Supporting Information: DFT

Pyrazinacene Conjugated Polymers:

A Breakthrough in Synthesis and Unraveling the Conjugation Continuum

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Contents

The default integration grid in Gaussian 16, Ultrafine, was used.

Optimized Geometry Coordinates

1.0 N6P-Br coordinates

Electronic Energy (EE:) -6702.104156 Hartree
EE + Thermal Free Energy Correction: -6701.808407 Hartree
E (Thermal): 249.536 kcal/mol
Entropy (S): 216.480 cal/mol-kelvin
Imaginary Freq: 0

0	1		
C	-5.24278	-0.71154	-0.00748
C	-4.04439	-1.40511	-0.01071
C	-4.04438	1.40512	0.010726
C	-5.24279	0.711554	0.007381
O	-6.43709	1.367568	-0.03341
O	-6.43711	-1.36752	0.033135
C	-7.14793	1.425925	1.217033
H	-8.06862	1.969417	1.010558
H	-7.3801	0.421506	1.577055
H	-6.56185	1.971334	1.962096
C	-7.14762	-1.42603	-1.21749
H	-8.06829	-1.96965	-1.01123
H	-7.37986	-0.42165	-1.57759
H	-6.56129	-1.97137	-1.96239
N	-1.63176	-1.4048	0.002421
C	-0.5271	-0.72147	0.001834
C	-0.5271	0.72147	-0.00157
N	-1.63175	1.404808	-0.00224
C	-2.80972	0.714181	-0.00088
C	-2.80972	-0.71417	0.000991
C	6.615609	-0.70689	0.009671
C	5.41973	-1.42676	0.019731
C	5.419731	1.426743	-0.0197
C	6.615611	0.706869	-0.00975
C	5.437849	2.847893	-0.04239
C	5.462511	4.050756	-0.0729
H	5.479646	5.112578	-0.09023
C	5.437851	-2.84792	0.04243
C	5.462513	-4.05078	0.07295
H	5.479655	-5.1126	0.090338
O	7.806144	1.375386	0.026392

O	7.806128	-1.37542	-0.02663
C	8.519767	1.422807	-1.22148
H	9.435475	1.977282	-1.02129
H	8.762124	0.416058	-1.56896
H	7.931009	1.95285	-1.97589
C	8.520029	-1.42269	1.221098
H	9.435884	-1.97685	1.020669
H	8.762153	-0.41589	1.568584
H	7.931598	-1.953	1.975572
N	3.0117	-1.40634	0.00701
C	1.907944	-0.72048	0.003585
C	1.907943	0.720466	-0.00332
N	3.0117	1.406328	-0.00683
C	4.187565	0.710466	-0.00305
C	4.187565	-0.71048	0.003163
N	0.689218	1.373937	-0.00496
N	0.689217	-1.37395	0.005325
H	0.69015	-2.38637	0.008691
H	0.690157	2.386367	-0.00839
Br	-4.06862	-3.30834	-0.02877
Br	-4.06861	3.308348	0.028837

2.0 N6P-Br dimer coordinates

N6P-Br Hg dimer: 0 degrees

Electronic Energy (EE:) -13556.085340 Hartree
EE + Thermal Free Energy Correction: -13555.497569 Hartree
E (Thermal): 489.762 kcal/mol
Entropy (S): 407.587 cal/mol-kelvin
Imaginary Freq: 0

0	1		
C	7.180255	-5.79034	0.601271
C	7.824736	-4.58459	0.382311
C	5.032704	-4.65181	0.697761
C	5.766826	-5.82397	0.763803
O	5.155687	-7.0307	0.933062
O	7.880807	-6.95412	0.716383
C	5.243033	-7.58144	2.260161
H	4.716856	-8.53399	2.22204
H	6.285183	-7.74174	2.544249

H	4.749674	-6.92101	2.978804
C	7.843703	-7.8092	-0.441
H	8.437487	-8.68475	-0.18303
H	6.818218	-8.10757	-0.6685
H	8.293068	-7.30436	-1.30082
N	7.735481	-2.18952	0.105647
C	7.014803	-1.11052	0.045663
C	5.580431	-1.1464	0.196945
N	4.942253	-2.2593	0.400068
C	5.672698	-3.41103	0.467583
C	7.092836	-3.37539	0.318572
C	6.735678	5.976424	-0.79999
C	7.495788	4.807831	-0.72631
C	4.654562	4.737132	-0.44864
C	5.329597	5.941624	-0.66282
C	3.242313	4.721553	-0.31394
C	8.909383	4.861485	-0.86352
C	10.10691	4.917679	-0.97002
H	11.16312	4.961461	-1.07281
O	4.627384	7.11319	-0.69472
O	7.352977	7.168728	-1.05251
C	4.424157	7.66792	-2.00618
H	3.865045	8.590713	-1.85798
H	5.379994	7.885134	-2.48793
H	3.836124	6.980966	-2.62183
C	7.517332	8.026408	0.090003
H	8.016132	8.922049	-0.2776
H	6.548618	8.289742	0.520647
H	8.147243	7.541794	0.84173
N	7.562811	2.417539	-0.44743
C	6.922323	1.305476	-0.24382
C	5.489636	1.269727	-0.09353
N	4.76717	2.348446	-0.15305
C	5.414623	3.532689	-0.36544
C	6.827251	3.566868	-0.51552
N	4.885923	0.044159	0.120109
N	7.617787	0.112686	-0.16711
H	8.624276	0.139122	-0.27339
H	3.879408	0.018465	0.226115
Br	9.716181	-4.56338	0.168888
Br	3.143479	-4.72115	0.917615

C	-3.24251	4.721557	0.3138
C	-4.65475	4.737066	0.448604
C	-5.32983	5.941523	0.66284
C	-5.41476	3.53259	0.365425
C	-6.7359	5.976258	0.80011
O	-4.62767	7.113127	0.694697
N	-4.76727	2.348382	0.152969
C	-6.82738	3.566702	0.515615
C	-7.49596	4.807629	0.72648
O	-7.35323	7.168528	1.052691
C	-4.42434	7.66782	2.006159
C	-5.48969	1.26963	0.09348
N	-7.56289	2.41734	0.447557
C	-8.90955	4.861217	0.863782
C	-7.51768	8.026234	-0.08979
H	-3.86528	8.590645	1.857934
H	-5.38013	7.884972	2.488016
H	-3.83621	6.980872	2.621724
C	-6.92237	1.30531	0.243874
N	-4.88594	0.044093	-0.12022
C	-10.1071	4.917357	0.970359
H	-8.01651	8.921841	0.277866
H	-6.549	8.289624	-0.52047
H	-8.14761	7.541611	-0.8415
N	-7.61778	0.11249	0.167194
C	-5.58039	-1.1465	-0.197
H	-3.87943	0.018445	-0.22629
C	-7.01476	-1.11069	-0.04562
H	-8.62427	0.138877	0.273561
N	-4.94218	-2.25937	-0.40017
N	-7.73539	-2.18972	-0.10555
C	-5.67257	-3.41113	-0.46764
C	-7.0927	-3.37556	-0.31852
C	-5.03254	-4.65188	-0.69786
C	-7.82455	-4.5848	-0.38221
C	-5.76661	-5.82408	-0.76385
Br	-3.14332	-4.72113	-0.91786
C	-7.18003	-5.79052	-0.60121
Br	-9.71598	-4.56368	-0.16864
O	-5.15542	-7.03077	-0.93316
O	-7.88053	-6.95433	-0.71627

C	-5.24286	-7.58154	-2.26024
C	-7.8433	-7.8094	0.441115
H	-4.71662	-8.53406	-2.22216
H	-6.28502	-7.74189	-2.54424
H	-4.7496	-6.92108	-2.97894
H	-8.43707	-8.68498	0.183196
H	-6.81779	-8.10773	0.668539
H	-8.29262	-7.30458	1.300968
H	-11.1633	4.961069	1.073202
C	2.031671	4.719161	-0.20168
Hg	-0.0001	4.716118	-0.0001
C	-2.03187	4.719182	0.201502

N6P-Br Hg dimer: 90 degrees

Electronic Energy (EE:) -13556.085282 Hartree
EE + Thermal Free Energy Correction: -13555.498444 Hartree
E (Thermal): 489.757 kcal/mol
Entropy (S): 409.537 cal/mol-kelvin
Imaginary Freq: 0

0	1		
C	9.922051	-4.20847	-2.01327
C	9.997024	-3.33443	-0.942
C	7.700725	-3.38271	-2.56145
C	8.757801	-4.23535	-2.83127
O	8.730495	-5.07491	-3.90495
O	10.92823	-5.08988	-2.27623
C	8.457213	-6.45454	-3.59804
H	8.477589	-6.98081	-4.55109
H	9.220399	-6.8607	-2.93097
H	7.465665	-6.55438	-3.14757
C	11.78403	-4.73319	-3.37739
H	12.51781	-5.53394	-3.45517
H	11.21137	-4.6604	-4.3043
H	12.29546	-3.78884	-3.17071
N	9.003126	-1.60496	0.415228
C	7.994323	-0.81715	0.636348
C	6.820777	-0.83277	-0.20299
N	6.717388	-1.63626	-1.21833
C	7.761945	-2.47715	-1.47601
C	8.924004	-2.46112	-0.64561

C	5.052234	4.32141	4.631055
C	6.124657	3.46257	4.383964
C	3.813072	3.453397	2.707226
C	3.908503	4.317669	3.800805
C	2.657687	3.462572	1.883825
C	7.266164	3.478026	5.230548
C	8.224192	3.490326	5.958967
H	9.075537	3.504317	6.593848
O	2.86133	5.141105	4.103816
O	5.124007	5.211504	5.664991
C	3.046269	6.522035	3.746745
H	2.138968	7.036596	4.060035
H	3.910916	6.94422	4.263458
H	3.165613	6.621198	2.66381
C	4.368467	4.851837	6.834628
H	4.528279	5.654943	7.552657
H	3.304979	4.768459	6.599605
H	4.739369	3.911242	7.252223
N	7.099083	1.737113	3.016559
C	6.994377	0.935652	1.999175
C	5.823463	0.921874	1.159549
N	4.813873	1.710436	1.378366
C	4.896466	2.563813	2.442101
C	6.051859	2.577453	3.269191
N	5.792021	0.037213	0.097131
N	8.025625	0.065034	1.697341
H	8.848182	0.076241	2.28751
H	4.968848	0.026313	-0.49217
Br	11.56364	-3.31676	0.139067
Br	6.153985	-3.43543	-3.66959
C	-2.65753	3.462357	-1.88394
C	-3.81295	3.453264	-2.70729
C	-3.90837	4.317546	-3.80086
C	-4.89639	2.563742	-2.44214
C	-5.05211	4.321333	-4.6311
O	-2.86118	5.140958	-4.10388
N	-4.81383	1.710376	-1.37839
C	-6.0518	2.577432	-3.26921
C	-6.12458	3.462548	-4.38398
O	-5.12387	5.211416	-5.66504
C	-3.04605	6.521868	-3.7467

C	-5.82345	0.921861	-1.15955
N	-7.09906	1.737141	-3.01655
C	-7.26609	3.478052	-5.23055
C	-4.36835	4.851726	-6.83468
H	-2.13876	7.036431	-4.06003
H	-3.91073	6.944113	-4.26331
H	-3.16529	6.620959	-2.66374
C	-6.99437	0.93568	-1.99916
N	-5.79203	0.037213	-0.09712
C	-8.22413	3.49039	-5.95896
H	-4.52819	5.654803	-7.55273
H	-3.30485	4.768374	-6.59968
H	-4.73924	3.911109	-7.25224
N	-8.02565	0.065108	-1.69731
C	-6.82082	-0.83273	0.20302
H	-4.96885	0.026282	0.492163
C	-7.99437	-0.81707	-0.63632
H	-8.84821	0.076334	-2.28748
N	-6.71746	-1.63621	1.218362
N	-9.00319	-1.60487	-0.4152
C	-7.76204	-2.47707	1.47605
C	-8.92409	-2.46101	0.645646
C	-7.70084	-3.38262	2.561497
C	-9.99714	-3.3343	0.942044
C	-8.75794	-4.23523	2.831325
Br	-6.1541	-3.43538	3.669637
C	-9.92219	-4.20833	2.013327
Br	-11.5637	-3.31661	-0.13904
O	-8.73066	-5.0748	3.905005
O	-10.9284	-5.0897	2.276273
C	-8.4574	-6.45443	3.598054
C	-11.7841	-4.73308	3.377544
H	-8.47776	-6.98072	4.551098
H	-9.22061	-6.86056	2.930999
H	-7.46587	-6.55427	3.147559
H	-12.5179	-5.53379	3.455271
H	-11.2114	-4.66045	4.304424
H	-12.2955	-3.78868	3.171019
H	-9.07545	3.504352	-6.59387
C	1.665918	3.475918	1.180678
Hg	0.000075	3.477726	-5.3E-05

C	-1.66575	3.475762	-1.1808

N6P-Br Hg dimer: 180 degrees

Electronic Energy (EE:) -13556.085424 Hartree
EE + Thermal Free Energy Correction: -13555.498501 Hartree
E (Thermal): 489.751 kcal/mol
Entropy (S): 409.337 cal/mol-kelvin
Imaginary Freq: 0

0	1		
C	-12.5899	1.513291	-0.54915
C	-12.1066	0.21965	-0.44812
C	-10.3272	2.394222	-0.40778
C	-11.6891	2.614718	-0.52544
O	-12.1897	3.874268	-0.67133
O	-13.9282	1.762707	-0.62062
C	-12.7916	4.435765	0.509666
H	-13.1427	5.425688	0.222491
H	-13.6322	3.823947	0.843443
H	-12.0487	4.529444	1.306796
C	-14.4207	2.099127	-1.9308
H	-15.489	2.272789	-1.81127
H	-13.9354	3.002484	-2.30608
H	-14.2618	1.26651	-2.62185
N	-10.2501	-1.30353	-0.21534
C	-8.96659	-1.47284	-0.1094
C	-8.05196	-0.35679	-0.10113
N	-8.46908	0.869521	-0.19838
C	-9.8137	1.079428	-0.3107
C	-10.7191	-0.02528	-0.31921
C	-3.45982	-5.97295	0.556897
C	-4.83724	-5.77322	0.449145
C	-3.02337	-3.5676	0.438247
C	-2.56182	-4.88154	0.550828
C	-2.10798	-2.48374	0.432776
C	-5.72605	-6.88221	0.459425
C	-6.47209	-7.82644	0.479829
H	-7.13333	-8.65756	0.48812
O	-1.22503	-5.11641	0.705224

O	-2.96538	-7.24453	0.625315
C	-0.54997	-5.60431	-0.4676
H	0.490028	-5.74641	-0.17734
H	-0.97827	-6.55415	-0.79498
H	-0.60562	-4.86532	-1.2723
C	-2.55344	-7.67115	1.935543
H	-2.18713	-8.68988	1.816905
H	-1.75613	-7.031	2.319808
H	-3.4056	-7.66848	2.621479
N	-6.67597	-4.23678	0.214986
C	-7.09103	-3.00946	0.11609
C	-6.17758	-1.89531	0.122191
N	-4.89307	-2.06254	0.227092
C	-4.42831	-3.3429	0.333236
C	-5.32971	-4.44138	0.326147
N	-6.70198	-0.62021	0.013399
N	-8.44369	-2.74537	-4.2E-05
H	-9.0845	-3.52919	-0.00499
H	-6.06044	0.162923	0.019469
Br	-13.3303	-1.23795	-0.48102
Br	-9.14089	3.882836	-0.37925
C	2.107865	2.483335	0.432712
C	3.023182	3.567256	0.438237
C	2.561528	4.881155	0.550823
C	4.428148	3.342664	0.333247
C	3.459453	5.972639	0.556938
O	1.224718	5.115928	0.705182
N	4.893007	2.062341	0.227074
C	5.329465	4.441219	0.326205
C	4.836889	5.773021	0.449221
O	2.964907	7.244174	0.62536
C	0.549662	5.603792	-0.46766
C	6.177531	1.895211	0.122193
N	6.675738	4.236717	0.215068
C	5.725607	6.882079	0.459543
C	2.552931	7.670761	1.935591
H	-0.49036	5.745802	-0.17744
H	0.977889	6.553668	-0.795
H	0.605399	4.864821	-1.27236
C	7.090891	3.009438	0.116147
N	6.702025	0.620158	0.013368

C	6.47158	7.82636	0.479975
H	2.186546	8.689459	1.816959
H	1.75567	7.030547	2.319848
H	3.405091	7.668148	2.621528
N	8.44357	2.745455	0.000042
C	8.052034	0.356847	-0.10114
H	6.06055	-0.16303	0.0194
C	8.96657	1.47297	-0.10935
H	9.084324	3.529318	-0.00487
N	8.46925	-0.86943	-0.19843
N	10.25009	1.303761	-0.21527
C	9.813887	-1.07923	-0.31073
C	10.71918	0.025544	-0.31918
C	10.32747	-2.39398	-0.40784
C	12.10676	-0.21927	-0.44807
C	11.68937	-2.61437	-0.52547
Br	9.141297	-3.88269	-0.37938
C	12.59016	-1.51287	-0.54913
Br	13.33035	1.238429	-0.48089
O	12.19015	-3.87388	-0.6714
O	13.92846	-1.76218	-0.6206
C	12.79206	-4.43535	0.509585
C	14.42101	-2.09855	-1.93078
H	13.14321	-5.42526	0.222396
H	13.63267	-3.8235	0.843342
H	12.0492	-4.52907	1.306734
H	15.48931	-2.2721	-1.81124
H	13.93582	-3.00196	-2.30605
H	14.26201	-1.26596	-2.62183
H	7.132743	8.657538	0.488199
C	-1.31769	-1.55983	0.426244
Hg	-1.1E-05	-0.00024	0.426407
C	1.317627	1.559382	0.42619

3.0 N6P-Ph coordinates

Electronic Energy (EE:) -2169.596377 Hartree
EE + Thermal Free Energy Correction: -2169.115848 Hartree
E (Thermal): 382.579 kcal/mol
Entropy (S): 273.804 cal/mol-kelvin
Imaginary Freq: 0

0	1		
C	4.793654	-0.70508	0.002504
C	3.596919	-1.43029	0.001949
C	3.596894	1.430358	-0.00195
C	4.793642	0.705163	-0.00249
O	5.985391	1.375554	0.034689
O	5.985418	-1.37545	-0.03465
C	6.695573	1.422156	-1.21459
H	7.612855	1.975772	-1.01785
H	6.936744	0.41534	-1.56275
H	6.105329	1.951779	-1.96835
C	6.695561	-1.42206	1.214645
H	7.612856	-1.97566	1.017931
H	6.936709	-0.41525	1.562832
H	6.1053	-1.9517	1.968379
N	1.187894	-1.406	-0.01197
C	0.083455	-0.7204	-0.00671
C	0.083442	0.720399	0.006687
N	1.187869	1.406024	0.011955
C	2.36413	0.710254	0.006011
C	2.364142	-0.71021	-0.00602
C	-7.062	-0.70643	-0.01545
C	-5.86559	-1.42594	-0.03165
C	-5.86561	1.425834	0.031659
C	-7.06201	0.706305	0.015463
C	-5.88441	2.846869	0.06642
C	-5.9111	4.049429	0.107475
H	-5.93045	5.110948	0.133968
C	-5.88436	-2.84697	-0.06641
C	-5.911	-4.04953	-0.10748
H	-5.92998	-5.11105	-0.13419
O	-8.25299	1.37553	-0.01533
O	-8.25296	-1.37568	0.01535
C	-8.96424	1.414503	1.233749
H	-9.88032	1.970578	1.039322
H	-9.20637	0.405394	1.574674
H	-8.3742	1.938978	1.991126
C	-8.96423	-1.41465	-1.23372
H	-9.8803	-1.97073	-1.03928
H	-9.20638	-0.40554	-1.57463
H	-8.3742	-1.93912	-1.9911

N	-3.45741	-1.40681	-0.01828
C	-2.35318	-0.72111	-0.0091
C	-2.3532	0.721066	0.009079
N	-3.45744	1.406755	0.018276
C	-4.63341	0.710272	0.009054
C	-4.6334	-0.71035	-0.00905
N	-1.13544	1.373004	0.015298
N	-1.13541	-1.37302	-0.01533
H	-1.13617	-2.38505	-0.02786
H	-1.13621	2.385035	0.027836
C	3.616261	2.844396	-0.00316
C	3.616312	-2.84433	0.003166
C	3.641693	-4.05431	0.011665
C	3.641611	4.054372	-0.01166
C	3.664341	5.47508	-0.01476
C	2.470778	6.209062	-0.14635
C	4.879298	6.173605	0.113841
C	2.496434	7.597986	-0.14968
H	1.534228	5.673972	-0.24504
C	4.895029	7.56279	0.109667
H	5.799637	5.612174	0.219442
C	3.706275	8.280064	-0.02223
H	1.569715	8.15138	-0.25198
H	5.837737	8.088753	0.21059
H	3.722482	9.363957	-0.02498
C	3.664488	-5.47502	0.014752
C	2.470954	-6.20905	0.146307
C	4.879479	-6.17349	-0.11383
C	2.496673	-7.59798	0.149626
H	1.534378	-5.67401	0.244975
C	4.895272	-7.56267	-0.10966
H	5.799796	-5.61202	-0.2194
C	3.706547	-8.28	0.022192
H	1.569976	-8.15141	0.251898
H	5.838007	-8.08859	-0.21057
H	3.722803	-9.36389	0.024934

4.0 N6P-Ph dimer coordinates

N6P- Ph Hg dimer: 20 degrees

Electronic Energy (EE:) -4491.069887 Hartree

EE + Thermal Free Energy Correction: -4490.114462 Hartree
E (Thermal): 755.831 kcal/mol
Entropy (S): 526.196 cal/mol-kelvin
Imaginary Freq: 0

0	1		
C	-9.6061	-3.97467	2.582794
C	-9.80361	-3.0821	1.523283
C	-7.34743	-3.12312	2.989528
C	-8.39432	-3.99666	3.303922
O	-8.25645	-4.85994	4.355987
O	-10.5901	-4.87084	2.89845
C	-7.99879	-6.22638	3.990501
H	-7.92342	-6.77837	4.926569
H	-8.8158	-6.62824	3.387063
H	-7.05306	-6.30273	3.445736
C	-11.3466	-4.552	4.078798
H	-12.0738	-5.35463	4.195034
H	-10.698	-4.50841	4.956564
H	-11.8717	-3.60098	3.948766
N	-8.9226	-1.31357	0.144396
C	-7.94379	-0.50483	-0.13455
C	-6.71202	-0.51675	0.612536
N	-6.5179	-1.33719	1.601888
C	-7.53073	-2.19883	1.9169
C	-8.74528	-2.18735	1.180256
C	-5.38701	4.757223	-4.23774
C	-6.42475	3.875709	-3.92812
C	-3.99563	3.874135	-2.42926
C	-4.18493	4.756814	-3.49599
C	-2.78279	3.887891	-1.69296
C	-1.74322	3.904835	-1.06254
C	-7.62631	3.888472	-4.68739
C	-8.63537	3.899692	-5.34343
H	-9.53111	3.912854	-5.91385
O	-3.17519	5.602863	-3.86012
O	-5.55009	5.665715	-5.24575
C	-3.35237	6.972544	-3.45961
H	-2.47868	7.50826	-3.82828
H	-4.25938	7.391748	-3.90073
H	-3.39159	7.047225	-2.36883
C	-4.88107	5.339039	-6.47567

H	-5.10613	6.152328	-7.16426
H	-3.80162	5.267876	-6.32381
H	-5.26919	4.400448	-6.88222
N	-7.26912	2.109154	-2.52652
C	-7.0768	1.290742	-1.53527
C	-5.84487	1.280772	-0.78528
N	-4.8665	2.09017	-1.06378
C	-5.04213	2.961843	-2.10157
C	-6.25595	2.971379	-2.8398
N	-5.72106	0.377832	0.252455
N	-8.06765	0.398612	-1.17391
H	-8.93164	0.406184	-1.70099
H	-4.85713	0.370932	0.779641
C	-6.14006	-3.15606	3.725003
C	-11.0242	-3.07668	0.809202
C	-12.0745	-3.07326	0.207853
C	-5.10583	-3.19306	4.352527
C	-3.89051	-3.22504	5.088079
C	-2.79716	-2.43014	4.696329
C	-3.75774	-4.05051	6.220087
C	-1.60977	-2.46359	5.416572
H	-2.8967	-1.79365	3.825591
C	-2.56633	-4.07731	6.934219
H	-4.59837	-4.66082	6.527129
C	-1.48897	-3.28601	6.536517
H	-0.77508	-1.84631	5.103889
H	-2.47732	-4.71708	7.805044
H	-0.56093	-3.30956	7.096223
C	-13.3027	-3.06834	-0.50673
C	-13.5543	-2.09268	-1.48928
C	-14.2888	-4.03789	-0.24565
C	-14.7564	-2.09004	-2.18565
H	-12.7969	-1.34555	-1.69255
C	-15.4878	-4.02733	-0.94728
H	-14.0971	-4.79296	0.507027
C	-15.727	-3.05522	-1.91827
H	-14.9376	-1.33263	-2.93999
H	-16.2388	-4.78057	-0.7371
H	-16.6638	-3.05023	-2.46375
Hg	0.000012	3.909835	0.000048
C	1.743245	3.904851	1.062627

C	2.782817	3.887896	1.693045
C	3.995663	3.874114	2.429349
C	4.184968	4.756762	3.4961
C	5.042155	2.961832	2.101627
C	5.387043	4.757151	4.23784
O	3.175224	5.602799	3.860258
N	4.866525	2.090189	1.063805
C	6.255983	2.971348	2.839848
C	6.424785	3.875647	3.928197
O	5.550125	5.665614	5.245884
C	3.352404	6.972494	3.459792
C	5.844897	1.280801	0.78528
N	7.269154	2.109133	2.526541
C	7.626351	3.88839	4.687455
C	4.881133	5.338889	6.475802
H	2.478714	7.508197	3.828489
H	4.259415	7.391682	3.90092
H	3.391614	7.047212	2.369019
C	7.076834	1.29075	1.535269
N	5.721088	0.377893	-0.25248
C	8.635413	3.899594	5.34349
H	5.10619	6.152159	7.164415
H	3.801675	5.267718	6.323952
H	5.269267	4.400289	6.882308
N	8.067679	0.398633	1.173872
C	6.712031	-0.5167	-0.61257
H	4.857149	0.371	-0.77966
C	7.943803	-0.5048	0.134511
H	8.931666	0.406178	1.700959
N	6.517901	-1.33712	-1.60193
N	8.922598	-1.31356	-0.14444
C	7.530718	-2.19878	-1.91695
C	8.745259	-2.18732	-1.18031
C	7.347397	-3.12306	-2.98959
C	9.803575	-3.0821	-1.52334
C	8.394278	-3.99661	-3.30399
C	6.140033	-3.15596	-3.72507
C	9.606056	-3.97465	-2.58285
C	11.02419	-3.07671	-0.80925
O	8.256402	-4.85987	-4.35607
C	5.105803	-3.19292	-4.3526

O	10.59	-4.87085	-2.89851
C	12.07449	-3.07331	-0.2079
C	7.998678	-6.22631	-3.9906
C	3.890493	-3.22485	-5.08816
C	11.34655	-4.552	-4.07883
C	13.30263	-3.06843	0.506672
H	7.92332	-6.77829	-4.92667
H	8.815648	-6.6282	-3.38713
H	7.052915	-6.30262	-3.44588
C	2.797212	-2.42983	-4.69647
C	3.757651	-4.05038	-6.22011
H	12.07377	-5.35465	-4.19508
H	10.69798	-4.50836	-4.95661
H	11.87166	-3.601	-3.94876
C	13.55436	-2.09275	1.489195
C	14.2887	-4.03802	0.245604
C	1.609815	-2.46321	-5.41672
H	2.896806	-1.79328	-3.82578
C	2.566241	-4.07713	-6.93425
H	4.598223	-4.6608	-6.52711
C	14.75639	-2.09014	2.185553
H	12.79697	-1.34558	1.692447
C	15.48776	-4.0275	0.947224
H	14.09698	-4.79311	-0.50705
C	1.488952	-3.2857	-6.5366
H	0.775183	-1.84584	-5.10408
H	2.477173	-4.71695	-7.80503
C	15.72698	-3.05538	1.918186
H	14.93772	-1.33272	2.939864
H	16.23873	-4.78078	0.737056
H	0.560911	-3.30921	-7.09631
H	16.66376	-3.05041	2.463662
H	9.531146	3.912739	5.913923

N6P-Ph Hg dimer: 90 degrees

Electronic Energy (EE:) -4491.069965 Hartree
EE + Thermal Free Energy Correction: -4490.114369 Hartree
E (Thermal): 755.827 kcal/mol
Entropy (S): 525.824 cal/mol-kelvin
Imaginary Freq: 0

0	1		
C	-12.2701	-2.16069	-1.20952
C	-11.9203	-0.83949	-0.90904
C	-9.94645	-2.90699	-1.02223
C	-11.2967	-3.17942	-1.26844
O	-11.6857	-4.46432	-1.53037
O	-13.574	-2.46275	-1.4921
C	-11.9842	-4.73974	-2.90964
H	-12.279	-5.78765	-2.94939
H	-12.8032	-4.10968	-3.2637
H	-11.0952	-4.58795	-3.529
C	-14.2852	-3.13051	-0.43595
H	-15.2914	-3.30473	-0.81507
H	-13.811	-4.08312	-0.1894
H	-14.3359	-2.49237	0.451322
N	-10.1903	0.749123	-0.37163
C	-8.93373	0.987072	-0.13827
C	-7.9425	-0.05772	-0.17837
N	-8.25473	-1.28919	-0.45342
C	-9.56901	-1.56741	-0.70388
C	-10.5469	-0.53796	-0.66181
C	-3.84633	5.728914	1.503154
C	-5.18958	5.457314	1.235258
C	-3.23219	3.380104	1.200552
C	-2.87746	4.701303	1.485845
C	-2.24837	2.357785	1.193997
C	-1.40423	1.482647	1.196275
C	-6.15021	6.504763	1.254802
C	-6.95402	7.400603	1.262866
H	-7.66811	8.186577	1.278218
O	-1.56601	5.016341	1.707717
O	-3.4661	7.000163	1.831231
C	-1.21659	5.237049	3.085209
H	-0.15514	5.481091	3.090337
H	-1.79112	6.066702	3.503041
H	-1.38353	4.327492	3.669705
C	-2.82212	7.735258	0.777048
H	-2.58449	8.712533	1.195088
H	-1.90539	7.234027	0.457928
H	-3.50164	7.858138	-0.0715

N	-6.88861	3.840074	0.691052
C	-7.20238	2.608017	0.420975
C	-6.21138	1.560678	0.387716
N	-4.95617	1.79696	0.629328
C	-4.59852	3.084117	0.917099
C	-5.57474	4.115835	0.947487
N	-6.62806	0.27853	0.087616
N	-8.51601	2.271569	0.157199
H	-9.21093	3.006987	0.18197
H	-5.93277	-0.45652	0.062854
C	-8.98306	-3.94043	-1.0835
C	-12.9096	0.169749	-0.85882
C	-13.7633	1.026274	-0.81083
C	-8.16048	-4.826	-1.14585
C	-7.18868	-5.86059	-1.21138
C	-5.81739	-5.56025	-1.1108
C	-7.57852	-7.20248	-1.37831
C	-4.86903	-6.57324	-1.17666
H	-5.51444	-4.52825	-0.9827
C	-6.62296	-8.20894	-1.44265
H	-8.63323	-7.43808	-1.45243
C	-5.2667	-7.89973	-1.34277
H	-3.81583	-6.32772	-1.09897
H	-6.93669	-9.23887	-1.57063
H	-4.52405	-8.68777	-1.39395
C	-14.7596	2.038105	-0.75925
C	-14.435	3.340164	-0.33507
C	-16.0875	1.757344	-1.13112
C	-15.4114	4.327019	-0.28495
H	-13.4136	3.559129	-0.0488
C	-17.0572	2.750835	-1.07788
H	-16.3404	0.757391	-1.46213
C	-16.7246	4.037538	-0.65507
H	-15.148	5.326038	0.043881
H	-18.0764	2.521578	-1.36807
H	-17.4839	4.810168	-0.61492
Hg	-0.00012	0.000754	1.1942
C	1.403935	-1.4812	1.196373
C	2.247943	-2.35646	1.194233
C	3.231551	-3.37898	1.200957
C	2.876521	-4.70006	1.486397

C	4.597964	-3.08332	0.917539
C	3.845171	-5.72788	1.503857
O	1.564998	-5.01477	1.708252
N	4.955912	-1.79627	0.629653
C	5.573951	-4.11524	0.948081
C	5.188489	-5.45661	1.23599
O	3.46465	-6.99902	1.832038
C	1.215482	-5.23537	3.085735
C	6.211186	-1.56029	0.38808
N	6.887897	-3.8398	0.691655
C	6.148888	-6.50427	1.25568
C	2.820552	-7.73407	0.777895
H	0.153955	-5.4791	3.090839
H	1.789753	-6.06519	3.503592
H	1.382679	-4.32586	3.67023
C	7.201947	-2.60784	0.421459
N	6.62816	-0.27825	0.087895
C	6.952503	-7.40028	1.263878
H	2.582795	-8.7113	1.195976
H	1.90388	-7.23273	0.458776
H	3.500032	-7.85707	-0.07066
N	8.515654	-2.27172	0.157658
C	7.942679	0.057673	-0.17809
H	5.933036	0.456946	0.06305
C	8.933667	-0.98735	-0.13793
H	9.210398	-3.0073	0.182472
N	8.255206	1.289058	-0.45322
N	10.19026	-0.74972	-0.37136
C	9.569544	1.566948	-0.70372
C	10.54715	0.537257	-0.66163
C	9.947303	2.906419	-1.02214
C	11.92064	0.838439	-0.90894
C	11.29756	3.178506	-1.26843
C	8.984151	3.940085	-1.08342
C	12.2708	2.159541	-1.20951
C	12.90972	-0.17104	-0.85874
O	11.68691	4.463303	-1.53046
C	8.161781	4.825844	-1.14578
O	13.57473	2.461268	-1.49215
C	13.76322	-1.02777	-0.81076
C	11.98542	4.738563	-2.90975

C	7.190155	5.860596	-1.21141
C	14.28613	3.12889	-0.43606
C	14.75925	-2.03982	-0.75926
H	12.28036	5.786424	-2.94959
H	12.80429	4.10835	-3.26377
H	11.09637	4.586849	-3.5291
C	5.818814	5.560496	-1.11077
C	7.580216	7.202405	-1.37847
H	15.29241	3.302786	-0.81521
H	13.81225	4.08166	-0.18957
H	14.33662	2.490799	0.451262
C	14.43439	-3.34184	-0.33515
C	16.08726	-1.75932	-1.13114
C	4.87063	6.573641	-1.17671
H	5.515689	4.528561	-0.98255
C	6.624829	8.209013	-1.44289
H	8.634965	7.437816	-1.45263
C	15.41059	-4.3289	-0.28511
H	13.41293	-3.5606	-0.04887
C	17.05672	-2.75303	-1.07798
H	16.3403	-0.75941	-1.4621
C	5.268512	7.900049	-1.34295
H	3.81738	6.328311	-1.09896
H	6.938731	9.23888	-1.57098
C	16.72382	-4.03968	-0.65524
H	15.147	-5.32788	0.043668
H	18.07596	-2.52397	-1.36819
H	4.526003	8.688208	-1.3942
H	17.48295	-4.81248	-0.61516
H	7.666388	-8.18644	1.279381

N6P-Ph Hg dimer: 180 degrees

Electronic Energy (EE:) -4491.069965 Hartree
EE + Thermal Free Energy Correction: -4490.114368 Hartree
E (Thermal): 755.827 kcal/mol
Entropy (S): 525.820 cal/mol-kelvin
Imaginary Freq: 0

0	1		
C	12.27025	2.160154	-1.20986
C	11.92027	0.83901	-0.90928

C	9.946661	2.906733	-1.02245
C	11.29688	3.178995	-1.26877
O	11.68607	4.46384	-1.53078
O	13.57413	2.46206	-1.49254
C	11.98454	4.739151	-2.91008
H	12.27954	5.786993	-2.94988
H	12.80335	4.108908	-3.26417
H	11.09544	4.587525	-3.52939
C	14.28547	3.129747	-0.43645
H	15.29172	3.30378	-0.81562
H	13.81147	4.082454	-0.18993
H	14.33606	2.491648	0.450861
N	10.1901	-0.74937	-0.37168
C	8.933544	-0.98717	-0.13824
C	7.942421	0.057725	-0.17837
N	8.254787	1.289155	-0.45349
C	9.569082	1.567212	-0.70402
C	10.54682	0.537649	-0.66195
C	3.84576	-5.72829	1.504073
C	5.189024	-5.45685	1.236089
C	3.231822	-3.37947	1.201121
C	2.876983	-4.70059	1.486656
C	2.248097	-2.35706	1.194459
C	1.404037	-1.48185	1.196664
C	6.149555	-6.50439	1.255761
C	6.953286	-7.4003	1.263944
H	7.667273	-8.18636	1.27939
O	1.565508	-5.01544	1.708636
O	3.465443	-6.99947	1.832334
C	1.216172	-5.23614	3.086149
H	0.154684	-5.48004	3.091356
H	1.790618	-6.06588	3.503918
H	1.38328	-4.32662	3.670658
C	2.821252	-7.73461	0.778313
H	2.583609	-8.71183	1.196473
H	1.904509	-7.23334	0.459281
H	3.500631	-7.85761	-0.07032
N	6.888188	-3.83986	0.691548
C	7.202058	-2.60787	0.421263
C	6.21116	-1.56044	0.387906
N	4.955934	-1.79657	0.629585

C	4.598171	-3.08365	0.917559
C	5.574294	-4.11546	0.94808
N	6.627951	-0.27837	0.087639
N	8.515701	-2.2716	0.15734
H	9.21055	-3.00708	0.182201
H	5.932732	0.456741	0.06283
C	8.983378	3.940277	-1.08371
C	12.90948	-0.17034	-0.85909
C	13.7631	-1.02696	-0.81114
C	8.160886	4.825925	-1.14604
C	7.189116	5.860544	-1.2116
C	5.817841	5.560281	-1.11048
C	7.578945	7.202365	-1.37907
C	4.869502	6.57328	-1.17635
H	5.514902	4.52833	-0.98194
C	6.6234	8.208832	-1.44343
H	8.633637	7.437909	-1.4536
C	5.267157	7.899707	-1.34301
H	3.816309	6.327827	-1.09823
H	6.937125	9.238712	-1.57183
H	4.524526	8.687756	-1.3942
C	14.75924	-2.0389	-0.75968
C	14.43458	-3.34089	-0.33535
C	16.08716	-1.75832	-1.13182
C	15.41089	-4.32786	-0.28536
H	13.41318	-3.55972	-0.04888
C	17.05673	-2.75192	-1.07869
H	16.34005	-0.75842	-1.46294
C	16.72402	-4.03856	-0.65573
H	15.14744	-5.32683	0.043592
H	18.0759	-2.5228	-1.36909
H	17.48324	-4.81127	-0.61568
Hg	-1.1E-05	0.000095	1.194527
C	-1.40407	1.482031	1.196673
C	-2.24815	2.357219	1.194459
C	-3.23191	3.379602	1.201097
C	-2.87711	4.70073	1.486645
C	-4.59824	3.083748	0.917506
C	-3.84591	5.728403	1.504046
O	-1.56565	5.015613	1.708665
N	-4.95597	1.796659	0.629526

C	-5.57439	4.115526	0.948007
C	-5.18916	5.45693	1.236029
O	-3.46564	6.999586	1.832332
C	-1.21635	5.236251	3.086199
C	-6.21118	1.560499	0.387815
N	-6.88827	3.839897	0.691446
C	-6.14972	6.50444	1.255683
C	-2.8214	7.734749	0.778358
H	-0.15487	5.480178	3.091447
H	-1.79083	6.065948	3.504
H	-1.38345	4.326693	3.670653
C	-7.20211	2.607905	0.42115
N	-6.62793	0.278418	0.087533
C	-6.95348	7.400334	1.263849
H	-2.58381	8.711974	1.196541
H	-1.90462	7.233505	0.459384
H	-3.50072	7.857739	-0.07032
N	-8.51573	2.271596	0.157194
C	-7.9424	-0.05772	-0.17845
H	-5.9327	-0.45668	0.062769
C	-8.93355	0.987144	-0.13834
H	-9.21061	3.007052	0.182064
N	-8.25473	-1.28917	-0.45352
N	-10.1901	0.749308	-0.37175
C	-9.56902	-1.56727	-0.70404
C	-10.5468	-0.53773	-0.66199
C	-9.94657	-2.90681	-1.02243
C	-11.9202	-0.83914	-0.9093
C	-11.2968	-3.17911	-1.26873
C	-8.98326	-3.94033	-1.08367
C	-12.2702	-2.1603	-1.20984
C	-12.9095	0.17019	-0.85913
O	-11.6859	-4.46398	-1.5307
C	-8.16074	-4.82596	-1.14599
O	-13.574	-2.46225	-1.4925
C	-13.7631	1.026786	-0.81118
C	-11.9844	-4.73934	-2.90999
C	-7.18895	-5.86056	-1.21154
C	-14.2854	-3.12991	-0.43638
C	-14.7593	2.038716	-0.75972
H	-12.2794	-5.78718	-2.94975

H	-12.8032	-4.10911	-3.26411
H	-11.0953	-4.58773	-3.5293
C	-5.81769	-5.56028	-1.11029
C	-7.57875	-7.20237	-1.37913
H	-15.2916	-3.30399	-0.81555
H	-13.8113	-4.08259	-0.18982
H	-14.336	-2.49177	0.450893
C	-14.4346	3.340701	-0.33535
C	-16.0872	1.758132	-1.1319
C	-4.86933	-6.57327	-1.17616
H	-5.51478	-4.52834	-0.98166
C	-6.62319	-8.20882	-1.44349
H	-8.63343	-7.43793	-1.45376
C	-15.4109	4.327655	-0.28534
H	-13.4132	3.559532	-0.04884
C	-17.0567	2.75172	-1.07876
H	-16.34	0.758238	-1.46306
C	-5.26696	-7.89969	-1.34294
H	-3.81615	-6.3278	-1.09795
H	-6.93689	-9.2387	-1.572
C	-16.7241	4.038348	-0.65576
H	-15.1475	5.326615	0.043641
H	-18.0759	2.522598	-1.36919
H	-4.52431	-8.68772	-1.39413
H	-17.4833	4.811056	-0.6157
H	-7.66748	8.186378	1.279281

5.0 N6P-Bu coordinates

Electronic Energy (EE:) -2021.972388 Hartree
EE + Thermal Free Energy Correction: -2021.431103 Hartree
E (Thermal): 422.764 kcal/mol
Entropy (S): 280.717 cal/mol-kelvin
Imaginary Freq: 0

0	1		
C	4.980516	0.706434	-0.0045
C	3.787342	1.43181	-0.0075
C	3.787373	-1.43174	0.00737
C	4.980529	-0.70634	0.00448
O	6.175563	-1.37288	-0.03392
O	6.175536	1.372997	0.034029

C	6.880797	-1.42475	1.21648
H	7.797551	-1.98029	1.022099
H	7.123361	-0.41941	1.568562
H	6.287032	-1.9547	1.967447
C	6.880885	1.424897	-1.21631
H	7.797617	1.980438	-1.02183
H	7.123493	0.419558	-1.56839
H	6.287187	1.954849	-1.96732
N	1.378947	1.405969	0.004956
C	0.275276	0.720075	0.002554
C	0.27529	-0.72009	-0.0029
N	1.378977	-1.40596	-0.00528
C	2.556499	-0.71091	-0.003
C	2.556484	0.710946	0.002741
C	-6.87125	0.706208	0.010347
C	-5.67464	1.425743	0.021571
C	-5.67463	-1.42585	-0.02159
C	-6.87125	-0.70633	-0.01025
C	-5.69349	-2.84716	-0.04613
C	-5.72027	-4.05002	-0.07836
H	-5.73912	-5.1117	-0.097
C	-5.6935	2.847051	0.04612
C	-5.72016	4.049912	0.078392
H	-5.7389	5.111587	0.097125
O	-8.0625	-1.37551	0.025635
O	-8.06251	1.375375	-0.02542
C	-8.77243	-1.4249	-1.22356
H	-9.68854	-1.97979	-1.0257
H	-9.01473	-0.41866	-1.57287
H	-8.18154	-1.95513	-1.97631
C	-8.77231	1.424773	1.223854
H	-9.68844	1.979665	1.026099
H	-9.01456	0.418532	1.573194
H	-8.18133	1.955001	1.97654
N	-3.2664	1.407017	0.008746
C	-2.16183	0.721485	0.004194
C	-2.16182	-0.72155	-0.00449
N	-3.26638	-1.4071	-0.00897
C	-4.44241	-0.71034	-0.00425
C	-4.44242	0.710237	0.004126
N	-0.94464	-1.37314	-0.00682

N	-0.94466	1.373101	0.006475
H	-0.94484	2.385182	0.011071
H	-0.9448	-2.38522	-0.01142
C	3.80523	-2.85192	0.013817
C	3.805143	2.851989	-0.01388
C	3.823971	4.059072	-0.02286
C	3.824148	-4.059	0.0229
C	3.835717	-5.5279	0.01811
C	3.83538	5.52797	-0.01797
C	2.78537	-6.05046	1.025547
H	1.786291	-5.69595	0.762713
H	2.776748	-7.14464	1.02543
H	3.011888	-5.70726	2.037597
C	5.24073	-6.03292	0.41855
H	5.998614	-5.6628	-0.27547
H	5.50438	-5.69394	1.423132
H	5.264285	-7.12676	0.406841
C	3.493005	6.032866	1.403943
H	3.492997	7.127005	1.42266
H	2.506409	5.681416	1.713888
H	4.225558	5.674686	2.13064
C	2.781023	6.050483	-1.02122
H	2.77221	7.144662	-1.02093
H	3.003642	5.707446	-2.03419
H	1.783041	5.695765	-0.75453
C	3.487835	-6.03298	-1.4024
H	2.500022	-5.68162	-1.70853
H	4.217533	-5.67485	-2.13199
H	3.487821	-7.12712	-1.42098
C	5.238751	6.033224	-0.42385
H	5.999366	5.663291	0.267276
H	5.498594	5.694242	-1.42942
H	5.262141	7.127073	-0.41229

6.0 N6P-Bu dimer coordinates

N6P-Bu Hg dimer: 30 degrees

Electronic Energy (EE:) -4195.822090 Hartree
EE + Thermal Free Energy Correction: -4194.744270 Hartree
E (Thermal): 836.200 kcal/mol
Entropy (S): 538.151 cal/mol-kelvin

Imaginary Freq: 0

0	1		
C	-6.55657	-5.14191	-2.35366
C	-5.71227	-4.05014	-2.14206
C	-8.42306	-4.0353	-1.21902
C	-7.89392	-5.13477	-1.89788
O	-8.69516	-6.21137	-2.16732
O	-6.0718	-6.2602	-2.9768
C	-8.47833	-7.35428	-1.32468
H	-9.18228	-8.11445	-1.66162
H	-7.45553	-7.72453	-1.4264
H	-8.68674	-7.10316	-0.2802
C	-6.46924	-6.40896	-4.3491
H	-6.01054	-7.33398	-4.69677
H	-7.55622	-6.47907	-4.43406
H	-6.09706	-5.57145	-4.94694
N	-5.41557	-1.84285	-1.22534
C	-5.9209	-0.82315	-0.59813
C	-7.28773	-0.81062	-0.14457
N	-8.08424	-1.81868	-0.33976
C	-7.58005	-2.90602	-0.99796
C	-6.23054	-2.91852	-1.44514
C	-4.99072	5.742367	2.07024
C	-4.46052	4.634022	1.404111
C	-7.17721	4.667954	2.277774
C	-6.33491	5.758857	2.502741
C	-8.52854	4.703508	2.717272
C	-9.67425	4.74778	3.083565
H	-10.6833	4.778683	3.413351
C	-3.10692	4.633745	0.978599
C	-1.94529	4.639246	0.619339
O	-6.80287	6.84352	3.190666
O	-4.21235	6.848696	2.267765
C	-7.12722	7.985947	2.380666
H	-7.47727	8.752701	3.070518
H	-6.2463	8.343516	1.842646
H	-7.92673	7.738371	1.676082
C	-3.71101	7.00989	3.605666
H	-3.12587	7.928516	3.598391
H	-4.53271	7.097868	4.319968

H	-3.06438	6.168893	3.873056
N	-4.80096	2.424358	0.505437
C	-5.59713	1.415432	0.309255
C	-6.9673	1.428949	0.761581
N	-7.47237	2.450467	1.38699
C	-6.65578	3.524522	1.606022
C	-5.30693	3.512092	1.160389
N	-7.74655	0.316123	0.514446
N	-5.13937	0.291093	-0.34846
H	-4.17908	0.281293	-0.66801
H	-8.70745	0.325793	0.832244
C	-9.76956	-4.04276	-0.76727
C	-4.36984	-4.07201	-2.60527
C	-3.2297	-4.08708	-3.00199
C	-10.9126	-4.04991	-0.37892
C	-12.3061	-4.04107	0.085834
C	-1.83634	-4.09933	-3.46696
C	-12.596	-2.69993	0.798082
H	-12.4411	-1.85889	0.118613
H	-13.6324	-2.67653	1.148337
H	-11.9366	-2.567	1.658737
C	-12.527	-5.2123	1.071496
H	-12.3268	-6.17095	0.587498
H	-11.8672	-5.12237	1.937465
H	-13.5624	-5.21407	1.425286
C	-1.10161	-5.30995	-2.8449
H	-0.06242	-5.33385	-3.18664
H	-1.105	-5.24833	-1.75439
H	-1.5832	-6.24687	-3.13348
C	-1.1434	-2.78778	-3.03107
H	-0.10248	-2.7825	-3.36804
H	-1.65049	-1.92017	-3.45928
H	-1.15571	-2.68595	-1.94362
C	-13.2498	-4.20171	-1.12908
H	-13.1138	-3.38197	-1.83799
H	-13.0528	-5.13979	-1.6527
H	-14.2923	-4.20207	-0.79627
C	-1.80975	-4.21397	-5.00917
H	-2.29499	-5.1354	-5.33915
H	-2.32765	-3.37056	-5.47154
H	-0.77553	-4.22179	-5.36627

Hg	-2.2E-05	4.641377	0.000049
C	1.945239	4.639273	-0.61926
C	3.106863	4.633778	-0.97854
C	4.460454	4.634063	-1.40409
C	4.990625	5.742409	-2.07024
C	5.306867	3.512131	-1.16041
C	6.334802	5.758896	-2.50279
O	4.212249	6.84874	-2.26773
N	4.800926	2.424398	-0.50543
C	6.655704	3.524555	-1.6061
C	7.177099	4.667986	-2.27787
O	6.802735	6.843559	-3.19073
C	3.710858	7.009942	-3.60561
C	5.597096	1.415466	-0.30929
N	7.472298	2.450497	-1.38711
C	8.528411	4.703534	-2.71744
C	7.127116	7.985986	-2.38075
H	3.125714	7.928562	-3.5983
H	4.532532	7.097934	-4.31994
H	3.064227	6.168941	-3.87298
C	6.967247	1.428979	-0.76168
N	5.139354	0.291122	0.348425
C	9.674101	4.747801	-3.08379
H	7.477156	8.752736	-3.07061
H	6.246209	8.343562	-1.8427
H	7.926639	7.738406	-1.67618
N	7.746505	0.316147	-0.51458
C	5.920906	-0.82311	0.598099
H	4.179073	0.28132	0.668009
C	7.287712	-0.81059	0.144489
H	8.707389	0.325821	-0.83241
N	5.41561	-1.84279	1.225353
N	8.08424	-1.81863	0.339671
C	6.230588	-2.91846	1.44514
C	7.580077	-2.90596	0.997899
C	5.71235	-4.05008	2.142087
C	8.423092	-4.03524	1.218925
C	6.556651	-5.14185	2.353648
C	4.369946	-4.07193	2.605389
C	7.893975	-5.13472	1.897805
C	9.769576	-4.04271	0.767116

O	6.071902	-6.26013	2.976811
C	3.229847	-4.08701	3.002216
O	8.69522	-6.21132	2.167205
C	10.91262	-4.04986	0.37872
C	6.469408	-6.40889	4.349091
C	1.836547	-4.09926	3.467364
C	8.478328	-7.35424	1.324587
C	12.30604	-4.04097	-0.08609
H	6.010694	-7.33389	4.696798
H	7.556384	-6.47902	4.433997
H	6.097278	-5.57136	4.946937
C	1.141814	-2.7904	3.026283
C	1.810275	-4.20771	5.010031
C	1.103377	-5.31335	2.850273
H	9.182303	-8.11441	1.661498
H	7.455539	-7.72448	1.426382
H	8.68668	-7.10314	0.280091
C	13.24988	-4.20123	1.128823
C	12.59581	-2.69994	-0.79864
C	12.52707	-5.21238	-1.0715
H	1.15382	-2.69294	1.938421
H	0.100932	-2.78512	3.363383
H	1.647829	-1.9204	3.450908
H	2.296754	-5.12717	5.343677
H	2.327129	-3.36177	5.46894
H	0.7761	-4.21544	5.367281
H	1.106552	-5.25612	1.759522
H	1.586263	-6.24846	3.142552
H	0.064258	-5.33729	3.192235
H	14.29232	-4.20153	0.795984
H	13.11379	-3.38136	1.837566
H	13.05298	-5.13922	1.652647
H	13.63214	-2.67651	-1.14894
H	11.93636	-2.56728	-1.65929
H	12.44083	-1.85877	-0.11934
H	12.32696	-6.17095	-0.58729
H	11.86721	-5.12271	-1.93747
H	13.5625	-5.21412	-1.42532
H	10.68311	4.778708	-3.41362

N6P-Bu Hg dimer: 90 degrees

Electronic Energy (EE:) -4195.821840 Hartree
EE + Thermal Free Energy Correction: -4194.745077 Hartree
E (Thermal): 836.190 kcal/mol
Entropy (S): 540.344 cal/mol-kelvin
Imaginary Freq: 0

0	1		
C	8.281598	-4.24666	-3.0761
C	7.24892	-3.35117	-2.79082
C	9.699375	-3.31712	-1.30925
C	9.490924	-4.22921	-2.34586
O	10.45715	-5.15468	-2.63512
O	8.141009	-5.13259	-4.11019
C	11.23295	-4.87337	-3.81094
H	11.94759	-5.69053	-3.90261
H	10.59604	-4.83586	-4.69776
H	11.77355	-3.9292	-3.69414
C	7.846108	-6.48188	-3.71544
H	7.766002	-7.05496	-4.63849
H	8.646835	-6.88931	-3.09379
H	6.893454	-6.52254	-3.17866
N	6.443455	-1.51953	-1.45039
C	6.646888	-0.67885	-0.48071
C	7.875011	-0.66831	0.271243
N	8.841101	-1.49981	0.018469
C	8.655041	-2.39717	-0.99642
C	7.44315	-2.40621	-1.74003
C	4.190158	4.73855	3.48259
C	3.990047	3.831325	2.438508
C	6.41445	3.834268	3.94411
C	5.389944	4.739992	4.227272
C	7.614158	3.848369	4.706384
C	8.621647	3.861268	5.364857
H	9.516285	3.87535	5.936936
C	2.779255	3.844715	1.698773
C	1.741198	3.861424	1.065812
O	5.564728	5.672699	5.211403
O	3.192656	5.609678	3.82187
C	4.889859	5.387446	6.448101
H	5.125288	6.215076	7.115904

H	3.809654	5.327438	6.296422
H	5.264154	4.454358	6.879596
C	3.390636	6.96394	3.381607
H	2.525197	7.523682	3.733838
H	4.303852	7.382096	3.810905
H	3.431274	7.006305	2.289115
N	4.83663	1.999377	1.121963
C	5.802779	1.167384	0.867716
C	7.032838	1.177148	1.622125
N	7.234892	2.018212	2.592461
C	6.234478	2.904344	2.879496
C	5.022956	2.894697	2.137728
N	8.009802	0.260399	1.288085
N	5.668241	0.240646	-0.14667
H	4.805746	0.232632	-0.67618
H	8.872765	0.268347	1.816807
C	10.92015	-3.31459	-0.58332
C	6.039895	-3.38048	-3.53554
C	5.011432	-3.40939	-4.16717
C	11.96008	-3.31226	0.029894
C	13.21539	-3.31024	0.792784
C	3.761929	-3.42579	-4.93942
C	13.61896	-1.85121	1.107862
H	12.84092	-1.35095	1.688627
H	14.54819	-1.83475	1.68542
H	13.7741	-1.28278	0.188003
C	14.32526	-3.99153	-0.04011
H	14.0522	-5.02106	-0.28217
H	14.49422	-3.45462	-0.97648
H	15.26313	-4.00493	0.523286
C	3.795535	-2.28378	-5.98279
H	2.868256	-2.28052	-6.56378
H	3.900278	-1.31308	-5.49318
H	4.634357	-2.41029	-6.67083
C	2.5663	-3.21748	-3.98114
H	1.628549	-3.21795	-4.54489
H	2.521268	-4.01461	-3.23556
H	2.653234	-2.2646	-3.45446
C	13.00725	-4.08781	2.114179
H	12.22255	-3.62586	2.717355
H	12.71902	-5.12238	1.915215

H	13.93422	-4.09212	2.695729
C	3.621674	-4.78485	-5.66257
H	4.464669	-4.955	-6.336
H	3.588719	-5.60673	-4.9435
H	2.698951	-4.80421	-6.25024
Hg	0.000003	3.865481	-3.2E-05
C	-1.74119	3.861408	-1.06588
C	-2.77924	3.84469	-1.69885
C	-3.99002	3.831272	-2.4386
C	-4.1901	4.738433	-3.48275
C	-5.02295	2.894672	-2.13779
C	-5.38988	4.739841	-4.22745
O	-3.19258	5.609527	-3.82207
N	-4.83665	1.999413	-1.12196
C	-6.23445	2.904281	-2.87958
C	-6.41439	3.834141	-3.94426
O	-5.56463	5.672492	-5.21164
C	-3.39055	6.963819	-3.38189
C	-5.80281	1.167439	-0.86769
N	-7.23487	2.018168	-2.59252
C	-7.61409	3.848207	-4.70656
C	-4.88978	5.387125	-6.44833
H	-2.52509	7.523522	-3.73412
H	-4.30374	7.381969	-3.81124
H	-3.43122	7.006249	-2.2894
C	-7.03284	1.177159	-1.62213
N	-5.6683	0.240763	0.146756
C	-8.62156	3.861077	-5.36505
H	-5.12516	6.21473	-7.11618
H	-3.80958	5.327061	-6.29665
H	-5.26413	4.454034	-6.87977
N	-8.00982	0.260429	-1.28807
C	-6.64693	-0.67875	0.480791
H	-4.80581	0.232774	0.676278
C	-7.87503	-0.66825	-0.2712
H	-8.87276	0.268336	-1.81682
N	-6.44351	-1.51939	1.4505
N	-8.84111	-1.49978	-0.01844
C	-7.44319	-2.4061	1.740125
C	-8.65505	-2.39712	0.996467
C	-7.24896	-3.35104	2.790938

C	-9.69936	-3.3171	1.309277
C	-8.28161	-4.24657	3.076184
C	-6.03997	-3.38028	3.535718
C	-9.49091	-4.22918	2.345895
C	-10.9201	-3.31461	0.583306
O	-8.14102	-5.13249	4.11028
C	-5.01156	-3.40913	4.167428
O	-10.4571	-5.15469	2.635125
C	-11.96	-3.3123	-0.02995
C	-7.846	-6.48176	3.715549
C	-3.76214	-3.42543	4.939811
C	-11.233	-4.87339	3.810909
C	-13.2153	-3.31025	-0.7929
H	-7.76589	-7.05483	4.638608
H	-8.64666	-6.88926	3.093857
H	-6.89331	-6.52235	3.178819
C	-2.56631	-3.21848	3.981481
C	-3.62257	-4.78393	5.664138
C	-3.79533	-2.28252	5.982194
H	-11.9476	-5.69058	3.902557
H	-10.5961	-4.83585	4.697752
H	-11.7736	-3.92924	3.694065
C	-13.0078	-4.09001	-2.11311
C	-13.6175	-1.85131	-1.11019
C	-14.3258	-3.98923	0.040982
H	-2.65276	-2.26601	3.453978
H	-1.62862	-3.2189	4.545333
H	-2.52157	-4.01627	3.236579
H	-4.46572	-4.95314	6.337617
H	-3.58991	-5.60644	4.945778
H	-2.69992	-4.80321	6.251922
H	-3.89961	-1.31219	5.491751
H	-4.63427	-2.40806	6.670277
H	-2.8681	-2.27915	6.563267
H	-13.9348	-4.09435	-2.69467
H	-12.2227	-3.6297	-2.71697
H	-12.7206	-5.12454	-1.91257
H	-14.5467	-1.83483	-1.68781
H	-13.7721	-1.28136	-0.19119
H	-12.8389	-1.35267	-1.69167
H	-14.0538	-5.01867	0.284568

H	-14.4943	-3.45077	0.976544
H	-15.2637	-4.00257	-0.52243
H	-9.51618	3.875143	-5.93716

N6P-Bu Hg dimer: 180 degrees

Electronic Energy (EE:) -4195.821945 Hartree
EE + Thermal Free Energy Correction: -4194.744886 Hartree
E (Thermal): 836.190 kcal/mol
Entropy (S): 539.722 cal/mol-kelvin
Imaginary Freq: 0

0	1		
C	-11.4037	2.937035	1.246348
C	-10.0485	2.700239	1.006784
C	-11.9676	0.576633	0.920909
C	-12.3506	1.889393	1.202963
O	-13.6614	2.164874	1.485491
O	-11.8337	4.214386	1.485399
C	-14.3946	2.781525	0.415287
H	-15.4046	2.937327	0.792874
H	-13.9493	3.740599	0.140432
H	-14.4297	2.11848	-0.4545
C	-12.1323	4.506082	2.859951
H	-12.4558	5.54612	2.883434
H	-12.9318	3.860112	3.230117
H	-11.2367	4.389986	3.477719
N	-8.31357	1.118864	0.46729
C	-7.96877	-0.10754	0.211188
C	-8.93201	-1.17771	0.180927
N	-10.1947	-0.97033	0.407455
C	-10.5871	0.310847	0.679903
C	-9.63609	1.367347	0.709819
C	-2.7754	-4.75791	-1.36834
C	-3.16433	-3.44285	-1.09873
C	-5.06951	-5.56754	-1.12441
C	-3.71828	-5.80892	-1.38136
C	-6.00407	-6.63848	-1.13894
C	-6.7857	-7.5538	-1.14271
H	-7.48061	-8.35681	-1.15431
C	-2.20443	-2.39796	-1.09479
C	-1.37782	-1.50621	-1.09827

O	-3.30475	-7.07399	-1.69393
O	-1.45491	-5.043	-1.57858
C	-2.64996	-7.78161	-0.62781
H	-2.38536	-8.75716	-1.03362
H	-1.74806	-7.25453	-0.30806
H	-3.33192	-7.91234	0.21764
C	-1.09133	-5.2665	-2.95152
H	-0.02415	-5.48449	-2.94795
H	-1.64256	-6.11355	-3.36599
H	-1.27662	-4.36636	-3.54509
N	-4.93068	-1.8961	-0.55673
C	-6.19303	-1.6882	-0.32532
C	-7.15765	-2.76106	-0.35181
N	-6.81133	-3.98777	-0.60673
C	-5.4894	-4.23319	-0.85291
C	-4.53932	-3.17733	-0.82768
N	-8.47998	-2.45532	-0.09793
N	-6.64366	-0.41397	-0.04358
H	-5.96748	0.338795	-0.02226
H	-9.15653	-3.20784	-0.11794
C	-12.9312	-0.46608	0.881894
C	-9.10935	3.764722	1.052238
C	-8.31164	4.669878	1.095162
C	-13.7504	-1.35206	0.844261
C	-14.7357	-2.44095	0.809824
C	-7.33441	5.766112	1.129833
C	-14.0039	-3.7813	0.569167
H	-13.2835	-3.97816	1.366184
H	-14.7249	-4.6039	0.542512
H	-13.4637	-3.76339	-0.38007
C	-15.744	-2.18601	-0.33505
H	-16.2732	-1.24222	-0.18455
H	-15.2345	-2.14176	-1.30029
H	-16.4819	-2.99316	-0.37091
C	-7.02974	6.219929	-0.31766
H	-6.29968	7.035051	-0.30827
H	-6.62011	5.395315	-0.90522
H	-7.93653	6.573527	-0.81339
C	-6.03339	5.269698	1.802148
H	-5.29191	6.074001	1.825395
H	-6.22397	4.946258	2.827987

H	-5.61124	4.425195	1.253036
C	-15.4877	-2.49151	2.160459
H	-14.7948	-2.67502	2.984585
H	-16.0029	-1.54802	2.353811
H	-16.2296	-3.29581	2.1465
C	-7.91839	6.951212	1.932453
H	-8.84497	7.308856	1.477888
H	-8.13577	6.654879	2.961294
H	-7.20214	7.778017	1.956251
Hg	0.00001	0.000126	-1.09604
C	1.377841	1.50646	-1.09826
C	2.204473	2.398187	-1.09479
C	3.164423	3.443032	-1.09876
C	2.775534	4.75812	-1.36828
C	4.539428	3.17743	-0.82783
C	3.718466	5.80909	-1.38133
O	1.455052	5.04329	-1.5784
N	4.930741	1.896169	-0.55698
C	5.489543	4.233253	-0.85307
C	5.069707	5.567635	-1.12447
O	3.304963	7.074189	-1.69382
C	1.091358	5.266856	-2.9513
C	6.193097	1.688202	-0.32567
N	6.811482	3.987763	-0.60697
C	6.004306	6.638534	-1.13903
C	2.650358	7.781822	-0.6276
H	0.024199	5.484896	-2.94764
H	1.6426	6.113887	-3.3658
H	1.276555	4.366718	-3.54492
C	7.157769	2.761029	-0.35215
N	6.643698	0.41393	-0.04407
C	6.785981	7.553824	-1.14281
H	2.385749	8.757389	-1.03335
H	1.748475	7.254772	-0.30773
H	3.332434	7.912503	0.217762
N	8.480095	2.455213	-0.09839
C	7.968775	0.107472	0.21083
H	5.967485	-0.3388	-0.02268
C	8.932055	1.177599	0.180596
H	9.156662	3.207721	-0.1183
N	8.313516	-1.11894	0.467018

N	10.19468	0.970197	0.40725
C	9.636014	-1.36746	0.709655
C	10.58703	-0.31099	0.67978
C	10.04837	-2.70035	1.006702
C	11.96757	-0.5768	0.920925
C	11.40348	-2.93718	1.246392
C	9.109159	-3.7648	1.052114
C	12.35045	-1.88957	1.203068
C	12.93115	0.465889	0.881991
O	11.83345	-4.21453	1.485515
C	8.311419	-4.66993	1.095002
O	13.66124	-2.16508	1.485751
C	13.75038	1.351831	0.844444
C	12.13188	-4.50622	2.860117
C	7.334174	-5.76615	1.129589
C	14.39451	-2.78169	0.415604
C	14.73576	2.440683	0.810171
H	12.45535	-5.54625	2.883658
H	12.93128	-3.86024	3.230417
H	11.2361	-4.39014	3.477734
C	6.03302	-5.26965	1.80158
C	7.917963	-6.95117	1.932463
C	7.02981	-6.22011	-0.31792
H	15.40448	-2.93749	0.793289
H	13.94927	-3.74076	0.14068
H	14.42976	-2.11862	-0.45416
C	15.48875	2.49012	2.160304
C	14.00387	3.781266	0.571104
C	15.74324	2.186579	-0.33563
H	5.610986	-4.4252	1.25229
H	5.291518	-6.07394	1.82476
H	6.223394	-4.9461	2.827423
H	8.844645	-7.30887	1.478133
H	8.135123	-6.65474	2.961321
H	7.201705	-7.77797	1.956188
H	6.620309	-5.39556	-0.90565
H	7.936694	-6.57377	-0.81341
H	6.299736	-7.03523	-0.3086
H	16.23067	3.294356	2.146439
H	14.79641	2.673052	2.98507
H	16.004	1.546424	2.352546

H	14.72493	4.603831	0.544561
H	13.46298	3.764141	-0.37775
H	13.28402	3.977565	1.3688
H	16.27241	1.242635	-0.18626
H	15.23296	2.14313	-1.30054
H	16.48117	2.993713	-0.37138
H	7.480934	8.356791	-1.15449

7.0 N4A coordinates

Electronic Energy (EE:) -1214.358769 Hartree
EE + Thermal Free Energy Correction: -1214.122436 Hartree
E (Thermal): 198.545 kcal/mol
Entropy (S): 170.507 cal/mol-kelvin
Imaginary Freq: 0

0	1		
C	3.782109	-0.94887	-0.07594
C	3.82127	0.517389	-0.15509
C	-3.20245	-0.67981	0.040111
C	-2.04481	-1.43957	0.032421
C	-1.94966	1.429839	-0.02916
C	-3.15499	0.748142	0.011872
C	-1.92338	2.849801	-0.05503
C	-1.91109	4.053057	-0.06546
H	-1.8887	5.11467	-0.08491
C	-2.11015	-2.85793	0.059172
C	-2.1732	-4.0595	0.070936
H	-2.2132	-5.12068	0.08984
O	-4.32844	1.441317	-0.02223
O	-4.41891	-1.29151	0.120398
C	-5.02377	1.541779	1.234016
H	-5.93048	2.108307	1.027751
H	-5.28112	0.551772	1.616215
H	-4.41279	2.083795	1.961437
C	-5.15326	-1.36445	-1.11524
H	-6.08955	-1.86642	-0.87638
H	-5.35537	-0.36497	-1.50656
H	-4.59956	-1.9559	-1.84988
N	0.349257	-1.49546	-0.00309
C	1.502184	-0.84141	-0.04781
C	1.548303	0.594882	-0.09715

N	0.442756	1.326965	-0.09578
C	-0.72534	0.672287	-0.04842
C	-0.77265	-0.76441	-0.00183
N	2.753814	1.245848	-0.15757
N	2.659018	-1.5818	-0.03251
O	5.037043	1.069284	-0.25041
O	4.917506	-1.67314	-0.14087
C	5.089805	2.503653	-0.37891
H	4.552909	2.823548	-1.27259
H	4.641722	2.98182	0.493021
H	6.148127	2.742265	-0.45466
C	5.888299	-1.52277	0.910657
H	5.446392	-1.80732	1.869897
H	6.690769	-2.21482	0.664174
H	6.275981	-0.50511	0.955269

8.0 N4A dimer coordinates

N4A Hg dimer: 0 degrees

Electronic Energy (EE:) -2580.596075 Hartree
EE + Thermal Free Energy Correction: -2580.128631 Hartree
E (Thermal): 387.765 kcal/mol
Entropy (S): 318.736 cal/mol-kelvin
Imaginary Freq: 0

0	1		
C	6.720799	4.229499	-0.69825
C	5.258339	4.14667	-0.81034
C	6.93866	-2.6467	0.545232
C	7.616053	-1.45231	0.363738
C	4.748373	-1.58202	0.232835
C	5.513181	-2.71097	0.482535
C	3.334281	-1.65922	0.174559
C	2.120844	-1.71133	0.125309
C	9.03387	-1.40769	0.428182
C	10.23604	-1.37907	0.473355
H	11.2963	-1.33692	0.518925
O	4.906739	-3.92425	0.625273
O	7.631585	-3.78588	0.834518
C	4.813348	-4.41123	1.976445
H	4.320913	-5.38023	1.91105

H	5.805874	-4.52646	2.417048
H	4.204383	-3.73294	2.580862
C	7.80149	-4.69731	-0.2658
H	8.361933	-5.54256	0.13074
H	6.833781	-5.03579	-0.64273
H	8.376203	-4.22193	-1.06574
N	7.505282	0.90269	-0.05973
C	6.773844	1.981927	-0.3032
C	5.340008	1.912934	-0.38641
N	4.688787	0.770262	-0.21918
C	5.420843	-0.32337	0.029763
C	6.855241	-0.25565	0.110024
N	4.607922	3.040947	-0.65365
N	7.429841	3.178229	-0.46174
O	4.62569	5.286922	-1.11109
O	7.365485	5.390628	-0.932
C	3.194813	5.214112	-1.27237
H	2.938832	4.519821	-2.07326
H	2.722667	4.878552	-0.34831
H	2.886933	6.226627	-1.52276
C	7.112773	6.503901	-0.05611
H	7.392547	6.243517	0.968778
H	7.757289	7.304434	-0.41312
H	6.070278	6.818863	-0.09926
Hg	0.082487	-1.74054	0.017403
C	-1.95673	-1.76567	-0.09413
C	-3.17065	-1.7448	-0.15189
C	-4.58534	-1.70479	-0.22358
C	-5.32001	-2.86067	-0.43471
C	-5.29041	-0.45529	-0.07752
C	-6.74611	-2.83287	-0.51174
O	-4.68511	-4.06457	-0.52745
N	-4.58756	0.664191	0.13377
C	-6.72547	-0.42513	-0.17302
C	-7.45432	-1.64874	-0.38365
O	-7.41037	-3.99644	-0.76426
C	-4.5487	-4.58534	-1.86236
C	-5.26548	1.797893	0.251946
N	-7.40464	0.723754	-0.05633
C	-8.87239	-1.64284	-0.46225
C	-7.5482	-4.88566	0.358909

H	-4.03669	-5.54082	-1.75946
H	-5.528	-4.7351	-2.32221
H	-3.94118	-3.90984	-2.47117
C	-6.69941	1.827091	0.151948
N	-4.55417	2.94887	0.487656
C	-10.0744	-1.64953	-0.5193
H	-8.08677	-5.75531	-0.01432
H	-6.56964	-5.18741	0.738252
H	-8.13236	-4.40702	1.150052
N	-7.37525	3.015223	0.261156
C	-5.21083	4.053268	0.602817
C	-6.67312	4.080144	0.467962
O	-4.50989	5.194915	0.75768
O	-7.24983	5.2858	0.546926
C	-4.73452	5.983741	1.940251
C	-8.67903	5.333689	0.367853
H	-4.49862	5.395879	2.83196
H	-4.04141	6.819075	1.865912
H	-5.75859	6.353533	1.986452
H	-8.95079	4.943855	-0.61368
H	-9.17989	4.741464	1.134699
H	-8.93996	6.385912	0.454351
H	-11.1348	-1.64251	-0.57789

N4A Hg dimer: 90 degrees

Electronic Energy (EE:) -2580.595852 Hartree
EE + Thermal Free Energy Correction: -2580.128996 Hartree
E (Thermal): 387.762 kcal/mol
Entropy (S): 319.963 cal/mol-kelvin
Imaginary Freq: 0

0	1		
C	-7.64248	2.846531	2.509961
C	-6.21107	3.168537	2.442309
C	-6.47251	-2.83587	-1.39005
C	-7.36219	-2.04775	-0.67918
C	-4.57915	-1.35865	-0.87663
C	-5.08976	-2.49201	-1.49063
C	-3.20417	-1.03166	-0.98548

C	-2.02642	-0.74534	-1.07755
C	-8.73329	-2.4058	-0.58855
C	-9.89176	-2.721	-0.50697
H	-10.9186	-2.98225	-0.43337
O	-4.25512	-3.3317	-2.16718
O	-6.91986	-3.94312	-2.04955
C	-4.32685	-3.24904	-3.60217
H	-3.61564	-3.9824	-3.97906
H	-5.332	-3.48868	-3.95532
H	-4.03307	-2.25032	-3.93772
C	-6.6417	-5.19796	-1.40217
H	-7.05332	-5.96728	-2.05367
H	-5.56567	-5.34485	-1.28561
H	-7.13902	-5.23994	-0.42902
N	-7.72847	-0.08949	0.649766
C	-7.23988	0.992023	1.241791
C	-5.84432	1.327546	1.156917
N	-4.98839	0.573304	0.481211
C	-5.47502	-0.52	-0.12059
C	-6.87074	-0.85721	-0.03406
N	-5.36224	2.444421	1.790068
N	-8.11489	1.794312	1.932751
O	-5.82044	4.254288	3.120825
O	-8.48166	3.59416	3.25536
C	-4.41185	4.558062	3.106896
H	-3.84137	3.72953	3.527941
H	-4.07055	4.741234	2.087266
H	-4.30925	5.451152	3.718988
C	-8.69072	4.967505	2.880596
H	-9.11302	5.019327	1.872912
H	-9.41402	5.35534	3.594826
H	-7.76696	5.543272	2.93792
Hg	-0.05471	-0.22794	-1.19381
C	1.916169	0.295456	-1.31007
C	3.095217	0.588812	-1.34414
C	4.473726	0.916622	-1.37037
C	4.98478	1.771561	-2.33374
C	5.374664	0.364588	-0.38887
C	6.372343	2.108837	-2.36903
O	4.149579	2.347459	-3.24606
N	4.886649	-0.45822	0.547471

C	6.774882	0.690305	-0.43558
C	7.266278	1.591095	-1.4455
O	6.822708	2.92235	-3.36647
C	4.18584	1.767704	-4.56281
C	5.743248	-0.95851	1.427598
N	7.636099	0.180112	0.454996
C	8.641927	1.940515	-1.49729
C	6.547911	4.324084	-3.19149
H	3.479208	2.340736	-5.16119
H	5.186708	1.84464	-4.9932
H	3.867273	0.722143	-4.52425
C	7.143159	-0.63434	1.377883
N	5.24875	-1.79039	2.401818
C	9.803736	2.251017	-1.54251
H	6.961409	4.820246	-4.06815
H	5.472559	4.50517	-3.1329
H	7.046368	4.697456	-2.29238
N	8.010361	-1.17721	2.290916
C	6.079313	-2.27916	3.259539
C	7.512836	-1.96679	3.184766
O	5.609316	-3.15774	4.167261
O	8.294837	-2.57007	4.088425
C	5.746732	-2.84509	5.565386
C	9.70971	-2.31213	3.996889
H	5.224288	-1.91134	5.792345
H	5.263872	-3.66504	6.092728
H	6.793821	-2.77842	5.859822
H	10.08996	-2.62812	3.024877
H	9.913046	-1.24853	4.127516
H	10.1563	-2.89658	4.797958
H	10.83292	2.510505	-1.57909

N4A Hg dimer: 180 degrees

Electronic Energy (EE:) -2580.596060 Hartree
EE + Thermal Free Energy Correction: -2580.128613 Hartree
E (Thermal): 387.765 kcal/mol
Entropy (S): 318.733 cal/mol-kelvin
Imaginary Freq: 0

0	1		
C	8.674395	-2.64207	-0.02553
C	7.327136	-3.22459	0.02125
C	5.836306	3.745845	0.057474
C	6.971066	2.951911	0.044701
C	4.338383	1.799605	0.051224
C	4.527672	3.173207	0.058598
C	3.032012	1.24966	0.050478
C	1.910864	0.780008	0.045767
C	8.26436	3.538148	0.045487
C	9.357273	4.041597	0.057032
H	10.32816	4.472148	0.05844
O	3.450388	4.006653	0.117383
O	5.955489	5.104172	0.023238
C	3.100344	4.651802	-1.12105
H	2.238217	5.27817	-0.89771
H	3.925606	5.267984	-1.48414
H	2.82356	3.904903	-1.87043
C	5.743259	5.772448	1.279974
H	5.867281	6.835078	1.077103
H	4.736531	5.579973	1.657203
H	6.491258	5.450973	2.010264
N	7.909285	0.749013	0.011354
C	7.729383	-0.56493	0.00972
C	6.412417	-1.14157	0.02946
N	5.323249	-0.38546	0.04673
C	5.497231	0.94277	0.046913
C	6.81484	1.519987	0.029113
N	6.254464	-2.50392	0.040523
N	8.846259	-1.3639	-0.02394
O	7.266878	-4.5612	0.066929
O	9.766408	-3.43226	0.021836
C	5.955529	-5.15004	0.162977
H	5.450156	-4.80456	1.065496
H	5.352015	-4.88268	-0.7054
H	6.12949	-6.22292	0.201756
C	10.00245	-4.33576	-1.07271
H	10.1281	-3.77192	-2.00155
H	10.93276	-4.84587	-0.83186
H	9.196098	-5.06251	-1.17276
Hg	0.043413	-0.04494	0.047707

C	-1.82538	-0.86863	0.048164
C	-2.95541	-1.31625	0.052224
C	-4.28071	-1.81781	0.052019
C	-4.52768	-3.18008	0.109495
C	-5.40321	-0.91425	-0.00658
C	-5.85969	-3.69585	0.109862
O	-3.48824	-4.05759	0.214938
N	-5.17188	0.403266	-0.05693
C	-6.74403	-1.43472	-0.02355
C	-6.96037	-2.85633	0.047646
O	-6.03769	-5.04766	0.125238
C	-3.14237	-4.74724	-0.99985
C	-6.22522	1.206401	-0.12117
N	-7.80436	-0.61854	-0.09131
C	-8.27675	-3.3895	0.050872
C	-5.85712	-5.67961	1.405562
H	-2.31424	-5.40638	-0.74388
H	-3.98689	-5.33519	-1.36602
H	-2.81738	-4.03227	-1.76099
C	-7.56482	0.684624	-0.14077
N	-5.99787	2.560301	-0.15533
C	-9.38845	-3.85011	0.065191
H	-6.02568	-6.74246	1.239356
H	-4.84437	-5.51657	1.78017
H	-6.59308	-5.30127	2.120718
N	-8.63638	1.536327	-0.22262
C	-7.02042	3.344485	-0.21717
C	-8.38512	2.803144	-0.2668
O	-6.79756	4.669276	-0.32946
O	-9.3707	3.70109	-0.3869
C	-7.32046	5.544096	0.686782
C	-10.7117	3.182652	-0.48604
H	-6.89972	5.278432	1.660808
H	-6.98492	6.541126	0.409396
H	-8.40928	5.513737	0.719769
H	-10.8025	2.531873	-1.35637
H	-10.9684	2.614417	0.40888
H	-11.3472	4.059309	-0.58786
H	-10.3738	-4.24623	0.067483

9.0 N4A dimer (0 degrees) radical anion coordinates

Electronic Energy (EE:) -2580.684830 Hartree
EE + Thermal Free Energy Correction: -2580.219399 Hartree
E (Thermal): 385.926 kcal/mol
Entropy (S): 316.809 cal/mol-kelvin
Imaginary Freq: 0

-1	2		
C	7.021856	4.152664	-0.30797
C	5.584926	4.183171	-0.35508
C	6.800541	-2.83649	0.21772
C	7.560786	-1.66625	0.141001
C	4.698221	-1.59133	0.06775
C	5.394431	-2.80125	0.172877
C	3.284258	-1.58176	0.039058
C	2.065533	-1.58724	0.024087
C	8.978348	-1.73152	0.177568
C	10.18149	-1.8039	0.195848
H	11.24145	-1.84296	0.222237
O	4.704116	-3.99026	0.197901
O	7.430253	-4.04749	0.382262
C	4.486113	-4.51806	1.511166
H	3.925655	-5.44427	1.379835
H	5.438224	-4.73002	2.006461
H	3.894994	-3.82098	2.113311
C	7.54187	-4.82653	-0.81352
H	8.065144	-5.74151	-0.53326
H	6.55384	-5.07346	-1.21127
H	8.128087	-4.29194	-1.56817
N	7.617182	0.723141	-0.03225
C	6.951404	1.8761	-0.13901
C	5.511586	1.911639	-0.18378
N	4.781955	0.797256	-0.11958
C	5.445015	-0.36553	-0.01192
C	6.88807	-0.40267	0.032539
N	4.857694	3.104408	-0.29331
N	7.67495	3.032655	-0.19941
O	5.005251	5.401089	-0.4698
O	7.735011	5.311763	-0.43433
C	3.573808	5.417779	-0.54096

H	3.221358	4.847623	-1.40256
H	3.132261	4.987786	0.360326
H	3.30457	6.468531	-0.63907
C	7.743773	6.153564	0.721071
H	8.194559	5.632175	1.572577
H	8.355593	7.018138	0.463453
H	6.7342	6.486566	0.977955
Hg	0.029697	-1.57356	-0.00781
C	-2.00992	-1.58754	-0.03795
C	-3.22844	-1.58423	-0.05061
C	-4.64253	-1.59677	-0.07455
C	-5.33795	-2.80764	-0.14589
C	-5.39303	-0.37038	-0.02379
C	-6.7462	-2.84552	-0.18293
O	-4.64977	-3.99707	-0.14569
N	-4.73246	0.796584	0.049906
C	-6.83378	-0.41048	-0.05992
C	-7.5073	-1.67532	-0.13165
O	-7.37567	-4.05879	-0.31626
C	-4.41567	-4.54422	-1.44896
C	-5.46118	1.909552	0.089474
N	-7.5633	0.718766	-0.01926
C	-8.92525	-1.74235	-0.15907
C	-7.46121	-4.8245	0.89111
H	-3.8587	-5.46909	-1.29675
H	-5.36202	-4.76188	-1.95287
H	-3.81575	-3.85675	-2.05302
C	-6.89882	1.869125	0.054466
N	-4.8055	3.109181	0.165748
C	-10.1283	-1.81604	-0.16912
H	-7.98606	-5.74422	0.630759
H	-6.46512	-5.06273	1.272818
H	-8.0357	-4.28291	1.649761
N	-7.62259	3.032089	0.096215
C	-5.52162	4.190444	0.203843
C	-6.96777	4.149869	0.167807
O	-4.95528	5.408341	0.279172
O	-7.60477	5.335287	0.21268
C	-3.52174	5.438088	0.314231
C	-9.03578	5.283056	0.175979
H	-3.10165	4.986036	-0.58634

H	-3.26048	6.493221	0.374654
H	-3.14305	4.894951	1.182249
H	-9.38411	4.807135	-0.74309
H	-9.42623	4.718459	1.025289
H	-9.36066	6.321352	0.220315
H	-11.1882	-1.86141	-0.18998

10.0 N6P-Br dimer (0 degrees) radical anion coordinates

Electronic Energy (EE:) -13556.154428 Hartree
EE + Thermal Free Energy Correction: -13555.571609 Hartree
E (Thermal): 487.418 kcal/mol
Entropy (S): 410.147 cal/mol-kelvin
Imaginary Freq: 0

-1	2		
C	-7.811	-5.72711	-0.38385
C	-8.37989	-4.46973	-0.22629
C	-5.60294	-4.72302	-0.45505
C	-6.4074	-5.85466	-0.49779
O	-5.86714	-7.10886	-0.60372
O	-8.58745	-6.8514	-0.4795
C	-5.91038	-7.66916	-1.924
H	-5.44608	-8.65239	-1.84983
H	-6.94303	-7.77119	-2.26734
H	-5.33926	-7.05052	-2.62279
C	-8.64566	-7.64325	0.715745
H	-9.29336	-8.48915	0.485597
H	-7.65109	-8.00176	0.991808
H	-9.08069	-7.06645	1.537785
N	-8.15915	-2.07419	-0.03747
C	-7.36346	-1.03848	-0.00054
C	-5.93461	-1.1688	-0.10877
N	-5.35569	-2.3319	-0.2509
C	-6.16075	-3.43524	-0.29378
C	-7.58284	-3.30496	-0.18573
C	-6.66052	6.061604	0.546829
C	-7.49756	4.932841	0.502367
C	-4.65639	4.67898	0.301603
C	-5.27151	5.938451	0.439472
C	-3.2494	4.585061	0.205722
C	-8.90553	5.081831	0.602084

C	-10.1012	5.2194	0.673735
H	-11.1539	5.330249	0.749304
O	-4.50102	7.076572	0.432948
O	-7.21489	7.30362	0.740956
C	-4.18346	7.5822	1.735367
H	-3.56818	8.468417	1.577767
H	-5.09381	7.856216	2.27641
H	-3.61285	6.843846	2.307181
C	-7.31966	8.102032	-0.44346
H	-7.78149	9.041145	-0.13708
H	-6.33227	8.297347	-0.86979
H	-7.95852	7.610182	-1.18436
N	-7.70812	2.541727	0.326573
C	-7.12107	1.380836	0.189949
C	-5.70516	1.251694	0.084295
N	-4.90791	2.289244	0.117301
C	-5.48476	3.516645	0.25707
C	-6.9052	3.645111	0.36422
N	-5.17499	-0.02177	-0.05871
N	-7.88739	0.22624	0.144916
H	-8.89197	0.321669	0.219947
H	-4.16957	-0.11143	-0.13477
Br	-10.2777	-4.32505	-0.06894
Br	-3.71241	-4.9228	-0.61267
C	3.249462	4.585018	-0.20599
C	4.656464	4.678929	-0.30171
C	5.271613	5.938397	-0.43949
C	5.48482	3.516585	-0.2571
C	6.660636	6.06154	-0.54667
O	4.501137	7.076524	-0.43303
N	4.907941	2.289186	-0.11743
C	6.905278	3.645042	-0.36406
C	7.497668	4.932771	-0.50211
O	7.215038	7.303554	-0.74072
C	4.183735	7.582179	-1.73548
C	5.705185	1.251628	-0.08435
N	7.708185	2.541653	-0.32633
C	8.905645	5.081752	-0.60165
C	7.319663	8.101956	0.443719
H	3.568441	8.468397	-1.57794
H	5.094156	7.856199	-2.27641

H	3.613194	6.843841	-2.30738
C	7.12111	1.380763	-0.18981
N	5.174979	-0.02183	0.05855
C	10.10135	5.219318	-0.67314
H	7.781535	9.041069	0.1374
H	6.332226	8.297273	0.869924
H	7.958428	7.610097	1.184689
N	7.887414	0.226161	-0.14469
C	5.934583	-1.16887	0.108694
H	4.169554	-0.11149	0.134471
C	7.363448	-1.03856	0.000673
H	8.892005	0.321583	-0.21957
N	5.355641	-2.33197	0.25072
N	8.159131	-2.07428	0.03771
C	6.160683	-3.43531	0.293692
C	7.582786	-3.30504	0.185863
C	5.602841	-4.72309	0.454851
C	8.379828	-4.46982	0.22652
C	6.40729	-5.85474	0.497682
Br	3.712291	-4.92286	0.612188
C	7.810904	-5.7272	0.383961
Br	10.2777	-4.32514	0.069469
O	5.867004	-7.10894	0.603499
O	8.58734	-6.8515	0.479696
C	5.910026	-7.66927	1.923783
C	8.64572	-7.64332	-0.71556
H	5.445731	-8.65249	1.849523
H	6.942621	-7.7713	2.267283
H	5.338791	-7.05063	2.622488
H	9.293381	-8.48923	-0.48533
H	7.651192	-8.00182	-0.99177
H	9.080871	-7.06651	-1.53752
H	11.15403	5.330221	-0.74852
C	-2.03313	4.537637	0.131171
Hg	0.000031	4.510369	-0.00016
C	2.03319	4.537603	-0.13148

11.0 N6P-Bu dimer (180 degrees) radical anion coordinates

Electronic Energy (EE:) -4195.886713 Hartree
EE + Thermal Free Energy Correction: -4194.814599 Hartree
E (Thermal): 833.721 kcal/mol

Entropy (S): 541.848 cal/mol-kelvin
Imaginary Freq: 0

-1	2		
C	-11.7009	2.904892	0.089732
C	-10.3175	2.677224	0.09113
C	-12.1733	0.508579	0.022177
C	-12.6129	1.83947	0.060434
O	-13.9612	2.107381	0.109886
O	-12.1775	4.195222	0.079261
C	-14.5293	2.51994	-1.13822
H	-15.5908	2.684999	-0.95056
H	-14.068	3.447072	-1.48892
H	-14.4131	1.735123	-1.89289
C	-12.6184	4.672426	1.35548
H	-12.9535	5.698263	1.198846
H	-13.4472	4.066847	1.732501
H	-11.7933	4.667583	2.074966
N	-8.49757	1.099762	0.048317
C	-8.10577	-0.1465	0.020636
C	-9.0405	-1.23822	-0.00524
N	-10.3325	-1.04514	-0.00277
C	-10.7722	0.250641	0.026583
C	-9.84558	1.333148	0.051813
C	-2.67872	-4.8177	-0.07295
C	-3.11534	-3.47929	-0.05178
C	-4.97675	-5.64881	-0.08699
C	-3.58964	-5.87881	-0.09943
C	-5.88275	-6.74131	-0.10309
C	-6.64424	-7.67621	-0.10298
H	-7.32096	-8.49347	-0.11588
C	-2.17645	-2.42301	-0.03859
C	-1.35684	-1.51999	-0.03654
O	-3.12211	-7.16814	-0.18129
O	-1.33337	-5.09545	-0.03005
C	-2.64648	-7.71059	1.056036
H	-2.32318	-8.72875	0.837122
H	-1.80341	-7.12898	1.437665
H	-3.45071	-7.73872	1.798651
C	-0.73913	-5.34111	-1.31034
H	0.317655	-5.53479	-1.12496

H	-1.19606	-6.21267	-1.78807
H	-0.83707	-4.46278	-1.95588
N	-4.96058	-1.92954	-0.0161
C	-6.25478	-1.73655	-0.01298
C	-7.18276	-2.821	-0.03675
N	-6.79447	-4.06977	-0.06296
C	-5.44932	-4.3053	-0.06671
C	-4.51974	-3.21965	-0.04205
N	-8.53527	-2.52179	-0.03242
N	-6.7596	-0.44686	0.014796
H	-6.10002	0.320221	0.033934
H	-9.19086	-3.29207	-0.04942
C	-13.1104	-0.55857	-0.01226
C	-9.4082	3.767933	0.12399
C	-8.63037	4.691365	0.157783
C	-13.9029	-1.4693	-0.0484
C	-14.8454	-2.59551	-0.07652
C	-7.66264	5.796336	0.181334
C	-14.0543	-3.92042	0.019189
H	-13.4767	-3.95941	0.945284
H	-14.7403	-4.77345	-0.00007
H	-13.3572	-4.01547	-0.81621
C	-15.6489	-2.56665	-1.39789
H	-16.2152	-1.63646	-1.48729
H	-14.9811	-2.64258	-2.25906
H	-16.3528	-3.40462	-1.43064
C	-7.14876	6.055499	-1.25493
H	-6.42152	6.873809	-1.25309
H	-6.66523	5.163631	-1.65923
H	-7.9732	6.325483	-1.91898
C	-6.47375	5.414497	1.093534
H	-5.73524	6.222224	1.11063
H	-6.81185	5.232785	2.116334
H	-5.98648	4.506223	0.733029
C	-15.8183	-2.48277	1.120448
H	-15.2724	-2.50743	2.066204
H	-16.3783	-1.54568	1.077392
H	-16.5301	-3.31467	1.10888
C	-8.3464	7.072514	0.72299
H	-9.19646	7.352342	0.096275
H	-8.71167	6.914694	1.74063

H	-7.63577	7.904977	0.736684
Hg	-5.1E-05	-0.00029	-0.03275
C	1.35673	1.519423	-0.03657
C	2.176301	2.422474	-0.03864
C	3.115087	3.478847	-0.0518
C	2.678334	4.817208	-0.07299
C	4.519512	3.219346	-0.04204
C	3.589154	5.878413	-0.09945
O	1.33296	5.094828	-0.03011
N	4.960479	1.929273	-0.01607
C	5.448987	4.305087	-0.06669
C	4.976285	5.648552	-0.08699
O	3.121492	7.167694	-0.18132
C	0.738717	5.340436	-1.31041
C	6.254697	1.736421	-0.01293
N	6.794157	4.069691	-0.06292
C	5.88218	6.741141	-0.10308
C	2.645794	7.710102	1.055997
H	-0.31809	5.534021	-1.12505
H	1.195585	6.212043	-1.78813
H	0.836753	4.462122	-1.95595
C	7.182574	2.820962	-0.03669
N	6.75965	0.446779	0.014869
C	6.643572	7.676111	-0.10295
H	2.322394	8.728226	0.837075
H	1.802778	7.128409	1.43762
H	3.450013	7.738318	1.798621
N	8.535113	2.521883	-0.03234
C	8.105845	0.146547	0.020694
H	6.100142	-0.32037	0.033998
C	9.040467	1.238359	-0.00519
H	9.190625	3.292225	-0.04936
N	8.497775	-1.09967	0.048364
N	10.3325	1.045408	-0.00273
C	9.845805	-1.33293	0.051842
C	10.77232	-0.25033	0.026604
C	10.31783	-2.67696	0.091138
C	12.17343	-0.50813	0.02217
C	11.70132	-2.90449	0.089707
C	9.408663	-3.76776	0.124012
C	12.61319	-1.83897	0.060402

C	13.11043	0.559115	-0.01228
O	12.17799	-4.19477	0.079213
C	8.630936	-4.69127	0.157818
O	13.96147	-2.10675	0.109819
C	13.90282	1.469925	-0.04841
C	12.61904	-4.67193	1.355412
C	7.663347	-5.79636	0.181352
C	14.52957	-2.51924	-1.13831
C	14.84527	2.596217	-0.07653
H	12.9542	-5.69774	1.198759
H	13.44777	-4.06627	1.732405
H	11.79389	-4.66718	2.07493
C	6.473821	-5.41419	1.092583
C	8.346941	-7.07215	0.724144
C	7.150417	-6.05639	-1.2551
H	15.59112	-2.6842	-0.95067
H	14.0684	-3.44641	-1.489
H	14.41327	-1.73442	-1.89296
C	15.81842	2.483375	1.120241
C	14.0541	3.921045	0.019507
C	15.64854	2.567609	-1.39805
H	5.986658	-4.50618	0.731269
H	5.735409	-6.22201	1.109651
H	6.811243	-5.23187	2.115498
H	9.197433	-7.35221	0.09812
H	8.711547	-6.91372	1.741928
H	7.636412	-7.9047	0.737848
H	6.667006	-5.16482	-1.66019
H	7.975326	-6.32661	-1.91847
H	6.423311	-6.87482	-1.25328
H	16.53015	3.315335	1.108672
H	15.27263	2.507851	2.066098
H	16.37842	1.546338	1.076946
H	14.74002	4.774133	0.000251
H	13.35685	4.016159	-0.81575
H	13.47666	3.959852	0.945711
H	16.21484	1.637478	-1.48769
H	14.98058	2.643608	-2.2591
H	16.35235	3.405644	-1.43081
H	7.320205	8.493448	-0.11582

12.0 N6P-Ph dimer (180 degrees) radical anion coordinates

Electronic Energy (EE:) -4491.141211 Hartree
EE + Thermal Free Energy Correction: -4490.189219 Hartree
E (Thermal): 753.284 kcal/mol
Entropy (S): 524.879 cal/mol-kelvin
Imaginary Freq: 0

-1	2		
C	12.55435	2.104505	-0.20491
C	12.14544	0.759218	-0.12524
C	10.23751	2.885636	-0.23145
C	11.62138	3.144189	-0.25334
O	12.06282	4.445525	-0.28801
O	13.89578	2.396276	-0.27405
C	12.48623	4.893125	-1.58198
H	12.7971	5.930933	-1.45862
H	13.32748	4.296053	-1.94404
H	11.65769	4.846074	-2.2959
C	14.46595	2.86182	0.955641
H	15.52206	3.041769	0.75258
H	13.98844	3.79038	1.279136
H	14.3722	2.099877	1.736201
N	10.3373	-0.83155	-0.0334
C	9.049274	-1.05328	-0.00597
C	8.093479	0.01289	-0.04562
N	8.45696	1.266795	-0.11502
C	9.795914	1.530409	-0.14625
C	10.74772	0.468911	-0.1039
C	3.709489	-5.80733	0.30834
C	5.087669	-5.54664	0.261491
C	3.181784	-3.42141	0.217567
C	2.773296	-4.76413	0.280311
C	2.219921	-2.38298	0.202625
C	1.384568	-1.49631	0.199547
C	6.018887	-6.61894	0.282643
C	6.80042	-7.53619	0.28777
H	7.49552	-8.33807	0.303628
O	1.434783	-5.06879	0.275976
O	3.271746	-7.10262	0.42712
C	0.882146	-5.33893	1.571332
H	-0.17417	-5.55602	1.412913

H	1.372627	-6.20247	2.028972
H	0.977547	-4.46286	2.220183
C	2.777633	-7.6823	-0.78725
H	2.477591	-8.70001	-0.5369
H	1.916319	-7.12415	-1.1627
H	3.56584	-7.71376	-1.54639
N	6.870507	-3.93105	0.163879
C	7.232483	-2.67812	0.09916
C	6.276047	-1.6101	0.065497
N	4.989431	-1.83233	0.100463
C	4.578214	-3.13241	0.168784
C	5.529935	-4.19461	0.20029
N	6.751398	-0.31464	-0.00705
N	8.574404	-2.34966	0.062429
H	9.248489	-3.10367	0.087631
H	6.076352	0.438763	-0.03233
C	9.310659	3.948134	-0.28681
C	13.10339	-0.27565	-0.07631
C	13.92902	-1.16197	-0.0255
C	8.513034	4.859057	-0.3466
C	7.562084	5.909654	-0.41065
C	6.184971	5.62416	-0.50039
C	7.968655	7.258449	-0.38722
C	5.253464	6.652333	-0.56522
H	5.866341	4.589079	-0.51873
C	7.029312	8.279836	-0.45235
H	9.025503	7.4856	-0.3142
C	5.668865	7.984127	-0.54194
H	4.197801	6.414074	-0.63523
H	7.359385	9.312943	-0.43221
H	4.938578	8.783849	-0.59275
C	14.88006	-2.21258	0.027269
C	14.46366	-3.54978	0.185386
C	16.26019	-1.94754	-0.07693
C	15.39552	-4.5783	0.237554
H	13.40405	-3.75997	0.265181
C	17.18444	-2.9832	-0.02329
H	16.588	-0.92264	-0.20298
C	16.75942	-4.30265	0.13428
H	15.05653	-5.60137	0.359431
H	18.24292	-2.76073	-0.10599

H	17.48378	-5.10838	0.175383
Hg	-1.9E-05	0.000071	0.195068
C	-1.38461	1.496449	0.199486
C	-2.21996	2.383122	0.202533
C	-3.18184	3.421529	0.217442
C	-2.77339	4.764266	0.280154
C	-4.57827	3.132501	0.168666
C	-3.70961	5.80744	0.308153
O	-1.43488	5.068956	0.275819
N	-4.98945	1.832407	0.100378
C	-5.53001	4.194671	0.200145
C	-5.08778	5.546717	0.261308
O	-3.2719	7.102742	0.426901
C	-0.88225	5.339107	1.571174
C	-6.27606	1.610148	0.065419
N	-6.87058	3.931079	0.163744
C	-6.01902	6.618994	0.282431
C	-2.77778	7.682403	-0.78748
H	0.174062	5.556229	1.412758
H	-1.37276	6.20264	2.028811
H	-0.97764	4.463046	2.220028
C	-7.23252	2.678139	0.099059
N	-6.75138	0.314668	-0.0071
C	-6.80058	7.536226	0.287536
H	-2.47778	8.700128	-0.53716
H	-1.91644	7.124268	-1.1629
H	-3.56598	7.713819	-1.54663
N	-8.57444	2.349651	0.062342
C	-8.09346	-0.01289	-0.04567
H	-6.07632	-0.43872	-0.03238
C	-9.04928	1.053253	-0.00603
H	-9.24854	3.103643	0.087527
N	-8.45691	-1.26681	-0.11506
N	-10.3373	0.831491	-0.03346
C	-9.79585	-1.53045	-0.14627
C	-10.7477	-0.46898	-0.10393
C	-10.2374	-2.88569	-0.23146
C	-12.1454	-0.75932	-0.12526
C	-11.6213	-3.14428	-0.25334
C	-9.31054	-3.94817	-0.28681
C	-12.5543	-2.10462	-0.20491

C	-13.1034	0.275529	-0.07634
O	-12.0627	-4.44563	-0.28799
C	-8.51288	-4.85906	-0.3466
O	-13.8957	-2.39642	-0.27404
C	-13.929	1.161811	-0.02552
C	-12.4861	-4.89325	-1.58195
C	-7.56186	-5.90959	-0.41077
C	-14.4658	-2.86196	0.955655
C	-14.8802	2.212334	0.027368
H	-12.7969	-5.93106	-1.45858
H	-13.3274	-4.2962	-1.94401
H	-11.6576	-4.84618	-2.29589
C	-6.18478	-5.624	-0.50057
C	-7.96834	-7.25841	-0.38737
H	-15.522	-3.04194	0.752603
H	-13.9883	-3.79051	1.279163
H	-14.3721	-2.10001	1.736204
C	-14.4639	3.549564	0.185531
C	-16.2603	1.947188	-0.07677
C	-5.2532	-6.65211	-0.56551
H	-5.86622	-4.5889	-0.51888
C	-7.02894	-8.27974	-0.4526
H	-9.02517	-7.48564	-0.3143
C	-15.3958	4.578001	0.237811
H	-13.4043	3.759841	0.265273
C	-17.1846	2.982761	-0.02301
H	-16.588	0.922263	-0.20285
C	-5.66851	-7.98393	-0.54227
H	-4.19756	-6.41378	-0.63558
H	-7.35894	-9.31287	-0.43249
C	-16.7597	4.302239	0.134604
H	-15.0569	5.601094	0.359723
H	-18.2431	2.760209	-0.10566
H	-4.93818	-8.7836	-0.59316
H	-17.4841	5.107909	0.175795
H	-7.49568	8.338109	0.303396