Electronic Supplementary Material (ESI) for Dalton Transactions

SUPLEMENTARY INFORMATION

O-O bond activation in H_2O_2 and $(CH_3)_3C$-OOH mediated by $[Ni(cyclam)(CH_3CN)_2](ClO_4)_2$: Different mechanisms to form the same Ni(III) product?

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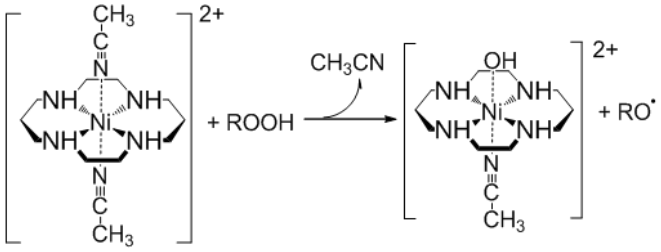
a) Homolysis



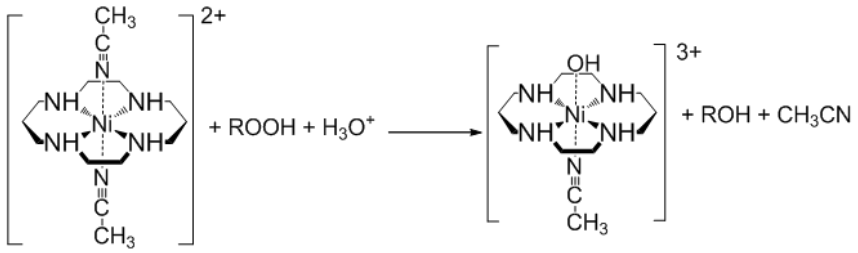
HOOH

	1	3
PBEPBE	0.0 (0.0)	+39.5 (-16.8)
BLYP	0.0 (0.0)	+16.1 (-34.7)
OLYP	0.0 (0.0)	+33.4 (-25.2)
OPBE	0.0 (0.0)	+41.5 (-5.7)
B3LYP	0.0 (0.0)	+78.8 (+25.6)
BHLYP	0.0 (0.0)	+148.9 (+108.5)

tBuOOH

	1	3
PBEPBE	0.0 (0.0)	-38.8 (-104.6)
BLYP	0.0 (0.0)	-66.4 (-125.4)
OLYP	0.0 (0.0)	-50.4 (-80.5)
OPBE	0.0 (0.0)	-0.9 (-40.2)
B3LYP	0.0 (0.0)	+7.2 (-57.2)
BHLYP	0.0 (0.0)	+101.7 (+53.1)

b) Heterolysis *(Acid media)*



HOOH

	1	4
PBEPBE	0.0 (0.0)	-126.8 (-148.8)
BLYP	0.0 (0.0)	-136.3 (-145.1)
OLYP	0.0 (0.0)	-66.4 (-73.7)
OPBE	0.0 (0.0)	-70.1 (-33.1)
B3LYP	0.0 (0.0)	-13.0 (-27.2)
BHLYP	0.0 (0.0)	181.2 (170.0)

tBuOOH

	1	4
PBEPBE	0.0 (0.0)	-142.3 (-164.9)
BLYP	0.0 (0.0)	-159.3 (-173.0)
OLYP	0.0 (0.0)	-91.1 (-68.1)
OPBE	0.0 (0.0)	-42.7 (+6.9)
B3LYP	0.0 (0.0)	-34.3 (-48.5)
BHLYP	0.0 (0.0)	+172.0 (162.1)

Figure S1

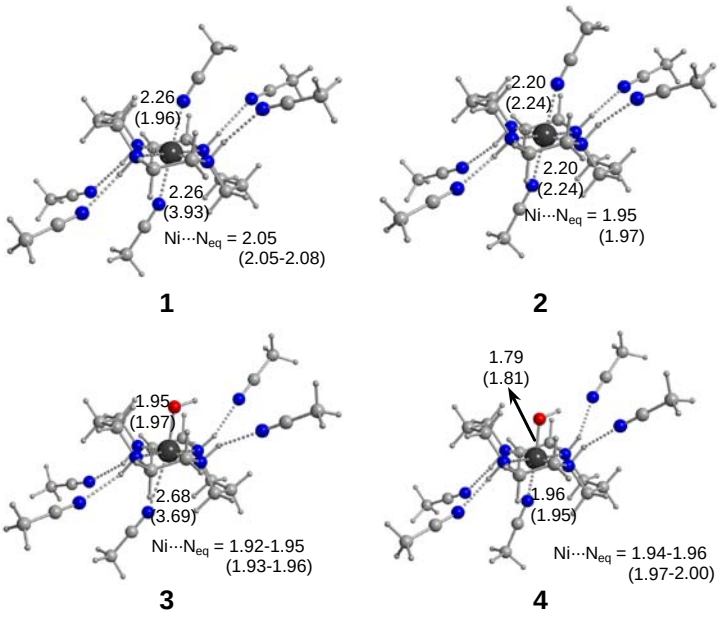


Figure S2

1-B3LYP

C	0.657570	0.525258	0.294978
C	0.455657	0.536805	2.963778
C	1.257706	0.862971	1.681015
H	0.433416	-0.540254	0.213373
H	1.408919	0.766605	-0.469587
H	1.080491	0.793496	3.830359
H	0.228873	-0.529840	3.025760
H	1.510630	1.932589	1.695415
H	2.214341	0.333438	1.755600
C	-4.516607	0.970237	-0.106631
C	-4.718460	0.981875	2.562172
C	-5.318720	0.644303	1.176152
H	-5.141460	0.713632	-0.973223
H	-4.289605	2.036832	-0.168650
H	-5.469834	0.740689	3.326765
H	-4.494067	2.047338	2.643770
H	-6.275216	1.174091	1.101576
H	-5.571904	-0.425257	1.161807
Ni	-2.030477	0.753376	1.428582
N	-0.587756	1.300028	0.048536
N	-0.816766	1.306328	3.008277
N	-3.473306	0.206814	2.808527
N	-3.244322	0.200479	-0.151063
H	-3.716627	-0.775546	2.669638
H	-3.503253	-0.781460	-0.042260
H	-0.557962	2.288316	2.899614
H	-0.344653	2.282454	0.187289
C	-2.828115	0.260005	4.153374
C	-1.658646	1.261950	4.239520
C	-2.402433	0.244623	-1.382296
C	-1.232916	1.246538	-1.296322
H	-3.005489	0.475832	-2.269476
H	-2.014103	-0.768171	-1.518847
H	-0.502233	1.010303	-2.080262
H	-1.596233	2.258226	-1.495873
H	-2.047010	2.274703	4.376267
H	-1.055585	1.030623	5.126664
H	-2.464731	-0.751718	4.352651
H	-3.558775	0.496010	4.937405
N	-4.423659	-2.785103	3.506003
C	-5.125069	-3.474373	4.124683
C	-6.004844	-4.341141	4.904067
H	-6.320277	-5.197005	4.300579
H	-5.480696	-4.706487	5.791813
H	-6.892395	-3.785887	5.220722
N	-4.060283	-2.787776	-1.026128
C	-4.651410	-3.451877	-1.774093
C	-5.392907	-4.285952	-2.716076
H	-4.847278	-4.359922	-3.661121
H	-5.526407	-5.290444	-2.304547
H	-6.377107	-3.849219	-2.908297
N	-0.000191	4.293732	3.882812
N	0.360923	4.292082	-0.652317
C	0.590358	4.958967	4.630223
C	1.061130	4.980662	-1.273127
C	1.330920	5.795051	5.571157
H	1.806969	6.625424	5.042018
H	0.652685	6.198704	6.328397
H	2.104555	5.203248	6.068747
C	1.939385	5.846556	-2.055200
H	2.827559	5.291678	-2.370767
H	1.414350	6.208837	-2.943678
H	2.253903	6.704463	-1.454143
N	-1.496007	-1.430849	1.471969
N	-2.564796	2.938023	1.385016
C	-2.505877	4.095166	1.395054
C	-1.554602	-2.587998	1.461387
C	-2.419620	5.547746	1.409327
H	-1.962278	5.868811	2.349384
H	-1.791955	5.875755	0.576064
H	-3.416080	5.988529	1.315263
C	-1.640432	-4.040588	1.446388
H	-2.272750	-4.368798	2.276050
H	-2.092323	-4.361625	0.503695
H	-0.644419	-4.481151	1.546063

E = -2919.14203486
G = -2918.598855
E + ΔG_{solv} = -2919.239134

2-B3LYP

C	0.632462	0.525593	0.322224
C	0.421168	0.532357	2.946920
C	1.260909	0.832687	1.692899
H	0.438805	-0.537989	0.180192
H	1.330077	0.850889	-0.458294
H	0.985246	0.860509	3.827776
H	0.206470	-0.530606	3.060323
H	1.554607	1.889699	1.713349
H	2.191084	0.260069	1.768931
C	-4.481513	0.975071	-0.090750
C	-4.692827	0.981820	2.533945
C	-5.321466	0.675205	1.163247
H	-5.045683	0.647181	-0.971645
H	-4.266242	2.037920	-0.204142
H	-5.390561	0.656766	3.314463
H	-4.498658	2.045292	2.676092
H	-6.251277	1.248417	1.087247
H	-5.615778	-0.381632	1.142736
Ni	-2.030285	0.753320	1.428095
N	-0.641881	1.286049	0.138390
N	-0.865052	1.293706	2.920437
N	-3.418836	0.220731	2.717620
N	-3.195691	0.213040	-0.064097
H	-3.669016	-0.767679	2.563901
H	-3.466051	-0.774345	0.054400
H	-0.595236	2.281244	2.802097
H	-0.392099	2.274581	0.291794
C	-2.787135	0.228856	4.086032
C	-1.705833	1.290433	4.170894
C	-2.354868	0.215706	-1.314493
C	-1.273546	1.277301	-1.230056
H	-2.989472	0.370764	-2.192755
H	-1.923482	-0.784254	-1.396294
H	-0.507677	1.120816	-1.996276
H	-1.688065	2.276419	-1.381115
H	-2.137210	2.290350	4.253191
H	-1.071204	1.135001	5.049066
H	-2.372638	-0.770340	4.236626
H	-3.552979	0.385000	4.852351
N	-4.535515	-2.477633	3.293113
C	-5.213280	-3.249043	3.837577
C	-6.063537	-4.216076	4.524068
H	-6.291370	-5.054948	3.859933
H	-5.555040	-4.595539	5.415414
H	-7.000917	-3.739911	4.827027
N	-4.171210	-2.504672	-0.836603
C	-4.743843	-3.257230	-1.512636
C	-5.461568	-4.200041	-2.364449
H	-4.927356	-4.331437	-3.310209

H	-5.544514	-5.170314	-1.865989
H	-6.466981	-3.822866	-2.574327
N	0.106933	4.012105	3.694903
N	0.475214	3.983931	-0.439509
C	0.678581	4.764725	4.371701
C	1.150793	4.755032	-0.987123
C	1.394561	5.708348	5.224039
H	1.841739	6.500187	4.615968
H	0.706106	6.158754	5.945345
H	2.189022	5.189976	5.769333
C	1.998416	5.721520	-1.677641
H	2.941025	5.249194	-1.970206
H	1.492783	6.088794	-2.575698
H	2.216112	6.568372	-1.020269
N	-1.468410	-1.409921	1.475887
N	-2.591624	2.917205	1.380360
C	-2.653648	4.075177	1.382264
C	-1.405410	-2.567831	1.474702
C	-2.741001	5.526901	1.389637
H	-1.855175	5.937058	1.883465
H	-2.789735	5.901669	0.362673
H	-3.638171	5.845297	1.929950
C	-1.315992	-4.019430	1.467687
H	-1.264541	-4.393794	2.494666
H	-2.202150	-4.431149	0.975807
H	-0.419457	-4.336602	0.925586

E = -2918.72751408
G = -2918.174726
E + ΔG_{solv} = -2919.030203

3-B3LYP-doublet

C	0.656900	0.333659	0.292561
C	0.394155	0.462350	2.888399
C	1.299145	0.630018	1.657357
H	0.315387	-0.702623	0.232454
H	1.400903	0.495961	-0.497255
H	0.965576	0.718599	3.788266
H	0.036194	-0.565534	2.984481
H	1.704359	1.649885	1.653081
H	2.157573	-0.039348	1.775738
C	-4.317369	0.831344	-0.231795
C	-4.575109	0.960178	2.365338
C	-5.172647	0.547602	1.011901
H	-4.841845	0.459558	-1.119251
H	-4.112961	1.897653	-0.335959
H	-5.267217	0.669144	3.163556
H	-4.388591	2.034006	2.410265
H	-6.121693	1.080667	0.891390
H	-5.421543	-0.521768	1.040429
Ni	-1.928899	0.876477	1.317823
N	-0.506432	1.236028	0.044087
N	-0.781745	1.377462	2.799716
N	-3.275915	0.256061	2.601240
N	-3.006098	0.117546	-0.135553
H	-3.460017	-0.743506	2.466802
H	-3.226580	-0.863937	0.061927
H	-0.403047	2.321843	2.666426
H	-0.188986	2.207109	0.168535
C	-2.694023	0.369232	3.979679
C	-1.663650	1.483652	4.005470
C	-2.163585	0.086198	-1.375824
C	-1.126496	1.194499	-1.318853
H	-2.791931	0.178680	-2.267094
H	-1.688205	-0.897258	-1.409233
H	-0.355644	1.060779	-2.086320
H	-1.593190	2.170365	-1.468632
H	-2.149037	2.458790	3.934871
H	-1.062334	1.458539	4.920433
H	-2.239469	-0.597392	4.211089
H	-3.485755	0.545904	4.714322
N	-4.705588	-2.329104	3.517397
C	-5.460255	-2.975376	4.119021
C	-6.409840	-3.785165	4.877481
H	-6.878492	-4.526071	4.223598
H	-5.894817	-4.304145	5.690921
H	-7.189260	-3.146717	5.303277
N	-4.220122	-2.553939	-1.099948
C	-4.811722	-3.284514	-1.782092
C	-5.555757	-4.200516	-2.642356
H	-4.863544	-4.793951	-3.246457
H	-6.165391	-4.875253	-2.034746
H	-6.212759	-3.635945	-3.310201
N	0.770157	3.799144	3.715664
N	0.136545	4.164749	-0.178447
C	1.284786	4.624730	4.349207
C	0.425782	5.223927	-0.554591
C	1.931749	5.661629	5.147576
H	2.911434	5.903184	4.725578
H	1.315299	6.565044	5.158239
H	2.066076	5.312850	6.175504
C	0.787345	6.555076	-1.029454
H	1.849916	6.740582	-0.848229
H	0.591271	6.634252	-2.102614
H	0.197201	7.311610	-0.504305
N	-1.431634	-2.127781	1.508019
C	-1.400226	-3.284958	1.599894
C	-1.360792	-4.738240	1.715610
H	-2.355500	-5.115167	1.969240
H	-1.042125	-5.180435	0.767369
H	-0.656649	-5.033472	2.498851
O	-2.632616	2.705200	1.204294
H	-1.968785	3.373568	0.976967

E = -2862.15809824
G = -2861.642310
E + ΔG_{solv} = -2862.267856

3-B3LYP-quartet

C	0.690382	0.245629	0.458180
C	0.280764	0.281246	3.041859
C	1.268039	0.427330	1.871162
H	0.183625	-0.721211	0.382687
H	1.511380	0.247374	-0.271138
H	0.836440	0.309172	3.988341
H	-0.246566	-0.676239	2.988228
H	1.775411	1.398124	1.945105
H	2.048243	-0.330420	2.001269
C	-4.220196	0.649881	-0.257858
C	-4.635504	0.876890	2.338622
C	-5.083665	0.325839	0.973841
H	-4.671742	0.167577	-1.131619
H	-4.166122	1.726441	-0.435804
H	-5.360618	0.560323	3.097152
H	-4.586733	1.969173	2.335156
H	-6.088973	0.712371	0.774241
H	-5.188718	-0.764332	1.053256
Ni	-1.919803	1.228734	1.390018
N	-0.289851	1.310366	0.101741
N	-0.715724	1.387633	3.033602
N	-3.286744	0.341422	2.693720
N	-2.823402	0.128954	-0.105995
H	-3.327389	-0.666442	2.529342
H	-2.896029	-0.846062	0.192573

H	-0.185417	2.268178	3.008685
H	0.155987	2.226098	0.184831
C	-2.812266	0.502572	4.099003
C	-1.645887	1.497733	4.192809
C	-1.962603	0.131463	-1.325555
C	-0.883685	1.221928	-1.260181
H	-2.572155	0.269487	-2.223546
H	-1.507013	-0.858492	-1.399420
H	-0.112876	1.022180	-2.015494
H	-1.314031	2.203534	-1.473194
H	-2.019637	2.525027	4.178901
H	-1.103230	1.351956	5.134879
H	-2.505355	-0.485031	4.451945
H	-3.627998	0.834522	4.748732
N	-4.780934	-2.253835	3.774758
C	-5.526659	-2.872045	4.416112
C	-6.466410	-3.646632	5.222769
H	-7.094235	-4.266598	4.576530
H	-5.922158	-4.293926	5.916313
H	-7.108788	-2.974077	5.798336
N	-4.059128	-2.497173	-1.496031
C	-4.580629	-3.202638	-2.257602
C	-5.237139	-4.086436	-3.217707
H	-4.488796	-4.644686	-3.787389
H	-5.885985	-4.794525	-2.694545
H	-5.844160	-3.499424	-3.912847
N	1.017553	3.791594	3.627344
N	-0.496933	4.572362	-0.164220
C	1.639572	4.592414	4.192190
C	-0.232661	5.602211	-0.631038
C	2.419574	5.599408	4.904723
H	3.338483	5.820469	4.354303
H	1.836383	6.518708	5.009690
H	2.683300	5.231430	5.900405
C	0.096128	6.895847	-1.218802
H	1.174665	7.069106	-1.163583
H	-0.215542	6.919974	-2.266976
H	-0.421656	7.692047	-0.676012
N	-1.674886	-2.349374	1.537069
C	-1.716342	-3.506754	1.624476
C	-1.765691	-4.960261	1.733429
H	-2.761413	-5.273040	2.059832
H	-1.548730	-5.414949	0.762707
H	-1.026479	-5.307493	2.461016
O	-2.510222	2.904946	1.189157
H	-1.858552	3.555643	0.847656

E = -2862.13275164
G =
E + ΔG_{solv} = -2862.239034

4-B3LYP-singlet

C	0.806111	0.174552	0.360043
C	0.512905	0.308871	2.973602
C	1.409102	0.498622	1.737541
H	0.559882	-0.880873	0.240908
H	1.542904	0.433008	-0.410357
H	1.063862	0.664219	3.852459
H	0.236150	-0.731146	3.147748
H	1.768861	1.534821	1.730337
H	2.298652	-0.126522	1.866851
C	-4.269383	1.039784	-0.242449
C	-4.553167	1.178323	2.359849
C	-5.170306	0.860251	0.989156
H	-4.829460	0.734106	-1.135044
H	-3.941596	2.070640	-0.367752
H	-5.295029	0.960871	3.138578
H	-4.249792	2.220931	2.448980
H	-6.039951	1.512482	0.859656
H	-5.560182	-0.165962	1.000594
Ni	-1.878678	0.621544	1.366361
N	-0.417074	0.997232	0.099484
N	-0.719786	1.146558	2.863126
N	-3.376523	0.299825	2.631886
N	-3.071246	0.151098	-0.157130
H	-3.705533	-0.672365	2.512802
H	-3.429947	-0.805581	-0.009273
H	-0.375769	2.107999	2.700964
H	-0.146458	1.981523	0.249228
C	-2.778852	0.333545	4.011154
C	-1.606403	1.295388	4.072206
C	-2.191329	0.033664	-1.370046
C	-1.008885	0.984286	-1.287617
H	-2.778311	0.233300	-2.272268
H	-1.864011	-1.007279	-1.416234
H	-0.238055	0.704552	-2.012915
H	-1.311684	2.012189	-1.497986
H	-1.946406	2.331922	4.069458
H	-1.016671	1.133217	4.979535
H	-2.474708	-0.689682	4.243403
H	-3.546472	0.621456	4.736637
N	-4.542651	-2.353719	3.215910
C	-5.305631	-3.034715	3.769016
C	-6.261953	-3.887840	4.465859
H	-6.369945	-4.840644	3.939074
H	-5.916248	-4.082211	5.485713
H	-7.237934	-3.394817	4.510136
N	-4.058355	-2.592559	-0.763563
C	-4.661721	-3.327039	-1.433516
C	-5.415656	-4.248544	-2.276526
H	-4.752524	-4.707114	-3.016399
H	-5.865658	-5.035930	-1.664537
H	-6.211092	-3.709006	-2.799731
N	0.592807	3.644898	3.517237
N	-0.198674	3.945224	-0.032197
C	1.098904	4.498240	4.121768
C	0.118418	4.988005	-0.435206
C	1.734004	5.568360	4.882804
H	2.710263	5.807254	4.450498
H	1.105554	6.463813	4.865405
H	1.874700	5.254678	5.921582
C	0.513893	6.294461	-0.943203
H	1.583722	6.451892	-0.774944
H	0.309362	6.355019	-2.016593
H	-0.049804	7.079070	-0.428925
N	-1.529434	-1.327162	1.506283
C	-1.530784	-2.482779	1.569134
C	-1.517005	-3.932230	1.642013
H	-1.628314	-4.250090	2.683552
H	-2.352412	-4.320670	1.051105
H	-0.573362	-4.319074	1.243024
O	-2.371822	2.360777	1.284814
H	-1.667435	2.953534	0.951458

E = -2861.71175102
G = -2861.181108
E + ΔG_{solv} = -2862.035764

4-B3LYP-triplet

C	1.119015	-0.078661	0.856645
C	0.575475	-0.156821	3.430426
C	1.612067	0.035274	2.309458

H	0.777853	-1.085167	0.612055
H	1.949650	0.168579	0.185016
H	1.063814	0.041934	4.392066
H	0.178393	-1.172109	3.461781
H	2.098026	1.009232	2.441482
H	2.399418	-0.712710	2.450197
C	-3.752675	1.280124	-0.103766
C	-4.271234	1.228066	2.464598
C	-4.782381	1.091851	1.022337
H	-4.253123	1.135124	-1.068868
H	-3.322690	2.286542	-0.105126
H	-5.105023	1.051700	3.154295
H	-3.872919	2.226586	2.667242
H	-5.574198	1.834821	0.878270
H	-5.261103	0.111761	0.902891
Ni	-1.619353	0.508532	1.653407
N	-0.002546	0.877400	0.576377
N	-0.557620	0.807022	3.281000
N	-3.211471	0.213699	2.759270
N	-2.652212	0.271149	0.002247
H	-3.634234	-0.706007	2.552805
H	-3.125389	-0.647545	-0.005653
H	-0.134014	1.735690	3.129450
H	0.313666	1.802220	0.885494
C	-2.749277	0.095587	4.192221
C	-1.521109	0.958493	4.428237
C	-1.666949	0.181919	-1.134066
C	-0.437841	1.035363	-0.861340
H	-2.147708	0.477580	-2.072302
H	-1.400627	-0.873638	-1.222129
H	0.381881	0.760398	-1.533019
H	-0.652497	2.095848	-1.011380
H	-1.787973	2.017296	4.472878
H	-1.029503	0.693050	5.369598
H	-2.528504	-0.961573	4.355901
H	-3.563659	0.370708	4.869993
N	-4.798808	-2.256108	3.121789
C	-5.643155	-2.905978	3.584169
C	-6.706696	-3.703522	4.186702
H	-6.935138	-4.568885	3.557420
H	-6.394643	-4.055419	5.174802
H	-7.610519	-3.096024	4.295511
N	-4.045257	-2.133849	-0.984339
C	-4.689301	-2.811215	-1.673575
C	-5.503351	-3.655903	-2.540663
H	-4.873198	-4.137734	-3.294229
H	-6.005521	-4.427697	-1.949959
H	-6.259839	-3.049172	-3.047777
N	0.651792	3.458410	2.848310
N	-1.383953	4.440560	-0.110942
C	1.202797	4.371795	3.312293
C	-1.324589	5.385432	-0.785225
C	1.894041	5.510326	3.903297
H	2.835632	5.692417	3.375619
H	1.265702	6.404062	3.837789
H	2.110957	5.305950	4.956823
C	-1.276739	6.586497	-1.606651
H	-0.244820	6.940228	-1.696066
H	-1.669505	6.374632	-2.605989
H	-1.885413	7.368874	-1.142056
N	-1.416276	-1.728740	1.620627
C	-1.464650	-2.887079	1.589778
C	-1.515425	-4.340763	1.561101
H	-2.347435	-4.688661	2.181092
H	-1.663846	-4.686514	0.533731
H	-0.579658	-4.757066	1.947770
O	-1.867693	2.627403	1.744453
H	-1.676938	3.334881	1.018928

E = -2861.69427227

tBuOOH·6H_2O-B3LYP

O	0.427913	-0.397039	0.317178
H	1.191679	0.232197	0.440991
O	-0.656977	0.588814	0.193744
O	2.275614	1.591606	0.496967
H	1.886927	2.144338	1.198197
H	2.025742	2.028933	-0.337090
H	-1.580242	4.905519	2.742443
O	-1.513895	4.344517	3.538448
H	-2.354323	4.401444	4.006842
H	-0.388991	2.998807	2.714561
O	0.106954	2.767813	1.904814
H	-0.344527	2.008078	1.488882
H	-0.342515	4.338869	1.096065
O	-0.855949	5.159688	0.914182
H	-0.215328	5.866574	0.765813
H	0.024050	1.559743	-1.278839
O	0.567192	2.208869	-1.773217
H	0.761374	1.810985	-2.631441
H	-1.659896	4.521680	-0.856760
O	-1.799556	3.985389	-1.654617
H	-0.936673	3.577567	-1.833880
C	-1.931546	-0.128715	0.089414
C	-1.951008	-0.928748	-1.216897
H	-2.898712	-1.468810	-1.309923
H	-1.856859	-0.263376	-2.081723
H	-1.134988	-1.654931	-1.237893
C	-2.117463	-1.027528	1.314838
H	-2.035234	-0.443733	2.237258
H	-3.112089	-1.484467	1.286384
H	-1.368729	-1.821706	1.340440
C	-2.953045	1.014462	0.067554
H	-3.949308	0.599464	-0.115165
H	-2.978031	1.537410	1.029354
H	-2.733784	1.746624	-0.716117

E = -767.511524333
G = -767.274162
E + ΔG_{solv} = -767.502017

tBuO$^{\bullet}$·6H_2O-B3LYP

O	-0.883451	1.196445	0.056055
H	-0.058483	1.579957	-0.375042
H	-1.635235	1.532499	-0.446297
O	3.399497	1.012779	0.463048
H	4.083986	0.397998	0.176924
O	1.167160	-2.508285	1.627816
O	1.329996	2.337809	-0.806114
H	1.368238	3.119156	-0.216963
H	2.111494	1.804861	-0.539661
H	2.971029	0.621871	1.264618
O	2.007582	0.070433	2.616274
H	1.240718	0.667360	2.713980
H	1.646995	-0.813836	2.423853
O	-0.170700	1.936160	2.521807
H	-0.872431	2.031712	3.176584
H	-0.594226	1.667252	1.660746
O	1.282262	4.112346	1.412211
H	0.814216	3.454309	1.964531
H	2.159355	4.217405	1.801014
C	-0.052199	-3.074132	1.296073
C	-0.126499	-4.311521	2.255492

H	-0.106531	-3.990665	3.299678
H	-1.071808	-4.826491	2.056042
H	0.705883	-4.993534	2.069407
C	-1.220761	-2.110585	1.567015
H	-1.119991	-1.208379	0.955469
H	-2.178136	-2.586533	1.327841
H	-1.235401	-1.817268	2.621876
C	-0.019313	-3.554113	-0.170361
H	0.823918	-4.231159	-0.332142
H	-0.949351	-4.074664	-0.421750
H	0.087199	-2.696460	-0.841225

E = -691.713991731
G = -691.494953
E + ΔG_{solv} = -691.706323

tBuOH·6H_2O-B3LYP

O	-0.539286	0.997674	0.188822
H	0.326303	1.349003	-0.224304
H	-0.020740	-0.760783	0.746205
H	-1.242643	1.155341	-0.453014
O	3.106904	-0.093581	0.727038
H	2.529401	-0.857037	0.564541
O	0.484955	-1.484904	1.170582
O	1.742066	1.877318	-0.636034
H	1.888461	2.718183	-0.154934
H	2.372049	1.224938	-0.244150
H	2.902725	0.124038	1.660811
O	1.720737	0.148326	3.198311
H	1.151927	0.937558	3.195836
H	1.188211	-0.541005	2.759148
O	-0.110060	2.356840	2.526419
H	-0.873868	2.659174	3.032533
H	-0.451957	1.897533	1.720413
O	1.715294	4.032636	1.172408
H	1.115582	3.583565	1.801997
H	2.481091	4.331366	1.676933
C	-0.258809	-2.726536	1.101654
C	0.634592	-3.772971	1.771841
H	0.846771	-3.490739	2.808095
H	0.146009	-4.752578	1.774283
H	1.586642	-3.863556	1.239215
C	-1.582727	-2.564626	1.863912
H	-2.201159	-1.781990	1.409079
H	-2.158548	-3.496520	1.852313
H	-1.392979	-2.290225	2.906603
C	-0.511569	-3.080020	-0.371150
H	0.435652	-3.160896	-0.913557
H	-1.043137	-4.033901	-0.458820
H	-1.120914	-2.310291	-0.859068

E = -692.393067497
G = -692.155600
E + ΔG_{solv} = -692.385918

HOOH·6H_2O-B3LYP

O	0.115941	2.219673	0.730372
H	0.909503	1.922958	0.218451
O	-0.982522	1.960242	-0.186055
H	-1.328364	1.049566	0.114461
O	2.173087	1.419799	-0.922999
H	2.955120	1.971690	-1.042153
H	1.686826	1.410677	-1.771352
H	-0.682739	2.050501	3.833130
O	-0.245953	1.341009	3.347496
H	-0.116414	1.674425	2.432539
H	-1.678081	-0.809436	1.212044
O	-1.850549	-0.418248	0.325485
H	-1.439279	-0.988578	-0.355148
H	-1.914035	-1.470583	3.510799
O	-1.239296	-1.177605	2.887821
H	-0.897937	-0.313327	3.213908
H	-0.452679	1.646199	-1.800948
O	0.002032	1.270242	-2.601630
H	-0.363503	1.707609	-3.380206
H	0.291321	-1.957011	-1.851880
O	-0.531703	-1.460655	-1.935928
H	-0.292790	-0.593967	-2.319225

E = -610.254681483
G = -610.121954
E + ΔG_{solv} = -610.255567

$OH^{\bullet}$·6H_2O-B3LYP

O	-0.832864	0.750481	0.595091
H	-0.023456	0.950783	0.010633
H	-0.528251	-0.830233	1.510328
H	-1.613808	0.848124	0.036521
O	3.330499	0.236830	0.637938
H	3.847507	-0.552693	0.442634
O	-0.123439	-1.494066	2.106787
H	-0.838922	-1.968175	2.545080
O	1.298863	1.389386	-0.731012
H	1.468037	2.329586	-0.537528
H	2.079753	0.903569	-0.365644
H	2.945681	0.124519	1.544074
O	1.996546	0.090792	3.001589
H	1.527548	0.938271	3.082607
H	1.290181	-0.572130	2.854665
O	0.129415	2.398132	2.558415
H	-0.461688	2.743230	3.238773
H	-0.409991	1.846623	1.941832
O	1.429113	3.990841	0.658672
H	1.035345	3.534537	1.450442

E = -534.433998046
G = -534.315335
E + ΔG_{solv} = -534.432573

OH^{-}·6H_2O-B3LYP

O	-0.697556	0.644751	0.882163
H	0.530570	1.094646	-0.323206
H	-0.141835	-0.621436	1.366722
H	-1.588113	0.659470	0.514843
O	2.962668	-0.516180	0.807501
H	2.167805	-1.071957	0.920561
O	0.420318	-1.419729	1.757842
H	-0.155468	-2.189223	1.812408
O	1.328580	1.356035	-0.850489
H	1.429834	3.195288	-0.225529
H	2.041131	0.818211	-0.458769
H	2.978504	-0.028019	1.651534
O	1.930927	0.384768	3.445168
H	1.409848	1.185043	3.224171
H	1.362708	-0.346839	3.139012
O	0.135168	2.411751	2.507089
H	-0.562577	2.690754	3.110183
H	-0.296028	1.737000	1.847545
O	1.333095	4.008448	0.311702
H	0.956487	3.665628	1.141443

E = -534.591867843
G = -534.472479
E + ΔG_{solv} = -534.650412

$H_2O \cdot 6H_2O$-B3LYP

O	-0.833215	0.743681	0.598063
H	-0.022830	0.930396	0.004905
H	-0.546130	-0.836791	1.498641
H	-1.616433	0.868726	0.048275
O	3.342235	0.215484	0.674053
H	3.853920	-0.581483	0.495408
O	-0.152905	-1.517269	2.085595
H	-0.877457	-1.972390	2.529086
O	1.289084	1.351655	-0.739580
H	1.457938	2.284515	-0.489613
H	2.059987	0.854570	-0.376801
H	2.931484	0.104690	1.569102
O	1.964547	0.055924	3.015084
H	1.486206	0.899700	3.091456
H	1.264147	-0.610121	2.854034
O	0.166700	2.370464	2.574316
H	-0.441204	2.763177	3.212440
H	-0.374806	1.846686	1.935911
O	1.574717	3.820903	0.588616
H	1.164509	3.470569	1.404709
H	2.475694	4.077262	0.820054

E = -535.131301537
G = -534.998444
E + ΔG_{solv} = -535.131371

$H_3O^+ \cdot 6H_2O$-B3LYP

O	-1.090631	0.647939	0.542085
H	0.411561	1.101937	-0.644062
H	-0.476519	-1.077010	1.075801
H	-2.006399	0.741303	0.245033
O	2.374414	-0.392438	0.872326
H	1.595964	-1.029224	1.083767
O	0.246472	-1.662351	1.382210
H	0.009851	-2.584019	1.215833
O	1.375730	1.204138	-0.773850
H	1.594591	2.126580	-0.539329
H	2.033765	0.257067	0.114132
H	2.549073	0.180740	1.674940
O	2.556854	1.439959	2.775768
H	1.639257	1.692000	3.009398
H	3.058407	1.337563	3.596862
O	-0.036383	2.496948	2.415628
H	-0.578477	2.983248	3.052894
H	-0.950990	1.293268	1.267998
O	1.956094	3.567524	0.762440
H	0.422868	3.158935	1.857734
H	2.681805	3.253078	1.327848
H	2.212347	4.441180	0.433517

E = -535.503712229
G = -535.356625
E + ΔG_{solv} = -535.563069

$6H_2O$-B3LYP

O	-0.664418	1.092432	0.627335
H	-0.035488	0.899801	-0.130878
H	-0.468290	-0.317231	1.833985
H	-1.528183	1.263563	0.233117
O	3.213965	-0.374012	0.035423
H	3.528612	-1.282856	-0.031064
O	-0.097167	-0.973650	2.459588
H	-0.737478	-1.083791	3.171631
O	1.094364	0.559037	-1.274132
H	1.428075	1.303783	-1.788942
H	1.894188	0.146997	-0.842926
H	3.025186	-0.198672	0.999544
O	2.476484	0.176702	2.547022
H	2.186610	1.110259	2.553877
H	1.651532	-0.330575	2.687955
O	1.105939	2.646708	2.185753
H	0.739464	3.233477	2.856981
H	0.353414	2.277419	1.681108

E = -458.680465003
G = -458.571194
E + ΔG_{solv} = -458.682190

CH_3CN-B3LYP

C	-1.642132	1.099995	-0.020948
N	-0.481021	1.100009	-0.020949
C	-3.103864	1.099991	-0.020937
H	-3.480708	2.111643	-0.197480
H	-3.480715	0.441291	-0.808785
H	-3.480738	0.747071	0.943438

E = -132.762593588
G = -132.741371
E + ΔG_{solv} = -132.764232

cis-stilbene-B3LYP

C	3.293278	1.508159	-1.096767
C	4.565880	1.073922	-0.725928
C	4.863392	0.815105	0.616816
C	3.878015	1.009266	1.588815
C	2.607443	1.453376	1.217809
C	2.284341	1.691335	-0.131742
H	3.079945	1.718672	-2.139394
H	5.330905	0.944928	-1.486703
H	5.855489	0.477160	0.902314
H	4.099786	0.822558	2.635933
H	1.848410	1.611396	1.980280
C	0.936973	2.196477	-0.465064
H	0.515224	2.855710	0.293584
C	0.164583	1.990318	-1.554249
H	-0.759524	2.566981	-1.592597
C	0.351857	1.087760	-2.708512
C	0.924449	-0.193312	-2.592212
C	-0.130344	1.485839	-3.969917
C	1.037096	-1.028833	-3.703471
H	1.271182	-0.537315	-1.623513
C	-0.009146	0.654223	-5.084812
H	-0.596787	2.462486	-4.074995
C	0.578387	-0.607502	-4.956682
H	1.476829	-2.015927	-3.589463
H	-0.379534	0.988501	-6.049988
H	0.667879	-1.260470	-5.820157

E = -540.730446613
G = -540.554150
E + ΔG_{solv} = -540.723266

Benzophenone-B3LYP

C	-1.096244	1.118413	0.229627

C	-1.919878	0.222749	0.917756
C	-1.364763	-0.856723	1.609561
C	0.023028	-1.033730	1.617296
C	0.846142	-0.136723	0.934770
C	0.292637	0.940780	0.225951
H	-1.522168	1.964679	-0.298176
H	-2.996085	0.371813	0.915259
H	-2.006204	-1.552074	2.143419
H	0.463429	-1.867428	2.156992
H	1.925015	-0.274648	0.949795
C	1.206550	1.886917	-0.481027
C	1.407076	1.931366	-1.960975
C	0.724578	1.033479	-2.939416
C	1.473803	0.031186	-3.575054
C	-0.630159	1.180121	-3.262096
C	0.873645	-0.824351	-4.500173
H	2.530578	-0.080363	-3.342543
C	-1.229503	0.326461	-4.192654
H	-1.203464	1.970527	-2.790497
C	-0.482733	-0.679681	-4.810858
H	1.463754	-1.599753	-4.980571
H	-2.280852	0.451196	-4.436687
H	-0.950565	-1.342075	-5.533580
O	0.633649	2.928448	-1.281287
H	2.385459	2.290550	-2.289655
H	2.059462	2.218186	0.116764

E = -615.931503868
G = -615.751802
E + ΔG_{solv} = -615.926701

1-OPBE

C	0.495800	0.904426	0.228000
C	0.392649	0.868655	2.866808
C	1.044191	1.383623	1.577669
H	0.595897	-0.182694	0.119154
H	1.091865	1.376584	-0.567802
H	0.921071	1.321465	3.720366
H	0.490771	-0.220456	2.956558
H	1.037965	2.484988	1.591362
H	2.106480	1.104160	1.616128
C	-4.477221	0.864765	0.034000
C	-4.580646	0.826029	2.655986
C	-5.282959	0.599372	1.311568
H	-5.157410	0.808616	-0.832776
H	-4.065903	1.883686	0.048984
H	-5.326281	0.744121	3.464789
H	-4.170034	1.844451	2.704873
H	-6.151394	1.272922	1.286724
H	-5.702910	-0.417703	1.280696
Ni	-2.085457	0.216949	1.433928
N	-0.931883	1.268186	0.069787
N	-1.046608	1.221320	2.923803
N	-3.486642	-0.145875	2.880947
N	-3.365168	-0.097595	-0.137035
H	-3.891204	-1.084412	2.821037
H	-3.763680	-1.039968	-0.142445
H	-1.106787	2.213809	2.689454
H	-1.009560	2.251333	0.337739
C	-2.776264	-0.075301	4.176060
C	-1.754608	1.063311	4.219778
C	-2.552711	0.023538	-1.367051
C	-1.536401	1.164242	-1.282454
H	-3.186218	0.159085	-2.258381
H	-2.037264	-0.937086	-1.486432
H	-0.765331	1.024670	-2.052161
H	-2.017849	2.124478	-1.504131
H	-2.248223	2.015921	4.446112
H	-1.045586	0.886441	5.039687
H	-2.272709	-1.042058	4.298879
H	-3.480068	0.027425	5.017744
N	-4.936054	-3.060431	3.492870
C	-5.639553	-3.849629	3.998131
C	-6.512520	-4.824592	4.625874
H	-6.249893	-5.837467	4.296580
H	-6.414429	-4.772033	5.717269
H	-7.556973	-4.624990	4.355977
N	-4.547931	-3.084191	-1.089486
C	-5.126026	-3.856526	-1.754844
C	-5.842952	-4.810686	-2.581045
H	-6.144201	-4.340516	-3.525382
H	-5.204102	-5.673636	-2.806047
H	-6.741946	-5.162350	-2.060016
N	0.232125	4.282633	5.085016
N	0.988581	4.279347	-1.770141
C	0.690582	4.969060	5.917555
C	1.659958	4.938730	-2.469422
C	1.259486	5.817652	6.950188
H	2.073679	6.425088	6.536138
H	0.491623	6.486866	7.357558
H	1.659444	5.203996	7.766816
C	2.492506	5.753535	-3.337243
H	3.271380	5.136908	-3.802595
H	1.884343	6.208312	-4.128856
H	2.975054	6.551975	-2.760197
N	-1.357580	-1.604893	1.437222
N	-2.140173	4.146479	1.395942
C	-2.143607	5.318078	1.394670
C	-1.076643	-2.738968	1.428991
C	-2.144780	6.767850	1.393793
H	-1.746593	7.142326	2.344921
H	-1.518225	7.140986	0.574207
H	-3.165729	7.146805	1.261621
C	-0.734712	-4.144124	1.414787
H	-0.718725	-4.537402	2.439309
H	-1.481946	-4.698077	0.832048
H	0.254235	-4.289777	0.961608

E = -2918.81663623
G = -2918.293139
E + ΔG_{solv} = -2918.912773

2-OPBE

C	0.620369	0.539972	0.327839
C	0.408572	0.549568	2.943753
C	1.245884	0.837674	1.693976
H	0.433303	-0.525978	0.172318
H	1.328739	0.870148	-0.447877
H	0.982186	0.886460	3.821223
H	0.199337	-0.515517	3.074633
H	1.570427	1.888180	1.716126
H	2.167995	0.245269	1.770284
C	-4.468736	0.957850	-0.087455
C	-4.680478	0.967550	2.528478
C	-5.306247	0.670361	1.162336
H	-5.042491	0.621227	-0.964941
H	-4.258864	2.022801	-0.218391
H	-5.389005	0.637723	3.304204
H	-4.492762	2.033372	2.684080
H	-6.227903	1.263478	1.086058
H	-5.631528	-0.379912	1.140195
Ni	-2.030191	0.753258	1.428161
N	-0.642511	1.295118	0.137556
N	-0.867789	1.304752	2.920519

N	-3.418052	0.211607	2.718589
N	-3.192800	0.201941	-0.064052
H	-3.665357	-0.776371	2.562757
H	-3.461067	-0.783582	0.062297
H	-0.600006	2.290441	2.794465
H	-0.395810	2.283243	0.293165
C	-2.777439	0.227752	4.071676
C	-1.716216	1.299779	4.153293
C	-2.344312	0.206262	-1.296751
C	-1.283038	1.278293	-1.215590
H	-2.969658	0.344705	-2.189530
H	-1.897645	-0.790870	-1.371763
H	-0.522978	1.135175	-1.996058
H	-1.713745	2.273851	-1.366978
H	-2.162903	2.296858	4.228840
H	-1.090826	1.160938	5.045972
H	-2.346696	-0.767877	4.222509
H	-3.537454	0.370431	4.852275
N	-4.680027	-2.587701	3.372581
C	-5.365806	-3.372360	3.910194
C	-6.213542	-4.341248	4.576926
H	-6.421879	-5.186963	3.909597
H	-5.719422	-4.717478	5.481708
H	-7.165358	-3.875988	4.863333
N	-4.334285	-2.617048	-0.957484
C	-4.917580	-3.380187	-1.630351
C	-5.638464	-4.321898	-2.464498
H	-5.117082	-4.456549	-3.420742
H	-5.713019	-5.295064	-1.963092
H	-6.651544	-3.950366	-2.664573
N	0.271446	4.123280	3.816262
N	0.618785	4.094855	-0.520012
C	0.852572	4.886988	4.490357
C	1.303207	4.878705	-1.060538
C	1.570282	5.829987	5.325745
H	2.011448	6.624030	4.710227
H	0.888531	6.284941	6.055526
H	2.374933	5.317332	5.868105
C	2.149269	5.846557	-1.730908
H	3.102822	5.382512	-2.013485
H	1.655485	6.216810	-2.638334
H	2.354202	6.696268	-1.067610
N	-1.464970	-1.410647	1.477510
N	-2.594935	2.918158	1.378713
C	-2.714387	4.082368	1.369542
C	-1.344478	-2.574739	1.486465
C	-2.877665	5.517454	1.360368
H	-2.042299	5.984125	1.898068
H	-2.890436	5.886734	0.326499
H	-3.821227	5.793595	1.849802
C	-1.179860	-4.009671	1.495319
H	-1.172571	-4.379824	2.528927
H	-2.011730	-4.476647	0.952501
H	-0.233312	-4.284495	1.010930

E = -2918.40913955
G =
E + ΔG_{solv} = -2918.711106

3-OPBE-doublet

C	0.637698	0.482870	0.377954
C	0.398790	0.522564	2.958125
C	1.295898	0.722694	1.736671
H	0.277993	-0.550011	0.290512
H	1.384349	0.644249	-0.415905
H	0.985187	0.716987	3.869995
H	0.031969	-0.510177	3.013705
H	1.736351	1.730127	1.762450
H	2.139531	0.024847	1.825581
C	-4.275520	0.825112	-0.082430
C	-4.510604	0.842385	2.500055
C	-5.097990	0.447338	1.147242
H	-4.790411	0.458043	-0.981976
H	-4.135966	1.909329	-0.154227
H	-5.180338	0.487676	3.296898
H	-4.386208	1.927783	2.581221
H	-6.075541	0.939887	1.055191
H	-5.307758	-0.633972	1.135010
Ni	-1.886610	0.982641	1.434728
N	-0.497701	1.412780	0.160564
N	-0.759902	1.449714	2.931137
N	-3.177946	0.217141	2.699046
N	-2.930543	0.197932	-0.026893
H	-3.283353	-0.782253	2.501734
H	-3.071408	-0.796859	0.171356
H	-0.385921	2.405527	2.854625
H	-0.141239	2.371005	0.283598
C	-2.597788	0.302540	4.071743
C	-1.639224	1.467228	4.132029
C	-2.110715	0.249827	-1.273363
C	-1.138746	1.401916	-1.183137
H	-2.756276	0.345228	-2.155991
H	-1.590982	-0.711446	-1.359508
H	-0.376825	1.350785	-1.974678
H	-1.661224	2.359864	-1.276642
H	-2.180916	2.418348	4.095906
H	-1.037779	1.451001	5.052511
H	-2.091933	-0.649393	4.270377
H	-3.393142	0.404318	4.821254
N	-4.883335	-2.602177	4.115611
C	-5.567221	-3.306542	4.756212
C	-6.415306	-4.176331	5.551628
H	-6.864219	-4.951396	4.918293
H	-5.827177	-4.661252	6.340561
H	-7.219689	-3.595221	6.019373
N	-4.525229	-2.597673	-1.722160
C	-5.157932	-3.260688	-2.453203
C	-5.942845	-4.079084	-3.360258
H	-5.297495	-4.514114	-4.133385
H	-6.432713	-4.892076	-2.810347
H	-6.714123	-3.469893	-3.847644
N	0.433119	4.247677	3.706239
N	0.719934	4.249392	-0.350823
C	0.827759	5.187453	4.283026
C	1.163085	5.219295	-0.834897
C	1.315636	6.350896	4.998959
H	2.358175	6.554085	4.724502
H	0.705336	7.228747	4.753074
H	1.263489	6.176936	6.080928
C	1.710689	6.420426	-1.435905
H	2.746395	6.569544	-1.106394
H	1.697350	6.334321	-2.529545
H	1.114834	7.293962	-1.143592
N	-1.605203	-2.692733	1.416524
C	-1.542125	-3.862871	1.400642
C	-1.466291	-5.310960	1.380244
H	-1.953380	-5.725101	2.271666
H	-1.970809	-5.699790	0.487060
H	-0.418689	-5.636356	1.365479
O	-2.672399	2.785117	1.345565
H	-2.025015	3.504053	1.378235

E = -2861.86954194

G = -2861.367376
E + ΔG_{solv} = -2861.978927

3-OPBE-quartet

C	0.815726	0.132880	0.787499
C	0.318975	0.443390	3.331450
C	1.338505	0.457391	2.188943
H	0.325992	-0.849602	0.783885
H	1.670947	0.063837	0.094566
H	0.851790	0.570352	4.288483
H	-0.201779	-0.522988	3.380092
H	1.868561	1.421659	2.181069
H	2.104642	-0.294297	2.425449
C	-4.036635	0.284679	-0.090642
C	-4.539886	0.794205	2.436851
C	-4.918981	0.070644	1.141933
H	-4.442997	-0.318684	-0.916293
H	-4.043075	1.335266	-0.404914
H	-5.282614	0.538222	3.208148
H	-4.543975	1.883505	2.307351
H	-5.932213	0.394891	0.866752
H	-5.005238	-1.008123	1.346935
Ni	-1.811417	1.192748	1.511568
N	-0.147204	1.137928	0.280038
N	-0.673530	1.527106	3.178863
N	-3.190571	0.370703	2.884790
N	-2.623824	-0.126294	0.140376
H	-3.179537	-0.647992	2.820467
H	-2.628742	-1.056794	0.573529
H	-0.154813	2.409418	3.074722
H	0.304466	2.053751	0.272823
C	-2.767413	0.704952	4.266818
C	-1.646633	1.744033	4.272653
C	-1.747269	-0.217199	-1.053788
C	-0.695447	0.893202	-1.072358
H	-2.341321	-0.178175	-1.975036
H	-1.269590	-1.204114	-1.037143
H	0.101193	0.634086	-1.787978
H	-1.140194	1.838742	-1.403833
H	-2.056946	2.748592	4.113227
H	-1.141285	1.745896	5.251250
H	-2.441585	-0.223932	4.749841
H	-3.612598	1.081559	4.857973
N	-4.809797	-2.427621	4.728930
C	-5.510079	-3.002076	5.473289
C	-6.378774	-3.711158	6.396096
H	-7.075089	-4.354162	5.843816
H	-5.783572	-4.335120	7.074142
H	-6.958895	-2.997248	6.993705
N	-4.293477	-2.176180	-3.128288
C	-4.772226	-2.710423	-4.055377
C	-5.365136	-3.371760	-5.204400
H	-4.584940	-3.842015	-5.815565
H	-6.069390	-4.145708	-4.874648
H	-5.905486	-2.643977	-5.822279
N	1.028624	4.144195	3.562872
N	-0.552087	4.695295	-0.349656
C	1.610310	5.038098	4.047201
C	-0.349543	5.711898	-0.895070
C	2.329997	6.144560	4.649091
H	3.144981	6.468703	3.990488
H	1.651251	6.989883	4.816825
H	2.756009	5.837332	5.612232
C	-0.099183	6.969562	-1.571291
H	0.970085	7.212179	-1.535647
H	-0.412679	6.902521	-2.620638
H	-0.663093	7.775375	-1.084583
N	-2.104986	-2.951907	1.483012
C	-2.162437	-4.114509	1.614878
C	-2.235755	-5.552868	1.779717
H	-3.079577	-5.811555	2.431258
H	-2.378210	-6.035994	0.805014
H	-1.309724	-5.930254	2.230652
O	-2.391010	2.846017	1.134008
H	-1.757733	3.476692	0.725990

E = -2861.84672411

4-OPBE-singlet

C	0.822253	0.217008	0.319916
C	0.556763	0.343959	2.927924
C	1.428696	0.550454	1.685973
H	0.618754	-0.849608	0.188956
H	1.554049	0.503632	-0.453232
H	1.122492	0.711759	3.798767
H	0.311778	-0.704901	3.116035
H	1.786029	1.590203	1.676593
H	2.330353	-0.065978	1.805442
C	-4.242970	1.022071	-0.220239
C	-4.497283	1.156881	2.375435
C	-5.131632	0.861698	1.014770
H	-4.828342	0.727805	-1.106895
H	-3.904302	2.052456	-0.358244
H	-5.246318	0.950984	3.157947
H	-4.183396	2.200204	2.475288
H	-5.980987	1.548098	0.895896
H	-5.566185	-0.148708	1.024106
Ni	-1.848999	0.590253	1.354757
N	-0.414056	0.995854	0.064532
N	-0.685342	1.147049	2.845350
N	-3.347154	0.265611	2.639372
N	-3.071682	0.120178	-0.159071
H	-3.693476	-0.701048	2.520699
H	-3.444558	-0.829844	-0.006214
H	-0.378136	2.117920	2.674591
H	-0.164097	1.993798	0.195434
C	-2.719287	0.289607	3.992558
C	-1.566856	1.265610	4.048102
C	-2.196719	-0.004674	-1.360276
C	-1.027166	0.953275	-1.300750
H	-2.783577	0.175704	-2.271941
H	-1.860592	-1.046307	-1.398843
H	-0.267339	0.669877	-2.042464
H	-1.342119	1.977699	-1.528150
H	-1.924281	2.299806	4.061235
H	-0.974348	1.107036	4.959299
H	-2.394986	-0.734234	4.208535
H	-3.471877	0.554364	4.748795
N	-4.697671	-2.404942	3.293092
C	-5.467976	-3.100721	3.838663
C	-6.419180	-3.959867	4.514456
H	-6.519979	-4.911791	3.977869
H	-6.082546	-4.164934	5.538802

H	-7.402199	-3.473389	4.557240
N	-4.283297	-2.642382	-0.872179
C	-4.912738	-3.384185	-1.527256
C	-5.688730	-4.300681	-2.338435
H	-5.049750	-4.766971	-3.099306
H	-6.124897	-5.088203	-1.710908
H	-6.501260	-3.762103	-2.842900
N	0.574216	3.795619	3.651971
N	-0.080523	3.947226	-0.118676
C	1.039049	4.664347	4.287006
C	0.261447	4.994139	-0.519110
C	1.613131	5.737622	5.073653
H	2.622235	5.973922	4.712847
H	0.988731	6.637032	4.999404
H	1.677628	5.439824	6.128017
C	0.683207	6.285776	-1.014296
H	1.756067	6.427506	-0.830028
H	0.496399	6.355159	-2.093839
H	0.125196	7.083089	-0.506257
N	-1.481498	-1.320853	1.487978
C	-1.403371	-2.484191	1.557063
C	-1.287681	-3.918394	1.640729
H	-1.333416	-4.236563	2.691124
H	-2.116547	-4.380886	1.088309
H	-0.333599	-4.247719	1.206438
O	-2.348991	2.332899	1.275391
H	-1.644584	2.919521	0.937670

E = -2861.43491722
G = -2860.914991
E + ΔG_{solv} = -2861.757796

4-OPBE-triplet

C	0.820139	0.028493	0.705379
C	0.285133	0.123220	3.232385
C	1.346587	0.146624	2.133356
H	0.290771	-0.919508	0.555443
H	1.671785	0.049360	0.005805
H	0.782479	0.231198	4.210725
H	-0.269241	-0.822682	3.245085
H	1.973152	1.043672	2.234804
H	2.018939	-0.705775	2.300870
C	-3.923858	0.850132	-0.368379
C	-4.485133	1.068581	2.163726
C	-4.907330	0.606729	0.772413
H	-4.347257	0.400371	-1.278862
H	-3.746735	1.915271	-0.554425
H	-5.265830	0.759650	2.875769
H	-4.364275	2.154979	2.237374
H	-5.838138	1.132236	0.518090
H	-5.169701	-0.460687	0.803653
Ni	-1.710157	0.998381	1.439003
N	-0.094727	1.146638	0.340045
N	-0.655630	1.256996	3.081142
N	-3.223263	0.413902	2.583111
N	-2.614023	0.179773	-0.127607
H	-3.357544	-0.594572	2.429768
H	-2.830939	-0.807195	0.072135
H	-0.083014	2.128457	3.007140
H	0.381191	2.030646	0.542829
C	-2.820484	0.546849	4.024492
C	-1.657008	1.502186	4.155155
C	-1.648711	0.154583	-1.276839
C	-0.564425	1.189559	-1.075390
H	-2.183959	0.333843	-2.217662
H	-1.240205	-0.860132	-1.329811
H	0.279534	1.015269	-1.760006
H	-0.935945	2.202776	-1.261676
H	-1.982678	2.542760	4.040036
H	-1.176841	1.409419	5.140754
H	-2.565976	-0.458455	4.377266
H	-3.672871	0.892491	4.621733
N	-5.057335	-2.056916	3.672225
C	-5.837149	-2.717063	4.249080
C	-6.799860	-3.529906	4.966269
H	-7.405004	-4.113015	4.260768
H	-6.283334	-4.219704	5.645126
H	-7.469241	-2.890737	5.555834
N	-3.998513	-2.399404	-1.429409
C	-4.550558	-3.152201	-2.139257
C	-5.235764	-4.079908	-3.018330
H	-4.726133	-4.127494	-3.989988
H	-5.247122	-5.084889	-2.576280
H	-6.271898	-3.753275	-3.178984
N	1.073186	3.612216	3.263187
N	-1.198963	4.776353	-0.009567
C	1.774667	4.425541	3.732129
C	-1.156382	5.866109	-0.435636
C	2.640084	5.429096	4.314205
H	3.184564	5.964032	3.525484
H	2.044956	6.150318	4.888998
H	3.366912	4.954212	4.986002
C	-1.095436	7.207963	-0.967534
H	-0.052751	7.548196	-1.016067
H	-1.525054	7.231584	-1.977661
H	-1.665352	7.890508	-0.323233
N	-1.582639	-2.554395	1.663207
C	-1.539103	-3.724228	1.737609
C	-1.488312	-5.168936	1.832155
H	-2.502461	-5.584157	1.772964
H	-0.887436	-5.582180	1.011695
H	-1.037366	-5.470987	2.786290
O	-2.234112	2.757473	1.332292
H	-1.720927	3.490208	0.822115

E = -2861.40966353
G = -2860.898557
E + ΔG_{solv} = -2861.725919

tBuOOH-6H_2O-OPBE

O	-0.264827	0.308031	-0.122845
H	-0.324731	0.731136	0.768672
O	-1.660101	0.088847	-0.414621
O	-0.264249	1.684687	2.316986
H	-0.158100	2.641086	2.115310
H	0.435964	1.481477	2.945404
H	0.247102	6.834305	3.292859
O	-0.689054	6.615169	3.444123
H	-1.174970	7.417704	3.228066
H	-0.518775	4.995654	2.144854
O	0.046947	4.396472	1.627145
H	-0.247699	4.499878	0.693630
H	1.617466	5.586720	2.020697
O	2.037111	6.380022	2.403685
H	2.798120	6.053900	2.895022
H	-1.896739	1.645238	-1.654560
O	-2.084646	2.466203	-2.144087
H	-3.043430	2.552947	-2.114177
H	-0.113974	4.949940	-1.650716
O	-0.796023	4.704771	-1.016875
H	-1.229394	3.914504	-1.406262
C	-1.936636	-1.332111	-0.512015
C	-1.105629	-1.962111	-1.633248

H	-1.358460	-3.023958	-1.747719
H	-1.294671	-1.457852	-2.589026
H	-0.036344	-1.886198	-1.408999
C	-1.682920	-2.015052	0.834362
H	-2.265108	-1.533504	1.629642
H	-1.970358	-3.072918	0.786104
H	-0.621309	-1.964105	1.099942
C	-3.429487	-1.336981	-0.857105
H	-3.784681	-2.370762	-0.943805
H	-4.015402	-0.837984	-0.075353
H	-3.617214	-0.834820	-1.814282

E = -767.118233354
G = -766.891854
E + ΔG_{solv} = -767.110221

tBuOH-6H_2O-OPBE

O	-0.380557	0.907259	-0.044785
H	0.490511	1.330274	-0.316931
H	0.018570	-1.020835	0.567494
H	-0.976459	1.080041	-0.781675
O	3.892172	0.863639	0.996140
H	4.551036	0.244458	0.666249
O	0.455368	-1.763541	1.022206
O	1.908778	2.132896	-0.616776
H	1.836774	2.972810	-0.126189
H	2.649921	1.666694	-0.177843
H	3.381561	0.363282	1.669975
O	2.224597	-0.459713	2.855548
H	1.674020	0.205972	3.283995
H	1.598253	-0.978343	2.310808
O	-0.461017	2.341586	2.451076
H	-1.341443	2.596507	2.746082
H	-0.601585	1.836235	1.624234
O	1.334430	4.319916	1.267594
H	0.732842	3.770627	1.804193
H	2.055377	4.556302	1.860688
C	-0.464057	-2.861947	1.141593
C	0.332885	-3.989340	1.801547
H	0.698921	-3.680881	2.788591
H	-0.290005	-4.882666	1.931028
H	1.199678	-4.258471	1.185525
C	-1.658672	-2.456066	2.018942
H	-2.214499	-1.623946	1.566368
H	-2.357675	-3.292624	2.149109
H	-1.318109	-2.138272	3.012359
C	-0.936220	-3.283319	-0.257794
H	-0.076798	-3.537405	-0.890251
H	-1.599045	-4.156877	-0.206948
H	-1.492573	-2.472921	-0.748190

E = -692.027253328
G = -691.798672
E + ΔG_{solv} = -692.017105

tBuO$^{\bullet}$-6H_2O-OPBE

O	-0.908359	1.580671	-0.035842
H	-0.065191	1.912795	-0.449483
H	-1.610446	2.049468	-0.499062
O	3.464315	1.006147	0.385988
H	3.980548	0.278352	0.025921
O	1.036188	-2.665599	1.663985
O	1.447860	2.607140	-0.913029
H	1.539470	3.370325	-0.316487
H	2.168062	2.011885	-0.626123
H	3.030810	0.644203	1.189230
O	2.037658	0.110870	2.674037
H	1.288856	0.725450	2.753011
H	1.636165	-0.754138	2.506840
O	-0.169434	2.167967	2.550555
H	-0.902599	2.250027	3.169017
H	-0.577477	1.961255	1.673655
O	1.445574	4.458179	1.461059
H	0.948182	3.811439	1.990184
H	2.304570	4.520517	1.892561
C	-0.117543	-3.306003	1.321928
C	-0.126123	-4.525650	2.317523
H	-0.149876	-4.172416	3.353550
H	-1.032430	-5.107249	2.107033
H	0.759080	-5.150762	2.164005
C	-1.369098	-2.438521	1.557157
H	-1.333924	-1.551879	0.912775
H	-2.287821	-2.993972	1.329168
H	-1.414689	-2.103554	2.600461
C	-0.044171	-3.840888	-0.125119
H	0.847151	-4.463934	-0.260238
H	-0.935093	-4.432058	-0.371675
H	0.014797	-2.997341	-0.823788

E = -691.349487358
G = -691.137354
E + ΔG_{solv} = -691.339864

CH_3CN-OPBE

C	-1.647814	1.100008	-0.020932
N	-0.475984	1.099996	-0.020979
C	-3.101857	1.099997	-0.020916
H	-3.481164	2.114173	-0.197928
H	-3.481137	0.439645	-0.810749
H	-3.481222	0.746181	0.945844

E = -132.703196577
G = -132.682621
E + ΔG_{solv} = -132.704546

6H_2O-OPBE

O	-0.738296	1.107760	0.572109
H	-0.106768	0.910569	-0.169352
H	-0.512277	-0.410338	1.856333
H	-1.590144	1.245993	0.145126
O	3.276332	-0.371869	0.015599
H	3.527395	-1.299250	-0.045446
O	-0.147606	-1.065284	2.479066
H	-0.780353	-1.111470	3.202859
O	1.088169	0.530620	-1.364231
H	1.433716	1.285370	-1.852867
H	1.880162	0.150470	-0.907295
H	3.088963	-0.214966	0.974625
O	2.549119	0.131066	2.631606
H	2.274454	1.062526	2.651713
H	1.711556	-0.353510	2.741602
O	1.118706	2.782630	2.240586
H	0.715984	3.349071	2.906369
H	0.377699	2.420004	1.726974

E = -458.430321304
G = -458.324508
E + ΔG_{solv} = -458.429634

H_2O-6H_2O-OPBE

O	-0.749662	0.790097	0.691191

H	0.125493	1.027084	0.242812
H	-0.413092	-0.451789	2.034605
H	-1.305822	0.434635	-0.010720
O	3.649819	-0.010845	0.628402
H	4.100972	-0.557924	-0.022917
O	-0.196955	-1.093965	2.744033
H	-0.546397	-0.697353	3.548792
O	1.514510	1.524706	-0.406157
H	1.647099	2.446219	-0.113512
H	2.285535	1.020361	-0.069654
H	3.300128	-0.644380	1.292324
O	2.545249	-1.791268	2.503866
H	2.933370	-1.793627	3.384656
H	1.596401	-1.583742	2.640809
O	-1.122699	3.385710	1.908235
H	-1.922724	3.837767	1.620518
H	-1.165037	2.499460	1.497544
O	1.367967	4.213341	0.710325
H	0.529442	4.069548	1.191342
H	1.992593	4.516314	1.377259

E = -534.839401647
G = -534.713237
E + ΔG_{solv} = -534.838387

HOOH-6H_2O-OPBE

O	0.064076	2.288563	0.711012
H	0.866082	2.020702	0.205405
O	-1.003590	1.984027	-0.201669
H	-1.324559	1.078624	0.110091
O	2.297075	1.554799	-0.930251
H	2.985487	2.217173	-1.052773
H	1.829341	1.502476	-1.781326
H	-0.690866	2.086478	3.917099
O	-0.200387	1.382636	3.479734
H	-0.098510	1.689715	2.559347
H	-1.709254	-0.822817	1.218887
O	-1.915568	-0.442175	0.340878
H	-1.516539	-1.033128	-0.320941
H	-1.928641	-1.492035	3.576902
O	-1.221586	-1.239065	2.974699
H	-0.889266	-0.381339	3.308331
H	-0.432509	1.621619	-1.913251
O	0.028568	1.259782	-2.705344
H	-0.353067	1.715917	-3.462924
H	0.236867	-2.128239	-1.942382
O	-0.583827	-1.630974	-2.024821
H	-0.321336	-0.777561	-2.407722

E = -609.922745474
G = -609.793950
E + ΔG_{solv} = -609.921061

$OH^{\bullet}$-6H_2O-OPBE

O	-0.760844	0.794574	0.713085
H	0.116195	1.073767	0.303968
H	-0.375958	-0.408942	2.108208
H	-1.261047	0.392631	-0.005686
O	3.669735	0.124707	0.659036
H	4.149596	-0.356796	-0.022849
O	-0.118757	-1.015259	2.833338
H	-0.343886	-0.540069	3.640176
O	1.526537	1.642140	-0.288994
H	1.645413	2.558150	0.008579
H	2.313186	1.145255	0.030122
H	3.329253	-0.567097	1.267736
O	2.560945	-1.821455	2.348499
H	2.984692	-2.015263	3.190680
H	1.637419	-1.578490	2.572329
O	-1.323297	3.350557	1.879905
H	-2.187989	3.728371	1.689434
H	-1.318313	2.464222	1.465928
O	1.076754	4.487968	0.881073
H	0.226431	4.199438	1.307331

E = -534.137442024
G = -534.025859
E + ΔG_{solv} = -534.134554

OH^--6H_2O-OPBE

O	-0.380279	0.633255	0.773997
H	-0.487498	1.549043	-0.502519
H	0.374616	-0.700325	0.678675
H	-1.269881	0.412359	1.073607
O	2.932009	-1.616057	2.571342
H	2.209441	-1.645242	1.901975
O	0.893852	-1.592990	0.617023
H	1.277441	-1.585029	-0.265879
O	-0.495095	2.175854	-1.313484
H	0.898415	3.449909	-0.651631
H	-0.124269	1.641591	-2.023220
H	3.189939	-0.687724	2.575802
O	1.325744	0.701815	4.940723
H	1.143230	1.189644	4.109541
H	1.555825	-0.181806	4.631278
O	0.788918	2.137882	2.494122
H	0.150802	2.833315	2.686001
H	0.297930	1.520684	1.822079
O	1.602084	3.946129	-0.190365
H	1.662841	3.476108	0.652825

E = -534.290839522
G = -534.182497
E + ΔG_{solv} = -534.341904

H_3O^+-6H_2O-OPBE

O	-1.262167	1.997179	1.508886
H	-0.085912	1.597665	0.615213
H	1.736154	-3.300526	-0.259837
H	-2.150876	1.840104	1.170914
O	2.246730	-0.204336	1.153625
H	2.279429	-1.119926	0.797937
O	2.413434	-2.814243	0.223993
H	3.254776	-3.179871	-0.072940
O	0.685078	1.263567	0.033053
H	1.155933	2.033419	-0.377583
H	1.385257	0.589489	0.576883
H	2.185344	-0.264078	2.133930
O	2.107248	-0.235582	3.915480
H	1.554873	-0.847981	4.415303
H	2.922942	-0.155239	4.423863
O	-1.195341	4.520392	2.712428
H	-1.357852	4.622585	3.657356
H	-1.273163	2.890264	1.915184
O	1.870591	3.385623	-1.142844
H	-1.474740	5.352254	2.313187
H	2.713326	3.759377	-0.859587
H	1.868593	3.448227	-2.105471

E = -535.225469727
G = -535.099010
E + ΔG_{solv} = -535.278572

cis-stilbene-OPBE

C	3.318523	1.553783	-1.090235
C	4.594299	1.127541	-0.715816
C	4.881947	0.837281	0.623604
C	3.882546	0.994221	1.590340
C	2.609160	1.431310	1.217692
C	2.293952	1.699447	-0.131688
H	3.114514	1.792939	-2.132554
H	5.372294	1.030057	-1.474309
H	5.879463	0.504555	0.912494
H	4.096312	0.782560	2.638833
H	1.838602	1.557286	1.980238
C	0.948670	2.193535	-0.468109
H	0.518610	2.855703	0.289337
C	0.169463	1.980675	-1.560102
H	-0.755716	2.563821	-1.593353
C	0.345645	1.078081	-2.709879
C	0.883040	-0.220586	-2.589238
C	-0.111947	1.487726	-3.980604
C	0.985227	-1.059522	-3.700655
H	1.206885	-0.577420	-1.612990
C	0.000480	0.652226	-5.094454
H	-0.550540	2.480575	-4.094629
C	0.553199	-0.626299	-4.960316
H	1.396935	-2.062611	-3.580473
H	-0.350480	0.998143	-6.067583
H	0.634927	-1.284214	-5.826165

E = -540.500555740
G = -540.327375
E + ΔG_{solv} = -540.493667

Benzophenone-OPBE

C	-1.112965	1.176784	0.331229
C	-1.924496	0.282040	1.036806
C	-1.367744	-0.845866	1.647637
C	0.011049	-1.071240	1.555901
C	0.823185	-0.175651	0.856153
C	0.267403	0.951660	0.226109
H	-1.545359	2.060709	-0.134857
H	-2.996147	0.471078	1.112511
H	-2.001761	-1.542899	2.196570
H	0.455613	-1.946060	2.032037
H	1.897866	-0.356710	0.794058
C	1.171664	1.900754	-0.487945
C	1.379445	1.941409	-1.964597
C	0.719606	1.034111	-2.947922
C	1.489504	0.031626	-3.563935
C	-0.630385	1.167403	-3.304719
C	0.915046	-0.835458	-4.496382
H	2.545794	-0.073550	-3.308957
C	-1.203023	0.302360	-4.242912
H	-1.225192	1.957723	-2.850913
C	-0.436192	-0.704149	-4.838244
H	1.524356	-1.612470	-4.959667
H	-2.253485	0.419714	-4.512430
H	-0.885156	-1.377584	-5.569042
O	0.609030	2.932102	-1.291464
H	2.367522	2.299102	-2.284160
H	2.031011	2.232387	0.111077

E = -615.675921028
G = -615.500244
E + ΔG_{solv} = -615.670731

1-BLYP

C	0.691566	0.519120	0.290306
C	0.484789	0.542025	2.981666
C	1.291123	0.868981	1.687148
H	0.467280	-0.553289	0.211603
H	1.448711	0.762634	-0.478511
H	1.112707	0.808674	3.852391
H	0.258246	-0.531025	3.050146
H	1.542691	1.945858	1.697213
H	2.255348	0.338780	1.765708
C	-4.546073	0.965143	-0.123219
C	-4.752791	0.988314	2.568151
C	-5.352632	0.638834	1.171330
H	-5.174058	0.698664	-0.993949
H	-4.318965	2.038058	-0.191860
H	-5.510033	0.745187	3.336997
H	-4.527876	2.060587	2.646875
H	-6.316477	1.169724	1.092759
H	-5.604933	-0.437872	1.161360
Ni	-2.030719	0.753171	1.429309
N	-0.568132	1.295730	0.032361
N	-0.803979	1.314020	3.026331
N	-3.493551	0.210915	2.825956
N	-3.257702	0.192465	-0.167652
H	-3.739713	-0.780896	2.695650
H	-3.518939	-0.797954	-0.060832
H	-0.543259	2.304599	2.919862
H	-0.322580	2.287692	0.162425
C	-2.843515	0.272525	4.186906
C	-1.654622	1.270410	4.272042
C	-2.406993	0.235432	-1.413270
C	-1.218157	1.233452	-1.328605
H	-3.015062	0.479698	-2.302398
H	-2.029193	-0.787649	-1.555216
H	-0.481388	0.978270	-2.110949
H	-1.569678	2.254101	-1.539439
H	-2.032225	2.293472	4.414613
H	-1.046479	1.025596	5.160965
H	-2.492016	-0.748249	4.397201
H	-3.580243	0.527334	4.969415
N	-4.483685	-2.795741	3.544260
C	-5.186206	-3.511709	4.154471
C	-6.062024	-4.407003	4.918822
H	-6.365860	-5.264183	4.297880
H	-5.535881	-4.783037	5.810170
H	-6.965746	-3.867522	5.242856
N	-4.118207	-2.808757	-1.072556
C	-4.716535	-3.487847	-1.820539
C	-5.462710	-4.335728	-2.757169
H	-4.924152	-4.408682	-3.714956
H	-5.584018	-5.348021	-2.341052
H	-6.460430	-3.908298	-2.943299
N	0.056632	4.315460	3.930661
N	0.419718	4.304342	-0.691615
C	0.654515	4.996247	4.677445
C	1.121349	5.018083	-1.305467
C	1.399878	5.846904	5.612202
H	1.876100	6.680013	5.072115
H	0.720676	6.259950	6.374343
H	2.182789	5.259729	6.117244
C	1.995998	5.910629	-2.074361
H	2.899251	5.370013	-2.397810
H	1.468488	6.283452	-2.966251
H	2.300735	6.770061	-1.456981
N	-1.498572	-1.381903	1.482192
N	-2.562459	2.888868	1.375991
C	-2.527027	4.059633	1.384306

C	-1.532145	-2.552699	1.472286
C	-2.472554	5.520545	1.397038
H	-2.017724	5.859051	2.340961
H	-1.851684	5.868223	0.556846
H	-3.484757	5.944356	1.304922
C	-1.583528	-4.013703	1.457341
H	-2.191185	-4.365074	2.305609
H	-2.051043	-4.351187	0.519251
H	-0.569066	-4.435238	1.533818

E = -2918.54520237
G = -2918.023931
E + ΔG_{solv} = -2918.641267

3-BLYP-doublet

C	0.661947	0.324475	0.308644
C	0.402577	0.425772	2.923974
C	1.314082	0.603954	1.684983
H	0.299825	-0.711911	0.242848
H	1.412459	0.482022	-0.486499
H	0.983935	0.651524	3.834950
H	0.020868	-0.603046	2.997270
H	1.734312	1.624969	1.691283
H	2.169792	-0.081999	1.794794
C	-4.346557	0.890670	-0.198615
C	-4.598539	0.995677	2.420356
C	-5.210233	0.605973	1.053327
H	-4.883040	0.537468	-1.095203
H	-4.116209	1.960212	-0.291144
H	-5.297944	0.705350	3.222266
H	-4.389347	2.071917	2.479479
H	-6.154037	1.164302	0.940454
H	-5.482820	-0.464499	1.070434
Ni	-1.932232	0.893276	1.355693
N	-0.499005	1.255203	0.059854
N	-0.768777	1.374441	2.861432
N	-3.297924	0.259411	2.649666
N	-3.035450	0.143549	-0.115372
H	-3.502783	-0.744286	2.506509
H	-3.275193	-0.844020	0.074448
H	-0.373115	2.326262	2.753646
H	-0.160999	2.230587	0.175677
C	-2.702084	0.348128	4.042933
C	-1.658466	1.462891	4.083867
C	-2.185440	0.108476	-1.371299
C	-1.133630	1.216366	-1.315481
H	-2.821433	0.209136	-2.264936
H	-1.717919	-0.885972	-1.405557
H	-0.359956	1.075067	-2.089059
H	-1.593465	2.203353	-1.461820
H	-2.137000	2.450134	4.031250
H	-1.049595	1.415164	5.001753
H	-2.252219	-0.632541	4.255113
H	-3.496486	0.519356	4.786502
N	-4.804645	-2.312512	3.547480
C	-5.545296	-3.013868	4.127960
C	-6.472239	-3.887912	4.855570
H	-6.911946	-4.630389	4.171491
H	-5.941427	-4.418101	5.661691
H	-7.284905	-3.292139	5.299902
N	-4.372939	-2.481305	-1.149528
C	-4.981951	-3.223752	-1.824378
C	-5.744046	-4.148896	-2.670606
H	-5.083107	-4.609400	-3.421480
H	-6.192748	-4.945231	-2.056572
H	-6.549489	-3.608928	-3.192625
N	0.689625	3.901501	3.716200
N	0.262160	4.168025	-0.237335
C	1.172222	4.770201	4.339527
C	0.596005	5.212750	-0.652741
C	1.775262	5.855443	5.120064
H	2.762953	6.115847	4.708600
H	1.129977	6.747352	5.090906
H	1.900505	5.543397	6.168735
C	1.010748	6.518566	-1.173249
H	2.085092	6.675762	-0.989322
H	0.825355	6.569448	-2.257614
H	0.441765	7.321176	-0.678381
N	-1.395102	-2.322995	1.501499
C	-1.253201	-3.486568	1.563468
C	-1.074702	-4.939719	1.640761
H	-2.053984	-5.435926	1.725065
H	-0.565757	-5.308580	0.736480
H	-0.466429	-5.201821	2.520623
O	-2.621909	2.777478	1.251236
H	-1.931878	3.447507	1.060286

E = -2861.63056095
G = -2861.135098
E + ΔG_{solv} = -2861.737982

4-BLYP-singlet

C	0.857847	0.181449	0.346688
C	0.565140	0.308629	2.984966
C	1.459836	0.518721	1.735401
H	0.619555	-0.883185	0.229485
H	1.599938	0.446964	-0.427126
H	1.123875	0.661564	3.869355
H	0.293647	-0.741190	3.151333
H	1.806789	1.566206	1.728628
H	2.364133	-0.098312	1.862755
C	-4.282924	1.041599	-0.251230
C	-4.563664	1.177912	2.375204
C	-5.187266	0.858920	0.993346
H	-4.856011	0.749515	-1.149710
H	-3.940886	2.076368	-0.369037
H	-5.316464	0.974168	3.158210
H	-4.243812	2.223575	2.461139
H	-6.058591	1.521305	0.865801
H	-5.584854	-0.171241	1.003870
Ni	-1.861801	0.602088	1.368342
N	-0.383484	0.997550	0.072541
N	-0.685746	1.146517	2.893447
N	-3.390831	0.278377	2.661753
N	-3.084117	0.131349	-0.185898
H	-3.731098	-0.701069	2.547269
H	-3.451647	-0.833939	-0.046785
H	-0.350936	2.122751	2.737960
H	-0.125772	1.996364	0.216776
C	-2.774003	0.313852	4.049938
C	-1.586612	1.276235	4.115181
C	-2.188984	0.019920	-1.408021
C	-0.988686	0.968189	-1.327066
H	-2.777302	0.232455	-2.315325
H	-1.869779	-1.030194	-1.459676
H	-0.215991	0.668479	-2.053226
H	-1.281189	2.003699	-1.549072
H	-1.921706	2.321330	4.126612
H	-0.993579	1.094934	5.025488
H	-2.476173	-0.718581	4.280737
H	-3.541051	0.610454	4.783609
N	-4.618226	-2.359656	3.252738
C	-5.388040	-3.052202	3.807519
C	-6.346478	-3.915920	4.501636

H	-6.459067	-4.870349	3.963320
H	-5.996953	-4.123949	5.525514
H	-7.329669	-3.421626	4.556143
N	-4.134048	-2.595252	-0.813875
C	-4.751504	-3.337996	-1.482930
C	-5.518161	-4.265044	-2.319314
H	-4.860443	-4.730919	-3.070435
H	-5.966978	-5.056564	-1.698471
H	-6.324273	-3.724500	-2.840822
N	0.585803	3.690651	3.553287
N	-0.159755	3.960948	-0.063376
C	1.082209	4.560115	4.166292
C	0.155856	5.015024	-0.473488
C	1.701474	5.644386	4.932499
H	2.683234	5.900016	4.503252
H	1.057969	6.538264	4.912747
H	1.843851	5.333624	5.979802
C	0.547268	6.327358	-0.986986
H	1.623201	6.494029	-0.817627
H	0.343426	6.386539	-2.068210
H	-0.023558	7.118031	-0.473830
N	-1.510255	-1.348819	1.503762
C	-1.482133	-2.516530	1.564282
C	-1.430050	-3.971815	1.634747
H	-1.517029	-4.299686	2.683393
H	-2.267512	-4.389493	1.052987
H	-0.477194	-4.339154	1.219044
O	-2.362896	2.378571	1.286913
H	-1.645900	2.978639	0.960346

E = -2861.21048743
G = -2860.700213
E + ΔG_{solv} = -2861.530848

4-BLYP-triplet

C	0.912448	-0.006840	0.732604
C	0.404596	-0.008259	3.317112
C	1.451200	0.098252	2.179553
H	0.425539	-0.973318	0.548104
H	1.754680	0.101263	0.026583
H	0.917523	0.128913	4.286636
H	-0.102284	-0.982035	3.328178
H	2.019192	1.036667	2.293989
H	2.179387	-0.717643	2.315918
C	-3.976901	0.983379	-0.279980
C	-4.512020	1.109246	2.305044
C	-4.975020	0.739369	0.876350
H	-4.433429	0.615424	-1.214115
H	-3.719694	2.045094	-0.400323
H	-5.306437	0.819612	3.014038
H	-4.307799	2.181773	2.425388
H	-5.881992	1.326028	0.656632
H	-5.282938	-0.320149	0.860856
Ni	-1.724269	0.868999	1.535929
N	-0.089631	1.089106	0.414736
N	-0.622332	1.086893	3.195895
N	-3.274605	0.332324	2.682289
N	-2.694366	0.196205	-0.083967
H	-3.503586	-0.667211	2.506533
H	-2.986942	-0.795245	0.039715
H	-0.094859	1.991084	3.098946
H	0.347589	1.993522	0.653838
C	-2.829285	0.370309	4.144235
C	-1.622294	1.292000	4.318852
C	-1.705354	0.168293	-1.246273
C	-0.577440	1.177091	-1.024174
H	-2.238182	0.378665	-2.186433
H	-1.325504	-0.860882	-1.301844
H	0.261797	0.989197	-1.714446
H	-0.919665	2.210208	-1.175849
H	-1.917035	2.350181	4.267033
H	-1.128523	1.116430	5.289393
H	-2.590451	-0.666552	4.418355
H	-3.667061	0.700321	4.776836
N	-4.861565	-2.108760	3.337246
C	-5.660327	-2.788454	3.866127
C	-6.657535	-3.633940	4.528948
H	-7.106793	-4.331967	3.804975
H	-6.186197	-4.214095	5.338091
H	-7.456197	-3.009748	4.960381
N	-3.970332	-2.263269	-1.157137
C	-4.536820	-3.003446	-1.871763
C	-5.243802	-3.924767	-2.765999
H	-4.540602	-4.364366	-3.491093
H	-5.710191	-4.736328	-2.185481
H	-6.031173	-3.387060	-3.317858
N	0.968675	3.517661	3.165801
N	-1.206403	4.595517	-0.100965
C	1.630178	4.381431	3.607486
C	-1.156957	5.654657	-0.604012
C	2.455551	5.456888	4.158784
H	3.247152	5.732071	3.443506
H	1.833909	6.342804	4.365071
H	2.926307	5.125851	5.098486
C	-1.090082	6.971493	-1.234984
H	-0.041926	7.237543	-1.446795
H	-1.655375	6.966010	-2.181021
H	-1.524999	7.730383	-0.564494
N	-1.538572	-2.123848	1.643059
C	-1.533846	-3.297248	1.699363
C	-1.520222	-4.759155	1.771000
H	-2.551194	-5.145647	1.747148
H	-0.962252	-5.175859	0.917221
H	-1.036977	-5.089392	2.704526
O	-2.195571	2.685501	1.515856
H	-1.719942	3.382276	0.920880

E = -2861.17755538
G = -2860.679667
E + ΔG_{solv} = -2861.492030

tBuOOH-6H_2O-BLYP

O	0.454907	-0.415351	0.349921
H	1.215548	0.244767	0.454477
O	-0.668696	0.591171	0.194555
O	2.307549	1.601844	0.492517
H	1.904424	2.159344	1.197289
H	2.033987	2.034759	-0.349938
H	-1.526043	4.949075	2.800154
O	-1.434964	4.399267	3.616077
H	-2.300947	4.408685	4.062443
H	-0.369603	3.023143	2.744061
O	0.114351	2.785203	1.914933
H	-0.351515	2.012030	1.513219
H	-0.361448	4.345419	1.107007
O	-0.881080	5.179692	0.932401
H	-0.226159	5.886399	0.777535
H	0.021831	1.555517	-1.289985
O	0.568783	2.220701	-1.782968
H	0.773292	1.816780	-2.647597
H	-1.668739	4.561086	-0.878886
O	-1.810345	4.037209	-1.697967
H	-0.941864	3.609623	-1.864268
C	-1.951103	-0.153877	0.078794

C	-1.944046	-0.973999	-1.228969
H	-2.889466	-1.531414	-1.328268
H	-1.846900	-0.314141	-2.106322
H	-1.113440	-1.694330	-1.230916
C	-2.147475	-1.044709	1.322887
H	-2.084036	-0.445378	2.245027
H	-3.143246	-1.515717	1.286076
H	-1.386506	-1.835901	1.369313
C	-2.983842	0.996430	0.029174
H	-3.979245	0.569880	-0.174050
H	-3.033609	1.527801	0.992957
H	-2.752575	1.729329	-0.759875

E = -767.269766402
G = -767.042308
E + ΔG_{solv} = -767.259768

tBuOH-6H_2O-BLYP

O	-0.351403	0.869746	0.004025
H	0.528674	1.320518	-0.315641
H	0.045574	-0.942367	0.505868
H	-1.024856	1.080058	-0.669392
O	3.741792	0.891070	1.008017
H	4.403187	0.227852	0.740107
O	0.479215	-1.693964	0.983631
O	1.858458	2.093192	-0.598113
H	1.779654	2.942234	-0.089637
H	2.616239	1.614456	-0.154286
H	3.165955	0.455310	1.708183
O	1.952543	-0.148433	2.791203
H	1.312917	0.582372	2.949694
H	1.436020	-0.813163	2.260812
O	-0.110594	2.006103	2.488893
H	-0.916527	2.124424	3.024757
H	-0.397597	1.605190	1.615717
O	1.344387	4.139801	1.300342
H	0.849452	3.514292	1.888221
H	2.120953	4.433092	1.812285
C	-0.452894	-2.817202	1.120890
C	0.350115	-3.920397	1.840871
H	0.693625	-3.568416	2.826766
H	-0.270624	-4.818548	1.989999
H	1.234426	-4.201263	1.247278
C	-1.675048	-2.378594	1.966432
H	-2.224185	-1.561421	1.468559
H	-2.376720	-3.217248	2.111338
H	-1.350545	-2.024429	2.957989
C	-0.890707	-3.279491	-0.290357
H	-0.010857	-3.552124	-0.893923
H	-1.559137	-4.154687	-0.229750
H	-1.434514	-2.476629	-0.816816

E = -692.152902430
G = -691.926221
E + ΔG_{solv} = -692.145541

tBuO$^{\bullet}$-6H2O-BLYP

O	-0.884489	1.236951	0.069192
H	-0.041209	1.620399	-0.369878
H	-1.637370	1.622456	-0.415834
O	3.390982	0.956080	0.446549
H	3.979472	0.264814	0.093716
O	1.170467	-2.501025	1.661802
O	1.345199	2.346291	-0.807863
H	1.391858	3.139791	-0.215370
H	2.120195	1.791228	-0.516170
H	2.951699	0.568023	1.260909
O	2.000722	0.045427	2.630181
H	1.234058	0.662617	2.722392
H	1.617559	-0.845442	2.442697
O	-0.145523	1.977705	2.530002
H	-0.853728	2.070518	3.193322
H	-0.583690	1.707579	1.657760
O	1.262603	4.180770	1.386557
H	0.809010	3.511346	1.958898
H	2.136491	4.329531	1.793477
C	-0.036759	-3.070003	1.298802
C	-0.114001	-4.342759	2.264026
H	-0.117216	-4.021894	3.314616
H	-1.057008	-4.861957	2.029695
H	0.738484	-5.010500	2.081712
C	-1.245114	-2.131952	1.568938
H	-1.154091	-1.217692	0.961381
H	-2.194080	-2.631194	1.312112
H	-1.278487	-1.845005	2.632064
C	0.015247	-3.562785	-0.180224
H	0.878377	-4.227420	-0.334179
H	-0.909192	-4.103245	-0.440850
H	0.114546	-2.695928	-0.851634

E = -691.481702340
G = -691.270725
E + ΔG_{solv} = -691.474184

CH_3CN-BLYP

C	-1.636798	1.099993	-0.020950
N	-0.462969	1.100011	-0.020949
C	-3.106038	1.099990	-0.020936
H	-3.487777	2.117927	-0.198576
H	-3.487785	0.437200	-0.813677
H	-3.487811	0.744880	0.949427

E = -132.712727687
G = -132.692920
E + ΔG_{solv} = -132.714184

6H_2O-BLYP

O	-0.655808	1.094534	0.632167
H	-0.024651	0.893788	-0.144534
H	-0.475804	-0.330506	1.822622
H	-1.528487	1.273834	0.236127
O	3.222551	-0.352040	0.035551
H	3.510062	-1.280467	-0.034991
O	-0.100049	-1.004487	2.446540
H	-0.731526	-1.084597	3.184216
O	1.084981	0.536480	-1.285185
H	1.413565	1.296508	-1.800442
H	1.904616	0.141872	-0.836725
H	3.020714	-0.185319	1.015122
O	2.478583	0.174440	2.558358
H	2.179083	1.117771	2.557647
H	1.639495	-0.337206	2.686145
O	1.124167	2.671632	2.178100
H	0.745227	3.228913	2.881802
H	0.360094	2.294239	1.672857

E = -458.568129427
G = -458.463635
E + ΔG_{solv} = -458.569683

H_2O-6H_2O-BLYP

O	-0.815186	0.743229	0.610033

H	0.006662	0.939231	-0.002275
H	-0.536232	-0.852229	1.477947
H	-1.609332	0.873780	0.059120
O	3.346469	0.221175	0.689878
H	3.825850	-0.601939	0.485534
O	-0.141485	-1.556972	2.056949
H	-0.878656	-1.972822	2.539379
O	1.298014	1.351414	-0.747020
H	1.460802	2.297152	-0.491553
H	2.074335	0.855387	-0.355772
H	2.925165	0.091487	1.593575
O	1.967415	0.019325	3.039064
H	1.487265	0.874424	3.119433
H	1.251604	-0.642693	2.852365
O	0.181745	2.382951	2.580267
H	-0.439185	2.783684	3.216449
H	-0.367387	1.849934	1.934068
O	1.539489	3.854753	0.557805
H	1.142028	3.498985	1.392518
H	2.446811	4.130090	0.785987

E = -534.999856858
G = -534.872830
E + ΔG_{solv} = -534.999654

HOOH-6H_2O-BLYP

O	0.525244	1.468826	0.762792
H	1.248806	1.795008	0.148438
O	-0.705789	1.793816	-0.029746
H	-1.261666	0.927524	0.154624
O	2.377911	2.070510	-1.176236
H	2.713339	2.966561	-1.363551
H	1.797262	1.818043	-1.938150
H	-0.673895	2.057034	3.736058
O	-0.191290	1.260728	3.447141
H	0.144400	1.469261	2.536380
H	-1.929286	-0.766406	1.189396
O	-2.050638	-0.391271	0.272473
H	-1.628706	-1.012922	-0.373650
H	-2.245681	-1.309565	3.522792
O	-1.541845	-1.096416	2.883894
H	-1.087953	-0.274013	3.221218
H	-0.301088	1.468596	-1.662163
O	0.118150	1.141823	-2.523489
H	-0.401270	1.523400	-3.256010
H	0.115493	-2.165532	-1.757297
O	-0.642452	-1.568121	-1.896586
H	-0.261057	-0.721706	-2.239346

E = -610.122534996
G = -609.996599
E + ΔG_{solv} = -610.122635

$OH^{\bullet}$-6H_2O-BLYP

O	-0.823197	0.746257	0.610419
H	-0.004220	0.955061	0.004044
H	-0.521042	-0.848129	1.496152
H	-1.616758	0.848626	0.052691
O	3.334219	0.265979	0.651589
H	3.829183	-0.543731	0.431829
O	-0.104147	-1.535808	2.078248
H	-0.826220	-1.977757	2.560266
O	1.291559	1.386800	-0.743197
H	1.447289	2.339629	-0.536233
H	2.082416	0.907573	-0.351247
H	2.938217	0.128941	1.565282
O	2.001003	0.061428	3.022618
H	1.527597	0.917993	3.111749
H	1.281025	-0.599505	2.848695
O	0.135594	2.417243	2.557291
H	-0.473911	2.786644	3.223155
H	-0.409708	1.856807	1.930602
O	1.405507	4.003892	0.622622
H	1.051660	3.540466	1.445321

E = -534.307228150
G = -534.194684
E + ΔG_{solv} = -534.305582

OH^--6H_2O-BLYP

O	-0.699863	0.646822	0.872400
H	0.521387	1.099216	-0.360424
H	-0.156022	-0.623796	1.365035
H	-1.614346	0.658000	0.537238
O	2.973653	-0.511878	0.807446
H	2.168666	-1.073484	0.922789
O	0.418676	-1.432741	1.764931
H	-0.152552	-2.220494	1.781699
O	1.331469	1.361632	-0.891114
H	1.431596	3.204103	-0.249303
H	2.045991	0.823865	-0.474033
H	2.983139	-0.024317	1.665225
O	1.937379	0.375886	3.490465
H	1.404045	1.179627	3.255610
H	1.364342	-0.365314	3.181065
O	0.146792	2.413932	2.518629
H	-0.558302	2.696796	3.128441
H	-0.300133	1.732872	1.848844
O	1.337493	4.032490	0.287655
H	0.962656	3.685194	1.129299

E = -534.466081304
G = -534.353255
E + ΔG_{solv} = -534.523649

H_3O^+-6H_2O-BLYP

O	-1.092448	0.651464	0.529314
H	0.414735	1.097423	-0.649357
H	-0.487782	-1.077514	1.084385
H	-2.015334	0.747482	0.222619
O	2.385304	-0.413617	0.872472
H	1.584980	-1.046115	1.090835
O	0.232914	-1.673681	1.411713
H	0.004386	-2.597460	1.194641
O	1.388675	1.192469	-0.800037
H	1.614005	2.122482	-0.555566
H	2.039122	0.249404	0.103306
H	2.557625	0.170160	1.683937
O	2.577248	1.436545	2.787496
H	1.650034	1.687749	3.030334
H	3.079351	1.317851	3.617717
O	-0.041807	2.493950	2.429195
H	-0.586670	2.985055	3.075582
H	-0.961358	1.305525	1.265175
O	1.943408	3.588364	0.752164
H	0.421661	3.168899	1.869958
H	2.691426	3.296446	1.318059
H	2.180183	4.475482	0.415035

E = -535.369177753
G = -535.228903
E + ΔG_{solv} = -535.428465

1-OLYP

C	0.561326	0.879377	0.226020
C	0.445804	0.869293	2.883889
C	1.106989	1.370303	1.583069
H	0.653852	-0.208920	0.127819
H	1.163256	1.342302	-0.569318
H	0.973195	1.329232	3.732889
H	0.537124	-0.219054	2.984679
H	1.104070	2.471100	1.585586
H	2.167088	1.084266	1.628761
C	-4.475926	0.888763	0.007976
C	-4.595021	0.869284	2.649631
C	-5.289882	0.629595	1.292910
H	-5.154195	0.823606	-0.858690
H	-4.063081	1.906000	0.016472
H	-5.347122	0.788167	3.451506
H	-4.186243	1.887420	2.695600
H	-6.159804	1.300385	1.258254
H	-5.703535	-0.389885	1.267314
Ni	-2.060635	0.214633	1.434746
N	-0.873959	1.251568	0.051893
N	-1.002846	1.230282	2.937190
N	-3.492682	-0.104723	2.896425
N	-3.356018	-0.082168	-0.157992
H	-3.896609	-1.044332	2.847220
H	-3.759201	-1.023281	-0.163899
H	-1.058170	2.221477	2.696008
H	-0.945212	2.238586	0.307566
C	-2.785178	-0.022559	4.205600
C	-1.721240	1.090461	4.242748
C	-2.534168	0.027186	-1.396642
C	-1.476100	1.143039	-1.313882
H	-3.166479	0.187364	-2.284004
H	-2.048918	-0.947609	-1.522080
H	-0.701901	0.965644	-2.071727
H	-1.924550	2.114548	-1.551798
H	-2.183043	2.058196	4.468290
H	-1.015705	0.888581	5.058977
H	-2.314219	-1.001441	4.353419
H	-3.494691	0.121314	5.035635
N	-4.897830	-3.039329	3.517237
C	-5.611707	-3.814210	4.030844
C	-6.501912	-4.776642	4.670978
H	-6.569543	-5.690868	4.068081
H	-6.123603	-5.037604	5.667374
H	-7.506860	-4.348808	4.776708
N	-4.556634	-3.037141	-1.114238
C	-5.138108	-3.809423	-1.777159
C	-5.863432	-4.767139	-2.605116
H	-5.463210	-4.763263	-3.626822
H	-5.765002	-5.778665	-2.191566
H	-6.927907	-4.503412	-2.642714
N	0.238038	4.213976	4.978139
N	0.976608	4.204174	-1.655453
C	0.699552	4.919032	5.793562
C	1.645669	4.882868	-2.338692
C	1.273578	5.794438	6.811253
H	1.893601	6.568275	6.341227
H	0.476133	6.282028	7.386227
H	1.899517	5.214040	7.500852
C	2.479644	5.725304	-3.190983
H	3.298779	5.135306	-3.621299
H	1.882315	6.146797	-4.009356
H	2.909485	6.549076	-2.607164
N	-1.360484	-1.658321	1.459113
N	-2.183567	4.120721	1.377092
C	-2.221228	5.291997	1.359563
C	-1.111858	-2.799505	1.461431
C	-2.265755	6.748739	1.338462
H	-1.848047	7.149628	2.270458
H	-1.678700	7.129634	0.493222
H	-3.301691	7.095604	1.236081
C	-0.808630	-4.221236	1.470034
H	-1.277057	-4.693937	2.342954
H	-1.203700	-4.689124	0.558773
H	0.276584	-4.379245	1.514598

E = -2918.93584214
G = -2918.413296
E + ΔG_{solv} = -2919.030506

3-OLYP-doublet

C	0.568986	0.449710	0.305972
C	0.370711	0.443698	2.911281
C	1.252131	0.653184	1.668674
H	0.195335	-0.574657	0.199511
H	1.306914	0.625242	-0.491936
H	0.978792	0.614769	3.812693
H	-0.015205	-0.580857	2.954587
H	1.708361	1.652799	1.706066
H	2.084381	-0.060831	1.730521
C	-4.412047	0.959400	-0.063661
C	-4.604933	0.943605	2.545315
C	-5.228252	0.594119	1.185489
H	-4.958497	0.620529	-0.955013
H	-4.236719	2.037013	-0.129250
H	-5.275767	0.593979	3.342542
H	-4.443458	2.020352	2.649707
H	-6.186488	1.126818	1.118153
H	-5.476731	-0.477460	1.160931
Ni	-1.965965	1.001732	1.427128
N	-0.566187	1.404593	0.119083
N	-0.779760	1.398776	2.929158
N	-3.282143	0.262176	2.717891
N	-3.078548	0.277673	-0.048019
H	-3.439095	-0.731602	2.520937
H	-3.263841	-0.716960	0.116732
H	-0.388409	2.347634	2.861703
H	-0.191386	2.353628	0.250744
C	-2.668315	0.303580	4.091292
C	-1.637989	1.416621	4.159846
C	-2.270606	0.325768	-1.316388
C	-1.232253	1.430153	-1.225809
H	-2.926874	0.477857	-2.182586
H	-1.803052	-0.657907	-1.433251
H	-0.483217	1.340088	-2.025331
H	-1.701725	2.414909	-1.309899
H	-2.122813	2.397419	4.174972
H	-1.015541	1.329779	5.061637
H	-2.213315	-0.677363	4.266369
H	-3.445033	0.441679	4.854015
N	-4.865848	-2.546238	3.783623
C	-5.549892	-3.297710	4.368063
C	-6.402804	-4.230324	5.097658
H	-6.823519	-4.976337	4.411797
H	-5.822853	-4.748805	5.871523
H	-7.228022	-3.690547	5.579066
N	-4.518302	-2.512361	-1.355206
C	-5.117462	-3.251107	-2.040388
C	-5.864606	-4.167883	-2.895261
H	-5.197836	-4.620470	-3.639997
H	-6.315511	-4.966467	-2.292894

H	-6.663774	-3.629220	-3.419939
N	0.464557	4.185927	3.717483
N	0.742001	4.222459	-0.385449
C	0.870672	5.122106	4.292725
C	1.217412	5.184031	-0.856108
C	1.374874	6.287075	5.010231
H	2.426545	6.464432	4.752231
H	0.788914	7.176324	4.745678
H	1.300185	6.124787	6.092930
C	1.808049	6.380929	-1.443089
H	2.810248	6.549967	-1.029502
H	1.890518	6.266187	-2.531291
H	1.181855	7.255770	-1.227093
N	-1.384002	-2.684618	1.446091
C	-1.263256	-3.850575	1.442453
C	-1.113968	-5.301303	1.437835
H	-2.092095	-5.780452	1.570354
H	-0.682725	-5.634585	0.485448
H	-0.451936	-5.617068	2.253984
O	-2.683608	2.863465	1.379642
H	-2.013387	3.564194	1.427727

E = -2861.99131903
G = -2861.488050
E + ΔG_{solv} = -2862.099118

3-OLYP-quartet

C	0.807500	0.248598	0.534378
C	0.378458	0.365416	3.122375
C	1.367711	0.480546	1.948210
H	0.316266	-0.730064	0.477127
H	1.644595	0.231285	-0.182411
H	0.940690	0.422499	4.068356
H	-0.136144	-0.603664	3.107827
H	1.882853	1.451319	1.995024
H	2.148989	-0.275305	2.108033
C	-4.126817	0.502617	-0.221299
C	-4.568492	0.792239	2.371048
C	-4.981361	0.182063	1.019241
H	-4.555458	-0.034943	-1.079016
H	-4.134835	1.574945	-0.446305
H	-5.282687	0.452462	3.135042
H	-4.590493	1.888179	2.343754
H	-6.000664	0.529349	0.801781
H	-5.060483	-0.910009	1.129859
Ni	-1.829958	1.297014	1.411359
N	-0.173581	1.291582	0.115910
N	-0.632092	1.458612	3.095043
N	-3.190653	0.353023	2.751427
N	-2.701667	0.068135	-0.057086
H	-3.152745	-0.655144	2.590555
H	-2.706868	-0.885092	0.316464
H	-0.118234	2.348674	3.059648
H	0.280603	2.206495	0.155508
C	-2.738398	0.565801	4.160045
C	-1.580559	1.575345	4.240103
C	-1.842961	0.047495	-1.280111
C	-0.761212	1.140794	-1.244866
H	-2.454264	0.172432	-2.181831
H	-1.389726	-0.947630	-1.345265
H	0.016138	0.909855	-1.989856
H	-1.190291	2.114312	-1.505551
H	-1.965817	2.600799	4.202806
H	-1.048100	1.457480	5.196164
H	-2.436656	-0.407964	4.561958
H	-3.567257	0.919935	4.785431
N	-5.016798	-2.427393	4.528287
C	-5.728352	-3.020090	5.247671
C	-6.616102	-3.754861	6.143712
H	-7.295500	-4.393592	5.565398
H	-6.031260	-4.386338	6.824296
H	-7.214788	-3.055456	6.740722
N	-4.204563	-2.669632	-2.404003
C	-4.695756	-3.308379	-3.255939
C	-5.307697	-4.102449	-4.316974
H	-4.535889	-4.640096	-4.881988
H	-6.005813	-4.833230	-3.889777
H	-5.859337	-3.451481	-5.006888
N	1.069312	4.052804	3.678951
N	-0.402212	4.848697	-0.238331
C	1.651967	4.912702	4.220673
C	-0.174263	5.894745	-0.714350
C	2.376303	5.982339	4.896946
H	3.231173	6.304068	4.288909
H	1.713929	6.841559	5.061588
H	2.747007	5.631070	5.868206
C	0.108260	7.194955	-1.308637
H	1.177566	7.425944	-1.223297
H	-0.170467	7.193267	-2.369998
H	-0.466193	7.975528	-0.793780
N	-2.035488	-2.731547	1.486145
C	-2.117415	-3.897679	1.568134
C	-2.223039	-5.346954	1.672155
H	-2.858471	-5.614810	2.525734
H	-2.666873	-5.756330	0.755837
H	-1.229829	-5.791141	1.814621
O	-2.381514	2.997400	1.149878
H	-1.731358	3.650116	0.807355

E = -2861.97027522
G = -2861.470704
E + ΔG_{solv} = -2862.076600

4-singlet-OLYP

C	0.854389	0.213563	0.323529
C	0.580107	0.342341	2.950085
C	1.455854	0.555230	1.700211
H	0.648655	-0.852488	0.199052
H	1.589038	0.497708	-0.446507
H	1.144379	0.709364	3.821039
H	0.336543	-0.707131	3.131828
H	1.805800	1.596780	1.689974
H	2.359283	-0.057610	1.822381
C	-4.273241	1.027135	-0.238536
C	-4.537308	1.160640	2.377050
C	-5.164544	0.855490	1.004751
H	-4.856621	0.727927	-1.123912
H	-3.943571	2.059383	-0.375000
H	-5.288571	0.947855	3.154521
H	-4.232305	2.205344	2.476241
H	-6.020802	1.532463	0.883767
H	-5.585319	-0.160151	1.013538
Ni	-1.851193	0.598191	1.356862
N	-0.391600	0.995683	0.051850
N	-0.675853	1.147200	2.875034
N	-3.370977	0.274731	2.656086
N	-3.082657	0.129887	-0.184290
H	-3.706137	-0.694230	2.536975
H	-3.445914	-0.823187	-0.033610
H	-0.371804	2.119197	2.710277
H	-0.142359	1.990662	0.181043
C	-2.747277	0.305254	4.025216
C	-1.563688	1.257920	4.090537
C	-2.201332	0.013479	-1.397885

C	-1.000385	0.947309	-1.329797
H	-2.786535	0.227710	-2.302410
H	-1.890520	-1.034124	-1.456192
H	-0.239761	0.631659	-2.056391
H	-1.283881	1.976083	-1.572588
H	-1.894904	2.299242	4.125632
H	-0.972339	1.063778	4.994829
H	-2.452411	-0.723370	4.255490
H	-3.501451	0.600219	4.767536
N	-4.703202	-2.433975	3.314948
C	-5.468351	-3.135519	3.861155
C	-6.418165	-4.005887	4.541588
H	-6.522332	-4.953574	3.997782
H	-6.072366	-4.218996	5.561419
H	-7.401394	-3.520669	4.596559
N	-4.278526	-2.660499	-0.891970
C	-4.909638	-3.403787	-1.544332
C	-5.691756	-4.326472	-2.356736
H	-5.053367	-4.796627	-3.115989
H	-6.129286	-5.111046	-1.726114
H	-6.503348	-3.787770	-2.862971
N	0.585274	3.810766	3.663950
N	-0.056150	3.994893	-0.135348
C	1.056494	4.685137	4.286911
C	0.284866	5.043339	-0.533817
C	1.641863	5.770895	5.062406
H	2.631549	6.029624	4.664509
H	0.996979	6.657981	5.017896
H	1.752752	5.467959	6.111636
C	0.707219	6.343796	-1.029729
H	1.781542	6.483824	-0.851936
H	0.513459	6.417267	-2.107907
H	0.153271	7.139984	-0.515206
N	-1.490845	-1.355765	1.491798
C	-1.426474	-2.520127	1.557309
C	-1.330566	-3.964360	1.636344
H	-1.375489	-4.284666	2.686159
H	-2.169043	-4.412383	1.086473
H	-0.383380	-4.305452	1.196025
O	-2.348437	2.360678	1.278578
H	-1.641972	2.954742	0.954917

E = -2861.55575084
G = -2861.037455
E + ΔG_{solv} = -2861.877307

tBuOOH-6H_2O-OLYP

O	0.397205	-0.523965	0.212662
H	1.121643	0.133298	0.366341
O	-0.737774	0.422699	0.083985
O	2.376958	1.515144	0.468173
H	2.057860	2.084617	1.186708
H	2.166479	2.006454	-0.343179
H	-1.594716	5.144116	3.034737
O	-1.575056	4.544994	3.801380
H	-2.445368	4.612899	4.213997
H	-0.396708	3.070627	2.848747
O	0.106074	2.848452	2.044871
H	-0.370012	2.110987	1.630122
H	-0.268910	4.607631	1.217133
O	-0.720016	5.462089	1.059112
H	-0.013492	6.116254	0.972526
H	0.027358	1.613857	-1.547241
O	0.559858	2.319444	-1.956077
H	0.742484	2.012548	-2.854699
H	-1.518947	5.019255	-1.011796
O	-1.644994	4.623355	-1.888257
H	-0.901476	4.006968	-1.976874
C	-1.979906	-0.348160	0.058601
C	-2.003705	-1.276844	-1.169414
H	-2.958885	-1.814693	-1.217386
H	-1.892400	-0.701495	-2.097087
H	-1.196651	-2.014620	-1.119028
C	-2.147327	-1.134978	1.370932
H	-2.116543	-0.461724	2.236630
H	-3.114034	-1.654151	1.377393
H	-1.354681	-1.880586	1.486465
C	-3.042479	0.760891	-0.064894
H	-4.035931	0.300414	-0.124819
H	-3.032975	1.426647	0.806664
H	-2.895157	1.367911	-0.965621

E = -767.222164200
G = -766.999078
E + ΔG_{solv} = -767.209675

tBuOH-6H_2O-OLYP

O	-0.474840	0.980989	0.011468
H	0.379406	1.371614	-0.338180
H	-0.082849	-1.027958	0.613028
H	-1.144177	1.214425	-0.645173
O	3.844293	0.857348	0.907503
H	4.496415	0.194260	0.648541
O	0.356475	-1.743881	1.106935
O	1.850908	2.144785	-0.732904
H	1.833709	2.993797	-0.251220
H	2.596035	1.658215	-0.321844
H	3.316501	0.442800	1.627759
O	2.083601	-0.189342	2.887443
H	1.489672	0.543206	3.114118
H	1.510534	-0.818819	2.406739
O	-0.132237	2.217775	2.599554
H	-0.932166	2.395085	3.111408
H	-0.438317	1.808727	1.761143
O	1.470080	4.342726	1.246324
H	0.970796	3.770409	1.858651
H	2.256644	4.616373	1.736388
C	-0.504844	-2.907670	1.146424
C	0.305228	-3.984620	1.886236
H	0.554378	-3.653543	2.902144
H	-0.264766	-4.918982	1.959865
H	1.242377	-4.192256	1.355208
C	-1.801425	-2.572221	1.914723
H	-2.365978	-1.778574	1.406334
H	-2.456075	-3.450646	1.990976
H	-1.568266	-2.228529	2.930303
C	-0.821077	-3.355018	-0.296277
H	0.106188	-3.557777	-0.846117
H	-1.434713	-4.265588	-0.305238
H	-1.374533	-2.575778	-0.838302

E = -692.120449956
G = -691.893372
E + ΔG_{solv} = -692.109800

tBuO$^{\bullet}$-6H_2O-OLYP

O	-0.948176	1.525562	-0.017808
H	-0.113383	1.847832	-0.453168

H	-1.665721	1.953299	-0.502800
O	3.480461	0.966175	0.373786
H	4.065482	0.266375	0.058098
O	1.033542	-2.635272	1.703553
O	1.429540	2.546190	-0.951080
H	1.534986	3.318418	-0.364755
H	2.158914	1.953667	-0.678586
H	3.050696	0.607530	1.182274
O	2.041091	0.086396	2.684393
H	1.299442	0.710715	2.777538
H	1.629770	-0.779343	2.524420
O	-0.156092	2.183168	2.575453
H	-0.871655	2.297110	3.214020
H	-0.590121	1.961951	1.715329
O	1.480064	4.428237	1.407495
H	0.989840	3.795696	1.964371
H	2.349296	4.507754	1.822438
C	-0.124594	-3.269910	1.337869
C	-0.155561	-4.513232	2.322743
H	-0.191942	-4.173568	3.362661
H	-1.062220	-5.085918	2.090716
H	0.728368	-5.140469	2.172671
C	-1.379127	-2.391306	1.567336
H	-1.327051	-1.496103	0.936143
H	-2.298119	-2.937236	1.317488
H	-1.438138	-2.071312	2.614746
C	-0.029564	-3.786263	-0.123965
H	0.859948	-4.412978	-0.253501
H	-0.920542	-4.367985	-0.392602
H	0.045579	-2.932456	-0.808479

E = -691.448289977
G = -691.237787
E + ΔG_{solv} = -691.438338

CH_3CN-OLYP

C	-1.642728	1.100004	-0.020937
N	-0.470618	1.100000	-0.020969
C	-3.103875	1.099995	-0.020922
H	-3.483974	2.114273	-0.197942
H	-3.483958	0.439578	-0.810828
H	-3.484023	0.746149	0.945939

E = -132.720607284
G = -132.700218
E + ΔG_{solv} = -132.721942

$6H_2O$-OLYP

O	-0.757980	1.122769	0.576185
H	-0.132285	0.925663	-0.169273
H	-0.536485	-0.415168	1.875218
H	-1.613835	1.277266	0.155807
O	3.300468	-0.385062	0.010200
H	3.595730	-1.302440	-0.050908
O	-0.160207	-1.070732	2.493208
H	-0.808824	-1.165442	3.202181
O	1.087229	0.533470	-1.387771
H	1.435875	1.276245	-1.898004
H	1.878882	0.145904	-0.938034
H	3.113974	-0.229237	0.969593
O	2.552735	0.133661	2.649327
H	2.277067	1.067390	2.671242
H	1.716885	-0.355174	2.768459
O	1.117517	2.778781	2.247440
H	0.734204	3.386503	2.892435
H	0.365859	2.424996	1.738072

E = -458.519928962
G = -458.416288
E + ΔG_{solv} = -458.519078

H_2O-$6H_2O$-OLYP

O	-0.910340	0.734607	0.547051
H	-0.107592	0.921957	-0.028374
H	-0.578871	-0.948791	1.511047
H	-1.672154	0.820893	-0.040954
O	3.454349	0.179393	0.671836
H	3.968587	-0.609886	0.460274
O	-0.186810	-1.639287	2.082062
H	-0.925309	-2.052285	2.546874
O	1.305808	1.362306	-0.832783
H	1.478517	2.291091	-0.584493
H	2.066922	0.872689	-0.455114
H	3.064956	0.011874	1.559885
O	2.080874	-0.154040	3.147936
H	1.663498	0.698050	3.343639
H	1.330278	-0.742201	2.930857
O	0.024589	2.550566	2.638382
H	-0.642072	3.003209	3.171307
H	-0.475753	1.994761	2.005525
O	1.589528	3.975139	0.545888
H	1.151602	3.654702	1.356939
H	2.485582	4.215601	0.815970

E = -534.942079141
G = -534.816880
E + ΔG_{solv} = -534.938474

HOOH-$6H_2O$-OLYP

O	0.115941	2.219673	0.730372
H	0.909503	1.922958	0.218451
O	-0.982522	1.960242	-0.186055
H	-1.328364	1.049566	0.114461
O	2.173087	1.419799	-0.922999
H	2.955120	1.971690	-1.042153
H	1.686826	1.410677	-1.771352
H	-0.682739	2.050501	3.833130
O	-0.245953	1.341009	3.347496
H	-0.116414	1.674425	2.432539
H	-1.678081	-0.809436	1.212044
O	-1.850549	-0.418248	0.325485
H	-1.439279	-0.988578	-0.355148
H	-1.914035	-1.470583	3.510799
O	-1.239296	-1.177605	2.887821
H	-0.897937	-0.313327	3.213908
H	-0.452679	1.646199	-1.800948
O	0.002032	1.270242	-2.601630
H	-0.363503	1.707609	-3.380206
H	0.291321	-1.957011	-1.851880
O	-0.531703	-1.460655	-1.935928
H	-0.292790	-0.593967	-2.319225

E = -610.254681483
G = -610.121954
E + ΔG_{solv} = -610.047743

$OH^{\bullet}$-$6H_2O$-OLYP

O	-0.788649	0.788627	0.691348
H	0.089675	1.069791	0.294100
H	-0.396463	-0.407441	2.128517
H	-1.280373	0.377256	-0.031986

O	3.709511	0.097374	0.637995
H	4.196264	-0.387286	-0.041034
O	-0.130002	-1.002801	2.860885
H	-0.364515	-0.525850	3.667707
O	1.543693	1.667181	-0.281554
H	1.663083	2.585093	0.018433
H	2.335957	1.168095	0.018671
H	3.370835	-0.589077	1.254315
O	2.566629	-1.842476	2.364935
H	2.987186	-2.086677	3.199020
H	1.645879	-1.592565	2.596563
O	-1.342573	3.372686	1.859197
H	-2.221911	3.749731	1.728254
H	-1.358048	2.484654	1.445840
O	1.088299	4.504551	0.873052
H	0.231588	4.227543	1.297637

E = -534.247652146
G = -534.138366
E + ΔG_{solv} = -534.244474

OH^--6H_2O-OLYP

O	-0.551508	0.656015	0.926765
H	0.295655	1.124332	-0.495006
H	0.176964	-0.509257	1.463070
H	-1.491354	0.484405	0.783769
O	3.178767	-0.931196	0.283031
H	2.370275	-1.111234	0.816708
O	0.808536	-1.259650	1.859952
H	0.335596	-2.092521	1.740393
O	0.900576	1.403784	-1.244176
H	1.527001	3.196316	-0.320312
H	1.614614	0.751637	-1.202337
H	3.544547	-0.136691	0.694307
O	1.002307	0.317862	4.551045
H	0.737079	1.135693	4.092828
H	0.998141	-0.333303	3.827722
O	0.061712	2.548884	2.609489
H	-0.730455	3.061436	2.813666
H	-0.252472	1.826222	1.950092
O	1.725792	3.916902	0.307382
H	1.294295	3.608776	1.123506

E = -534.399195162
G = -534.289520
E + ΔG_{solv} = -534.451747

H_3O^+-6H_2O-OLYP

O	-1.156108	0.730224	0.469511
H	0.556204	1.141750	-0.591819
H	-0.538433	-1.411807	0.989412
H	-2.039582	0.859086	0.095132
O	2.369513	-0.496229	1.020257
H	1.593458	-1.147293	1.111283
O	0.225271	-1.930718	1.293356
H	0.091464	-2.844339	1.004720
O	1.528137	1.172853	-0.686007
H	1.777977	2.102566	-0.533137
H	2.094956	0.200923	0.287131
H	2.461732	0.009631	1.898781
O	2.498197	0.996612	3.137530
H	1.690317	1.533549	3.254032
H	2.797551	0.716289	4.013300
O	0.153182	2.689439	2.596719
H	-0.320280	3.209543	3.262278
H	-1.101748	1.337090	1.228497
O	1.895208	3.997406	0.386219
H	0.592327	3.341516	2.021195
H	2.791965	4.234798	0.668766
H	1.618348	4.735474	-0.178180

E = -535.317940322
G = -535.181347
E + ΔG_{solv} = -535.372624

1-PBEPBE

C	0.669348	0.527227	0.316003
C	0.444922	0.547585	2.984657
C	1.257692	0.870992	1.706703
H	0.444104	-0.547061	0.234606
H	1.432787	0.768125	-0.450351
H	1.067232	0.809288	3.863479
H	0.215334	-0.527307	3.049859
H	1.509104	1.949939	1.719499
H	2.223692	0.343585	1.791890
C	-4.505835	0.959593	-0.126964
C	-4.730200	0.980074	2.541697
C	-5.318680	0.636455	1.151013
H	-5.128140	0.697924	-1.005797
H	-4.276045	2.034436	-0.192239
H	-5.493649	0.739308	3.308084
H	-4.504734	2.054315	2.623106
H	-6.284529	1.164141	1.065830
H	-5.570362	-0.442433	1.138289
Ni	-2.030457	0.753524	1.428861
N	-0.574144	1.302129	0.060999
N	-0.827564	1.318248	3.013112
N	-3.486866	0.204892	2.796575
N	-3.233470	0.188722	-0.155292
H	-3.731645	-0.787249	2.656610
H	-3.497289	-0.802026	-0.044891
H	-0.563841	2.309048	2.902928
H	-0.329585	2.294342	0.200744
C	-2.840239	0.257811	4.142273
C	-1.687183	1.278966	4.233644
C	-2.373859	0.227694	-1.375822
C	-1.220751	1.248824	-1.284701
H	-2.970359	0.438720	-2.283479
H	-1.966991	-0.789921	-1.493195
H	-0.482833	1.032465	-2.080206
H	-1.604938	2.264607	-1.473472
H	-2.094089	2.296533	4.351275
H	-1.090693	1.067774	5.141266
H	-2.455976	-0.758009	4.330713
H	-3.578136	0.473890	4.937875
N	-4.392428	-2.760396	3.443508
C	-5.093882	-3.462024	4.071462
C	-5.961120	-4.334546	4.852213
H	-6.276244	-5.200050	4.247738
H	-5.428766	-4.700344	5.744817
H	-6.859390	-3.785457	5.177084
N	-4.046496	-2.759179	-0.954619
C	-4.657658	-3.419231	-1.709283
C	-5.413940	-4.239010	-2.646851
H	-4.878789	-4.310681	-3.607264
H	-5.551221	-5.254344	-2.241841
H	-6.405676	-3.793941	-2.826700
N	-0.013378	4.265281	3.811901
N	0.328731	4.267667	-0.590712
C	0.598242	4.925933	4.565664
C	1.028036	4.968617	-1.221817

C	1.354914	5.747068	5.501720
H	1.839220	6.582584	4.971556
H	0.685969	6.157806	6.274885
H	2.133802	5.142660	5.993650
C	1.892617	5.840276	-2.006481
H	2.791439	5.291811	-2.330880
H	1.358371	6.202346	-2.899476
H	2.206988	6.708245	-1.405157
N	-1.499878	-1.306638	1.483817
N	-2.560870	2.813894	1.373806
C	-2.497799	3.984112	1.387060
C	-1.562652	-2.476863	1.470182
C	-2.406319	5.432503	1.406091
H	-1.941595	5.751618	2.353140
H	-1.770156	5.763520	0.569282
H	-3.405745	5.886655	1.313059
C	-1.653731	-3.925268	1.450674
H	-2.294428	-4.256289	2.284021
H	-2.113149	-4.244529	0.501097
H	-0.654741	-4.379212	1.549235

E = -2917.03580773
G = -2916.508909
E + ΔG_{solv} = -2917.135223

3-PBEBPE-doublet

C	0.698667	0.320872	0.290073
C	0.448468	0.448096	2.887094
C	1.345870	0.628912	1.651030
H	0.360629	-0.726145	0.235953
H	1.442902	0.487989	-0.511501
H	1.026331	0.712335	3.792317
H	0.098932	-0.591764	2.984644
H	1.738896	1.662858	1.643882
H	2.222039	-0.030872	1.766190
C	-4.264130	0.858238	-0.210737
C	-4.512632	0.976057	2.386298
C	-5.127329	0.585828	1.031988
H	-4.808039	0.521940	-1.112414
H	-4.014786	1.927694	-0.293103
H	-5.218914	0.710212	3.194105
H	-4.284472	2.052270	2.430466
H	-6.070187	1.146451	0.916739
H	-5.404971	-0.485710	1.054400
Ni	-1.881605	0.826689	1.329063
N	-0.472468	1.214469	0.047934
N	-0.736922	1.352149	2.803952
N	-3.239005	0.226382	2.613450
N	-2.981902	0.095342	-0.123409
H	-3.456808	-0.776921	2.474716
H	-3.237045	-0.890333	0.067275
H	-0.365372	2.311985	2.670642
H	-0.163472	2.200242	0.175831
C	-2.634503	0.317954	3.985107
C	-1.620058	1.447809	4.011712
C	-2.130151	0.048809	-1.357971
C	-1.106477	1.170792	-1.310526
H	-2.756987	0.115434	-2.263869
H	-1.639243	-0.937567	-1.364459
H	-0.336677	1.051441	-2.093870
H	-1.592684	2.149335	-1.448129
H	-2.122923	2.424036	3.935625
H	-1.014032	1.434442	4.934574
H	-2.156526	-0.654616	4.184744
H	-3.420860	0.466397	4.745123
N	-4.595425	-2.417263	3.375998
C	-5.374043	-3.046055	3.989622
C	-6.339909	-3.825490	4.752935
H	-6.834729	-4.564077	4.102223
H	-5.835556	-4.357910	5.575214
H	-7.108755	-3.162567	5.181330
N	-4.172678	-2.593621	-0.948253
C	-4.768764	-3.310785	-1.661132
C	-5.508168	-4.199091	-2.548455
H	-4.831192	-4.638010	-3.298838
H	-5.974575	-5.013901	-1.972055
H	-6.300029	-3.639702	-3.072015
N	0.711904	3.834113	3.610830
N	0.120695	4.128205	-0.118657
C	1.202186	4.683098	4.254947
C	0.395850	5.202710	-0.499360
C	1.810861	5.736406	5.055879
H	2.798192	6.003849	4.646651
H	1.170044	6.632660	5.055708
H	1.940830	5.395610	6.095565
C	0.734679	6.536294	-0.972846
H	1.801973	6.743033	-0.793678
H	0.534731	6.616687	-2.053420
H	0.130360	7.290796	-0.444028
N	-1.379608	-2.047829	1.499899
C	-1.526966	-3.208412	1.592907
C	-1.712817	-4.646091	1.710065
H	-2.734017	-4.857419	2.065363
H	-1.566063	-5.128646	0.730627
H	-0.988546	-5.067890	2.425293
O	-2.568845	2.696234	1.217468
H	-1.871303	3.348751	1.001408

E = -2860.17141471
G = -2859.671445
E + ΔG_{solv} = -2860.282083

4-PBEPBE-singlet

C	0.808178	0.181215	0.354552
C	0.527233	0.302786	2.972144
C	1.416581	0.505526	1.731207
H	0.559970	-0.883176	0.233439
H	1.550888	0.439782	-0.423768
H	1.091933	0.648999	3.858237
H	0.248152	-0.747121	3.140966
H	1.769873	1.553158	1.726352
H	2.320078	-0.114953	1.854397
C	-4.260404	1.040606	-0.214768
C	-4.529794	1.171839	2.389178
C	-5.158493	0.858249	1.020687
H	-4.835109	0.756700	-1.117135
H	-3.914224	2.077515	-0.327963
H	-5.279578	0.973834	3.179195
H	-4.205212	2.219176	2.473403
H	-6.033604	1.517680	0.896869
H	-5.554681	-0.174720	1.031430
Ni	-1.866317	0.606114	1.380052
N	-0.411532	1.005987	0.099358
N	-0.700717	1.146338	2.878206
N	-3.371839	0.274641	2.658070
N	-3.079469	0.134148	-0.146989
H	-3.714380	-0.707098	2.534879
H	-3.448370	-0.833514	-0.002984
H	-0.352271	2.123708	2.724138
H	-0.144502	2.005113	0.252902
C	-2.750678	0.298278	4.026374
C	-1.593008	1.281139	4.083842
C	-2.191859	0.020763	-1.353707

C	-1.025869	0.994630	-1.277303
H	-2.781392	0.200351	-2.269546
H	-1.843539	-1.023620	-1.387466
H	-0.256342	0.738350	-2.025937
H	-1.355963	2.027609	-1.470388
H	-1.954290	2.320319	4.075075
H	-0.999367	1.132808	5.001968
H	-2.422510	-0.731919	4.238036
H	-3.515298	0.562308	4.777593
N	-4.533659	-2.349263	3.152003
C	-5.310661	-3.036597	3.703336
C	-6.270183	-3.888627	4.387544
H	-6.375739	-4.849400	3.857758
H	-5.935262	-4.087140	5.418953
H	-7.255683	-3.395671	4.424670
N	-4.069685	-2.570265	-0.704372
C	-4.683026	-3.304650	-1.386526
C	-5.437853	-4.216045	-2.231963
H	-4.774385	-4.678272	-2.981355
H	-5.896210	-5.012519	-1.623335
H	-6.238126	-3.669786	-2.758039
N	0.539227	3.656758	3.445940
N	-0.157252	3.908950	0.000634
C	1.032985	4.526645	4.060140
C	0.166180	4.957075	-0.418180
C	1.644546	5.604428	4.821146
H	2.632848	5.854160	4.401803
H	1.005543	6.502068	4.790735
H	1.775008	5.299605	5.872482
C	0.564359	6.252819	-0.937585
H	1.642399	6.413515	-0.771229
H	0.360014	6.307228	-2.019710
H	0.000382	7.052981	-0.430042
N	-1.520343	-1.308576	1.508785
C	-1.527284	-2.477162	1.563551
C	-1.518252	-3.922286	1.624560
H	-1.654315	-4.255563	2.667093
H	-2.348514	-4.308043	1.009135
H	-0.562442	-4.317342	1.240209
O	-2.367943	2.366018	1.298525
H	-1.638980	2.961856	0.993261

E = -2859.75597895
G = -2859.243588
E + ΔG_{solv} = -2860.079481

tBuOOH-6H_2O-PBEPBE

O	0.444537	-0.380035	0.349099
H	1.217631	0.270681	0.455510
O	-0.644092	0.627486	0.213052
O	2.269595	1.595377	0.488696
H	1.861163	2.152034	1.190158
H	1.984420	2.021008	-0.353553
H	-1.550257	4.853771	2.709369
O	-1.456049	4.320231	3.535741
H	-2.337059	4.274049	3.942978
H	-0.378005	3.010008	2.709716
O	0.117641	2.768461	1.887497
H	-0.343114	1.992466	1.484035
H	-0.384459	4.258698	1.083696
O	-0.926293	5.079096	0.897992
H	-0.290645	5.799396	0.741307
H	0.014228	1.547312	-1.236002
O	0.568057	2.196341	-1.744374
H	0.774169	1.766602	-2.593286
H	-1.670319	4.448741	-0.851198
O	-1.811668	3.919506	-1.665836
H	-0.933307	3.521110	-1.844400
C	-1.926310	-0.087210	0.097095
C	-1.941160	-0.876240	-1.217948
H	-2.888791	-1.430726	-1.315139
H	-1.856115	-0.197543	-2.083091
H	-1.110375	-1.597729	-1.243651
C	-2.120900	-0.994675	1.316575
H	-2.043216	-0.413023	2.249791
H	-3.122263	-1.454102	1.278617
H	-1.366190	-1.794230	1.340463
C	-2.937207	1.068452	0.080002
H	-3.939491	0.659258	-0.127300
H	-2.975425	1.575773	1.058721
H	-2.700957	1.819993	-0.693526

E = -766.628185598
G = -766.396936
E + ΔG_{solv} = -766.619359

tBuOH-6H_2O-PBEPBE

O	-0.461934	0.948258	0.176690
H	0.436304	1.341230	-0.226102
H	0.051486	-0.753515	0.681757
H	-1.160391	1.103325	-0.482562
O	3.171069	0.027475	0.792510
H	2.715883	-0.801244	0.541048
O	0.556277	-1.493939	1.111746
O	1.762870	1.879629	-0.584120
H	1.855535	2.730839	-0.078748
H	2.403792	1.237564	-0.146931
H	2.830691	0.170169	1.719584
O	1.686849	0.103615	3.139456
H	1.092386	0.887452	3.133627
H	1.169028	-0.590123	2.661416
O	-0.130293	2.278924	2.478145
H	-0.922639	2.558183	2.967921
H	-0.446149	1.811120	1.643893
O	1.619114	4.012169	1.182990
H	1.013642	3.526939	1.800514
H	2.397416	4.265579	1.707874
C	-0.248863	-2.704960	1.098852
C	0.626279	-3.781610	1.749861
H	0.895206	-3.492264	2.779221
H	0.092552	-4.745116	1.788647
H	1.556847	-3.922118	1.175837
C	-1.532394	-2.471540	1.915093
H	-2.138139	-1.663247	1.469709
H	-2.154332	-3.382363	1.945294
H	-1.283992	-2.188098	2.951320
C	-0.582635	-3.071346	-0.357003
H	0.341628	-3.201170	-0.943303
H	-1.160782	-4.009682	-0.406332
H	-1.185333	-2.278802	-0.833943

E = -691.577324185
G = -691.346295
E + ΔG_{solv} = -691.570311

tBuO$^{\bullet}$-6H_2O-PBEPBE

O	-0.830377	1.121892	0.048579
H	0.025290	1.525430	-0.374403
H	-1.576664	1.499320	-0.447994
O	3.347190	0.931925	0.512237
H	3.910000	0.222834	0.159689
O	1.225325	-2.450416	1.622201

O	1.345560	2.240246	-0.777229
H	1.364818	3.036458	-0.184562
H	2.120767	1.698836	-0.452101
H	2.889772	0.553013	1.324731
O	1.952606	0.042392	2.639721
H	1.167442	0.640676	2.700123
H	1.599353	-0.856857	2.431067
O	-0.183083	1.892704	2.466991
H	-0.908040	1.983238	3.108345
H	-0.592769	1.604558	1.579659
O	1.220425	4.049698	1.362064
H	0.748194	3.382870	1.922976
H	2.096053	4.162759	1.770935
C	-0.001854	-2.975633	1.294595
C	-0.064784	-4.256580	2.224984
H	-0.022388	-3.960215	3.282959
H	-1.026817	-4.752498	2.014519
H	0.767404	-4.936667	1.994676
C	-1.171068	-2.028595	1.634461
H	-1.095513	-1.108981	1.029851
H	-2.139901	-2.510574	1.420205
H	-1.146112	-1.754917	2.702244
C	-0.024751	-3.430620	-0.184649
H	0.814906	-4.112107	-0.391334
H	-0.972943	-3.942666	-0.418063
H	0.066974	-2.548794	-0.838677

E = -690.902177348
G = -690.689036
E + ΔG_{solv} = -690.895474

CH_3CN-PBEPBE

C	-1.642734	1.100005	-0.020938
N	-0.468987	1.099999	-0.020965
C	-3.102801	1.099997	-0.020928
H	-3.484876	2.118162	-0.198621
H	-3.484861	0.437046	-0.813855
H	-3.484917	0.744791	0.949647

E = -132.590353562
G = -132.570386
E + ΔG_{solv} = -132.591818

$6H_2O$-PBEPBE

O	-0.621193	1.072687	0.647852
H	0.017538	0.879400	-0.136373
H	-0.437439	-0.313233	1.793077
H	-1.493703	1.246548	0.255362
O	3.174159	-0.341864	0.054520
H	3.409262	-1.282431	-0.015590
O	-0.061451	-0.990644	2.414847
H	-0.677021	-1.050388	3.164350
O	1.086757	0.553300	-1.231848
H	1.415391	1.331978	-1.713590
H	1.909022	0.152377	-0.777081
H	2.971520	-0.165990	1.038840
O	2.458252	0.191099	2.527816
H	2.148785	1.131999	2.509931
H	1.618844	-0.323319	2.650401
O	1.130175	2.637966	2.131635
H	0.755104	3.171326	2.852116
H	0.362811	2.248579	1.639113

E = -458.178273284
G = -458.071443
E + ΔG_{solv} = -458.180543

H_2O-$6H_2O$-PBEPBE

O	-0.778181	0.741259	0.637709
H	0.051367	0.948084	0.009880
H	-0.492157	-0.810845	1.460193
H	-1.577606	0.866795	0.097890
O	3.289379	0.268533	0.698430
H	3.746238	-0.562047	0.484657
O	-0.090337	-1.525039	2.025158
H	-0.815888	-1.918910	2.537465
O	1.272754	1.344346	-0.711809
H	1.429452	2.291869	-0.451923
H	2.052556	0.855853	-0.306606
H	2.866459	0.138660	1.606264
O	1.950080	0.053236	3.006940
H	1.458476	0.902148	3.079279
H	1.241507	-0.614587	2.805644
O	0.196974	2.354857	2.553391
H	-0.423510	2.756105	3.185665
H	-0.350887	1.816471	1.904332
O	1.542785	3.792585	0.571302
H	1.132672	3.435477	1.399904
H	2.464058	4.005498	0.799989

E = -534.546326505
G = -534.416891
E + ΔG_{solv} = -534.546723

HOOH-$6H_2O$-PBEPBE

O	0.553326	1.325562	0.709562
H	1.274427	1.721598	0.129750
O	-0.665623	1.747186	-0.010353
H	-1.270761	0.891617	0.160913
O	2.337269	2.092271	-1.157681
H	2.576886	3.020834	-1.318961
H	1.745309	1.819094	-1.904790
H	-0.668023	2.040624	3.559581
O	-0.162380	1.239976	3.338321
H	0.193199	1.399219	2.422151
H	-1.925760	-0.721690	1.192968
O	-2.056658	-0.348381	0.272693
H	-1.629694	-0.968562	-0.374654
H	-2.238968	-1.235913	3.458046
O	-1.528511	-1.053415	2.820893
H	-1.057310	-0.231288	3.143233
H	-0.292373	1.437977	-1.579243
O	0.126585	1.113859	-2.450488
H	-0.400461	1.488626	-3.177736
H	0.113119	-2.102201	-1.601935
O	-0.646213	-1.532629	-1.813944
H	-0.259396	-0.689187	-2.159346

E = -609.601178968
G = -609.471739
E + ΔG_{solv} = -609.601690

$OH^{\bullet}$-6H2O-PBEPBE

O	-0.780434	0.748877	0.640586
H	0.047939	0.966402	0.021050
H	-0.477868	-0.805412	1.474354
H	-1.577809	0.855071	0.093483
O	3.279109	0.280205	0.660399
H	3.723088	-0.552247	0.427843
O	-0.060406	-1.505719	2.043214
H	-0.776199	-1.918113	2.554700
O	1.276485	1.376733	-0.699017

H	1.425725	2.329827	-0.484620
H	2.069236	0.898986	-0.294920
H	2.879433	0.152697	1.578682
O	1.980997	0.084731	2.990645
H	1.499260	0.937015	3.070140
H	1.265738	-0.580158	2.803896
O	0.165068	2.385780	2.535119
H	-0.442715	2.756007	3.198369
H	-0.380548	1.821591	1.905150
O	1.392076	3.943137	0.618665
H	1.037892	3.482999	1.444157

E = -533.848847888
G = -533.733885
E + ΔG_{solv} = -533.847963

OH^--6H_2O-PBEPBE

OH--6H2O-PBEPBE

O	-0.679164	0.649550	0.880815
H	0.536328	1.096401	-0.331272
H	-0.152337	-0.594902	1.357003
H	-1.589360	0.664334	0.542308
O	2.941858	-0.460801	0.811840
H	2.156832	-1.050622	0.905466
O	0.427373	-1.407611	1.757638
H	-0.155866	-2.179350	1.835180
O	1.352975	1.358617	-0.847863
H	1.427972	3.154236	-0.223454
H	2.057414	0.822338	-0.410097
H	2.912965	0.009212	1.680770
O	1.934527	0.377477	3.413577
H	1.398093	1.183390	3.191652
H	1.350229	-0.358477	3.111475
O	0.169562	2.391877	2.502472
H	-0.524445	2.666254	3.124488
H	-0.286927	1.709942	1.832096
O	1.319086	3.987453	0.303028
H	0.948950	3.639094	1.144776

E = -534.011007562
G = -533.895780
E + ΔG_{solv} = -534.070545

H_3O^+-6H_2O-PBEPBE

O	-1.058234	0.653880	0.531074
H	0.399599	1.093817	-0.611792
H	-0.464815	-1.015747	1.092404
H	-1.979069	0.748097	0.225395
O	2.378239	-0.391489	0.852778
H	1.571785	-1.013553	1.092626
O	0.246471	-1.615517	1.434149
H	0.020696	-2.534833	1.206034
O	1.369652	1.197136	-0.782785
H	1.596167	2.119290	-0.510210
H	2.011887	0.278765	0.084049
H	2.560979	0.194790	1.653542
O	2.565994	1.489021	2.739246
H	1.633411	1.692755	3.001790
H	3.086483	1.388214	3.557846
O	-0.049024	2.458426	2.398462
H	-0.599075	2.952323	3.034654
H	-0.925491	1.309414	1.266786
O	1.931448	3.505927	0.783208
H	0.421521	3.129758	1.840029
H	2.630129	3.154168	1.378655
H	2.230902	4.383721	0.481035

E = -534.918298298
G = -534.774995
E + ΔG_{solv} = -534.979504

1-BHLYP

C	0.634650	0.522509	0.300576
C	0.431606	0.523245	2.953218
C	1.229468	0.850366	1.680133
H	0.409880	-0.534442	0.215963
H	1.384210	0.760284	-0.454296
H	1.055813	0.765972	3.813229
H	0.200628	-0.534650	3.006369
H	1.480859	1.912074	1.699032
H	2.178265	0.323600	1.752802
C	-4.492220	0.983790	-0.096679
C	-4.695203	0.984616	2.555968
C	-5.290132	0.656875	1.176429
H	-5.116428	0.741089	-0.956696
H	-4.261095	2.041648	-0.149893
H	-5.444772	0.746959	3.310869
H	-4.470245	2.041529	2.640585
H	-6.238812	1.183853	1.103770
H	-5.541730	-0.404787	1.157588
Ni	-2.030301	0.753451	1.428279
N	-0.594671	1.298180	0.057136
N	-0.822828	1.295649	3.003085
N	-3.466014	0.208715	2.799313
N	-3.237882	0.211225	-0.146453
H	-3.707661	-0.762341	2.654158
H	-3.497250	-0.760040	-0.038805
H	-0.563547	2.266957	2.895622
H	-0.353191	2.269297	0.202134
C	-2.824141	0.255198	4.129611
C	-1.660911	1.249612	4.219106
C	-2.399801	0.257006	-1.362474
C	-1.236529	1.251399	-1.273165
H	-2.993554	0.487448	-2.245717
H	-2.012104	-0.747533	-1.497985
H	-0.514460	1.020619	-2.054909
H	-1.599096	2.255885	-1.466611
H	-2.048636	2.254110	4.354822
H	-1.067158	1.019036	5.102313
H	-2.461524	-0.749324	4.322798
H	-3.546192	0.485763	4.911434
N	-4.368476	-2.777871	3.480804
C	-5.062359	-3.444295	4.106991
C	-5.941149	-4.289932	4.903053
H	-6.263730	-5.143284	4.315889
H	-5.414580	-4.642438	5.783737
H	-6.813123	-3.724078	5.213912
N	-4.007832	-2.771471	-0.995908
C	-4.589865	-3.421781	-1.741611
C	-5.326918	-4.246056	-2.689493
H	-4.773436	-4.322045	-3.619551
H	-5.471449	-5.240269	-2.279997
H	-6.296071	-3.800585	-2.888136
N	-0.052954	4.277695	3.853016
N	0.305979	4.284871	-0.627421
C	0.527667	4.928805	4.599120
C	0.998859	4.950774	-1.255271
C	1.262674	5.754657	5.547215
H	1.733638	6.582658	5.027993
H	0.584519	6.145222	6.298705
H	2.028602	5.160935	6.035083
C	1.876374	5.795739	-2.053455

H	2.749494	5.230601	-2.362394
H	1.349462	6.144763	-2.935320
H	2.197179	6.651372	-1.468643
N	-1.505169	-1.460033	1.464606
N	-2.555291	2.967186	1.391726
C	-2.473064	4.109080	1.403703
C	-1.587187	-2.601931	1.451981
C	-2.357062	5.555907	1.419938
H	-1.901652	5.859411	2.356449
H	-1.722941	5.864199	0.595660
H	-3.337665	6.009432	1.321608
C	-1.702914	-4.048764	1.434920
H	-2.343149	-4.356970	2.254498
H	-2.151260	-4.352406	0.495059
H	-0.723030	-4.502182	1.540633

E = -2918.18543726
G = -2917.617312
E + ΔG_{solv} = -2918.284094

3-BHLYP-Doublet

C	0.678659	0.325352	0.291238
C	0.413045	0.472416	2.880747
C	1.301050	0.648812	1.649532
H	0.397893	-0.718313	0.219098
H	1.409844	0.534192	-0.487105
H	0.971212	0.787412	3.758852
H	0.111279	-0.559253	3.014817
H	1.664860	1.675549	1.634166
H	2.177354	0.018256	1.773602
C	-4.308844	0.846585	-0.242820
C	-4.569951	0.990508	2.338872
C	-5.165561	0.584718	0.993139
H	-4.840063	0.492992	-1.123850
H	-4.081354	1.899443	-0.341035
H	-5.269522	0.725607	3.128681
H	-4.358334	2.050924	2.371578
H	-6.098807	1.127506	0.868487
H	-5.430255	-0.473313	1.025133
Ni	-1.939927	0.813121	1.306311
N	-0.516633	1.163399	0.052241
N	-0.793504	1.318487	2.767997
N	-3.302261	0.259283	2.582324
N	-3.028248	0.104671	-0.145926
H	-3.510847	-0.725785	2.459984
H	-3.270242	-0.862035	0.043382
H	-0.462016	2.260792	2.592173
H	-0.237780	2.132454	0.189581
C	-2.718542	0.367367	3.944578
C	-1.663094	1.446611	3.964851
C	-2.184019	0.057459	-1.366907
C	-1.122218	1.130199	-1.303135
H	-2.795898	0.168698	-2.257596
H	-1.735290	-0.929650	-1.399530
H	-0.356807	0.972654	-2.058946
H	-1.559488	2.109009	-1.462556
H	-2.122001	2.425233	3.896105
H	-1.066673	1.406519	4.871937
H	-2.290555	-0.601338	4.180468
H	-3.495987	0.569654	4.675850
N	-4.503893	-2.464077	3.437448
C	-5.261221	-3.053568	4.067293
C	-6.221326	-3.800357	4.868250
H	-6.700364	-4.558737	4.257979
H	-5.714284	-4.279190	5.699420
H	-6.978800	-3.126918	5.255559
N	-4.013063	-2.713453	-0.949046
C	-4.598320	-3.404338	-1.654579
C	-5.339791	-4.279311	-2.552202
H	-4.667776	-4.704839	-3.290155
H	-5.802501	-5.081564	-1.987125
H	-6.112813	-3.713043	-3.061171
N	0.773028	3.690075	3.738201
N	0.141038	4.075826	-0.178052
C	1.275586	4.506348	4.368407
C	0.407814	5.134435	-0.529009
C	1.912911	5.541108	5.170326
H	2.881676	5.788974	4.749510
H	1.291438	6.430311	5.184536
H	2.048554	5.187069	6.186885
C	0.744505	6.477513	-0.976622
H	1.791831	6.679016	-0.777647
H	0.561844	6.565131	-2.042522
H	0.133253	7.203133	-0.450278
N	-1.443311	-1.769141	1.500826
C	-1.586809	-2.904811	1.568217
C	-1.779090	-4.341823	1.655314
H	-2.564004	-4.548820	2.374953
H	-2.072232	-4.723620	0.683255
H	-0.858396	-4.821097	1.971243
O	-2.606782	2.614397	1.195950
H	-1.997307	3.302395	0.940649

E = -2861.19946118
G =
E + ΔG_{solv} = -2861.314249

4-BHLYP-singlet

C	0.754599	0.170251	0.372378
C	0.452988	0.320985	2.963362
C	1.353886	0.487422	1.741070
H	0.504513	-0.875394	0.253068
H	1.485277	0.424267	-0.392136
H	0.990937	0.686189	3.834517
H	0.172995	-0.707362	3.148822
H	1.723503	1.511660	1.730755
H	2.227648	-0.143950	1.876956
C	-4.263430	1.036406	-0.251956
C	-4.558276	1.183405	2.328191
C	-5.164242	0.860752	0.966199
H	-4.806301	0.713760	-1.137671
H	-3.950540	2.061522	-0.386036
H	-5.289339	0.951950	3.099781
H	-4.273268	2.221673	2.418407
H	-6.032066	1.500177	0.830936
H	-5.542748	-0.161455	0.980207
Ni	-1.904026	0.644619	1.355488
N	-0.455794	0.995591	0.120732
N	-0.766369	1.154781	2.824974
N	-3.373650	0.328201	2.591669
N	-3.063035	0.169574	-0.140554
H	-3.689099	-0.635291	2.472844
H	-3.413851	-0.775723	0.015021
H	-0.415191	2.098079	2.652677
H	-0.173554	1.963629	0.272639
C	-2.800387	0.367309	3.966981
C	-1.640351	1.327914	4.023074
C	-2.195655	0.043515	-1.345342
C	-1.027577	0.994466	-1.259769
H	-2.779115	0.232467	-2.241447
H	-1.863168	-0.987538	-1.384022
H	-0.256317	0.727839	-1.976372
H	-1.335981	2.013224	-1.463726
H	-1.982459	2.354849	4.002578

H	-1.054780	1.184395	4.925646
H	-2.492479	-0.644426	4.206221
H	-3.570516	0.652315	4.677434
N	-4.455221	-2.361647	3.195474
C	-5.204255	-3.030171	3.754298
C	-6.152603	-3.875099	4.465488
H	-6.244967	-4.831866	3.961659
H	-5.808627	-4.038730	5.481873
H	-7.124433	-3.392266	4.492081
N	-3.988954	-2.601073	-0.726544
C	-4.577084	-3.327395	-1.395287
C	-5.319342	-4.247497	-2.244843
H	-4.648615	-4.705201	-2.965125
H	-5.776046	-5.023063	-1.638460
H	-6.097371	-3.708304	-2.776077
N	0.617578	3.594005	3.506508
N	-0.235525	3.937634	-0.009723
C	1.139184	4.422535	4.106149
C	0.085099	4.969045	-0.399477
C	1.800089	5.471385	4.868835
H	2.766780	5.693167	4.428274
H	1.189443	6.368550	4.865233
H	1.944205	5.144053	5.893542
C	0.489543	6.274192	-0.895796
H	1.553509	6.414163	-0.732537
H	0.278920	6.343339	-1.958424
H	-0.060371	7.049730	-0.371785
N	-1.553734	-1.298605	1.507259
C	-1.581140	-2.439923	1.576336
C	-1.603107	-3.885884	1.659114
H	-1.677302	-4.186289	2.699804
H	-2.468458	-4.244473	1.110489
H	-0.694344	-4.292468	1.224548
O	-2.391127	2.343208	1.266426
H	-1.704526	2.933356	0.931607

E = -2860.72068969
G = -2860.165364
E + ΔG_{solv} = -2861.048289

tBuOOH-6H_2O-BHLYP

O	0.403758	-0.390325	0.265650
H	1.169184	0.200033	0.418936
O	-0.644089	0.580299	0.188618
O	2.254126	1.581343	0.503667
H	1.886682	2.126550	1.204325
H	2.026397	2.025065	-0.317968
H	-1.664394	4.858700	2.676666
O	-1.631307	4.278124	3.443485
H	-2.420756	4.414206	3.957917
H	-0.411840	2.971191	2.688487
O	0.103216	2.752107	1.904136
H	-0.326330	2.006609	1.470506
H	-0.318420	4.345826	1.088204
O	-0.827479	5.148432	0.894703
H	-0.205014	5.857217	0.754628
H	0.037249	1.562762	-1.283437
O	0.577113	2.198010	-1.771541
H	0.770777	1.809441	-2.621072
H	-1.651922	4.482361	-0.842301
O	-1.784962	3.931301	-1.615418
H	-0.927068	3.550432	-1.808799
C	-1.913704	-0.106243	0.102269
C	-1.971752	-0.880744	-1.205554
H	-2.924932	-1.395769	-1.288813
H	-1.879891	-0.207474	-2.054354
H	-1.177071	-1.617296	-1.252899
C	-2.083655	-1.017156	1.307515
H	-1.973506	-0.453200	2.229961
H	-3.077733	-1.456164	1.293447
H	-1.351108	-1.815780	1.303419
C	-2.919835	1.034746	0.119676
H	-3.918565	0.633468	-0.028532
H	-2.905264	1.549666	1.077215
H	-2.720128	1.762598	-0.661937

E = -767.071656392
G = -766.823261
E + ΔG_{solv} = -767.062252

tBuOH-6H_2O-BHLYP

O	-0.571204	0.992247	0.168667
H	0.275752	1.330217	-0.232418
H	-0.039571	-0.754082	0.755052
H	-1.265550	1.142356	-0.467481
O	3.064432	-0.154732	0.707963
H	2.442873	-0.875291	0.587419
O	0.463426	-1.464847	1.172741
O	1.735035	1.863354	-0.640686
H	1.898239	2.687546	-0.165530
H	2.355515	1.209470	-0.279615
H	2.929277	0.091794	1.630637
O	1.710882	0.156972	3.197758
H	1.155802	0.939791	3.197313
H	1.189019	-0.523021	2.761564
O	-0.125942	2.342478	2.526781
H	-0.874321	2.645378	3.033749
H	-0.466136	1.894557	1.734292
O	1.752900	3.981933	1.203302
H	1.146609	3.549197	1.815756
H	2.497827	4.294294	1.708493
C	-0.250300	-2.701497	1.103340
C	0.646474	-3.728416	1.773862
H	0.845731	-3.445014	2.803850
H	0.175882	-4.707879	1.772097
H	1.596227	-3.802906	1.251273
C	-1.570400	-2.560287	1.852812
H	-2.192421	-1.792119	1.397340
H	-2.127714	-3.493664	1.838536
H	-1.390476	-2.284013	2.888293
C	-0.489668	-3.059145	-0.358718
H	0.454680	-3.128511	-0.891441
H	-1.005225	-4.012346	-0.446005
H	-1.100675	-2.302479	-0.847036

E = -691.993330626
G = -691.744974
E + ΔG_{solv} = -691.986568

tBuO$^{\bullet}$-6H_2O-BHLYP

O	-0.933420	0.978758	-0.008920
H	-0.112758	1.279993	-0.454151
H	-1.659505	1.216563	-0.578523
O	3.439987	1.487590	0.959376
H	4.375566	1.324829	1.034120
O	1.129559	-2.386910	1.490588
O	1.340667	2.015343	-0.960697
H	1.358741	2.829052	-0.437602
H	2.133849	1.560231	-0.665919
H	2.988059	0.920085	1.613071
O	1.901457	0.127741	2.702159
H	1.116803	0.683940	2.766494
H	1.609985	-0.736415	2.399379

O	-0.276118	1.933567	2.443565
H	-0.976337	2.118707	3.062711
H	-0.680593	1.625598	1.612373
O	1.660451	3.754549	1.208800
H	1.010367	3.344421	1.785016
H	2.465940	3.244214	1.328243
C	-0.105008	-2.997726	1.287407
C	0.004083	-4.318116	2.067890
H	0.172852	-4.130154	3.123839
H	-0.929598	-4.863056	1.959056
H	0.815868	-4.926641	1.683395
C	-1.235554	-2.126923	1.824464
H	-1.258338	-1.176310	1.298964
H	-2.196426	-2.617779	1.688992
H	-1.095596	-1.938491	2.886008
C	-0.258538	-3.267664	-0.209259
H	0.563843	-3.876077	-0.572230
H	-1.193840	-3.787969	-0.398824
H	-0.271437	-2.332224	-0.760986

E = -691.321607389
G = -691.091312
E + ΔG_{solv} = -691.312793

CH_3CN-BHLYP

C	-1.646460	1.099997	-0.020946
N	-0.499579	1.100006	-0.020947
C	-3.103037	1.099993	-0.020939
H	-3.473359	2.104650	-0.196261
H	-3.473365	0.445844	-0.803337
H	-3.473379	0.749509	0.936770

E = -132.678684974
G = -132.655714
E + ΔG_{solv} = -132.680543

$6H_2O$-BHLYP

O	-0.684769	1.095074	0.620587
H	-0.060148	0.910700	-0.116302
H	-0.469871	-0.306826	1.856783
H	-1.537837	1.257982	0.227669
O	3.218867	-0.405295	0.029558
H	3.574440	-1.286747	-0.029510
O	-0.103369	-0.942973	2.483377
H	-0.756699	-1.096797	3.158720
O	1.105383	0.583169	-1.277117
H	1.447319	1.309635	-1.790862
H	1.880544	0.149933	-0.866840
H	3.043024	-0.220375	0.974729
O	2.478208	0.176870	2.543389
H	2.199383	1.098982	2.560698
H	1.670299	-0.325660	2.700194
O	1.083541	2.626214	2.203862
H	0.735146	3.256548	2.826688
H	0.343350	2.268957	1.699753

E = -458.426816373
G = -458.312483
E + ΔG_{solv} = -458.428429

H_2O-$6H_2O$-BHLYP

O	-0.772920	0.735666	0.592945
H	-0.018173	0.992315	-0.007133
H	-0.154574	-0.837743	1.364331
H	-1.574533	0.775520	0.078062
O	2.918654	-0.333599	0.663086
H	2.360221	-1.108224	0.733649
O	0.400993	-1.487581	1.817332
H	-0.118792	-2.274996	1.948988
O	1.328100	1.424789	-0.749686
H	1.559230	2.318882	-0.468821
H	2.014837	0.836693	-0.394282
H	2.891872	0.041026	1.553129
O	2.038433	0.402196	3.250017
H	1.478978	1.181210	3.210104
H	1.446470	-0.342018	3.114866
O	0.077540	2.462745	2.568117
H	-0.564664	2.852377	3.155192
H	-0.399998	1.897249	1.939098
O	1.634931	3.837575	0.650806
H	1.170281	3.526151	1.435972
H	2.449302	4.240114	0.937981

E = -534.834421860
G = -534.693631
E + ΔG_{solv} = -534.834855

$HOOH$-$6H_2O$-BHLYP

O	0.539753	1.090195	0.487430
H	1.240356	1.525885	-0.032866
O	-0.642613	1.695699	-0.038842
H	-1.313287	0.978292	0.130659
O	2.287977	2.010128	-1.344500
H	2.727438	2.848650	-1.450879
H	1.717719	1.869224	-2.109744
H	-0.228601	1.768467	3.590320
O	-0.036381	0.911164	3.220792
H	0.272661	1.058464	2.317809
H	-2.340109	-0.632919	1.149815
O	-2.249988	-0.317583	0.238209
H	-1.732205	-0.965938	-0.252016
H	-2.032933	-1.662976	3.418520
O	-2.133182	-0.848690	2.935262
H	-1.388164	-0.273301	3.166354
H	-0.428277	1.543547	-1.863650
O	0.003286	1.279325	-2.691595
H	-0.551465	1.557749	-3.415046
H	0.475386	-0.869324	-0.572666
O	-0.055975	-1.332554	-1.221620
H	-0.013406	-0.778324	-2.002766

E = -609.915841150
G = -609.774492
E + ΔG_{solv} = -609.914059

$OH^{\bullet}$-6H2O-BHLYP

O	-0.787359	0.750249	0.596710
H	-0.032781	1.021595	0.008215
H	-0.142856	-0.830626	1.356297
H	-1.582928	0.769102	0.071204
O	2.929150	-0.270360	0.647871
H	2.379370	-1.051050	0.721258
O	0.433901	-1.465476	1.802426
H	-0.061529	-2.268174	1.936220
O	1.329626	1.470728	-0.726463
H	1.572510	2.371092	-0.494950
H	2.023866	0.888562	-0.369768
H	2.917728	0.094369	1.542426
O	2.049504	0.440421	3.235042
H	1.492178	1.220466	3.205767
H	1.457425	-0.302639	3.094426

O	0.029801	2.488445	2.563289
H	-0.591838	2.835078	3.197903
H	-0.450650	1.901340	1.956837
O	1.531554	4.004467	0.746454
H	1.049395	3.590818	1.490733

E = -534.147960325
G = -534.021593
E + ΔG_{solv} = -534.146592

OH^--6H_2O-BHLYP

O	-0.705260	0.641243	0.889921
H	0.539490	1.090560	-0.292744
H	-0.128738	-0.633894	1.371852
H	-1.570061	0.659948	0.493143
O	2.957331	-0.529557	0.807854
H	2.171587	-1.075005	0.920157
O	0.419134	-1.416205	1.752674
H	-0.156539	-2.168817	1.831960
O	1.324956	1.349836	-0.813917
H	1.431419	3.196865	-0.203759
H	2.034197	0.812279	-0.450390
H	2.983573	-0.037127	1.633702
O	1.925518	0.395733	3.407042
H	1.418610	1.191333	3.199653
H	1.363222	-0.325468	3.106489
O	0.117926	2.416523	2.498893
H	-0.573047	2.691243	3.092828
H	-0.295399	1.750928	1.851929
O	1.334381	3.992329	0.334558
H	0.953765	3.655666	1.150051

E = -534.289541906
G = -534.162619
E + ΔG_{solv} = -534.348499

H_3O^+-6H_2O-BHLYP

O	-1.098690	0.642816	0.552804
H	0.410355	1.112631	-0.649449
H	-0.472340	-1.096165	1.064887
H	-2.005972	0.732861	0.266066
O	2.364515	-0.376859	0.875351
H	1.612672	-1.018770	1.075016
O	0.254772	-1.667196	1.343871
H	0.010396	-2.584073	1.240225
O	1.363694	1.218902	-0.748728
H	1.576609	2.133299	-0.532034
H	2.033398	0.256778	0.131554
H	2.541037	0.182656	1.668836
O	2.541401	1.441927	2.770257
H	1.637477	1.700418	2.995535
H	3.043318	1.358686	3.579905
O	-0.031868	2.508689	2.407752
H	-0.572073	2.986477	3.035634
H	-0.951688	1.277813	1.267122
O	1.976140	3.560400	0.770601
H	0.418568	3.159113	1.853045
H	2.680595	3.228887	1.332612
H	2.247343	4.419076	0.448115

E = -535.210495590
G = -535.055823
E + ΔG_{solv} = -535.269474