Electronic Supporting Information

Computational Study of C(sp^3)-O Bond Formation at a Pd^{IV} Centre

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Table of Contents

I. Computational Details

Gaussian 09[1] was used at the B3LYP[2] level of density functional theory (DFT) for geometry optimisation. The Stuttgart/Dresden ECP (SDD) was used to describe Pd,[3] and the 6-31G(d) basis set was used for other atoms to form basis set BS1. Computation was carried out for acetonitrile as the solvent utilizing the IEFPCM (SCRF) model. To further refine energies obtained from the B3LYP/BS1 calculations, we carried out single point energy calculations for all structures at the B3LYP-D3 level.[4] These calculations employed a larger basis set (BS2) utilizing the quadrupole-ξ valence polarized def2-QZVP[5] basis set on Pd along with the corresponding ECP and the 6-311+G(2d,p) basis set on other atoms. All thermodynamic data were calculated at the standard state (298.15 K and 1 atm). To estimate the corresponding Gibbs free energies in acetonitrile (ΔG), entropy corrections were calculated at the B3LYP/BS1 level and added to the single point potential energies, adjusted by the method developed by Okuno.[6] All transition structures contained one imaginary frequency, exhibiting atom displacements consistent with the anticipated reaction pathway. The nature of transition structures was confirmed by intrinsic reaction coordinate (IRC) searches, vibrational frequency calculations, and potential energy surface scans. In calculations, the translational contribution to the entropy is calculated on the basis of the Thacker-Tetrode equation.[7] However, this contribution is suppressed upon going from the gas phase to a solvent, leading to an inadequate estimation of the Gibbs free energy changes, especially where the number of reactants is different from that of products, on the basis that the free space available for molecule movement is much smaller in solution than in the gas phase.

1. Gaussian 09, revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr. J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.
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3. H. Andrae, U. Haussermann, M. Dolg, H. Stoll and H. Preuss, H. *Theor. Chim. Acta* 1990, 77, 123.
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5. F. Weigend, F. Furche and R. Ahlrichs, *J. Chem. Phys*., 2003, 119, 12753.
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7. Gurney, R. W. Introduction to Statistical Mechanics 1st ed. McGraw-Hill Book Company, New York, 1949

Figure SI-1. Conformational analysis for structure **1b** showing the effect of rotation of the acetate group beneath the 'Pd(bpy)FC$_{Ar}$' square-plane to give conformer **1b_I** and connecting transition structures. Energies ΔG (ΔH) in kcal/mol.

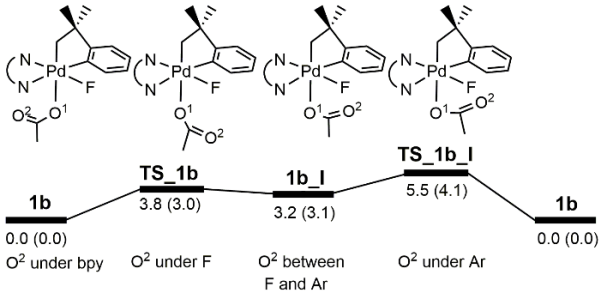


Figure SI-2. Conformational analysis for structure **1c** showing the effect of rotation of the difluoroacetate group beneath the 'Pd(bpy)FC$_{Ar}$' square-plane to give conformer **1c_I** and connecting transition structures. Energies ΔG (ΔH) in kcal/mol.

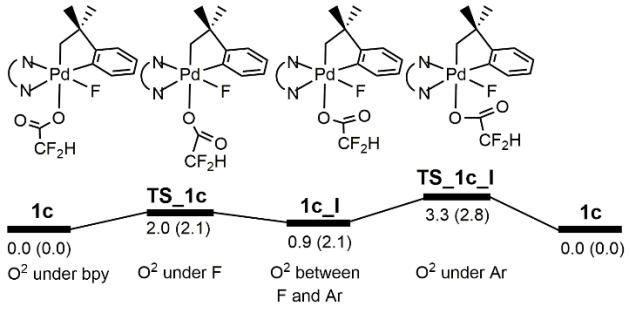


Figure SI-3. Conformational analysis for structure **1d** showing the effect of rotation of the nitrate group beneath the 'Pd(bpy)FC$_{Ar}$' square-plane to give conformer **1d_I** and **1d_II** connecting transition structures. Energies ΔG (ΔH) in kcal/mol.

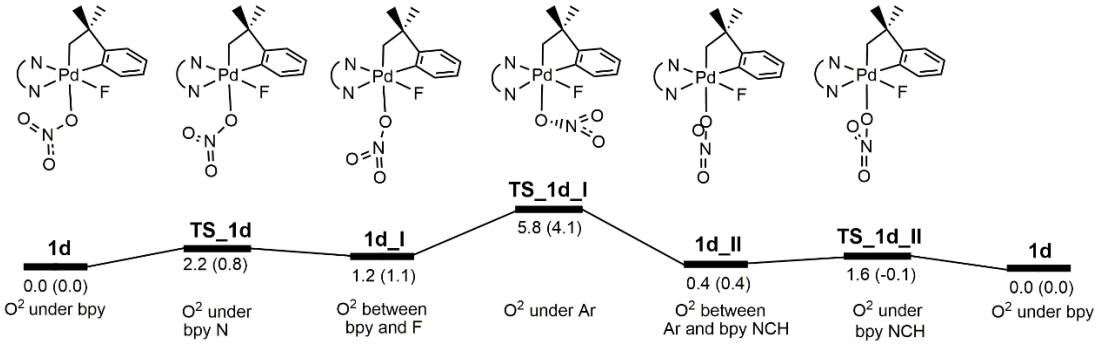


Figure SI-4. Conformational analysis for structure **1e** showing the effect of rotation of the phenoxide group beneath the 'Pd(bpy)FC$_{Ar}$' square-plane to give conformer **1e_I** and **1e_II** connecting transition structures. Energies ΔG (ΔH) in kcal/mol.

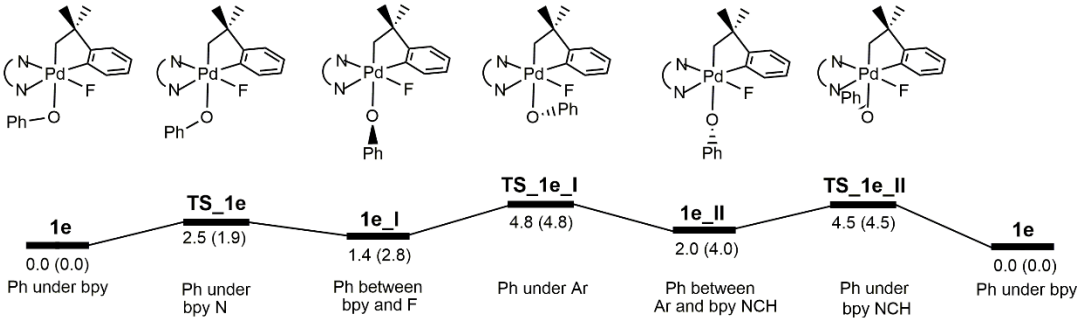


Figure SI-5. Energy profile for exchange of difluoroacetate and acetonitrile ligands for **1c**, and C-O coupling by the S_N2 mechanism to give the Pd^{II} product **4c**. Angle Pd···C···O 152.8º (**TS_3_DFA**). Energies ΔG (ΔH) in kcal/mol.

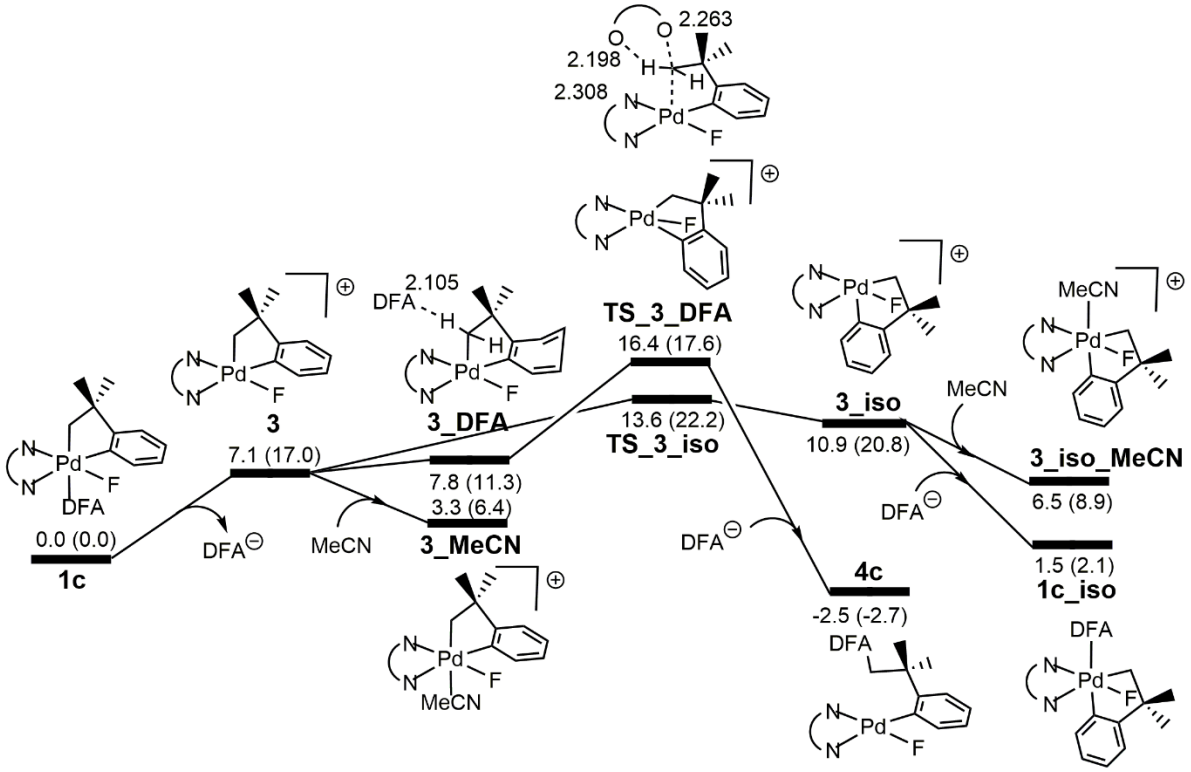


Figure SI-6. Energy profile for exchange of nitrate and acetonitrile ligands for **1d**, and C-O coupling by the S_N2 mechanism to give the Pd^{II} product **4d**. Angle Pd···C···O 151.3º (**TS_3_NO3**). Energies ΔG (ΔH) in kcal/mol.

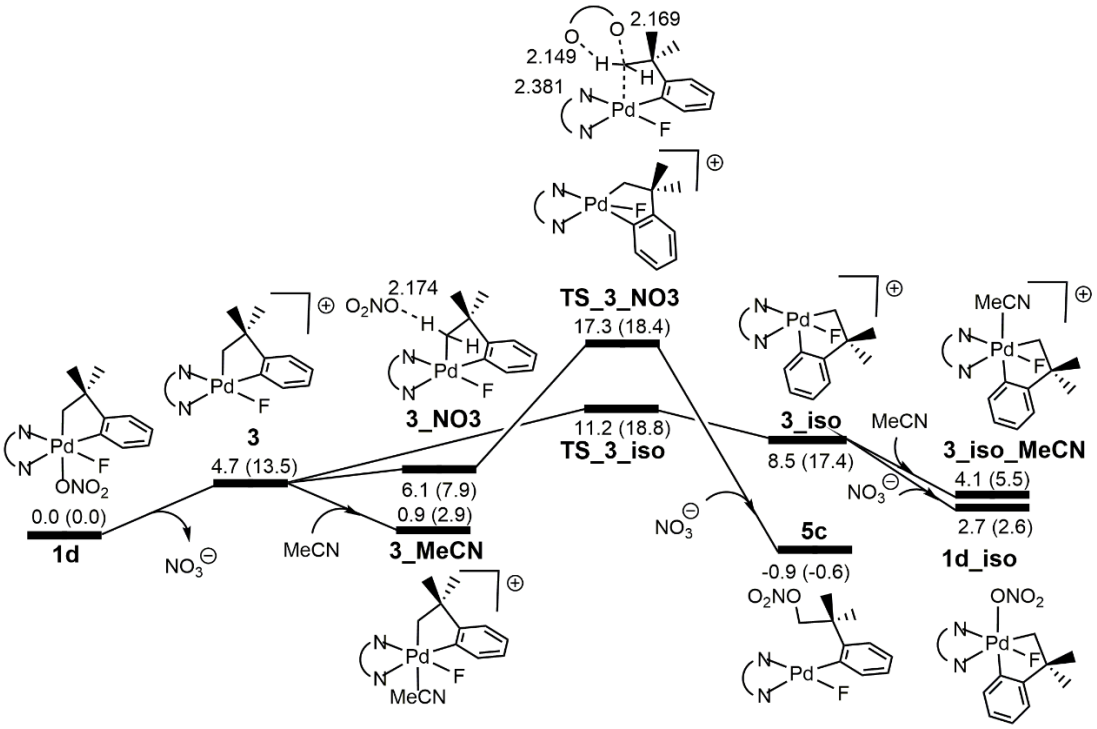
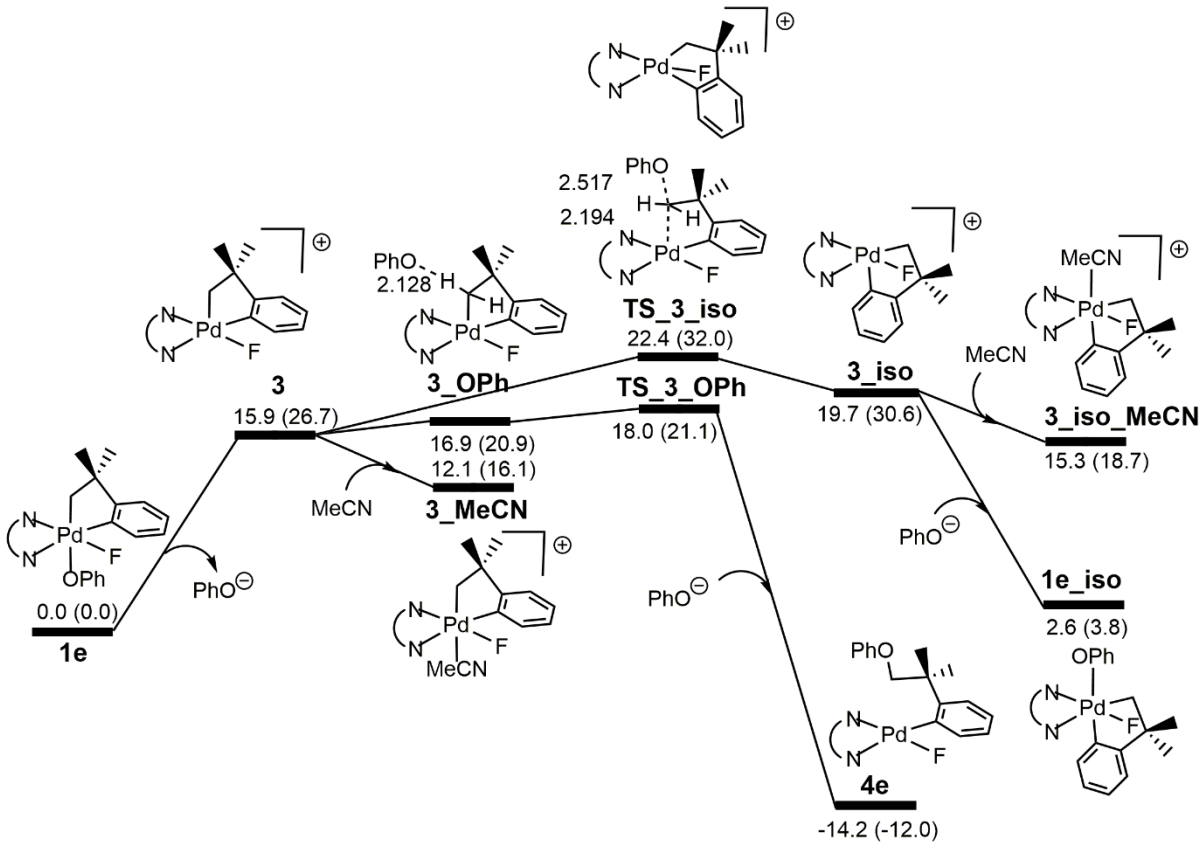


Figure SI-7. Energy profile for exchange of phenoxide and acetonitrile ligands for **1e**, and C-O coupling by the S_N2 mechanism to give the Pd^{II} product **4e**. Angle Pd···C···O 153.0º (**TS_3_OPh**)

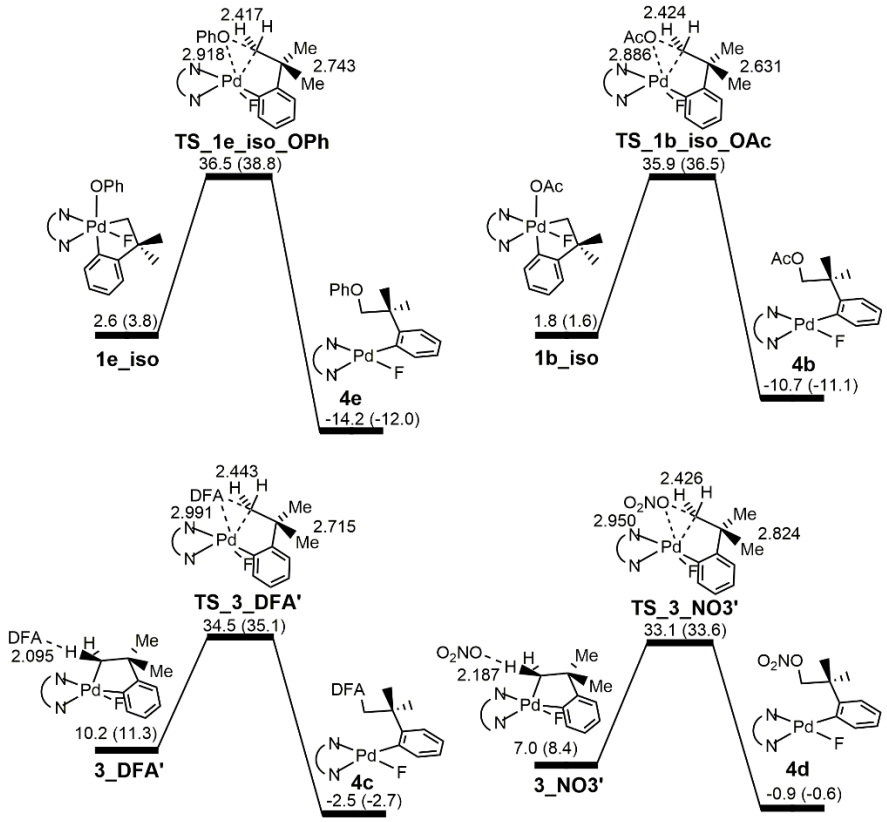


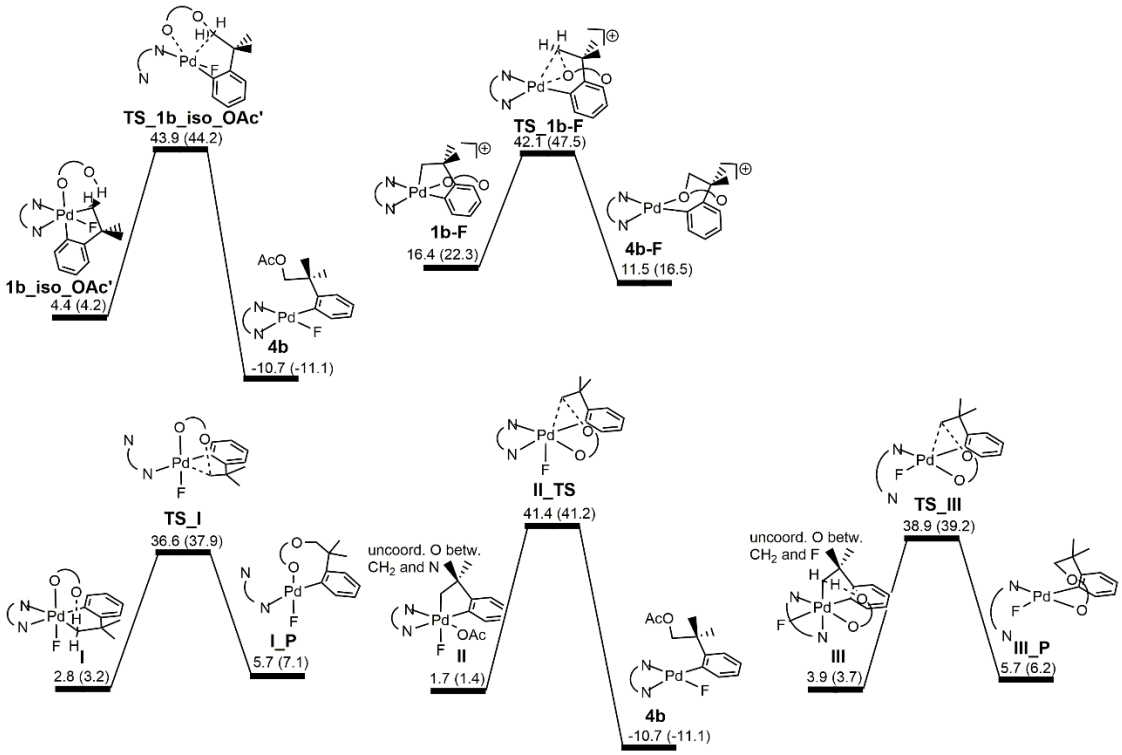
IX. Survey of high energy concerted C-O coupling

Although both experimental and computational studies implicate an outer-sphere S_N2 mechanism for C(sp^3)-O coupling in this system, we have explored a range of alternative mechanisms for C-O coupling in order to provide guidance for future studies of carbon-heteroatom coupling involving "M(CH_2CMe_2-*o*-C_6H_4-*C*,*C*')" and related substrates (Figure below). These pathways examined inner-sphere mechanisms,

Computation for **1b_iso_OAc'**, **I**, and **III** reveal monodentate bpy in five-coordinate transition structures. The transition structure **TS_1e_iso_OAc'** involves the acetate group acting in a similar bridging role to that computed for trifluoroacetate in the Me-DFA coupling step that occurs from $[Pd^{IV}Me(DFA)_2(bis(NHC))]^+$ as part of a mechanism for CH activation of methane by $Pd^{II}Br_2${bis(NHC)} (bis(NHC) = 1,1'-dimethyl-3,3'-methylenediimidazolin-2,2'-ylidene) (D. Munz, D. Meyer and T. Strassner, *Organometallics,* 2013, 32, 3469). However, all transition structures examined for the alternative pathways shown are substantially higher than found for the S_N2 process, by $\Delta\Delta G^{‡}$ = 13.5 (NO_3), 15.3 (DFA), 16.1-23.4 (OAc), and 15.5 (OPh) kcal/mol.

Energies ΔG in kcal/mol referenced to appropriate **1b-d** or **1e_MeCN**.



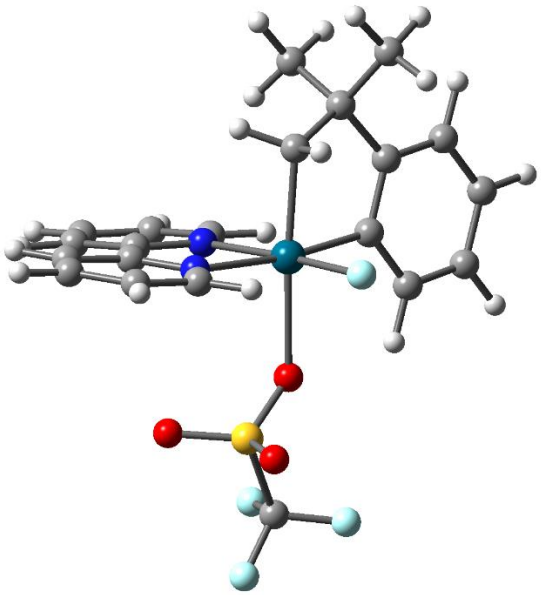


X. Energies of calculated species, and Gaussview structures

1a

Zero-point correction=	0.384567 (Hartree/Particle)
Thermal correction to Energy=	0.414995
Thermal correction to Enthalpy=	0.415939
Thermal correction to Gibbs Free Energy=	0.321146
Sum of electronic and zero-point Energies=	-2072.524706
Sum of electronic and thermal Energies=	-2072.494278
Sum of electronic and thermal Enthalpies=	-2072.493334
Sum of electronic and thermal Free Energies=	-2072.588128

E(RB3LYP) = -2073.58220328



Pd	-0.609090	0.125454	-0.575732
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C	-0.859537	0.166606	2.437770
H	-1.392742	-0.756193	2.250031
C	-0.634036	0.630351	3.728944
H	-1.000254	0.058360	4.573475
C	0.060364	1.825779	3.896454
H	0.254613	2.221187	4.887789
C	0.516666	2.508741	2.772182
C	1.406795	3.883731	0.226260
C	1.848422	4.384733	-0.998143
H	2.349690	5.346228	-1.038198
C	1.638375	3.645781	-2.161253
H	1.968415	4.005133	-3.129302
C	0.982447	2.420611	-2.057426
H	0.775935	1.794721	-2.919557
C	0.764028	2.643626	0.258209
C	0.269170	1.997145	1.496268
H	1.562576	4.457742	1.131126
H	1.076465	3.427678	2.889580
N	0.565161	1.943907	-0.880642
C	-2.364972	1.145870	-0.924604
H	-2.236617	2.132359	-0.473407
H	-2.314104	1.208695	-2.012439
C	-1.870613	-1.396932	-0.208684
C	-1.424175	-2.704722	-0.023256
C	-3.232156	-1.067140	-0.207078
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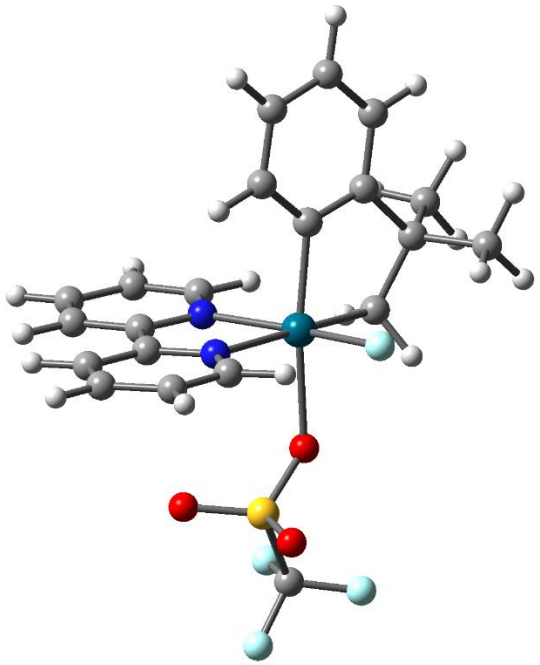
H	-0.364025	-2.933556	-0.053740
C	-4.159958	-2.094659	0.020339
C	-3.730875	-3.407345	0.226242
H	-2.033838	-4.737746	0.354275
H	-5.223716	-1.869794	0.033594
H	-4.462132	-4.192054	0.400135
C	-3.614846	0.390462	-0.421360
C	-4.714957	0.536019	-1.501482
H	-4.921407	1.595163	-1.695214
H	-4.408809	0.065727	-2.442062
H	-5.650614	0.070477	-1.172829
F	-0.626945	-0.412284	-2.460023
C	-4.129241	1.009620	0.899025
H	-5.012115	0.470359	1.258811
H	-3.369750	0.973177	1.685754
H	-4.411016	2.058202	0.745023
C	3.525067	-2.344040	0.248485
S	2.694671	-0.810538	-0.397618
F	3.093556	-3.425793	-0.414225
F	3.258498	-2.505527	1.552138
F	4.852399	-2.245443	0.092078
O	1.249888	-1.176029	-0.161933
O	3.076741	-0.741465	-1.820803
O	3.188989	0.278666	0.467189

1a_iso

Zero-point correction=	0.384456 (Hartree/Particle)
Thermal correction to Energy=	0.414911
Thermal correction to Enthalpy=	0.415855
Thermal correction to Gibbs Free Energy=	0.320616
Sum of electronic and zero-point Energies=	-2072.520309
Sum of electronic and thermal Energies=	-2072.489854
Sum of electronic and thermal Enthalpies=	-2072.488909
Sum of electronic and thermal Free Energies=	-2072.584149

E(RB3LYP) = --2073.57700871



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H	-1.089725	-0.770767	2.677160
C	-0.461048	0.923398	3.845087
H	-0.731368	0.465939	4.789618
C	0.084345	2.201705	3.774417
H	0.260429	2.783187	4.673110
C	0.398593	2.732284	2.526703
C	0.993070	3.781609	-0.236399
C	1.229388	4.166723	-1.555765
H	1.633312	5.151763	-1.765538
C	0.944170	3.281648	-2.594629
H	1.116447	3.548466	-3.631178
C	0.425586	2.029505	-2.271523
H	0.178961	1.287243	-3.023839
C	0.473525	2.508171	0.014136
C	0.174237	1.984786	1.368190
H	1.214675	4.467714	0.571129
H	0.818387	3.727258	2.456567
N	0.198537	1.668355	-1.005068
C	-1.216591	-2.131329	0.310808
H	-0.573633	-2.824244	-0.235560
H	-0.958023	-2.163809	1.371550
C	-2.529408	0.113690	-0.361611
C	-3.023342	1.394495	-0.592693
C	-3.365188	-0.987510	-0.136363
C	-4.410462	1.589920	-0.597509
H	-2.360345	2.234189	-0.768084
C	-4.750217	-0.763669	-0.145448
C	-5.269168	0.512213	-0.372927
H	-4.809485	2.584397	-0.777937
H	-5.428524	-1.596112	0.023884
H	-6.344868	0.664405	-0.375214
C	-2.722893	-2.354572	0.048877
C	-3.328856	-3.120315	1.247778
H	-2.792402	-4.063725	1.403052
H	-3.265862	-2.533994	2.171492
H	-4.382212	-3.365433	1.071590
F	-0.702608	-0.997354	-2.169573
C	-2.920396	-3.192493	-1.237699
H	-3.986656	-3.328013	-1.451673

H	-2.448941	-2.700818	-2.092120
H	-2.470263	-4.185425	-1.114469
C	4.016143	-1.799284	0.244275
S	2.872582	-0.502878	-0.440711
O	3.209423	-0.414733	-1.873791
O	3.136843	0.700111	0.372246
F	3.835890	-2.965896	-0.388463
F	3.786449	-1.979937	1.552291
F	5.289471	-1.414395	0.082106
O	1.539270	-1.154065	-0.161152

1b

Zero-point correction=	0.406981 (Hartree/Particle)
Thermal correction to Energy=	0.434037
Thermal correction to Enthalpy=	0.434982
Thermal correction to Gibbs Free Energy=	0.349113
Sum of electronic and zero-point Energies=	-1339.551296
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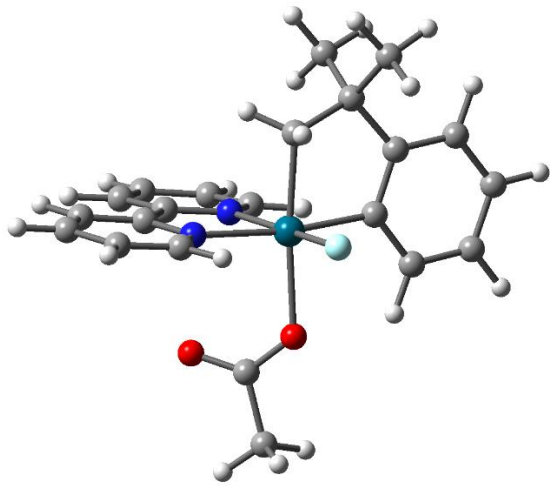

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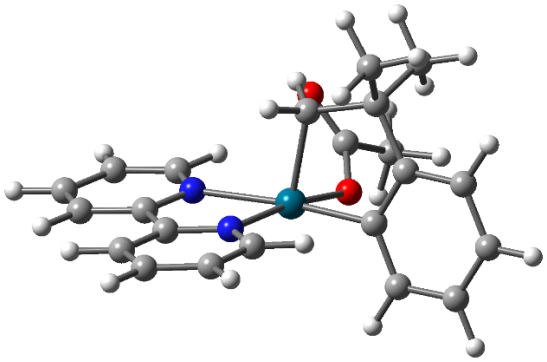
H	1.193104	0.641755	2.192041
C	-0.286384	0.108539	3.679288
H	0.329170	0.408666	4.519410
C	-1.563350	-0.418323	3.854491
H	-1.980747	-0.545714	4.847798
C	-2.308054	-0.774904	2.733538
C	-3.808703	-1.471578	0.206715
C	-4.440067	-1.690924	-1.017343
H	-5.435594	-2.122111	-1.041762
C	-3.783078	-1.355361	-2.200036
H	-4.243315	-1.510963	-3.169262
C	-2.501446	-0.813813	-2.112768
H	-1.924027	-0.538936	-2.989949
C	-2.528615	-0.910827	0.219415
C	-1.772162	-0.603654	1.455247
H	-4.313626	-1.736149	1.127362
H	-3.308881	-1.168979	2.854772
N	-1.904995	-0.601154	-0.937090
C	0.840168	-1.806799	-0.685760
H	0.146476	-2.419060	-0.103387
H	0.731124	-2.030854	-1.748588
C	2.050158	0.565505	-0.237240
C	2.518855	1.876577	-0.152658
C	2.905068	-0.536837	-0.099891
C	3.877852	2.098746	0.100590

H	1.830226	2.704698	-0.284329
C	4.264037	-0.291259	0.152065
C	4.747052	1.014973	0.253162
H	4.253485	3.116545	0.172608
H	4.951298	-1.126218	0.268868
H	5.802505	1.186219	0.447924
C	2.305558	-1.934328	-0.199547
C	3.084444	-2.803332	-1.215707
H	2.608733	-3.785870	-1.319635
H	3.107581	-2.327072	-2.202104
H	4.118143	-2.967345	-0.890718
F	0.584325	0.250049	-2.545697
C	2.348381	-2.625849	1.183690
H	3.378522	-2.710438	1.547400
H	1.773227	-2.066413	1.928841
H	1.928132	-3.636964	1.118547
C	-1.642804	4.284727	-0.464168
H	-0.757044	4.820576	-0.104856
H	-1.715622	4.468379	-1.542063
H	-2.531934	4.683282	0.030331
C	-1.496070	2.782719	-0.193899
O	-2.339212	2.191482	0.498620
O	-0.450064	2.256891	-0.745534

1b-F

Zero-point correction=	0.405596	(Hartree/Particle)
Thermal correction to Energy=	0.431176	
Thermal correction to Enthalpy=	0.432121	
Thermal correction to Gibbs Free Energy=	0.349386	
Sum of electronic and zero-point Energies=	-1239.542868	
Sum of electronic and thermal Energies=	-1239.517288	
Sum of electronic and thermal Enthalpies=	-1239.516344	
Sum of electronic and thermal Free Energies=	-1239.599078	

E(RB3LYP) = -1240.38239437



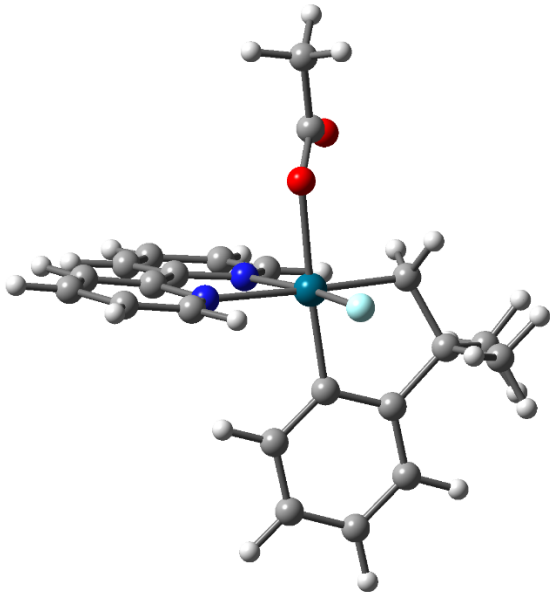
Pd	-0.040080	0.245983	-0.382448
N	-2.175000	0.761545	-0.073240
N	-0.913754	-1.629505	-0.096660
C	1.803365	-0.462148	-0.731235
C	-0.224297	-2.785450	-0.086648
C	-0.848837	-4.020654	0.037549
C	-2.235444	-4.056777	0.154800
C	-2.947562	-2.860558	0.146672
C	-2.271768	-1.644231	0.020234
H	0.849919	-2.705326	-0.182556
H	-0.249791	-4.923691	0.040895
H	-2.760980	-5.000557	0.253968
H	-4.025264	-2.878858	0.239944
C	-2.730269	1.982424	-0.068000
C	-4.108078	2.173891	0.013139
C	-4.931939	1.054918	0.094438
C	-4.356170	-0.214342	0.098485
C	-2.966814	-0.335921	0.013744

H	-2.043070	2.817397	-0.103877
H	-4.512861	3.179461	0.014204
H	-6.009834	1.160865	0.158120
H	-4.989481	-1.089243	0.165072
C	2.684305	-0.505562	0.353048
C	3.970653	-1.019443	0.133162
C	4.348965	-1.461519	-1.136585
C	3.451235	-1.396611	-2.206267
C	2.160447	-0.890386	-2.007002
C	2.195298	0.054495	1.679368
H	4.682270	-1.069923	0.953456
H	5.348999	-1.856133	-1.292200
H	3.748863	-1.736774	-3.194341
H	1.457640	-0.838814	-2.835019
C	2.456158	-0.923870	2.851981
C	2.901595	1.398657	1.973174
C	0.669428	0.262145	1.587058
H	2.030914	-0.530452	3.782260
H	2.014837	-1.907002	2.657142
H	3.531841	-1.055251	3.009785
H	2.538313	1.826453	2.914709
H	3.982098	1.245511	2.063739
H	2.727369	2.123106	1.173538
H	0.311306	1.244182	1.893998
H	0.085905	-0.550328	2.019394
O	0.745751	2.024240	-0.932958
C	0.579888	3.154372	-0.280136
O	0.009852	3.274038	0.803990
C	1.183044	4.338249	-1.021620
H	2.252818	4.172634	-1.184767
H	0.713526	4.444083	-2.005158
H	1.035564	5.252860	-0.444790

1b_iso

Zero-point correction=	0.407101 (Hartree/Particle)
Thermal correction to Energy=	0.434087
Thermal correction to Enthalpy=	0.435032
Thermal correction to Gibbs Free Energy=	0.349506
Sum of electronic and zero-point Energies=	-1339.549638
Sum of electronic and thermal Energies=	-1339.522651
Sum of electronic and thermal Enthalpies=	-1339.521707
Sum of electronic and thermal Free Energies=	-1339.607233

E(RB3LYP) = -1340.43849290

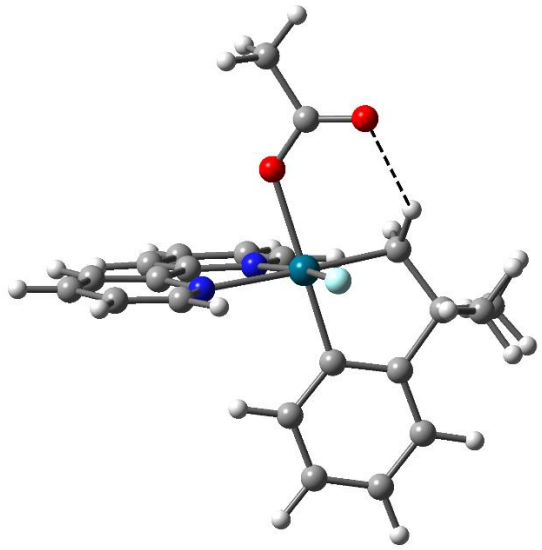


Pd	0.145171	0.327435	-0.555553
N	-1.605470	-0.971899	-0.957849
N	-0.683002	0.087472	1.341196
C	1.507824	-1.098219	-0.129132
F	0.765216	0.325634	-2.418823
C	-0.140621	0.563761	2.471411
C	-0.737510	0.398994	3.715901
C	-1.948335	-0.283710	3.788526
C	-2.508953	-0.785295	2.618068
C	-1.860910	-0.596948	1.393681
H	0.797541	1.089653	2.373695
H	-0.253375	0.801983	4.597932
H	-2.448638	-0.432494	4.739634
H	-3.443103	-1.330366	2.659290
C	-1.984551	-1.419811	-2.157455
C	-3.198177	-2.078353	-2.347334
C	-4.032298	-2.256769	-1.244283
C	-3.633795	-1.781369	0.004417
C	-2.397845	-1.135774	0.120460
H	-1.289676	-1.232371	-2.970144
H	-3.477317	-2.433591	-3.333007
H	-4.988465	-2.758848	-1.350534
H	-4.283612	-1.909941	0.860957
C	2.819969	-0.635566	0.050747
C	3.822339	-1.573050	0.341755
C	3.521165	-2.932679	0.449247
C	2.209616	-3.375352	0.264784
C	1.195203	-2.454078	-0.025608
C	3.082308	0.853243	-0.138010
H	4.848116	-1.240199	0.482192
H	4.310192	-3.644767	0.676115
H	1.970106	-4.432797	0.344419
H	0.177410	-2.804781	-0.166651
C	3.957374	1.434863	0.996719
C	3.798473	1.076631	-1.492206
C	1.719858	1.583875	-0.133758
H	4.064478	2.519345	0.874551
H	3.515629	1.244178	1.981691
H	4.963941	1.001231	0.987462
H	4.011127	2.143352	-1.638264
H	4.750379	0.533968	-1.523261
H	3.168020	0.732244	-2.315818
H	1.642072	2.347277	-0.910598
H	1.463216	2.032183	0.826061
O	-1.221606	1.922290	-1.097503
C	-1.431838	2.958678	-0.347181
O	-0.924657	3.173036	0.764207
C	-2.410716	3.967094	-0.956299
H	-3.376309	3.486072	-1.148422
H	-2.557511	4.817670	-0.286592
H	-2.031129	4.325674	-1.919635

1b_iso_OAc'

Zero-point correction=	0.407015 (Hartree/Particle)
Thermal correction to Energy=	0.434022
Thermal correction to Enthalpy=	0.434966
Thermal correction to Gibbs Free Energy=	0.349523
Sum of electronic and zero-point Energies=	-1339.547246
Sum of electronic and thermal Energies=	-1339.520239
Sum of electronic and thermal Enthalpies=	-1339.519295
Sum of electronic and thermal Free Energies=	-1339.604738

E(RB3LYP) = -1340.43433849



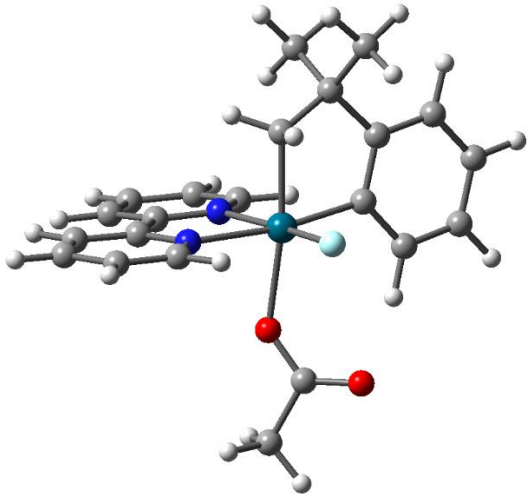
Pd	0.130623	0.452514	-0.261540
N	-1.655297	-0.534215	-1.134485
N	-0.680451	-0.548726	1.385293
C	1.478505	-1.024968	-0.516558
F	0.696123	1.212017	-1.980657
C	-0.110817	-0.624597	2.598243
C	-0.714756	-1.267471	3.673151
C	-1.957987	-1.861855	3.478666
C	-2.543161	-1.799702	2.217709
C	-1.891856	-1.139360	1.171860
H	0.858844	-0.160179	2.709494
H	-0.208749	-1.296185	4.631163
H	-2.463869	-2.375240	4.289496
H	-3.500400	-2.274741	2.046290
C	-2.055125	-0.439891	-2.404748
C	-3.302609	-0.902853	-2.820221
C	-4.148969	-1.465469	-1.865689
C	-3.727787	-1.555512	-0.539386
C	-2.457582	-1.078374	-0.198372
H	-1.349916	0.026150	-3.085788
H	-3.598001	-0.815752	-3.859835
H	-5.132033	-1.830166	-2.145412
H	-4.387406	-1.982737	0.205333
C	2.806327	-0.681459	-0.220619
C	3.798552	-1.658504	-0.389445
C	3.471701	-2.940151	-0.838503
C	2.144182	-3.263364	-1.126703
C	1.138557	-2.301426	-0.965022
C	3.085478	0.750716	0.216485
H	4.836056	-1.416861	-0.171058
H	4.253278	-3.685003	-0.962624
H	1.884624	-4.258983	-1.477708
H	0.108749	-2.559737	-1.191685
C	4.051150	0.812797	1.422728
C	3.704199	1.538400	-0.963612
C	1.739989	1.383983	0.629902
H	4.161241	1.848437	1.765748
H	3.684261	0.211363	2.262431
H	5.048917	0.447352	1.153775
H	3.918243	2.570716	-0.658695
H	4.645381	1.078216	-1.286650
H	3.011048	1.561643	-1.807325
H	1.605636	2.420210	0.320326
H	1.552053	1.300920	1.703315
O	-0.116710	3.910818	0.047654
C	-1.175906	3.291339	0.226282

O	-1.346782	2.008371	0.162540
C	-2.462026	4.058088	0.557625
H	-2.266358	5.130776	0.627284
H	-3.216494	3.878198	-0.216656
H	-2.881047	3.702680	1.505692

1b_I

Zero-point correction=	0.406968 (Hartree/Particle)
Thermal correction to Energy=	0.434051
Thermal correction to Enthalpy=	0.434996
Thermal correction to Gibbs Free Energy=	0.349199
Sum of electronic and zero-point Energies=	-1339.547767
Sum of electronic and thermal Energies=	-1339.520684
Sum of electronic and thermal Enthalpies=	-1339.519740
Sum of electronic and thermal Free Energies=	-1339.605536

E(RB3LYP) = -1340.43600799



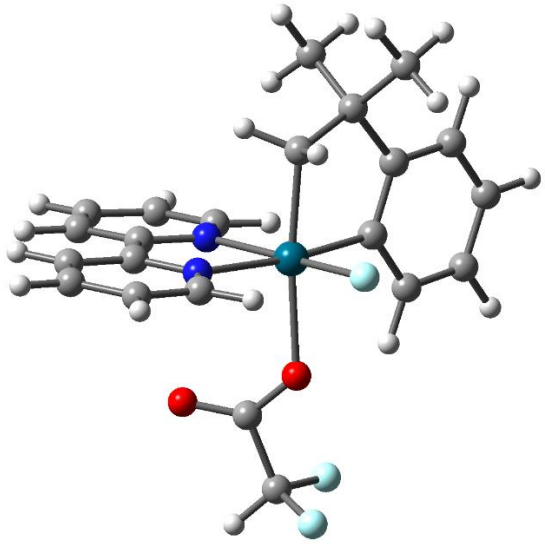
Pd	0.050811	0.252691	-0.518440
N	-0.557691	-0.618105	1.255095
C	0.210453	-0.691241	2.354653
H	1.228612	-0.340680	2.247960
C	-0.269313	-1.186943	3.562173
H	0.388676	-1.228481	4.422401
C	-1.592022	-1.617067	3.627258
H	-2.004052	-2.010685	4.550475
C	-2.389674	-1.528422	2.489842
C	-3.989655	-1.289668	-0.062682
C	-4.654113	-1.078883	-1.270482
H	-5.683345	-1.403470	-1.383725
C	-3.987724	-0.453136	-2.323145
H	-4.474152	-0.272120	-3.274975
C	-2.664224	-0.061880	-2.127842
H	-2.079653	0.426975	-2.900929
C	-2.663259	-0.864828	0.064471
C	-1.859385	-1.018744	1.301463
H	-4.503503	-1.779145	0.755157
H	-3.423936	-1.844421	2.532041
N	-2.033302	-0.266526	-0.968778
C	0.690570	-1.550516	-1.294287
H	-0.053808	-2.294257	-0.998134
H	0.608102	-1.337789	-2.361368
C	2.001340	0.444933	-0.058051
C	2.539445	1.627706	0.450645
C	2.796504	-0.684846	-0.300763
C	3.904783	1.674347	0.759456
H	1.912134	2.505480	0.568298
C	4.162127	-0.614340	0.015744

C	4.711948	0.553663	0.546939
H	4.334206	2.590370	1.158002
H	4.801126	-1.477396	-0.156601
H	5.771397	0.591080	0.786620
C	2.128969	-1.929326	-0.870705
C	2.882008	-2.442235	-2.122243
H	2.353431	-3.296350	-2.562229
H	2.959227	-1.657177	-2.882511
H	3.895213	-2.773715	-1.868383
F	0.426628	1.020281	-2.286515
C	2.101575	-3.056117	0.188262
H	3.117521	-3.323214	0.499573
H	1.544653	-2.756966	1.081880
H	1.626132	-3.954975	-0.222910
C	-1.692715	4.184220	1.047916
H	-2.686300	4.022926	0.613961
H	-1.750693	3.893255	2.102765
H	-1.437886	5.244542	0.977701
C	-0.654751	3.323732	0.314539
O	0.282423	3.873018	-0.287138
O	-0.877476	2.054462	0.409467

1c

Zero-point correction=	0.392726 (Hartree/Particle)
Thermal correction to Energy=	0.420977
Thermal correction to Enthalpy=	0.421921
Thermal correction to Gibbs Free Energy=	0.332482
Sum of electronic and zero-point Energies=	-1538.031060
Sum of electronic and thermal Energies=	-1538.002809
Sum of electronic and thermal Enthalpies=	-1538.001865
Sum of electronic and thermal Free Energies=	-1538.091304

E(RB3LYP) = -1538.98576203



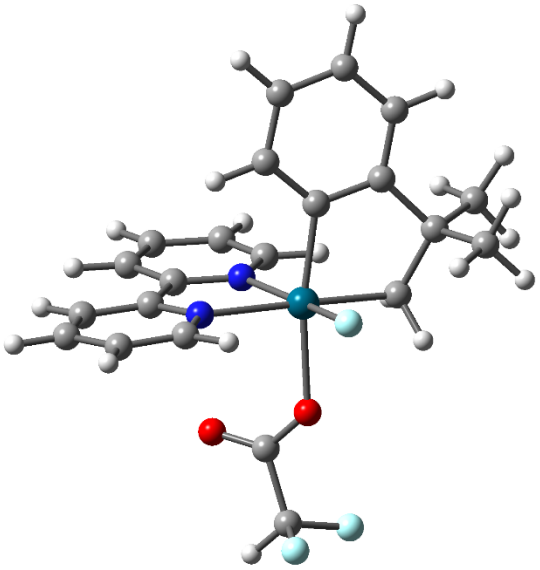
Pd	0.157412	-0.147323	-0.627458
N	-0.426740	-0.592932	1.300997
C	0.287566	-0.278736	2.393958
H	1.236711	0.210746	2.219332
C	-0.161194	-0.564644	3.678924
H	0.450442	-0.292922	4.531441
C	-1.390898	-1.200030	3.829109
H	-1.773844	-1.444642	4.814280
C	-2.133590	-1.514566	2.694371
C	-3.643964	-2.093727	0.142326
C	-4.274947	-2.271751	-1.088464
H	-5.243169	-2.759669	-1.132808
C	-3.653925	-1.821047	-2.252447

H	-4.115951	-1.941629	-3.225746
C	-2.407840	-1.206959	-2.140929
H	-1.860351	-0.837539	-3.002338
C	-2.397879	-1.461081	0.180999
C	-1.641745	-1.195330	1.426979
H	-4.122922	-2.444855	1.047659
H	-3.098362	-1.993956	2.798612
N	-1.809714	-1.037471	-0.958384
C	1.083121	-1.980734	-0.810115
H	0.490169	-2.691835	-0.229403
H	0.946061	-2.165450	-1.877060
C	2.014747	0.484004	-0.201470
C	2.313452	1.830074	0.013353
C	2.999504	-0.511590	-0.166844
C	3.637660	2.193025	0.288115
H	1.528646	2.578568	-0.025431
C	4.320301	-0.123429	0.107669
C	4.637368	1.217370	0.333516
H	3.883893	3.237601	0.462081
H	5.107214	-0.873217	0.146182
H	5.665230	1.500214	0.544758
C	2.576710	-1.957782	-0.394347
C	3.409700	-2.603635	-1.527037
H	3.064757	-3.626611	-1.719274
H	3.317333	-2.029062	-2.455153
H	4.471294	-2.654361	-1.260256
F	0.571650	0.148418	-2.524251
C	2.772517	-2.776250	0.903872
H	3.821668	-2.766585	1.219327
H	2.170146	-2.372865	1.725078
H	2.476618	-3.820523	0.746050
C	-1.622014	3.926724	0.107818
H	-2.433278	4.335325	0.715551
C	-1.554449	2.384419	0.161108
O	-2.314801	1.806424	0.947110
O	-0.670182	1.900668	-0.625145
F	-0.431035	4.439481	0.568565
F	-1.774997	4.361017	-1.181714

1c_iso

Zero-point correction=	0.392493 (Hartree/Particle)
Thermal correction to Energy=	0.420813
Thermal correction to Enthalpy=	0.421757
Thermal correction to Gibbs Free Energy=	0.331397
Sum of electronic and zero-point Energies=	-1538.027576
Sum of electronic and thermal Energies=	-1537.999255
Sum of electronic and thermal Enthalpies=	-1537.998311
Sum of electronic and thermal Free Energies=	-1538.088671

E(RB3LYP) = -1538.98223746



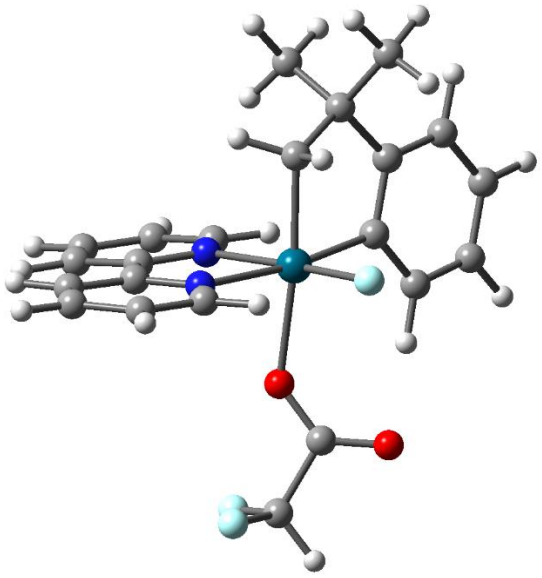
Pd	0.214540	0.371073	-0.352316
N	-0.166374	-0.728580	1.379977
C	0.315044	-0.432774	2.596653
H	0.943056	0.443482	2.672466
C	0.038790	-1.202986	3.721191
H	0.452821	-0.914650	4.680427
C	-0.759404	-2.332827	3.572393
H	-0.994190	-2.965930	4.421541
C	-1.250572	-2.647322	2.308735
C	-2.316584	-3.174654	-0.459587
C	-2.714278	-3.354807	-1.783912
H	-3.388970	-4.165643	-2.038768
C	-2.242348	-2.488667	-2.769685
H	-2.531949	-2.599114	-3.808634
C	-1.381201	-1.461842	-2.387818
H	-0.975166	-0.744994	-3.094745
C	-1.448594	-2.122641	-0.149716
C	-0.951291	-1.831404	1.215428
H	-2.687878	-3.842012	0.307844
H	-1.865235	-3.528150	2.175848
N	-1.002168	-1.297393	-1.117538
C	1.294819	1.939329	0.423098
H	0.840540	2.807826	-0.057519
H	1.055124	1.957287	1.488905
C	2.028933	-0.496467	-0.462035
C	2.218812	-1.830638	-0.818799
C	3.108355	0.350699	-0.171630
C	3.520970	-2.342326	-0.886088
H	1.376518	-2.476211	-1.045958
C	4.404092	-0.182582	-0.244572
C	4.610296	-1.517906	-0.597266
H	3.676240	-3.381280	-1.165319
H	5.260170	0.452113	-0.028507
H	5.621231	-1.913225	-0.647988
C	2.810928	1.810684	0.146595
C	3.588488	2.301458	1.389836
H	3.301231	3.331183	1.633634
H	3.384908	1.673279	2.264755
H	4.669818	2.294462	1.212122
F	0.526056	1.147850	-2.126295
C	3.198727	2.687337	-1.069044
H	4.263927	2.577918	-1.303135
H	2.612604	2.401461	-1.945866
H	3.006122	3.745116	-0.849945
C	-3.674264	2.572701	0.229146
H	-4.620665	2.358633	0.732434

C	-2.667330	1.407086	0.345183
O	-3.018416	0.411376	0.988616
O	-1.563742	1.641372	-0.258388
F	-3.132475	3.708140	0.776575
F	-3.929842	2.842032	-1.090788

1c_I

Zero-point correction=	0.392459 (Hartree/Particle)
Thermal correction to Energy=	0.420845
Thermal correction to Enthalpy=	0.421789
Thermal correction to Gibbs Free Energy=	0.330531
Sum of electronic and zero-point Energies=	-1538.028229
Sum of electronic and thermal Energies=	-1537.999842
Sum of electronic and thermal Enthalpies=	-1537.998898
Sum of electronic and thermal Free Energies=	-1538.090156

E(RB3LYP) = -1538.98231851



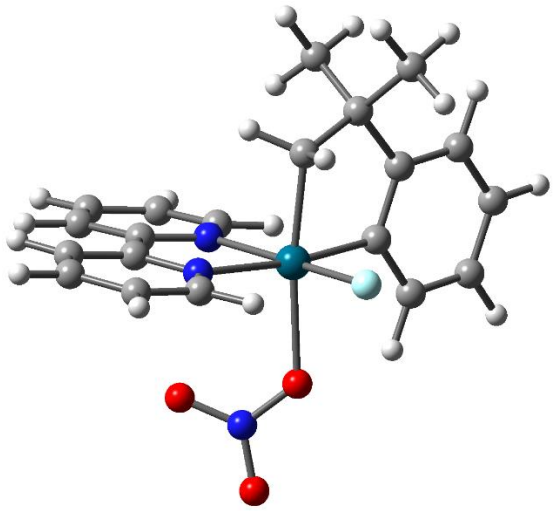
Pd	0.240704	-0.023916	-0.576310
N	-0.205292	-0.764791	1.301838
C	0.474232	-0.442398	2.415030
H	1.353262	0.173036	2.275564
C	0.074693	-0.870551	3.676306
H	0.656384	-0.587463	4.545865
C	-1.070799	-1.655127	3.782085
H	-1.415211	-2.008968	4.748088
C	-1.781508	-1.975412	2.628636
C	-3.201060	-2.604683	0.036567
C	-3.820203	-2.772497	-1.201687
H	-4.700249	-3.401898	-1.283953
C	-3.300193	-2.130066	-2.324320
H	-3.757110	-2.236732	-3.301645
C	-2.162851	-1.339999	-2.166463
H	-1.698508	-0.814367	-2.994893
C	-2.068288	-1.789582	0.123032
C	-1.338667	-1.517345	1.385009
H	-3.598581	-3.106707	0.909733
H	-2.684092	-2.568624	2.699070
N	-1.574601	-1.182789	-0.977611
C	1.429577	-1.638634	-1.056591
H	0.917095	-2.524188	-0.672325
H	1.360618	-1.600796	-2.144812
C	2.011909	0.811585	-0.119086
C	2.142170	2.162110	0.206814
C	3.119011	-0.047384	-0.171640
C	3.410922	2.664957	0.520944

H	1.278046	2.817524	0.187970
C	4.380467	0.478411	0.147204
C	4.525562	1.822638	0.495093
H	3.523738	3.715123	0.778613
H	5.256261	-0.165640	0.121445
H	5.509763	2.213585	0.739129
C	2.882482	-1.504851	-0.544102
C	3.834734	-1.955826	-1.678239
H	3.602910	-2.982943	-1.984120
H	3.737854	-1.305623	-2.554527
H	4.880020	-1.935286	-1.350013
F	0.482963	0.569096	-2.429841
C	3.106611	-2.417082	0.684546
H	4.129125	-2.315540	1.064408
H	2.419084	-2.172399	1.500273
H	2.949786	-3.467851	0.412160
C	-2.741239	3.342563	0.186746
H	-2.859865	4.408252	-0.025880
C	-1.398943	2.777506	-0.331630
O	-0.701373	3.529236	-1.024335
O	-1.197018	1.570193	0.033398
F	-3.777170	2.660787	-0.405714
F	-2.854465	3.149592	1.539165

1d

Zero-point correction=	0.371999 (Hartree/Particle)
Thermal correction to Energy=	0.398034
Thermal correction to Enthalpy=	0.398978
Thermal correction to Gibbs Free Energy=	0.314795
Sum of electronic and zero-point Energies=	-1391.404305
Sum of electronic and thermal Energies=	-1391.378270
Sum of electronic and thermal Enthalpies=	-1391.377326
Sum of electronic and thermal Free Energies=	-1391.461509

E(RB3LYP) = -1392.27844519



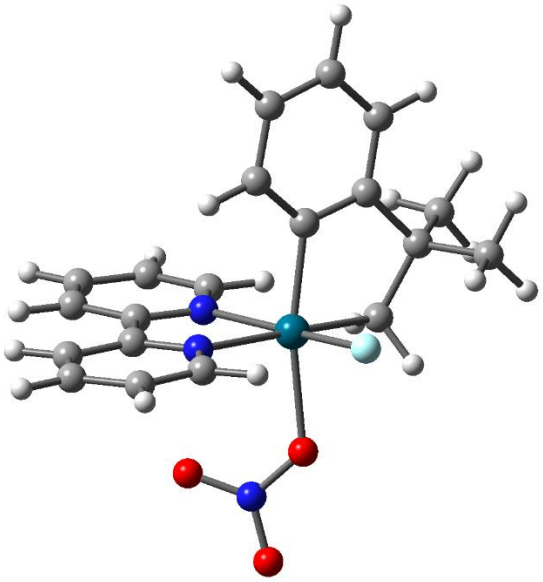
Pd	0.123787	0.143776	-0.630171
N	-0.513400	-0.129293	1.312511
C	0.216382	0.184596	2.395532
H	1.211670	0.564973	2.207317
C	-0.273919	0.030780	3.687892
H	0.351322	0.297996	4.531867
C	-1.562354	-0.469247	3.856670
H	-1.979260	-0.607974	4.848576
C	-2.319749	-0.784136	2.731485
C	-3.841840	-1.401128	0.194461
C	-4.478008	-1.586513	-1.032841
H	-5.481786	-1.997512	-1.063400
C	-3.816120	-1.243249	-2.210596

H	-4.280684	-1.372501	-3.181526
C	-2.524282	-0.728306	-2.116437
H	-1.942358	-0.449044	-2.989138
C	-2.550368	-0.867627	0.215391
C	-1.784077	-0.600243	1.455064
H	-4.351457	-1.671886	1.110640
H	-3.328912	-1.157437	2.848700
N	-1.922304	-0.549596	-0.937393
C	0.826124	-1.793957	-0.712784
H	0.127401	-2.399535	-0.131196
H	0.700690	-1.990049	-1.778600
C	2.046682	0.564492	-0.225990
C	2.516475	1.872750	-0.111537
C	2.898094	-0.542361	-0.112821
C	3.875950	2.085365	0.147420
H	1.835019	2.709852	-0.223335
C	4.257389	-0.306334	0.144434
C	4.742443	0.996383	0.275065
H	4.253195	3.100348	0.243387
H	4.942692	-1.145113	0.242537
H	5.797998	1.161170	0.473936
C	2.294545	-1.934640	-0.242940
C	3.057269	-2.776396	-1.294543
H	2.577374	-3.753925	-1.422186
H	3.072590	-2.270511	-2.266017
H	4.092962	-2.952461	-0.983552
F	0.572253	0.295382	-2.534395
C	2.348594	-2.666194	1.119037
H	3.383094	-2.769209	1.464405
H	1.789514	-2.124098	1.888789
H	1.919739	-3.671698	1.030500
O	-2.183105	2.243907	0.553495
O	-0.444025	2.325535	-0.794257
N	-1.443285	2.903394	-0.199959
O	-1.617586	4.111898	-0.415762

1d_iso

Zero-point correction=	0.372016 (Hartree/Particle)
Thermal correction to Energy=	0.397987
Thermal correction to Enthalpy=	0.398931
Thermal correction to Gibbs Free Energy=	0.314997
Sum of electronic and zero-point Energies=	-1391.400622
Sum of electronic and thermal Energies=	-1391.374650
Sum of electronic and thermal Enthalpies=	-1391.373706
Sum of electronic and thermal Free Energies=	-1391.457640

E(RB3LYP) = -1392.27429702



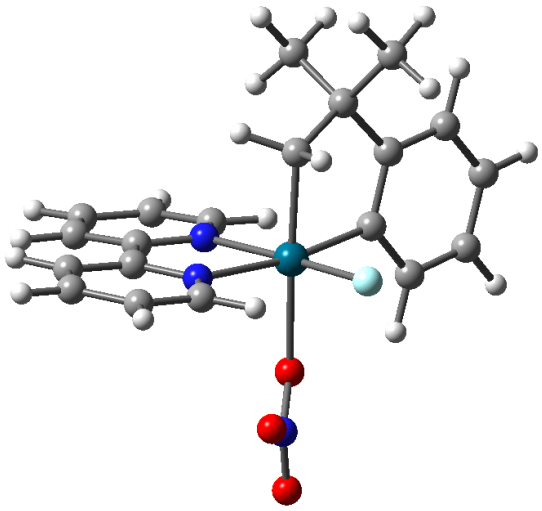
Pd	0.192625	0.564630	-0.373043
N	-0.575635	-0.265588	1.379445
C	-0.033145	-0.123962	2.598269
H	0.870413	0.464782	2.664504
C	-0.585522	-0.699759	3.737231
H	-0.106396	-0.548485	4.697476
C	-1.740955	-1.462697	3.601800
H	-2.202452	-1.934101	4.463021
C	-2.298972	-1.619717	2.336322
C	-3.443577	-1.832133	-0.441705
C	-3.868409	-1.896035	-1.768480
H	-4.784263	-2.422607	-2.016483
C	-3.112330	-1.280507	-2.765143
H	-3.413621	-1.309709	-3.806172
C	-1.945378	-0.616095	-2.392335
H	-1.304820	-0.112376	-3.109462
C	-2.262526	-1.146806	-0.140599
C	-1.708111	-1.010813	1.227093
H	-4.033062	-2.304452	0.333924
H	-3.193443	-2.216533	2.214336
N	-1.543595	-0.560887	-1.119591
C	1.770364	1.649096	0.383968
H	1.676166	2.605641	-0.133856
H	1.542483	1.793305	1.442799
C	1.559734	-0.911598	-0.421724
C	1.238992	-2.228773	-0.743182
C	2.871024	-0.515182	-0.126779
C	2.258015	-3.189513	-0.767412
H	0.220488	-2.520887	-0.975104
C	3.874263	-1.495653	-0.155477
C	3.571947	-2.821645	-0.471076
H	2.017699	-4.219295	-1.018356
H	4.901732	-1.218739	0.067276
H	4.362713	-3.566632	-0.487139
C	3.133951	0.959199	0.147587
C	4.022543	1.164955	1.395953
H	4.127676	2.234431	1.613166
H	3.594025	0.676492	2.278583
H	5.028821	0.760268	1.239920
F	0.777879	1.126994	-2.157219
C	3.833750	1.588883	-1.081410
H	4.782176	1.081353	-1.291658
H	3.191320	1.516660	-1.962488
H	4.049820	2.647823	-0.892532
O	-2.714952	1.756728	0.746218

O	-0.961991	2.473991	-0.376675
N	-2.127541	2.683280	0.159215
O	-2.607521	3.820782	0.055747

1d_I

Zero-point correction=	0.371890 (Hartree/Particle)
Thermal correction to Energy=	0.397941
Thermal correction to Enthalpy=	0.398886
Thermal correction to Gibbs Free Energy=	0.314782
Sum of electronic and zero-point Energies=	-1391.403142
Sum of electronic and thermal Energies=	-1391.377090
Sum of electronic and thermal Enthalpies=	-1391.376146
Sum of electronic and thermal Free Energies=	-1391.460250

E(RB3LYP) = -1392.27653180



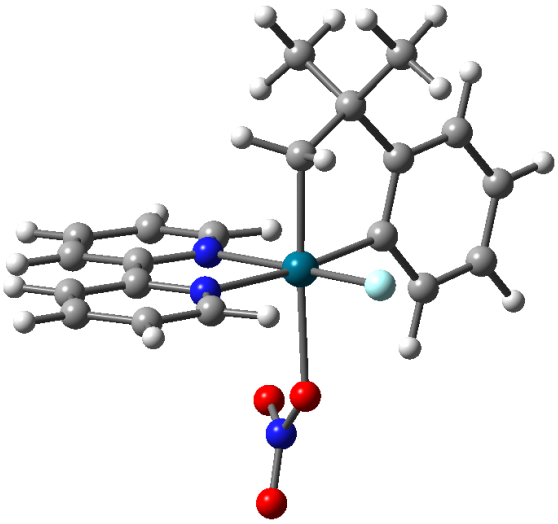
Pd	0.080635	0.428357	-0.341013
N	-0.443999	-0.942744	1.114373
C	0.350928	-1.273987	2.146496
H	1.335961	-0.826139	2.152740
C	-0.062944	-2.143498	3.149554
H	0.613708	-2.383110	3.961535
C	-1.344197	-2.684315	3.076837
H	-1.702753	-3.368595	3.838467
C	-2.171149	-2.327907	2.015030
C	-3.833735	-1.463107	-0.362404
C	-4.533540	-0.946068	-1.451866
H	-5.533157	-1.306488	-1.671692
C	-3.939664	0.030467	-2.250439
H	-4.455394	0.455062	-3.104322
C	-2.653284	0.458273	-1.928018
H	-2.130959	1.217394	-2.499634
C	-2.545805	-0.986917	-0.098360
C	-1.708732	-1.445260	1.035642
H	-4.288213	-2.224371	0.259103
H	-3.176135	-2.725842	1.957362
N	-1.987015	-0.041980	-0.884468
C	0.752114	-1.035918	-1.628632
H	0.054584	-1.872329	-1.539710
H	0.610359	-0.521791	-2.580441
C	2.034600	0.573396	0.112005
C	2.538681	1.578205	0.936988
C	2.868031	-0.372382	-0.500299
C	3.916707	1.628686	1.180669
H	1.868550	2.305270	1.383896
C	4.245835	-0.302286	-0.243597
C	4.766307	0.689040	0.590841
H	4.320764	2.404512	1.826105
H	4.918028	-1.025269	-0.699715

H	5.836022	0.729200	0.777950
C	2.223866	-1.438763	-1.376462
C	2.931628	-1.546240	-2.748512
H	2.414837	-2.271858	-3.387618
H	2.940843	-0.579320	-3.263224
H	3.967625	-1.883923	-2.633628
F	0.429231	1.714756	-1.778155
C	2.290115	-2.814340	-0.671748
H	3.329373	-3.102554	-0.479388
H	1.762091	-2.802150	0.287219
H	1.834331	-3.588068	-1.301506
O	-1.519686	3.766833	1.883483
O	-0.479177	1.995719	1.181654
N	-1.369741	2.923388	0.985550
O	-2.031391	2.937453	-0.065645

1d_II

Zero-point correction=	0.371846 (Hartree/Particle)
Thermal correction to Energy=	0.397907
Thermal correction to Enthalpy=	0.398851
Thermal correction to Gibbs Free Energy=	0.314775
Sum of electronic and zero-point Energies=	-1391.403551
Sum of electronic and thermal Energies=	-1391.377491
Sum of electronic and thermal Enthalpies=	-1391.376547
Sum of electronic and thermal Free Energies=	-1391.460622

E(RB3LYP) = -1392.27770940



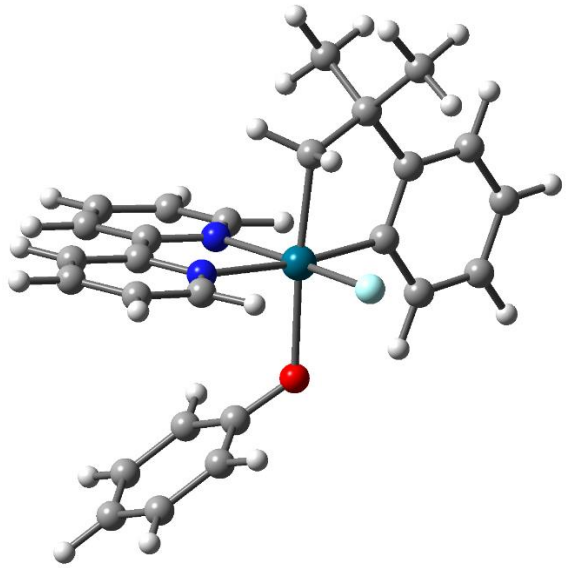
Pd	0.074185	-0.122528	-0.656795
N	-0.593629	0.291111	1.251875
C	0.152530	0.898326	2.188922
H	1.167581	1.141253	1.906471
C	-0.348024	1.202391	3.449699
H	0.293425	1.687765	4.176057
C	-1.669865	0.874864	3.740427
H	-2.097012	1.097657	4.712449
C	-2.446808	0.260897	2.761718
C	-3.996679	-1.071707	0.529513
C	-4.627179	-1.636276	-0.578886
H	-5.658525	-1.964864	-0.503171
C	-3.925272	-1.773937	-1.775570
H	-4.385078	-2.207220	-2.656516
C	-2.601570	-1.340073	-1.819209
H	-1.990765	-1.417142	-2.713137
C	-2.667492	-0.654524	0.413429
C	-1.893658	-0.026676	1.511360
H	-4.538798	-0.965170	1.460736
H	-3.480039	0.013725	2.968872

N	-2.003378	-0.799667	-0.753855
C	0.717988	-1.996407	-0.080212
H	-0.004099	-2.355891	0.656604
H	0.594613	-2.530499	-1.023560
C	2.008936	0.347194	-0.401165
C	2.521060	1.597932	-0.743968
C	2.826955	-0.681421	0.084082
C	3.889241	1.841039	-0.575536
H	1.866510	2.375124	-1.121450
C	4.195825	-0.416741	0.245366
C	4.722955	0.834033	-0.081191
H	4.298624	2.814362	-0.833816
H	4.854970	-1.193497	0.625667
H	5.785397	1.022031	0.048215
C	2.177837	-2.013723	0.434388
C	2.913484	-3.191264	-0.250223
H	2.399266	-4.136284	-0.039100
H	2.949921	-3.053919	-1.336436
H	3.941208	-3.282231	0.118335
F	0.524309	-0.616444	-2.500396
C	2.202171	-2.232816	1.965392
H	3.231138	-2.235367	2.341271
H	1.653176	-1.446871	2.493934
H	1.746072	-3.196961	2.220596
O	-0.362026	3.107477	0.148138
O	-0.695448	1.787751	-1.581485
N	-0.891387	2.912700	-0.961878
O	-1.599368	3.762598	-1.522767

1e

Zero-point correction=	0.449512 (Hartree/Particle)
Thermal correction to Energy=	0.477627
Thermal correction to Enthalpy=	0.478571
Thermal correction to Gibbs Free Energy=	0.389143
Sum of electronic and zero-point Energies=	-1417.878698
Sum of electronic and thermal Energies=	-1417.850584
Sum of electronic and thermal Enthalpies=	-1417.849640
Sum of electronic and thermal Free Energies=	-1417.939068

E(RB3LYP) = -1418.83307676



Pd	0.474197	-0.082690	-0.624002
N	-0.084390	-0.152404	1.359664
C	0.530112	0.537599	2.335753
H	1.392763	1.117764	2.036350
C	0.087904	0.510260	3.653467

H	0.617794	1.081397	4.407007
C	-1.031173	-0.258492	3.966338
H	-1.404481	-0.308614	4.983727
C	-1.675833	-0.959111	2.951566
C	-2.959739	-2.422611	0.635557
C	-3.496841	-3.015066	-0.506555
H	-4.359977	-3.667164	-0.421375
C	-2.916947	-2.764361	-1.749455
H	-3.308828	-3.207571	-2.657986
C	-1.807530	-1.922814	-1.804009
H	-1.301555	-1.684782	-2.734196
C	-1.847065	-1.585664	0.505658
C	-1.194125	-0.891609	1.640970
H	-3.404927	-2.616997	1.603251
H	-2.556187	-1.547180	3.177117
N	-1.296968	-1.357834	-0.706436
C	1.709553	-1.739209	-0.430441
H	1.224542	-2.425236	0.269505
H	1.661431	-2.145732	-1.442520
C	2.198164	0.917610	-0.396157
C	2.271941	2.304000	-0.528264
C	3.333252	0.134174	-0.147390
C	3.513563	2.935367	-0.387542
H	1.370301	2.872301	-0.733012
C	4.567967	0.788008	-0.008851
C	4.658297	2.176436	-0.127258
H	3.583405	4.016115	-0.484803
H	5.466649	0.209210	0.191773
H	5.622939	2.665271	-0.018331
C	3.154101	-1.372865	-0.005549
C	4.143083	-2.140667	-0.914836
H	3.967869	-3.220630	-0.840528
H	4.022631	-1.845107	-1.962997
H	5.182875	-1.951969	-0.624127
F	0.848339	-0.137308	-2.554073
C	3.397846	-1.794906	1.462884
H	4.410585	-1.528445	1.785672
H	2.689650	-1.308514	2.142045
H	3.282393	-2.880217	1.572096
O	-0.698930	1.761189	-0.890842
C	-2.000137	1.857010	-0.657164
C	-2.960383	1.603649	-1.672863
C	-2.499568	2.276761	0.604550
C	-4.324895	1.770350	-1.440689
H	-2.602236	1.285749	-2.649677
C	-3.866943	2.441740	0.827345
H	-1.784514	2.487598	1.396735
C	-4.794326	2.190355	-0.189871
H	-5.031204	1.573993	-2.245320
H	-4.212146	2.773402	1.804971
H	-5.858610	2.321351	-0.013681

1e_iso

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Zero-point correction=                           0.449702 (Hartree/Particle)
Thermal correction to Energy=                    0.477748
Thermal correction to Enthalpy=                  0.478692
Thermal correction to Gibbs Free Energy=         0.390450
Sum of electronic and zero-point Energies=          -1417.875600
Sum of electronic and thermal Energies=             -1417.847554
Sum of electronic and thermal Enthalpies=           -1417.846610
Sum of electronic and thermal Free Energies=        -1417.934852
E(RB3LYP) =  -1418.83019794
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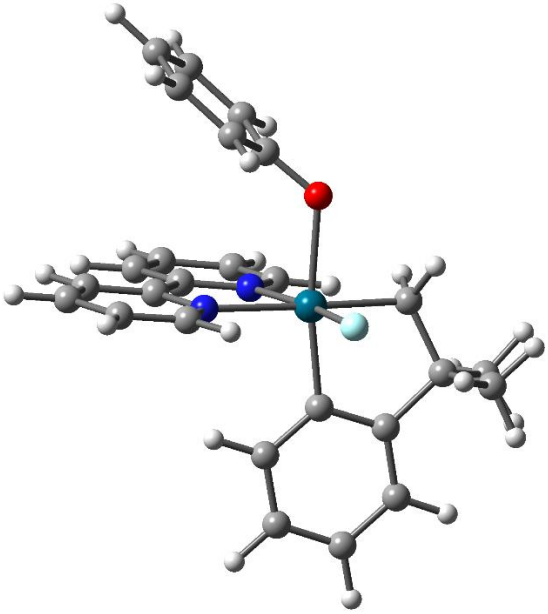


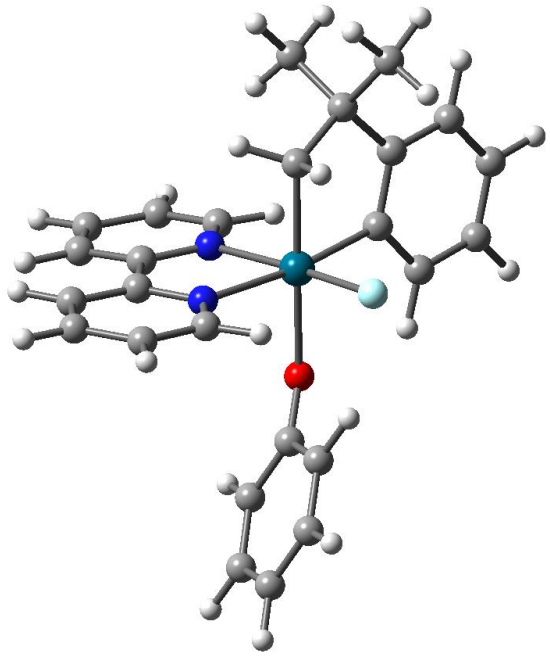
Pd	-0.500885	-0.407589	-0.478664
N	0.176025	0.085204	1.433212
C	-0.279878	-0.458567	2.573035
H	-1.073254	-1.186512	2.480983
C	0.222359	-0.115453	3.822907
H	-0.183311	-0.588768	4.709535
C	1.236140	0.836152	3.894378
H	1.655381	1.134092	4.849587
C	1.703741	1.409052	2.716360
C	2.629853	2.572395	0.094121
C	2.950737	3.076941	-1.165222
H	3.739990	3.814930	-1.265647
C	2.253811	2.626539	-2.285910
H	2.478128	2.996896	-3.279958
C	1.251348	1.676168	-2.102207
H	0.669628	1.273364	-2.925449
C	1.609184	1.621602	0.202764
C	1.164346	1.024394	1.485156
H	3.171815	2.918591	0.965202
H	2.485548	2.156410	2.755474
N	0.944626	1.201001	-0.892355
C	-1.808551	-1.928558	-0.037413
H	-1.522055	-2.709278	-0.744567
H	-1.546183	-2.252205	0.972320
C	-2.148688	0.738382	-0.206422
C	-2.131393	2.133359	-0.172310
C	-3.346890	0.021452	-0.060358
C	-3.330082	2.835241	0.009990
H	-1.202914	2.684436	-0.284787
C	-4.537075	0.741766	0.120313
C	-4.530859	2.137954	0.156480
H	-3.318941	3.922075	0.035335
H	-5.478403	0.208622	0.231362
H	-5.462413	2.679354	0.298756
C	-3.288842	-1.498474	-0.161936
C	-4.101239	-2.183366	0.961636
H	-3.981247	-3.271965	0.906178
H	-3.770706	-1.853014	1.953232
H	-5.171446	-1.964906	0.871210
F	-1.008311	-0.633293	-2.363721
C	-3.854754	-1.940690	-1.533082
H	-4.893390	-1.609980	-1.650089
H	-3.255695	-1.519050	-2.343765
H	-3.835810	-3.034783	-1.617278

O	1.047211	-1.910775	-0.732184
C	2.342986	-1.727438	-0.509140
C	3.228725	-1.368572	-1.558925
C	2.918819	-1.942604	0.770165
C	4.599323	-1.238663	-1.340134
H	2.810588	-1.205861	-2.549840
C	4.291914	-1.811039	0.979937
H	2.264231	-2.231392	1.589581
C	5.146496	-1.456937	-0.069763
H	5.249332	-0.967905	-2.170075
H	4.699563	-1.990962	1.972976
H	6.215659	-1.356910	0.096720

1e_I

Zero-point correction=	0.449699 (Hartree/Particle)
Thermal correction to Energy=	0.477742
Thermal correction to Enthalpy=	0.478686
Thermal correction to Gibbs Free Energy=	0.390112
Sum of electronic and zero-point Energies=	-1417.878989
Sum of electronic and thermal Energies=	-1417.850946
Sum of electronic and thermal Enthalpies=	-1417.850001
Sum of electronic and thermal Free Energies=	-1417.938576

E(RB3LYP) = -1418.82977878



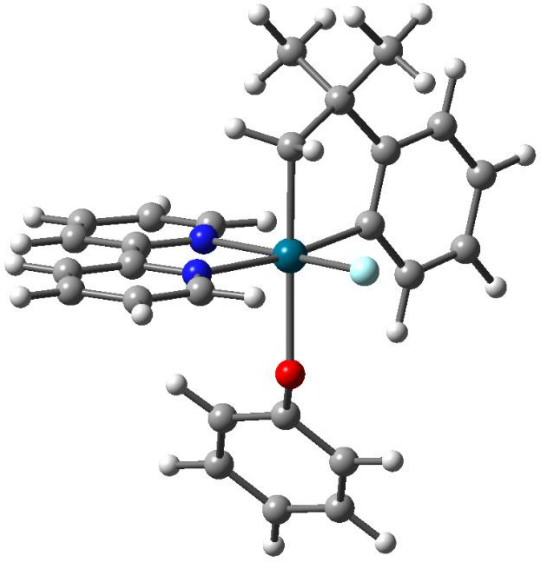
Pd	-0.311277	-0.209153	-0.388722
N	-0.286193	1.200645	1.116625
C	-1.073114	1.145546	2.203886
H	-1.797780	0.342297	2.226969
C	-0.966991	2.064645	3.242309
H	-1.626255	1.981918	4.098676
C	-0.008811	3.070685	3.147379
H	0.103939	3.807838	3.935320
C	0.817539	3.114723	2.027968
C	2.522906	3.080730	-0.469730
C	3.296925	2.932527	-1.620207
H	4.056760	3.669756	-1.858240
C	3.083913	1.837572	-2.456342
H	3.666801	1.690946	-3.358688
C	2.091631	0.922489	-2.108925
H	1.866021	0.050134	-2.712794
C	1.546786	2.121782	-0.181556
C	0.672871	2.163122	1.014918

H	2.680931	3.932654	0.179804
H	1.580041	3.879161	1.950861
N	1.353275	1.068847	-1.005215
C	-1.637602	0.890794	-1.539541
H	-1.361508	1.944707	-1.442688
H	-1.379478	0.527346	-2.536185
C	-1.983572	-1.171720	0.158613
C	-1.949135	-2.321503	0.946931
C	-3.184170	-0.648543	-0.341255
C	-3.152260	-2.962622	1.266134
H	-0.996730	-2.698504	1.305120
C	-4.378299	-1.307543	-0.009236
C	-4.363308	-2.454441	0.787640
H	-3.139266	-3.857757	1.883240
H	-5.327522	-0.923769	-0.376111
H	-5.297710	-2.952287	1.033309
C	-3.119693	0.622744	-1.179751
C	-3.922155	0.472213	-2.494193
H	-3.813092	1.372595	-3.110432
H	-3.567662	-0.386245	-3.075458
H	-4.991136	0.333134	-2.296169
F	-0.178207	-1.457154	-1.907069
C	-3.701562	1.810799	-0.377690
H	-4.746646	1.624553	-0.105812
H	-3.140427	1.985721	0.546026
H	-3.665330	2.729347	-0.976267
O	0.978531	-1.379422	0.945891
C	2.213401	-1.785430	0.694449
C	2.636251	-2.263625	-0.575184
C	3.178449	-1.794632	1.738016
C	3.938980	-2.720815	-0.775081
H	1.911970	-2.267537	-1.383694
C	4.474339	-2.262365	1.525676
H	2.874952	-1.435566	2.719598
C	4.873012	-2.729516	0.267443
H	4.227806	-3.082172	-1.761007
H	5.183198	-2.258837	2.352058
H	5.884914	-3.090779	0.104384

1e_II

Zero-point correction=	0.449523 (Hartree/Particle)
Thermal correction to Energy=	0.477720
Thermal correction to Enthalpy=	0.478664
Thermal correction to Gibbs Free Energy=	0.389041
Sum of electronic and zero-point Energies=	-1417.876598
Sum of electronic and thermal Energies=	-1417.848401
Sum of electronic and thermal Enthalpies=	-1417.847457
Sum of electronic and thermal Free Energies=	-1417.937080

E(RB3LYP) = -1418.83178112



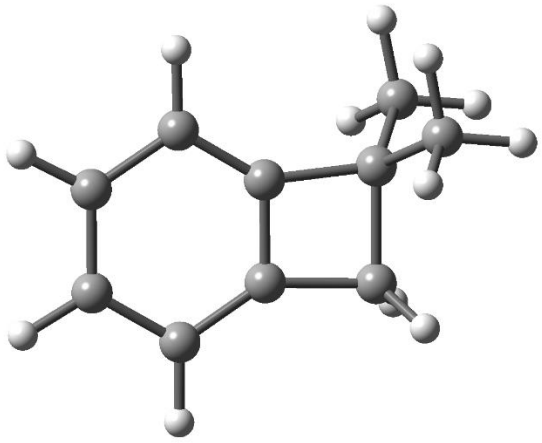
Pd	0.209256	-0.443458	-0.673461
N	-0.575087	-0.334471	1.229517
C	-0.009684	0.355642	2.234418
H	0.930345	0.841016	2.008751
C	-0.591814	0.442466	3.494470
H	-0.095893	1.008886	4.274154
C	-1.803695	-0.206213	3.715342
H	-2.288981	-0.164031	4.684664
C	-2.396017	-0.908490	2.668788
C	-3.570484	-2.365372	0.293215
C	-4.042568	-2.963729	-0.874573
H	-4.977238	-3.514726	-0.858786
C	-3.307087	-2.848112	-2.053288
H	-3.644997	-3.299333	-2.979386
C	-2.110408	-2.133938	-2.018555
H	-1.481458	-2.006412	-2.894061
C	-2.363999	-1.659289	0.252922
C	-1.770954	-0.962801	1.420080
H	-4.138404	-2.454685	1.210771
H	-3.345512	-1.404773	2.822991
N	-1.663861	-1.562397	-0.897261
C	1.218295	-2.196489	-0.218237
H	0.571505	-2.771153	0.450133
H	1.246611	-2.665920	-1.203101
C	1.998107	0.388244	-0.287312
C	2.258844	1.743026	-0.493089
C	2.994873	-0.492426	0.159304
C	3.539395	2.242255	-0.223906
H	1.481589	2.409487	-0.852049
C	4.271481	0.028549	0.421390
C	4.543182	1.384860	0.232978
H	3.747773	3.298268	-0.377436
H	5.060737	-0.630921	0.774593
H	5.537918	1.770556	0.440247
C	2.629043	-1.956656	0.369437
C	3.627600	-2.890560	-0.355444
H	3.317414	-3.936668	-0.246884
H	3.677727	-2.656334	-1.424591
H	4.636392	-2.798027	0.062743
F	0.805567	-0.691365	-2.530129
C	2.640375	-2.290941	1.879979
H	3.630432	-2.111325	2.313677
H	1.916483	-1.680891	2.430264
H	2.386496	-3.346048	2.039367
O	-0.922550	1.311191	-1.382615
C	-1.141550	2.506725	-0.864231

C	-0.673611	3.675173	-1.527823
C	-1.895888	2.712292	0.323234
C	-0.941489	4.952326	-1.036936
H	-0.108032	3.546327	-2.448449
C	-2.153786	3.994340	0.808279
H	-2.295583	1.845915	0.843254
C	-1.679978	5.128492	0.138758
H	-0.569983	5.820100	-1.578981
H	-2.740929	4.109776	1.717700
H	-1.886353	6.124579	0.520730

2

Zero-point correction=	0.190804 (Hartree/Particle)
Thermal correction to Energy=	0.199687
Thermal correction to Enthalpy=	0.200631
Thermal correction to Gibbs Free Energy=	0.157567
Sum of electronic and zero-point Energies=	-388.066790
Sum of electronic and thermal Energies=	-388.057907
Sum of electronic and thermal Enthalpies=	-388.056963
Sum of electronic and thermal Free Energies=	-388.100027

E(RB3LYP) = -388.389954723

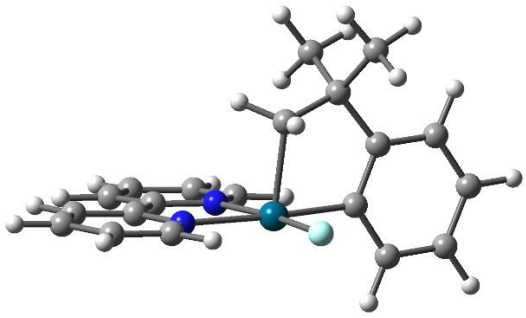


C	0.960783	1.500463	0.000593
H	1.244630	2.075417	-0.888769
H	1.243995	2.074203	0.890968
C	-0.451806	0.937338	0.000196
C	-1.798515	1.278000	0.000002
C	-0.019951	-0.388998	0.000290
C	-2.707735	0.205406	-0.000016
H	-2.151707	2.306413	-0.000104
C	-0.905931	-1.459195	0.000164
C	-2.272787	-1.128999	0.000047
H	-3.775427	0.410857	-0.000096
H	-0.585429	-2.498279	0.000340
H	-3.014225	-1.924307	-0.000027
C	1.467557	-0.010174	0.000092
C	2.234885	-0.412709	1.264384
H	3.224587	0.060606	1.284054
H	1.695672	-0.113001	2.170376
H	2.381856	-1.499167	1.302837
C	2.233423	-0.411856	-1.265448
H	2.379852	-1.498346	-1.305059
H	1.693334	-0.111069	-2.170557
H	3.223322	0.061029	-1.285783

3

Zero-point correction=	0.356045 (Hartree/Particle)
Thermal correction to Energy=	0.377607
Thermal correction to Enthalpy=	0.378551
Thermal correction to Gibbs Free Energy=	0.305798

Sum of electronic and zero-point Energies= -1110.955369
Sum of electronic and thermal Energies= -1110.933807
Sum of electronic and thermal Enthalpies= -1110.932863
Sum of electronic and thermal Free Energies= -1111.005615
E(RB3LYP) = -1111.69400690



Pd	-0.008681	-0.614525	-0.551351
N	-0.693569	1.309451	-0.240644
C	0.077356	2.409125	-0.326744
H	1.125577	2.243293	-0.536753
C	-0.438408	3.688813	-0.156279
H	0.221502	4.544943	-0.232436
C	-1.797242	3.829687	0.112143
H	-2.236049	4.811122	0.256494
C	-2.597067	2.691646	0.185740
C	-4.194835	0.122777	0.305738
C	-4.840914	-1.113627	0.284898
H	-5.902664	-1.170034	0.500830
C	-4.115949	-2.266335	-0.012291
H	-4.587031	-3.242151	-0.038394
C	-2.753462	-2.141541	-0.276273
H	-2.123289	-2.993526	-0.510128
C	-2.827176	0.176815	0.026877
C	-2.032886	1.428253	0.000880
H	-4.755890	1.018996	0.538586
H	-3.657507	2.790582	0.377708
N	-2.138887	-0.953696	-0.254835
C	0.531108	-0.915277	1.431853
H	-0.269893	-0.436930	1.997508
H	0.437885	-2.000988	1.435231
C	1.942222	-0.195712	-0.732398
C	2.517681	0.010757	-1.984272
C	2.690984	-0.180219	0.448756
C	3.892104	0.268442	-2.058901
H	1.915936	-0.025934	-2.889446
C	4.066497	0.075780	0.353144
C	4.660076	0.299868	-0.891131
H	4.356920	0.438276	-3.026293
H	4.678319	0.099105	1.251399
H	5.726841	0.496596	-0.949807
C	1.949265	-0.405997	1.757700
C	2.633288	-1.500296	2.617022
H	2.047454	-1.703523	3.520598
H	2.741697	-2.433258	2.054284
H	3.628343	-1.170329	2.933712
F	0.430633	-2.479845	-0.906579
C	1.874681	0.905311	2.573139
H	2.880852	1.263376	2.814266
H	1.359913	1.696922	2.020089
H	1.338001	0.740308	3.514629

3_DFA

```
Zero-point correction=                           0.391430 (Hartree/Particle)
 Thermal correction to Energy=                    0.420530
 Thermal correction to Enthalpy=                  0.421474
  Thermal correction to Gibbs Free Energy=         0.326571
 Sum of electronic and zero-point Energies=          -1538.003104
 Sum of electronic and thermal Energies=             -1537.974004
 Sum of electronic and thermal Enthalpies=           -1537.973059
 Sum of electronic and thermal Free Energies=        -1538.067962
 E(RB3LYP) =  -1538.96736395
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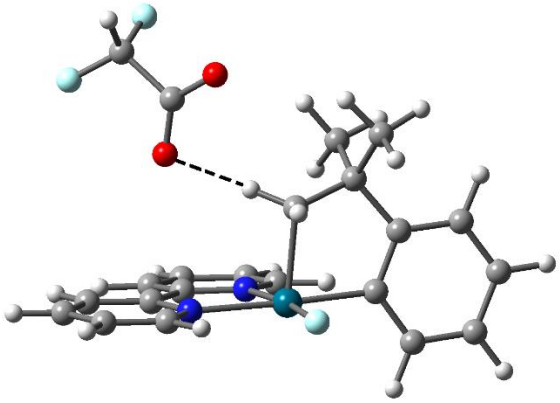
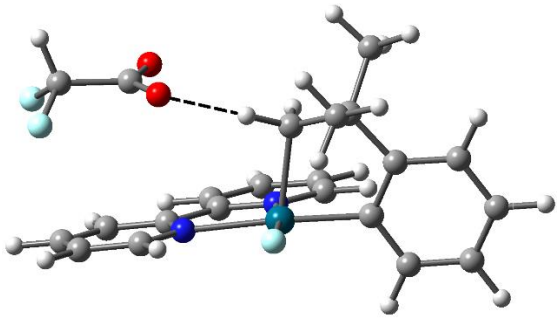


Pd	-1.159316	-1.059079	-0.421843
N	-0.213093	-0.871762	1.404331
C	-0.774580	-0.318281	2.494837
H	-1.766434	0.093906	2.364013
C	-0.124418	-0.277072	3.722547
H	-0.616815	0.180089	4.572884
C	1.150112	-0.829754	3.820389
H	1.691040	-0.815157	4.760621
C	1.724509	-1.414562	2.694956
C	2.827965	-2.649517	0.163057
C	3.210052	-3.246344	-1.037777
H	4.195646	-3.690903	-1.129305
C	2.322529	-3.263744	-2.113071
H	2.587283	-3.719139	-3.060496
C	1.071582	-2.674434	-1.946368
H	0.329056	-2.645141	-2.737296
C	1.557154	-2.078320	0.261529
C	1.028371	-1.432760	1.484957
H	3.518095	-2.627108	0.996836
H	2.707290	-1.862759	2.762800
N	0.710239	-2.105615	-0.790804
C	-0.537772	0.808506	-1.139058
H	0.504979	0.848242	-0.808882
H	-0.644041	0.565225	-2.196854
C	-2.823714	-0.025744	-0.004512
C	-3.983036	-0.668096	0.428140
C	-2.778943	1.356601	-0.228216
C	-5.131633	0.095681	0.670734
H	-4.000870	-1.745523	0.576228
C	-3.940193	2.104173	0.015452
C	-5.105908	1.477944	0.463390
H	-6.040794	-0.390600	1.014466
H	-3.937299	3.179525	-0.145508
H	-5.997944	2.070362	0.647702
C	-1.453989	1.953279	-0.679945
C	-1.625053	2.891278	-1.902853
H	-0.642365	3.228881	-2.247820
H	-2.134487	2.380912	-2.727383
H	-2.210549	3.776161	-1.629789
F	-1.917721	-1.458937	-2.175842
C	-0.795811	2.755400	0.466833

H	-1.450615	3.575758	0.781221
H	-0.602733	2.127474	1.341700
H	0.156120	3.172855	0.124610
C	4.227926	2.588712	-0.372445
H	4.749945	2.986509	-1.248348
C	2.828626	2.013613	-0.719457
O	2.512130	0.925933	-0.178127
O	2.173168	2.747400	-1.498217
F	4.069056	3.625313	0.527268
F	5.040769	1.665142	0.231991

3_DFA'

Zero-point correction= 0.391523 (Hartree/Particle)
Thermal correction to Energy= 0.420328
Thermal correction to Enthalpy= 0.421273
Thermal correction to Gibbs Free Energy= 0.330120
Sum of electronic and zero-point Energies= -1538.004150
Sum of electronic and thermal Energies= -1537.975345
Sum of electronic and thermal Enthalpies= -1537.974401
Sum of electronic and thermal Free Energies= -1538.065553
E(RB3LYP) = -1538.96708789



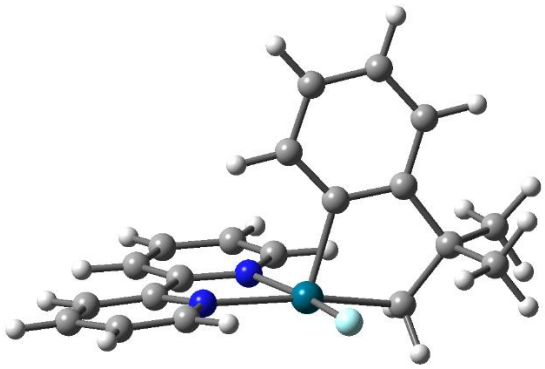
Pd	-0.436940	0.102736	-0.741228
N	1.696242	0.258003	-1.110452
N	0.079181	1.723432	0.441542
C	-2.422842	0.356477	-0.679162
F	-0.734091	-1.336651	-2.069439
C	-0.776725	2.414691	1.215883
C	-0.376031	3.484217	2.008844
C	0.966548	3.854142	1.998920
C	1.854455	3.147526	1.192719
C	1.395773	2.081783	0.413848
H	-1.810544	2.093932	1.184108
H	-1.108137	4.005489	2.614975
H	1.321263	4.679972	2.606609
H	2.901555	3.422033	1.175822
C	2.395880	-0.496787	-1.963881
C	3.737787	-0.246108	-2.241907
C	4.357827	0.825239	-1.601757
C	3.625753	1.610413	-0.712394
C	2.281670	1.302803	-0.482595
H	1.845287	-1.308078	-2.427731
H	4.274958	-0.876769	-2.941493
H	5.401330	1.054616	-1.792421
H	4.100062	2.449196	-0.218264
C	-3.259783	-0.503507	0.054130
C	-4.650443	-0.332230	-0.030518
C	-5.204787	0.677120	-0.820646
C	-4.370763	1.534075	-1.540084
C	-2.982764	1.369135	-1.468705
C	-2.627923	-1.618449	0.875955
H	-5.316189	-0.988508	0.523355
H	-6.284198	0.792715	-0.868775
H	-4.792862	2.323187	-2.157598
H	-2.336575	2.034249	-2.038125

C	-3.427920	-1.911028	2.203464
C	-2.528888	-2.929205	0.061110
C	-1.326399	-1.215479	1.459691
H	-2.923599	-2.667660	2.811035
H	-3.577895	-1.007931	2.801465
H	-4.408115	-2.311581	1.925349
H	-2.058139	-3.721715	0.653686
H	-3.533675	-3.258310	-0.223702
H	-1.936342	-2.748144	-0.838073
H	-0.785552	-1.970685	2.001969
H	-1.175726	-0.205403	1.817901
O	0.791267	-2.134421	0.659253
C	1.702055	-1.695859	1.424325
O	1.627417	-0.881103	2.360211
C	3.123488	-2.266785	1.169451
H	3.475794	-2.889130	1.998806
F	3.192665	-3.004422	0.019610
F	4.000682	-1.217404	1.026952

3_iso

Zero-point correction=	0.355864	(Hartree/Particle)
Thermal correction to Energy=	0.377434	
Thermal correction to Enthalpy=	0.378378	
Thermal correction to Gibbs Free Energy=	0.305473	
Sum of electronic and zero-point Energies=	-1110.949638	
Sum of electronic and thermal Energies=	-1110.928068	
Sum of electronic and thermal Enthalpies=	-1110.927124	
Sum of electronic and thermal Free Energies=	-1111.000028	

E(RM06) = -1111.68764279



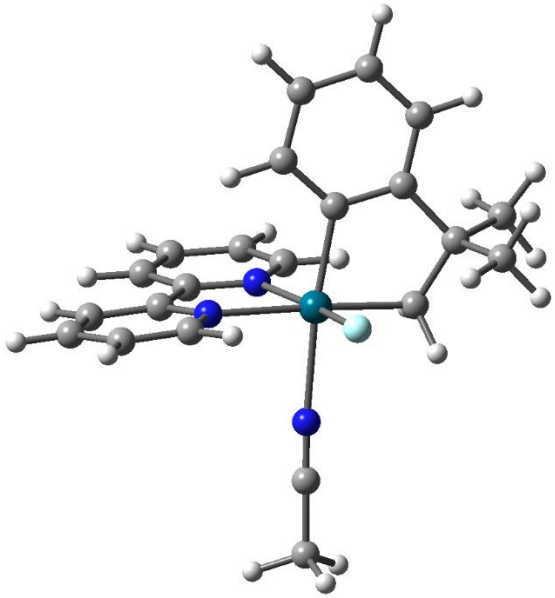
Pd	0.095850	-0.451467	-0.796016
N	-0.837940	1.368154	-0.383212
C	-0.239172	2.569861	-0.444763
H	0.812178	2.578579	-0.694766
C	-0.917986	3.757278	-0.197102
H	-0.386260	4.699208	-0.262008
C	-2.269045	3.695301	0.130250
H	-2.836184	4.598435	0.328441
C	-2.887824	2.450734	0.212199
C	-4.099038	-0.307679	0.366029
C	-4.543127	-1.626902	0.460459
H	-5.583916	-1.829443	0.690526
C	-3.645914	-2.673904	0.255632
H	-3.958096	-3.709948	0.320113
C	-2.321778	-2.360439	-0.043835
H	-1.568924	-3.120401	-0.226673
C	-2.755319	-0.065734	0.068675
C	-2.159278	1.287115	-0.041469
H	-4.796125	0.506326	0.519034
H	-3.934246	2.387346	0.480740
N	-1.900566	-1.093689	-0.127105
C	1.845943	0.220640	-1.665522
H	1.882183	-0.356503	-2.594020

H	1.659831	1.271408	-1.898791
C	1.210450	-0.296628	0.863630
C	0.610770	-0.447258	2.106102
C	2.572724	-0.068668	0.666417
C	1.435267	-0.358121	3.236211
H	-0.452463	-0.628254	2.214958
C	3.367182	0.017382	1.820091
C	2.804453	-0.124640	3.089739
H	0.996233	-0.473208	4.223029
H	4.434656	0.195302	1.719984
H	3.437528	-0.053546	3.969291
C	3.083347	0.016012	-0.761443
C	4.053099	1.202780	-0.961618
H	4.335771	1.283824	-2.017395
H	3.598508	2.150852	-0.653423
H	4.973116	1.062423	-0.383422
F	0.717011	-2.262943	-1.118807
C	3.808483	-1.300890	-1.127868
H	4.663314	-1.467244	-0.463079
H	3.127400	-2.151255	-1.047869
H	4.183419	-1.248612	-2.157334

3_iso_MeCN

Zero-point correction=	0.403541 (Hartree/Particle)
Thermal correction to Energy=	0.430040
Thermal correction to Enthalpy=	0.430984
Thermal correction to Gibbs Free Energy=	0.346089
Sum of electronic and zero-point Energies=	-1243.677312
Sum of electronic and thermal Energies=	-1243.650813
Sum of electronic and thermal Enthalpies=	-1243.649869
Sum of electronic and thermal Free Energies=	-1243.734764

E(RB3LYP) = -1244.51318005



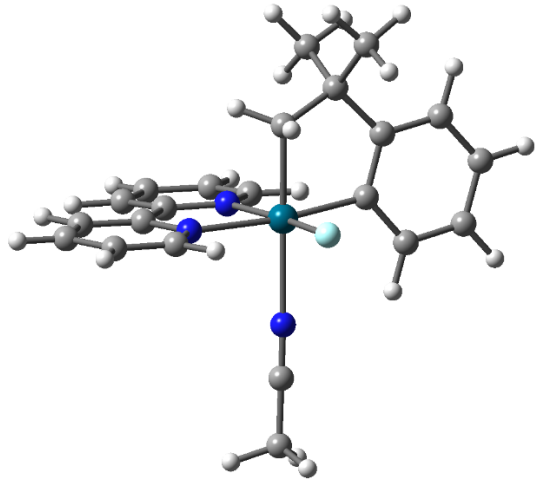
Pd	0.120846	0.575107	-0.283114
N	-0.663969	-0.398162	1.395056
C	-0.091696	-0.415544	2.609798
H	0.856001	0.094033	2.709942
C	-0.669626	-1.055100	3.700536
H	-0.164391	-1.036628	4.659042
C	-1.886036	-1.706846	3.521362
H	-2.370605	-2.218993	4.345718
C	-2.474229	-1.702246	2.259912
C	-3.653563	-1.597040	-0.511655
C	-4.081334	-1.538088	-1.837847
H	-5.035674	-1.973008	-2.115985

C	-3.278841	-0.918088	-2.794554
H	-3.580830	-0.854510	-3.833767
C	-2.065595	-0.368971	-2.383970
H	-1.393076	0.138697	-3.068044
C	-2.420666	-1.031358	-0.172182
C	-1.850891	-1.044599	1.196658
H	-4.278610	-2.072084	0.233771
H	-3.413027	-2.217186	2.102965
N	-1.659464	-0.433303	-1.112553
C	1.717223	1.577879	0.563674
H	1.602295	2.597230	0.188870
H	1.520229	1.565400	1.637963
C	1.487651	-0.877576	-0.497344
C	1.144969	-2.158685	-0.920171
C	2.805474	-0.505350	-0.204598
C	2.159948	-3.114697	-1.055374
H	0.118300	-2.426984	-1.144278
C	3.802079	-1.482526	-0.347059
C	3.483256	-2.775146	-0.767334
H	1.907878	-4.118604	-1.385902
H	4.836640	-1.228988	-0.130352
H	4.269595	-3.517547	-0.870752
C	3.073629	0.939418	0.190725
C	4.022070	1.044821	1.407409
H	4.123916	2.091569	1.716548
H	3.648025	0.469332	2.261507
H	5.023794	0.675557	1.161113
F	0.665665	1.327032	-2.005781
C	3.704461	1.689743	-1.007289
H	4.652316	1.223415	-1.298327
H	3.026890	1.679717	-1.864000
H	3.908931	2.732560	-0.734402
C	-2.639571	4.522487	0.499881
H	-2.567922	5.183865	-0.368185
H	-2.258024	5.043623	1.382478
H	-3.687309	4.255174	0.663856
C	-1.855746	3.318195	0.264729
N	-1.232716	2.361758	0.079450

3_MeCN

Zero-point correction=	0.403252 (Hartree/Particle)
Thermal correction to Energy=	0.429929
Thermal correction to Enthalpy=	0.430873
Thermal correction to Gibbs Free Energy=	0.344984
Sum of electronic and zero-point Energies=	-1243.680869
Sum of electronic and thermal Energies=	-1243.654192
Sum of electronic and thermal Enthalpies=	-1243.653248
Sum of electronic and thermal Free Energies=	-1243.739137

E(RB3LYP) = -1244.51716272

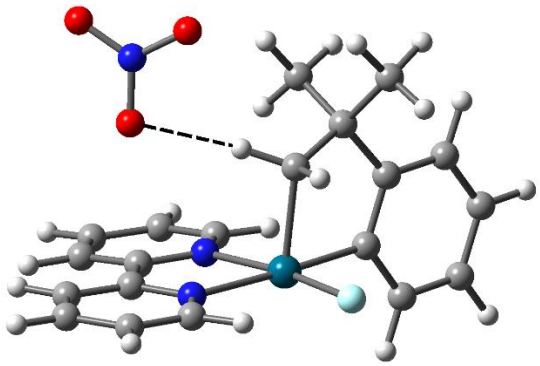


Pd	0.055034	0.333740	-0.522703
N	-0.562536	-0.467826	1.284005
C	0.197985	-0.493033	2.392608
H	1.206196	-0.113659	2.289318
C	-0.279147	-0.979018	3.604803
H	0.370592	-0.981640	4.472085
C	-1.587156	-1.452672	3.664881
H	-1.994842	-1.842304	4.591577
C	-2.376677	-1.414056	2.518555
C	-3.957692	-1.266783	-0.057175
C	-4.612430	-1.095918	-1.276815
H	-5.631141	-1.449806	-1.395908
C	-3.950465	-0.472501	-2.333434
H	-4.429668	-0.322922	-3.294167
C	-2.640690	-0.041578	-2.131716
H	-2.060836	0.446942	-2.908290
C	-2.645319	-0.805303	0.077561
C	-1.852124	-0.911726	1.325483
H	-4.467866	-1.754181	0.764067
H	-3.399914	-1.764381	2.557112
N	-2.018785	-0.207444	-0.960313
C	0.738962	-1.480568	-1.213804
H	0.012990	-2.222159	-0.873473
H	0.636046	-1.301999	-2.284863
C	1.997730	0.603788	-0.067219
C	2.496322	1.822790	0.391318
C	2.829309	-0.501068	-0.292661
C	3.865654	1.937457	0.660197
H	1.839197	2.673390	0.539076
C	4.198335	-0.363427	-0.018860
C	4.712039	0.844884	0.455615
H	4.264619	2.880911	1.023349
H	4.868655	-1.204242	-0.179006
H	5.774917	0.934286	0.662285
C	2.191183	-1.791360	-0.786948
C	2.933181	-2.352811	-2.024875
H	2.414765	-3.238273	-2.410814
H	2.985486	-1.606632	-2.824896
H	3.954649	-2.653099	-1.767125
F	0.447470	1.067362	-2.296517
C	2.206184	-2.859134	0.331607
H	3.233143	-3.081607	0.640254
H	1.654582	-2.525405	1.215936
H	1.749518	-3.790629	-0.023591
C	-1.740010	4.740389	0.738538
H	-1.534780	5.447761	-0.069957
H	-1.289294	5.110344	1.663947
H	-2.821729	4.653398	0.874540
C	-1.179309	3.438130	0.405571
N	-0.728576	2.405086	0.143760

3_NO3

Zero-point correction=	0.371350 (Hartree/Particle)
Thermal correction to Energy=	0.397983
Thermal correction to Enthalpy=	0.398928
Thermal correction to Gibbs Free Energy=	0.311866
Sum of electronic and zero-point Energies=	-1391.382850
Sum of electronic and thermal Energies=	-1391.356217
Sum of electronic and thermal Enthalpies=	-1391.355272
Sum of electronic and thermal Free Energies=	-1391.442334

E(RB3LYP) = -1392.26581873

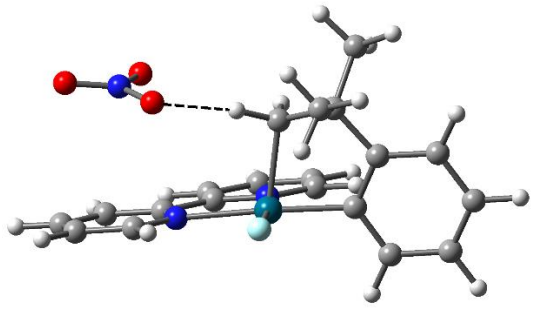


Pd	-0.496417	-1.102874	-0.408819
N	0.334275	-0.552631	1.396817
C	-0.378324	-0.180670	2.476382
H	-1.449639	-0.113187	2.341835
C	0.220566	0.098607	3.699129
H	-0.395214	0.395648	4.539983
C	1.604544	-0.014199	3.804751
H	2.109369	0.196950	4.741453
C	2.339442	-0.412114	2.691304
C	3.791365	-1.273329	0.183138
C	4.351879	-1.737043	-1.006514
H	5.429174	-1.833076	-1.093389
C	3.522169	-2.069693	-2.076612
H	3.924538	-2.432446	-3.015554
C	2.146274	-1.922618	-1.916549
H	1.438207	-2.157943	-2.704640
C	2.403200	-1.151426	0.275545
C	1.689900	-0.683311	1.485936
H	4.433143	-1.006626	1.013122
H	3.414011	-0.518090	2.764693
N	1.614600	-1.479104	-0.771857
C	-0.562300	0.832088	-1.203578
H	0.400825	1.255662	-0.908396
H	-0.593527	0.525622	-2.249579
C	-2.411159	-0.684184	0.012649
C	-3.274041	-1.669602	0.489993
C	-2.843229	0.621356	-0.249930
C	-4.610751	-1.335339	0.740672
H	-2.919406	-2.682571	0.667021
C	-4.185932	0.936514	0.004118
C	-5.060910	-0.034381	0.497285
H	-5.294268	-2.090724	1.119211
H	-4.553129	1.942385	-0.184529
H	-6.098642	0.224449	0.688765
C	-1.807792	1.614290	-0.755039
C	-2.312383	2.386377	-2.002164
H	-1.517288	3.026707	-2.399498
H	-2.634952	1.698226	-2.790685
H	-3.158084	3.030572	-1.737704
F	-1.093287	-1.792787	-2.133822
C	-1.444496	2.634671	0.348306

H	-2.329235	3.212183	0.638063
H	-1.059506	2.140057	1.245034
H	-0.676526	3.322896	-0.019203
O	1.492443	3.541706	-1.327985
N	2.307139	3.140549	-0.451898
O	3.118251	3.940738	0.074065
O	2.307389	1.921676	-0.102370

3_NO3'

Zero-point correction= 0.371094 (Hartree/Particle)
Thermal correction to Energy= 0.397815
Thermal correction to Enthalpy= 0.398760
Thermal correction to Gibbs Free Energy= 0.312253
Sum of electronic and zero-point Energies= -1391.383095
Sum of electronic and thermal Energies= -1391.356374
Sum of electronic and thermal Enthalpies= -1391.355429
Sum of electronic and thermal Free Energies= -1391.441937
E(RB3LYP) = -1392.26482394



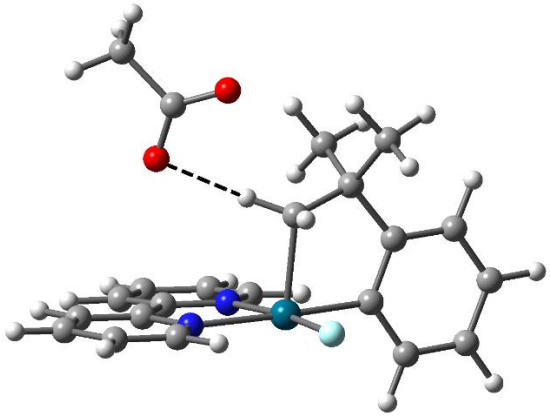
Pd	-0.390388	0.106952	-0.773181
N	1.765356	0.257537	-0.972384
N	0.008437	1.821594	0.314442
C	-2.391461	0.130717	-0.623931
F	-0.539550	-1.444920	-1.940281
C	-0.930817	2.571910	0.917784
C	-0.617384	3.740705	1.601960
C	0.715348	4.139688	1.663287
C	1.686996	3.361996	1.038179
C	1.320587	2.197171	0.361199
H	-1.949626	2.215590	0.838619
H	-1.408403	4.313703	2.071431
H	1.000564	5.044484	2.189404
H	2.725848	3.663418	1.076267
C	2.546519	-0.603022	-1.631792
C	3.929490	-0.439438	-1.688451
C	4.494532	0.655769	-1.038397
C	3.672938	1.551919	-0.354012
C	2.295528	1.324782	-0.333527
H	2.035592	-1.430659	-2.110175
H	4.539058	-1.155937	-2.226695
H	5.567512	0.816034	-1.058514
H	4.108699	2.402862	0.154296
C	-2.970117	-0.783667	0.265546
C	-4.367148	-0.820985	0.362766
C	-5.153038	0.030216	-0.419628
C	-4.555690	0.930419	-1.305813
C	-3.159269	0.985982	-1.411923
C	-2.013342	-1.690809	1.021565
H	-4.846850	-1.516198	1.047301
H	-6.235609	-0.009835	-0.336342
H	-5.168809	1.588206	-1.916095
H	-2.691374	1.687179	-2.099362
C	-2.386912	-1.824493	2.520445
C	-1.979997	-3.095430	0.376694
C	-0.630667	-1.030882	0.976081

H	-1.619092	-2.391672	3.058781
H	-2.492983	-0.843992	2.996640
H	-3.333083	-2.365911	2.629171
H	-1.286933	-3.746737	0.922515
H	-2.975396	-3.552223	0.409390
H	-1.652912	-3.031551	-0.663145
H	0.235458	-1.694884	0.897920
H	-0.496019	-0.260507	1.735360
O	1.955752	-2.974972	0.469697
O	2.614118	-1.420169	1.861947
O	4.069788	-2.786267	0.979274
N	2.883966	-2.392113	1.106020

3_OAc

Zero-point correction=	0.405646 (Hartree/Particle)
Thermal correction to Energy=	0.433559
Thermal correction to Enthalpy=	0.434503
Thermal correction to Gibbs Free Energy=	0.344571
Sum of electronic and zero-point Energies=	-1339.519944
Sum of electronic and thermal Energies=	-1339.492030
Sum of electronic and thermal Enthalpies=	-1339.491086
Sum of electronic and thermal Free Energies=	-1339.581018

E(RB3LYP) = -1340.41614296



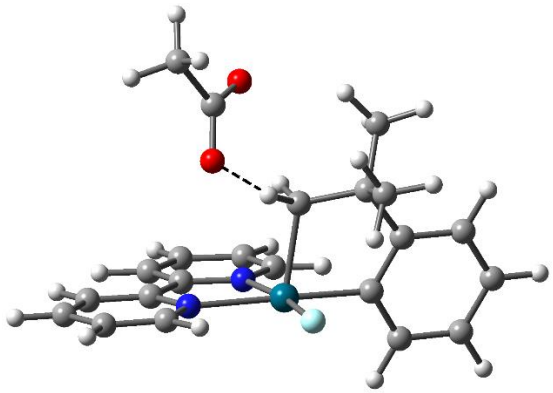
Pd	-0.477251	-0.941052	-0.697541
N	0.250593	-1.047037	1.234484
C	-0.517689	-1.024180	2.338756
H	-1.581308	-0.910120	2.177178
C	0.016830	-1.142278	3.616639
H	-0.642299	-1.117774	4.476549
C	1.395144	-1.288067	3.751152
H	1.851167	-1.379644	4.731240
C	2.188272	-1.324711	2.607338
C	3.767547	-1.400237	0.029618
C	4.389433	-1.481040	-1.215698
H	5.469230	-1.570651	-1.274519
C	3.617133	-1.442795	-2.375972
H	4.067678	-1.502977	-3.360090
C	2.235560	-1.321634	-2.246235
H	1.569935	-1.281135	-3.102486
C	2.376825	-1.281027	0.086380
C	1.601369	-1.205536	1.346192
H	4.365084	-1.422482	0.932208
H	3.259044	-1.452723	2.698586
N	1.643975	-1.247629	-1.048704
C	-0.452411	1.170077	-0.768754
H	0.489481	1.391040	-0.256317
H	-0.377856	1.243522	-1.854066
C	-2.401171	-0.626702	-0.256356
C	-3.304424	-1.686218	-0.168701
C	-2.803743	0.705388	-0.096435

C	-4.648688	-1.414080	0.112804
H	-2.972761	-2.711772	-0.316053
C	-4.155366	0.959288	0.180530
C	-5.069016	-0.092056	0.286391
H	-5.361158	-2.231228	0.190305
H	-4.498884	1.982237	0.313898
H	-6.112487	0.121522	0.501726
C	-1.736676	1.787959	-0.191617
C	-2.161058	2.924572	-1.157513
H	-1.339659	3.639678	-1.258395
H	-2.411984	2.528062	-2.147753
H	-3.037502	3.453840	-0.767030
F	-0.985741	-1.003354	-2.585316
C	-1.458961	2.398109	1.202027
H	-2.368791	2.856202	1.606029
H	-1.120733	1.638788	1.914438
H	-0.682017	3.163123	1.114673
C	3.271135	4.177516	0.568846
H	4.258927	3.704787	0.565173
H	3.290102	5.077302	-0.053643
H	3.061512	4.485700	1.601962
C	2.180287	3.186823	0.100331
O	2.321197	1.983818	0.468721
O	1.229621	3.666297	-0.578430

3_OAc'

Zero-point correction=	0.405806 (Hartree/Particle)
Thermal correction to Energy=	0.433620
Thermal correction to Enthalpy=	0.434564
Thermal correction to Gibbs Free Energy=	0.345285
Sum of electronic and zero-point Energies=	-1339.519556
Sum of electronic and thermal Energies=	-1339.491742
Sum of electronic and thermal Enthalpies=	-1339.490798
Sum of electronic and thermal Free Energies=	-1339.580077

E(RB3LYP) = -1339.92425944



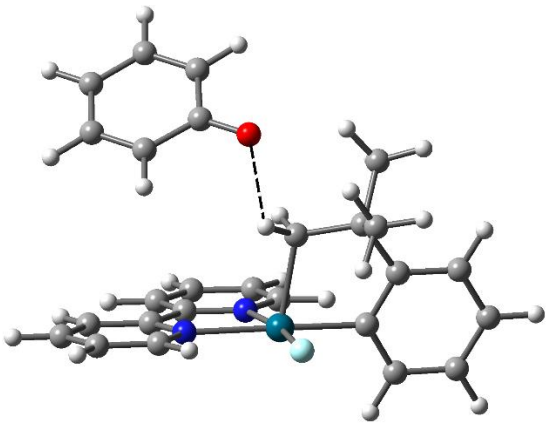
Pd	0.352142	-0.511711	-0.860794
N	-1.792374	-0.755474	-1.105596
N	-0.104908	-1.784108	0.712075
C	2.331341	-0.403887	-0.554697
F	0.560372	0.590824	-2.459790
C	0.795819	-2.274046	1.582041
C	0.438619	-3.138437	2.611064
C	-0.898777	-3.502611	2.741645
C	-1.831567	-2.995538	1.839994
C	-1.420898	-2.132048	0.822653
H	1.820345	-1.957590	1.435550
H	1.200359	-3.507696	3.287743
H	-1.217858	-4.172347	3.533145
H	-2.873778	-3.273351	1.930378
C	-2.535256	-0.195393	-2.065869
C	-3.909219	-0.411534	-2.150082

C	-4.509137	-1.234032	-1.198248
C	-3.728641	-1.817316	-0.199795
C	-2.355478	-1.561385	-0.176702
H	-1.997763	0.433282	-2.768032
H	-4.485299	0.055894	-2.940440
H	-5.576883	-1.424644	-1.227852
H	-4.191892	-2.457473	0.540200
C	2.809826	0.771679	0.041279
C	4.189322	0.894028	0.254736
C	5.059663	-0.130474	-0.128497
C	4.564442	-1.291482	-0.727728
C	3.186954	-1.433843	-0.943852
C	1.782156	1.843698	0.372451
H	4.589151	1.791578	0.719997
H	6.127247	-0.021586	0.042372
H	5.242551	-2.085800	-1.028550
H	2.799204	-2.338552	-1.406990
C	2.021335	2.487320	1.763652
C	1.798678	2.948275	-0.709610
C	0.412202	1.163896	0.439477
H	1.171359	3.124931	2.023588
H	2.130653	1.722532	2.540845
H	2.931338	3.098001	1.749796
H	1.057164	3.719384	-0.472188
H	2.786031	3.421907	-0.753903
H	1.563135	2.527059	-1.689325
H	-0.454048	1.733360	0.080828
H	0.219942	0.669492	1.390365
O	-2.076041	2.994383	-0.086784
C	-2.131984	3.384635	1.115948
C	-3.186125	4.469282	1.442274
H	-3.996771	4.478307	0.707323
H	-3.599455	4.325420	2.446227
H	-2.705660	5.456847	1.426845
O	-1.398913	3.009953	2.072851

3_OPh

Zero-point correction=	0.447972 (Hartree/Particle)
Thermal correction to Energy=	0.476921
Thermal correction to Enthalpy=	0.477865
Thermal correction to Gibbs Free Energy=	0.384996
Sum of electronic and zero-point Energies=	-1417.845952
Sum of electronic and thermal Energies=	-1417.817003
Sum of electronic and thermal Enthalpies=	-1417.816058
Sum of electronic and thermal Free Energies=	-1417.908927

E(RB3LYP) = -1418.80200933



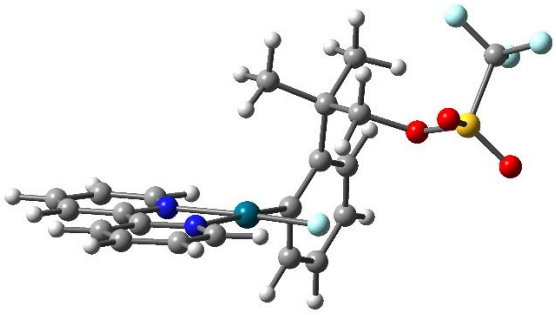
Pd	-1.020982	-0.831885	-0.673484
N	-0.282751	-1.450590	1.165179
C	-0.936863	-1.317656	2.332535
H	-1.904903	-0.836048	2.284706

C	-0.408762	-1.773569	3.535387
H	-0.974321	-1.644097	4.450805
C	0.840756	-2.387489	3.524755
H	1.286726	-2.756727	4.442149
C	1.519292	-2.524150	2.315974
C	2.873341	-2.716623	-0.383820
C	3.400666	-2.758579	-1.674607
H	4.380702	-3.192936	-1.842483
C	2.662784	-2.241407	-2.738348
H	3.042038	-2.258711	-3.753693
C	1.410708	-1.692743	-2.469192
H	0.776843	-1.272661	-3.243418
C	1.610556	-2.152435	-0.184900
C	0.945532	-2.046773	1.135925
H	3.445023	-3.116669	0.443974
H	2.490694	-3.001119	2.295288
N	0.910780	-1.653082	-1.229297
C	-0.492056	1.205952	-0.304219
H	-0.044859	1.110753	0.683770
H	0.254454	1.371015	-1.077123
C	-2.797622	-0.153797	-0.050435
C	-3.851906	-1.022392	0.232241
C	-2.940930	1.237934	0.039326
C	-5.087887	-0.490211	0.622630
H	-3.723659	-2.099849	0.153352
C	-4.183332	1.751998	0.436062
C	-5.248526	0.894127	0.723927
H	-5.917531	-1.156919	0.843053
H	-4.324231	2.826881	0.518467
H	-6.205925	1.308344	1.028397
C	-1.741231	2.093771	-0.344417
C	-1.934995	2.680204	-1.761872
H	-1.068566	3.296091	-2.025805
H	-2.037891	1.878015	-2.496977
H	-2.832333	3.308569	-1.796447
F	-1.560395	-0.450202	-2.515968
C	-1.503509	3.250928	0.660163
H	-2.313149	3.987050	0.595815
H	-1.461433	2.878165	1.690327
H	-0.554048	3.738590	0.420810
O	1.460071	3.091162	-0.735270
C	2.554620	2.741800	-0.143281
C	3.427106	1.728221	-0.668330
C	2.992884	3.343350	1.085634
C	4.611180	1.366001	-0.029771
H	3.141736	1.251440	-1.605447
C	4.180681	2.973567	1.709602
H	2.364629	4.120436	1.518835
C	5.008823	1.980083	1.166198
H	5.239168	0.593281	-0.472719
H	4.470066	3.466353	2.637621
H	5.934862	1.695019	1.658702

4a

Zero-point correction=	0.386071 (Hartree/Particle)
Thermal correction to Energy=	0.416498
Thermal correction to Enthalpy=	0.417442
Thermal correction to Gibbs Free Energy=	0.321043
Sum of electronic and zero-point Energies=	-2072.515122
Sum of electronic and thermal Energies=	-2072.484695
Sum of electronic and thermal Enthalpies=	-2072.483751
Sum of electronic and thermal Free Energies=	-2072.580150

E(RB3LYP) = -2073.56621639

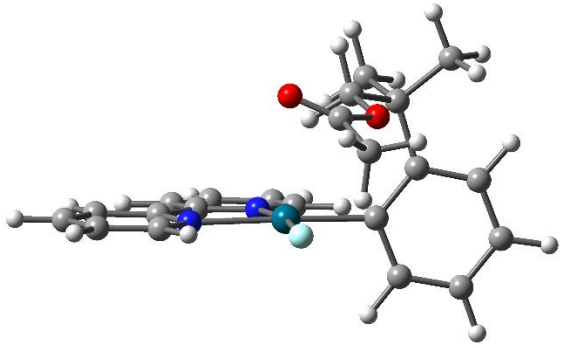


Pd	0.500394	1.072151	0.172049
N	2.464533	0.225091	0.201495
N	1.476000	2.347265	1.482662
C	-1.279472	2.035483	0.159520
F	-0.192014	-0.263121	-1.132054
C	0.919680	3.401550	2.106008
C	1.631543	4.221157	2.976335
C	2.974806	3.940079	3.211404
C	3.556474	2.849672	2.569636
C	2.792241	2.060078	1.706955
H	-0.124115	3.582344	1.885106
H	1.132567	5.058012	3.451877
H	3.564648	4.555913	3.882251
H	4.599875	2.617384	2.741693
C	2.850557	-0.856219	-0.486761
C	4.152307	-1.347519	-0.420322
C	5.070737	-0.682320	0.391016
C	4.665456	0.443356	1.106951
C	3.342454	0.882238	0.995012
H	2.079215	-1.316375	-1.095971
H	4.431529	-2.226127	-0.991046
H	6.094792	-1.032798	0.469278
H	5.374994	0.963338	1.738510
C	-2.485007	1.677744	0.823478
C	-3.598499	2.525077	0.668241
C	-3.563469	3.678527	-0.117563
C	-2.390167	4.015926	-0.785772
C	-1.268148	3.194492	-0.639262
C	-2.633931	0.393066	1.679724
H	-4.529960	2.284750	1.167466
H	-4.452114	4.298431	-0.205751
H	-2.340132	4.903912	-1.411913
H	-0.353367	3.471947	-1.159926
C	-1.527756	0.297580	2.759627
C	-3.987428	0.302523	2.419196
H	-1.675392	-0.593162	3.381816
H	-0.528464	0.247339	2.317789
H	-1.568899	1.177919	3.410332
H	-4.010503	-0.612448	3.021678
H	-4.122737	1.150799	3.097991
H	-4.840888	0.267382	1.737076
O	-3.597673	-0.833066	-0.198803
S	-4.036341	-2.182579	-0.926348
C	-5.400312	-2.735900	0.222967
F	-5.949942	-3.847038	-0.261880
F	-4.889554	-2.979880	1.433273
F	-6.322572	-1.779764	0.314491
O	-2.991674	-3.199471	-0.869618
O	-4.673690	-1.808490	-2.180495
C	-2.479687	-0.851122	0.790723
H	-1.563055	-0.841567	0.202163
H	-2.565630	-1.764846	1.382759

4b

Zero-point correction=	0.409695 (Hartree/Particle)
Thermal correction to Energy=	0.436356
Thermal correction to Enthalpy=	0.437300
Thermal correction to Gibbs Free Energy=	0.352035
Sum of electronic and zero-point Energies=	-1339.574100
Sum of electronic and thermal Energies=	-1339.547439
Sum of electronic and thermal Enthalpies=	-1339.546494
Sum of electronic and thermal Free Energies=	-1339.631759

E(RB3LYP) = -1340.46099185

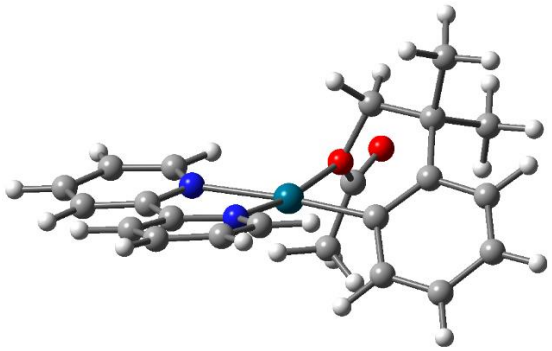


Pd	-0.364427	0.114817	-0.626657
N	-2.229046	1.141788	-0.393567
N	-1.581190	-1.399876	0.091591
C	1.326845	-0.968248	-0.862290
F	0.542753	1.689907	-1.446040
C	-1.212966	-2.683908	0.254456
C	-2.090096	-3.666646	0.701995
C	-3.403716	-3.307793	0.993527
C	-3.794070	-1.982880	0.817575
C	-2.870501	-1.039196	0.360685
H	-0.182039	-2.910802	0.015638
H	-1.739018	-4.686090	0.815814
H	-4.117913	-4.044095	1.347121
H	-4.814787	-1.689625	1.028888
C	-2.437576	2.435875	-0.664004
C	-3.666390	3.049729	-0.431963
C	-4.700530	2.281334	0.101815
C	-4.480213	0.933283	0.381554
C	-3.222765	0.380127	0.120292
H	-1.582777	2.964726	-1.073358
H	-3.801593	4.100424	-0.663093
H	-5.671628	2.723048	0.300660
H	-5.278790	0.331930	0.797937
C	2.411433	-1.141999	0.041393
C	3.505557	-1.915811	-0.395170
C	3.561622	-2.503868	-1.659983
C	2.501727	-2.326625	-2.544490
C	1.405247	-1.561598	-2.136757
C	2.434949	-0.584100	1.490436
H	4.351299	-2.069173	0.265155
H	4.432014	-3.090289	-1.943929
H	2.522668	-2.768788	-3.538132
H	0.585199	-1.418872	-2.838400
C	1.469575	-1.407868	2.378137
C	3.836954	-0.650885	2.138641
C	1.961757	0.873947	1.566412
H	1.493224	-1.049681	3.415145
H	0.438961	-1.341755	2.019116
H	1.764788	-2.462807	2.378782
H	3.801721	-0.174461	3.125286
H	4.169504	-1.682251	2.292018
H	4.589892	-0.128933	1.540147

H	2.021044	1.234291	2.599330
H	0.929462	0.980173	1.222881
O	2.806647	1.697298	0.735292
C	2.442473	2.985754	0.613577
O	1.550465	3.498930	1.265519
C	3.260777	3.693216	-0.437257
H	2.828827	3.453360	-1.415718
H	3.213936	4.772539	-0.282681
H	4.299061	3.352161	-0.432172

4b-F

Zero-point correction= 0.408066 (Hartree/Particle)
Thermal correction to Energy= 0.433122
Thermal correction to Enthalpy= 0.434067
Thermal correction to Gibbs Free Energy= 0.352675
Sum of electronic and zero-point Energies= -1239.556270
Sum of electronic and thermal Energies= -1239.531214
Sum of electronic and thermal Enthalpies= -1239.530269
Sum of electronic and thermal Free Energies= -1239.611661
E(RB3LYP) = -1240.39358232



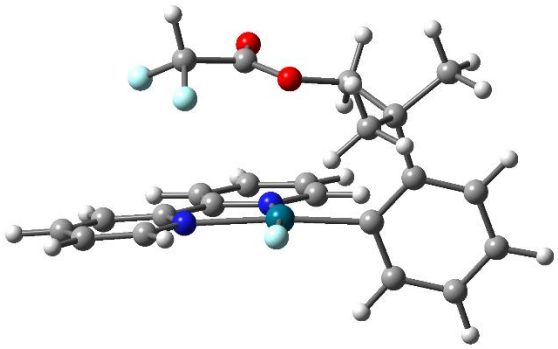
Pd	-0.197078	0.060316	-0.111057
N	-2.041205	1.185744	0.111617
N	-1.596433	-1.461040	0.099113
C	1.431247	-1.070773	-0.430478
C	-1.310823	-2.765255	0.261723
C	-2.294327	-3.733763	0.436918
C	-3.627831	-3.337570	0.446400
C	-3.927607	-1.984989	0.306115
C	-2.898783	-1.054253	0.145118
H	-0.263476	-3.031238	0.239620
H	-2.004660	-4.770638	0.563091
H	-4.425103	-4.061888	0.575372
H	-4.958304	-1.656500	0.340792
C	-2.172359	2.519108	0.148052
C	-3.413191	3.150491	0.133871
C	-4.557316	2.357537	0.071876
C	-4.425041	0.970516	0.051622
C	-3.147207	0.403902	0.085067
H	-1.252435	3.091254	0.196714
H	-3.470634	4.232457	0.166473
H	-5.543750	2.808529	0.046042
H	-5.309201	0.347186	0.009927
C	2.678007	-0.852783	0.200351
C	3.709506	-1.776126	-0.074069
C	3.562397	-2.819499	-0.984501
C	2.358992	-2.966039	-1.672992
C	1.306051	-2.096418	-1.385366
C	3.047281	0.329552	1.132188
H	4.665075	-1.670612	0.430772
H	4.390382	-3.499664	-1.164428
H	2.232003	-3.749717	-2.415328
H	0.365159	-2.225031	-1.914302
C	3.333362	-0.182228	2.566429

C	4.317764	1.034159	0.584964
C	1.941390	1.389274	1.297580
H	3.576581	0.651714	3.236188
H	2.466353	-0.711782	2.977086
H	4.184165	-0.869513	2.569629
H	4.575941	1.892622	1.214677
H	5.177193	0.359512	0.579108
H	4.171216	1.394182	-0.437998
H	2.359655	2.333609	1.645389
H	1.156348	1.067889	1.983441
O	1.224238	1.660343	0.041447
C	1.618629	2.726415	-0.762174
O	2.413505	3.536619	-0.361250
C	0.958318	2.694474	-2.110108
H	1.327258	1.828664	-2.671282
H	-0.126721	2.590610	-2.023130
H	1.203284	3.610810	-2.647442

4c

Zero-point correction=	0.395141 (Hartree/Particle)
Thermal correction to Energy=	0.423064
Thermal correction to Enthalpy=	0.424008
Thermal correction to Gibbs Free Energy=	0.334904
Sum of electronic and zero-point Energies=	-1538.040118
Sum of electronic and thermal Energies=	-1538.012195
Sum of electronic and thermal Enthalpies=	-1538.011251
Sum of electronic and thermal Free Energies=	-1538.100355

E(RB3LYP) = -1538.99223040



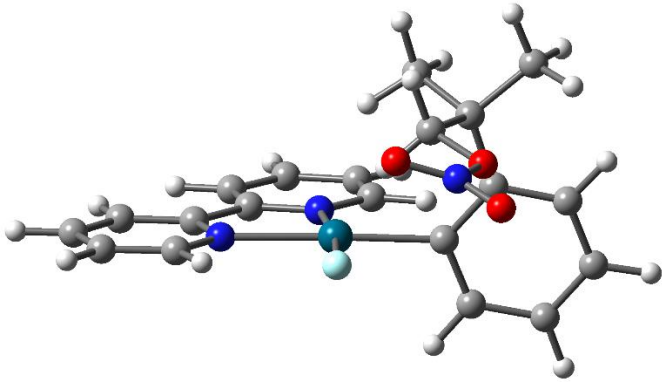
Pd	-0.117958	0.305230	-0.917516
N	2.003102	0.149306	-1.132945
N	0.538151	1.643285	0.519547
C	-2.097976	0.694056	-0.738062
F	-0.468501	-0.973225	-2.403341
C	-0.252535	2.369683	1.330312
C	0.251586	3.252488	2.280107
C	1.632198	3.391204	2.397113
C	2.456353	2.645095	1.558593
C	1.893795	1.774528	0.621862
H	-1.317564	2.231453	1.196104
H	-0.433295	3.811518	2.907711
H	2.065537	4.067830	3.126223
H	3.532009	2.741398	1.636137
C	2.632198	-0.632068	-2.018198
C	4.020383	-0.649831	-2.130178
C	4.763940	0.175550	-1.287311
C	4.104900	0.987983	-0.365686
C	2.708352	0.955483	-0.306461
H	1.982222	-1.240821	-2.637979
H	4.499028	-1.294055	-2.859334
H	5.847574	0.191689	-1.344256
H	4.677259	1.633554	0.288861
C	-3.118123	-0.062333	-0.097924

C	-4.429482	0.451090	-0.121808
C	-4.760339	1.648761	-0.759160
C	-3.765443	2.379186	-1.401854
C	-2.453505	1.896221	-1.380586
C	-2.861869	-1.440138	0.570151
H	-5.229351	-0.091859	0.368281
H	-5.789519	1.999026	-0.748267
H	-3.997515	3.312374	-1.910293
H	-1.680792	2.480738	-1.877135
C	-4.075492	-1.937964	1.392881
C	-2.608438	-2.485547	-0.545470
C	-1.677620	-1.358042	1.581665
H	-3.825503	-2.900236	1.853568
H	-4.347885	-1.241889	2.195181
H	-4.956285	-2.099636	0.764888
H	-2.381729	-3.469557	-0.118673
H	-3.521745	-2.580410	-1.145160
H	-1.795380	-2.180726	-1.206521
H	-1.955127	-1.788088	2.547993
H	-1.351727	-0.332043	1.748551
O	-0.528906	-2.119743	1.110527
C	0.608368	-1.948024	1.766523
O	0.787123	-1.255325	2.746274
C	1.745387	-2.788605	1.161721
H	1.896453	-3.723148	1.710893
F	1.505021	-3.087160	-0.145953
F	2.891822	-2.053831	1.226955

4d

Zero-point correction=	0.373837 (Hartree/Particle)
Thermal correction to Energy=	0.399675
Thermal correction to Enthalpy=	0.400619
Thermal correction to Gibbs Free Energy=	0.315904
Sum of electronic and zero-point Energies=	-1391.410870
Sum of electronic and thermal Energies=	-1391.385032
Sum of electronic and thermal Enthalpies=	-1391.384088
Sum of electronic and thermal Free Energies=	-1391.468803

E(RB3LYP) = -1392.28106607



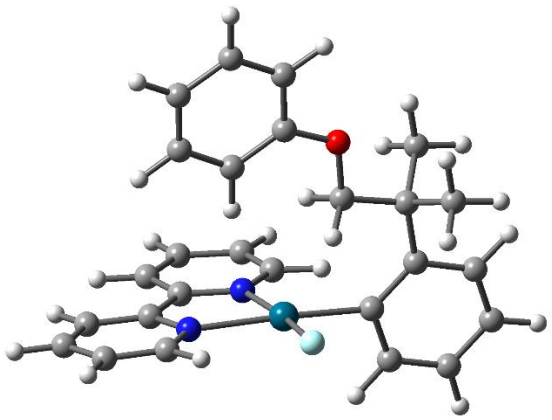
Pd	-0.295108	0.123314	-0.425749
N	-2.182445	1.108223	-0.210592
N	-1.541719	-1.471397	0.017188
C	1.402265	-0.944055	-0.694434
F	0.678607	1.798494	-0.880602
C	-1.157541	-2.756458	0.119330
C	-2.047293	-3.785735	0.410654
C	-3.390443	-3.473649	0.604566
C	-3.794267	-2.144955	0.501815
C	-2.855899	-1.152577	0.207619
H	-0.105044	-2.946396	-0.044718
H	-1.683070	-4.804524	0.480322
H	-4.115797	-4.247727	0.832304
H	-4.834993	-1.885691	0.650384

C	-2.385006	2.425458	-0.335197
C	-3.644069	2.997643	-0.168057
C	-4.716759	2.160468	0.136976
C	-4.502123	0.788871	0.266535
C	-3.211618	0.281230	0.087463
H	-1.500960	3.008302	-0.573575
H	-3.773177	4.068868	-0.274870
H	-5.713452	2.567007	0.274797
H	-5.331355	0.134299	0.504316
C	2.492114	-1.110068	0.203447
C	3.568226	-1.918079	-0.210849
C	3.607449	-2.537067	-1.461765
C	2.550741	-2.355003	-2.349144
C	1.466271	-1.564588	-1.956320
C	2.554247	-0.429697	1.596429
H	4.410972	-2.072350	0.453089
H	4.463248	-3.149735	-1.733909
H	2.562205	-2.818233	-3.333229
H	0.642624	-1.432696	-2.655788
C	1.299070	-0.761258	2.439689
C	3.779092	-0.862570	2.433569
C	2.589111	1.103492	1.440451
H	1.367507	-0.295739	3.430282
H	0.380493	-0.413568	1.958629
H	1.222148	-1.845365	2.578530
H	3.747859	-0.358938	3.406355
H	3.767862	-1.941800	2.618536
H	4.729119	-0.603138	1.959059
H	2.603618	1.593504	2.418262
H	1.771433	1.481816	0.826128
O	3.839889	1.428941	0.751128
O	3.253394	3.572075	1.033234
O	5.094018	3.028300	-0.018665
N	4.065455	2.785478	0.580891

4e

Zero-point correction=	0.452161	(Hartree/Particle)
Thermal correction to Energy=	0.480299	
Thermal correction to Enthalpy=	0.481243	
Thermal correction to Gibbs Free Energy=	0.391413	
Sum of electronic and zero-point Energies=	-1417.908799	
Sum of electronic and thermal Energies=	-1417.880662	
Sum of electronic and thermal Enthalpies=	-1417.879718	
Sum of electronic and thermal Free Energies=	-1417.969547	

E(RB3LYP) = -1418.85791762

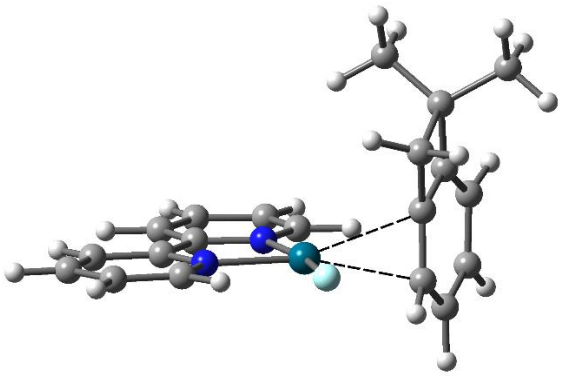


Pd	-0.346362	-0.883220	-0.814556
N	-0.174116	-2.008646	0.915235
C	-1.130248	-2.151679	1.850681
H	-2.065910	-1.647432	1.647191
C	-0.942800	-2.901196	3.007922

H	-1.747742	-2.981590	3.729795
C	0.283517	-3.530464	3.205829
H	0.469492	-4.123180	4.095415
C	1.277159	-3.386792	2.240708
C	3.320525	-2.988172	0.043205
C	4.193483	-2.718074	-1.009840
H	5.185888	-3.157139	-1.015451
C	3.779478	-1.884539	-2.048398
H	4.430900	-1.652697	-2.883617
C	2.494658	-1.348889	-1.994820
H	2.097317	-0.695486	-2.764970
C	2.045334	-2.414361	0.035544
C	1.032951	-2.620540	1.098311
H	3.635764	-3.637140	0.850811
H	2.237418	-3.866969	2.381090
N	1.659078	-1.609135	-0.981832
C	-0.636052	2.012378	0.151104
H	-0.265868	1.212948	0.804068
H	-0.330123	1.796597	-0.876786
C	-2.296102	-0.391267	-0.604398
C	-3.140941	-1.461393	-0.975587
C	-2.891544	0.827378	-0.189848
C	-4.532551	-1.372041	-0.941010
H	-2.693355	-2.400118	-1.297009
C	-4.303180	0.887419	-0.154275
C	-5.119341	-0.178886	-0.520006
H	-5.144451	-2.221193	-1.237003
H	-4.784189	1.805791	0.170769
H	-6.200586	-0.074675	-0.475598
C	-2.165760	2.129132	0.249826
C	-2.607843	3.299775	-0.665085
H	-2.088249	4.219617	-0.381320
H	-2.370806	3.081370	-1.713312
H	-3.683556	3.484873	-0.595876
F	-0.259726	0.147212	-2.520538
C	-2.530250	2.448575	1.721604
H	-3.606199	2.602247	1.846177
H	-2.230481	1.625860	2.382480
H	-2.017521	3.356564	2.052813
O	-0.053789	3.258419	0.570924
C	1.303437	3.378450	0.539079
C	2.184332	2.357734	0.150839
C	1.816528	4.626296	0.932874
C	3.563475	2.598447	0.159652
H	1.811281	1.387767	-0.157313
C	3.190334	4.848596	0.936100
H	1.119613	5.404551	1.230139
C	4.076409	3.835408	0.548789
H	4.237039	1.801319	-0.145283
H	3.571902	5.819277	1.242221
H	5.148155	4.011405	0.550962

5

Zero-point correction=	0.356240	(Hartree/Particle)
Thermal correction to Energy=	0.378241	
Thermal correction to Enthalpy=	0.379185	
Thermal correction to Gibbs Free Energy=	0.304025	
Sum of electronic and zero-point Energies=	-1110.965414	
Sum of electronic and thermal Energies=	-1110.943413	
Sum of electronic and thermal Enthalpies=	-1110.942469	
Sum of electronic and thermal Free Energies=	-1111.017629	
E(RB3LYP) = -1111.70033245		

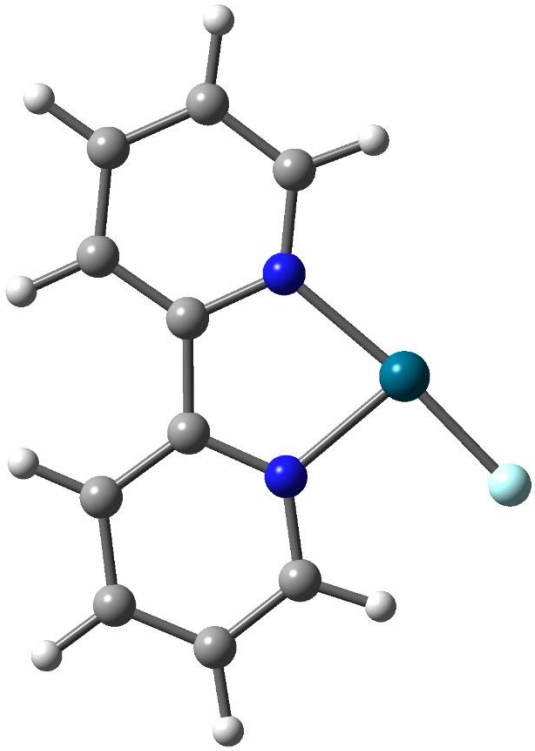


Pd	-0.278634	-0.680543	-0.532043
N	-0.756251	1.285153	-0.145805
C	0.068380	2.336679	-0.248152
H	1.082296	2.124584	-0.556917
C	-0.345314	3.638036	0.023965
H	0.362703	4.452694	-0.074492
C	-1.663030	3.854991	0.415079
H	-2.021491	4.854995	0.634384
C	-2.524031	2.764458	0.521728
C	-4.224191	0.233502	0.691548
C	-4.886873	-0.992809	0.732265
H	-5.932422	-1.031978	1.018758
C	-4.197299	-2.159065	0.404610
H	-4.679270	-3.129556	0.426263
C	-2.856962	-2.064809	0.041117
H	-2.246503	-2.918123	-0.229856
C	-2.879758	0.269900	0.321106
C	-2.052867	1.483736	0.237164
H	-4.750017	1.145249	0.946013
H	-3.553446	2.910982	0.823995
N	-2.231933	-0.879680	0.004613
C	2.464983	-1.737120	0.885916
H	1.575303	-2.065536	1.429241
H	3.089491	-2.610318	0.668236
C	2.243455	-0.837404	-0.329524
C	1.832993	-0.818959	-1.677878
C	3.020011	0.206754	0.217479
C	2.217504	0.325813	-2.434896
H	1.426404	-1.690758	-2.179467
C	3.442639	1.282553	-0.536011
C	2.997423	1.335344	-1.883161
H	1.930909	0.381153	-3.480807
H	4.108124	2.049777	-0.149619
H	3.297456	2.173021	-2.506225
C	3.258054	-0.525083	1.542116
C	4.728643	-0.817840	1.855464
H	4.807685	-1.514927	2.698133
H	5.241376	-1.261618	0.994782
H	5.258009	0.102433	2.129128
F	-0.160131	-2.608122	-0.830216
C	2.539288	0.092266	2.748388
H	3.010207	1.038555	3.039180
H	1.484477	0.291233	2.526224
H	2.586062	-0.587765	3.607383

6

Zero-point correction=	0.163938 (Hartree/Particle)
Thermal correction to Energy=	0.175217
Thermal correction to Enthalpy=	0.176162
Thermal correction to Gibbs Free Energy=	0.125662
Sum of electronic and zero-point Energies=	-722.885026
Sum of electronic and thermal Energies=	-722.873746
Sum of electronic and thermal Enthalpies=	-722.872802

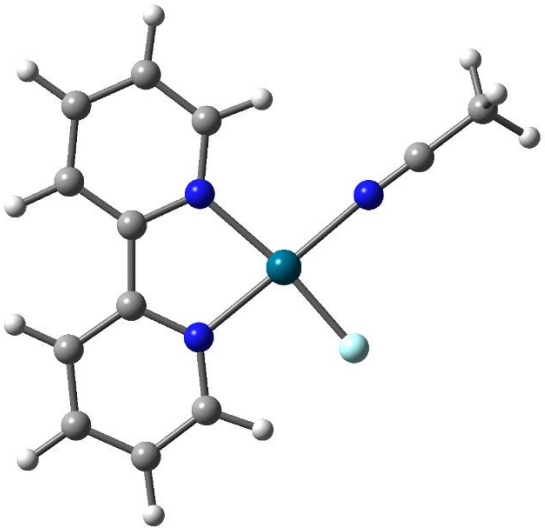
Sum of electronic and thermal Free Energies= -722.923302
E(RB3LYP) = -723.289167209



Pd	0.380286	-1.449870	-0.000069
N	-1.346416	-0.394675	-0.000487
C	-2.572362	-0.936159	-0.000354
H	-2.618396	-2.019875	-0.000648
C	-3.718418	-0.144842	0.000119
H	-4.694604	-0.615207	0.000164
C	-3.575158	1.241373	0.000453
H	-4.447432	1.886020	0.000919
C	-2.297136	1.800395	0.000296
C	0.650511	2.727500	-0.000013
C	2.018924	2.998457	0.000053
H	2.365465	4.026238	0.000217
C	2.930741	1.944223	-0.000036
H	4.000509	2.117152	-0.000038
C	2.449236	0.638672	-0.000161
H	3.086147	-0.237280	-0.000140
C	0.215392	1.403618	-0.000184
C	-1.186532	0.959039	-0.000193
H	-0.067270	3.538530	0.000082
H	-2.170904	2.876122	0.000596
N	1.130127	0.394407	-0.000236
F	2.119573	-2.296606	0.000801

7

Zero-point correction= 0.211670 (Hartree/Particle)
Thermal correction to Energy= 0.227853
Thermal correction to Enthalpy= 0.228797
Thermal correction to Gibbs Free Energy= 0.165565
Sum of electronic and zero-point Energies= -855.635209
Sum of electronic and thermal Energies= -855.619025
Sum of electronic and thermal Enthalpies= -855.618081
Sum of electronic and thermal Free Energies= -855.681314
E(RB3LYP) = -856.135460203



Pd	0.655896	-0.708320	0.000551
N	0.099193	1.254824	0.000404
C	0.930874	2.308928	0.000805
H	1.989978	2.086448	0.001407
C	0.459281	3.618386	0.000579
H	1.165902	4.440085	0.000907
C	-0.916393	3.836299	-0.000024
H	-1.318056	4.843823	-0.000199
C	-1.779490	2.741684	-0.000351
C	-3.455434	0.177336	-0.001088
C	-4.097635	-1.061018	-0.001167
H	-5.181453	-1.106774	-0.001741
C	-3.338919	-2.230297	-0.000527
H	-3.804014	-3.209155	-0.000561
C	-1.950789	-2.128361	0.000135
H	-1.284948	-2.983433	0.000577
C	-2.062189	0.222256	-0.000361
C	-1.251271	1.451733	-0.000137
H	-4.035164	1.091928	-0.001627
H	-2.851840	2.892580	-0.000735
N	-1.344012	-0.932928	0.000212
F	0.928676	-2.640591	0.000895
C	5.277143	-0.262230	-0.002135
H	5.639209	-0.166668	1.025547
H	5.708269	-1.159051	-0.456235
H	5.581238	0.617107	-0.577244
C	3.826913	-0.366550	-0.000738
N	2.674682	-0.443021	0.000324

DFA$^-$

Zero-point correction=	0.034516 (Hartree/Particle)
Thermal correction to Energy=	0.039900
Thermal correction to Enthalpy=	0.040844
Thermal correction to Gibbs Free Energy=	0.004438
Sum of electronic and zero-point Energies=	-427.032607
Sum of electronic and thermal Energies=	-427.027223
Sum of electronic and thermal Enthalpies=	-427.026279
Sum of electronic and thermal Free Energies=	-427.062685

E(RB3LYP) = -427.262203620

C	-0.630987	-0.150704	0.362401
H	-0.792916	-0.521674	1.380604
C	0.873633	0.069818	0.038201
O	1.205098	1.197767	-0.390605
O	1.568583	-0.952553	0.261103
F	-1.154368	-1.092873	-0.506297
F	-1.384789	0.986793	0.200941

F^-

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 Zero-point correction=                           0.000000 (Hartree/Particle)
 Thermal correction to Energy=                    0.001416
 Thermal correction to Enthalpy=                  0.002360
 Thermal correction to Gibbs Free Energy=        -0.014159
 Sum of electronic and zero-point Energies=            -99.891852
 Sum of electronic and thermal Energies=               -99.890436
 Sum of electronic and thermal Enthalpies=             -99.889492
 Sum of electronic and thermal Free Energies=          -99.906011
 E(RB3LYP) =  -100.022609716
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I

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 Zero-point correction=                           0.406938 (Hartree/Particle)
 Thermal correction to Energy=                    0.434092
 Thermal correction to Enthalpy=                  0.435036
 Thermal correction to Gibbs Free Energy=         0.348633
 Sum of electronic and zero-point Energies=         -1339.550184
 Sum of electronic and thermal Energies=            -1339.523030
 Sum of electronic and thermal Enthalpies=          -1339.522086
 Sum of electronic and thermal Free Energies=       -1339.608490
 E(RB3LYP) =  -1340.43599523
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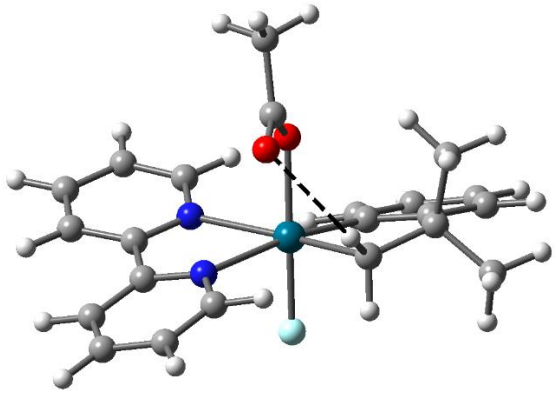


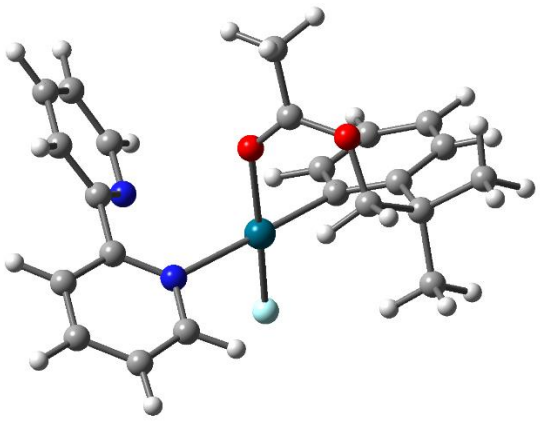
Pd	0.176010	-0.083051	-0.267056
N	-1.512610	1.497448	0.025910
N	-1.797836	-1.168127	-0.420217
C	1.915743	0.912438	-0.449698
F	0.022686	0.020987	-2.236022
C	-1.869087	-2.474953	-0.701410
C	-3.041067	-3.090714	-1.133125
C	-4.181078	-2.304963	-1.289315
C	-4.112035	-0.946520	-0.991898
C	-2.902163	-0.399443	-0.545967
H	-0.955095	-3.042587	-0.572884
H	-3.048291	-4.153900	-1.346242
H	-5.112554	-2.739144	-1.638359
H	-4.987391	-0.321895	-1.119693
C	-1.342542	2.751910	0.461685
C	-2.401708	3.624342	0.702441
C	-3.697665	3.159638	0.492312
C	-3.883238	1.846375	0.067998
C	-2.767715	1.029602	-0.157778
H	-0.319258	3.065581	0.632665
H	-2.206254	4.632365	1.051051
H	-4.555107	3.800358	0.671743
H	-4.886534	1.459720	-0.059615
C	3.091317	0.152236	-0.372770
C	4.322433	0.805649	-0.523325
C	4.374984	2.179831	-0.768643
C	3.193097	2.913377	-0.887755
C	1.954558	2.275377	-0.738686

C	2.930221	-1.338280	-0.131577
H	5.247223	0.237062	-0.459934
H	5.336680	2.672646	-0.883692
H	3.225693	3.977914	-1.105306
H	1.043030	2.846745	-0.875312
C	3.829418	-2.178530	-1.069564
C	3.284165	-1.680977	1.333476
C	1.461089	-1.678198	-0.456639
H	3.624020	-3.247210	-0.934255
H	3.652399	-1.925021	-2.120674
H	4.891190	-2.016708	-0.851873
H	3.119748	-2.747675	1.529886
H	4.339081	-1.459219	1.532120
H	2.676895	-1.099774	2.030969
H	1.031939	-2.435409	0.201186
H	1.318916	-1.928960	-1.510218
O	-0.402676	-2.088529	2.182564
C	-0.009663	-0.978585	2.540515
O	0.379393	-0.002841	1.755218
C	0.074710	-0.590459	4.014463
H	1.073960	-0.214114	4.255456
H	-0.638085	0.213903	4.227591
H	-0.156118	-1.452434	4.643619

I_P

Zero-point correction=	0.408257 (Hartree/Particle)
Thermal correction to Energy=	0.435486
Thermal correction to Enthalpy=	0.436430
Thermal correction to Gibbs Free Energy=	0.348358
Sum of electronic and zero-point Energies=	-1339.549821
Sum of electronic and thermal Energies=	-1339.522592
Sum of electronic and thermal Enthalpies=	-1339.521648
Sum of electronic and thermal Free Energies=	-1339.609720

E(RB3LYP) = -1340.43116247



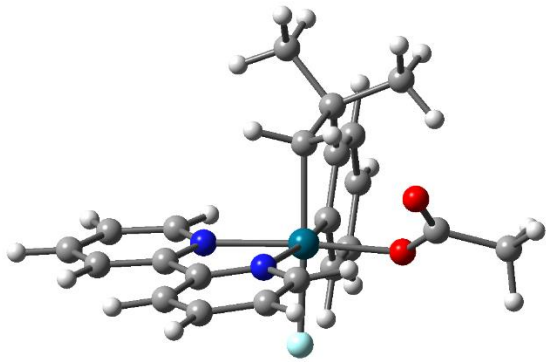
Pd	0.062990	-0.294421	-0.643150
N	-2.464772	1.498300	-0.902907
N	-1.927604	-1.305129	-0.443202
C	1.827917	0.628684	-0.800454
F	0.086087	-0.753518	-2.575469
C	-1.912129	-2.640709	-0.599397
C	-3.035864	-3.443210	-0.422961
C	-4.235807	-2.830632	-0.066468
C	-4.261598	-1.447080	0.089542
C	-3.091228	-0.703054	-0.108606
H	-0.953924	-3.071842	-0.870596
H	-2.963018	-4.516158	-0.563000
H	-5.138836	-3.415768	0.077289
H	-5.185292	-0.936508	0.338455
C	-2.498729	2.832979	-0.806978
C	-3.167235	3.519313	0.209203

C	-3.839568	2.773384	1.176005
C	-3.818169	1.382092	1.086086
C	-3.116535	0.782046	0.031171
H	-1.967429	3.379735	-1.583140
H	-3.158495	4.604114	0.235401
H	-4.368872	3.262334	1.988363
H	-4.319623	0.771879	1.830000
C	3.062814	0.208081	-0.245760
C	4.167074	1.072730	-0.378090
C	4.082002	2.301067	-1.035498
C	2.868426	2.702232	-1.589280
C	1.756889	1.864007	-1.465731
C	3.266592	-1.176505	0.413835
H	5.126608	0.787382	0.037835
H	4.962770	2.933655	-1.111381
H	2.780855	3.654104	-2.108198
H	0.808204	2.182645	-1.891987
C	3.310236	-2.257903	-0.695575
C	4.570081	-1.266299	1.237959
C	2.101700	-1.574988	1.339312
H	3.418540	-3.261502	-0.264572
H	2.397952	-2.232795	-1.299792
H	4.165013	-2.079866	-1.356511
H	4.631279	-2.247981	1.721048
H	5.458309	-1.163405	0.607980
H	4.611935	-0.500594	2.019823
H	2.359315	-2.479127	1.895478
H	1.181943	-1.755084	0.780529
O	1.847847	-0.584762	2.376930
C	0.793355	0.210923	2.333516
O	-0.009805	0.306614	1.396881
C	0.626880	1.011098	3.594503
H	1.569417	1.505838	3.846488
H	-0.164469	1.749692	3.467884
H	0.375169	0.337727	4.420986

II

Zero-point correction=	0.407274 (Hartree/Particle)
Thermal correction to Energy=	0.434240
Thermal correction to Enthalpy=	0.435184
Thermal correction to Gibbs Free Energy=	0.349873
Sum of electronic and zero-point Energies=	-1339.548874
Sum of electronic and thermal Energies=	-1339.521908
Sum of electronic and thermal Enthalpies=	-1339.520964
Sum of electronic and thermal Free Energies=	-1339.606275

E(RB3LYP) = -1340.43895590



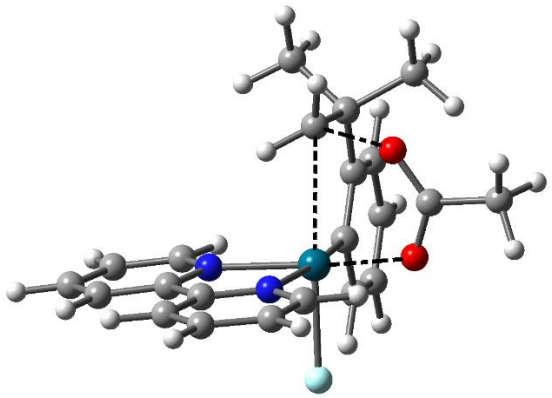
Pd	-0.016035	0.244458	-0.353001
N	-2.149026	0.772756	0.070923
N	-0.890343	-1.618986	-0.038619
C	1.826395	-0.476375	-0.655133
F	-0.630116	0.075362	-2.346873
C	-0.206340	-2.775409	-0.073832

C	-0.826557	-4.011187	0.070165
C	-2.205813	-4.046298	0.256006
C	-2.912801	-2.848444	0.287099
C	-2.239503	-1.632008	0.133179
H	0.861880	-2.695627	-0.221886
H	-0.229951	-4.915502	0.036905
H	-2.728152	-4.989543	0.376712
H	-3.984773	-2.863278	0.433298
C	-2.706011	1.990838	0.083781
C	-4.084490	2.179517	0.175157
C	-4.906106	1.058633	0.257132
C	-4.326917	-0.208429	0.248771
C	-2.936111	-0.324222	0.152947
H	-2.014790	2.823501	0.047064
H	-4.492254	3.184234	0.182316
H	-5.984047	1.161832	0.328300
H	-4.957847	-1.085779	0.309345
C	2.664964	-0.528325	0.463022
C	3.953577	-1.058013	0.287274
C	4.375531	-1.508794	-0.965735
C	3.518248	-1.433629	-2.067899
C	2.228807	-0.909608	-1.916625
C	2.137743	0.031254	1.778258
H	4.634465	-1.114575	1.133524
H	5.376202	-1.916522	-1.082313
H	3.848718	-1.779930	-3.044078
H	1.541842	-0.837834	-2.753416
C	2.345562	-0.967752	2.940113
C	2.885312	1.344827	2.108403
C	0.617367	0.307247	1.621304
H	1.917564	-0.566302	3.866499
H	1.860379	-1.927339	2.727963
H	3.409760	-1.157248	3.121317
H	2.515398	1.769927	3.049386
H	3.960981	1.164436	2.217295
H	2.743619	2.086504	1.317120
H	0.324109	1.300496	1.960319
H	0.012465	-0.453464	2.121729
O	-0.025150	3.354097	0.793912
C	0.662808	3.167646	-0.212910
O	0.850997	2.029711	-0.827788
C	1.411350	4.311964	-0.891582
H	1.218302	5.249720	-0.366891
H	2.487374	4.108083	-0.893474
H	1.094130	4.403436	-1.935647

II_TS

Zero-point correction=	0.405358 (Hartree/Particle)
Thermal correction to Energy=	0.432387
Thermal correction to Enthalpy=	0.433332
Thermal correction to Gibbs Free Energy=	0.347777
Sum of electronic and zero-point Energies=	-1339.483045
Sum of electronic and thermal Energies=	-1339.456016
Sum of electronic and thermal Enthalpies=	-1339.455072
Sum of electronic and thermal Free Energies=	-1339.540626

E(RB3LYP) = -1340.37362184

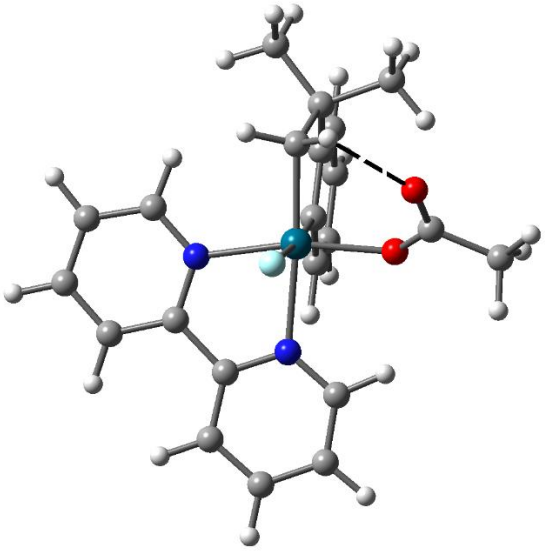


Pd	-0.123235	0.233372	-0.511244
N	-2.182702	0.811996	-0.123557
N	-0.989677	-1.586511	0.157250
C	1.718066	-0.496797	-0.753783
F	-0.830291	-0.273835	-2.636151
C	-0.352339	-2.766819	0.222298
C	-0.999569	-3.952307	0.557720
C	-2.365131	-3.910693	0.827973
C	-3.031939	-2.691139	0.748133
C	-2.326765	-1.532143	0.407213
H	0.706694	-2.745644	-0.003142
H	-0.437339	-4.878371	0.601766
H	-2.908747	-4.811666	1.092941
H	-4.095910	-2.648683	0.943611
C	-2.701109	2.031341	-0.311192
C	-4.044912	2.316724	-0.082648
C	-4.873323	1.284998	0.355783
C	-4.338085	0.011505	0.536231
C	-2.979043	-0.205544	0.280720
H	-2.008731	2.789547	-0.660760
H	-4.422793	3.319844	-0.245829
H	-5.925616	1.463697	0.551757
H	-4.977275	-0.796169	0.869962
C	2.707869	-0.469149	0.246873
C	3.950301	-1.071938	-0.033229
C	4.211330	-1.677720	-1.260895
C	3.223341	-1.692045	-2.249208
C	1.983671	-1.103324	-1.991788
C	2.510377	0.217760	1.602304
H	4.733170	-1.065223	0.721541
H	5.181341	-2.133285	-1.442793
H	3.416165	-2.157842	-3.213206
H	1.188708	-1.096826	-2.733276
C	2.775061	-0.799881	2.770660
C	3.494046	1.399661	1.757497
C	1.097773	0.626927	1.905379
H	2.614123	-0.331844	3.747650
H	2.131454	-1.680764	2.687977
H	3.817302	-1.131848	2.728941
H	3.338702	1.913069	2.713091
H	4.526782	1.039840	1.729404
H	3.366142	2.126868	0.952539
H	0.988742	1.256514	2.778351
H	0.327551	-0.129725	1.840872
O	0.785095	2.586855	1.201404
C	0.789712	2.921082	-0.016475
O	0.565002	2.143143	-0.997474
C	1.110708	4.368316	-0.349912
H	0.839850	5.025849	0.478206
H	2.190461	4.455505	-0.519225
H	0.596282	4.675320	-1.263042

III

Zero-point correction=	0.406938	(Hartree/Particle)
Thermal correction to Energy=	0.434092	
Thermal correction to Enthalpy=	0.435036	
Thermal correction to Gibbs Free Energy=	0.348633	
Sum of electronic and zero-point Energies=	-1339.550184	
Sum of electronic and thermal Energies=	-1339.523030	
Sum of electronic and thermal Enthalpies=	-1339.522086	
Sum of electronic and thermal Free Energies=	-1339.608490	

E(RB3LYP) = -1340.43514890



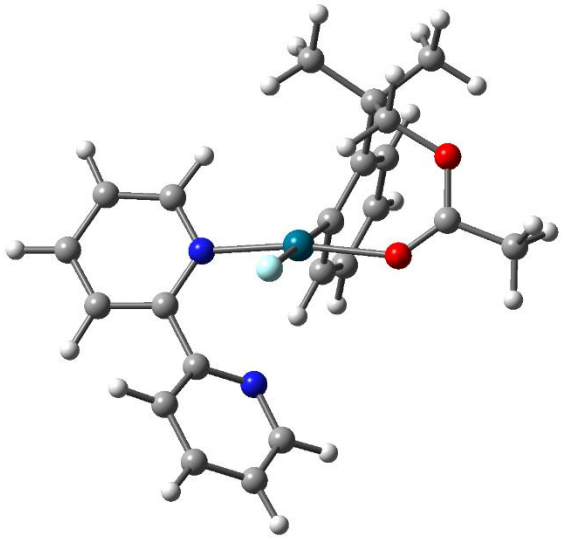
Pd	-0.098549	0.323473	-0.478132
N	1.799268	1.032632	0.445163
N	1.179630	-1.327984	-0.719120
C	-0.937019	-0.565817	1.126450
F	0.715766	1.078096	-2.222097
C	0.810767	-2.515358	-1.222106
C	1.704515	-3.564868	-1.405329
C	3.035338	-3.373430	-1.046536
C	3.418325	-2.146241	-0.513916
C	2.476948	-1.124854	-0.353547
H	-0.232067	-2.629935	-1.481103
H	1.350513	-4.503055	-1.816711
H	3.766072	-4.165783	-1.169893
H	4.446592	-1.988361	-0.215489
C	2.005403	2.242582	0.970949
C	3.277165	2.682426	1.334630
C	4.356987	1.826825	1.122164
C	4.137170	0.568580	0.563046
C	2.830817	0.191757	0.232159
H	1.118650	2.857061	1.090461
H	3.410615	3.668943	1.764372
H	5.364796	2.132717	1.383902
H	4.975395	-0.093209	0.385463
C	-2.194202	-1.150059	0.907220
C	-2.821322	-1.811168	1.974322
C	-2.210519	-1.885606	3.227802
C	-0.961739	-1.294284	3.432182
C	-0.320224	-0.632430	2.377582
C	-2.832837	-0.976565	-0.465825
H	-3.797488	-2.267874	1.827955
H	-2.709854	-2.402378	4.043137
H	-0.482471	-1.346137	4.406689
H	0.651551	-0.176960	2.543107
C	-3.365973	-2.316020	-1.026776
C	-4.014730	0.016319	-0.351610

C	-1.765599	-0.412649	-1.436894
H	-3.761319	-2.173116	-2.039471
H	-2.577183	-3.075742	-1.071938
H	-4.178391	-2.712556	-0.407416
H	-4.485148	0.167438	-1.330786
H	-4.776777	-0.366080	0.337114
H	-3.675071	0.987324	0.019292
H	-2.108542	0.452157	-2.002396
H	-1.359556	-1.164712	-2.117885
O	-2.093370	2.696044	-1.829876
C	-1.710629	2.876240	-0.676907
O	-1.036701	2.039110	0.079266
C	-1.998569	4.181155	0.065687
H	-2.650762	4.816726	-0.536796
H	-2.470502	3.977523	1.032023
H	-1.059852	4.710418	0.263435

III_P

Zero-point correction=	0.408803	(Hartree/Particle)
Thermal correction to Energy=	0.435801	
Thermal correction to Enthalpy=	0.436745	
Thermal correction to Gibbs Free Energy=	0.350027	
Sum of electronic and zero-point Energies=	-1339.548232	
Sum of electronic and thermal Energies=	-1339.521235	
Sum of electronic and thermal Enthalpies=	-1339.520291	
Sum of electronic and thermal Free Energies=	-1339.607009	

E(RB3LYP) = -1340.43284659



Pd	-0.085930	-0.337662	-0.491597
N	-2.551926	-0.843440	1.148222
N	-1.352795	1.311615	-0.421254
C	1.153374	0.449896	0.888124
F	-1.283846	-1.188849	-1.924813
C	-0.875750	2.532654	-0.735615
C	-1.685509	3.654241	-0.871524
C	-3.055151	3.514672	-0.662700
C	-3.549704	2.261815	-0.313691
C	-2.684467	1.166898	-0.195754
H	0.193267	2.599605	-0.878507
H	-1.239961	4.607568	-1.132904
H	-3.724171	4.364534	-0.752497
H	-4.604409	2.124915	-0.104592
C	-3.052301	-2.015156	1.557877
C	-4.243541	-2.558361	1.072660
C	-4.954374	-1.836763	0.114645
C	-4.448070	-0.612131	-0.317298

C	-3.236115	-0.155596	0.218604
H	-2.474683	-2.541595	2.314915
H	-4.599625	-3.515252	1.440323
H	-5.884499	-2.220069	-0.294120
H	-4.968040	-0.034435	-1.074130
C	2.528322	0.775891	0.723210
C	3.228996	1.245036	1.854308
C	2.632625	1.391129	3.106074
C	1.288205	1.062949	3.264926
C	0.569410	0.599137	2.161309
C	3.295787	0.729716	-0.626075
H	4.276633	1.508353	1.764210
H	3.220581	1.756013	3.944537
H	0.801053	1.163100	4.232527
H	-0.477950	0.336136	2.284789
C	3.011742	2.023355	-1.430689
C	4.827890	0.614718	-0.436306
C	2.862920	-0.425601	-1.541284
H	3.619566	2.058748	-2.343234
H	1.960376	2.086451	-1.727461
H	3.252832	2.904047	-0.827195
H	5.306883	0.463668	-1.410319
H	5.255856	1.526224	-0.009821
H	5.096443	-0.227252	0.209139
H	3.456648	-0.413930	-2.458086
H	1.805290	-0.367602	-1.809353
O	3.149561	-1.726326	-0.955895
C	2.188281	-2.489491	-0.465825
O	0.998220	-2.173880	-0.363448
C	2.685737	-3.844577	-0.048515
H	3.554874	-3.734730	0.606664
H	1.894520	-4.391928	0.463633
H	3.006834	-4.402641	-0.934528

MeCN

Zero-point correction=	0.045851	(Hartree/Particle)
Thermal correction to Energy=	0.049728	
Thermal correction to Enthalpy=	0.050672	
Thermal correction to Gibbs Free Energy=	0.022615	
Sum of electronic and zero-point Energies=	-132.708607	
Sum of electronic and thermal Energies=	-132.704730	
Sum of electronic and thermal Enthalpies=	-132.703785	
Sum of electronic and thermal Free Energies=	-132.731843	

E(RB3LYP) = -132.804605207

C	0.000000	0.000000	-1.226191
H	0.000000	1.008806	-1.582857
H	0.873651	-0.504403	-1.582857
H	-0.873651	-0.504403	-1.582857
C	0.000000	0.000000	0.313809
N	0.000000	0.000000	1.460409

NO_3^-

Zero-point correction=	0.014208	(Hartree/Particle)
Thermal correction to Energy=	0.017364	
Thermal correction to Enthalpy=	0.018308	
Thermal correction to Gibbs Free Energy=	-0.011293	
Sum of electronic and zero-point Energies=	-280.413786	
Sum of electronic and thermal Energies=	-280.410630	
Sum of electronic and thermal Enthalpies=	-280.409686	
Sum of electronic and thermal Free Energies=	-280.439286	

E(RB3LYP) = -280.560776389

N	0.000050	0.000078	0.000102
O	0.252702	1.236409	-0.000030
O	0.944596	-0.837060	-0.000030

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O    -1.197342   -0.399418   -0.000030
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OAc^-

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 Zero-point correction=                           0.048771 (Hartree/Particle)
 Thermal correction to Energy=                    0.053141
 Thermal correction to Enthalpy=                  0.054085
 Thermal correction to Gibbs Free Energy=         0.021546
 Sum of electronic and zero-point Energies=           -228.546618
 Sum of electronic and thermal Energies=              -228.542249
 Sum of electronic and thermal Enthalpies=            -228.541304
 Sum of electronic and thermal Free Energies=         -228.573843
 E(RB3LYP) =  -228.711699301

C    -1.353618   -0.000084   -0.003908
H    -1.758629   -0.895048   -0.489224
H    -1.758644    0.894736   -0.489505
H    -1.713296    0.000086    1.034936
C     0.200463   -0.000006   -0.012527
O     0.759435   -1.130955    0.002746
O     0.759253    1.131051    0.002554
```

OPh^-

```
 Zero-point correction=                           0.091354 (Hartree/Particle)
 Thermal correction to Energy=                    0.096542
 Thermal correction to Enthalpy=                  0.097486
 Thermal correction to Gibbs Free Energy=         0.062549
 Sum of electronic and zero-point Energies=           -306.876198
 Sum of electronic and thermal Energies=              -306.871011
 Sum of electronic and thermal Enthalpies=            -306.870066
 Sum of electronic and thermal Free Energies=         -306.905003
 E(RB3LYP) =  -307.096970193

C    -1.828459    0.000003    0.000014
C    -1.103494   -1.202175    0.000033
C     0.287963   -1.210825   -0.000033
C     1.076236    0.000015   -0.000444
C     0.287972    1.210826   -0.000045
C    -1.103501    1.202164    0.000049
H    -2.915725   -0.000008    0.000087
H    -1.640523   -2.151846    0.000173
H     0.829159   -2.157447    0.000163
H     0.829123    2.157475    0.000142
H    -1.640511    2.151845    0.000177
O     2.354772   -0.000008    0.000227
```

OTf^-

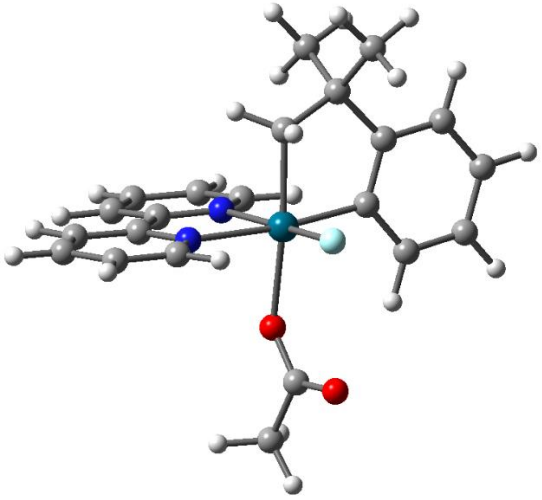
```
 Zero-point correction=                           0.027187 (Hartree/Particle)
 Thermal correction to Energy=                    0.034345
 Thermal correction to Enthalpy=                  0.035290
 Thermal correction to Gibbs Free Energy=        -0.005262
 Sum of electronic and zero-point Energies=           -961.546685
 Sum of electronic and thermal Energies=              -961.539527
 Sum of electronic and thermal Enthalpies=            -961.538583
 Sum of electronic and thermal Free Energies=         -961.579134
 E(RB3LYP) =  -961.865471100

C    -0.949099   -0.000085    0.000228
S     0.905890    0.000053    0.000011
F    -1.430736   -1.240522    0.197267
F    -1.430709    0.449238   -1.172649
F    -1.430882    0.790986    0.975763
O     1.242442    1.425562   -0.226745
O     1.243862   -0.516572    1.347464
O     1.242609   -0.908698   -1.121341
```

TS_1b

Zero-point correction=	0.406655 (Hartree/Particle)
Thermal correction to Energy=	0.433036
Thermal correction to Enthalpy=	0.433980
Thermal correction to Gibbs Free Energy=	0.349468
Sum of electronic and zero-point Energies=	-1339.546873
Sum of electronic and thermal Energies=	-1339.520492
Sum of electronic and thermal Enthalpies=	-1339.519548
Sum of electronic and thermal Free Energies=	-1339.604060

E(RB3LYP) = -1340.43522839



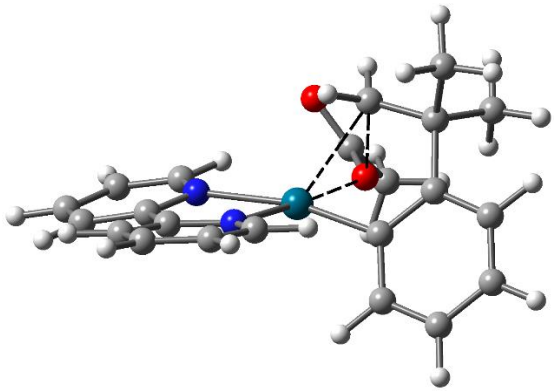
Pd	0.065077	0.271860	-0.472837
N	-0.556830	-0.757255	1.209578
C	0.199413	-0.924292	2.306279
H	1.214862	-0.555635	2.244784
C	-0.289302	-1.532834	3.457467
H	0.359555	-1.648889	4.317819
C	-1.609332	-1.975977	3.467558
H	-2.028243	-2.455475	4.345960
C	-2.395762	-1.787862	2.334235
C	-3.968190	-1.318720	-0.206762
C	-4.617885	-0.999793	-1.398825
H	-5.644802	-1.314062	-1.554162
C	-3.939697	-0.280529	-2.381927
H	-4.414276	-0.014955	-3.319770
C	-2.620040	0.093837	-2.134949
H	-2.026257	0.650415	-2.853240
C	-2.645148	-0.904839	-0.023648
C	-1.855578	-1.168553	1.203905
H	-4.490723	-1.881950	0.556249
H	-3.428602	-2.111535	2.335937
N	-2.003999	-0.212769	-0.989954
C	0.759854	-1.454586	-1.368527
H	0.056497	-2.248046	-1.102166
H	0.646925	-1.186932	-2.420136
C	1.996124	0.496154	0.019758
C	2.482190	1.657011	0.621883
C	2.841613	-0.566583	-0.327746
C	3.848012	1.751548	0.914780
H	1.810680	2.476864	0.852011
C	4.206983	-0.451966	-0.023290
C	4.706297	0.695963	0.595130
H	4.236717	2.650392	1.386878
H	4.886619	-1.263050	-0.274513
H	5.766588	0.768372	0.822337
C	2.224060	-1.791170	-0.992221
C	2.984968	-2.165224	-2.286905
H	2.494342	-3.008845	-2.786903

H	3.012009	-1.320822	-2.984338
H	4.017056	-2.462569	-2.069585
F	0.476802	1.157702	-2.174342
C	2.264893	-2.998569	-0.026045
H	3.296240	-3.238644	0.255460
H	1.703375	-2.798481	0.892178
H	1.829544	-3.884435	-0.504387
C	-1.627905	3.997109	1.564086
H	-2.653944	3.619905	1.644668
H	-1.148256	3.835702	2.535939
H	-1.654900	5.067705	1.346267
C	-0.872736	3.235824	0.464436
O	-0.440352	3.851227	-0.520671
O	-0.764268	1.968090	0.701034

TS_1b-F

Zero-point correction=	0.404041 (Hartree/Particle)
Thermal correction to Energy=	0.429337
Thermal correction to Enthalpy=	0.430281
Thermal correction to Gibbs Free Energy=	0.348206
Sum of electronic and zero-point Energies=	-1239.505298
Sum of electronic and thermal Energies=	-1239.480002
Sum of electronic and thermal Enthalpies=	-1239.479058
Sum of electronic and thermal Free Energies=	-1239.561132

E(RB3LYP) = -1240.34033464



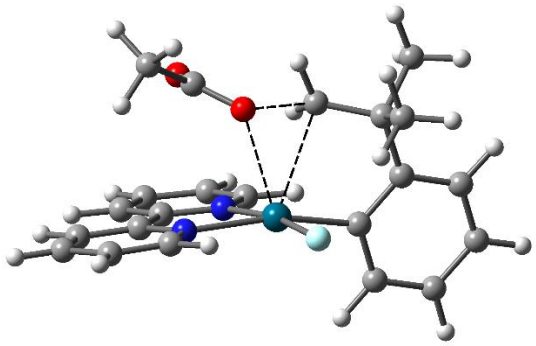
Pd	0.100094	-0.153516	-0.201992
N	2.180532	-0.905641	-0.011831
N	1.179953	1.598068	0.146426
C	-1.595999	0.814130	-0.674202
C	0.622071	2.800833	0.380849
C	1.376230	3.931432	0.674717
C	2.761904	3.813235	0.732475
C	3.340840	2.567940	0.505775
C	2.533610	1.464749	0.215237
H	-0.456082	2.847183	0.322270
H	0.874774	4.875276	0.855218
H	3.386056	4.670630	0.961039
H	4.414810	2.453861	0.573243
C	2.617796	-2.166786	-0.148192
C	3.967503	-2.485610	-0.281951
C	4.898997	-1.451364	-0.281301
C	4.452535	-0.140535	-0.129742
C	3.083966	0.106618	0.012638
H	1.859841	-2.938569	-0.127194
H	4.267359	-3.522207	-0.386648
H	5.958647	-1.655319	-0.394691
H	5.165603	0.674066	-0.134513
C	-2.786925	0.636244	0.051609
C	-3.923754	1.364673	-0.334549
C	-3.892195	2.224547	-1.432017
C	-2.714666	2.369205	-2.168237

C	-1.567425	1.667729	-1.784327
C	-2.871742	-0.374704	1.193582
H	-4.850847	1.250645	0.221947
H	-4.786373	2.773171	-1.713960
H	-2.682480	3.025178	-3.034101
H	-0.649580	1.794801	-2.353301
C	-3.279840	0.324265	2.536753
C	-3.892581	-1.488887	0.874900
C	-1.526946	-0.939164	1.525741
H	-3.276222	-0.385065	3.371304
H	-2.613915	1.159036	2.774013
H	-4.298565	0.710889	2.432570
H	-3.923579	-2.224925	1.686315
H	-4.895519	-1.066024	0.767939
H	-3.635328	-1.999343	-0.055465
H	-1.452747	-1.957203	1.888958
H	-0.805063	-0.270892	1.991169
O	-1.104376	-1.842447	-0.378030
C	-0.731429	-3.107460	-0.179230
O	-0.096972	-3.493436	0.793250
C	-1.220306	-4.027582	-1.281221
H	-2.306164	-3.942859	-1.388217
H	-0.772701	-3.732850	-2.236251
H	-0.948713	-5.058730	-1.049776

TS_1b_iso_OAc

Zero-point correction=	0.404501 (Hartree/Particle)
Thermal correction to Energy=	0.431869
Thermal correction to Enthalpy=	0.432813
Thermal correction to Gibbs Free Energy=	0.345876
Sum of electronic and zero-point Energies=	-1339.488675
Sum of electronic and thermal Energies=	-1339.461308
Sum of electronic and thermal Enthalpies=	-1339.460363
Sum of electronic and thermal Free Energies=	-1339.547301

E(RB3LYP) = -1340.38058927



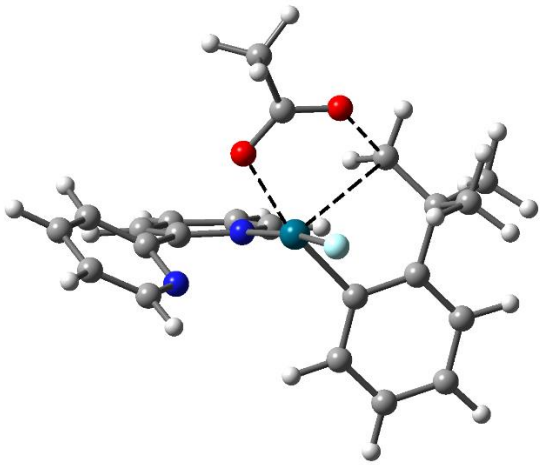
Pd	-0.205195	-0.025737	-0.718947
N	1.933787	-0.172669	-1.046985
N	0.506016	1.579217	0.385402
C	-2.143102	0.478534	-0.708425
F	-0.661722	-1.451935	-2.018705
C	-0.264027	2.436175	1.079326
C	0.261500	3.500311	1.804071
C	1.641455	3.686731	1.806512
C	2.442016	2.805722	1.084800
C	1.859561	1.751017	0.377020
H	-1.330991	2.255458	1.038334
H	-0.405503	4.160925	2.346143
H	2.092220	4.505134	2.358070
H	3.516149	2.940628	1.075833
C	2.540554	-1.085219	-1.812101
C	3.921565	-1.091179	-1.998653
C	4.679725	-0.112771	-1.355902
C	4.042346	0.836918	-0.558566

C	2.651164	0.786103	-0.421722
H	1.884352	-1.814054	-2.275949
H	4.382940	-1.842932	-2.629331
H	5.758321	-0.084082	-1.472597
H	4.627266	1.598825	-0.058734
C	-3.071673	-0.248333	0.056701
C	-4.434057	0.072507	-0.045608
C	-4.869447	1.099634	-0.886477
C	-3.943063	1.823200	-1.638947
C	-2.581921	1.508395	-1.549680
C	-2.559392	-1.383716	0.932772
H	-5.170266	-0.479112	0.532920
H	-5.928952	1.333254	-0.948601
H	-4.273120	2.624525	-2.295676
H	-1.863714	2.069172	-2.144678
C	-3.373361	-1.516188	2.270700
C	-2.617111	-2.735956	0.184677
C	-1.198469	-1.095058	1.469942
H	-2.949199	-2.293241	2.913400
H	-3.409379	-0.573147	2.824080
H	-4.398238	-1.813931	2.026216
H	-2.227130	-3.543954	0.814370
H	-3.655485	-2.969006	-0.074369
H	-2.021544	-2.671603	-0.728083
H	-0.749968	-1.878479	2.053551
H	-0.959798	-0.094975	1.807643
O	0.773671	-2.307264	0.752476
C	1.713135	-2.005754	1.574192
O	1.749426	-1.011863	2.326092
C	2.903009	-2.982283	1.570950
H	3.569192	-2.729781	0.736821
H	3.470328	-2.899127	2.502253
H	2.571138	-4.014760	1.427324

TS_1b_iso_OAc'

Zero-point correction=	0.404967 (Hartree/Particle)
Thermal correction to Energy=	0.432077
Thermal correction to Enthalpy=	0.433021
Thermal correction to Gibbs Free Energy=	0.346651
Sum of electronic and zero-point Energies=	-1339.486904
Sum of electronic and thermal Energies=	-1339.459794
Sum of electronic and thermal Enthalpies=	-1339.458850
Sum of electronic and thermal Free Energies=	-1339.545220

E(RB3LYP) = -1340.36858109



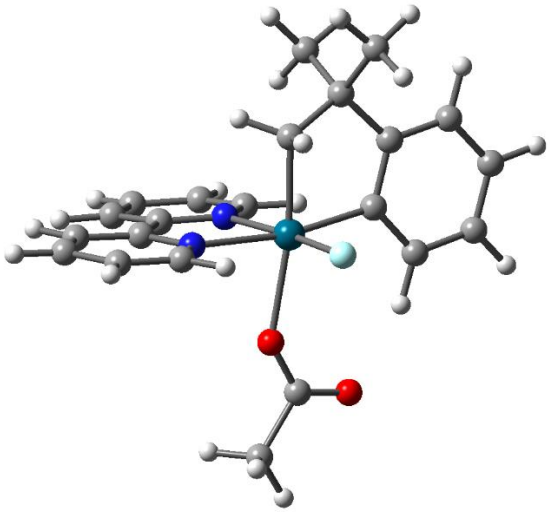
Pd	0.093630	0.338374	-0.332748
N	-2.319951	-0.505033	-1.372581
N	-0.717618	-1.179541	0.890084
C	1.617379	-0.811444	-0.853875

F	0.699101	1.662983	-1.696395
C	0.044170	-1.881967	1.750898
C	-0.467608	-2.838177	2.619963
C	-1.835687	-3.096706	2.591289
C	-2.624493	-2.399791	1.681499
C	-2.049935	-1.445362	0.833392
H	1.106754	-1.673981	1.729559
H	0.201292	-3.363570	3.292237
H	-2.278699	-3.839017	3.247279
H	-3.684271	-2.610640	1.600426
C	-3.055360	0.089336	-2.318773
C	-4.387244	0.464599	-2.133097
C	-4.977326	0.211571	-0.895499
C	-4.220694	-0.406216	0.099210
C	-2.891390	-0.750054	-0.180153
H	-2.554958	0.270245	-3.267316
H	-4.938773	0.941637	-2.936537
H	-6.007363	0.495216	-0.702258
H	-4.647554	-0.594756	1.078270
C	2.886117	-0.441086	-0.363432
C	3.999047	-1.199818	-0.770015
C	3.863430	-2.295987	-1.623947
C	2.600876	-2.660388	-2.093100
C	1.483217	-1.913969	-1.706363
C	3.079561	0.795481	0.530312
H	4.995057	-0.936256	-0.426688
H	4.744135	-2.861031	-1.917650
H	2.484144	-3.513506	-2.757355
H	0.499250	-2.191408	-2.077424
C	4.189901	0.541265	1.615882
C	3.504316	2.016700	-0.320900
C	1.919742	1.146446	1.424059
H	4.294955	1.403722	2.280697
H	3.980014	-0.348814	2.216751
H	5.152320	0.400545	1.115856
H	3.669591	2.894553	0.314863
H	4.438071	1.790749	-0.846465
H	2.720299	2.237502	-1.047229
H	2.147351	1.965189	2.088960
H	1.342844	0.366811	1.905249
O	0.589359	2.810335	1.174715
C	-0.658751	2.799807	0.931753
O	-1.310495	1.835853	0.436328
C	-1.418578	4.084623	1.232544
H	-0.870116	4.715359	1.934636
H	-1.555738	4.638123	0.296138
H	-2.409567	3.850631	1.631258

TS_1b_I

Zero-point correction=	0.406941 (Hartree/Particle)
Thermal correction to Energy=	0.433237
Thermal correction to Enthalpy=	0.434181
Thermal correction to Gibbs Free Energy=	0.350637
Sum of electronic and zero-point Energies=	-1339.545844
Sum of electronic and thermal Energies=	-1339.519548
Sum of electronic and thermal Enthalpies=	-1339.518604
Sum of electronic and thermal Free Energies=	-1339.602148

E(RB3LYP) = -1340.43368080



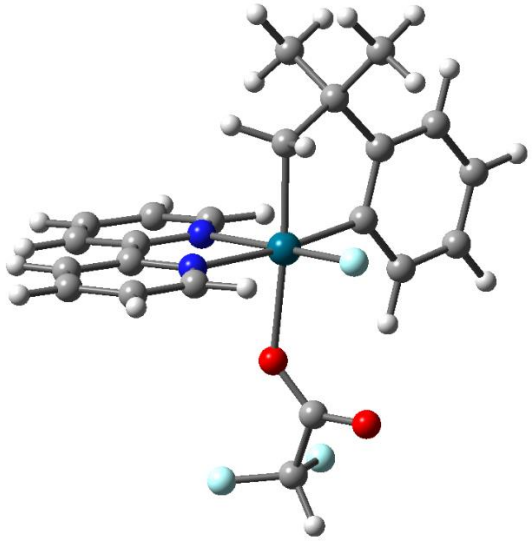
Pd	0.070838	0.138094	-0.584691
N	-0.558458	-0.261176	1.339246
C	0.187275	-0.018759	2.431014
H	1.198142	0.322680	2.251127
C	-0.306458	-0.192438	3.719129
H	0.333183	0.015400	4.569024
C	-1.619151	-0.629730	3.876794
H	-2.041665	-0.776082	4.865208
C	-2.392799	-0.870945	2.744922
C	-3.934052	-1.387834	0.197975
C	-4.580175	-1.520255	-1.030800
H	-5.592548	-1.909005	-1.068858
C	-3.916863	-1.152354	-2.200472
H	-4.389499	-1.239488	-3.172314
C	-2.613712	-0.667728	-2.096248
H	-2.033509	-0.366492	-2.963010
C	-2.629296	-0.885087	0.226732
C	-1.849518	-0.678668	1.471728
H	-4.444394	-1.678227	1.107790
H	-3.419834	-1.194714	2.853676
N	-2.000533	-0.543519	-0.917232
C	0.713074	-1.797726	-0.904626
H	-0.034330	-2.448979	-0.444648
H	0.631289	-1.837026	-1.992411
C	2.030019	0.425226	-0.185524
C	2.569913	1.693072	0.025102
C	2.827560	-0.729299	-0.190800
C	3.947308	1.811432	0.256127
H	1.920421	2.566165	0.023958
C	4.203740	-0.584666	0.041983
C	4.761106	0.676127	0.263264
H	4.379486	2.794752	0.426942
H	4.844795	-1.463132	0.049109
H	5.829469	0.770409	0.440010
C	2.147275	-2.072380	-0.405567
C	2.877130	-2.918967	-1.475766
H	2.328094	-3.849106	-1.664884
H	2.961274	-2.370970	-2.420661
H	3.886164	-3.191218	-1.146497
F	0.485267	0.509599	-2.466092
C	2.115080	-2.868068	0.920747
H	3.130720	-3.053523	1.287520
H	1.569803	-2.327708	1.701067
H	1.625282	-3.838299	0.772532
C	-2.027374	4.221558	-0.270547
H	-2.433352	4.168725	-1.287152
H	-2.811034	3.867806	0.408883
H	-1.784335	5.260072	-0.032893

C	-0.784633	3.327762	-0.154876
O	0.303401	3.838408	0.161738
O	-1.018319	2.085399	-0.410331

TS_1c

Zero-point correction=	0.392119 (Hartree/Particle)
Thermal correction to Energy=	0.419781
Thermal correction to Enthalpy=	0.420726
Thermal correction to Gibbs Free Energy=	0.331117
Sum of electronic and zero-point Energies=	-1538.027478
Sum of electronic and thermal Energies=	-1537.999816
Sum of electronic and thermal Enthalpies=	-1537.998871
Sum of electronic and thermal Free Energies=	-1538.088480

E(RB3LYP) = -1538.98126941



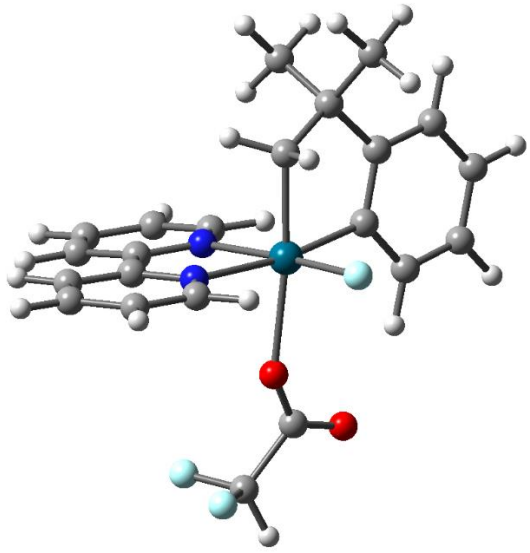
Pd	0.139228	-0.221456	-0.593761
N	-0.501220	-0.540765	1.346356
C	0.187714	-0.165385	2.436695
H	1.162947	0.268566	2.259284
C	-0.319897	-0.319665	3.722245
H	0.273320	-0.003778	4.572515
C	-1.585537	-0.879433	3.876829
H	-2.015879	-1.017022	4.863123
C	-2.302864	-1.255653	2.744445
C	-3.731603	-2.022205	0.192295
C	-4.321658	-2.286846	-1.043271
H	-5.301150	-2.751921	-1.084515
C	-3.645849	-1.951990	-2.215829
H	-4.075871	-2.142398	-3.192607
C	-2.387956	-1.361449	-2.108341
H	-1.799351	-1.075693	-2.974458
C	-2.469437	-1.421743	0.225958
C	-1.748104	-1.075936	1.474619
H	-4.251986	-2.284762	1.104814
H	-3.294204	-1.677327	2.849483
N	-1.829001	-1.109464	-0.921412
C	1.054166	-2.065291	-0.697442
H	0.423370	-2.753439	-0.129039
H	0.962189	-2.261252	-1.766519
C	1.999829	0.408608	-0.168113
C	2.324399	1.757026	-0.011840
C	2.970356	-0.598686	-0.071939
C	3.652140	2.112176	0.255588
H	1.565017	2.526857	-0.088719
C	4.295077	-0.220130	0.194825

C	4.634767	1.124230	0.355917
H	3.912755	3.160014	0.381133
H	5.067515	-0.980770	0.279571
H	5.665742	1.399785	0.561032
C	2.524044	-2.048252	-0.212874
C	3.386522	-2.804169	-1.251728
H	3.015080	-3.827433	-1.383049
H	3.359911	-2.301245	-2.224587
H	4.431406	-2.869339	-0.928129
F	0.569189	-0.049028	-2.498624
C	2.636976	-2.767939	1.151982
H	3.669664	-2.754963	1.517339
H	2.005470	-2.290516	1.908649
H	2.323684	-3.814873	1.058730
C	-1.500724	3.998587	-0.131337
H	-1.799297	4.840581	-0.761074
C	-0.916125	2.821490	-0.944352
O	-0.453696	3.100460	-2.056283
O	-0.935908	1.711273	-0.311312
F	-2.570185	3.616387	0.630086
F	-0.520541	4.431700	0.736338

TS_1c_I

Zero-point correction=	0.392272 (Hartree/Particle)
Thermal correction to Energy=	0.419917
Thermal correction to Enthalpy=	0.420861
Thermal correction to Gibbs Free Energy=	0.332283
Sum of electronic and zero-point Energies=	-1538.026549
Sum of electronic and thermal Energies=	-1537.998904
Sum of electronic and thermal Enthalpies=	-1537.997959
Sum of electronic and thermal Free Energies=	-1538.086538

E(RB3LYP) = -1538.98027432



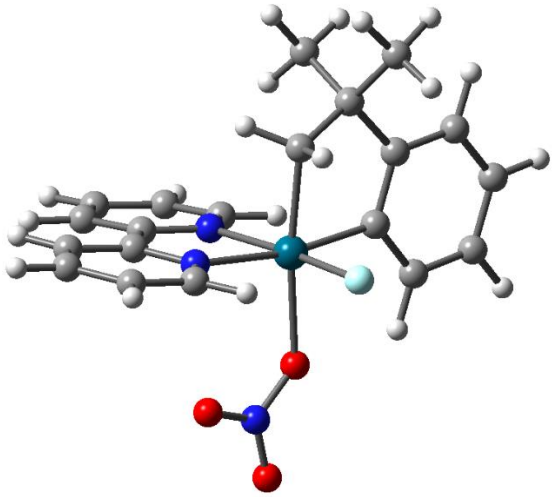
Pd	0.298805	-0.116872	-0.623573
N	-0.272825	-0.421283	1.336347
C	0.347992	0.136031	2.390443
H	1.241079	0.706599	2.171033
C	-0.126033	-0.008411	3.689543
H	0.409263	0.457944	4.508443
C	-1.284317	-0.752797	3.897726
H	-1.686159	-0.888084	4.896278
C	-1.931749	-1.319248	2.803132
C	-3.208464	-2.505761	0.333208
C	-3.750376	-2.951774	-0.872027
H	-4.632273	-3.583977	-0.865744

C	-3.152144	-2.580896	-2.075372
H	-3.548425	-2.907342	-3.030252
C	-2.016328	-1.774041	-2.027637
H	-1.494747	-1.447818	-2.922136
C	-2.071138	-1.692724	0.304802
C	-1.415668	-1.142834	1.516627
H	-3.668656	-2.795439	1.269544
H	-2.841976	-1.885947	2.950695
N	-1.501814	-1.351599	-0.870455
C	1.469399	-1.812433	-0.673257
H	0.917194	-2.580216	-0.125966
H	1.441816	-2.014145	-1.745207
C	2.072643	0.770777	-0.264047
C	2.220406	2.157029	-0.227549
C	3.164032	-0.095923	-0.105563
C	3.495032	2.694533	-0.002788
H	1.357485	2.805874	-0.354912
C	4.430324	0.466138	0.116223
C	4.595671	1.851393	0.167960
H	3.622049	3.773898	0.034355
H	5.292868	-0.183009	0.247777
H	5.583447	2.271035	0.339707
C	2.903644	-1.594210	-0.144509
C	3.881271	-2.315918	-1.103309
H	3.631541	-3.381327	-1.172162
H	3.834518	-1.885461	-2.109565
H	4.914140	-2.239900	-0.745770
F	0.665012	0.095197	-2.537461
C	3.057286	-2.198784	1.270881
H	4.071646	-2.038429	1.652366
H	2.356564	-1.748019	1.980753
H	2.870276	-3.279276	1.247177
C	-2.909502	3.135012	-0.263780
H	-3.076936	4.211732	-0.350554
C	-1.423649	2.744761	-0.439859
O	-0.596554	3.654483	-0.285758
O	-1.252755	1.506822	-0.687494
F	-3.710716	2.490547	-1.165893
F	-3.311275	2.732880	0.990933

TS_1d

Zero-point correction=	0.371662 (Hartree/Particle)
Thermal correction to Energy=	0.396946
Thermal correction to Enthalpy=	0.397890
Thermal correction to Gibbs Free Energy=	0.315890
Sum of electronic and zero-point Energies=	-1391.402425
Sum of electronic and thermal Energies=	-1391.377141
Sum of electronic and thermal Enthalpies=	-1391.376197
Sum of electronic and thermal Free Energies=	-1391.458197

E(RB3LYP) = -1392.27606672

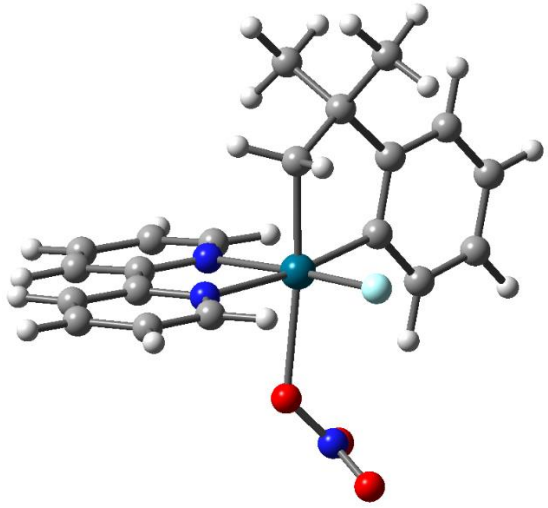


Pd	0.113183	0.297294	-0.515908
N	-0.472796	-0.444375	1.317583
C	0.273742	-0.352659	2.431835
H	1.260063	0.075929	2.310455
C	-0.190704	-0.783907	3.669288
H	0.446585	-0.692132	4.541040
C	-1.470801	-1.326832	3.748786
H	-1.867591	-1.677386	4.695686
C	-2.247440	-1.406461	2.595980
C	-3.799972	-1.506712	-0.005924
C	-4.446804	-1.436342	-1.239352
H	-5.440628	-1.856970	-1.352440
C	-3.807540	-0.826628	-2.317931
H	-4.281029	-0.754222	-3.290526
C	-2.529786	-0.306008	-2.122015
H	-1.970260	0.182322	-2.913441
C	-2.519611	-0.959188	0.118605
C	-1.737159	-0.952193	1.377265
H	-4.289815	-1.983993	0.833627
H	-3.251422	-1.807570	2.649135
N	-1.917650	-0.374996	-0.938319
C	0.803188	-1.532134	-1.179435
H	0.084405	-2.282418	-0.841840
H	0.713752	-1.376514	-2.255763
C	2.065293	0.591207	-0.097542
C	2.573797	1.822759	0.314305
C	2.896226	-0.519407	-0.303666
C	3.948487	1.947222	0.550671
H	1.910249	2.669685	0.451101
C	4.270654	-0.372089	-0.062976
C	4.793454	0.850757	0.362037
H	4.353376	2.902076	0.876496
H	4.938339	-1.217667	-0.209252
H	5.860639	0.947407	0.542999
C	2.251587	-1.829828	-0.733884
C	2.994041	-2.465907	-1.934195
H	2.467802	-3.366259	-2.272440
H	3.055705	-1.766295	-2.774829
H	4.012331	-2.761882	-1.658371
F	0.461482	0.995314	-2.314786
C	2.257424	-2.832520	0.443835
H	3.281955	-3.042147	0.769929
H	1.703867	-2.444590	1.304622
H	1.796704	-3.780751	0.141125
O	-2.503645	2.391907	-0.221680
O	-0.348289	2.385730	0.232381
N	-1.500843	2.985398	0.211618
O	-1.544845	4.149744	0.637705

TS_1d_I

Zero-point correction=	0.371998 (Hartree/Particle)
Thermal correction to Energy=	0.397230
Thermal correction to Enthalpy=	0.398174
Thermal correction to Gibbs Free Energy=	0.316601
Sum of electronic and zero-point Energies=	-1391.398835
Sum of electronic and thermal Energies=	-1391.373603
Sum of electronic and thermal Enthalpies=	-1391.372659
Sum of electronic and thermal Free Energies=	-1391.454232

E(RB3LYP) = -1392.27106641



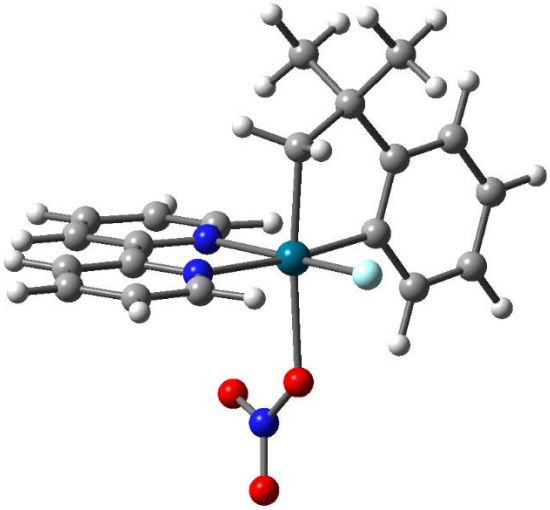
Pd	0.021956	0.267639	-0.491885
N	-0.631143	-0.589642	1.266589
C	0.141433	-0.739884	2.356376
H	1.176959	-0.444356	2.250972
C	-0.357712	-1.243014	3.552693
H	0.303223	-1.347673	4.405159
C	-1.702285	-1.598953	3.617072
H	-2.128644	-1.996808	4.531835
C	-2.503514	-1.429678	2.490908
C	-4.107309	-1.004020	-0.040990
C	-4.763980	-0.704576	-1.234530
H	-5.812832	-0.957041	-1.350714
C	-4.065749	-0.082216	-2.268287
H	-4.546141	0.167898	-3.207339
C	-2.718203	0.214531	-2.071307
H	-2.109208	0.696313	-2.829744
C	-2.755730	-0.671890	0.089865
C	-1.954741	-0.915687	1.313714
H	-4.646861	-1.488670	0.763018
H	-3.554099	-1.686117	2.533955
N	-2.094707	-0.077451	-0.926912
C	0.519144	-1.548041	-1.336695
H	-0.269122	-2.238375	-1.028672
H	0.409539	-1.278709	-2.387878
C	1.994699	0.310057	-0.067825
C	2.625126	1.425487	0.481611
C	2.711958	-0.843758	-0.416533
C	4.007999	1.386560	0.702608
H	2.059951	2.308881	0.760300
C	4.095920	-0.860984	-0.188262
C	4.740602	0.246308	0.365743
H	4.505633	2.250378	1.136008
H	4.674647	-1.744949	-0.444929
H	5.813654	0.217734	0.534766

C	1.940154	-2.028140	-0.979248
C	2.593252	-2.571675	-2.273713
H	1.981195	-3.374051	-2.701840
H	2.699117	-1.780358	-3.023600
H	3.586371	-2.985964	-2.068426
F	0.453418	1.101865	-2.209814
C	1.877807	-3.166730	0.065830
H	2.885711	-3.507119	0.326466
H	1.384183	-2.842768	0.987573
H	1.322930	-4.023595	-0.334889
O	0.343997	3.434535	1.597746
O	-0.905061	2.249851	0.238019
N	-0.294844	3.355254	0.528741
O	-0.388350	4.311597	-0.257028

TS_1d_II

Zero-point correction=	0.371835 (Hartree/Particle)
Thermal correction to Energy=	0.397052
Thermal correction to Enthalpy=	0.397997
Thermal correction to Gibbs Free Energy=	0.316413
Sum of electronic and zero-point Energies=	-1391.403242
Sum of electronic and thermal Energies=	-1391.378024
Sum of electronic and thermal Enthalpies=	-1391.377080
Sum of electronic and thermal Free Energies=	-1391.458663

E(RB3LYP) = -1392.27755517



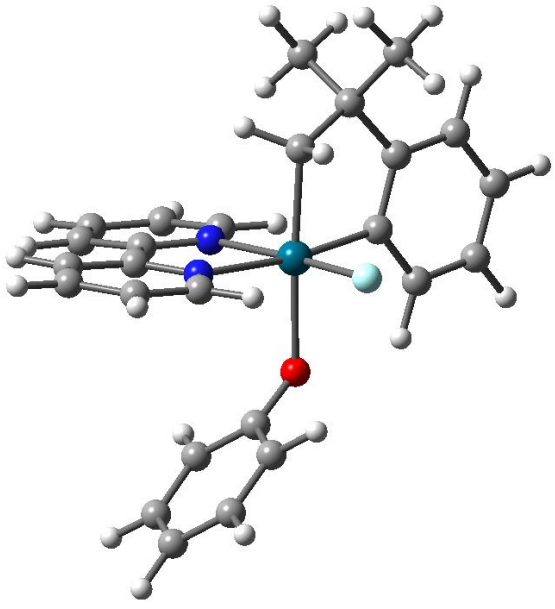
Pd	0.085020	-0.009525	-0.669815
N	-0.550664	0.040259	1.292960
C	0.204888	0.479290	2.312125
H	1.212976	0.782374	2.063196
C	-0.276201	0.545619	3.614691
H	0.372212	0.902827	4.406302
C	-1.587724	0.149245	3.862703
H	-1.999642	0.185701	4.865645
C	-2.374296	-0.290016	2.801472
C	-3.956072	-1.199580	0.387919
C	-4.602734	-1.557251	-0.794669
H	-5.631369	-1.901275	-0.764168
C	-3.920120	-1.469781	-2.007299
H	-4.392694	-1.738946	-2.945087
C	-2.599570	-1.025284	-1.992269
H	-2.003396	-0.934062	-2.894684
C	-2.630552	-0.758863	0.328893
C	-1.841689	-0.336045	1.510687
H	-4.482525	-1.266966	1.331654
H	-3.400265	-0.587031	2.976986
N	-1.985498	-0.683228	-0.855726

C	0.781017	-1.938382	-0.429357
H	0.069432	-2.444488	0.227165
H	0.673924	-2.297138	-1.454049
C	2.009779	0.456502	-0.350399
C	2.487360	1.759763	-0.483218
C	2.854160	-0.615006	-0.032427
C	3.846654	2.010777	-0.261156
H	1.815201	2.565509	-0.759184
C	4.213379	-0.341765	0.185417
C	4.705152	0.960363	0.075111
H	4.229820	3.023525	-0.356262
H	4.893238	-1.151223	0.440463
H	5.760455	1.154219	0.247029
C	2.240912	-2.004200	0.082667
C	3.008294	-3.026093	-0.791216
H	2.521158	-4.007368	-0.747072
H	3.038918	-2.703281	-1.837566
H	4.038746	-3.150284	-0.440209
F	0.520945	-0.173457	-2.575373
C	2.270078	-2.484376	1.552695
H	3.298555	-2.529638	1.927228
H	1.703205	-1.814559	2.206912
H	1.835425	-3.487888	1.634829
O	-0.955011	2.889116	0.718029
O	-0.631144	2.045520	-1.289786
N	-1.087408	2.983646	-0.515980
O	-1.636858	3.955991	-1.056025

TS_1e

Zero-point correction=	0.449425 (Hartree/Particle)
Thermal correction to Energy=	0.476615
Thermal correction to Enthalpy=	0.477559
Thermal correction to Gibbs Free Energy=	0.392184
Sum of electronic and zero-point Energies=	-1417.878616
Sum of electronic and thermal Energies=	-1417.851426
Sum of electronic and thermal Enthalpies=	-1417.850482
Sum of electronic and thermal Free Energies=	-1417.935857

E(RB3LYP) = -1418.83209944



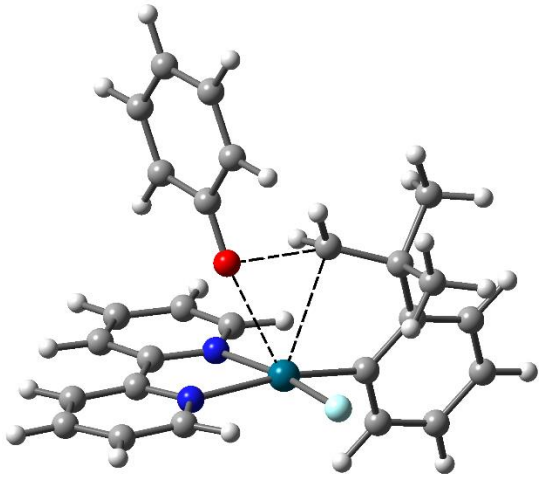
Pd	-0.405576	-0.252658	-0.464777
N	-0.104113	0.988790	1.154277
C	-0.824187	0.925877	2.286898
H	-1.648479	0.224865	2.287731
C	-0.531299	1.712300	3.395569

H	-1.143011	1.629001	4.286454
C	0.549063	2.588744	3.325799
H	0.809489	3.218595	4.169835
C	1.303286	2.641149	2.157142
C	2.811128	2.664216	-0.467634
C	3.477920	2.542023	-1.686139
H	4.306453	3.203653	-1.917050
C	3.070265	1.570211	-2.598965
H	3.566163	1.446872	-3.555161
C	1.996869	0.749653	-2.257169
H	1.621469	-0.024790	-2.917827
C	1.744790	1.803496	-0.189616
C	0.966894	1.827275	1.071801
H	3.118807	3.422030	0.242004
H	2.158116	3.302468	2.095950
N	1.361528	0.871053	-1.088275
C	-1.649335	1.102668	-1.426310
H	-1.237015	2.102484	-1.263434
H	-1.499658	0.802252	-2.465331
C	-2.152167	-1.050436	0.116963
C	-2.218712	-2.262471	0.803132
C	-3.303669	-0.341057	-0.251514
C	-3.472822	-2.778199	1.151660
H	-1.302601	-2.784928	1.059430
C	-4.550679	-0.876277	0.107969
C	-4.635345	-2.084348	0.803581
H	-3.538213	-3.720928	1.689557
H	-5.462998	-0.347321	-0.158047
H	-5.609525	-2.484778	1.071945
C	-3.128047	0.984828	-0.982910
C	-4.025259	1.056768	-2.241096
H	-3.837048	1.987435	-2.789678
H	-3.826090	0.215344	-2.913920
H	-5.088383	1.037926	-1.975239
F	-0.516032	-1.365366	-2.082952
C	-3.499656	2.155164	-0.041377
H	-4.537556	2.068497	0.299476
H	-2.855857	2.178493	0.843988
H	-3.393253	3.113825	-0.563857
O	0.766349	-1.762069	0.620537
C	2.082157	-1.884981	0.523173
C	2.714130	-2.394143	-0.643123
C	2.925583	-1.560753	1.618966
C	4.095783	-2.573330	-0.698525
H	2.089737	-2.649179	-1.495770
C	4.306394	-1.748294	1.554849
H	2.463016	-1.175595	2.525449
C	4.907807	-2.255059	0.397196
H	4.545581	-2.971174	-1.606596
H	4.919840	-1.496590	2.418205
H	5.983729	-2.400408	0.349984

TS_1e_iso_OPh

Zero-point correction=	0.447268 (Hartree/Particle)
Thermal correction to Energy=	0.475627
Thermal correction to Enthalpy=	0.476571
Thermal correction to Gibbs Free Energy=	0.386470
Sum of electronic and zero-point Energies=	-1417.821229
Sum of electronic and thermal Energies=	-1417.792871
Sum of electronic and thermal Enthalpies=	-1417.791926
Sum of electronic and thermal Free Energies=	-1417.882027

E(RB3LYP) = -1418.77230327

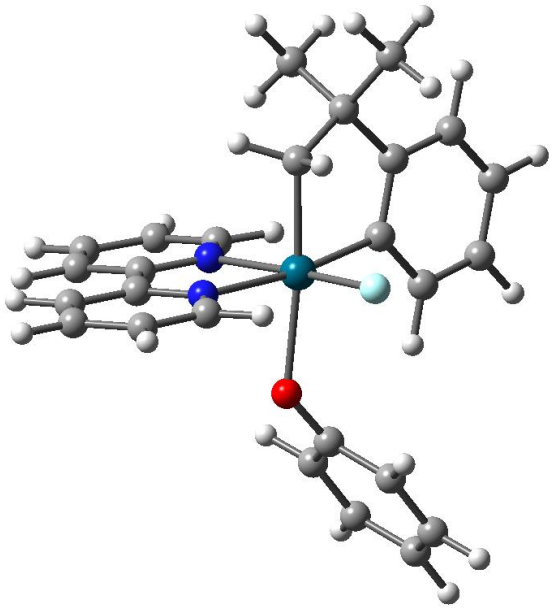


Pd	0.712602	-0.825441	-0.649561
N	-1.169218	-1.725533	-1.202494
N	-0.039853	-1.372041	1.199898
C	2.568453	-0.384980	-0.046930
F	1.250853	-0.510086	-2.533704
C	0.573456	-1.164729	2.378619
C	0.001861	-1.520945	3.595867
C	-1.256426	-2.116743	3.591680
C	-1.894060	-2.336723	2.373235
C	-1.272532	-1.958441	1.180013
H	1.552073	-0.704881	2.328231
H	0.540773	-1.330480	4.517042
H	-1.738417	-2.408579	4.518915
H	-2.872764	-2.799173	2.354932
C	-1.633337	-1.858325	-2.447514
C	-2.866815	-2.448846	-2.717655
C	-3.626205	-2.912867	-1.644852
C	-3.136955	-2.772984	-0.346313
C	-1.892601	-2.166050	-0.150354
H	-0.985042	-1.473420	-3.228283
H	-3.214908	-2.539745	-3.740595
H	-4.591052	-3.381037	-1.811450
H	-3.722067	-3.134454	0.490196
C	3.039533	0.939547	0.020263
C	4.376835	1.165215	0.385396
C	5.235407	0.104216	0.681351
C	4.765126	-1.207987	0.616825
C	3.434905	-1.446042	0.253150
C	2.104818	2.078553	-0.364283
H	4.762505	2.179346	0.441898
H	6.265513	0.306036	0.963056
H	5.424821	-2.042038	0.844207
H	3.073052	-2.471360	0.203026
C	2.396458	3.386562	0.458482
C	2.239265	2.414356	-1.869073
C	0.678372	1.834771	0.019928
H	1.665843	4.167586	0.227650
H	2.391097	3.200081	1.536301
H	3.383076	3.768107	0.173811
H	1.579579	3.248256	-2.139395
H	3.270447	2.707967	-2.093174
H	1.975958	1.538259	-2.465529
H	-0.009987	2.569420	-0.365484
H	0.450819	1.458567	1.010798
O	-1.501315	1.075345	-0.698680
C	-2.229762	2.014503	-0.161180
C	-2.835887	1.856308	1.123719
C	-2.444850	3.265800	-0.816950
C	-3.624433	2.856762	1.681647

H	-2.683384	0.916331	1.649334
C	-3.232095	4.262272	-0.244230
H	-1.990629	3.412675	-1.794742
C	-3.831453	4.068435	1.006164
H	-4.083848	2.697601	2.655274
H	-3.383005	5.199299	-0.776442
H	-4.446245	4.847108	1.449146
F	4.000682	-1.217404	1.026952

TS_1e_I

Zero-point correction=	0.449351 (Hartree/Particle)
Thermal correction to Energy=	0.476706
Thermal correction to Enthalpy=	0.477650
Thermal correction to Gibbs Free Energy=	0.391222
Sum of electronic and zero-point Energies=	-1417.875902
Sum of electronic and thermal Energies=	-1417.848547
Sum of electronic and thermal Enthalpies=	-1417.847603
Sum of electronic and thermal Free Energies=	-1417.934031
E(RB3LYP) =	-1418.82744517



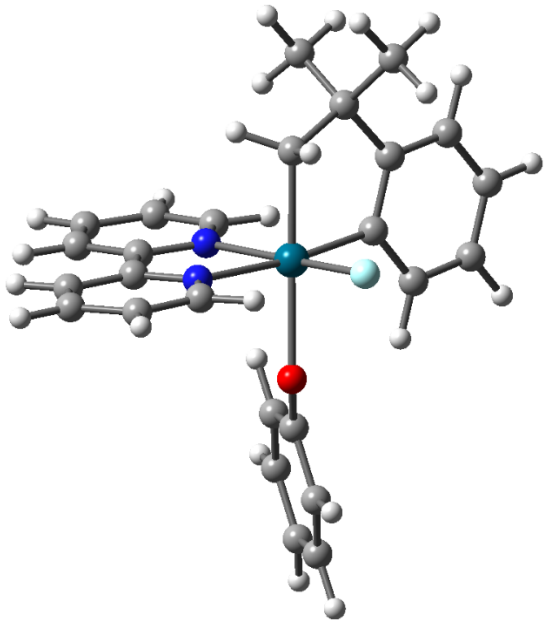
Pd	0.217629	0.191443	-0.590544
N	0.979187	0.063185	1.322836
C	0.324077	0.471579	2.422596
H	-0.626628	0.961028	2.257050
C	0.832589	0.279801	3.702699
H	0.267642	0.627801	4.559726
C	2.062611	-0.357799	3.843278
H	2.494231	-0.524042	4.824619
C	2.735310	-0.788525	2.703268
C	4.070248	-1.672660	0.139706
C	4.576893	-2.073502	-1.096004
H	5.540942	-2.568821	-1.148782
C	3.838239	-1.834070	-2.253997
H	4.200918	-2.134557	-3.230535
C	2.607155	-1.191905	-2.131241
H	1.974569	-0.972200	-2.985633
C	2.825874	-1.035885	0.187903
C	2.177279	-0.576230	1.439632
H	4.641323	-1.857633	1.040947
H	3.687062	-1.295312	2.798339
N	2.128720	-0.809172	-0.945083
C	1.097871	2.039070	-0.926145
H	2.085279	2.008099	-0.457759
H	1.196044	2.007748	-2.012751

C	-1.392360	1.328729	-0.171450
C	-2.657788	0.794145	0.070058
C	-1.175829	2.715778	-0.183436
C	-3.731001	1.656230	0.328572
H	-2.818356	-0.278520	0.060650
C	-2.264464	3.562357	0.076509
C	-3.533011	3.038692	0.332306
H	-4.717889	1.242650	0.521182
H	-2.120474	4.640289	0.078199
H	-4.364943	3.709294	0.530825
C	0.236035	3.226609	-0.442504
C	0.247121	4.315749	-1.542102
H	1.276426	4.623163	-1.762259
H	-0.205476	3.943834	-2.467965
H	-0.304402	5.208287	-1.225607
F	-0.340331	0.216733	-2.474347
C	0.826103	3.826897	0.855655
H	0.210739	4.659218	1.215085
H	0.881812	3.080559	1.654637
H	1.838803	4.207391	0.674469
O	-0.460056	-1.897724	-0.292437
C	-1.656785	-2.441665	-0.158477
C	-2.460519	-2.785227	-1.279924
C	-2.178673	-2.771994	1.122483
C	-3.693684	-3.417802	-1.125146
H	-2.085333	-2.553157	-2.273985
C	-3.411803	-3.406975	1.266379
H	-1.582277	-2.525048	1.998599
C	-4.184180	-3.737071	0.146540
H	-4.277831	-3.668860	-2.008737
H	-3.774110	-3.648627	2.264067
H	-5.144764	-4.231821	0.262076

TS_1e_II

Zero-point correction=	0.449371 (Hartree/Particle)
Thermal correction to Energy=	0.476703
Thermal correction to Enthalpy=	0.477647
Thermal correction to Gibbs Free Energy=	0.391179
Sum of electronic and zero-point Energies=	-1417.875372
Sum of electronic and thermal Energies=	-1417.848040
Sum of electronic and thermal Enthalpies=	-1417.847096

Sum of electronic and 1418.82792905

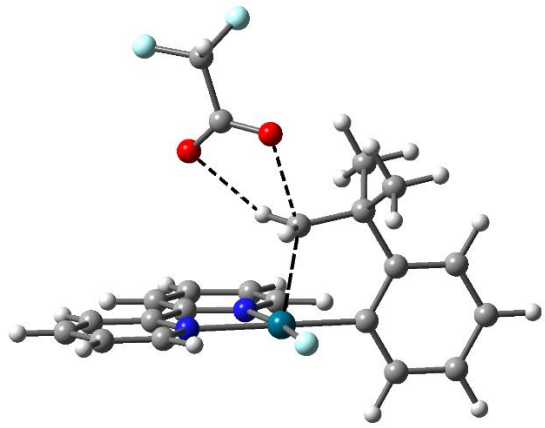


Pd	0.290281	-0.319377	-0.650270
N	-0.258713	-0.645730	1.317845
C	0.259393	0.019278	2.365332
H	1.021590	0.751678	2.133673
C	-0.158776	-0.210077	3.671021
H	0.289201	0.351860	4.482301
C	-1.150822	-1.161608	3.895547
H	-1.505900	-1.368604	4.899531
C	-1.685914	-1.850087	2.810890
C	-2.747757	-3.263319	0.357128
C	-3.157971	-3.856440	-0.836558
H	-3.932827	-4.616013	-0.823023
C	-2.567647	-3.466607	-2.037801
H	-2.862507	-3.906614	-2.983787
C	-1.577729	-2.485721	-2.000267
H	-1.075784	-2.128569	-2.893974
C	-1.748301	-2.285803	0.319216
C	-1.227591	-1.583982	1.517269
H	-3.205216	-3.563606	1.291453
H	-2.457385	-2.591934	2.971835
N	-1.189539	-1.921847	-0.854086
C	1.828806	-1.690133	-0.470473
H	1.479107	-2.462817	0.219307
H	1.862739	-2.087400	-1.486352
C	1.762534	1.007380	-0.329667
C	1.561180	2.385598	-0.410427
C	3.030081	0.461752	-0.080251
C	2.645239	3.247629	-0.204771
H	0.576527	2.789680	-0.619351
C	4.102668	1.343969	0.124203
C	3.913059	2.725626	0.064590
H	2.495326	4.322998	-0.260052
H	5.095357	0.948057	0.325886
H	4.755328	3.393749	0.223639
C	3.172626	-1.054646	-0.032487
C	4.280007	-1.532727	-1.002551
H	4.343174	-2.627483	-0.997817
H	4.071500	-1.205067	-2.026910
H	5.261300	-1.141105	-0.711848
F	0.736287	-0.218637	-2.560824
C	3.534197	-1.514419	1.399879
H	4.477486	-1.065325	1.730131
H	2.758385	-1.234467	2.120325
H	3.648918	-2.604695	1.431991
O	-1.413254	0.988010	-1.121482
C	-1.983095	2.069738	-0.628008
C	-2.824415	2.855913	-1.466762
C	-1.838131	2.517153	0.712946
C	-3.475201	3.991692	-0.992791
H	-2.951779	2.538292	-2.499506
C	-2.492085	3.660719	1.174978
H	-1.203911	1.951857	1.387122
C	-3.318832	4.412034	0.334616
H	-4.111344	4.559692	-1.669580
H	-2.352180	3.965932	2.210776

TS_3_DFA

Zero-point correction=	0.391190	(Hartree/Particle)
Thermal correction to Energy=	0.419487	
Thermal correction to Enthalpy=	0.420431	
Thermal correction to Gibbs Free Energy=	0.329063	
Sum of electronic and zero-point Energies=	-1537.998795	
Sum of electronic and thermal Energies=	-1537.970498	
Sum of electronic and thermal Enthalpies=	-1537.969554	
Sum of electronic and thermal Free Energies=	-1538.060922	

E(RB3LYP) = -1538.95619899

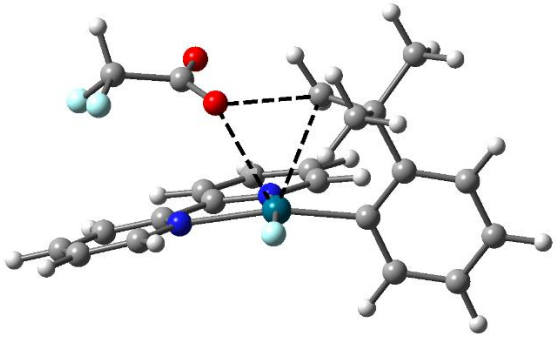


Pd	-0.979484	-0.913146	-0.712762
N	-0.435813	-1.431817	1.221419
C	-1.114673	-1.082389	2.328575
H	-1.997900	-0.476925	2.171402
C	-0.713730	-1.470563	3.602583
H	-1.294978	-1.162045	4.463873
C	0.432819	-2.249632	3.732050
H	0.779812	-2.571274	4.708365
C	1.135131	-2.616353	2.586593
C	2.539442	-3.335719	0.005767
C	3.103262	-3.611661	-1.239651
H	4.004939	-4.212057	-1.302385
C	2.502081	-3.112048	-2.393980
H	2.913516	-3.306722	-3.377884
C	1.345648	-2.347074	-2.258464
H	0.819634	-1.925446	-3.109040
C	1.378670	-2.559750	0.069002
C	0.687180	-2.200269	1.330942
H	3.004218	-3.722256	0.904054
H	2.026893	-3.223662	2.673400
N	0.807978	-2.084891	-1.061980
C	-0.054856	1.196887	-0.579570
H	0.632204	0.836403	0.172619
H	0.239734	1.080800	-1.613618
C	-2.614549	0.120970	-0.261106
C	-3.852833	-0.522801	-0.154829
C	-2.507444	1.508897	-0.088423
C	-5.002577	0.214346	0.145602
H	-3.924231	-1.598111	-0.304978
C	-3.672206	2.234739	0.214238
C	-4.907383	1.596150	0.331944
H	-5.963369	-0.287222	0.230175
H	-3.618515	3.311085	0.357288
H	-5.794522	2.178427	0.566414
C	-1.148741	2.211333	-0.228137
C	-1.231422	3.262959	-1.363854
H	-0.270047	3.767992	-1.477110
H	-1.495559	2.787435	-2.315330
H	-1.997543	4.011484	-1.137204
F	-1.369403	-0.618522	-2.620365
C	-0.783697	2.903386	1.109078
H	-1.557201	3.625849	1.388435
H	-0.698700	2.171920	1.921096
H	0.168315	3.429434	1.010570
C	3.862099	3.166326	-0.044187
H	4.095962	3.579041	-1.029479
C	2.671975	2.173176	-0.073917
O	2.788603	1.087783	0.517584
O	1.677412	2.646441	-0.711968
F	3.531048	4.211551	0.789302
F	4.985597	2.581225	0.464824

TS_3_DFA'

Zero-point correction=	0.389961	(Hartree/Particle)
Thermal correction to Energy=	0.418521	
Thermal correction to Enthalpy=	0.419466	
Thermal correction to Gibbs Free Energy=	0.329142	
Sum of electronic and zero-point Energies=	-1537.970346	
Sum of electronic and thermal Energies=	-1537.941785	
Sum of electronic and thermal Enthalpies=	-1537.940841	
Sum of electronic and thermal Free Energies=	-1538.031164	

E(RB3LYP) = -1538.92740685



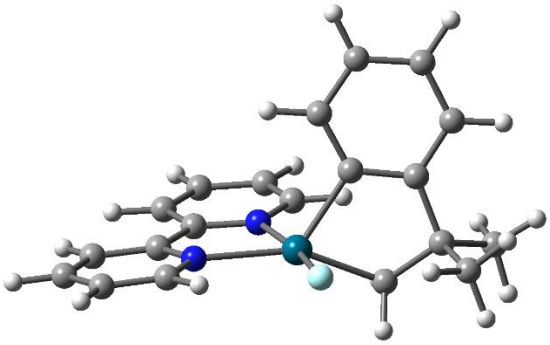
Pd	-0.436940	0.102736	-0.741228
N	1.696242	0.258003	-1.110452
N	0.079181	1.723432	0.441542
C	-2.422842	0.356477	-0.679162
F	-0.734091	-1.336651	-2.069439
C	-0.776725	2.414691	1.215883
C	-0.376031	3.484217	2.008844
C	0.966548	3.854142	1.998920
C	1.854455	3.147526	1.192719
C	1.395773	2.081783	0.413848
H	-1.810544	2.093932	1.184108
H	-1.108137	4.005489	2.614975
H	1.321263	4.679972	2.606609
H	2.901555	3.422033	1.175822
C	2.395880	-0.496787	-1.963881
C	3.737787	-0.246108	-2.241907
C	4.357827	0.825239	-1.601757
C	3.625753	1.610413	-0.712394
C	2.281670	1.302803	-0.482595
H	1.845287	-1.308078	-2.427731
H	4.274958	-0.876769	-2.941493
H	5.401330	1.054616	-1.792421
H	4.100062	2.449196	-0.218264
C	-3.259783	-0.503507	0.054130
C	-4.650443	-0.332230	-0.030518
C	-5.204787	0.677120	-0.820646
C	-4.370763	1.534075	-1.540084
C	-2.982764	1.369135	-1.468705
C	-2.627923	-1.618449	0.875955
H	-5.316189	-0.988508	0.523355
H	-6.284198	0.792715	-0.868775
H	-4.792862	2.323187	-2.157598
H	-2.336575	2.034249	-2.038125
C	-3.427920	-1.911028	2.203464
C	-2.528888	-2.929205	0.061110
C	-1.326399	-1.215479	1.459691
H	-2.923599	-2.667660	2.811035
H	-3.577895	-1.007931	2.801465
H	-4.408115	-2.311581	1.925349
H	-2.058139	-3.721715	0.653686
H	-3.533675	-3.258310	-0.223702
H	-1.936342	-2.748144	-0.838073

H	-0.785552	-1.970685	2.001969
H	-1.175726	-0.205403	1.817901
O	0.791267	-2.134421	0.659253
C	1.702055	-1.695859	1.424325
O	1.627417	-0.881103	2.360211
C	3.123488	-2.266785	1.169451
H	3.475794	-2.889130	1.998806
F	3.192665	-3.004422	0.019610
F	4.000682	-1.217404	1.026952

TS_3_iso

Zero-point correction=	0.355648 (Hartree/Particle)
Thermal correction to Energy=	0.376507
Thermal correction to Enthalpy=	0.377451
Thermal correction to Gibbs Free Energy=	0.306644
Sum of electronic and zero-point Energies=	-1110.947968
Sum of electronic and thermal Energies=	-1110.927109
Sum of electronic and thermal Enthalpies=	-1110.926165
Sum of electronic and thermal Free Energies=	-1110.996971

E(RB3LYP) = -1111.68449988



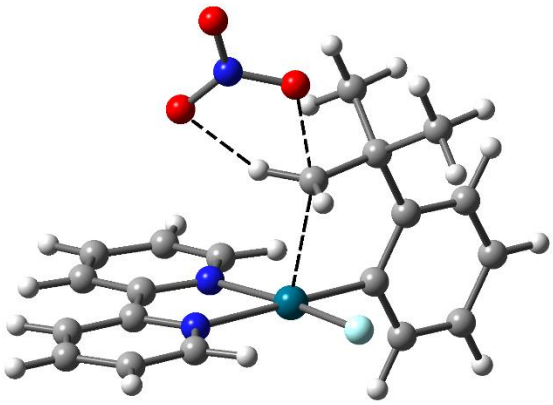
Pd	-0.015203	-0.608746	-0.410503
N	0.855656	1.272618	-0.387562
C	0.174672	2.421368	-0.546716
H	-0.895792	2.336968	-0.673905
C	0.794897	3.665043	-0.537467
H	0.198800	4.559840	-0.672296
C	2.172586	3.719110	-0.348733
H	2.695513	4.669343	-0.335758
C	2.877277	2.532433	-0.162634
C	4.274702	-0.113729	0.236241
C	4.809680	-1.381645	0.467205
H	5.878556	-1.495624	0.614496
C	3.966877	-2.491186	0.505789
H	4.350386	-3.489270	0.683661
C	2.602676	-2.291245	0.304890
H	1.885867	-3.106026	0.312322
C	2.896060	0.015900	0.050925
C	2.206617	1.308012	-0.178322
H	4.929707	0.747409	0.201681
H	3.946399	2.563410	0.002120
N	2.095208	-1.072972	0.087771
C	-1.592232	-0.203813	-1.706794
H	-1.365132	0.802533	-2.063776
H	-1.388075	-0.938829	-2.490823
C	-1.476049	-0.065931	0.873535
C	-1.117362	0.160186	2.195718
C	-2.785054	0.008397	0.394016
C	-2.140903	0.483658	3.097950
H	-0.087755	0.090952	2.533114
C	-3.784919	0.339147	1.319373
C	-3.464029	0.573372	2.658252
H	-1.892747	0.662404	4.140225
H	-4.818007	0.411901	0.989254

H	-4.250509	0.827978	3.362647
C	-2.989626	-0.317886	-1.070551
C	-3.551722	-1.750616	-1.222769
H	-3.686547	-1.989090	-2.284967
H	-2.869222	-2.481779	-0.784828
H	-4.526787	-1.832568	-0.730160
F	-0.569718	-2.470569	-0.362866
C	-3.938528	0.678157	-1.776388
H	-4.956557	0.589954	-1.381236
H	-3.609583	1.714770	-1.645269
H	-3.981469	0.463243	-2.850169
N	-1.232716	2.361758	0.079450

TS_3_NO3

Zero-point correction=	0.370481 (Hartree/Particle)
Thermal correction to Energy=	0.396592
Thermal correction to Enthalpy=	0.397536
Thermal correction to Gibbs Free Energy=	0.311663
Sum of electronic and zero-point Energies=	-1391.373238
Sum of electronic and thermal Energies=	-1391.347127
Sum of electronic and thermal Enthalpies=	-1391.346183
Sum of electronic and thermal Free Energies=	-1391.432055

E(RB3LYP) = -1392.24766541



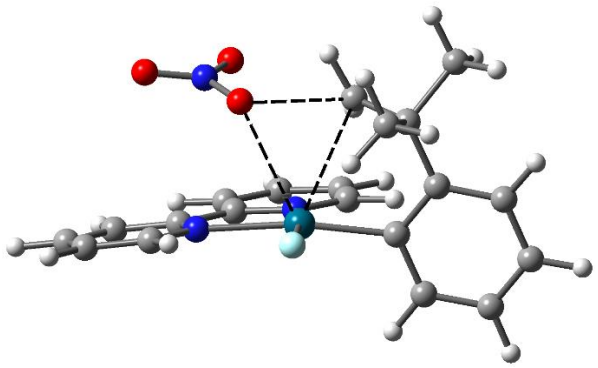
Pd	-0.072034	-0.694706	-0.878512
N	0.634529	-1.370815	0.951687
C	-0.137525	-1.827319	1.954173
H	-1.203952	-1.823554	1.770021
C	0.391710	-2.279088	3.158541
H	-0.274420	-2.635664	3.935724
C	1.773205	-2.256831	3.329638
H	2.225227	-2.597958	4.255011
C	2.575838	-1.789557	2.291815
C	4.179525	-0.773196	-0.060571
C	4.821253	-0.285203	-1.198590
H	5.904230	-0.221550	-1.221876
C	4.063004	0.116307	-2.297257
H	4.528237	0.500086	-3.198094
C	2.675933	0.013136	-2.216530
H	2.019901	0.303200	-3.030963
C	2.783975	-0.848111	-0.046654
C	1.991445	-1.349921	1.101907
H	4.765439	-1.087874	0.793862
H	3.651424	-1.768169	2.411438
N	2.063856	-0.454918	-1.122841
C	-0.745184	1.451131	-0.095353
H	-0.000229	1.325778	0.674837
H	-0.419749	1.763784	-1.077313
C	-2.006472	-1.023480	-0.552380
C	-2.553859	-2.279924	-0.841996
C	-2.819021	0.014867	-0.070286

C	-3.915214	-2.521758	-0.635722
H	-1.918639	-3.074001	-1.229158
C	-4.185315	-0.245159	0.135197
C	-4.729913	-1.499192	-0.142478
H	-4.334474	-3.499291	-0.860571
H	-4.836298	0.538976	0.513312
H	-5.789333	-1.675129	0.023827
C	-2.238206	1.408466	0.227674
C	-2.964641	2.457709	-0.654213
H	-2.579524	3.460454	-0.456557
H	-2.828337	2.231514	-1.717562
H	-4.038242	2.452797	-0.443000
F	-0.521646	-0.073279	-2.697279
C	-2.435395	1.741135	1.728023
H	-3.498955	1.730372	1.984871
H	-1.928503	1.006242	2.363851
H	-2.033757	2.732435	1.951043
O	-0.394907	3.525242	0.344513
N	0.751048	3.753925	0.906051
O	1.072899	4.937688	1.089981
O	1.484689	2.801087	1.241815

TS_3_NO3’

Zero-point correction=	0.369343 (Hartree/Particle)
Thermal correction to Energy=	0.395743
Thermal correction to Enthalpy=	0.396687
Thermal correction to Gibbs Free Energy=	0.311642
Sum of electronic and zero-point Energies=	-1391.346756
Sum of electronic and thermal Energies=	-1391.320356
Sum of electronic and thermal Enthalpies=	-1391.319412
Sum of electronic and thermal Free Energies=	-1391.404456

E(RB3LYP) = -1392.22261284



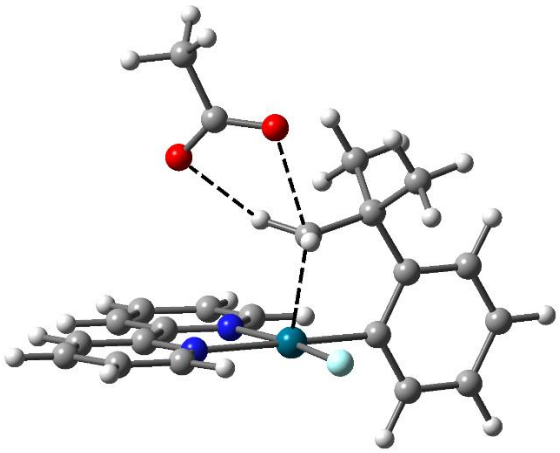
Pd	-0.162206	-0.051912	-0.760838
N	1.959950	-0.327776	-0.996557
N	0.586297	1.557287	0.305998
C	-2.092553	0.490238	-0.750795
F	-0.646377	-1.567707	-1.941200
C	-0.159207	2.468498	0.956897
C	0.399302	3.524423	1.669228
C	1.786121	3.644049	1.705898
C	2.561953	2.708196	1.027127
C	1.947057	1.666100	0.328857
H	-1.232115	2.338401	0.890830
H	-0.248453	4.229215	2.177955
H	2.261321	4.452053	2.252182
H	3.641454	2.788051	1.046878
C	2.537411	-1.305734	-1.701386
C	3.917561	-1.367913	-1.881076
C	4.706382	-0.377815	-1.297280
C	4.100434	0.636714	-0.556826
C	2.709064	0.639279	-0.420297
H	1.856078	-2.037592	-2.122671

H	4.354961	-2.172321	-2.461755
H	5.785203	-0.390173	-1.414237
H	4.708906	1.408666	-0.102457
C	-3.063817	-0.166012	0.029832
C	-4.409897	0.213038	-0.100052
C	-4.793706	1.227881	-0.978573
C	-3.829379	1.883700	-1.744314
C	-2.485959	1.510875	-1.628107
C	-2.642732	-1.302293	0.954801
H	-5.176836	-0.282631	0.488117
H	-5.841524	1.504352	-1.058065
H	-4.116289	2.676353	-2.431032
H	-1.739324	2.021612	-2.233078
C	-3.522696	-1.365327	2.272081
C	-2.727142	-2.676164	0.245896
C	-1.335796	-1.079072	1.593177
H	-3.172014	-2.148575	2.949022
H	-3.547376	-0.408602	2.799944
H	-4.541465	-1.624546	1.967739
H	-2.415115	-3.483470	0.917956
H	-3.760272	-2.861412	-0.064778
H	-2.079699	-2.663065	-0.633636
H	-0.950234	-1.866129	2.218842
H	-0.980398	-0.084404	1.829295
O	0.667958	-2.294230	0.967147
O	1.503872	-0.971750	2.502993
O	2.754987	-2.483050	1.545400
N	1.659911	-1.906969	1.687337

TS_3_OAc

Zero-point correction=	0.405626 (Hartree/Particle)
Thermal correction to Energy=	0.432619
Thermal correction to Enthalpy=	0.433563
Thermal correction to Gibbs Free Energy=	0.346996
Sum of electronic and zero-point Energies=	-1339.519515
Sum of electronic and thermal Energies=	-1339.492522
Sum of electronic and thermal Enthalpies=	-1339.491578
Sum of electronic and thermal Free Energies=	-1339.578145

E(RM06) = -1340.41199468



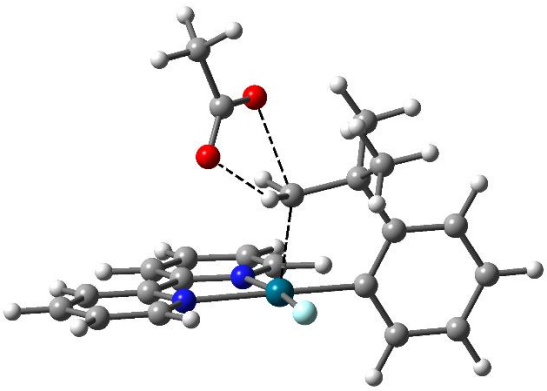
Pd	-0.287422	-0.779857	-0.856119
N	0.382151	-1.352804	1.020816
C	-0.417132	-1.621331	2.068498
H	-1.479050	-1.502528	1.897779
C	0.082314	-2.029819	3.300491
H	-0.603234	-2.233818	4.114831
C	1.460009	-2.165794	3.449166
H	1.889052	-2.482915	4.393805
C	2.288807	-1.890934	2.364190
C	3.951158	-1.234458	-0.075006

C	4.619006	-0.933989	-1.261962
H	5.702934	-0.971482	-1.295257
C	3.886179	-0.585742	-2.395597
H	4.372481	-0.346124	-3.334366
C	2.496844	-0.548223	-2.298335
H	1.858912	-0.284086	-3.135727
C	2.555051	-1.179560	-0.048801
C	1.734908	-1.481504	1.149261
H	4.517656	-1.500097	0.808564
H	3.361066	-1.998771	2.465376
N	1.860658	-0.838220	-1.158179
C	-0.486387	1.353946	-0.307133
H	0.313725	1.342998	0.426827
H	-0.191597	1.677260	-1.298821
C	-2.234809	-0.776409	-0.453176
C	-3.007294	-1.928413	-0.625606
C	-2.807219	0.429176	-0.026184
C	-4.377959	-1.890901	-0.347463
H	-2.548361	-2.851572	-0.973476
C	-4.184230	0.448532	0.250117
C	-4.962318	-0.699878	0.093066
H	-4.982811	-2.784821	-0.476931
H	-4.656408	1.367552	0.588492
H	-6.026181	-0.663502	0.311976
C	-1.925578	1.670523	0.130585
C	-2.469905	2.811797	-0.765617
H	-1.827264	3.689771	-0.674065
H	-2.497226	2.500107	-1.816183
H	-3.488299	3.083426	-0.467296
F	-0.719384	-0.336837	-2.721183
C	-1.917393	2.126235	1.609665
H	-2.932556	2.365608	1.944224
H	-1.524615	1.338967	2.263479
H	-1.290452	3.014803	1.715563
C	2.311912	4.752707	0.982206
H	3.381259	4.552142	1.097121
H	2.153996	5.498252	0.197334
H	1.946843	5.178863	1.925691
C	1.539230	3.452343	0.684207
O	2.006537	2.378493	1.139812
O	0.460357	3.594292	0.022103

TS_3_OAc'

Zero-point correction=	0.405391	(Hartree/Particle)
Thermal correction to Energy=	0.432493	
Thermal correction to Enthalpy=	0.433437	
Thermal correction to Gibbs Free Energy=	0.345967	
Sum of electronic and zero-point Energies=	-1339.518869	
Sum of electronic and thermal Energies=	-1339.491766	
Sum of electronic and thermal Enthalpies=	-1339.490822	
Sum of electronic and thermal Free Energies=	-1339.578292	

E(RB3LYP) = -1340.41011924

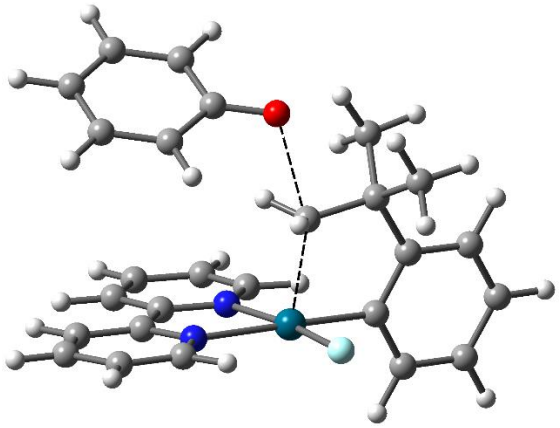


Pd	0.147159	-0.552165	-0.879633
N	-2.020233	-0.477583	-1.009058
N	-0.409252	-1.767831	0.707840
C	2.118693	-0.735220	-0.686011
F	0.451948	0.537584	-2.484310
C	0.451863	-2.402874	1.522759
C	0.025589	-3.218284	2.565655
C	-1.342182	-3.378823	2.770261
C	-2.235167	-2.724629	1.925082
C	-1.753813	-1.918271	0.891325
H	1.503070	-2.245123	1.319151
H	0.758712	-3.709066	3.195274
H	-1.714575	-4.004856	3.574208
H	-3.300891	-2.845099	2.071206
C	-2.724995	0.201729	-1.920298
C	-4.118360	0.196707	-1.925732
C	-4.780752	-0.539891	-0.945257
C	-4.041435	-1.247521	0.002653
C	-2.645787	-1.201136	-0.052274
H	-2.139608	0.752333	-2.649383
H	-4.661124	0.757285	-2.678287
H	-5.865029	-0.567214	-0.913551
H	-4.553418	-1.820804	0.765172
C	2.802525	0.283099	-0.008880
C	4.199496	0.186349	0.097112
C	4.887090	-0.893587	-0.460279
C	4.189871	-1.898645	-1.136310
C	2.797655	-1.817499	-1.252788
C	2.016534	1.463835	0.564267
H	4.759734	0.961177	0.614557
H	5.968468	-0.948973	-0.367355
H	4.723154	-2.738448	-1.574531
H	2.251141	-2.594563	-1.783234
C	2.349408	1.642357	2.067565
C	2.381094	2.753264	-0.209727
C	0.508100	1.204124	0.425655
H	1.767600	2.470524	2.475544
H	2.113041	0.731710	2.631088
H	3.415385	1.854768	2.202931
H	1.831818	3.600609	0.209313
H	3.455107	2.955478	-0.133384
H	2.126668	2.654113	-1.270258
H	-0.100179	1.843464	-0.206582
H	-0.002085	0.806548	1.295568
O	-1.565149	3.402801	-0.198314
C	-1.132663	3.785598	0.916330
C	-1.656876	5.122518	1.477705
H	-2.598204	5.408511	1.000188
H	-1.792341	5.066060	2.562398
H	-0.918298	5.910303	1.281306
O	-0.264088	3.197361	1.640341

TS_3_OPh

Zero-point correction=	0.447566 (Hartree/Particle)
Thermal correction to Energy=	0.475843
Thermal correction to Enthalpy=	0.476787
Thermal correction to Gibbs Free Energy=	0.385483
Sum of electronic and zero-point Energies=	-1417.845882
Sum of electronic and thermal Energies=	-1417.817606
Sum of electronic and thermal Enthalpies=	-1417.816662
Sum of electronic and thermal Free Energies=	-1417.907966

E(RB3LYP) = -1418.80070200



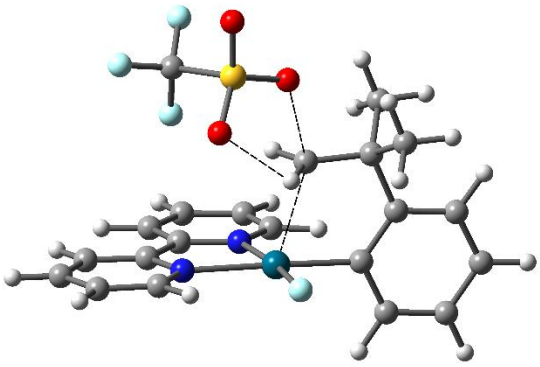
Pd	-0.938662	-0.846153	-0.730760
N	-0.304313	-1.445047	1.150738
C	-1.031650	-1.321947	2.275253
H	-2.006666	-0.866113	2.161705
C	-0.566605	-1.753319	3.512804
H	-1.190248	-1.632040	4.390913
C	0.697265	-2.333030	3.584476
H	1.096223	-2.682270	4.530972
C	1.451172	-2.461986	2.420413
C	2.963830	-2.658457	-0.193934
C	3.567893	-2.703190	-1.450418
H	4.562961	-3.122960	-1.555441
C	2.886426	-2.206912	-2.560776
H	3.325640	-2.226268	-3.551667
C	1.612611	-1.675741	-2.371069
H	1.020626	-1.270149	-3.185269
C	1.682278	-2.113436	-0.075591
C	0.937319	-2.010797	1.202784
H	3.491761	-3.041821	0.670137
H	2.434092	-2.913122	2.464090
N	1.037826	-1.633540	-1.164124
C	-0.448405	1.263168	-0.377420
H	0.215237	1.120164	0.467200
H	0.059083	1.389405	-1.324797
C	-2.757863	-0.220197	-0.222382
C	-3.828762	-1.114187	-0.145090
C	-2.931175	1.152116	-0.003497
C	-5.105533	-0.634917	0.169705
H	-3.676721	-2.175788	-0.329054
C	-4.218556	1.615462	0.311190
C	-5.295814	0.731091	0.397155
H	-5.943453	-1.324604	0.231857
H	-4.384622	2.675553	0.487049
H	-6.285084	1.109440	0.640545
C	-1.726879	2.082532	-0.127956
C	-1.929707	3.054277	-1.315311
H	-1.058191	3.707921	-1.403031
H	-2.055219	2.501448	-2.252761
H	-2.823123	3.669396	-1.160282
F	-1.378310	-0.441697	-2.601498
C	-1.535390	2.890935	1.179455
H	-2.397249	3.542408	1.361447
H	-1.430136	2.222019	2.042089
H	-0.632657	3.499305	1.089608
O	1.165573	3.194180	-0.433532
C	2.338143	2.807659	-0.034604
C	3.227864	2.061606	-0.875279
C	2.835003	3.105214	1.276620
C	4.492024	1.665136	-0.443835
H	2.890363	1.820842	-1.882257
C	4.103094	2.708647	1.692493

H	2.189284	3.672972	1.944343
C	4.949669	1.982759	0.842315
H	5.134360	1.103228	-1.120834
H	4.440428	2.966962	2.695711
H	5.937865	1.674133	1.173131

TS_3_OTf

Zero-point correction=	0.383429 (Hartree/Particle)
Thermal correction to Energy=	0.413841
Thermal correction to Enthalpy=	0.414785
Thermal correction to Gibbs Free Energy=	0.318786
Sum of electronic and zero-point Energies=	-2072.493171
Sum of electronic and thermal Energies=	-2072.462759
Sum of electronic and thermal Enthalpies=	-2072.461815
Sum of electronic and thermal Free Energies=	-2072.557814

E(RB3LYP) = -2073.54786225



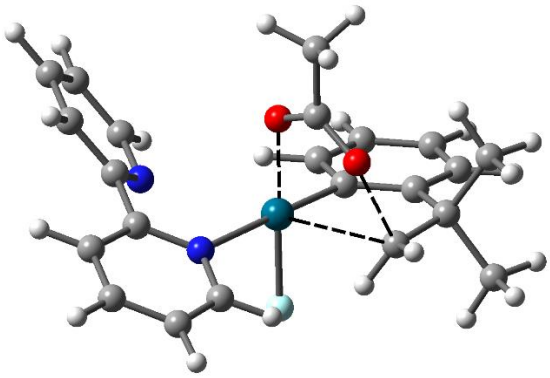
Pd	1.074785	0.765546	-0.871462
N	0.888593	1.799918	0.915825
C	1.734509	1.701679	1.957019
H	2.560563	1.013763	1.832014
C	1.568700	2.436551	3.126429
H	2.278673	2.319760	3.937169
C	0.486524	3.307599	3.219074
H	0.322099	3.898397	4.114065
C	-0.389286	3.415033	2.141450
C	-2.192657	3.535971	-0.284855
C	-2.951600	3.518480	-1.454880
H	-3.831884	4.147709	-1.536414
C	-2.570587	2.690864	-2.509958
H	-3.136755	2.651885	-3.433683
C	-1.432782	1.902100	-2.354090
H	-1.073014	1.233092	-3.129113
C	-1.062042	2.719211	-0.195789
C	-0.175178	2.653167	0.990728
H	-2.485577	4.177568	0.536742
H	-1.232902	4.090972	2.198901
N	-0.707668	1.921708	-1.229915
C	0.269343	-1.442832	-0.009265
H	-0.150135	-0.805650	0.753145
H	-0.147744	-1.414745	-1.005025
C	2.772851	-0.190432	-0.453645
C	3.983396	0.475533	-0.699208
C	2.784152	-1.507753	0.036905
C	5.208047	-0.148702	-0.449257
H	3.971126	1.491772	-1.088083
C	4.024823	-2.122142	0.286988
C	5.225027	-1.453672	0.048843
H	6.138416	0.379100	-0.643738
H	4.059473	-3.139028	0.669052
H	6.169018	-1.953015	0.250023
C	1.485808	-2.300945	0.300230

C	1.462635	-3.550920	-0.616497
H	0.559923	-4.139896	-0.439654
H	1.491515	-3.258847	-1.671936
H	2.333233	-4.181727	-0.416098
F	1.077977	-0.067899	-2.663103
C	1.432483	-2.719481	1.792336
H	2.298601	-3.337397	2.044807
H	1.444034	-1.839173	2.445192
H	0.527469	-3.295101	1.998529
O	-1.219210	-2.752269	0.481106
O	-2.498103	-1.814041	-1.458293
C	-3.301022	-1.200191	0.984400
O	-3.476094	-3.642517	-0.025457
F	-2.505732	-0.112398	1.016798
F	-4.507847	-0.829339	0.546036
F	-3.415606	-1.676699	2.227485
S	-2.579590	-2.485813	-0.149723

TS_I

Zero-point correction=	0.404542 (Hartree/Particle)
Thermal correction to Energy=	0.431885
Thermal correction to Enthalpy=	0.432829
Thermal correction to Gibbs Free Energy=	0.344910
Sum of electronic and zero-point Energies=	-1339.497554
Sum of electronic and thermal Energies=	-1339.470212
Sum of electronic and thermal Enthalpies=	-1339.469268
Sum of electronic and thermal Free Energies=	-1339.557186

E(RB3LYP) = -1340.37840901



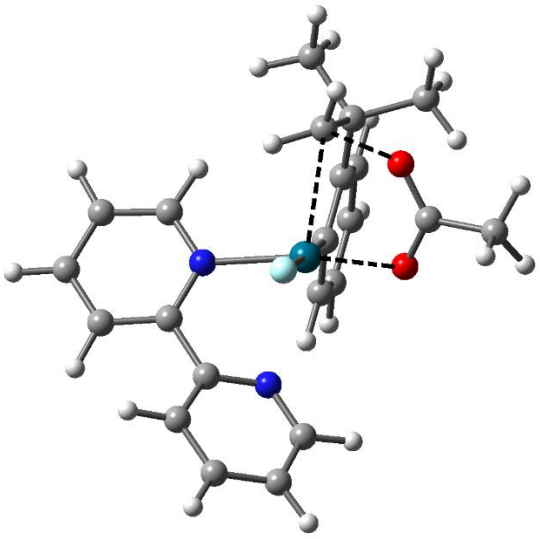
Pd	0.151387	-0.042253	-0.476234
N	-2.144112	1.648784	-0.647453
N	-1.791335	-1.161104	-0.631929
C	1.863290	0.967576	-0.394329
F	0.468249	-0.307786	-2.439571
C	-1.739297	-2.460737	-0.967868
C	-2.868280	-3.268922	-1.068268
C	-4.113490	-2.698323	-0.811803
C	-4.176343	-1.349930	-0.470695
C	-2.996535	-0.599253	-0.384757
H	-0.750819	-2.863935	-1.159300
H	-2.764850	-4.312845	-1.343048
H	-5.022162	-3.287414	-0.886797
H	-5.133355	-0.871152	-0.297424
C	-2.181857	2.959378	-0.379136
C	-3.096443	3.541636	0.500383
C	-4.017743	2.711133	1.136295
C	-3.994336	1.344733	0.861228
C	-3.042913	0.850026	-0.041799
H	-1.448230	3.573676	-0.896223
H	-3.080196	4.611861	0.678177
H	-4.740685	3.116000	1.837951
H	-4.688138	0.672855	1.354939

C	3.106505	0.349373	-0.162777
C	4.268174	1.142189	-0.184801
C	4.210445	2.513696	-0.428527
C	2.974828	3.122582	-0.658466
C	1.812618	2.346688	-0.643114
C	3.222146	-1.142838	0.148415
H	5.237977	0.682881	-0.007260
H	5.124936	3.100714	-0.439042
H	2.913756	4.191203	-0.850369
H	0.852917	2.822595	-0.830019
C	4.170441	-1.849541	-0.891668
C	3.793099	-1.374815	1.563892
C	1.960114	-1.909280	-0.089641
H	4.231278	-2.927337	-0.707698
H	3.838068	-1.679413	-1.919633
H	5.177676	-1.435301	-0.781920
H	3.856110	-2.445822	1.786631
H	4.799446	-0.952538	1.640252
H	3.164673	-0.902993	2.322118
H	1.939047	-2.913920	0.310306
H	1.500605	-1.818865	-1.069006
O	0.831230	-1.860312	1.741482
C	0.235299	-0.854223	2.222569
O	-0.128930	0.169641	1.559471
C	-0.048749	-0.845477	3.714162
H	0.814629	-0.411011	4.231866
H	-0.926433	-0.235121	3.936626
H	-0.190419	-1.862866	4.084074

TS_III

Zero-point correction=	0.404906 (Hartree/Particle)
Thermal correction to Energy=	0.431990
Thermal correction to Enthalpy=	0.432934
Thermal correction to Gibbs Free Energy=	0.346631
Sum of electronic and zero-point Energies=	-1339.492284
Sum of electronic and thermal Energies=	-1339.465199
Sum of electronic and thermal Enthalpies=	-1339.464255
Sum of electronic and thermal Free Energies=	-1339.550559

E(RB3LYP) = -1340.37649822



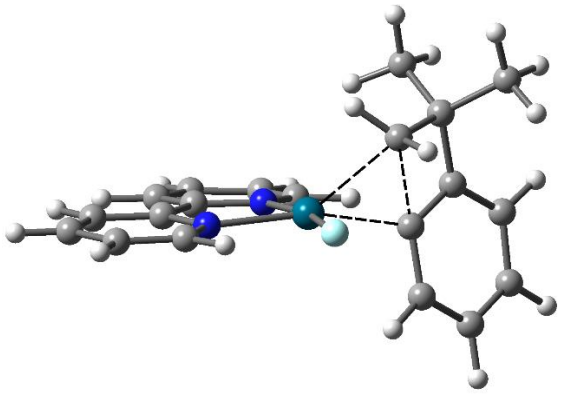
Pd	-0.004444	0.459967	-0.229278
N	2.339498	0.582717	1.077427
N	1.117704	-1.296743	-0.651799
C	-1.147660	-0.561480	1.051067
F	1.130126	1.473701	-1.616461
C	0.550104	-2.403339	-1.160781

C	1.272880	-3.534052	-1.523263
C	2.652807	-3.524656	-1.334861
C	3.243914	-2.391355	-0.785043
C	2.460191	-1.280453	-0.449364
H	-0.526832	-2.381637	-1.275707
H	0.756175	-4.393397	-1.935403
H	3.257413	-4.387647	-1.594535
H	4.309339	-2.370525	-0.588604
C	2.868716	1.655612	1.675082
C	4.157766	2.122034	1.410869
C	4.927266	1.434991	0.472956
C	4.385929	0.314200	-0.155096
C	3.083072	-0.080770	0.174961
H	2.232807	2.160957	2.398373
H	4.539636	2.997904	1.924931
H	5.931042	1.767475	0.226604
H	4.955834	-0.222748	-0.905336
C	-2.466767	-0.930471	0.715699
C	-3.218972	-1.671400	1.646023
C	-2.689633	-2.042659	2.880904
C	-1.383455	-1.673653	3.210771
C	-0.622432	-0.940763	2.296410
C	-3.123599	-0.491878	-0.595996
H	-4.239777	-1.961024	1.408218
H	-3.294585	-2.615011	3.579160
H	-0.958288	-1.954911	4.171533
H	0.396981	-0.658428	2.546116
C	-3.750060	-1.721800	-1.354456
C	-4.258920	0.519621	-0.316802
C	-2.168645	0.011626	-1.636312
H	-4.193440	-1.415915	-2.307424
H	-3.012250	-2.507110	-1.542510
H	-4.548445	-2.145175	-0.737517
H	-4.708760	0.872282	-1.251262
H	-5.040980	0.044971	0.283214
H	-3.885677	1.384381	0.235951
H	-2.633010	0.460904	-2.502386
H	-1.311545	-0.594492	-1.906173
O	-2.059763	2.197905	-1.543788
C	-1.611587	2.785152	-0.525018
O	-0.862920	2.247897	0.354753
C	-1.953187	4.252022	-0.323726
H	-2.887875	4.503493	-0.827946
H	-2.020651	4.488029	0.740829
H	-1.149143	4.858453	-0.756413

TS_CC

Zero-point correction=	0.354954 (Hartree/Particle)
Thermal correction to Energy=	0.376206
Thermal correction to Enthalpy=	0.377151
Thermal correction to Gibbs Free Energy=	0.305220
Sum of electronic and zero-point Energies=	-1110.923590
Sum of electronic and thermal Energies=	-1110.902337
Sum of electronic and thermal Enthalpies=	-1110.901393
Sum of electronic and thermal Free Energies=	-1110.973324

E(RB3LYP) = -1111.66030943



Pd	-0.209105	-0.772821	-0.052371
N	-0.654584	1.251859	-0.057723
C	0.219395	2.264352	-0.190110
H	1.261130	1.991214	-0.284087
C	-0.179672	3.597342	-0.209338
H	0.568323	4.374549	-0.314153
C	-1.534227	3.893943	-0.092434
H	-1.882161	4.921314	-0.096906
C	-2.446870	2.846881	0.012764
C	-4.283186	0.425954	0.140094
C	-5.022083	-0.756743	0.117506
H	-6.103792	-0.718241	0.190474
C	-4.362676	-1.979267	0.000715
H	-4.904892	-2.917419	-0.022349
C	-2.973115	-1.982011	-0.083324
H	-2.381683	-2.886706	-0.165720
C	-2.892433	0.361696	0.044574
C	-1.991445	1.528412	0.016567
H	-4.788476	1.379166	0.231735
H	-3.507184	3.055845	0.077508
N	-2.273013	-0.840018	-0.060857
C	1.633284	-1.210751	1.321436
H	0.789792	-1.204087	2.018484
H	1.974142	-2.225705	1.136605
C	1.872721	-0.578270	-0.561227
C	1.920947	-0.872340	-1.931218
C	2.924518	0.104444	0.070441
C	2.971378	-0.318634	-2.676409
H	1.162708	-1.472875	-2.422583
C	3.984440	0.619782	-0.672874
C	3.976737	0.436276	-2.060593
H	3.003685	-0.486686	-3.749251
H	4.817842	1.118986	-0.185965
H	4.783591	0.844530	-2.662373
C	2.738803	-0.166462	1.545110
C	3.979862	-0.837668	2.173754
H	3.748030	-1.205999	3.179200
H	4.331923	-1.678065	1.566546
H	4.795514	-0.111564	2.259549
F	-0.125483	-2.720171	-0.188992
C	2.297025	1.023439	2.411954
H	3.059051	1.809910	2.398885
H	1.353582	1.456861	2.069484
H	2.159802	0.701138	3.450654