

Supporting Information:

A simple model for calculating atomic charges in molecules

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Dipole moments in D

Molecule	Exp.	Den.	Mul.	Low.	Hir.	I-H	CM5	ESP	NPA	AIM	ACP	
PMol001	fulvene	0.424	0.698	1.043	0.653	0.612	0.801	0.654	0.687	0.304	0.646	0.627
PMol002	propane	0.084	0.090	0.062	0.206	0.030	0.139	0.010	0.055	0.046	0.092	0.060
PMol003	isobutane	0.132	0.133	0.005	0.356	0.037	0.163	0.001	0.113	0.123	0.115	0.087
PMol004	cyclopropene	0.454	0.481	0.658	0.193	0.525	0.730	0.443	0.466	0.659	0.180	0.574
PMol005	propene	0.366	0.417	0.595	0.569	0.349	0.422	0.399	0.415	0.319	0.387	0.377
PMol006	propyne	0.784	0.825	0.215	1.121	0.813	0.825	0.909	0.813	0.464	0.836	0.836
PMol007	1,3-pentadiyne	1.207	1.344	0.291	1.666	1.353	1.285	1.450	1.327	0.987	1.443	1.367
PMol008	ammonia	1.472	1.740	1.231	0.734	0.516	1.796	1.544	1.797	1.944	1.898	1.295
PMol009	water	1.855	2.076	1.771	0.863	0.864	2.493	1.812	2.133	2.564	3.166	1.458
PMol010	Z-diimine	2.917	2.923	1.704	1.129	0.883	1.977	2.631	2.820	2.512	2.772	2.129
PMol011	hydroxylamine	0.590	0.591	0.883	0.234	0.521	0.739	0.641	0.592	1.176	1.729	0.434
PMol012	nitrogen_monoxide	0.159	0.120	0.310	0.555	0.169	0.322	0.145	0.095	1.018	2.289	0.304
PMol013	nitrogen_dioxide	0.316	0.328	0.793	0.218	0.475	1.136	0.248	0.535	1.080	1.607	0.576
PMol014	nitroxyl	1.620	1.675	1.581	0.600	0.891	1.388	1.574	1.613	2.036	3.116	1.433
PMol015	methylamine	1.310	1.370	0.983	0.684	0.352	1.313	1.245	1.339	1.586	1.835	1.157
PMol016	dimethylamine	1.010	0.960	0.649	0.458	0.217	0.789	1.023	0.939	1.286	1.697	0.958
PMol017	trimethylamine	0.612	0.499	0.393	0.224	0.060	0.204	0.910	0.545	1.136	1.595	0.807
PMol018	ethylamine	1.304	1.346	0.762	0.837	0.313	1.211	1.255	1.324	1.699	1.798	1.197
PMol019	propylamine	1.170	1.412	0.760	0.609	0.347	1.268	1.274	1.390	1.701	1.869	1.244
PMol020	cyclopropylamine	1.190	1.296	0.823	0.945	0.467	1.411	1.212	1.255	1.400	1.717	1.109
PMol021	isopropylamine	1.190	1.298	0.860	0.538	0.351	1.405	1.191	1.284	1.399	1.719	1.187
PMol022	aziridine	1.890	1.717	1.414	0.790	0.662	1.688	1.829	1.708	2.230	3.210	1.881
PMol023	piperidine_(NH_equatoria	0.820	0.828	0.689	0.557	0.195	0.877	0.985	0.872	1.170	1.591	0.955
PMol024	piperidine_(NH_axial)	1.190	1.190	0.942	0.510	0.245	0.778	1.106	1.135	1.473	1.846	1.165
PMol025	1,2,3,6-Tetrahydropyridi	0.990	0.982	0.814	1.034	0.350	0.969	1.093	1.012	1.271	1.631	0.961
PMol026	1,2,3,6-Tetrahydropyridi	1.007	0.989	0.460	0.814	0.184	0.738	0.926	0.930	1.515	1.538	1.059
PMol027	aniline	1.530	1.669	1.753	2.259	1.360	1.482	1.650	1.746	1.519	1.450	1.125
PMol028	pyrrole	1.767	1.914	1.500	2.527	1.555	2.021	1.524	1.897	1.720	1.057	1.102
PMol029	pyridine	2.215	2.236	1.644	0.426	1.102	1.702	2.050	2.233	2.383	4.199	2.177
PMol030	2-methylpyridine	1.850	1.855	1.110	0.735	0.824	1.510	1.680	1.841	1.992	3.684	1.856
PMol031	4-methylpyridine	2.700	2.749	2.253	1.397	1.617	1.970	2.648	2.735	2.841	4.794	2.661
PMol032	indole	2.100	2.188	2.014	2.614	1.887	2.124	1.838	2.155	1.815	1.197	1.473
PMol033	quinoline	2.290	2.066	1.289	0.482	1.015	1.668	1.921	2.059	2.231	3.868	2.051
PMol034	isoquinoline	2.730	2.590	1.601	0.853	1.494	2.054	2.428	2.574	2.735	4.670	2.543
PMol035	imidazole	3.800	3.764	2.627	2.525	2.356	3.335	3.315	3.760	3.732	3.519	3.037
PMol036	pyridazine	4.220	4.210	2.719	0.746	2.067	2.841	3.803	4.083	4.176	7.267	4.006
PMol037	pyrimidine	2.334	2.343	1.566	0.449	1.152	1.824	2.159	2.348	2.565	4.477	2.293
PMol038	2-methylpyrimidine	1.676	1.650	0.824	0.617	0.653	1.623	1.516	1.665	1.765	3.597	1.702

PMol039	hydrogen_cyanide	2.985	3.030	1.062	0.372	1.655	2.666	2.673	2.992	2.814	7.450	2.768
PMol040	acetonitrile	3.925	4.010	2.270	1.794	2.716	3.531	3.824	4.020	3.452	8.983	3.835
PMol041	malonic_dinitrile	3.730	3.834	2.212	1.341	2.458	3.389	3.649	3.860	3.275	8.937	3.693
PMol042	propionitrile	4.050	4.113	2.382	1.896	2.848	3.628	3.962	4.087	3.529	9.200	3.943
PMol043	butanenitrile(anti)	3.910	4.093	2.346	1.805	2.812	3.656	3.928	4.055	3.494	9.147	3.923
PMol044	butanenitrile(gauche)	3.730	4.246	2.450	2.158	3.037	3.759	4.158	4.251	3.675	9.386	4.099
PMol045	cyclopropane_carbonitril	4.131	4.384	2.744	2.114	3.144	3.886	4.211	4.371	3.807	9.454	4.212
PMol046	isobutyronitrile	4.290	4.136	2.397	2.056	2.900	3.579	4.039	4.127	3.604	9.283	3.970
PMol047	cyclobutane_carbonitrile	4.040	4.356	2.865	2.129	3.157	3.879	4.236	4.320	3.719	9.652	4.215
PMol048	t-butyl_cyanide	3.950	4.131	2.448	2.212	2.925	3.444	4.099	4.148	3.669	9.323	3.965
PMol049	pentanenitrile	4.120	4.363	2.558	2.178	3.144	3.911	4.255	4.367	3.719	9.521	4.212
PMol050	benzonitrile	4.180	4.711	2.413	2.285	3.513	4.327	4.564	4.712	4.170	9.955	4.583
PMol051	2-methylaziridine(cis)	1.770	1.812	1.398	1.130	0.814	1.727	2.016	1.809	2.436	3.393	2.041
PMol052	2-methylaziridine(trans)	1.570	1.647	1.433	0.500	0.615	1.720	1.725	1.569	2.123	3.159	1.863
PMol053	E-ethanimine	2.058	2.054	1.137	0.239	1.015	2.029	1.951	2.038	2.422	4.654	2.074
PMol054	Z-ethanimine	2.560	2.566	1.734	1.128	1.336	2.222	2.431	2.536	2.745	5.037	2.444
PMol055	Z-N-ethylidene_methanami	1.498	1.464	0.414	0.350	0.687	1.224	1.567	1.470	1.826	4.025	1.586
PMol056	N-methylformaldimine	1.530	1.484	0.900	0.433	0.540	1.032	1.557	1.483	1.764	3.965	1.529
PMol057	diazomethane	1.500	1.668	1.709	0.169	0.728	0.968	1.837	1.680	1.116	3.574	1.809
PMol058	methyl_azide	2.170	2.366	2.199	0.779	1.251	1.881	2.381	2.411	2.197	3.276	2.405
PMol059	E-2-butenenitrile	4.750	4.822	3.188	2.810	3.618	4.305	4.711	4.836	4.273	9.986	4.663
PMol060	Z-2-butenenitrile	4.080	4.310	2.645	2.290	3.108	4.014	4.148	4.310	4.034	9.240	4.182
PMol061	cianoacetylene	3.732	3.880	2.787	1.387	2.603	3.512	3.597	3.890	3.682	8.537	3.683
PMol062	acrylonitrile	3.920	4.010	2.219	1.753	2.808	3.614	3.855	4.020	3.605	9.070	3.882
PMol063	methacrylonitrile	3.690	4.043	2.140	1.895	2.845	3.431	3.926	4.049	3.509	9.231	3.879
PMol064	2-cyanopyridine	5.780	5.842	3.627	2.220	3.935	5.151	5.656	5.835	5.510	12.367	5.708
PMol065	3-cyanopyridine	3.660	4.012	2.211	1.965	2.988	3.640	3.877	3.994	3.574	8.517	3.906
PMol066	4-cyanopyridine	1.960	2.090	0.610	1.445	2.012	2.226	2.115	2.081	1.396	5.336	2.012
PMol067	cyanimide	4.280	4.659	2.219	2.932	3.171	4.270	4.351	4.679	3.888	6.836	3.953
PMol068	cyanoallene	4.280	4.463	2.787	2.311	3.303	4.049	4.325	4.501	4.087	9.535	4.362
PMol069	cyclopentadiene-1-carbon	4.250	4.698	2.648	2.390	3.553	4.342	4.566	4.692	4.223	9.846	4.612
PMol070	methylaminonitrile	2.640	2.661	1.613	1.796	2.419	2.220	2.651	2.669	1.860	7.241	2.650
PMol071	methanol	1.700	1.684	1.711	0.687	0.776	1.940	1.597	1.680	2.567	3.593	1.460
PMol072	ethanol	1.440	1.586	1.488	0.439	0.712	2.000	1.496	1.551	2.474	3.435	1.466
PMol073	ethylene_glycol	2.404	2.371	2.280	1.266	1.298	2.818	2.381	2.358	3.689	5.261	2.419
PMol074	propargyl_alcohol	1.130	1.393	1.843	0.879	0.567	1.677	1.276	1.410	2.560	3.229	1.245
PMol075	2-propanol	1.580	1.639	1.496	0.957	0.815	1.723	1.637	1.649	2.815	3.579	1.467
PMol076	1-propanol(trans)	1.550	1.477	1.369	0.477	0.691	1.859	1.485	1.491	2.514	3.370	1.413
PMol077	1-propanol(gauche)	1.580	1.512	1.405	0.651	0.727	1.974	1.506	1.496	2.414	3.277	1.553
PMol078	1,2-propanediol(CH3-gauc	2.320	2.213	2.013	1.119	1.211	2.797	2.244	2.189	3.514	4.980	2.412
PMol079	1,2-propanediol(CH3-anti	2.568	2.535	2.404	1.293	1.526	2.706	2.641	2.555	4.087	5.601	2.630

PMol080	1-butanol	1.660	1.543	1.409	0.390	0.705	1.971	1.477	1.514	2.464	3.435	1.457
PMol081	cyclopropanol(gauche)	1.460	1.520	1.390	0.867	0.683	1.875	1.458	1.489	2.433	3.608	1.398
PMol082	cyclobutanol	1.620	1.510	1.398	0.639	0.665	1.823	1.419	1.479	2.364	3.478	1.389
PMol083	phenol	1.224	1.319	0.972	1.541	0.625	1.531	1.304	1.309	1.954	3.640	1.122
PMol084	methyl_propyl_ether	1.107	1.052	1.230	0.282	0.601	1.163	1.336	1.089	2.414	3.498	1.354
PMol085	dimethyl_ether	1.300	1.240	1.561	0.042	0.688	1.208	1.445	1.290	2.508	3.796	1.400
PMol086	diethylether	1.150	1.299	1.382	0.155	0.717	1.109	1.434	1.343	2.574	3.655	1.410
PMol087	vinyl_methyl_ether	0.965	0.925	1.002	1.187	0.641	0.747	1.005	0.961	1.674	3.737	0.828
PMol088	tetrahydrofuran	1.750	1.595	1.732	0.135	0.923	1.317	1.637	1.577	2.827	4.311	1.668
PMol089	anisole	1.380	1.280	1.404	1.312	0.972	1.190	1.388	1.305	2.037	3.592	1.312
PMol090	tetrahydropyran	1.580	1.461	1.855	0.113	0.820	1.206	1.515	1.452	2.654	3.964	1.517
PMol091	1,3-dioxane	2.060	2.042	2.454	0.333	1.195	2.017	2.241	2.039	3.851	5.617	2.218
PMol092	3,4-dihydro-2,4-pyran	1.400	1.343	1.629	1.193	0.778	0.944	1.300	1.310	1.978	4.282	1.226
PMol093	oxetane	1.940	1.944	1.908	0.064	1.200	1.739	1.913	1.968	3.178	4.927	1.985
PMol094	3-methyleneoxetane	1.630	1.556	1.459	0.450	0.894	1.351	1.529	1.548	3.121	4.784	1.631
PMol095	formaldehyde	2.332	2.308	1.793	0.137	1.474	2.366	2.160	2.309	3.298	6.510	2.349
PMol096	acetaldehyde	2.750	2.820	2.524	0.850	1.957	2.714	2.672	2.827	3.879	6.994	2.806
PMol097	propanal	2.520	2.726	2.576	0.843	1.857	2.638	2.564	2.708	3.797	6.856	2.774
PMol098	butanal	2.720	3.020	2.641	1.032	2.183	2.909	2.899	3.030	4.004	7.281	2.989
PMol099	E-2-butenal	3.670	4.194	3.910	2.168	3.293	4.085	3.992	4.199	5.235	8.141	4.104
PMol100	acetone	2.880	3.026	2.618	1.105	2.116	2.861	2.862	3.044	4.191	7.146	2.969
PMol101	2-butanone	2.779	2.892	2.573	0.792	1.999	2.746	2.731	2.894	4.093	6.960	2.955
PMol102	cyclopentanone	3.300	3.175	2.772	0.871	2.271	3.100	2.952	3.201	3.807	7.468	3.056
PMol103	acetophenone	3.020	3.154	2.346	0.979	2.252	3.235	2.896	3.175	4.229	7.013	3.107
PMol104	cyclobutane-1,2-dione	3.831	3.969	3.749	1.003	2.794	3.291	3.768	4.029	4.856	10.133	3.949
PMol105	cyclobutanone	2.890	3.018	2.635	0.906	2.177	2.787	2.857	3.083	3.549	7.318	2.992
PMol106	cyclopropanone	2.670	2.968	2.395	0.897	2.106	2.453	2.783	3.001	3.339	7.196	2.926
PMol107	cyclopentadienone	3.132	3.279	2.808	0.695	2.369	3.304	2.970	3.307	4.127	7.132	3.212
PMol108	4-cyclopentene-1,3-dione	1.680	1.755	0.953	0.098	1.327	2.055	1.547	1.759	2.252	3.639	1.756
PMol109	3-cyclopentenone	2.790	2.813	2.117	0.085	2.013	2.911	2.577	2.862	3.672	7.098	2.807
PMol110	cyclohexanone	2.870	3.334	2.856	1.096	2.399	3.339	3.125	3.346	4.232	7.558	3.217
PMol111	formic_acid(s-cis)	1.425	1.530	1.085	1.695	1.353	1.310	1.387	1.525	1.618	3.515	1.466
PMol112	formic_acid(s-trans)	3.787	3.958	3.102	1.612	2.469	4.404	3.753	3.928	5.102	8.407	3.586
PMol113	acetic_acid	1.700	1.734	1.332	1.215	1.588	1.377	1.562	1.760	1.990	4.420	1.726
PMol114	glyoxylic_acid(trans)	1.860	1.953	1.436	1.987	1.253	2.511	1.975	1.967	2.500	4.141	1.853
PMol115	propionic_acid(cis)	1.460	1.611	1.258	0.865	1.455	1.254	1.420	1.600	1.909	4.377	1.661
PMol116	acrylic_acid(s-cis)	1.460	1.560	1.050	0.500	1.454	1.269	1.318	1.567	1.952	4.349	1.656
PMol117	acrylic_acid(s-trans)	2.020	2.172	1.682	1.639	1.940	1.964	1.881	2.215	2.552	4.825	1.938
PMol118	2-methoxyethanoic_acid(g	4.720	5.111	4.304	2.235	3.554	5.529	5.050	5.161	6.482	10.448	4.947
PMol119	acetoacetic_acid	2.300	2.381	2.011	1.019	1.623	2.510	2.415	2.394	3.055	5.629	2.311
PMol120	methyl_acetate	1.720	1.877	1.369	1.151	1.515	1.969	1.642	1.866	2.008	3.552	1.658

PMol121	methyl_formate	1.770	1.903	1.664	1.573	1.509	1.960	1.668	1.914	2.015	3.106	1.581
PMol122	ethyl_formate(cis)	1.810	1.963	1.745	1.771	1.545	1.980	1.728	1.928	2.123	3.063	1.605
PMol123	ethyl_formate(trans)	1.980	2.168	2.065	2.011	1.768	2.004	1.953	2.195	2.343	3.509	1.700
PMol124	ethyl_acetate	1.780	2.038	1.705	1.571	1.670	1.966	1.833	2.067	2.258	3.795	1.692
PMol125	pentyl_formate	1.900	2.370	2.328	2.198	1.961	2.224	2.146	2.370	2.462	3.701	1.867
PMol126	diethyl_carbonate	1.100	0.495	0.247	1.189	0.781	0.562	0.299	0.530	0.503	0.846	0.270
PMol127	maleic_anhydride	3.940	4.209	3.245	0.278	2.955	4.182	3.926	4.210	5.714	10.878	4.251
PMol128	\beta-propiolactone	4.180	4.269	3.666	1.367	3.061	4.102	4.077	4.311	5.487	9.824	4.188
PMol129	\gamma-butyrolactone	4.270	4.682	4.107	1.521	3.343	4.562	4.456	4.724	6.049	10.517	4.518
PMol130	2-methoxyethanol_(gauche)	2.360	1.997	1.749	0.692	0.966	2.216	2.079	2.036	3.269	4.498	1.901
PMol131	benzyl_alcohol	1.710	1.760	1.598	1.359	1.033	2.022	1.839	1.736	2.475	3.167	1.792
PMol132	diketene	3.530	3.567	3.229	0.438	2.473	3.221	3.415	3.599	5.058	10.352	3.649
PMol133	3-oxetanone	0.887	1.011	0.475	0.729	0.880	0.865	0.875	1.059	0.288	2.279	0.951
PMol134	2-furanone	4.905	5.044	4.376	1.941	3.718	5.135	4.742	5.064	6.678	10.776	4.952
PMol135	ketene	1.422	1.480	0.916	0.574	0.914	1.133	1.514	1.520	2.127	8.631	1.752
PMol136	methylketene	1.790	1.879	1.445	0.438	1.234	1.628	1.868	1.867	2.385	8.972	2.073
PMol137	formamide	3.965	3.959	3.264	2.415	2.890	3.739	3.596	3.930	4.738	6.733	3.409
PMol138	acetamide	3.902	3.885	2.966	2.138	2.827	3.626	3.546	3.894	4.685	6.951	3.387
PMol139	N-methylformamide	4.260	4.187	4.048	2.335	3.219	4.165	3.924	4.189	5.214	7.969	4.105
PMol140	N,N-dimethylformamide	4.085	4.004	3.882	2.410	3.077	3.932	3.825	4.005	5.064	7.299	3.921
PMol141	E-N-methylacetamide	4.171	4.095	3.894	2.187	3.132	4.208	3.854	4.168	5.270	8.083	4.037
PMol142	Z-N-methylacetamide	3.887	3.886	2.884	2.075	2.795	3.798	3.513	3.844	4.701	6.357	3.310
PMol143	N,N-dimethylacetamide	3.898	3.837	3.592	2.198	2.902	3.927	3.674	3.866	5.032	7.286	3.768
PMol144	benzamide	3.642	3.642	2.551	1.787	2.657	3.668	3.352	3.657	4.550	6.798	3.346
PMol145	phenylurea	3.857	3.923	2.676	2.805	2.997	3.771	3.851	3.925	4.584	5.344	3.473
PMol146	nitromethane	3.460	3.572	3.786	1.725	2.581	3.251	3.452	3.571	4.449	6.266	3.421
PMol147	nitroethane	3.230	3.724	3.933	1.868	2.642	3.400	3.530	3.741	4.642	6.495	3.450
PMol148	1-nitropropane	3.660	3.851	4.081	2.115	2.818	3.589	3.719	3.895	4.770	6.697	3.590
PMol149	2-nitropropane	3.730	3.824	3.775	2.109	2.723	3.433	3.630	3.859	4.865	6.607	3.529
PMol150	nitrobenzene	4.220	4.636	4.709	2.618	3.512	4.601	4.274	4.678	5.750	8.008	4.340
PMol151	methyl_nitrate	3.100	3.008	3.265	1.198	1.980	2.800	2.795	3.071	3.807	5.284	2.618
PMol152	acetyl_cyanide	3.450	3.524	2.700	1.483	2.485	2.850	3.442	3.530	3.902	8.555	3.349
PMol153	dimethylnitrosamine	4.010	4.220	4.646	2.325	3.037	3.547	4.002	4.146	5.081	6.494	3.992
PMol154	formaldoxime	0.303	0.246	0.529	0.947	0.223	0.940	0.242	0.236	1.006	3.118	0.525
PMol155	fulminic_acid	3.099	3.148	2.829	0.696	2.336	3.099	3.090	3.165	4.287	9.271	3.444
PMol156	1,4-dihydrooxazole	1.770	1.760	1.482	1.318	0.862	1.484	1.719	1.806	1.709	1.428	1.605
PMol157	oxazole	1.503	1.554	0.876	1.415	0.810	1.473	1.488	1.579	1.438	1.983	1.472
PMol158	isoxazole	2.950	3.003	2.216	1.306	1.395	1.887	2.816	2.907	3.424	8.310	3.015
PMol159	morpholine	1.550	1.554	1.384	0.662	0.880	1.186	1.447	1.559	2.098	2.758	1.020
PMol160	uracil	4.440	4.455	3.946	2.161	3.468	4.660	4.048	4.488	5.636	9.196	4.443
PMol205	difluoroborane	0.971	0.873	1.326	2.048	0.663	1.045	0.947	0.909	2.175	1.895	1.215

PMol206	chloroborane	0.750	0.499	1.040	4.668	0.194	0.318	0.170	0.580	0.749	2.414	0.754
PMol207	hydroxyborane	1.506	1.612	1.391	2.883	0.866	1.869	1.529	1.575	2.132	2.540	1.352
PMol208	difluorohydroxyborane	1.860	1.998	2.280	1.245	1.269	2.164	2.004	1.951	2.568	3.026	1.783
PMol209	dihydroxyborane	1.470	1.571	1.448	2.781	0.766	1.906	1.483	1.525	2.252	2.646	1.418
PMol210	dihydroxyfluoroborane	1.818	1.401	0.533	0.296	0.261	2.535	1.292	1.322	2.047	2.893	1.279
PMol211	boranamine	1.844	1.973	1.669	3.313	1.402	1.435	1.810	1.928	1.016	0.921	0.324
PMol212	difluoroboranamine	2.595	2.698	3.050	1.647	1.971	2.146	2.712	2.713	3.201	2.864	1.557
PMol213	difluoro(methyl)borane	1.668	1.664	2.378	0.191	1.157	1.086	1.844	1.698	2.311	1.239	1.621
PMol214	ethynyl difluoroborane	1.876	1.954	2.426	0.140	1.354	1.949	1.873	1.990	2.631	0.882	2.155
PMol215	difluoro(vinyl)borane	1.740	2.044	2.378	0.697	1.496	1.789	2.127	2.100	2.670	1.288	2.223
PMol216	difluoro(ethyl)borane	1.690	1.666	2.329	0.172	1.123	1.175	1.854	1.709	2.204	1.259	1.778
PMol217	diaminoborane	1.250	1.360	0.690	2.705	0.858	0.812	1.190	1.397	0.500	0.590	0.047
PMol218	BH3B ₁ CO_adduct	1.698	1.313	2.095	4.002	1.424	1.619	1.165	1.311	0.486	5.672	0.078
PMol219	BH3 ₁ NH3_adduct	5.216	5.408	4.718	6.071	4.678	5.250	5.192	5.360	5.397	5.691	4.510
PMol220	BF3 ₁ NH3_adduct	5.903	6.009	5.823	5.445	5.239	5.531	6.128	6.029	7.158	7.048	5.445
PMol221	hydrogen_fluoride	1.826	1.921	1.762	0.794	0.974	2.290	1.278	1.945	2.405	3.125	1.369
PMol222	fluorocyclohexane(axial)	1.810	1.784	2.069	0.600	1.257	1.544	1.763	1.783	3.344	4.426	1.870
PMol223	fluorocyclohexane(equato)	2.110	2.134	2.365	0.686	1.563	1.988	2.061	2.160	3.594	4.961	2.119
PMol224	1,2-difluoroethane(gauch)	2.670	2.675	3.185	0.131	1.837	2.643	2.584	2.686	4.855	6.879	2.781
PMol225	1-fluoropropane(gauche)	1.900	1.834	2.145	0.443	1.270	1.685	1.755	1.816	3.236	4.511	1.883
PMol226	1-fluoropropane(trans)	2.050	1.933	2.200	0.572	1.417	1.689	1.915	1.964	3.397	4.696	1.958
PMol227	fluoromethane	1.858	1.811	2.265	0.150	1.220	1.707	1.696	1.809	3.125	4.494	1.801
PMol228	1,1-difluoroethane	2.270	2.226	2.516	0.681	1.531	1.883	2.123	2.245	3.711	5.846	2.168
PMol229	fluoroethane	1.937	1.900	2.242	0.514	1.327	1.710	1.815	1.897	3.314	4.607	1.894
PMol230	2-fluoropropane	1.958	1.930	2.204	0.729	1.353	1.645	1.858	1.955	3.464	4.639	1.909
PMol231	difluoromethane	1.978	1.881	2.177	0.341	1.257	1.944	1.801	1.926	3.243	5.305	1.957
PMol232	trifluoromethane	1.651	1.580	1.578	0.650	1.050	1.815	1.534	1.643	2.668	4.896	1.705
PMol233	1,1,1-trifluoroethane	2.347	2.318	2.357	0.501	1.602	1.603	2.209	2.353	3.613	6.283	2.112
PMol234	pentafluoroethane	1.540	1.517	1.599	0.543	0.996	1.589	1.494	1.530	2.724	4.843	1.633
PMol235	1,1,1,2,2,3,3-heptafluor	1.620	1.476	1.535	0.460	0.978	1.581	1.470	1.498	2.490	4.688	1.579
PMol236	2-fluoro-2-methylpropane	1.960	1.936	2.175	0.743	1.348	1.545	1.869	1.972	3.603	4.640	1.890
PMol237	1,2-difluoroethene	2.420	2.279	3.051	0.807	1.577	2.348	2.353	2.224	4.757	7.790	2.639
PMol238	3-fluoropropene(eclipsed)	1.765	1.724	2.082	0.074	1.179	1.721	1.659	1.714	3.194	4.328	1.879
PMol239	3-fluoropropene(gauche)	1.939	1.860	2.116	0.358	1.351	1.733	1.816	1.915	3.386	4.624	1.898
PMol240	1,1-difluoro-1-propene	0.889	1.606	1.992	0.530	1.040	1.106	1.629	1.623	2.739	6.858	1.585
PMol241	fluoroethene	1.468	1.357	1.761	0.343	0.921	1.241	1.380	1.330	2.757	4.870	1.499
PMol242	2-fluoropropene	1.610	1.575	1.869	0.792	1.129	1.245	1.592	1.588	2.936	4.972	1.630
PMol243	cis-1-fluoro-1-propene	1.460	1.413	1.877	0.832	0.979	1.312	1.435	1.351	2.851	4.799	1.595
PMol244	1,1-difluoroethene	1.389	1.190	1.498	0.699	0.730	0.580	1.267	1.221	2.393	6.493	1.306
PMol245	1,1-difluoroallene	2.070	1.941	2.343	0.012	1.459	1.768	1.986	1.978	3.139	6.929	2.089
PMol246	trifluoroethene	1.320	1.242	1.623	0.806	0.834	1.173	1.296	1.221	2.592	5.198	1.446

PMol247	3,3,3-trifluoropropene	2.450	2.431	2.181	0.618	1.730	2.094	2.280	2.486	3.834	6.522	2.221
PMol248	fluoroallene	1.970	1.746	2.304	0.491	1.303	1.640	1.757	1.801	3.118	5.167	1.847
PMol249	fluorobenzene	1.600	1.480	1.781	0.156	1.055	1.444	1.532	1.523	2.945	5.229	1.637
PMol250	(trifluoromethyl)benzene	2.860	2.850	2.395	0.702	2.100	2.707	2.666	2.905	4.206	7.157	2.602
PMol251	ortho-fluorotoluene	1.370	1.198	1.387	1.035	0.811	1.121	1.249	1.234	2.705	4.837	1.405
PMol252	meta-fluorotoluene	1.860	1.715	2.092	0.849	1.311	1.529	1.823	1.759	3.139	5.455	1.852
PMol253	para-fluorotoluene	2.000	1.880	2.431	0.698	1.451	1.600	2.005	1.917	3.300	5.654	2.001
PMol254	1,3-difluorobenzene	1.510	1.461	1.745	0.218	1.028	1.444	1.508	1.500	2.941	5.260	1.621
PMol255	1,2,3,4-tetrafluorobenze	2.420	2.348	2.582	0.738	1.625	1.860	2.474	2.360	4.876	9.228	2.686
PMol256	1,2-difluorobenzene	2.460	2.452	2.870	0.469	1.735	2.165	2.570	2.498	4.980	9.125	2.762
PMol257	fluoroacetylene	0.721	0.542	1.239	1.353	0.300	0.248	0.743	0.578	1.740	7.228	0.894
PMol258	acetyl_fluoride	2.960	2.990	2.609	1.002	2.157	2.686	2.824	3.004	3.875	7.405	2.847
PMol259	3,3,3-trifluoropropyne	2.317	2.370	3.367	0.200	1.701	2.353	2.179	2.411	3.809	5.996	2.331
PMol260	tetrafluoropropyne	1.710	1.968	2.350	1.778	1.579	1.945	1.612	1.996	2.176	1.113	1.573
PMol261	carbonyl_fluoride	0.950	1.095	0.109	0.756	0.756	1.388	0.861	1.064	0.764	1.773	0.971
PMol262	bis(trifluoromethyl)ethe	0.540	0.039	0.184	0.256	0.143	0.444	0.063	0.037	0.188	0.358	0.155
PMol263	cyanic_fluoride	2.120	2.321	0.157	1.862	1.321	2.253	1.871	2.311	0.918	2.084	1.761
PMol264	trifluoroacetonitrile	1.262	1.348	0.235	0.956	0.758	0.742	1.294	1.289	0.177	2.470	1.201
PMol265	1-fluoro-4-nitrobenzene	2.870	3.302	3.108	2.981	2.608	3.300	2.897	3.295	2.945	2.875	2.840
PMol322	SiH	0.119	0.086	0.350	0.633	0.893	1.917	0.359	0.917	2.546	5.190	0.381
PMol323	SiS	1.730	1.769	2.153	1.129	2.061	3.686	1.675	2.903	6.087	10.908	1.888
PMol324	silyl_radical	0.051	0.093	0.200	0.347	0.478	1.451	0.061	0.745	1.210	4.418	0.070
PMol325	silylmethyl_radical	0.618	0.677	0.163	0.101	0.306	0.173	0.417	0.658	0.566	1.078	0.604
PMol326	methylsilane	0.735	0.801	0.421	0.143	0.316	0.027	0.506	0.768	0.634	0.853	0.642
PMol327	dimethylsilane	0.713	0.772	0.356	0.284	0.250	0.062	0.484	0.766	0.785	1.170	0.609
PMol328	ethylsilane	0.810	0.870	0.457	0.091	0.355	0.262	0.574	0.837	0.722	0.904	0.708
PMol329	trimethylsilane	0.525	0.560	0.216	0.360	0.137	0.120	0.353	0.591	0.714	1.151	0.433
PMol330	vinylsilane	0.657	0.729	0.142	0.344	0.298	0.433	0.439	0.695	0.743	1.176	0.630
PMol331	phenylsilane	0.845	0.959	0.237	0.466	0.477	0.866	0.618	0.908	0.758	0.999	0.852
PMol332	SiO	3.098	3.104	2.885	1.589	2.854	5.314	2.871	3.834	8.529	10.368	2.704
PMol333	disiloxane	0.240	0.215	0.338	0.201	0.234	0.838	0.521	0.199	1.425	0.809	0.438
PMol334	methyl_silyl_ether	1.150	1.109	1.366	0.545	0.714	1.424	1.317	1.111	2.563	3.190	1.301
PMol335	hexamethyldisiloxane	0.780	0.467	0.713	0.140	0.277	1.015	0.826	0.478	1.299	0.141	0.748
PMol336	methoxytrimethylsilane	1.180	1.005	1.136	0.039	0.542	1.461	1.235	1.040	2.114	3.285	1.203
PMol337	methylsilanol	1.650	1.709	1.468	1.224	0.753	1.842	1.575	1.659	2.383	2.276	1.420
PMol338	silanediol	0.965	1.121	0.581	1.819	0.430	0.554	0.705	1.013	0.471	1.364	0.546
PMol339	silanone	3.816	3.670	3.297	1.110	2.638	4.239	3.360	3.725	6.111	5.398	3.106
PMol340	silanole	1.321	1.369	1.259	1.241	0.629	1.901	1.331	1.321	2.670	2.530	1.093
PMol341	fluorosilane	1.268	1.279	2.068	0.295	1.107	1.489	1.519	1.306	3.437	2.136	1.460
PMol342	difluorosilane	1.540	1.473	2.216	0.667	1.241	1.811	1.715	1.531	3.754	2.544	1.665
PMol343	trifluorosilane	1.260	1.318	1.898	0.837	1.119	1.668	1.570	1.375	3.125	2.191	1.537

PMol344	fluoromethylsilane	1.710	1.729	2.290	0.492	1.314	1.437	1.840	1.725	3.242	2.000	1.831
PMol345	difluoromethylsilane	2.110	2.122	2.698	0.733	1.631	1.691	2.275	2.145	3.462	2.190	2.243
PMol346	trifluoromethylsilane	2.339	2.360	2.765	0.327	1.838	1.572	2.549	2.397	2.798	1.638	2.508
PMol347	fluorodisilane	1.230	1.271	2.037	0.387	1.203	1.406	1.612	1.271	3.510	2.751	1.532
PMol348	1,1,1-trifluorodisilane	2.030	2.120	2.164	0.285	2.051	2.134	2.450	2.187	3.611	8.513	2.318
PMol349	chlorosilane	1.310	1.229	2.207	2.330	0.865	1.345	1.031	1.386	2.455	3.059	1.133
PMol350	dichlorosilane	1.170	1.121	2.210	3.090	0.810	1.403	1.003	1.291	2.569	3.333	1.151
PMol351	trichlorosilane	0.860	0.758	1.694	2.983	0.593	1.115	0.777	0.911	2.112	2.709	0.930
PMol352	chloro(methyl)silane	1.940	1.824	2.563	2.185	1.166	1.354	1.459	1.921	2.379	2.940	1.619
PMol353	trichloro(methyl)silane	1.910	1.907	2.769	2.363	1.242	0.919	1.658	1.974	1.644	2.359	1.820
PMol354	(chloromethyl)silane	1.626	1.671	1.898	1.588	0.962	0.837	1.231	1.767	2.246	3.371	1.525
PMol355	dichloro(ethyl)silane	2.040	2.065	2.850	2.865	1.295	1.548	1.699	2.150	2.294	3.082	1.807
PMol356	chlorotrimethylsilane	2.080	2.140	2.806	1.727	1.321	1.162	1.694	2.280	1.921	2.253	1.888
PMol357	dichloromethylsilane	1.995	1.956	2.878	2.798	1.266	1.335	1.630	2.067	2.351	3.078	1.810
PMol358	trichlorofluorosilane	0.490	0.575	0.446	2.423	0.638	0.370	0.908	0.532	1.558	0.240	0.654
PMol359	iodomethylsilane	1.862	1.956	2.195	0.419	1.285	1.336	1.244	2.146	1.540	2.258	1.264
PMol360	phosphine	0.574	0.617	0.616	0.057	0.149	0.396	0.752	0.628	0.092	5.671	0.860
PMol361	methylphosphine	1.100	1.169	0.587	1.098	0.281	0.673	0.880	1.125	0.806	5.727	1.157
PMol362	dimethyl_methylphosphona	2.288	2.248	1.769	1.868	1.992	2.246	2.063	2.228	2.194	3.232	2.061
PMol363	hypophosphorous_acid	2.650	2.685	2.537	1.885	2.315	2.788	2.696	2.709	4.149	3.529	2.697
PMol364	trimethylphosphine	1.218	1.189	0.083	1.210	0.223	1.358	0.823	1.139	1.872	6.534	0.976
PMol365	dimethylphosphine	1.230	1.263	0.323	1.252	0.233	0.996	0.872	1.266	1.381	6.056	1.134
PMol366	PH	0.429	0.454	0.347	0.260	0.192	0.432	0.346	0.437	0.792	3.558	0.366
PMol367	CH2PH2	0.503	0.429	0.244	1.749	0.337	1.068	0.512	0.457	1.634	6.170	0.674
PMol368	CH3CH(PH2)CH3	1.249	1.248	0.575	1.449	0.309	0.666	0.936	1.226	0.807	5.626	1.276
PMol369	CH3PH	1.297	1.315	0.706	1.244	0.237	0.597	0.887	1.280	1.131	5.125	1.157
PMol370	(CH3)3PH2	1.226	1.221	0.536	1.445	0.314	0.635	0.941	1.207	0.839	5.556	1.292
PMol371	CH3CH(PH)CH3	1.414	1.409	0.766	1.620	0.223	0.662	0.940	1.378	1.199	4.943	1.256
PMol372	phosphorus_mononitride	2.747	2.879	1.808	2.669	1.816	3.664	2.305	2.893	5.992	9.975	2.465
PMol373	phosphorus_oxychloride	2.540	2.497	1.730	4.054	2.193	2.827	2.782	2.501	4.262	3.081	2.550
PMol374	thiophosphoryl_fluorid	0.640	0.554	0.045	0.121	0.407	1.297	0.257	0.645	1.179	0.301	0.345
PMol375	hypophosphorous_acid(=Mo	2.650	2.685	2.537	1.885	2.315	2.788	2.696	2.709	4.149	3.529	2.697
PMol376	methylphosphonic_acid	1.526	1.459	1.340	1.670	1.849	0.919	1.324	1.535	1.016	1.558	1.591
PMol377	phosphine_oxide	3.666	3.599	3.888	2.130	2.801	4.227	3.739	3.637	6.417	5.310	3.688
PMol378	OPH	2.374	2.368	2.694	1.763	2.051	3.910	2.277	2.429	6.270	9.151	2.223
PMol379	hydroxyphosphane	0.768	0.839	1.440	0.949	1.018	3.034	0.979	0.812	3.955	8.481	0.709
PMol380	trimethylphosphine_oxide	4.407	4.289	4.321	2.147	3.375	4.129	4.435	4.346	5.769	4.822	4.462
PMol381	PO	2.072	2.107	2.337	1.746	1.923	3.559	1.983	2.137	6.421	9.075	1.985
PMol382	phosphorus_trichloride	0.560	0.565	2.142	1.267	1.090	2.573	0.619	0.625	3.457	7.123	0.832
PMol383	phosphorus_trifluoride	1.030	1.089	2.711	0.547	1.613	3.921	1.421	1.098	6.370	9.128	1.517
PMol384	phosphoryl_fluoride	1.869	1.854	0.860	1.839	1.440	2.209	1.717	1.860	1.755	2.037	1.657

PMol1385	FCP	0.279	0.062	0.471	0.740	0.150	0.196	0.205	0.012	4.165	11.718	0.210
PMol1386	CH3P(O)(OCH3)(SCH3)	1.622	1.582	1.342	3.363	2.009	2.468	2.011	1.557	3.564	4.553	1.739
PMol1387	CH3P(O)(SCH3)2	1.590	1.578	1.743	4.579	2.182	2.766	2.232	1.534	4.964	5.105	1.915
PMol1388	OP(OCH3)(SCH3)2	2.851	2.885	2.944	4.629	2.976	4.211	3.615	2.823	7.143	8.860	3.235
PMol1389	trimethylphosphine_sulfi	4.796	4.691	5.075	1.254	3.653	4.181	4.343	4.896	4.003	3.772	4.694
PMol1390	PS	0.626	0.664	1.232	0.450	0.754	1.320	0.443	0.692	2.491	7.285	0.525
PMol1391	SP(CH3)(OCH3)2	2.521	2.481	2.270	0.799	1.968	2.692	1.728	2.555	2.217	4.760	1.974
PMol1392	SH	0.779	0.864	0.963	0.038	0.312	0.617	0.732	0.960	0.571	0.047	0.775
PMol1393	CH2SH	0.858	0.879	0.811	2.673	0.467	0.931	0.777	0.913	1.215	0.935	0.917
PMol1394	ethenethiol	0.759	0.753	0.364	2.607	0.194	0.330	0.572	0.807	0.605	0.429	0.846
PMol1395	methanethiol	1.520	1.549	1.428	1.432	0.547	0.625	1.125	1.617	0.672	0.517	1.501
PMol1396	ethanethiol_(gauche)	1.610	1.633	1.486	1.598	0.573	0.664	1.166	1.683	0.735	0.692	1.589
PMol1397	ethanethiol_(trans)	1.580	1.635	1.403	1.529	0.586	0.821	1.142	1.657	0.731	0.871	1.591
PMol1398	1-propane_thiol	1.600	1.695	1.518	1.465	0.645	0.742	1.239	1.741	0.753	0.735	1.646
PMol1399	2-methyl-2-propane_thiol	1.660	1.657	1.543	1.601	0.528	0.507	1.148	1.752	0.801	0.950	1.641
PMol1400	HSSH	1.122	1.218	1.284	0.125	0.416	0.841	1.019	1.285	1.029	0.147	1.106
PMol1401	CH3SSH	1.720	1.747	1.659	1.548	0.579	0.603	1.234	1.759	0.812	0.576	1.595
PMol1402	2-propanethiol	1.682	1.647	1.578	1.692	0.545	0.484	1.172	1.729	0.799	0.757	1.611
PMol1403	thioacetone	2.899	2.852	3.074	0.706	1.864	2.059	2.512	2.949	1.268	1.128	2.778
PMol1404	CH3S_radical	1.699	1.708	1.595	1.532	0.668	0.457	1.189	1.746	0.355	0.450	1.506
PMol1405	1,3-dithiane	2.162	2.124	1.838	2.472	0.699	0.585	1.567	2.182	0.385	0.586	2.166
PMol1406	(CH3)3CS_radical	1.897	1.851	1.767	1.740	0.620	0.220	1.206	1.904	0.439	0.881	1.617
PMol1407	ethyl_methyl_sulfide	1.593	1.585	1.220	1.793	0.436	0.259	1.077	1.608	0.119	0.228	1.478
PMol1408	ethyl_methyl_sulfide	1.560	1.557	1.099	1.857	0.417	0.270	1.047	1.550	0.123	0.334	1.480
PMol1409	dimethyl_sulfide	1.554	1.538	1.179	1.731	0.431	0.108	1.069	1.559	0.056	0.062	1.452
PMol1410	diethyl_sulfide	1.540	1.569	1.037	1.975	0.394	0.424	1.023	1.494	0.121	0.085	1.503
PMol1411	hydrogen_sulfide	0.978	1.111	1.318	0.223	0.456	1.051	1.044	1.265	1.215	0.177	1.171
PMol1412	thietane	1.850	1.941	1.492	2.206	0.750	0.682	1.424	1.999	0.283	0.675	1.980
PMol1413	thiacyclohexane	1.781	1.782	1.584	2.060	0.565	0.458	1.230	1.746	0.203	0.564	1.728
PMol1414	dimethyl_disulfide	2.011	2.007	1.710	2.181	0.594	0.086	1.331	2.047	0.309	0.293	1.827
PMol1415	thiophene	0.550	0.452	0.076	4.067	0.392	0.795	0.194	0.446	1.830	0.801	0.668
PMol1416	2-methylthiophene	0.674	0.632	0.700	4.211	0.634	0.896	0.522	0.645	1.829	1.093	0.763
PMol1417	2,5-dihydrothiophene	1.750	1.755	1.032	2.591	0.641	0.699	1.197	1.761	0.518	0.482	1.848
PMol1418	3-methylthiophene	0.914	0.847	0.381	3.388	0.140	0.525	0.634	0.848	1.512	0.466	1.005
PMol1419	carbon_monosulfide	1.958	1.932	0.601	4.080	0.642	1.223	0.477	1.857	1.283	5.275	0.303
PMol1420	methyl_isothiocyanate	3.453	3.874	4.987	0.583	3.247	3.904	3.784	3.937	2.380	2.992	4.049
PMol1421	carbon_oxide_sulfide	0.715	0.812	0.366	1.844	0.493	0.546	0.589	0.674	2.659	10.203	0.727
PMol1422	thioformaldehyde	1.649	1.688	1.743	1.936	0.940	1.114	1.463	1.743	0.279	2.735	1.704
PMol1423	propanethial_S-oxide	3.350	3.966	4.450	2.656	3.210	4.410	3.956	3.943	6.160	8.715	4.050
PMol1424	thioacetaldehyde	2.330	2.458	2.646	1.339	1.577	1.827	2.158	2.519	1.001	1.845	2.416
PMol1425	methylthiocyanate	3.340	4.280	2.505	3.777	3.183	3.739	4.028	4.274	4.514	11.182	4.038

PMol426	thiazole	1.650	1.642	1.304	4.096	1.257	2.080	1.770	1.628	3.754	5.168	1.518
PMol427	methanesulfonic_acid	3.805	3.803	3.780	2.054	2.893	3.573	3.792	3.794	4.763	8.025	3.768
PMol428	methyl_methanesulfenate	1.964	1.970	2.001	1.892	0.918	1.392	1.753	2.006	2.925	4.323	1.856
PMol429	methyl_methanesulfinate	2.706	2.654	3.160	2.228	2.341	4.184	2.695	2.592	5.848	8.234	2.856
PMol430	methane_sulfonamide	3.526	3.405	3.605	2.111	2.964	2.813	3.273	3.408	4.288	7.113	3.246
PMol431	dicyanogen_sulfide	3.020	3.083	0.811	3.455	2.221	3.233	2.874	2.953	3.858	11.197	2.689
PMol432	dimethyl_sulfone	4.470	4.464	4.647	2.135	3.432	4.174	4.506	4.483	5.910	9.872	4.628
PMol433	dimethyl_sulfoxide	3.960	3.912	4.417	2.612	3.100	4.513	3.893	3.931	6.589	9.219	4.061
PMol434	HCl	1.109	1.232	1.418	0.276	0.745	1.536	1.088	1.378	1.578	1.716	1.207
PMol435	chloromethane	1.893	1.898	2.039	1.427	1.141	1.224	1.501	1.967	1.562	2.613	1.788
PMol436	dichloromethane	1.600	1.642	1.863	2.044	0.988	1.336	1.394	1.806	1.447	2.603	1.764
PMol437	trichloromethane	1.040	1.078	1.293	1.946	0.671	1.081	1.018	1.260	1.005	1.970	1.354
PMol438	chloroethane	2.050	2.073	2.151	1.405	1.259	1.389	1.625	2.141	1.808	2.898	1.910
PMol439	1,1-dichloroethane	2.060	2.052	2.226	2.010	1.223	1.232	1.660	2.140	1.835	3.306	1.966
PMol440	1,1,1-trichloroethane	1.755	1.801	1.888	1.995	1.024	0.487	1.454	1.862	1.499	3.286	1.627
PMol441	pentachloroethane	0.920	0.887	1.255	2.035	0.566	0.847	0.913	1.015	0.972	1.857	1.266
PMol442	cyclopropylchloride	1.780	1.911	1.875	1.844	1.158	1.147	1.498	1.996	1.505	2.843	1.830
PMol443	1-chloropropane(gauche)	2.020	2.056	2.133	1.534	1.205	1.417	1.577	2.101	1.788	2.851	1.906
PMol444	1-chloropropane(trans)	1.950	2.143	2.161	1.231	1.372	1.434	1.748	2.216	1.877	2.999	1.994
PMol445	1,3-dichloropropane	2.080	1.843	2.005	1.725	1.112	1.560	1.517	1.926	1.727	2.463	1.937
PMol446	2-chloropropane	2.170	2.178	2.257	1.330	1.307	1.296	1.691	2.279	2.046	3.042	1.966
PMol447	1-chloro-2-methylpropane	2.000	2.059	2.135	1.281	1.280	1.333	1.675	2.125	1.907	2.874	1.941
PMol448	2-chlorobutane	2.040	2.141	2.223	1.440	1.243	1.284	1.633	2.226	2.017	2.951	1.956
PMol449	1-chlorobutane	2.050	2.229	2.207	1.325	1.445	1.560	1.812	2.285	1.911	3.111	2.074
PMol450	2-chloro-2-methylpropane	2.130	2.246	2.401	1.148	1.323	1.098	1.734	2.358	2.174	3.128	1.989
PMol451	1-chloropentane	2.160	2.244	2.159	1.139	1.489	1.536	1.862	2.310	1.964	3.140	2.098
PMol452	chlorocyclohexane(axial)	1.910	2.126	2.177	1.429	1.226	1.352	1.626	2.175	2.027	2.947	1.957
PMol453	chlorocyclohexane(equato)	2.440	2.447	2.468	1.337	1.560	1.737	1.929	2.521	2.098	3.397	2.209
PMol454	chloroethene	1.450	1.366	1.409	2.255	0.783	0.876	1.116	1.432	1.099	2.588	1.458
PMol455	1,1-dichloroethene	1.340	1.230	1.326	2.809	0.627	0.360	0.989	1.298	0.891	3.018	1.304
PMol456	Z-1,2-dichloroethene	1.900	1.778	2.172	4.136	1.006	1.249	1.563	1.908	1.513	3.470	2.246
PMol457	1-chloropropene(cis)	1.670	1.598	1.641	2.349	0.931	1.073	1.270	1.584	1.372	2.742	1.629
PMol458	1-chloropropene(trans)	1.970	1.884	1.974	1.587	1.263	1.243	1.644	1.958	1.446	3.148	1.906
PMol459	2-chloropropene	1.647	1.594	1.678	2.135	0.940	0.774	1.294	1.697	1.284	2.828	1.570
PMol460	3-chloropropene	1.940	1.846	1.915	1.855	1.072	1.422	1.445	1.895	1.701	2.493	1.851
PMol461	chlorobenzene	1.690	1.667	1.597	2.229	1.025	1.199	1.355	1.764	1.314	3.030	1.728
PMol462	1,2-dichlorobenzene	2.500	2.363	2.119	4.278	1.416	1.597	1.989	2.527	1.898	4.789	2.673
PMol463	1,3-dichlorobenzene	1.720	1.563	1.495	2.365	0.926	1.113	1.260	1.655	1.256	2.927	1.643
PMol464	ortho-chlorotoluene	1.560	1.415	1.302	2.870	0.728	0.828	1.037	1.498	1.114	2.721	1.456
PMol465	para-chlorotoluene	2.210	2.135	2.320	1.315	1.487	1.410	1.895	2.241	1.722	3.529	2.157
PMol466	chloroacetylene	0.444	0.266	1.102	3.579	0.092	0.162	0.198	0.337	0.002	2.279	0.590

PMol1467	3-chloropropyne	1.680	1.692	2.489	1.898	1.011	1.258	1.346	1.807	1.648	2.517	1.710
PMol1468	chlorofluoromethane	1.820	1.791	2.083	1.832	1.156	1.731	1.637	1.888	2.817	4.393	1.900
PMol1469	chlorodifluoromethane	1.420	1.421	1.539	1.947	0.948	1.608	1.401	1.523	2.687	4.603	1.618
PMol1470	fluorotrifluoromethane	0.460	0.367	0.490	1.694	0.256	0.403	0.431	0.301	2.141	2.993	0.137
PMol1471	chloropentafluoroethane	0.520	0.498	0.550	2.097	0.391	0.581	0.588	0.414	1.992	3.121	0.193
PMol1472	1-chloro-1-fluoroethane	2.068	2.199	2.444	1.683	1.434	1.633	1.950	2.273	3.194	4.950	2.136
PMol1473	1,1-dichloro-2-fluoropro	2.430	1.934	2.371	2.082	1.281	1.187	1.773	1.976	2.800	4.809	1.943
PMol1474	chlorotrifluoromethane	0.500	0.395	0.471	1.800	0.272	0.355	0.460	0.334	1.723	3.043	0.113
PMol1475	dichlorofluoromethane	1.290	1.256	1.463	2.256	0.829	1.374	1.242	1.406	2.435	3.846	1.497
PMol1476	1-chloro-1,1-difluoroeth	2.140	2.189	2.279	1.560	1.463	1.314	2.014	2.240	3.427	5.798	2.022
PMol1477	acetylchloride	2.720	2.824	2.729	1.592	2.023	2.375	2.644	2.852	3.656	7.147	2.743
PMol1478	phosgene	1.170	1.318	0.678	2.703	0.997	1.588	1.294	1.241	2.695	4.991	1.095
PMol1479	para-chlorophenol	2.110	2.252	2.090	0.776	1.521	1.868	2.024	2.308	1.773	2.207	1.909
PMol1480	cyanogen_chloride	2.833	3.044	0.756	4.275	2.063	2.855	2.776	2.923	2.998	6.120	2.446
PMol1481	1-chloro-2-nitrobenzene	4.640	4.867	4.635	2.893	3.685	4.811	4.601	4.939	5.968	9.157	4.997
PMol1482	1-chloro-3-nitrobenzene	3.730	3.978	4.103	4.301	3.051	4.054	3.699	3.976	5.141	6.898	3.687
PMol1483	1-chloro-4-nitrobenzene	2.830	3.308	3.460	5.217	2.802	3.716	3.237	3.262	4.757	5.306	2.913
PMol1587	HBr	0.827	0.919	1.313	0.328	0.612	1.189	0.912	1.110	1.340	0.818	0.828
PMol1588	bromomethane	1.820	1.895	1.807	1.208	1.020	0.882	1.242	1.983	1.149	1.608	1.685
PMol1589	dibromomethane	1.430	1.499	1.564	1.778	0.793	0.828	1.050	1.641	0.872	1.376	1.543
PMol1590	bromoform	0.990	0.898	1.044	1.640	0.485	0.751	0.711	1.118	0.456	0.917	1.107
PMol1591	bromoethane	2.040	2.151	2.043	1.154	1.169	1.152	1.392	2.259	1.458	2.016	1.917
PMol1592	1-bromopropane	2.180	2.238	2.081	0.978	1.292	1.232	1.523	2.349	1.519	2.124	2.013
PMol1593	2-bromopropane	2.210	2.302	2.238	1.064	1.228	1.093	1.467	2.448	1.697	2.223	2.063
PMol1594	1-bromobutane	2.080	2.335	2.141	1.067	1.377	1.366	1.599	2.411	1.558	2.246	2.106
PMol1595	2-bromobutane	2.230	2.281	2.227	1.148	1.164	1.086	1.409	2.393	1.685	2.154	2.064
PMol1596	1-bromopentane	2.200	2.357	2.106	0.876	1.429	1.353	1.658	2.457	1.612	2.297	2.140
PMol1597	1-bromoheptane	2.160	2.409	2.122	0.832	1.483	1.402	1.711	2.511	1.650	2.359	2.190
PMol1598	bromoethene	1.420	1.423	1.161	2.015	0.697	0.660	0.876	1.536	0.688	1.431	1.386
PMol1599	bromobenzene	1.700	1.775	1.528	1.986	0.965	1.059	1.134	1.929	0.907	1.902	1.750
PMol1600	bromoacetylene	0.230	0.166	0.532	3.468	0.311	0.463	0.194	0.250	0.600	0.023	0.224
PMol1601	3-bromopropyne	1.540	1.665	2.209	1.735	0.872	0.945	1.068	1.830	1.228	1.551	1.665
PMol1602	bromotrifluoromethane	0.650	0.436	0.565	1.491	0.387	0.544	0.743	0.317	1.967	4.156	0.131
PMol1603	dibromodifluoromethane	0.660	0.465	0.642	1.615	0.413	0.645	0.804	0.377	2.728	4.735	0.175
PMol1604	hydrogen_iodide	0.448	0.462	0.930	0.127	0.496	0.889	0.748	0.746	0.745	0.605	0.402
PMol1605	iodine_monofluoride	1.948	2.066	3.327	3.019	1.721	2.502	2.127	1.846	4.777	5.352	1.553
PMol1606	iodine_monochloride	1.240	1.167	2.105	0.719	0.909	1.266	1.182	1.007	2.551	3.489	0.822
PMol1607	iodine_monobromide	0.726	0.750	1.455	0.767	0.491	0.671	0.615	0.738	1.577	2.137	0.570
PMol1608	cyanic_iodide	3.670	3.816	2.701	4.754	2.719	3.549	3.752	3.599	4.766	10.330	3.462
PMol1609	iodomethane	1.641	1.684	1.204	1.566	0.950	0.651	1.054	1.836	0.372	0.086	1.487
PMol1610	iodoacetylene	0.025	0.151	0.735	3.987	0.466	0.704	0.497	0.030	1.683	2.479	0.108

PMol611	iodoethene	1.311	1.254	0.540	2.372	0.659	0.532	0.711	1.414	0.205	0.484	1.220
PMol612	iodoethane	1.976	2.019	1.561	1.457	1.135	1.009	1.239	2.180	0.754	0.666	1.773
PMol613	iodopropane	2.040	2.121	1.616	1.298	1.263	1.109	1.375	2.273	0.777	0.790	1.872
PMol614	iodobenzene	1.700	1.647	0.846	2.384	0.934	0.972	0.970	1.819	0.015	0.159	1.620

DEN. reference data

Mul.	Low.	Hir.	I-H	CM5	ESP	NPA	AIM	ACP							
Deviation							-0.193	-0.622	-0.689	-0.187	-0.155	0.030	0.520	2.243	-0.084
Abs. dev.							0.482	1.151	0.717	0.447	0.223	0.056	0.919	2.475	0.186
Disp.							0.673	1.425	0.806	0.606	0.292	0.108	1.209	3.184	0.274

Exp. reference data

Den.	Mul.	Low.	Hir.	I-H	CM5	ESP	NPA	AIM	ACP						
Deviation						0.039	-0.153	-0.583	-0.649	-0.148	-0.116	0.070	0.559	2.282	-0.045
Abs. dev.						0.109	0.455	1.112	0.679	0.446	0.221	0.132	0.919	2.501	0.177
Disp.						0.163	0.633	1.379	0.766	0.604	0.295	0.196	1.216	3.225	0.273

Number of molecules 411

M E T A L S

Dipole moments in D

Molecule		Exp.	Den.	Mul.	Low.	Hir.	I-H	CM5	ESP	NPA	AIM	ACP
Met001	LiF	6.327	6.032	5.530	4.476	4.279	6.963	5.418	6.058	6.990	6.660	4.946
Met003	LiS	6.893	6.806	6.652	3.891	4.768	8.873	5.756	6.877	8.860	9.024	6.785
Met004	LiCl	7.129	6.859	6.662	4.164	5.026	8.773	5.924	6.965	8.807	8.645	6.352
Met005	LiBr	7.268	7.086	7.339	4.404	5.200	9.338	5.883	7.507	9.453	9.390	6.834
Met006	LiI	7.428	7.336	7.885	4.640	5.644	10.000	6.102	7.724	10.246	10.405	7.297
Met007	LiOH	4.497	4.109	3.981	3.528	3.396	5.526	4.133	4.085	5.095	4.200	3.878
Met008	LiSH	6.840	6.736	6.554	4.203	4.869	9.068	5.841	6.843	8.957	9.104	6.961
Met009	LiNH2	4.790	4.387	4.441	3.551	3.693	5.864	4.448	4.369	5.588	5.536	4.721
Met010	LiCH3	5.703	5.516	6.071	4.630	4.674	7.556	4.915	5.424	6.712	8.572	6.074
Met011	LiCH3O	3.684	3.585	4.271	3.726	3.186	5.675	3.573	3.462	4.557	4.944	4.015
Met012	LiOCH3	5.271	5.040	4.165	5.143	4.231	5.747	5.071	4.977	5.236	3.689	4.463
Met013	LiC2H	6.024	5.909	8.571	5.420	5.161	7.268	5.549	5.850	8.416	9.891	6.186
Met014	LiC3H5	3.796	3.574	5.188	3.782	3.123	6.705	4.070	3.624	6.447	6.944	4.840
Met015	LiC2H2F	4.451	4.242	6.249	3.931	3.811	6.549	4.749	4.165	7.117	6.866	4.986
Met016	LiC2H6N	5.646	5.437	4.753	4.917	4.610	6.425	5.433	5.303	6.336	5.761	5.369
Met017	CH3HNLi	5.001	4.923	4.526	4.621	4.274	6.196	5.035	4.901	6.064	5.788	5.083
Met018	(CH3)2NLi	5.553	5.491	4.798	4.995	4.659	6.499	5.420	5.357	6.448	5.888	5.435

Met019	CH3-OLi	5.069	4.982	4.105	5.058	4.171	5.692	5.009	4.911	5.208	3.732	4.428
Met020	Li+_CH3	6.447	6.576	7.227	6.349	5.773	7.895	5.944	6.595	7.738	7.670	6.662
Met021	Li+_C2H5	7.867	7.974	8.625	7.780	7.197	9.365	7.377	7.874	9.317	9.094	8.211
Met022	Li+_C2H3	6.612	6.712	7.597	6.630	5.896	8.329	6.187	6.728	8.407	8.099	6.902
Met023	Li+_propene	7.727	7.822	8.713	7.796	6.915	9.574	7.282	7.643	9.542	9.274	8.157
Met024	Li+_propyne	7.270	7.393	8.515	7.312	6.377	9.003	6.822	7.296	9.158	8.654	7.492
Met025	Li(NH3)+	4.532	4.556	5.193	4.725	4.323	5.332	4.385	4.511	5.161	4.854	4.862
Met026	Li+_N(CH3)H2	6.495	6.554	6.915	7.026	6.091	7.340	6.334	6.507	7.275	6.556	6.614
Met027	Li+_N(CH3)2H	6.724	6.792	7.181	7.138	6.166	7.847	6.516	6.677	7.665	6.795	6.852
Met028	Li+_N(CH3)3	6.751	6.818	7.192	6.897	6.028	8.195	6.478	6.730	7.805	6.809	6.895
Met029	C5H5N-Li+	8.508	8.557	9.311	9.562	8.002	9.562	8.482	8.482	9.630	6.822	8.455
Met030	HCN-Li+	4.898	4.909	6.428	6.370	4.675	5.439	4.945	4.891	5.476	0.512	4.780
Met031	CH3CN-Li+	6.849	6.887	7.623	7.821	6.453	7.769	6.743	6.865	8.029	1.711	6.665
Met032	Li(H2O)+	3.995	3.987	4.344	4.443	3.850	4.204	3.847	3.969	4.178	3.267	4.013
Met033	Li+_CH3OH	6.085	6.147	5.942	6.904	5.644	6.546	5.912	6.091	6.204	4.788	5.929
Met037	Li+_O(CH3)2	6.373	6.462	5.985	7.094	5.722	7.228	6.129	6.357	6.489	4.758	6.165
Met038	Li+CH2Cl2	4.516	4.673	4.895	6.646	3.804	6.532	4.148	4.657	6.621	5.189	4.489
Met036	Li+S(CH3)2	7.767	7.886	8.437	8.814	7.197	10.043	7.478	7.687	10.395	10.027	8.275
Met037	Li+CH3F	6.194	6.259	5.930	7.140	5.682	6.855	6.090	6.209	5.935	4.439	5.872
Met038	BeClF	0.273	0.296	0.106	3.322	0.342	0.472	0.342	0.174	0.720	1.538	0.138
Met039	BeBrF	0.386	0.367	0.123	3.670	0.519	0.458	0.584	0.266	0.793	1.947	0.051
Met040	BeBrCl	0.122	0.064	0.320	0.334	0.183	0.028	0.240	0.039	0.030	0.411	0.078
Met041	Be=CH2	3.349	2.909	0.238	1.119	2.193	4.703	2.927	2.897	7.695	8.778	3.353
Met042	BeFCH3	1.303	1.293	1.409	0.858	0.833	0.594	1.386	1.320	1.120	0.655	0.741
Met043	BeClCH3	1.109	1.052	2.066	2.507	0.527	0.874	1.069	1.160	1.822	0.855	0.885
Met044	BeBrCH3	1.048	1.046	1.755	2.830	0.393	0.844	0.872	1.195	1.860	1.312	0.847
Met045	BeCl+	8.065	7.851	4.678	2.022	6.140	10.438	7.436	7.962	11.840	12.768	7.899
Met046	BeS	5.466	5.122	1.275	1.084	3.232	7.210	4.827	5.392	10.602	12.116	5.627
Met047	Be=NH	4.386	3.871	0.320	0.758	2.287	5.457	3.640	3.704	8.609	8.341	3.994
Met048	Be=NF	5.529	5.217	1.247	0.961	3.311	6.401	5.434	4.872	11.272	11.985	5.319
Met049	CH3BeH	0.551	0.595	0.506	0.492	0.100	0.108	0.461	0.550	0.924	1.398	0.284
Met050	BeH(CH=CH2)	0.747	0.777	0.517	0.389	0.048	0.475	0.375	0.727	1.154	1.494	0.082
Met051	BeH(OH)	1.688	1.816	1.248	1.419	0.755	1.454	0.273	1.772	0.334	2.453	1.009
Met052	BeCN(OH)	4.644	4.750	2.615	2.164	3.291	3.918	4.176	4.718	4.732	11.201	4.588
Met053	BeH(NO2)	2.794	2.782	3.221	1.408	2.709	3.134	3.941	2.883	4.599	4.529	3.181
Met054	BeHF	0.679	0.680	0.762	0.185	0.847	0.748	1.771	0.691	1.938	0.654	0.958
Met055	CH3BeF	1.256	1.265	1.365	0.813	0.828	0.564	1.385	1.292	1.070	0.670	0.735
Met056	BeHCl	0.436	0.350	0.556	3.043	0.508	0.873	1.409	0.503	2.696	2.159	1.042
Met057	BeH(SH)	0.685	0.744	0.912	2.963	0.401	1.173	1.313	0.924	2.699	2.271	1.444
Met058	Be(OH)(SH)	1.794	1.889	2.142	1.771	0.897	2.643	1.654	2.026	2.964	4.362	2.140
Met059	NaF	8.156	7.844	6.877	4.888	5.786	8.700	7.247	7.831	8.724	8.404	6.546

Met060	NaS	8.608	8.092	6.856	2.477	5.959	9.676	7.227	8.122	9.897	9.869	8.409
Met061	NaCl	9.001	8.622	7.371	2.945	6.588	10.205	7.847	8.690	10.357	10.064	8.253
Met062	NaBr	9.118	8.808	7.989	2.888	6.727	10.579	7.824	9.026	10.948	10.608	8.736
Met063	NaI	9.236	8.922	7.964	2.762	7.062	11.018	7.948	9.212	11.573	11.322	9.288
Met064	NaOH	6.633	6.169	5.492	3.620	5.108	7.702	6.279	6.111	6.922	6.125	5.966
Met065	NaSH	8.524	7.998	6.663	2.819	6.070	9.833	7.349	8.065	9.890	9.910	8.590
Met066	NaCH3	6.346	5.619	6.583	4.077	4.948	7.372	5.496	5.564	6.695	8.146	6.844
Met067	NaC2H	7.799	7.549	11.872	5.709	6.717	8.884	7.406	7.434	10.030	11.099	8.247
Met068	NaC2H2F	6.983	6.659	8.907	4.158	5.988	8.784	7.385	6.453	9.204	9.052	7.103
Met069	NaC2H6N	7.836	7.511	6.851	5.292	6.562	8.373	7.738	7.322	8.084	7.468	7.688
Met070	(CH3)HNNa	6.765	6.604	6.119	4.683	5.822	7.750	7.059	6.575	7.536	7.155	7.051
Met071	(CH3)2NNa	7.530	7.423	6.760	5.193	6.470	8.305	7.706	7.238	8.055	7.429	7.632
Met072	CH3-ONa	7.566	7.419	6.327	5.604	6.368	8.208	7.656	7.271	7.271	5.965	6.883
Met073	Na(OH)	6.425	6.148	5.465	3.576	5.082	7.675	6.278	6.083	6.889	6.105	5.947
Met074	NaS	8.160	8.061	6.844	2.421	5.923	9.645	7.220	8.089	9.865	9.823	8.379
Met075	Na+CH3	4.182	4.267	4.028	2.813	3.531	5.416	3.844	4.250	5.237	5.117	4.497
Met076	Na+C2H5	6.204	6.287	6.068	4.791	5.610	7.532	5.968	6.131	7.447	7.158	6.719
Met077	Na+C2H3	5.156	5.217	4.875	3.600	4.409	6.650	4.917	5.213	6.696	6.307	5.551
Met078	Na+propyne	6.386	6.457	6.073	4.859	5.498	7.923	6.181	6.322	8.061	7.433	6.747
Met079	Na(NH3)+	2.666	2.676	3.083	1.573	2.443	3.447	2.731	2.619	3.168	2.784	3.118
Met080	Na+N(CH3)H2	5.111	5.153	5.122	4.376	4.756	5.965	5.235	5.091	5.752	4.981	5.418
Met081	Na+N(CH3)2H	6.061	6.114	5.968	5.049	5.587	7.186	6.198	6.003	6.842	5.908	6.408
Met082	Na+N(CH3)3	6.626	6.682	6.380	5.176	6.011	8.054	6.741	6.549	7.494	6.432	7.003
Met083	C5H5N-Na+	8.268	8.287	8.716	7.929	7.851	9.309	8.588	8.204	9.227	6.408	8.448
Met084	HCN-Na+	3.083	3.083	5.220	3.197	2.928	3.644	3.419	3.055	3.619	1.386	3.117
Met085	CH3CN-Na+	5.226	5.248	6.540	4.846	4.892	6.148	5.435	5.216	6.314	0.035	5.205
Met086	Na(H2O)+	2.415	2.370	2.650	1.626	2.259	2.613	2.482	2.360	2.423	1.511	2.485
Met087	Na+CH3OH	4.932	4.960	4.675	4.480	4.539	5.356	5.038	4.922	4.821	3.443	4.855
Met088	Na+O(CH3)2	5.963	6.012	5.455	5.216	5.375	6.761	6.041	5.900	5.790	4.109	5.829
Met089	Na+OC(CH3)2	6.569	6.597	6.628	6.131	6.143	7.411	6.877	6.596	6.216	2.775	6.124
Met090	Na+HCON(CH3)2	7.275	7.296	6.768	6.579	6.775	8.068	7.609	7.218	7.215	5.644	6.905
Met091	Na+CH2Cl2	5.470	5.527	4.283	4.123	4.665	7.142	5.263	5.439	7.274	5.795	5.476
Met092	Na+S(CH3)2	7.382	7.456	6.628	6.229	6.856	9.342	7.321	7.262	9.767	9.277	8.049
Met093	MgClF	0.075	0.122	0.274	3.014	0.123	0.958	0.302	0.137	1.090	1.378	0.126
Met094	MgBrF	0.201	0.284	0.004	3.462	0.289	1.098	0.640	0.143	1.344	1.743	0.040
Met095	MgBrCl	0.156	0.158	0.320	0.424	0.165	0.144	0.335	0.054	0.235	0.363	0.090
Met096	Mg=CH2	3.405	3.253	3.679	3.349	3.309	5.728	3.752	4.075	7.618	7.824	3.338
Met097	MgFCH3	1.923	2.026	2.123	1.266	1.280	1.015	2.009	2.051	1.588	0.286	1.207
Met098	MgClCH3	2.114	2.127	2.169	1.660	1.365	1.958	1.906	2.292	2.847	1.800	1.524
Met099	MgBrCH3	2.077	2.094	2.668	2.033	1.298	2.138	1.672	2.377	3.141	2.245	1.548
Met100	CH3MgH	0.422	0.434	1.887	0.716	0.776	0.350	1.049	0.317	0.707	1.531	0.438

Met101	MgH(CH=CH2)	0.375	0.393	1.708	1.069	1.043	0.282	1.359	0.325	1.481	2.120	0.568
Met102	MgH(CN)	3.558	3.512	3.528	2.090	3.667	3.159	5.044	3.573	5.039	9.587	4.312
Met103	MgH(NH2)	0.649	0.784	1.704	0.122	0.473	0.605	1.119	0.801	0.269	0.303	0.361
Met104	MgH(OH)	0.508	0.632	1.888	0.138	0.622	0.376	1.231	0.572	0.104	1.091	0.183
Met105	MgCN(OH)	4.015	4.084	1.899	1.889	3.006	3.345	3.758	4.047	4.819	10.586	4.455
Met106	MgH(ONO)	0.730	0.749	2.236	0.873	0.606	0.428	2.802	0.584	0.320	0.380	0.231
Met107	MgH(NO2)	3.796	3.733	6.033	2.960	4.268	4.212	5.621	3.941	5.154	5.954	4.281
Met108	MgHF	1.501	1.512	3.856	1.737	1.917	1.310	2.931	1.535	2.221	1.702	1.544
Met109	MgHCl	1.615	1.574	3.831	1.037	1.957	2.186	2.785	1.860	3.407	3.188	1.804
Met110	Mg(OH)(SH)	1.550	1.635	1.366	1.752	0.669	2.631	1.158	1.887	3.074	4.012	1.989
Met111	AlH=NH	2.787	2.689	1.902	0.684	2.082	3.951	2.479	3.327	5.070	5.345	2.607
Met112	AlH2NH2	1.079	1.286	0.576	2.115	0.566	0.681	0.739	1.176	0.248	0.487	0.511
Met113	AlH2OH	1.233	1.297	1.160	1.717	0.628	1.902	1.282	1.242	2.382	2.349	1.010
Met114	AlH=PH	2.949	2.792	1.587	1.435	2.052	4.183	2.705	3.423	4.321	6.515	2.884
Met115	AlH2SH	0.947	0.936	1.277	3.482	0.443	1.443	0.952	1.112	2.215	2.802	1.110
Met116	AlH=S	3.938	3.787	2.503	1.939	2.885	5.385	3.161	4.424	5.790	7.771	3.416
Met117	AlF	1.530	1.481	2.690	0.607	2.571	4.051	2.451	2.508	6.726	7.333	2.304
Met118	AlCl	1.622	1.521	2.775	2.030	2.567	3.951	2.193	2.746	7.122	8.656	2.331
Met119	AlBr	1.746	1.702	3.013	1.737	2.566	3.920	1.973	2.929	7.110	8.946	2.289
Met120	AlS	3.857	3.754	2.904	1.183	3.382	6.252	3.100	4.916	8.763	11.361	3.495
Met121	AlF2	1.925	1.887	2.585	0.270	2.344	4.769	2.222	2.882	6.141	7.023	2.125
Met122	AlF2O	0.164	0.159	0.172	0.091	0.273	0.142	0.052	0.160	0.140	0.278	0.354
Met123	AlCl+	5.610	5.624	4.756	0.437	5.174	7.940	4.717	6.182	9.992	11.660	5.078
Met124	AlCl2	1.588	1.528	2.269	2.705	2.036	4.421	1.644	2.544	5.705	8.177	1.818
Met125	AlCl2-	0.795	0.849	2.113	3.935	1.140	2.418	0.802	1.079	5.412	7.845	0.699
Met126	AlClF+	0.210	0.244	0.145	2.586	0.329	1.585	0.032	0.602	0.988	2.554	0.387
Met127	AlClF	1.772	1.724	2.453	2.886	2.215	4.719	2.011	2.807	6.054	7.700	1.995
Met128	AlF2Cl	0.504	0.506	0.461	3.426	0.672	0.265	0.981	0.357	0.372	0.949	0.613
Met129	AlFCl2	0.485	0.486	0.472	3.297	0.634	0.121	0.928	0.343	0.653	0.853	0.581

DEN. reference data

Mul.	Low.	Hir.	I-H	CM5	ESP	NPA	AIM	ACP							
Deviation							0.030	-0.726	-0.625	1.030	-0.038	0.076	1.440	1.364	0.040
Abs. dev.							0.843	1.519	0.756	1.161	0.435	0.178	1.538	2.069	0.334
Disp.							1.196	2.107	0.935	1.391	0.595	0.316	2.083	2.873	0.426
xDisp.							1.319	2.544	1.000	1.472	0.737	0.396	2.189	3.044	0.547

Exp. reference data

Den.	Mul.	Low.	Hir.	I-H	CM5	ESP	NPA	AIM	ACP						
Deviation						-0.063	-0.033	-0.789	-0.688	0.967	-0.101	0.014	1.378	1.302	-0.022
Abs. dev.						0.121	0.884	1.591	0.814	1.085	0.467	0.219	1.465	2.020	0.329
Disp.						0.179	1.253	2.219	1.039	1.310	0.637	0.341	2.003	2.809	0.424

Number of molecules 129