

Supporting Information

For

G4 Accuracy at DFT Cost: Unlocking Accurate Redox Potentials for Organic Molecules using Systematic Error Cancellation

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XYZ coordinates of geometries optimized at SMD/B3LYP/6-31G(2df,p) level of theory

(1) 2,6-dimethoxyphenol

0 1				1 2			
6	-0.032992	2.096984	0.000000	6	-0.033900	2.075048	-0.000001
6	1.191680	1.432690	0.000000	6	1.213717	1.430184	-0.000000
6	1.201977	0.038039	0.000000	6	1.245450	0.052782	-0.000000
6	0.000386	-0.680773	0.000000	6	0.002203	-0.680496	0.000000
6	-1.222972	-0.001089	-0.000000	6	-1.263618	0.014298	0.000000
6	-1.236936	1.396220	0.000000	6	-1.258351	1.397845	-0.000000
8	0.000625	-2.054114	0.000000	8	-0.007914	-1.988371	-0.000001
1	0.927155	-2.334879	0.000000	1	0.907258	-2.329179	-0.000006
1	2.117791	1.991627	0.000000	1	2.124506	2.011777	-0.000001
1	-0.049920	3.181224	0.000000	1	-0.048358	3.159174	-0.000001
8	2.319882	-0.753374	0.000000	8	2.310296	-0.744542	0.000001
6	3.593231	-0.113123	-0.000000	6	3.621419	-0.151047	0.000001
1	3.725047	0.505248	0.894553	1	3.755778	0.458013	0.897506
1	4.332961	-0.914862	-0.000000	1	4.318531	-0.986963	0.000001
1	3.725047	0.505248	-0.894553	1	3.755779	0.458012	-0.897505
1	-2.175376	1.933760	0.000000	1	-2.182535	1.957306	-0.000000
8	-2.333135	-0.800515	-0.000000	8	-2.319338	-0.787602	0.000000
6	-3.606157	-0.161173	-0.000000	6	-3.631646	-0.197065	0.000000
1	-4.344463	-0.964662	-0.000000	1	-4.325320	-1.036027	0.000001
1	-3.743256	0.457335	0.894117	1	-3.770818	0.411359	0.897302
1	-3.743256	0.457335	-0.894117	1	-3.770818	0.411358	-0.897301

0 2				6	2.890332	-0.874735	-0.000106
6	0.000000	-2.037317	-0.000000	8	3.923024	-0.235048	-0.000287
6	-1.229244	-1.365935	-0.000000	1	2.891488	-1.979057	-0.000179
6	-1.244450	0.016497	-0.000000				
6	0.000000	0.788037	-0.000000	0 2			
6	1.244450	0.016497	-0.000000	6	-1.353535	-0.218178	0.000053
6	1.229244	-1.365935	-0.000000	6	-0.129481	-0.887672	0.000049
8	0.000000	2.039277	-0.000000	6	1.054049	-0.158699	0.000011
1	-2.148570	-1.935470	0.000000	6	1.028684	1.320989	-0.000006
1	0.000000	-3.121776	-0.000000	6	-0.278982	1.948305	0.000011
8	-2.344499	0.788455	0.000000	6	-1.418761	1.208156	0.000036
6	-3.622379	0.145190	0.000000	8	2.089071	1.972418	-0.000033
1	-3.747768	-0.471962	0.895106	1	-0.118653	-1.970949	0.000065
1	-4.358785	0.948863	0.000000	8	2.279446	-0.673204	-0.000009
1	-3.747768	-0.471962	-0.895106	6	2.437322	-2.101077	-0.000024
1	2.148570	-1.935470	-0.000000	1	1.986499	-2.535199	-0.896567
8	2.344499	0.788455	0.000000	1	3.512355	-2.276049	-0.000034
6	3.622379	0.145190	0.000000	1	1.986511	-2.535217	0.896517
1	4.358785	0.948863	0.000000	1	-2.395737	1.677266	0.000043
1	3.747768	-0.471962	0.895107	1	-0.296122	3.032537	-0.000002
1	3.747768	-0.471962	-0.895106	6	-2.588113	-1.012934	0.000065
				8	-3.711477	-0.533846	-0.000108
				1	-2.438266	-2.108679	0.000014
(2) 2-methoxy-4-formylphenol							
0 1				(3) 2-methoxyphenol			
6	1.420104	-0.182569	0.000180	0 1			
6	0.201676	-0.886993	0.000126	6	-1.376879	-1.654724	-0.000062
6	-0.996685	-0.194923	0.000251	6	-0.002878	-1.389414	-0.000082
6	-0.984408	1.217498	0.000013	6	0.445137	-0.073302	0.000065
6	0.222753	1.913334	0.000042	6	-0.484857	0.984325	0.000032
6	1.421570	1.217458	0.000137	6	-1.844863	0.713551	0.000065
8	-2.151408	1.908855	-0.000297	6	-2.292977	-0.609985	0.000035
1	-2.881673	1.271082	-0.000641	1	-2.541475	1.544974	0.000098
1	0.216695	-1.970469	0.000117	1	-3.358081	-0.813722	0.000098
8	-2.245739	-0.743051	0.000496	8	-0.046825	2.284137	-0.000054
6	-2.352722	-2.166213	-0.000353	1	0.921164	2.264573	-0.000855
1	-1.889135	-2.595276	0.894503	1	0.706564	-2.207150	-0.000219
1	-3.420649	-2.386589	-0.000509	1	-1.717554	-2.684192	-0.000125
1	-1.888985	-2.594236	-0.895600	8	1.753708	0.328508	0.000154
1	2.366080	1.748830	0.000224	6	2.762478	-0.677812	-0.000010
1	0.195929	2.997136	-0.000074	1	2.693703	-1.306528	-0.894607
6	2.668959	-0.940569	0.000107	1	3.716085	-0.148130	0.000155
8	3.791360	-0.452205	-0.000359	1	2.693571	-1.306819	0.894401
1	2.540549	-2.041404	0.000234				
1 2				1 2			
6	1.548895	-0.249728	-0.000005	6	-1.301671	-1.682747	-0.000075
6	0.435333	-1.044177	0.000004	6	0.048448	-1.418788	-0.000126
6	-0.866487	-0.477293	0.000027	6	0.468722	-0.080697	-0.000008
6	-0.988066	0.977609	-0.000074	6	-0.518156	0.990288	-0.000000
6	0.184118	1.760506	0.000294	6	-1.888603	0.684648	0.000114
6	1.418144	1.175900	0.000348	6	-2.270461	-0.632398	0.000065
8	-2.121095	1.648782	-0.000424	1	-2.602131	1.498921	0.000172
1	-2.922382	1.106258	-0.000560	1	-3.322405	-0.891276	0.000123
1	0.507494	-2.125971	0.000111	8	-0.128865	2.246536	-0.000087
8	-1.835362	-1.359096	0.000392	1	0.843937	2.311831	-0.000561
6	-3.254910	-1.083794	-0.000107	1	0.775093	-2.219504	-0.000202
1	-3.532020	-0.547844	-0.912136	1	-1.645233	-2.710306	-0.000060
1	-3.724355	-2.065381	0.000400	8	1.708522	0.349588	0.000123
1	-3.532390	-0.546953	0.911310	6	2.808915	-0.589075	0.000050
1	2.317317	1.780037	0.000623	1	2.762188	-1.206175	-0.899423
1	0.058162	2.836077	0.000698	1	3.705925	0.026347	0.000059

1	2.762207	-1.206220	0.899493	0 2			
0 2				6	-0.002841	1.493802	0.000039
6	1.244334	-1.676545	-0.000000	6	-1.384116	1.740021	0.000002
6	-0.107728	-1.344679	-0.000000	6	-2.274379	0.692796	-0.000040
6	-0.485594	-0.006165	-0.000000	6	-1.803855	-0.675577	0.000017
6	0.526792	1.062638	-0.000000	6	-0.370306	-0.889166	-0.000100
6	1.908163	0.643471	0.000000	6	0.507664	0.174532	-0.000045
6	2.250669	-0.681232	0.000000	8	-2.603720	-1.647297	0.000081
1	2.654634	1.430539	0.000000	1	-1.741414	2.763693	0.000007
1	3.292999	-0.979959	0.000000	1	-3.346942	0.853081	-0.000099
8	0.185404	2.269404	0.000000	1	-0.030153	-1.917811	-0.000189
1	-0.853475	-2.128832	-0.000000	1	0.698179	2.319640	0.000097
1	1.529959	-2.722505	0.000000	6	1.997276	-0.010256	-0.000021
8	-1.744935	0.441910	-0.000000	8	2.730578	0.967166	0.000026
6	-2.814589	-0.511993	0.000000	6	2.554789	-1.408922	0.000019
1	-2.773726	-1.138850	0.895648	1	3.644200	-1.363878	0.000009
1	-3.732694	0.074975	0.000000	1	2.207948	-1.958478	0.881375
1	-2.773726	-1.138851	-0.895647	1	2.207927	-1.958574	-0.881279
(4) 3-hydroxy-acetophenone				(5) 3-methoxyphenol			
0 1				0 1			
6	0.113575	1.543719	0.000021	6	-0.694111	1.183522	0.000131
6	-1.247159	1.825462	0.000035	6	-0.759650	-0.212051	0.000139
6	-2.184128	0.795910	0.000013	6	0.412731	-0.976380	0.000041
6	-1.752307	-0.532032	0.000020	6	1.649732	-0.341511	-0.000125
6	-0.389397	-0.825090	-0.000003	6	1.735220	1.054660	-0.000098
6	0.550489	0.212660	0.000009	6	0.561368	1.795523	0.000088
8	-2.711365	-1.508817	-0.000051	1	2.708557	1.530928	-0.000231
1	-2.286229	-2.376731	-0.000056	1	0.617080	2.879295	0.000091
1	-1.588024	2.855172	0.000033	8	2.825243	-1.047150	-0.000127
1	-3.248180	1.005035	0.000018	1	2.625214	-1.992053	0.000530
1	-0.077167	-1.863574	-0.000019	1	-1.590552	1.787844	0.000382
1	0.846280	2.340880	-0.000006	1	0.344863	-2.059489	-0.000046
6	2.018795	-0.062341	-0.000004	8	-1.923481	-0.928935	0.000353
8	2.824179	0.861107	-0.000085	6	-3.152220	-0.206677	-0.000343
6	2.494683	-1.494466	0.000062	1	-3.247594	0.418941	-0.894830
1	3.585143	-1.512500	0.000272	1	-3.942155	-0.959473	0.000040
1	2.119017	-2.024810	0.881219	1	-3.247930	0.420175	0.893254
1	2.119353	-2.024725	-0.881291	1 2			
1 2				6	-0.675773	1.197112	0.000039
6	0.069277	1.506706	0.000017	6	-0.750342	-0.247858	0.000029
6	-1.313860	1.793134	0.000134	6	0.410776	-1.025311	0.000035
6	-2.225544	0.773043	0.000121	6	1.632540	-0.382581	-0.000010
6	-1.746263	-0.572983	-0.000018	6	1.718094	1.057604	-0.000041
6	-0.342627	-0.863852	0.000126	6	0.559444	1.819853	0.000020
6	0.555580	0.172955	0.000058	1	2.703060	1.508619	-0.000129
8	-2.546138	-1.604501	-0.000228	1	0.620572	2.900616	0.000049
1	-3.487553	-1.349994	-0.000488	8	2.802600	-1.009835	-0.000005
1	-1.643725	2.824450	0.000254	1	2.678705	-1.972617	-0.000072
1	-3.295895	0.946777	0.000152	1	-1.584794	1.782524	0.000047
1	-0.046672	-1.905012	0.000257	1	0.339551	-2.106063	0.000023
1	0.788880	2.316693	-0.000100	8	-1.894449	-0.897729	0.000037
6	2.048869	-0.039923	-0.000025	6	-3.161756	-0.199965	-0.000063
8	2.781745	0.933147	-0.000333	1	-3.253844	0.411166	-0.899891
6	2.573493	-1.446305	0.000203	1	-3.912459	-0.988130	-0.000024
1	3.663283	-1.426561	0.000027	1	-3.253896	0.411268	0.899684
1	2.211755	-1.985922	0.882072	0 2			
1	2.211529	-1.986244	-0.881390	6	0.590008	1.162297	-0.000000
				6	0.722535	-0.249649	-0.000000

6	-0.404754	-1.042681	0.000000	6	3.520825	0.569618	0.782666
6	-1.721934	-0.459711	0.000000	1	3.651944	-0.465774	1.110792
6	-1.821583	0.990162	0.000000	1	4.510587	1.001723	0.610933
6	-0.684656	1.757825	-0.000000	1	3.034777	1.125872	1.589518
1	-2.813790	1.426546	0.000000				
1	-0.751038	2.840083	-0.000000	0 2			
8	-2.757209	-1.177760	-0.000000	6	1.296683	-0.035272	-0.348171
1	1.468031	1.794146	-0.000000	6	0.158330	0.770808	-0.237096
1	-0.316647	-2.123062	0.000000	6	-1.091081	0.204998	-0.026223
8	1.922894	-0.886108	-0.000000	6	-1.253253	-1.251526	0.082215
6	3.117659	-0.101463	0.000000	6	-0.048261	-2.034985	-0.040447
1	3.182269	0.525343	0.895487	6	1.168746	-1.448097	-0.245532
1	3.939775	-0.818130	0.000000	8	-2.383484	-1.765553	0.267167
1	3.182270	0.525344	-0.895486	1	0.267584	1.845025	-0.319817
				8	-2.238591	0.886275	0.093713
(6) 4-ethyl-2-methoxyphenol				6	-2.203165	2.315468	0.006788
0 1				1	-1.831896	2.635578	-0.971508
6	1.363958	0.197277	0.341483	1	-3.234256	2.644161	0.136567
6	0.290145	-0.703896	0.252746	1	-1.576259	2.736719	0.798590
6	-1.004836	-0.245819	0.044413	1	2.061255	-2.058945	-0.338173
6	-1.250894	1.134169	-0.081892	1	-0.157331	-3.111870	0.033747
6	-0.196972	2.028680	0.007619	6	2.655807	0.581763	-0.536933
6	1.102509	1.560575	0.218728	1	3.230162	-0.022710	-1.248116
8	-2.529503	1.592191	-0.286291	1	2.547869	1.582058	-0.967175
1	-3.109646	0.818202	-0.324743	6	3.440828	0.676571	0.785112
1	0.478953	-1.766283	0.352669	1	3.585546	-0.312979	1.229878
8	-2.125574	-1.027767	-0.050678	1	4.426346	1.118659	0.609516
6	-1.967680	-2.440072	0.050565	1	2.909777	1.300162	1.511173
1	-1.556555	-2.723520	1.025832				
1	-2.966946	-2.863611	-0.059587	(7) 4-ethylphenol			
1	-1.318373	-2.823379	-0.744329	0 1			
1	1.918521	2.272870	0.290270	6	-0.910019	-0.011727	-0.346727
1	-0.402502	3.089842	-0.085039	6	-0.180414	-1.199388	-0.234712
6	2.773619	-0.318625	0.527960	6	1.196412	-1.192131	-0.024331
1	3.384545	0.460921	0.996114	6	1.873104	0.023315	0.079223
1	2.764407	-1.170961	1.217299	6	1.167567	1.221920	-0.032640
6	3.431900	-0.750418	-0.792388	6	-0.207350	1.194444	-0.243128
1	3.490693	0.088937	-1.493523	1	1.703703	2.161886	0.042120
1	4.448190	-1.120221	-0.619859	1	-0.745862	2.133707	-0.332812
1	2.858838	-1.549420	-1.274763	8	3.229522	0.094291	0.285705
				1	3.582007	-0.802734	0.348244
1 2				1	1.749401	-2.123505	0.054875
6	1.329381	0.042391	-0.341365	1	-0.695863	-2.152079	-0.317552
6	0.197823	0.836598	-0.231994	6	-2.410052	-0.028565	-0.535081
6	-1.047092	0.240292	-0.037140	1	-2.711180	0.831427	-1.144131
6	-1.151164	-1.205555	0.050882	1	-2.697490	-0.927486	-1.092014
6	-0.000262	-2.001863	-0.072394	6	-3.178995	0.005658	0.795616
6	1.208208	-1.388232	-0.261134	1	-4.260475	-0.006002	0.623304
8	-2.323341	-1.771797	0.246333	1	-2.925407	-0.859677	1.417392
1	-3.019729	-1.094192	0.325902	1	-2.936525	0.908982	1.365615
1	0.283268	1.912939	-0.298374				
8	-2.206594	0.854879	0.084341	1 2			
6	-2.269398	2.296823	0.033351	6	-0.899119	-0.018826	-0.351351
1	-1.907064	2.646823	-0.935733	6	-0.168346	-1.236633	-0.224103
1	-3.321846	2.541607	0.161244	6	1.180845	-1.229730	-0.015262
1	-1.673127	2.719230	0.845146	6	1.856422	0.023369	0.081498
1	2.107435	-1.986147	-0.357992	6	1.142950	1.254760	-0.033527
1	-0.103269	-3.078019	-0.012696	6	-0.204735	1.221099	-0.243774
6	2.689503	0.646531	-0.514401	1	1.699171	2.180674	0.044908
1	3.218369	0.103136	-1.306174	1	-0.766262	2.143236	-0.339633
1	2.591189	1.688537	-0.828785	8	3.150664	0.105757	0.276214

1	3.564435	-0.773303	0.335978	1	0.428010	2.206039	-0.034902
1	1.755191	-2.145028	0.075120	1	-2.077567	2.136116	-0.046344
1	-0.703350	-2.175953	-0.303871	1	-1.933754	-2.191853	0.045060
6	-2.374440	-0.040251	-0.552447	6	2.143833	0.165118	0.005352
1	-2.673560	0.821616	-1.156426	8	2.645233	1.276475	0.055397
1	-2.662120	-0.955514	-1.077171	6	2.964967	-1.088329	-0.054343
6	-3.117171	0.019142	0.806536	1	2.756874	-1.719092	0.816906
1	-4.195076	0.006603	0.624776	1	2.707356	-1.670206	-0.945798
1	-2.857406	-0.839735	1.431257	1	4.022678	-0.826182	-0.074270
1	-2.864775	0.933777	1.349937	1	0.545043	-2.116588	0.055375
0 2				0 2			
6	0.844844	0.015103	-0.350120	6	0.594312	0.063232	-0.000092
6	0.125997	1.228477	-0.225232	6	-0.062579	-1.191079	-0.000089
6	-1.227358	1.233452	-0.007539	6	-1.431022	-1.260011	-0.000005
6	-1.968904	-0.006534	0.103149	6	-2.239271	-0.053303	0.000025
6	-1.211877	-1.235220	-0.028006	6	-1.535637	1.217601	-0.000002
6	0.140884	-1.209562	-0.245220	6	-0.169845	1.258769	-0.000031
1	-1.758150	-2.169396	0.048871	8	-3.491441	-0.108672	0.000062
1	0.694202	-2.138325	-0.345192	1	0.518940	-2.104724	-0.000136
8	-3.212036	-0.015923	0.303369	1	-1.952954	-2.210422	0.000005
1	-1.785145	2.159379	0.085056	1	-2.135169	2.121249	0.000017
1	0.667538	2.165639	-0.309515	6	2.084699	0.176234	-0.000014
6	2.333276	0.024217	-0.547903	8	2.608363	1.283340	0.000021
1	2.625285	-0.837870	-1.156721	6	2.914057	-1.080511	0.000071
1	2.624159	0.929434	-1.090499	1	2.688099	-1.689450	0.881768
6	3.092029	-0.026979	0.793460	1	2.687918	-1.689666	-0.881434
1	4.171649	-0.021213	0.615782	1	3.971431	-0.814494	-0.000042
1	2.842332	0.836316	1.418098	1	0.358074	2.204564	-0.000022
1	2.841060	-0.934302	1.351633	(9) 4-methoxyphenol			
(8) 4-hydroxy-acetophenone				0 1			
0 1				6	0.925356	-0.287019	0.000097
6	0.662138	0.068418	0.000087	6	0.414244	1.012130	0.000160
6	-0.114903	1.238374	0.000019	6	-0.966035	1.216925	0.000161
6	-1.497285	1.181537	-0.000043	6	-1.841115	0.134987	-0.000009
6	-2.137749	-0.064113	-0.000024	6	-1.329777	-1.165010	-0.000010
6	-1.383173	-1.241665	0.000042	6	0.043327	-1.371900	0.000103
6	0.000695	-1.170318	-0.000002	1	-2.009224	-2.012049	-0.000035
8	-3.491864	-0.184632	0.000008	1	0.448840	-2.377769	0.000150
1	-3.895592	0.693986	-0.000253	8	-3.193203	0.396599	-0.000284
1	0.385930	2.199426	-0.000015	1	-3.673098	-0.441264	0.000402
1	-2.093226	2.088840	0.000005	1	-1.367341	2.224508	0.000258
1	-1.895340	-2.196980	0.000103	1	1.072664	1.870893	0.000359
6	2.139626	0.183619	-0.000041	8	2.263130	-0.598739	0.000021
8	2.686922	1.283904	0.000037	6	3.191322	0.479552	-0.000203
6	2.971215	-1.078546	-0.000065	1	4.183396	0.024545	-0.000428
1	2.748648	-1.688270	0.881732	1	3.080502	1.105106	-0.893828
1	2.747905	-1.689017	-0.881013	1	3.080906	1.105159	0.893433
1	4.029128	-0.813068	-0.000737				
1	0.568700	-2.092926	-0.000026	1 2			
				6	0.913295	-0.280058	0.000287
1 2				6	0.406465	1.050076	0.000626
6	0.640862	0.057413	0.004857	6	-0.944861	1.247684	0.000416
6	-0.109244	1.267015	-0.018953	6	-1.829935	0.133514	-0.000065
6	-1.471575	1.239041	-0.024961	6	-1.325984	-1.196045	0.000159
6	-2.134622	-0.029400	-0.001949	6	0.021760	-1.396285	0.000385
6	-1.390910	-1.253464	0.027989	1	-2.022896	-2.026787	-0.000028
6	-0.025892	-1.197804	0.032000	1	0.451123	-2.390549	0.000473
8	-3.436384	-0.010291	-0.010356	8	-3.122737	0.403267	-0.000639
1	-3.823942	-0.905244	0.003689	1	-3.657136	-0.408372	-0.001081

1	-1.371632	2.243137	0.000543				
1	1.081418	1.894593	0.001020	1 2			
8	2.192080	-0.585090	-0.000061	6	1.180334	0.668662	0.020248
6	3.196225	0.454747	-0.000650	6	1.398097	-0.143935	1.165969
1	4.148309	-0.072160	-0.000990	6	2.445037	-1.031689	1.231473
1	3.096680	1.066369	-0.899640	6	3.315686	-1.157384	0.132366
1	3.097600	1.066553	0.898359	6	3.109863	-0.377870	-1.025636
				6	2.053518	0.505263	-1.078293
0 2				1	2.618757	-1.639307	2.111471
6	0.861457	0.280582	0.000000	1	1.912984	1.093874	-1.974973
6	0.355041	-1.039611	-0.000000	1	0.729037	-0.061710	2.013891
6	-1.001606	-1.243420	-0.000000	1	3.793857	-0.481952	-1.861700
6	-1.942184	-0.143678	-0.000000	6	-0.000142	1.641327	-0.000094
6	-1.376570	1.190895	-0.000000	6	-1.180294	0.668507	-0.020317
6	-0.026527	1.388388	-0.000000	6	-2.053679	0.505321	1.078260
1	-2.065760	2.028585	-0.000000	6	-1.397798	-0.144554	-1.165866
1	0.404406	2.383531	-0.000000	6	-3.109922	-0.377747	1.025730
8	-3.187681	-0.337020	0.000000	1	-1.913029	1.094224	1.974734
1	-1.410288	-2.248332	-0.000000	6	-2.444620	-1.032306	-1.231242
1	1.031368	-1.884404	-0.000000	1	-0.728519	-0.062471	-2.013642
8	2.164612	0.590786	0.000000	6	-3.315635	-1.157554	-0.132245
6	3.137445	-0.463153	0.000000	1	-3.794127	-0.481870	1.861642
1	4.106927	0.034309	0.000000	1	-2.618338	-1.640401	-2.110925
1	3.037780	-1.081917	0.896191	8	4.322349	-2.033558	0.237612
1	3.037781	-1.081917	-0.896191	1	4.854412	-2.042392	-0.572628
				8	-4.322253	-2.033522	-0.237476
				1	-4.854524	-2.042427	0.572667
(10) bisphenol-A				6	-0.016795	2.552317	-1.242433
0 1				1	0.884147	3.173047	-1.262995
6	1.257009	0.582239	0.000299	1	-0.072519	2.000935	-2.182551
6	1.421070	-0.394012	0.994174	1	-0.885990	3.213618	-1.189541
6	2.551836	-1.199183	1.054705	6	0.016363	2.552496	1.242025
6	3.562752	-1.046321	0.103400	1	0.885731	3.213578	1.189290
6	3.423883	-0.088385	-0.896814	1	-0.884398	3.173493	1.262228
6	2.283267	0.712696	-0.940027	1	0.071666	2.001279	2.182266
1	2.655024	-1.948442	1.834266				
1	2.209311	1.448289	-1.731687				
1	0.642769	-0.535745	-1.737488	0 2			
1	4.209010	0.025735	-1.636566	6	-1.300818	0.550746	-0.005927
6	-0.000594	1.470234	0.010263	6	-1.414730	-0.435705	-1.025221
6	-1.255320	0.578485	0.001744	6	-2.493341	-1.272170	-1.098809
6	-2.285830	0.692551	0.937835	6	-3.567604	-1.190520	-0.130519
6	-1.411591	-0.384646	-1.007707	6	-3.432770	-0.183495	0.899414
6	-3.423865	-0.113380	0.876719	6	-2.339099	0.646977	0.947830
1	-2.219626	1.416859	1.740525	1	-2.577465	-2.021555	-1.878914
6	-2.537174	-1.193144	-1.085545	1	-2.276549	1.386541	1.736009
1	-0.628756	-0.511675	-1.748943	1	-0.617961	-0.523338	-1.756296
6	-3.553425	-1.058652	-0.136813	1	-4.227989	-0.109349	1.633914
1	-4.211150	-0.008618	1.617879	6	-0.079367	1.472128	-0.005092
1	-2.639702	-1.932891	-1.872309	6	1.186388	0.596800	0.006072
8	4.701731	-1.813524	0.111609	6	2.198047	0.698033	-0.952075
1	4.660947	-2.423419	0.859571	6	1.363509	-0.341181	1.035845
8	-4.647188	-1.881414	-0.249880	6	3.343148	-0.095175	-0.888452
1	-5.265313	-1.682773	0.465442	1	2.110919	1.402348	-1.770216
6	-0.068038	2.397492	-1.223390	6	2.496003	-1.139555	1.112525
1	0.775831	3.094627	-1.243885	1	0.595822	-0.453814	1.795210
1	-0.071421	1.834941	-2.161194	6	3.495701	-1.017268	0.144798
1	-0.988108	2.988619	-1.184183	1	4.118839	-0.000548	-1.642849
6	0.063772	2.372326	1.262537	1	2.617504	-1.860241	1.913862
1	0.983392	2.964912	1.237236	8	-4.565265	-1.956867	-0.180660
1	-0.780608	3.068337	1.295446	8	4.596795	-1.826147	0.258678
1	0.065536	1.790951	2.188799	1	5.202847	-1.639574	-0.470293

6	-0.041306	2.406994	1.222508	1	1.018535	-1.432829	-2.130350
1	-0.903168	3.081453	1.235437	17	5.603811	-0.828484	-0.155435
1	-0.023345	1.851061	2.163699				
1	0.863241	3.020272	1.177775	0 2			
6	-0.170394	2.361408	-1.267913	6	-2.420483	-1.595706	0.697177
1	-1.098573	2.939633	-1.242120	6	-3.472912	-0.884206	0.130092
1	0.664906	3.067525	-1.298788	6	-3.336515	0.446695	-0.244833
1	-0.161462	1.775600	-2.190477	6	-2.108113	1.068105	-0.049730
				6	-1.037606	0.370410	0.509786
				6	-1.202459	-0.957337	0.892182
				1	-4.160843	0.992859	-0.683871
				1	-0.373998	-1.486456	1.348487
				1	-2.548217	-2.629212	0.992725
				8	0.126387	1.064946	0.779329
				17	-5.017408	-1.678499	-0.113789
				17	-1.904868	2.735501	-0.522312
				6	1.346974	0.540660	0.506571
				6	1.595051	-0.182373	-0.745795
				6	2.377797	0.827566	1.386029
				6	2.951827	-0.639853	-0.964571
				6	3.667030	0.383621	1.121896
				1	2.163493	1.391912	2.285593
				6	3.928897	-0.356392	-0.057270
				1	3.146329	-1.193996	-1.874265
				1	4.469121	0.591894	1.818400
				8	0.692183	-0.365670	-1.589231
				17	5.570432	-0.903376	-0.334313
(11) triclosan				(12) 3-chlorophenol			
0 1				0 1			
6	-2.181262	-1.713238	0.291873	6	0.562485	1.415519	-0.000228
6	-3.391279	-1.053940	0.118950	6	-0.772713	1.815954	0.000023
6	-3.451117	0.330058	0.004186	6	-1.804844	0.883460	0.000088
6	-2.267079	1.053149	0.061235	6	-1.501347	-0.479651	0.000110
6	-1.032558	0.414587	0.231900	6	-0.171724	-0.908533	0.000017
6	-1.004697	-0.973648	0.350078	6	0.831275	0.051189	-0.000473
1	-4.395372	0.841306	-0.129521	8	-2.465547	-1.448253	-0.000485
1	-0.058599	-1.480236	0.494715	1	-3.337911	-1.031688	0.002622
1	-2.148567	-2.791435	0.384523	1	-1.009998	2.874287	0.000291
8	0.077576	1.212280	0.303546	1	-2.842538	1.200918	0.000632
17	-4.881519	-1.979555	0.043391	1	1.366906	2.139541	-0.000128
17	-2.324530	2.794739	-0.083487	1	0.056394	-1.966718	0.000601
6	1.341730	0.637330	0.254045	17	2.507808	-0.488114	0.000155
6	1.840946	0.155317	-0.964986				
6	2.132830	0.641756	1.391595				
6	3.145497	-0.334272	-1.018455				
6	3.440424	0.162013	1.346811				
1	1.718327	1.031161	2.314133				
6	3.919640	-0.321616	0.136249				
1	3.538687	-0.709809	-1.956134				
1	4.062469	0.164335	2.232078				
8	1.018155	0.191452	-2.045106				
1	1.475922	-0.179882	-2.811537				
17	5.563863	-0.938142	0.050880				
1 2				1 2			
6	-2.452874	-1.565343	0.698081	6	-0.517201	1.400330	-0.000370
6	-3.522871	-0.833244	0.185025	6	0.826704	1.814960	0.000007
6	-3.384615	0.493127	-0.210906	6	1.832206	0.884603	0.000450
6	-2.137566	1.092077	-0.095199	6	1.491114	-0.510230	0.000072
6	-1.051494	0.361386	0.396198	6	0.135530	-0.945104	0.000263
6	-1.210987	-0.959820	0.805592	6	-0.837742	0.011789	-0.000026
1	-4.224040	1.052228	-0.602245	8	2.402176	-1.445724	-0.000360
1	-0.371552	-1.500031	1.226707	1	3.310716	-1.089980	-0.000524
1	-2.589342	-2.589001	1.021618	1	1.054439	2.873256	0.000016
8	0.135298	1.045994	0.573843	1	2.880583	1.161813	0.000762
17	-5.088464	-1.593321	0.046476	1	-1.315973	2.132382	-0.000965
17	-1.923776	2.746943	-0.580799	1	-0.077433	-2.005810	0.000458
6	1.351951	0.544125	0.374387	17	-2.509024	-0.437880	0.000045
6	1.669982	-0.429147	-0.650712				
6	2.382405	1.103655	1.151403				
6	2.995159	-0.852164	-0.800810				
6	3.673800	0.679867	0.993406				
1	2.115934	1.849764	1.888919				
6	3.965970	-0.312018	0.012572				
1	3.229657	-1.585801	-1.562329				
1	4.470491	1.081190	1.605954				
8	0.692257	-0.838230	-1.433422				

0 2				(14) 2,4-dinitrophenol			
6	-0.440208	1.393125	-0.000000	0 1			
6	0.915384	1.763824	-0.000000	6	1.384247	0.147578	0.000079
6	1.902206	0.808334	0.000000	6	0.304288	-0.710985	-0.000027
6	1.566197	-0.602072	0.000000	6	-0.976698	-0.168928	-0.000019
6	0.159254	-0.960200	-0.000000	6	-1.183827	1.234857	0.000061
6	-0.787433	0.027431	-0.000000	6	-0.051949	2.069937	0.000320
8	2.455233	-1.488959	0.000000	6	1.216913	1.540313	0.000263
1	1.167848	2.818072	-0.000000	1	-0.213120	3.140687	0.000406
1	2.954190	1.070255	0.000001	1	2.084869	2.185522	0.000351
1	-1.216725	2.148249	-0.000000	8	-2.379974	1.808410	-0.000305
1	-0.100250	-2.011615	-0.000000	1	-3.051922	1.088110	-0.000459
17	-2.490548	-0.393879	0.000000	7	2.726045	-0.411241	-0.000034
				8	2.851618	-1.634150	0.000175
(13) 2,4,6-trichlorophenol				8	3.676671	0.368360	-0.000414
0 1				1	0.439600	-1.782306	-0.000199
6	-1.611359	-0.048557	0.000000	7	-2.094598	-1.083766	-0.000069
6	-0.898058	-1.239996	0.000000	8	-3.245191	-0.610263	0.000033
6	0.488604	-1.175241	0.000000	8	-1.882800	-2.287806	0.000081
6	1.186351	0.040255	0.000000				
6	0.417963	1.212289	0.000000	1 2			
6	-0.969706	1.183922	0.000000	6	1.383631	0.158536	0.006034
1	-1.402200	-2.197059	0.000000	6	0.274960	-0.723780	-0.022303
1	-1.532316	2.107884	0.000000	6	-0.974893	-0.187041	-0.007263
8	2.531220	0.135014	0.000000	6	-1.155590	1.242881	0.041735
1	2.922793	-0.751235	0.000000	6	0.004560	2.092973	0.088177
17	1.422147	-2.657365	0.000000	6	1.266821	1.545885	0.061336
17	-3.363116	-0.099693	0.000000	1	-0.164371	3.161775	0.135678
17	1.239746	2.752603	0.000000	1	2.150809	2.168435	0.087183
				8	-2.308280	1.807431	0.038271
1 2				1	-3.012838	1.088283	-0.008070
6	-1.606336	-0.046333	0.000000	7	2.728152	-0.441930	-0.006017
6	-0.890059	-1.265761	0.000000	8	2.815024	-1.606570	0.353975
6	0.475207	-1.219998	-0.000000	8	3.652628	0.267893	-0.366215
6	1.168771	0.040552	0.000000	1	0.426875	-1.794375	-0.062167
6	0.395155	1.256055	-0.000000	7	-2.133933	-1.075221	-0.046846
6	-0.972773	1.212217	-0.000000	8	-3.254954	-0.544471	-0.048816
1	-1.418817	-2.209766	0.000000	8	-1.949035	-2.271881	-0.075825
1	-1.559666	2.121171	-0.000000				
8	2.458813	0.148018	0.000000	0 2			
1	2.915126	-0.716383	0.000000	6	1.345925	0.140930	-0.007962
17	1.424319	-2.658344	-0.000000	6	0.221749	-0.704110	-0.002692
17	-3.312311	-0.104565	0.000000	6	-1.016228	-0.133008	0.014535
17	1.239349	2.748818	-0.000000	6	-1.208940	1.321308	0.069535
				6	0.011869	2.113664	0.066290
0 2				6	1.256830	1.535822	0.023982
6	-1.567590	0.000000	0.000000	1	-0.112486	3.188910	0.111980
6	-0.896240	1.233918	0.000000	1	2.157962	2.133285	0.018830
6	0.474432	1.230862	0.000000	8	-2.321455	1.862566	0.156494
6	1.267839	0.000000	0.000000	7	2.672801	-0.483561	-0.049424
6	0.474432	-1.230862	-0.000000	8	2.726989	-1.707814	-0.081750
6	-0.896240	-1.233918	-0.000000	8	3.649996	0.255425	-0.047880
8	2.506027	-0.000000	0.000000	1	0.344324	-1.777881	-0.028167
1	-1.455427	2.160389	0.000000	7	-2.176275	-1.021181	-0.027129
1	-1.455427	-2.160389	-0.000000	8	-3.171323	-0.632636	-0.624221
17	1.346742	2.723268	-0.000000	8	-2.075796	-2.109885	0.528744
17	-3.298023	0.000000	0.000000				
17	1.346742	-2.723268	-0.000000				

(15) 2,5-dimethylphenol	1	3.536299	-0.300089	-0.879839	
0 1					
6 1.134011 -1.316929 -0.007581	(16) 2-chlorophenol				
6 -0.238430 -1.560018 -0.001452	0 1				
6 -1.172112 -0.523495 0.002496	6 -1.829921 -1.282263 -0.000031				
6 -0.672288 0.789389 -0.000725	6 -2.353586 0.010730 -0.000138				
6 0.697060 1.041278 -0.006588	6 -1.510607 1.115406 -0.000363				
6 1.620501 -0.007479 -0.007870	6 -0.124022 0.946224 0.000311				
1 1.034052 2.073436 -0.011534	6 0.385837 -0.356890 0.000505				
8 -1.505482 1.884480 -0.001084	6 -0.450651 -1.467043 0.000470				
1 -2.424784 1.590908 -0.001031	1 -0.020414 -2.461406 0.000620				
1 -0.601186 -2.583936 -0.002745	8 0.660861 2.058123 0.000272				
1 1.829788 -2.149975 -0.012981	1 1.592882 1.796754 0.000712				
6 -2.655770 -0.786368 0.006051	1 -3.427393 0.162317 -0.000902				
1 -3.145544 -0.354452 0.888396	1 -1.903783 2.125802 -0.000976				
1 -3.149442 -0.358318 -0.876042	1 -2.487150 -2.143941 -0.000073				
1 -2.856882 -1.860218 0.008763	17 2.132745 -0.573029 -0.000357				
6 3.101191 0.279060 0.008913					
1 3.361943 1.078969 -0.691741	1 2				
1 3.430987 0.605389 1.003010	6 -1.727477 -1.358735 0.000223				
1 3.679946 -0.610264 -0.254888	6 -2.345722 -0.077184 -0.000228				
	6 -1.583634 1.054391 -0.000321				
1 2	6 -0.165289 0.938376 -0.000096				
6 1.091247 -1.312641 -0.000098	6 0.452097 -0.372243 -0.000080				
6 -0.277301 -1.570311 -0.000127	6 -0.335284 -1.500724 0.000288				
6 -1.195375 -0.535033 -0.000024	1 0.116390 -2.484208 0.000474				
6 -0.658257 0.814986 -0.000023	8 0.623756 1.972611 0.000453				
6 0.732890 1.069936 0.000104	1 0.126904 2.812581 0.000560				
6 1.618587 0.025300 0.000037	1 -3.426437 -0.009626 -0.000369				
1 1.061422 2.102161 0.000211	1 -2.014592 2.048934 -0.000507				
8 -1.446763 1.865143 -0.000160	1 -2.347925 -2.247131 0.000554				
1 -2.390194 1.628925 -0.000141	17 2.163968 -0.470866 -0.000180				
1 -0.632215 -2.593978 -0.000183					
1 1.790597 -2.142176 -0.000142	0 2				
6 -2.668603 -0.756354 0.000164	6 1.712765 -1.343636 -0.000000				
1 -3.134591 -0.299625 0.883255	6 2.343908 -0.082260 0.000000				
1 -3.134914 -0.299623 -0.882734	6 1.592604 1.062788 0.000000				
1 -2.897639 -1.822311 0.000249	6 0.142214 1.020482 0.000000				
6 3.099651 0.221710 0.000063	6 -0.453974 -0.315423 0.000000				
1 3.366045 1.279595 0.000310	6 0.314381 -1.456180 -0.000000				
1 3.544295 -0.260046 0.878854	1 -0.153167 -2.433352 -0.000000				
1 3.544263 -0.259622 -0.878979	8 -0.548910 2.060921 -0.000000				
	1 3.426697 -0.028186 0.000000				
0 2	1 2.043995 2.048918 0.000000				
6 1.038947 -1.306772 0.000066	1 2.311906 -2.247231 -0.000000				
6 -0.343419 -1.524371 0.000058	17 -2.185267 -0.420126 0.000000				
6 -1.237702 -0.471048 0.000027					
6 -0.706938 0.892324 0.000048	(17) 2-phenylphenol				
6 0.730384 1.067356 -0.000083	0 1				
6 1.593977 0.001862 -0.000035	6 -2.709263 -1.499954 -0.392794				
1 1.096310 2.089409 -0.000198	6 -3.474518 -0.370631 -0.104556				
8 -1.481321 1.883327 0.000111	6 -2.850853 0.829810 0.213860				
1 -0.717809 -2.543284 0.000072	6 -1.458222 0.915543 0.237761				
1 1.710179 -2.160079 0.000148	6 -0.663463 -0.208512 -0.063040				
6 -2.720727 -0.664498 -0.000105	6 -1.321866 -1.408892 -0.366016				
1 -3.177977 -0.191223 0.876600	1 -0.719807 -2.279971 -0.603109				
1 -3.177641 -0.192369 -0.877612	8 -0.928280 2.130997 0.590435				
1 -2.979564 -1.725453 0.000536	1 0.033885 2.056652 0.652250				
6 3.088533 0.175646 -0.000037	1 -4.558007 -0.422350 -0.122935				
1 3.366276 1.232095 -0.000862	1 -3.427218 1.715845 0.456934				
1 3.536176 -0.298619 0.880625	1 -3.187347 -2.440760 -0.641468				

6	0.821561	-0.153048	-0.045612	(18)	4-nitrophenol		
6	1.556750	-1.139628	0.629544	0	1		
6	1.528277	0.858217	-0.717086	6	0.690287	0.000391	0.000017
6	2.947776	-1.115684	0.635296	6	0.014553	1.223330	-0.000011
1	1.028180	-1.923255	1.161806	6	-1.366530	1.230807	-0.000236
6	2.921732	0.883311	-0.706502	6	-2.070978	0.017858	-0.000529
1	0.986621	1.614462	-1.276249	6	-1.382011	-1.203876	-0.000015
6	3.636635	-0.102078	-0.030330	6	0.000488	-1.213411	0.000090
1	3.495223	-1.887640	1.166066	1	-1.941174	-2.133295	0.000371
1	3.446288	1.670860	-1.237232	1	0.547548	-2.146153	0.000312
1	4.721146	-0.082553	-0.022685	8	-3.420283	0.085965	0.000238
				1	-3.796326	-0.805398	0.000869
1	2			1	-1.919427	2.162355	-0.000100
6	-2.667108	-1.521643	-0.327639	7	2.135290	-0.008294	0.000127
6	-3.465456	-0.356179	-0.152132	8	2.733427	1.070557	0.000252
6	-2.877222	0.849042	0.109767	8	2.721126	-1.093909	-0.000275
6	-1.468563	0.924078	0.215222	1	0.573340	2.149046	0.000039
6	-0.629325	-0.240346	-0.028581				
6	-1.289220	-1.457423	-0.253373	1	2		
1	-0.700279	-2.347270	-0.436041	6	0.665271	0.002193	0.002168
8	-0.982288	2.085453	0.602550	6	0.012155	1.243412	-0.111107
1	-0.019400	2.065346	0.744501	6	-1.354200	1.256523	-0.117095
1	-4.544096	-0.435232	-0.216946	6	-2.064828	0.013482	-0.000171
1	-3.448667	1.753134	0.278462	6	-1.370353	-1.236636	0.118664
1	-3.150600	-2.466016	-0.548368	6	-0.004696	-1.234072	0.114512
6	0.823659	-0.157407	-0.034491	1	-1.945090	-2.151113	0.207222
6	1.587306	-1.219032	0.504453	1	0.565476	-2.148729	0.200405
6	1.504849	0.947045	-0.600420	8	-3.359821	0.091110	-0.010604
6	2.969518	-1.159368	0.506094	1	-3.797464	-0.779130	0.061636
1	1.081886	-2.062330	0.959275	1	-1.927880	2.170061	-0.207463
6	2.890617	0.987288	-0.610498	7	2.135909	-0.007840	0.000191
1	0.950174	1.737875	-1.092344	8	2.688497	-1.051673	-0.316728
6	3.627211	-0.057871	-0.050724	8	2.704221	1.028253	0.313823
1	3.542167	-1.968337	0.944927	1	0.590338	2.152865	-0.196890
1	3.398720	1.828979	-1.066566				
1	4.710807	-0.018882	-0.053382	0	2		
				6	-0.620073	-0.000003	-0.000000
0	2			6	0.047567	-1.237337	0.000001
6	2.690537	-1.484733	0.338385	6	1.416884	-1.244144	-0.000011
6	3.493297	-0.347336	0.100662	6	2.169426	0.000001	0.000000
6	2.899931	0.854888	-0.169917	6	1.416881	1.244143	0.000011
6	1.458086	0.991857	-0.235211	6	0.047565	1.237333	-0.000002
6	0.641960	-0.200025	0.044718	1	1.978396	2.170951	0.000022
6	1.297694	-1.398429	0.307464	1	-0.526225	2.153673	-0.000016
1	0.713636	-2.285523	0.525981	8	3.420763	0.000002	0.000001
8	0.944897	2.092162	-0.556510	1	1.978401	-2.170950	-0.000022
1	4.573617	-0.435558	0.135954	7	-2.081960	-0.000000	0.000001
1	3.478926	1.750772	-0.366507	8	-2.660385	1.083747	-0.000010
1	3.160561	-2.435722	0.563242	8	-2.660394	-1.083743	0.000011
6	-0.827266	-0.129972	0.029893	1	-0.526220	-2.153678	0.000014
6	-1.520743	0.978777	0.548930				
6	-1.578275	-1.201878	-0.486366	(19)	4-cyanophenol		
6	-2.910701	1.007423	0.553839	0	1		
1	-0.964823	1.805588	0.970405	6	-1.078508	-0.001639	-0.000130
6	-2.967460	-1.164068	-0.490504	6	-0.365784	-1.211043	0.000036
1	-1.064746	-2.056448	-0.912819	6	1.018792	-1.201765	-0.000075
6	-3.640329	-0.059658	0.031361	6	1.706749	0.017623	-0.000329
1	-3.426232	1.866067	0.970931	6	1.002035	1.227464	-0.000117
1	-3.525764	-1.996325	-0.905793	6	-0.381129	1.217985	0.000078
1	-4.724733	-0.031220	0.031160	8	3.062290	0.085583	0.000311
				1	3.433277	-0.807375	-0.000126

1	-0.903724	-2.151705	0.000121
1	1.577595	-2.131781	0.000077
1	1.553333	2.160327	-0.000045
1	-0.931864	2.151194	0.000126
6	-2.500552	-0.010959	-0.000136
7	-3.662366	-0.018760	0.000199

1 2			
6	-1.057753	-0.000647	-0.000071
6	-0.353623	-1.239939	-0.000153
6	1.009693	-1.239561	-0.000194
6	1.703256	0.013910	-0.000042
6	0.992755	1.258752	-0.000184
6	-0.370586	1.245812	-0.000156
8	3.001126	0.090229	0.000394
1	3.432744	-0.784922	0.000268
1	-0.912540	-2.166796	-0.000213
1	1.586308	-2.157342	-0.000320
1	1.565430	2.177441	-0.000324
1	-0.939212	2.166594	-0.000237
6	-2.472970	-0.010772	0.000113
7	-3.635213	-0.017448	0.000257

0 2			
6	1.008454	0.000000	-0.000000
6	0.312198	1.236007	-0.000000
6	-1.055353	1.242548	0.000000
6	-1.809159	0.000000	0.000000
6	-1.055353	-1.242548	0.000000
6	0.312198	-1.236007	-0.000000
8	-3.061327	0.000000	0.000000
1	0.877791	2.159958	-0.000000
1	-1.617408	2.169367	0.000000
1	-1.617409	-2.169367	0.000000
1	0.877791	-2.159958	-0.000000
6	2.427520	-0.000000	0.000000
7	3.589547	0.000000	0.000000

(20) 2-methoxy-5-nitroaniline

0 1			
6	-0.590833	-1.351490	0.006620
6	0.798929	-1.323687	0.008031
6	1.479927	-0.107161	0.011718
6	0.772057	1.127024	0.012917
6	-0.615073	1.089146	0.002472
6	-1.276885	-0.142521	0.003225
1	1.348623	-2.255034	0.006264
1	-1.181879	2.010560	-0.006648
7	1.482084	2.314918	0.077812
1	2.419592	2.257903	-0.295828
1	0.977486	3.121771	-0.264188
7	-2.722565	-0.155278	-0.004346
8	-3.309081	-1.241711	-0.010007
8	-3.325040	0.922226	-0.004981
1	-1.127668	-2.289046	0.006246
8	2.825972	0.020822	0.011178
6	3.627437	-1.162877	-0.019648
1	3.427420	-1.747397	-0.923268
1	4.662038	-0.819183	-0.026184
1	3.449592	-1.778357	0.867814

1 2			
6	-0.560614	-1.340098	-0.000667
6	0.819371	-1.334509	-0.000548
6	1.507913	-0.117470	0.000142
6	0.762169	1.128959	0.000149
6	-0.657511	1.096770	0.000143
6	-1.276288	-0.121516	-0.000185
1	1.361137	-2.269906	-0.000864
1	-1.216484	2.023032	0.000433
7	1.422367	2.277284	0.000082
1	2.436142	2.288526	-0.000210
1	0.927194	3.162384	-0.000325
7	-2.740514	-0.167349	0.000066
8	-3.277415	-1.269897	0.001170
8	-3.350761	0.895690	-0.000759
1	-1.105849	-2.273821	-0.001095
8	2.813558	0.035932	0.000517
6	3.679303	-1.120168	-0.000042
1	3.502924	-1.713692	-0.899672
1	4.690051	-0.717167	0.000259
1	3.502804	-1.714515	0.899070

(21) 2-methoxyaniline

0 1			
6	1.327302	-1.706421	-0.003740
6	-0.036906	-1.394365	0.007169
6	-0.449582	-0.066684	0.016388
6	0.498844	0.981648	0.013116
6	1.853637	0.647584	-0.005070
6	2.268772	-0.684835	-0.010592
1	3.329001	-0.914362	-0.024243
1	2.584440	1.451098	-0.015166
7	0.061891	2.306076	0.083396
1	0.725116	2.966950	-0.300771
1	-0.861069	2.442617	-0.307719
1	-0.770138	-2.190881	0.007253
1	1.637026	-2.745622	-0.009289
8	-1.758859	0.346499	0.025019
6	-2.772173	-0.650935	-0.022448
1	-3.723017	-0.115386	-0.027197
1	-2.692865	-1.258873	-0.931146
1	-2.730218	-1.306010	0.855412

1 2			
6	1.268717	-1.714510	-0.000180
6	-0.082756	-1.408342	-0.000163
6	-0.479567	-0.072106	0.000115
6	0.525440	0.973843	0.000024
6	1.903242	0.618985	0.000206
6	2.261698	-0.699587	0.000117
1	3.307968	-0.979853	0.000274
1	2.637822	1.416230	0.000334
7	0.134601	2.242008	-0.000247
1	0.815079	2.991561	-0.000532
1	-0.849366	2.479646	-0.000581
1	-0.822702	-2.196789	-0.000348
1	1.575103	-2.754082	-0.000436
8	-1.729378	0.371395	0.000356
6	-2.814475	-0.574545	-0.000021
1	-3.721328	0.027854	0.000340
1	-2.771849	-1.195611	-0.898195

1	-2.771703	-1.196604	0.897438	1	3.083620	-1.128712	0.897698
				1	3.086694	-1.127006	-0.888974
(22) 3-methoxyaniline							
0	1			1	2		
6	0.266456	1.663794	0.004375	6	0.929807	-0.280468	0.000163
6	0.827406	0.380212	0.000344	6	0.049152	-1.397187	-0.000008
6	0.014150	-0.751084	-0.005557	6	-1.300591	-1.210497	-0.000185
6	-1.384803	-0.611316	-0.010064	6	-1.835568	0.114501	-0.000027
6	-1.947577	0.672221	-0.002938	6	-0.944956	1.230011	-0.000032
6	-1.117073	1.790123	0.003389	6	0.410274	1.038402	0.000102
1	0.919482	2.528502	0.010798	1	1.075186	1.891092	0.000189
1	0.439474	-1.746866	-0.006332	1	-1.363012	2.230422	-0.000209
1	-3.026969	0.783476	-0.001850	7	-3.153453	0.307052	0.000133
1	-1.559947	2.781273	0.011320	1	-3.543972	1.240645	-0.000138
7	-2.194410	-1.743139	-0.080715	1	-3.792949	-0.477201	-0.000266
1	-1.770579	-2.582410	0.292742	1	0.482798	-2.389853	-0.000036
1	-3.127682	-1.607012	0.284919	1	-1.984089	-2.051942	-0.000374
8	2.196259	0.331880	0.006665	8	2.222974	-0.576226	0.000312
6	2.824282	-0.945885	-0.001248	6	3.201299	0.480412	-0.000239
1	3.898441	-0.752814	0.001244	1	4.166972	-0.022811	-0.001500
1	2.559823	-1.528914	0.888358	1	3.095558	1.094913	-0.897618
1	2.561710	-1.516681	-0.899320	1	3.097376	1.094135	0.897882
				(24) 2-chloroaniline			
1	2			0	1		
6	0.682311	1.174163	-0.000039	6	-1.832268	-1.299109	0.006020
6	0.769773	-0.251848	0.000105	6	-2.354299	-0.005194	0.000970
6	-0.381513	-1.009857	0.000232	6	-1.512139	1.097993	-0.003220
6	-1.638937	-0.364493	0.000130	6	-0.113276	0.953713	-0.007893
6	-1.725437	1.073035	0.000137	6	0.382365	-0.360754	-0.001661
6	-0.566636	1.809511	-0.000006	6	-0.451364	-1.472106	0.005868
1	1.582742	1.773328	-0.000140	1	-0.015061	-2.464076	0.013149
1	-0.325329	-2.091675	0.000344	7	0.716442	2.060577	-0.077282
1	-2.704056	1.538049	0.000169	1	0.286243	2.917111	0.245663
1	-0.608100	2.891798	-0.000055	1	1.641910	1.931464	0.309022
7	-2.765021	-1.071667	-0.000228	1	-1.922559	2.103143	-0.003012
1	-2.746333	-2.084492	-0.000841	1	-3.428292	0.148347	0.005020
1	-3.667398	-0.611040	-0.000549	1	-2.485844	-2.163532	0.011047
8	1.936510	-0.916318	0.000317	17	2.129082	-0.610809	-0.002377
6	3.170727	-0.183099	-0.000296				
1	3.954363	-0.940573	-0.000473	1	2		
1	3.257351	0.435974	-0.897753	6	-1.765191	-1.339024	0.000245
1	3.258101	0.436374	0.896776	6	-2.361781	-0.060480	-0.000177
				6	-1.579688	1.061068	-0.000351
(23) 4-methoxyaniline				6	-0.151740	0.944022	0.000009
0	1			6	0.431588	-0.373756	-0.000043
6	0.943870	0.285449	-0.000375	6	-0.370666	-1.489355	0.000253
6	0.069422	1.376323	0.000266	1	0.072139	-2.477091	0.000488
6	-1.304129	1.181190	-0.004264	7	0.593206	2.037121	0.000352
6	-1.849938	-0.112026	-0.010219	1	0.153675	2.952281	0.001021
6	-0.965789	-1.195029	-0.005935	1	1.606681	2.002451	0.000418
6	0.417220	-1.006162	-0.002316	1	-2.003271	2.058915	-0.000916
1	1.065571	-1.873014	0.002860	1	-3.440940	0.028434	-0.000435
1	-1.363051	-2.205837	-0.005063	1	-2.388581	-2.225270	0.000549
7	-3.237737	-0.306006	-0.084021	17	2.154866	-0.532613	-0.000188
1	-3.537084	-1.186574	0.316739				
1	-3.765973	0.456792	0.321768	(25) 4-chloroaniline			
1	0.483144	2.379253	0.007906	0	1		
1	-1.968977	2.039889	-0.002081	6	-0.969490	0.000030	-0.001205
8	2.287645	0.585574	0.004509	6	-0.283180	1.209668	-0.001528
6	3.202442	-0.502584	0.005159	6	1.106595	1.205839	-0.004365
1	4.200461	-0.060304	0.007327				

6	1.826216	0.000105	-0.008595	1	-1.198835	2.163354	-0.001103
6	1.106551	-1.205773	-0.004370	6	-2.869177	0.000094	0.001228
6	-0.283105	-1.209696	-0.001551	1	-3.244012	-0.530674	0.885347
1	-0.825001	2.148112	0.004012	1	-3.283867	1.009173	-0.008318
1	1.645840	2.147866	-0.002433	1	-3.246798	-0.549585	-0.869826
1	1.646028	-2.147673	-0.002539				
1	-0.824949	-2.148123	0.004023				
7	3.214315	-0.000094	-0.075708	(27) diethylamine			
1	3.652203	0.837011	0.285780	0 1			
1	3.651938	-0.837124	0.286279	7	0.124658	-0.303691	-0.000000
17	-2.733399	-0.000027	0.004971	1	-0.646275	-0.969556	-0.000000
				6	-0.002112	0.507721	1.213422
1 2				1	0.842821	1.207342	1.242809
6	-0.961188	-0.000009	-0.000048	1	-0.914224	1.131478	1.198246
6	-0.278719	1.233840	-0.000136	6	-0.002112	-0.353011	2.469779
6	1.089878	1.238669	-0.000107	1	0.919158	-0.939598	2.548337
6	1.805564	-0.000005	0.000004	1	-0.087962	0.271208	3.364715
6	1.089882	-1.238683	-0.000100	1	-0.847615	-1.050994	2.466748
6	-0.278714	-1.233854	-0.000089	6	-0.002112	0.507721	-1.213422
1	-0.837012	2.161121	-0.000201	1	0.842821	1.207342	-1.242809
1	1.648369	2.167413	-0.000195	1	-0.914224	1.131478	-1.198246
1	1.648397	-2.167416	-0.000142	6	-0.002112	-0.353011	-2.469779
1	-0.836986	-2.161146	-0.000121	1	-0.847615	-1.050994	-2.466748
7	3.131302	0.000024	0.000213	1	-0.087962	0.271208	-3.364715
1	3.653352	0.869791	0.000531	1	0.919158	-0.939598	-2.548337
1	3.653233	-0.869805	-0.000259	1 2			
17	-2.685217	0.000007	0.000103	7	0.001753	0.178093	0.066761
				1	0.013441	1.194870	0.175684
(26) 4-methylaniline				6	1.240075	-0.490616	-0.215566
0 1				1	1.234152	-1.439190	0.335725
6	1.399393	0.000968	-0.010998	1	1.195215	-0.776618	-1.281768
6	0.670629	-1.193692	-0.008615	6	2.458674	0.367247	0.073318
6	-0.719871	-1.201950	0.003743	1	2.523920	0.609882	1.137014
6	-1.442701	0.000166	0.013469	1	3.355307	-0.187299	-0.211846
6	-0.720965	1.202150	0.003635	1	2.429891	1.295839	-0.503765
6	0.670283	1.194501	-0.008578	6	-1.254903	-0.499896	0.219729
1	1.201750	2.142265	-0.021845	1	-1.307624	-0.801440	1.281667
1	-1.260716	2.144853	-0.000464	1	-1.207491	-1.428510	-0.356973
7	-2.838336	-0.000913	0.088410	6	-2.444930	0.377546	-0.139359
1	-3.267050	0.831850	-0.295406	1	-2.431538	0.638160	-1.200465
1	-3.265817	-0.833775	-0.296566	1	-3.362974	-0.174117	0.074136
1	-1.259390	-2.144801	-0.000161	1	-2.448065	1.296084	0.454533
1	1.202499	-2.141308	-0.021938				
6	2.908010	-0.000284	0.004095	(28) piperidine			
1	3.311424	0.922529	-0.423902	0 1			
1	3.303526	-0.082660	1.024955	6	0.006250	0.742584	1.261143
1	3.313453	-0.843713	-0.564046	6	-0.645031	1.326427	0.000000
				6	0.006250	0.742584	-1.261143
1 2				6	0.006250	-0.790230	-1.212818
6	-1.377545	0.011257	-0.000484	6	0.006250	-0.790230	1.212818
6	-0.652497	1.227092	-0.000833	1	-0.513540	1.087846	-2.163127
6	0.717138	1.236287	-0.000793	1	-1.715671	1.078374	0.000000
6	1.430628	-0.002360	-0.000015	1	-0.575925	2.420020	0.000000
6	0.706699	-1.236129	-0.000795	1	1.044212	1.095739	1.335669
6	-0.659536	-1.214564	-0.000875	1	-0.513540	1.087846	2.163127
1	-1.215167	-2.145790	-0.001190	1	-1.029077	-1.153659	-1.259154
1	1.263096	-2.166610	-0.001259	1	0.524305	-1.198949	-2.086467
7	2.758624	-0.007579	0.001199	1	-1.029077	-1.153659	1.259154
1	3.276671	-0.878806	0.002340	1	0.524305	-1.198949	2.086467
1	3.283766	0.859387	0.002316	1	1.044212	1.095739	-1.335669
1	1.280524	2.162541	-0.001299	7	0.623090	-1.355373	-0.000000

1	1.598346	-1.059542	-0.000000	6	-3.894038	0.600131	-0.072076
1 2				1	-4.476193	-1.344983	0.653008
6	0.009541	0.754311	1.263318	1	-2.176686	-2.231957	0.709146
6	-0.649279	1.303832	0.000000	1	-0.703197	1.510867	-0.808379
6	0.009541	0.754311	-1.263318	1	-2.983423	2.402004	-0.817432
6	0.009541	-0.814387	-1.232839	1	-4.903154	0.996101	-0.089392
6	0.009541	-0.814387	1.232839	7	-0.000016	-1.003603	0.000502
1	-0.526418	1.042528	-2.171096	1	-0.000007	-2.013369	0.000216
1	-1.717053	1.057447	0.000000	6	1.265561	-0.420823	0.015737
1	-0.566078	2.396777	0.000000	6	1.515355	0.889372	0.455488
1	1.044436	1.097987	1.349536	6	2.358583	-1.214177	-0.377403
1	-0.526418	1.042528	2.171096	6	2.816326	1.386432	0.472265
1	-1.029286	-1.157913	-1.249730	1	0.703502	1.510690	0.809269
1	0.569520	-1.228501	-2.069056	6	3.651901	-0.709792	-0.344833
1	-1.029286	-1.157913	1.249730	1	2.176359	-2.231957	-0.709285
1	0.569520	-1.228501	2.069056	6	3.894046	0.600037	0.071517
1	1.044436	1.097987	-1.349536	1	2.983807	2.401853	0.817451
7	0.606210	-1.224661	-0.000000	1	4.475898	-1.344991	-0.653991
1	1.589854	-1.491885	-0.000000	1	4.903169	0.996011	0.088443
(29) pyrrolidine				1 2			
0 1				6	-3.623960	-0.743253	0.325956
6	0.777093	1.024336	-0.069960	6	-2.337806	-1.245005	0.326298
6	-0.776524	1.024715	-0.070210	6	-1.254902	-0.406185	-0.027824
6	-1.155150	-0.450571	0.197118	6	-1.496874	0.923721	-0.438506
6	1.154941	-0.451233	0.196920	6	-2.793586	1.403986	-0.439337
1	1.163124	1.348144	-1.041015	6	-3.858501	0.585044	-0.047730
1	1.196651	1.694127	0.685824	1	-4.450371	-1.382224	0.613869
1	-1.162011	1.348107	-1.041617	1	-2.138096	-2.270751	0.617021
1	-1.196094	1.695150	0.685004	1	-0.688205	1.541752	-0.802128
1	-1.328401	-0.604577	1.268702	1	-2.983678	2.419274	-0.767127
1	-2.056918	-0.768125	-0.330893	1	-4.870038	0.974438	-0.054312
1	1.328459	-0.605580	1.268409	7	-0.000043	-0.970571	0.000220
1	2.056304	-0.769224	-0.331508	1	-0.000059	-1.989128	0.000285
7	-0.000400	-1.276814	-0.208353	6	1.254869	-0.406200	0.028033
1	-0.000476	-1.283806	-1.227639	6	1.496981	0.923684	0.438732
1 2				6	2.337717	-1.245003	-0.326347
6	0.741518	1.018966	0.208264	6	2.793694	1.403910	0.439329
6	-0.742013	1.018606	-0.208374	1	0.688361	1.541691	0.802514
6	-1.199504	-0.408472	0.113079	6	3.623885	-0.743283	-0.326255
6	1.199756	-0.408038	-0.112706	1	2.137918	-2.270731	-0.617080
1	1.334516	1.759543	-0.327361	6	3.858534	0.584982	0.047452
1	0.842104	1.200375	1.281810	1	2.983895	2.419172	0.767144
1	-0.842492	1.199591	-1.282019	1	4.450209	-1.382274	-0.614379
1	-1.335332	1.759135	0.326927	1	4.870060	0.974396	0.053852
1	-1.553846	-0.511939	1.153899	(31) n-methylaniline			
1	-1.984052	-0.833061	-0.521378	0 1			
1	1.983898	-0.832344	0.522435	6	1.360187	1.348463	0.015308
1	1.554930	-0.511327	-1.153196	6	-0.002346	1.059930	0.073095
7	0.000209	-1.192150	-0.000395	6	-0.446916	-0.273704	0.076325
1	0.000266	-2.211292	0.000065	6	0.519016	-1.296727	0.006057
(30) diphenylamine				6	1.872100	-0.995110	-0.055568
0 1				6	2.309711	0.331901	-0.049615
6	-3.652071	-0.709753	0.344248	1	1.677151	2.386993	0.015839
6	-2.358782	-1.214143	0.377296	1	-0.718537	1.871480	0.118252
6	-1.265563	-0.420788	-0.015354	1	0.187662	-2.331297	-0.000181
6	-1.515169	0.889462	-0.455026	1	2.592843	-1.805226	-0.111446
6	-2.816142	1.386535	-0.472287	1	3.367563	0.564702	-0.097974
				7	-1.790059	-0.607496	0.184761
				1	-1.994431	-1.537013	-0.154296

6	-2.820947	0.365861	-0.136632	6	-3.707065	0.225159	0.000102
1	-2.686215	0.829783	-1.124795	1	-3.893637	-0.371592	0.897058
1	-3.789400	-0.137169	-0.121610	1	-4.338316	1.112493	0.000240
1	-2.851063	1.166545	0.609065	1	-3.893603	-0.371317	-0.897045
				1	1.822409	-2.428804	-0.000051
1 2				8	2.303369	0.230076	0.000232
6	1.340623	1.374363	-0.000006	6	3.512847	-0.547056	0.000171
6	-0.005656	1.097891	-0.000019	1	4.322118	0.181527	0.000382
6	-0.434936	-0.262822	0.000023	1	3.562660	-1.169660	0.897520
6	0.530951	-1.317133	-0.000014	1	3.562816	-1.169347	-0.897386
6	1.870136	-1.011826	0.000001	8	-0.064096	1.753207	0.000138
6	2.285263	0.330989	0.000017	6	1.085471	2.637157	-0.000385
1	1.678806	2.403625	-0.000010	1	1.678663	2.469182	-0.898264
1	-0.737671	1.894814	-0.000068	1	0.649531	3.634472	-0.000386
1	0.181940	-2.343931	-0.000011	1	1.679525	2.469285	0.896899
1	2.607183	-1.805865	-0.000006				
1	3.343225	0.566553	0.000028	(33) 1,2,4-trimethoxybenzene			
7	-1.731443	-0.588763	0.000002	0 1			
1	-1.953199	-1.580160	-0.000096	6	1.622252	0.014954	-0.000057
6	-2.851750	0.336631	0.000014	6	0.669556	1.046143	-0.000004
1	-2.818558	0.971402	-0.889623	6	-0.683793	0.748139	0.000082
1	-3.770918	-0.245085	0.000052	6	-1.109810	-0.602508	0.000141
1	-2.818490	0.971425	0.889619	6	-0.157233	-1.607699	0.000090
				6	1.214677	-1.311136	-0.000028
(32) 1,2,3-trimethoxybenzene				1	-0.464115	-2.645495	0.000118
0 1				1	1.928907	-2.123021	-0.000097
6	1.216584	-1.653444	0.154804	8	-2.467809	-0.795319	0.000226
6	1.215605	-0.275422	-0.081555	6	-2.935658	-2.138840	-0.000242
6	0.000005	0.412359	-0.203849	1	-2.602765	-2.679943	0.893438
6	-1.215389	-0.275773	-0.081902	1	-4.025343	-2.078346	-0.000505
6	-1.216007	-1.653848	0.154406	1	-2.602287	-2.679470	-0.894027
6	0.000375	-2.320844	0.269685	8	-1.681078	1.679832	0.000120
1	-2.145526	-2.198424	0.248653	6	-1.304014	3.053801	-0.000102
1	0.000536	-3.389970	0.453594	1	-0.723674	3.307756	-0.894315
8	-2.335879	0.491004	-0.213230	1	-2.236515	3.620196	-0.000085
6	-3.601075	-0.157526	-0.107044	1	-0.723491	3.307963	0.893926
1	-3.732019	-0.619267	0.877799	1	1.018333	2.070088	-0.000050
1	-4.349328	0.624924	-0.242321	8	2.929730	0.432886	-0.000187
1	-3.725449	-0.918181	-0.885653	6	3.939873	-0.569309	0.000094
1	2.146267	-2.197701	0.249374	1	4.892866	-0.037397	0.000136
8	2.335882	0.491685	-0.212170	1	3.878008	-1.201272	0.893796
6	3.601104	-0.157011	-0.107649	1	3.878233	-1.201529	-0.893446
1	4.349291	0.625296	-0.244120				
1	3.733394	-0.618574	0.877111	1 2			
1	3.724233	-0.917865	-0.886260	6	1.615027	0.052410	-0.000035
8	-0.000133	1.764111	-0.490944	6	0.662025	1.085170	-0.000015
6	-0.000781	2.604231	0.671569	6	-0.678184	0.771570	-0.000065
1	0.893664	2.432499	1.280512	6	-1.091507	-0.622795	-0.000158
1	-0.001453	3.635241	0.310899	6	-0.117054	-1.641883	-0.000161
1	-0.895095	2.431300	1.280367	6	1.214909	-1.319458	-0.000106
				1	-0.421970	-2.679070	-0.000275
1 2				1	1.959026	-2.103873	-0.000157
6	0.963094	-1.773876	-0.000100	8	-2.391173	-0.816587	-0.000284
6	1.133214	-0.400668	0.000048	6	-2.924599	-2.158825	0.000352
6	-0.040158	0.449571	0.000027	1	-2.600020	-2.688027	0.898922
6	-1.361149	-0.161494	0.000033	1	-4.005582	-2.033058	0.001218
6	-1.483246	-1.537029	-0.000174	1	-2.601464	-2.688144	-0.898681
6	-0.324492	-2.318117	-0.000242	8	-1.681838	1.640516	-0.000011
1	-2.454889	-2.009311	-0.000254	6	-1.374243	3.044624	0.000088
1	-0.427374	-3.397441	-0.000377	1	-0.807288	3.308567	-0.896917
8	-2.356897	0.717797	0.000228	1	-2.337620	3.552202	-0.000042

1	-0.807531	3.308569	0.897233	1	1.842839	2.368092	0.000000
1	1.009424	2.108489	0.000111	1	-0.523218	3.132081	-0.000000
8	2.880537	0.439543	0.000039	8	2.638543	-0.045177	0.000000
6	3.944378	-0.533964	0.000130	6	2.984877	-1.427267	-0.000000
1	4.862644	0.051076	0.000384	1	2.604793	-1.934337	-0.894047
1	3.892639	-1.152920	0.898611	1	4.075447	-1.463460	-0.000000
1	3.893028	-1.152681	-0.898543	1	2.604793	-1.934337	0.894047
(34) 1,2-dimethoxybenzene				1	-2.375880	1.502452	-0.000000
0 1				8	-1.986411	-1.205394	0.000000
6	-0.693562	2.291407	-0.000000	6	-3.360726	-0.829531	0.000000
6	-1.395303	1.080234	-0.000001	1	-3.616592	-0.249880	-0.894031
6	-0.707627	-0.127798	-0.000001	1	-3.926933	-1.762345	0.000000
6	0.707699	-0.127179	-0.000000	1	-3.616592	-0.249880	0.894031
6	1.394747	1.081068	0.000001	1	0.469346	-1.714040	0.000000
6	0.692259	2.291869	0.000001	1 2			
1	2.477004	1.088530	0.000002	6	-1.348511	1.160509	-0.000000
1	1.244134	3.225376	0.000002	6	-1.036187	-0.249263	0.000000
8	1.294015	-1.362180	-0.000000	6	0.287728	-0.697858	0.000000
6	2.717572	-1.418614	0.000000	6	1.299963	0.245084	0.000000
1	3.136805	-0.943391	0.894131	6	0.996852	1.656567	0.000000
1	2.974651	-2.479058	-0.000000	6	-0.320920	2.086919	0.000000
1	3.136805	-0.943391	-0.894129	1	1.828468	2.350943	0.000000
8	-1.293274	-1.362680	-0.000003	1	-0.545742	3.145893	0.000000
6	-2.716811	-1.419653	0.000002	8	2.596268	-0.018901	0.000000
1	-3.135907	-0.944348	0.894123	6	3.035402	-1.389971	-0.000000
1	-3.135913	-0.944351	-0.894116	1	2.673744	-1.898886	-0.897326
1	-2.973636	-2.480164	0.000005	1	4.123024	-1.345629	-0.000000
1	-2.477589	1.087158	-0.000002	1	2.673744	-1.898886	0.897326
1	-1.246127	3.224518	-0.000000	1	-2.380377	1.483688	-0.000000
1 2				8	-1.968153	-1.180437	-0.000000
6	-0.711437	2.272396	0.000000	6	-3.371462	-0.836792	0.000000
6	-1.426471	1.098692	-0.000000	1	-3.620059	-0.270077	-0.899491
6	-0.730082	-0.122400	-0.000000	1	-3.893218	-1.792036	0.000000
6	0.729914	-0.123004	-0.000000	1	-3.620059	-0.270077	0.899491
6	1.427390	1.097368	0.000000	1	0.478365	-1.761398	0.000000
6	0.713424	2.271734	0.000000	(36) 1,4-dimethoxybenzene			
1	2.508420	1.104865	0.000000	0 1			
1	1.239075	3.219113	0.000000	6	-0.939388	-1.034806	-0.000000
8	1.273969	-1.316242	-0.000000	6	-1.370484	0.294860	-0.000000
6	2.712082	-1.459296	0.000000	6	-0.423222	1.319596	-0.000000
1	3.129857	-1.001102	0.898946	6	0.939388	1.034806	0.000000
1	2.888679	-2.532982	0.000000	6	1.370484	-0.294860	-0.000000
1	3.129857	-1.001102	-0.898946	6	0.423222	-1.319596	-0.000000
8	-1.275069	-1.315248	-0.000000	1	0.765584	-2.348743	-0.000000
6	-2.713349	-1.457801	0.000000	1	-1.648085	-1.852532	-0.000000
1	-3.130939	-0.999511	0.898970	8	-2.686523	0.686541	-0.000000
1	-3.130940	-0.999513	-0.898970	6	-3.679809	-0.332575	0.000000
1	-2.890411	-2.531369	0.000001	1	-3.608669	-0.963481	0.893874
1	-2.507470	1.107094	-0.000000	1	-4.641349	0.183855	0.000001
1	-1.236157	3.220290	0.000000	1	-3.608670	-0.963481	-0.893873
(35) 1,3-dimethoxybenzene				1	-0.765584	2.348743	0.000000
0 1				8	2.686523	-0.686541	0.000000
6	-1.352797	1.152936	-0.000000	6	3.679809	0.332575	0.000000
6	-1.050580	-0.208181	0.000000	1	4.641349	-0.183855	0.000000
6	0.280738	-0.648992	0.000000	1	3.608670	0.963481	-0.893874
6	1.312257	0.284523	0.000000	1	3.608670	0.963481	0.893874
6	1.024549	1.657592	0.000000	1	1.648085	1.852532	0.000000
6	-0.297494	2.070624	0.000000				

1 2				6	-4.022435	-0.069361	-0.534006
6	-0.933995	-1.071040	-0.000000	6	0.834665	-0.453394	-0.106792
6	-1.360824	0.284957	-0.000000	6	2.020084	0.394498	-0.021191
6	-0.403409	1.343294	-0.000000	6	0.971160	-1.850371	-0.048725
6	0.933995	1.071040	0.000000	6	3.289877	-0.193198	0.114630
6	1.360824	-0.284957	-0.000000	6	2.228045	-2.390007	0.087001
6	0.403409	-1.343294	-0.000000	6	3.385609	-1.562809	0.167424
1	0.773264	-2.361320	-0.000000	6	2.861348	2.630004	-0.006757
1	-1.655905	-1.876055	-0.000000	1	-2.456018	1.149568	-1.343561
8	-2.619848	0.668150	-0.000000	1	-1.541278	-1.150491	-1.206587
6	-3.683043	-0.309521	0.000000	1	-1.684458	-1.105616	0.581487
1	-3.622009	-0.926656	0.898815	1	-4.758132	0.736430	-0.657575
1	-4.602679	0.272378	0.000000	1	-4.070833	-0.715339	-1.415039
1	-3.622010	-0.926657	-0.898814	1	0.098503	-2.485198	-0.109891
1	-0.773264	2.361320	-0.000000	1	4.172539	0.428067	0.174681
8	2.619848	-0.668150	0.000000	1	-1.758380	1.759100	0.833201
6	3.683043	0.309521	0.000000	1	2.347631	-3.465847	0.133902
1	4.602679	-0.272378	0.000000	1	4.357863	-2.029317	0.272480
1	3.622010	0.926657	-0.898814	1	-4.258551	-0.306871	1.370243
1	3.622009	0.926657	0.898815	1	3.539156	2.480539	-0.849782
1	1.655905	1.876055	0.000000	1	3.389961	2.514179	0.941679
				1	2.387049	3.607501	-0.065033

(37) 3,2-methoxy-phenoxy-1,2-propanediol

0 1			
8	0.263359	-1.030029	-0.786232
8	1.777958	0.389471	1.249072
8	4.192047	0.505402	-0.130348
8	-0.338016	1.524873	-0.377989
6	2.258178	-0.780564	0.585406
6	1.120856	-1.702641	0.158160
6	3.166573	-0.375651	-0.576457
6	-1.015981	-0.726545	-0.375685
6	-1.356340	0.628152	-0.198505
6	-1.974742	-1.714055	-0.190499
6	-2.662974	0.969284	0.145956
6	-3.279875	-1.371677	0.166101
6	-3.618490	-0.033123	0.327009
6	-0.622110	2.911152	-0.178242
1	2.859162	-1.320067	1.327088
1	1.526729	-2.594941	-0.330279
1	0.539880	-2.012664	1.031139
1	2.562122	0.094862	-1.365528
1	3.655421	-1.258194	-1.000991
1	-1.687989	-2.750095	-0.336035
1	-2.939554	2.006356	0.283753
1	1.163764	0.840883	0.643105
1	-4.022495	-2.148865	0.307209
1	-4.631011	0.246233	0.597352
1	3.741757	1.154293	0.427984
1	0.317860	3.434656	-0.355890
1	-0.961872	3.102427	0.844966
1	-1.377123	3.261396	-0.889359
1 2			
8	-0.293724	0.200914	-0.236812
8	-2.646713	1.399625	0.718011
8	-4.332935	-0.877795	0.595137
8	1.774096	1.680779	-0.080425
6	-2.637013	0.560795	-0.433100
6	-1.559813	-0.506972	-0.323065

(38) anisole

0 1			
6	-0.037735	1.058968	0.000330
6	-0.451353	-0.275664	0.000345
6	0.501026	-1.302322	0.000055
6	1.854932	-0.994158	-0.000255
6	2.279152	0.336626	-0.000185
6	1.327762	1.351660	0.000033
1	1.641350	2.390672	0.000044
1	-0.759245	1.865408	0.000592
8	-1.758429	-0.678304	0.000486
6	-2.767538	0.327151	-0.000546
1	-2.704101	0.957460	-0.894861
1	-3.720660	-0.204265	-0.000802
1	-2.705006	0.958275	0.893269
1	0.157844	-2.331134	0.000026
1	3.336805	0.575386	-0.000337
1	2.582972	-1.798944	-0.000485
1 2			
6	-0.043265	1.103624	0.000320
6	-0.450646	-0.265534	0.000086
6	0.517722	-1.325410	0.000082
6	1.850621	-1.015807	-0.000164
6	2.252172	0.336335	-0.000227
6	1.297012	1.383180	0.000081
1	1.636673	2.411626	0.000098
1	-0.782432	1.893068	0.000667
8	-1.694005	-0.659477	0.000508
6	-2.789508	0.290937	-0.000518
1	-2.736758	0.905483	-0.900785
1	-3.688402	-0.321246	-0.000905
1	-2.737724	0.905738	0.899654
1	0.151383	-2.344489	0.000137
1	3.307768	0.582294	-0.000522
1	2.596887	-1.800605	-0.000372

(39) 3-amino-L-tyrosine				7	2.013172	-1.157968	-1.155634
0	1			7	-3.177078	1.889716	-0.564319
8	3.882731	1.399464	0.568723	6	1.129741	0.004573	0.907403
8	-4.333510	-0.502531	-0.280514	6	2.023402	0.104144	-0.334853
8	4.316720	-0.627996	-0.322802	6	-0.342709	-0.123225	0.597138
7	1.962944	-1.068402	-1.209783	6	-1.066982	0.973955	0.166087
7	-3.200621	1.951861	-0.434385	6	-0.994940	-1.385100	0.734298
6	1.201552	0.068659	0.894833	6	-2.432694	0.858334	-0.144081
6	2.067086	0.176912	-0.371962	6	-2.323643	-1.539207	0.443131
6	-0.272921	-0.105591	0.612108	6	3.518770	0.383695	0.011377
6	-1.048441	0.985879	0.201524	6	-3.123110	-0.436952	-0.012397
6	-0.879370	-1.357543	0.721196	1	1.318077	0.916011	1.479964
6	-2.405828	0.857348	-0.093633	1	1.461900	-0.842782	1.516896
6	-2.236262	-1.510384	0.421678	1	1.672875	0.907485	-0.985337
6	3.570982	0.340714	-0.011348	1	-0.587594	1.943354	0.063898
6	-2.993137	-0.420365	0.021372	1	-0.413104	-2.232629	1.083843
1	1.385402	0.985025	1.461765	1	-2.819336	-2.498184	0.551585
1	1.568270	-0.769221	1.498189	1	1.597881	-1.949284	-0.659927
1	1.739677	1.017852	-0.983080	1	3.034796	-1.332641	-1.298730
1	-0.591638	1.968039	0.110610	1	-2.791822	2.814416	-0.675469
1	-0.301898	-2.215253	1.051567	1	-4.154271	1.725052	-0.758305
1	-2.715444	-2.481675	0.505300	1	1.532507	-1.049227	-2.048439
1	1.210068	-1.691382	-0.907883	(40) 3-methoxy-L-tyrosine			
1	2.900393	-1.507844	-1.086212	0	1		
1	-2.681195	2.715144	-0.848637	8	-4.566412	-0.326460	0.467343
1	-4.004751	1.705894	-0.996919	8	4.071131	-1.157152	0.263286
1	-4.619484	-1.420864	-0.195240	8	-3.933867	1.411539	-0.825193
1	1.824834	-0.855203	-2.198152	7	-2.250669	-0.897181	1.363201
1	2			6	-1.413039	-0.206457	-0.906754
8	3.776074	1.328822	0.793985	6	-2.237909	0.194433	0.326244
8	-4.348450	-0.420723	-0.281008	6	0.047499	-0.463191	-0.612395
8	4.409606	-0.384581	-0.530156	6	0.904570	0.610918	-0.316575
7	2.082350	-1.175978	-1.159927	6	0.563554	-1.757076	-0.609033
7	-3.097396	1.915648	-0.565155	6	2.241836	0.384139	-0.023954
6	1.176170	-0.010382	0.896136	6	1.910157	-1.991741	-0.314245
6	2.076016	0.086050	-0.340474	6	-3.725001	0.460758	-0.046671
6	-0.297530	-0.113071	0.583342	6	2.750057	-0.931168	-0.022251
6	-1.007300	0.979712	0.154220	1	-1.528017	0.613607	-1.620678
6	-0.975117	-1.362931	0.729699	1	-1.863341	-1.097559	-1.357753
6	-2.389727	0.872460	-0.146670	1	-1.815262	1.085579	0.790310
6	-2.320635	-1.506746	0.450620	1	0.514003	1.621505	-0.321958
6	3.567784	0.374803	0.022032	1	-0.083860	-2.595168	-0.846840
6	-3.050867	-0.405288	0.011521	1	2.315987	-2.997475	-0.314173
1	1.369932	0.895894	1.474031	1	-1.622141	-1.672089	1.140816
1	1.489558	-0.865291	1.503867	1	-3.249331	-1.203009	1.355318
1	1.730263	0.887603	-0.995819	1	4.484334	-0.297273	0.428993
1	-0.534617	1.949139	0.036685	1	-2.013384	-0.549340	2.292567
1	-0.410971	-2.221787	1.077084	8	3.169248	1.343338	0.274038
1	-2.822816	-2.459851	0.571529	6	2.745800	2.704490	0.289201
1	1.681885	-1.974120	-0.662628	1	1.963859	2.865760	1.039301
1	3.107028	-1.334519	-1.304160	1	3.627835	3.290884	0.549720
1	-2.661065	2.822005	-0.679652	1	2.378058	3.014103	-0.695226
1	-4.083630	1.825027	-0.773993	1	2		
1	-4.729365	-1.302219	-0.144326	8	-4.621763	-0.020805	0.587466
1	1.598512	-1.075364	-2.052172	8	4.042558	-1.138754	0.248047
0	2			8	-3.762696	1.436527	-0.907433
8	3.742292	1.347991	0.767195	7	-2.432905	-1.161764	1.197045
8	-4.348579	-0.526459	-0.290215	6	-1.379203	-0.214631	-0.905128
8	4.352340	-0.392172	-0.531847	6	-2.251228	0.051493	0.328497

6	0.074289	-0.434402	-0.590073	6	0.700161	0.550107	-0.350442
6	0.894762	0.643809	-0.289218	6	0.298250	-1.790457	-0.628813
6	0.612540	-1.764918	-0.596585	6	2.044007	0.270752	-0.070514
6	2.238489	0.423009	0.004597	6	1.621155	-2.080347	-0.351965
6	1.929304	-2.012746	-0.314758	6	-3.938940	0.584964	-0.008066
6	-3.690388	0.538651	-0.049623	6	2.531761	-1.057872	-0.062045
6	2.771368	-0.929477	-0.013129	1	-1.732993	0.709260	-1.552567
1	-1.488689	0.672254	-1.533793	1	-2.099535	-1.012242	-1.452538
1	-1.780595	-1.072567	-1.453081	1	-2.014773	0.922634	0.917631
1	-1.796981	0.821894	0.954690	1	0.378579	1.583574	-0.347042
1	0.494185	1.649082	-0.289588	1	-0.381515	-2.605747	-0.856947
1	-0.051824	-2.586986	-0.838261	1	1.986523	-3.100423	-0.355826
1	2.346923	-3.011533	-0.322142	1	-3.650359	-1.065983	1.440057
1	-2.232908	-2.031723	0.698501	1	-2.082730	-0.970550	2.102914
1	-3.453985	-1.124328	1.417192	1	4.285473	-0.557057	0.378531
1	4.496574	-0.294288	0.427225	1	-2.361961	-1.936422	0.786071
1	-1.868451	-1.136643	2.046753	7	2.921365	1.376161	0.202240
8	3.141846	1.333162	0.305203	8	2.480408	2.520477	0.180222
6	2.775390	2.729297	0.350654	8	4.120952	1.142605	0.457421
1	1.997583	2.880875	1.102223				
1	3.686724	3.254958	0.628146	1 2			
1	2.430288	3.049821	-0.634847	8	-4.108272	1.385632	-0.920747
				8	3.844074	-1.323614	0.180224
0 2				8	-4.911392	0.102686	0.505737
8	-4.532982	-0.058737	0.665434	7	-2.555876	-0.965862	1.380453
8	4.084135	-1.093119	0.294065	6	-1.651782	-0.310197	-0.881004
8	-3.827173	1.239931	-1.038836	6	-2.463479	0.121363	0.354036
7	-2.252238	-0.951516	1.342614	6	-0.186455	-0.550681	-0.591826
6	-1.339547	-0.290010	-0.918974	6	0.671420	0.506006	-0.341632
6	-2.182322	0.124200	0.292513	6	0.344102	-1.854606	-0.579480
6	0.119331	-0.501147	-0.603319	6	2.026642	0.275891	-0.079144
6	0.937074	0.598756	-0.310075	6	1.680798	-2.093185	-0.323679
6	0.665758	-1.810643	-0.588422	6	-3.862547	0.533964	-0.020790
6	2.275856	0.417631	-0.002478	6	2.560204	-1.035068	-0.064126
6	1.984337	-2.021472	-0.289254	1	-1.763603	0.495186	-1.612681
6	-3.659773	0.468288	-0.076282	1	-2.109002	-1.207994	-1.307530
6	2.871444	-0.927799	0.021045	1	-1.992364	0.979282	0.841426
1	-1.454610	0.516929	-1.647692	1	0.314647	1.527917	-0.347632
1	-1.764734	-1.198068	-1.358497	1	-0.312562	-2.694540	-0.782103
1	-1.747113	1.002624	0.772925	1	2.081275	-3.099856	-0.319077
1	0.509322	1.593548	-0.330896	1	-2.984090	-1.811095	0.985344
1	0.017227	-2.648253	-0.824345	1	-3.119341	-0.670341	2.184935
1	2.413490	-3.017599	-0.277637	1	4.303265	-0.469144	0.337563
1	-1.996711	-1.871140	0.976089	1	-1.620142	-1.211315	1.721048
1	-3.267943	-0.952635	1.589214	7	2.868245	1.415256	0.172388
1	-1.671702	-0.754858	2.157829	8	2.383892	2.541266	0.155253
8	3.141760	1.395474	0.289625	8	4.079437	1.225933	0.403868
6	2.673735	2.749532	0.299065				
1	1.884246	2.881014	1.045188	0 2			
1	3.538531	3.357756	0.563760	8	-3.985771	1.237697	-1.165122
1	2.304376	3.038865	-0.689454	8	3.808155	-1.312595	0.350101
				8	-4.748361	0.176954	0.675679
(41) 3-nitro-L-tyrosine				7	-2.517438	-0.799396	1.411582
0 1				6	-1.591559	-0.380729	-0.903589
8	-4.052290	1.497881	-0.847490	6	-2.396462	0.178162	0.275669
8	3.802320	-1.393998	0.200683	6	-0.145812	-0.630852	-0.584558
8	-4.852274	-0.012944	0.624416	6	0.722007	0.461932	-0.338277
7	-2.622968	-1.060175	1.242467	6	0.372783	-1.940852	-0.517379
6	-1.646854	-0.172503	-0.914012	6	2.044628	0.258674	-0.060623
6	-2.485396	0.130542	0.331737	6	1.692445	-2.165316	-0.219788
6	-0.192210	-0.470371	-0.628420	6	-3.857088	0.568370	-0.124341

6	2.626190	-1.082575	0.035807	1	-1.820350	-2.021016	0.632334
1	-1.673860	0.368862	-1.696299	1	-3.085691	-1.255962	1.426821
1	-2.061722	-1.301739	-1.260790	1	4.690947	0.365406	0.598388
1	-1.915331	1.071164	0.679684	1	-1.483577	-1.139092	1.997631
1	0.340109	1.474598	-0.391808	9	3.034963	1.907701	0.576711
1	-0.291285	-2.777337	-0.707286				
1	2.097239	-3.168729	-0.151677	0 2			
1	-3.526968	-0.715159	1.668098	8	-4.337413	-0.371665	0.537751
1	-1.914507	-0.572855	2.202752	8	4.355686	-0.449443	0.302714
1	-2.327324	-1.761642	1.122271	8	-3.704712	1.320676	-0.814183
7	2.881257	1.435752	0.138975	7	-2.007329	-1.154667	1.175617
8	2.349806	2.446688	0.595464	6	-1.112235	-0.035800	-0.907631
8	4.066685	1.367189	-0.168168	6	-2.004046	0.092733	0.334269
				6	0.354858	-0.150792	-0.594316
(42) 3-fluoro-L-tyrosine				6	1.065092	0.977538	-0.134765
0 1				6	1.032358	-1.386356	-0.746851
8	-4.357499	-0.523244	0.438132	6	2.395094	0.861974	0.158994
8	4.365463	-0.531360	0.267602	6	2.364967	-1.510001	-0.452697
8	-3.834110	1.353584	-0.699331	6	-3.496675	0.378445	-0.028001
7	-2.001572	-1.088547	1.209468	6	3.135955	-0.384195	0.023123
6	-1.185355	0.016342	-0.901450	1	-1.298762	0.865307	-1.497929
6	-2.063942	0.146455	0.350504	1	-1.440164	-0.897815	-1.497007
6	0.289784	-0.124624	-0.605015	1	-1.652883	0.905865	0.972114
6	1.031662	0.976280	-0.155331	1	0.570089	1.935314	-0.016617
6	0.945460	-1.348890	-0.754437	1	0.473023	-2.242898	-1.108331
6	2.373187	0.825946	0.127932	1	2.889346	-2.452102	-0.568446
6	2.301959	-1.488971	-0.462771	1	-1.602358	-1.959695	0.692982
6	-3.565786	0.352114	-0.008445	1	-3.030836	-1.314487	1.323213
6	3.035289	-0.396368	-0.014880	1	-1.524392	-1.036068	2.066167
1	-1.375879	0.914035	-1.495115	9	3.083060	1.913493	0.586835
1	-1.530286	-0.842557	-1.487423				
1	-1.729081	0.986016	0.960892	(43) L-tyrosine			
1	0.574761	1.951948	-0.027440	0 1			
1	0.390273	-2.210410	-1.111628	8	-3.707988	1.338616	-0.378396
1	2.804760	-2.442021	-0.583071	8	4.615654	-0.041133	0.437323
1	-1.399495	-1.817255	0.822302	8	-4.033229	-0.822545	0.182313
1	-3.000066	-1.400340	1.218925	7	-1.650815	-1.313108	0.925224
1	4.708676	0.319690	0.572724	6	-0.924247	0.359251	-0.810637
1	-1.690415	-0.889649	2.160385	6	-1.832591	0.085529	0.397292
9	3.099264	1.878759	0.555035	6	0.551269	0.247540	-0.503274
				6	1.215324	1.248425	0.218265
1 2				6	1.290217	-0.867069	-0.909026
8	-4.383636	-0.254024	0.620210	6	2.565463	1.143144	0.525895
8	4.308460	-0.472768	0.279802	6	2.645205	-0.989356	-0.606769
8	-3.696007	1.273191	-0.895986	6	-3.339868	0.221079	0.031953
7	-2.076932	-1.188675	1.168618	6	3.284996	0.018472	0.112949
6	-1.150498	-0.069135	-0.910939	1	-1.175701	1.367132	-1.150819
6	-2.038442	0.060712	0.336514	1	-1.192112	-0.333465	-1.616294
6	0.306899	-0.160826	-0.594191	1	-1.597816	0.774484	1.209118
6	1.000516	0.980334	-0.132555	1	0.666433	2.128446	0.540672
6	1.003618	-1.399793	-0.750185	1	0.802802	-1.652310	-1.479967
6	2.328557	0.876702	0.153462	1	3.208645	-1.859223	-0.931053
6	2.334018	-1.509335	-0.462821	1	-0.935373	-1.842099	0.422177
6	-3.527015	0.394374	-0.033803	1	-2.598164	-1.730303	0.778789
6	3.035458	-0.367441	0.001562	1	4.988032	-0.859447	0.083683
1	-1.347475	0.836626	-1.492890	1	-1.416869	-1.326978	1.918058
1	-1.469448	-0.935109	-1.497176	1	3.075716	1.923924	1.079252
1	-1.679051	0.861068	0.986401				
1	0.495569	1.931453	-0.012710	1 2			
1	0.451466	-2.260559	-1.108388	8	-3.527144	1.344518	-0.619368
1	2.882261	-2.436146	-0.575608	8	4.546773	0.071089	0.477263

8	-4.119180	-0.557443	0.446859	1	0.607281	2.143978	0.392624
7	-1.755943	-1.410070	0.872895	1	0.607122	-2.143821	0.392970
6	-0.881090	0.224821	-0.854463	1	2.991454	2.147759	-0.270285
6	-1.803062	-0.001749	0.352612	1	2.991296	-2.147880	-0.269950
6	0.568631	0.161576	-0.505955	1	4.193026	-0.000135	-0.606236
6	1.158047	1.190031	0.287041	1	-3.851770	0.894489	0.720038
6	1.374515	-0.921679	-0.951453	1	-3.851836	-0.893905	0.720562
6	2.482916	1.152850	0.609713	1	-4.454377	-0.000104	-0.695520
6	2.703182	-0.983517	-0.637310				
6	-3.305195	0.296358	0.010206	1 2			
6	3.277663	0.060980	0.147824	16	-2.026289	-0.558026	-0.428891
1	-1.132375	1.227876	-1.215532	6	0.276942	-0.251485	0.571608
1	-1.121244	-0.495425	-1.641047	6	-1.067617	-0.595890	1.132330
1	-1.522876	0.650464	1.181909	6	0.735227	1.085172	0.569366
1	0.538408	2.013796	0.622710	6	1.091563	-1.274159	0.020972
1	0.918652	-1.700654	-1.551512	6	1.993671	1.377538	0.082866
1	3.336390	-1.798684	-0.969563	6	2.348133	-0.969468	-0.467409
1	-1.402602	-2.070987	0.177201	6	2.801768	0.353875	-0.440491
1	-2.763575	-1.616798	1.050411	6	-2.627629	1.141713	-0.514413
1	5.024271	-0.701096	0.124120	1	-1.130799	-1.607753	1.529820
1	-1.201785	-1.506510	1.724439	1	-1.470248	0.132659	1.834030
1	2.961109	1.925172	1.199275	1	0.105107	1.864793	0.982178
				1	0.726863	-2.295508	0.013232
0 2				1	2.362333	2.396240	0.106910
8	-3.540296	1.346161	-0.563930	1	2.980055	-1.752673	-0.868906
8	4.608901	-0.030886	0.453693	1	3.784085	0.594732	-0.831338
8	-4.053521	-0.647769	0.360002	1	-1.788126	1.835936	-0.588340
7	-1.677644	-1.356538	0.916791	1	-3.225484	1.353666	0.374600
6	-0.839767	0.254282	-0.841963	1	-3.235512	1.202536	-1.418903
6	-1.766155	0.039299	0.361537				
6	0.623296	0.176472	-0.504164	(45)	2-hydroxyethyl benzyl sulfide		
6	1.227346	1.190290	0.281924	0 1			
6	1.411893	-0.905758	-0.954927	16	1.237098	-0.303729	-0.443166
6	2.555421	1.133509	0.608658	8	4.013638	1.305696	-0.252110
6	2.745644	-0.988560	-0.641459	6	-1.355652	-0.174386	0.465254
6	-3.269110	0.274435	0.007982	6	0.036539	-0.477331	0.948224
6	3.386625	0.032937	0.161129	6	2.800701	-0.722412	0.426734
1	-1.084075	1.250202	-1.223076	6	-2.173136	-1.192917	-0.036241
1	-1.088553	-0.472073	-1.622108	6	-1.852162	1.133133	0.500830
1	-1.501382	0.720410	1.172003	6	3.994805	-0.116392	-0.303142
1	0.618242	2.023017	0.619925	6	-3.460005	-0.911960	-0.489312
1	0.944519	-1.675485	-1.561012	6	-3.138751	1.416286	0.048520
1	3.359681	-1.814440	-0.984273	6	-3.946283	0.394048	-0.448417
1	-1.193179	-2.001830	0.289739	1	0.339734	0.213314	1.738473
1	-2.685567	-1.628282	0.985250	1	0.107077	-1.500159	1.325132
1	-1.226234	-1.393903	1.830806	1	2.743127	-0.316519	1.440761
1	3.028217	1.906662	1.204790	1	2.909314	-1.808913	0.485972
				1	-1.798007	-2.211484	-0.064591
(44) benzyl methyl sulfide				1	-1.226427	1.929904	0.891540
0 1				1	4.029324	-0.475766	-1.342023
16	-2.071918	-0.000187	-0.679239	1	4.911943	-0.453288	0.190885
6	0.443697	0.000089	0.434775	1	-4.084054	-1.713565	-0.870594
6	-1.009158	0.000174	0.827428	1	-3.511860	2.434412	0.087811
6	1.130028	1.204096	0.242432	1	-4.949511	0.613271	-0.798381
6	1.129941	-1.204004	0.242624	1	3.190328	1.614474	-0.652144
6	2.472181	1.205344	-0.130145				
6	2.472090	-1.205405	-0.129955	1 2			
6	3.147010	-0.000070	-0.318503	16	1.229806	-0.980578	-0.339443
6	-3.713641	0.000108	0.107534	8	3.016503	1.381011	-1.037010
1	-1.257191	-0.888483	1.413451	6	-1.182242	-0.665257	0.357447
1	-1.257193	0.889110	1.413026	6	-0.108581	-1.648321	0.714721

6	2.135191	0.132710	0.787879
6	-1.980797	-0.886145	-0.792092
6	-1.393977	0.488174	1.145820
6	3.398454	0.617563	0.096133
6	-2.995131	-0.002017	-1.109554
6	-2.412605	1.362864	0.821577
6	-3.212775	1.123601	-0.307139
1	0.192327	-1.632645	1.760858
1	-0.317398	-2.662803	0.378244
1	1.479902	0.972522	1.032429
1	2.362745	-0.432164	1.695028
1	-1.802488	-1.766990	-1.399396
1	-0.772831	0.659009	2.017819
1	4.034042	-0.230800	-0.186613
1	3.953622	1.222866	0.827081
1	-3.620499	-0.180885	-1.976151
1	-2.598181	2.233654	1.439395
1	-4.003400	1.820904	-0.560714
1	3.798006	1.499468	-1.589566

(46) thioanisole

0 1

16	1.819313	-0.718308	0.000115
6	0.108821	-0.233123	0.000142
6	-0.328006	1.095165	0.000172
6	-0.837851	-1.268349	-0.000036
6	-1.694389	1.377209	0.000064
6	-2.196452	-0.974812	-0.000119
6	-2.634054	0.350387	-0.000081
6	2.724043	0.856526	-0.000256
1	0.381998	1.912502	0.000332
1	-0.508603	-2.302894	-0.000127
1	-2.019012	2.412764	0.000035
1	-2.915726	-1.787357	-0.000216
1	-3.694520	0.576986	-0.000194
1	2.506503	1.439744	0.896426
1	2.506087	1.439676	-0.896886
1	3.781585	0.583491	-0.000525

1 2

16	1.755915	-0.703415	-0.000021
6	0.117801	-0.214649	-0.000058
6	-0.315820	1.136683	-0.000048
6	-0.829432	-1.282125	0.000007
6	-1.666565	1.400452	0.000004
6	-2.174588	-0.991630	0.000012
6	-2.598842	0.345788	0.000028
6	2.749505	0.802886	0.000060
1	0.400415	1.947451	-0.000130
1	-0.482617	-2.309520	0.000077
1	-2.015275	2.426016	-0.000001
1	-2.902677	-1.793506	0.000021
1	-3.659026	0.572025	0.000083
1	2.543287	1.383908	0.900976
1	2.543693	1.383801	-0.901014
1	3.785205	0.460040	0.000303