Supporting Information (ESI-2)

Electrophilicity and Nucleophilicity of Commonly Used Aldehydes

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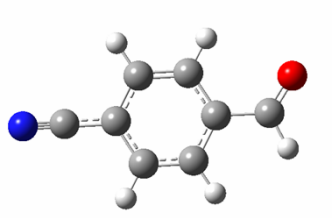
Optimized Geometry:

4-Cyano Benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -437.932572817 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

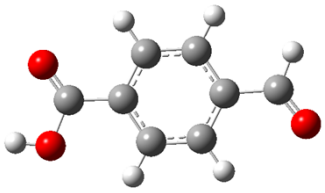
C	-0.862180	1.253105	-0.000003
C	0.522973	1.353948	0.000013
C	1.317314	0.202905	0.000036
C	0.714987	-1.062363	0.000039
C	-0.665395	-1.175035	0.000022
C	-1.460026	-0.014969	-0.000001
C	2.796554	0.333976	0.000065
O	3.566110	-0.598486	-0.000086
C	-2.887541	-0.129061	-0.000017
N	-4.039185	-0.221110	-0.000030
H	-1.483787	2.139602	-0.000020
H	0.993303	2.331900	0.000010
H	1.347229	-1.942221	0.000057
H	-1.141523	-2.147607	0.000025
H	3.170073	1.378951	-0.000098



4-formylbenzoic acid

E(RB+HF-LYP/6-311+G(d,p)) = -534.303751 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

C	0	-0.264697	-1.126435	-0.000024
C	0	-1.033053	0.047355	-0.000092
C	0	-0.406261	1.297541	-0.000047
C	0	0.980729	1.372942	0.000065
C	0	1.749833	0.204088	0.000133
C	0	1.119997	-1.047022	0.000083
C	0	3.231068	0.304680	0.000275
O	0	3.984938	-0.641251	-0.000241
H	0	-0.759185	-2.088738	-0.000057
H	0	-1.018497	2.190504	-0.000102
H	0	1.472987	2.340179	0.000099
H	0	1.732471	-1.940753	0.000142
H	0	3.624366	1.342740	-0.000286
C	0	-2.523802	0.016653	-0.000222
O	0	-3.231730	0.995397	0.000012
O	0	-3.026173	-1.241851	0.000098
H	0	-3.991304	-1.161107	0.000218

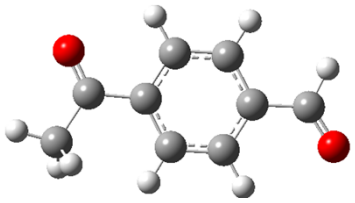


4-Acetyl Benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -498.3577321 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

C	0.265444	-1.099611	-0.000092
C	1.023894	0.081777	-0.000018

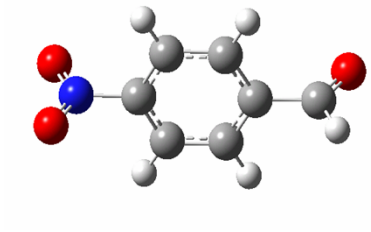
C	0.366612	1.318852	0.000017
C	-1.020418	1.372551	0.000021
C	-1.772942	0.191960	-0.000018
C	-1.121507	-1.046996	-0.000083
C	-3.254715	0.267464	0.000013
O	-3.993282	-0.691009	0.000069
H	0.757261	-2.064331	-0.000160
H	0.964821	2.221445	0.000060
H	-1.528452	2.331948	0.000057
H	-1.717730	-1.951746	-0.000122
H	-3.665484	1.298724	-0.000013
C	2.530370	0.075991	0.000005
O	3.145826	1.124056	-0.000060
H	4.330517	-1.064695	0.000025
C	3.258427	-1.253254	0.000106
H	2.993827	-1.844172	-0.881796
H	2.993906	-1.843958	0.882173



4-Nitro Benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -550.207130540 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

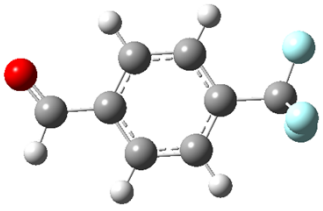
C	1.702829	0.005690	-0.202846
C	1.007922	-1.205443	-0.163598
C	-0.381062	-1.215162	-0.068768
C	-1.046849	0.000380	-0.018794
C	-0.385043	1.218483	-0.057864
C	1.003939	1.214135	-0.153240
H	1.546851	-2.145334	-0.199639
H	-0.930890	-2.147456	-0.032001
H	-0.937888	2.148620	-0.012684
H	1.539702	2.156117	-0.181395
C	3.205581	0.008596	-0.304170
O	3.937112	-0.016868	0.652330
H	3.620762	0.035424	-1.334049
N	-2.526646	-0.002485	0.077814
O	-3.010820	-0.006806	1.198826
O	-3.150783	-0.000082	-0.972312



4-Trifluromethyl Benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -682.8159086 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

C	0	-0.069716	1.152306	-0.000033
C	0	0.708352	-0.007667	-0.000035
C	0	0.108149	-1.268536	-0.000023
C	0	-1.277950	-1.364084	-0.000012
C	0	-2.065713	-0.207989	-0.000012

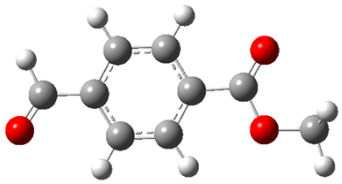


C	0	-1.454971	1.050490	-0.000025
C	0	2.214284	0.073057	0.000002
C	0	-3.545825	-0.330084	-0.000005
O	0	-4.311426	0.605861	0.000038
H	0	0.408329	2.122879	-0.000047
H	0	0.718888	-2.163172	-0.000032
H	0	-1.753505	-2.339467	-0.000006
H	0	-2.079288	1.935880	-0.000028
H	0	-3.925071	-1.373157	0.000051
F	0	2.745555	-0.538877	1.085436
F	0	2.666837	1.343472	-0.000379
F	0	2.745652	-0.539573	-1.084988

Methyl-4-formylbenzoate

E(RB+HF-LYP/6-311+G(d,p)) = -573.6142568 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

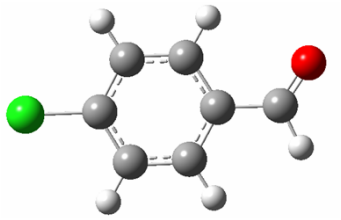
C	0	-0.078016	-1.009061	-0.000363
C	0	0.585450	0.227070	-0.000189
C	0	-0.149960	1.416344	0.000120
C	0	-1.538619	1.370190	0.000285
C	0	-2.202682	0.138772	0.000094
C	0	-1.464287	-1.051779	-0.000251
C	0	-3.685884	0.108888	0.000270
O	0	-4.355362	-0.899063	-0.000008
H	0	0.499878	-1.923546	-0.000580
H	0	0.381589	2.359561	0.000218
H	0	-2.113828	2.290696	0.000567
H	0	-1.995571	-1.996067	-0.000413
H	0	-4.168706	1.108628	0.000395
C	0	2.076741	0.330866	-0.000316
O	0	2.686061	1.375454	-0.000516
O	0	2.675424	-0.876467	0.000000
C	0	4.115983	-0.866116	0.000650
H	0	4.492033	-0.358107	-0.888136
H	0	4.412138	-1.912535	0.000030
H	0	4.491129	-0.359068	0.890326



4-Chloro Benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -805.291395750 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

C	0.548932	-1.170791	0.000016
C	1.325617	-0.010013	0.000002
C	0.745532	1.255811	-0.000001
C	-0.641830	1.355176	0.000011
C	-1.439836	0.206678	0.000026
C	-0.833197	-1.056760	0.000026
Cl	3.072906	-0.151136	-0.000015
C	-2.914049	0.338241	0.000043
O	-3.691147	-0.590040	-0.000057

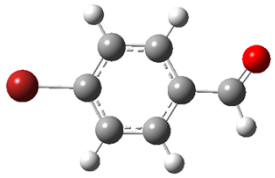


H	1.028828	-2.141022	0.000018
H	1.370167	2.139580	-0.000015
H	-1.109311	2.334810	0.000009
H	-1.462567	-1.938927	0.000037
H	-3.284357	1.385136	-0.000077

4-Bromo Benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -2919.2108878 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

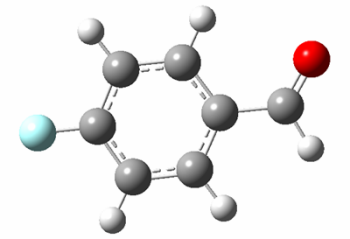
C	-0.106989	-1.137475	0.000099
C	0.649040	0.037304	0.000028
C	0.046173	1.292887	0.000008
C	-1.343408	1.366876	0.000057
C	-2.120256	0.204285	0.000135
C	-1.491437	-1.047931	0.000150
C	-3.596857	0.309023	0.000214
O	-4.356453	-0.633633	-0.000314
H	0.386104	-2.100871	0.000115
H	0.650819	2.190349	-0.000047
H	-1.828484	2.338018	0.000043
H	-2.104560	-1.941548	0.000211
H	-3.986336	1.348908	-0.000403
Br	2.557614	-0.083303	-0.000044



4-Fluro Benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -444.9378314 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

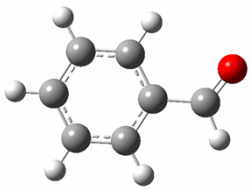
C	0.957744	-1.224763	0.000000
C	1.751589	-0.082177	0.000000
C	1.223844	1.200705	0.000000
C	-0.160360	1.338434	0.000000
C	-0.989767	0.211452	-0.000001
C	-0.420446	-1.070316	-0.000001
C	-2.458521	0.384123	-0.000002
O	-3.262715	-0.521275	0.000002
H	1.425907	-2.201122	0.000000
H	1.887401	2.056053	0.000001
H	-0.601806	2.329874	-0.000001
H	-1.076686	-1.932467	-0.000001
H	-2.798967	1.441312	0.000003
F	3.093486	-0.229800	0.000001



Benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -345.6690893 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

C	1.614576	-1.230837	0.000000
C	1.328003	0.131759	0.000000
C	0.000000	0.572485	0.000000

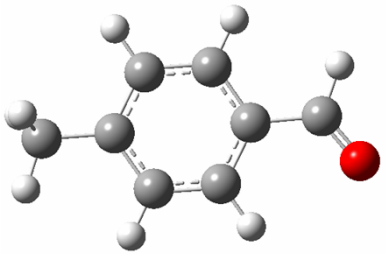


C	-1.044848	-0.362139	0.000000
C	-0.757771	-1.720629	0.000000
C	0.571167	-2.155469	0.000000
C	-0.283761	2.025400	0.000000
O	-1.390181	2.517583	0.000000
H	2.643434	-1.571636	0.000000
H	2.133050	0.860233	0.000000
H	-2.066646	-0.001202	0.000000
H	-1.563573	-2.445740	0.000000
H	0.791076	-3.217233	0.000000
H	0.619914	2.671495	0.000000

4-Methyl Benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -384.997623681 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

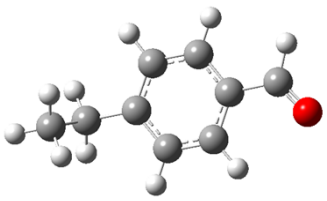
C	-0.919131	-1.199330	-0.000011
C	-1.754629	-0.072690	-0.000008
C	-1.161925	1.197152	-0.000006
C	0.220331	1.335571	-0.000003
C	1.046543	0.205131	-0.000003
C	0.462692	-1.067790	-0.000009
C	-3.255575	-0.215553	0.000014
C	2.514500	0.370698	0.000001
O	3.319060	-0.535699	0.000014
H	-1.363630	-2.189125	-0.000017
H	-1.791782	2.081046	-0.000008
H	0.667495	2.325176	-0.000004
H	1.108729	-1.938127	-0.000012
H	-3.557674	-1.264374	-0.000255
H	-3.695694	0.262154	0.880915
H	-3.695777	0.262638	-0.880581
H	2.859014	1.427069	-0.000005



4-Ethyl Benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -424.3216763 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

C	0	-0.496522	-1.126580	-0.316993
C	0	-1.291310	0.030940	-0.347136
C	0	-0.664577	1.273773	-0.200905
C	0	0.712806	1.359199	-0.025730
C	0	1.495225	0.200476	0.005986
C	0	0.876955	-1.048592	-0.142787
C	0	-2.791802	-0.068211	-0.497155
C	0	2.957317	0.308692	0.190952
O	0	3.726096	-0.627189	0.233304
H	0	-0.967761	-2.096968	-0.437675
H	0	-1.261126	2.179871	-0.229286
H	0	1.188313	2.329367	0.083701
H	0	1.491888	-1.940874	-0.122778
H	0	-3.035692	-0.913868	-1.147798

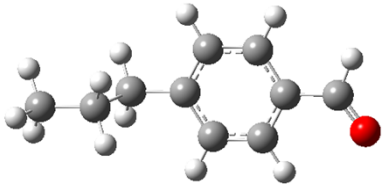


H	0	-3.167277	0.830493	-0.995928
H	0	3.332338	1.349440	0.295194
C	0	-3.514235	-0.240785	0.851622
H	0	-3.315173	0.605559	1.514256
H	0	-4.595422	-0.310460	0.704724
H	0	-3.182000	-1.148523	1.362032

4-Propyl Benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -463.6463683 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

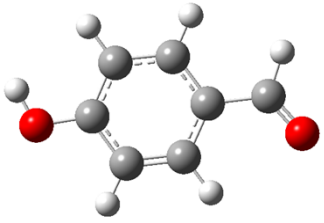
C	0	0.013145	-1.075530	-0.412405
C	0	-0.747219	0.105108	-0.443971
C	0	-0.092585	1.324450	-0.234856
C	0	1.277697	1.364881	0.001783
C	0	2.025356	0.183458	0.033644
C	0	1.379265	-1.042435	-0.177358
C	0	-2.240613	0.053398	-0.660959
C	0	3.480368	0.243798	0.283789
O	0	4.220495	-0.714767	0.330447
H	0	-0.479132	-2.028112	-0.581189
H	0	-0.661639	2.248051	-0.263034
H	0	1.774729	2.317444	0.159587
H	0	1.967487	-1.952532	-0.156516
H	0	-2.480735	-0.758344	-1.356423
H	0	-2.574636	0.982271	-1.135405
H	0	3.879202	1.269786	0.435561
C	0	-3.032762	-0.155942	0.646037
H	0	-2.790279	0.653586	1.343142
H	0	-2.694835	-1.081739	1.124122
C	0	-4.545101	-0.210787	0.416852
H	0	-5.082151	-0.357261	1.357692
H	0	-4.911882	0.716452	-0.034462
H	0	-4.815392	-1.033863	-0.251990



4-Hydroxy Benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -420.9186684 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

C	0	0.170512	1.331820	-0.000037
C	0	-1.211640	1.187018	0.000006
C	0	-1.767392	-0.095253	0.000022
C	0	-0.940599	-1.227664	-0.000005
C	0	0.432679	-1.070800	-0.000048
C	0	1.007118	0.211526	-0.000068

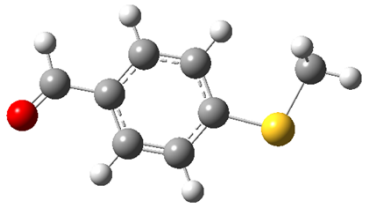


H	0	0.605432	2.326480	-0.000050
H	0	-1.857088	2.060292	0.000028
H	0	-1.400198	-2.208517	0.000007
H	0	1.089336	-1.932923	-0.000072
C	0	2.469768	0.388834	-0.000124
O	0	3.283531	-0.510744	0.000110
H	0	2.804463	1.448869	0.000130
O	0	-3.111216	-0.311240	0.000066
H	0	-3.583151	0.528785	0.000067

4-Mercapto Benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -783.208119 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

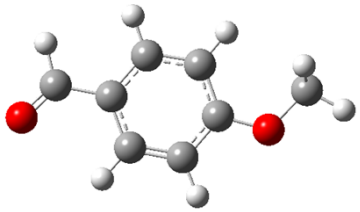
C	0	-0.921702	1.300682	-0.000030
C	0	0.449712	1.065760	-0.000040
C	0	0.930540	-0.249468	-0.000019
C	0	0.012606	-1.318978	0.000009
C	0	-1.347304	-1.075034	0.000015
C	0	-1.833845	0.242620	-0.000003
H	0	-1.288245	2.322951	-0.000046
H	0	1.130578	1.906094	-0.000064
H	0	0.380472	-2.339214	0.000029
H	0	-2.057545	-1.893618	0.000038
C	0	-3.281812	0.519927	0.000004
O	0	-4.154028	-0.322724	0.000028
H	0	-3.543453	1.599923	-0.000012
C	0	3.511179	0.912231	0.000077
H	0	4.572845	0.664349	0.000131
H	0	3.283702	1.489463	-0.896662
H	0	3.283591	1.489388	0.896836
S	0	2.647127	-0.690249	-0.000035



4-Methoxy Benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -460.2281 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

C	-0.541256	1.278108	-0.000178
C	0.830948	1.040114	-0.000234
C	1.293936	-0.280614	-0.000174
C	0.377759	-1.348622	-0.000134
C	-0.978434	-1.096551	-0.000097
C	-1.458613	0.225706	-0.000081
H	-0.903264	2.301887	-0.000201
H	1.519350	1.873937	-0.000427
H	0.766777	-2.359633	-0.000182
H	-1.694378	-1.910094	-0.000087

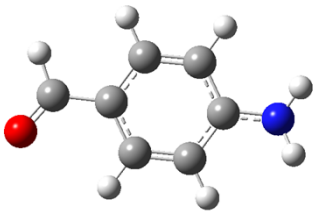


C	-2.903104	0.511019	0.000136
O	-3.782114	-0.325265	0.000254
H	-3.158003	1.592835	0.000173
O	2.602778	-0.634740	-0.000034
C	3.596534	0.386065	0.000351
H	4.552527	-0.133903	0.000595
H	3.522799	1.011944	-0.894689
H	3.522260	1.011717	0.895527

4-Amino Benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -401.0499374 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

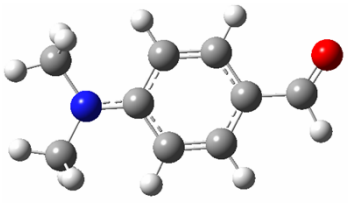
C	0.934406	-1.209460	-0.005868
C	1.773380	-0.075212	-0.004133
C	1.185989	1.202700	-0.003292
C	-0.193172	1.334360	-0.001269
C	-1.028389	0.209383	-0.000800
C	-0.439142	-1.065837	-0.003175
C	-2.487632	0.374293	0.003753
O	-3.299102	-0.530007	0.006788
H	1.379205	-2.199424	-0.012216
H	1.819716	2.083427	-0.007749
H	-0.635397	2.326163	0.000893
H	-1.086056	-1.935545	-0.002330
H	-2.829581	1.432192	0.004292
N	3.146506	-0.220738	-0.052494
H	3.713038	0.570492	0.209297
H	3.533710	-1.113441	0.209666



4-(dimethylamino) Benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -479.6774014 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

C	0.170709	-1.144144	-0.006247
C	0.990540	0.016316	-0.008475
C	0.343837	1.276897	-0.003321
C	-1.038209	1.358896	-0.000062
C	-1.841061	0.211194	-0.000191
C	-1.205746	-1.040918	-0.002892
C	-3.302199	0.329153	0.003901
O	-4.087112	-0.599739	0.004224
H	0.620664	-2.127119	-0.007257
H	0.923783	2.188973	-0.001284
H	-1.509719	2.337430	0.003524
H	-1.820666	-1.933766	-0.001651
H	-3.677031	1.376138	0.006371
N	2.361013	-0.082482	-0.015774

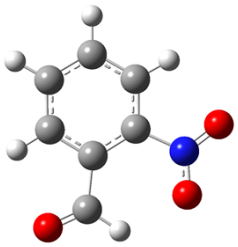


C	3.182795	1.118270	0.006823
C	3.005349	-1.387558	0.009923
H	2.747768	-1.952895	0.913559
H	4.085103	-1.251509	-0.005123
H	2.730042	-1.991633	-0.861994
H	2.988357	1.756240	-0.862666
H	4.232677	0.832437	-0.016545
H	3.012739	1.712347	0.912931

2-nitro Benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -550.2186827 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

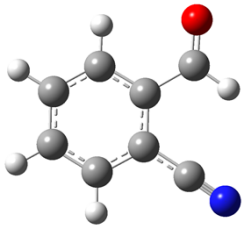
1	6	0	-1.917411	1.698072	-0.000073
2	6	0	-0.719864	2.409444	-0.000037
3	6	0	0.488814	1.724007	0.000012
4	6	0	0.500378	0.331143	0.000022
5	6	0	-0.696334	-0.416839	0.000013
6	6	0	-1.895209	0.309697	-0.000037
7	6	0	-0.852779	-1.920677	0.000149
8	8	0	-1.950348	-2.431617	0.000068
9	7	0	1.856488	-0.293549	-0.000010
10	8	0	1.936763	-1.515383	-0.000386
11	8	0	2.822378	0.455026	0.000263
12	1	0	-2.865494	2.222982	-0.000117
13	1	0	-0.720964	3.492801	-0.000055
14	1	0	1.431831	2.251445	0.000026
15	1	0	-2.815221	-0.261706	-0.000035
16	1	0	0.058519	-2.523960	0.000406



2-formyl Benzonitrile

E(RB+HF-LYP/6-311+G(d,p)) = -437.9303849 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

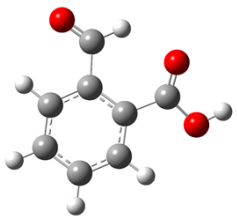
C	-2.261594	0.636821	0.000037
C	-2.295246	-0.759235	-0.000046
C	-1.112320	-1.489428	-0.000068
C	0.120318	-0.821896	0.000009
C	0.159189	0.587968	0.000065
C	-1.042088	1.302231	0.000077
C	1.451939	1.328180	0.000133
O	1.527310	2.535551	-0.000207
H	-3.186834	1.201028	0.000063
H	-3.245144	-1.280795	-0.000087
H	-1.131440	-2.572040	-0.000137
H	-0.990651	2.384470	0.000117
H	2.363164	0.702038	0.000536
C	1.322669	-1.602460	-0.000001
N	2.273604	-2.258884	-0.000011



2-formyl Benzoic acid

E(RB+HF-LYP/6-311+G(d,p)) = -534.2964382 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

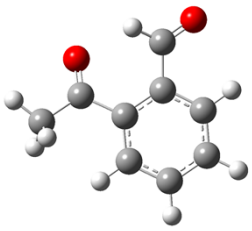
1	6	0	0.246699	-1.766376	0.034522
2	6	0	0.427576	-0.378300	-0.008996
3	6	0	-0.703205	0.468939	-0.042497
4	6	0	-1.979221	-0.103508	-0.012985
5	6	0	-2.147538	-1.481617	0.047257
6	6	0	-1.030874	-2.315516	0.066591
7	1	0	-2.832432	0.563086	-0.046458
8	1	0	-3.145146	-1.904960	0.072307
9	1	0	-1.152430	-3.391686	0.108757
10	6	0	-0.635304	1.960817	-0.185650
11	8	0	-1.601735	2.670004	-0.008430
12	1	0	0.331033	2.386974	-0.486431
13	1	0	1.115298	-2.410297	0.058970
14	6	0	1.813437	0.170918	0.056105
15	8	0	2.115039	1.290304	0.399378
16	8	0	2.751808	-0.743000	-0.296711
17	1	0	3.613363	-0.313714	-0.187118



2-acetyl Benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -498.3503244 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

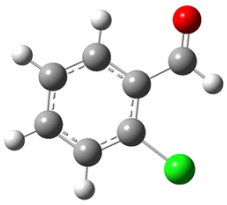
1	6	0	-0.298014	-1.750890	-0.063472
2	6	0	-0.427287	-0.357499	-0.002345
3	6	0	0.742633	0.434374	0.064485
4	6	0	1.994421	-0.188253	0.043606
5	6	0	2.105779	-1.571733	-0.040403
6	6	0	0.955234	-2.356036	-0.090057
7	1	0	2.875340	0.439675	0.103197
8	1	0	3.084597	-2.037117	-0.059397
9	1	0	1.031469	-3.435479	-0.152814
10	6	0	0.731376	1.922413	0.246807
11	8	0	1.697353	2.611551	0.002860
12	1	0	-0.187062	2.364139	0.658707
13	1	0	-1.182554	-2.372920	-0.117455
14	6	0	-1.789338	0.269723	-0.094346
15	8	0	-1.925003	1.400333	-0.522836
16	6	0	-2.997345	-0.540185	0.339615
17	1	0	-2.836128	-1.025126	1.305334
18	1	0	-3.858086	0.124573	0.392448
19	1	0	-3.211119	-1.324302	-0.393568



2-Chloro Benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -805.2873169 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

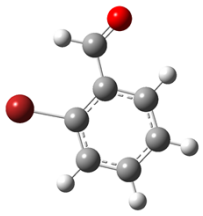
1	6	0	-2.245278	0.860749	-0.000005
2	6	0	-2.371918	-0.529909	0.000019
3	6	0	-1.241151	-1.341169	0.000019
4	6	0	0.021274	-0.755110	-0.000004
5	6	0	0.175367	0.638623	-0.000028
6	6	0	-0.982288	1.432233	-0.000028
7	6	0	1.500411	1.315476	-0.000053
8	8	0	1.631409	2.519946	0.000055
9	1	0	-3.127956	1.488982	-0.000006
10	1	0	-3.353866	-0.989107	0.000036
11	1	0	-1.331338	-2.419854	0.000037
12	1	0	-0.848818	2.507732	-0.000046
13	1	0	2.382000	0.653281	0.000063
14	17	0	1.417070	-1.830939	-0.000003



2-Bromo Benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -2919.2067547 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

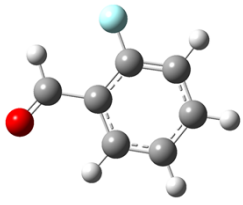
1	6	0	2.646077	-1.112151	-0.000008
2	6	0	1.679279	-2.119046	0.000039
3	6	0	0.324590	-1.796725	0.000038
4	6	0	-0.060632	-0.459183	-0.000007
5	6	0	0.890655	0.570282	-0.000063
6	6	0	2.249405	0.215964	-0.000056
7	35	0	-1.950439	-0.093875	-0.000002
8	6	0	0.541622	2.017519	-0.000140
9	8	0	1.369110	2.901928	0.000127
10	1	0	3.699240	-1.366743	-0.000007
11	1	0	1.975747	-3.161856	0.000077
12	1	0	-0.426332	-2.575838	0.000074
13	1	0	2.973690	1.022319	-0.000100
14	1	0	-0.535829	2.252373	0.000177



2-Fluro Benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -444.9346659 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	1.353062	-1.629785	0.000000
2	6	0	2.233096	-0.543140	0.000001
3	6	0	1.747386	0.761633	0.000001
4	6	0	0.375153	0.954931	0.000000
5	6	0	-0.534812	-0.104152	-0.000002
6	6	0	-0.016218	-1.408331	-0.000002
7	6	0	-2.000644	0.124230	-0.000003
8	8	0	-2.815677	-0.772866	0.000003
9	1	0	1.741034	-2.641177	-0.000001
10	1	0	3.303886	-0.711305	0.000002
11	1	0	2.407745	1.619661	0.000003
12	1	0	-0.722086	-2.230508	-0.000003

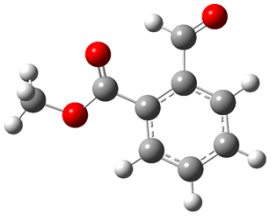


13	1	0	-2.322434	1.180266	0.000006
14	9	0	-0.091652	2.225964	-0.000001

Methyl 2-formylbenzoate

E(RB+HF-LYP/6-311+G(d,p)) = -498.3503244 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

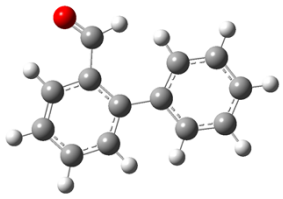
1	6	0	-0.298014	-1.750890	-0.063472
2	6	0	-0.427287	-0.357499	-0.002345
3	6	0	0.742633	0.434374	0.064485
4	6	0	1.994421	-0.188253	0.043606
5	6	0	2.105779	-1.571733	-0.040403
6	6	0	0.955234	-2.356036	-0.090057
7	1	0	2.875340	0.439675	0.103197
8	1	0	3.084597	-2.037117	-0.059397
9	1	0	1.031469	-3.435479	-0.152814
10	6	0	0.731376	1.922413	0.246807
11	8	0	1.697353	2.611551	0.002860
12	1	0	-0.187062	2.364139	0.658707
13	1	0	-1.182554	-2.372920	-0.117455
14	6	0	-1.789338	0.269723	-0.094346
15	8	0	-1.925003	1.400333	-0.522836
16	6	0	-2.997345	-0.540185	0.339615
17	1	0	-2.836128	-1.025126	1.305334
18	1	0	-3.858086	0.124573	0.392448
19	1	0	-3.211119	-1.324302	-0.393568



Biphenyl 2-carbaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -576.7557779 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-3.190499	-1.274368	0.000071
2	6	0	-2.161132	-2.209379	0.000134
3	6	0	-0.839727	-1.789191	0.000074
4	6	0	-0.438236	-0.434955	-0.000042
5	6	0	-1.514318	0.514069	-0.000151
6	6	0	-2.849285	0.063841	-0.000064
7	6	0	1.052250	-0.169454	-0.000033
8	6	0	1.651348	1.104950	0.000114
9	6	0	3.032290	1.288537	0.000156
10	6	0	3.895469	0.200482	0.000038
11	6	0	3.341248	-1.075750	-0.000104
12	6	0	1.962561	-1.251246	-0.000129
13	6	0	-1.434984	2.010491	-0.000408
14	8	0	-2.415063	2.727514	0.000187
15	1	0	-4.229640	-1.581322	0.000114
16	1	0	-2.378120	-3.271858	0.000247
17	1	0	-0.096906	-2.569443	0.000164
18	1	0	-3.617908	0.825849	-0.000153
19	1	0	1.061101	2.001287	0.000276
20	1	0	3.425271	2.299010	0.000293

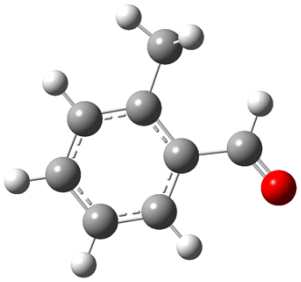


21	1	0	4.970003	0.341184	0.000071
22	1	0	3.982410	-1.950150	-0.000194
23	1	0	1.615357	-2.272261	-0.000248
24	1	0	-0.452979	2.489428	-0.000001

2-methyl benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -384.9934865 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

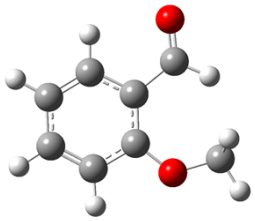
1	6	0	-1.372506	-1.668265	0.000003
2	6	0	-2.241528	-0.576731	0.000001
3	6	0	-1.737639	0.721755	-0.000005
4	6	0	-0.361808	0.971786	-0.000007
5	6	0	0.510886	-0.138984	0.000000
6	6	0	-0.003941	-1.443727	0.000002
7	6	0	1.983880	0.030338	0.000017
8	8	0	2.779573	-0.885947	-0.000012
9	6	0	0.131090	2.402426	0.000001
10	1	0	-1.762134	-2.679610	0.000005
11	1	0	-3.314392	-0.735222	0.000002
12	1	0	-2.426047	1.560381	-0.000012
13	1	0	0.700268	-2.267481	0.000005
14	1	0	2.351909	1.073394	0.000004
15	1	0	-0.714462	3.092052	-0.000140
16	1	0	0.738710	2.626264	0.881277
17	1	0	0.738955	2.626207	-0.881118



2-methoxy benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -460.2128601 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

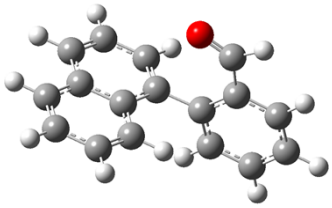
1	6	0	-2.407977	0.485445	0.000128
2	6	0	-2.350852	-0.914989	0.000013
3	6	0	-1.130119	-1.558794	-0.000094
4	6	0	0.081536	-0.840840	-0.000117
5	6	0	0.042312	0.576229	-0.000059
6	6	0	-1.229317	1.198694	0.000094
7	8	0	1.151968	-1.681552	-0.000166
8	6	0	2.514545	-1.279366	0.000276
9	6	0	1.196492	1.512264	-0.000252
10	8	0	1.073181	2.721631	0.000052
11	1	0	-3.361511	0.999326	0.000229
12	1	0	-3.263042	-1.501261	0.000030
13	1	0	-1.065182	-2.639804	-0.000143
14	1	0	-1.234809	2.281616	0.000147
15	1	0	3.084413	-2.207694	0.000889
16	1	0	2.765876	-0.706723	-0.897123
17	1	0	2.765044	-0.705996	0.897460
18	1	0	2.208300	1.088041	-0.000516



2-(naphthalen-2-yl) benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -730.4473298 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

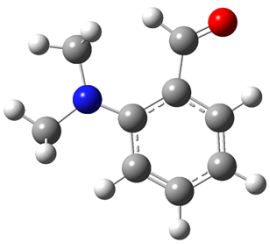
1	6	0	1.936158	0.208326	-1.606538
2	6	0	1.334454	0.274400	-0.346719
3	6	0	2.105431	-0.096409	0.779075
4	6	0	3.431886	-0.516538	0.606963
5	6	0	4.012648	-0.578926	-0.653848
6	6	0	3.257242	-0.211574	-1.764241
7	1	0	1.353298	0.489312	-2.476379
8	1	0	4.009395	-0.792778	1.483995
9	1	0	5.039217	-0.906252	-0.769577
10	1	0	3.692545	-0.250896	-2.756655
11	6	0	-0.080856	0.753731	-0.259790
12	6	0	-1.170609	-0.171891	-0.226470
13	6	0	-0.335206	2.108228	-0.272646
14	6	0	-0.984074	-1.579673	-0.242615
15	6	0	-2.507980	0.337371	-0.179324
16	6	0	-1.656513	2.606076	-0.223956
17	1	0	0.494759	2.805529	-0.302829
18	6	0	-2.057231	-2.438424	-0.208116
19	1	0	0.022441	-1.978207	-0.283719
20	6	0	-3.592964	-0.577509	-0.143740
21	6	0	-2.719616	1.740475	-0.174355
22	1	0	-1.821553	3.677607	-0.222944
23	6	0	-3.376535	-1.934001	-0.156704
24	1	0	-1.892813	-3.510148	-0.219608
25	1	0	-4.603316	-0.183293	-0.105884
26	1	0	-3.736557	2.116368	-0.133578
27	1	0	-4.215002	-2.620820	-0.128188
28	6	0	1.607507	-0.053077	2.178069
29	8	0	0.508085	0.288197	2.545576
30	1	0	2.370451	-0.375519	2.920492



2-(dimethylamino) benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -479.6584272 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	2.064601	-1.681964	-0.000529
2	6	0	0.863006	-2.394805	-0.000241
3	6	0	-0.350122	-1.735182	0.000035
4	6	0	-0.457831	-0.314926	0.000029
5	6	0	0.782461	0.415546	-0.000045
6	6	0	1.997240	-0.306210	-0.000415
7	6	0	-2.027707	1.642816	-0.000963
8	6	0	0.985207	1.888627	0.000612
9	8	0	2.085528	2.413707	0.000383
10	1	0	3.019603	-2.192700	-0.000756
11	1	0	0.867856	-3.479675	-0.000272
12	1	0	-1.244282	-2.337715	0.000137
13	1	0	2.901510	0.289548	-0.000486

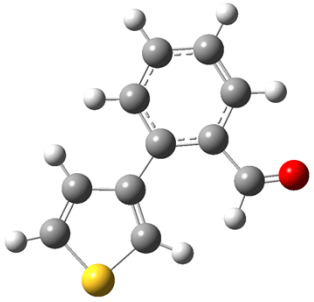


14	1	0	-3.107172	1.780096	-0.001937
15	1	0	-1.633284	2.143568	0.889610
16	1	0	-1.631854	2.142484	-0.891494
17	1	0	0.107677	2.541311	0.001928
18	7	0	-1.736734	0.218418	0.000032
19	6	0	-2.888826	-0.680265	0.000925
20	1	0	-2.908855	-1.321705	-0.887175
21	1	0	-2.907836	-1.321169	0.889423
22	1	0	-3.798631	-0.084452	0.001282

2-(thiophen-3-yl) benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -897.5261245 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

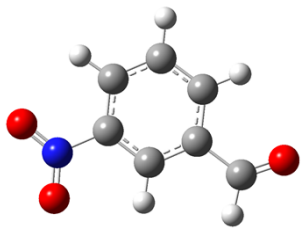
1	6	0	1.297460	3.259698	0.000000
2	6	0	-0.091481	3.168156	0.000000
3	6	0	-0.709477	1.925700	0.000000
4	6	0	0.000000	0.706192	0.000000
5	6	0	1.423639	0.818939	0.000000
6	6	0	2.030688	2.087302	0.000000
7	6	0	-0.820528	-0.544688	0.000000
8	6	0	-0.400473	-1.859920	0.000000
9	16	0	-1.692733	-3.002216	0.000000
10	6	0	-2.862243	-1.731925	0.000000
11	6	0	-2.267752	-0.509465	0.000000
12	6	0	2.400908	-0.306442	0.000000
13	8	0	3.604996	-0.149497	0.000000
14	1	0	1.794296	4.222590	0.000000
15	1	0	-0.702781	4.063851	0.000000
16	1	0	-1.788157	1.916542	0.000000
17	1	0	3.113228	2.111926	0.000000
18	1	0	0.591881	-2.268367	0.000000
19	1	0	-3.917387	-1.957125	0.000000
20	1	0	-2.862255	0.390329	0.000000
21	1	0	2.010488	-1.329586	0.000000



3-nitro benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -550.2293617 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	0.473782	2.043629	-0.000016
2	6	0	-0.807933	1.493139	0.000035
3	6	0	-0.942077	0.108941	-0.000014
4	6	0	0.158507	-0.738704	-0.000010
5	6	0	1.435695	-0.177455	0.000029
6	6	0	1.590213	1.216051	0.000007
7	6	0	2.623472	-1.070960	0.000006
8	8	0	3.767688	-0.681981	-0.000023
9	1	0	0.592789	3.120312	-0.000011

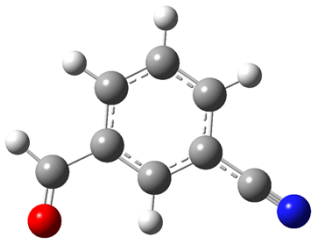


10	1	0	-1.693639	2.113728	0.000023
11	1	0	2.593281	1.626017	-0.000033
12	1	0	2.389157	-2.155160	0.000068
13	7	0	-2.301382	-0.481527	-0.000005
14	8	0	-2.386915	-1.702247	-0.000002
15	8	0	-3.252461	0.287931	-0.000011
16	1	0	0.011634	-1.811684	0.000048

3-formyl benzonitrile

E(RB+HF-LYP/6-311+G(d,p)) = -437.9322139 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

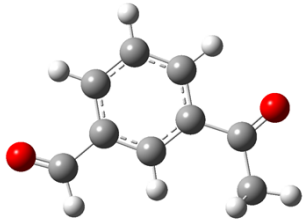
1	6	0	0.156855	2.132355	0.000052
2	6	0	-1.094410	1.519128	-0.000025
3	6	0	-1.197505	0.125095	-0.000098
4	6	0	-0.042867	-0.661897	-0.000088
5	6	0	1.211335	-0.047816	-0.000009
6	6	0	1.308551	1.355569	0.000061
7	6	0	-2.538548	-0.514729	-0.000200
8	8	0	-2.728668	-1.708209	0.000187
9	1	0	0.236266	3.212683	0.000106
10	1	0	-1.996996	2.121964	-0.000033
11	1	0	-0.136529	-1.740947	-0.000145
12	1	0	-3.390074	0.197063	0.000253
13	6	0	2.403967	-0.842528	-0.000001
14	7	0	3.369404	-1.476733	0.000007
15	1	0	2.286585	1.820980	0.000122



3-acetyl benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -498.3582385 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	0.927410	0.198299	-0.000039
2	6	0	-0.160839	-0.679732	-0.000066
3	6	0	-1.470306	-0.191760	-0.000008
4	6	0	-1.699759	1.189958	0.000032
5	6	0	-0.623212	2.069714	0.000056
6	6	0	0.680117	1.578048	0.000044
7	1	0	-0.004793	-1.753226	-0.000089
8	1	0	-2.722664	1.548047	0.000063
9	1	0	-0.796118	3.139691	0.000108
10	1	0	1.530148	2.249697	0.000091
11	6	0	-2.603579	-1.146900	-0.000009
12	8	0	-3.772125	-0.832935	-0.000032
13	1	0	-2.306087	-2.217165	0.000005
14	6	0	2.355339	-0.274370	-0.000024
15	8	0	3.267426	0.529100	-0.000130
16	6	0	2.633047	-1.764829	0.000120
17	1	0	3.710538	-1.919340	0.000250

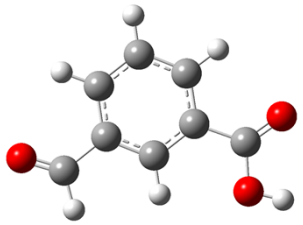


18	1	0	2.198534	-2.243714	0.882627
19	1	0	2.198725	-2.243882	-0.882391

3-formyl benzoicacid

E(RB+HF-LYP/6-311+G(d,p)) = -534.3046204 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

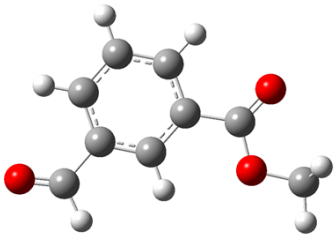
1	6	0	0.934295	0.162251	-0.000069
2	6	0	-0.163593	-0.702626	-0.000028
3	6	0	-1.460314	-0.186717	0.000061
4	6	0	-1.661908	1.200662	0.000103
5	6	0	-0.571059	2.061184	0.000062
6	6	0	0.724152	1.545447	-0.000021
7	1	0	-0.005369	-1.774859	-0.000062
8	1	0	-2.677980	1.577780	0.000170
9	1	0	-0.723642	3.133981	0.000096
10	1	0	1.586282	2.201264	-0.000051
11	6	0	-2.614644	-1.117933	0.000109
12	8	0	-3.775194	-0.775740	0.000063
13	1	0	-2.341053	-2.193772	-0.000047
14	6	0	2.336779	-0.335562	-0.000155
15	8	0	3.319074	0.367291	-0.000107
16	8	0	2.414161	-1.689727	-0.000018
17	1	0	3.355188	-1.919227	0.000024



Methyl 3-formyl benzoate

E(RB+HF-LYP/6-311+G(d,p)) = -573.6150233Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

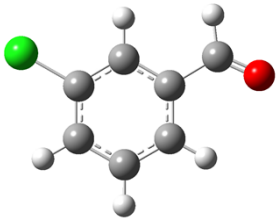
1	6	0	0.494090	0.473866	0.000060
2	6	0	-0.431177	-0.573413	0.000071
3	6	0	-1.800190	-0.299824	0.000008
4	6	0	-2.249220	1.028216	-0.000063
5	6	0	-1.330423	2.070160	-0.000065
6	6	0	0.036867	1.795688	-0.000005
7	1	0	-0.082238	-1.599336	0.000115
8	1	0	-3.316467	1.216775	-0.000094
9	1	0	-1.673295	3.098202	-0.000125
10	1	0	0.766489	2.596282	-0.000008
11	6	0	-2.765452	-1.424852	0.000028
12	8	0	-3.969416	-1.301710	-0.000024
13	1	0	-2.299783	-2.432779	0.000112
14	6	0	1.968375	0.240654	0.000082
15	8	0	2.797704	1.120680	0.000070
16	8	0	2.280709	-1.071552	0.000052
17	6	0	3.686838	-1.383998	-0.000153
18	1	0	4.166547	-0.975226	0.889921
19	1	0	3.741477	-2.470193	-0.002008
20	1	0	4.167044	-0.972045	-0.888477



3-chloro benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -805.290435 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

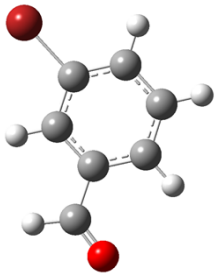
1	6	0	0.014120	-1.991930	0.000000
2	6	0	-1.200567	-1.301830	0.000000
3	6	0	-1.194344	0.089932	0.000000
4	6	0	0.000000	0.800293	0.000000
5	6	0	1.210946	0.100666	0.000000
6	6	0	1.217559	-1.299691	0.000000
7	17	0	-2.720166	0.961435	0.000000
8	6	0	2.482254	0.866167	0.000000
9	8	0	3.584774	0.368890	0.000000
10	1	0	0.007715	-3.075741	0.000000
11	1	0	-2.141701	-1.836961	0.000000
12	1	0	-0.008278	1.884282	0.000000
13	1	0	2.168569	-1.818152	0.000000
14	1	0	2.358515	1.969419	0.000000



3-bromo benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -2919.2101408 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	2.295973	-0.115145	0.000000
2	6	0	1.357926	0.920666	0.000000
3	6	0	0.000000	0.612089	0.000000
4	6	0	-0.432319	-0.709301	0.000000
5	6	0	0.514189	-1.738873	0.000000
6	6	0	1.882167	-1.440379	0.000000
7	6	0	0.043894	-3.146444	0.000000
8	8	0	0.769785	-4.113934	0.000000
9	1	0	3.352537	0.126711	0.000000
10	1	0	1.679583	1.954340	0.000000
11	1	0	-1.491107	-0.941172	0.000000
12	1	0	2.595251	-2.255700	0.000000
13	1	0	-1.059831	-3.265935	0.000000
14	35	0	-1.291591	2.028502	0.000000

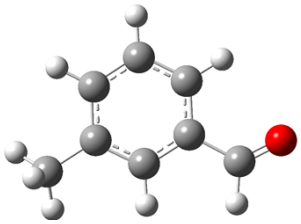


3-methyl benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -384.9968886 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-1.558226	-0.318783	-0.010342
2	6	0	-0.301785	-0.929896	-0.010127
3	6	0	0.874466	-0.173406	-0.000991

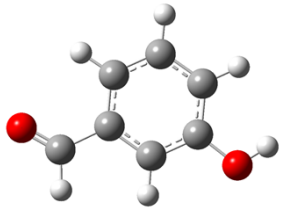
4	6	0	0.807576	1.225291	0.005851
5	6	0	-0.434193	1.845364	0.001498
6	6	0	-1.602869	1.079676	-0.007722
7	1	0	-0.231521	-2.014482	-0.019164
8	1	0	1.728333	1.796155	0.010233
9	1	0	-0.501876	2.927471	0.001553
10	1	0	-2.566474	1.579560	-0.015321
11	6	0	2.181256	-0.869399	-0.002918
12	8	0	3.261501	-0.321847	0.006526
13	1	0	2.112787	-1.978310	-0.013624
14	6	0	-2.825825	-1.138390	0.010899
15	1	0	-3.634014	-0.635795	-0.525302
16	1	0	-2.674252	-2.118802	-0.445854
17	1	0	-3.167390	-1.303757	1.038390



3-hydroxy benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -420.915852 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

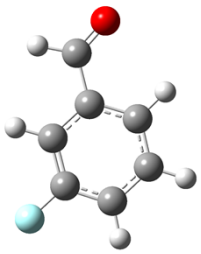
1	6	0	1.553181	-0.394204	0.000014
2	6	0	0.285160	-0.975032	0.000013
3	6	0	-0.850471	-0.163844	-0.000009
4	6	0	-0.729076	1.232572	-0.000033
5	6	0	0.536481	1.801362	0.000005
6	6	0	1.678148	0.995650	0.000015
7	1	0	0.198232	-2.056282	0.000038
8	1	0	-1.625263	1.839986	-0.000063
9	1	0	0.649599	2.879418	0.000005
10	1	0	2.664487	1.450528	0.000028
11	6	0	-2.186613	-0.807453	-0.000012
12	8	0	-3.240923	-0.213179	0.000021
13	1	0	-2.164237	-1.917738	0.000059
14	8	0	2.629528	-1.237003	-0.000072
15	1	0	3.447482	-0.728767	0.000381



3-fluro benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -444.9363205 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	1.650490	-0.903496	0.000000
2	6	0	0.634810	-1.862918	0.000000
3	6	0	-0.684096	-1.435703	0.000000
4	6	0	-1.025752	-0.094006	0.000000
5	6	0	0.000000	0.857235	0.000000
6	6	0	1.340389	0.450820	0.000000
7	6	0	-0.356457	2.297605	0.000000
8	8	0	0.443165	3.205069	0.000000
9	1	0	2.685251	-1.225322	0.000000
10	1	0	0.852857	-2.923768	0.000000

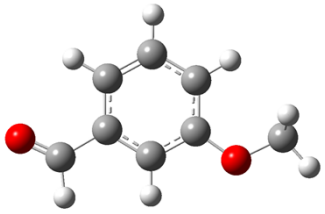


11	1	0	-2.069445	0.200148	0.000000
12	1	0	2.115708	1.206869	0.000000
13	1	0	-1.447408	2.503958	0.000000
14	9	0	-1.670955	-2.362184	0.000000

3-methoxy benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -460.2252286 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

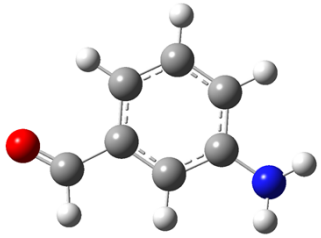
1	6	0	1.124563	-0.225035	0.000074
2	6	0	-0.101947	-0.898765	-0.000007
3	6	0	-1.296483	-0.182794	-0.000126
4	6	0	-1.284339	1.220769	-0.000164
5	6	0	-0.067414	1.881915	-0.000082
6	6	0	1.140073	1.171929	0.000035
7	1	0	-0.102065	-1.983591	0.000024
8	1	0	-2.224559	1.757532	-0.000256
9	1	0	-0.038168	2.965719	-0.000110
10	1	0	2.074658	1.716805	0.000090
11	6	0	-2.575927	-0.931194	-0.000215
12	8	0	-3.675388	-0.424697	-0.000270
13	1	0	-2.463881	-2.036220	-0.000114
14	8	0	2.234947	-1.014667	0.000172
15	6	0	3.514784	-0.393585	0.000428
16	1	0	3.659466	0.220977	0.895339
17	1	0	4.238374	-1.206702	0.000585
18	1	0	3.659837	0.220955	-0.894438



3-amino benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -401.0456223 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

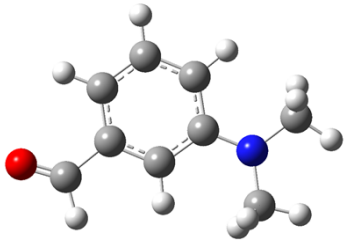
1	6	0	1.565237	-0.363795	-0.006128
2	6	0	0.292870	-0.950941	-0.007872
3	6	0	-0.858769	-0.161104	-0.002078
4	6	0	-0.765363	1.235850	0.003418
5	6	0	0.494690	1.821049	0.003017
6	6	0	1.647228	1.036987	-0.002339
7	1	0	0.197536	-2.033553	-0.017798
8	1	0	-1.671164	1.828513	0.008357
9	1	0	0.591482	2.901019	0.007371
10	1	0	2.622887	1.512945	-0.007070
11	6	0	-2.179283	-0.832561	-0.001381
12	8	0	-3.249196	-0.265897	0.007871
13	1	0	-2.131606	-1.942953	-0.009435
14	7	0	2.716163	-1.148504	-0.067567
15	1	0	3.567986	-0.712447	0.252541
16	1	0	2.623646	-2.099727	0.256216



3-(dimethylamino) benzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -479.6726988 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

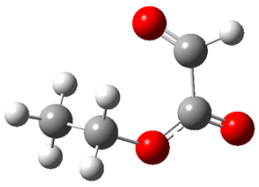
1	6	0	0.885899	0.137897	-0.067635
2	6	0	-0.256283	-0.689813	-0.044331
3	6	0	-1.542707	-0.148179	-0.009356
4	6	0	-1.741369	1.236351	0.015123
5	6	0	-0.624540	2.060572	0.010494
6	6	0	0.664851	1.532401	-0.024489
7	1	0	-0.156376	-1.767789	-0.054073
8	1	0	-2.748609	1.631451	0.044207
9	1	0	-0.745735	3.137961	0.038764
10	1	0	1.502337	2.216069	-0.019462
11	6	0	-2.694673	-1.078729	0.007650
12	8	0	-3.859528	-0.748382	0.034723
13	1	0	-2.417314	-2.155271	-0.007030
14	7	0	2.165601	-0.393914	-0.140281
15	6	0	3.312024	0.474342	0.077105
16	6	0	2.354726	-1.823679	0.046495
17	1	0	3.323510	0.920524	1.082490
18	1	0	4.224916	-0.106172	-0.049374
19	1	0	3.335890	1.284746	-0.656705
20	1	0	1.797254	-2.394021	-0.701651
21	1	0	3.409643	-2.061773	-0.083262
22	1	0	2.043943	-2.168247	1.043942



Ethylglyoxalate

E(RB+HF-LYP/6-311+G(d,p)) = -381.802647 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

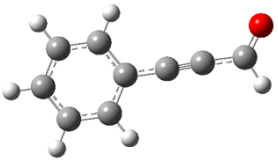
1	6	0	0.985268	-0.499358	-0.004863
2	8	0	1.945163	-1.146874	-0.340918
3	8	0	-0.217235	-1.050904	0.139978
4	6	0	-2.296272	0.066200	-0.519217
5	6	0	-1.396356	-0.343461	0.629910
6	6	0	1.220475	1.012175	0.179143
7	8	0	0.425921	1.874546	-0.087125
8	1	0	-3.218983	0.496840	-0.119539
9	1	0	-2.559262	-0.799821	-1.130282
10	1	0	-1.812735	0.816572	-1.145752
11	1	0	-1.883143	-1.076948	1.273492
12	1	0	-1.097628	0.510338	1.236334
13	1	0	2.262261	1.225542	0.480421



3-phenyl propynal

E(RB+HF-LYP/6-311+G(d,p)) = -421.8331326 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

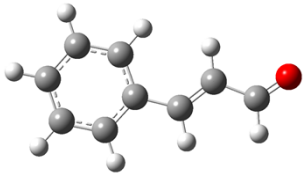
1	6	0	-2.471235	1.290470	0.000220
2	6	0	-3.257536	0.137757	0.000187
3	6	0	-2.654177	-1.120415	-0.000052
4	6	0	-1.269068	-1.230375	-0.000235
5	6	0	-0.468165	-0.073632	-0.000213
6	6	0	-1.085320	1.191033	-0.000011
7	6	0	0.949041	-0.177565	-0.000343
8	6	0	2.159513	-0.238717	-0.000070
9	6	0	3.589516	-0.364776	0.000631
10	8	0	4.361269	0.572067	-0.000401
11	1	0	-2.939788	2.267759	0.000408
12	1	0	-4.338462	0.219726	0.000344
13	1	0	-3.264832	-2.015848	-0.000084
14	1	0	-0.793992	-2.203806	-0.000394
15	1	0	-0.467503	2.080626	-0.000024
16	1	0	3.959008	-1.407671	0.002272



Cinamaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -423.0928986 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

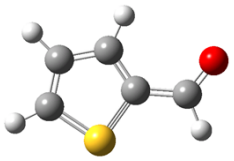
1	6	0	-2.308401	1.366361	-0.000002
2	6	0	-3.239741	0.325201	-0.000005
3	6	0	-2.798959	-0.996315	-0.000009
4	6	0	-1.435560	-1.273340	-0.000003
5	6	0	-0.485396	-0.238096	0.000007
6	6	0	-0.947877	1.090303	0.000008
7	6	0	0.933757	-0.585861	0.000011
8	6	0	1.994998	0.243755	0.000011
9	6	0	3.357336	-0.288667	0.000020
10	8	0	4.363381	0.391284	-0.000027
11	1	0	-2.647672	2.395951	0.000000
12	1	0	-4.301068	0.545528	-0.000017
13	1	0	-3.515545	-1.809607	-0.000012
14	1	0	-1.094917	-2.303556	-0.000003
15	1	0	-0.239715	1.910170	0.000014
16	1	0	1.142568	-1.655161	0.000011
17	1	0	1.902562	1.324711	0.000009
18	1	0	3.425797	-1.398353	-0.000006



Thiophene-2-carbaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -666.4313764 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

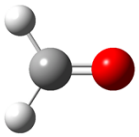
1	6	0	1.278258	-0.043079	0.000000
2	6	0	1.305770	-1.458089	0.000000
3	6	0	0.048912	-2.010664	0.000000
4	16	0	-1.188394	-0.812387	0.000000
5	6	0	0.000000	0.470370	0.000000
6	6	0	-0.404814	1.875828	0.000000
7	8	0	0.374835	2.805906	0.000000
8	1	0	2.152018	0.594306	0.000000
9	1	0	2.212383	-2.048137	0.000000
10	1	0	-0.218286	-3.056639	0.000000
11	1	0	-1.499255	2.055229	0.000000



Formaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -114.5417558 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

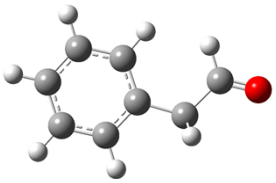
1	1	0	-1.114929	0.939531	0.000002
2	6	0	-0.527455	0.000000	-0.000001
3	8	0	0.674324	0.000000	0.000000
4	1	0	-1.114930	-0.939530	0.000002



Phenyl acetaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -384.9811675Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-1.809859	1.360552	0.000017
2	6	0	-2.756487	0.341814	-0.000173
3	6	0	-2.329094	-0.986022	-0.000187
4	6	0	-0.969894	-1.281012	-0.000016
5	6	0	-0.003285	-0.265335	0.000174
6	6	0	-0.445652	1.060842	0.000192
7	6	0	1.458276	-0.680077	0.000383
8	6	0	2.540600	0.382168	0.000079
9	8	0	3.715582	0.106041	-0.000440
10	1	0	-2.127136	2.397425	0.000033
11	1	0	-3.814665	0.576793	-0.000309
12	1	0	-3.054519	-1.791940	-0.000334
13	1	0	-0.649384	-2.318442	-0.000035
14	1	0	0.258210	1.883181	0.000354
15	1	0	1.663174	-1.318266	0.868905
16	1	0	1.663306	-1.318829	-0.867679

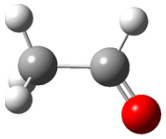


17	1	0	2.228720	1.444178	-0.000225

acetaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -153.8804044 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

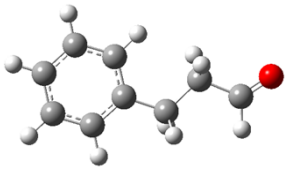
1	6	0	1.170743	-0.134891	-0.000010
2	6	0	-0.238989	0.409414	-0.000009
3	8	0	-1.224320	-0.286057	0.000001
4	1	0	1.916481	0.661686	-0.000640
5	1	0	1.314289	-0.767606	0.880678
6	1	0	1.313909	-0.768734	-0.879941
7	1	0	-0.340643	1.515968	0.000009



3-phenyl propanal

E(RB+HF-LYP/6-311+G(d,p)) = -424.3083375 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

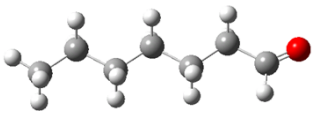
1	6	0	-2.274453	1.409570	-0.000002
2	6	0	-3.275773	0.444259	-0.000050
3	6	0	-2.923768	-0.906272	-0.000042
4	6	0	-1.583607	-1.277391	0.000015
5	6	0	-0.562710	-0.315915	0.000066
6	6	0	-0.929486	1.032568	0.000055
7	6	0	0.881049	-0.787073	0.000147
8	6	0	1.954680	0.301193	-0.000099
9	6	0	3.366406	-0.254306	-0.000145
10	8	0	4.358943	0.429671	0.000089
11	1	0	-2.534375	2.462386	-0.000009
12	1	0	-4.319359	0.737637	-0.000096
13	1	0	-3.694194	-1.669407	-0.000084
14	1	0	-1.321255	-2.331285	0.000017
15	1	0	-0.171245	1.806221	0.000092
16	1	0	1.032536	-1.434172	0.873249
17	1	0	1.032508	-1.434535	-0.872689
18	1	0	1.867895	0.954994	-0.875379
19	1	0	1.868048	0.955305	0.874956
20	1	0	3.453869	-1.364300	-0.000443



Heptanal

E(RB+HF-LYP/6-311+G(d,p)) = -350.5023384 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

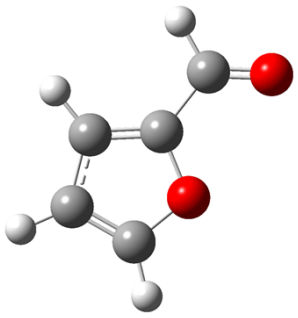
1	6	0	-4.326403	-0.316947	-0.000255
2	6	0	-3.037631	0.509837	-0.000101
3	6	0	-1.767806	-0.348560	0.000005
4	6	0	-0.473369	0.471419	0.000157
5	6	0	0.794929	-0.388193	0.000260
6	6	0	2.083464	0.437724	0.000423
7	6	0	3.352079	-0.392108	0.000636
8	8	0	4.465591	0.070873	-0.000926
9	1	0	-5.212157	0.324263	-0.000327
10	1	0	-4.383158	-0.961363	-0.883332
11	1	0	-4.383338	-0.961407	0.882779
12	1	0	-3.026773	1.169532	0.876217
13	1	0	-3.026594	1.169571	-0.876386
14	1	0	-1.778639	-1.009043	-0.876965
15	1	0	-1.778817	-1.009079	0.876944
16	1	0	-0.462259	1.131919	0.876801
17	1	0	-0.462085	1.131959	-0.876451
18	1	0	0.785271	-1.048034	-0.876532
19	1	0	0.785090	-1.048078	0.877014
20	1	0	2.129469	1.100113	0.873767
21	1	0	2.129695	1.100164	-0.872867
22	1	0	3.207999	-1.496530	-0.000001



Furan-2-carbaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -343.4469717 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

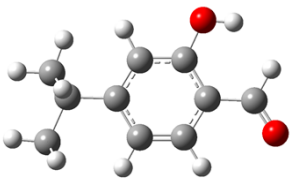
1	6	0	0.000000	0.367510	0.000000
2	6	0	-1.371491	0.305790	0.000000
3	6	0	-1.715509	-1.074275	0.000000
4	6	0	-0.529650	-1.751550	0.000000
5	6	0	0.896852	1.512543	0.000000
6	8	0	2.107750	1.463194	0.000000
7	1	0	-2.042427	1.151010	0.000000
8	1	0	-2.701913	-1.509073	0.000000
9	1	0	0.355811	2.481202	0.000000
10	1	0	-0.282389	-2.800453	0.000000
11	8	0	0.515963	-0.898543	0.000000



4-tert-butyl-2-hydroxybenzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -578.2100112 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-0.147768	-1.354385	-0.000084
2	6	0	-0.867765	-0.144225	-0.000062
3	6	0	-0.141942	1.047972	-0.000062
4	6	0	1.251749	1.058258	-0.000039
5	6	0	1.970841	-0.155256	-0.000016
6	6	0	1.234697	-1.351792	-0.000058

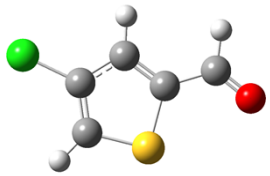


7	8	0	1.833322	2.293601	-0.000014
8	6	0	3.437617	-0.212935	0.000029
9	8	0	4.098992	-1.230351	0.000022
10	1	0	-0.668279	-2.301514	-0.000135
11	1	0	-0.638942	2.010057	-0.000077
12	1	0	1.791583	-2.281537	-0.000058
13	1	0	3.973325	0.764786	0.000147
14	1	0	2.793391	2.225491	-0.000109
15	6	0	-2.405195	-0.095164	0.000012
16	6	0	-3.036701	-1.499626	-0.000698
17	1	0	-4.125833	-1.407070	-0.000672
18	1	0	-2.755663	-2.074136	-0.887423
19	1	0	-2.755748	-2.075054	0.885462
20	6	0	-2.892779	0.654015	-1.262553
21	1	0	-3.986048	0.693500	-1.276656
22	1	0	-2.521608	1.680525	-1.297067
23	1	0	-2.559857	0.146197	-2.171837
24	6	0	-2.892497	0.652713	1.263437
25	1	0	-3.985774	0.691752	1.278128
26	1	0	-2.558952	0.144248	2.172143
27	1	0	-2.521657	1.679316	1.298656

4-chlorofuran-2-carbaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -1126.0518687 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

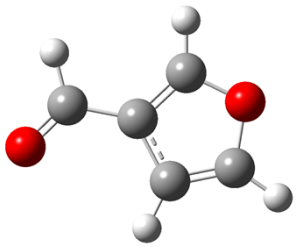
1	6	0	1.104711	0.187134	0.000000
2	6	0	0.000000	1.007941	0.000000
3	6	0	-1.207879	0.269760	0.000000
4	6	0	-1.019254	-1.086892	0.000000
5	6	0	2.504279	0.603453	0.000000
6	8	0	3.451935	-0.152745	0.000000
7	1	0	0.050011	2.088467	0.000000
8	1	0	2.645297	1.703293	0.000000
9	1	0	-1.776840	-1.855127	0.000000
10	16	0	0.653762	-1.498915	0.000000
11	17	0	-2.781487	1.022329	0.000000



Furan-3-carbaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -343.4460185 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	0.696634	1.115441	-0.000001
2	6	0	-0.297874	0.175191	0.000001
3	6	0	0.366503	-1.103288	0.000003
4	6	0	1.691693	-0.834774	0.000001
5	1	0	-0.107661	-2.070931	0.000005
6	1	0	2.578500	-1.445053	0.000002
7	8	0	1.908208	0.522058	-0.000002
8	1	0	0.691082	2.193267	-0.000007
9	6	0	-1.733352	0.451596	0.000002

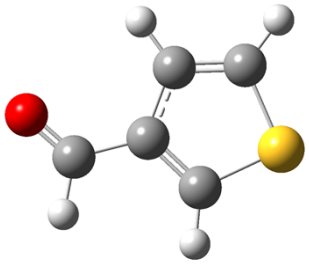


10	8	0	-2.595846	-0.400853	-0.000005
11	1	0	-2.002449	1.528082	0.000028

Thiophene-3-carbaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -666.45796816452 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

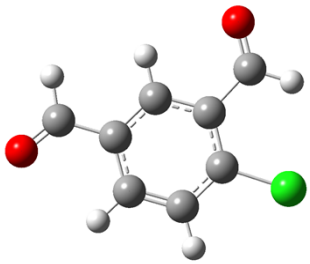
1	6	0	0.388358	-1.107240	0.000015
2	6	0	-0.615165	-0.165890	0.000045
3	6	0	-0.107974	1.174941	0.000037
4	6	0	1.251409	1.216950	0.000008
5	1	0	-0.748398	2.045922	0.000055
6	1	0	1.898648	2.080574	-0.000002
7	16	0	1.946859	-0.379332	-0.000030
8	1	0	0.286292	-2.182585	0.000015
9	6	0	-2.039494	-0.526310	0.000075
10	8	0	-2.950670	0.273466	-0.000085
11	1	0	-2.243727	-1.617028	0.000007



4-chloroisophthalaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = - 918.6431634 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-1.685729	0.033658	0.000019
2	6	0	-0.684129	0.997511	0.000010
3	6	0	0.671449	0.643147	0.000001
4	6	0	0.992265	-0.721605	0.000001
5	6	0	-0.001947	-1.703184	0.000010
6	6	0	-1.334579	-1.325611	0.000019
7	1	0	-0.925884	2.055782	0.000009
8	1	0	0.280306	-2.748150	0.000010
9	1	0	-2.121563	-2.070710	0.000026
10	6	0	1.689682	1.730756	-0.000006
11	8	0	1.397572	2.905543	0.000001
12	1	0	2.744124	1.409676	-0.000006
13	6	0	-3.110495	0.446965	0.000026
14	8	0	-4.044102	-0.322226	-0.000039
15	1	0	-3.275475	1.543726	-0.000050
16	17	0	2.661861	-1.262746	-0.000010

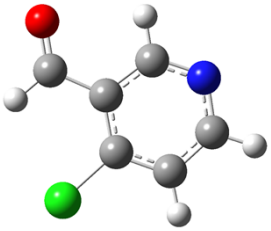


4-chloronicotinaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = - -821.3247923 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	0.908722	1.460937	0.000142
2	6	0	-0.214517	0.615346	0.000135
3	6	0	0.034761	-0.761210	0.000018
4	6	0	1.344915	-1.223720	-0.000095

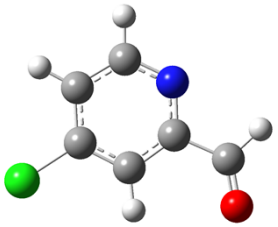
5	6	0	2.369642	-0.281739	-0.000070
6	7	0	2.169895	1.042123	0.000057
7	1	0	3.404234	-0.611801	-0.000170
8	17	0	-1.267117	-1.936570	-0.000048
9	1	0	1.561462	-2.283724	-0.000217
10	1	0	0.738886	2.532849	0.000273
11	6	0	-1.573895	1.219197	0.000350
12	8	0	-1.769204	2.413642	-0.000467
13	1	0	-2.416987	0.507507	0.001373



4-chloropicolinaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = - -821.3303733 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

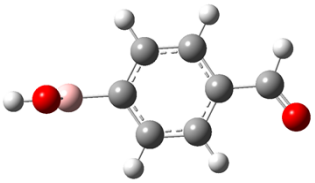
1	6	0	1.268224	0.173897	-0.000008
2	6	0	0.135928	-0.645023	-0.000007
3	6	0	-1.102250	-0.020126	-0.000001
4	6	0	-1.174283	1.370049	0.000005
5	6	0	0.023072	2.085497	0.000004
6	7	0	1.226315	1.511921	-0.000003
7	1	0	0.245850	-1.721481	-0.000012
8	1	0	0.004195	3.171374	0.000008
9	6	0	2.636653	-0.428778	-0.000017
10	8	0	2.850555	-1.617471	0.000014
11	1	0	3.449603	0.322249	0.000033
12	17	0	-2.569668	-0.971187	0.000001
13	1	0	-2.127995	1.881264	0.000010



4-formylphenylboronic acid

E(RB+HF-LYP/6-311+G(d,p)) = - -521.7411331 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

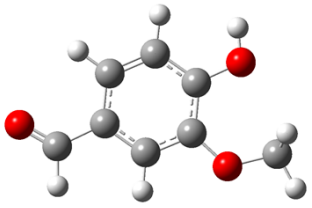
1	6	0	1.185535	-1.055388	0.000091
2	6	0	-0.199935	-1.134075	0.000097
3	6	0	-0.995746	0.025569	-0.000003
4	6	0	-0.353352	1.271542	-0.000111
5	6	0	1.035723	1.357491	-0.000120
6	6	0	1.814431	0.196335	-0.000019
7	1	0	1.799515	-1.948570	0.000168
8	1	0	-0.672068	-2.111226	0.000181
9	1	0	-0.939555	2.184649	-0.000189
10	1	0	1.521788	2.328601	-0.000205
11	5	0	-2.567680	-0.074862	0.000006
12	8	0	-3.208479	-0.115707	1.209035
13	1	0	-4.168798	-0.178814	1.181581
14	8	0	-3.208461	-0.116189	-1.209015
15	1	0	-4.168781	-0.179280	-1.181551
16	6	0	3.289562	0.307231	-0.000029
17	8	0	4.059016	-0.628548	0.000061
18	1	0	3.672386	1.350272	-0.000110



4-hydroxy-3-methoxybenzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = - -535.4651711 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

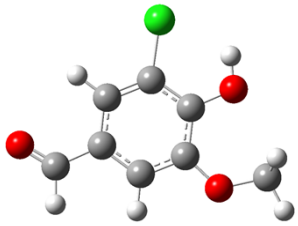
1	6	0	0.861012	-0.478981	0.000009
2	6	0	-0.428225	-1.015678	-0.000066
3	6	0	-1.568785	-0.212894	-0.000160
4	6	0	-1.430422	1.180748	-0.000169
5	6	0	-0.161041	1.728301	-0.000098
6	6	0	0.987534	0.924549	-0.000021
7	1	0	-0.515673	-2.097180	-0.000050
8	1	0	-2.314339	1.805815	-0.000237
9	1	0	-0.032902	2.807631	-0.000114
10	6	0	-2.901758	-0.846193	-0.000249
11	8	0	-3.956366	-0.247949	-0.000078
12	1	0	-2.884700	-1.956844	0.000016
13	8	0	1.860623	-1.404309	0.000075
14	6	0	3.251900	-1.063353	0.000506
15	1	0	3.524763	-0.497094	0.891922
16	1	0	3.768568	-2.022180	0.000591
17	1	0	3.525293	-0.496960	-0.890659
18	8	0	2.235525	1.490742	0.000011
19	1	0	2.149433	2.449951	-0.000036



phthalaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = - -459.017076 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

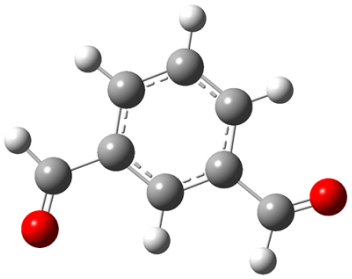
1	6	0	0.832084	-1.078310	0.000028
2	6	0	-0.464212	-1.595825	0.000008
3	6	0	-1.588430	-0.772176	-0.000045
4	6	0	-1.437048	0.618541	-0.000072
5	6	0	-0.157739	1.131480	-0.000060
6	6	0	0.995510	0.323028	-0.000025
7	1	0	-0.570543	-2.675066	0.000040
8	1	0	-2.306961	1.261491	-0.000105
9	6	0	-2.936544	-1.377913	-0.000065
10	8	0	-3.975618	-0.755475	-0.000204
11	1	0	-2.941571	-2.488088	-0.000145
12	8	0	1.817735	-2.014309	0.000057
13	6	0	3.217418	-1.700315	0.000546
14	1	0	3.500402	-1.140479	0.892358
15	1	0	3.712461	-2.670162	0.000623
16	1	0	3.501000	-1.140309	-0.890965
17	8	0	2.240831	0.865027	-0.000067
18	1	0	2.158481	1.829815	-0.000090
19	17	0	0.089231	2.880576	-0.00011



isophthalaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = - -459.0251025 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

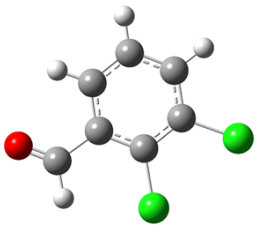
1	6	0	1.092986	-0.207483	-0.000020
2	6	0	-0.206745	-0.706544	-0.000027
3	6	0	-1.296335	0.172517	-0.000016
4	6	0	-1.069003	1.551708	0.000002
5	6	0	0.233173	2.056004	0.000009
6	6	0	1.310642	1.180769	-0.000002
7	1	0	-0.395042	-1.775500	-0.000040
8	1	0	-1.915559	2.231615	0.000011
9	1	0	0.400766	3.126544	0.000023
10	1	0	2.331381	1.545132	0.000002
11	6	0	-2.685899	-0.345720	-0.000023
12	8	0	-2.981760	-1.518762	0.000035
13	1	0	-3.472877	0.437375	0.000057
14	6	0	2.241134	-1.149245	-0.000033
15	8	0	3.403226	-0.813073	0.000039
16	1	0	1.959887	-2.222522	0.000012



2,3-dichlorobenzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = - -1264.9034065 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-0.370261	2.408207	0.000015
2	6	0	0.925118	1.897676	0.000008
3	6	0	1.137682	0.520790	-0.000002
4	6	0	0.048237	-0.358176	-0.000005
5	6	0	-1.260193	0.154851	0.000003
6	6	0	-1.452056	1.541523	0.000012
7	6	0	-2.470458	-0.718455	0.000002
8	8	0	-3.598691	-0.279725	0.000030
9	1	0	-0.524298	3.480432	0.000023
10	1	0	1.782483	2.558793	0.000010
11	1	0	-2.287656	-1.804818	0.000011
12	17	0	0.331454	-2.085496	-0.000018
13	1	0	-2.472133	1.906012	0.000018
14	17	0	2.782824	-0.066335	-0.000011

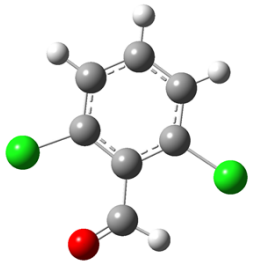


2,6-dichlorobenzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = - -1264.8977441Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-0.925817	1.902598	0.000026
2	6	0	0.350424	2.451582	0.000034
3	6	0	1.471239	1.629011	0.000009
4	6	0	1.296887	0.252080	-0.000025
5	6	0	0.022708	-0.355061	-0.000036

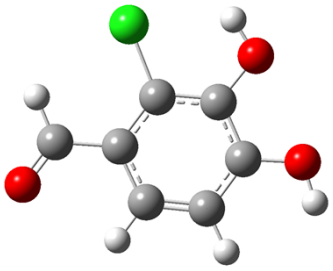
6	6	0	-1.086283	0.520252	-0.000008
7	6	0	-0.089260	-1.845533	-0.000085
8	8	0	-1.118098	-2.478237	0.000187
9	1	0	-1.802843	2.536187	0.000045
10	1	0	0.472926	3.528316	0.000062
11	1	0	2.470232	2.043885	0.000017
12	1	0	0.882553	-2.363751	0.000052
13	17	0	2.772116	-0.714943	-0.000048
14	17	0	-2.731967	-0.064370	-0.000020



2-chloro-3,4-dihydroxybenzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = - -955.7791275 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

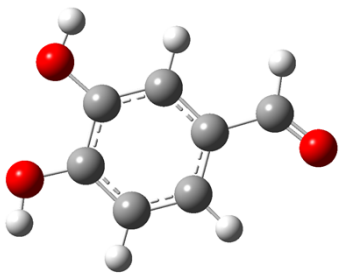
1	6	0	1.180557	0.466155	-0.000092
2	6	0	-0.208941	0.581305	-0.000053
3	6	0	-1.056423	-0.539041	0.000053
4	6	0	-0.462754	-1.805405	0.000113
5	6	0	0.915326	-1.948217	0.000074
6	6	0	1.743221	-0.825828	-0.000028
7	1	0	-1.115805	-2.669231	0.000194
8	6	0	-2.534093	-0.441408	0.000109
9	8	0	-3.269880	-1.405989	0.000388
10	1	0	-2.951512	0.580101	0.000229
11	8	0	2.031072	1.518159	-0.000186
12	8	0	3.096691	-0.895603	-0.000070
13	1	0	3.375511	-1.817962	-0.000012
14	1	0	1.519801	2.338923	-0.000235
15	17	0	-0.853876	2.226306	-0.000142
16	1	0	1.363483	-2.936935	0.000123



3,4-dihydroxybenzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = - -496.159875 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-1.120983	0.772920	0.000112
2	6	0	0.222286	1.119962	0.000040
3	6	0	1.225598	0.140086	-0.000075
4	6	0	0.867338	-1.211180	-0.000123
5	6	0	-0.473851	-1.565672	-0.000053
6	6	0	-1.474648	-0.590358	0.000064
7	1	0	0.501500	2.171065	0.000074
8	1	0	1.645869	-1.963721	-0.000212
9	6	0	2.641023	0.552448	-0.000147
10	8	0	3.589062	-0.203323	-0.000235
11	1	0	2.800502	1.652619	-0.000089
12	8	0	-2.140270	1.679259	0.000224
13	8	0	-2.799599	-0.886682	0.000139
14	1	0	-2.919011	-1.842631	0.000078

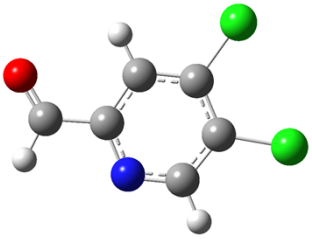


15	1	0	-1.779680	2.572059	0.000308
16	1	0	-0.763311	-2.612656	-0.000087

3,4-dichloropicolinaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = - -1280.9469025 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

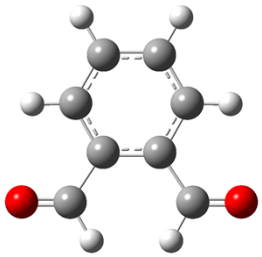
1	6	0	-1.731785	-0.390149	-0.000006
2	6	0	-0.945717	0.761999	-0.000005
3	6	0	0.435590	0.621084	-0.000002
4	6	0	0.972056	-0.671722	0.000000
5	6	0	0.093703	-1.761173	-0.000001
6	7	0	-1.227182	-1.630776	-0.000004
7	1	0	-1.416363	1.736703	-0.000007
8	1	0	0.497312	-2.768446	0.000000
9	6	0	-3.221907	-0.292723	-0.000013
10	8	0	-3.828548	0.751838	0.000015
11	1	0	-3.729098	-1.276456	0.000030
12	17	0	1.449934	2.031724	-0.000001
13	17	0	2.682723	-0.966722	0.000004



Phthalaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = - 459.017076 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

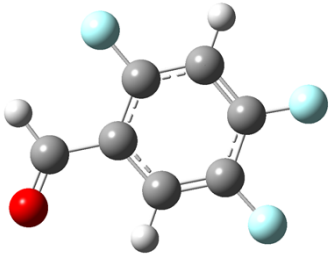
1	6	0	0.699122	2.227955	-0.000003
2	6	0	1.392296	1.025991	-0.000041
3	6	0	0.707521	-0.197189	-0.000047
4	6	0	-0.707523	-0.197181	-0.000015
5	6	0	-1.392284	1.026006	0.000021
6	6	0	-0.699096	2.227963	0.000028
7	1	0	1.242690	3.165693	0.000003
8	1	0	2.475179	1.004426	-0.000067
9	1	0	-2.475167	1.004454	0.000044
10	1	0	-1.242654	3.165706	0.000058
11	6	0	-1.531966	-1.439782	-0.000020
12	8	0	-2.743331	-1.433673	0.000020
13	1	0	-0.993405	-2.402543	-0.000038
14	6	0	1.531949	-1.439802	-0.000092
15	8	0	2.743314	-1.433694	0.000096
16	1	0	0.993379	-2.402558	0.000083



2,4,5-trifluorobenzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = - -643.4608948 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	1.178762	-0.904247	-0.000008
2	6	0	1.633352	0.416706	0.000001
3	6	0	0.744278	1.478296	0.000013

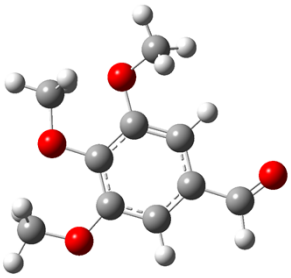


4	6	0	-0.610935	1.186286	0.000016
5	6	0	-1.100735	-0.120702	0.000007
6	6	0	-0.171708	-1.172407	-0.000005
7	6	0	-2.555002	-0.416269	0.000012
8	8	0	-3.002078	-1.541539	-0.000033
9	1	0	-3.222062	0.462658	-0.000013
10	1	0	-0.529899	-2.194834	-0.000012
11	9	0	-1.478985	2.219814	0.000029
12	9	0	2.949765	0.653020	-0.000003
13	9	0	2.080228	-1.899606	-0.000020
14	1	0	1.101442	2.499463	0.000021

3,4,5-trimethoxybenzaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = - -689.2583075 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-0.598253	-1.379437	0.034773
2	6	0	0.747818	-1.761819	0.045622
3	6	0	1.751798	-0.799858	-0.033019
4	6	0	1.425933	0.562376	-0.123944
5	6	0	0.092020	0.934652	-0.134234
6	6	0	-0.925922	-0.024369	-0.055632
7	1	0	0.990649	-2.816763	0.116147
8	1	0	2.222158	1.293495	-0.184102
9	6	0	3.166164	-1.243080	-0.018732
10	8	0	4.124353	-0.505979	-0.081249
11	1	0	3.304201	-2.342620	0.056060
12	8	0	-1.503740	-2.394313	0.115958
13	6	0	-2.890004	-2.075004	0.109796
14	1	0	-3.179015	-1.571660	-0.818968
15	1	0	-3.413276	-3.026692	0.182025
16	1	0	-3.158360	-1.447521	0.966379
17	8	0	-2.291039	0.401272	-0.069259
18	8	0	-0.265402	2.316210	-0.226134
19	6	0	-2.345598	1.826841	-0.167632
20	1	0	-1.849177	2.261733	0.674587
21	1	0	-1.861189	2.140990	-1.068497
22	1	0	-3.367254	2.144483	-0.182595
23	6	0	0.723777	3.110130	0.434258
24	1	0	1.602151	3.164402	-0.174358
25	1	0	0.340334	4.095914	0.595818
26	1	0	0.968999	2.664125	1.375451

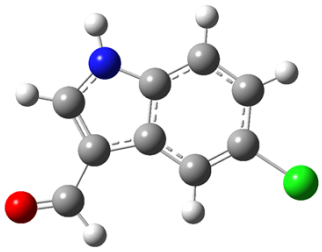


5-chloro-1H-indole-3-carbaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -936.8967041 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-1.889584	-0.308931	0.000133
2	6	0	-2.538261	0.911605	0.000147

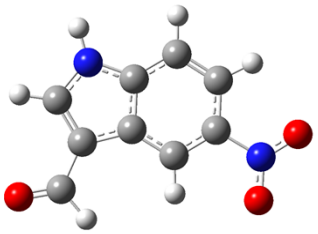
3	7	0	-1.620177	1.919129	-0.000070
4	6	0	-0.338044	1.387289	-0.000018
5	6	0	-0.470623	-0.023248	0.000068
6	6	0	0.902159	2.023781	-0.000121
7	6	0	2.037097	1.225870	-0.000097
8	6	0	1.913769	-0.173560	-0.000001
9	6	0	0.687374	-0.815885	0.000071
10	1	0	-3.598601	1.108572	0.000211
11	1	0	0.989000	3.104239	-0.000205
12	1	0	3.021906	1.673831	-0.000155
13	1	0	0.638056	-1.896767	0.000122
14	1	0	-1.841779	2.901924	0.000656
15	6	0	-2.552159	-1.606047	0.000092
16	8	0	-3.758330	-1.769724	-0.000296
17	1	0	-1.873112	-2.482835	0.000423
18	17	0	3.386002	-1.141784	0.000009



5-nitro-1H-indole-3-carbaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -681.8387813 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

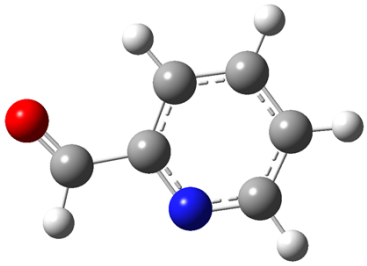
1	6	0	-2.102678	-0.332597	0.000285
2	6	0	-2.807279	0.852601	0.000099
3	7	0	-1.935599	1.906443	-0.000225
4	6	0	-0.634710	1.440930	-0.000177
5	6	0	-0.699355	0.022179	0.000052
6	6	0	0.572810	2.143227	-0.000333
7	6	0	1.743855	1.406227	-0.000230
8	6	0	1.682477	0.002500	-0.000063
9	6	0	0.492097	-0.708875	0.000075
10	1	0	-3.875608	1.000442	0.000117
11	1	0	0.600676	3.226384	-0.000532
12	1	0	2.710768	1.888469	-0.000271
13	1	0	0.515836	-1.789615	0.000188
14	7	0	2.951173	-0.753636	0.000021
15	8	0	3.996304	-0.113349	0.001377
16	8	0	2.887769	-1.977447	-0.001320
17	1	0	-2.205244	2.877626	0.000061
18	6	0	-2.703693	-1.663560	0.000465
19	8	0	-3.900397	-1.876792	-0.000105
20	1	0	-1.986005	-2.508037	0.001216



Picolinaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -361.7090596 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-0.498484	-0.199953	-0.000040
2	6	0	-0.010744	1.109978	-0.000033
3	6	0	1.365714	1.298897	0.000001

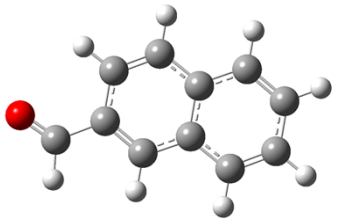


4	6	0	2.193113	0.177810	0.000027
5	6	0	1.607494	-1.089207	0.000018
6	7	0	0.288749	-1.284558	-0.000015
7	1	0	1.787597	2.297744	0.000007
8	1	0	-0.710698	1.936373	-0.000056
9	1	0	3.272193	0.277135	0.000055
10	1	0	2.225697	-1.982490	0.000038
11	6	0	-1.965519	-0.474380	-0.000078
12	8	0	-2.816390	0.384695	0.000072
13	1	0	-2.214354	-1.553285	0.000108

2-naphthaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -499.3477623 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	3.282150	0.361864	-0.000013
2	6	0	2.231904	1.250724	-0.000007
3	6	0	0.891823	0.789593	0.000003
4	6	0	0.649362	-0.621513	0.000006
5	6	0	1.754596	-1.512078	-0.000001
6	6	0	3.042539	-1.031889	-0.000010
7	1	0	-0.028583	2.748863	0.000007
8	1	0	4.302295	0.728829	-0.000021
9	1	0	2.418219	2.319415	-0.000010
10	6	0	-0.219059	1.680727	0.000009
11	6	0	-0.691114	-1.079241	0.000015
12	1	0	1.566726	-2.580637	0.000002
13	1	0	3.880103	-1.719908	-0.000015
14	6	0	-1.748463	-0.192143	0.000022
15	6	0	-1.503871	1.208483	0.000018
16	1	0	-0.883746	-2.148647	0.000018
17	1	0	-2.354047	1.879860	0.000024
18	6	0	-3.131014	-0.714672	0.000033
19	8	0	-4.131098	-0.030494	-0.000054
20	1	0	-3.205301	-1.822951	-0.000021

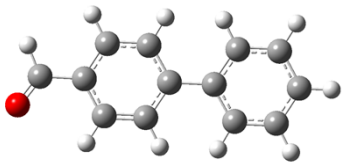


biphenyl-4-carbaldehyde

E(RB+HF-LYP/6-311+G(d,p)) = -576 .7779192 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	0.062942	0.068554	0.000001
2	6	0	-0.618032	1.299173	0.000015
3	6	0	-2.005077	1.358886	0.000015
4	6	0	-2.770866	0.189884	0.000002
5	6	0	-2.110606	-1.045163	-0.000012
6	6	0	-0.727125	-1.100290	-0.000013
7	1	0	-0.068013	2.229936	0.000026
8	1	0	-2.701402	-1.953758	-0.000022
9	1	0	-0.258412	-2.074845	-0.000025

10	6	0	-4.245412	0.271676	0.000004
11	8	0	-4.995241	-0.680715	-0.000013
12	1	0	-4.649444	1.306747	0.000049
13	1	0	-2.500941	2.324891	0.000027
14	6	0	1.552783	0.002182	0.000000
15	6	0	2.233444	-1.228177	0.000017
16	6	0	2.341033	1.166722	-0.000017
17	6	0	3.623077	-1.291999	0.000016
18	1	0	1.683286	-2.159231	0.000031
19	6	0	3.730631	1.105978	-0.000018
20	1	0	1.876623	2.143639	-0.000031
21	6	0	4.382950	-0.124822	-0.000001
22	1	0	4.111788	-2.259795	0.000030
23	1	0	4.304267	2.025999	-0.000032
24	1	0	5.465725	-0.173482	-0.000002



Int. 1

Cartesian Coordinates (Angstroms):

1	6	0	2.266639	1.029964	-0.288614
2	6	0	0.938344	0.677767	-0.480612
3	6	0	0.533335	-0.658436	-0.379606
4	6	0	1.486464	-1.642225	-0.098167
5	6	0	2.821641	-1.311595	0.095298
6	6	0	3.196726	0.027771	-0.003578
7	1	0	2.596815	2.057173	-0.361352
8	1	0	0.188284	1.420917	-0.721468
9	1	0	1.174233	-2.679169	-0.027990
10	1	0	3.569173	-2.061352	0.314880
11	6	0	-0.938602	-1.026516	-0.566755
12	8	0	-1.595776	-0.964037	0.680177
13	1	0	-0.999261	-2.067060	-0.951895
14	8	0	-1.631918	-0.139314	-1.330285
15	25	0	-2.985794	0.241391	0.170707
16	8	0	-3.393267	0.074686	1.698886
17	8	0	-2.772429	1.788494	-0.072852
18	8	0	-4.179650	-0.324015	-0.690432
19	7	0	4.605006	0.388779	0.187495
20	8	0	5.408607	-0.510032	0.436006
21	8	0	4.921094	1.573330	0.090985

Frequency Data:

NImag=0

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.127133 (Hartree/Particle)

Thermal correction to Energy= 0.141233

Thermal correction to Enthalpy= 0.142177

Thermal correction to Gibbs Free Energy= 0.082993

Sum of electronic and zero-point Energies= -954.994316

Sum of electronic and thermal Energies= -954.980215

Sum of electronic and thermal Enthalpies= -954.979271
Sum of electronic and thermal Free Energies= -955.038456

TS 1

Cartesian Coordinates (Angstroms):

1	6	0	2.774464	1.232274	0.307684
2	6	0	1.498715	1.752472	0.147948
3	6	0	0.458136	0.955361	-0.345531
4	6	0	0.703649	-0.385679	-0.661342
5	6	0	1.974454	-0.924040	-0.497448
6	6	0	2.998185	-0.104661	-0.024348
7	1	0	3.590492	1.832900	0.684935
8	1	0	1.275970	2.779324	0.409979
9	1	0	-0.111013	-1.006368	-1.011689
10	1	0	2.179576	-1.961168	-0.723909
11	6	0	-0.907976	1.600417	-0.538336
12	8	0	-1.903062	0.680403	-1.018934
13	1	0	-1.104377	1.577171	-1.801339
14	8	0	-1.185929	2.645116	0.063686
15	25	0	-2.914087	-0.618629	0.216330
16	8	0	-2.242852	-2.006330	-0.150896
17	8	0	-2.560494	-0.072927	1.652869
18	8	0	-4.423894	-0.468528	-0.218092
19	7	0	4.347773	-0.662109	0.134322
20	8	0	5.232936	0.074664	0.566939
21	8	0	4.531965	-1.837177	-0.175353

Frequency Data:

NImag=1 (-1037.67)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.119831 (Hartree/Particle)
Thermal correction to Energy= 0.134887
Thermal correction to Enthalpy= 0.135831
Thermal correction to Gibbs Free Energy= 0.074337
Sum of electronic and zero-point Energies= -954.971297
Sum of electronic and thermal Energies= -954.956241
Sum of electronic and thermal Enthalpies= -954.955297
Sum of electronic and thermal Free Energies= -955.016791

Int. 2

Cartesian Coordinates (Angstroms):

1	6	0	-2.533150	-1.085202	-0.275207
2	6	0	-1.203117	-0.721854	-0.473186
3	6	0	-0.798403	0.609390	-0.350373
4	6	0	-1.753824	1.577539	-0.041521
5	6	0	-3.091340	1.235574	0.160647

6	6	0	-3.461514	-0.097905	0.039644
7	1	0	-2.848273	-2.117337	-0.369811
8	1	0	-0.455441	-1.461014	-0.735059
9	1	0	-1.450663	2.616496	0.047255
10	1	0	-3.831491	1.988428	0.402861
11	6	0	0.669605	0.987148	-0.544173
12	8	0	1.352457	0.939460	0.690388
13	1	0	0.721123	2.026935	-0.934212
14	8	0	1.368611	0.103787	-1.311730
15	25	0	2.763954	-0.223338	0.153423
16	8	0	3.190405	-0.057394	1.678397
17	8	0	2.609813	-1.777401	-0.101346
18	8	0	3.922888	0.397164	-0.720341
19	17	0	-5.162179	-0.549596	0.280909

Frequency Data:

NImag=0
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.115284 (Hartree/Particle)
Thermal correction to Energy= 0.128010
Thermal correction to Enthalpy= 0.128954
Thermal correction to Gibbs Free Energy= 0.073399
Sum of electronic and zero-point Energies= -1210.057688
Sum of electronic and thermal Energies= -1210.044962
Sum of electronic and thermal Enthalpies= -1210.044018
Sum of electronic and thermal Free Energies= -1210.099573

TS 2

Cartesian Coordinates (Angstroms):

1	6	0	3.028527	1.081102	0.401553
2	6	0	1.767565	1.649123	0.242818
3	6	0	0.715155	0.916763	-0.313308
4	6	0	0.935049	-0.407720	-0.698613
5	6	0	2.189689	-0.994058	-0.537089
6	6	0	3.222375	-0.238052	0.004141
7	1	0	3.845841	1.647070	0.831465
8	1	0	1.573244	2.667462	0.557653
9	1	0	0.113895	-0.988270	-1.099972
10	1	0	2.357958	-2.025576	-0.820308
11	6	0	-0.629908	1.606806	-0.493321
12	8	0	-1.655937	0.724180	-0.992370
13	1	0	-0.835553	1.642572	-1.746285
14	8	0	-0.883054	2.642661	0.138327
15	25	0	-2.693571	-0.598458	0.187722
16	8	0	-2.027409	-1.986724	-0.190721
17	8	0	-2.381252	-0.095173	1.649734
18	8	0	-4.191713	-0.427674	-0.284062
19	17	0	4.825182	-0.971985	0.198828

Frequency Data:

NImag=1 (-1000.66)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.108045 (Hartree/Particle)
Thermal correction to Energy= 0.121733
Thermal correction to Enthalpy= 0.122677
Thermal correction to Gibbs Free Energy= 0.064723
Sum of electronic and zero-point Energies= -1210.035983
Sum of electronic and thermal Energies= -1210.022295
Sum of electronic and thermal Enthalpies= -1210.021351
Sum of electronic and thermal Free Energies= -1210.079305

Int. 3

Cartesian Coordinates (Angstroms):

1	6	0	-1.887198	-0.923237	-0.397620
2	6	0	-0.541115	-0.599558	-0.560587
3	6	0	-0.090487	0.708595	-0.371346
4	6	0	-1.013789	1.696873	-0.031060
5	6	0	-2.366884	1.396978	0.137400
6	6	0	-2.776975	0.085331	-0.050295
7	1	0	-2.234608	-1.938270	-0.543884
8	1	0	0.182516	-1.354238	-0.845155
9	1	0	-0.674553	2.718734	0.110570
10	1	0	-3.079267	2.167183	0.404462
11	6	0	1.394019	1.039351	-0.520875
12	8	0	2.046353	0.913094	0.724489
13	1	0	1.491184	2.092277	-0.864140
14	8	0	2.077083	0.164277	-1.311624
15	25	0	3.426825	-0.277235	0.166076
16	8	0	3.824788	-0.192400	1.705202
17	8	0	3.222543	-1.812083	-0.159617
18	8	0	4.626496	0.336760	-0.655513
19	35	0	-4.686841	-0.355942	0.169401

Frequency Data:
NImag=0
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.114527 (Hartree/Particle)
Thermal correction to Energy= 0.127564
Thermal correction to Enthalpy= 0.128508
Thermal correction to Gibbs Free Energy= 0.071547
Sum of electronic and zero-point Energies= -762.994464
Sum of electronic and thermal Energies= -762.981427
Sum of electronic and thermal Enthalpies= -762.980483
Sum of electronic and thermal Free Energies= -763.037445

TS 3

Cartesian Coordinates (Angstroms):

1	6	0	2.306252	1.387056	0.363469
2	6	0	1.004091	1.863852	0.230508
3	6	0	0.000270	1.066183	-0.324994
4	6	0	0.309810	-0.231687	-0.737250
5	6	0	1.606265	-0.729563	-0.602198
6	6	0	2.583228	0.093808	-0.061568
7	1	0	3.083467	2.006024	0.793520
8	1	0	0.741503	2.859832	0.566859
9	1	0	-0.471891	-0.864413	-1.138796
10	1	0	1.840879	-1.741281	-0.906919
11	6	0	-1.394772	1.658951	-0.472066
12	8	0	-2.360489	0.714003	-0.975226
13	1	0	-1.622002	1.704796	-1.721202
14	8	0	-1.712431	2.660372	0.185324
15	25	0	-3.276709	-0.708440	0.191811
16	8	0	-2.512731	-2.032925	-0.228215
17	8	0	-2.978733	-0.212971	1.659401
18	8	0	-4.790804	-0.641930	-0.254028
19	35	0	4.419897	-0.594227	0.118223

Frequency Data:

NImag=1 (-1002.47)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.107239 (Hartree/Particle)
Thermal correction to Energy= 0.121270
Thermal correction to Enthalpy= 0.122214
Thermal correction to Gibbs Free Energy= 0.062314
Sum of electronic and zero-point Energies= -762.972658
Sum of electronic and thermal Energies= -762.958627
Sum of electronic and thermal Enthalpies= -762.957683
Sum of electronic and thermal Free Energies= -763.017583

Int. 4

Cartesian Coordinates (Angstroms):

1	6	0	3.143204	1.460160	0.058332
2	6	0	1.860215	1.002593	-0.231877
3	6	0	1.589902	-0.368547	-0.268224
4	6	0	2.628849	-1.269260	-0.028716
5	6	0	3.916326	-0.815264	0.260919
6	6	0	4.176868	0.553756	0.306446
7	1	0	3.342128	2.527259	0.086027
8	1	0	1.048683	1.688500	-0.444098
9	1	0	2.424491	-2.335616	-0.066096
10	1	0	4.714538	-1.527422	0.447502

11	1	0	5.177255	0.912368	0.528160
12	6	0	0.173344	-0.865608	-0.551383
13	8	0	-0.566384	-0.954462	0.648828
14	1	0	0.234780	-1.880799	-1.000300
15	8	0	-0.577355	-0.006991	-1.300408
16	25	0	-2.053365	0.106637	0.109924
17	8	0	-2.528849	-0.193505	1.600873
18	8	0	-2.030172	1.682122	-0.042373
19	8	0	-3.114740	-0.556815	-0.853454

Frequency Data:

NImag= 0
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.124752 (Hartree/Particle)
Thermal correction to Energy= 0.136245
Thermal correction to Enthalpy= 0.137189
Thermal correction to Gibbs Free Energy= 0.085013
Sum of electronic and zero-point Energies= -750.420271
Sum of electronic and thermal Energies= -750.408777
Sum of electronic and thermal Enthalpies= -750.407833
Sum of electronic and thermal Free Energies= -750.460010

TS 4

Cartesian Coordinates (Angstroms):

1	6	0	3.804266	0.238910	0.553034
2	6	0	2.684897	1.028049	0.301644
3	6	0	1.540186	0.471125	-0.277587
4	6	0	1.526488	-0.889878	-0.595822
5	6	0	2.644910	-1.681049	-0.335429
6	6	0	3.788248	-1.120072	0.233018
7	1	0	4.687084	0.679941	1.005676
8	1	0	2.666006	2.080748	0.557805
9	1	0	0.630218	-1.325296	-1.019391
10	1	0	2.618355	-2.740390	-0.569771
11	1	0	4.657993	-1.738185	0.432926
12	6	0	0.355040	1.385822	-0.558044
13	8	0	-0.810569	0.678074	-1.038806
14	1	0	0.194032	1.369081	-1.816238
15	8	0	0.280410	2.494137	-0.007623
16	25	0	-2.118701	-0.324012	0.177980
17	8	0	-1.696205	-1.839591	-0.017682
18	8	0	-1.806860	0.263624	1.608747
19	8	0	-3.535572	0.050876	-0.415310

Frequency Data:

NImag= 1 (-997.23)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.

Zero-point correction= 0.117589 (Hartree/Particle)
Thermal correction to Energy= 0.130035
Thermal correction to Enthalpy= 0.130979
Thermal correction to Gibbs Free Energy= 0.076386
Sum of electronic and zero-point Energies= -750.398846
Sum of electronic and thermal Energies= -750.386401
Sum of electronic and thermal Enthalpies= -750.385457
Sum of electronic and thermal Free Energies= -750.440049

Int. 5

Cartesian Coordinates (Angstroms):

1	6	0	-2.603210	-0.873322	-0.250756
2	6	0	-1.253400	-0.570970	-0.442584
3	6	0	-0.778958	0.731664	-0.309145
4	6	0	-1.692750	1.740895	0.006568
5	6	0	-3.040791	1.460148	0.201492
6	6	0	-3.500143	0.146961	0.074454
7	1	0	-2.937488	-1.897000	-0.362902
8	1	0	-0.545904	-1.347252	-0.709110
9	1	0	-1.340937	2.763854	0.105419
10	1	0	-3.752053	2.240365	0.448993
11	6	0	0.704835	1.036521	-0.489941
12	8	0	1.395876	0.904854	0.735193
13	1	0	0.813911	2.086643	-0.839024
14	8	0	1.359393	0.148276	-1.294449
15	25	0	2.754102	-0.287079	0.132194
16	8	0	3.198163	-0.207746	1.660656
17	8	0	2.546981	-1.823530	-0.191742
18	8	0	3.929066	0.333739	-0.721812
19	8	0	-4.852202	-0.040694	0.279077
20	6	0	-5.362393	-1.356236	0.182060
21	1	0	-6.430194	-1.282024	0.390532
22	1	0	-5.219942	-1.774297	-0.822059
23	1	0	-4.897310	-2.026466	0.915032

Frequency Data:

NImag= 0
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.156981 (Hartree/Particle)
Thermal correction to Energy= 0.171126
Thermal correction to Enthalpy= 0.172070
Thermal correction to Gibbs Free Energy= 0.113622
Sum of electronic and zero-point Energies= -864.943678
Sum of electronic and thermal Energies= -864.929533
Sum of electronic and thermal Enthalpies= -864.928589
Sum of electronic and thermal Free Energies= -864.987037

TS 5

Cartesian Coordinates (Angstroms):

1	6	0	3.033876	0.876507	0.326568
2	6	0	1.789591	1.494135	0.190766
3	6	0	0.707422	0.825514	-0.377666
4	6	0	0.884394	-0.495535	-0.808462
5	6	0	2.114975	-1.124365	-0.674966
6	6	0	3.196424	-0.439833	-0.112165
7	1	0	3.852447	1.423718	0.776487
8	1	0	1.636925	2.509013	0.538606
9	1	0	0.040881	-1.034116	-1.221985
10	1	0	2.255701	-2.152098	-0.989645
11	6	0	-0.610095	1.567715	-0.525722
12	8	0	-1.690291	0.721861	-0.985754
13	1	0	-0.851832	1.609016	-1.768510
14	8	0	-0.809021	2.618496	0.103235
15	25	0	-2.747386	-0.540944	0.229390
16	8	0	-2.138399	-1.962761	-0.119093
17	8	0	-2.408167	-0.020858	1.680268
18	8	0	-4.245547	-0.331820	-0.231203
19	6	0	5.494710	-0.505812	0.557763
20	1	0	5.299438	-0.223792	1.599362
21	1	0	6.306374	-1.233213	0.529512
22	1	0	5.792304	0.388164	-0.003972
23	8	0	4.377002	-1.144051	-0.028866

Frequency Data:

NImag= 1 (-987.13)
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
1 imaginary frequencies ignored.
Zero-point correction= 0.149793 (Hartree/Particle)
Thermal correction to Energy= 0.164892
Thermal correction to Enthalpy= 0.165837
Thermal correction to Gibbs Free Energy= 0.105095
Sum of electronic and zero-point Energies= -864.922475
Sum of electronic and thermal Energies= -864.907376
Sum of electronic and thermal Enthalpies= -864.906432
Sum of electronic and thermal Free Energies= -864.967173

Int. 6

Cartesian Coordinates (Angstroms):

1	6	0	2.249985	0.959702	-0.275149
2	6	0	0.896065	0.673034	-0.448631
3	6	0	0.436402	-0.641343	-0.481559
4	6	0	1.377128	-1.666901	-0.365688
5	6	0	2.731445	-1.394616	-0.207571
6	6	0	3.195435	-0.069864	-0.150022

7	1	0	2.560696	1.996354	-0.238896
8	1	0	0.172193	1.471604	-0.561972
9	1	0	1.043746	-2.700013	-0.412458
10	1	0	3.439136	-2.215068	-0.158396
11	6	0	-1.049920	-0.944804	-0.633015
12	8	0	-1.689085	-0.967752	0.626654
13	1	0	-1.163441	-1.948980	-1.097676
14	8	0	-1.749081	0.020240	-1.300094
15	25	0	-3.100739	0.243076	0.213634
16	8	0	-3.471485	-0.006210	1.743691
17	8	0	-2.962826	1.811495	0.041053
18	8	0	-4.290641	-0.334050	-0.650386
19	7	0	4.592765	0.181626	-0.018674
20	6	0	5.257230	-0.463274	1.109039
21	1	0	6.341200	-0.425744	0.963231
22	1	0	5.020446	0.026299	2.070693
23	1	0	4.963269	-1.508306	1.184798
24	6	0	5.037206	1.551644	-0.196023
25	1	0	4.730990	2.225899	0.624377
26	1	0	6.129724	1.562898	-0.246397
27	1	0	4.650245	1.955526	-1.133082

Frequency Data:

NImag= 0
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.197190 (Hartree/Particle)
Thermal correction to Energy= 0.212871
Thermal correction to Enthalpy= 0.213816
Thermal correction to Gibbs Free Energy= 0.152286
Sum of electronic and zero-point Energies= -884.347285
Sum of electronic and thermal Energies= -884.331604
Sum of electronic and thermal Enthalpies= -884.330660
Sum of electronic and thermal Free Energies= -884.392190

TS 6

Cartesian Coordinates (Angstroms):

1	6	0	2.659915	1.220498	0.331532
2	6	0	1.375407	1.753574	0.241279
3	6	0	0.337473	1.042903	-0.358165
4	6	0	0.618278	-0.225739	-0.877162
5	6	0	1.896013	-0.762007	-0.795982
6	6	0	2.947579	-0.052908	-0.187190
7	1	0	3.428917	1.799663	0.826392
8	1	0	1.152959	2.728431	0.659466
9	1	0	-0.179146	-0.799501	-1.332768
10	1	0	2.078787	-1.740924	-1.223182
11	6	0	-1.038134	1.679425	-0.441326
12	8	0	-2.054766	0.771930	-0.935088

13	1	0	-1.308018	1.776583	-1.673113
14	8	0	-1.313302	2.669332	0.254730
15	25	0	-2.963029	-0.660220	0.205982
16	8	0	-2.204990	-1.989199	-0.212151
17	8	0	-2.685868	-0.188946	1.686303
18	8	0	-4.475149	-0.591100	-0.252204
19	7	0	4.252659	-0.610481	-0.147417
20	6	0	5.323347	0.228023	0.357633
21	1	0	5.257468	0.421396	1.443550
22	1	0	6.278367	-0.267560	0.163671
23	1	0	5.329467	1.188162	-0.161183
24	6	0	4.367452	-1.988833	0.318135
25	1	0	3.613480	-2.621133	-0.144881
26	1	0	5.351358	-2.382094	0.046144
27	1	0	4.252092	-2.069918	1.413023

Frequency Data:

NImag= 1 (-982.10)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

1 imaginary frequencies ignored.

Zero-point correction= 0.190042 (Hartree/Particle)

Thermal correction to Energy= 0.206760

Thermal correction to Enthalpy= 0.207705

Thermal correction to Gibbs Free Energy= 0.142884

Sum of electronic and zero-point Energies= -884.326716

Sum of electronic and thermal Energies= -884.309997

Sum of electronic and thermal Enthalpies= -884.309053

Sum of electronic and thermal Free Energies= -884.373873