

Supporting Information

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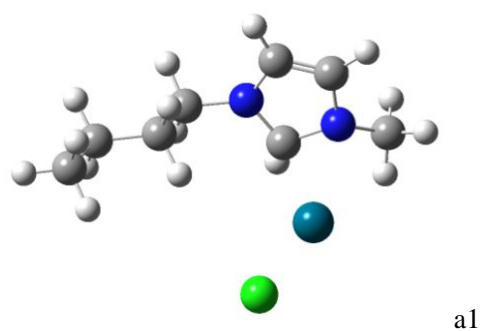
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Page 33-34. The B3LYP optimized structures of $[\text{Bmim}^+\cdot\text{PF}_6^-]\text{-Pd}$ and $[\text{Bmim}^+\cdot\text{PF}_6^-]\text{-Pd}_2$ complex in simulated $[\text{Bmim}^+\cdot\text{PF}_6^-]$ solvent.

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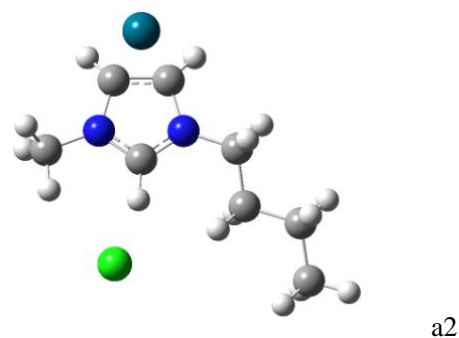


HF=-1010.5065043

Zero-point correction= 0.224596

Cartesian coordinate:

C	0.824590	-0.863568	0.786310
N	-0.133561	-1.754623	0.294160
C	0.374394	-2.371642	-0.833742
C	1.664412	-2.003017	-1.008243
N	1.995516	-1.066454	0.005575
C	-1.537061	-1.743478	0.708255
C	-2.415093	-0.777477	-0.099873
C	-3.863849	-0.757715	0.404622
C	-4.750832	0.195698	-0.403322
C	3.347222	-1.058941	0.589384
Cl	-0.332860	2.824150	0.047042
H	-0.241501	-3.017264	-1.442802
H	2.384229	-2.281858	-1.761519
H	3.395532	-0.289944	1.360995
H	3.588777	-2.039546	1.016850
H	4.066954	-0.812542	-0.194352
H	0.900319	-0.744351	1.866324
H	-1.553943	-1.474344	1.770492
H	-1.910828	-2.771836	0.630402
H	-1.983349	0.229268	-0.048087
H	-2.394519	-1.076452	-1.157490
H	-4.285082	-1.773608	0.369891
H	-3.874160	-0.456136	1.461595
H	-5.776089	0.205931	-0.016733
H	-4.362885	1.219613	-0.362604
H	-4.793825	-0.102166	-1.458073
Pd	1.034839	0.939197	-0.125937

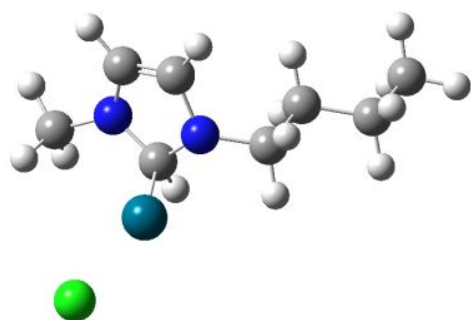


HF=-1010.4798166

Zero-point correction= 0.225271

Cartesian coordinate:

C	0.370098	0.792933	0.406856
N	0.273636	-0.536965	0.509813
C	-1.019484	-0.880163	0.957362
C	-1.700113	0.350081	1.152319
N	-0.776015	1.353060	0.801010
C	1.313498	-1.489803	0.078729
C	2.733316	-0.966454	0.310350
C	3.787025	-1.976749	-0.165641
C	5.216236	-1.474738	0.065541
C	-1.005867	2.800916	0.790659
Cl	2.299373	2.844617	-0.813367
H	-1.161939	-1.819527	1.477992
H	-2.487455	0.581128	1.859784
H	-0.103559	3.274432	0.387583
H	-1.863052	3.027598	0.151543
H	-1.200746	3.150952	1.808673
H	1.214950	1.407302	-0.012131
H	1.150282	-1.713520	-0.982123
H	1.139945	-2.413966	0.641105
H	2.876509	-0.013315	-0.215405
H	2.869255	-0.761448	1.380746
H	3.643722	-2.937164	0.351115
H	3.639437	-2.176423	-1.236151
H	5.952173	-2.201772	-0.295223
H	5.388631	-0.528146	-0.458342
H	5.408204	-1.304261	1.131677
Pd	-2.613202	-0.708243	-0.498183

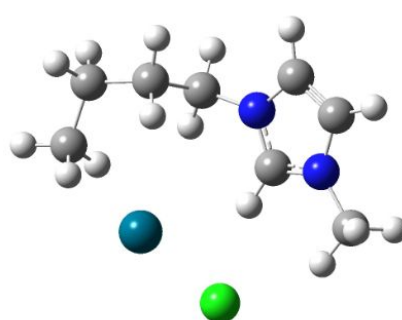


a3

HF= -1010.5054663

Cartesian coordinate:

C	-0.058990	0.685425	-0.585896
N	0.693970	0.204896	0.518188
C	0.778556	1.267118	1.457813
C	0.143035	2.341173	0.938221
N	-0.294313	2.043755	-0.341538
C	1.806095	-0.762726	0.367575
C	3.117563	-0.124090	-0.103037
C	4.244278	-1.158534	-0.236293
C	5.564068	-0.540532	-0.709778
C	-1.272245	2.808633	-1.099537
Cl	-3.504386	-1.169436	-0.471881
H	1.260714	1.125498	2.412222
H	-0.060108	3.302118	1.387993
H	-2.293056	2.488566	-0.859169
H	-1.149685	3.869926	-0.870373
H	-1.099617	2.658835	-2.169270
H	0.204599	0.389024	-1.600247
H	1.466405	-1.529732	-0.333246
H	1.932704	-1.249309	1.340459
H	2.952877	0.369764	-1.070774
H	3.415874	0.662441	0.602668
H	4.398011	-1.654987	0.731990
H	3.934713	-1.945431	-0.937900
H	6.347708	-1.301048	-0.794711
H	5.450520	-0.067120	-1.692418
H	5.917092	0.226313	-0.009742
Pd	-1.344260	-0.658778	0.227686

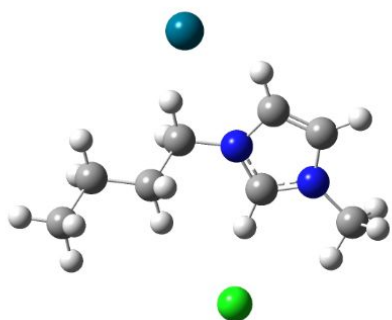


a4

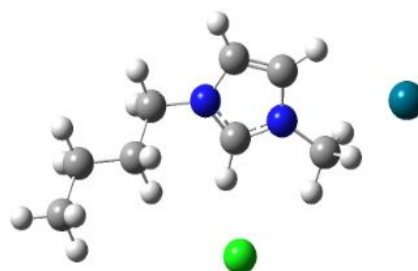
HF=-1010.4897019

Cartesian coordinate:

C	-1.666072	0.013631	0.357420
N	-1.546243	1.344842	0.449989
C	-2.735496	1.928512	0.046827
C	-3.584908	0.915095	-0.287187
N	-2.895566	-0.270751	-0.089920
C	-0.272707	2.016315	0.774733
C	0.456993	2.507295	-0.485574
C	1.962159	2.730876	-0.246731
C	2.771004	1.428190	-0.138102
C	-3.379978	-1.635142	-0.331190
Cl	0.137466	-2.732134	0.094257
H	-2.873936	2.998172	0.034670
H	-4.603994	0.934038	-0.640337
H	-2.520814	-2.308998	-0.259278
H	-4.135577	-1.898435	0.413727
H	-3.810883	-1.689962	-1.333468
H	-0.871987	-0.720051	0.536065
H	0.329883	1.260248	1.286810
H	-0.490131	2.833578	1.469821
H	0.338825	1.746081	-1.266195
H	-0.012346	3.431729	-0.847196
H	2.352709	3.321946	-1.084662
H	2.113021	3.345237	0.652876
H	3.843754	1.627261	-0.049628
H	2.502763	0.844102	0.776939
H	2.636499	0.811319	-1.050451
Pd	1.579391	-0.805157	-0.019646



a5



a6

HF= -1010.4539754

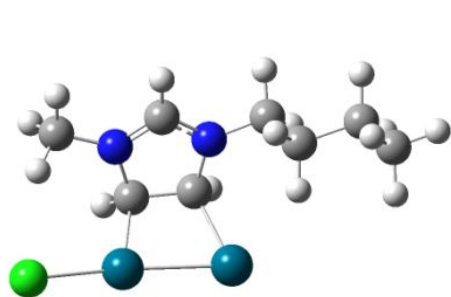
Cartesian coordinate:

C	-1.809147	-0.797934	-0.280299
N	-0.480168	-0.619941	-0.292627
C	0.138036	-1.795162	0.105878
C	-0.851687	-2.696400	0.366397
N	-2.053638	-2.051284	0.122483
C	0.173352	0.653103	-0.644844
C	-0.343199	1.829186	0.186455
C	0.350554	3.142382	-0.198691
C	-0.154286	4.330500	0.626871
C	-3.412370	-2.581305	0.294975
Cl	-4.314847	0.950488	-0.176569
H	1.223723	-1.872741	0.164577
H	-0.804855	-3.720287	0.702658
H	-4.104854	-1.736627	0.202991
H	-3.618643	-3.331614	-0.472896
H	-3.498920	-3.031340	1.286751
H	-2.625963	-0.045097	-0.449807
H	0.028909	0.828649	-1.715625
H	1.265239	0.499411	-0.477939
H	-1.429524	1.924071	0.048772
H	-0.174534	1.612515	1.249672
H	1.438308	3.036078	-0.069485
H	0.182658	3.341966	-1.266154
H	0.346694	5.257928	0.328558
H	-1.232804	4.469797	0.494092
H	0.032878	4.177390	1.696517
Pd	3.032896	-0.464697	-0.005880

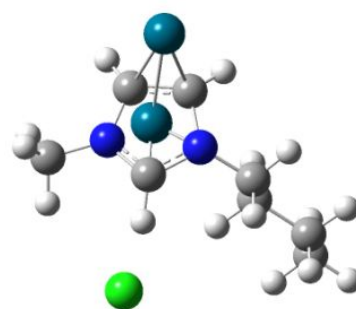
HF=- 1010.4531344

Cartesian coordinate:

C	0.875472	-0.011358	-0.496560
N	1.506113	-1.194571	-0.474653
C	0.578895	-2.195770	-0.225757
C	-0.635570	-1.589607	-0.093072
N	-0.424299	-0.232769	-0.262195
C	2.960633	-1.353143	-0.668287
C	3.773634	-0.488785	0.301496
C	5.282855	-0.634398	0.062864
C	6.109546	0.224504	1.025696
C	-1.416801	0.842496	-0.170655
Cl	1.328295	3.013392	-0.285919
H	0.860283	-3.235397	-0.165772
H	-1.622094	-1.983340	0.107795
H	-0.877836	1.802215	-0.208907
H	-2.113589	0.782125	-1.024819
H	-1.931252	0.779050	0.811197
H	1.291670	1.021250	-0.596865
H	3.192243	-1.095851	-1.707192
H	3.180272	-2.416265	-0.531901
H	3.480750	0.563321	0.189099
H	3.525705	-0.779028	1.331170
H	5.574579	-1.689829	0.165642
H	5.515043	-0.348590	-0.972429
H	7.181678	0.112309	0.831053
H	5.856413	1.285469	0.921691
H	5.926620	-0.061250	2.068499
Pd	-3.790569	-0.102959	0.225781



b1



b2

HF= -1137.2692609

Zero-point correction= 0.225783

Cartesian coordinate:

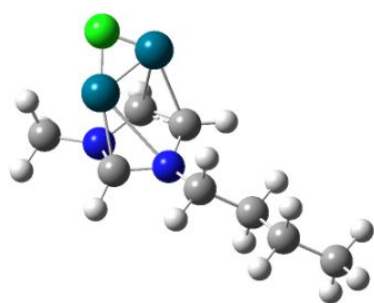
C	0.435350	2.310584	-0.284536
N	1.221906	1.360302	-0.770819
C	0.403411	0.301806	-1.358779
C	-0.991778	0.752985	-1.098484
N	-0.848472	2.061907	-0.484820
C	2.681787	1.341374	-0.669969
C	3.207929	0.632530	0.584497
C	4.739649	0.554936	0.608753
C	5.274593	-0.150231	1.859723
C	-1.965439	2.917225	-0.095909
Cl	-3.780351	0.174882	1.259377
H	0.690145	0.103330	-2.399908
H	-1.712489	0.739820	-1.919420
H	-2.658615	2.335784	0.523353
H	-1.583110	3.777293	0.459030
H	-2.486568	3.267763	-0.993088
H	0.800692	3.181368	0.245805
H	3.032825	2.379623	-0.702681
H	3.052896	0.844395	-1.573016
H	2.843784	1.160969	1.476387
H	2.770535	-0.375739	0.619690
H	5.090564	0.025288	-0.288283
H	5.161699	1.568738	0.550835
H	6.369000	-0.195133	1.850649
H	4.968660	0.374650	2.772524
H	4.897628	-1.177787	1.925496
Pd	-1.733023	-0.567285	0.240236
Pd	0.596094	-1.539369	-0.510651

HF=-1137.209471

Zero-point correction= 0.224076

Cartesian coordinate:

C	0.380238	-0.875068	-1.069050
C	0.736330	0.282079	-1.804573
N	0.164347	1.371911	-1.156474
C	-0.468073	0.971001	-0.028971
N	-0.401594	-0.404523	0.047926
H	0.171433	-1.868100	-1.450456
H	1.036100	0.364269	-2.839828
C	0.214008	2.770764	-1.573841
H	-0.711131	3.245818	-1.228717
H	1.089860	3.271141	-1.148387
H	0.265740	2.809304	-2.664437
H	-1.277798	1.589921	0.422481
C	-1.536004	-1.197552	0.605885
H	-1.812591	-0.721488	1.549236
C	-2.738035	-1.236263	-0.343070
H	-1.143516	-2.194419	0.828312
C	-3.906478	-2.023842	0.267109
H	-3.054804	-0.203408	-0.541347
H	-2.443081	-1.692438	-1.299095
C	-5.127517	-2.059064	-0.657996
H	-3.586952	-3.050461	0.499852
H	-4.188703	-1.559629	1.221523
H	-5.952691	-2.615625	-0.199969
H	-5.481678	-1.044900	-0.872789
H	-4.888657	-2.541777	-1.613850
Pd	2.448080	-0.738055	-0.695405
Pd	1.035169	0.223674	1.643596
Cl	-3.053944	2.547604	0.065151



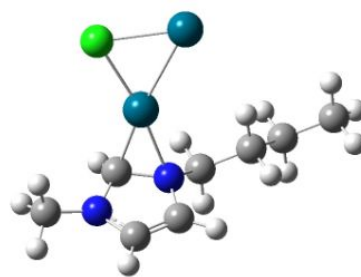
b3

HF = -1137.2617027

Zero-point correction = 0.224328

Cartesian coordinate:

C	-0.710271	1.386362	0.797608
C	0.469944	1.449894	1.577278
N	0.735399	0.139782	2.009512
C	-0.081053	-0.737526	1.306139
N	-1.108488	0.037692	0.783333
H	-1.456766	2.159345	0.670835
H	0.825750	2.278126	2.178619
C	1.979263	-0.253066	2.651492
H	1.863589	-1.250037	3.084913
H	2.808523	-0.265930	1.935801
H	2.201337	0.456107	3.454716
H	-0.339647	-1.706232	1.774734
C	-2.175807	-0.500633	-0.060567
H	-2.215204	-1.579308	0.125167
C	-3.541701	0.130977	0.229428
H	-1.900636	-0.365755	-1.114279
C	-4.653116	-0.492038	-0.626877
H	-3.776656	0.011068	1.295596
H	-3.502460	1.211059	0.034314
C	-6.026802	0.134335	-0.366131
H	-4.395927	-0.383974	-1.689521
H	-4.699596	-1.572677	-0.431523
H	-6.798405	-0.330959	-0.989167
H	-6.326112	0.013477	0.682109
H	-6.021551	1.208272	-0.588548
Pd	0.998047	1.690743	-0.512773
Pd	0.966185	-1.766197	-0.191678
Cl	2.025172	-0.256697	-1.801128

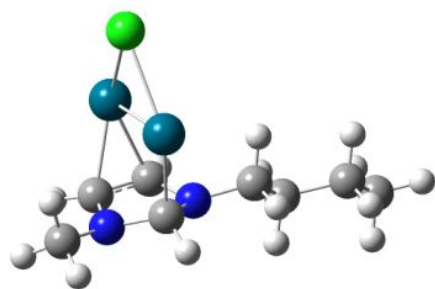


b4

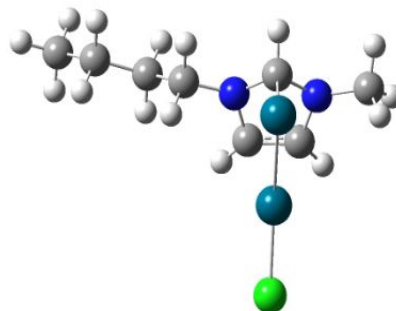
HF = - 1137.2546635

Cartesian coordinate:

C	0.000000	0.000000	0.000000
N	0.000000	0.000000	1.340665
C	1.310483	0.000000	1.792281
C	2.111241	-0.002764	0.689105
N	1.273152	-0.007396	-0.413342
C	-1.229362	-0.044543	2.157080
C	-2.099473	-1.261747	1.826481
C	-3.399821	-1.267498	2.641228
C	-4.280241	-2.479496	2.319948
C	1.650982	-0.055658	-1.831526
Cl	-1.900825	-0.814079	-2.249060
H	1.555215	0.001338	2.842886
H	3.185940	-0.005877	0.595630
H	0.741570	-0.276263	-2.402538
H	2.073064	0.905472	-2.136750
H	2.387976	-0.848479	-1.978502
H	-0.865884	-0.108197	-0.705871
H	-1.779565	0.885943	1.983425
H	-0.910073	-0.052195	3.203610
H	-2.333415	-1.262911	0.753201
H	-1.524830	-2.175626	2.028607
H	-3.166767	-1.253845	3.716205
H	-3.960055	-0.345258	2.434259
H	-5.207897	-2.457607	2.902225
H	-4.547260	-2.498748	1.257653
H	-3.762095	-3.418094	2.550660
Pd	-0.550884	-0.774235	-4.064635
Pd	1.656585	-1.959953	-3.918857



b5



b6

$HF=-1137.2615505$

Cartesian coordinate:

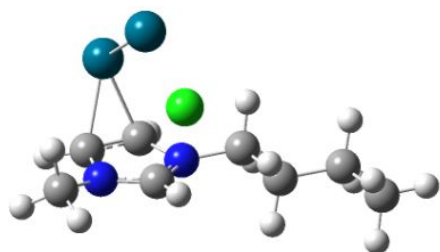
C	0.807215	0.936090	1.231940
C	-0.339173	1.750515	1.290360
N	-0.554219	2.263693	0.017686
C	0.211236	1.471100	-0.903072
N	1.272111	0.962439	-0.078638
H	1.464425	0.668030	2.047630
H	-0.759361	2.244459	2.157189
C	-1.791438	2.916370	-0.376633
H	-1.621987	3.477823	-1.299367
H	-2.594650	2.187219	-0.542612
H	-2.088511	3.617124	0.408755
H	0.548568	2.009843	-1.791754
C	2.276160	0.039093	-0.608968
H	2.412738	0.299098	-1.663778
C	3.616630	0.132882	0.126537
H	1.883685	-0.986958	-0.577938
C	4.676105	-0.789230	-0.493232
H	3.967279	1.173446	0.108227
H	3.484134	-0.137279	1.183279
C	6.021690	-0.723804	0.236427
H	4.305169	-1.823272	-0.488053
H	4.817773	-0.519854	-1.549241
H	6.756876	-1.389083	-0.229320
H	6.433574	0.292622	0.220225
H	5.918752	-1.024110	1.286280
Pd	-1.003680	-0.406949	1.307736
Pd	-1.042625	-0.279650	-1.335858
Cl	-2.276131	-2.087445	-0.033495

$HF=-1137.2302613$

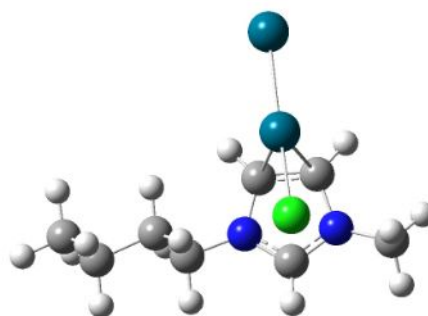
$S=3$

Cartesian coordinate:

C	-0.483189	0.678824	1.164687
C	0.643812	0.196143	1.836752
N	0.583813	-1.191548	1.810486
C	-0.363705	-1.554713	0.817694
N	-1.214101	-0.421611	0.731699
H	-0.915697	1.666703	1.214545
H	1.290566	0.719800	2.526010
C	1.693787	-2.046733	2.198825
H	1.334979	-3.073429	2.306631
H	2.500461	-2.022468	1.455422
H	2.080012	-1.707403	3.163787
H	-0.859856	-2.518284	0.957611
C	-2.354361	-0.344980	-0.183537
H	-2.662077	-1.375042	-0.390826
C	-3.528722	0.446378	0.401852
H	-2.027459	0.094237	-1.136275
C	-4.732085	0.475170	-0.550962
H	-3.819523	0.001675	1.362764
H	-3.214223	1.477175	0.613433
C	-5.911942	1.276979	0.007967
H	-4.422056	0.902115	-1.514612
H	-5.054091	-0.554641	-0.760600
H	-6.755343	1.277280	-0.690941
H	-6.264637	0.855774	0.957183
H	-5.630310	2.320815	0.191136
Pd	1.329668	0.926336	-0.262201
Pd	0.656824	-1.684169	-1.022473
Cl	2.215945	3.136806	-0.183251



b7



b8

$HF=-1137.2388897$

Cartesian coordinate:

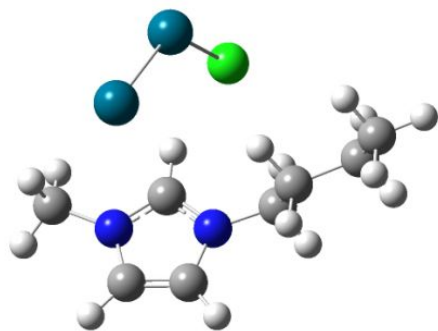
C	-0.194550	-2.192943	-0.283961
C	-1.111510	-2.095405	0.786698
N	-0.441161	-1.392782	1.806149
C	0.762666	-1.023395	1.355970
N	0.978295	-1.537429	0.142677
H	-0.121007	-2.954467	-1.049628
H	-1.922557	-2.761395	1.051379
C	-1.084945	-0.832963	2.991266
H	-0.319139	-0.542426	3.711550
H	-1.665592	0.048560	2.704819
H	-1.735109	-1.590446	3.435378
H	1.412105	-0.331458	1.865591
C	2.100314	-1.217093	-0.756637
H	1.699790	-0.555892	-1.533604
C	3.281953	-0.551567	-0.053859
H	2.405254	-2.157075	-1.231473
C	4.441155	-0.303297	-1.030713
H	2.954838	0.406121	0.369986
H	3.629540	-1.185877	0.774037
C	5.631966	0.389732	-0.360786
H	4.766837	-1.258300	-1.466931
H	4.082131	0.313490	-1.865439
H	6.442585	0.558829	-1.077797
H	5.340328	1.362349	0.051678
H	6.033769	-0.215635	0.460971
Pd	-1.788903	-0.793156	-0.851053
Pd	-1.064718	1.705892	-0.395897
Cl	0.678857	2.138284	1.272324

$HF=-1137.2253017$

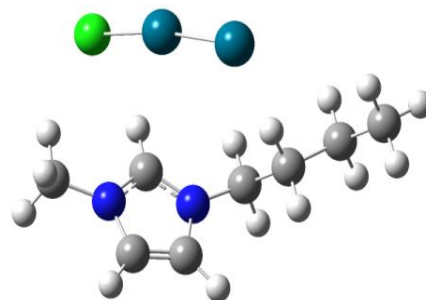
$S=3$

Cartesian coordinate:

C	0.000000	0.000000	0.000000
N	0.000000	0.000000	1.337290
C	1.327104	0.000000	1.779040
C	2.126365	0.092103	0.631877
N	1.249893	0.157652	-0.456152
C	-1.179640	-0.217217	2.188051
C	-1.249019	-1.635777	2.765384
C	-2.532168	-1.849886	3.579437
C	-2.607596	-3.254716	4.187142
C	1.643238	-0.065738	-1.845464
Cl	0.620534	-3.025121	-0.221160
H	1.570520	0.224320	2.805788
H	3.152131	0.414158	0.534060
H	1.707760	-1.145790	-2.014904
H	0.897012	0.378812	-2.507486
H	2.608799	0.412486	-2.019485
H	-0.871008	-0.139916	-0.619734
H	-2.056847	-0.003946	1.568938
H	-1.151463	0.535436	2.984344
H	-1.179468	-2.357064	1.942987
H	-0.369919	-1.809314	3.399389
H	-2.594415	-1.099134	4.380898
H	-3.406674	-1.683450	2.933944
H	-3.534185	-3.389678	4.755942
H	-2.574863	-4.023303	3.406644
H	-1.766752	-3.436514	4.866759
Pd	2.315344	-2.047410	1.379065
Pd	4.280055	-1.702321	3.027810



b9



b10

HF=-1137.2243095 S=3

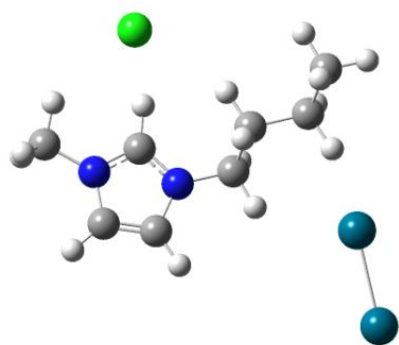
Cartesian coordinate:

C	0.000000	0.000000	0.000000
N	0.000000	0.000000	1.338926
C	1.310343	0.000000	1.782496
C	2.108510	0.020384	0.677745
N	1.271609	0.037748	-0.425062
C	-1.218335	-0.095576	2.171170
C	-1.384229	-1.487427	2.787867
C	-2.692417	-1.595076	3.583078
C	-2.884442	-2.981331	4.206733
C	1.679372	-0.082003	-1.824745
Cl	-3.158122	-0.238163	-0.943179
H	1.559289	-0.003302	2.831767
H	3.182615	0.032811	0.580466
H	0.883820	0.310252	-2.459154
H	2.593121	0.494172	-1.982931
H	1.841453	-1.137676	-2.065973
H	-0.901939	-0.001792	-0.610952
H	-2.057877	0.129848	1.507610
H	-1.151629	0.683425	2.938287
H	-1.379553	-2.227671	1.977111
H	-0.529245	-1.714380	3.441025
H	-2.709782	-0.829609	4.372620
H	-3.533540	-1.373384	2.913829
H	-3.826569	-3.035272	4.763026
H	-2.906455	-3.759086	3.434663
H	-2.070997	-3.222746	4.902271
Pd	-2.279479	-2.483409	-1.360017
Pd	0.010411	-3.417944	-0.711381

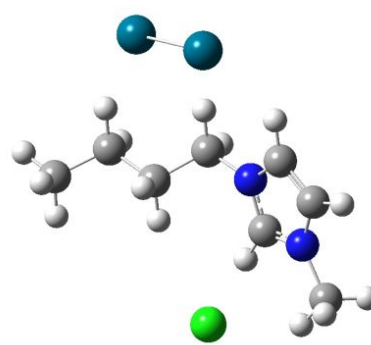
HF=-1137.130968

Cartesian coordinate:

C	0.000000	0.000000	0.000000
N	0.000000	0.000000	1.340665
C	1.310483	0.000000	1.792281
C	2.111241	-0.002764	0.689105
N	1.273152	-0.007396	-0.413342
C	-1.229362	-0.044543	2.157080
C	-2.099473	-1.261747	1.826481
C	-3.399821	-1.267498	2.641228
C	-4.280241	-2.479496	2.319948
C	1.650982	-0.055658	-1.831526
Cl	-1.900825	-0.814079	-2.249060
H	1.555215	0.001338	2.842886
H	3.185940	-0.005877	0.595630
H	0.741570	-0.276263	-2.402538
H	2.073064	0.905472	-2.136750
H	2.387976	-0.848479	-1.978502
H	-0.865884	-0.108197	-0.705871
H	-1.779565	0.885943	1.983425
H	-0.910073	-0.052195	3.203610
H	-2.333415	-1.262911	0.753201
H	-1.524830	-2.175626	2.028607
H	-3.166767	-1.253845	3.716205
H	-3.960055	-0.345258	2.434259
H	-5.207897	-2.457607	2.902225
H	-4.547260	-2.498748	1.257653
H	-3.762095	-3.418094	2.550660
Pd	-3.236096	-1.859298	-0.775062
Pd	-4.987695	-3.292858	0.355294



b11



b12

HF=-1137.191115

S=3

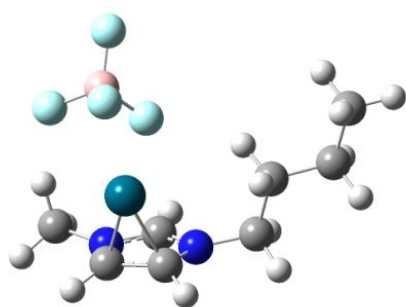
Cartesian coordinate:

C	0.000000	0.000000	0.000000
N	0.000000	0.000000	1.340665
C	1.310483	0.000000	1.792281
C	2.111241	-0.002764	0.689105
N	1.273152	-0.007396	-0.413342
C	-1.229362	-0.044543	2.157080
C	-2.099473	-1.261747	1.826481
C	-3.399821	-1.267498	2.641228
C	-4.280241	-2.479496	2.319948
C	1.650982	-0.055658	-1.831526
Cl	-1.900825	-0.814079	-2.249060
H	1.555215	0.001338	2.842886
H	3.185940	-0.005877	0.595630
H	0.741570	-0.276263	-2.402538
H	2.073064	0.905472	-2.136750
H	2.387976	-0.848479	-1.978502
H	-0.865884	-0.108197	-0.705871
H	-1.779565	0.885943	1.983425
H	-0.910073	-0.052195	3.203610
H	-2.333415	-1.262911	0.753201
H	-1.524830	-2.175626	2.028607
H	-3.166767	-1.253845	3.716205
H	-3.960055	-0.345258	2.434259
H	-5.207897	-2.457607	2.902225
H	-4.547260	-2.498748	1.257653
H	-3.762095	-3.418094	2.550660
Pd	0.724771	0.116984	4.521848
Pd	-1.568229	-1.027168	4.716709

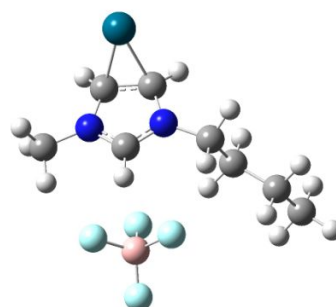
HF=-1137.1905779

Cartesian coordinate:

C	0.000000	0.000000	0.000000
N	0.000000	0.000000	1.340665
C	1.310483	0.000000	1.792281
C	2.111241	-0.002764	0.689105
N	1.273152	-0.007396	-0.413342
C	-1.229362	-0.044543	2.157080
C	-2.099473	-1.261747	1.826481
C	-3.399821	-1.267498	2.641228
C	-4.280241	-2.479496	2.319948
C	1.650982	-0.055658	-1.831526
Cl	-1.900825	-0.814079	-2.249060
H	1.555215	0.001338	2.842886
H	3.185940	-0.005877	0.595630
H	0.741570	-0.276263	-2.402538
H	2.073064	0.905472	-2.136750
H	2.387976	-0.848479	-1.978502
H	-0.865884	-0.108197	-0.705871
H	-1.779565	0.885943	1.983425
H	-0.910073	-0.052195	3.203610
H	-2.333415	-1.262911	0.753201
H	-1.524830	-2.175626	2.028607
H	-3.166767	-1.253845	3.716205
H	-3.960055	-0.345258	2.434259
H	-5.207897	-2.457607	2.902225
H	-4.547260	-2.498748	1.257653
H	-3.762095	-3.418094	2.550660
Pd	0.724771	0.116984	4.521848
Pd	-1.568229	-1.027168	4.716709



c1



c2

HF=-974.8521801

Zero-point correction= 0.239798

Cartesian coordinate:

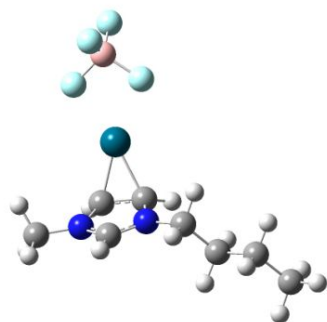
C	-0.013923	-1.585426	1.527132
N	-0.910212	-1.761360	0.557853
C	-0.218841	-1.997573	-0.669146
C	1.166787	-2.001277	-0.324244
N	1.223050	-1.779943	1.078128
C	-2.342984	-1.469806	0.680527
C	-2.710047	-0.069975	0.166602
C	-4.180409	0.272212	0.439698
C	-4.565393	1.656495	-0.093513
C	2.443947	-1.458003	1.819492
F	1.178324	1.956142	-0.928552
B	1.287224	2.056084	0.524851
F	1.134368	3.363100	0.897471
F	0.261357	1.239407	1.084209
F	2.531770	1.522797	0.887166
H	-0.723069	-2.596982	-1.419185
H	1.969748	-2.572020	-0.775809
H	2.714308	-0.416745	1.620296
H	2.261626	-1.607843	2.886059
H	3.238633	-2.134353	1.495907
H	-0.253314	-1.255165	2.526874
H	-2.601046	-1.574086	1.739982
H	-2.886389	-2.249628	0.134867
H	-2.042282	0.662950	0.633551
H	-2.508702	-0.024955	-0.911532
H	-4.830182	-0.490485	-0.013901
H	-4.369360	0.232207	1.522188
H	-5.614668	1.885490	0.122852
H	-3.947805	2.439203	0.361370
H	-4.426579	1.714300	-1.179611
Pd	0.694911	-0.224263	-1.338304

HF=-974.8452665

Zero-point correction= 0.240373

Cartesian coordinate:

C	0.056628	-0.759279	-0.355790
N	0.260097	0.551902	-0.251529
C	1.342905	0.778294	0.620376
C	1.784427	-0.506504	1.035270
N	0.930882	-1.426225	0.397354
C	-0.669787	1.568939	-0.781268
C	-1.639168	2.064573	0.298942
C	-2.783265	2.881914	-0.315395
C	-3.735087	3.444495	0.744892
C	0.917213	-2.879479	0.570355
F	-2.291783	-1.117132	1.040479
B	-2.867266	-1.622613	-0.153233
F	-4.158537	-2.037040	0.029570
F	-2.775152	-0.595631	-1.139154
F	-2.029940	-2.695926	-0.605075
H	1.394649	1.715309	1.160043
H	2.255875	-0.790850	1.967930
H	-0.057034	-3.240137	0.235126
H	1.725324	-3.340667	-0.004591
H	1.045892	-3.108121	1.631255
H	-0.708433	-1.228040	-0.958327
H	-1.233964	1.079116	-1.575077
H	-0.069947	2.377539	-1.210875
H	-2.049498	1.186373	0.807028
H	-1.097570	2.667503	1.042588
H	-2.377596	3.705652	-0.921458
H	-3.338237	2.224743	-0.996409
H	-4.555882	4.002809	0.281238
H	-4.174681	2.637639	1.342217
H	-3.213711	4.124483	1.430467
Pd	3.306735	0.405953	-0.202662

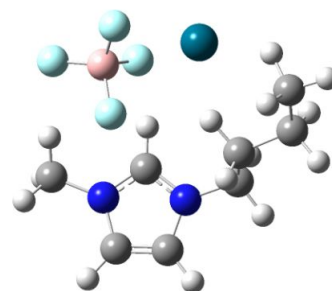


c3

HF=-974.8497923

Cartesian coordinate:

C	-0.960138	0.468092	-0.843405
C	-0.210633	1.701200	-0.935481
N	-0.677099	2.504936	0.158869
C	-1.576018	1.815109	0.855848
N	-1.812989	0.630404	0.302152
H	-1.374200	-0.104632	-1.667123
H	0.050509	2.245410	-1.838850
C	-0.107974	3.792483	0.529937
H	-0.689317	4.228908	1.344982
H	0.930752	3.662354	0.847363
H	-0.139219	4.466379	-0.331269
H	-2.004591	2.145942	1.792173
C	-2.716269	-0.397137	0.829097
H	-3.050105	-0.063929	1.817409
C	-3.920946	-0.662702	-0.081332
H	-2.125038	-1.308010	0.971282
C	-4.846324	-1.742841	0.496561
H	-4.477902	0.273048	-0.224836
H	-3.569441	-0.976441	-1.072769
C	-6.053635	-2.029252	-0.402199
H	-4.273327	-2.667656	0.648130
H	-5.194521	-1.430290	1.491139
H	-6.694885	-2.801635	0.035357
H	-6.664459	-1.129941	-0.546532
H	-5.736913	-2.379851	-1.391617
Pd	1.027578	0.136205	-0.446203
B	3.417720	-1.257437	0.332979
F	4.302863	-1.858138	-0.518686
F	3.744438	-1.356673	1.659852
F	3.257246	0.148540	-0.028414
F	2.077420	-1.795396	0.116616

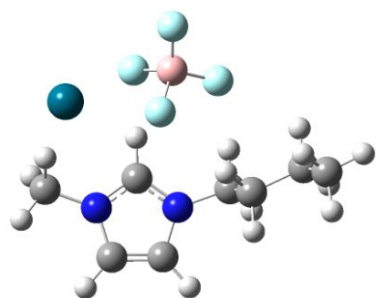


c4

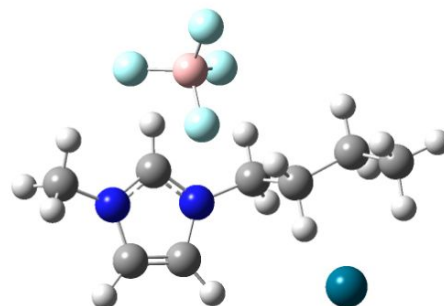
HF=-974.8229145

Cartesian coordinate:

C	-2.245667	0.365612	0.551148
N	-2.145962	1.675519	0.294425
C	-3.204553	2.049866	-0.516233
C	-3.953770	0.932808	-0.734010
N	-3.336789	-0.107007	-0.059601
C	-0.989241	2.511143	0.684864
C	0.271071	2.126227	-0.095537
C	1.511220	2.922935	0.333478
C	2.806301	2.260139	-0.157478
C	-3.743190	-1.519172	-0.068539
F	-0.565482	-1.185745	-0.845858
B	-0.111662	-2.088477	0.144981
F	1.236027	-2.416758	-0.098580
F	-0.208104	-1.430935	1.409547
F	-0.929575	-3.214787	0.151529
H	-3.327392	3.063689	-0.862840
H	-4.857266	0.786528	-1.304376
H	-2.858177	-2.148610	0.049385
H	-4.461143	-1.706312	0.734497
H	-4.206769	-1.734861	-1.032712
H	-1.526307	-0.230918	1.108282
H	-0.837192	2.378392	1.760440
H	-1.285811	3.551329	0.517548
H	0.476205	1.051905	0.050903
H	0.089113	2.258528	-1.169774
H	1.450053	3.950738	-0.050863
H	1.543196	3.001466	1.429254
H	3.679671	2.900548	0.008412
H	3.018467	1.329243	0.447773
H	2.761981	2.028581	-1.228188
Pd	2.408046	-0.362625	-0.181790



c5



c6

HF=-974.8198901

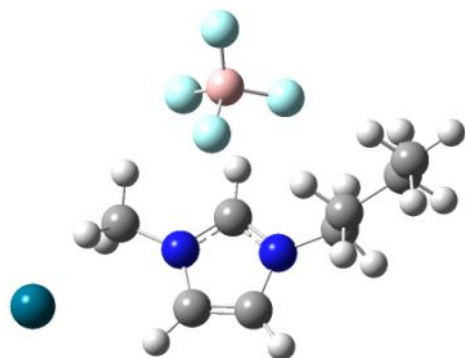
Cartesian coordinate:

C	0.000000	0.000000	0.000000
N	0.000000	0.000000	1.334582
C	1.313468	0.000000	1.773832
C	2.106731	0.012098	0.665659
N	1.263474	0.010451	-0.433271
C	-1.215151	-0.212246	2.149537
C	-1.369630	-1.682036	2.554948
C	-2.762051	-1.953176	3.138691
C	-2.924840	-3.401124	3.610724
C	1.637481	-0.072828	-1.849339
F	-0.868829	-2.619678	-0.599696
B	-1.926365	-2.003102	-1.309531
F	-2.751958	-2.913786	-1.910455
F	-2.638076	-1.177751	-0.385084
F	-1.336932	-1.116750	-2.270956
H	1.565287	-0.013074	2.822444
H	3.180388	0.019397	0.562803
H	0.768368	-0.447478	-2.393326
H	1.937326	0.910805	-2.220805
H	2.465851	-0.776245	-1.953129
H	-0.873988	-0.045452	-0.632910
H	-2.054973	0.084276	1.520904
H	-1.156589	0.458563	3.012717
H	-1.222652	-2.293523	1.659266
H	-0.590179	-1.951354	3.282383
H	-2.963266	-1.267465	3.975288
H	-3.503505	-1.735181	2.359857
H	-3.933190	-3.577230	4.001139
H	-2.758491	-4.101757	2.784625
H	-2.210645	-3.645028	4.407216
Pd	0.691022	-2.552495	-2.420256

HF=-974.8205848

Cartesian coordinate:

C	2.076675	-1.028332	0.741988
N	0.833592	-1.170333	1.207589
C	0.335680	-2.387385	0.770588
C	1.320773	-2.982824	0.040278
N	2.400388	-2.114209	0.034869
C	0.071744	-0.080366	1.849796
C	-0.839825	0.617921	0.837757
C	-1.515212	1.864021	1.413756
C	-2.530232	2.462166	0.436752
C	3.662645	-2.259278	-0.698437
F	1.680621	0.919622	-1.246833
B	2.635531	1.695165	-0.544050
F	2.888929	2.890865	-1.158996
F	2.138848	1.880466	0.783291
F	3.824858	0.903331	-0.424370
H	-0.666621	-2.710596	1.003467
H	1.347711	-3.932048	-0.471014
H	4.082969	-1.259437	-0.822418
H	4.349790	-2.907533	-0.147815
H	3.451413	-2.691403	-1.678520
H	2.705248	-0.159784	0.869745
H	0.809862	0.628097	2.227193
H	-0.485714	-0.509104	2.688488
H	-0.238619	0.877680	-0.037849
H	-1.629513	-0.113379	0.510087
H	-2.014651	1.620027	2.362347
H	-0.736883	2.604702	1.638273
H	-3.061019	3.315186	0.873563
H	-2.042326	2.798477	-0.484345
H	-3.291003	1.701880	0.157311
Pd	-3.232369	-0.463715	-0.621699

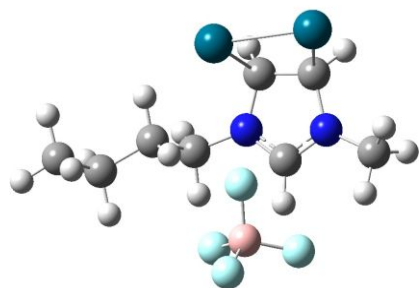


c7

HF=-974.816674

Cartesian coordinate:

C	0.404428	-0.279902	-0.986815
N	1.046347	-1.440498	-0.838398
C	0.168979	-2.361642	-0.288012
C	-1.025274	-1.726195	-0.118080
N	-0.853533	-0.425087	-0.560532
C	2.508165	-1.584108	-1.004504
C	3.238497	-1.455489	0.337380
C	4.751461	-1.301891	0.134768
C	5.513636	-1.234226	1.461987
C	-1.813247	0.675792	-0.470622
F	1.498982	1.315712	1.031620
B	1.871716	2.212448	0.001050
F	2.504923	3.325734	0.481519
F	2.695555	1.490430	-0.916328
F	0.676316	2.557490	-0.715818
H	0.468379	-3.373526	-0.065789
H	-1.974116	-2.063714	0.273677
H	-1.262576	1.613021	-0.582825
H	-2.576385	0.586558	-1.258471
H	-2.252318	0.678912	0.551889
H	0.838175	0.639125	-1.350630
H	2.817101	-0.776073	-1.668325
H	2.695370	-2.544420	-1.495510
H	2.845463	-0.571253	0.848795
H	3.023110	-2.333420	0.963370
H	5.139679	-2.133648	-0.471818
H	4.925025	-0.380617	-0.435466
H	6.587840	-1.100789	1.292971
H	5.163199	-0.393003	2.070636
H	5.378793	-2.152155	2.047879
Pd	-4.160584	-0.136880	0.342203



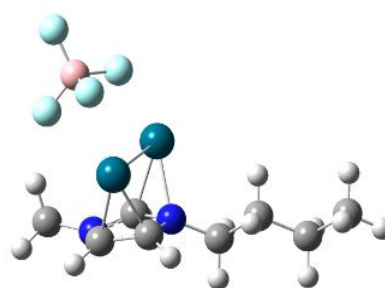
d1

$HF=-1101.603601$

Zero-point correction= 0.240084

Cartesian coordinate:

C	-0.426160	1.247115	1.357743
N	-0.462350	-0.058071	1.606754
C	0.854211	-0.603259	1.439757
C	1.725052	0.560143	1.199079
N	0.813180	1.672264	1.158864
C	-1.702453	-0.838790	1.730502
C	-2.050279	-1.593595	0.441718
C	-3.450107	-2.217791	0.493579
C	-3.773868	-3.037291	-0.759382
C	1.146114	3.058076	0.827789
F	-1.396529	1.206284	-1.174034
B	-2.469497	2.044535	-0.753156
F	-3.285649	2.387540	-1.796650
F	-3.177161	1.340511	0.264296
F	-1.892064	3.195305	-0.132396
H	1.143060	-1.365668	2.167508
H	2.605406	0.718436	1.834934
H	0.226281	3.559772	0.522530
H	1.599011	3.559058	1.690155
H	1.847046	3.062122	-0.009259
H	-1.296918	1.885013	1.293771
H	-2.496642	-0.124690	1.949912
H	-1.584629	-1.519852	2.581477
H	-1.992418	-0.882478	-0.387012
H	-1.295613	-2.392787	0.274429
H	-3.549930	-2.851272	1.387052
H	-4.174448	-1.399788	0.594889
H	-4.788030	-3.448490	-0.710585
H	-3.707297	-2.416557	-1.660217
H	-3.078702	-3.878720	-0.876751
Pd	2.699337	0.211143	-0.571368
Pd	0.871599	-1.659850	-0.321720



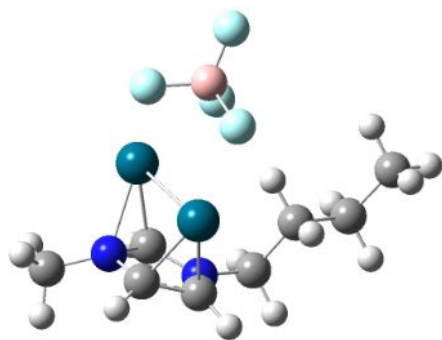
d2

$HF=-1101.5972545$

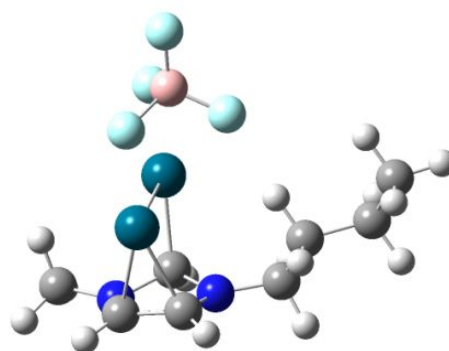
Zero-point correction= 0.239555

Cartesian coordinate:

C	-0.529860	1.244513	-1.465908
N	-1.417851	0.856734	-0.454966
C	-0.951516	1.491958	0.785068
C	0.155249	2.304220	0.414391
N	0.314471	2.212785	-0.980013
C	-2.870744	0.680676	-0.698110
C	-3.488552	-0.400628	0.186987
C	-4.991273	-0.571430	-0.076741
C	-5.621207	-1.661881	0.796158
C	1.535851	2.609247	-1.676562
F	2.397420	-1.094082	1.274935
B	2.858375	-1.275759	-0.079749
F	3.967273	-2.062643	-0.102645
F	1.781675	-1.943482	-0.816018
F	3.045251	-0.020588	-0.655906
H	-1.714645	1.715739	1.521489
H	0.524586	3.193292	0.910862
H	2.319113	1.863846	-1.512316
H	1.322777	2.702010	-2.745128
H	1.854751	3.582614	-1.295120
H	-0.819308	1.243819	-2.511403
H	-2.984301	0.418091	-1.754186
H	-3.360543	1.650623	-0.534583
H	-2.961108	-1.345552	0.000864
H	-3.324941	-0.154693	1.244449
H	-5.506171	0.383454	0.100159
H	-5.149105	-0.814334	-1.136995
H	-6.691292	-1.765358	0.586847
H	-5.149029	-2.634772	0.615899
H	-5.509589	-1.430361	1.862134
Pd	0.760502	0.526974	1.489632
Pd	-0.099017	-0.783695	-0.876684



d3



d4

HF = -1101.5933729

Cartesian coordinate:

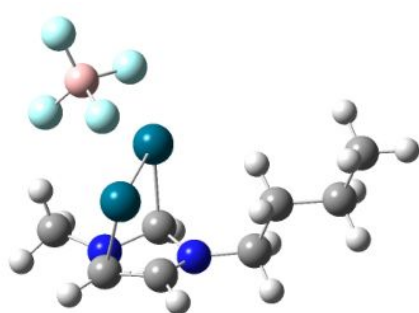
C	-0.333904	-1.731358	-1.152385
N	0.662749	-2.058878	-0.246818
C	0.130108	-2.051705	1.060405
C	-1.280806	-1.914443	0.935114
N	-1.560506	-1.766442	-0.470120
C	2.088039	-2.043228	-0.559542
C	2.815789	-0.759595	-0.131137
C	4.281484	-0.765851	-0.586677
C	5.049557	0.478572	-0.128798
C	-2.853059	-2.176260	-1.053357
F	-0.290208	2.158073	1.221061
B	-0.241760	2.733262	-0.104954
F	0.176487	4.014007	-0.038745
F	0.629518	1.921769	-0.910596
F	-1.522164	2.548652	-0.690846
H	0.667931	-2.610414	1.818073
H	-2.047077	-2.375695	1.546767
H	-3.441437	-1.294445	-1.292763
H	-2.683962	-2.767407	-1.957406
H	-3.390041	-2.789723	-0.323916
H	-0.257475	-2.135969	-2.161824
H	2.183045	-2.196058	-1.640899
H	2.544405	-2.915565	-0.072191
H	2.289207	0.117062	-0.527627
H	2.768568	-0.676810	0.962597
H	4.782825	-1.665964	-0.200953
H	4.322146	-0.839179	-1.682981
H	6.086568	0.455183	-0.482053
H	4.584621	1.394423	-0.510925
H	5.069949	0.549675	0.965201
Pd	-0.509821	-0.116381	1.724199
Pd	-0.931747	0.178610	-1.189968

HF = -1101.5765968

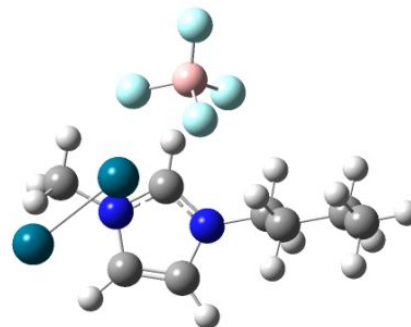
S = 3

Cartesian coordinate:

C	0.778190	-1.805699	-1.387139
N	1.756897	-1.665206	-0.434651
C	1.227400	-2.024564	0.777471
C	-0.051062	-2.557455	0.549022
N	-0.245272	-2.551726	-0.824853
C	2.962182	-0.871158	-0.617875
C	2.786935	0.582959	-0.143714
C	4.006836	1.444654	-0.485724
C	3.862087	2.883801	0.018049
C	-1.512911	-2.683341	-1.485233
F	-1.490257	1.464112	1.367169
B	-1.810264	1.871597	0.029670
F	-2.350385	3.088856	0.017440
F	-0.277472	2.339346	-0.774117
F	-2.900332	0.946564	-0.428755
H	1.906618	-2.335568	1.566099
H	-0.564633	-3.305588	1.143256
H	-2.116366	-1.761142	-1.326454
H	-1.348143	-2.804563	-2.554123
H	-2.030129	-3.558748	-1.088611
H	0.829247	-1.468421	-2.408936
H	3.210760	-0.905923	-1.683825
H	3.787789	-1.360692	-0.083700
H	1.879543	1.022643	-0.580928
H	2.625806	0.584741	0.943387
H	4.914508	0.992092	-0.057172
H	4.152557	1.449555	-1.575275
H	4.738929	3.484355	-0.249317
H	2.976556	3.363144	-0.412196
H	3.755255	2.912479	1.109111
Pd	-0.196775	-0.568450	1.529022
Pd	-0.921492	0.209473	-0.856368



d5



d6

HF=-1101.5758162

S=3

Cartesian coordinate:

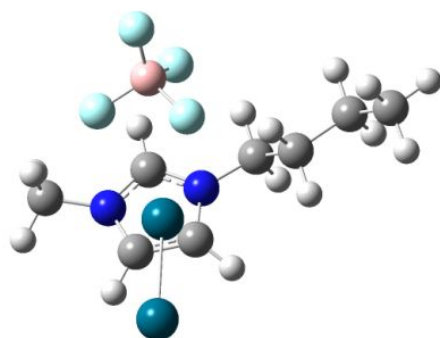
C	-0.851498	1.537651	-1.379316
N	-1.807955	1.483093	-0.302556
C	-1.163819	1.872529	0.864325
C	0.032222	2.521547	0.485011
N	0.104704	2.511819	-0.896393
C	-3.050272	0.721037	-0.353743
C	-2.947948	-0.734073	0.131116
C	-4.282033	-1.480813	0.011988
C	-4.190911	-2.931366	0.498358
C	1.342234	2.798166	-1.616058
F	1.877410	-1.304100	1.388523
B	2.570121	-1.488299	0.120739
F	3.597483	-2.362107	0.265735
F	1.581535	-2.003933	-0.802441
F	2.957732	-0.220518	-0.327776
H	-1.728079	2.009727	1.778387
H	0.611232	3.234818	1.058391
H	2.080712	2.000910	-1.472852
H	1.117105	2.900696	-2.680292
H	1.747917	3.746708	-1.251699
H	-1.293034	1.796191	-2.345842
H	-3.396684	0.749960	-1.392568
H	-3.790971	1.264955	0.246836
H	-2.169792	-1.242990	-0.456644
H	-2.603779	-0.744178	1.174016
H	-5.054305	-0.948771	0.586514
H	-4.614977	-1.466116	-1.035645
H	-5.154265	-3.443387	0.398437
H	-3.449106	-3.495603	-0.078926
H	-3.894636	-2.977675	1.553087
Pd	0.546657	0.498692	1.240466
Pd	0.181801	-0.310685	-1.332317

HF=-1101.5671191

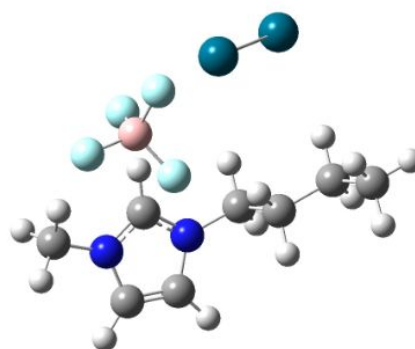
S=3

Cartesian coordinate:

C	0.894920	1.426224	1.442276
N	1.634100	2.128180	0.576084
C	0.875770	3.187935	0.110807
C	-0.338967	3.113103	0.726464
N	-0.302333	2.009676	1.559713
C	2.980571	1.727981	0.114403
C	2.931030	0.902641	-1.175060
C	4.338707	0.501526	-1.637415
C	4.311840	-0.338690	-2.918517
C	-1.412347	1.475619	2.354930
F	1.233290	-1.955105	-0.053862
B	1.436477	-1.915935	1.371968
F	1.718375	-3.152716	1.865725
F	2.467878	-0.980422	1.632065
F	0.226376	-1.384633	1.930619
H	1.259547	3.892075	-0.610346
H	-1.214956	3.736314	0.642160
H	-1.085861	0.536342	2.800905
H	-1.695579	2.195305	3.127077
H	-2.252703	1.266798	1.683357
H	1.216205	0.516984	1.929226
H	3.422231	1.137899	0.918654
H	3.562154	2.646972	-0.010186
H	2.336862	0.001966	-0.987000
H	2.425835	1.477312	-1.963762
H	4.949476	1.402053	-1.798086
H	4.827080	-0.069888	-0.836887
H	5.324976	-0.620065	-3.225708
H	3.737327	-1.259982	-2.770078
H	3.851963	0.213664	-3.747130
Pd	-3.122863	0.152358	-0.829195
Pd	-0.909131	-1.047601	-0.462999



d7



d8

HF=-1101.5686789

S=3

Cartesian coordinate:

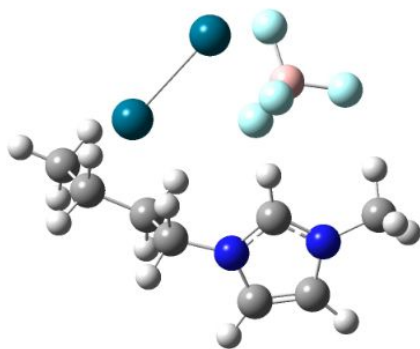
C	1.462520	-1.414202	1.579672
N	1.281691	-0.095682	1.703683
C	-0.087548	0.169424	1.687297
C	-0.730127	-1.068844	1.582588
N	0.279004	-2.034949	1.565379
C	2.373906	0.901529	1.710886
C	2.185089	1.990499	0.651837
C	3.395519	2.932653	0.597880
C	3.217427	4.046713	-0.438181
C	0.077595	-3.456597	1.274686
F	1.174617	-0.339727	-1.413884
B	2.242038	-1.327611	-1.431334
F	2.758067	-1.427540	-2.690376
F	3.210795	-0.897844	-0.490246
F	1.687720	-2.539895	-0.976995
H	-0.473421	1.126013	1.998287
H	-1.750710	-1.338967	1.805322
H	0.250158	-3.620783	0.210469
H	0.790350	-4.045778	1.856291
H	-0.936680	-3.727095	1.568414
H	2.414368	-1.884562	1.397628
H	3.286521	0.342617	1.503287
H	2.431353	1.326939	2.719279
H	2.038154	1.502689	-0.314953
H	1.277975	2.572435	0.868894
H	3.569393	3.375300	1.589454
H	4.291963	2.347468	0.353232
H	4.095532	4.700948	-0.468846
H	3.073203	3.629746	-1.441281
H	2.345025	4.670162	-0.205783
Pd	-3.387314	0.747248	-0.214375
Pd	-0.953672	-0.033914	-0.457429

HF=-1101.5635594

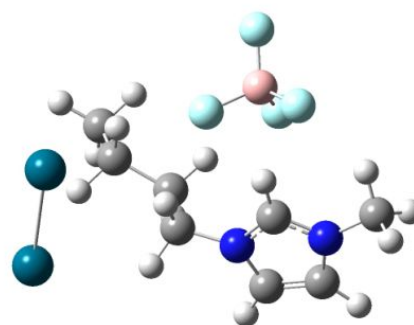
S=3

Cartesian coordinate:

C	2.564591	0.514561	-0.834990
N	2.312338	1.812555	-0.641663
C	3.512353	2.468667	-0.424152
C	4.499128	1.531867	-0.500317
N	3.885522	0.316980	-0.754180
C	0.958925	2.387912	-0.493564
C	0.505594	2.406168	0.970209
C	-0.904516	2.992732	1.115234
C	-1.393198	2.983484	2.566643
C	4.542261	-0.993297	-0.869409
F	1.525317	-0.883487	1.308736
B	1.315285	-2.133279	0.693809
F	0.178985	-2.751254	1.252436
F	1.022344	-1.886160	-0.697700
F	2.451131	-2.921203	0.776845
H	3.556815	3.529384	-0.234395
H	5.569097	1.620251	-0.397937
H	3.899083	-1.755329	-0.423089
H	4.737984	-1.222973	-1.920050
H	5.485255	-0.951459	-0.322142
H	1.828113	-0.268779	-0.981365
H	0.280219	1.775575	-1.094772
H	0.986792	3.392267	-0.927916
H	0.532015	1.377880	1.349311
H	1.220250	2.991072	1.566722
H	-0.921826	4.019783	0.721874
H	-1.599700	2.403328	0.495885
H	-2.399008	3.410409	2.643413
H	-1.433885	1.960154	2.956716
H	-0.729929	3.566851	3.217575
Pd	-1.478917	-1.296747	0.215501
Pd	-2.940291	0.430173	-0.939170



d9



d10

HF = -1101.5581654

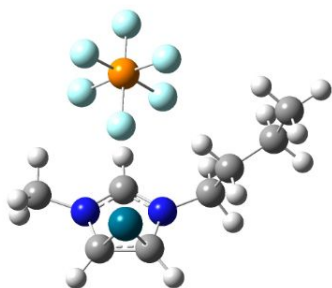
Cartesian coordinate:

C	2.286811	-0.480606	-0.710969
N	2.650053	0.805956	-0.732386
C	4.031628	0.877365	-0.679356
C	4.495943	-0.403157	-0.632481
N	3.390223	-1.235898	-0.649698
C	1.701734	1.933580	-0.664369
C	1.483252	2.425217	0.769983
C	0.310345	3.411052	0.843711
C	0.045339	3.914474	2.264706
C	3.394046	-2.703814	-0.576559
F	0.799336	-0.778417	1.649136
B	0.102675	-1.940509	1.285569
F	-1.081300	-2.082057	1.974781
F	-0.228275	-1.799104	-0.146036
F	0.934679	-3.057039	1.382464
H	4.554590	1.820475	-0.675615
H	5.501162	-0.791334	-0.587481
H	2.526513	-3.025591	0.004560
H	3.368489	-3.128829	-1.583484
H	4.307753	-3.018305	-0.069518
H	1.267746	-0.853291	-0.705912
H	0.737726	1.564532	-1.073193
H	2.079803	2.721278	-1.323701
H	1.269074	1.554810	1.399276
H	2.400192	2.899150	1.148808
H	0.484910	4.262064	0.170508
H	-0.605938	2.890404	0.471251
H	-0.810079	4.598089	2.285043
H	-0.174777	3.079663	2.939357
H	0.914093	4.452413	2.664918
Pd	-2.450009	-1.159032	-0.346826
Pd	-1.483276	1.361022	-0.723809

HF = -1101.555155

Cartesian coordinate:

C	2.776916	1.022740	-0.647672
N	1.686611	1.630524	-0.174609
C	2.061841	2.849914	0.364446
C	3.409604	2.965948	0.193333
N	3.835942	1.810224	-0.440849
C	0.375165	0.962256	-0.057079
C	0.181502	0.336741	1.329237
C	-0.955708	-0.690026	1.310470
C	-1.336558	-1.223056	2.693618
C	5.212841	1.416413	-0.758422
F	3.153463	-1.054695	1.212802
B	3.033750	-1.949669	0.121784
F	3.210631	-3.253489	0.496088
F	1.743151	-1.740902	-0.460815
F	3.992557	-1.549280	-0.865591
H	1.346791	3.517497	0.818598
H	4.092503	3.755836	0.463434
H	5.220045	0.332114	-0.884732
H	5.550759	1.917718	-1.669453
H	5.859521	1.691150	0.077266
H	2.816795	0.036745	-1.086724
H	0.361144	0.177313	-0.815025
H	-0.411393	1.690110	-0.290061
H	1.109845	-0.168764	1.612484
H	-0.031486	1.121018	2.068529
H	-1.889881	-0.162475	0.885244
H	-0.621012	-1.529515	0.674389
H	-2.135396	-1.967141	2.620414
H	-0.471082	-1.699458	3.169079
H	-1.684831	-0.413723	3.346385
Pd	-3.227215	1.201988	0.042099
Pd	-2.255193	-1.204066	-0.852979



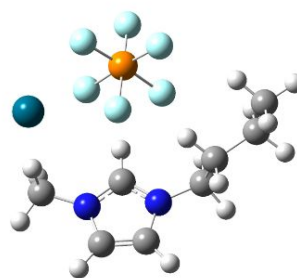
e1

HF=-1491.0546162

Zero-point correction= 0.244218

Cartesian coordinate:

N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.384600
C	1.302300	0.000000	1.786300
N	2.077500	-0.008500	0.638300
C	1.266800	-0.010400	-0.423200
C	3.539100	-0.098100	0.552900
C	-1.166300	-0.185800	-0.892400
C	-1.523600	-1.667600	-1.056600
C	-2.510100	-1.893700	-2.210100
C	-2.715500	-3.385000	-2.495200
H	-0.915400	-0.001900	1.955000
H	1.739900	0.004700	2.772100
H	3.794700	-0.430300	-0.454200
H	3.990600	0.874500	0.765500
H	3.889700	-0.836500	1.276500
H	1.582700	-0.072100	-1.452800
H	-0.883500	0.239000	-1.856600
H	-1.989100	0.405600	-0.478800
H	-0.602200	-2.215700	-1.266000
H	-1.937500	-2.057000	-0.115800
H	-3.472600	-1.408700	-1.991600
H	-2.106100	-1.414300	-3.110800
H	-3.429700	-3.534700	-3.312300
H	-1.765000	-3.845200	-2.785700
H	-3.099200	-3.914400	-1.614100
P	2.028000	-2.268700	-3.033400
F	0.830200	-1.102300	-3.058800
F	1.669000	-2.513400	-1.430100
F	3.208700	-3.360400	-2.936800
F	2.366000	-1.943600	-4.573600
F	3.078200	-1.067700	-2.540400
F	0.928600	-3.386600	-3.438700
Pd	0.939100	-2.300100	0.940100



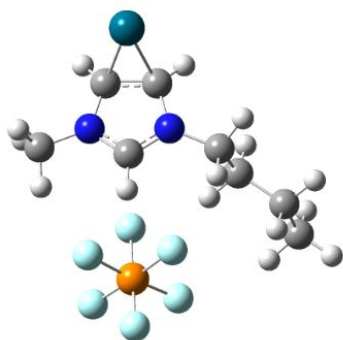
e2

HF=-1491.0292233

Zero-point correction= 0.243750

Cartesian coordinate:

N	1.652290	2.221160	0.467554
C	1.445716	3.384968	-0.250643
C	0.115669	3.674946	-0.171290
N	-0.470765	2.682674	0.595896
C	0.477672	1.811755	0.960307
C	-1.902714	2.494406	0.832217
C	2.909080	1.445121	0.548623
C	3.124052	0.573748	-0.694360
C	4.253166	-0.445137	-0.487301
C	4.341660	-1.439330	-1.650032
H	2.253884	3.903419	-0.741653
H	-0.457085	4.492274	-0.579853
H	-2.303652	1.740039	0.100602
H	-2.056432	2.117808	1.843342
H	-2.407449	3.453492	0.709949
H	0.308273	0.896435	1.505433
H	2.824156	0.815842	1.435035
H	3.722450	2.160636	0.705562
H	2.193820	0.038255	-0.897024
H	3.337737	1.210805	-1.564114
H	5.214056	0.072250	-0.352113
H	4.054464	-1.000260	0.438238
H	5.160743	-2.150788	-1.497959
H	3.408729	-2.007974	-1.729594
H	4.515229	-0.927961	-2.605178
P	-0.034485	-1.729695	0.546673
F	1.279166	-1.022736	1.276618
F	-0.015987	-0.484175	-0.571136
F	-1.358044	-2.334755	-0.183871
F	-0.059087	-2.882753	1.667195
F	-1.001562	-0.761755	1.494917
F	0.952063	-2.578617	-0.414016
Pd	-2.701675	-0.035118	-0.790596

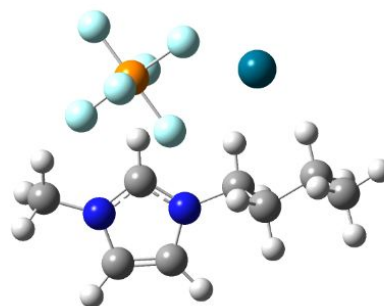


e3

HF=-1491.0508914

Cartesian coordinate:

N	0.995419	0.715447	-0.202123
C	2.115472	0.714007	0.652313
C	2.316525	-0.640451	1.029552
N	1.296135	-1.369381	0.388381
C	0.550423	-0.532958	-0.333077
C	1.026574	-2.801066	0.527828
C	0.278682	1.905853	-0.706509
C	-0.704496	2.461502	0.331821
C	-1.668721	3.484855	-0.283415
C	-2.769399	3.891083	0.702398
H	2.348985	1.612025	1.210438
H	2.740098	-1.031732	1.946352
H	0.004246	-2.984933	0.194437
H	1.738056	-3.382761	-0.064958
H	1.117308	-3.074981	1.581791
H	-0.304504	-0.825044	-0.923950
H	-0.265581	1.584375	-1.595621
H	1.034855	2.637243	-1.007831
H	-1.283526	1.625012	0.729653
H	-0.151457	2.913342	1.167789
H	-1.116947	4.371050	-0.629201
H	-2.135854	3.031884	-1.167145
H	-3.444695	4.629689	0.256521
H	-3.362412	3.013952	0.983326
H	-2.349729	4.330043	1.616385
P	-2.936033	-0.948655	-0.096379
F	-2.153434	0.100768	-1.134386
F	-1.764779	-0.611600	1.034781
F	-3.618435	-1.993104	0.924803
F	-4.010555	-1.277658	-1.250633
F	-1.931449	-2.149572	-0.675454
F	-3.818673	0.288226	0.467193
Pd	3.961660	0.005385	-0.216920

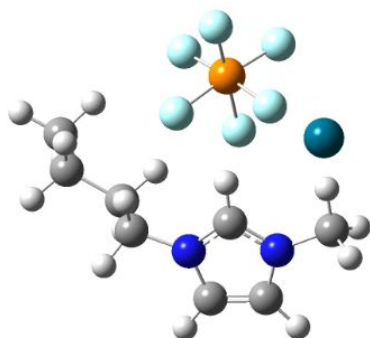


e4

HF=-1491.0291629

Cartesian coordinate:

N	1.169955	2.265274	-0.430816
C	2.022914	3.293097	-0.065400
C	3.274067	2.761241	0.026958
N	3.164087	1.414873	-0.278045
C	1.882544	1.139962	-0.550139
C	4.253096	0.431553	-0.299236
C	-0.298610	2.342536	-0.564757
C	-1.006767	2.492339	0.784342
C	-2.524707	2.329903	0.629800
C	-3.273157	2.434338	1.960448
H	1.668640	4.298222	0.099214
H	4.219502	3.213570	0.281829
H	3.812565	-0.563282	-0.240664
H	4.839752	0.543581	-1.214863
H	4.891441	0.595047	0.571396
H	1.480090	0.168928	-0.812021
H	-0.629241	1.400666	-1.043048
H	-0.523786	3.172600	-1.242247
H	-0.626949	1.718153	1.458983
H	-0.775442	3.471527	1.228120
H	-2.914647	3.072439	-0.079998
H	-2.721966	1.323149	0.179238
H	-4.349799	2.296954	1.815115
H	-2.929391	1.667111	2.663265
H	-3.120581	3.415219	2.428722
P	0.552257	-2.107122	0.437916
F	0.546193	-1.441471	-1.104465
F	0.186026	-0.592299	1.010833
F	0.570480	-2.679075	1.941524
F	0.933023	-3.539342	-0.192162
F	2.152937	-1.702909	0.537173
F	-1.046124	-2.416489	0.280425
Pd	-2.108727	-0.346818	-0.901995

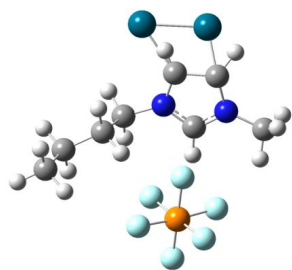


e5

HF= -1490.991762

Cartesian coordinate:

N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.384146
C	1.302720	0.000000	1.786473
N	2.078910	-0.001479	0.640036
C	1.268209	-0.008954	-0.422291
C	3.541302	-0.093029	0.570650
C	-1.172848	-0.150861	-0.889425
C	-1.603415	-1.615462	-1.028484
C	-2.632733	-1.802377	-2.151754
C	-2.927429	-3.283365	-2.412787
H	-0.915184	-0.002029	1.954744
H	1.739950	-0.000782	2.772306
H	3.823900	-0.211493	-0.475229
H	3.991404	0.808807	0.993156
H	3.865947	-0.981724	1.119284
H	1.585253	-0.070827	-1.450833
H	-0.873331	0.244973	-1.861017
H	-1.968727	0.483768	-0.487397
H	-0.715629	-2.211195	-1.253970
H	-2.009719	-1.976805	-0.073656
H	-3.561381	-1.265571	-1.910046
H	-2.233821	-1.352403	-3.070200
H	-3.673602	-3.402160	-3.205917
H	-2.014325	-3.801320	-2.726597
H	-3.311471	-3.781550	-1.514012
P	1.942516	-2.302335	-3.139883
F	0.791198	-1.111141	-3.118698
F	1.532880	-2.606739	-1.506479
F	3.074640	-3.455667	-3.023980
F	2.331281	-1.954082	-4.654429
F	3.021541	-1.185913	-2.564435
F	0.818307	-3.374382	-3.575704
Pd	2.979891	-3.869801	-0.066657



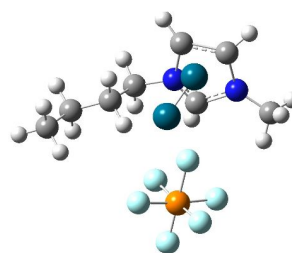
f1

HF = -1617.8118535

Zero-point correction = 0.244381

Cartesian coordinate:

N	-0.255351	0.549192	1.748194
C	-1.638326	0.635735	1.374665
C	-2.085055	-0.760084	1.226663
N	-0.889307	-1.531423	1.443690
C	0.130115	-0.722280	1.693680
C	-0.761003	-2.980687	1.294482
C	0.661865	1.692963	1.881202
C	1.020162	2.322838	0.529611
C	2.152307	3.352373	0.634134
C	2.598635	3.848287	-0.745111
H	-2.235629	1.346451	1.951361
H	-2.959241	-1.111940	1.788945
H	0.298050	-3.224702	1.204048
H	-1.205281	-3.492781	2.154594
H	-1.269653	-3.289464	0.379183
H	1.154905	-1.048167	1.793691
H	1.567229	1.312570	2.356154
H	0.189726	2.415165	2.557158
H	1.325834	1.523703	-0.147778
H	0.115895	2.808659	0.103756
H	1.846182	4.197812	1.266818
H	3.004233	2.870361	1.131075
H	3.412181	4.576740	-0.658676
H	2.956324	3.007157	-1.348937
H	1.773679	4.332180	-1.284045
P	2.869986	-1.121901	-0.440644
F	2.852043	-0.148289	0.916181
F	1.267368	-0.723100	-0.677781
F	2.814352	-2.084033	-1.732841
F	4.405251	-1.504574	-0.140182
F	2.350379	-2.364905	0.533515
F	3.297423	0.164985	-1.334188
Pd	-2.853469	-0.931991	-0.666376
Pd	-1.719687	1.433833	-0.516214



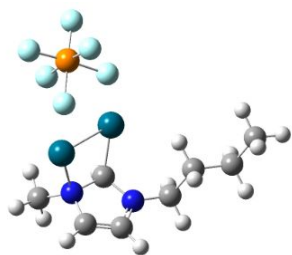
f2

HF = -1617.7933549

Zero-point correction = 0.244599

Cartesian coordinate:

N	-1.211225	1.569392	1.532727
C	-2.456378	1.146979	0.999727
C	-2.665405	-0.168214	1.498923
N	-1.530355	-0.459278	2.297166
C	-0.689440	0.571582	2.243577
C	-1.214960	-1.762425	2.880296
C	-0.487336	2.793397	1.152846
C	0.022042	2.759524	-0.293003
C	0.898980	3.975911	-0.616841
C	1.471115	3.906844	-2.036838
H	-3.196226	1.900899	0.759622
H	-3.603124	-0.655691	1.737864
H	-0.140372	-1.816534	3.055256
H	-1.767672	-1.908037	3.813468
H	-1.486971	-2.539180	2.162860
H	0.319516	0.559135	2.625746
H	0.353205	2.885448	1.844911
H	-1.161615	3.640851	1.322836
H	0.602430	1.844615	-0.431183
H	-0.832502	2.714851	-0.981151
H	0.321993	4.903594	-0.489482
H	1.727273	4.019601	0.103425
H	2.106785	4.773228	-2.250536
H	2.076635	3.002213	-2.163466
H	0.671386	3.884963	-2.787514
P	2.325816	-0.601630	0.627401
F	2.069015	0.889685	1.294130
F	2.558774	0.104466	-0.822141
F	2.458154	-2.073630	-0.034436
F	1.946118	-1.265267	2.083307
F	0.662044	-0.646281	0.268409
F	3.885052	-0.539595	0.994993
Pd	-2.227984	-0.282288	-0.590282
Pd	-0.014865	-1.316022	-1.878705



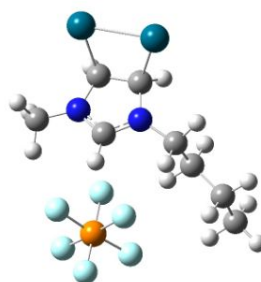
f3

HF = -1617.8006883

Zero-point correction = 0.243804

Cartesian coordinate:

N	-2.897809	-0.883475	0.037912
C	-2.933061	-1.783167	-0.994351
C	-1.895819	-2.649694	-0.899348
N	-1.091215	-2.281657	0.227871
C	-1.729716	-1.088902	0.830254
C	-0.737761	-3.373099	1.176552
C	-3.842126	0.204438	0.260980
C	-3.441426	1.539345	-0.384936
C	-4.458126	2.654235	-0.110894
C	-4.051879	3.991646	-0.739325
H	-3.697197	-1.728141	-1.757535
H	-1.636962	-3.503630	-1.505254
H	-0.099994	-2.965113	1.961700
H	-1.649616	-3.801858	1.608415
H	-0.188886	-4.148107	0.638380
H	-1.938089	-1.219490	1.902897
H	-3.949112	0.330760	1.346254
H	-4.815011	-0.125574	-0.121688
H	-2.449142	1.827693	-0.000666
H	-3.319473	1.395714	-1.466946
H	-5.443678	2.352393	-0.493871
H	-4.576496	2.780168	0.974817
H	-4.793462	4.769141	-0.526458
H	-3.085815	4.334180	-0.350198
H	-3.959325	3.906043	-1.828462
P	2.958471	1.018935	-0.054738
F	1.419469	1.706433	0.127639
F	2.264283	-0.090121	-1.173146
F	4.373055	0.288416	-0.265844
F	3.541801	2.065674	1.012658
F	2.559396	-0.034628	1.133767
F	3.202346	2.011970	-1.293833
Pd	-0.410581	0.434660	0.749967
Pd	0.659379	-1.474459	-0.578783

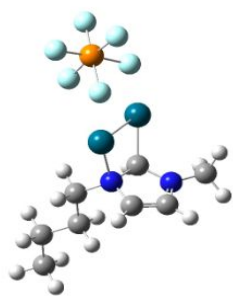


f4

HF = -1617.8084551

Cartesian coordinate:

N	0.214197	0.732755	-0.232900
C	1.362207	0.698810	0.622025
C	1.566678	-0.731249	0.920593
N	0.514431	-1.396655	0.214349
C	-0.219994	-0.505035	-0.441010
C	0.192856	-2.822470	0.289638
C	-0.545614	1.940756	-0.620223
C	-1.499194	2.397580	0.491126
C	-2.495298	3.453135	-0.008416
C	-3.560655	3.772801	1.045551
H	1.355085	1.430000	1.436184
H	1.696936	-1.058343	1.958299
H	-0.837916	-2.956778	-0.041201
H	0.877110	-3.405703	-0.332659
H	0.282056	-3.144839	1.330829
H	-1.076954	-0.753924	-1.050092
H	-1.118056	1.675434	-1.510298
H	0.180818	2.712081	-0.893348
H	-2.054893	1.524305	0.840025
H	-0.924514	2.791397	1.341928
H	-1.964151	4.368871	-0.306664
H	-2.991645	3.062356	-0.905721
H	-4.259440	4.534012	0.681300
H	-4.134206	2.870385	1.283090
H	-3.109945	4.148573	1.972863
P	-3.703857	-0.977279	-0.147349
F	-2.961448	0.155105	-1.124143
F	-2.475405	-0.747436	0.953938
F	-4.345991	-2.102790	0.811986
F	-4.836772	-1.196470	-1.270826
F	-2.739585	-2.125737	-0.875426
F	-4.545098	0.210254	0.566829
Pd	3.035355	1.318155	-0.384441
Pd	3.418340	-1.219321	0.192672

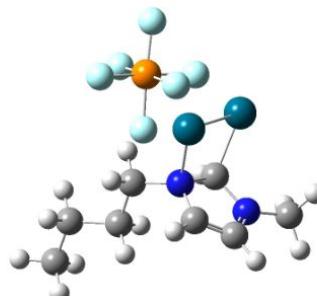


f5

HF=-1617.7972908

Cartesian coordinate:

N	1.874956	-0.040737	0.549631
C	2.425577	0.540941	1.735879
C	2.558977	1.876191	1.541953
N	2.181271	2.208408	0.269062
C	1.675265	1.063572	-0.414951
C	2.128684	3.555544	-0.270397
C	2.518022	-1.291708	0.025682
C	3.999259	-1.131148	-0.331260
C	4.604652	-2.448343	-0.839065
C	6.086836	-2.315886	-1.204582
H	2.669920	-0.071433	2.589601
H	2.873160	2.632391	2.248063
H	2.257625	3.512423	-1.356421
H	1.174998	4.048484	-0.051207
H	2.945731	4.146398	0.154036
H	2.161873	0.876522	-1.384132
H	1.928340	-1.603570	-0.840275
H	2.391465	-2.056351	0.798562
H	4.114695	-0.355845	-1.100860
H	4.552486	-0.783191	0.550773
H	4.484241	-3.223873	-0.070023
H	4.039608	-2.795295	-1.714930
H	6.491043	-3.269325	-1.560992
H	6.235465	-1.573277	-1.997756
H	6.683085	-2.002855	-0.339009
Pd	-0.288977	1.145685	-0.875976
Pd	-0.094676	-0.489689	1.081568
P	-3.260170	-0.633343	-0.204460
F	-3.825800	-2.039853	0.327041
F	-4.382508	0.200104	0.587117
F	-2.584173	0.838602	-0.697261
F	-1.999189	-1.384961	-0.931306
F	-4.122406	-0.681577	-1.556934
F	-2.289300	-0.535156	1.215102

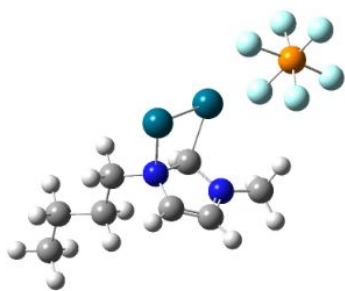


f6

HF=-1617.7911301

Cartesian coordinate:

N	-1.466096	0.398441	0.435141
C	-1.592550	0.428800	1.862648
C	-2.416291	-0.576190	2.240912
N	-2.895078	-1.236423	1.137189
C	-2.276195	-0.728037	-0.036593
C	-3.692825	-2.448654	1.166132
C	-1.590714	1.701978	-0.304219
C	-2.933799	2.406512	-0.092415
C	-2.998487	3.735684	-0.859910
C	-4.330580	4.466937	-0.663403
H	-1.067539	1.169941	2.444494
H	-2.681808	-0.891729	3.240274
H	-4.293897	-2.507662	0.253494
H	-3.068429	-3.347466	1.234947
H	-4.368725	-2.412587	2.025137
H	-2.977775	-0.458054	-0.837383
H	-1.416510	1.476323	-1.359472
H	-0.761946	2.329978	0.035657
H	-3.754426	1.753764	-0.421110
H	-3.086556	2.588977	0.979130
H	-2.172473	4.382469	-0.534629
H	-2.836487	3.546980	-1.929948
H	-4.346917	5.409853	-1.220160
H	-5.173856	3.858629	-1.012431
H	-4.503104	4.700673	0.394039
Pd	-1.066827	-2.037467	-1.020020
Pd	0.461546	-0.278801	0.151833
P	3.477010	0.564272	0.077483
F	4.581808	-0.116297	-0.867428
F	4.279089	1.945185	0.221686
F	4.139743	-0.061343	1.404554
F	2.655363	1.110641	-1.223942
F	2.225285	1.166943	1.029346
F	2.531503	-0.886478	-0.053427

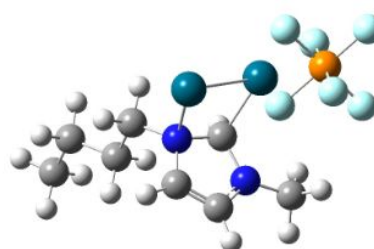


f7

$HF = -1617.7880308$

Cartesian coordinate:

N	-2.175242	0.223140	0.441250
C	-2.512792	0.251952	1.829417
C	-1.649442	-0.556904	2.495170
N	-0.796772	-1.163580	1.616406
C	-1.044514	-0.696128	0.299343
C	0.280577	-2.092119	1.955219
C	-3.295434	0.083825	-0.548987
C	-4.124277	-1.193167	-0.373407
C	-5.259146	-1.273092	-1.405777
C	-6.105480	-2.541716	-1.256034
H	-3.319501	0.869001	2.192222
H	-1.565222	-0.723770	3.560027
H	0.330645	-2.876611	1.194426
H	1.246966	-1.583775	1.990048
H	0.053703	-2.546972	2.922467
H	-1.203733	-1.484324	-0.450576
H	-2.839682	0.129574	-1.541220
H	-3.927919	0.969586	-0.436463
H	-3.476194	-2.073943	-0.474339
H	-4.540764	-1.223362	0.641409
H	-5.903473	-0.388268	-1.307366
H	-4.834344	-1.232580	-2.418137
H	-6.906116	-2.570489	-2.002722
H	-5.495334	-3.443404	-1.386115
H	-6.570943	-2.594048	-0.264510
Pd	0.549800	0.256717	-0.428261
Pd	-1.258348	2.111287	0.085086
P	3.601076	-0.496328	-0.267441
F	2.737896	0.800860	-0.946704
F	2.242715	-1.449021	-0.600166
F	2.882650	-0.124045	1.173328
F	4.321623	-1.769794	0.401004
F	4.820274	0.494955	0.058915
F	4.172193	-0.844368	-1.730234

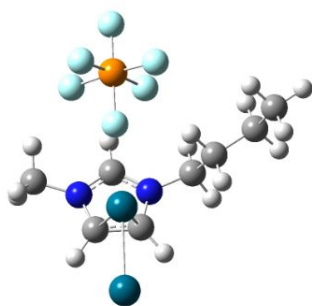


f8

$HF = -1617.7855287$

Cartesian coordinate:

N	2.043669	-0.049009	0.342650
C	2.723467	-0.319441	1.569115
C	1.814211	-0.274461	2.574861
N	0.582897	0.061938	2.076409
C	0.650076	0.191585	0.677338
C	-0.625108	0.296868	2.867419
C	2.680389	0.899789	-0.632658
C	2.883325	2.311430	-0.072972
C	3.540937	3.236935	-1.107941
C	3.752770	4.658428	-0.576375
H	3.779909	-0.536350	1.583010
H	1.953075	-0.486540	3.625679
H	-1.328804	0.873716	2.269082
H	-1.100061	-0.649145	3.143591
H	-0.355784	0.852780	3.770173
H	0.198094	1.093073	0.252249
H	2.037568	0.911030	-1.516149
H	3.637718	0.457366	-0.924245
H	1.915186	2.731736	0.228964
H	3.504321	2.262452	0.830853
H	4.506584	2.811761	-1.416018
H	2.917302	3.272663	-2.011431
H	4.222948	5.294794	-1.333608
H	2.799906	5.122067	-0.295532
H	4.399098	4.659400	0.309633
P	-3.291392	0.724085	-0.238328
F	-2.380051	0.175146	-1.517572
F	-1.974529	1.622984	0.238193
F	-4.079843	1.211397	1.082893
F	-4.505097	-0.234326	-0.687910
F	-2.644121	-0.558616	0.660804
F	-3.828597	1.955871	-1.119960
Pd	-0.512379	-1.137181	-0.312225
Pd	1.992545	-1.975459	-0.591590

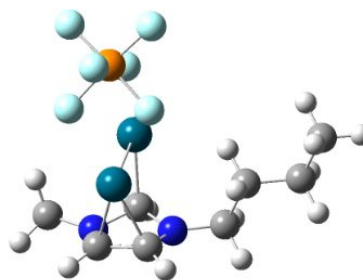


f9

HF=-1617.7854566

Cartesian coordinate:

N	0.124115	0.501311	1.895051
C	-1.211782	0.362728	1.468101
C	-1.439384	-1.030256	1.337136
N	-0.224082	-1.652935	1.686268
C	0.678385	-0.710122	1.960051
C	0.065581	-3.085002	1.573633
C	0.862498	1.774611	1.998466
C	1.028965	2.470349	0.642055
C	2.005232	3.651191	0.722146
C	2.261382	4.268827	-0.656715
H	-1.930237	1.143515	1.681381
H	-2.372021	-1.571019	1.439138
H	1.103179	-3.202640	1.260784
H	-0.117492	-3.588125	2.527600
H	-0.584216	-3.505736	0.804816
H	1.730688	-0.893095	2.108982
H	1.840699	1.527963	2.414692
H	0.329730	2.406003	2.718571
H	1.410405	1.738383	-0.071597
H	0.049650	2.813411	0.280638
H	1.625075	4.415443	1.415566
H	2.957038	3.292136	1.135636
H	2.969333	5.102352	-0.591640
H	2.680227	3.518614	-1.336709
H	1.334345	4.651141	-1.101973
P	3.027255	-0.810083	-0.647385
F	3.083716	0.143883	0.714367
F	1.355021	-0.605998	-0.648527
F	2.884911	-1.762678	-1.940853
F	4.621917	-1.007012	-0.587097
F	2.799863	-2.108948	0.356300
F	3.152866	0.521674	-1.564834
Pd	-1.317323	-0.162477	-0.635637
Pd	-3.994098	0.152086	-0.479097



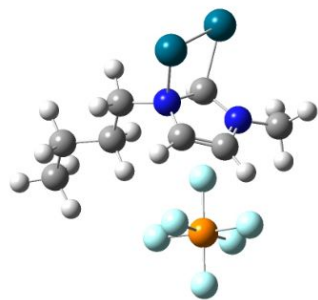
f10

HF=-1617.7774573

S=3

Cartesian coordinate:

N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.435142
C	1.421858	0.000000	1.819982
N	2.120547	-0.089312	0.564699
C	1.250203	-0.129948	-0.433939
C	3.565097	-0.240020	0.392499
C	-1.194915	-0.132963	-0.849521
C	-1.797182	-1.542648	-0.805028
C	-2.888601	-1.757246	-1.861140
C	-3.360940	-3.214178	-1.902359
H	-0.696828	0.699675	1.903493
H	1.800747	0.777942	2.494827
H	3.755152	-0.600005	-0.619234
H	4.070942	0.715739	0.565883
H	3.931199	-0.984358	1.102268
H	1.517387	-0.295677	-1.467160
H	-0.879575	0.095381	-1.868531
H	-1.913226	0.629514	-0.526927
H	-0.993160	-2.261504	-0.971473
H	-2.219451	-1.725858	0.206504
H	-3.737306	-1.082268	-1.679831
H	-2.469732	-1.491811	-2.840506
H	-4.134266	-3.357246	-2.664902
H	-2.520258	-3.874888	-2.140609
H	-3.781713	-3.527230	-0.937940
P	1.574623	-2.899309	-2.542807
F	0.558257	-1.603389	-2.819950
F	1.270119	-2.715985	-0.912675
F	2.581283	-4.113818	-2.210890
F	1.864494	-3.004194	-4.123544
F	2.810104	-1.800235	-2.370592
F	0.297553	-3.897278	-2.644538
Pd	1.193596	-1.513736	-1.188619
Pd	2.052475	-1.872642	0.330000

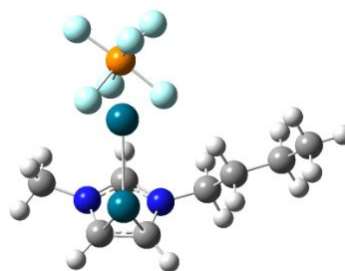


f11

HF=-1617.7748618

Cartesian coordinate:

N	0.863660	0.614027	0.428991
C	0.269187	0.085901	1.588641
C	-0.070306	-1.215840	1.338523
N	0.271131	-1.530079	0.065164
C	0.861103	-0.431383	-0.567765
C	-0.149031	-2.746549	-0.631312
C	0.571441	2.036642	0.018905
C	-0.860571	2.239053	-0.483207
C	-1.186439	3.727184	-0.675488
C	-2.576915	3.916738	-1.294865
H	0.040505	0.710184	2.437106
H	-0.588865	-1.916531	1.973058
H	-0.121125	-2.555366	-1.705515
H	0.522720	-3.575984	-0.393232
H	-1.174606	-2.966227	-0.333201
H	0.426231	-0.154178	-1.534456
H	1.315224	2.300785	-0.736863
H	0.768423	2.644947	0.907204
H	-0.999875	1.706230	-1.430300
H	-1.569625	1.791334	0.216209
H	-1.141321	4.236377	0.297949
H	-0.426984	4.207732	-1.310220
H	-2.856586	4.975735	-1.322167
H	-2.602022	3.534929	-2.322151
H	-3.335666	3.367246	-0.728304
Pd	2.773904	-0.804311	-1.202549
Pd	2.881042	0.549090	1.119355
P	-3.475169	-0.662403	0.149641
F	-2.824362	-2.054871	0.781024
F	-2.119914	-0.531537	-0.812281
F	-2.673297	0.185811	1.323779
F	-4.756867	-0.803460	1.119995
F	-4.024281	0.737476	-0.469348
F	-4.195811	-1.521097	-1.015668



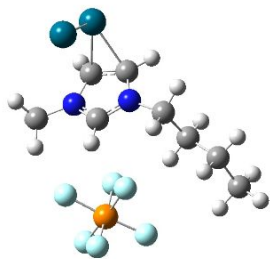
f12

HF=-1617.7745241

S=3

Cartesian coordinate:

N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.411809
C	1.364469	0.000000	1.802299
N	2.106313	-0.007971	0.601499
C	1.261318	-0.057457	-0.427560
C	3.559161	-0.155186	0.493693
C	-1.181741	-0.206966	-0.857779
C	-1.749529	-1.627563	-0.738278
C	-2.748476	-1.944580	-1.858676
C	-3.196051	-3.409683	-1.819703
H	-0.851481	0.416995	1.935111
H	1.811569	0.426842	2.691667
H	3.785033	-0.647159	-0.452540
H	4.048186	0.821781	0.554194
H	3.903728	-0.791677	1.310635
H	1.552510	-0.226516	-1.452413
H	-0.852243	-0.022741	-1.881656
H	-1.920829	0.556672	-0.590484
H	-0.916180	-2.329606	-0.797421
H	-2.225905	-1.753134	0.244240
H	-3.620301	-1.277027	-1.796419
H	-2.262141	-1.747571	-2.822840
H	-3.904760	-3.628543	-2.626061
H	-2.329992	-4.070007	-1.938437
H	-3.685767	-3.654542	-0.868595
P	1.748717	-3.067073	-2.154676
F	0.706781	-1.845260	-2.599175
F	1.398032	-2.711311	-0.557393
F	2.779772	-4.204034	-1.658050
F	2.084602	-3.346205	-3.704246
F	2.948472	-1.920650	-2.080107
F	0.505104	-4.110190	-2.167009
Pd	0.502333	-1.921344	2.260311
Pd	2.603840	-2.086098	0.404134

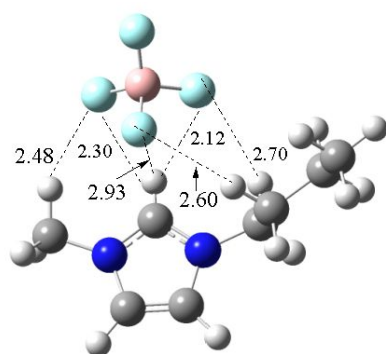


f13

HF=-1617.7699427

Cartesian coordinate:

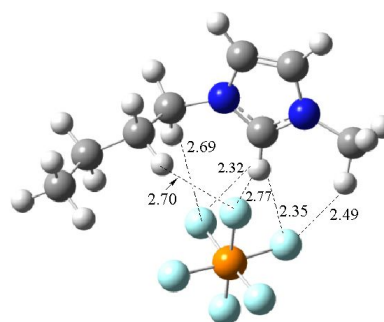
N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.394067
C	1.346561	0.000000	1.791222
N	2.096474	-0.014935	0.615033
C	1.263688	0.011521	-0.427627
C	3.556547	-0.055059	0.504794
C	-1.176037	-0.160517	-0.883587
C	-1.560991	-1.636044	-1.048721
C	-2.553471	-1.842170	-2.201254
C	-2.787744	-3.329282	-2.487333
H	-0.881788	-0.297555	1.944033
H	1.790522	-0.305428	2.728776
H	3.804806	-0.406840	-0.497485
H	3.973113	0.939914	0.683617
H	3.945559	-0.758764	1.243920
H	1.568119	0.000097	-1.463022
H	-0.891818	0.260028	-1.848938
H	-1.982340	0.447679	-0.462906
H	-0.650276	-2.200426	-1.261135
H	-1.982151	-2.020869	-0.108842
H	-3.505962	-1.338782	-1.981125
H	-2.140591	-1.369786	-3.101654
H	-3.504016	-3.464550	-3.305161
H	-1.845963	-3.807707	-2.777275
H	-3.182532	-3.851702	-1.606825
P	1.973544	-2.239682	-3.016488
F	0.782811	-1.066706	-3.049545
F	1.633400	-2.453555	-1.401656
F	3.148480	-3.337608	-2.911786
F	2.294592	-1.947827	-4.566971
F	3.037264	-1.036450	-2.558947
F	0.861591	-3.358890	-3.385206
Pd	1.094772	3.801685	0.503935
Pd	0.490653	2.059673	2.288167



Sum of electronic and zero-point Energies=
 -847.884985

Cartesian coordinate:

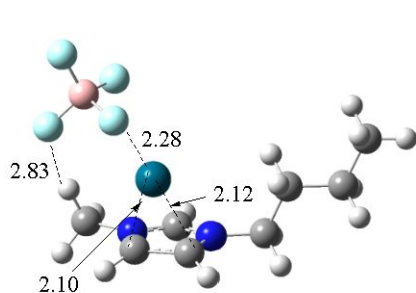
N	0.079366	-1.706499	0.477622
C	0.415822	-2.915111	-0.103697
C	1.719788	-2.827539	-0.481843
N	2.158112	-1.563807	-0.130896
C	1.149172	-0.907904	0.448859
C	3.506688	-1.021195	-0.337408
C	-1.259745	-1.307679	0.958707
C	-2.177170	-0.875976	-0.187208
C	-3.557081	-0.450960	0.328448
C	-4.501582	-0.029775	-0.800726
H	-0.290010	-3.723426	-0.195800
H	2.364715	-3.545138	-0.960665
H	3.461562	0.058936	-0.213863
H	4.195846	-1.457806	0.386532
H	3.832180	-1.258683	-1.349798
H	1.178635	0.106861	0.812047
H	-1.108061	-0.488108	1.661471
H	-1.669646	-2.159236	1.506646
H	-1.705323	-0.043781	-0.718975
H	-2.287730	-1.702966	-0.898354
H	-4.007475	-1.275659	0.893809
H	-3.437509	0.379576	1.033398
H	-5.476745	0.268396	-0.407157
H	-4.093438	0.817373	-1.359659
H	-4.663862	-0.849223	-1.507731
B	0.633799	2.453006	-0.011379
F	0.086807	1.888876	1.179294
F	2.002004	2.062038	-0.081812
F	-0.052532	1.926129	-1.122848
F	0.530405	3.847051	0.025047



Sum of electronic and zero-point Energies=
 -1364.088823

Cartesian coordinate:

N	2.062948	1.019182	0.435745
C	2.871659	1.808802	-0.361651
C	2.160766	2.926743	-0.669117
N	0.926256	2.801677	-0.058681
C	0.894919	1.642478	0.602722
C	-0.172449	3.773580	-0.115887
C	2.389826	-0.327721	0.947013
C	2.401252	-1.380454	-0.163053
C	2.722054	-2.774351	0.389350
C	2.755473	-3.845430	-0.704162
H	3.870215	1.514257	-0.637196
H	2.422277	3.788590	-1.259927
H	-1.094964	3.267388	0.160181
H	0.026849	4.599468	0.568116
H	-0.257034	4.148860	-1.135144
H	0.053806	1.258808	1.153586
H	1.637009	-0.565927	1.698662
H	3.359821	-0.258326	1.445463
H	1.423717	-1.387901	-0.654193
H	3.144776	-1.106362	-0.920319
H	3.688090	-2.749543	0.907503
H	1.972871	-3.044436	1.142165
H	2.983125	-4.828582	-0.284389
H	1.791237	-3.915803	-1.215912
H	3.517435	-3.619689	-1.456507
P	-2.121764	-0.515688	-0.031818
F	-0.987103	-0.813572	1.138657
F	-0.907754	-0.088667	-1.062151
F	-3.228694	-0.183795	-1.185944
F	-3.309009	-0.914034	1.018622
F	-2.191947	1.057541	0.491301
F	-2.017515	-2.063403	-0.536658

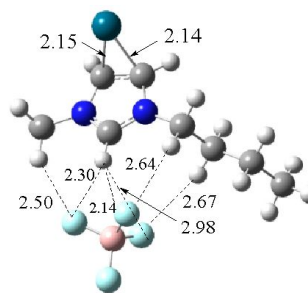


c1 in solution

Sum of electronic and zero-point Energies= -974.641466

Cartesian coordinate:

C	1.166716	1.934928	1.051365
N	1.858792	1.357650	0.075407
C	1.055290	1.313696	-1.099107
C	-0.163893	1.957703	-0.747106
N	-0.027686	2.325833	0.614159
C	3.212060	0.799880	0.197285
C	3.221562	-0.725453	0.334424
C	4.647581	-1.279638	0.431000
C	4.680645	-2.803590	0.576090
C	-1.090181	2.925007	1.420045
F	-2.327725	-1.445215	-0.678719
B	-3.049238	-1.227949	0.573227
F	-4.099731	-2.149040	0.620853
F	-2.155653	-1.425398	1.630933
F	-3.532733	0.089811	0.572691
H	1.564458	1.320335	-2.058594
H	-0.825102	2.551444	-1.371816
H	-1.918100	2.219596	1.507588
H	-0.698841	3.163665	2.408253
H	-1.434659	3.841162	0.937967
H	1.510002	2.038335	2.070506
H	3.681326	1.273186	1.063154
H	3.767401	1.113553	-0.690902
H	2.650241	-1.007889	1.225783
H	2.705939	-1.166504	-0.524796
H	5.212440	-0.984921	-0.461253
H	5.159555	-0.820254	1.284928
H	5.708154	-3.170195	0.642245
H	4.152719	-3.126470	1.478441
H	4.206378	-3.292872	-0.279920
Pd	-0.529338	-0.086161	-1.026532

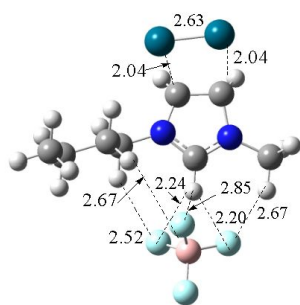


c2 in solution

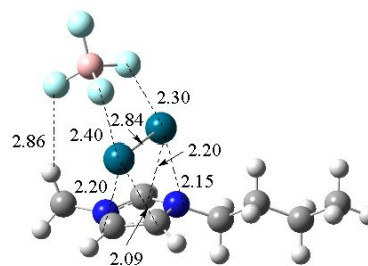
Sum of electronic and zero-point Energies= -974.634528

Cartesian coordinate:

C	0.050267	-0.744228	-0.048160
N	0.358259	0.549518	-0.061232
C	1.558405	0.744822	0.657594
C	1.946807	-0.538920	1.117225
N	0.952139	-1.426850	0.652930
C	-0.473354	1.605195	-0.665903
C	-1.381747	2.290260	0.358287
C	-2.231924	3.389797	-0.288807
C	-3.144738	4.097332	0.716398
C	0.929946	-2.874099	0.866745
F	-3.376378	-0.774173	0.888043
B	-3.311833	-1.614782	-0.238941
F	-4.581421	-2.104709	-0.569130
F	-2.770545	-0.881244	-1.335540
F	-2.426013	-2.696126	0.033952
H	1.754898	1.711633	1.109724
H	2.507781	-0.799269	2.009719
H	-0.058883	-3.246103	0.604457
H	1.690604	-3.356589	0.250807
H	1.128597	-3.079694	1.919282
H	-0.801478	-1.175076	-0.551685
H	-1.071173	1.130590	-1.444920
H	0.205748	2.316947	-1.140670
H	-2.032450	1.534738	0.809807
H	-0.771033	2.721253	1.160329
H	-1.575743	4.126208	-0.768305
H	-2.840055	2.950241	-1.087606
H	-3.742031	4.872512	0.229254
H	-3.834409	3.390293	1.186673
H	-2.563354	4.575008	1.511143
Pd	3.353404	0.148432	-0.351769



d1 in solution



d2 in solution

Sum of electronic and zero-point Energies= -1101.393270

Total free energy in solution: with all non electrostatic terms
 (a.u.) = -1064.421315

Cartesian coordinate:

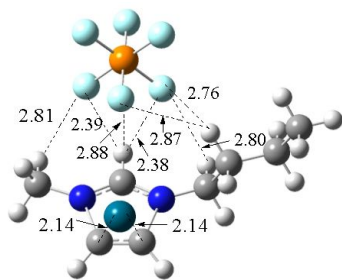
C	0.699539	-1.051973	0.988382
N	0.355361	0.191965	1.288660
C	-1.078817	0.295155	1.339670
C	-1.561793	-1.072501	1.084155
N	-0.359790	-1.838654	0.877856
C	1.299100	1.304864	1.466464
C	1.467495	2.157806	0.206699
C	2.441116	3.319897	0.426984
C	2.628134	4.181479	-0.824810
C	-0.302712	-3.275612	0.615751
F	3.247606	-0.588951	-1.432281
B	3.859643	-1.439978	-0.492089
F	5.162856	-1.765319	-0.886154
F	3.875728	-0.793149	0.776244
F	3.076907	-2.624388	-0.361404
H	-1.466980	0.866822	2.191804
H	-2.281321	-1.536670	1.772212
H	0.741082	-3.571919	0.522280
H	-0.769823	-3.816178	1.441888
H	-0.826347	-3.505872	-0.312390
H	1.716933	-1.380771	0.835899
H	2.256434	0.867622	1.752940
H	0.929033	1.905121	2.302537
H	1.826081	1.518459	-0.606147
H	0.481970	2.548367	-0.097503
H	2.084469	3.945844	1.253800
H	3.411042	2.916480	0.739599
H	3.331487	4.997588	-0.640086
H	3.017093	3.586912	-1.656597
H	1.680573	4.625134	-1.146166
Pd	-2.730673	-0.974788	-0.582349
Pd	-1.774092	1.443296	-0.194752

Sum of electronic and zero-point Energies= -1101.381257

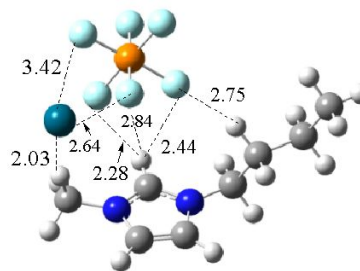
Total free energy in solution: with all non electrostatic terms
 (a.u.) = -1065.619966

Cartesian coordinate:

C	-0.651955	1.413288	-1.390871
N	-1.478637	0.888758	-0.403288
C	-1.028886	1.446146	0.870911
C	0.020425	2.341643	0.556270
N	0.167335	2.353092	-0.836759
C	-2.925151	0.628545	-0.637846
C	-3.450010	-0.550911	0.173857
C	-4.944919	-0.791360	-0.069807
C	-5.491251	-1.972684	0.736735
C	1.302836	2.944344	-1.534635
F	2.523837	-1.064236	1.199446
B	2.995794	-1.332579	-0.130292
F	3.979791	-2.310540	-0.078668
F	1.885466	-1.839719	-0.913063
F	3.454006	-0.153172	-0.710214
H	-1.772386	1.550767	1.651819
H	0.371290	3.194068	1.127852
H	2.180003	2.296587	-1.454906
H	1.044253	3.083577	-2.584787
H	1.522282	3.915454	-1.090003
H	-0.936060	1.444765	-2.440093
H	-3.038503	0.440720	-1.707267
H	-3.467921	1.548391	-0.393224
H	-2.875609	-1.444626	-0.095598
H	-3.277607	-0.374541	1.241162
H	-5.505964	0.115381	0.185052
H	-5.114831	-0.968372	-1.138322
H	-6.556309	-2.122814	0.542764
H	-4.971516	-2.900703	0.480281
H	-5.368052	-1.808348	1.811495
Pd	0.718543	0.489436	1.506597
Pd	-0.101312	-0.673032	-0.952459



e1 in solution



e2 in solution

Sum of electronic and zero-point Energies= -1490.839593

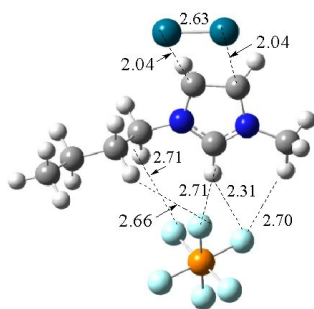
Cartesian coordinate:

N	-1.234910	0.416912	1.421182
C	-2.522239	0.073702	0.949390
C	-2.527788	-1.339386	0.838070
N	-1.244621	-1.760136	1.249499
C	-0.515759	-0.692436	1.563775
C	-0.768921	-3.142359	1.241804
C	-0.755757	1.785351	1.670586
C	-0.505178	2.570548	0.381053
C	-0.038649	4.000946	0.674204
C	0.220341	4.809058	-0.600257
H	-3.351882	0.739174	1.170677
H	-3.361805	-2.025962	0.949884
H	0.181843	-3.192818	1.768233
H	-1.501456	-3.774736	1.744812
H	-0.631256	-3.481429	0.214374
H	0.526564	-0.719282	1.836260
H	0.162661	1.698914	2.253019
H	-1.505951	2.279960	2.294318
H	0.249666	2.043530	-0.209292
H	-1.426120	2.594859	-0.211847
H	-0.790602	4.513851	1.286038
H	0.877296	3.965799	1.275430
H	0.553865	5.822906	-0.363925
H	0.992997	4.337598	-1.214594
H	-0.685979	4.889819	-1.208415
P	2.809438	-0.534131	-0.287221
F	2.300463	0.539505	0.864488
F	1.293809	-0.535601	-0.928480
F	3.296956	-1.616620	-1.413797
F	4.304778	-0.537758	0.380758
F	2.362312	-1.772658	0.715811
F	3.231437	0.705809	-1.264586
Pd	-2.645626	-0.472050	-1.118933

Sum of electronic and zero-point Energies= -1490.807592

Cartesian coordinate:

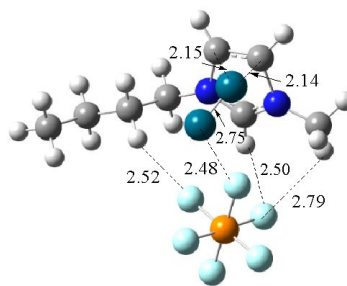
N	1.919067	-1.864518	-0.755788
C	1.714141	-3.084831	-0.137940
C	0.408245	-3.414357	-0.326908
N	-0.165679	-2.393146	-1.061421
C	0.767218	-1.468421	-1.303267
C	-1.586179	-2.267421	-1.391568
C	3.172642	-1.084030	-0.746437
C	3.474805	-0.497630	0.633823
C	4.768350	0.325284	0.625360
C	5.092978	0.921978	1.997514
H	2.505320	-3.612558	0.367270
H	-0.154158	-4.277192	-0.011941
H	-2.135547	-1.884155	-0.496594
H	-1.701465	-1.561780	-2.210577
H	-1.975624	-3.243457	-1.677134
H	0.604860	-0.541297	-1.825807
H	3.052775	-0.290588	-1.484386
H	3.972157	-1.746864	-1.086442
H	2.634425	0.132589	0.939402
H	3.559806	-1.307968	1.366820
H	5.601525	-0.305591	0.293585
H	4.677163	1.131538	-0.111257
H	6.018517	1.502336	1.964518
H	4.293620	1.587254	2.336713
H	5.217650	0.138212	2.750940
P	-0.428942	2.042988	-0.467387
F	1.129275	1.621759	-0.817576
F	-0.561351	0.673451	0.462913
F	-1.983939	2.415536	-0.133031
F	-0.289916	3.370271	-1.408656
F	-0.921220	1.158468	-1.777907
F	0.079656	2.879213	0.836749
Pd	-2.738182	-0.700291	1.044571



f1 in solution

Sum of electronic and zero-point Energies= -1617.598348

N	-0.379376	0.521317	1.521653
C	-1.796815	0.383983	1.314335
C	-2.019334	-1.066208	1.193855
N	-0.701153	-1.636351	1.308335
C	0.192029	-0.673149	1.472715
C	-0.392387	-3.063631	1.254836
C	0.331048	1.794376	1.701560
C	0.521925	2.569857	0.396100
C	1.237093	3.906056	0.621373
C	1.422078	4.703255	-0.672539
H	-2.419007	0.982698	1.990785
H	-2.778542	-1.556734	1.818170
H	0.669734	-3.203614	1.447389
H	-0.977148	-3.588901	2.012853
H	-0.632488	-3.461157	0.268310
H	1.256415	-0.837679	1.534885
H	1.298989	1.560889	2.147169
H	-0.242772	2.380777	2.425363
H	1.089117	1.950940	-0.305015
H	-0.466799	2.751102	-0.059474
H	0.672922	4.506289	1.345211
H	2.216581	3.713969	1.074263
H	1.939588	5.647125	-0.482779
H	2.011846	4.139436	-1.401126
H	0.458007	4.939074	-1.133843
P	3.572083	-0.796289	-0.375243
F	3.215412	0.193695	0.903822
F	2.090505	-0.466504	-1.012319
F	3.898884	-1.795549	-1.627466
F	5.029216	-1.129613	0.291741
F	2.903990	-2.058670	0.464159
F	4.212726	0.469930	-1.184112
Pd	-2.870610	-1.375935	-0.631320
Pd	-2.330356	1.192860	-0.479099



f2 in solution

Sum of electronic and zero-point Energies= -1617.570645

N	-1.843789	0.950660	1.523377
C	-2.608395	-0.209235	1.255625
C	-1.925403	-1.276111	1.891548
N	-0.794529	-0.694511	2.508183
C	-0.774983	0.606970	2.235881
C	0.252498	-1.436456	3.206881
C	-2.145261	2.300876	1.026322
C	-2.031200	2.409036	-0.496319
C	-2.360298	3.821539	-0.991408
C	-2.240183	3.952158	-2.512492
H	-3.672032	-0.103395	1.064857
H	-2.337165	-2.188935	2.311073
H	0.916421	-0.731275	3.702570
H	-0.207923	-2.091531	3.947485
H	0.824085	-2.025486	2.489721
H	0.029361	1.273493	2.502137
H	-1.450150	2.984380	1.518101
H	-3.155234	2.553257	1.363050
H	-1.014996	2.133574	-0.792733
H	-2.709742	1.685705	-0.960854
H	-3.376415	4.092681	-0.680480
H	-1.687863	4.541142	-0.509570
H	-2.475059	4.967831	-2.841363
H	-1.225670	3.718124	-2.848440
H	-2.926004	3.269324	-3.023458
P	2.599294	0.858636	0.292104
F	1.283852	1.839010	0.194546
F	2.741403	0.869646	-1.334903
F	3.885189	-0.146768	0.412248
F	2.417875	0.818212	1.931811
F	1.589042	-0.468524	0.185958
F	3.579179	2.160250	0.417830
Pd	-1.717294	-1.488003	-0.223717
Pd	0.575505	-1.673096	-1.728635

The Gaussian03 program allows the definition of an arbitrary solvent in the PCM model by specification of the parameters available for user input. The text pasted below is from <http://www.ccl.net/cgi-bin/ccl/message-new?2009+05+14+009>

- *From:* Madi <madi7sk[#]gmail.com>
 - *Subject:* CCL:G: Dioxane in PCM with G03
 - *Date:* Thu, 14 May 2009 17:17:29 -0400
-

Sent to CCL by: Madi [madi7sk{:}gmail.com]

Hi,

I was trying to specify DMF using the PCM model in gaussian and was trouble getting it to work. I wrote to gaussian and their reply was very helpful. I am attaching it here for your reference. After you are done specifying all the parameters, make sure you deliberately leave a blank line.

Hope this helps

madi

Regarding the specification of the DMF solvent, even though only the solvents listed in the Gaussian documentation of the SCRF keyword are available through the "Solvent=" option, a different solvent may be explicitly defined in the PCM input. However, please, note that it is not possible to input all parameters that define an arbitrary solvent. Specifically, one cannot define all of the terms necessary to calculate the non-electrostatic contributions. For this reason, there are two recommended alternatives:

1) Check in the list of solvents provided for the SCRF keyword whether there is a solvent similar enough to the one you would like to use in your calculation and provide this name in the "Solvent" option of the SCRF keyword. Then, add also the "Read" option to provide the modifications of "EPS", "RSOLV", "Density", and "VMOL". This way, you would be introducing the parameters for your desired

solvent, for the cases of parameters that are available for user input, and the program would be using the closest possible parameters for those other parameters that are not available for user input. (Note: if no solvent is specified, then the program defaults to water). So, probably, your best choice here would be to select a solvent with similar properties to DMF (such as Acetonitrile, DMSO, Acetone, Nitromethane) and then give the corresponding "EPS", "RSOLV", "Density", and "VMOL" parameters for DMF.

2) Alternatively, you can use the options "NoDis NoRep NoCav" in order to prevent the use of the parameters for the internally stored solvent (water, by default), so the non-electrostatic contributions to the solvation energy will not be computed. Note also that this is true if the default "UA0" radii are used, the electrostatic terms are then correctly computed this way. If this is not the case, and the UAHF or UAKS radii are used, then there is a dependency of the radius with the type of solvent so it would not be correct to use a modified water as a model for a solvent with properties different than water. Thus, if UAHF or UAKS radii are used, then one has to still do what it was explained in the previous paragraph, 1), (that is to use the "Solvent=" option to select, from the list of predefined solvents, a solvent similar to the one you are interested in). For the calculation of only the electrostatic part, you can define the solvent by defining the dielectric constant using the "EPS" option, the solvent radius using the "RSOLV" option, and the dielectric constant at infinite frequency using the "EPSINF". EPSINF is the dielectric constant at infinite frequency. It is an experimentally measured value. The value of EPSINF will not affect the results of ground-state energy calculation of $\Delta G(\text{solv})$, so you do not need to worry about getting a non-standard value. EPSINF is only necessary when performing excited state PCM calculations. Other than EPS, RSOLV usually makes the biggest difference in the result. As for choosing a value of RSOLV, our developers recommended a couple of references they use for this parameter:

* O. Sinanoglu in "Molecular Interactions" Z. Ratajczack and Orville-Thomas eds, Wiley 1982 vol. 3 chap. 6

* M.H. Abraham and A. Nasehzadeh J. Chem. Soc. Faraday Trans. 1 1981, 77, 340.

If the desired RSOLV parameter is not found there, the molar volume may give some hints for RSOLV values for new solvents, even though attention must be paid to the chemical nature of the solvent, because strong interactions modify, to some extent, the definition of the hard sphere analogue of the solvent molecular volume. Thus, although a simple approximation, the Stearn-Eyring formula (Stearn, Eyring J. Chem. Phys. 1937, 5, 113) can be used to derive a value for RSOLV, given the molar volume of the solvent. Finally, about other parameters, which only affect the non-electrostatic terms, the DENSITY is a "number density", i.e. number of particles per volume, and the units are Angstroms⁻³. Taking the density of the solvent in "g * cm⁻³", divide by the molar weight of the solvent and multiply by Avogadro's number to transform the grams into number of particles, and, finally, divide by 10²⁴ to transform cm⁻³ into Angstrom⁻³. Although the density and the molar volume are obviously related, these two quantities are used by the program to compute two different energy contributions and, unfortunately, they were introduced in the code as two independent parameters. Thus, the user needs to provide both the density ("DENSITY" PCM keyword) and the molar volume ("VMOL" PCM keyword) in order to set the desired modifications, so the two of them are consistent with each other. The units of the density are Angstrom⁻³ while the units of the molar volume are cm³. So, from the value of the density of the solvent in "g * cm⁻³", take the inverse of the density and then divide by the molar weight of the solvent in order to get the molar volume in cm³. Enter this parameter in your input file with the "VMOL" PCM keyword. The following input will use the standard parameters for the solvent given in "Solvent=<Solvent>", and modify those given in the additional PCM options (the values given below are not representative of any particular solvent and they are only given as an example of how to use these keywords):

```
%<Link 0 commands>
#P SCRF=(PCM,Solvent=<Solvent>,READ) <Method>/<BasisSet>
<Title>
<Charge Multiplicity>
```

<Coordinates>

EPS=6.0

RSOLV=1.6

DENSITY=0.045

VMOL=19.05