Supplementary information for a paper in Chemical Physics Letters, xxx (2015) yyy.

Choosing a density functional for static molecular polarizabilities

Taozhe Wu, Yulia N. Kalugina and Ajit J. Thakkar

Department of Chemistry, University of New Brunswick, Fredericton, NB E3B 5A3, Canada

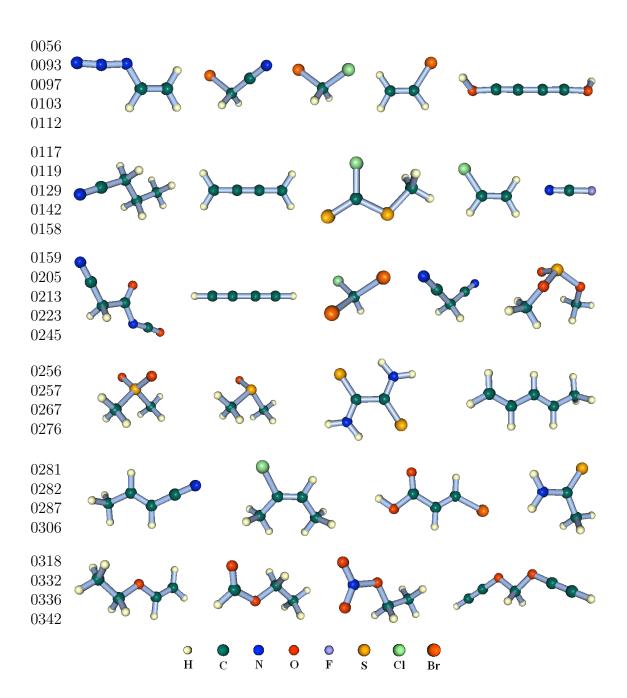
Molecules in T145 Pages 2–7 display ball-and-stick representations of the 145 molecules in T145. The molecules are ordered by their TABS ID number. The ID numbers increase from left to right. The number of molecules in a row and on a page varies because an attempt has been made to keep the atoms to the same size for each molecule. The color legend for the eight different types of atoms is given at the bottom of each page. Further details of these structures are given in the supplementary material to the TABS database paper. It lists, among other quantities, the TABS identification number, chemical name, point group, dipole moment, and Cartesian coordinates for each molecule.

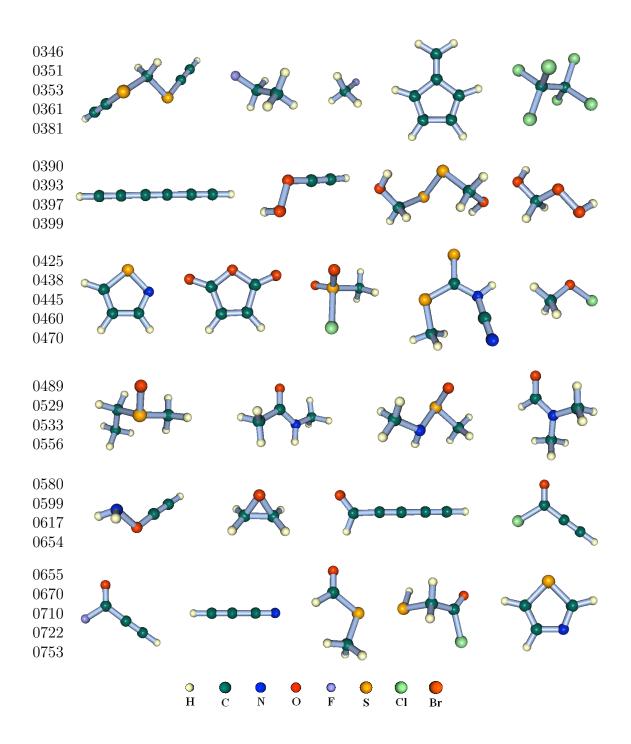
Polarizabilities Pages 8–22 list the calculated polarizabilities in atomic units. The ID number can be used to find the relevant structural diagram for the molecule on pages 2–7. The SI value of one atomic unit of the dipole polarizability α is $1.648\,777\times10^{-41}\,\mathrm{C^2}\,\mathrm{m^2}\,\mathrm{J^{-1}}$ on the basis of the 2010 CODATA recommendations for the fundamental physical constants.³

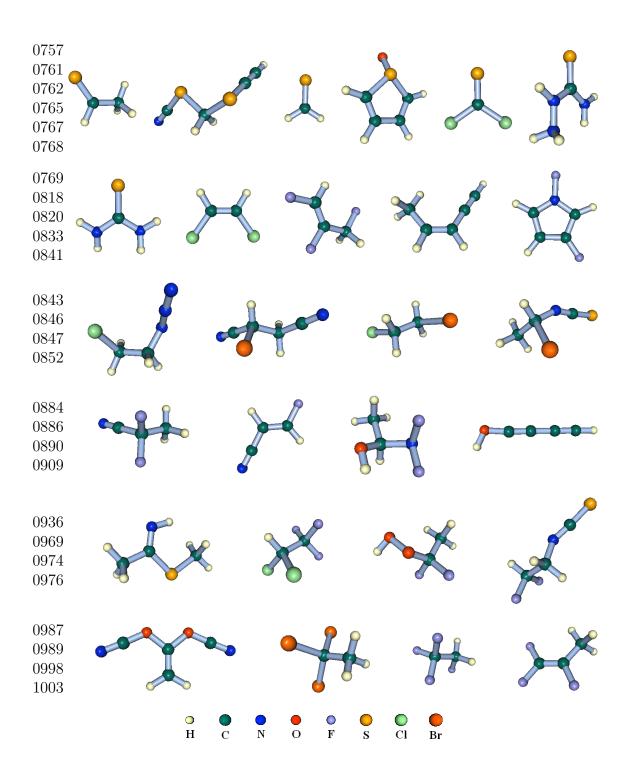
¹Available online as a 1642 page PDF file at http://dx.doi.org/10.1016/j.comptc.2014.05.010.

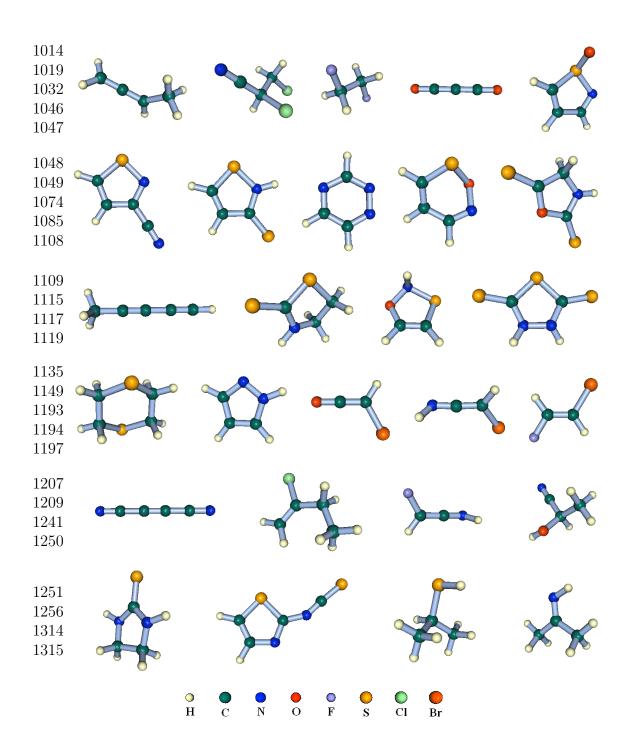
²S. A. Blair, A. J. Thakkar, Comput. Theor. Chem. 1043 (2014) 13.

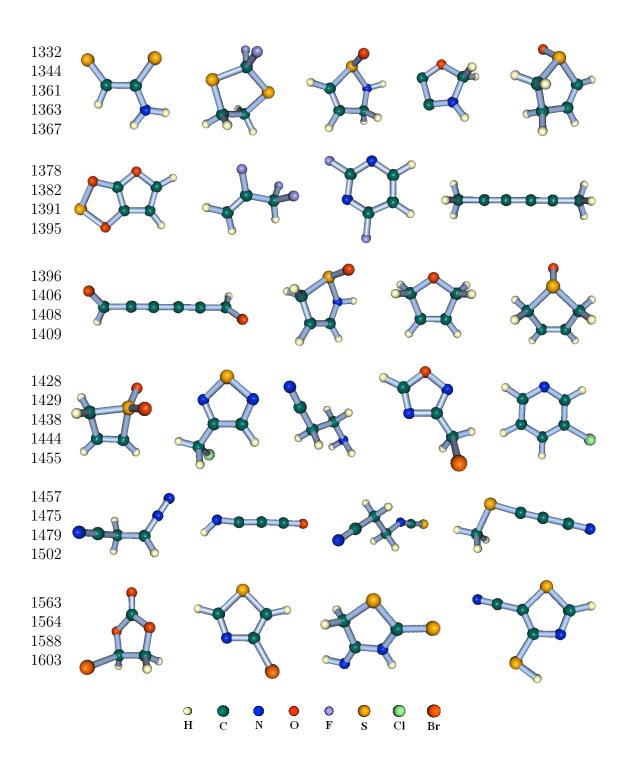
³P. J. Mohr, B. N. Taylor, D. B. Newell, Rev. Mod. Phys. 84 (2012) 1527.

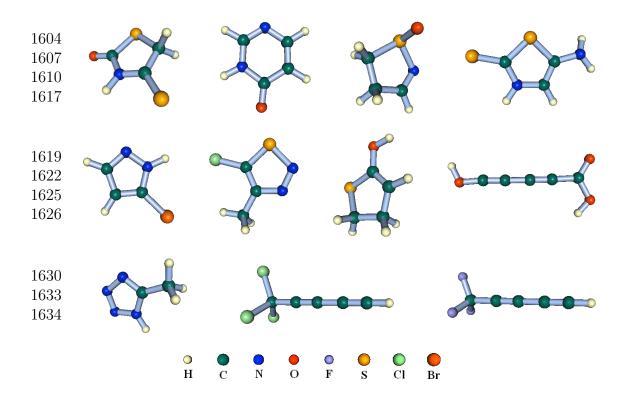












ID	HF	MP2	CCSD(T)
0056	54.392	54.554	54.319
0093	49.138	49.815	50.010
0097	48.852	50.330	50.360
0103	47.508	47.657	47.521
0112	57.508	59.757	59.585
0117	51.584	53.190	53.103
0119	61.631	57.647	56.635
0129	83.094	87.305	87.131
0142	40.182	40.450	40.239
0158	17.326	17.876	18.028
0159	59.555	64.564	64.337
0205	48.239	47.092	46.911
0213	69.066	71.282	71.413
0223	41.078	41.291	41.717
0245	54.462	59.485	59.151
0256	49.655	54.579	54.029
0257	49.960	54.093	53.551
0267	86.782	93.141	92.702
0276	69.930	68.337	67.463
0281	54.672	54.561	54.422
0282	64.054	65.489	65.170
0287	65.404	68.587	68.509
0306	56.894	60.907	60.476
0318	56.738	58.962	58.364
0332	42.972	46.527	46.236
0336	47.377	50.994	50.959
0342	65.216	67.471	67.214
0346	99.451	101.935	101.446
0351	27.176	28.744	28.588
0353	15.864	16.846	16.773
0361	74.176	71.830	70.979
0381	101.789	106.926	106.750
0390	82.167	80.994	80.271
0393	36.286	36.577	36.700
0397	75.623	80.846	80.455
0399	30.035	32.223	32.296
0425	56.935	58.763	58.300
0438	51.656	54.053	54.080
0445	53.183	57.988	57.567
0460	92.280	98.201	97.975
0470	34.026	35.078	35.178
0489	61.298	65.958	65.358
0529	47.310	51.553	51.192
0533	58.318	63.374	62.833
0556	47.840	52.179	51.783
0580	38.502	39.650	39.526
0599	26.984	28.512	28.256
0617	66.604	66.886	66.829
0654	50.669	52.472	52.551
0655	36.562	37.620	37.720

ID	HF	MP2	CCSD(T)
0670	39.415	38.670	38.854
0710	48.560	51.992	51.761
0722	60.706	64.501	64.234
0753	56.738	58.731	58.396
0757	47.361	47.671	47.502
0761	90.553	93.123	93.079
0762	34.553	33.666	33.646
0765	65.491	68.611	67.916
0767	61.573	63.277	63.530
0768	62.023	68.597	68.239
0769	53.152	58.611	58.313
0818	52.531	53.477	53.316
0820	38.439	40.183	39.926
0833	62.372	61.458	61.074
0841	53.446	55.196	55.043
0843	60.751	63.484	63.311
			75.135
0846	73.304	74.639	
0847	61.965	64.153	64.067
0852	89.895	95.559	94.885
0884	40.030	41.908	42.045
0886	41.537	41.740	41.708
0890	41.353	44.370	44.348
0909	53.147	53.790	53.553
0936	65.048	68.681	68.348
0969	52.766	56.185	56.132
0974	36.719	39.369	39.408
0976	67.736	72.874	72.216
0987	60.413	62.981	63.197
0989	88.182	90.889	91.357
0998	27.751	30.514	30.434
1003	38.435	40.346	40.162
1014	53.545	53.002	52.468
1019	65.909	68.022	68.138
1032	27.145	29.097	28.975
1046	43.321	47.740	46.884
1047	59.994	63.649	63.063
1048	73.027	74.768	74.666
1049	87.733	93.935	93.152
1074	51.716	53.538	52.962
1085	62.678	64.997	64.603
1108	91.079	97.608	97.624
1109	62.722	62.433	62.019
1115	84.222	90.429	89.716
1117	52.591	54.884	54.521
1119	106.635	116.097	115.896
1135	83.867	87.859	87.246
1149	46.999	48.741	48.399
1193	47.033	49.145	48.870
1194	55.132	56.463	56.429
1197	46.537	47.396	47.320

ID	HF	MP2	CCSD(T)
1207	60.505	59.681	60.112
1209	62.900	64.574	64.167
1241	34.350	35.280	35.104
1250	43.750	45.649	45.666
1251	72.068	78.605	78.067
1256	106.563	114.075	112.564
1314	58.680	61.398	60.864
1315	45.030	46.908	46.673
1332	78.107	80.032	80.271
1344	71.848	76.242	75.764
1361	62.076	66.253	65.681
1363	43.720	48.798	48.861
1367	66.472	70.222	69.561
1378	68.013	71.729	71.306
1382	38.901	40.663	40.403
1391	55.155	59.180	58.389
1395	77.415	78.011	77.659
1396	86.416	88.516	88.525
1406	62.377	66.780	66.076
1408	48.608	50.041	49.650
1409	66.484	70.115	69.437
1428	55.668	59.902	59.280
1429	78.269	81.367	81.069
1438	48.458	50.851	50.799
1444	69.351	72.642	72.434
1455	75.491	78.253	77.330
1457	56.230	56.770	56.941
1475	52.616	57.505	56.730
1479	82.145	86.555	86.006
1502	77.924	79.780	79.592
1563	62.609	67.153	67.214
1564	78.096	81.037	80.970
1588	93.337	100.557	100.186
1603	94.645	98.358	97.864
1604	85.372	92.336	91.970
1607	60.967	65.137	64.526
1610	61.526	65.864	65.351
1617	94.521	103.147	102.065
1619	67.412	69.997	69.957
1622	78.128	81.537	81.519
1625	68.364	71.616	70.964
1626	74.823	79.279	79.066
1630	48.592	51.418	51.330
1633	106.337	109.191	108.792
1634	62.255	63.662	63.556

ID	LSDA	PBE	HCTH	N12	revTPSS	tHCTH	M11-L	MN12-L
0056	56.885	56.773	56.323	56.094	56.163	56.168	58.116	57.226
0093	52.985	52.876	52.244	51.974	52.071	52.020	53.267	52.131
0097	53.220	52.949	52.058	51.677	52.010	51.859	53.813	51.707
0103	50.430	50.260	49.796	49.450	49.352	49.455	51.276	50.148
0112	65.759	65.739	64.733	64.463	64.963	64.865	67.247	64.508
0117	56.916	56.373	55.889	55.521	55.526	55.780	57.220	56.451
0119	60.311	60.176	59.909	60.000	59.680	60.067	64.014	62.877
0129	91.249	90.540	89.185	88.006	89.036	88.907	93.763	88.482
0142	42.766	42.444	41.852	41.531	41.861	41.830	44.285	42.455
0158	18.949	18.965	18.638	18.441	18.772	18.595	18.971	18.553
0159	67.890	67.602	66.618	66.084	66.715	66.449	67.047	65.840
0205	50.772	50.749	50.313	50.392	50.318	50.352	53.376	51.901
0213	75.837	75.605	74.460	73.920	74.125	73.938	75.597	72.982
0223	44.268	44.135	43.642	43.461	43.644	43.601	44.908	43.970
0245	62.998	62.606	61.902	60.895	61.522	61.613	62.375	60.555
0256	57.216	56.944	56.409	55.816	56.126	56.123	56.558	55.708
0257	57.300	57.012	56.747	55.969	55.844	56.116	57.107	55.973
0267	94.701	94.377	93.125	92.028	93.059	93.009	98.698	93.571
0276	74.349	73.761	73.414	73.150	72.629	73.389	76.904	75.409
0281	59.092	58.699	58.195	57.990	57.890	58.192	60.363	59.168
0282	70.241	69.554	68.743	68.318	68.422	68.732	71.626	69.497
0287	74.086	73.947	72.994	72.482	72.676	72.511	73.295	71.855
0306	63.341	62.995	62.317	61.651	61.807	61.995	66.239	63.009
0318	63.039	62.520	62.158	61.419	61.372	61.744	63.574	62.474
0332	49.487	49.088	48.554	47.871	48.193	48.307	49.081	48.088
0336	53.789	53.424	52.728	52.148	52.623	52.576	53.246	52.191
0342	72.666	72.551	71.737	71.184	71.517	71.485	74.778	72.056
0346	109.628	109.073	107.739	107.196	107.494	107.637	114.046	108.542
0351	30.855	30.574	30.293	29.837	30.017	30.127	30.690	30.205
0353	18.062	17.940	17.731	17.409	17.632	17.645	17.951	17.594
0361	75.038	74.871	74.662	74.481	74.240	74.624	79.018	77.308
0381	113.390	112.567	110.139	109.218	111.203	110.300	114.461	108.158
0390	90.763	90.707	89.957	90.200	89.787	90.140	94.775	91.805
0393	39.762	39.826	39.406	39.203	39.378	39.288	41.440	39.706
0397	86.427	85.625	84.239	83.087	83.946	83.953	87.771	83.206
0399	35.069	34.976	34.480	33.856	34.420	34.262	34.728	33.782
0425	60.206	59.993	59.499	58.816	59.244	59.285	62.204	59.823
0438	56.681	56.709	56.011	55.561	56.228	55.861	57.036	56.192
0445	59.821	59.525	58.583	58.053	58.843	58.520	59.805	57.802
0460	102.828	102.220	100.823	99.676	100.694	100.561	104.721	100.093
0470	37.690	37.372	36.786	36.309	36.714	36.672	38.448	36.702
0489	70.021	69.453	69.020	68.107	68.101	68.462	69.779	68.508
0529	54.952	54.517	54.003	53.300	53.482	53.687	54.621	53.578
0533	67.466	67.025	66.619	65.587	65.651	65.943	67.274	65.601
0556	55.482	54.943	54.401	53.693	53.780	54.078	54.848	54.035
0580	42.583	42.630	42.222	41.965	42.088	42.041	44.601	42.790
0599	29.964	29.805	29.583	29.220	29.361	29.452	30.090	29.502
0617	74.702	74.600	73.869	73.830	73.733	73.877	76.464	74.513
0654	56.248	56.021	55.122	54.750	55.353	55.065	57.114	54.748
0655	40.425	40.430	39.849	39.559	40.035	39.763	40.787	39.838
0000	10.720	40.40U	00.043	00.003	40.000	00.100	40.101	00.000

ID	LSDA	PBE	HCTH	N12	revTPSS	tHCTH	M11-L	MN12-L
0670	41.562	41.544	41.118	41.074	41.206	41.116	42.801	41.830
0710	54.643	54.159	53.431	52.685	53.197	53.217	55.152	52.967
0722	68.566	67.962	66.725	65.971	66.882	66.635	69.441	66.008
0753	60.706	60.459	59.906	59.221	59.642	59.670	62.741	60.153
0757	51.150	50.703	50.199	49.730	49.641	49.966	53.842	51.132
0761	99.944	99.424	98.123	97.456	98.036	98.023	102.717	98.084
0762	35.316	35.097	34.629	34.270	34.657	34.651	37.708	35.772
0765	71.606	71.417	70.881	70.219	70.504	70.618	73.206	71.247
0767	66.877	66.461	65.183	64.340	65.515	65.069	68.707	64.579
0768	72.244	72.033	71.169	70.226	70.593	70.734	75.311	70.794
0769	61.102	60.908	60.138	59.382	59.744	59.773	63.786	60.048
0818	56.715	56.283	55.258	54.807	55.518	55.313	58.451	55.558
0820	43.087	42.992	42.383	41.769	42.448	42.289	43.521	42.421
0833	66.501	66.116	65.658	65.596	65.238	65.687	69.119	67.604
0841	57.383	57.390	56.820	56.199	56.803	56.627	58.671	57.036
0843	66.412	65.955	65.064	64.545	64.998	64.915	67.388	65.299
0846	79.979	79.706	78.748	78.405	78.593	78.519	80.365	78.735
0847	68.311	67.888	66.803	66.388	66.702	66.609	68.891	66.378
0852	99.693	99.162	97.938	96.816	97.479	97.449	100.426	96.855
0884	45.103	44.897	44.261	43.772	44.326	44.117	44.809	43.995
0886	44.850	44.785	44.248	43.959	44.329	44.218	45.605	44.600
0890	47.652	47.336	46.673	45.940	46.573	46.435	47.032	46.058
0909	58.617	58.595	57.868	57.761	57.970	57.927	60.712	58.697
0936	73.101	72.355	71.527	70.810	71.019	71.276	74.207	71.591
0969	59.746	59.420	58.105	57.328	58.689	58.028	59.862	57.188
0974	42.223	42.065	41.382	40.686	41.526	41.201	41.634	40.770
0976	75.153	74.784	73.667	72.556	73.681	73.402	76.433	73.532
0987	67.711	67.515	66.539	65.927	66.674	66.404	67.576	65.742
0989	96.580	96.386	95.318	94.732	94.448	94.475	95.575	93.648
0998	32.710	32.653	32.023	31.368	32.245	31.860	32.096	31.388
1003	43.267	43.125	42.513	41.959	42.557	42.429	43.194	42.319
1014	56.314	55.928	55.642	55.513	55.087	55.631	58.457	57.442
1019	72.642	72.082	70.808	70.346	71.139	70.860	73.810	70.780
1032	31.198	31.050	30.659	30.119	30.579	30.510	31.189	30.495
1046	45.165	45.150	44.488	44.120	44.819	44.362	44.781	44.496
1047	66.415	66.264	65.693	65.041	65.378	65.429	67.407	65.509
1048	78.344	78.205	77.464	76.840	77.391	77.342	80.237	77.578
1049	96.027	95.635	94.568	93.284	94.073	94.189	100.868	94.665
1074	55.140	55.030	54.604	54.211	54.341	54.439	56.273	54.772
1085	68.219	67.977	67.321	66.512	66.961	67.026	70.329	67.360
1108	101.989	101.593	100.210	98.603	100.076	99.820	104.580	99.210
1109	68.811	68.463	67.829	67.879	67.485	67.938	71.395	69.410
1115	93.408	92.782	91.683	90.521	91.250	91.357	96.781	91.790
1117	57.644	57.475	56.857	56.042	56.591	56.553	60.312	57.194
1119	118.474	117.895	116.224	114.428	116.059	115.758	122.631	115.098
1135	93.070	92.073	91.069	90.157	90.281	90.745	96.520	91.872
1149	50.061	49.965	49.626	49.214	49.398	49.428	51.500	50.227
1193	50.605	50.576	49.020	49.506	49.797	49.428	50.813	49.647
1193	58.898	58.878	58.234	57.961	57.974	57.937	59.820	58.319
1194	50.272	50.230	49.572		49.422	49.298	50.694	49.473
1191	50.212	50.250	45.512	49.117	43.422	43.230	50.094	45.413

ID	LSDA	PBE	HCTH	N12	revTPSS	tHCTH	M11-L	MN12-L
1207	66.645	66.618	65.888	65.895	66.016	65.949	67.540	66.176
1209	68.748	68.051	67.245	66.785	66.992	67.192	70.088	68.036
1241	36.788	36.795	36.366	36.059	36.392	36.287	37.880	36.707
1250	49.057	48.732	48.184	47.762	48.040	48.049	49.114	48.235
1251	81.860	81.394	80.546	79.490	79.961	80.151	84.506	80.528
1256	118.966	118.542	117.234	115.986	116.989	116.941	121.353	116.076
1314	65.399	64.576	63.919	63.272	63.281	63.682	66.648	64.355
1315	50.389	49.895	49.578	49.166	48.933	49.297	50.606	49.919
1332	84.857	84.482	83.438	82.420	83.198	83.267	88.621	84.253
1344	80.399	79.935	78.809	77.636	78.712	78.491	82.296	78.339
1361	69.795	69.522	68.982	68.118	68.448	68.587	70.643	68.752
1363	54.410	54.021	53.867	52.825	52.036	52.669	55.197	52.634
1367	73.903	73.545	73.024	72.296	72.446	72.668	74.986	73.255
1378	75.698	75.692	74.872	73.740	74.604	74.479	77.493	74.047
1382	43.526	43.426	42.798	42.183	42.895	42.652	43.770	42.744
1391	61.240	61.182	60.427	59.713	60.473	60.223	61.117	59.736
1395	87.479	86.774	85.926	85.965	85.229	86.162	90.104	87.447
1396	102.138	101.917	100.761	100.605	100.445	100.742	102.718	100.130
1406	69.766	69.528	68.994	68.126	68.519	68.607	70.741	68.818
1408	53.453	53.123	52.813	52.304	52.276	52.616	54.555	53.506
1409	73.754	73.396	72.907	72.170	72.294	72.553	74.918	73.184
1428	62.276	62.175	61.625	61.114	61.494	61.441	62.605	61.377
1429	85.169	84.729	83.645	82.748	83.566	83.487	86.758	83.032
1438	55.074	54.692	54.186	53.681	53.813	53.936	55.237	54.084
1444	76.571	76.403	75.551	74.999	75.225	75.181	76.887	74.890
1455	81.537	81.186	80.328	79.768	80.155	80.227	83.381	80.428
1457	59.554	59.375	58.768	58.511	58.745	58.669	60.421	59.352
1475	54.583	54.584	53.862	53.529	54.225	53.750	54.813	54.349
1479	89.838	89.293	88.148	87.323	87.984	87.979	91.692	88.474
1502	86.769	86.345	85.335	84.875	85.165	85.265	88.576	85.353
1563	70.955	70.811	69.850	69.003	69.651	69.376	70.160	68.439
1564	84.608	84.453	83.562	82.740	83.143	83.051	85.874	82.785
1588	104.359	103.792	102.452	101.186	102.277	102.086	106.806	101.984
1603	104.077	103.591	102.362	101.439	102.210	102.166	106.286	101.771
1604	95.720	95.236	93.852	92.583	93.849	93.500	97.845	93.098
1607	66.881	66.787	66.184	65.621	66.022	65.958	67.630	66.321
1610	69.232	68.926	68.383	67.633	67.833	67.989	69.782	67.998
1617	106.687	106.286	105.096	103.727	104.550	104.515	110.921	104.606
1619	72.916	72.903	72.201	71.688	71.877	71.799	73.626	71.857
1622	85.868	85.341	84.195	83.354	84.080	84.015	87.093	83.538
1625	75.591	75.131	74.412	73.587	73.969	74.112	77.731	74.875
1626	89.143	88.956	87.560	87.187	87.801	87.532	88.602	86.133
1630	54.069	53.830	53.266	52.795	52.990	53.076	54.566	53.081
1633	121.522	120.846	118.927	118.611	119.069	119.000	123.389	117.220
1634	70.486	70.432	69.427	69.042	69.679	69.378	71.100	69.099
1001	10.400	10.402	00.421	00.042	00.019	00.010	, 1.100	00.000

ID	PBE0	mPW1PW	B3LYP	B3PW91	B97-2	M06	M06-2X	MO6-HF	SOGGA11X	·	BMK	TPSSh
0056	55.295	55.195	56.002	55.317	55.277	55.974	54.870	54.960	55.360	55.695	55.174	55.634
0093	51.048	50.915	51.731	51.173	51.024	51.445	50.643	49.906	50.585	51.556	51.002	51.487
0097	50.969	50.840	51.756	51.139	50.874	51.908	50.764	49.780	50.469	51.467	51.033	51.382
0103	48.668	48.517	49.361	48.743	48.621	49.427	48.273	47.173	48.320	49.090	48.720	48.935
0112	62.452	62.356	63.360	62.813	62.600	62.684	60.990	60.280	61.752	63.611	61.966	63.658
0117	54.348	54.154	54.817	54.374	54.292	54.389	53.706	53.805	53.971	54.897	53.803	54.840
0119	59.477	59.394	60.222	59.407	59.495	60.997	58.752	58.113	59.897	59.815	59.419	59.538
0129	87.276	87.045	88.469	87.472	87.058	88.826	86.875	85.910	86.469	88.017	86.945	87.849
0142	41.154	41.055	41.731	41.223	41.079	42.046	40.865	40.419	41.026	41.512	41.150	41.400
0158	18.230	18.196	18.464	18.288	18.228	18.320	17.954	17.798	18.179	18.427	18.205	18.450
0159	64.462	64.313	65.179	64.710	64.470	64.821	63.516	63.043	63.857	65.302	63.915	65.448
0205	49.343	49.239	50.081	49.430	49.418	49.174	48.738	49.177	49.203	49.992	49.639	49.794
0213	72.473	72.267	73.599	72.744	72.377	73.604	72.044	70.267	71.402	73.265	72.486	73.185
0223	42.678	42.586	43.114	42.750	42.687	42.872	42.284	42.252	42.566	43.112	42.577	43.073
0245	59.492	59.268	60.106	59.638	59.462	59.876	58.218	56.853	58.697	60.187	57.999	60.400
0256	54.215	54.030	54.846	54.323	54.192	54.591	53.305	53.058	53.529	54.885	53.291	55.109
0257	54.031	53.795	54.836	54.054	53.976	54.566	53.030	52.668	53.184	54.681	52.903	54.878
0267	91.022	90.846	92.432	91.229	90.951	92.565	90.711	91.404	90.957	91.855	90.436	91.700
0276	71.467	71.260	72.257	71.503	71.508	72.334	70.071	69.346	71.191	72.249	70.658	72.001
0281	56.715	56.568	57.302	56.805	56.740	57.146	55.811	55.348	56.468	57.351	56.254	57.225
0282	67.046	66.842	67.741	67.137	66.941	67.921	66.226	65.753	66.392	67.733	66.410	67.610
0287	70.206	70.024	71.266	70.536	70.251	71.162	68.803	66.786	69.152	71.212	69.479	71.360
0306	60.258	60.080	61.209	60.318	60.184	61.346	59.736	59.843	60.035	60.833	59.561	60.825
0318	59.866	59.618	60.580	59.881	59.815	60.307	58.726	58.010	59.336	60.506	58.868	60.538
0332	46.721	46.535	47.212	46.807	46.661	46.972	45.790	45.004	46.129	47.253	45.803	47.364
0336	50.976	50.834	51.513	51.113	50.940	51.502	50.149	49.383	50.499	51.557	50.331	51.707
0342	69.219	69.008	70.266	69.383	69.287	69.520	68.032	67.503	68.769	70.271	68.850	70.259
0346	104.609	104.338	106.080	104.861	104.619	105.836	103.644	103.477	103.664	106.047	104.215	105.868
0351	29.197	29.072	29.484	29.219	29.139	29.200	28.616	28.320	28.819	29.492	28.633	29.541
0353	17.112	17.046	17.298	17.139	17.078	17.188	16.738	16.353	16.895	17.275	16.734	17.328
0361	73.473	73.330	74.372	73.385	73.521	74.875	72.825	72.449	74.023	74.050	73.419	73.803
0381	107.902	107.673	109.176	108.326	107.624	109.920	107.239	106.803	106.399	109.112	107.256	109.251
0390	87.103	86.940	88.462	87.497	87.419	86.366	84.827	84.776	86.013	88.739	86.670	88.494
0393	38.044	37.983	38.740	38.183	38.141	38.435	37.247	36.732	37.927	38.647	37.910	38.694
0397	81.309	81.033	82.458	81.502	81.160	82.872	80.293	79.393	80.263	82.354	80.299	82.406
0399	32.740	32.642	33.273	32.875	32.767	33.337	31.877	30.889	32.472	33.247	31.990	33.534
0425	58.344	58.186	59.085	58.368	58.293	59.094	58.058	57.753	58.402	58.792	58.340	58.646
0438	54.490	54.395	55.186	54.649	54.513	55.159	53.642	52.843	54.246	55.102	54.083	55.293
0445	57.142	57.030	57.904	57.339	57.085	57.900	56.674	56.424	56.610	57.765	56.773	57.886
0460	98.138	97.888	99.389	98.408	98.028	99.298	97.361	96.823	97.179	99.167	97.450	99.130
0470	35.775	35.668	36.269	35.866	35.699	36.448	35.321	34.449	35.482	36.128	35.495	36.148
0489	66.092	65.798	66.906	66.119	66.005	66.690	65.026	64.711	65.149	66.868	64.842	67.012
0529	51.695	51.481	52.269	51.794	51.652	51.907	50.673	50.166	50.992	52.346	50.661	52.503
0533	63.399	63.111	64.285	63.450	63.346	64.020	62.162	61.342	62.445	64.203	61.991	64.454
0556	52.209	51.988	52.779	52.304	52.135	52.440	51.159	50.277	51.429	52.799	51.126	52.912
0580	40.608	40.511	41.364	40.721	40.687	40.991	39.876	39.451	40.500	41.244	40.417	41.319
0599	28.581	28.479	28.923	28.612	28.560	28.726	28.171	27.853	28.326	28.874	28.166	28.937
0617	71.192	71.056	72.285	71.546	71.412	70.888	69.233	68.541	70.294	72.507	70.600	72.457
0654	53.671	53.562	54.479	53.904	53.670	54.133	52.971	52.482	53.123	54.407	53.635	54.394
0655	38.701	38.623	39.242	38.836	38.728	38.774	38.012	37.791	38.416	39.231	38.571	39.299
0000	55.701	00.020	00.242	55.550	00.120	00.114	00.012	01.131	50.410	00.201	00.011	00.200

ID	PBE0	mPW1PW	B3LYP	B3PW91	B97-2	M06	M06-2X		SOGGA11X	•	BMK	TPSSh
0670	40.389	40.311	40.933	40.473	40.429	40.288	39.904	40.013	40.285	40.857	40.545	40.746
0710	51.908	51.732	52.579	52.032	51.805	52.586	51.323	50.669	51.327	52.456	51.531	52.411
0722	64.863	64.689	65.790	65.112	64.752	65.848	64.160	63.568	64.105	65.661	64.480	65.658
0753	58.541	58.380	59.329	58.597	58.502	59.336	58.139	57.703	58.523	59.073	58.530	58.939
0757	48.810	48.647	49.502	48.823	48.720	49.643	48.285	47.731	48.523	49.211	48.404	49.055
0761	95.370	95.131	96.603	95.634	95.364	96.578	94.479	94.005	94.505	96.595	94.892	96.510
0762	34.343	34.257	34.845	34.360	34.269	35.114	34.272	33.876	34.550	34.508	34.477	34.358
0765	68.727	68.545	69.596	68.823	68.755	69.792	67.785	66.743	68.380	69.498	68.097	69.535
0767	64.132	63.993	65.120	64.368	63.961	65.622	63.857	62.617	63.556	64.682	64.228	64.582
0768	67.869	67.685	69.183	68.117	67.909	69.364	66.833	66.341	67.374	68.830	66.604	69.022
0769	57.684	57.535	58.823	57.852	57.671	59.029	57.002	56.921	57.498	58.386	56.847	58.506
0818	54.420	54.305	55.171	54.571	54.291	55.751	54.070	53.372	54.082	54.929	54.407	54.810
0820	41.056	40.948	41.467	41.152	41.032	41.630	40.239	39.317	40.632	41.523	40.352	41.666
0833	64.066	63.896	64.834	64.111	64.103	64.480	63.069	62.966	63.842	64.821	63.710	64.596
0841	55.403	55.278	56.055	55.454	55.398	56.008	54.862	54.328	55.286	55.927	55.048	55.994
0843	63.609	63.437	64.349	63.662	63.476	64.412	63.247	63.293	63.286	64.147	63.236	64.128
0846	76.733	76.528	77.583	76.890	76.715	77.183	76.020	75.462	76.104	77.585	76.432	77.539
0847	65.099	64.918	66.067	65.300	65.003	66.032	64.601	63.670	64.271	65.841	64.866	65.773
0852	95.161	94.883	96.518	95.444	95.054	95.891	94.460	93.740	93.948	96.162	94.507	96.099
0884	42.881	42.758	43.311	42.981	42.852	43.023	42.134	41.894	42.488	43.375	42.393	43.489
0886	43.178	43.099	43.699	43.291	43.211	43.713	42.480	41.836	43.016	43.669	42.895	43.684
0890	44.856	44.706	45.339	44.961	44.810	45.288	43.997	43.183	44.369	45.408	44.096	45.603
0909	56.226	56.122	57.066	56.446	56.336	56.261	55.149	54.983	55.818	57.129	56.131	57.053
0936	69.255	69.007	70.080	69.366	69.154	70.194	68.394	67.860	68.548	70.043	68.548	69.978
0969	56.674	56.544	57.409	56.896	56.535	57.700	56.044	55.280	55.970	57.299	56.239	57.499
0974	39.843	39.726	40.296	39.957	39.804	40.261	39.017	38.325	39.445	40.319	39.160	40.597
0976	71.866	71.673	72.749	72.010	71.712	72.638	71.285	70.930	71.342	72.463	71.188	72.522
0987	64.420	64.263	65.199	64.654	64.460	64.897	63.344	62.390	63.869	65.292	63.809	65.435
0989	92.493	92.192	93.738	92.736	92.405	93.512	91.825	89.822	91.097	93.446	92.255	93.388
0998	30.793	30.710	31.140	30.912	30.754	31.176	30.028	29.226	30.346	31.170	30.183	31.426
1003	41.194	41.089	41.602	41.302	41.165	41.622	40.374	39.670	40.703	41.662	40.515	41.794
1014	54.356	54.203	54.997	54.336	54.351	55.253	53.517	53.093	54.249	54.858	53.844	54.662
1019	69.298	69.136	70.152	69.485	69.187	70.266	68.818	68.656	68.736	70.068	69.025	70.029
1032	29.508	29.403	29.805	29.562	29.466	29.735	28.865	28.255	29.142	29.834	28.870	29.972
1046	44.353	44.294	44.797	44.394	44.226	44.626	44.535	44.623	44.486	44.467	44.787	44.446
1047	63.548	63.383	64.366	63.678	63.586	64.514	62.586	61.334	63.145	64.289	62.840	64.387
1048	75.710	75.552	76.625	75.871	75.757	76.351	74.923	74.410	75.526	76.499	75.477	76.402
1049	91.924	91.718	93.404	92.134	91.871	93.681	91.490	91.447	91.446	92.808	91.418	92.651
1074	53.285	53.165	53.918	53.335	53.301	54.181	52.737	51.916	53.412	53.743	53.007	53.712
1085	65.442	65.265	66.303	65.543	65.427	66.500	64.619	63.329	65.163	66.093	64.898	66.055
1108	97.034	96.796	98.575	97.395	96.985	98.533	96.189	95.061	96.159	98.122	96.120	98.242
1109	65.931	65.764	66.749	66.103	66.023	65.709	64.697	64.786	65.326	66.912	65.615	66.661
1115	89.180	88.937	90.449	89.342	89.057	90.803	88.706	88.375	88.611	90.043	88.567	89.939
1117	55.117	54.957	55.924	55.199	55.096	56.257	54.511	53.328	54.946	55.696	54.766	55.722
1119	113.215	112.953	114.938	113.557	113.074	115.503	112.956	112.711	112.304	114.302	112.762	114.190
1135	88.353	88.041	89.433	88.399	88.176	89.704	87.659	87.373	87.448	89.259	87.551	89.103
1149	48.393	48.268	49.055	48.408	48.404	49.024	48.019	47.704	48.634	48.837	48.281	48.807
1193	48.905	48.784	49.576	49.037	48.845	49.578	48.675	47.658	48.494	49.310	49.043	49.254
1194	56.899	56.774	57.772	57.043	56.880	57.869	56.458	55.181	56.490	57.440	56.894	57.361
1197	48.385	48.255	49.040	48.511	48.341	49.179	47.894	46.561	47.908	48.849	48.262	48.826

ID	PBE0	mPW1PW	B3LYP	B3PW91	B97-2	M06	M06-2X	MO6-HE	SOGGA11X	+HCTHhyb	BMK	TPSSh
1207	63.992	63.903	64.864	64.314	64.187	63.530	62.356	61.825	63.323	65.037	63.636	64.981
1209	65.677	65.468	66.366	65.735	65.558	66.457	65.002	64.727	65.161	66.317	65.154	66.195
1241	35.495	35.430	35.996	35.558	35.494	36.077	35.031	34.466	35.465	35.838	35.234	35.874
1250	46.609	46.460	47.121	46.691	46.597	46.861	45.878	45.603	46.313	47.167	46.046	47.232
1251	77.639	77.414	78.830	77.814	77.609	78.861	76.823	76.429	77.162	78.517	76.543	78.587
1256	113.644	113.407	115.359	114.141	113.724	114.747	112.020	110.421	112.410	115.116	112.673	115.088
1314	62.011	61.751	62.703	62.017	61.862	62.442	61.320	61.488	61.401	62.611	61.274	62.480
1315	47.722	47.523	48.247	47.742	47.676	47.931	46.862	46.677	47.304	48.247	46.959	48.247
1332	81.206	81.024	82.498	81.400	81.169	82.591	80.334	79.737	80.797	82.068	80.552	81.937
1344	76.490		77.422	76.631	76.355							77.385
		76.247				77.651	75.728	75.014	75.649	77.308	75.834	
1361	66.302	66.078	67.164	66.414 49.642	66.323	67.206	65.183	64.123	65.720	67.129	65.282	67.297
1363	49.482	49.229	50.353		49.578	50.155	47.985	45.940	48.653	50.324	48.015	50.598
1367	70.407	70.176	71.263	70.484	70.402	71.322	69.373	68.681	69.800	71.243	69.486	71.355
1378	72.159	71.962	73.113	72.358	72.215	73.152	70.999	69.328	71.562	73.051	71.243	73.227
1382	41.429	41.317	41.895	41.524	41.405	42.018	40.559	39.741	41.059	41.908	40.828	42.063
1391	58.692	58.566	59.364	58.848	58.697	59.493	57.796	56.771	58.379	59.320	58.114	59.464
1395	82.988	82.752	83.852	83.275	83.112	82.740	81.074	80.705	81.860	84.360	82.012	84.051
1396	95.608	95.440	97.142	96.360	96.060	95.114	91.808	89.574	93.697	97.863	93.890	98.033
1406	66.489	66.269	67.363	66.580	66.500	67.397	65.532	64.683	65.996	67.275	65.566	67.423
1408	50.988	50.808	51.556	51.035	50.987	51.405	50.066	49.253	50.619	51.548	50.255	51.579
1409	70.328	70.091	71.196	70.397	70.318	71.240	69.346	68.715	69.729	71.148	69.422	71.242
1428	59.532	59.384	60.257	59.668	59.582	60.218	58.716	58.120	59.088	60.270	58.799	60.468
1429	81.660	81.456	82.685	81.826	81.587	82.850	81.022	80.458	81.217	82.474	81.173	82.392
1438	51.980	51.791	52.607	52.090	52.002	52.245	51.074	50.826	51.536	52.692	51.229	52.802
1444	73.254	73.059	74.216	73.456	73.265	74.117	72.397	70.975	72.573	74.118	72.785	74.139
1455	78.395	78.223	79.351	78.556	78.390	79.818	77.645	76.676	78.043	79.213	78.038	79.126
1457	57.563	57.445	58.147	57.603	57.538	57.838	57.390	58.158	57.595	58.026	57.539	58.011
1475	53.599	53.533	54.204	53.634	53.477	54.105	53.792	53.865	53.955	53.776	54.064	53.761
1479	86.173	85.947	87.206	86.312	86.050	86.842	85.709	85.910	85.701	86.938	85.626	86.824
1502	82.913	82.721	84.005	83.206	82.960	83.301	81.523	80.770	81.937	83.996	82.178	83.929
1563	67.425	67.225	68.318	67.663	67.394	68.155	66.516	64.888	66.453	68.225	66.732	68.450
1564	81.431	81.202	82.547	81.620	81.382	82.578	80.842	79.403	80.719	82.252	81.427	82.137
1588	99.400	99.152	100.856	99.708	99.332	101.034	98.627	98.013	98.610	100.519	98.770	100.561
1603	99.713	99.489	101.004	100.020	99.713	100.869	98.560	97.564	98.915	100.862	99.222	100.733
1604	91.171	90.944	92.450	91.471	91.077	92.498	90.492	89.821	90.374	92.161	90.671	92.230
1607	64.299	64.151	65.113	64.420	64.318	65.212	63.542	62.905	64.171	64.969	63.762	65.065
1610	65.758	65.544	66.613	65.863	65.760	66.591	64.742	63.830	65.137	66.561	64.793	66.726
1617	101.433	101.178	103.083	101.723	101.408	103.516	100.578	100.020	100.577	102.620	100.563	102.681
1619	70.240	70.055	71.189	70.394	70.254	71.243	69.634	68.307	69.856	70.978	70.138	70.966
1622	82.153	81.946	83.118	82.358	82.069	83.425	81.405	80.370	81.564	82.996	81.791	82.908
1625	72.087	71.863	73.028	72.165	72.027	73.212	71.250	70.585	71.611	72.863	71.337	72.888
1626	83.362	83.223	84.681	84.011	83.652	83.343	80.536	78.947	81.895	85.213	82.099	85.532
1630	51.558	51.425	52.158	51.662	51.574	52.267	50.870	50.116	51.504	52.128	51.095	52.161
1633	114.563	114.335	116.374	115.253	114.716	115.408	112.250	111.417	112.431	116.724	113.683	116.661
1634	66.960	66.816	67.851	67.262	67.074	66.696	65.271	65.009	66.033	68.115	66.381	68.235

ID	LC-rTPSS	LC-wPBE	LC-N12		LC-tHCTH	M11	CAM-B3LYP	wB97XD	wB97	wB97X
0056	53.819	53.935	53.434	54.690	55.537	54.845	55.328	55.201	54.919	55.101
0093	49.077	49.506	48.664	49.857	50.676	50.886	50.867	51.074	50.530	50.867
0097	48.921	49.326	48.383	49.557	50.509	51.171	50.808	51.032	50.235	50.714
0103	46.766	47.122	46.444	47.735	48.540	48.437	48.543	48.730	48.170	48.525
0112	59.182	59.836	58.488	59.405	60.400	61.337	61.714	61.911	60.863	61.302
0117	52.459	52.663	51.826	53.034	53.687	53.843	54.021	54.086	53.528	53.841
0119	58.129	58.057	57.944	59.441	60.617	58.659	59.787	59.677	59.241	59.582
0129	83.848	84.271	82.165	84.653	86.084	86.801	86.789	86.704	85.151	86.079
0142	39.846	39.945	39.283	40.331	41.140	40.975	41.154	41.183	40.606	40.968
0158	17.880	18.022	17.661	17.974	18.237	18.178	18.306	18.375	18.415	18.406
0159	62.238	62.778	61.512	62.541	63.350	63.735	64.060	64.211	63.800	63.985
0205	46.877	47.067	46.341	47.606	48.667	48.308	49.020	49.085	48.096	48.621
0213	69.005	69.737	68.231	70.012	71.240	72.553	71.923	72.295	71.074	71.776
0223	41.384	41.600	40.993	41.778	42.420	42.364	42.573	42.681	42.395	42.569
0245	57.219	57.732	56.246	57.716	58.180	58.192	59.032	59.056	58.638	58.864
0256	52.267	52.681	51.543	52.743	53.142	53.482	53.896	53.919	53.482	53.702
0257	51.531	51.918	50.617	52.477	52.849	52.989	53.611	53.434	52.665	53.090
0267	87.707	88.213	86.221	88.724	90.294	90.302	90.764	90.841	89.375	90.223
0276	68.312	68.454	67.777	69.543	70.638	69.965	70.875	70.855	69.719	70.311
0281	54.540	54.769	54.074	55.227	56.062	55.839	56.355	56.431	55.755	56.116
0282	64.502	64.732	63.610	65.102	66.036	66.421	66.588	66.597	65.586	66.138
0287	66.658	67.460	66.053	67.536	68.483	69.055	69.517	69.781	68.801	69.284
0306	57.779	58.117	56.786	58.546	59.363	59.687	59.964	59.962	58.985	59.523
0318	57.488	57.782	56.656	58.509	59.140	58.778	59.519	59.478	58.778	59.167
0332	45.070	45.417	44.382	45.506	45.862	45.911	46.458	46.469	46.110	46.301
0336	49.523	49.843	48.891	49.788	50.312	50.357	50.795	50.816	50.609	50.709
0342	65.966	66.475	64.853	66.862	68.026	67.743	68.724	68.854	67.887	68.377
0346	98.827	99.326	97.083	99.979	101.864	102.891	103.218	103.291	100.930	102.148
0351	28.336	28.493	27.878	28.647	28.812	28.788	29.109	29.086	28.910	29.015
0353	16.728	16.842	16.452	16.882	16.933	16.868	17.130	17.101	17.079	17.099
0361	71.186	71.177	70.745	72.734	74.024	72.456	73.458	73.449	72.705	73.174
0381	103.329	103.839	101.048	103.231	105.159	107.654	106.814	106.980	104.755	105.969
0390	80.451	81.056	79.651	81.450	83.127	83.830	85.277	85.304	82.633	83.846
0393	36.193	36.475	35.767	36.705	37.413	37.132	37.894	37.947	37.342	37.651
0393	77.502	78.047	75.954	78.354	79.602	80.246	80.555	80.573	79.124	79.916
			30.950							32.510
0399 0425	31.443	31.744 56.749		31.711 57.483	32.012 58.420	31.980 57.648	32.610 58.313	32.628 58.286	32.403	58.123
	56.566		55.723						57.744	
0438	52.815	53.182	52.261	53.271	53.993	53.668	54.374	54.453	54.148	54.322
0445	55.521	55.903	54.786	55.875	56.697	57.066	57.114	57.140	56.647	56.950
0460	94.103	94.736	92.493	94.969	96.394	97.206	97.383	97.442	95.881	96.737
0470	34.487	34.646	33.915	34.782	35.305	35.194	35.668	35.666	35.191	35.473
0489	63.222	63.632	62.153	64.194	64.736	65.032	65.527	65.437	64.544	65.035
0529	49.486	49.861	48.742	49.968	50.354	50.741	51.204	51.220	50.591	50.898
0533	60.280	60.744	59.176	61.277	61.767	61.920	62.757	62.627	61.689	62.192
0556	50.026	50.407	49.293	50.545	50.916	51.265	51.753	51.707	51.083	51.393
0580	38.566	38.839	38.000	39.132	39.831	39.602	40.380	40.422	39.729	40.083
0599	27.694	27.831	27.322	28.049	28.265	28.208	28.524	28.466	28.273	28.382
0617	66.383	66.961	65.744	67.126	68.326	68.701	69.973	70.075	68.226	69.067
0654	51.324	51.691	50.527	51.722	52.747	53.022	53.344	53.478	52.545	53.048
0655	37.320	37.608	36.794	37.628	38.258	38.046	38.590	38.687	38.371	38.540

ID	LC-rTPSS	LC-wPBE	LC-N12	LC-HCTH	LC-tHCTH	M11	CAM-B3LYP	wB97XD	wB97	wB97X
0670	38.771	38.961	38.379	39.305	40.093	39.799	40.261	40.337	39.778	40.101
0710	49.848	50.180	48.983	50.399	51.129	51.434	51.633	51.634	50.852	51.303
0722	62.048	62.436	60.839	62.491	63.631	64.429	64.371	64.439	63.240	63.900
0753	56.483	56.717	55.631	57.362	58.339	57.730	58.404	58.403	57.722	58.151
0757	46.947	47.084	46.199	47.724	48.477	48.199	48.612	48.573	47.844	48.269
0761	90.607	91.102	89.057	91.531	93.199	94.043	94.271	94.371	92.517	93.503
0762	33.530	33.519	33.052	34.073	34.828	34.205	34.497	34.521	34.156	34.414
0765	65.921	66.318	65.069	66.870	67.737	67.386	68.288	68.328	67.474	67.934
0767	61.802	62.117	60.575	62.215	63.501	64.074	63.936	64.001	62.856	63.551
0768	64.103	64.789	63.064	64.826	65.683	66.669	67.185	67.332	65.748	66.528
0769	54.841	55.380	53.945	55.516	56.313	57.035	57.332	57.400	56.237	56.836
0818	52.584	52.784	51.729	52.956	54.075	54.345	54.319	54.409	53.513	54.053
0820	40.085	40.365	39.428	40.266	40.641	40.542	40.964	41.000	41.037	41.006
0833	61.230	61.415	60.667	62.230	63.300	62.857	63.605	63.657	62.598	63.150
0841	53.725	53.983	52.944	54.332	55.065	54.563	55.281	55.315	54.983	55.178
0843	61.688	61.901	60.820	62.310	63.279	63.319	63.443	63.359	62.844	63.171
0846	73.636	74.189	72.885	74.516	75.701	76.114	76.173	76.459	75.631	76.098
0847	62.211	62.677	61.420	63.008	64.119	64.924	64.657	64.869	63.763	64.389
0852	90.976	91.671	89.603	92.264	93.694	94.390	94.429	94.430	92.957	93.811
0884	41.690	41.975	41.032	41.916	42.409	42.401	42.745	42.825	42.729	42.786
0886	41.904	42.152	41.461	42.327	43.008	42.628	43.109	43.191	42.980	43.102
0890	43.477	43.796	42.754	43.717	44.132	44.125	44.666	44.725	44.565	44.645
0909	53.279	53.712	52.651	53.774	54.808	55.084	55.676	55.812	54.763	55.257
0936	66.163	66.556	65.149	66.910	67.810	68.366	68.651	68.714	67.503	68.150
0969	54.995	55.353	53.766	54.999	55.916	56.575	56.509	56.585	56.087	56.381
0974	38.826	39.118	38.105	38.950	39.327	39.312	39.769	39.780	39.819	39.802
0976	69.885	70.306	68.627	70.440	71.398	71.497	71.777	71.689	71.229	71.540
0987	62.093	62.612	61.223	62.571	63.565	63.494	64.051	64.198	63.783	63.994
0989	87.944	88.931	87.139	89.451	90.680	92.234	91.587	92.081	90.675	91.469
0998	30.256	30.545	29.625	30.230	30.445	30.461	30.802	30.837	31.081	30.938
1003	40.292	40.579	39.672	40.437	40.820	40.817	41.121	41.146	41.199	41.157
1014	52.450	52.546	52.020	53.452	54.263	53.434	54.200	54.112	53.472	53.849
1019	66.680	66.977	65.586	67.069	68.354	68.997	68.892	69.021	67.948	68.556
1032	28.750	28.961	28.254	28.925	29.063	29.071	29.438	29.468	29.432	29.446
1046	44.630	44.751	44.198	44.946	45.574	44.738	44.924	44.896	45.395	45.247
1047	60.939	61.384	60.155	61.727	62.481	62.239	63.134	63.170	62.452	62.834
1048	72.830	73.187	71.867	73.731	74.946	74.498	75.281	75.334	74.436	74.954
1049	88.374	88.897	86.827	89.572	91.021	91.146	91.581	91.547	90.023	90.933
1074	51.904	52.165	51.463	52.682	53.412	52.519	53.335	53.371	53.159	53.326
1085	62.697	63.079	61.737	63.584	64.521	64.201	65.073	65.108	64.175	64.715
1108	93.192	93.843	91.466	94.246	95.674	95.823	96.398	96.296	94.980	95.702
1109	62.175	62.534	61.510	62.865	63.964	64.396	65.036	65.097	63.634	64.331
1115	85.489	85.991	83.973	86.502	87.769	88.540	88.636	88.629	87.075	87.941
1117	52.745	53.045	51.849	53.454	54.280	54.131	54.796	54.848	54.035	54.488
1119	108.705	109.508	106.536	109.870	111.611	112.682	112.658	112.689	110.731	111.875
1135	84.325	84.656	82.843	85.416	86.677	87.493	87.503	87.501	85.767	86.719
1149	46.782	46.961	46.279	47.582	48.320	47.579	48.356	48.398	47.938	48.218
1193	47.344	47.788	46.960	48.067	48.835	48.922	48.880	49.082	48.765	48.992
1194	54.762	55.254	54.417	55.759	56.670	56.582	56.815	56.969	56.374	56.746
1197	46.729	47.178	46.281	47.405	48.146	48.201	48.280	48.497	48.189	48.394

ID	LC-rTPSS	LC-wPBE	LC-N12	I С-НСТН	LC-tHCTH	M11	CAM-B3LYP	wB97XD	wB97	wB97X
1207	60.125	60.647	59.654	60.680	61.784	62.287	63.047	63.198	61.790	62.448
1209	63.263	63.461	62.340	63.916	64.907	65.154	65.287	65.334	64.382	64.921
1241	34.630	34.833	34.279	35.068	35.571	35.155	35.605	35.599	35.499	35.580
1250	44.936	45.212	44.331	45.379	45.958	45.984	46.369	46.449	46.048	46.271
1251	74.081	74.694	72.936	74.981	75.891	76.829	77.077	77.143	75.703	76.443
1256	107.618	108.381	105.983	108.826	110.578	111.010	112.196	112.004	109.705	110.875
1314	59.349	59.565	58.284	60.148	60.994	61.425	61.504	61.506	60.399	61.024
1315	45.800	46.030	45.270	46.457	46.920	46.901	47.393	47.418	46.784	47.125
1332	77.569	77.890	76.264	78.626	80.010	79.714	80.576	80.571	79.049	79.852
1344	73.420	73.846	71.863	74.015	74.985	75.711	75.879	75.920	74.850	75.443
1361	63.398	63.841	62.473	64.275	64.938	64.854	65.747	65.769	64.931	65.368
1363	45.728	46.448	45.085	46.439	46.737	47.208	48.381	48.595	47.407	47.932
1367	67.482	67.856	66.542	68.439	69.186	69.143	69.855	69.834	68.942	69.414
1378	68.935	69.487	67.691	69.660	70.522	70.382	71.508	71.576	70.695	71.143
1382	40.454	40.724	39.763	40.720	41.199	40.831	41.392	41.446	41.503	41.476
1391	57.269	57.739	56.545	57.734	58.416	57.960	58.655	58.732	58.704	58.733
1395	77.817	78.347	77.019	78.337	79.486	80.902	81.395	81.479	79.509	80.374
1396	87.633	88.720	86.897	88.257	89.627	91.148	93.082	93.284	90.260	91.509
1406	63.650	64.085	62.711	64.586	65.280	65.212	66.005	66.017	65.185	65.628
1408	48.995	49.198	48.406	49.660	50.160	50.001	50.634	50.607	50.012	50.316
1409	67.430	67.788	66.521	68.434	69.160	69.129	69.796	69.779	68.857	69.345
1428	57.450	57.841	56.796	58.027	58.630	58.669	59.227	59.267	58.837	59.044
1429	78.714	79.070	77.388	79.574	80.865	80.719	81.244	81.225	80.228	80.829
1438	49.629	49.968	48.965	50.213	50.826	51.069	51.501	51.633	50.900	51.273
1444	70.168	70.813	69.479	71.168	72.164	72.400	72.761	72.989	72.194	72.630
1455	75.588	75.938	74.669	76.504	77.730	77.381	78.040	78.104	77.122	77.686
1457	56.243	56.346	55.732	56.831	57.664	57.377	57.500	57.483	57.347	57.449
1475	53.643	53.775	53.752	54.141	54.913	53.906	54.240	54.188	54.584	54.502
1479	83.257	83.666	82.014	84.099	85.441	85.681	85.844	85.763	84.834	85.402
1502	78.326	78.909	77.202	79.061	80.349	81.351	81.833	81.847	80.043	80.956
1563	64.802	65.519	63.938	65.505	66.254	66.878	67.019	67.210	66.679	66.973
1564	77.957	78.596	76.935	79.151	80.384	80.634	80.914	81.114	80.010	80.656
1588	95.184	95.840	93.615	96.154	97.566	98.335	98.662	98.697	97.051	97.939
1603	95.175	95.799	93.734	96.167	97.741	98.191	98.820	98.857	97.137	98.060
1604	87.596	88.226	86.035	88.345	89.636	90.370	90.572	90.661	89.340	90.061
1607	62.269	62.678	61.686	62.997	63.791	63.389	64.176	64.256	63.774	64.056
1610	62.209	63.405	62.119	63.825	64.440	64.512	65.245	65.203	64.412	64.827
1617	96.484	97.309	94.747	97.627	99.007	100.276	100.569	100.578	98.572	99.652
1619	67.351	67.920	66.702	68.426	69.435	69.425	69.873	70.137	69.323	69.789
1622	79.091	79.557	77.868	79.778	80.996	81.318	81.656	81.721	80.646	81.254
1625	68.972	69.330	67.861	69.867	70.820	71.173	71.542	71.529	70.397	71.007
1626	77.820	78.837	76.934	78.056	70.820	80.606	81.756	81.985	80.178	80.886
1630		50.106						51.432	51.026	
1633	49.754	107.548	49.279	50.263 107.284	50.895 109.340	50.784	51.335	112.394	108.930	51.240 110.573
	106.715		104.932	64.011	65.032	111.800	112.281			
1634	63.650	64.200	62.665	04.011	05.032	65.314	66.202	66.316	65.396	65.788

ID	N12-SX	MN12-SX	HSE06	HISS
0056	55.062	57.218	55.367	54.410
0093	50.672	52.097	51.174	49.886
0097	50.562	52.126	51.132	49.777
0103	48.320	49.879	48.815	47.699
0112	61.988	64.340	62.566	60.456
0117	53.934	56.055	54.390	52.928
0119	59.420	62.128	59.554	59.003
0129	86.446	89.730	87.479	85.244
0142	40.912	42.540	41.219	40.294
0158	18.025	18.563	18.231	17.765
0159	63.888	65.773	64.521	62.558
0205	49.145	51.455	49.427	48.244
0213	71.924	73.470	72.759	70.713
0223	42.389	43.901	42.696	41.637
0245	58.589	60.398	59.575	57.491
0256	53.589	55.614	54.286	52.514
0257	53.435	55.932	54.134	52.273
0267	90.020	94.645	91.196	88.820
0207	71.229	74.195	71.606	70.052
0270	56.448	58.553	56.780	55.395
0282	66.626	69.299	67.152	65.432
0287	69.724	71.370	70.430	68.147
0306	59.525	63.583	60.383	58.521
0318	59.284	61.815	59.947	58.179
0332	46.130	47.849	46.764	45.203
0336	50.445	52.107	51.013	49.508
0342	68.488	71.456	69.316	67.033
0346	103.914	108.710	104.887	101.836
0351	28.854	30.007	29.216	28.336
0353	16.886	17.509	17.119	16.607
0361	73.256	76.710	73.585	72.539
0381	107.085	109.654	108.146	105.084
0390	87.009	90.514	87.412	84.837
0393	37.678	39.524	38.097	36.798
0397	80.207	83.853	81.500	78.775
0399	32.225	33.637	32.779	31.449
0425	57.824	60.109	58.425	57.220
0438	54.120	55.987	54.545	53.132
0445	56.558	58.344	57.224	55.620
0460	97.076	100.787	98.340	95.563
0470	35.379	36.867	35.829	34.740
0489	65.383	68.272	66.208	64.062
0529	51.065	53.265	51.762	49.940
0533	62.597	65.477	63.522	61.203
0556	51.587	53.690	52.277	50.486
0580	40.185	42.509	40.665	39.221
0599	28.283	29.448	28.603	27.795
0617	70.986	73.610	71.379	69.074
0654	53.320	54.935	53.761	52.164
0655	38.387	39.667	38.737	37.632

ID	N12-SX	MN12-SX	HSE06	HISS
0670	40.194	41.632	40.431	39.485
0710	51.346	53.257	51.993	50.476
0722	64.229	66.440	65.000	62.993
0753	58.020	60.413	58.632	57.289
0757	48.325	51.280	48.906	47.662
0761	94.691	98.342	95.587	92.861
0762	33.991	35.872	34.400	33.841
0765	68.209	71.000	68.843	67.066
0767	63.606	65.634	64.277	62.678
0768	66.839	71.519	68.043	65.277
0769	56.874	60.870	57.821	55.640
0818	54.104	56.035	54.518	53.212
0820	40.621	42.199	41.090	40.033
0833	63.784	66.810	64.170	62.655
0841	54.880	57.151	55.456	54.194
0843	63.114	65.826	63.698	62.149
0846	76.195	78.516	76.888	74.860
0847	64.586	66.619	65.314	63.485
0852	94.244	97.487	95.446	92.838
0884	42.438	43.862	42.905	41.671
0886	42.923	44.317	43.219	42.222
0890	44.242	45.898	44.889	43.402
0909	55.882	58.282	56.329	54.660
0936	68.580	71.585	69.379	67.256
0969	56.093	57.800	56.758	55.128
0974	39.275	40.717	39.871	38.587
0976	71.022	74.187	71.959	70.115
0987	63.767	65.512	64.486	62.532
0989	91.806	93.753	92.871	90.341
0998	30.341	31.402	30.810	29.856
1003	40.787	42.104	41.224	40.182
1014	54.134	56.745	54.433	53.318
1019	68.805	71.230	69.411	67.520
1032	29.120	30.381	29.525	28.617
1046	43.987	45.033	44.342	43.835
1047	63.024	65.347	63.652	61.868
1048	75.194	77.627	75.828	74.101
1049	90.965	95.661	92.147	89.727
1074	52.903	54.776	53.327	52.178
1085	64.815	67.528	65.544	63.756
1108	95.884	99.990	97.294	94.509
1109	65.675	68.670	66.062	64.191
1115	88.240	92.754	89.372	86.860
1117	54.449	57.374	55.208	53.579
1119	111.842	116.822	113.479	110.242
1135	87.478	92.322	88.546	86.021
1149	47.983	50.183	48.444	47.298
1193	48.507	49.791	49.027	47.907
1194	56.541	58.328	57.054	55.694
1197	47.996	49.297	48.516	47.360

ID	N12-SX	MN12-SX	HSE06	HISS
1207	63.864	65.444	64.130	62.261
1209	65.224	67.871	65.777	64.113
1241	35.203	36.697	35.525	34.703
1250	46.165	47.974	46.647	45.208
1251	76.689	81.115	77.794	75.194
1256	112.873	116.499	114.005	110.945
1314	61.372	64.283	62.121	60.307
1315	47.318	49.433	47.778	46.317
1332	80.296	84.591	81.424	79.330
1344	75.599	78.890	76.632	74.440
1361	65.589	68.456	66.419	64.324
1363	48.746	52.142	49.582	46.865
1367	69.811	72.919	70.532	68.531
1378	71.230	74.026	72.286	70.059
1382	40.974	42.483	41.466	40.381
1391	58.157	59.717	58.743	57.304
1395	82.690	86.388	83.173	80.564
1396	95.416	98.412	95.937	92.118
1406	65.749	68.681	66.603	64.570
1408	50.562	52.963	51.052	49.650
1409	69.714	72.868	70.452	68.491
1428	58.995	61.252	59.616	57.927
1429	80.965	83.637	81.814	79.811
1438	51.472	53.678	52.042	50.244
1444	72.638	74.844	73.437	71.382
1455	77.936	80.574	78.528	76.714
1457	57.212	59.572	57.603	56.471
1475	53.167	54.936	53.599	52.898
1479	85.408	89.078	86.298	84.125
1502	82.529	85.310	83.101	80.690
1563	66.656	68.509	67.587	65.479
1564	80.786	83.104	81.657	79.632
1588	98.407	102.684	99.641	96.772
1603	99.000	102.176	99.918	97.306
1604	90.165	93.835	91.360	88.741
1607	63.789	66.241	64.373	62.719
1610	65.127	67.864	65.872	63.849
1617	100.342	105.882		98.449
1619	69.710	71.802	70.413	68.605
1622	81.517	84.003	82.283	80.181
1625	71.427	75.076	72.220	70.174
1626	82.891	85.177	83.591	80.321
1630	51.088	53.031	51.596	50.093
1633	114.155	117.346	114.953	110.969
1634	66.478	68.598	67.076	65.000