.325871
42	6	0	-6.152740	-2.146788	-0.027580
43	1	0	-6.674565	-3.054290	0.269411
44	1	0	-6.580199	-1.292513	0.505511
45	1	0	-6.264764	-2.000156	-1.105824

Structure 45b (^{2}E ax-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 1091.3835187
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.408822	0.459134	-0.440338
2	6	0	-2.484330	-0.914597	-0.203785
3	6	0	-3.697567	-1.510498	0.098804

4	6	0	-4.863691	-0.741087	0.176111
5	6	0	-4.798610	0.634103	-0.057476
6	6	0	-3.571805	1.216670	-0.366363
7	1	0	-1.586304	-1.518555	-0.259767
8	1	0	-3.767862	-2.576720	0.279835
9	1	0	-5.683916	1.254151	-0.010896
10	1	0	-3.526488	2.285431	-0.551878
11	6	0	-1.105565	1.150199	-0.729301
12	1	0	-1.251061	1.895580	-1.522526
13	7	0	-0.510393	1.845124	0.404030
14	8	0	-0.119543	0.213555	-1.174385
15	6	0	1.154108	0.843280	-1.002298
16	6	0	0.860003	2.059308	-0.082836
17	1	0	1.564134	2.137853	0.742814
18	1	0	0.894755	2.978971	-0.670563
19	1	0	1.521369	1.166642	-1.983183
20	6	0	2.106640	-0.204814	-0.444065
21	1	0	1.844226	-0.422672	0.598988
22	6	0	3.567212	0.254499	-0.465839
23	1	0	3.770089	0.759733	-1.420140
24	6	0	4.515755	-0.952642	-0.396762
25	1	0	4.555878	-1.393778	-1.396951
26	6	0	5.927286	-0.568457	0.020508
27	1	0	6.606238	-1.403701	-0.173988
28	1	0	6.273398	0.302953	-0.537686
29	8	0	2.009517	-1.391144	-1.228714
30	1	0	1.067689	-1.543773	-1.374227
31	8	0	3.747637	1.193276	0.585670
32	1	0	4.475483	0.884371	1.143089
33	8	0	4.091392	-1.921632	0.555841
34	1	0	3.276214	-2.302581	0.207411
35	8	0	5.958295	-0.222535	1.406031
36	1	0	5.580633	-0.979644	1.872109
37	6	0	-0.541479	1.062962	1.644744
38	1	0	0.060393	1.581217	2.392300
39	1	0	-1.565308	1.004653	2.017606
40	1	0	-0.154603	0.041429	1.534335
41	8	0	-6.000134	-1.411794	0.476812
42	6	0	-7.208143	-0.666026	0.528514
43	1	0	-7.424877	-0.198821	-0.436742
44	1	0	-7.993346	-1.380340	0.767365
45	1	0	-7.167258	0.101725	1.306752

Structure 45c ($^5C_2$ ec-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1091.3637063
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.005663	1.415543	0.505570
2	6	0	-1.020231	2.485598	0.055667
3	6	0	-1.736412	0.140244	-0.298109
4	1	0	-1.166424	3.389244	0.651392
5	1	0	-1.180041	2.736771	-1.007781
6	1	0	-3.033355	1.754657	0.358038
7	1	0	-1.933464	0.352918	-1.361381
8	8	0	-0.378219	-0.228768	-0.137287
9	7	0	0.325696	1.971433	0.299806
10	6	0	-2.573882	-1.068458	0.113993
11	1	0	-2.303633	-1.899732	-0.544849
12	6	0	-4.079507	-0.834441	-0.004725
13	1	0	-4.380049	-0.024056	0.676431
14	6	0	-4.566620	-0.516474	-1.407331
15	1	0	-4.161696	-1.269031	-2.099866
16	1	0	-4.220103	0.469544	-1.727334
17	8	0	-2.298084	-1.512238	1.430096
18	1	0	-2.222461	-0.718657	1.977482
19	8	0	-4.745585	-2.028150	0.369127
20	1	0	-4.300116	-2.346129	1.163018
21	8	0	-5.973373	-0.487661	-1.447758
22	1	0	-6.264837	-1.276663	-0.977880
23	8	0	-1.829908	1.178583	1.896062
24	1	0	-0.870916	1.205491	2.030625
25	6	0	1.332696	2.997281	0.062492
26	1	0	1.382041	3.296349	-0.997939
27	1	0	1.080573	3.877739	0.655056
28	1	0	2.314643	2.640432	0.369379
29	6	0	1.922376	0.202717	-0.324494
30	6	0	2.241048	-0.441687	0.874358
31	6	0	2.892814	0.317055	-1.305563
32	6	0	3.508444	-0.946689	1.081896
33	1	0	1.471834	-0.560391	1.628295

34	6	0	4.179899	-0.184988	-1.111063
35	1	0	2.654010	0.807154	-2.244047
36	6	0	4.488667	-0.818478	0.089835
37	1	0	3.774804	-1.457593	1.998605
38	1	0	4.915787	-0.081015	-1.896334
39	6	0	0.542178	0.768346	-0.515997
40	1	0	0.384729	1.020309	-1.585687
41	8	0	5.700376	-1.346974	0.389751
42	6	0	6.711342	-1.271074	-0.593227
43	1	0	7.586350	-1.751759	-0.162336
44	1	0	6.416949	-1.800159	-1.505300
45	1	0	6.950973	-0.230765	-0.835961

Structure 45c ($^5C_2$ ax-ec) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1091.3599418
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.912024	1.636130	-0.083486
2	6	0	-0.788986	2.507289	-0.661677
3	6	0	-1.644410	0.178212	-0.482155
4	1	0	-0.899817	3.528905	-0.295187
5	1	0	-0.881521	2.527928	-1.754633
6	1	0	-2.880755	1.954392	-0.472047
7	1	0	-1.684336	0.110863	-1.581472
8	8	0	-0.336931	-0.175738	-0.047473
9	7	0	0.551824	2.019067	-0.331568
10	6	0	-2.603815	-0.875852	0.077026
11	1	0	-2.167162	-1.845591	-0.185101
12	6	0	-3.995242	-0.783080	-0.549305
13	1	0	-3.912740	-0.719089	-1.644003
14	6	0	-4.827456	-2.003621	-0.192736
15	1	0	-4.791053	-2.142154	0.891990
16	1	0	-4.422693	-2.892447	-0.690111
17	8	0	-2.701691	-0.855627	1.482366
18	1	0	-3.148947	-0.027379	1.703055
19	8	0	-4.620897	0.377314	-0.035469
20	1	0	-5.567524	0.248520	-0.167077
21	8	0	-6.149209	-1.721795	-0.636819
22	1	0	-6.757816	-2.325789	-0.208394
23	8	0	-1.975527	1.774834	1.329308
24	1	0	-1.305925	1.185402	1.695868
25	6	0	1.009217	2.313680	1.028321
26	1	0	0.717577	1.553432	1.764719
27	1	0	2.098300	2.381533	1.044138
28	1	0	0.594338	3.270445	1.343507
29	6	0	2.018485	0.050407	-0.398097
30	6	0	2.185727	-1.111291	0.353681
31	6	0	3.142330	0.694040	-0.901541
32	6	0	3.453802	-1.614163	0.593633
33	1	0	1.313665	-1.613763	0.751320
34	6	0	4.421793	0.199235	-0.669448
35	1	0	3.013705	1.609399	-1.469977
36	6	0	4.578529	-0.965488	0.082590
37	1	0	3.604850	-2.514292	1.176468
38	1	0	5.275936	0.724575	-1.074234
39	6	0	0.654188	0.624765	-0.693115
40	1	0	0.462631	0.566512	-1.776350
41	8	0	5.776537	-1.538162	0.369567
42	6	0	6.938595	-0.905756	-0.121011
43	1	0	7.042178	0.106074	0.284485
44	1	0	7.776401	-1.514589	0.211082
45	1	0	6.935283	-0.859992	-1.214983

Structure 45c ($^5C_2$ ec-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 1091.3850528
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.001794	1.430133	0.498235
2	6	0	-1.011555	2.493919	0.046191
3	6	0	-1.740378	0.151804	-0.302534
4	1	0	-1.154317	3.400871	0.637615
5	1	0	-1.168283	2.740689	-1.017824

6	1	0	-3.027529	1.774497	0.351339
7	1	0	-1.940752	0.362167	-1.364897
8	8	0	-0.381825	-0.223693	-0.145222
9	7	0	0.332015	1.973180	0.295403
10	6	0	-2.578274	-1.054337	0.117823
11	1	0	-2.305960	-1.891758	-0.532424
12	6	0	-4.085121	-0.826478	-0.004675
13	1	0	-4.389230	-0.002173	0.657321
14	6	0	-4.572411	-0.544301	-1.414108
15	1	0	-4.166071	-1.309216	-2.091621
16	1	0	-4.231916	0.435502	-1.757703
17	8	0	-2.304346	-1.483386	1.441662
18	1	0	-2.211945	-0.680304	1.973603
19	8	0	-4.748535	-2.014964	0.398012
20	1	0	-4.306638	-2.306113	1.204517
21	8	0	-5.982328	-0.524835	-1.456671
22	1	0	-6.268951	-1.308379	-0.974177
23	8	0	-1.823011	1.194844	1.891688
24	1	0	-0.863139	1.228320	2.023955
25	6	0	1.342848	2.997749	0.068867
26	1	0	1.400648	3.304614	-0.988567
27	1	0	1.089190	3.876072	0.664675
28	1	0	2.323388	2.641901	0.382808
29	6	0	1.922016	0.195961	-0.328841
30	6	0	2.232157	-0.465508	0.863088
31	6	0	2.901957	0.325118	-1.300053
32	6	0	3.497859	-0.976275	1.072451
33	1	0	1.460912	-0.590250	1.614375
34	6	0	4.187125	-0.180400	-1.102875
35	1	0	2.671917	0.830672	-2.232648
36	6	0	4.486669	-0.834244	0.090311
37	1	0	3.753150	-1.500236	1.985491
38	1	0	4.929618	-0.064655	-1.880642
39	6	0	0.544948	0.771321	-0.522496
40	1	0	0.390783	1.023665	-1.591433
41	8	0	5.694963	-1.367759	0.388792
42	6	0	6.717785	-1.263750	-0.583539
43	1	0	7.591945	-1.749476	-0.154644
44	1	0	6.439527	-1.776810	-1.509707
45	1	0	6.957203	-0.217783	-0.800368

Structure 45c ($^5C_2$ ax-ec) (M06-2X, Benzene)

Energy (Hartrees): = - 1091.3805371
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.913894	1.633142	-0.078696
2	6	0	-0.791608	2.512758	-0.644889
3	6	0	-1.645927	0.181349	-0.495541
4	1	0	-0.901740	3.530239	-0.266554
5	1	0	-0.887001	2.544840	-1.737032
6	1	0	-2.881295	1.957514	-0.465733
7	1	0	-1.686446	0.127177	-1.594750
8	8	0	-0.336789	-0.176668	-0.064256
9	7	0	0.551410	2.021390	-0.323005
10	6	0	-2.603286	-0.880450	0.051116
11	1	0	-2.181764	-1.845888	-0.247508
12	6	0	-4.006544	-0.760110	-0.544573
13	1	0	-3.942386	-0.636757	-1.635029
14	6	0	-4.827977	-2.000969	-0.240048
15	1	0	-4.777859	-2.199862	0.834997
16	1	0	-4.428563	-2.861188	-0.789192
17	8	0	-2.672370	-0.897249	1.459809
18	1	0	-3.124174	-0.078883	1.706769
19	8	0	-4.628435	0.370270	0.041409
20	1	0	-5.577419	0.234648	-0.068156
21	8	0	-6.159575	-1.705248	-0.646488
22	1	0	-6.754813	-2.335348	-0.233775
23	8	0	-1.982663	1.752865	1.337406
24	1	0	-1.300467	1.172688	1.695896
25	6	0	1.015155	2.306698	1.035421
26	1	0	0.702094	1.563465	1.780996
27	1	0	2.106207	2.343881	1.053333
28	1	0	0.634189	3.280032	1.344588
29	6	0	2.017842	0.051771	-0.409012
30	6	0	2.189184	-1.061074	0.413017
31	6	0	3.139815	0.652232	-0.968445
32	6	0	3.457396	-1.557979	0.666948
33	1	0	1.321140	-1.532760	0.855535
34	6	0	4.419373	0.162732	-0.724485
35	1	0	3.014128	1.529523	-1.595026

36	6	0	4.580150	-0.952239	0.099794
37	1	0	3.606896	-2.419751	1.306264
38	1	0	5.271018	0.653670	-1.175904
39	6	0	0.653962	0.630051	-0.701692
40	1	0	0.463544	0.586030	-1.785174
41	8	0	5.777065	-1.512134	0.405801
42	6	0	6.937937	-0.926092	-0.149503
43	1	0	7.060835	0.109875	0.182657
44	1	0	7.777056	-1.517746	0.211508
45	1	0	6.919615	-0.960745	-1.243607

Structure 45c ($^5C_2$ ec-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 1091.3922323
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.998907	1.422098	0.492362
2	6	0	-1.022651	2.480412	0.004345
3	6	0	-1.741116	0.132470	-0.288301
4	1	0	-1.158138	3.401037	0.575639
5	1	0	-1.199609	2.697137	-1.061601
6	1	0	-3.027406	1.758748	0.352527
7	1	0	-1.937688	0.328296	-1.352511
8	8	0	-0.379340	-0.240538	-0.118514
9	7	0	0.332812	1.977143	0.239849
10	6	0	-2.583066	-1.063007	0.147308
11	1	0	-2.315723	-1.912043	-0.489794
12	6	0	-4.087429	-0.829289	0.015376
13	1	0	-4.389903	0.003541	0.665967
14	6	0	-4.559093	-0.556417	-1.399735
15	1	0	-4.146399	-1.323135	-2.070457
16	1	0	-4.214592	0.422085	-1.740122
17	8	0	-2.315862	-1.469593	1.483137
18	1	0	-2.199379	-0.652816	1.990165
19	8	0	-4.760257	-2.012525	0.429561
20	1	0	-4.340189	-2.277378	1.256797
21	8	0	-5.973754	-0.541138	-1.457387
22	1	0	-6.260942	-1.323807	-0.973365
23	8	0	-1.798658	1.208142	1.891087
24	1	0	-0.836077	1.235336	2.005417
25	6	0	1.321226	3.001340	-0.080960
26	1	0	1.337917	3.239920	-1.156428
27	1	0	1.071782	3.910647	0.468154
28	1	0	2.318428	2.680312	0.220800
29	6	0	1.920662	0.192993	-0.329263
30	6	0	2.288973	-0.274597	0.936613
31	6	0	2.849072	0.149834	-1.357350
32	6	0	3.560623	-0.766297	1.161486
33	1	0	1.565057	-0.251650	1.744161
34	6	0	4.139283	-0.341417	-1.148004
35	1	0	2.573658	0.507946	-2.344307
36	6	0	4.498099	-0.798250	0.119245
37	1	0	3.860176	-1.131298	2.137109
38	1	0	4.841618	-0.361432	-1.970778
39	6	0	0.538757	0.750472	-0.539734
40	1	0	0.374721	0.962159	-1.613851
41	8	0	5.718314	-1.288634	0.438112
42	6	0	6.698589	-1.327559	-0.588993
43	1	0	7.600453	-1.727564	-0.130257
44	1	0	6.387601	-1.982635	-1.408178
45	1	0	6.903290	-0.325842	-0.978359

Structure 45c ($^5C_2$ ax-ec) (M06-2X, DMSO)

Energy (Hartrees): = - 1091.3861727
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.912424	1.618397	-0.071340
2	6	0	-0.795085	2.502169	-0.637639
3	6	0	-1.647884	0.172416	-0.502373
4	1	0	-0.900069	3.518147	-0.253159
5	1	0	-0.901531	2.535551	-1.728062
6	1	0	-2.879479	1.947108	-0.455645
7	1	0	-1.691381	0.130118	-1.600483

8	8	0	-0.335777	-0.191894	-0.076225
9	7	0	0.553118	2.008418	-0.329753
10	6	0	-2.610244	-0.887921	0.031874
11	1	0	-2.222670	-1.852462	-0.310635
12	6	0	-4.024219	-0.715202	-0.525609
13	1	0	-3.974391	-0.495496	-1.600603
14	6	0	-4.840021	-1.977718	-0.317625
15	1	0	-4.775010	-2.274938	0.733984
16	1	0	-4.447774	-2.783090	-0.947634
17	8	0	-2.645149	-0.949308	1.444192
18	1	0	-3.103244	-0.143888	1.719887
19	8	0	-4.639334	0.362058	0.166131
20	1	0	-5.589434	0.213618	0.079921
21	8	0	-6.180614	-1.652255	-0.672187
22	1	0	-6.763762	-2.317552	-0.294646
23	8	0	-1.979550	1.726920	1.348543
24	1	0	-1.293407	1.145999	1.699203
25	6	0	1.021150	2.282044	1.030185
26	1	0	0.692109	1.547191	1.777244
27	1	0	2.113397	2.298070	1.049010
28	1	0	0.662761	3.264459	1.338353
29	6	0	2.016389	0.040475	-0.424176
30	6	0	2.202175	-1.001055	0.484546
31	6	0	3.130164	0.583073	-1.056518
32	6	0	3.474192	-1.482984	0.754626
33	1	0	1.343451	-1.432697	0.983373
34	6	0	4.413508	0.110212	-0.796965
35	1	0	2.999053	1.397811	-1.761745
36	6	0	4.589137	-0.930006	0.119232
37	1	0	3.627696	-2.289481	1.462275
38	1	0	5.257057	0.556346	-1.306738
39	6	0	0.651334	0.615895	-0.716776
40	1	0	0.459494	0.576568	-1.798912
41	8	0	5.790673	-1.460422	0.451272
42	6	0	6.944128	-0.915257	-0.172388
43	1	0	7.052541	0.149838	0.052437
44	1	0	7.793081	-1.457539	0.239189
45	1	0	6.913882	-1.060614	-1.256464

Structure 45d ($^5C_2$ ec-ax) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1091.3579982
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.690264	1.203752	-0.966476
2	6	0	-0.449381	1.954504	-1.449497
3	6	0	-1.291108	0.272313	0.185169
4	1	0	-0.752028	2.704121	-2.184523
5	1	0	0.250348	1.254891	-1.929589
6	1	0	-2.133928	0.637931	-1.787885
7	1	0	-0.552910	-0.451645	-0.190212
8	8	0	-0.709515	1.056668	1.220081
9	7	0	0.101162	2.640709	-0.290663
10	6	0	-2.444793	-0.504344	0.813314
11	1	0	-2.026742	-1.136663	1.603810
12	6	0	-3.178852	-1.409645	-0.175607
13	1	0	-3.639598	-0.795855	-0.964177
14	6	0	-2.317513	-2.484174	-0.815490
15	1	0	-1.768021	-3.013129	-0.022960
16	1	0	-1.591716	-2.044140	-1.503905
17	8	0	-3.402539	0.325710	1.445308
18	1	0	-3.535302	1.085639	0.862434
19	8	0	-4.195964	-2.101964	0.528369
20	1	0	-4.620411	-1.447464	1.095354
21	8	0	-3.111865	-3.370998	-1.567480
22	1	0	-3.865874	-3.585113	-1.007161
23	8	0	-2.664605	2.139810	-0.525226
24	1	0	-2.170880	2.753164	0.038362
25	6	0	0.945603	3.795009	-0.526286
26	1	0	1.888907	3.585348	-1.047267
27	1	0	0.388829	4.525131	-1.118436
28	1	0	1.189080	4.257914	0.432730
29	6	0	1.592357	0.759303	0.570883
30	6	0	2.487359	0.834251	-0.486058
31	6	0	1.764112	-0.269979	1.506912
32	6	0	3.532250	-0.081593	-0.625437
33	1	0	2.383565	1.606658	-1.236713
34	6	0	2.790464	-1.184388	1.384886
35	1	0	1.066270	-0.349228	2.333204
36	6	0	3.687079	-1.096012	0.314008
37	1	0	4.204431	0.010242	-1.467431

38	1	0	2.927894	-1.982710	2.103528
39	6	0	0.453122	1.753857	0.802780
40	1	0	0.714110	2.388856	1.654250
41	8	0	4.660531	-2.037724	0.278364
42	6	0	5.588681	-1.981580	-0.784682
43	1	0	6.278842	-2.806540	-0.625652
44	1	0	5.091320	-2.104636	-1.752097
45	1	0	6.142650	-1.037387	-0.776860

Structure 45d ($^5C_2$ ax-ax) (M06-2X, Gas Phase)

Energy (Hartrees): = - 1091.3603633
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.479351	1.263950	0.984350
2	6	0	0.198488	2.007961	1.374907
3	6	0	1.121663	0.266847	-0.121708
4	1	0	0.438139	2.795542	2.091145
5	1	0	-0.484745	1.301605	1.860797
6	1	0	1.886384	0.731645	1.846117
7	1	0	0.381365	-0.439832	0.279224
8	8	0	0.549351	0.996835	-1.205626
9	7	0	-0.492769	2.608996	0.231587
10	6	0	2.272328	-0.555963	-0.705870
11	1	0	1.859111	-1.071902	-1.579627
12	6	0	2.790307	-1.602674	0.280983
13	1	0	1.947773	-2.144388	0.733472
14	6	0	3.696694	-2.601692	-0.418298
15	1	0	4.451529	-2.048147	-0.985271
16	1	0	3.109025	-3.226342	-1.100718
17	8	0	3.341950	0.229070	-1.182446
18	1	0	3.767641	0.596136	-0.395826
19	8	0	3.526611	-0.918911	1.277922
20	1	0	4.100780	-1.578636	1.684159
21	8	0	4.290093	-3.382760	0.611937
22	1	0	5.051084	-3.844015	0.255738
23	8	0	2.478312	2.175298	0.546965
24	1	0	2.354394	2.282661	-0.403834
25	6	0	0.047245	3.885666	-0.227247
26	1	0	0.937630	3.794654	-0.861408
27	1	0	-0.722750	4.414474	-0.794730
28	1	0	0.312682	4.494049	0.637263
29	6	0	-1.771566	0.650059	-0.556320
30	6	0	-2.789181	0.915323	0.348226
31	6	0	-1.809652	-0.552117	-1.270669
32	6	0	-3.823918	0.003981	0.561159
33	1	0	-2.769417	1.850846	0.895300
34	6	0	-2.827094	-1.465349	-1.071259
35	1	0	-1.022500	-0.764037	-1.986057
36	6	0	-3.842468	-1.193888	-0.148553
37	1	0	-4.598064	0.242347	1.277739
38	1	0	-2.867161	-2.400743	-1.615492
39	6	0	-0.669696	1.662057	-0.841236
40	1	0	-0.934680	2.223980	-1.740381
41	8	0	-4.793877	-2.153229	-0.016870
42	6	0	-5.832710	-1.919648	0.909853
43	1	0	-6.473872	-2.797245	0.872155
44	1	0	-5.438947	-1.800772	1.924533
45	1	0	-6.414283	-1.032365	0.639637

Structure 716d ($^5C_2$ ec-ax) (M06-2X, Benzene)

Energy (Hartrees): = - 1091.3790078
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.694078	1.205658	-0.959517
2	6	0	-0.449543	1.945757	-1.446054
3	6	0	-1.295235	0.262021	0.182068
4	1	0	-0.744817	2.699966	-2.179304
5	1	0	0.241256	1.240374	-1.929658
6	1	0	-2.151178	0.651474	-1.780999
7	1	0	-0.570754	-0.468417	-0.206056
8	8	0	-0.695920	1.031143	1.219287
9	7	0	0.110666	2.623091	-0.286717

10	6	0	-2.453272	-0.503259	0.817151
11	1	0	-2.036906	-1.152255	1.595011
12	6	0	-3.220039	-1.382781	-0.170597
13	1	0	-3.677970	-0.752847	-0.947313
14	6	0	-2.389824	-2.468630	-0.830034
15	1	0	-1.843442	-3.021420	-0.052126
16	1	0	-1.662139	-2.036920	-1.521303
17	8	0	-3.387798	0.341214	1.469966
18	1	0	-3.495601	1.116163	0.900866
19	8	0	-4.245338	-2.060016	0.540592
20	1	0	-4.657747	-1.396497	1.106500
21	8	0	-3.213156	-3.332225	-1.583856
22	1	0	-3.962394	-3.540173	-1.014480
23	8	0	-2.653727	2.152389	-0.499514
24	1	0	-2.137615	2.773090	0.036833
25	6	0	0.958426	3.774646	-0.526277
26	1	0	1.873610	3.568129	-1.096341
27	1	0	0.387294	4.530076	-1.072227
28	1	0	1.252017	4.207128	0.433046
29	6	0	1.606355	0.734947	0.560434
30	6	0	2.498421	0.812152	-0.499755
31	6	0	1.786173	-0.292529	1.497237
32	6	0	3.549795	-0.096812	-0.638475
33	1	0	2.389707	1.582193	-1.252423
34	6	0	2.818633	-1.200959	1.375411
35	1	0	1.093248	-0.375220	2.327400
36	6	0	3.714591	-1.107799	0.303912
37	1	0	4.221421	-0.001704	-1.480931
38	1	0	2.960446	-1.995181	2.098443
39	6	0	0.467395	1.729853	0.798830
40	1	0	0.733581	2.359769	1.652220
41	8	0	4.696114	-2.039269	0.269987
42	6	0	5.650271	-1.953503	-0.771900
43	1	0	6.353206	-2.766651	-0.602994
44	1	0	5.182718	-2.080801	-1.753339
45	1	0	6.187579	-1.000371	-0.740101

Structure 45d ($^5C_2$ ax-ax) (M06-2X, Benece)

Energy (Hartrees): = - 1091.3806826
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.483069	1.256794	0.983338
2	6	0	0.208023	2.007353	1.378708
3	6	0	1.117642	0.262051	-0.121886
4	1	0	0.452479	2.795219	2.093073
5	1	0	-0.471845	1.302522	1.870998
6	1	0	1.887397	0.723085	1.845514
7	1	0	0.375637	-0.440985	0.280918
8	8	0	0.546508	0.996820	-1.204388
9	7	0	-0.487634	2.609679	0.238339
10	6	0	2.261601	-0.569118	-0.706707
11	1	0	1.838908	-1.108204	-1.561492
12	6	0	2.800688	-1.592087	0.294639
13	1	0	1.967093	-2.105727	0.793095
14	6	0	3.668104	-2.625236	-0.403203
15	1	0	4.412029	-2.104997	-1.014807
16	1	0	3.049191	-3.262662	-1.044616
17	8	0	3.321148	0.212274	-1.215174
18	1	0	3.773371	0.567534	-0.437998
19	8	0	3.582412	-0.887691	1.244530
20	1	0	4.171778	-1.542344	1.638658
21	8	0	4.289217	-3.383693	0.628331
22	1	0	5.040512	-3.852927	0.258189
23	8	0	2.489384	2.161372	0.543639
24	1	0	2.353076	2.280934	-0.404166
25	6	0	0.047869	3.889316	-0.216774
26	1	0	0.945734	3.807984	-0.842220
27	1	0	-0.719522	4.412698	-0.793136
28	1	0	0.297711	4.502737	0.649521
29	6	0	-1.778062	0.658878	-0.558806
30	6	0	-2.779885	0.906733	0.369122
31	6	0	-1.835084	-0.527430	-1.298738
32	6	0	-3.814546	-0.005436	0.580696
33	1	0	-2.750967	1.829591	0.937166
34	6	0	-2.853643	-1.440980	-1.102795
35	1	0	-1.062615	-0.729805	-2.032647
36	6	0	-3.851525	-1.187737	-0.155140
37	1	0	-4.575068	0.218941	1.316567
38	1	0	-2.903501	-2.363193	-1.669154
39	6	0	-0.670235	1.667542	-0.837955

40	1	0	-0.931761	2.234812	-1.734676
41	8	0	-4.804367	-2.143137	-0.026665
42	6	0	-5.815744	-1.932140	0.939646
43	1	0	-6.458242	-2.809639	0.901845
44	1	0	-5.392618	-1.840096	1.945218
45	1	0	-6.409394	-1.041812	0.708710

Structure 45d ($^5C_2$ ec-ax) (M06-2X, DMSO)

Energy (Hartrees): = - 1091.3850941
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.689616	1.208535	-0.963505
2	6	0	-0.442164	1.947485	-1.439922
3	6	0	-1.300591	0.264190	0.180071
4	1	0	-0.727572	2.702514	-2.176025
5	1	0	0.251958	1.241503	-1.916159
6	1	0	-2.141008	0.653149	-1.786571
7	1	0	-0.580546	-0.469640	-0.207895
8	8	0	-0.701165	1.027309	1.224377
9	7	0	0.108290	2.624998	-0.274417
10	6	0	-2.464490	-0.495859	0.808260
11	1	0	-2.057564	-1.139903	1.595091
12	6	0	-3.219757	-1.382941	-0.180597
13	1	0	-3.661167	-0.761759	-0.972698
14	6	0	-2.379561	-2.476946	-0.810242
15	1	0	-1.841562	-3.016103	-0.017812
16	1	0	-1.647650	-2.051544	-1.499643
17	8	0	-3.408154	0.358705	1.441755
18	1	0	-3.486502	1.135541	0.868581
19	8	0	-4.261792	-2.047759	0.523867
20	1	0	-4.689177	-1.369272	1.060745
21	8	0	-3.195338	-3.359794	-1.559460
22	1	0	-3.950417	-3.556398	-0.993229
23	8	0	-2.651788	2.160873	-0.507084
24	1	0	-2.128850	2.791912	0.011690
25	6	0	0.970222	3.768330	-0.516109
26	1	0	1.865141	3.553154	-1.113130
27	1	0	0.398715	4.539960	-1.038465
28	1	0	1.293690	4.178471	0.443445
29	6	0	1.601456	0.728869	0.562889
30	6	0	2.500055	0.813542	-0.492907
31	6	0	1.776896	-0.306336	1.491721
32	6	0	3.553128	-0.094103	-0.632805
33	1	0	2.396413	1.586227	-1.243435
34	6	0	2.810337	-1.215747	1.367858
35	1	0	1.083215	-0.398062	2.320433
36	6	0	3.713098	-1.114212	0.301963
37	1	0	4.228035	0.008808	-1.472082
38	1	0	2.944178	-2.014813	2.087854
39	6	0	0.465013	1.726984	0.805674
40	1	0	0.736855	2.351994	1.660579
41	8	0	4.695518	-2.044522	0.262988
42	6	0	5.666155	-1.929666	-0.767663
43	1	0	6.376052	-2.737560	-0.602657
44	1	0	5.211526	-2.044174	-1.756011
45	1	0	6.188874	-0.970249	-0.711347

Structure 45d ($^5C_2$ ax-ax) (M06-2X, DMSO)

Energy (Hartrees): = - 1091.3856841
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.476675	1.238976	0.987980
2	6	0	0.204088	1.995310	1.380472
3	6	0	1.113104	0.252674	-0.122886
4	1	0	0.446692	2.780377	2.098800
5	1	0	-0.478860	1.289473	1.866665
6	1	0	1.864969	0.695241	1.852120
7	1	0	0.374729	-0.453858	0.278653
8	8	0	0.542014	0.989969	-1.205188
9	7	0	-0.486778	2.604038	0.238577
10	6	0	2.254864	-0.578900	-0.705284
11	1	0	1.821937	-1.160995	-1.525541

12	6	0	2.837338	-1.552491	0.321828
13	1	0	2.027471	-1.998589	0.913811
14	6	0	3.614090	-2.658348	-0.368916
15	1	0	4.321454	-2.210806	-1.074891
16	1	0	2.924668	-3.312211	-0.913531
17	8	0	3.289900	0.204178	-1.267945
18	1	0	3.800219	0.521960	-0.510536
19	8	0	3.712340	-0.817211	1.166083
20	1	0	4.330646	-1.466075	1.526005
21	8	0	4.299570	-3.369101	0.656553
22	1	0	4.996590	-3.892647	0.250024
23	8	0	2.497533	2.137867	0.565631
24	1	0	2.373037	2.263511	-0.383104
25	6	0	0.073056	3.872951	-0.222322
26	1	0	0.981886	3.772756	-0.828922
27	1	0	-0.675727	4.395249	-0.823461
28	1	0	0.310255	4.494836	0.641963
29	6	0	-1.782845	0.654465	-0.555336
30	6	0	-2.799872	0.918450	0.352991
31	6	0	-1.829891	-0.545709	-1.273681
32	6	0	-3.841276	0.013199	0.564287
33	1	0	-2.780348	1.846864	0.912394
34	6	0	-2.854639	-1.454142	-1.077854
35	1	0	-1.044949	-0.770508	-1.987690
36	6	0	-3.869554	-1.182370	-0.152401
37	1	0	-4.611980	0.251771	1.285410
38	1	0	-2.890823	-2.386751	-1.628899
39	6	0	-0.673021	1.660947	-0.837429
40	1	0	-0.938536	2.229407	-1.732259
41	8	0	-4.826044	-2.132059	-0.021442
42	6	0	-5.843504	-1.905957	0.942678
43	1	0	-6.486527	-2.783311	0.914765
44	1	0	-5.420416	-1.799788	1.946132
45	1	0	-6.433117	-1.017629	0.697753