

ELECTRONIC SUPPLEMENTARY INFORMATION FOR

**Understanding alkali-metal driven hydrophosphorylation:
mechanism and challenges in the Pudovik reaction**

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SUPPORTING INFORMATION

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1. Alkali metal cation/proton exchange between M-HMDs and R₂P(O)H

Figure S1 depicts the Gibbs energy profile for the three alkali cations (M = Li, Na, K; R = Mes) and **Figure S2** the influence of the P-substituent (M = K; R = Mes, Mes/Ph, Ph, Cy and OEt).

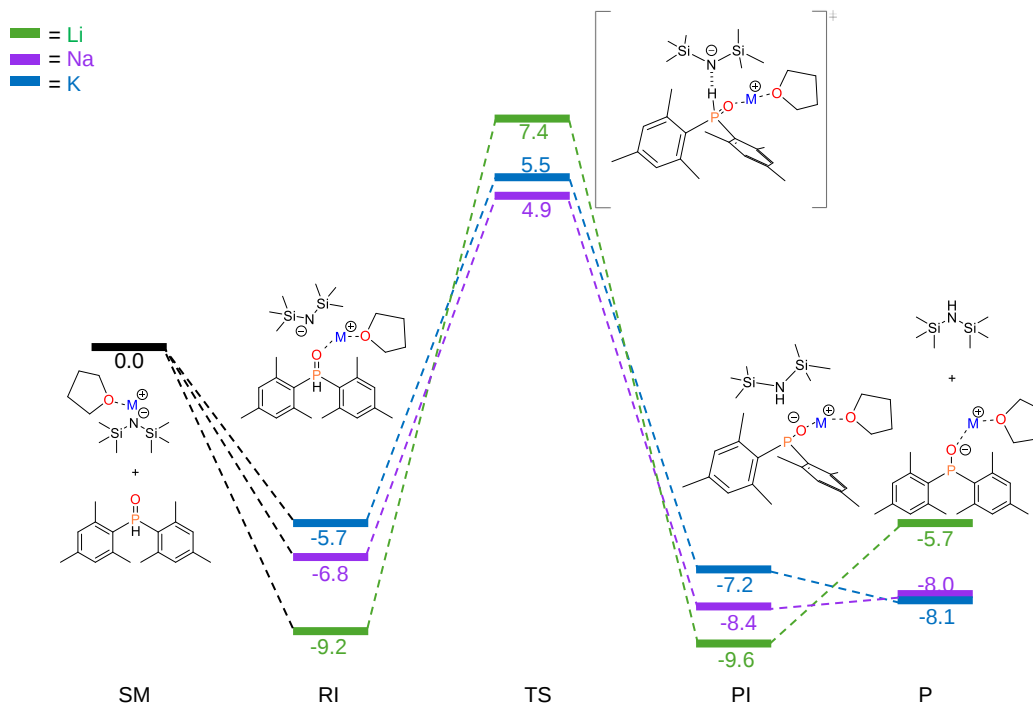


Figure S1: Gibbs energy profile in THF (ΔG_{THF} kcal mol⁻¹) at 298 K for the proton transfer step for the generation of M-OPMes₂ active species considering monosolvated structures (M = Li (green), Na (purple), K (blue)).

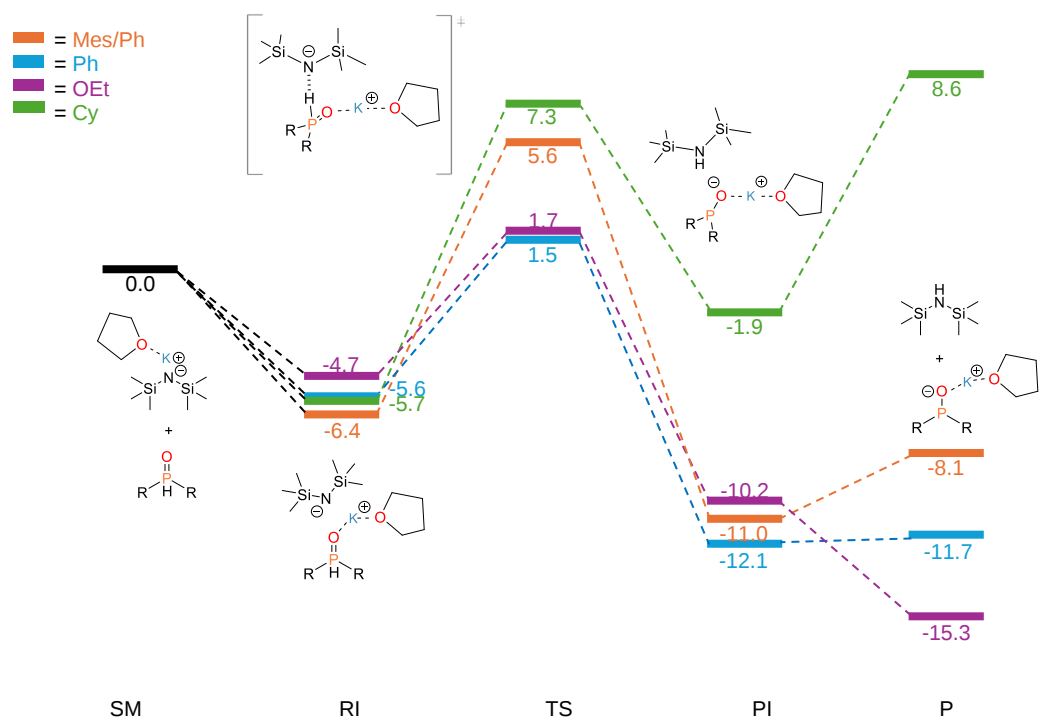


Figure S2: Gibbs energy profile in THF (ΔG_{THF} kcal mol⁻¹) at 298 K for the proton transfer step for the generation of K-OPR₂ active species considering monosolvated structures (R = Mes/Ph (orange), Ph (blue), Cy (green), OEt (purple)).

2. Markovnikov vs. anti-Markovnikov addition

The Gibbs energy profile comparing both the addition of the P-nucleophile to the terminal (anti-Markovnikov) and internal (Markovnikov) carbon of the triple bond is depicted in **Figure S3**, whilst the optimized structures for the transition states are illustrated in **Figure S4**.

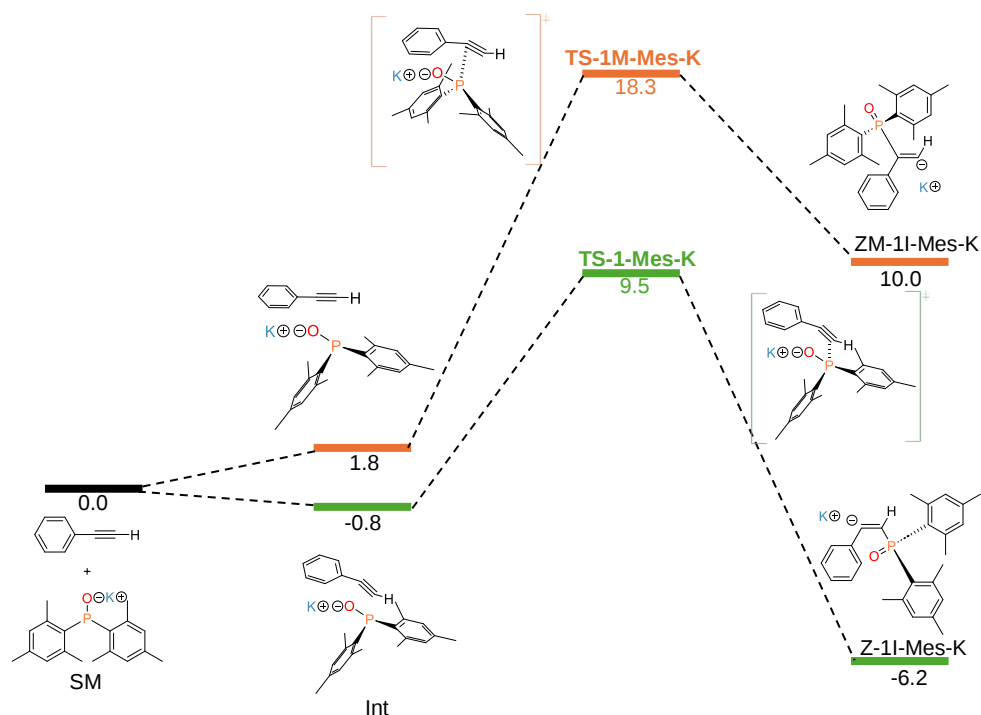


Figure S3: Computed Gibbs energy profile in THF (ΔG_{THF} kcal mol⁻¹) at 298 K for the two nucleophilic attacks leading to formation of anti-Markovnikov intermediate (**TS-1-Mes-K**; green) and the formation of the Markovnikov intermediate (**TS-1M-Mes-K**; orange) in the case of potassium metal-mediated Pudovik reaction (SM = starting materials, Int = initial intermediate).

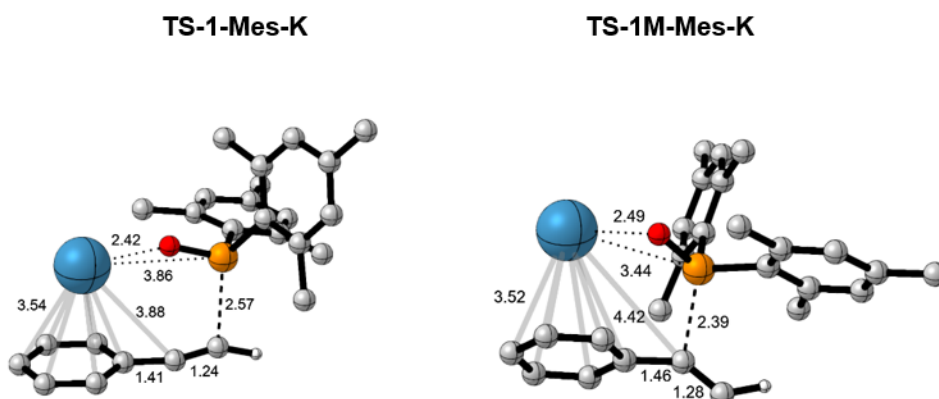


Figure S4: Optimised structures for the transition states for Markovnikov (right) vs anti-Markovnikov (left) additions. Certain hydrogen atoms are omitted for clarity reasons. The distances presented are given in Å.

3. Comparison of Mes₂P(O)H and H-HMDS as protonating agents

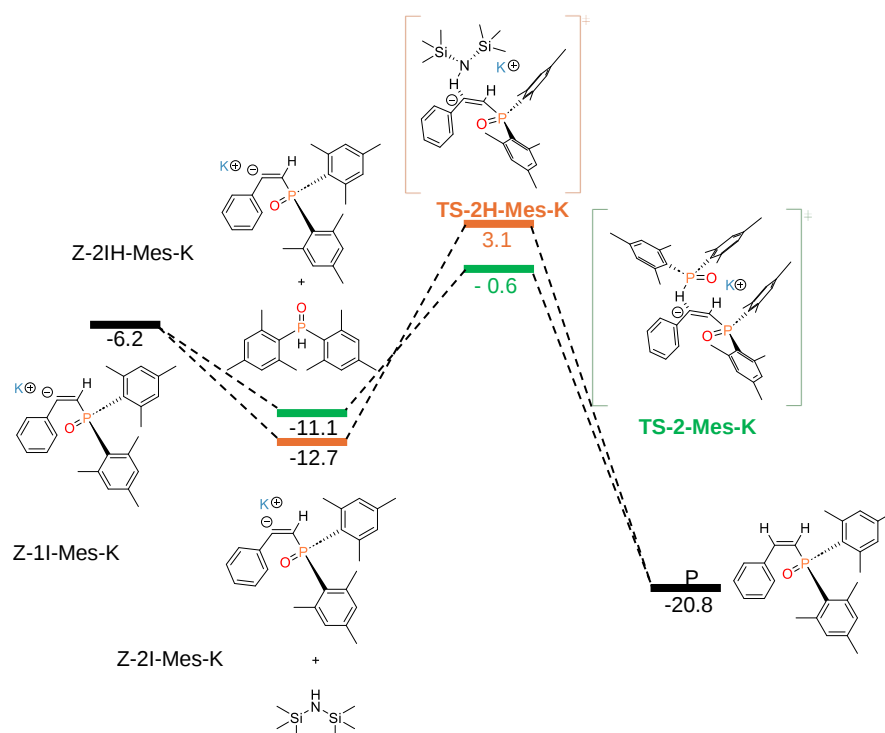


Figure S5: Computed Gibbs energy diagram comparing H-HMDS (orange) vs Mes₂P(O)H (green) as possible proton donors for the proton step in potassium metal-mediated Pudovik reaction which yields the Z-dimesityl(styryl)phosphine oxide.

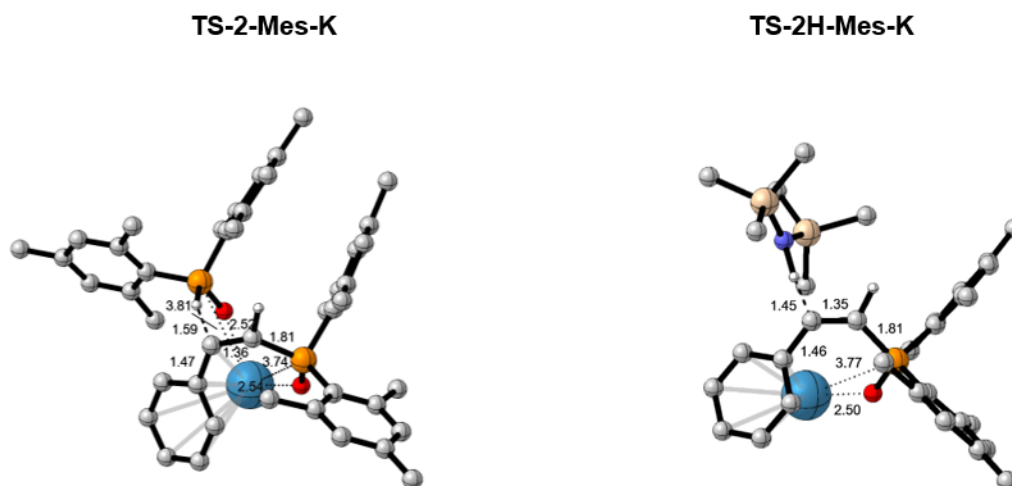


Figure S6: Optimised structures of the transition states involved in the protonation step for potassium metal-mediated Pudovik reaction for formation of Z-dimesityl(styryl)phosphine oxide. Left: Mes₂-P(O)H as the proton donor (**TS-2-Mes-K**); right: H-HMDS as the proton donor (**TS-2H-Mes-K**). Certain H atoms are omitted for clarity reasons. The distances presented are given in Å.

4. Influence of explicit THF solvent molecules in the nucleophilic addition and protonation steps

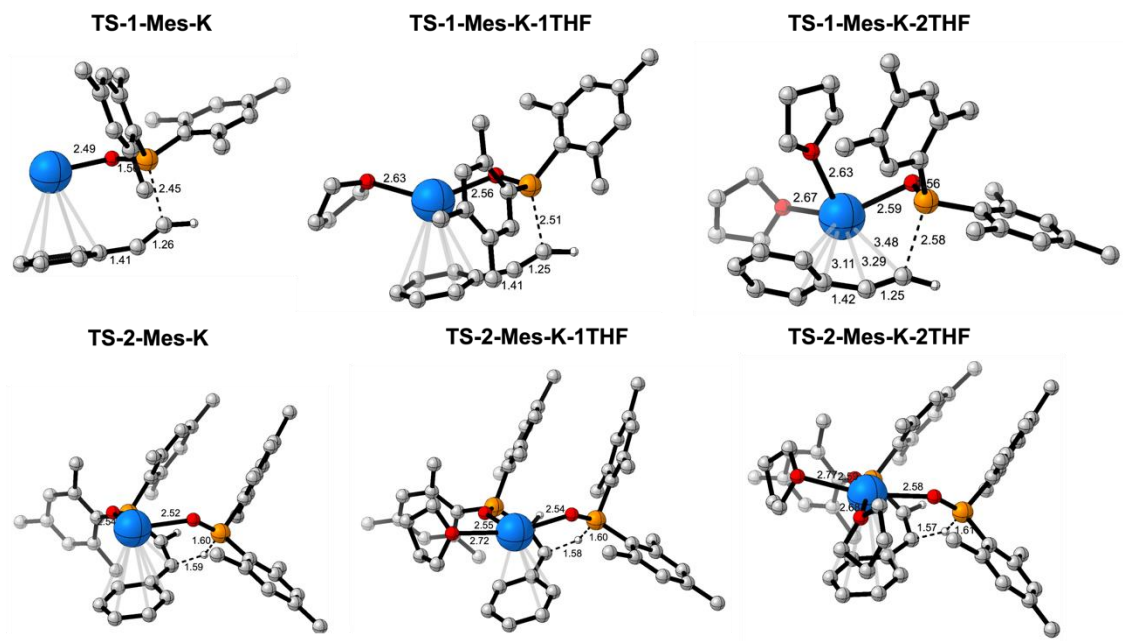


Figure S7: Optimised structures of the transition states for the nucleophilic addition (TS-1-Mes) and protonation (TS-2-Mes) steps for the potassium metal-mediated formation of Z-dimesityl(styryl)phosphine oxide. Left: no explicit THF molecules solvating the cation; middle: one explicit THF molecules solvating the cation; right: two explicit THF molecules solvating the cation.

5. Bishydrophosphorylation with Mes₂P(O)H

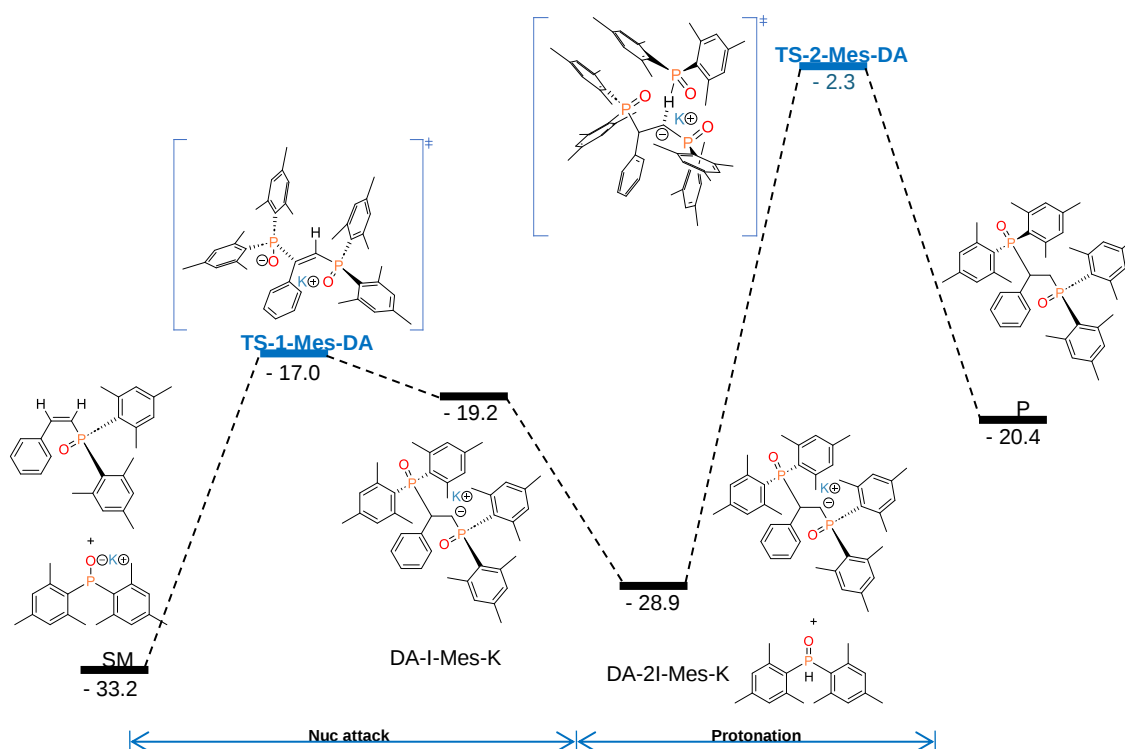


Figure S8: Computed Gibbs energy profile in THF (ΔG_{THF} kcal mol⁻¹) at 298 K for the second addition steps of the bishydrophosphorylation of phenylacetylene catalysed by potassium dimesityl phosphinite.

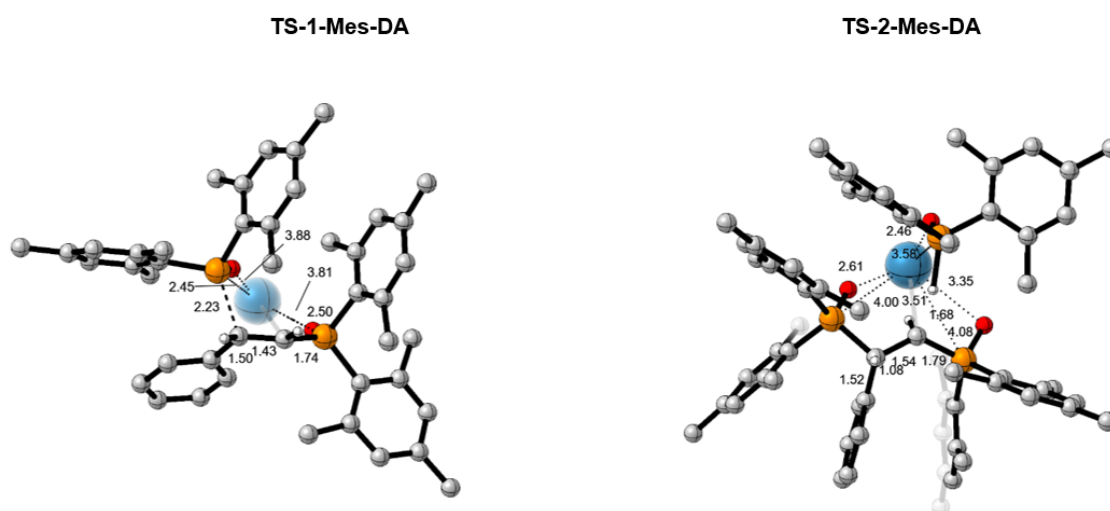


Figure S9: Optimised structures for the transition states involved in the potassium-mediated hydrophosphorylation of phenylacetylene yielding bishydrophosphorylated alkane from Z-dimesityl(styryl)phosphine oxide. Certain H atoms are omitted for clarity reasons. The distances presented are given in Å.

6. Influence of the alkali metal cation in the hydrophosphorylation reaction catalysed by M-OPMes₂

6.1 Sodium (Na-OPMes₂)

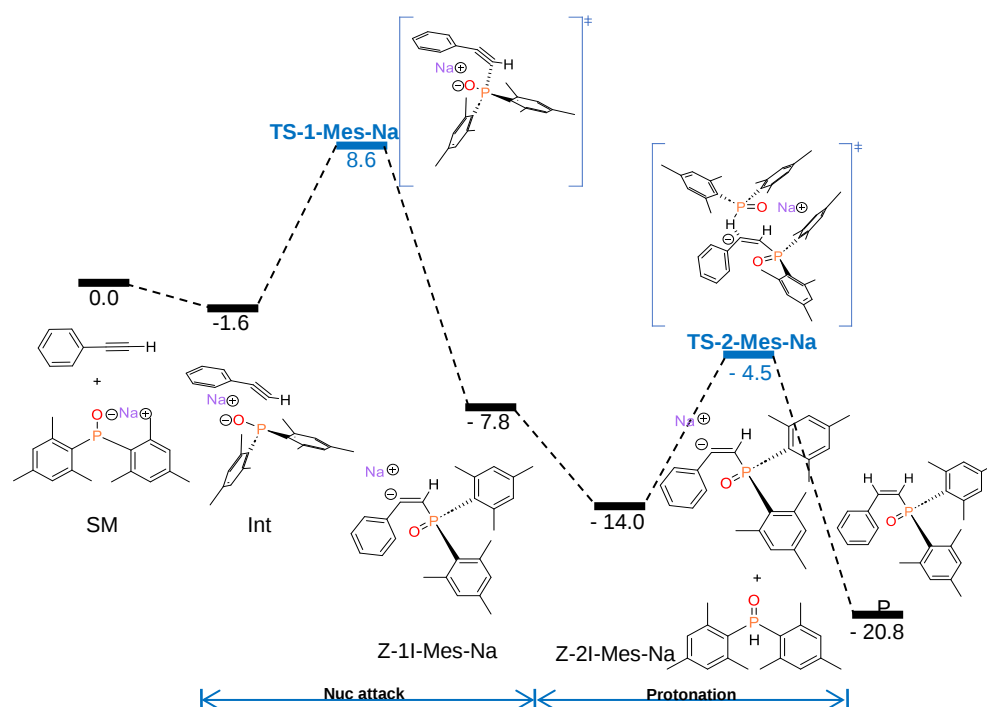


Figure S10: Computed Gibbs energy profile in THF (ΔG_{THF} kcal mol⁻¹) at 298 K for the hydrophosphorylation of phenylacetylene generating Z-dimesityl(styryl)phosphine oxide, catalysed by sodium dimesitylphosphinite.

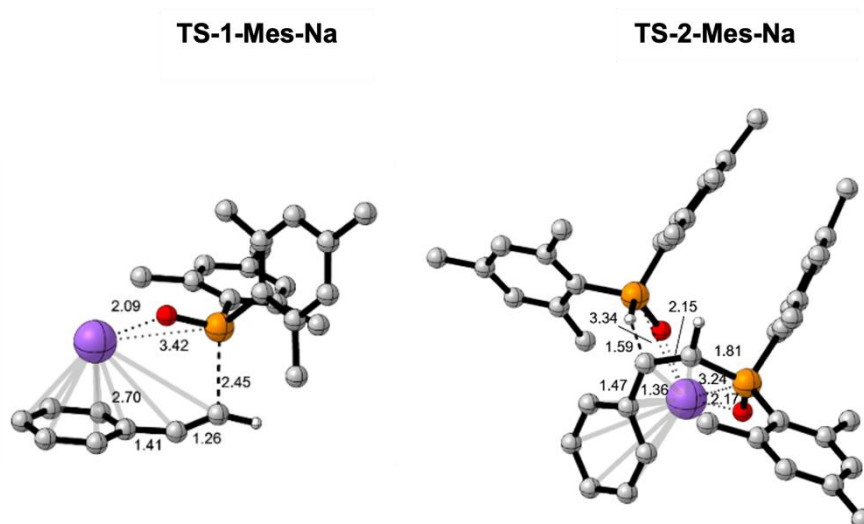


Figure S11: Optimised structures for the transition states involved in the sodium metal-mediated Pudovik reaction for formation of Z-dimesityl(styryl)phosphine oxide. Certain H atoms are omitted for clarity reasons. The distances presented are given in Å.

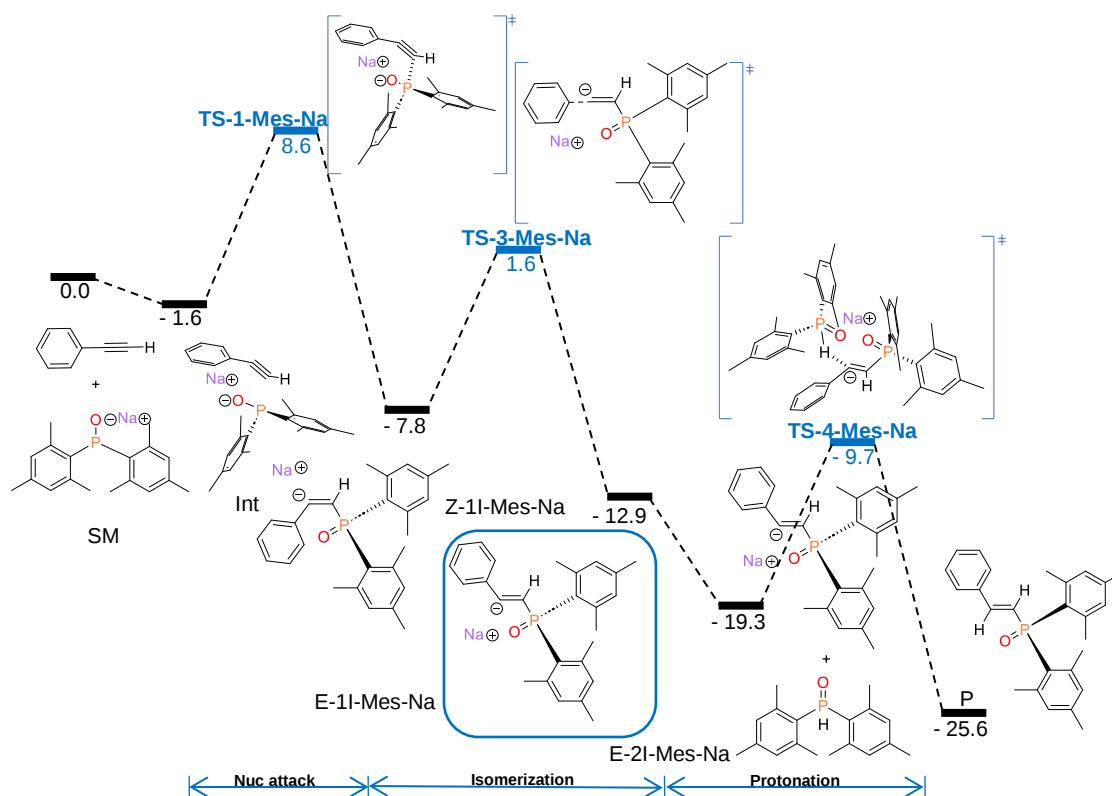


Figure S12: Computed Gibbs energy profile in THF (ΔG_{THF} kcal mol⁻¹) at 298 K for the hydrophosphorylation of phenylacetylene generating *E*-dimesityl(styryl)phosphine oxide, catalysed by sodium dimesitylphosphinite.

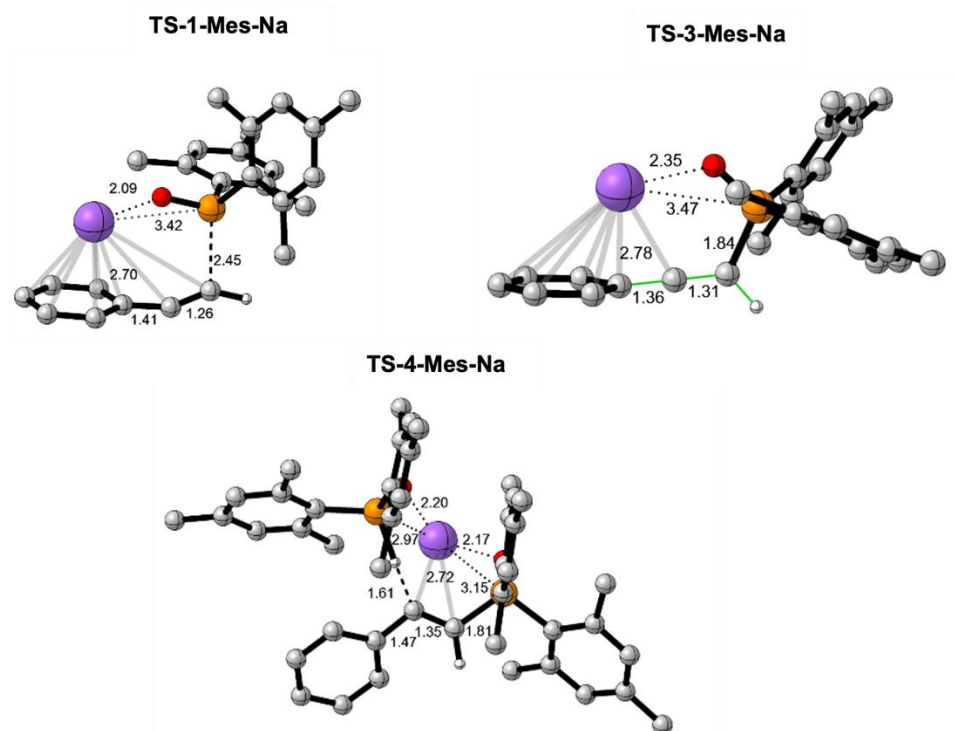


Figure S13: Optimised structures for the transition states involved in the sodium metal-mediated formation of *E*-dimesityl(styryl)phosphine.

6.2 Lithium (Li-OPMe_2)

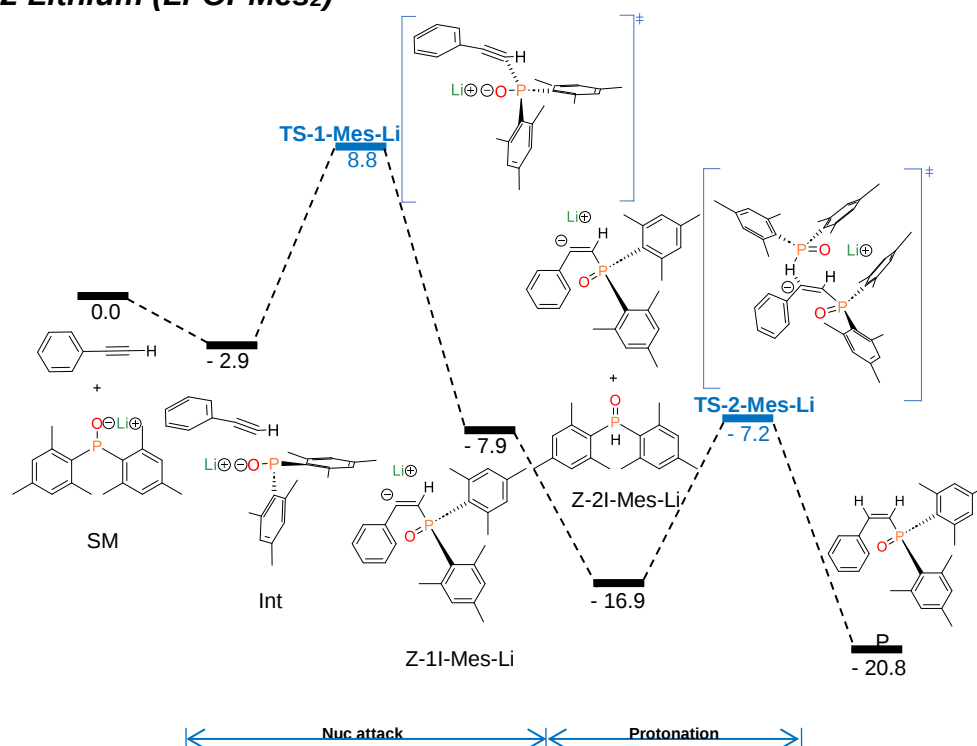


Figure S14: Computed Gibbs energy profile in THF (ΔG_{THF} kcal mol⁻¹) at 298 K for the hydrophosphorylation of phenylacetylene generating Z-dimesityl(styryl)phosphine oxide, catalysed by lithium dimesitylphosphinite.

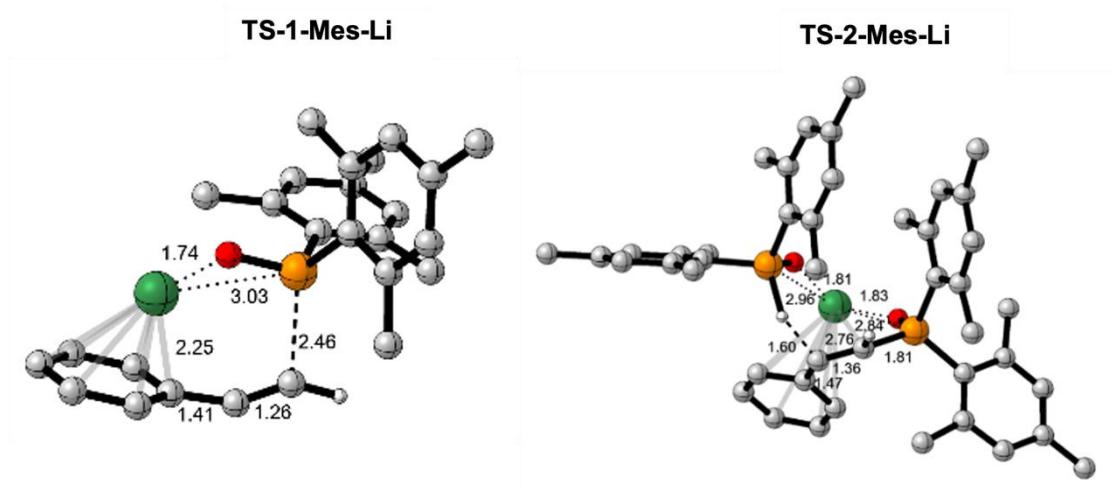


Figure S15: Optimised structures for the transition states involved in the lithium metal-mediated formation of Z-dimesityl(styryl)phosphine oxide. Certain H atoms are omitted for clarity reasons. The distances presented are given in Å.

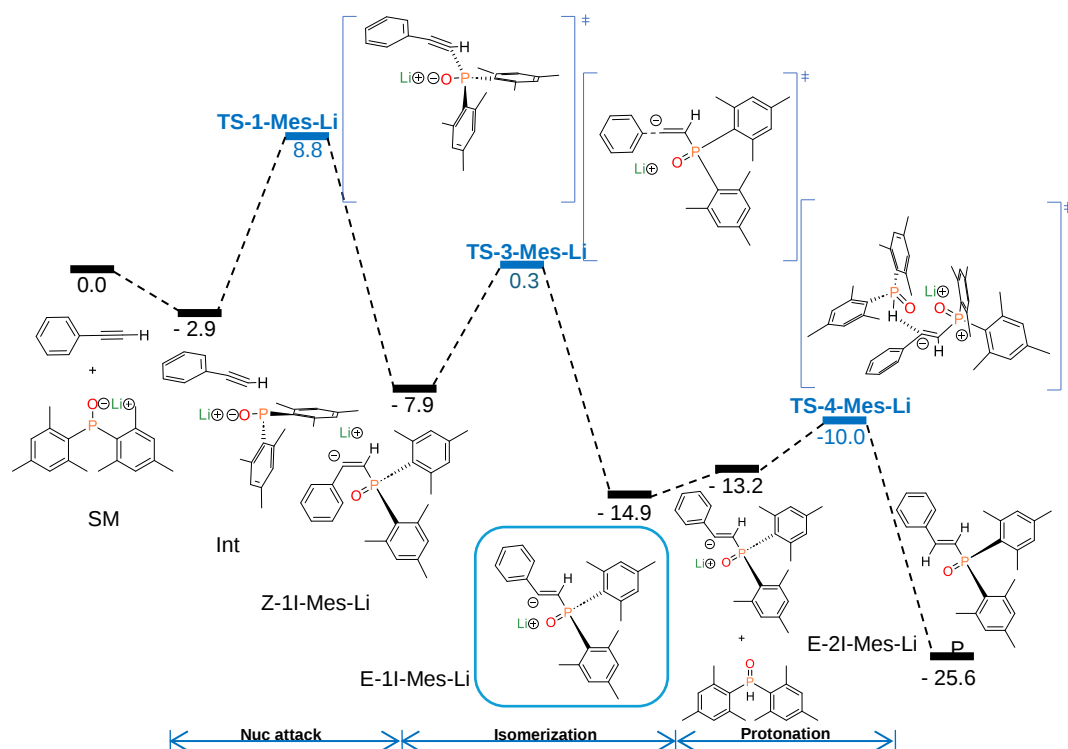


Figure S16: Computed Gibbs energy profile in THF (ΔG_{THF} kcal mol⁻¹) at 298 K for the hydrophosphorylation of phenylacetylene generating *E*-dimesityl(styryl)phosphine oxide, catalysed by lithium dimesitylphosphinite.

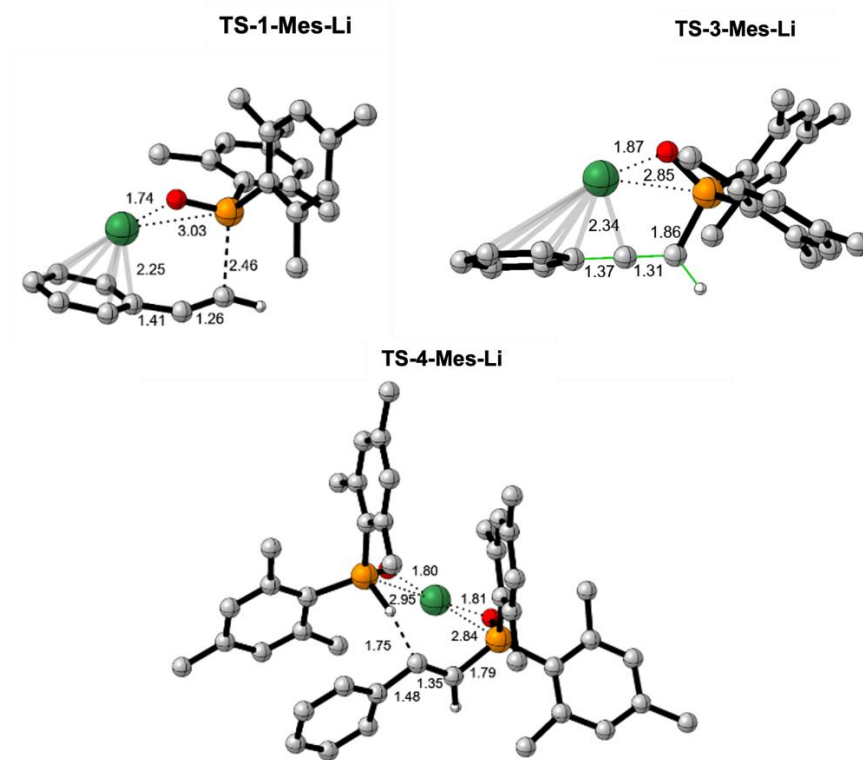


Figure S17: Optimised structures for the transition states involved in the lithium metal-mediated formation of *E*-dimesityl(styryl)phosphine.

7. Dimesitylphosphine oxide as a nucleophile

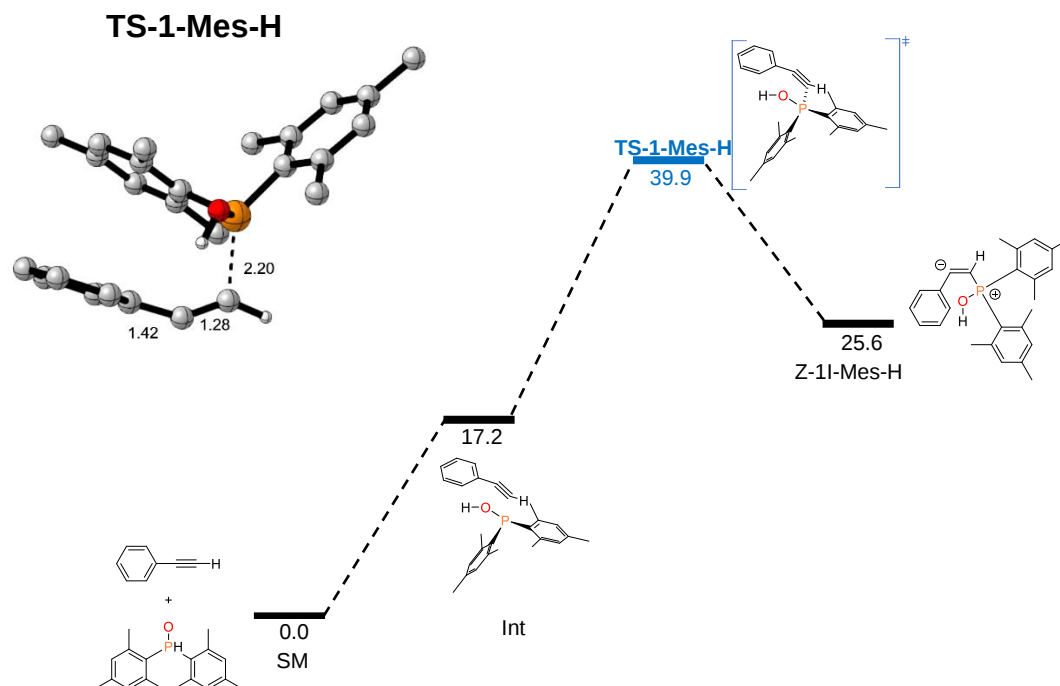


Figure S18: Computed Gibbs energy profile in THF (ΔG_{THF} kcal mol⁻¹) at 298 K for the nucleophilic addition step with Mes₂P(O)H as a nucleophile.

8. Influence of the P-bound group R in the hydrophosphorylation reaction catalysed by K-OPR₂

8.1 R = Ph (K-OPPh₂)

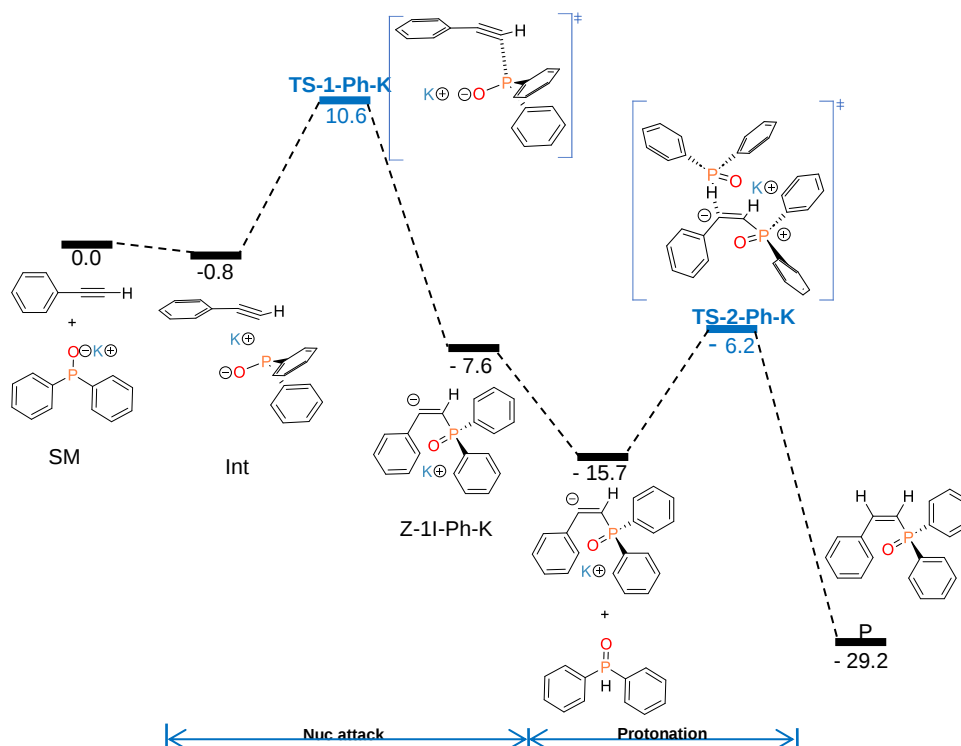


Figure S19: Computed Gibbs energy profile in THF (ΔG_{THF} kcal mol⁻¹) at 298 K for the hydrophosphorylation of phenylacetylene generating Z-diphenyl(styryl)phosphine oxide, catalysed by potassium diphenylphosphinite.

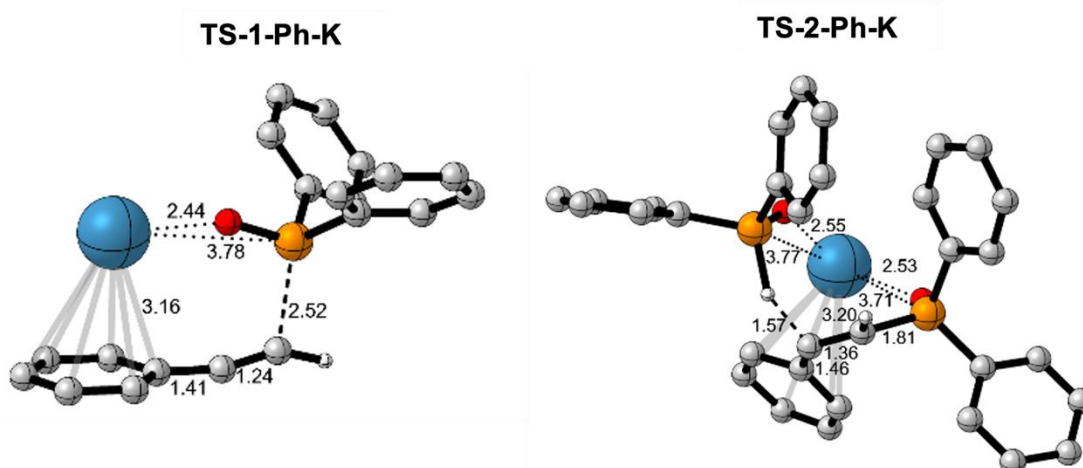


Figure S20: Optimised structures for the transition states of the potassium metal-mediated formation of Z-diphenyl(styryl)phosphine oxide. Certain H atoms are omitted for clarity reasons. The distances presented are given in Å.

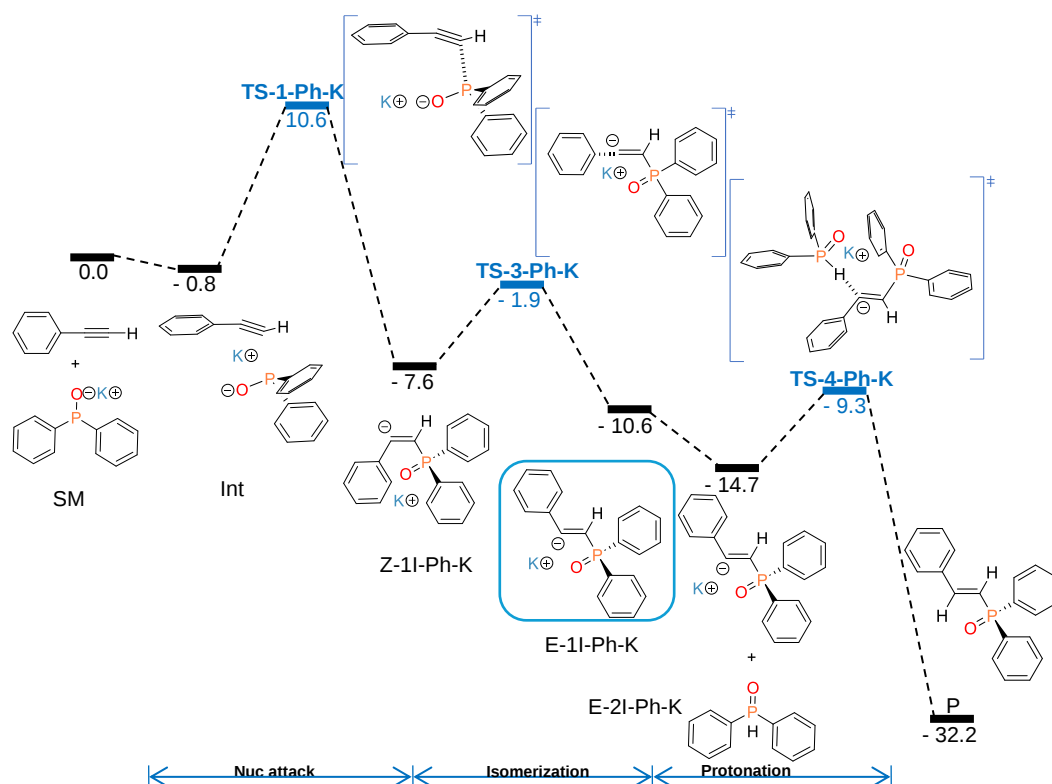


Figure S21: Computed Gibbs energy profile in THF (ΔG_{THF} kcal mol⁻¹) at 298 K for the hydrophosphorylation of phenylacetylene generating *E*-diphenyl(styryl)phosphine oxide, catalysed by potassium diphenylphosphinite.

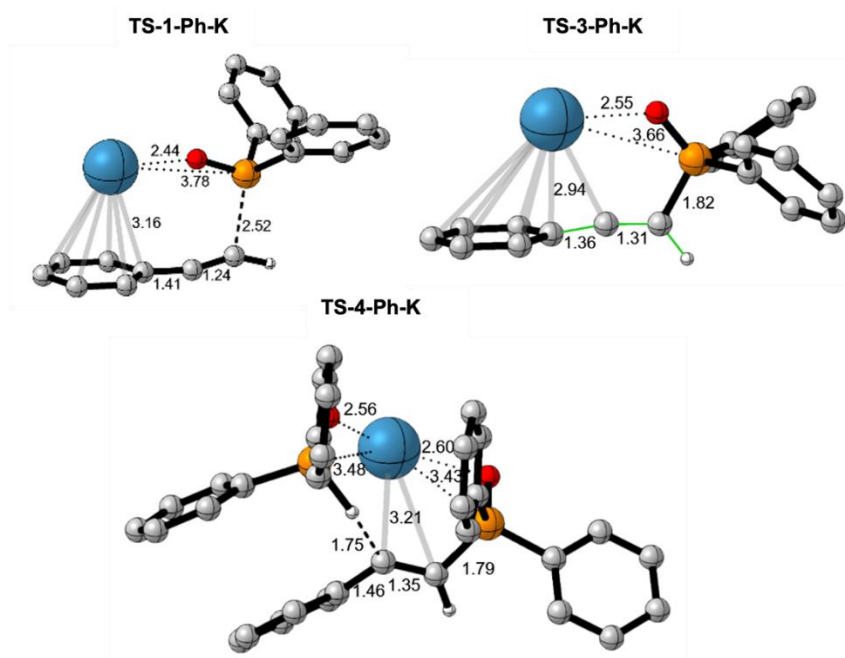


Figure S22: Optimised structures for the transition states of the potassium metal-mediated formation of *E*-diphenyl(styryl)phosphine oxide.

8.2 R = Cy (K-OPCy₂)

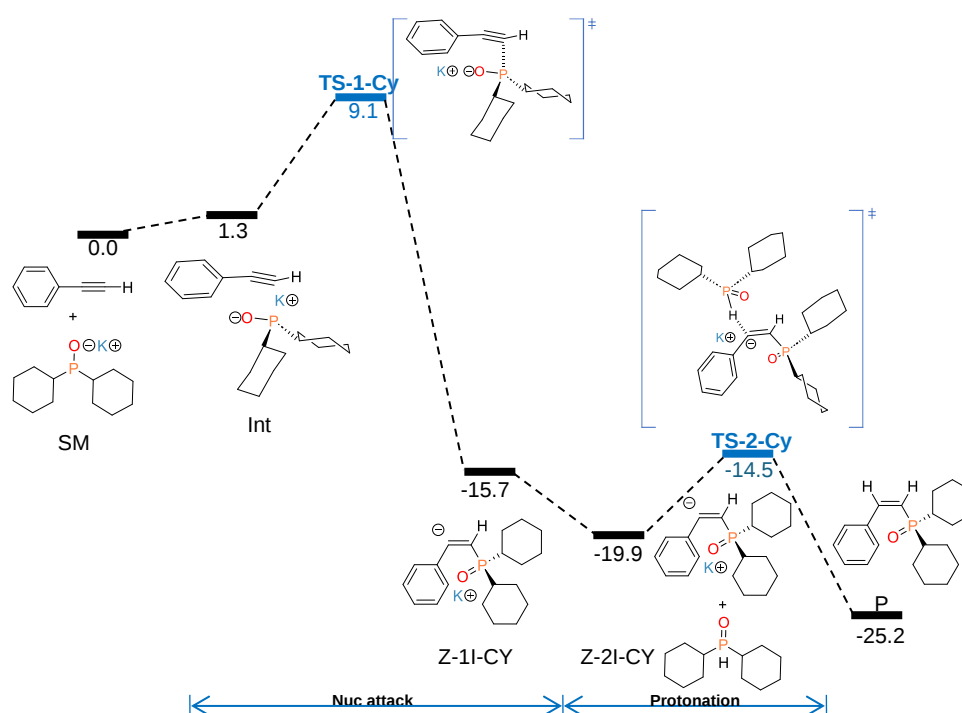


Figure S23: Computed Gibbs energy profile in THF (ΔG_{THF} kcal mol⁻¹) at 298 K for the hydrophosphorylation of phenylacetylene generating Z-dicyclohexyl(styryl)phosphine oxide, catalysed by potassium dicyclohexylphosphinite.

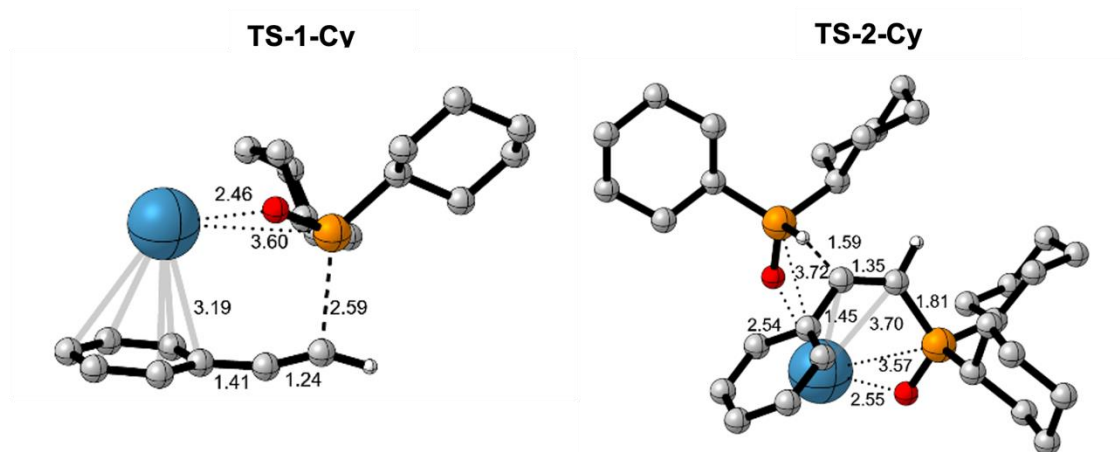


Figure S24: Optimised structures for the transition states of the potassium metal-mediated formation of Z-dicyclohexyl(styryl)phosphine oxide. Certain H atoms are omitted for clarity reasons. The distances presented are given in Å.

8.3 $R = \text{OEt}$ (K-OP(OEt)_2)

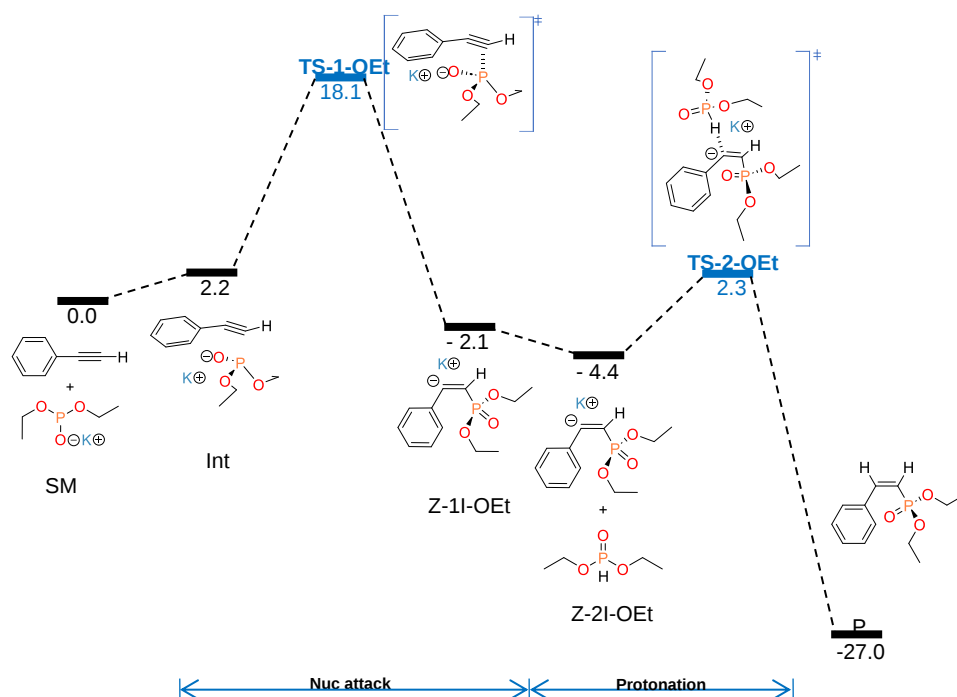


Figure S25: Computed Gibbs energy profile in THF (ΔG_{THF} kcal mol⁻¹) at 298 K for the hydrophosphorylation of phenylacetylene generating Z-diethoxy(styryl)phosphine oxide, catalysed by potassium diethoxyphosphinite.

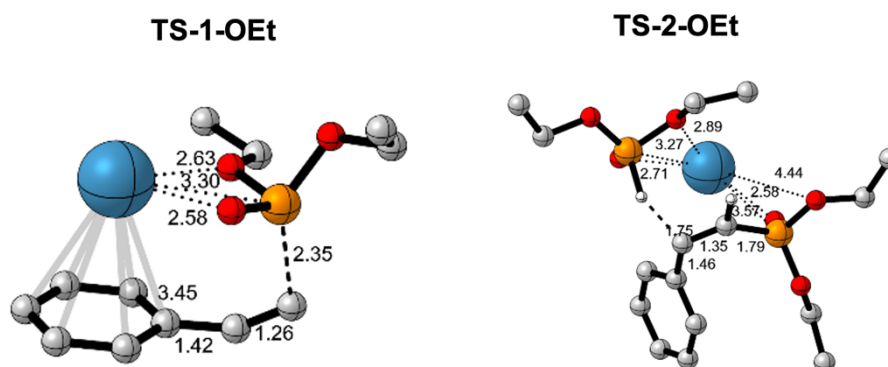


Figure S26: Optimised structures for the transition states of the potassium metal-mediated formation of Z-diethoxy(styryl)phosphine oxide. Certain H atoms are omitted for clarity reasons. The distances presented are given in Å.

9. Formation of bisphosphorylated alkane product with $\text{Ph}_2\text{P}(\text{O})\text{H}$

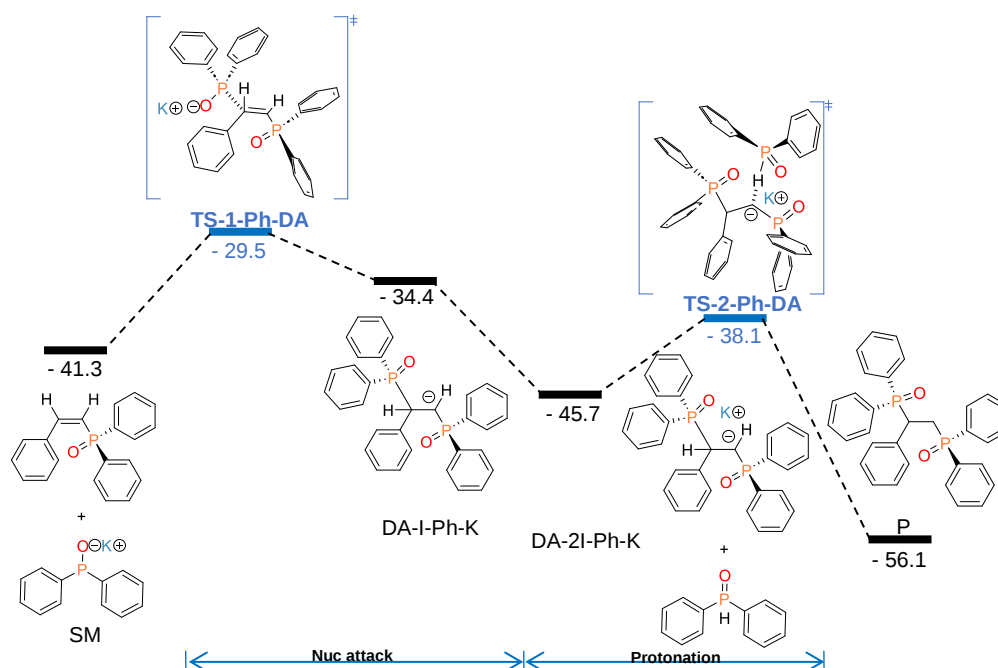


Figure S27: Computed Gibbs energy profile in THF (ΔG_{THF} kcal mol⁻¹) at 298 K for the second addition steps of the bishydrophosphorylation of phenylacetylene catalysed by potassium diphenyl phosphinite.

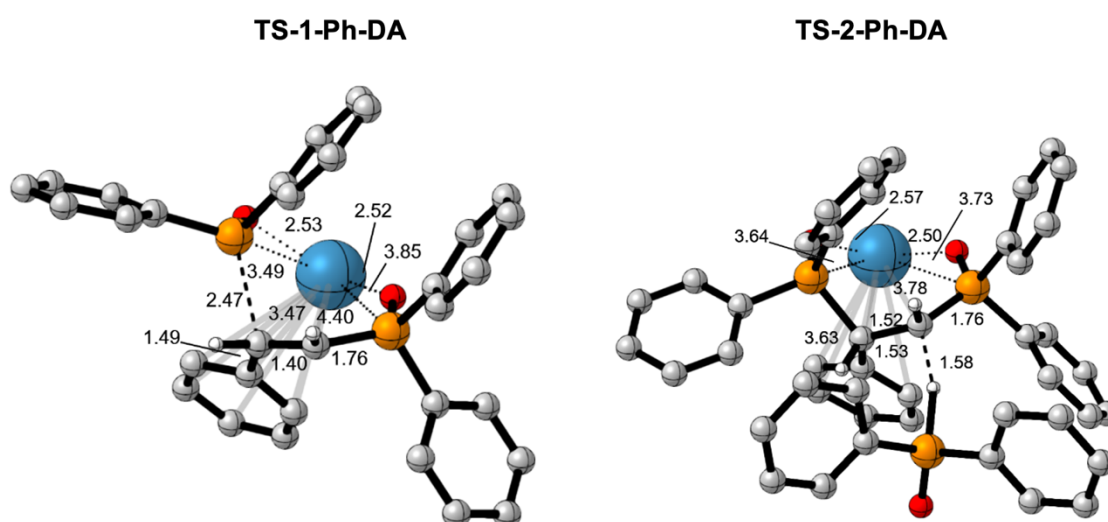


Figure S28: Optimised structures for the transition states involved in the potassium-mediated hydrophosphorylation of phenylacetylene yielding bishydrophosphorylated alkane from Z-diphenyl(styryl)phosphine oxide. Certain H atoms are omitted for clarity reasons. The distances presented are given in Å.

10. Cartesian coordinates (Å) and energies (hartrees) for all computed molecules.

Cartesian coordinates (Å), absolute energies in THF solvent (hartrees), and 3-D views of all the optimized geometries.

Absolute Gibbs energies in THF solvent, $G(\text{BS2})$, were calculated at 298.15 K by adding the thermal and entropic corrections obtained with BS1 to the BS2 energies in solvent, $E(\text{BS2})$:

$$G(\text{BS2}) = E(\text{BS2}) + G(\text{BS1}) - E(\text{BS1})$$

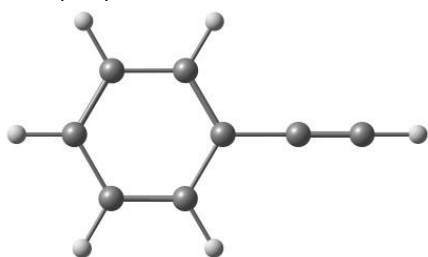
Small molecules

Phenylacetylene

$E(\text{BS1}) = -308.429740$

$E(\text{BS2}) = -308.545380$

$G_{298.15}(\text{BS2}) = -308.466185$



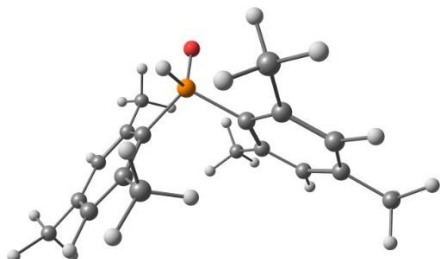
C	-3.232779	0.000018	-0.000000
C	-2.021644	-0.000023	-0.000009
H	-4.300986	-0.000012	0.000064
C	-0.592071	-0.000039	-0.000043
C	0.119087	-1.214969	0.000014
C	0.119028	1.214928	0.000010
C	1.511689	-1.209492	0.000013
C	1.511636	1.209533	0.000008
C	2.211184	0.000039	-0.000013
H	-0.428804	-2.151583	0.000008
H	-0.428916	2.151511	0.000034
H	2.052493	-2.151045	0.000006
H	2.052370	2.151126	0.000012
H	3.297057	0.000043	-0.000010

OP(H)Mes₂

$E(\text{BS1}) = -1116.517798$

$E(\text{BS2}) = -1116.832927$

$G_{298.15}(\text{BS2}) = -1116.521587$



C	-3.653408	-0.004912	-0.651915
C	-2.530538	0.823586	-0.531488
C	-1.470810	0.414780	0.314002
C	-1.577781	-0.804674	1.032325
C	-2.717902	-1.595398	0.870273
C	-3.766026	-1.217925	0.027479

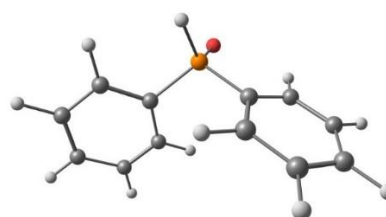
H	-4.465859	0.315693	-1.299399
H	-2.789071	-2.528404	1.423781
C	1.558791	-0.054112	-1.225079
C	1.478662	0.480591	0.082109
C	2.561736	0.312592	0.978170
C	3.671307	-0.431523	0.564612
C	3.750404	-1.001109	-0.708464
C	2.689419	-0.787752	-1.592416
H	4.500309	-0.560589	1.255785
H	2.745179	-1.194550	-2.599108
O	-0.029578	2.853987	0.026939
P	0.015925	1.450169	0.582574
H	0.102335	1.412783	1.987649
C	2.584101	0.905029	2.369581
H	1.848761	0.431620	3.029230
H	3.569118	0.762390	2.820752
H	2.374954	1.979349	2.364830
C	0.468424	0.154600	-2.247276
H	0.820349	-0.125898	-3.243183
H	-0.417977	-0.446914	-2.022765
H	0.154061	1.201075	-2.284393
C	4.941427	-1.828892	-1.115641
H	4.751248	-2.895600	-0.941269
H	5.165176	-1.709901	-2.180162
H	5.832256	-1.557526	-0.541884
C	-0.508413	-1.297875	1.979640
H	-0.830693	-2.223263	2.462837
H	0.434931	-1.499345	1.463879
H	-0.294265	-0.571128	2.771033
C	-2.523478	2.099090	-1.342123
H	-2.142729	2.947314	-0.774611
H	-1.877282	2.001150	-2.221863
H	-3.533259	2.318160	-1.699913
C	-4.971939	-2.102718	-0.154082
H	-4.792895	-2.849282	-0.938271
H	-5.209258	-2.648416	0.764295
H	-5.851489	-1.523404	-0.449618

OP(H)Ph₂

$E(\text{BS1}) = -880.568853$

$E(\text{BS2}) = -880.816328$

$G_{298.15}(\text{BS2}) = -880.659572$



15	-0.000978	1.398413	0.329066
6	-1.443686	0.332923	0.064754
6	-2.527689	0.389967	0.950650

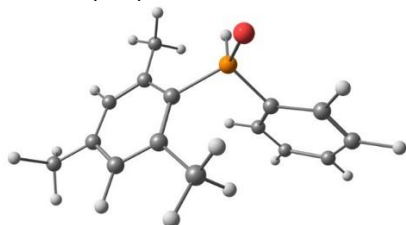
6	-1.497807	-0.520403	-1.048146
6	-3.656681	-0.399427	0.726975
6	-2.627285	-1.305447	-1.269882
6	-3.706155	-1.245490	-0.382350
1	-2.488425	1.047875	1.814822
1	-0.654247	-0.575130	-1.730503
1	-4.493732	-0.355555	1.417250
1	-2.666175	-1.967505	-2.129648
1	-4.584090	-1.860773	-0.555670
6	1.436117	0.292301	0.218533
6	1.477459	-0.922143	0.918468
6	2.519523	0.676653	-0.579335
6	2.598927	-1.743717	0.818882
6	3.638956	-0.151559	-0.680998
6	3.678884	-1.359222	0.017958
1	0.634672	-1.228429	1.532085
1	2.474025	1.618995	-1.116160
1	2.630568	-2.684206	1.360768
1	4.477379	0.145658	-1.303876
1	4.550035	-2.003021	-0.060502
8	0.114639	2.616736	-0.551037
1	-0.125825	1.685389	1.710688

OP(H)(Mes)Ph

E (BS1) = -998.544859

E (BS2) = -998.826174

G298.15 (BS2) = -998.591971



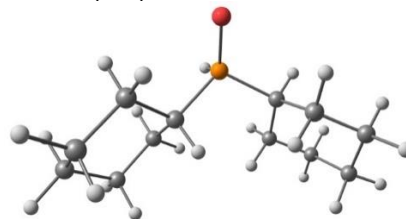
6	-4.170449	-0.662509	-0.178769
6	-3.147982	0.196319	-0.585456
6	-1.955058	0.258807	0.143290
6	-1.789873	-0.539932	1.283096
6	-2.814103	-1.395031	1.688381
6	-4.004007	-1.457255	0.957178
1	-5.093602	-0.712812	-0.748544
1	-3.260392	0.812998	-1.471723
1	-0.860241	-0.504885	1.844080
1	-2.683272	-2.016367	2.569388
1	-4.798924	-2.126792	1.272401
6	1.144464	-0.645151	-0.957633
6	0.916814	0.521126	-0.187991
6	1.910956	0.987298	0.703718
6	3.102809	0.264213	0.818740
6	3.344036	-0.892535	0.072974
6	2.352742	-1.329366	-0.810339
1	3.865581	0.619234	1.507112
1	2.524105	-2.224600	-1.402983
8	-0.919031	2.005103	-1.767258
15	-0.654867	1.409816	-0.404655
1	-0.629062	2.364281	0.631109
6	1.749796	2.235004	1.544630
1	0.937152	2.139449	2.272723
1	2.668893	2.433511	2.101149
1	1.536496	3.117558	0.932734
6	0.113298	-1.185119	-1.920624
1	0.570637	-1.901417	-2.607872
1	-0.691494	-1.702754	-1.386695
1	-0.347535	-0.388116	-2.509704
6	4.652784	-1.629568	0.189849
1	5.106115	-1.485941	1.174981
1	4.522999	-2.702654	0.020264
1	5.370442	-1.266569	-0.556807

OP(H)Cy₂

E (BS1) = -887.857680

E (BS2) = -888.088540

G298.15 (BS2) = -887.793072



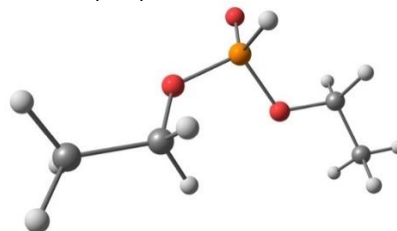
15	-0.009577	1.212063	-0.821589
8	-0.125387	2.686049	-0.509088
6	1.652314	0.507035	-0.483216
6	1.780826	-0.976208	-0.870905
6	3.210235	-1.479981	-0.626353
6	3.642521	-1.246682	0.826983
6	3.500444	-0.228598	1.222937
6	2.075754	0.743522	0.977650
1	2.321867	1.092008	-1.131205
1	1.499063	-1.123539	-1.920039
1	1.086479	-1.572894	-0.265537
1	3.277041	-2.544934	-0.878038
1	3.897903	-0.950600	-1.300053
1	4.676389	-1.580810	0.973211
1	3.015810	-1.859416	1.490357
1	3.770549	0.368745	2.276201
1	4.204356	0.831368	0.632665
1	2.003713	1.808873	1.218376
1	1.381087	0.216814	1.646270
6	-1.258185	0.129432	0.006040
6	-1.816861	-0.934544	-0.957785
6	-2.833897	-1.838048	-0.248313
6	-3.964799	-1.019185	0.386405
6	-3.412683	0.058602	1.328199
6	-2.398323	0.963608	0.617084
1	-0.732702	-0.382351	0.823684
1	-1.008199	-1.538311	-1.382432
1	-2.305832	-0.426339	-1.800055
1	-3.241874	-2.567580	-0.957899
1	-2.317723	-2.412126	0.533842
1	-4.654334	-1.679122	0.926032
1	-4.548065	-0.535800	-0.409839
1	-4.231216	0.664685	1.734264
1	-2.922967	-0.425516	2.184905
1	-1.991445	1.707938	1.307587
1	-2.904596	1.522544	-0.180717
1	-0.192637	0.900122	-2.197395

OP(H)OEt₂

E (BS1) = -726.169173

E (BS2) = -726.390271

G298.15 (BS2) = -726.270402



15	-0.007335	0.910892	0.224974
8	0.326848	2.258718	-0.296742
1	-0.052601	0.819750	1.629852
8	0.968257	-0.301711	-0.200904
6	2.373041	-0.206776	0.158716
1	2.457859	0.038087	1.225186
1	2.827902	0.604135	-0.418381
6	3.023745	-1.538266	-0.144859
1	2.929005	-1.781843	-1.207331
1	2.562429	-2.339320	0.440587
1	4.088339	-1.493537	0.106058
8	-1.430112	0.364793	-0.272472
6	-1.899740	-0.932929	0.185707

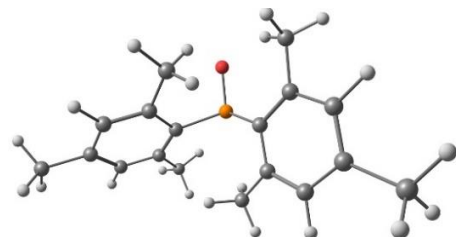
1	-1.698223	-1.035039	1.259469
1	-1.339509	-1.708543	-0.344286
6	-3.382867	-1.020883	-0.099054
1	-3.579438	-0.906574	-1.169279
1	-3.930571	-0.243700	0.442205
1	-3.760179	-1.998075	0.219202

[OPMes₂]⁻

E (BS1) = -1115.989571

E (BS2) = -1116.307964

G_{298.15}(BS2) = -1116.007906



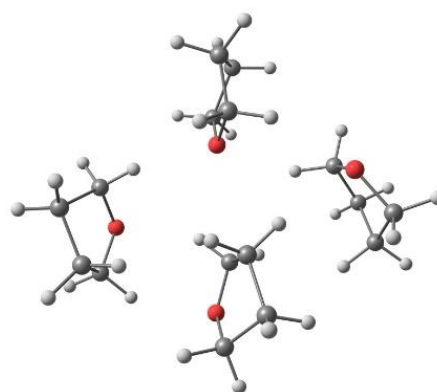
C	-2.721153	-1.801689	-0.151669
C	-1.592649	-1.223651	0.431564
C	-1.432354	0.191667	0.473576
P	0.002129	0.887297	1.514093
O	0.029809	2.445208	1.426557
C	1.440395	0.293820	0.412601
C	2.468241	-0.509666	0.956242
H	4.361489	-1.477481	0.617806
C	3.585674	-0.853815	0.176126
C	3.734621	-0.412766	-1.136181
C	2.733623	0.415026	-1.659143
H	2.836833	0.795796	-2.674567
C	1.609340	0.775842	-0.912907
C	-2.481415	0.977879	-0.066570
C	-3.609096	0.356101	-0.631205
H	-4.396989	0.988598	-1.039320
C	-3.752248	-1.026834	-0.695848
H	-2.802998	-2.887760	-0.173686
C	-0.554694	-2.148490	1.018102
H	-0.933092	-3.173792	1.076163
H	0.363664	-2.157890	0.423110
H	-0.269250	-1.827415	2.025579
C	-2.458512	2.492193	-0.115249
H	-1.731428	2.897929	0.590258
H	-2.168486	2.839110	-1.116642
H	-3.459768	2.895548	0.080063
C	-4.969412	-1.673093	-1.310293
H	-5.529750	-2.260998	-0.572304
H	-5.651317	-0.924520	-1.725254
H	-4.694599	-2.360776	-2.119606
C	2.433612	-1.048541	2.370083
H	1.795723	-0.442140	3.015291
H	2.037577	-2.071467	2.398225
H	3.443015	-1.083756	2.794190
C	4.934865	-0.794520	-1.967004
H	5.651538	-1.383365	-1.386589
H	4.643074	-1.390591	-2.840737
H	5.457120	0.091330	-2.347870
C	0.595380	1.701284	-1.538743
H	-0.303614	1.155962	-1.845754
H	0.286763	2.445606	-0.799585
H	1.008771	2.196477	-2.423528

(THF)₄

E (BS1) = -929.937599

E (BS2) = -930.274918

G_{298.15}(BS2) = -929.866329



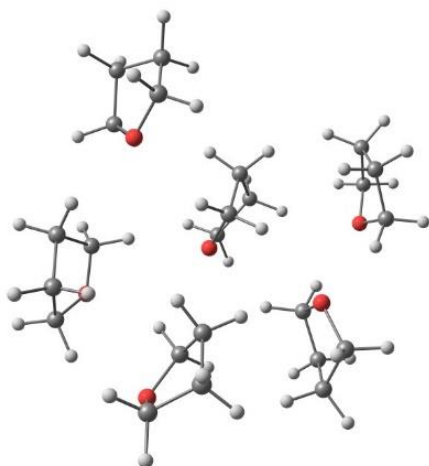
C	0.272276	-2.877629	1.166921
C	0.146274	-1.393173	0.797927
C	-0.272497	-1.457394	-0.674614
O	-0.922634	-2.735149	-0.866975
C	-0.862916	-3.490311	0.348257
H	-0.702915	-4.544264	0.093925
H	0.174538	-3.072967	2.238717
H	1.236843	-3.276178	0.831633
H	-0.641739	-0.923033	1.395819
H	1.065921	-0.824143	0.943016
H	-0.960765	-0.658693	-0.958496
H	0.602151	-1.416072	-1.338940
H	-1.818900	-3.412791	0.890183
O	-3.272538	0.206948	-1.327638
C	-3.323184	1.252416	-0.337846
C	-4.153058	0.707119	0.828514
H	-2.298025	1.488502	-0.027685
H	-3.767348	2.147186	-0.791722
C	-3.870901	-0.798335	0.735311
H	-3.865298	1.147299	1.787538
H	-5.219712	0.902110	0.668827
C	-3.811337	-1.007213	-0.777989
H	-2.901120	-1.031200	1.187529
H	-4.632399	-1.417800	1.217536
H	-3.161329	-1.836358	-1.071435
H	-4.819543	-1.179336	-1.187162
O	3.272203	0.134654	0.805861
C	3.161404	0.559874	-0.569672
H	2.097697	0.672327	-0.800497
H	3.646166	1.537820	-0.681394
H	3.473575	-1.721897	1.670864
H	4.995355	-1.005442	1.089992
H	2.751966	-2.222613	-0.600342
H	4.495668	-2.521287	-0.746234
C	3.741942	-1.762020	-0.520631
C	3.926126	-1.140002	0.861394
C	3.833270	-0.524030	-1.424331
H	3.338314	-0.655526	-2.390218
H	4.882761	-0.272092	-1.611818
C	0.418772	2.162580	1.202930
O	0.036655	1.710351	-0.111861
C	0.140292	2.794278	-1.050232
C	0.939772	3.890287	-0.345448
C	0.517649	3.687034	1.116167
H	-0.334612	1.821055	1.920888
H	1.381836	1.709124	1.466469
H	0.620897	2.421279	-1.961009
H	-0.868796	3.143827	-1.312839
H	2.014688	3.710206	-0.458408
H	0.715254	4.888186	-0.731478
H	1.227470	4.101252	1.837256
H	-0.461381	4.146196	1.294455

(THF)₆

E (BS1) = -1394.914151

E (BS2) = -1395.416760

G_{298.15}(BS2) = -1394.791895



C	-1.155687	-3.711197	1.852128
C	-0.886454	-2.453037	1.015705
C	-1.297190	-2.903280	-0.389746
O	-2.266692	-3.963309	-0.219018
C	-2.408652	-4.263395	1.173851
H	-2.527260	-5.347325	1.285373
H	-1.305595	-3.507209	2.916264
H	-0.327704	-4.422717	1.751823
H	-1.527676	-1.631912	1.353285
H	0.149062	-2.111986	1.055809
H	-1.742568	-2.102409	-0.983381
H	-0.439232	-3.311236	-0.942553
H	-3.313291	-3.779561	1.575056
O	-3.717700	-0.916365	-1.876365
C	-3.532348	0.399184	-1.313121
C	-4.464720	0.494819	-0.099614
H	-2.480696	0.506246	-1.024007
H	-3.762571	1.148290	-2.081473
C	-4.585217	-0.975161	0.324217
H	-4.053020	1.145970	0.674257
H	-5.447060	0.881010	-0.396428
C	-4.582185	-1.686534	-1.027859
H	-3.709171	-1.274999	0.908732
H	-5.481442	-1.189750	0.913623
H	-4.191162	-2.706441	-0.977156
H	-5.598046	-1.711392	-1.455419
O	2.520090	-1.855931	0.784099
C	2.475186	-1.930645	-0.662931
H	1.449915	-1.713651	-0.976565
H	3.138045	-1.162277	-1.070666
H	2.206970	-3.297491	2.224938

H	3.875560	-3.201669	1.615243
H	1.438465	-4.382974	0.191707
H	3.060869	-5.089815	0.325777
C	2.508837	-4.152792	0.212547
C	2.814852	-3.153236	1.325692
C	2.908570	-3.351936	-1.034545
H	2.426634	-3.705673	-1.949987
H	3.993632	-3.397735	-1.180658
C	0.246874	0.840203	0.302261
O	-0.140387	0.110736	-0.880768
C	0.398768	0.753566	-2.046857
C	1.422083	1.771116	-1.539855
C	0.808278	2.172333	-0.192595
H	-0.637428	0.965776	0.931955
H	1.004147	0.258665	0.842819
H	0.835482	-0.011288	-2.698615
H	-0.416979	1.246753	-2.595904
H	2.394123	1.293067	-1.383178
H	1.552322	2.610571	-2.229117
H	1.530230	2.608297	0.503053
H	-0.008292	2.884964	-0.337870
C	4.901601	0.498693	0.553774
O	4.727387	0.699729	-0.852627
C	5.147687	2.042508	-1.099596
C	4.656216	2.870588	0.105320
C	4.431691	1.805798	1.211273
H	4.724072	2.357513	-2.056707
H	5.392310	3.625601	0.394249
H	3.723256	3.388683	-0.131567
H	4.987558	2.022982	2.127379
H	3.371907	1.736385	1.471737
H	5.965803	0.313495	0.773495
H	4.314094	-0.374949	0.842165
H	6.246147	2.081443	-1.174905
C	-1.761149	3.710311	1.917151
O	-2.350103	2.889745	0.895133
C	-2.792871	3.713567	-0.198272
C	-2.674817	5.163380	0.279424
C	-1.509875	5.074207	1.274713
H	-3.817223	3.430975	-0.462095
H	-2.495085	5.861063	-0.542737
H	-3.590934	5.470358	0.796070
H	-0.552286	5.074655	0.742496
H	-1.497213	5.886862	2.005858
H	-0.847859	3.221117	2.271761
H	-2.457384	3.795444	2.764559
H	-2.151058	3.527061	-1.070508

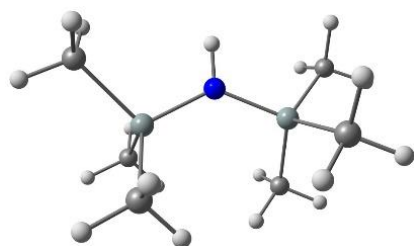
Generation of active species

H-HMDS

E (BS1) = -874.023677

E (BS2) = -874.194263

G_{298.15} (BS2) = -873.999944



N	-0.000012	-0.000180	-0.819686
Si	-1.588015	0.010090	-0.088885
Si	1.588004	-0.010127	-0.088892
C	-2.108011	-1.712189	0.481596

H	-2.115023	-2.421559	-0.354481
H	-1.420636	-2.102971	1.240530
H	-3.114259	-1.701599	0.918788
C	-1.591243	1.155209	1.408332
H	-2.581638	1.174900	1.879333
H	-0.875898	0.828254	2.171429
H	-1.334538	2.182065	1.125386
C	-2.808783	0.625270	-1.385672
H	-2.799128	-0.012035	-2.278298
H	-3.832826	0.624359	-0.993874
H	-2.573568	1.647714	-1.702865
C	1.591615	-1.155025	1.408506
H	1.335184	-2.181992	1.125709
H	2.582014	-1.174381	1.879517
H	0.876172	-0.828158	2.171551
C	2.107688	1.712330	0.481304
H	1.420354	2.103077	1.240289
H	3.113999	1.701992	0.918357
H	2.114436	2.421585	-0.354871
C	2.808759	-0.625295	-1.385695
H	3.832813	-0.624329	-0.993930
H	2.573590	-1.647764	-1.702847

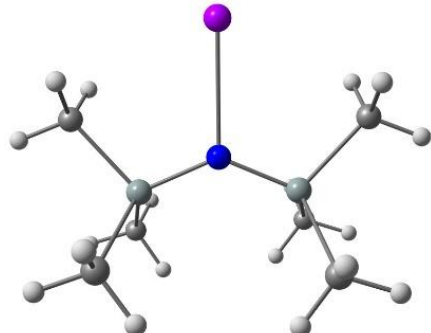
H	2.799040	0.011985	-2.278337
H	-0.000006	-0.001170	-1.834926

K-HMDS

E (BS1) = -1473.346239

E (BS2) = -1473.559964

G_{298.15} (BS2) = -1473.381086



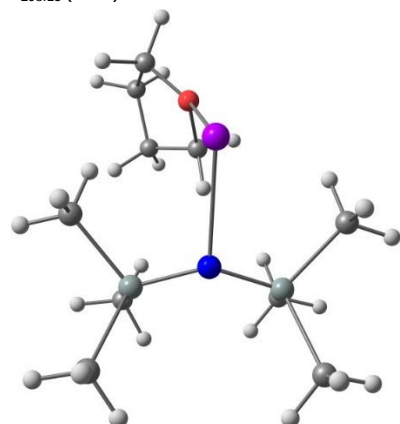
N	-0.000580	0.183756	0.046697
Si	1.544652	-0.486228	0.008860
Si	-1.548834	-0.479066	0.004455
C	1.957563	-1.479229	-1.564088
H	1.320218	-2.368089	-1.648412
H	1.793951	-0.877034	-2.466911
H	3.001124	-1.820893	-1.577025
C	2.843632	0.917885	0.074217
H	3.867111	0.521699	0.066401
H	2.766645	1.589609	-0.793598
H	2.749702	1.521222	0.988722
C	1.962402	-1.639132	1.466610
H	1.328952	-2.535051	1.450871
H	3.007199	-1.976544	1.446073
H	1.792910	-1.139602	2.428835
C	-1.895188	-1.645970	-1.461263
H	-1.287074	-2.556430	-1.390274
H	-2.947083	-1.958364	-1.503532
H	-1.651256	-1.166887	-2.417766
C	-2.837351	0.928690	-0.139965
H	-2.703174	1.515513	-1.060173
H	-3.862057	0.536501	-0.167296
H	-2.792962	1.615492	0.718228
C	-2.045220	-1.454417	1.564000
H	-3.080792	-1.816944	1.518758
H	-1.396407	-2.328271	1.702980
H	-1.949387	-0.834570	2.464704
K	0.009998	2.765237	0.004688

K-HMDS·(THF)

E (BS1) = -1705.851044

E (BS2) = -1706.146436

G_{298.15} (BS2) = -1705.857096



N	1.245857	-0.138389	0.427293
Si	2.079217	1.090433	-0.358546
Si	0.890446	-1.755463	0.139922

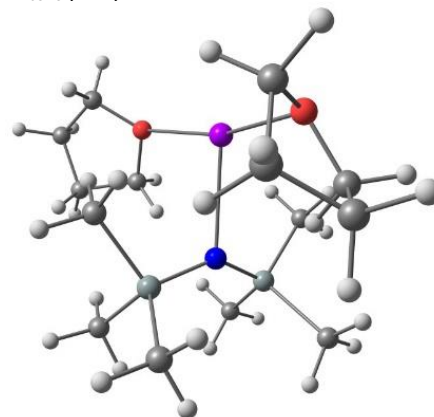
C	1.814869	1.190292	-2.244465
H	2.185550	0.289585	-2.748396
H	0.751238	1.288911	-2.494710
H	2.337852	2.050030	-2.684130
C	1.499965	2.790469	0.309213
H	2.038444	3.615957	-0.173669
H	0.430955	2.963978	0.118140
H	1.680882	2.893403	1.389261
C	3.967292	1.073800	-0.106312
H	4.407418	0.155996	-0.517111
H	4.463095	1.924149	-0.593031
H	4.224254	1.105563	0.960357
C	0.517217	-2.208358	-1.674505
H	1.421433	-2.128041	-2.290686
H	0.148464	-3.238133	-1.772082
H	-0.234334	-1.543553	-2.115046
C	-0.669312	-2.254885	1.134667
H	-1.534144	-1.626855	0.885378
H	-0.962223	-3.293527	0.935585
H	-0.494190	-2.184644	2.218661
C	2.233745	-2.987074	0.695511
H	1.932226	-4.031473	0.539098
H	3.166581	-2.826586	0.139920
H	2.466354	-2.865157	1.761333
K	-0.517844	0.881326	2.092694
O	-2.518610	0.940900	0.395627
C	-2.020315	0.813834	-0.960170
C	-2.908768	-0.236295	-1.616050
H	-2.107512	1.784856	-1.466991
H	-0.965804	0.532077	-0.900222
C	-4.264711	0.045140	-0.953361
H	-2.930355	-0.142866	-2.704712
H	-2.556206	-1.241362	-1.361486
C	-3.858104	0.401160	0.478697
H	-4.751160	0.899853	-1.435491
H	-4.950778	-0.804862	-0.987671
H	-4.512039	1.148906	0.939413
H	-3.835645	-0.487945	1.122432

K-HMDS·(THF)₂

E (BS1) = -1938.354092

E (BS2) = -1938.731324

G_{298.15} (BS2) = -1938.334405



N	-0.223848	0.988151	0.145352
Si	-0.213347	2.333241	-0.853573
Si	-0.037399	0.629266	1.771855
C	1.235584	3.542029	-0.575334
H	1.194483	3.982780	0.428436
H	2.201674	3.029071	-0.664598
H	1.232528	4.369422	-1.297459
C	-0.064979	1.776599	-2.679980
H	-0.072118	2.632197	-3.367415
H	0.872940	1.233714	-2.865482
H	-0.903187	1.130262	-2.977955
C	-1.795975	3.394182	-0.786258
H	-1.949737	3.804251	0.220189

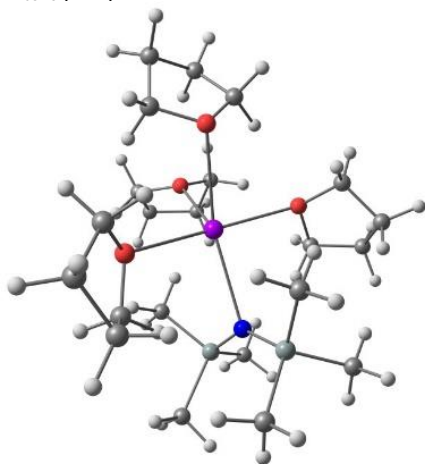
H	-1.767002	4.239841	-1.486259
H	-2.682173	2.793488	-1.028861
C	1.388377	1.539902	2.653280
H	1.167907	2.611261	2.742667
H	1.561508	1.158071	3.668414
H	2.329742	1.449492	2.099135
C	0.329592	-1.239610	1.979504
H	1.230585	-1.536897	1.427914
H	0.493066	-1.509606	3.030576
H	-0.507020	-1.857313	1.623738
C	-1.576139	0.958819	2.848387
H	-1.443648	0.624817	3.886271
H	-1.807118	2.031691	2.875624
H	-2.459980	0.449305	2.445663
K	0.003659	-1.239133	-1.291226
O	2.635616	-1.425141	-1.045356
C	3.144180	-0.143790	-0.595312
C	4.079355	-0.467035	0.564445
H	3.684934	0.337167	-1.422340
H	2.286066	0.474844	-0.316594
C	4.673984	-1.811243	0.121669
H	4.831831	0.309867	0.721911
H	3.506245	-0.586173	1.489908
C	3.474508	-2.489852	-0.543754
H	5.474199	-1.649263	-0.608583
H	5.077174	-2.402617	0.947666
H	3.755015	-3.141003	-1.378323
H	2.896404	-3.079768	0.180076
C	-3.294716	-0.580369	-0.948094
O	-2.589981	-1.833644	-1.175282
C	-3.057825	-2.822368	-0.238091
C	-3.642788	-2.030562	0.925713
C	-4.280629	-0.839435	0.196348
H	-2.210535	-3.458412	0.040379
H	-4.357746	-2.612856	1.512822
H	-2.841974	-1.688676	1.589054
H	-5.264975	-1.118594	-0.194164
H	-4.401147	0.039433	0.834681
H	-3.789591	-0.282676	-1.878916
H	-2.549061	0.174096	-0.673145
H	-3.821687	-3.453155	-0.715167

K-HMDS·(THF)₄

E (BS1) = -2403.357119

E (BS2) = -2403.895830

G_{298.15} (BS2) = -2403.281424



N	2.121805	-0.368719	0.305664
Si	2.354865	-0.699262	1.929191
Si	3.028416	-0.088621	-1.071885
C	3.845199	0.174948	2.741062
H	4.791899	-0.172315	2.308607
H	3.797983	1.260366	2.587837
H	3.895142	-0.004488	3.823341
C	0.823863	-0.161277	2.939424
H	0.922527	-0.411512	4.003472

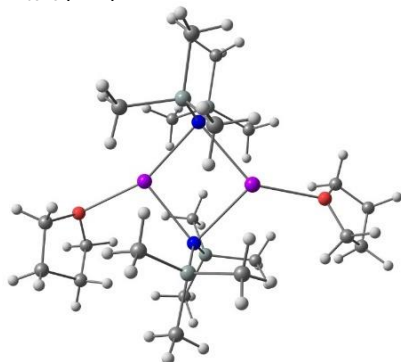
H	0.652022	0.920398	2.870875
H	-0.077017	-0.665986	2.572815
C	2.565719	-2.553752	2.333412
H	3.439452	-2.972969	1.818234
H	2.695740	-2.737927	3.408312
H	1.690461	-3.128824	2.003878
C	4.471684	1.145500	-0.870184
H	5.247063	0.732620	-0.212715
H	4.951457	1.383724	-1.829075
H	4.139540	2.089230	-0.423298
C	1.916648	0.641089	-2.449714
H	1.478854	1.601238	-2.144214
H	2.477103	0.824757	-3.376421
H	1.092986	-0.039258	-2.704578
C	3.838787	-1.637170	-1.840205
H	4.343519	-1.420959	-2.791724
H	4.591527	-2.053154	-1.157314
H	3.103671	-2.428402	-2.026666
K	-0.486885	0.315601	-0.191812
O	0.001688	2.924119	0.396886
C	1.375801	3.076591	0.825864
C	1.994414	4.067014	-0.154790
H	1.393715	3.472501	1.852117
H	1.837626	2.085399	0.810116
C	0.813218	5.006491	-0.433550
H	2.868147	4.577480	0.259727
H	2.299217	3.549977	-1.071232
C	-0.375795	4.039967	-0.437180
H	0.710488	5.735105	0.378206
H	0.903706	5.553830	-1.375497
H	-1.290906	4.490213	-0.038325
H	-0.586992	3.665845	-1.447372
C	0.124897	-3.043994	-0.850389
O	-0.825055	-2.101732	-1.420972
C	-0.918462	-2.307154	-2.842082
C	0.357793	-3.046031	-3.231375
C	0.582817	-3.941256	-2.004288
H	-1.026022	-1.330066	-3.323223
H	0.250424	-3.606491	-4.163947
H	1.183758	-2.336485	-3.343522
H	-0.042792	-4.838159	-2.072149
H	1.622364	-4.257854	-1.887374
H	-0.376682	-3.603129	-0.052114
H	0.946780	-2.460184	-0.421365
H	-1.810851	-2.907808	-3.071860
C	-3.412882	2.154300	-0.775336
O	-2.720185	1.163669	-1.561876
C	-3.602989	0.049706	-1.829188
C	-4.855982	0.282802	-0.984728
C	-4.897407	1.813085	-0.886719
H	-3.084117	-0.878615	-1.576886
H	-5.750341	-0.148913	-1.440466
H	-4.720111	-0.151733	0.009346
H	-5.320244	2.245858	-1.800123
H	-5.474642	2.177786	-0.032136
H	-3.160920	3.143349	-1.168626
H	-3.074271	2.095930	0.268413
H	-3.835324	0.040719	-2.902575
C	-2.884741	-1.961502	1.308640
O	-2.549698	-0.567220	1.346827
C	-2.887542	-0.100243	2.663886
C	-2.719581	-1.308872	3.614968
C	-2.421177	-2.492489	2.663594
H	-3.923125	0.267191	2.665260
H	-1.905065	-1.150358	4.324940
H	-3.636294	-1.477828	4.186385
H	-1.346656	-2.697886	2.630816
H	-2.936758	-3.411629	2.953598
H	-2.381559	-2.395571	0.443038
H	-3.972787	-2.080916	1.187492
H	-2.221156	0.733679	2.896815

[(K-HMDS)·(THF)]₂

E (BS1) = -3411.766716

E (BS2) = -3412.346123

G_{298.15} (BS2) = -3411.741184



N	0.604834	1.464042	0.155424
Si	1.077791	1.940184	1.703944
Si	0.216522	2.342948	-1.232772
C	2.310272	0.691314	2.448715
H	1.891955	-0.322379	2.472654
H	3.244946	0.658182	1.876535
H	2.572399	0.949759	3.482831
C	1.890909	3.653652	1.863374
H	2.243199	3.831611	2.887791
H	2.751811	3.762588	1.194193
H	1.182179	4.454314	1.618316
C	-0.370611	1.986829	2.959924
H	-0.756757	0.990541	3.215246
H	-0.049398	2.435832	3.908943
H	-1.206711	2.591257	2.583611
C	1.348246	3.813812	-1.655380
H	2.399494	3.506360	-1.705287
H	1.084123	4.247514	-2.628913
H	1.276387	4.613297	-0.909511
C	-1.556177	3.052265	-1.219665
H	-1.678331	3.762464	-0.392067
H	-1.794407	3.583908	-2.150331
H	-2.312410	2.268757	-1.091342
C	0.278024	1.215479	-2.772769
H	-0.068613	1.753083	-3.664567
H	1.295872	0.867765	-2.997241
H	-0.364083	0.333445	-2.666292
K	-1.688463	-0.073623	0.746382
N	-0.524314	-2.461164	0.032067
Si	-0.049870	-3.253529	1.441578
Si	-1.167828	-2.917446	-1.457610
C	-0.719539	-5.013023	1.709530
H	-1.815670	-5.032198	1.682919
H	-0.361294	-5.705992	0.939475
H	-0.405710	-5.411577	2.683027
C	1.851690	-3.417432	1.604986
H	2.122674	-4.012895	2.486684
H	2.282493	-3.921489	0.729281
H	2.358830	-2.450642	1.726402
C	-0.578546	-2.270215	2.992052
H	-1.672579	-2.190806	3.064131
H	-0.234776	-2.761036	3.911636
H	-0.157580	-1.257019	3.005856
C	-1.904026	-4.666753	-1.579362
H	-2.686691	-4.828039	-0.828619
H	-2.352143	-4.839468	-2.566514
H	-1.139798	-5.437896	-1.426509
C	0.109135	-2.823747	-2.880366
H	0.994114	-3.434967	-2.656402
H	-0.315793	-3.203950	-3.818639
H	0.444543	-1.799892	-3.091118
C	-2.581162	-1.742930	-1.984918
H	-2.964915	-2.002219	-2.980044
H	-3.427474	-1.808421	-1.288210
H	-2.264953	-0.693075	-2.039748
K	1.715562	-0.913302	-0.620613
O	-4.081716	1.056503	0.502705
C	-4.989554	0.889565	-0.613441

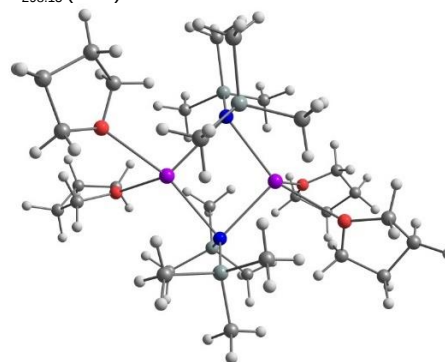
C	-5.991050	2.040933	-0.518339
H	-4.411313	0.934206	-1.544582
H	-5.454970	-0.097820	-0.538963
C	-5.158011	3.137516	0.159574
H	-6.377626	2.332813	-1.497952
H	-6.837742	1.759779	0.117231
C	-4.326494	2.326646	1.148490
H	-4.504495	3.627633	-0.569695
H	-5.764399	3.900706	0.653750
H	-3.361124	2.784554	1.385426
H	-4.872564	2.152850	2.085538
O	4.257596	-0.323853	-1.242027

[K-HMDS]·(THF)₂

E (BS1) = -3876.770408

E (BS2) = -3877.510956

G_{298.15} (BS2) = -3876.693058



N	0.591486	-1.579680	-0.940615
Si	0.631932	-1.622524	-2.627338
Si	0.833195	-2.847350	0.147797
C	1.389499	-0.035075	-3.362154
H	0.832774	0.861313	-3.067030
H	2.425272	0.102471	-3.030624
H	1.389856	-0.065396	-4.459885
C	1.627159	-3.050195	-3.406889
H	1.598240	-3.014637	-4.503919
H	2.681059	-3.004970	-3.104962
H	1.241745	-4.030283	-3.100220
C	-1.117300	-1.751923	-3.395555
H	-1.736829	-0.872215	-3.173663
H	-1.081665	-1.838536	-4.489836
H	-1.641357	-2.636897	-3.010853
C	2.618747	-3.518246	0.197092
H	3.332778	-2.706835	0.381746
H	2.758546	-4.272454	0.983163
H	2.893615	-3.982376	-0.757812
C	-0.303916	-4.355185	-0.119636
H	-0.142131	-4.811130	-1.104537
H	-0.151271	-5.137644	0.636089
H	-1.351869	-4.035757	-0.067389
C	0.448874	-2.268872	1.924794
H	0.721160	-3.032442	2.665088
H	0.976778	-1.349073	2.201175
H	-0.622769	-2.081280	2.047014
K	-1.874199	-0.398060	-0.246968
N	-0.794667	2.060524	0.514837
Si	-0.862020	3.106975	-0.802686
Si	-0.953412	2.227618	2.183113
C	-1.796512	4.747776	-0.547761
H	-2.805993	4.584067	-0.154014
H	-1.274242	5.404077	0.158557
H	-1.895230	5.297576	-1.493037
C	0.864735	3.633177	-1.445451
H	0.778264	4.379640	-2.246484
H	1.461344	4.085632	-0.641845
H	1.441664	2.799153	-1.865656
C	-1.702474	2.275464	-2.300613
H	-2.735710	1.994980	-2.071135
H	-1.725452	2.943473	-3.171292

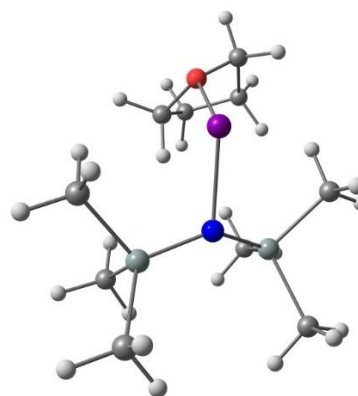
H	-1.173594	1.367942	-2.612760
C	-1.893228	3.766782	2.798401
H	-2.905554	3.812761	2.378528
H	-1.991234	3.759597	3.892003
H	-1.382369	4.696038	2.520871
C	0.723685	2.263355	3.101292
H	1.341126	3.100218	2.748010
H	0.587679	2.391521	4.183658
H	1.302881	1.341982	2.960339
C	-1.889799	0.747323	2.945609
H	-1.991539	0.862168	4.032746
H	-2.903336	0.651369	2.535162
H	-1.360932	-0.197406	2.776788
K	1.662823	0.717956	0.089745
O	-3.199313	-2.448707	0.845565
C	-3.240662	-3.067239	2.149827
C	-4.631662	-3.688491	2.275046
H	-2.452709	-3.829108	2.201358
H	-3.036932	-2.300813	2.903878
C	-4.954959	-4.037178	0.815576
H	-4.640923	-4.553967	2.942384
H	-5.346785	-2.950599	2.655502
C	-4.355638	-2.844330	0.075287
H	-4.445418	-4.962009	0.523406
H	-6.024421	-4.153837	0.621820
H	-4.026505	-3.081395	-0.941724
H	-5.056478	-2.001292	0.031248
O	3.417498	0.067030	2.031984
C	4.392809	1.110927	2.188436
C	5.737356	0.401743	2.457501
H	4.389065	1.702718	1.270838
H	4.105295	1.753513	3.032068
C	5.330291	-1.056631	2.792054
H	6.387162	0.437433	1.579398
H	6.268245	0.878833	3.285295
C	3.808206	-0.975198	2.934903
H	5.590992	-1.728183	1.968795
H	5.807945	-1.433299	3.699987
H	3.281227	-1.884519	2.644916
H	3.517428	-0.704147	3.961163
C	-5.300517	0.614473	-1.714086
O	-4.372933	0.585274	-0.608664
C	-4.521730	1.780679	0.192978
C	-5.314260	2.757058	-0.670740
C	-6.225354	1.806791	-1.461070
H	-3.521213	2.133359	0.456705
H	-5.863710	3.489856	-0.074194
H	-4.642490	3.295619	-1.347449
H	-7.079974	1.503368	-0.846338
H	-6.605822	2.239908	-2.389620
H	-5.828850	-0.343746	-1.753465
H	-4.733261	0.738353	-2.645955
H	-5.066454	1.529124	1.113576
C	4.659501	-0.389213	-1.180088
O	4.005534	0.903948	-1.181913
C	4.864493	1.880237	-1.795570
C	6.274850	1.326958	-1.624115
C	6.036346	-0.177803	-1.821848
H	4.694936	2.838947	-1.297288
H	6.984426	1.750157	-2.339758
H	6.638202	1.530067	-0.610448
H	6.000431	-0.414661	-2.890298
H	6.805348	-0.802156	-1.359973
H	4.038495	-1.103193	-1.730436
H	4.730198	-0.721196	-0.140375
H	4.605966	1.986869	-2.858780

Na-HMDS·(THF)

E (BS1) = -1268.249159

E (BS2) = -1268.514342

G_{298.15} (BS2) = -1268.224267



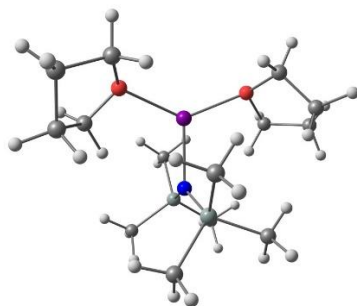
N	1.070341	0.159066	0.535710
Si	0.726304	1.733058	0.032673
Si	2.019654	-1.092745	-0.081930
C	0.016296	1.871406	-1.730779
H	0.764479	1.588352	-2.481159
H	-0.846668	1.209774	-1.870368
H	-0.309045	2.893986	-1.963418
C	-0.594464	2.475901	1.195090
H	-0.846422	3.508874	0.923446
H	-1.535395	1.909090	1.171357
H	-0.237730	2.493230	2.234120
C	2.202913	2.932332	0.086046
H	2.991293	2.614201	-0.608011
H	1.918492	3.956949	-0.187603
H	2.648095	2.967450	1.088259
C	1.930112	-1.319042	-1.970948
H	2.356690	-0.453687	-2.493034
H	2.484506	-2.206547	-2.303330
H	0.894079	-1.428168	-2.314578
C	1.431689	-2.743911	0.678926
H	0.396257	-2.978249	0.394776
H	2.048220	-3.590768	0.351922
H	1.487012	-2.720734	1.777272
C	3.870505	-0.958489	0.338653
H	4.449923	-1.806324	-0.049811
H	4.302478	-0.041662	-0.082151
H	4.026374	-0.919845	1.424358
Na	-0.541502	-0.624162	1.846011
O	-2.440636	-1.105624	0.751433
C	-2.116733	-1.412364	-0.638324
C	-3.159801	-0.685188	-1.492542
H	-1.102660	-1.045913	-0.825922
H	-2.137560	-2.498418	-0.769133
C	-3.636125	0.442284	-0.565379
H	-2.732105	-0.317388	-2.428360
H	-3.992316	-1.353401	-1.734987
C	-3.601089	-0.242433	0.794522
H	-2.931493	1.279630	-0.585111
H	-4.631145	0.816876	-0.817932
H	-3.480004	0.443878	1.638199
H	-4.499363	-0.851232	0.961662

Na-HMDS·(THF)₂

E (BS1) = -1500.757523

E (BS2) = -1501.103577

G_{298.15} (BS2) = -1500.705602



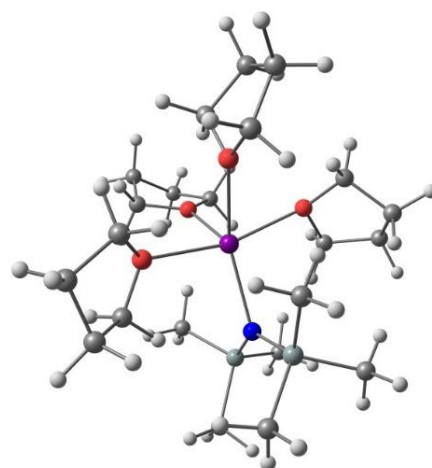
N	-0.231203	1.053656	0.126000
Si	-0.684565	2.249995	-0.966560
Si	-0.421753	0.797673	1.777760
C	0.326941	3.859050	-0.842389
H	0.217204	4.314808	0.149841
H	1.397041	3.665344	-0.991113
H	0.019764	4.606756	-1.585510
C	-0.412736	1.599672	-2.742137
H	-0.657073	2.353983	-3.500860
H	0.635893	1.312750	-2.905448
H	-1.040725	0.722504	-2.952049
C	-2.513261	2.778579	-0.870772
H	-2.733805	3.261598	0.089510
H	-2.782719	3.489137	-1.663430
H	-3.182789	1.913818	-0.959710
C	0.384972	2.113249	2.894466
H	-0.091090	3.092254	2.755016
H	0.309291	1.861144	3.960561
H	1.449463	2.234068	2.656729
C	0.402936	-0.857924	2.256051
H	1.480383	-0.830332	2.049645
H	0.281372	-1.083939	3.323182
H	-0.021746	-1.706810	1.703344
C	-2.234289	0.675314	2.356324
H	-2.317504	0.409567	3.418552
H	-2.755198	1.630788	2.216067
H	-2.785457	-0.078968	1.782144
Na	0.387044	-0.828930	-0.927172
O	2.622050	-1.054237	-1.071257
C	3.252182	0.232529	-0.821574
C	4.117970	0.025422	0.415481
H	3.853393	0.503913	-1.698287
H	2.458602	0.971476	-0.678549
C	4.562776	-1.434602	0.252752
H	4.952274	0.729761	0.459662
H	3.514768	0.145177	1.321812
C	3.310793	-2.092228	-0.327632
H	5.393068	-1.501825	-0.458258
H	4.874262	-1.900634	1.190827
H	3.528808	-2.919829	-1.009098
H	2.644194	-2.454297	0.465850
C	-2.592537	-1.457030	-1.176741
O	-1.361983	-2.240346	-1.195503
C	-1.506349	-3.384543	-0.323087
C	-2.622210	-3.011982	0.645119
C	-3.564304	-2.208272	-0.262553
H	-0.540522	-3.566597	0.158957
H	-3.096566	-3.889158	1.092222
H	-2.230846	-2.378525	1.447330
H	-4.197830	-2.884907	-0.845340
H	-4.212097	-1.523997	0.290880
H	-2.957364	-1.358790	-2.203653
H	-2.343551	-0.465706	-0.784543
H	-1.771353	-4.265992	-0.921938

Na-HMDS·(THF)₄

E (BS1) = -1965.760560

E (BS2) = -1966.268465

G_{298.15} (BS2) = -1965.649309



N	1.952053	-0.065243	-0.033258
Si	2.901331	0.305394	1.306552
Si	2.365633	-0.641882	-1.557541
C	4.568618	1.150151	0.910684
H	5.239863	0.474961	0.364878
H	4.426971	2.041601	0.286911
H	5.095188	1.465332	1.821709
C	1.985091	1.489970	2.483639
H	2.507126	1.606015	3.442574
H	1.876768	2.488535	2.043370
H	0.977792	1.111759	2.687171
C	3.372058	-1.196476	2.393239
H	3.837601	-1.990175	1.794983
H	4.081534	-0.921056	3.185302
H	2.492408	-1.632853	2.882397
C	3.537573	0.476498	-2.567571
H	4.528346	0.543129	-2.102197
H	3.680895	0.105512	-3.591496
H	3.144216	1.498398	-2.638647
C	0.798031	-0.802343	-2.637064
H	0.318649	0.175059	-2.775423
H	1.029710	-1.197206	-3.634619
H	0.060733	-1.475758	-2.185465
C	3.195536	-2.361408	-1.572991
H	3.349740	-2.747883	-2.589524
H	4.179796	-2.319355	-1.088296
H	2.598006	-3.098977	-1.024484
Na	-0.398679	0.087352	-0.011544
O	-0.534367	2.337020	-0.756868
C	0.715830	3.065658	-0.712342
C	0.858922	3.720853	-2.083357
H	0.656026	3.821813	0.082798
H	1.500463	2.343465	-0.476100
C	-0.605412	3.989750	-2.455358
H	1.476583	4.622355	-2.053880
H	1.308210	3.018701	-2.794742
C	-1.293665	2.736982	-1.914852
H	-0.970528	4.883713	-1.936934
H	-0.768533	4.123401	-3.528234
H	-2.332878	2.901361	-1.614166
H	-1.272875	1.927006	-2.653293
C	0.260484	-2.822831	1.220751
O	-0.871922	-2.200550	0.559700
C	-1.475147	-3.144247	-0.338609
C	-0.362689	-4.123778	-0.696770
C	0.385271	-4.238240	0.639406
H	-1.872324	-2.586691	-1.187203
H	-0.744152	-5.080564	-1.063662
H	0.286983	-3.689649	-1.463583
H	-0.109999	-4.970190	1.286561
H	1.429320	-4.540484	0.522953
H	0.079979	-2.830177	2.301660
H	1.130453	-2.199373	1.002473
H	-2.307489	-3.661460	0.162834
C	-3.626174	0.115612	-0.382634

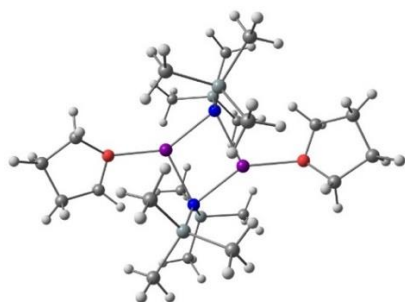
O	-2.469372	-0.070155	-1.207054
C	-2.965834	-0.400295	-2.509494
C	-4.230094	-1.257117	-2.278272
C	-4.571679	-1.020521	-0.783873
H	-2.167825	-0.915520	-3.047282
H	-5.039974	-0.940265	-2.940406
H	-4.035113	-2.314491	-2.474238
H	-5.620518	-0.757559	-0.624173
H	-4.352415	-1.914428	-0.193579
H	-4.076746	1.097778	-0.594865
H	-3.294230	0.091567	0.655459
H	-3.213103	0.523763	-3.051252
C	-1.542466	-0.159966	3.150074
O	-1.389230	0.692028	1.993802
C	-1.803481	2.037668	2.307498
C	-2.624343	1.918485	3.588330
C	-1.905680	0.769386	4.309323
H	-2.359150	2.428442	1.452136
H	-2.640928	2.848813	4.161823
H	-3.657536	1.636708	3.354909
H	-0.998088	1.140407	4.797592
H	-2.522528	0.272064	5.062127
H	-0.607463	-0.704251	3.309053
H	-2.337790	-0.886435	2.944387
H	-0.912937	2.660314	2.460129

[(Na-HMDS)·(THF)]₂

E (BS1) = -2536.573615

E (BS2) = -2537.092583

G_{298.15} (BS2) = -2536.484827



N	1.090106	1.459177	-0.170174
Si	1.547741	1.990660	1.376158
Si	1.253490	2.188730	-1.695956
C	1.880997	0.494662	2.510384
H	1.033196	-0.194926	2.578567
H	2.749353	-0.075538	2.159672
H	2.103245	0.821646	3.534065
C	3.136603	3.027904	1.490066
H	3.405869	3.201680	2.540055
H	3.982834	2.516871	1.015197
H	3.032826	4.007164	1.011564
C	0.184937	3.022353	2.219973
H	-0.755270	2.462865	2.310629
H	0.467469	3.343229	3.231045
H	-0.026983	3.924496	1.631282
C	2.487532	3.626834	-1.831400
H	3.498915	3.331086	-1.530661
H	2.543703	3.987521	-2.866609
H	2.191797	4.476336	-1.204871
C	-0.404113	2.913108	-2.312971
H	-0.770897	3.680277	-1.617975
H	-0.287612	3.389559	-3.295091
H	-1.198559	2.164004	-2.428287
C	1.792345	0.914780	-3.001239
H	1.829278	1.356429	-4.005325
H	2.792073	0.522000	-2.777556
H	1.104811	0.063232	-3.051338
Na	-1.213429	0.864150	-0.151380
N	-1.088792	-1.470493	-0.167951
Si	-1.547098	-2.002313	1.377938

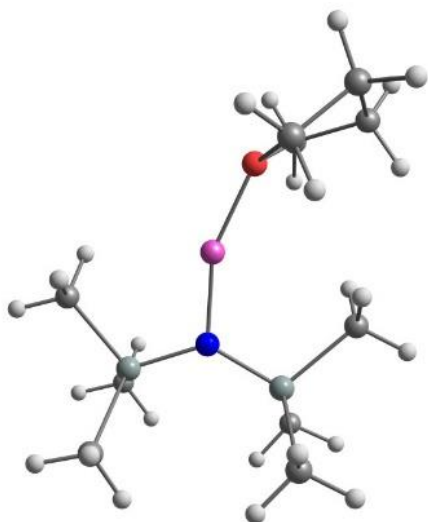
Si	-1.256531	-2.193135	-1.696390
C	-3.129358	-3.049746	1.490129
H	-3.978633	-2.543833	1.015123
H	-3.018996	-4.028063	1.011168
H	-3.398072	-3.225736	2.539899
C	-0.180507	-3.025605	2.225824
H	-0.462444	-3.344340	3.237735
H	0.034148	-3.928983	1.639966
H	0.758102	-2.463315	2.315057
C	-1.894406	-0.506704	2.508925
H	-2.769883	0.052204	2.157545
H	-2.111302	-0.833151	3.533928
H	-1.054849	0.193303	2.574093
C	-2.479923	-3.640186	-1.832432
H	-3.492120	-3.353431	-1.525836
H	-2.538036	-3.996696	-2.868985
H	-2.174792	-4.490121	-1.211006
C	0.403083	-2.901780	-2.326281
H	0.779056	-3.669889	-1.637214
H	0.284440	-3.374293	-3.310029
H	1.191601	-2.146655	-2.442779
C	-1.814635	-0.917063	-2.991685
H	-1.844224	-1.350661	-3.999516
H	-2.820794	-0.543022	-2.764763
H	-1.141592	-0.053558	-3.034551
Na	1.214601	-0.875839	-0.155074
O	-3.344060	1.583775	-0.137359
C	-4.331000	0.546303	-0.372685
C	-5.374635	0.722913	0.724819
H	-4.766888	0.694031	-1.368657
H	-3.815125	-0.416878	-0.349206
C	-5.360667	2.244279	0.932051
H	-6.353105	0.335255	0.430762
H	-5.058402	0.208462	1.638478
C	-3.877971	2.578992	0.771040
H	-5.949797	2.738532	0.152167
H	-5.749145	2.553061	1.905586
H	-3.697140	3.569498	0.343699
H	-3.342063	2.503533	1.725599
O	3.351364	-1.582305	-0.144354
C	3.896164	-2.566609	0.769669
C	5.372083	-2.206662	0.940788
H	3.351899	-2.498645	1.720000
H	3.735782	-3.561070	0.343249
C	5.364579	-0.686777	0.722100
H	5.756905	-2.502127	1.919892
H	5.975857	-2.697292	0.169895
C	4.326380	-0.534623	-0.383931
H	5.034003	-0.169661	1.629143
H	6.339267	-0.286850	0.431913
H	3.797327	0.421507	-0.373075
H	4.771098	-0.686441	-1.375448

Li-HMDS·(THF)

E (BS1) = -113.500051

E (BS2) = -1113.753595

G_{298.15} (BS2) = -1113.463413



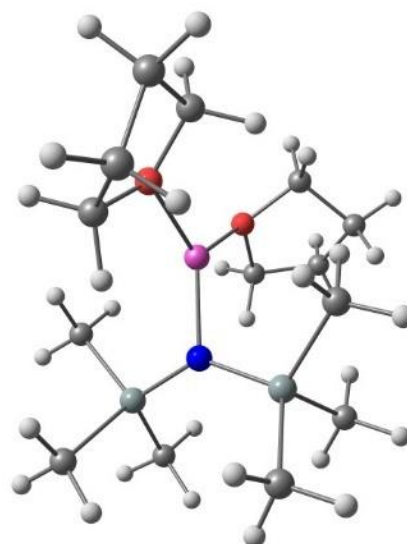
N	-0.933004	-0.088058	-0.004552
Si	-2.234310	-1.180372	-0.013586
Si	-0.900851	1.610180	0.027903
C	-1.528812	-2.940718	0.170071
H	-0.828839	-3.180415	-0.643419
H	-0.992851	-3.060399	1.121540
H	-2.315913	-3.704680	0.145432
C	-3.481265	-0.929626	1.399151
H	-4.236909	-1.725460	1.426042
H	-2.978836	-0.913479	2.374052
H	-4.014111	0.023201	1.290755
C	-3.245047	-1.168269	-1.623867
H	-2.603217	-1.357353	-2.493597
H	-4.034274	-1.931363	-1.621224
H	-3.727168	-0.195955	-1.782112
C	-1.920422	2.435148	-1.348768
H	-2.991959	2.239546	-1.217806
H	-1.786449	3.524659	-1.362569
H	-1.637472	2.052010	-2.336896
C	0.898639	2.194613	-0.186234
H	1.316711	1.852652	-1.141535
H	0.979595	3.288662	-0.167317
H	1.538800	1.809680	0.618219
C	-1.516089	2.360563	1.663448
H	-1.421310	3.454262	1.676527
H	-2.571406	2.119214	1.839295
H	-0.947598	1.968120	2.516093
Li	0.707093	-0.939643	-0.014032
O	2.559772	-1.121525	-0.032689
C	3.321540	-0.796682	1.169845
C	4.678728	-0.303203	0.673759
H	2.778651	-0.016657	1.715577
H	3.378050	-1.695268	1.788851
C	4.334668	0.292513	-0.698828
H	5.122421	0.422444	1.359154
H	5.372208	-1.142963	0.561876
C	3.292496	-0.689439	-1.216226
H	3.894000	1.288129	-0.586579
H	5.196942	0.364266	-1.365755
H	2.574908	-0.252066	-1.915902
H	3.753246	-1.569955	-1.677767

Li-HMDS·(THF)₂

E (BS1) = -1346.013093

E (BS2) = -1346.346999

G_{298.15} (BS2) = -1345.943449



N	-0.819736	0.652210	0.085688
Si	-1.786659	1.441943	-1.052045
Si	-1.020359	0.301550	1.725461
C	-1.881629	3.328329	-0.813689
H	-2.319744	3.581032	0.159922
H	-0.881624	3.779359	-0.844842
H	-2.489238	3.817471	-1.586433
C	-1.045713	1.160815	-2.785203
H	-1.617718	1.674286	-3.568369
H	-0.014485	1.535174	-2.840336
H	-1.026045	0.094037	-3.044801
C	-3.589098	0.831295	-1.120437
H	-4.111572	1.040961	-0.178420
H	-4.161200	1.311961	-1.924967
H	-3.634912	-0.252756	-1.283288
C	-1.520243	1.789589	2.801555
H	-2.517885	2.155950	2.528015
H	-1.545567	1.540323	3.870515
H	-0.819954	2.623884	2.670749
C	0.632516	-0.342392	2.423759
H	1.411253	0.427024	2.352859
H	0.551155	-0.634416	3.478446
H	0.987702	-1.224006	1.874482
C	-2.312325	-1.053709	2.077752
H	-2.398897	-1.280430	3.148662
H	-3.305479	-0.749545	1.724365
H	-2.058395	-1.987976	1.562613
Li	0.653209	-0.275369	-0.665853
O	2.379104	0.512290	-0.838455
C	2.372331	1.949621	-0.600865
C	3.423650	2.182000	0.477477
H	2.633428	2.455132	-1.538105
H	1.357227	2.223562	-0.305166
C	4.454870	1.090405	0.158721
H	3.837119	3.192735	0.439513
H	2.990468	2.021069	1.470640
C	3.564795	-0.082069	-0.247172
H	5.087875	1.397835	-0.680468
H	5.099732	0.841453	1.005060
H	4.019541	-0.747986	-0.985357
H	3.260631	-0.671436	0.626080
C	-0.850371	-2.567964	-1.311080
O	0.532218	-2.129417	-1.140223
C	1.267272	-3.141893	-0.415056
C	0.215344	-3.858475	0.419584
C	-0.979801	-3.891189	-0.545312
H	2.040609	-2.638498	0.170236
H	0.539474	-4.852752	0.736829
H	-0.022640	-3.266693	1.309046
H	-0.890515	-4.741510	-1.228675
H	-1.940206	-3.967697	-0.029889
H	-1.050883	-2.675666	-2.381079
H	-1.481824	-1.776984	-0.899586

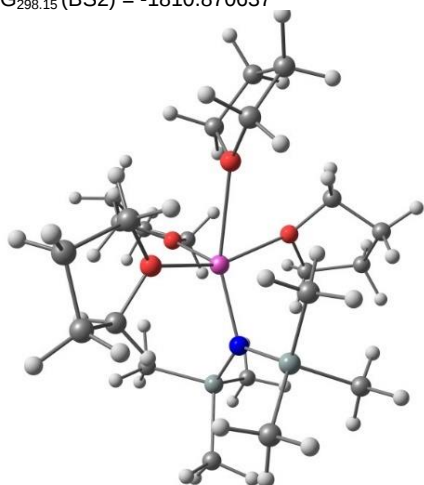
H	1.749174	-3.822337	-1.129102
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Li-HMDS·(THF)₄

E (BS1) = -1810.998760

E (BS2) = -1811.495333

G_{298.15} (BS2) = -1810.870637



N	1.787668	-0.128694	-0.127780
Si	2.924677	0.182572	1.082136
Si	2.052763	-0.694684	-1.696796
C	4.678322	0.612836	0.457055
H	5.128360	-0.215947	-0.103687
H	4.664488	1.486441	-0.205944
H	5.353530	0.844920	1.291720
C	2.421341	1.650700	2.187581
H	3.019957	1.691765	3.106989
H	2.551546	2.608246	1.669673
H	1.367430	1.570917	2.468784
C	3.213479	-1.259221	2.305433
H	3.501046	-2.180544	1.782986
H	4.017922	-1.019439	3.013799
H	2.318391	-1.486470	2.896776
C	3.167679	0.400609	-2.794518
H	4.206360	0.412649	-2.445525
H	3.176314	0.048493	-3.835080
H	2.813841	1.439341	-2.803147
C	0.404799	-0.779534	-2.650265
H	0.006984	0.230271	-2.801218
H	0.530754	-1.243045	-3.637114
H	-0.351179	-1.352794	-2.105677
C	2.832236	-2.434534	-1.796092
H	2.937410	-2.789264	-2.830245
H	3.834391	-2.436578	-1.347817
H	2.234975	-3.174672	-1.251653
Li	-0.209281	0.142288	0.052689
O	-0.371313	2.059749	-0.822791
C	0.781138	2.924902	-0.751619
C	0.689321	3.811263	-1.986835
H	0.725436	3.526803	0.166669
H	1.654725	2.276164	-0.703429
C	-0.827223	4.019435	-2.093670
H	1.251663	4.742753	-1.879888
H	1.066678	3.276950	-2.866399
C	-1.369217	2.647632	-1.680222
H	-1.150981	4.790228	-1.385224
H	-1.162778	4.311854	-3.092326
H	-2.318707	2.703374	-1.139959
H	-1.505441	1.995692	-2.549235
C	0.253093	-2.782124	1.142187
O	-0.803929	-2.025438	0.503344
C	-1.625682	-2.929365	-0.247143
C	-0.687040	-4.050615	-0.676137
C	0.188211	-4.211475	0.575614
H	-2.063862	-2.367506	-1.069398
H	-1.218086	-4.965407	-0.953886

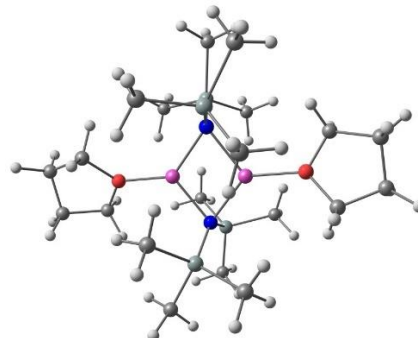
H	-0.084868	-3.723702	-1.529955
H	-0.293478	-4.890296	1.287364
H	1.182760	-4.607846	0.354154
H	0.101411	-2.766654	2.227813
H	1.179809	-2.264056	0.899728
H	-2.437028	-3.319382	0.387545
C	-3.541188	-0.069809	0.237566
O	-2.576320	-0.006011	-0.817406
C	-3.321314	-0.022335	-2.036772
C	-4.453544	-1.033211	-1.806948
C	-4.681221	-0.975385	-0.274326
H	-2.636425	-0.292327	-2.843151
H	-5.348338	-0.774670	-2.379138
H	-4.139139	-2.034709	-2.113142
H	-5.658272	-0.557437	-0.017862
H	-4.621159	-1.973097	0.167304
H	-3.916838	0.941470	0.453799
H	-3.028664	-0.451472	1.119308
H	-3.730811	0.978580	-2.241290
C	-0.863710	-0.029781	3.029107
O	-0.877858	0.756484	1.818492
C	-1.455688	2.053903	2.068802
C	-2.175563	1.921914	3.407586
C	-1.273601	0.925781	4.149441
H	-2.110412	2.301309	1.232232
H	-2.279389	2.881175	3.921183
H	-3.175158	1.496782	3.262581
H	-0.394119	1.439874	4.551953
H	-1.776112	0.409466	4.971314
H	0.138646	-0.445295	3.158746
H	-1.574100	-0.856122	2.913728
H	-0.651895	2.798994	2.118809

[(Li-HMDS)·(THF)₂]₂

E (BS1) = -2227.074775

E (BS2) = -2227.571136

G_{298.15} (BS2) = -2226.950347

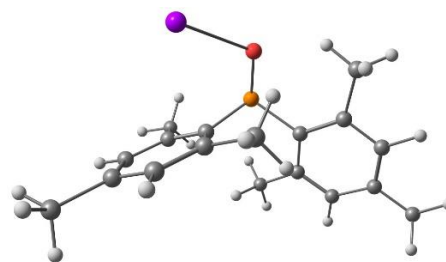


N	0.446414	1.546944	-0.062941
Si	0.902560	2.239502	1.436599
Si	0.403308	2.327571	-1.590031
C	1.659685	0.910762	2.572548
H	1.076118	-0.012545	2.625774
H	2.667099	0.645910	2.233187
H	1.745864	1.293159	3.597499
C	2.239280	3.591718	1.392907
H	2.595894	3.780507	2.414128
H	3.108604	3.294028	0.794927
H	1.872376	4.542192	0.994332
C	-0.560809	3.011833	2.370676
H	-1.342504	2.275102	2.584955
H	-0.247830	3.448988	3.327674
H	-1.017340	3.812622	1.775351
C	1.047024	4.112999	-1.664596
H	2.112690	4.188706	-1.426411
H	0.908352	4.505305	-2.680645
H	0.503023	4.776439	-0.982577
C	-1.369474	2.460575	-2.273900
H	-1.931639	3.213953	-1.707859
H	-1.357909	2.780191	-3.323901

H	-1.936447	1.526809	-2.219080
C	1.431545	1.376502	-2.873893
H	1.275869	1.772420	-3.885557
H	2.500796	1.464912	-2.648575
H	1.188725	0.309958	-2.900619
Li	-1.163476	0.322834	-0.036565
N	-0.454039	-1.545445	-0.064994
Si	-0.906685	-2.228595	1.440295
Si	-0.398364	-2.340126	-1.584764
C	-2.246071	-3.578580	1.412343
H	-3.119671	-3.283199	0.819693
H	-1.883936	-4.531893	1.016201
H	-2.594788	-3.761122	2.437431
C	0.558183	-2.998518	2.374245
H	0.246717	-3.431450	3.333648
H	1.012914	-3.802027	1.781199
H	1.340758	-2.261530	2.584129
C	-1.655427	-0.890792	2.570786
H	-2.661750	-0.621589	2.231753
H	-1.742128	-1.268111	3.597570
H	-1.066467	0.029262	2.618821
C	-1.116729	-4.096530	-1.663133
H	-2.187436	-4.125792	-1.436818
H	-0.983451	-4.497341	-2.676508
H	-0.609996	-4.780776	-0.973248
C	1.384508	-2.546141	-2.223222
H	1.908990	-3.309612	-1.634059
H	1.388611	-2.877459	-3.268764
H	1.978064	-1.628785	-2.162079
C	-1.341101	-1.356758	-2.908010
H	-1.239090	-1.824141	-3.895795
H	-2.411283	-1.315980	-2.673320
H	-0.983300	-0.327106	-2.997812
Li	1.156791	-0.321082	-0.024121
O	-3.017519	0.696125	0.003561
C	-4.032226	-0.255908	-0.403938
C	-5.318110	0.212527	0.269532
H	-4.116884	-0.225995	-1.496110
H	-3.705011	-1.251895	-0.099592
C	-5.119616	1.734327	0.306537
H	-6.208345	-0.096900	-0.283296
H	-5.384815	-0.187423	1.287215
C	-3.633619	1.848063	0.630035
H	-5.331015	2.170338	-0.675947
H	-5.742833	2.236169	1.050628
H	-3.157376	2.746556	0.232604
H	-3.452412	1.795283	1.709580
O	3.011169	-0.696955	0.011682
C	3.628271	-1.840573	0.652502
C	5.113040	-1.733001	0.322135
H	3.451399	-1.771988	1.731882
H	3.149298	-2.743760	0.269641
C	5.313240	-0.212020	0.266725
H	5.738329	-2.227019	1.069720
H	5.319969	-2.180786	-0.656003
C	4.025887	0.250177	-0.408204
H	5.383904	0.199556	1.279490
H	6.201994	0.089899	-0.292617
H	3.700221	1.249578	-0.113388
H	4.106954	0.208374	-1.500021

K-OPMe₂

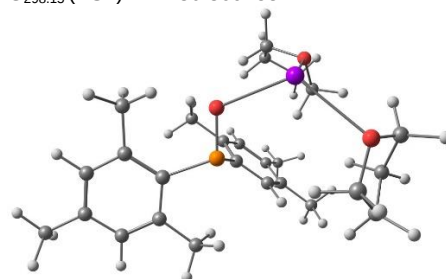
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E (BS2) = -1716.207622
G_{298.15} (BS2) = -1715.911211



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C	-3.316656	-1.655724	0.103790
C	-2.088989	-1.206599	0.592082
C	-1.712012	0.159870	0.457658
P	-0.139274	0.694847	1.349315
O	0.222001	2.191320	0.977255
C	1.153359	-0.269169	0.337102
C	2.167862	-0.978354	1.029627
H	4.021825	-2.056690	0.876263
C	3.253317	-1.518605	0.325131
C	3.381926	-1.381849	-1.059484
C	2.388345	-0.668001	-1.737428
H	2.470857	-0.533339	-2.814547
C	1.286408	-0.116296	-1.068215
C	-2.640931	1.043441	-0.142496
C	-3.872555	0.551467	-0.605929
H	-4.568151	1.251918	-1.065855
C	-4.231846	-0.789835	-0.505578
H	-3.570618	-2.708871	0.212296
C	-1.186476	-2.212688	1.265374
H	-1.716226	-3.153759	1.439396
H	-0.296663	-2.431711	0.666489
H	-0.830350	-1.838249	2.231866
C	-2.381646	2.518780	-0.368174
H	-1.594382	2.895181	0.283938
H	-2.056075	2.695619	-1.402944
H	-3.304197	3.093003	-0.225736
C	-5.559870	-1.295437	-1.011317
H	-6.178970	-1.682839	-0.192639
H	-6.124972	-0.502007	-1.509334
H	-5.430061	-2.116425	-1.726617
C	2.135010	-1.173213	2.529987
H	2.012071	-0.226875	3.064156
H	1.300102	-1.812119	2.834825
H	3.059791	-1.646149	2.874378
C	4.541689	-1.998908	-1.799744
H	5.433527	-2.059394	-1.168322
H	4.302068	-3.020378	-2.121667
H	4.793307	-1.427368	-2.698648
C	0.282844	0.667109	-1.885249
H	-0.626964	0.085374	-2.062035
H	-0.024516	1.573483	-1.359190
H	0.702458	0.937192	-2.859551

K-OPMe₂(THF)₂

E (BS1) = -2180.871423
E (BS2) = -2181.383942
G_{298.15} (BS2) = -2180.869453



K	-1.633901	-1.907674	-2.175127
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O	0.614069	-0.859674	-1.788627

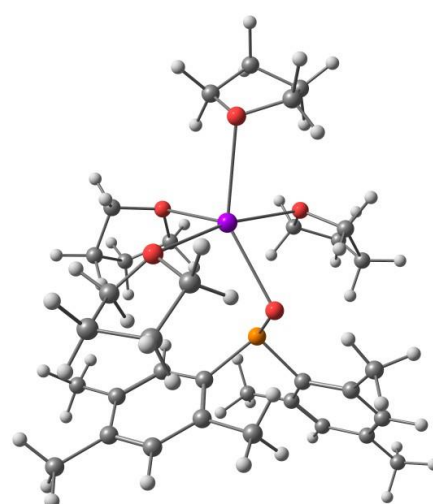
C	0.434808	1.861491	0.079873
C	0.318235	0.538777	0.557043
C	-0.297755	2.872191	0.714996
C	-1.133663	2.631795	1.810870
C	-1.243732	1.315725	2.300354
C	-0.525159	0.304726	1.652540
H	-0.214380	3.890811	0.339865
H	-0.620286	-0.714337	2.021660
C	3.441303	-0.610087	1.204391
C	4.814244	-0.462140	1.406832
C	2.891734	-0.540112	-0.108566
C	3.787012	-0.344567	-1.188378
C	5.163487	-0.212423	-0.938152
C	5.702148	-0.259832	0.344500
H	5.202933	-0.516940	2.422376
H	5.829913	-0.063330	-1.786475
O	-2.891368	-3.034219	-0.146824
C	-2.084436	-3.386481	1.007747
C	-4.109549	-2.417654	0.308275
C	-2.781764	-2.774519	2.234375
H	-2.008032	-4.477967	1.071775
H	-1.080977	-2.973778	0.850260
C	-3.728288	-1.734727	1.614764
H	-4.454624	-1.734514	-0.473722
H	-4.882166	-3.183991	0.467466
H	-2.065717	-2.336645	2.933927
H	-3.356194	-3.537170	2.769635
H	-3.192096	-0.804950	1.404123
H	-4.592153	-1.507610	2.244624
O	-2.904178	0.442983	-2.227776
C	-1.973556	1.301345	-2.931827
C	-3.197627	1.092760	-0.977952
C	-2.216869	2.737425	-2.415101
H	-0.949106	0.967492	-2.723297
H	-2.178826	1.186651	-4.000562
C	-3.315575	2.569233	-1.343362
H	-4.117380	0.653835	-0.583621
H	-2.382140	0.927525	-0.262786
H	-2.529196	3.411701	-3.216392
H	-1.303084	3.138234	-1.972553
H	-4.304891	2.769842	-1.767072
H	-3.167707	3.223126	-0.480494
C	1.324035	2.202492	-1.087714
H	2.378927	2.192157	-0.791142
H	1.207441	1.457159	-1.877285
H	1.096890	3.197346	-1.482944
C	-1.906967	3.760226	2.443688
H	-2.987426	3.570958	2.422558
H	-1.635499	3.895475	3.498105
H	-1.720852	4.705379	1.926270
C	-2.124374	0.998689	3.482616
H	-3.176521	1.237701	3.283246
H	-2.065309	-0.061247	3.743025
H	-1.834965	1.577859	4.368128
C	2.576542	-0.838038	2.421806
H	1.848119	-1.639369	2.253155
H	3.191085	-1.106603	3.286222
H	1.999175	0.054411	2.683239
C	3.355930	-0.223796	-2.635245
H	4.091561	-0.702275	-3.292185
H	2.365696	-0.649410	-2.794887
H	3.307312	0.832857	-2.930791
C	7.181885	-0.101302	0.590073
H	7.398737	0.821247	1.143045
H	7.580184	-0.929975	1.187162
H	7.740673	-0.064168	-0.349625

K-OPMe₂(THF)₄

E (BS1) = -2645.876836

E (BS2) = -2646.549644

G_{298.15} (BS2) = -2645.817797

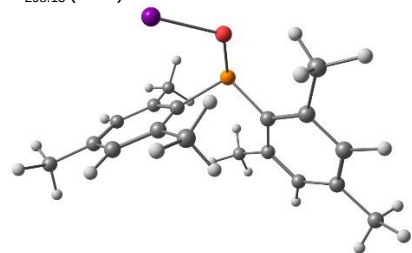


K	-2.109140	-0.096467	-0.522669
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O	0.311904	-0.604198	-1.289969
C	2.537419	1.784507	-1.038022
C	1.869905	1.204878	0.061507
C	2.867094	3.144657	-0.983072
C	2.579436	3.952781	0.122507
C	1.933435	3.374319	1.232360
C	1.584410	2.021028	1.165608
H	3.368711	3.594780	-1.838147
H	1.061892	1.580197	2.012146
C	3.502776	-1.602839	1.122436
C	4.585604	-2.479304	1.198108
C	2.686553	-1.558477	-0.045753
C	3.001765	-2.447105	-1.102420
C	4.094673	-3.322048	-0.977290
C	4.904880	-3.354801	0.153486
H	5.192431	-2.486056	2.102048
H	4.313794	-3.994823	-1.805307
O	-2.800585	0.854310	1.892017
C	-1.809562	0.547323	2.904974
C	-3.110270	2.260294	1.934801
C	-1.486505	1.869408	3.611724
H	-2.216568	-0.210168	3.583229
H	-0.929936	0.130130	2.400031
C	-1.885668	2.916156	2.561738
H	-3.322160	2.591957	0.913732
H	-4.008557	2.424304	2.547387
H	-0.435157	1.930697	3.903652
H	-2.098186	1.984875	4.512619
H	-1.095428	3.026624	1.813466
H	-2.103155	3.898462	2.988987
O	-1.788746	2.318231	-1.769271
C	-1.071719	1.950977	-2.975567
C	-1.068649	3.391335	-1.141907
C	-0.127570	3.126295	-3.309386
H	-0.510082	1.027771	-2.791341
H	-1.823170	1.776907	-3.752851
C	-0.531073	4.219533	-2.303474
H	-1.768536	3.928420	-0.496205
H	-0.247588	2.995343	-0.531843
H	-0.228244	3.453736	-4.347360
H	0.910962	2.831571	-3.144902
H	-1.326241	4.852548	-2.711914
H	0.307625	4.856223	-2.010071
C	2.887647	0.975007	-2.259539
H	3.691672	0.263746	-2.038687
H	2.022406	0.387514	-2.575984
H	3.221497	1.616741	-3.080541
C	2.946692	5.414653	0.116186
H	2.064265	6.052856	0.249436
H	3.636314	5.662379	0.932801
H	3.426502	5.696939	-0.824981
C	1.602286	4.196338	2.452379
H	0.912676	5.016522	2.215931

H	1.136878	3.580480	3.226170
H	2.498734	4.657171	2.885214
C	3.238591	-0.711169	2.312226
H	2.175535	-0.705992	2.579551
H	3.812808	-1.045688	3.181354
H	3.510175	0.329345	2.108210
C	2.243703	-2.509163	-2.413008
H	2.060719	-3.552466	-2.697631
H	1.302882	-1.963364	-2.353584
H	2.842982	-2.063467	-3.218269
C	6.082712	-4.290983	0.259174
H	7.029821	-3.738352	0.297335
H	6.032529	-4.897627	1.171105
H	6.129303	-4.971469	-0.596190
C	-4.817455	-1.945218	-1.783750
O	-4.671734	-0.630854	-1.214125
C	-5.500414	-0.530306	-0.029480
C	-6.145029	-1.909646	0.176029
C	-5.216212	-2.841706	-0.617371
H	-6.242206	0.262467	-0.179357
H	-6.217650	-2.174444	1.234108
H	-7.153965	-1.927659	-0.249297
H	-4.325454	-3.092104	-0.033161
H	-5.706846	-3.763143	-0.942478
H	-3.865507	-2.219465	-2.250261
H	-5.593199	-1.930085	-2.563638
H	-4.856998	-0.246903	0.811452
C	-1.284284	-3.440293	-0.624230
O	-2.006137	-2.678766	0.376911
C	-1.513990	-3.014108	1.689088
C	-0.824239	-4.365652	1.531682
C	-0.212809	-4.231897	0.129802
H	-2.365501	-3.024999	2.376683
H	-0.079958	-4.546829	2.311779
H	-1.561207	-5.176498	1.557105
H	0.716971	-3.657570	0.177344
H	0.001735	-5.193137	-0.344713
H	-0.850101	-2.740588	-1.343366
H	-2.000709	-4.101349	-1.128802
H	-0.798036	-2.248323	2.013994

Na-OPMe₂

E (BS1) = -1278.251341
E (BS2) = -1278.569838
G_{298.15} (BS2) = -178.272635

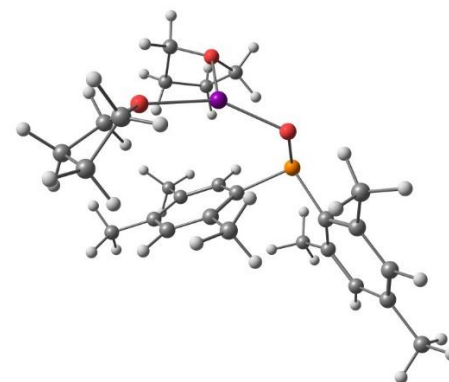


11	1.910319	2.898402	-0.252024
6	-2.990988	-1.780819	0.224056
6	-1.809551	-1.186162	0.674981
6	-1.569631	0.197850	0.456446
15	-0.046955	0.926418	1.288105
8	0.156771	2.431334	0.808632
6	1.323414	0.019122	0.333876
6	2.405064	-0.525173	1.073779
1	4.325521	-1.486447	0.990575
6	3.509835	-1.068424	0.404536
6	3.599091	-1.082860	-0.989722
6	2.544260	-0.522386	-1.714957
1	2.593188	-0.512676	-2.802272
6	1.414093	0.017968	-1.084505
6	-2.583366	0.953031	-0.184758
6	-3.760019	0.317320	-0.608080
1	-4.522225	0.917688	-1.102636
6	-3.986572	-1.046123	-0.425150

1	-3.140611	-2.845293	0.395384
6	-0.811089	-2.061155	1.395243
1	-1.255073	-3.028933	1.645471
1	0.083663	-2.247049	0.792489
1	-0.471850	-1.592180	2.325908
6	-2.470826	2.431157	-0.495739
1	-1.797392	2.943705	0.188979
1	-2.068531	2.583438	-1.506959
1	-3.461699	2.897561	-0.476421
6	-5.274446	-1.693701	-0.868756
1	-6.040669	-1.635703	-0.084027
1	-5.685732	-1.202333	-1.756810
1	-5.130731	-2.753652	-1.101512
6	2.416849	-0.548985	2.587110
1	2.250086	0.443992	3.014329
1	1.630264	-1.196338	2.987644
1	3.377194	-0.922949	2.954407
6	4.781678	-1.703444	-1.689437
1	5.684811	-1.651176	-1.073791
1	4.596490	-2.763557	-1.905219
1	4.986663	-1.210370	-2.644803
6	0.324826	0.589653	-1.966910
1	-0.501785	-0.118677	-2.082732
1	-0.105799	1.498850	-1.543410
1	0.715135	0.811506	-2.965040

Na-OPMe₂·(THF)₂

E (BS1) = -1743.278337
E (BS2) = -1743.758165
G_{298.15} (BS2) = -1743.241227



Na	1.366120	-0.407388	-1.878055
P	-1.319982	0.977911	-1.001037
O	-0.718496	0.039646	-2.128420
C	-0.233352	-0.829215	1.041305
C	-0.338778	0.486726	0.534191
C	0.631194	-1.066696	2.117984
C	1.407529	-0.062568	2.706685
C	1.318829	1.248018	2.197011
C	0.452212	1.485240	1.124048
H	0.706117	-2.077752	2.513318
H	0.378743	2.498179	0.732864
C	-3.657490	1.070933	0.572123
C	-4.979092	0.789515	0.921140
C	-3.022430	0.358585	-0.485452
C	-3.784148	-0.611324	-1.180147
C	-5.115298	-0.853615	-0.801656
C	-5.733626	-0.176042	0.245578
H	-5.435630	1.346142	1.737899
H	-5.679298	-1.605856	-1.351061
O	2.698394	1.357119	-2.365137
C	2.126775	2.657585	-2.068747
C	4.056213	1.370919	-1.889492
C	2.974296	3.258905	-0.925592
H	2.164045	3.276222	-2.972714
H	1.079824	2.498409	-1.798686
C	3.972498	2.137363	-0.575563
H	4.386511	0.334044	-1.800963

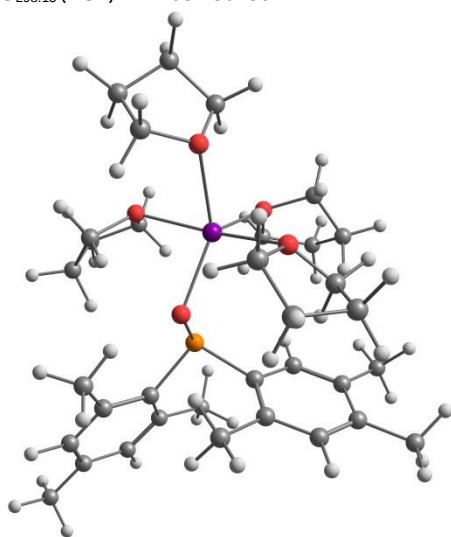
H	4.700279	1.888009	-2.615366
H	2.359543	3.544046	-0.069923
H	3.503652	4.150450	-1.273045
H	3.561579	1.486631	0.202835
H	4.941422	2.515180	-0.239655
O	2.774032	-1.942905	-1.038757
C	2.458875	-3.352361	-1.078469
C	3.566186	-1.655848	0.145059
C	2.509343	-3.808464	0.373436
H	1.476148	-3.463188	-1.546215
H	3.204964	-3.875805	-1.691422
C	3.670968	-2.971003	0.929277
H	4.545382	-1.278103	-0.165054
H	3.044844	-0.878741	0.709879
H	2.673987	-4.884804	0.465873
H	1.575012	-3.552345	0.879105
H	4.626279	-3.463421	0.722470
H	3.599110	-2.806506	2.007019
C	-1.021649	-1.974471	0.455286
H	-2.068066	-1.939621	0.776713
H	-1.024829	-1.917775	-0.635561
H	-0.608550	-2.937978	0.767210
C	2.337423	-0.388330	3.846939
H	3.382790	-0.180935	3.585775
H	2.113365	0.213773	4.735827
H	2.263003	-1.442153	4.128611
C	2.139853	2.366902	2.785912
H	3.216043	2.177719	2.687682
H	1.919966	3.316895	2.291928
H	1.940976	2.492408	3.857200
C	-2.937069	2.140695	1.359563
H	-2.377644	2.817406	0.703559
H	-3.648064	2.735332	1.940745
H	-2.209068	1.712369	2.056123
C	-3.241936	-1.465987	-2.306582
H	-4.021634	-1.648805	-3.054544
H	-2.366516	-1.014750	-2.771357
H	-2.933565	-2.448691	-1.923879
C	-7.162152	-0.458038	0.639026
H	-7.228532	-0.817561	1.673257
H	-7.780442	0.445615	0.577110
H	-7.611824	-1.216879	-0.008071

Na-OPMe₂(THF)₄

E (BS1) = -2208.282041

E (BS2) = -2208.923538

G_{298.15} (BS2) = -2208.186736



Na	-1.920077	-0.362919	-0.178137
P	1.134353	-0.393055	0.275594
O	0.144796	-0.644627	-0.929581
C	2.162934	1.931155	-1.157521

C	1.679432	1.388189	0.051607
C	2.326807	3.318684	-1.252135
C	2.041746	4.191765	-0.195739
C	1.573760	3.653159	1.018542
C	1.398171	2.268027	1.105981
H	2.688901	3.738702	-2.189143
H	1.016085	1.853746	2.036815
C	3.755199	-1.148936	0.995258
C	4.922837	-1.911231	0.956639
C	2.766744	-1.285450	-0.023494
C	3.009108	-2.226020	-1.053245
C	4.193832	-2.982412	-1.044923
C	5.166071	-2.843469	-0.059257
H	5.660652	-1.780500	1.746575
H	4.354155	-3.698570	-1.849740
O	-2.531778	0.580073	1.852036
C	-1.653223	0.569741	3.005980
C	-3.181538	1.862607	1.770469
C	-1.629104	2.006638	3.553453
H	-2.033696	-0.148885	3.740170
H	-0.670471	0.236113	2.659860
C	-2.181153	2.834575	2.383111
H	-3.410914	2.048551	0.719473
H	-4.119676	1.842382	2.344481
H	-0.623446	2.311030	3.854043
H	-2.285193	2.097589	4.425037
H	-1.387865	3.052570	1.662738
H	-2.640245	3.775458	2.697846
O	-2.165383	1.666726	-1.444906
C	-1.906621	1.182169	-2.785235
C	-1.470252	2.914599	-1.244039
C	-0.982077	2.209005	-3.449897
H	-1.435234	0.196955	-2.720117
H	-2.868240	1.093349	-3.303367
C	-1.250781	3.484429	-2.640724
H	-2.094251	3.547646	-0.607213
H	-0.517608	2.728609	-0.739917
H	-1.188148	2.319554	-4.517860
H	0.061195	1.907399	-3.329758
H	-2.157301	3.987094	-2.996720
H	-0.421465	4.195649	-2.671246
C	2.485488	1.054354	-2.339800
H	3.394657	0.469788	-2.160624
H	1.673965	0.341777	-2.504132
H	2.640358	1.649646	-3.244793
C	2.223115	5.678735	-0.363088
H	1.281555	6.219701	-0.205969
H	2.940056	6.083293	0.362115
H	2.586455	5.921960	-1.365359
C	1.243446	4.545088	2.188642
H	0.439859	5.252012	1.946573
H	0.921567	3.956163	3.051750
H	2.107136	5.147144	2.496873
C	3.587593	-0.178783	2.140783
H	2.586752	-0.249824	2.582496
H	4.326142	-0.373615	2.924021
H	3.706749	0.859227	1.814131
C	2.075077	-2.460113	-2.223173
H	1.928996	-3.534703	-2.387473
H	1.114389	-1.971802	-2.067765
H	2.516677	-2.058272	-3.144897
C	6.431197	-3.664673	-0.070219
H	7.322721	-3.026308	-0.092729
H	6.510885	-4.289060	0.828177
H	6.470038	-4.325658	-0.941109
C	-4.136923	-2.126480	-1.800026
O	-4.029070	-0.888801	-1.068651
C	-5.017724	-0.866182	-0.008679
C	-5.837058	-2.152629	-0.154333
C	-4.848657	-3.092114	-0.859710
H	-5.622268	0.041025	-0.112270
H	-6.181262	-2.532248	0.811238
H	-6.714711	-1.979847	-0.786610
H	-4.131166	-3.495707	-0.139898
H	-5.334319	-3.915755	-1.389513

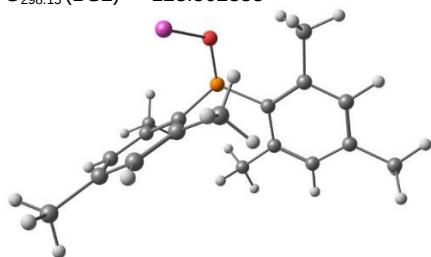
H	-3.129133	-2.442173	-2.082917
H	-4.720017	-1.958223	-2.716715
H	-4.488378	-0.825197	0.949453
C	-1.167450	-3.475798	-0.287598
O	-1.895820	-2.630707	0.637716
C	-1.437283	-2.879745	1.984075
C	-0.666239	-4.195776	1.924511
C	-0.045742	-4.121310	0.522967
H	-2.310009	-2.906067	2.644095
H	0.074938	-4.277893	2.723944
H	-1.351680	-5.047936	1.997157
H	0.834120	-3.470981	0.531671
H	0.248329	-5.095410	0.123060
H	-0.793593	-2.843940	-1.094609
H	-1.860046	-4.228750	-0.686586
H	-0.777783	-2.060989	2.292837

Li-OPMes₂

E (BS1) = -1123.496016

E (BS2) = -1123.803069

G_{298.15} (BS2) = -123.502838



Li	1.433023	2.762325	-1.129838
C	-2.741494	-1.682798	0.683791
C	-1.607377	-0.910164	0.944366
C	-1.481448	0.390856	0.387295
P	0.004038	1.401068	0.923686
O	0.102013	2.701072	-0.009769
C	1.417509	0.349732	0.221950
C	2.552064	0.128642	1.047339
H	4.530131	-0.695365	1.181569
C	3.672866	-0.531119	0.532304
C	3.726664	-0.979869	-0.791392
C	2.618677	-0.740766	-1.605142
H	2.638531	-1.075436	-2.640245
C	1.469499	-0.092273	-1.126126
C	-2.560306	0.898016	-0.376572
C	-3.684011	0.089225	-0.605345
H	-4.500169	0.493924	-1.200828
C	-3.795061	-1.205619	-0.100943
H	-2.806466	-2.680122	1.115155
C	-0.536943	-1.503549	1.830278
H	-0.916398	-2.385361	2.354428
H	0.347106	-1.806456	1.260196
H	-0.196382	-0.783631	2.583012
C	-2.583084	2.277245	-1.001209
H	-2.159343	3.037823	-0.347063
H	-1.992314	2.308361	-1.924846
H	-3.610504	2.550050	-1.262488
C	-5.011240	-2.056423	-0.368377
H	-5.515315	-2.338376	0.563910
H	-5.736535	-1.529222	-0.994971
H	-4.741853	-2.989190	-0.878479
C	2.598751	0.579479	2.491211
H	2.404690	1.651499	2.592456
H	1.847174	0.067105	3.100188
H	3.581347	0.368816	2.923474
C	4.936535	-1.713881	-1.311077
H	5.865504	-1.260039	-0.950591
H	4.936502	-2.757605	-0.972378
H	4.959907	-1.723103	-2.404620
C	0.317286	0.083124	-2.093484
H	-0.439736	-0.694194	-1.947250
H	-0.196534	1.037704	-1.965179

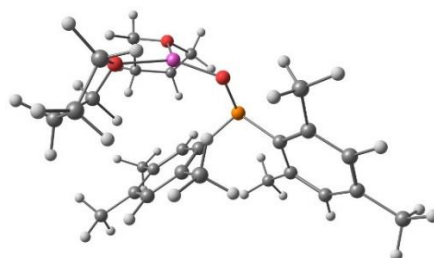
H	0.671598	0.012102	-3.126278
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Li-OPMes₂·(THF)₂

E (BS1) = -1588.533013

E (BS2) = -1589.000357

G_{298.15} (BS2) = -1588.479535



Li	1.380839	1.744267	-0.971017
P	-0.997736	1.120918	0.527958
O	-0.398023	1.762377	-0.799560
C	-0.237875	-1.561391	-0.385865
C	-0.139597	-0.547913	0.592714
C	0.572254	-2.696545	-0.257080
C	1.488164	-2.864788	0.787817
C	1.600444	-1.850377	1.758270
C	0.781533	-0.722332	1.636006
H	0.494534	-3.479662	-1.009025
H	0.860374	0.057611	2.390913
C	-3.411173	-0.112202	1.272666
C	-4.770788	-0.420723	1.189531
C	-2.769280	0.596944	0.220278
C	-3.555661	1.010812	-0.882450
C	-4.920750	0.686360	-0.918569
C	-5.550614	-0.032189	0.096309
H	-5.233803	-0.972564	2.005753
H	-5.506613	1.008623	-1.777484
O	2.524702	2.740833	0.215700
C	2.061265	3.036132	1.559053
C	3.937844	2.479700	0.321651
C	3.009128	2.279716	2.516850
H	2.110786	4.119922	1.714393
H	1.020258	2.713114	1.619252
C	4.050755	1.627413	1.580245
H	4.254654	1.994996	-0.602218
H	4.476255	3.431361	0.430781
H	2.474042	1.533824	3.108448
H	3.486245	2.977877	3.209552
H	3.768027	0.595357	1.350921
H	5.060211	1.625720	1.998722
O	2.512780	0.689289	-2.102813
C	2.062682	0.360315	-3.442439
C	3.127028	-0.479666	-1.484795
C	2.018048	-1.161930	-3.491195
H	1.090878	0.837080	-3.596928
H	2.781046	0.769473	-4.163355
C	3.186997	-1.548332	-2.574878
H	4.113752	-0.194219	-1.111822
H	2.498935	-0.787574	-0.646248
H	2.122973	-1.544853	-4.509276
H	1.074764	-1.523833	-3.076582
H	4.135255	-1.488709	-3.119127
H	3.089724	-2.553612	-2.158238
C	-1.173384	-1.449529	-1.562642
H	-2.217254	-1.572269	-1.258067
H	-1.088371	-0.461930	-2.022270
H	-0.951787	-2.213885	-2.313033
C	2.352461	-4.097419	0.853570
H	3.418828	-3.843365	0.806825
H	2.203586	-4.645948	1.791690
H	2.132477	-4.778738	0.027202
C	2.584445	-1.965732	2.894764
H	3.615834	-2.052983	2.531012
H	2.531814	-1.091564	3.549489
H	2.393322	-2.855287	3.507590

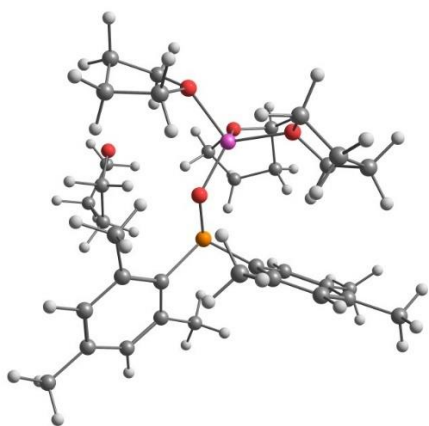
C	-2.659194	-0.569044	2.501417
H	-2.008491	0.220819	2.894283
H	-3.356441	-0.862903	3.291491
H	-2.012428	-1.426077	2.287620
C	-3.006361	1.760699	-2.076763
H	-3.820197	2.257923	-2.614582
H	-2.246426	2.487416	-1.794922
H	-2.522089	1.073217	-2.781357
C	-7.021880	-0.358849	0.036713
H	-7.202930	-1.425267	0.214337
H	-7.584567	0.191028	0.801609
H	-7.448276	-0.101467	-0.937329

Li-OPMe₂(THF)₄

E (BS1) = -2053.533953

E (BS2) = -2054.163460

G_{298.15} (BS2) = -2053.423635



Li	-0.431462	-2.156921	-0.302739
P	0.137756	0.783338	0.416638
O	0.206557	-0.468884	-0.552379
C	-2.216347	1.700949	-1.048767
C	-1.599519	1.447931	0.194547
C	-3.581233	2.012525	-1.068167
C	-4.360428	2.089627	0.091983
C	-3.746695	1.848783	1.336424
C	-2.384816	1.530453	1.353163
H	-4.060444	2.197542	-2.028012
H	-1.913688	1.324804	2.312670
C	1.233609	3.369606	0.480516
C	2.123654	4.390207	0.144844
C	1.143067	2.193724	-0.321079
C	1.983011	2.106822	-1.458034
C	2.877161	3.151743	-1.747773
C	2.967297	4.301348	-0.968401
H	2.168358	5.275497	0.776785
H	3.516872	3.054869	-2.623657
O	-0.260639	-2.925202	1.522273
C	0.678112	-2.272355	2.407479
C	-1.415564	-3.228547	2.319922
C	-0.170271	-1.525316	3.459920
H	1.312684	-3.038107	2.870483
H	1.297520	-1.620208	1.794547
C	-1.621194	-1.969650	3.157645
H	-2.231285	-3.474645	1.639662
H	-1.203247	-4.101171	2.955102
H	-0.054265	-0.444552	3.356059
H	0.132327	-1.810470	4.471336
H	-2.135578	-1.210922	2.560414
H	-2.209337	-2.156484	4.059952
O	-2.334475	-2.470486	-0.810814
C	-2.570089	-2.604306	-2.233564
C	-3.410823	-1.699135	-0.208481
C	-3.640166	-1.572414	-2.573378
H	-1.626289	-2.437602	-2.756480
H	-2.911900	-3.626536	-2.440264
C	-4.479089	-1.553296	-1.290141

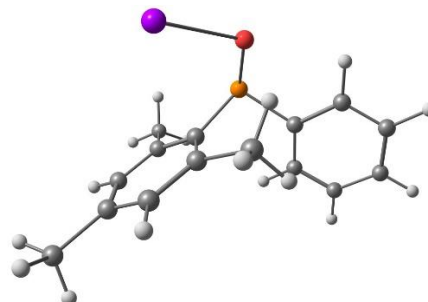
H	-3.766853	-2.235027	0.675423
H	-3.010068	-0.730738	0.095718
H	-4.211257	-1.845733	-3.464380
H	-3.181093	-0.593427	-2.737732
H	-5.167452	-2.405442	-1.271471
H	-5.057445	-0.635200	-1.166581
C	-1.447029	1.621516	-2.341202
H	-0.719729	2.437052	-2.415377
H	-0.880139	0.688506	-2.381788
H	-2.114822	1.683556	-3.205581
C	-5.830508	2.410004	0.003880
H	-6.444476	1.603190	0.423223
H	-6.081153	3.317245	0.567367
H	-6.139930	2.563151	-1.033613
C	-4.537092	1.911610	2.618666
H	-5.372943	1.200922	2.615311
H	-3.904456	1.680861	3.480343
H	-4.972863	2.905756	2.778531
C	0.379980	3.560970	1.711870
H	0.403212	2.675545	2.357893
H	0.725650	4.421178	2.292522
H	-0.671175	3.727088	1.454987
C	1.963481	0.955033	-2.440301
H	2.977625	0.732281	-2.789919
H	1.510157	0.068699	-2.003054
H	1.374783	1.223265	-3.327698
C	3.929448	5.413544	-1.303007
H	3.398047	6.342632	-1.543627
H	4.592642	5.636989	-0.458847
H	4.554656	5.154891	-2.162673
C	1.099759	-2.847371	-2.674964
O	0.673588	-3.386927	-1.399280
C	1.821406	-3.932248	-0.691422
C	2.942344	-4.015913	-1.722893
C	2.625102	-2.820877	-2.631760
H	1.531145	-4.900345	-0.274516
H	3.926862	-3.948726	-1.253663
H	2.885919	-4.953525	-2.287014
H	2.972479	-1.892213	-2.171445
H	3.067643	-2.900321	-3.628152
H	0.654760	-1.856379	-2.790145
H	0.731077	-3.505646	-3.471929
H	2.097686	-3.255788	0.121464
C	3.599914	-0.595339	0.369320
O	3.791993	-1.829653	1.095123
C	4.301056	-1.545593	2.406309
C	4.802847	-0.102349	2.363116
C	3.811316	0.533590	1.380216
H	5.084109	-2.274914	2.642749
H	4.806515	0.370623	3.349063
H	5.820943	-0.064897	1.958703
H	2.867645	0.765113	1.884678
H	4.177988	1.449524	0.911399
H	2.597943	-0.603481	-0.064886
H	4.340912	-0.544255	-0.441574
H	3.495391	-1.655760	3.148030

K-OP(Mes)Ph

E (BS1) = -1597.889026

E (BS2) = -1598.205057

G_{298.15} (BS2) = -1597.985678



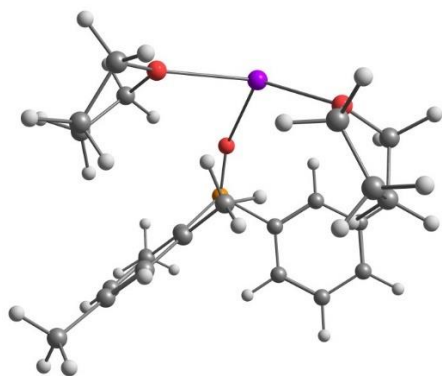
K	1.575685	2.793315	-0.379899
C	-3.389287	-2.120298	-0.096497
C	-2.275136	-1.479026	0.445137
C	-2.148935	-0.081714	0.385674
P	-0.747475	0.817055	1.217056
O	-0.668026	2.240439	0.530871
C	0.672953	-0.170548	0.439892
C	1.636225	-0.767441	1.288703
H	3.518476	-1.800127	1.409767
C	2.788701	-1.347669	0.741537
C	3.031875	-1.355244	-0.634362
C	2.075548	-0.769283	-1.470201
H	2.238721	-0.767289	-2.546690
C	0.902562	-0.195696	-0.961042
C	-3.179612	0.656250	-0.213024
C	-4.298522	0.018610	-0.753680
H	-5.084654	0.606365	-1.221800
C	-4.407456	-1.373058	-0.699111
H	-3.464048	-3.204168	-0.054662
C	1.466822	-0.800859	2.792823
H	1.375431	0.204824	3.214870
H	0.562089	-1.342004	3.086973
H	2.322587	-1.294117	3.263719
C	4.270145	-2.000970	-1.203289
H	5.093012	-1.994050	-0.482027
H	4.079315	-3.048501	-1.469398
H	4.604905	-1.492950	-2.113297
C	-0.095983	0.378359	-1.944968
H	-0.880171	-0.354051	-2.166123
H	-0.598586	1.258184	-1.535756
H	0.390870	0.633223	-2.892683
H	-1.485894	-2.071135	0.903905
H	-5.275826	-1.872107	-1.120185
H	-3.077328	1.737103	-0.266887

K-OP(Mes)Ph.(THF)₂

E (BS1) = -2062.899422

E (BS2) = -2063.377753

G_{298.15} (BS2) = -2062.941721



K	1.277823	-2.111978	-1.674373
C	-3.578168	2.021944	0.727444
C	-2.664640	2.118234	-0.331344
C	-1.475146	1.351343	-0.312808
P	-0.309567	1.473045	-1.792664
O	0.145417	0.014611	-2.175701
C	1.138657	2.204557	-0.861936
C	2.436860	1.792817	-1.204768
H	4.557060	2.035521	-0.891565
C	3.561688	2.375875	-0.615806
C	3.409812	3.390603	0.332120
H	4.281353	3.844265	0.795576
C	2.123304	3.819031	0.677058
H	1.994416	4.605619	1.416588
C	1.003503	3.236128	0.082654
H	0.010282	3.572202	0.370084
C	-1.238677	0.508104	0.798619

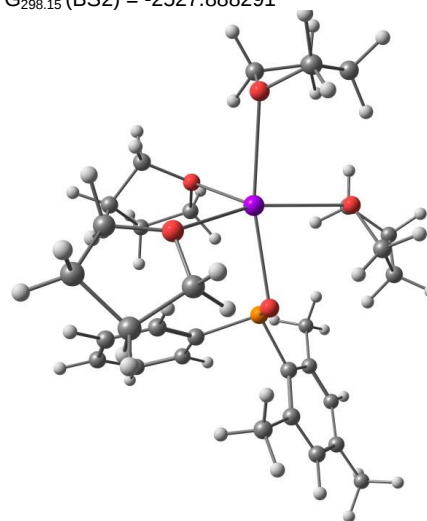
C	-2.165863	0.450277	1.845858
H	-1.954800	-0.191417	2.699873
C	-3.350028	1.191236	1.826442
H	-4.487234	2.619086	0.694796
H	2.553990	0.998008	-1.937580
O	-1.081358	-3.151013	-1.049196
C	-2.116349	-2.350385	-1.671397
C	-3.219855	-2.159179	-0.607690
H	-1.641384	-1.419290	-1.991082
H	-2.500703	-2.888938	-2.548566
C	-2.759091	-3.035633	0.580227
H	-3.315186	-1.112255	-0.314196
H	-4.186590	-2.492465	-0.994828
C	-1.722577	-3.960361	-0.056802
H	-2.285992	-2.416107	1.347053
H	-3.578900	-3.589042	1.045752
H	-0.952977	-4.319149	0.632212
H	-2.203112	-4.828871	-0.533377
C	-0.024960	-0.382446	0.899004
H	-0.252283	-1.364659	0.472460
H	0.832568	0.030576	0.372254
H	0.249914	-0.538104	1.946569
C	-4.356684	1.075535	2.943344
H	-5.003125	0.199467	2.803009
H	-3.865098	0.959525	3.914923
H	-5.005711	1.955135	2.990857
C	-2.989768	3.075271	-1.459152
H	-2.282862	3.911102	-1.499871
H	-2.943378	2.585220	-2.435940
H	-3.992817	3.493200	-1.328397
C	4.040959	-1.162004	0.496610
O	3.004597	-2.144176	0.327641
C	2.633788	-2.620183	1.638671
C	3.088022	-1.543714	2.650407
C	3.648277	-0.412996	1.763984
H	3.123241	-3.584008	1.827720
H	2.263389	-1.201480	3.280009
H	3.866355	-1.944975	3.305575
H	2.875097	0.323093	1.531030
H	4.492846	0.108074	2.221718
H	4.062243	-0.539959	-0.400835
H	5.015378	-1.660928	0.608905
H	1.551241	-2.776240	1.635941

K-OP(Mes)Ph.(THF)₄

E (BS1) = -2527.901648

E (BS2) = -2528.540988

G_{298.15} (BS2) = -2527.888291



K	-1.907568	-0.405540	-0.557129
P	1.342581	-0.075507	0.237899
O	0.605597	-0.059226	-1.156161
C	0.685500	2.663692	0.156857
C	1.561967	1.714389	0.704813
C	0.722142	3.999306	0.565307

C	1.631418	4.409544	1.543262
C	2.508410	3.471918	2.101699
C	2.472524	2.140160	1.686828
H	0.039612	4.720795	0.122037
H	3.169760	1.425704	2.118695
C	3.799655	-1.363767	0.857020
C	5.126662	-1.747845	0.622111
C	3.156857	-0.473296	-0.034463
C	3.886512	0.028895	-1.138893
C	5.206117	-0.387221	-1.346702
C	5.844743	-1.279933	-0.480683
H	5.608703	-2.432007	1.317742
H	5.752527	0.004828	-2.202911
O	-2.375632	0.530397	1.906973
C	-1.352181	0.608602	2.921403
C	-3.229828	1.669372	2.076315
C	-1.206265	2.102481	3.289650
H	-1.659016	0.009993	3.789817
H	-0.445551	0.175416	2.491556
C	-2.275249	2.807043	2.425682
H	-3.784425	1.814727	1.145208
H	-3.948772	1.484119	2.889364
H	-0.204318	2.475659	3.069906
H	-1.399040	2.253882	4.355457
H	-1.820854	3.199895	1.512927
H	-2.773560	3.629025	2.946481
O	-2.251599	1.861036	-1.961597
C	-1.288862	1.895753	-3.046008
C	-2.715488	3.192777	-1.668543
C	-0.929073	3.368449	-3.233316
H	-0.440755	1.268959	-2.753927
H	-1.763126	1.484564	-3.948245
C	-2.230191	4.072358	-2.821489
H	-3.805859	3.169277	-1.568909
H	-2.286400	3.519137	-0.711716
H	-0.622453	3.593188	-4.258220
H	-0.111651	3.648543	-2.560950
H	-2.951350	4.051268	-3.646050
H	-2.085281	5.112504	-2.517707
C	3.107091	-1.909161	2.088257
H	2.140753	-2.358544	1.844563
H	3.730018	-2.664644	2.577027
H	2.903229	-1.120916	2.822007
C	3.284393	1.045849	-2.077440
H	3.863951	1.120085	-3.003015
H	2.244527	0.790880	-2.296851
H	3.273526	2.037909	-1.608836
C	7.256580	-1.741423	-0.743256
H	7.766702	-2.018815	0.185149
H	7.269844	-2.623542	-1.397680
H	7.846485	-0.963164	-1.239297
C	-4.894135	-2.281839	-1.290888
O	-4.516995	-1.200233	-0.428508
C	-4.899249	-1.598250	0.900635
C	-4.752940	-3.136881	0.955050
C	-4.501832	-3.542906	-0.518887
H	-5.939157	-1.294257	1.086133
H	-3.919106	-3.436486	1.595486
H	-5.661394	-3.596382	1.354140
H	-3.441119	-3.751140	-0.679639
H	-5.085449	-4.415212	-0.825077
H	-4.367263	-2.153694	-2.240746
H	-5.977899	-2.247816	-1.482437
H	-4.246656	-1.068696	1.597945
C	-0.092070	-3.239355	-1.475635
O	-1.153353	-3.022340	-0.508682
C	-0.728888	-3.482030	0.788586
C	0.389685	-4.483569	0.517982
C	1.078127	-3.855467	-0.702266
H	-1.597455	-3.914870	1.293989
H	1.057900	-4.605602	1.374621
H	-0.032202	-5.462504	0.263889
H	1.770781	-3.071249	-0.384839
H	1.634856	-4.579383	-1.303217
H	0.177631	-2.275411	-1.916561

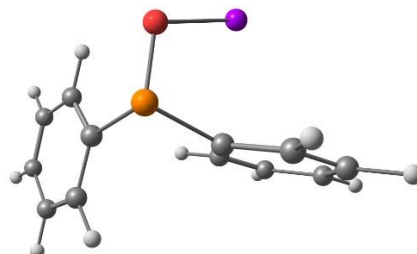
H	-0.477694	-3.916662	-2.247840
H	-0.360142	-2.630529	1.377919
H	3.226152	3.784338	2.856294
H	1.661311	5.446515	1.865751
H	-0.022177	2.335234	-0.596610

K-OPPh₂

E (BS1) = -1479.916549

E (BS2) = -1480.199113

G_{298.15} (BS2) = -1480.057225



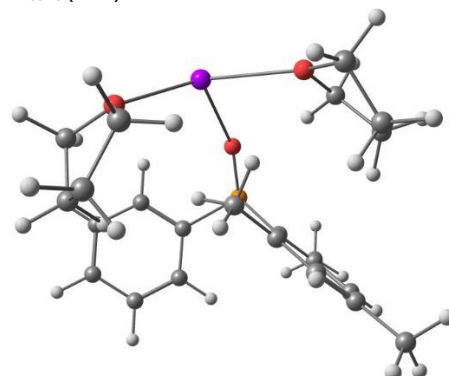
K	-1.696250	2.052051	0.988087
C	3.398428	-1.621616	-0.046747
C	2.241851	-1.246701	-0.729937
C	1.690751	0.033090	-0.559869
P	0.181425	0.575584	-1.507441
O	-0.153474	2.016517	-0.954602
C	-1.056038	-0.531722	-0.596732
C	-2.314648	-0.710018	-1.199824
H	-4.330757	-1.451925	-1.006546
C	-3.367322	-1.328249	-0.519102
C	-3.180617	-1.790438	0.787044
C	-1.933016	-1.639898	1.400436
H	-1.775397	-2.007222	2.411442
C	-0.884768	-1.017490	0.713910
C	2.339124	0.935044	0.293011
C	3.502452	0.566573	0.975391
H	3.995607	1.277049	1.634757
C	4.033540	-0.714205	0.809554
H	3.809385	-2.619045	-0.180762
H	1.755287	-1.957376	-1.395867
H	4.938653	-1.003765	1.336249
H	-3.996519	-2.272033	1.318228
H	-2.471693	-0.348081	-2.214216
H	0.079055	-0.908116	1.203934
H	1.913118	1.929432	0.404741

K-OPPh₂·(THF)₂

E (BS1) = -1944.926731

E (BS2) = -1945.371268

G_{298.15} (BS2) = -1945.009931



K	0.632238	1.480168	-1.520346
C	-3.860677	-2.200437	0.331416
C	-2.474045	-2.348485	0.319337
C	-1.697463	-1.803034	-0.717344
P	0.145442	-2.087413	-0.840908
O	0.643217	-1.004140	-1.871167
C	0.566780	-1.433903	0.878682

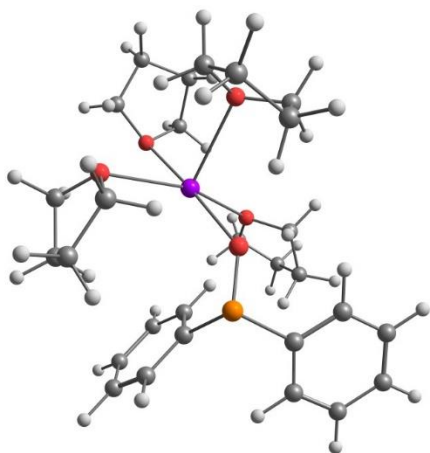
C	-0.006942	-0.283234	1.451549
H	-0.042457	1.084261	3.117127
C	0.419473	0.197650	2.691051
C	1.432222	-0.468026	3.390630
H	1.762861	-0.097490	4.356897
C	2.006855	-1.616250	2.843803
H	2.789339	-2.143101	3.383481
C	1.573775	-2.090126	1.601003
H	2.024461	-2.987187	1.181481
C	-2.356291	-1.121059	-1.750047
H	-1.757914	-0.709480	-2.559453
C	-3.747239	-0.974827	-1.746554
H	-4.239714	-0.441156	-2.556082
C	-4.504514	-1.511500	-0.703828
H	-5.585056	-1.399394	-0.696476
H	-4.443453	-2.620060	1.147606
H	-1.985563	-2.885865	1.129576
H	-0.807183	0.232660	0.927902
O	3.225942	1.383696	-0.952101
C	3.782856	0.466797	-1.926875
C	4.969566	-0.184924	-1.227275
H	3.022003	-0.279697	-2.193196
H	4.055346	1.047672	-2.813646
C	4.432096	-0.322687	0.203154
H	5.244006	-1.142451	-1.677681
H	5.841979	0.477633	-1.254471
C	3.616019	0.961508	0.378193
H	3.776159	-1.194219	0.273268
H	5.215736	-0.419631	0.958978
H	2.719461	0.808087	0.987445
H	4.211029	1.766278	0.828025
C	-1.335335	3.111583	1.098673
O	-1.388998	2.621308	-0.254689
C	-2.777725	2.400765	-0.552513
C	-3.338652	1.773592	0.720492
C	-2.543501	2.490963	1.837499
H	-2.834953	1.753824	-1.429832
H	-4.418897	1.911461	0.811103
H	-3.130441	0.701037	0.722319
H	-3.139255	3.272871	2.315595
H	-2.227918	1.789939	2.613368
H	-1.395482	4.208066	1.089025
H	-0.367630	2.819906	1.514379
H	-3.265444	3.360922	-0.779151

K-OPPh₂·(THF)₄

E (BS1) = -2409.933220

E (BS2) = -2410.536921

G_{298.15} (BS2) = -2409.961941



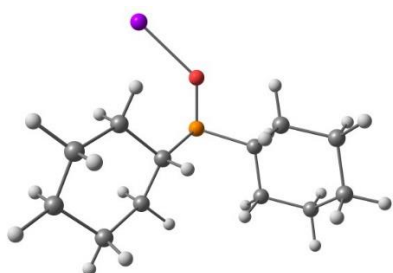
K	-1.281881	-0.133825	-0.210039
P	2.023575	0.901961	1.467936
O	0.722214	0.014992	1.389551
C	1.699567	1.200614	-1.376429
C	2.144470	1.790117	-0.180551

C	1.714972	1.908185	-2.578920
C	2.189406	3.224685	-2.610061
C	2.647672	3.820041	-1.433528
C	2.617120	3.107930	-0.229460
H	1.364940	1.434387	-3.493095
H	2.955602	3.586037	0.687272
C	4.638416	0.053440	0.563837
C	5.668081	-0.878616	0.421527
C	3.417527	-0.304962	1.157456
C	3.269059	-1.619516	1.625604
C	4.296316	-2.555138	1.486846
C	5.500479	-2.188822	0.880400
H	6.600663	-0.585388	-0.054300
H	4.157193	-3.571213	1.848442
O	-2.345773	2.174561	0.723663
C	-1.501637	2.576031	1.834880
C	-2.390129	3.255547	-0.220760
C	-0.714922	3.818150	1.367005
H	-2.133052	2.795117	2.704381
H	-0.846052	1.730866	2.063342
C	-1.002611	3.881256	-0.143259
H	-2.643183	2.836188	-1.198757
H	-3.171332	3.976960	0.064022
H	0.351528	3.725691	1.582773
H	-1.087452	4.719026	1.864432
H	-0.284928	3.268906	-0.697156
H	-0.971017	4.897799	-0.544136
O	-0.000808	-1.953501	-1.726710
C	0.942910	-2.608986	-0.843020
C	0.484452	-1.998773	-3.086113
C	2.252147	-2.667596	-1.622823
H	1.003564	-2.014001	0.072085
H	0.573188	-3.617312	-0.607160
C	1.751714	-2.858428	-3.061801
H	-0.301854	-2.407391	-3.729784
H	0.699786	-0.973163	-3.412133
H	2.905922	-3.472585	-1.279853
H	2.793794	-1.722277	-1.519582
H	1.501935	-3.910138	-3.239885
H	2.475818	-2.545617	-3.818522
C	-3.544858	-1.560999	-2.372064
O	-3.329074	-0.186884	-2.003562
C	-4.542314	0.327037	-1.406871
C	-5.460938	-0.882822	-1.142385
C	-4.524950	-2.089665	-1.330402
H	-5.003595	1.052035	-2.088401
H	-5.906372	-0.846666	-0.144967
H	-6.273639	-0.911686	-1.874672
H	-3.994454	-2.309381	-0.399066
H	-5.049682	-2.989481	-1.662898
H	-2.572277	-2.061098	-2.367894
H	-3.968490	-1.617349	-3.386225
H	-4.262074	0.851802	-0.488055
C	-1.848490	-2.466206	2.346782
O	-2.695808	-1.624607	1.547145
C	-3.401694	-0.747003	2.449773
C	-2.550442	-0.654482	3.738361
C	-1.320135	-1.537850	3.435508
H	-4.397593	-1.161523	2.653920
H	-2.264763	0.376376	3.961992
H	-3.113899	-1.039385	4.593393
H	-0.502042	-0.939812	3.020655
H	-0.964358	-2.082584	4.314703
H	-1.074003	-2.874738	1.691688
H	-2.435384	-3.298964	2.764392
H	-3.522219	0.214541	1.943508
H	3.018383	4.841607	-1.450431
H	2.201866	3.779199	-3.544172
H	1.341613	0.175721	-1.360925
H	4.780141	1.065999	0.193850
H	6.300872	-2.914773	0.767322
H	2.325867	-1.903979	2.083700

K-OPCy₂

E (BS1) = -1487.188599

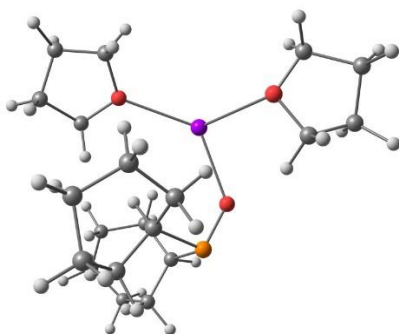
E (BS2) = -1487.455302
G298.15 (BS2) = -1487.176479



15	-0.051275	0.716494	-1.042660
8	-0.572514	2.001257	-0.274965
19	-2.755144	2.961819	-0.002126
6	1.771264	0.596839	-0.529626
6	2.459054	-0.712801	-0.936486
6	3.961055	-0.680782	-0.612470
6	4.206376	-0.362451	0.869249
6	3.508151	0.939288	1.288098
6	2.010145	0.897510	0.955325
1	2.244396	1.409696	-1.104806
1	2.304929	-0.912626	-2.004948
1	2.001428	-1.549915	-0.391914
1	4.429973	-1.637521	-0.876408
1	4.444909	0.088349	-1.231196
1	5.282875	-0.303366	1.073178
1	3.816142	-1.189002	1.480821
1	3.660054	1.121560	2.360292
1	3.972109	1.783022	0.757112
1	1.516257	1.840177	1.213338
1	1.535762	0.116734	1.567048
6	-0.730717	-0.787110	-0.072302
6	-0.887250	-2.010166	-0.988839
6	-1.475804	-3.218124	-0.245321
6	-2.814461	-2.865580	0.416191
6	-2.677832	-1.642301	1.332254
6	-2.075418	-0.446267	0.582991
1	-0.032247	-1.049137	0.735716
1	0.075270	-2.277161	-1.439922
1	-1.551005	-1.743368	-1.824539
1	-1.604181	-4.064497	-0.932170
1	-0.766696	-3.545924	0.528255
1	-3.202383	-3.722982	0.979885
1	-3.553126	-2.644540	-0.368089
1	-3.654513	-1.374816	1.757403
1	-2.024766	-1.897523	2.178676
1	-1.937936	0.400532	1.265972
1	-2.787651	-0.128045	-0.198081

K-OPCy₂·(THF)₂

E (BS1) = -1952.176905
E (BS2) = -1952.607439
G_{298.15} (BS2) = -1952.115749

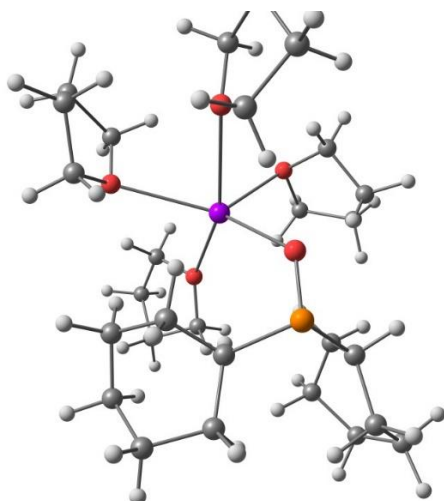


K	1.500680	0.091276	-1.315257
C	-1.905597	0.688514	3.359369
C	-2.146937	-0.369631	2.257501

C	-0.960410	-0.496093	1.273296
P	-0.751468	-2.217038	0.486224
O	0.507355	-2.024815	-0.459558
C	-2.200228	-2.229887	-0.749742
C	-3.573533	-2.517818	-0.108915
H	-4.515767	-2.874836	-2.008363
C	-4.703411	-2.264600	-1.114996
C	-4.777212	-0.770024	-1.509000
H	-5.147958	-0.682775	-2.537638
C	-3.408701	-0.065045	-1.385797
H	-3.379591	0.815073	-2.039760
C	-2.256513	-1.018638	-1.715386
H	-1.298262	-0.484802	-1.697151
C	0.334476	-0.107528	2.004511
H	1.215148	-0.343209	1.400788
C	0.328204	1.384966	2.389380
H	1.045363	1.557553	3.201970
C	-1.081958	1.860071	2.813966
H	-1.008860	2.666983	3.552207
H	-2.864604	1.039247	3.758584
H	-3.053648	-0.103130	1.704662
H	-3.599064	-3.552462	0.251302
O	0.516020	2.537534	-1.115503
C	-0.889383	2.880516	-1.094586
C	-0.969635	4.257126	-0.440866
H	-1.264510	2.903777	-2.126373
H	-1.425588	2.103340	-0.544140
C	0.353116	4.895203	-0.886588
H	-1.852127	4.816813	-0.760400
H	-0.997576	4.158902	0.649527
C	1.312854	3.708549	-0.818752
H	0.271022	5.261912	-1.915533
H	0.673157	5.723072	-0.249091
H	2.129863	3.766616	-1.545188
H	1.741533	3.598397	0.185899
H	-5.506230	-0.252037	-0.873994
H	-5.668579	-2.595698	-0.713314
H	-3.737991	-1.886929	0.770995
H	-1.940268	-3.111199	-1.352890
H	-1.368001	0.237899	4.203444
H	-1.608410	2.281538	1.947862
H	0.670126	1.980702	1.534791
H	0.428426	-0.728622	2.905639
H	-2.347428	-1.342187	2.726979
H	-3.279492	0.308524	-0.364414
H	-1.098990	0.223952	0.452969
H	-2.378877	-1.365422	-2.750603
C	3.621031	-1.784719	0.561342
O	3.762549	-0.485492	-0.066915
C	5.117336	-0.327621	-0.543685
C	5.844604	-1.648131	-0.248468
C	4.686057	-2.646141	-0.104117
H	5.581373	0.529691	-0.042447
H	6.553317	-1.913707	-1.037094
H	6.396365	-1.575860	0.694650
H	4.337308	-2.981891	-1.087782
H	4.946871	-3.526749	0.488747
H	2.590684	-2.117902	0.396167
H	3.809212	-1.689550	1.640822
H	5.078796	-0.115930	-1.620296

K-OPCy₂·(THF)₄

E (BS1) = -2417.184318
E (BS2) = -2417.774168
G_{298.15} (BS2) = -2417.062141



K	1.019658	0.063427	0.433774
C	-2.826557	-2.868352	-2.672642
C	-3.056716	-1.371723	-2.349642
C	-1.815197	-0.698014	-1.723938
P	-1.650874	1.176303	-1.990850
O	-0.358129	1.525766	-1.139375
C	-3.053846	1.840535	-0.894147
C	-4.460702	1.719244	-1.513646
H	-5.328691	3.066680	-0.081215
C	-5.536261	2.062982	-0.475392
C	-5.543290	1.037596	0.683613
H	-5.859402	1.536448	1.608096
C	-4.161750	0.379900	0.892262
H	-4.076588	0.007436	1.920138
C	-3.022875	1.353997	0.577703
H	-2.047236	0.905706	0.798555
C	-0.558206	-1.394753	-2.269438
H	0.344365	-0.829779	-2.018629
C	-0.464321	-2.845374	-1.755980
H	0.182172	-3.430375	-2.422205
C	-1.862509	-3.502061	-1.662931
H	-1.787917	-4.584594	-1.818145
H	-3.784313	-3.401884	-2.682316
H	-3.905932	-1.283088	-1.664974
H	-4.536361	2.380297	-2.384517
O	-0.340684	-1.576066	2.080535
C	-1.693080	-2.069802	2.130973
C	-1.569521	-3.568055	2.386069
H	-2.233550	-1.570350	2.947306
H	-2.182711	-1.821959	1.186857
C	-0.338426	-3.622704	3.301026
H	-2.469165	-3.991755	2.839689
H	-1.372063	-4.095595	1.446340
C	0.552949	-2.531249	2.703988
H	-0.620534	-3.369706	4.328808
H	0.154053	-4.598418	3.310345
H	1.154338	-2.008784	3.456208
H	1.221046	-2.927250	1.931441
H	-6.287341	0.256149	0.486180
H	-6.528757	2.113813	-0.939125
H	-4.642027	0.705419	-1.886028
H	-2.805537	2.911489	-0.884145
H	-2.405674	-2.975998	-3.680545
H	-2.272058	-3.362758	-0.654463
H	0.014358	-2.859288	-0.768843
H	-0.603797	-1.388562	-3.366840
H	-3.345001	-0.843378	-3.268523
H	-4.071326	-0.496953	0.242483
H	-1.829434	-0.853742	-0.635463
H	-3.112546	2.214333	1.254259
C	2.746979	1.761176	-1.998682
O	3.184304	1.224841	-0.725875
C	4.413329	1.862166	-0.322305
C	4.764630	2.870490	-1.424953

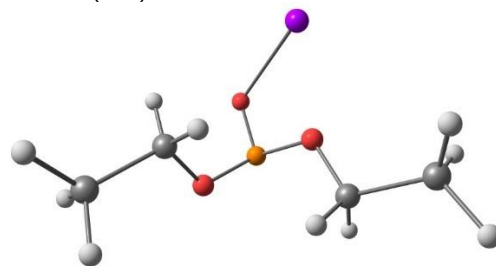
C	3.402234	3.133991	-2.083731
H	5.188428	1.099461	-0.186191
H	5.238260	3.770834	-1.025014
H	5.450041	2.418328	-2.150069
H	2.824667	3.861849	-1.502297
H	3.483265	3.499343	-3.110987
H	1.651515	1.777024	-1.986035
H	3.102569	1.106178	-2.808553
H	4.242283	2.354791	0.642686
C	0.173928	1.771952	3.288685
O	1.383790	1.808714	2.493631
C	1.455392	3.076006	1.809300
C	0.003589	3.500976	1.622426
C	-0.616682	3.047923	2.953881
H	1.991772	2.913401	0.871430
H	-0.100240	4.575775	1.447610
H	-0.421114	2.958140	0.770067
H	-0.455930	3.808099	3.725773
H	-1.689742	2.856665	2.884043
H	0.442903	1.713893	4.350299
H	-0.370564	0.857877	3.024833
H	2.016884	3.798777	2.420450
C	3.101808	-2.312629	-1.270221
O	2.703341	-2.071599	0.096639
C	3.870897	-1.815531	0.907750
C	5.081683	-2.126394	0.026054
C	4.542056	-1.820538	-1.377896
H	3.816431	-2.439336	1.805674
H	5.955561	-1.528106	0.296849
H	5.351436	-3.184988	0.108146
H	4.548653	-0.742975	-1.561450
H	5.096357	-2.322540	-2.175067
H	2.412627	-1.779947	-1.930943
H	3.025321	-3.387882	-1.481001
H	3.867644	-0.761652	1.216541

K-OPOEt₂

E (BS1) = -1325.532053

E (BS2) = -1325.782432

G298.15 (BS2) = -1325.677617



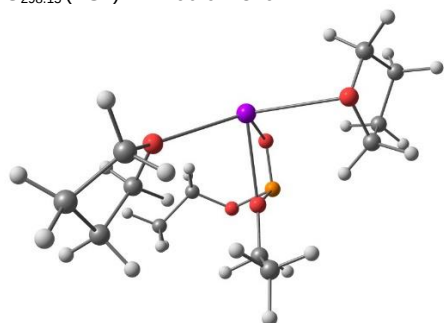
15	0.289447	-0.141896	-1.410978
8	0.125453	-1.635705	-1.068160
19	-1.538510	-1.734359	0.830202
8	-0.892062	0.508695	-0.275897
6	-0.947855	1.925071	-0.154350
1	-0.896608	2.393849	-1.149046
1	-0.080773	2.288885	0.415403
6	-2.239635	2.321549	0.540082
1	-2.293536	1.882878	1.543597
1	-3.107213	1.978902	-0.034047
1	-2.303821	3.410494	0.644124
8	1.670056	0.420729	-0.601423
6	1.937816	-0.050573	0.721156
1	1.907717	-1.147956	0.738158
1	1.163955	0.315632	1.412845
6	3.303129	0.450247	1.156561
1	3.336928	1.544806	1.147178
1	4.082811	0.078896	0.483520
1	3.532220	0.107360	2.172235

K-OP(OEt)₂·(THF)₂

E (BS1) = -1790.537044

E (BS2) = -1790.949457

G_{298.15} (BS2) = -1790.627849



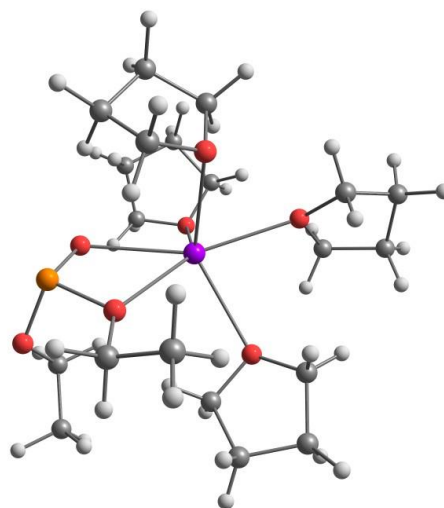
K	0.508356	0.929115	-1.035765
O	-1.995772	1.811964	-0.853881
C	-2.878369	0.691594	-0.596118
C	-3.933724	1.203962	0.382494
H	-3.329977	0.375081	-1.545556
H	-2.277049	-0.127856	-0.197400
C	-4.017358	2.691750	0.013513
H	-4.884980	0.676317	0.278045
H	-3.586066	1.086683	1.414312
C	-2.558180	3.018751	-0.297092
H	-4.636155	2.828669	-0.880058
H	-4.422485	3.316359	0.813689
H	-2.435720	3.825610	-1.026431
H	-2.007934	3.286340	0.615839
P	0.773361	-2.202425	0.191891
O	1.219841	-1.576141	-1.143234
O	-0.561202	-3.197367	-0.127882
C	-1.502009	-2.830816	-1.141258
H	-1.311263	-1.811671	-1.495731
H	-1.366516	-3.496554	-2.005099
H	-3.113054	-3.977294	-0.259825
H	-3.080441	-2.276771	0.236064
H	-3.648987	-2.717226	-1.389217
C	-0.714793	-0.942089	2.107239
H	-1.721410	-1.371421	1.999870
O	-0.102253	-0.816584	0.831466
H	-0.138966	-1.631974	2.742947
C	-2.919084	-2.956747	-0.606547
C	-0.794258	0.428146	2.761965
H	0.208263	0.834627	2.933777
H	-1.340656	1.129543	2.122451
H	-1.312323	0.369689	3.726007
C	3.102644	0.737737	1.124397
O	2.792917	1.730637	0.118541
C	3.866154	1.774423	-0.852244
C	4.900161	0.729270	-0.414466
C	4.059483	-0.229712	0.440159
H	4.273648	2.790543	-0.890030
H	5.378597	0.242772	-1.268231
H	5.680796	1.197888	0.194336
H	3.484164	-0.914552	-0.190984
H	4.653102	-0.809705	1.151590
H	2.163584	0.276118	1.439515
H	3.569234	1.227666	1.990947
H	3.451177	1.536626	-1.841981

K-OP(OEt)₂·(THF)₄

E (BS1) = -2255.538958

E (BS2) = -2256.112665

G_{298.15} (BS2) = -2255.573618



K	0.240102	-0.001519	-0.096320
O	-0.770920	2.467953	-0.640823
C	-2.175607	2.335122	-0.966863
C	-2.903782	3.448231	-0.207123
H	-2.286921	2.441481	-2.053106
H	-2.505458	1.337306	-0.670853
C	-1.799570	4.498810	-0.021033
H	-3.771899	3.822746	-0.755167
H	-3.245899	3.083631	0.766580
C	-0.572875	3.618085	0.199616
H	-1.677892	5.093327	-0.933334
H	-1.984129	5.179412	0.814217
H	0.367810	4.094647	-0.088320
H	-0.496029	3.303135	1.250696
P	-2.402788	-2.161241	0.444504
O	-1.152650	-2.289124	-0.444175
O	-3.725928	-1.888097	-0.584995
C	-3.543382	-1.136124	-1.787457
H	-2.570597	-0.631793	-1.785464
H	-3.538271	-1.827024	-2.642577
H	-5.642077	-0.633101	-1.957610
H	-4.673031	0.583885	-1.110829
H	-4.561546	0.432947	-2.877868
C	-3.143030	0.036435	1.865536
H	-3.916596	0.560689	1.285497
O	-2.168600	-0.509672	0.989112
H	-3.652526	-0.765380	2.422228
C	-4.670491	-0.128319	-1.942023
C	-2.473417	0.996186	2.837005
H	-1.748425	0.467997	3.465147
H	-1.941113	1.785297	2.295847
H	-3.215465	1.470282	3.489955
C	0.566728	-1.836048	2.868500
O	1.451409	-0.932622	2.180659
C	2.628395	-1.659888	1.769861
C	2.337237	-3.156588	1.995750
C	0.815519	-3.190455	2.215504
H	3.493550	-1.317098	2.351256
H	2.657245	-3.768803	1.148374
H	2.861602	-3.514996	2.887491
H	0.277289	-3.226522	1.263394
H	0.492629	-4.027535	2.840594
H	-0.450594	-1.463075	2.733490
H	0.807468	-1.852228	3.942792
H	2.815892	-1.424198	0.717105
C	0.954175	-2.084980	-2.808816
O	1.504596	-0.826167	-2.385518
C	2.926788	-1.002987	-2.249257
C	3.171146	-2.513424	-2.013823
C	1.752587	-3.119212	-2.022883
H	3.249240	-0.373498	-1.416503
H	3.780247	-2.931581	-2.820439
H	3.693551	-2.701338	-1.071953

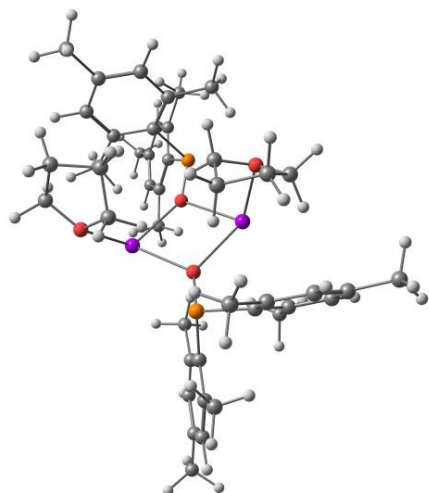
H	1.716473	-4.115742	-2.472165
H	1.336152	-3.180828	-1.013469
H	1.088927	-2.207722	-3.895207
H	-0.106215	-2.086160	-2.553254
H	3.429870	-0.658817	-3.163183
C	2.702072	2.472764	-1.076683
O	2.494984	1.522005	-0.006881
C	3.110209	2.004363	1.201925
C	4.123534	3.051828	0.750954
C	3.398135	3.682337	-0.446033
H	3.553686	1.152488	1.723044
H	4.366339	3.768529	1.539660
H	5.050303	2.566447	0.425180
H	2.660144	4.411643	-0.094892
H	4.068674	4.185769	-1.147018
H	1.732672	2.712548	-1.523691
H	3.331467	2.000463	-1.841086
H	2.344004	2.449232	1.852995

[K-OPMes₂]₂

E (BS1) = -3896.797826

E (BS2) = -3897.648924

G_{298.15} (BS2) = -3896.811973



K	-0.424218	-0.005675	1.937852
C	-6.022804	-3.090639	-1.440475
C	-5.335639	-1.890673	-1.256123
C	-3.963820	-1.891119	-0.869524
P	-3.101902	-0.209328	-0.868085
O	-1.618104	-0.366644	-0.325232
C	-3.985441	0.617082	0.588254
C	-4.520710	1.916334	0.415009
H	-5.429414	3.619399	1.361300
C	-5.021978	2.622889	1.519245
C	-5.003875	2.093943	2.808903
C	-4.481301	0.806570	2.974539
H	-4.463995	0.364471	3.969407
C	-3.987811	0.063639	1.896489
C	-3.329490	-3.146912	-0.715178
C	-4.057073	-4.331483	-0.916736
H	-3.544176	-5.282207	-0.777269
C	-5.402188	-4.334038	-1.273584
H	-7.072201	-3.054191	-1.727664
O	-0.204466	2.638113	1.947345
C	-1.377232	3.373078	2.380974
C	-1.795865	4.253274	1.200167
H	-2.163495	2.652654	2.637003
H	-1.122773	3.947139	3.278184
C	-1.222699	3.483865	0.003435
H	-2.878801	4.381677	1.153869
H	-1.330161	5.242064	1.273178
C	0.095035	2.979293	0.575404
H	-1.861831	2.632761	-0.245741

H	-1.092135	4.101195	-0.887915
H	0.488595	2.085777	0.084025
H	0.872094	3.754143	0.548855
C	-6.094628	-0.604524	-1.478652
H	-7.056526	-0.801245	-1.960729
H	-6.288846	-0.078985	-0.538194
H	-5.528939	0.086528	-2.113290
C	-1.875809	-3.330856	-0.319282
H	-1.419973	-2.382298	-0.049438
H	-1.791418	-4.019379	0.529487
H	-1.308561	-3.786772	-1.143925
C	-6.167134	-5.617141	-1.480293
H	-6.538514	-5.699807	-2.509036
H	-5.541149	-6.491496	-1.279470
H	-7.042259	-5.671360	-0.821682
C	-4.611472	2.598057	-0.932528
H	-3.803013	2.299437	-1.600931
H	-5.550606	2.340421	-1.437401
H	-4.593958	3.686003	-0.816595
C	-5.490029	2.893421	3.991034
H	-6.187705	3.677955	3.683437
H	-5.991980	2.256802	4.726778
H	-4.652976	3.383173	4.505588
C	-3.486597	-1.334286	2.184984
H	-4.259408	-2.081522	1.975013
H	-2.635746	-1.596452	1.558118
H	-3.209759	-1.439281	3.239749
K	0.471456	-1.166860	-1.617017
C	6.523077	-2.347897	1.785983
C	5.532078	-1.367108	1.714236
C	4.225644	-1.691598	1.254655
P	2.918920	-0.343026	1.355003
O	1.607220	-0.848382	0.620123
C	3.616609	0.916487	0.137242
C	3.675004	2.277084	0.534246
H	4.119754	4.292581	-0.059912
C	4.079753	3.253958	-0.382306
C	4.437722	2.935804	-1.696206
C	4.365878	1.597342	-2.082517
H	4.631825	1.323694	-3.101597
C	3.956903	0.590956	-1.195810
C	3.954911	-3.045030	0.932435
C	4.979442	-4.000435	1.031146
H	4.749059	-5.033386	0.775886
C	6.271572	-3.679482	1.441053
H	7.515998	-2.065324	2.131518
O	0.361529	0.638166	-3.547527
C	1.469469	1.075933	-4.368796
C	1.588606	2.592709	-4.170905
H	2.370100	0.552259	-4.028939
H	1.276033	0.797699	-5.410795
C	0.882396	2.812266	-2.825752
H	2.628400	2.924603	-4.169898
H	1.057863	3.125236	-4.967084
C	-0.239957	1.784935	-2.906452
H	1.555649	2.573847	-1.996744
H	0.514244	3.832596	-2.695050
H	-0.637749	1.455169	-1.943484
H	-1.076948	2.153199	-3.516648
C	5.895661	0.033685	2.145857
H	6.861669	0.041472	2.658797
H	5.957404	0.722507	1.297706
H	5.144958	0.443959	2.830517
C	2.614492	-3.559943	0.444596
H	1.779205	-3.005921	0.868623
H	2.536895	-3.468382	-0.648552
H	2.515485	-4.625499	0.676694
C	7.355111	-4.724291	1.535462
H	7.717636	-4.832909	2.564985
H	6.995838	-5.702527	1.202763
H	8.222615	-4.457369	0.920068
C	3.323405	2.730533	1.935047
H	2.314620	2.429704	2.229144
H	4.008613	2.313377	2.679490
H	3.382163	3.821383	2.003813

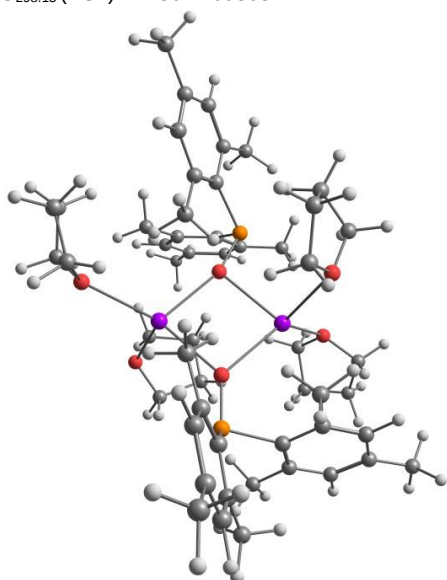
C	4.858555	4.014063	-2.662657
H	4.024078	4.687363	-2.893682
H	5.660293	4.633218	-2.244437
H	5.216722	3.589493	-3.604870
C	3.918487	-0.826965	-1.718620
H	4.879071	-1.332989	-1.570551
H	3.172329	-1.420125	-1.194292
H	3.706033	-0.838739	-2.793489

[K-OPMe₂(THF)]₂

E (BS1) = -4361.810992

E (BS2) = -4362.822573

G_{298.15} (BS2) = -4361.769368



K	0.766112	-0.966791	1.151003
C	6.096809	3.517606	-0.685715
C	5.474083	2.296484	-0.971133
C	4.076781	2.140333	-0.787478
P	3.305688	0.505756	-1.319500
O	1.822627	0.431329	-0.768668
C	4.211330	-0.681844	-0.158601
C	4.715541	-1.889434	-0.697564
H	5.669455	-3.772336	-0.286019
C	5.280386	-2.854589	0.149447
C	5.351586	-2.674926	1.531604
C	4.830567	-1.489760	2.060779
H	4.859258	-1.330498	3.137616
C	4.268023	-0.498380	1.247363
C	3.332819	3.277740	-0.375813
C	3.995868	4.478614	-0.095801
H	3.406191	5.331548	0.236865
C	5.379284	4.623199	-0.229633
H	7.172421	3.602586	-0.828824
O	0.868949	-3.630321	1.502205
C	2.058815	-4.186331	2.115185
C	2.653295	-5.181309	1.102316
H	2.741444	-3.357023	2.326508
H	1.786176	-4.666983	3.061868
C	1.953759	-4.797047	-0.210519
H	3.739986	-5.103132	1.042008
H	2.396955	-6.208631	1.380171
C	0.585224	-4.366893	0.299300
H	2.460971	-3.947936	-0.680419
H	1.902387	-5.619008	-0.929463
H	0.031560	-3.709651	-0.373065
H	-0.045282	-5.238142	0.529173
C	6.341689	1.169117	-1.480137
H	7.308912	1.551358	-1.819796
H	6.529700	0.415446	-0.709028
H	5.867842	0.648838	-2.320067
C	1.821755	3.296218	-0.243631

H	1.436610	2.372085	0.181136
H	1.504105	4.147024	0.367391
H	1.357054	3.421641	-1.231865
C	6.063779	5.922796	0.112987
H	5.514792	6.783713	-0.285083
H	6.133156	6.062783	1.199810
H	7.081783	5.954995	-0.287345
C	4.678590	-2.192571	-2.180194
H	3.672802	-2.087964	-2.595381
H	5.323285	-1.514859	-2.749735
H	5.020243	-3.215218	-2.367714
C	5.927917	-3.735339	2.435236
H	6.429552	-4.520267	1.862006
H	6.653799	-3.310782	3.137551
H	5.143179	-4.211834	3.036259
C	3.729298	0.740963	1.926455
H	4.466289	1.551172	1.920911
H	2.841992	1.118048	1.419396
H	3.473344	0.525791	2.967779
K	-0.415696	1.113962	-1.810233
C	-6.061458	1.194170	2.312269
C	-5.124013	0.221332	1.953611
C	-3.875242	0.596857	1.391490
P	-2.605259	-0.746767	1.058989
O	-1.473783	-0.146259	0.126116
C	-3.536778	-1.858649	-0.136898
C	-3.486277	-3.258286	0.072279
H	-3.959119	-5.199838	-0.718327
C	-4.005513	-4.126922	-0.895211
C	-4.580532	-3.656413	-2.079322
C	-4.623563	-2.275067	-2.277316
H	-5.062903	-1.883825	-3.193240
C	-4.108775	-1.375172	-1.335176
C	-3.582080	1.981437	1.297054
C	-4.549121	2.924198	1.676378
H	-4.301900	3.981281	1.594517
C	-5.803685	2.559532	2.164923
H	-7.014388	0.874216	2.729935
O	-1.699372	3.317118	-2.664638
C	-1.652806	4.634800	-2.086107
C	-3.113798	5.020240	-1.754457
H	-1.001880	4.583957	-1.209854
H	-1.210397	5.332115	-2.809855
C	-3.952422	3.865198	-2.351441
H	-3.273403	5.112925	-0.677875
H	-3.369217	5.978049	-2.215136
C	-2.972451	3.203922	-3.318285
H	-4.241381	3.156559	-1.570254
H	-4.859658	4.213092	-2.851841
H	-3.162779	2.144349	-3.501864
H	-2.944535	3.731696	-4.283669
C	-5.480893	-1.225464	2.200838
H	-6.344957	-1.299623	2.867631
H	-5.722205	-1.754864	1.274340
H	-4.648048	-1.765425	2.665056
C	-2.263494	2.540385	0.802447
H	-1.419082	1.916585	1.086340
H	-2.254672	2.612163	-0.288950
H	-2.119224	3.553362	1.191643
C	-6.839561	3.594392	2.525273
H	-7.392996	3.311659	3.427082
H	-6.382747	4.573619	2.698709
H	-7.577403	3.715697	1.721403
C	-2.893134	-3.868500	1.324415
H	-1.882300	-3.505858	1.527646
H	-3.491059	-3.629192	2.210793
H	-2.855639	-4.958640	1.235146
C	-5.105928	-4.614072	-3.119408
H	-5.696651	-5.416040	-2.663473
H	-5.736011	-4.101473	-3.852342
H	-4.284847	-5.093403	-3.667683
C	-4.185816	0.100513	-1.647758
H	-5.023571	0.576117	-1.127150
H	-3.278315	0.609678	-1.322580
H	-4.327018	0.260885	-2.720703

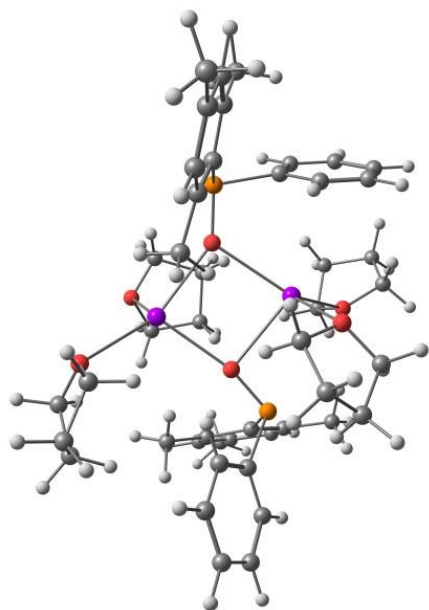
O	0.612001	0.334587	3.498045
C	0.611275	1.774094	3.354947
C	-0.467191	-0.068486	4.366223
C	-0.535193	2.300843	4.226535
H	1.588953	2.163393	3.656845
H	0.459843	2.015589	2.296467
C	-1.463914	1.083713	4.338319
H	-0.881907	-1.005153	3.980624
H	-0.076274	-0.240996	5.379367
H	-1.023272	3.171356	3.780835
H	-0.161682	2.586981	5.215508
H	-2.104682	1.001417	3.456732
H	-2.101194	1.107753	5.226338
O	-0.327014	-0.552942	-3.992452
C	0.919152	-1.267706	-3.914328
C	-1.339190	-1.533486	-3.715268
C	0.758448	-2.261198	-2.746682
H	1.094690	-1.793871	-4.864018
H	1.717341	-0.537446	-3.761213
C	-0.779730	-2.359965	-2.550340
H	-2.265898	-1.006317	-3.482502
H	-1.505609	-2.156724	-4.607011
H	1.244938	-1.859298	-1.855064
H	1.213436	-3.226319	-2.982267
H	-1.082285	-1.910238	-1.601044
H	-1.150756	-3.387202	-2.570287

[K-OP(Mes)Ph·(THF)]₂

E (BS1) = -4125.865321

E (BS2) = -4126.809028

G_{298.15} (BS2) = -4125.911853



K	-0.687003	1.136408	0.882854
C	-6.766985	-1.633791	-0.367685
C	-5.888727	-0.659966	-0.853466
C	-4.486919	-0.885461	-0.842832
P	-3.400013	0.453875	-1.600319
O	-1.886750	0.142535	-1.264309
C	-3.786949	1.805575	-0.349301
C	-3.724417	3.141144	-0.773917
H	-3.794707	5.223963	-0.216144
C	-3.836412	4.197002	0.136217
C	-4.004938	3.931157	1.497364
C	-4.064974	2.605295	1.941009
H	-4.198894	2.389795	2.998103
C	-3.958854	1.556040	1.023937
C	-4.020597	-2.141958	-0.382134
C	-4.934565	-3.086158	0.107755
H	-4.553093	-4.039084	0.470217
C	-6.310445	-2.852951	0.137572

H	-7.836374	-1.431478	-0.386439
O	0.305223	3.569104	1.441842
C	-0.440112	4.562638	2.179106
C	-0.688295	5.740326	1.210190
H	-1.365358	4.089549	2.518782
H	0.139541	4.873032	3.057323
C	-0.152833	5.220294	-0.137991
H	-1.744959	6.011138	1.161060
H	-0.126085	6.622188	1.530854
C	0.908001	4.225521	0.314911
H	-0.939294	4.694128	-0.688872
H	0.249947	6.013404	-0.773408
H	1.165503	3.460318	-0.417581
H	1.831322	4.737350	0.623339
C	-6.485707	0.626782	-1.376974
H	-7.547671	0.492802	-1.603461
H	-6.399500	1.439487	-0.647959
H	-5.981496	0.968242	-2.287850
C	-2.567508	-2.570225	-0.433573
H	-1.904547	-1.795988	-0.057176
H	-2.421558	-3.488782	0.142425
H	-2.273385	-2.786993	-1.469055
C	-7.266971	-3.871654	0.704857
H	-6.847601	-4.881791	0.663029
H	-7.497136	-3.657511	1.757090
H	-8.218159	-3.873631	0.161989
K	0.142443	-1.230158	-1.949431
C	5.019604	-2.853373	2.795614
C	4.468245	-1.652552	2.347752
C	3.224761	-1.630355	1.695104
P	2.369553	-0.044683	1.256330
O	1.299935	-0.441933	0.153967
C	3.755931	0.821991	0.343096
C	4.144010	2.108311	0.783363
H	5.327117	3.854400	0.361227
C	5.037389	2.865247	0.012549
C	5.562966	2.387587	-1.189947
C	5.196158	1.101763	-1.600886
H	5.610482	0.700285	-2.524172
C	4.315383	0.313291	-0.853907
C	2.545562	-2.844981	1.514008
C	3.090783	-4.048190	1.969038
H	2.549595	-4.979151	1.820463
C	4.331439	-4.057654	2.611099
H	5.988791	-2.852896	3.287928
O	0.777970	-3.780576	-2.420824
C	0.510898	-4.702378	-1.337527
C	1.733976	-5.618531	-1.242618
H	0.368835	-4.125526	-0.414316
H	-0.416896	-5.241361	-1.554420
C	2.852478	-4.728748	-1.802075
H	1.920633	-5.953824	-0.219798
H	1.598619	-6.502131	-1.875455
C	2.120007	-3.984788	-2.912949
H	3.198314	-4.026777	-1.037367
H	3.711514	-5.293737	-2.172809
H	2.553071	-3.007320	-3.148058
H	2.081848	-4.578753	-3.836577
C	3.634295	2.705181	2.079232
H	2.543342	2.778449	2.099034
H	3.923559	2.097166	2.943304
H	4.049741	3.707517	2.224654
C	6.479608	3.238036	-2.033223
H	6.958956	4.021395	-1.438391
H	7.264195	2.636546	-2.503820
H	5.925710	3.733286	-2.841368
C	4.004875	-1.082937	-1.338543
H	4.598995	-1.823193	-0.790824
H	2.956313	-1.324673	-1.162395
H	4.238164	-1.192185	-2.401881
O	-1.126868	-0.300343	3.111909
C	-0.987519	-1.684593	2.718260
C	-0.265548	-0.021775	4.239073
C	-0.322227	-2.387071	3.898889
H	-1.983173	-2.069504	2.480404

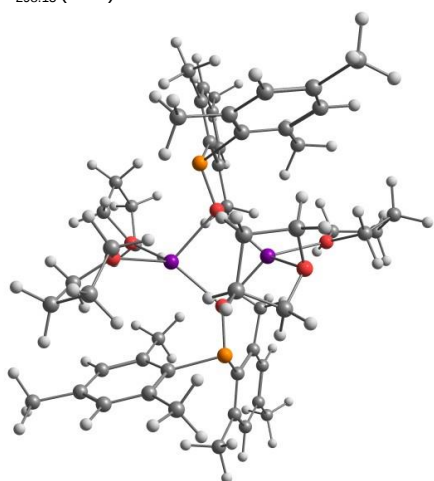
H	-0.358983	-1.737760	1.819611
C	0.578949	-1.277923	4.458841
H	0.345922	0.857762	4.008138
H	-0.896223	0.205435	5.108459
H	0.238120	-3.273797	3.591635
H	-1.073411	-2.686973	4.637973
H	1.501519	-1.215024	3.875718
H	0.840180	-1.422053	5.510500
O	0.783258	0.384304	-4.084565
C	-0.228878	1.409251	-4.068427
C	2.001917	1.051750	-3.723743
C	0.144523	2.361007	-2.911235
H	-0.226369	1.933525	-5.034492
H	-1.196250	0.922034	-3.929214
C	1.606413	1.970357	-2.564743
H	2.739916	0.290969	-3.463598
H	2.378876	1.629025	-4.581911
H	-0.528548	2.193227	-2.067907
H	0.060114	3.406359	-3.219497
H	1.652811	1.414651	-1.623737
H	2.274035	2.830653	-2.478515
H	-4.093184	4.748869	2.206920
H	-3.593232	3.355708	-1.832811
H	-4.017178	0.529290	1.376570
H	5.014583	-0.723290	2.493842
H	4.758647	-4.991581	2.964998
H	1.589080	-2.831721	0.999492

[Na-OPMes₂·(THF)]₂

E (BS1) = -3486.624405

E (BS2) = -3487.572885

G_{298.15} (BS2) = -3486.513026



Na	0.663581	-1.138689	0.511861
C	5.924050	3.492863	-0.000664
C	5.247079	2.398878	-0.552833
C	3.868675	2.199237	-0.287974
P	3.012121	0.779728	-1.170750
O	1.570475	0.578531	-0.532277
C	3.972056	-0.678104	-0.462430
C	4.430763	-1.674905	-1.356094
H	5.453446	-3.554007	-1.565012
C	5.101211	-2.802164	-0.862240
C	5.328388	-2.987293	0.502383
C	4.853815	-2.008764	1.380047
H	5.007174	-2.136486	2.450216
C	4.178384	-0.869300	0.926451
C	3.192252	3.175921	0.488568
C	3.908801	4.254101	1.022342
H	3.373757	4.983868	1.627498
C	5.278161	4.428981	0.806591
H	6.984119	3.614916	-0.215174
O	0.833717	-3.387432	0.106873
C	1.932581	-4.155481	0.654083
C	2.390689	-5.123190	-0.457277
H	2.708516	-3.447184	0.947226

H	1.586594	-4.692892	1.544753
C	1.606978	-4.648395	-1.694284
H	3.471045	-5.084829	-0.607446
H	2.116434	-6.152050	-0.205272
C	0.348718	-4.074396	-1.056739
H	2.151204	-3.853457	-2.214435
H	1.396642	-5.452505	-2.404290
H	-0.186632	-3.351754	-1.671445
H	-0.347199	-4.872703	-0.758737
C	6.036049	1.457526	-1.432847
H	6.978796	1.919260	-1.740833
H	6.272826	0.518883	-0.922284
H	5.476897	1.192752	-2.337186
C	1.704230	3.143510	0.770278
H	1.375655	2.188790	1.178865
H	1.439658	3.941933	1.470633
H	1.128762	3.302456	-0.147730
C	6.026156	5.579937	1.431301
H	5.413931	6.487411	1.461942
H	6.315316	5.352405	2.465780
H	6.943911	5.806557	0.879856
C	4.245307	-1.569513	-2.854407
H	3.206464	-1.371161	-3.127551
H	4.841312	-0.755290	-3.280427
H	4.555398	-2.498821	-3.341972
C	6.004418	-4.230247	1.022108
H	6.561088	-4.743741	0.232684
H	6.698898	-3.998775	1.836599
H	5.267773	-4.939848	1.420694
C	3.703753	0.121587	1.962559
H	4.402400	0.958705	2.060991
H	2.734570	0.542706	1.694837
H	3.620508	-0.360815	2.939695
Na	-0.431181	1.247352	-1.163371
C	-5.210580	-0.092136	3.582378
C	-4.640454	-0.662690	2.440503
C	-3.407661	-0.176200	1.930841
P	-2.630610	-1.145961	0.527390
O	-1.359682	-0.355300	0.001811
C	-3.884017	-0.869441	-0.852969
C	-4.194997	-1.977929	-1.676414
H	-5.203344	-2.665586	-3.445969
C	-4.985584	-1.802831	-2.819890
C	-5.499650	-0.555582	-3.178971
C	-5.192829	0.533100	-2.359097
H	-5.576472	1.517868	-2.619718
C	-4.397116	0.400194	-1.213807
C	-2.759505	0.867474	2.639802
C	-3.366276	1.407789	3.782515
H	-2.854984	2.211394	4.309281
C	-4.593279	0.954831	4.270234
H	-6.158538	-0.483998	3.946641
O	-1.345402	3.350505	-1.253786
C	-1.677963	4.348639	-0.265721
C	-2.110685	5.570415	-1.066645
H	-2.495897	3.979730	0.367000
H	-0.796827	4.513146	0.357310
C	-2.849402	4.916951	-2.242580
H	-2.737987	6.250486	-0.484861
H	-1.232484	6.121513	-1.420833
C	-2.011503	3.663302	-2.506042
H	-3.865522	4.642162	-1.940641
H	-2.915661	5.558106	-3.125051
H	-2.613170	2.802506	-2.810345
H	-1.240563	3.836401	-3.263883
C	-5.372493	-1.806013	1.778099
H	-6.165378	-2.187042	2.428309
H	-5.828347	-1.504269	0.829678
H	-4.691417	-2.633892	1.548022
C	-1.424856	1.459982	2.239683
H	-0.667910	0.692132	2.090839
H	-1.491539	2.014460	1.301195
H	-1.078084	2.155988	3.009876
C	-5.234400	1.576916	5.485282
H	-5.706651	0.820346	6.121068

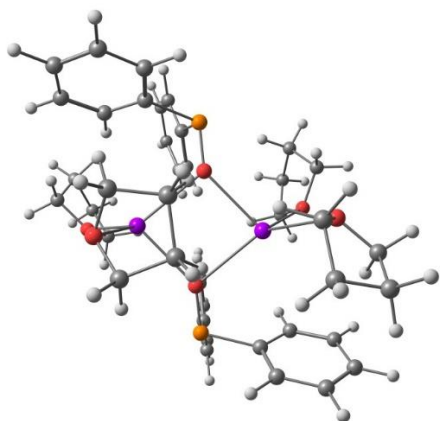
H	-4.501633	2.120108	6.089826
H	-6.018367	2.291036	5.201172
C	-3.690797	-3.374031	-1.379584
H	-2.600166	-3.410139	-1.309913
H	-4.077460	-3.751393	-0.427445
H	-4.003091	-4.066294	-2.167532
C	-6.372501	-0.390765	-4.397453
H	-6.182377	-1.176621	-5.134759
H	-7.436276	-0.443116	-4.131823
H	-6.208519	0.578521	-4.879283
C	-4.117687	1.647481	-0.411982
H	-4.699175	1.665540	0.514548
H	-3.066948	1.713865	-0.134484
H	-4.378993	2.538410	-0.988849
O	0.685083	-1.551700	2.780829
C	0.901604	-0.758988	3.960040
C	-0.103865	-2.680332	3.197006
C	-0.367219	-0.915105	4.825324
H	1.788626	-1.134191	4.488358
H	1.095385	0.265411	3.638427
C	-1.125357	-2.098153	4.173690
H	-0.538913	-3.125445	2.301208
H	0.547741	-3.417745	3.689302
H	-0.977793	-0.010184	4.808759
H	-0.099701	-1.121630	5.864994
H	-1.996681	-1.734754	3.625453
H	-1.462318	-2.839991	4.902446
O	-0.610693	0.863812	-3.477911
C	0.563437	0.185221	-3.962294
C	-1.692012	-0.059301	-3.707363
C	0.398266	-1.277187	-3.516487
H	0.596613	0.266418	-5.058295
H	1.438521	0.680609	-3.536743
C	-1.131442	-1.424470	-3.292411
H	-2.546224	0.265802	-3.113270
H	-1.966288	-0.038264	-4.772157
H	0.944378	-1.446012	-2.585074
H	0.785969	-1.971158	-4.266773
H	-1.346709	-1.585038	-2.235305
H	-1.575294	-2.240243	-3.868140

[K-OPPh₂·(THF)]₂

E (BS1) = -3889.923288

E (BS2) = -3890.798253

G_{298.15} (BS2) = -3890.056873



K	1.628912	-0.497204	0.940375
C	2.145982	5.121815	-2.067864
C	2.506778	3.823790	-2.429380
C	1.831875	2.714184	-1.896197
P	2.273238	0.978715	-2.419283
O	1.275274	0.061293	-1.601193
C	3.891016	0.857649	-1.465191
C	4.815015	-0.111365	-1.890190
H	6.700461	-1.096557	-1.536150
C	5.996813	-0.347671	-1.182813

C	6.276248	0.384932	-0.026322
C	5.367885	1.351790	0.415666
H	5.579094	1.926357	1.313993
C	4.189395	1.586113	-0.298895
C	0.775872	2.942974	-1.004994
C	0.405919	4.241144	-0.641249
H	-0.412905	4.398713	0.056317
C	1.091112	5.335670	-1.172158
H	2.682585	5.970122	-2.484715
O	3.136369	-2.466161	1.981383
C	4.536917	-2.130370	2.136591
C	5.324657	-3.076358	1.212836
H	4.663816	-1.080222	1.853263
H	4.821355	-2.242473	3.189340
C	4.239816	-3.625216	0.272644
H	6.124035	-2.555028	0.682809
H	5.770523	-3.892287	1.790476
C	3.037619	-3.674176	1.206861
H	4.048954	-2.923357	-0.547009
H	4.489842	-4.600770	-0.152436
H	2.067672	-3.671880	0.704436
H	3.083925	-4.552621	1.867843
K	-1.227312	-0.460407	-1.607555
C	-4.801047	1.808865	2.583110
C	-4.205873	0.549467	2.511000
C	-2.935946	0.383610	1.932891
P	-2.050852	-1.257050	1.950690
O	-0.850072	-1.052333	0.938648
C	-3.314934	-2.249927	0.981049
C	-3.324059	-3.639874	1.175829
H	-4.137191	-5.547216	0.582189
C	-4.145250	-4.473896	0.412334
C	-4.979005	-3.927377	-0.565971
C	-4.989779	-2.544133	-0.770421
H	-5.643189	-2.110731	-1.523487
C	-4.167967	-1.716451	-0.001245
C	-2.274400	1.521122	1.446933
C	-2.860305	2.788076	1.529442
H	-2.330721	3.657641	1.149323
C	-4.128019	2.935918	2.095647
H	-5.788956	1.916546	3.023242
O	-2.962417	1.316082	-2.604433
C	-2.775676	2.677531	-2.144445
C	-4.169907	3.219558	-1.800410
H	-2.125645	2.648127	-1.265498
H	-2.272442	3.255746	-2.926746
C	-4.991479	1.937875	-1.596979
H	-4.152929	3.859079	-0.915281
H	-4.573521	3.799019	-2.637103
C	-4.370714	1.019548	-2.642247
H	-4.829072	1.535881	-0.591394
H	-6.064354	2.084059	-1.747020
H	-4.495975	-0.047736	-2.439342
H	-4.770123	1.232823	-3.644673
O	1.750989	1.211985	3.006248
C	1.156402	2.508083	2.762418
C	1.200217	0.643839	4.213116
C	0.230109	2.794191	3.948733
H	1.955035	3.249176	2.650139
H	0.599478	2.461681	1.820561
C	-0.110265	1.384758	4.453160
H	1.072783	-0.432964	4.060153
H	1.906444	0.796252	5.041500
H	-0.653247	3.364285	3.650597
H	0.761381	3.358423	4.722570
H	-0.909714	0.945006	3.850386
H	-0.415623	1.363843	5.502527
O	-1.033638	-2.813302	-2.958749
C	0.355045	-3.000582	-3.280020
C	-1.331699	-3.810465	-1.968200
C	1.049518	-3.342156	-1.948056
H	0.452604	-3.820762	-4.006270
H	0.720002	-2.077072	-3.735638
C	-0.113138	-3.819629	-1.032719
H	-2.267071	-3.530409	-1.481303

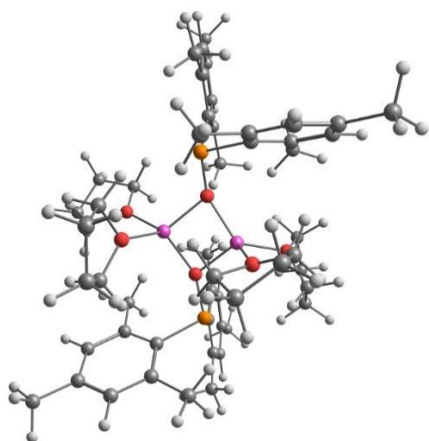
H	-1.468721	-4.786381	-2.458017
H	1.525602	-2.442598	-1.550910
H	1.816408	-4.108883	-2.085540
H	-0.273515	-3.119203	-0.207354
H	0.060339	-4.813130	-0.610864
H	-5.620085	-4.571988	-1.160481
H	-2.677381	-4.073236	1.936118
H	-4.199971	-0.641830	-0.156791
H	-4.735516	-0.317112	2.901189
H	-4.587920	3.917726	2.161030
H	0.252464	2.085318	-0.592685
H	0.805993	6.346932	-0.896157
H	3.326234	3.668418	-3.128793
H	7.195220	0.206504	0.524725
H	4.607417	-0.682412	-2.793148
H	3.496476	2.346052	0.052911
H	-1.287055	1.397137	1.011484

[Li-OPMe₂(THF)₂]₂

E (BS1) = -3177.132013

E (BS2) = -3178.057272

G_{298.15} (BS2) = -3176.985872



Li	-0.260683	-0.139936	-1.242143
C	-5.890152	2.251817	2.079084
C	-5.108542	1.174946	1.660176
C	-3.823918	1.393152	1.081374
P	-2.798635	-0.156917	0.799400
O	-1.373921	0.255471	0.210989
C	-3.713455	-0.914512	-0.661774
C	-4.067202	-2.284050	-0.585831
H	-4.989350	-3.950192	-1.580849
C	-4.724820	-2.897753	-1.658994
C	-5.037407	-2.202713	-2.829743
C	-4.656517	-0.861877	-2.909513
H	-4.867183	-0.303052	-3.819233
C	-4.005196	-0.210849	-1.853587
C	-3.372415	2.731018	0.965939
C	-4.185600	3.782655	1.422305
H	-3.812409	4.800848	1.324298
C	-5.445413	3.574670	1.975215
H	-6.869543	2.051720	2.510005
O	-0.341158	-1.993805	-1.888377
C	-1.203432	-2.587745	-2.886946
C	-1.334527	-4.069099	-2.511109
H	-2.161711	-2.064688	-2.888337
H	-0.723465	-2.454591	-3.862953
C	-0.089408	-4.314665	-1.645573
H	-2.240927	-4.226797	-1.920025
H	-1.385535	-4.714022	-3.392122
C	0.036692	-2.985931	-0.913435
H	-0.200619	-5.161618	-0.962978
H	0.792973	-4.487997	-2.271875
H	-0.642535	-2.929781	-0.056692
H	1.041793	-2.740488	-0.572520

C	-5.672251	-0.214452	1.841423
H	-6.593598	-0.184757	2.429953
H	-5.898669	-0.692222	0.882769
H	-4.957622	-0.867326	2.355576
C	-2.066759	3.140406	0.318154
H	-2.247885	3.478035	-0.710517
H	-1.624412	3.987454	0.852675
H	-1.359091	2.316999	0.275573
C	-6.302454	4.720462	2.451587
H	-5.807086	5.682573	2.291453
H	-7.264149	4.745880	1.925010
H	-6.528505	4.633203	3.521292
C	-3.737964	-3.141565	0.615901
H	-2.673915	-3.098051	0.858673
H	-4.278970	-2.823645	1.512355
H	-3.998835	-4.186204	0.421006
C	-5.765664	-2.878633	-3.963654
H	-6.850041	-2.876462	-3.793649
H	-5.583719	-2.369861	-4.915062
H	-5.458527	-3.924204	-4.069168
C	-3.622160	1.233833	-2.044663
H	-4.330289	1.903872	-1.546502
H	-2.637713	1.429482	-1.625514
H	-3.608551	1.489996	-3.107812
Li	0.193746	-0.127321	1.239851
C	5.432192	2.793106	-2.037421
C	4.821793	1.571267	-1.743069
C	3.531659	1.533224	-1.148359
P	2.726262	-0.153039	-1.003285
O	1.348672	0.013758	-0.223966
C	3.830906	-0.983145	0.271426
C	4.260724	-2.308568	0.008953
H	5.248492	-4.052690	0.783047
C	4.935786	-3.033012	0.999044
C	5.212571	-2.487060	2.254807
C	4.797064	-1.176971	2.500123
H	5.004653	-0.728912	3.469785
C	4.113432	-0.420684	1.539007
C	2.875640	2.766217	-0.903766
C	3.524558	3.969287	-1.221591
H	3.005133	4.904746	-1.022431
C	4.801891	4.013098	-1.780070
H	6.422781	2.788558	-2.488666
O	0.299997	0.955605	2.882846
C	-0.357262	2.220690	3.140594
C	-0.086864	2.544717	4.612795
H	0.078960	2.969277	2.472358
H	-1.419767	2.118296	2.908982
C	1.207941	1.767791	4.890684
H	0.003912	3.619784	4.786761
H	-0.897068	2.163383	5.243569
C	0.979042	0.504504	4.071989
H	2.075504	2.315252	4.505532
H	1.370088	1.557294	5.950985
H	1.892839	-0.006871	3.767027
H	0.338861	-0.204558	4.612275
C	5.570332	0.305218	-2.084752
H	6.440614	0.525527	-2.709535
H	5.920171	-0.217368	-1.188645
H	4.928506	-0.398203	-2.627716
C	1.496162	2.883097	-0.294824
H	0.778807	2.221783	-0.773967
H	1.496433	2.602996	0.761986
H	1.140142	3.915338	-0.369079
C	5.482238	5.322531	-2.091436
H	5.921036	5.317657	-3.095564
H	4.781224	6.160439	-2.032293
H	6.299555	5.525040	-1.387474
C	4.020742	-2.997687	-1.317256
H	2.989462	-2.889971	-1.660475
H	4.654827	-2.579062	-2.106823
H	4.251027	-4.064481	-1.238866
C	5.924990	-3.296380	3.309357
H	5.335125	-4.173474	3.602198
H	6.888720	-3.668704	2.942938

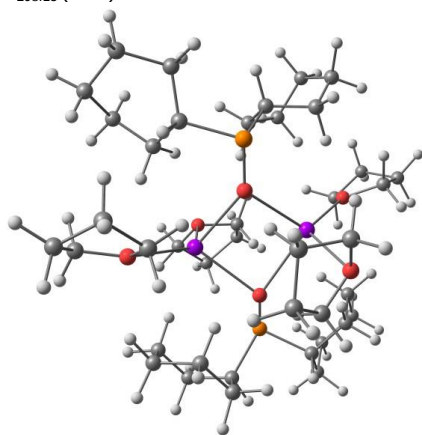
H	6.112608	-2.703176	4.208926
C	3.692201	0.978885	1.912871
H	4.258969	1.728851	1.354182
H	2.636355	1.141524	1.692370
H	3.858909	1.158071	2.978707
O	-0.260346	0.806982	-2.982703
C	-0.493246	2.185783	-3.316980
C	0.582279	0.280785	-4.024346
C	0.817234	2.695705	-3.942888
H	-1.324038	2.243813	-4.032507
H	-0.781061	2.704469	-2.402427
C	1.578111	1.402460	-4.334037
H	1.044199	-0.627798	-3.638207
H	-0.038126	0.038557	-4.898972
H	1.398029	3.276311	-3.223753
H	0.611059	3.334889	-4.805363
H	2.471181	1.288947	-3.716545
H	1.882066	1.390936	-5.383935
O	0.306456	-1.887385	2.201649
C	-0.706423	-2.495611	3.014963
C	1.472201	-2.709335	2.352431
C	-0.536396	-4.007050	2.794541
H	-0.532373	-2.234021	4.068832
H	-1.667602	-2.086883	2.699664
C	0.947521	-4.153292	2.360326
H	2.148664	-2.476882	1.534022
H	1.965448	-2.465361	3.303308
H	-1.206020	-4.359588	2.005914
H	-0.767119	-4.568934	3.703246
H	1.019090	-4.594787	1.362964
H	1.525905	-4.780128	3.043802

[K-OPCy₂·(THF)]₂

E (BS1) = -3904.452209

E (BS2) = -3905.294086

G_{298.15} (BS2) = -3904.276167



K	-0.919404	-1.287202	-0.796480
P	-2.735858	1.563505	1.213437
O	-1.525894	0.604057	0.819653
O	-2.957594	-2.896579	-0.164058
C	-4.071787	-3.549226	-0.809008
C	-5.053120	-3.908027	0.307705
H	-4.521266	-2.850903	-1.528139
H	-3.694594	-4.419864	-1.355564
C	-4.795384	-2.790886	1.328704
H	-6.087186	-3.944781	-0.045932
H	-4.799743	-4.882699	0.739856
C	-3.284270	-2.606900	1.217623
H	-5.312988	-1.873224	1.028202
H	-5.109425	-3.047992	2.343997
H	-2.944325	-1.591499	1.438953
H	-2.746183	-3.313565	1.863722
K	1.017441	1.014857	1.096948
P	2.811668	-2.052411	-0.556099
O	1.549154	-1.335406	0.103768
O	2.326166	3.195586	0.239178
C	2.989276	3.586711	-0.979362

C	3.307826	5.066397	-0.801131
H	3.904398	2.993608	-1.105814
H	2.314577	3.376461	-1.812006
C	3.652009	5.126314	0.693874
H	4.124152	5.400478	-1.446553
H	2.421025	5.672490	-1.016643
C	2.664850	4.122875	1.298645
H	4.682676	4.793714	0.856080
H	3.540934	6.123940	1.125989
H	3.090426	3.563478	2.139653
H	1.741487	4.609893	1.632347
O	-0.005248	-0.065241	-3.031272
C	1.072938	0.798310	-2.594974
C	0.433552	-0.856917	-4.157852
C	2.099284	0.789817	-3.724620
H	0.650930	1.785266	-2.389787
H	1.503972	0.376607	-1.678697
C	1.941254	-0.634861	-4.273420
H	0.168811	-1.905112	-3.976561
H	-0.097880	-0.515086	-5.056273
H	3.109776	0.997914	-3.363230
H	1.840709	1.532280	-4.488063
H	2.476006	-1.336255	-3.624644
H	2.301488	-0.750994	-5.298972
O	1.110467	0.025325	3.629802
C	-0.105327	0.371423	4.317255
C	1.147604	-1.417609	3.443807
C	-1.105158	-0.697108	3.894143
H	0.062891	0.366149	5.405626
H	-0.389525	1.384831	4.014358
C	-0.223591	-1.955623	3.889030
H	1.344584	-1.605267	2.383085
H	1.971167	-1.831468	4.038541
H	-1.456441	-0.462456	2.884258
H	-1.961123	-0.771101	4.570851
H	-0.593739	-2.727765	3.210126
H	-0.163190	-2.387499	4.893994
C	-0.173139	-4.911005	-0.369058
C	0.398449	-4.229218	0.881513
C	1.922492	-4.382335	0.983720
C	2.654717	-3.939926	-0.297283
C	2.062586	-4.651993	-1.527095
C	0.547160	-4.459260	-1.647054
H	-1.247859	-4.710594	-0.439784
H	-0.053027	-6.000026	-0.272087
H	-0.079728	-4.642464	1.778711
H	0.174720	-3.159709	0.862896
H	2.290677	-3.818437	1.849155
H	2.158188	-5.440099	1.180700
H	3.705038	-4.254110	-0.219291
H	2.561378	-4.297279	-2.437483
H	2.268165	-5.731213	-1.454087
H	0.160002	-5.009640	-2.513727
H	0.347113	-3.398439	-1.847589
C	5.945665	0.436095	-0.174703
C	5.993361	-0.916226	-0.897652
C	5.595933	-2.076254	0.029202
C	4.232900	-1.849436	0.713435
C	4.214071	-0.483136	1.412775
C	4.572043	0.668689	0.466364
H	6.187068	1.247873	-0.872934
H	6.714957	0.457881	0.611210
H	6.995163	-1.092329	-1.308981
H	5.299339	-0.887959	-1.746401
H	5.585659	-3.013917	-0.542159
H	6.370716	-2.195744	0.801721
H	4.094540	-2.618699	1.485282
H	3.238417	-0.324941	1.878851
H	4.944022	-0.493405	2.237068
H	4.554312	1.624361	1.003770
H	3.815864	0.740960	-0.325670
C	-4.187178	0.999779	0.124513
C	-5.269804	2.073815	-0.043834
H	-7.182303	1.088279	0.269136
C	-6.585010	1.460827	-0.572013

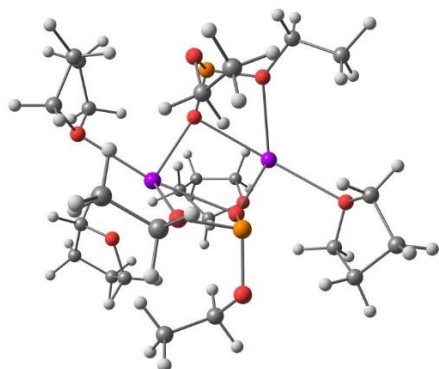
C	-6.327472	0.306850	-1.571425
H	-6.323428	-0.653537	-1.038460
C	-4.973031	0.479815	-2.266883
H	-4.841776	-0.268510	-3.058452
C	-3.821639	0.373194	-1.245289
H	-2.922930	0.833819	-1.663620
H	-5.454563	2.595653	0.903568
H	-7.140837	0.248529	-2.303556
H	-7.182431	2.245221	-1.053297
H	-4.912069	2.835395	-0.747072
H	-4.634973	0.202372	0.735244
H	-4.947810	1.459204	-2.762520
H	-3.596151	-0.685610	-1.087100
C	-2.301705	3.228842	0.411768
C	-1.332553	4.008440	1.315995
H	-1.918673	6.098396	1.245517
C	-1.132952	5.458573	0.826400
C	-1.150788	5.558496	-0.717174
H	-2.166579	5.787322	-1.064499
C	-0.705884	4.233522	-1.343793
H	-0.593413	4.330685	-2.430619
C	-1.710810	3.110995	-1.011241
H	-1.214045	2.138224	-1.100834
H	-1.685024	4.004950	2.353912
H	-0.516523	6.387654	-1.051958
H	-0.180992	5.843734	1.213572
H	-0.359529	3.500290	1.323909
H	-3.238642	3.800369	0.380899
H	0.280330	3.970368	-0.946105
H	-2.525217	3.118723	-1.744746

[K-OP(OEt)₂·(THF)]₂

E (BS1) = -3581.139736

E (BS2) = -3581.950213

G_{298.15} (BS2) = -3581.285191



K	-1.384965	-0.013350	0.451773
K	1.925253	0.279821	-1.564261
P	0.011452	3.159989	-1.267451
O	-0.441045	1.681538	-1.360492
O	-3.686244	1.405804	0.519153
C	-3.884764	2.383499	1.553708
C	-3.429919	3.701675	0.939113
H	-4.947808	2.420091	1.837812
H	-3.304021	2.070849	2.426532
C	-3.946613	3.561660	-0.502165
H	-3.840065	4.572450	1.458335
H	-2.337735	3.765850	0.942276
C	-3.823421	2.051684	-0.772122
H	-4.991981	3.880974	-0.566765
H	-3.364343	4.149467	-1.216552
H	-4.704824	1.646676	-1.283285
H	-2.927339	1.818417	-1.355376
O	0.897891	-1.638078	-3.213912
C	-0.250114	-2.065112	-2.451209
C	-1.392755	-1.180259	-2.940169
H	-0.455771	-3.126829	-2.651712
H	0.004358	-1.956757	-1.392330

C	-1.084634	-1.101878	-4.442579
H	-2.375387	-1.601356	-2.721903
H	-1.316862	-0.183350	-2.492774
C	0.449828	-1.066341	-4.466002
H	-1.453990	-1.997066	-4.954147
H	-1.523077	-0.225636	-4.926660
H	0.876129	-1.639632	-5.296372
H	0.829780	-0.037979	-4.529802
O	1.726835	2.897417	-1.375510
C	2.597570	4.007490	-1.172715
H	2.221349	4.636309	-0.356404
H	2.638275	4.629834	-2.079479
C	3.983213	3.484124	-0.832013
H	4.378743	2.867049	-1.647095
H	3.949920	2.873797	0.076979
H	4.680270	4.313345	-0.666220
O	-0.032306	3.595554	0.374853
C	0.377063	2.655132	1.377141
H	0.858858	1.786124	0.921396
H	-0.517788	2.299526	1.903193
C	1.319777	3.307864	2.371601
H	0.855483	4.186031	2.833211
H	2.245172	3.626473	1.881643
H	1.578819	2.596121	3.163723
P	1.520452	-0.850401	2.105158
O	1.168232	-0.902140	0.598211
O	1.598376	-2.460327	2.630748
C	0.754439	-3.455804	2.036862
H	0.491601	-3.151637	1.017198
H	1.350782	-4.374094	1.968022
H	-0.232635	-3.954024	3.898406
H	-1.137555	-2.818819	2.877002
H	-1.068620	-4.544931	2.450113
C	-0.173242	-0.248279	4.126748
H	-0.239651	-1.223238	4.629259
O	-0.050016	-0.434368	2.720925
H	0.717924	0.260909	4.523962
C	-0.498563	-3.705598	2.865344
C	-1.418054	0.574367	4.413744
H	-1.340861	1.566207	3.956194
H	-2.309437	0.076704	4.014905
H	-1.554350	0.703222	5.493448
O	-2.977450	-2.106173	0.019897
C	-2.673563	-3.507443	-0.100940
H	-1.604285	-3.605455	-0.307118
C	-3.577327	-4.019344	-1.217154
H	-3.145223	-3.783247	-2.195614
H	-3.742121	-5.098482	-1.162089
C	-4.852126	-3.197465	-0.974187
H	-5.483208	-3.103974	-1.861571
H	-5.447999	-3.656456	-0.178251
C	-4.296718	-1.844154	-0.513573
H	-4.193514	-1.140437	-1.348138
H	-4.906606	-1.369199	0.260640
H	-2.893881	-4.016427	0.847433
O	4.298311	-0.905824	-1.085379
C	4.867637	-0.339887	0.110615
H	5.568606	0.443549	-0.191165
C	5.518006	-1.512995	0.835268
H	6.496278	-1.733173	0.393773
H	5.652146	-1.321244	1.903228
C	4.519191	-2.645103	0.549442
H	4.976242	-3.637544	0.588523
H	3.698359	-2.615168	1.270544
C	4.001995	-2.305672	-0.855819
H	4.506556	-2.881965	-1.639861
H	2.921728	-2.466766	-0.937828
H	4.077409	0.107931	0.730841

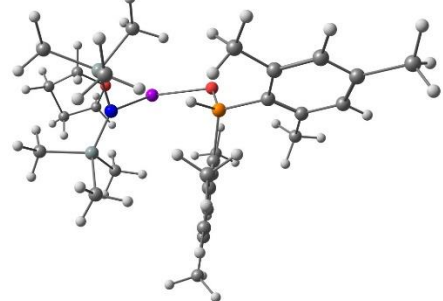
Metalation-deprotonation of phosphane oxides

K-RI

E (BS1) = -2822.408394

E (BS2) = -2823.011239

G_{298.15} (BS2) = -2822.384803



N	1.863400	-0.674398	0.819858
Si	1.676556	-2.265769	1.320204
Si	2.564416	0.697399	1.488217
C	1.023143	-3.323642	-0.131726
H	0.139724	-2.875311	-0.601918
H	1.792097	-3.437020	-0.910198
H	0.749497	-4.337631	0.187243
C	3.273069	-3.146743	1.889307
H	3.090766	-4.200747	2.139748
H	4.046081	-3.122254	1.111214
H	3.694809	-2.667288	2.781327
C	0.459196	-2.516958	2.767404
H	-0.501684	-2.030615	2.569971
H	0.259303	-3.576485	2.976089
H	0.860883	-2.071892	3.687073
C	1.610019	1.487766	2.935828
H	1.467900	0.768001	3.752089
H	2.136941	2.357396	3.351909
H	0.618768	1.825328	2.616545
C	2.685399	2.071444	0.163760
H	1.688880	2.339899	-0.208969
H	3.132075	2.988755	0.568658
H	3.305636	1.768748	-0.690220
C	4.337535	0.452895	2.155895
H	4.821307	1.405036	2.412655
H	4.328332	-0.161258	3.065523
H	4.976472	-0.060339	1.428552
K	1.622736	-0.418907	-1.817492
O	4.209666	-0.639474	-2.433272
C	4.747673	-1.510570	-1.401098
C	6.159163	-1.000926	-1.105218
H	4.097702	-1.434130	-0.522088
H	4.730556	-2.541238	-1.771046
C	6.049931	0.487125	-1.465407
H	6.445951	-1.173015	-0.064742
H	6.892527	-1.495360	-1.751296
C	5.130556	0.441997	-2.681983
H	5.573231	1.041630	-0.650796
H	7.013895	0.952232	-1.687321
H	4.551863	1.359875	-2.829582
H	5.695720	0.235114	-3.601669
C	-0.873839	3.747583	-0.423036
C	-1.021224	2.442683	-0.915806
C	-1.483159	1.431905	-0.044462
C	-1.786420	1.757466	1.306534
C	-1.633843	3.072694	1.741415
C	-1.171692	4.085966	0.893466
H	-0.515054	4.517896	-1.101877
H	-1.867876	3.310842	2.775905
C	-4.388698	-0.003060	-1.262114
C	-3.449060	-0.755438	-0.517661
C	-3.871901	-1.901931	0.199080
C	-5.228687	-2.240763	0.188592
C	-6.175653	-1.491571	-0.513193

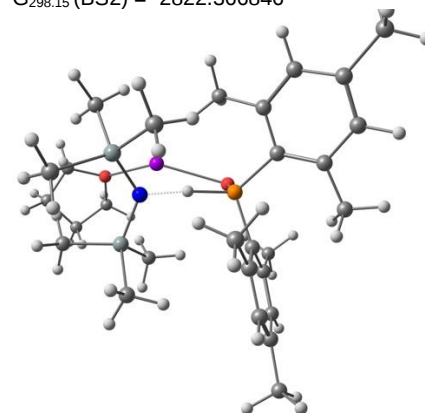
C	-5.732242	-0.383929	-1.240785
H	-5.550704	-3.120837	0.739185
H	-6.449197	0.196888	-1.815668
O	-0.978608	-0.717058	-1.832716
P	-1.682063	-0.315787	-0.543124
H	-1.167784	-0.980628	0.575334
C	-2.927166	-2.782967	0.984522
H	-2.540624	-2.270560	1.871015
H	-3.449810	-3.679361	1.326689
H	-2.064689	-3.108009	0.395100
C	-3.994371	1.193015	-2.093201
H	-4.820588	1.492048	-2.742790
H	-3.732683	2.051626	-1.467201
H	-3.132309	0.975319	-2.728951
C	-7.635974	-1.859114	-0.478766
H	-8.158371	-1.299573	0.307592
H	-8.129537	-1.623382	-1.426455
H	-7.775416	-2.923717	-0.270254
C	-2.230070	0.724430	2.314709
H	-2.503303	1.209137	3.254811
H	-3.095249	0.148870	1.973687
H	-1.421155	0.017880	2.531976
C	-0.660378	2.239846	-2.373075
H	0.394138	2.499461	-2.535186
H	-0.831453	1.223442	-2.718484
H	-1.243919	2.921847	-3.001024
C	-0.983049	5.488962	1.406982
H	-1.868834	5.835749	1.949977
H	-0.139214	5.535055	2.106035
H	-0.782069	6.189825	0.592264

K-TS

E (BS1) = -2822.394906

E (BS2) = -2822.991582

G_{298.15} (BS2) = -2822.366846



N	1.135769	-0.433688	1.119653
Si	1.213063	-1.805238	2.144122
Si	2.005502	1.036478	1.283463
C	2.071724	-3.269111	1.268494
H	1.530134	-3.625650	0.383334
H	3.087266	-2.990194	0.955831
H	2.169262	-4.131039	1.941359
C	2.180118	-1.575404	3.762313
H	2.020538	-2.438789	4.421437
H	3.258281	-1.488514	3.591975
H	1.855231	-0.682427	4.309072
C	-0.517888	-2.385171	2.667787
H	-1.239802	-2.398937	1.846095
H	-0.479883	-3.396090	3.093729
H	-0.922470	-1.721936	3.441939
C	1.274796	2.261337	2.533426
H	1.116324	1.785490	3.508818
H	1.950704	3.112739	2.687506
H	0.313215	2.660382	2.196855
C	2.059575	1.944480	-0.388717

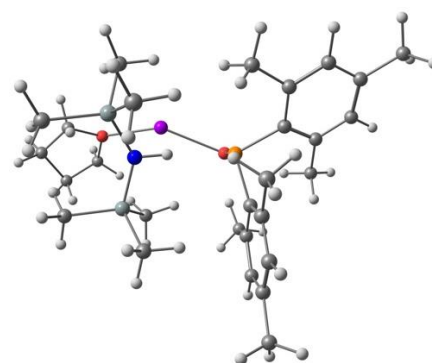
H	1.074776	2.013336	-0.859932
H	2.423372	2.969508	-0.243615
H	2.748730	1.473194	-1.100478
C	3.821918	0.804823	1.800533
H	4.400812	1.713948	1.592465
H	3.914476	0.600130	2.872346
H	4.297417	-0.023334	1.264769
K	1.802633	-1.161872	-1.530223
O	4.369508	-0.889133	-2.050834
C	5.319853	-1.423157	-1.099412
C	6.376261	-0.325146	-0.859196
H	4.764903	-1.681925	-0.191358
H	5.764379	-2.339450	-1.505513
C	5.780633	0.911435	-1.556097
H	6.555197	-0.157019	0.205274
H	7.326185	-0.605116	-1.323685
C	4.947366	0.278452	-2.662736
H	5.129259	1.464900	-0.873550
H	6.543395	1.593204	-1.940635
H	4.127655	0.905847	-3.024720
H	5.571874	-0.016649	-3.518475
C	-1.915516	4.089715	-0.844491
C	-1.676775	2.784836	-1.294632
C	-1.705471	1.720973	-0.364553
C	-1.997283	1.995649	0.994980
C	-2.250933	3.310401	1.393830
C	-2.200426	4.377189	0.491176
H	-1.889865	4.902541	-1.566936
H	-2.484890	3.505806	2.437907
C	-4.078057	-0.624817	-0.739353
C	-2.731148	-1.064479	-0.744997
C	-2.476059	-2.461707	-0.707379
C	-3.530766	-3.367313	-0.581697
C	-4.858890	-2.940371	-0.508268
C	-5.104954	-1.571571	-0.609590
H	-3.308425	-4.431402	-0.547426
H	-6.134100	-1.220286	-0.600271
O	-0.504715	-0.124304	-2.151696
P	-1.215697	-0.000160	-0.779662
H	-0.118284	-0.313286	0.372233
C	-1.082315	-3.026111	-0.861052
H	-0.363895	-2.495453	-0.235633
H	-1.054642	-4.079147	-0.570683
H	-0.750789	-2.949897	-1.902939
C	-4.506108	0.815321	-0.905193
H	-5.573331	0.856128	-1.140610
H	-4.343282	1.408033	-0.000799
H	-3.964497	1.310633	-1.712780
C	-5.983179	-3.926577	-0.324255
H	-6.106270	-4.186222	0.735001
H	-6.935693	-3.517451	-0.673606
H	-5.789534	-4.859052	-0.864045
C	-2.067400	0.898497	2.030542
H	-2.312501	1.312980	3.012074
H	-2.828680	0.151656	1.781267
H	-1.111849	0.373263	2.111865
C	-1.465181	2.573221	-2.774460
H	-0.597585	1.943255	-2.973012
H	-2.322556	2.050656	-3.217525
H	-1.360098	3.534208	-3.286277
C	-2.426505	5.793319	0.954995
H	-3.225686	5.846723	1.701574
H	-1.521661	6.202272	1.422429
H	-2.690705	6.450086	0.121008

K-PI

E (BS1) = -2822.420507

E (BS2) = -2823.015462

G_{298.15} (BS2) = -2822.387144



N	1.708544	-0.154490	1.136945
Si	2.090359	-1.332601	2.374094
Si	2.294281	1.453466	0.740282
C	1.983811	-3.056003	1.597196
H	1.002992	-3.239080	1.141090
H	2.763120	-3.206001	0.838723
H	2.126725	-3.834979	2.356039
C	3.827749	-1.098375	3.054815
H	4.048188	-1.914488	3.754025
H	4.593235	-1.118609	2.273132
H	3.930013	-0.158425	3.606093
C	0.855535	-1.239386	3.794498
H	-0.164862	-1.441848	3.451611
H	1.092255	-1.969382	4.578325
H	0.860479	-0.242857	4.251311
C	1.333244	2.780023	1.665351
H	1.463768	2.673239	2.749136
H	1.668850	3.785923	1.384650
H	0.262970	2.713909	1.449340
C	2.059288	1.689677	-1.118054
H	1.068745	1.363401	-1.446749
H	2.165208	2.744395	-1.396995
H	2.815602	1.129510	-1.680411
C	4.126884	1.636796	1.130630
H	4.485633	2.578665	0.696746
H	4.325899	1.676535	2.205646
H	4.727368	0.828573	0.704312
K	1.485055	-1.565579	-1.428502
O	4.043262	-1.491350	-2.064037
C	4.944584	-1.676008	-0.944323
C	6.197779	-0.845775	-1.250466
H	4.434340	-1.324616	-0.041554
H	5.160909	-2.743796	-0.830639
C	5.682950	0.185724	-2.265414
H	6.617397	-0.390395	-0.349966
H	6.969451	-1.473282	-1.707557
C	4.664733	-0.636278	-3.045794
H	5.184696	1.015435	-1.753587
H	6.471387	0.592222	-2.903696
H	3.878400	-0.040994	-3.519614
H	5.152248	-1.251630	-3.814691
C	-1.727787	3.863974	-0.761504
C	-1.564841	2.528989	-1.168678
C	-1.807020	1.478560	-0.250062
C	-2.225379	1.832885	1.065300
C	-2.407776	3.171164	1.415687
C	-2.153325	4.213128	0.516425
H	-1.526537	4.651851	-1.485900
H	-2.735500	3.408503	2.426143
C	-4.086869	-0.784869	-1.310736
C	-3.026124	-1.141829	-0.443941
C	-3.211511	-2.238365	0.430739
C	-4.446822	-2.899110	0.471966
C	-5.512434	-2.522640	-0.347454
C	-5.304266	-1.471096	-1.244291
H	-4.573854	-3.735313	1.156433
H	-6.108782	-1.179845	-1.917223
O	-0.794955	-0.549951	-1.983280
P	-1.337735	-0.322036	-0.517157

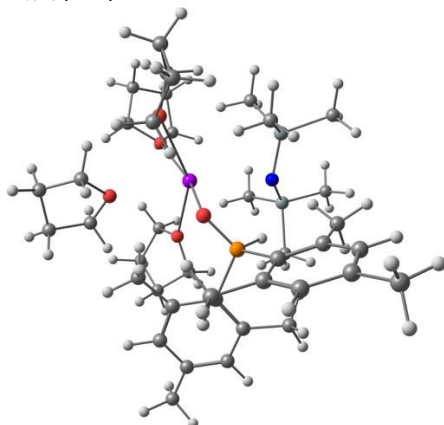
H	0.705335	-0.224295	0.892869
C	-2.110068	-2.750647	1.332782
H	-1.817193	-2.012487	2.083914
H	-2.435283	-3.653416	1.858956
H	-1.207357	-2.997312	0.765674
C	-3.934759	0.312362	-2.334085
H	-4.727578	0.254171	-3.086044
H	-3.982707	1.302304	-1.869147
H	-2.964668	0.232650	-2.828246
C	-6.846398	-3.221320	-0.266140
H	-7.553732	-2.651531	0.350310
H	-7.301337	-2.332754	-1.255909
H	-6.751237	-4.215629	0.180682
C	-2.451429	0.790012	2.132521
H	-2.675634	1.260977	3.093788
H	-3.275398	0.114820	1.883500
H	-1.558853	0.166870	2.259652
C	-1.182764	2.316111	-2.618853
H	-0.822554	1.302403	-2.793712
H	-2.056571	2.476321	-3.264119
H	-0.425047	3.046111	-2.925899
C	-2.304774	5.653703	0.935557
H	-3.252895	5.822127	1.458624
H	-1.503375	5.953520	1.623000
H	-2.268768	6.326363	0.073440

K-RI-4THF

E (BS1) = -3519.908191

E (BS2) = -3520.750980

G_{298.15} (BS2) = -3519.797956



N	-0.044621	-1.796873	1.996939
Si	-0.111346	-1.091175	3.521465
Si	-0.519469	-3.321607	1.471804
C	-1.791536	-0.273983	3.914573
H	-2.046664	0.443437	3.129453
H	-2.587213	-1.029150	3.953179
H	-1.793789	0.258395	4.875786
C	0.211115	-2.247561	5.010924
H	0.269133	-1.682993	5.951882
H	-0.588240	-2.989974	5.127297
H	1.153654	-2.797783	4.899466
C	1.191697	0.286833	3.714400
H	1.198817	0.963794	2.854711
H	1.020637	0.893197	4.613892
H	2.195904	-0.145091	3.803143
C	0.077451	-4.814647	2.504171
H	-0.365211	-4.825643	3.506952
H	-0.181917	-5.766390	2.020407
H	1.167543	-4.796817	2.629733
C	0.135134	-3.655125	-0.284747
H	1.229908	-3.725711	-0.284438
H	-0.256154	-4.594863	-0.695394
H	-0.132583	-2.846060	-0.969073
C	-2.422172	-3.537999	1.378900
H	-2.720915	-4.508513	0.959131
H	-2.856069	-3.468633	2.385248

H	-2.892343	-2.755083	0.773043
K	-1.400225	-0.233294	-0.077084
O	-4.055639	-0.284973	0.383580
C	-4.910208	-0.598005	1.486438
C	-5.836537	-1.694116	0.954773
H	-4.278366	-0.905886	2.320907
H	-5.480469	0.296858	1.782785
C	-5.983045	-1.333448	-0.545551
H	-5.354779	-2.668958	1.070134
H	-6.793501	-1.720150	1.482521
C	-4.889655	-0.267188	-0.783399
H	-5.829545	-2.211895	-1.177621
H	-6.973415	-0.929369	-0.772429
H	-4.249539	-0.466775	-1.642860
H	-5.332986	0.732114	-0.901124
C	5.558378	-1.060945	-2.208580
C	4.383828	-0.378642	-1.896014
C	3.652563	-0.750257	-0.739015
C	4.099973	-1.826367	0.062582
C	5.283491	-2.484939	-0.300866
C	6.029188	-2.117176	-1.419445
H	6.115003	-0.768874	-3.095940
H	5.625950	-3.312510	0.315322
C	3.234732	2.295024	0.937953
C	2.385723	1.893859	-0.123673
C	1.691122	2.878488	-0.872997
C	1.837578	4.223161	-0.510013
C	2.631788	4.631111	0.563347
C	3.333633	3.650468	1.265776
H	1.305838	4.975310	-1.087733
H	3.980364	3.943022	2.089139
O	0.984028	-0.194376	-1.376852
P	2.085460	0.101813	-0.373780
H	1.746244	-0.330958	0.919100
C	0.797436	2.584256	-2.056147
H	-0.101955	2.036261	-1.773616
H	0.493912	3.526013	-2.522181
H	1.302239	1.978359	-2.810016
C	4.074585	1.314664	1.719261
H	4.513657	1.801676	2.593238
H	3.494287	0.463180	2.077197
H	4.890387	0.917464	1.106463
C	2.707969	6.081641	0.962335
H	1.883325	6.340862	1.638381
H	3.642128	6.304746	1.485808
H	2.632355	6.740392	0.091771
C	3.400947	-2.299522	1.316605
H	3.710975	-1.699944	2.181950
H	2.310583	-2.246980	1.276716
H	3.683889	-3.334152	1.529906
C	3.918395	0.726057	-2.812598
H	2.892474	0.548391	-3.147427
H	3.934461	1.700125	-2.313391
H	4.559186	0.788973	-3.695403
C	7.303740	-2.834320	-1.781996
H	7.493971	-3.675979	-1.110769
H	7.262987	-3.218017	-2.807717
H	8.164553	-2.157183	-1.728190
C	-2.749295	3.009981	-1.672957
O	-2.408623	1.633531	-1.926823
C	-2.508478	1.358426	-3.337105
C	-3.295445	2.523076	-3.933063
C	-2.842113	3.686146	-3.040711
H	-2.986627	0.384612	-3.459914
H	-3.079461	2.675396	-4.993817
H	-4.372407	2.353880	-3.819425
H	-1.856488	4.043637	-3.358648
H	-3.532269	4.533929	-3.040466
H	-1.985341	3.439853	-1.021542
H	-3.713474	3.043861	-1.149491
H	-1.497614	1.305109	-3.763718
C	-0.633927	2.971949	2.001486
O	-1.587828	2.108915	1.373140
C	-2.875136	2.633626	1.727710
C	-2.717029	4.169374	1.743832

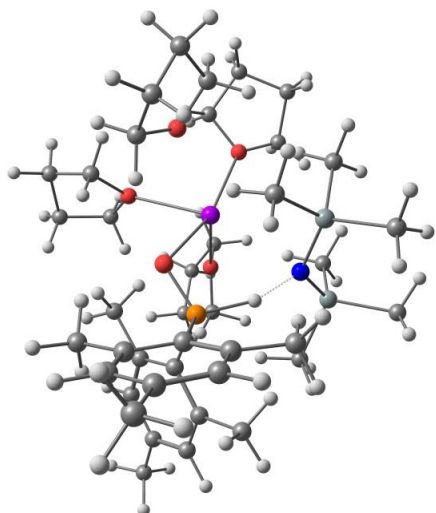
C	-1.180500	4.382723	1.765107
H	-3.157026	2.261610	2.723055
H	-3.165762	4.627039	0.858495
H	-3.202602	4.599783	2.623661
H	-0.827310	4.759686	0.801092
H	-0.858214	5.083102	2.540172
H	0.339280	2.786885	1.547131
H	-0.578058	2.742646	3.075583
H	-3.592991	2.252420	1.001302
C	-2.819515	-2.971665	-2.401119
O	-2.043859	-1.755724	-2.370001
C	-1.052886	-1.780278	-3.422459
C	-0.938342	-3.241472	-3.846207
C	-2.380056	-3.734171	-3.654450
H	-0.133593	-1.350456	-3.019340
H	-0.578292	-3.349832	-4.873052
H	-0.257538	-3.778717	-3.179313
H	-2.995417	-3.445801	-4.514128
H	-2.456999	-4.817130	-3.526619
H	-3.883615	-2.712457	-2.410228
H	-2.610388	-3.541113	-1.489496
H	-1.402518	-1.160951	-4.260374

K-TS-4THF

E (BS1) = -3519.903606

E (BS2) = -3520.741449

G_{298.15} (BS2) = -3519.787872



N	0.376183	-0.914216	2.248806
Si	0.059251	0.158619	3.538189
Si	-0.011034	-2.576360	2.210775
C	-1.773795	0.657230	3.661352
H	-2.122723	1.083634	2.716576
H	-2.397007	-0.214906	3.891801
H	-1.943085	1.401162	4.451489
C	0.498878	-0.512367	5.266794
H	0.412730	0.274931	6.027869
H	-0.166392	-1.329991	5.568712
H	1.526337	-0.894334	5.301495
C	1.062975	1.757892	3.350497
H	1.050924	2.140955	2.327378
H	0.672772	2.544355	4.008849
H	2.110673	1.595549	3.626865
C	0.797407	-3.634808	3.571596
H	0.378333	-3.420062	4.560957
H	0.648866	-4.705586	3.377891
H	1.877476	-3.456497	3.628034
C	0.526833	-3.337397	0.560335
H	1.616310	-3.373709	0.460108
H	0.154691	-4.365586	0.474606
H	0.147112	-2.760598	-0.285267
C	-1.883202	-2.920027	2.372945

H	-2.098118	-3.994367	2.296681
H	-2.257505	-2.581701	3.346818
H	-2.474912	-2.411882	1.603622
K	-1.526194	-0.212920	-0.119870
O	-4.120171	-0.546953	0.495148
C	-4.912526	-0.718614	1.672993
C	-5.648878	-2.035840	1.435907
H	-4.239199	-0.722871	2.531462
H	-5.618705	0.120541	1.777067
C	-5.925526	-1.999465	-0.086251
H	-4.988628	-2.871034	1.688728
H	-6.559753	-2.123058	2.033918
C	-4.949263	-0.922381	-0.617349
H	-5.747538	-2.973317	-0.549329
H	-6.960519	-1.715818	-0.296431
H	-4.287589	-1.271883	-1.410965
H	-5.493500	-0.039587	-0.980077
C	5.189346	-1.337863	-2.388908
C	4.042613	-0.650664	-1.993144
C	3.516037	-0.855917	-0.687786
C	4.163294	-1.765359	0.175566
C	5.312700	-2.438715	-0.269921
C	5.843143	-2.240907	-1.540723
H	5.582672	-1.169231	-3.389224
H	5.800910	-3.136030	0.407683
C	3.322247	2.254625	0.682734
C	2.332432	1.787526	-0.219324
C	1.616499	2.737529	-0.992338
C	1.923958	4.099306	-0.855619
C	2.896798	4.567505	0.027150
C	3.586578	3.622451	0.788507
H	1.374523	4.815927	-1.462212
H	4.348866	3.954943	1.489609
O	0.853690	-0.365078	-1.279539
P	1.927212	-0.024857	-0.226807
H	1.339477	-0.432332	1.170961
C	0.500037	2.398304	-1.956822
H	-0.421524	2.146242	-1.426278
H	0.286525	3.267913	-2.585879
H	0.734007	1.543863	-2.587193
C	4.119033	1.318299	1.557257
H	4.618096	1.874499	2.355187
H	3.484835	0.563591	2.025952
H	4.886509	0.788064	0.984953
C	3.170742	6.041702	0.180209
H	2.628282	6.454804	1.040323
H	4.234997	6.235639	0.348043
H	2.854877	6.601146	-0.705364
C	3.731844	-2.050562	1.597159
H	4.444050	-1.606478	2.303515
H	2.743673	-1.668377	1.844531
H	3.735007	-3.129258	1.783297
C	3.397430	0.292883	-2.979282
H	2.336844	0.058522	-3.095467
H	3.459223	1.331038	-2.636738
H	3.890313	0.228357	-3.953042
C	7.073525	-2.977458	-2.005264
H	7.510733	-3.573786	-1.199611
H	6.838664	-3.654400	-2.835606
H	7.838997	-2.281950	-2.368062
C	-3.082648	2.425643	-2.555774
O	-2.725358	1.056654	-2.291125
C	-2.451401	0.373752	-3.530660
C	-2.974216	1.287013	-4.637823
C	-2.746169	2.675229	-4.025538
H	-2.937070	-0.604356	-3.496764
H	-2.450664	1.136262	-5.585567
H	-4.044050	1.115142	-4.802627
H	-1.695320	2.966031	-4.131409
H	-3.367289	3.457728	-4.469308
H	-2.527873	3.066116	-1.867561
H	-4.157549	2.557090	-2.367515
H	-1.368451	0.219374	-3.619254
C	-1.277496	3.461599	1.173687
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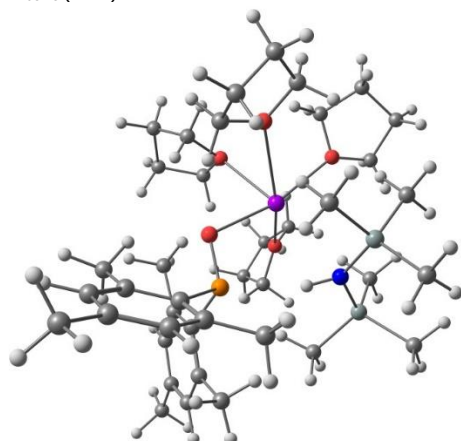
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H	-3.749949	2.494685	1.881815
H	-3.962677	4.475427	-0.358940
H	-4.043046	4.756767	1.382189
H	-1.642172	4.855845	-0.433991
H	-1.806091	5.588612	1.169581
H	-0.251658	3.332153	0.829593
H	-1.286068	3.484368	2.273166
H	-4.006830	2.122997	0.164284
C	-2.571893	-3.671669	-1.416000
O	-1.965661	-2.419013	-1.792653
C	-0.970117	-2.642622	-2.819734
C	-0.698849	-4.144671	-2.815559
C	-2.070532	-4.711162	-2.421081
H	-0.102730	-2.024284	-2.576176
H	-0.347022	-4.504603	-3.786290
H	0.051194	-4.394822	-2.059739
H	-2.731043	-4.746590	-3.294820
H	-2.020132	-5.714137	-1.988986
H	-3.660277	-3.554348	-1.428549
H	-2.263187	-3.918814	-0.393835
H	-1.380862	-2.325914	-3.788331

K-PI-4THF

E (BS1) = -3519.929536

E (BS2) = -3520.764074

G_{298.15} (BS2) = -3519.809704



N	-0.335282	-0.731246	2.527026
Si	-0.626097	0.607399	3.614338
Si	-0.853086	-2.394904	2.642779
C	-2.355269	1.309701	3.342878
H	-2.487673	1.608991	2.300040
H	-3.119329	0.563141	3.587453
H	-2.534566	2.186033	3.978401
C	-0.517464	0.089892	5.428516
H	-0.624250	0.965697	6.081310
H	-1.310281	-0.616015	5.700839
H	0.444860	-0.381406	5.657152
C	0.684029	1.915988	3.272924
H	0.815081	2.094216	2.202857
H	0.422143	2.869028	3.747560
H	1.654532	1.603929	3.673406
C	-0.230669	-3.264360	4.199894
H	-0.659229	-2.840620	5.113854
H	-0.486595	-4.331239	4.177087
H	0.860434	-3.186372	4.276363
C	-0.197504	-3.318283	1.143223
H	0.895639	-3.312875	1.105091
H	-0.525312	-4.364297	1.174893
H	-0.563814	-2.879647	0.213128
C	-2.741423	-2.453855	2.623634
H	-3.101978	-3.489416	2.660715
H	-3.173679	-1.924784	3.480777

H	-3.136594	-1.992224	1.712476
K	-1.515519	-0.095259	-0.340521
O	-4.180575	-0.242540	0.043577
C	-5.190554	-0.079586	1.044914
C	-6.065708	-1.342867	0.952077
H	-4.690581	0.049968	2.005455
H	-5.778143	0.824828	0.826822
C	-5.795859	-1.871378	-0.483555
H	-5.758588	-2.078998	1.699488
H	-7.119874	-1.109344	1.121934
C	-4.852331	-0.819187	-1.084279
H	-5.302742	-2.846239	-0.446770
H	-6.709475	-1.977715	-1.074199
H	-4.092970	-1.218218	-1.757710
H	-5.416465	-0.036583	-1.613694
C	5.148161	-1.869544	-1.995189
C	4.095903	-1.018375	-1.655013
C	3.487088	-1.113466	-0.374468
C	3.960404	-2.100630	0.518671
C	5.021901	-2.939478	0.138438
C	5.632807	-2.839690	-1.108169
H	5.601465	-1.778144	-2.980977
H	5.372149	-3.691929	0.842909
C	3.522305	2.042048	1.000545
C	2.631006	1.646575	-0.038552
C	2.128465	2.663471	-0.889453
C	2.508745	4.001428	-0.682044
C	3.383693	4.387121	0.329059
C	3.885460	3.379323	1.160474
H	2.101939	4.761358	-1.347710
H	4.568822	3.644012	1.965599
O	0.947962	-0.360048	-1.136480
P	1.949964	-0.110772	0.052042
H	0.494449	-0.584520	1.931009
C	1.213286	2.412876	-2.069402
H	0.649508	1.489073	-1.955875
H	0.537776	3.262584	-2.211346
H	1.801464	2.314832	-2.991534
C	4.092414	1.036759	1.969570
H	4.594517	1.538855	2.801654
H	3.304701	0.396889	2.378724
H	4.816279	0.373346	1.485860
C	3.780855	5.828294	0.528557
H	3.578102	6.161708	1.553301
H	4.853865	5.975675	0.353486
H	3.238499	6.489602	-0.153772
C	3.402417	-2.306315	1.911132
H	4.079556	-1.891077	2.667778
H	2.435798	-1.820983	2.038947
H	3.295176	-3.373896	2.131122
C	3.624326	-0.010610	-2.673439
H	2.533691	-0.031242	-2.735052
H	3.910696	1.005675	-2.382185
H	4.057035	-0.216122	-3.657372
C	6.770865	-3.746555	-1.504793
H	7.024115	-4.444632	-0.701602
H	6.520159	-4.334837	-2.395723
H	7.672415	-3.171255	-1.747573
C	-2.327554	2.249643	-3.189497
O	-2.309212	0.857588	-2.812868
C	-1.666080	0.084957	-3.845015
C	-1.745541	0.942990	-5.103514
C	-1.575184	2.352662	-4.520590
H	-2.189380	-0.870674	-3.921670
H	-0.978656	0.682478	-5.837918
H	-2.729136	0.837520	-5.575541
H	-0.514831	2.558191	-4.344546
H	-1.975248	3.141857	-5.162650
H	-1.864951	2.833152	-2.390891
H	-3.374321	2.565025	-3.293904
H	-0.624243	-0.108717	-3.557859
C	-1.142330	3.622012	0.629618
O	-1.970729	2.534575	0.200577
C	-3.299129	3.065505	0.077725
C	-3.135135	4.530230	-0.385913

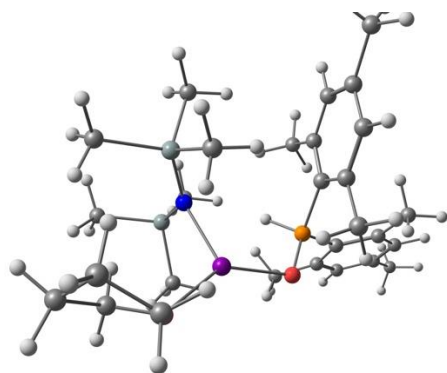
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H	-3.432758	4.655537	-1.429958
H	-3.754583	5.197741	0.218932
H	-1.109278	4.834630	-1.159804
H	-1.430989	5.768849	0.307877
H	-0.103320	3.343378	0.452459
H	-1.287972	3.797540	1.705779
H	-3.841119	2.427680	-0.621844
C	-2.572997	-3.691059	-1.573065
O	-1.759693	-2.518411	-1.777424
C	-0.578450	-2.870391	-2.536243
C	-0.382292	-4.363615	-2.301431
C	-1.833951	-4.864342	-2.234693
H	0.232149	-2.229882	-2.178972
H	0.195472	-4.836935	-3.100087
H	0.133133	-4.536253	-1.352504
H	-2.219917	-5.033847	-3.245597
H	-1.946734	-5.793121	-1.669263
H	-3.564512	-3.524540	-2.008648
H	-2.692723	-3.837611	-0.492810
H	-0.758781	-2.669745	-3.602120

Na-RI

E (BS1) = -2384.812135

E (BS2) = -2385.383582

G_{298.15} (BS2) = -2384.755973



N	-1.878353	-0.576132	-0.914229
Si	-1.772948	-2.086858	-1.652391
Si	-2.672878	0.850734	-1.332977
C	-1.354041	-3.405578	-0.336037
H	-0.507909	-3.104999	0.293019
H	-2.213753	-3.581205	0.324489
H	-1.091196	-4.371674	-0.785367
C	-3.366610	-2.712954	-2.493213
H	-3.255162	-3.743698	-2.855638
H	-4.218615	-2.696732	-1.802451
H	-3.634764	-2.091339	-3.356400
C	-0.435223	-2.221755	-3.005591
H	0.561026	-1.962059	-2.629819
H	-0.373975	-3.233399	-3.428475
H	-0.654940	-1.533609	-3.832162
C	-1.966615	1.749917	-2.857027
H	-2.012826	1.112716	-3.749486
H	-2.516850	2.673012	-3.084179
H	-0.917166	2.023136	-2.699975
C	-2.554851	2.103109	0.098251
H	-1.519268	2.421167	0.252280
H	-3.147922	3.004984	-0.101662
H	-2.922723	1.684559	1.044102
C	-4.539019	0.653447	-1.687004
H	-5.031035	1.623800	-1.836913
H	-4.716153	0.054878	-2.588622
H	-5.051911	0.148870	-0.859340
Na	-1.497380	-0.758864	1.311824
O	-3.427123	-1.119533	2.451710
C	-4.380511	-1.783982	1.571754
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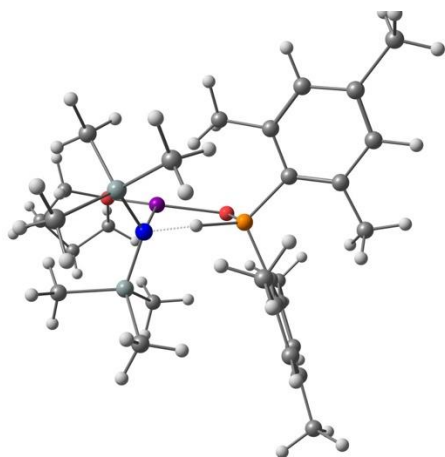
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C	-5.330430	0.274535	2.337273
H	-6.345427	-1.078780	0.920447
H	-6.292635	-1.656062	2.596190
C	-4.090974	-0.049477	3.162699
H	-5.067598	0.928839	1.500207
H	-6.109662	0.760763	2.929525
H	-3.387501	0.784109	3.254909
H	-4.358510	-0.395684	4.169844
C	0.821807	3.778725	0.739180
C	0.944274	2.434881	1.109568
C	1.314848	1.492365	0.125241
C	1.551307	1.912488	-1.207240
C	1.409970	3.264247	-1.525691
C	1.040853	4.213985	-0.568371
H	0.542192	4.503751	1.499352
H	1.592932	3.582014	-2.548923
C	4.310840	0.066116	0.882454
C	3.238863	-0.782633	0.518321
C	3.503395	-2.125883	0.137990
C	4.824371	-2.572352	0.085369
C	5.898707	-1.737086	0.404471
C	5.617175	-0.432528	0.811442
H	5.017293	-3.602403	-0.203723
H	6.437999	0.222011	1.092801
O	0.689682	-0.748178	1.716366
P	1.486446	-0.276257	0.501957
H	1.021247	-0.866897	-0.678926
C	2.402235	-3.108684	-0.185796
H	1.873274	-2.852258	-1.109662
H	2.815051	-4.112133	-0.311666
H	1.656572	-3.150773	0.612952
C	4.137620	1.487362	1.362680
H	5.082258	1.856682	1.769548
H	3.836723	2.159095	0.554076
H	3.384580	1.566587	2.149660
C	7.317067	-2.233934	0.305790
H	7.658589	-2.228320	-0.736917
H	8.002228	-1.605332	0.881226
H	7.404394	-3.263377	0.667475
C	1.937221	0.952333	-2.307149
H	2.217586	1.503114	-3.208096
H	2.783226	0.315045	-2.030833
H	1.098026	0.297936	-2.566452
C	0.647179	2.082244	2.548994
H	-0.394611	1.757213	2.658883
H	1.268774	1.273718	2.931745
H	0.780304	2.963596	3.182357
C	0.861954	5.659960	-0.948812
H	1.638527	5.988190	-1.646968
H	-0.104281	5.810709	-1.446158
H	0.887173	6.311133	-0.070703

Na-TS

E (BS1) = -2384.796994

E (BS2) = -2385.361701

G_{298.15} (BS2) = -2384.737246



N	1.366401	-0.306277	1.076663
Si	1.468561	-1.590131	2.222372
Si	2.147764	1.226490	1.187617
C	2.351170	-3.105552	1.485924
H	1.904867	-3.440040	0.541821
H	3.406668	-2.880216	1.291284
H	2.322266	-3.957769	2.177145
C	2.417371	-1.180761	3.814308
H	2.298438	-1.996508	4.539227
H	3.490846	-1.055769	3.637563
H	2.048079	-0.264873	4.289903
C	-0.255894	-2.149222	2.788526
H	-0.967584	-2.275434	1.967309
H	-0.192712	-3.106956	3.320696
H	-0.688334	-1.420118	3.483637
C	1.400090	2.409295	2.465985
H	1.308736	1.934899	3.450001
H	2.029164	3.300783	2.586269
H	0.404246	2.748726	2.164005
C	2.036151	2.120828	-0.486381
H	1.006535	2.209576	-0.844521
H	2.433330	3.138217	-0.379931
H	2.630176	1.642720	-1.275680
C	4.001996	1.107965	1.582715
H	4.498864	2.066050	1.382197
H	4.181892	0.862295	2.634335
H	4.499296	0.343943	0.975210
Na	1.703385	-0.794548	-1.239384
O	3.728903	-1.119809	-2.145644
C	4.790726	-1.603938	-1.277586
C	5.999005	-0.683069	-1.509151
H	4.421948	-1.554368	-0.249316
H	5.001741	-2.649367	-1.524151
C	5.380595	0.545826	-2.194529
H	6.508156	-0.436866	-0.574369
H	6.722602	-1.163085	-2.175005
C	4.261407	-0.088371	-3.007772
H	4.960415	1.232629	-1.452828
H	6.092526	1.094407	-2.816027
H	3.442581	0.591518	-3.260316
H	4.641543	-0.542904	-3.932322
C	-2.038383	3.961190	-1.052229
C	-1.741199	2.637727	-1.401515
C	-1.682048	1.658319	-0.385048
C	-1.953163	2.027162	0.955709
C	-2.263021	3.355819	1.254581
C	-2.296180	4.344049	0.265254
H	-2.080999	4.710625	-1.839280
H	-2.479629	3.625204	2.285803
C	-3.897885	-0.889318	-0.630846
C	-2.522069	-1.225326	-0.649400
C	-2.155827	-2.599698	-0.620665
C	-3.138838	-3.584126	-0.517113
C	-4.497376	-3.262746	-0.450221
C	-4.848391	-1.916039	-0.522550
H	-2.834941	-4.628083	-0.492108

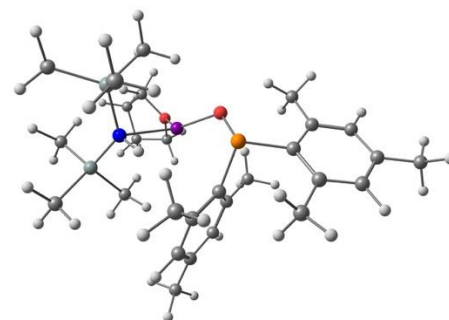
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O	-0.295640	-0.207605	-1.996811
P	-1.091865	-0.054977	-0.666939
H	0.041087	-0.248943	0.477264
C	-0.719562	-3.055443	-0.745416
H	-0.055121	-2.480275	-0.099511
H	-0.621843	-4.105869	-0.460230
H	-0.362002	-2.943228	-1.774521
C	-4.437201	0.517167	-0.755338
H	-5.515902	0.483095	-0.930948
H	-4.266561	1.112677	0.145494
H	-3.978806	1.057800	-1.585254
C	-5.540643	-4.340601	-0.307117
H	-5.509819	-4.786249	0.694881
H	-6.547998	-3.945195	-0.464457
H	-5.375462	-5.152775	-1.023485
C	-1.942545	1.011753	2.073565
H	-2.232739	1.478128	3.018727
H	-2.635142	0.185562	1.880392
H	-0.948837	0.575335	2.202114
C	-1.555083	2.306624	-2.861933
H	-0.627366	1.759127	-3.033989
H	-2.361357	1.653346	-3.218307
H	-1.571145	3.217946	-3.466267
C	-2.585527	5.780203	0.618868
H	-3.377437	5.854708	1.371420
H	-1.696202	6.267332	1.038572
H	-2.891338	6.354795	-0.260231

Na-PI

E (BS1) = -2384.824830

E (BS2) = -2385.386296

G_{298.15} (BS2) = -2384.758460



N	2.224518	0.516366	1.111473
Si	2.440873	-0.184533	2.726527
Si	3.353417	1.328719	0.025139
C	1.919792	-1.993368	2.707622
H	0.871956	-2.068933	2.392199
H	2.540559	-2.598199	2.035792
H	2.006808	-2.427984	3.710889
C	4.233062	-0.064386	3.287483
H	4.304329	-0.419751	4.322960
H	4.901586	-0.685899	2.684294
H	4.609018	0.963999	3.265443
C	1.327090	0.746745	3.921597
H	0.274277	0.643902	3.634717
H	1.431178	0.347637	4.937790
H	1.570142	1.814738	3.955284
C	3.540632	3.141399	0.499857
H	3.933662	3.248182	1.517595
H	4.220303	3.669465	-0.179772
H	2.570712	3.651819	0.461502
C	2.622707	1.218331	-1.705892
H	1.582896	1.555129	-1.723319
H	3.184569	1.846918	-2.406960
H	2.659797	0.194476	-2.091913
C	5.025560	0.467460	0.028180
H	5.594385	0.796055	-0.850242
H	5.622674	0.702494	0.913166
H	4.924885	-0.620951	-0.035518

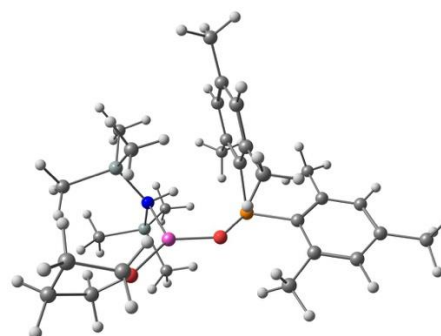
Na	0.995728	-1.150580	-0.169599
O	2.269058	-2.534523	-1.390298
C	3.428152	-3.147097	-0.763734
C	4.506899	-3.260478	-1.854721
H	3.732463	-2.499111	0.063291
H	3.141246	-4.122321	-0.356311
C	3.985939	-2.340563	-2.971885
H	5.492633	-2.964820	-1.487021
H	4.574262	-4.291232	-2.215107
C	2.478633	-2.491829	-2.817586
H	4.280102	-1.301914	-2.787778
H	4.337749	-2.632039	-3.964478
H	1.894175	-1.657401	-3.214490
H	2.119146	-3.425194	-3.272123
C	-0.932694	1.593093	-2.667443
C	-1.334370	0.719473	-1.648835
C	-1.310075	1.144713	-0.295716
C	-0.825158	2.447471	-0.013082
C	-0.430735	3.290954	-1.060927
C	-0.487232	2.889042	-2.397200
H	-0.967784	1.248170	-3.699359
H	-0.066892	4.288356	-0.823267
C	-4.507195	0.532989	0.546686
C	-3.519189	-0.490866	0.572099
C	-3.948368	-1.825582	0.365090
C	-5.303787	-2.087610	0.104445
C	-6.266851	-1.083871	0.039602
C	-5.841480	0.227776	0.271753
H	-5.607916	-3.120902	-0.054238
H	-6.570365	1.036246	0.250891
O	-0.818916	-1.239337	0.959084
P	-1.788554	0.000376	1.141784
H	1.327659	1.005049	1.085283
C	-3.029640	-3.030113	0.371680
H	-2.168671	-2.887191	1.021650
H	-3.587416	-3.925021	0.667252
H	-2.630043	-3.219817	-0.633740
C	-4.161401	1.976458	0.823313
H	-5.068280	2.568828	0.975143
H	-3.540941	2.067723	1.721547
H	-3.596962	2.429060	0.002158
C	-7.715038	-1.391729	-0.248643
H	-8.365101	-1.066070	0.572658
H	-8.061885	-0.874924	-1.151828
H	-7.873245	-2.464317	-0.395268
C	-0.730151	2.999687	1.392828
H	-0.102166	3.895589	1.408464
H	-1.714798	3.281909	1.780976
H	-0.316693	2.276461	2.097775
C	-1.796160	-0.663397	-2.050534
H	-1.535309	-1.403014	-1.292879
H	-2.884778	-0.698014	-2.166499
H	-1.351990	-0.954558	-3.008049
C	-0.009576	3.794667	-3.503113
H	-0.154595	4.849187	-3.249169
H	1.062448	3.648878	-3.689833
H	-0.533511	3.591553	-4.442182

Li-Ri

E (BS1) = -2230.078785

E (BS2) = -2230.628156

G_{298.15} (BS2) = -2229.997265



N	2.213742	0.270694	0.879355
Si	2.690341	-0.322581	2.484758
Si	3.126101	1.248109	-0.288618
C	1.829244	-1.979669	2.735576
H	0.749909	-1.891963	2.564914
H	2.219579	-2.750397	2.059418
H	1.976981	-2.343051	3.759534
C	4.551817	-0.552272	2.589083
H	4.793694	-1.009962	3.556221
H	4.944775	-1.209323	1.807910
H	5.087455	0.400941	2.535039
C	2.138555	0.878800	3.822849
H	1.047574	0.945093	3.880701
H	2.501784	0.550393	4.804316
H	2.529755	1.886285	3.641818
C	3.280183	3.022568	0.322226
H	3.800229	3.071794	1.285895
H	3.840761	3.640113	-0.390179
H	2.291416	3.477379	0.446307
C	2.153074	1.213675	-1.894105
H	1.134355	1.580438	-1.749970
H	2.631917	1.846025	-2.651502
H	2.088477	0.200396	-2.305367
C	4.837203	0.527951	-0.586853
H	5.264104	1.005467	-1.477564
H	5.525986	0.708063	0.242628
H	4.807102	-0.548348	-0.776547
Li	1.242092	-1.345171	-0.019167
O	2.234597	-2.648616	-0.973703
C	3.552405	-3.138652	-0.615629
C	4.350470	-3.241515	-1.929175
H	3.982467	-2.423659	0.088960
H	3.447547	-4.106702	-0.115629
C	3.477533	-2.487195	-2.948013
H	5.350320	-2.812013	-1.832207
H	4.459473	-4.288882	-2.224706
C	2.077045	-2.737693	-2.407797
H	3.697037	-1.414966	-2.931621
H	3.603398	-2.852812	-3.969922
H	1.330935	-1.996868	-2.704665
H	1.712111	-3.738228	-2.673502
C	-1.295421	2.405601	-2.369640
C	-1.533782	1.256555	-1.613031
C	-1.294108	1.266177	-0.212090
C	-0.793829	2.452059	0.371776
C	-0.551784	3.582234	-0.427515
C	-0.801092	3.584324	-1.796723
H	-1.485741	2.377478	-3.441015
H	-0.162667	4.482567	0.043927
C	-4.241239	0.156326	0.929487
C	-3.241699	-0.749008	0.485010
C	-3.659588	-2.007093	-0.019802
C	-5.029730	-2.290334	-0.118623
C	-6.017590	-1.385510	0.270867
C	-5.595793	-0.167082	0.806455
H	-5.330070	-3.259043	-0.513801
H	-6.338543	0.550820	1.149572
O	-0.520133	-1.330052	0.070241
P	-1.454761	-0.297444	0.836023
H	1.280948	0.684766	0.956973

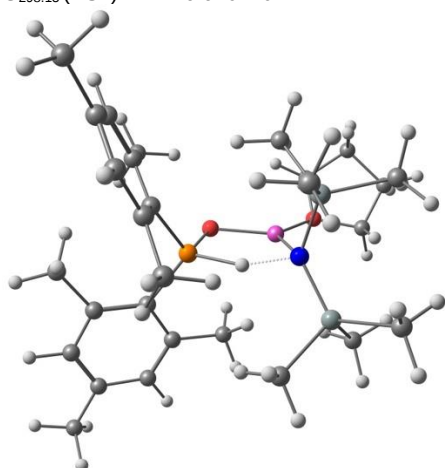
C	-2.712650	-3.093330	-0.484960
H	-1.867938	-3.223838	0.190622
H	-3.253727	-4.040288	-0.581230
H	-2.280633	-2.855995	-1.462831
C	-3.892075	1.486931	1.553906
H	-4.760507	1.909644	2.067559
H	-3.081800	1.386739	2.284079
H	-3.556061	2.212935	0.807150
C	-7.482760	-1.706413	0.113576
H	-7.656768	-2.786914	0.101374
H	-8.077523	-1.274010	0.924966
H	-7.879993	-1.302376	-0.826950
C	-0.519804	2.599153	1.852633
H	0.415467	3.141769	2.024336
H	-1.318936	3.172806	2.338514
H	-0.466502	1.634113	2.355532
C	-2.028736	0.023591	-2.328599
H	-1.509847	-0.860911	-1.954784
H	-3.099613	-0.132147	-2.161651
H	-1.866898	0.112291	-3.407286
C	-0.515233	4.794692	-2.648582
H	-0.268860	5.666156	-2.035224
H	0.330796	4.610781	-3.322511
H	-1.374381	5.052470	-3.278045

Li-TS

E (BS1) = -2230.049125

E (BS2) = -2230.600806

G_{298.15} (BS2) = -2229.970220



N	1.594075	-0.295299	0.969402
Si	1.777965	-1.546409	2.152106
Si	2.357356	1.259126	1.026713
C	2.506171	-3.128429	1.392414
H	2.046040	-3.392460	0.434217
H	3.582182	-3.013851	1.218932
H	2.375143	-3.984273	2.066805
C	2.913030	-1.123640	3.611752
H	2.844443	-1.914997	4.369490
H	3.963764	-1.050867	3.312650
H	2.636183	-0.181621	4.097979
C	0.099867	-1.981640	2.926788
H	-0.693594	-2.147658	2.191841
H	0.181622	-2.890961	3.535510
H	-0.235182	-1.175387	3.590012
C	1.713037	2.393162	2.401813
H	1.731873	1.902369	3.381487
H	2.324990	3.301378	2.475553
H	0.683478	2.708631	2.203928
C	2.052240	2.185707	-0.599723
H	0.994781	2.418140	-0.747079
H	2.599484	3.136807	-0.578900
H	2.399193	1.641246	-1.484866
C	4.242710	1.169067	1.223354
H	4.682580	2.165181	1.085010

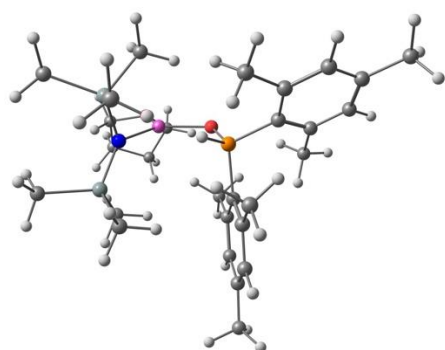
H	4.542814	0.815915	2.214915
H	4.699684	0.504294	0.482115
Li	1.554671	-0.702643	-1.028092
O	3.024394	-1.266622	-2.073607
C	4.259139	-1.696032	-1.432622
C	5.398974	-0.949966	-2.144183
H	4.176873	-1.436227	-0.375994
H	4.343015	-2.782768	-1.524936
C	4.675163	0.179823	-2.895079
H	6.144101	-0.578199	-1.436878
H	5.904073	-1.612627	-2.853341
C	3.348873	-0.479386	-3.244513
H	4.504319	1.036135	-2.234791
H	5.217836	0.522808	-3.779305
H	2.522118	0.214552	-3.414019
H	3.442386	-1.143073	-4.113539
C	-1.883509	3.893174	-1.142946
C	-1.613625	2.543325	-1.395466
C	-1.549396	1.644602	-0.307941
C	-1.786985	2.114534	1.005681
C	-2.063352	3.468812	1.209693
C	-2.101615	4.379037	0.148768
H	-1.933930	4.581597	-1.983429
H	-2.253380	3.819855	2.221265
C	-3.802101	-0.878111	-0.476593
C	-2.431052	-1.237833	-0.485916
C	-2.087283	-2.618546	-0.455963
C	-3.088938	-3.586453	-0.377122
C	-4.442684	-3.243799	-0.331008
C	-4.769914	-1.890599	-0.392050
H	-2.802234	-4.635272	-0.352549
H	-5.818401	-1.603096	-0.383818
O	-0.110524	-0.307934	-1.748948
P	-0.986254	-0.088510	-0.471559
H	0.181464	-0.234021	0.628754
C	-0.657434	-3.098853	-0.543313
H	0.003987	-2.525688	0.105430
H	-0.584936	-4.146904	-0.241871
H	-0.269434	-3.003793	-1.562450
C	-4.322598	0.537132	-0.583828
H	-5.407098	0.519237	-0.720999
H	-4.111426	1.131347	0.308850
H	-3.886814	1.070203	-1.430635
C	-5.505644	-4.305664	-0.216956
H	-5.489931	-4.771955	0.775917
H	-6.504766	-3.889804	-0.373846
H	-5.348880	-5.106054	-0.948371
C	-1.780540	1.180990	2.193641
H	-2.074348	1.713947	3.101840
H	-2.473057	0.343356	2.057420
H	-0.788329	0.753006	2.359585
C	-1.441606	2.093678	-2.824784
H	-0.455392	1.654018	-2.986661
H	-2.167064	1.313971	-3.083523
H	-1.586381	2.933285	-3.510257
C	-2.354247	5.844003	0.396060
H	-3.052550	5.995020	1.225304
H	-1.423235	6.362578	0.658548
H	-2.762315	6.335185	-0.492236

Li-PI

E (BS1) = -2230.068917

E (BS2) = -2230.627883

G_{298.15} (BS2) = -2229.996602



N	-2.223207	-0.918186	-0.713547
Si	-1.994958	-2.486423	-1.311924
Si	-2.883147	0.427679	-1.502278
C	-1.122103	-3.534950	0.021271
H	-0.205553	-3.067712	0.399668
H	-1.786023	-3.690849	0.882741
H	-0.852451	-4.528101	-0.359074
C	-3.594899	-3.441330	-1.706700
H	-3.387295	-4.478960	-2.000631
H	-4.258204	-3.472499	-0.833072
H	-4.155347	-2.973849	-2.524705
C	-0.950398	-2.574567	-2.903816
H	-0.044336	-1.964424	-2.822918
H	-0.643226	-3.599055	-3.151250
H	-1.522348	-2.191124	-3.758475
C	-1.736777	1.198510	-2.813070
H	-1.462118	0.465190	-3.581289
H	-2.209589	2.048081	-3.323888
H	-0.810814	1.565217	-2.358661
C	-3.263367	1.817897	-0.261886
H	-2.354682	2.165732	0.240691
H	-3.709408	2.688281	-0.760130
H	-3.969207	1.483871	0.507757
C	-4.521164	0.075171	-2.412765
H	-4.970173	0.993231	-2.814477
H	-4.368865	-0.608353	-3.257269
H	-5.258029	-0.390213	-1.746406
Li	-1.524789	-0.882666	1.062319
O	-2.636742	-1.062448	2.607279
C	-4.065626	-1.069094	2.339572
C	-4.656907	0.139655	3.094425
H	-4.174532	-1.009919	1.254771
H	-4.484945	-2.018017	2.690913
C	-3.419955	0.883823	3.634500
H	-5.265062	0.769227	2.440642
H	-5.290169	-0.199600	3.919137
C	-2.401102	-0.240419	3.768268
H	-3.064393	1.619569	2.906658
H	-3.609489	1.395125	4.581681
H	-1.357454	0.077815	3.736521
H	-2.570624	-0.832398	4.678110
C	0.470117	3.888137	0.194148
C	0.509070	2.561777	0.638578
C	1.107949	1.586376	-0.196584
C	1.642946	1.966669	-1.453579
C	1.581961	3.306405	-1.843657
C	0.995427	4.283305	-1.037254
H	0.010010	4.635240	0.835438
H	1.994770	3.588454	-2.808700
C	3.729173	-0.139901	1.349167
C	2.870162	-0.752019	0.403981
C	3.340000	-1.836558	-0.377783
C	4.665769	-2.254294	-0.219063
C	5.535402	-1.644501	0.686813
C	5.043094	-0.595556	1.468508
H	5.024349	-3.085867	-0.819925
H	5.696366	-0.122084	2.196949
O	0.281039	-0.564626	1.435340
P	1.149364	-0.183090	0.236961
H	0.713858	-0.789632	-0.946667

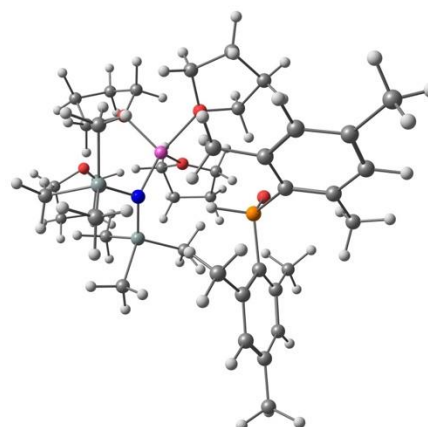
C	2.486125	-2.574195	-1.383505
H	2.214023	-1.938405	-2.231416
H	3.034606	-3.431848	-1.779730
H	1.558056	-2.950883	-0.946420
C	3.267757	0.975254	2.253045
H	4.051539	1.239135	2.966726
H	3.010449	1.876229	1.687946
H	2.381568	0.678326	2.821250
C	6.967610	-2.093306	0.811378
H	7.630297	-1.441164	0.228534
H	7.308615	-2.054431	1.850541
H	7.100387	-3.113417	0.440481
C	2.246521	0.973719	-2.417092
H	2.631218	1.489364	-3.299711
H	3.071427	0.411364	-1.971288
H	1.498843	0.249500	-2.760597
C	-0.108191	2.267833	1.986250
H	-0.949423	1.580542	1.898821
H	0.600773	1.808583	2.676942
H	-0.472005	3.195126	2.436077
C	0.900026	5.714132	-1.497161
H	1.732058	5.978267	-2.156499
H	-0.027608	5.877558	-2.060059
H	0.893890	6.406603	-0.650326

Li-RI-4THF

E (BS1) = -2927.548875

E (BS2) = -2928.352046

G_{298.15} (BS2) = -2927.386314



N	0.895081	0.173449	1.371395
Si	1.047295	-0.417331	2.963338
Si	1.175983	1.822872	1.036600
C	-0.332101	0.080195	4.189660
H	-0.423295	1.166790	4.291192
H	-1.314117	-0.305760	3.896131
H	-0.113843	-0.323779	5.187986
C	1.040550	-2.319625	3.019563
H	1.723580	-2.751980	2.283243
H	1.335449	-2.683062	4.012512
H	0.038128	-2.711083	2.816298
C	2.633327	0.144532	3.875945
H	2.596038	1.219352	4.092189
H	2.748113	-0.373106	4.837746
H	3.541522	-0.035638	3.292051
C	0.478925	3.049980	2.325586
H	0.937620	2.935880	3.314610
H	0.658356	4.084237	2.001240
H	-0.604813	2.933224	2.445428
C	0.389881	2.399869	-0.595064
H	0.283604	1.585413	-1.311206
H	-0.607189	2.810821	-0.411182
H	0.982075	3.195460	-1.063986
C	3.029654	2.274927	0.935430
H	3.171294	3.318014	0.622269
H	3.508583	2.157718	1.914282
H	3.571256	1.638107	0.229814

Li	1.341165	-1.121826	-0.094128
O	0.149602	-2.701596	-0.664540
C	0.224555	-4.041540	-0.148323
C	-1.111828	-4.700811	-0.524831
H	1.063596	-4.564158	-0.625891
H	0.409706	-3.977892	0.922670
C	-1.611099	-3.862445	-1.730125
H	-0.971176	-5.755652	-0.774811
H	-1.822302	-4.645079	0.303189
C	-0.503630	-2.821546	-1.943846
H	-1.766894	-4.466290	-2.627896
H	-2.554718	-3.367339	-1.489386
H	0.229089	-3.168676	-2.686381
H	-0.880733	-1.837240	-2.214972
C	6.522607	1.083950	0.783727
O	6.105447	0.379546	-0.394250
C	6.593066	1.128985	-1.507577
C	6.349023	2.587648	-1.122505
C	6.621658	2.580395	0.399063
H	6.052948	0.799932	-2.398480
H	6.991884	3.281962	-1.670193
H	5.306879	2.851558	-1.322915
H	7.617664	2.970194	0.626912
H	5.891240	3.185257	0.940602
H	7.496669	0.698958	1.118723
H	5.784948	0.884176	1.564540
H	7.667914	0.935462	-1.658265
C	3.268362	0.012649	-2.160694
O	1.920199	-0.413819	-1.916180
C	1.182301	-0.109218	-3.117750
C	1.824398	1.167692	-3.702940
C	3.116255	1.355848	-2.871803
H	0.134765	0.008942	-2.840892
H	2.042795	1.035896	-4.766182
H	1.160699	2.029473	-3.602051
H	3.986480	1.598950	-3.486707
H	2.986818	2.150494	-2.133143
H	3.770408	-0.720395	-2.810223
H	3.796468	0.058235	-1.210476
H	1.282497	-0.951803	-3.815634
C	4.089193	-1.802604	1.085089
O	3.006007	-2.219503	0.215198
C	3.513749	-3.092100	-0.816941
C	5.024655	-2.882560	-0.825438
C	5.312008	-2.613029	0.656833
H	3.016672	-2.826413	-1.752468
H	5.559749	-3.749549	-1.222244
H	5.290624	-2.002128	-1.415914
H	5.363511	-3.554500	1.215049
H	6.239464	-2.059296	0.813770
H	3.791159	-1.987730	2.118468
H	4.244245	-0.730497	0.944462
H	3.263479	-4.129997	-0.563157
C	-3.689202	4.236557	-1.026855
C	-3.210735	2.961074	-1.350170
C	-3.125895	1.986641	-0.325074
C	-3.482285	2.336032	1.001196
C	-3.948688	3.625445	1.270590
C	-4.070980	4.589417	0.268386
H	-3.751736	4.980963	-1.816656
H	-4.214535	3.881344	2.293226
C	-4.995796	-0.880607	-0.983415
C	-3.792905	-0.900087	-0.235873
C	-3.585633	-1.915221	0.728432
C	-4.593049	-2.863122	0.942351
C	-5.794464	-2.844163	0.231656
C	-5.972222	-1.847208	-0.731618
H	-4.427329	-3.640310	1.684261
H	-6.891956	-1.825128	-1.311057
O	-1.898903	0.085353	-2.025537
P	-2.473215	0.302097	-0.638285
H	-1.522998	0.148066	0.388946
C	-2.317599	-2.035191	1.536413
H	-2.192360	-1.192959	2.219335
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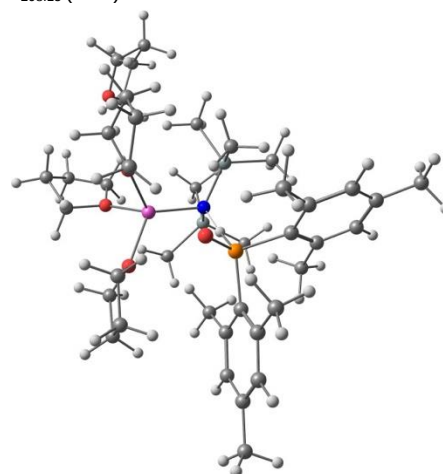
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H	-5.324007	1.150406	-1.662445
H	-4.438412	0.135861	-2.799501
C	-6.875192	-3.857827	0.504421
H	-7.608693	-3.462392	1.218573
H	-7.420070	-4.116213	-0.408847
H	-6.463248	-4.775920	0.933307
C	-3.344671	1.376099	2.157085
H	-3.616769	1.866574	3.094607
H	-3.985967	0.497521	2.038738
H	-2.315435	1.021345	2.259103
C	-2.776110	2.728444	-2.778432
H	-2.915772	3.644383	-3.359204
H	-1.725658	2.435653	-2.828439
H	-3.340367	1.927557	-3.259790
C	-4.607804	5.963506	0.574252
H	-5.703376	5.977861	0.510289
H	-4.338000	6.280938	1.586119
H	-4.229688	6.706826	-0.133744

Li-TS-4THF

E (BS1) = -2927.533139

E (BS2) = -2928.328606

G_{298.15} (BS2) = -2927.361565



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Si	0.870191	-0.072456	2.748803
Si	1.081945	1.938637	0.574263
C	-0.336476	0.600820	4.058338
H	-0.482414	1.682071	3.970138
H	-1.322311	0.128165	4.036101
H	0.087804	0.408087	5.052913
C	0.918362	-1.949480	3.034660
H	1.442030	-2.475052	2.232860
H	1.450260	-2.153740	3.972700
H	-0.079672	-2.383159	3.132673
C	2.548770	0.568583	3.386577
H	2.543708	1.655367	3.522009
H	2.748946	0.122982	4.369587
H	3.387882	0.319985	2.733057
C	0.471059	3.336913	1.708810
H	0.856896	3.256359	2.730965
H	0.790032	4.310972	1.314503
H	-0.623524	3.351138	1.760875
C	0.456859	2.378735	-1.159209
H	0.043239	1.520697	-1.688106
H	-0.325631	3.140183	-1.101505
H	1.275416	2.793842	-1.756821
C	2.972389	2.140387	0.499489
H	3.206450	3.023288	-0.109116
H	3.414218	2.301459	1.485965
H	3.479182	1.283720	0.047885

Li	1.116835	-1.166662	-0.236543
O	-0.102108	-2.777911	-0.534188
C	-0.128184	-4.034827	0.164034
C	-1.492280	-4.663500	-0.165223
H	0.688900	-4.668237	-0.204642
H	0.029677	-3.835687	1.222599
C	-1.927425	-3.944943	-1.467994
H	-1.400754	-5.745470	-0.292384
H	-2.213830	-4.479679	0.633456
C	-0.742916	-3.031713	-1.802307
H	-2.137845	-4.641129	-2.284210
H	-2.823881	-3.346175	-1.292451
H	-0.026016	-3.536128	-2.466789
H	-1.040338	-2.065567	-2.204563
C	6.414415	0.644616	1.076848
O	5.945475	0.356306	-0.253840
C	6.249545	1.461589	-1.124199
C	6.662253	2.620446	-0.217270
C	7.310787	1.877873	0.958179
H	5.366671	1.684198	-1.729862
H	7.335200	3.323385	-0.715325
H	5.777082	3.167667	0.122630
H	8.335184	1.583499	0.703971
H	7.339853	2.462550	1.881378
H	6.939740	-0.235625	1.462386
H	5.553168	0.844892	1.728654
H	7.068725	1.173126	-1.798944
C	3.190215	-0.374828	-2.364289
O	1.818554	-0.650434	-2.044922
C	1.089378	-0.489046	-3.280212
C	1.786830	0.661984	-4.032636
C	3.129416	0.846720	-3.281560
H	0.052095	-0.293336	-3.011550
H	1.939611	0.401400	-5.083361
H	1.188597	1.575136	-3.996782
H	3.991287	0.895843	-3.952100
H	3.111723	1.760288	-2.681985
H	3.620785	-1.238250	-2.892583
H	3.739508	-0.221382	-1.437006
H	1.158112	-1.425862	-3.850803
C	3.886105	-1.874183	1.047989
O	2.749417	-2.275049	0.239637
C	3.153075	-3.301404	-0.695307
C	4.675162	-3.229416	-0.749900
C	5.020065	-2.834632	0.691383
H	2.656982	-3.099497	-1.646530
H	5.122337	-4.177508	-1.060032
H	5.000902	-2.446360	-1.440109
H	4.998933	-3.714240	1.344086
H	5.998544	-2.358687	0.781771
H	3.597333	-1.924018	2.099469
H	4.138035	-0.844567	0.789145
H	2.822036	-4.277173	-0.319613
C	-3.369266	4.209562	-1.190975
C	-2.940605	2.891315	-1.418674
C	-2.863349	1.989671	-0.331516
C	-3.227879	2.459603	0.958951
C	-3.652660	3.776106	1.137623
C	-3.729474	4.676450	0.069576
H	-3.416041	4.888673	-2.040270
H	-3.922178	4.108618	2.137976
C	-4.765562	-0.790933	-0.842423
C	-3.610144	-0.807877	-0.020508
C	-3.533530	-1.754865	1.023008
C	-4.606147	-2.625141	1.257163
C	-5.759814	-2.599207	0.473781
C	-5.812374	-1.679155	-0.577672
H	-4.527417	-3.347279	2.066768
H	-6.691114	-1.656666	-1.218873
O	-1.695106	-0.096305	-1.865614
P	-2.148302	0.268951	-0.434413
H	-0.831688	0.253115	0.575875
C	-2.315195	-1.878259	1.898442
H	-2.256425	-1.061365	2.620963
H	-2.342360	-2.812905	2.464752

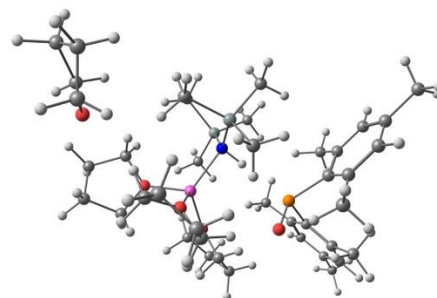
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H	-5.078055	1.171931	-1.694495
H	-3.992771	0.139535	-2.619706
C	-6.916143	-3.525862	0.750200
H	-7.716965	-3.005478	1.290892
H	-7.352398	-3.908418	-0.178442
H	-6.607769	-4.379081	1.361480
C	-3.164422	1.564446	2.169317
H	-3.271011	2.145248	3.089092
H	-3.954403	0.806251	2.153188
H	-2.210624	1.038374	2.216930
C	-2.609561	2.542629	-2.854403
H	-2.006560	3.338970	-3.304311
H	-2.081812	1.595294	-2.931586
H	-3.531932	2.470082	-3.444881
C	-4.180260	6.098168	0.288762
H	-5.200135	6.134563	0.690131
H	-3.535237	6.611800	1.011472
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Li-PI-4THF

E (BS1) = -2927.555875

E (BS2) = -2928.349987

G_{298.15} (BS2) = -2927.381205



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Si	1.198585	1.915741	0.721827
C	-0.427616	0.380894	4.042154
H	-0.575428	1.460583	3.949201
H	-1.389097	-0.107577	3.862327
H	-0.147077	0.171658	5.082608
C	0.903955	-2.140520	2.987191
H	1.679388	-2.587425	2.360154
H	1.070519	-2.466811	4.021173
H	-0.063610	-2.537762	2.667366
C	2.563613	0.376362	3.587268
H	2.532791	1.455876	3.767002
H	2.747958	-0.107465	4.554450
H	3.419990	0.166440	2.943495
C	0.540351	3.203843	1.938447
H	0.938073	3.087359	2.951872
H	0.811180	4.209693	1.592207
H	-0.553722	3.163308	1.991669
C	0.473460	2.321685	-0.966374
H	0.019672	1.456555	-1.451281
H	-0.307900	3.079609	-0.859508
H	1.244433	2.730249	-1.627445
C	3.075981	2.079811	0.657356
H	3.324036	3.011409	0.133876
H	3.524533	2.139230	1.652513
H	3.558566	1.260462	0.119201
Li	1.350178	-1.285067	-0.183519
O	0.117021	-2.833588	-0.434981
C	0.301006	-4.172678	0.056207
C	-1.085513	-4.819717	-0.031542
H	1.015404	-4.698546	-0.591599
H	0.709793	-4.113220	1.063739
C	-1.772331	-4.051519	-1.191333
H	-1.010040	-5.894210	-0.218456

H	-1.634080	-4.678367	0.902708
C	-0.751012	-2.973546	-1.586338
H	-2.002461	-4.700567	-2.040393
H	-2.705392	-3.594379	-0.856025
H	-0.141202	-3.306410	-2.438311
H	-1.187188	-1.993900	-1.794545
C	6.627332	0.771358	0.778793
O	5.971923	0.515439	-0.477748
C	6.146901	1.645913	-1.352415
C	6.657430	2.788753	-0.476458
C	7.474041	2.029076	0.576486
H	5.190568	1.867342	-1.833153
H	7.242859	3.519619	-1.040361
H	5.817371	3.307619	-0.003019
H	8.459309	1.765895	0.175978
H	7.618739	2.587986	1.504687
H	7.222759	-0.106100	1.051707
H	5.866580	0.927210	1.555948
H	6.875914	1.387573	-2.134130
C	3.182263	-0.311301	-2.391583
O	1.850358	-0.633675	-1.963105
C	1.011814	-0.498497	-3.134452
C	1.610130	0.672043	-3.939567
C	3.003217	0.904013	-3.301304
H	-0.011249	-0.333546	-2.787686
H	1.685835	0.413515	-4.999058
H	0.986779	1.565096	-3.856573
H	3.805208	0.980986	-4.039919
H	3.003828	1.819031	-2.703243
H	3.599351	-1.160798	-2.952009
H	3.797157	-0.137451	-1.509655
H	1.067530	-1.433962	-3.707924
C	4.121100	-1.836892	1.111048
O	3.017378	-2.263001	0.267842
C	3.494391	-3.224210	-0.706191
C	5.005470	-3.037355	-0.747647
C	5.310794	-2.712084	0.719316
H	2.985752	-3.022645	-1.650691
H	5.522027	-3.928744	-1.112625
H	5.273773	-2.186917	-1.380858
H	5.325156	-3.629114	1.318411
H	6.261983	-2.194840	0.857588
H	3.826024	-1.958543	2.155412
H	4.312965	-0.781737	0.905865
H	3.232898	-4.233498	-0.367410
C	-3.314591	4.306293	-1.017771
C	-2.981635	2.972819	-1.313176
C	-3.029075	1.991236	-0.292529
C	-3.424716	2.416308	1.007721
C	-3.759211	3.748200	1.255881
C	-3.706855	4.721442	0.251484
H	-3.264478	5.039674	-1.821500
H	-4.059458	4.035146	2.262412
C	-4.979749	-0.701207	-1.025702
C	-3.859383	-0.782610	-0.162112
C	-3.850413	-1.793902	0.826561
C	-4.955278	-2.646183	0.971586
C	-6.077832	-2.544170	0.149650
C	-6.062606	-1.569625	-0.852913
H	-4.928148	-3.415950	1.740394
H	-6.913912	-1.488392	-1.526814
O	-1.883891	-0.036458	-1.919482
P	-2.302877	0.251699	-0.432282
H	-0.250169	0.132600	0.900214
C	-2.668790	-2.018850	1.742565
H	-2.579358	-1.225209	2.489250
H	-2.779546	-2.963866	2.283270
H	-1.729007	-2.043826	1.187922
C	-5.028395	0.290992	-2.160472
H	-5.840727	0.051438	-2.853532
H	-5.185990	1.309940	-1.792468
H	-4.075969	0.285506	-2.695477
C	-7.269577	-3.450186	0.333333
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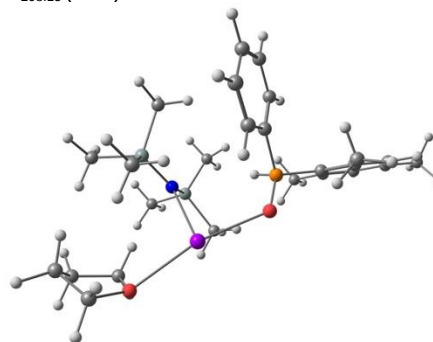
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H	-2.570665	0.849125	2.203892
C	-2.616098	2.682319	-2.754214
H	-1.993008	3.488396	-3.158970
H	-2.105565	1.724572	-2.848451
H	-3.521838	2.640284	-3.374102
C	-4.054032	6.159554	0.545103
H	-5.071782	6.253295	0.942993
H	-3.379257	6.589288	1.295810
H	-3.988268	6.777426	-0.355381

K-OP(Mes)Ph-RI

E (BS1) = -2704.432517

E (BS2) = -2705.002195

G_{298.15} (BS2) = -2704.456326



N	1.898763	-0.165726	0.788827
Si	1.540729	-1.463304	1.788551
Si	2.547763	1.365302	1.017350
C	0.868976	-2.912497	0.735260
H	0.017867	-2.617868	0.109012
H	1.653901	-3.296798	0.068143
H	0.539313	-3.757191	1.353668
C	3.024892	-2.205485	2.732392
H	2.739779	-3.079235	3.334106
H	3.816869	-2.523874	2.042759
H	3.466192	-1.467984	3.414520
C	0.246031	-1.094703	3.144531
H	-0.601874	-0.524127	2.748733
H	-0.148272	-2.002629	3.619697
H	0.696416	-0.481999	3.936558
C	1.496579	2.531077	2.096132
H	1.497432	2.192344	3.140445
H	1.863599	3.566111	2.087462
H	0.455058	2.542620	1.760549
C	2.752198	2.245924	-0.670150
H	1.789816	2.373494	-1.181018
H	3.181161	3.249223	-0.551205
H	3.425915	1.692335	-1.337881
C	4.287843	1.387383	1.802946
H	4.733348	2.391450	1.810276
H	4.249766	1.040635	2.843621
H	4.975796	0.722502	1.267014
K	1.561234	-0.650358	-1.797500
O	4.107234	-1.372547	-2.221448
C	4.569784	-1.885606	-0.941019
C	5.996140	-1.361482	-0.758002
H	3.897141	-1.502482	-0.165429
H	4.514357	-2.979370	-0.963118
C	5.985926	-0.078983	-1.601601
H	6.231832	-1.182227	0.294159
H	6.726446	-2.072921	-1.158305
C	5.103283	-0.490995	-2.775507
H	5.518053	0.739084	-1.044811
H	6.982141	0.240065	-1.919012
H	4.590134	0.348616	-3.256527
H	5.683143	-1.026915	-3.540577
C	-0.913328	3.909465	-0.565013

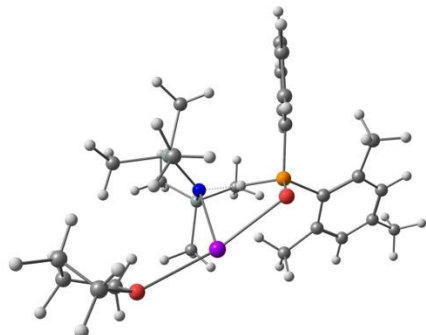
C	-0.997381	2.553900	-0.884983
C	-1.706307	1.681035	-0.053553
C	-2.338604	2.169833	1.097516
C	-2.255110	3.525275	1.413380
C	-1.541184	4.394677	0.583529
H	-0.356489	4.583573	-1.208752
H	-2.743723	3.903028	2.306316
C	-4.420393	-0.000718	-1.304666
C	-3.504264	-0.594851	-0.401154
C	-3.940978	-1.588893	0.504548
C	-5.292864	-1.953005	0.497208
C	-6.213498	-1.373234	-0.377267
C	-5.755877	-0.401353	-1.274000
H	-5.631370	-2.716824	1.192191
H	-6.456582	0.052992	-1.970397
O	-1.030269	-0.419484	-1.748126
P	-1.763624	-0.087343	-0.457709
H	-1.204448	-0.690467	0.674728
C	-3.021444	-2.284386	1.484315
H	-2.623296	-1.595765	2.236219
H	-3.565558	-3.070072	2.013869
H	-2.164621	-2.751477	0.989412
C	-3.998830	1.062813	-2.290849
H	-4.763713	1.195140	-3.060034
H	-3.856534	2.028201	-1.792676
H	-3.057026	0.808815	-2.784193
C	-7.663955	-1.779921	-0.366028
H	-8.305491	-0.936009	-0.086196
H	-7.987724	-2.111873	-1.358888
H	-7.846197	-2.592627	0.341888
H	-2.897744	1.497688	1.742342
H	-1.473883	5.449026	0.834304
H	-0.521762	2.167480	-1.780460

K-OP(Mes)Ph-TS

E (BS1) = -2704.41863268

E (BS2) = -2704.982358

G_{298.15} (BS2) = -2704.437182



N	1.171072	0.063241	0.896941
Si	1.027428	-0.746140	2.403089
Si	2.012483	1.536224	0.627641
C	1.621231	-2.549846	2.272990
H	1.151012	-3.095532	1.447199
H	2.705761	-2.576303	2.108647
H	1.415922	-3.111482	3.193654
C	2.026731	-0.008703	3.841144
H	1.790572	-0.540506	4.772268
H	3.106815	-0.094129	3.681097
H	1.795762	1.050496	4.003242
C	-0.775807	-0.748847	3.004997
H	-1.482674	-1.132044	2.262522
H	-0.894421	-1.351285	3.914763
H	-1.084583	0.275545	3.248362
C	1.175232	3.080472	1.344273
H	0.935925	2.943162	2.405763
H	1.834339	3.955258	1.265806
H	0.243972	3.319526	0.824681
C	2.182374	1.839927	-1.246781
H	1.242353	1.681563	-1.787378
H	2.492184	2.875988	-1.430888

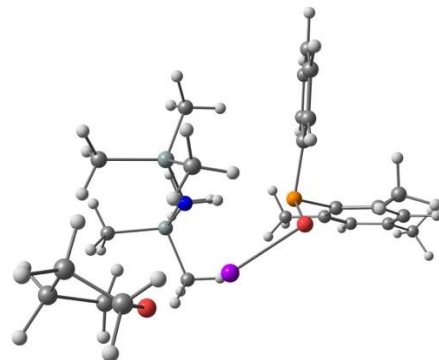
H	2.957679	1.204304	-1.696015
C	3.787827	1.567970	1.310231
H	4.366442	2.367255	0.828596
H	3.802416	1.762850	2.387615
H	4.315833	0.624405	1.139369
K	1.459421	-1.212580	-1.596509
O	4.037674	-1.715998	-1.736762
C	4.595566	-1.933527	-0.414654
C	5.963539	-1.240033	-0.399771
H	3.907180	-1.495440	0.316786
H	4.662646	-3.010961	-0.229797
C	5.832828	-0.206669	-1.528261
H	6.183105	-0.789070	0.571027
H	6.758102	-1.956105	-0.632913
C	4.973651	-0.961885	-2.534334
H	5.303700	0.683895	-1.174606
H	6.795226	0.100682	-1.945062
H	4.401175	-0.315365	-3.206727
H	5.579088	-1.649783	-3.141002
C	-1.807479	4.295588	-1.056184
C	-1.545167	2.965856	-1.392480
C	-1.831602	1.940134	-0.485557
C	-2.359533	2.259420	0.774448
C	-2.627044	3.586150	1.107343
C	-2.351693	4.607406	0.191651
H	-1.587775	5.087771	-1.766587
H	-3.042920	3.826911	2.081602
C	-4.161297	-0.360238	-0.907142
C	-2.848169	-0.801861	-0.606761
C	-2.664946	-2.124502	-0.133256
C	-3.775663	-2.927119	0.141641
C	-5.078597	-2.473533	-0.072802
C	-5.244130	-1.199505	-0.621323
H	-3.615736	-3.934382	0.519215
H	-6.248405	-0.848970	-0.848269
O	-0.770567	0.089893	-2.293213
P	-1.339432	0.225875	-0.858958
H	-0.156903	0.044136	0.206685
C	-1.296637	-2.750257	0.009185
H	-0.544687	-2.031525	0.330442
H	-1.308788	-3.562910	0.739602
H	-0.978258	-3.182063	-0.950028
C	-4.468201	0.965406	-1.565459
H	-5.445567	0.916113	-2.053815
H	-4.498924	1.786876	-0.843290
H	-3.726462	1.229019	-2.321861
C	-6.267989	-3.331729	0.272077
H	-6.583189	-3.161695	1.309536
H	-7.124633	-3.103913	-0.369335
H	-6.035488	-4.396464	0.173881
H	-2.568650	1.468022	1.489478
H	-2.554756	5.641614	0.454071
H	-1.125179	2.709944	-2.360590

K-OP(Mes)Ph-PI

E (BS1) = -2704.449410

E (BS2) = -2705.011426

G_{298.15} (BS2) = -2704.463541



N	1.575063	-0.369238	1.065648
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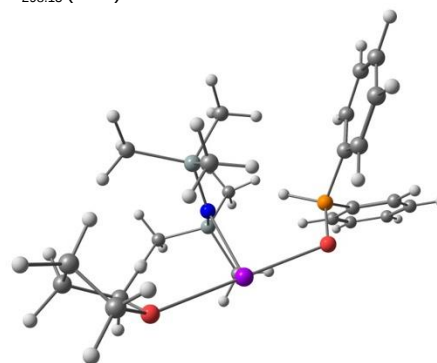
Si	1.876733	-1.864174	1.925792
Si	2.212669	1.264578	1.150646
C	1.477650	-3.274525	0.727642
H	0.475656	-3.163576	0.293611
H	2.211718	-3.328417	-0.087323
H	1.498078	-4.246193	1.235564
C	3.668936	-2.022431	2.476194
H	3.821247	-3.024010	2.897500
H	4.380548	-1.900333	1.654238
H	3.924454	-1.298213	3.255683
C	0.766642	-2.016530	3.440488
H	-0.291176	-1.934128	3.169122
H	0.908166	-2.978169	3.948761
H	0.985858	-1.220666	4.162258
C	1.202578	2.318244	2.339955
H	1.303769	1.950273	3.368189
H	1.526535	3.365909	2.324829
H	0.139292	2.295562	2.080653
C	2.103542	2.004279	-0.584465
H	1.106910	1.870499	-1.017292
H	2.310002	3.080842	-0.567993
H	2.840162	1.542756	-1.251672
C	4.016332	1.260555	1.688035
H	4.428372	2.270373	1.569216
H	4.134256	0.981453	2.739776
H	4.628625	0.581481	1.087568
K	1.287907	-0.938897	-1.807935
O	3.861876	-0.774795	-2.396538
C	4.635817	-1.324494	-1.301030
C	5.979273	-0.586850	-1.302311
H	4.078622	-1.148004	-0.375577
H	4.742964	-2.404918	-1.445730
C	5.641031	0.726213	-2.022862
H	6.364915	-0.435877	-0.290962
H	6.724450	-1.150873	-1.872352
C	4.625776	0.255555	-3.057890
H	5.175642	1.435825	-1.330853
H	6.511752	1.204249	-2.478467
H	3.929750	1.033336	-3.385396
H	5.123017	-0.167365	-3.941699
C	-1.597242	4.234071	0.030368
C	-1.425310	2.953631	-0.501569
C	-1.905855	1.823380	0.173713
C	-2.571985	2.007649	1.396985
C	-2.748650	3.284312	1.929342
C	-2.254950	4.404254	1.250313
H	-1.220123	5.100022	-0.508459
H	-3.270395	3.409566	2.874790
C	-4.174880	-0.117709	-1.449652
C	-3.219376	-0.562151	-0.502984
C	-3.571452	-1.600998	0.386570
C	-4.848855	-2.174632	0.315430
C	-5.792204	-1.755970	-0.624282
C	-5.433586	-0.724351	-1.498799
H	-5.108407	-2.971507	1.009257
H	-6.156845	-0.375570	-2.234160
O	-0.932771	0.298790	-1.912354
P	-1.479376	0.125722	-0.443059
H	0.565889	-0.318658	0.839283
C	-2.613852	-2.117678	1.439658
H	-2.340447	-1.338642	2.158664
H	-3.065119	-2.944098	1.997230
H	-1.677893	-2.473130	0.997729
C	-3.879983	1.029059	-2.386092
H	-4.584873	1.042875	-3.223285
H	-3.971189	1.986499	-1.858465
H	-2.854029	0.969102	-2.757981
C	-7.156567	-2.394270	-0.704511
H	-7.952649	-1.644417	-0.628895
H	-7.297619	-2.912476	-1.660946
H	-7.303931	-3.124866	0.096102
H	-2.959218	1.143982	1.933425
H	-2.385627	5.398233	1.668848
H	-0.927592	2.809868	-1.456145

K-OPPh₂-RI

E (BS1) = -2586.455402

E (BS2) = -2586.990703

G_{298.15} (BS2) = -2586.522614



N	1.334593	-0.624527	0.703410
Si	1.050083	-2.233298	1.079199
Si	1.585647	0.806214	1.542780
C	0.530479	-3.170288	-0.505892
H	-0.317723	-2.696061	-1.015310
H	1.366852	-3.214727	-1.219216
H	0.243083	-4.209265	-0.299181
C	2.565953	-3.189957	1.730185
H	2.336761	-4.242226	1.946191
H	3.386115	-3.173570	1.000987
H	2.945926	-2.738703	2.655609
C	-0.314089	-2.528964	2.382315
H	-1.219588	-1.948792	2.169873
H	-0.604936	-3.585158	2.459607
H	0.039176	-2.217114	3.373829
C	0.207376	1.276964	2.773427
H	0.117326	0.526607	3.568945
H	0.396312	2.245546	3.255553
H	-0.766612	1.345117	2.275919
C	1.679993	2.266462	0.311143
H	0.737551	2.383521	-0.239779
H	1.865699	3.218561	0.824569
H	2.491344	2.137071	-0.417251
C	3.199841	0.869496	2.556822
H	3.387122	1.861391	2.989612
H	3.160798	0.152987	3.387741
H	4.069230	0.604002	1.944227
K	1.381528	-0.172428	-1.928363
O	4.040744	-0.005230	-2.042609
C	4.543436	-0.852684	-0.971985
C	5.771532	-0.138972	-0.400299
H	3.746348	-0.955518	-0.226668
H	4.778257	-1.838527	-1.388388
C	5.490176	1.330883	-0.742893
H	5.883795	-0.316983	0.672195
H	6.684840	-0.476059	-0.902177
C	4.821249	1.203869	-2.107503
H	4.793003	1.765014	-0.019116
H	6.391223	1.949001	-0.773924
H	4.148576	2.033718	-2.348393
H	5.567875	1.117560	-2.910008
C	-2.403192	4.167122	-0.412103
C	-2.051817	2.892203	-0.859314
C	-2.450661	1.763226	-0.134790
C	-3.202518	1.913015	1.039687
C	-3.547576	3.187893	1.484875
C	-3.147587	4.314421	0.759545
H	-2.095487	5.042554	-0.976166
H	-4.127674	3.303955	2.395272
C	-4.616080	-0.473609	-1.146768
C	-3.385069	-0.931803	-0.653386
C	-3.275533	-2.239580	-0.158442
C	-4.388898	-3.080382	-0.156214
C	-5.611584	-2.620208	-0.648890
C	-5.724863	-1.317782	-1.144235

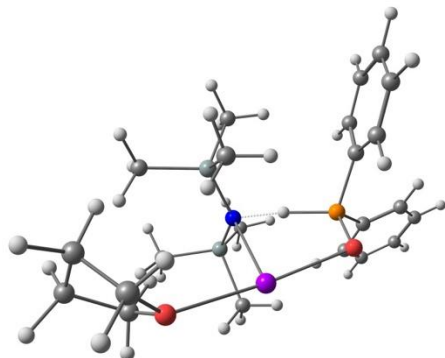
H	-4.301901	-4.090615	0.232083
H	-6.677581	-0.960655	-1.523358
O	-1.199865	0.188221	-2.041432
P	-1.918022	0.126623	-0.700887
H	-1.097768	-0.382467	0.325775
H	-3.517246	1.038015	1.601392
H	-3.417991	5.306471	1.108936
H	-1.472634	2.761888	-1.767961
H	-4.707106	0.541900	-1.520879
H	-6.478319	-3.274556	-0.644585
H	-2.326163	-2.598095	0.225289

K-OPPh₂-TS

E (BS1) = -2586.448665

E (BS2) = -2586.978444

G_{298.15} (BS2) = -2586.511239



N	0.834618	-0.555814	0.771836
Si	0.937760	-2.216374	1.143507
Si	1.388401	0.849131	1.568156
C	0.842276	-3.195176	-0.491641
H	0.015554	-2.865349	-1.133502
H	1.777905	-3.089226	-1.059642
H	0.703139	-4.269832	-0.320432
C	2.540990	-2.786595	1.984871
H	2.539868	-3.878597	2.100726
H	3.431461	-2.518635	1.405245
H	2.653017	-2.352428	2.984446
C	-0.470977	-2.808247	2.271315
H	-1.451933	-2.480161	1.911303
H	-0.498577	-3.901015	2.370247
H	-0.341651	-2.390471	3.278116
C	0.185251	1.511172	2.876378
H	0.016671	0.766388	3.664413
H	0.567717	2.420992	3.357027
H	-0.788750	1.753604	2.438370
C	1.593471	2.237325	0.279757
H	0.663491	2.409197	-0.276389
H	1.858236	3.188626	0.757879
H	2.393059	2.013720	-0.437760
C	3.060738	0.664300	2.448068
H	3.439320	1.644040	2.767571
H	2.970778	0.042561	3.346276
H	3.820689	0.206593	1.807682
K	1.338548	-0.209259	-1.968293
O	3.969428	0.055944	-1.987577
C	4.474867	-0.832962	-0.957948
C	5.716278	-0.154304	-0.373467
H	3.691511	-0.957102	-0.201773
H	4.689456	-1.808425	-1.407054
C	5.443665	1.330214	-0.654419
H	5.842329	-0.376380	0.689077
H	6.617184	-0.481598	-0.902758
C	4.759403	1.263761	-2.015181
H	4.758592	1.742002	0.093704
H	6.350141	1.940444	-0.671566
H	4.088128	2.104827	-2.215025
H	5.493964	1.199983	-2.829770
C	-2.484376	4.154887	-0.495724
C	-2.098308	2.891345	-0.948910

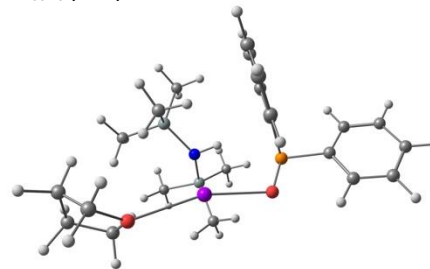
C	-2.383855	1.748983	-0.190695
C	-3.058457	1.887455	1.032609
C	-3.445323	3.148878	1.483554
C	-3.156268	4.285304	0.721029
H	-2.262042	5.035699	-1.091776
H	-3.970600	3.247573	2.429202
C	-4.519707	-0.468149	-0.872783
C	-3.218736	-0.954540	-0.670147
C	-3.034520	-2.329842	-0.459441
C	-4.125791	-3.199490	-0.440312
C	-5.416240	-2.703169	-0.635135
C	-5.611010	-1.336815	-0.853578
H	-3.968688	-4.260576	-0.269272
H	-6.613580	-0.948199	-1.008319
O	-1.201582	0.257687	-2.198547
P	-1.745429	0.133125	-0.755585
H	-0.545361	-0.301442	0.202489
H	-3.286851	1.007362	1.627778
H	-3.455530	5.267394	1.075558
H	-1.578244	2.773682	-1.895042
H	-4.679665	0.592374	-1.039709
H	-6.267494	-3.377576	-0.616411
H	-2.035765	-2.723949	-0.305934

K-OPPh₂-PI

E (BS1) = -2586.477232

E (BS2) = -2587.004796

G_{298.15} (BS2) = -2586.533000



N	1.148174	-0.735370	1.052259
Si	1.370727	-2.481678	0.949548
Si	2.021474	0.584393	1.816438
C	1.015775	-3.031604	-0.822249
H	0.048416	-2.645418	-1.167967
H	1.803362	-2.701672	-1.513484
H	0.980468	-4.126015	-0.886108
C	3.126555	-2.985794	1.396524
H	3.226230	-4.068845	1.252382
H	3.879417	-2.501343	0.767313
H	3.366945	-2.770167	2.442372
C	0.147964	-3.325366	2.104647
H	-0.875668	-3.020750	1.858114
H	0.204510	-4.417662	2.024395
H	0.338140	-3.052696	3.149516
C	1.373309	0.896433	3.556938
H	1.522229	0.015280	4.192131
H	1.886727	1.742273	4.030256
H	0.302077	1.122647	3.543930
C	1.751860	2.134685	0.770740
H	0.690413	2.313101	0.568915
H	2.133015	3.022572	1.289251
H	2.289794	2.071717	-0.182750
C	3.865927	0.229504	1.895539
H	4.391498	1.147397	2.186259
H	4.109628	-0.536311	2.637446
H	4.269787	-0.092263	0.932496
K	0.768425	0.102551	-1.722276
O	3.302768	0.435931	-2.373481
C	4.246598	-0.590083	-1.982488
C	5.569711	0.126548	-1.656611
H	3.828113	-1.107954	-1.113803
H	4.355018	-1.313719	-2.798392
C	5.154208	1.602189	-1.533876
H	6.031267	-0.261461	-0.745239

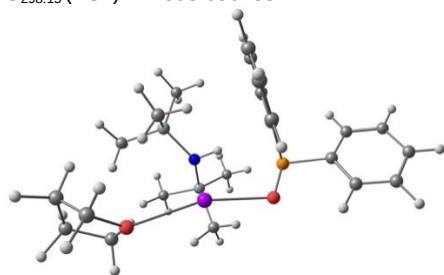
H	6.282301	0.001290	-2.477357
C	4.006337	1.681928	-2.531577
H	4.787849	1.820582	-0.525923
H	5.965795	2.295453	-1.768459
H	3.297565	2.492359	-2.337996
H	4.376939	1.774964	-3.562524
C	-1.810317	3.412655	-0.212087
C	-1.989674	2.081733	-0.592346
C	-2.092261	1.062543	0.369714
C	-2.004732	1.412601	1.723934
C	-1.833843	2.746034	2.111563
C	-1.732539	3.748367	1.144664
H	-1.737118	4.190507	-0.968467
H	-1.769301	3.000386	3.166171
C	-4.568750	-0.752594	-1.794209
C	-4.096046	-0.627570	-0.482549
C	-5.023731	-0.480449	0.559549
C	-6.392331	-0.443144	0.293534
C	-6.855502	-0.564534	-1.021515
C	-5.939565	-0.720220	-2.064333
H	-7.100803	-0.321301	1.109110
H	-6.294380	-0.815955	-3.087872
O	-1.589640	-0.812506	-1.575342
P	-2.262143	-0.736345	-0.155993
H	0.142260	-0.552398	1.103959
H	-2.063017	0.633941	2.481762
H	-1.590579	4.783069	1.443376
H	-2.059902	1.812714	-1.644959
H	-3.839832	-0.870221	-2.591774
H	-7.921893	-0.541483	-1.228413
H	-4.671956	-0.386924	1.585404

K-OPCy₂-RI

E (BS1) = -2593.744378

E (BS2) = -2594.263178

G_{298.15} (BS2) = -2593.656188



N	1.721536	-0.018728	0.983338
Si	1.757435	-1.324233	2.030069
Si	1.636714	1.652812	1.032077
C	1.528376	-2.948531	1.041759
H	0.587466	-2.964890	0.476464
H	2.355819	-3.100743	0.333547
H	1.513638	-3.827162	1.699335
C	3.400620	-1.559876	2.969205
H	3.399245	-2.456600	3.603316
H	4.242435	-1.649862	2.270392
H	3.608948	-0.698779	3.617216
C	0.406262	-1.332125	3.378870
H	-0.597780	-1.224964	2.951426
H	0.416056	-2.256058	3.972436
H	0.550195	-0.495453	4.074470
C	0.315318	2.366442	2.211589
H	0.609777	2.212239	3.257726
H	0.163899	3.445212	2.071853
H	-0.653205	1.873820	2.075797
C	1.226029	2.334047	-0.710035
H	0.297116	1.912129	-1.113305
H	1.107717	3.425234	-0.703600
H	2.032659	2.109001	-1.421245
C	3.256866	2.527194	1.529919
H	3.185046	3.620796	1.456626
H	3.525492	2.284778	2.566317

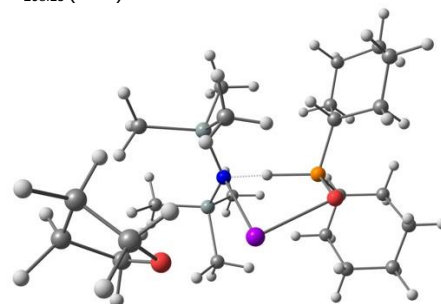
H	4.092803	2.205812	0.896957
K	1.327752	-0.881413	-1.519943
O	3.882546	-0.554607	-2.233451
C	4.652464	-0.673436	-1.004161
C	5.717711	0.425568	-1.055943
H	3.962841	-0.529927	-0.163970
H	5.079683	-1.681099	-0.956070
C	5.074901	1.467880	-1.981898
H	5.946412	0.817495	-0.061615
H	6.645498	0.047468	-1.498566
C	4.351981	0.578952	-2.988263
H	4.352805	2.076272	-1.428259
H	5.800840	2.133561	-2.456075
H	3.487830	1.058503	-3.460480
H	5.034441	0.237781	-3.779991
O	-1.244167	-0.584239	-1.468614
P	-1.900818	-0.240634	-0.134391
H	-0.970521	-0.208659	0.925853
C	-3.490417	-3.731844	-1.393066
C	-4.113155	-2.359088	-1.681187
C	-4.394191	-1.596452	-0.379603
C	-3.135095	-1.448383	0.495919
C	-2.476212	-2.823291	0.747128
C	-2.215107	-3.602554	-0.549369
H	-3.270031	-4.252590	-2.332532
H	-4.220373	-4.351211	-0.852139
H	-5.045304	-2.476246	-2.246270
H	-3.426157	-1.773969	-2.303301
H	-4.833695	-0.617099	-0.592048
H	-5.139342	-2.151728	0.206379
H	-3.420719	-1.022013	1.466891
H	-1.547866	-2.702759	1.316130
H	-3.158230	-3.403379	1.383190
H	-1.817337	-4.594375	-0.304330
H	-1.451288	-3.080519	-1.136326
C	-3.323332	1.825487	-1.424994
C	-3.729516	3.304990	-1.402106
C	-4.584963	3.635045	-0.171434
C	-3.879445	3.233012	1.130640
C	-3.476830	1.752072	1.113386
C	-2.604069	1.454026	-0.117035
H	-2.673284	1.613191	-2.279211
H	-4.219990	1.204928	-1.544536
H	-4.271247	3.557796	-2.321131
H	-2.821194	3.923377	-1.388557
H	-4.828520	4.703814	-0.155054
H	-5.539615	3.094831	-0.243001
H	-4.526524	3.433495	1.992491
H	-2.976487	3.844823	1.261895
H	-2.944627	1.493910	2.036324
H	-4.380892	1.131181	1.079148
H	-1.704495	2.081950	-0.048619

K-OPCy₂-TS

E (BS1) = -2593.730006

E (BS2) = -2594.242213

G_{298.15} (BS2) = -2593.635458



N	1.086333	0.192465	1.038386
Si	1.529138	-0.927676	2.250097
Si	1.496711	1.827553	0.749313
C	1.776835	-2.649318	1.465827

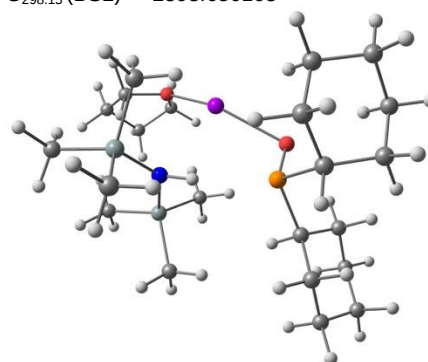
H	0.911281	-2.974726	0.874881
H	2.664129	-2.665202	0.818377
H	1.934677	-3.417295	2.233518
C	3.146592	-0.547971	3.163300
H	3.386279	-1.356136	3.866759
H	3.993361	-0.447255	2.475071
H	3.077444	0.379843	3.742150
C	0.180580	-1.098080	3.573470
H	-0.801215	-1.287046	3.125273
H	0.387816	-1.911600	4.280098
H	0.098097	-0.169031	4.151648
C	0.370357	3.051574	1.662776
H	0.477771	2.934456	2.748635
H	0.611345	4.093855	1.417073
H	-0.684911	2.888844	1.422110
C	1.308775	2.171735	-1.114683
H	0.348982	1.811470	-1.504269
H	1.366702	3.245103	-1.333689
H	2.112233	1.690124	-1.687159
C	3.269118	2.318813	1.212020
H	3.498010	3.319909	0.823433
H	3.409047	2.351503	2.297977
H	4.012574	1.627695	0.804570
K	1.249728	-1.134588	-1.448783
O	3.814663	-0.784193	-2.00918
C	4.621049	-0.841532	-0.796647
C	5.763880	0.161281	-0.991360
H	3.982266	-0.569713	0.050844
H	4.975116	-1.868109	-0.654437
C	5.185215	1.133436	-2.029726
H	6.044417	0.649014	-0.054493
H	6.649167	-0.340652	-1.395011
C	4.368842	0.192024	-2.906912
H	4.528108	1.864485	-1.547926
H	5.952858	1.670507	-2.592497
H	3.539412	0.678726	-3.429360
H	5.002474	-0.313523	-3.648988
O	-1.289498	-0.712374	-1.651069
P	-1.673757	-0.260422	-0.208353
H	-0.263004	-0.025528	0.649599
C	-3.398415	-3.827236	-1.096036
C	-4.071082	-2.475008	-1.370126
C	-4.214731	-1.662490	-0.076182
C	-2.860483	-1.439878	0.623979
C	-2.180229	-2.802510	0.878355
C	-2.043369	-3.643053	-0.399361
H	-3.270083	-4.385846	-2.031514
H	-4.054831	-4.433457	-0.454369
H	-5.057321	-2.628565	-1.825589
H	-3.459361	-1.907322	-2.079525
H	-4.710459	-0.708468	-0.274644
H	-4.869713	-2.212292	0.617212
H	-3.039488	-0.964826	1.598322
H	-1.200451	-2.657067	1.343722
H	-2.788777	-3.359028	1.605920
H	-1.603193	-4.618296	-0.156400
H	-1.363208	-3.132580	-1.090257
C	-3.442449	1.559328	-1.544320
C	-3.954503	3.003508	-1.632240
C	-4.692361	3.413770	-0.349915
C	-3.818181	3.209156	0.895230
C	-3.299971	1.766406	0.983360
C	-2.554893	1.377538	-0.302985
H	-2.876085	1.285180	-2.439853
H	-4.300618	0.878497	-1.495626
H	-4.612582	3.120888	-2.502208
H	-3.100598	3.678148	-1.788638
H	-5.019370	4.458582	-0.415925
H	-5.602644	2.805008	-0.251455
H	-4.381423	3.464836	1.801118
H	-2.960234	3.894653	0.852531
H	-2.645014	1.650770	1.855745
H	-4.150343	1.089462	1.134241
H	-1.718109	2.083559	-0.416320

K-OPCy₂-PI

E (BS1) = -2593.747193

E (BS2) = -2594.257337

G_{298.15} (BS2) = -2593.650108



N	1.365674	0.162073	1.196677
Si	1.987815	-1.001342	2.340704
Si	1.646404	1.851173	0.835220
C	1.947180	-2.702135	1.506380
H	0.941324	-2.945113	1.139756
H	2.656122	-2.763501	0.670051
H	2.223905	-3.494355	2.212519
C	3.758282	-0.617826	2.849126
H	4.130585	-1.420526	3.497705
H	4.435544	-0.547002	1.992039
H	3.827696	0.317940	3.412755
C	0.890843	-1.075162	3.871425
H	-0.149589	-1.279730	3.592069
H	1.212436	-1.859218	4.567678
H	0.905090	-0.120085	4.409738
C	0.515079	2.949992	1.868714
H	0.748974	2.860263	2.936308
H	0.606842	4.007429	1.591942
H	-0.532327	2.657253	1.734621
C	1.235194	2.110794	-0.992394
H	0.251329	1.698311	-1.245060
H	1.222401	3.176789	-1.249208
H	1.984055	1.633392	-1.634847
C	3.439412	2.336317	1.138940
H	3.619398	3.341028	0.736996
H	3.680752	2.362878	2.206331
H	4.142494	1.654251	0.652663
K	1.081865	-1.190532	-1.379153
O	3.518603	-0.634027	-2.267903
C	4.463367	-0.723487	-1.172144
C	5.592125	0.264659	-1.487496
H	3.934793	-0.454356	-0.251846
H	4.814934	-1.757264	-1.085750
C	4.913724	1.256661	-2.443502
H	5.987002	0.737624	-0.584880
H	6.416675	-0.246245	-1.994866
C	3.984018	0.338002	-3.227338
H	4.331224	1.995153	-1.882801
H	5.620431	1.785874	-3.087530
H	3.108982	0.842093	-3.647961
H	4.519479	-0.174302	-4.038653
O	-1.366334	-0.609870	-1.487823
P	-1.785439	-0.259467	0.000357
H	0.346366	-0.012739	1.060533
C	-3.272761	-3.871337	-1.171752
C	-3.937834	-2.543434	-1.559858
C	-4.327845	-1.741169	-0.310538
C	-3.116352	-1.469151	0.599926
C	-2.450813	-2.809514	0.978509
C	-2.063963	-3.637394	-0.255591
H	-2.966558	-4.423009	-2.069978
H	-4.003977	-4.505171	-0.647700
H	-4.823652	-2.732521	-2.180254
H	-3.230002	-1.945167	-2.142886
H	-4.813832	-0.804292	-0.596876

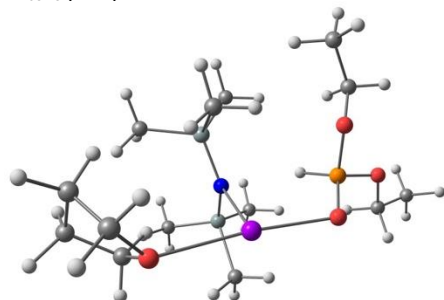
H	-5.077575	-2.314429	0.260047
H	-3.468995	-1.001534	1.530330
H	-1.565882	-2.625108	1.601655
H	-3.149391	-3.398816	1.592220
H	-1.625064	-4.594920	0.053077
H	-1.303231	-3.090073	-0.824290
C	-3.501408	1.600815	-1.428994
C	-4.007076	3.047204	-1.522043
C	-4.856135	3.417839	-0.296940
C	-4.097809	3.169289	1.015088
C	-3.579732	1.725006	1.096319
C	-2.720357	1.379515	-0.126376
H	-2.862845	1.342116	-2.279776
H	-4.363141	0.923404	-1.469907
H	-4.587824	3.194448	-2.441981
H	-3.144690	3.727151	-1.581789
H	-5.178864	4.464801	-0.356666
H	-5.770614	2.807156	-0.300544
H	-4.743728	3.394068	1.873520
H	-3.243586	3.858775	1.074449
H	-3.008350	1.578087	2.022690
H	-4.438278	1.041810	1.145856
H	-1.890449	2.105609	-0.143562

K-OP(OEt)₂-RI

E (BS1) = -2432.053112

E (BS2) = -2432.561609

G_{298.15} (BS2) = -2432.131907



N	-0.527418	0.452101	0.705132
Si	-0.431538	2.097436	1.010197
Si	-0.890176	-0.943896	1.558222
C	-0.468586	3.069611	-0.636983
H	0.351420	2.756505	-1.297565
H	-1.417082	2.932894	-1.175244
H	-0.352934	4.148947	-0.474372
C	-1.843687	2.816500	2.072237
H	-1.787471	3.910230	2.154642
H	-2.825196	2.565660	1.650860
H	-1.815491	2.410356	3.091251
C	1.180553	2.662174	1.862883
H	2.056082	2.459273	1.233026
H	1.179590	3.738125	2.082573
H	1.333709	2.131829	2.811359
C	0.416684	-1.452610	2.851630
H	0.439524	-0.723632	3.672503
H	0.216781	-2.436608	3.296011
H	1.423498	-1.479256	2.421138
C	-1.043923	-2.409896	0.339488
H	-0.131994	-2.524745	-0.259929
H	-1.213204	-3.363126	0.856410
H	-1.891898	-2.273011	-0.346017
C	-2.529549	-0.909724	2.534367
H	-2.775890	-1.889183	2.966377
H	-2.474591	-0.192529	3.363092
H	-3.370198	-0.605782	1.900926
K	-0.799050	0.037628	-1.916604
O	-3.462427	0.062344	-1.978831
C	-3.902481	0.873061	-0.855410
C	-5.143219	0.179940	-0.288367
H	-3.086575	0.906385	-0.124784
H	-4.103854	1.887730	-1.214670

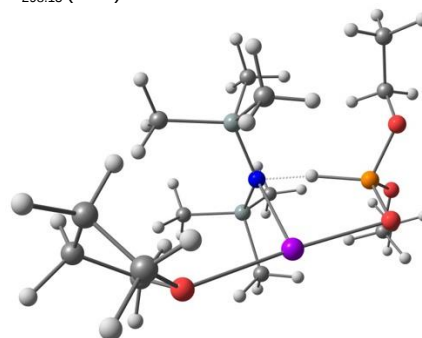
C	-4.908773	-1.284789	-0.683216
H	-5.236039	0.326443	0.790675
H	-6.051832	0.560709	-0.766948
C	-4.267606	-1.131103	-2.058469
H	-4.207013	-1.758808	0.010725
H	-5.825738	-1.878924	-0.712807
H	-3.617438	-1.966988	-2.337991
H	-5.028855	-1.007010	-2.841563
O	1.810931	0.207181	-2.030140
P	2.555315	-0.233395	-0.810998
H	2.068684	0.298260	0.385912
O	2.526747	-1.827120	-0.648089
C	3.287101	-2.456589	0.423504
H	4.321965	-2.555890	0.084675
H	3.276482	-1.811842	1.309195
C	2.663401	-3.801031	0.723192
H	1.639092	-3.685918	1.085799
H	2.652319	-4.430861	-0.171684
H	3.250242	-4.309562	1.495063
O	4.137794	0.076189	-0.812080
C	4.563370	1.467826	-0.799352
H	4.316579	1.916260	-1.766798
H	4.014787	2.005936	-0.016509
C	6.052386	1.497684	-0.536132
H	6.594346	0.951005	-1.313675
H	6.403922	2.534303	-0.532789
H	6.284032	1.049453	0.434708

K-OP(OEt)₂-TS

E (BS1) = -2432.047986

E (BS2) = -2432.549429

G_{298.15} (BS2) = -2432.121741



N	0.167300	-0.118969	0.767082
Si	0.045718	-1.643078	1.520057
Si	0.692994	1.398686	1.338290
C	0.128996	-2.988076	0.170395
H	-0.589208	-2.802667	-0.639156
H	1.135117	-3.049614	-0.268101
H	-0.098330	-3.983419	0.571976
C	1.412370	-2.050181	2.770178
H	1.313542	-3.079512	3.139083
H	2.409988	-1.951654	2.326404
H	1.370043	-1.385254	3.640623
C	-1.612811	-1.854857	2.421794
H	-2.452043	-1.561944	1.780522
H	-1.789138	-2.884928	2.756350
H	-1.648384	-1.208256	3.307864
C	-0.491690	2.205455	2.584533
H	-0.515918	1.623139	3.514644
H	-0.186267	3.226814	2.845937
H	-1.518132	2.251191	2.207007
C	0.838952	2.564114	-0.160390
H	-0.075062	2.561985	-0.766496
H	1.022484	3.601372	0.146314
H	1.679649	2.278797	-0.809118
C	2.386137	1.390114	2.197404
H	2.737970	2.414101	2.380106
H	2.338036	0.884150	3.168495
H	3.147476	0.879657	1.600300
K	0.911627	-0.467582	-1.893261

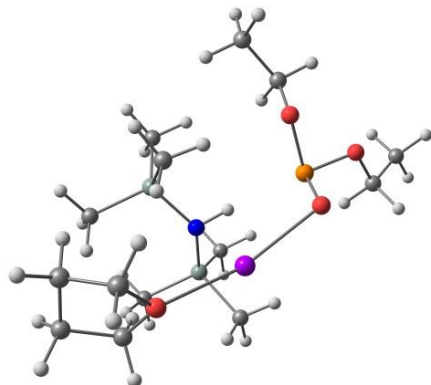
O	3.533240	-0.638126	-1.749933
C	3.923121	-1.166055	-0.455302
C	5.147912	-0.359669	-0.010818
H	3.080068	-1.033899	0.232663
H	4.128907	-2.236790	-0.556748
C	4.985414	0.953003	-0.791009
H	5.172769	-0.216926	1.072246
H	6.070465	-0.866580	-0.311810
C	4.406295	0.453224	-2.108897
H	4.269067	1.612462	-0.289813
H	5.924685	1.495479	-0.924452
H	3.814252	1.200869	-2.646772
H	5.195819	0.086217	-2.779298
O	-1.634359	-0.104651	-2.468383
P	-2.233739	0.232391	-1.117468
H	-1.149542	0.061080	0.015016
O	-2.784215	1.773178	-1.149057
C	-3.470249	2.277968	0.017881
H	-4.545716	2.127944	-0.125114
H	-3.172768	1.709889	0.907740
C	-3.135747	3.746180	0.185435
H	-2.064828	3.884193	0.361271
H	-3.417026	4.310356	-0.709475
H	-3.683068	4.159555	1.039378
O	-3.662198	-0.543555	-0.845457
C	-3.664870	-1.985427	-0.912030
H	-3.574506	-2.293390	-1.959856
H	-2.804630	-2.390478	-0.365360
C	-4.957598	-2.487671	-0.302954
H	-5.821720	-2.078514	-0.835774
H	-4.999536	-3.580344	-0.363267
H	-5.029540	-2.196120	0.749558

K-OP(OEt)₂-PI

E (BS1) = -2432.075815

E (BS2) = -2432.573847

G_{298.15} (BS2) = -2432.140688



H	1.090466	2.900607	1.497216
H	1.621262	2.050015	0.051698
C	2.624485	0.080960	2.402183
H	3.009834	0.966140	2.923047
H	2.660712	-0.754659	3.107791
H	3.308185	-0.142476	1.579027
K	0.678618	0.209318	-1.977744
O	3.257318	0.722415	-1.867698
C	4.070670	-0.327382	-1.289010
C	5.238844	0.366106	-0.569008
H	3.437833	-0.894542	-0.598077
H	4.409683	-1.001894	-2.083300
C	4.749351	1.815768	-0.423886
H	5.466974	-0.105697	0.389801
H	6.140806	0.332291	-1.187728
C	3.924137	1.987994	-1.692169
H	4.107843	1.922013	0.456674
H	5.565903	2.538420	-0.351178
H	3.156286	2.764275	-1.626888
H	4.563797	2.195524	-2.561678
O	-1.800687	0.692839	-2.110313
P	-2.492477	0.444252	-0.757671
H	-0.673782	-0.610926	0.461919
O	-2.608960	2.001382	-0.089964
C	-3.303262	2.094837	1.151515
H	-4.381161	2.191293	0.964658
H	-3.166230	1.174202	1.741247
C	-2.788843	3.291336	1.933158
H	-1.726913	3.176478	2.171385
H	-2.911661	4.212319	1.353236
H	-3.342766	3.401665	2.872414
O	-4.167209	0.301009	-1.035441
C	-4.632320	-1.003999	-1.360822
H	-4.534794	-1.181336	-2.442538
H	-4.019872	-1.769306	-0.854942
C	-6.084140	-1.140554	-0.935054
H	-6.704341	-0.387451	-1.432523
H	-6.472055	-2.132092	-1.194821
H	-6.180817	-1.001637	0.146852

N	0.302538	-0.826998	0.723686
Si	0.527093	-2.561399	0.610423
Si	0.874293	0.430090	1.807435
C	0.493170	-3.026826	-1.225104
H	-0.409187	-2.647527	-1.721835
H	1.379040	-2.655831	-1.758339
H	0.488981	-4.116261	-1.350677
C	2.175348	-3.102551	1.334056
H	2.319589	-4.172405	1.139069
H	3.020102	-2.569217	0.886309
H	2.218350	-2.957159	2.417866
C	-0.887130	-3.456483	1.473888
H	-1.853340	-3.138231	1.064455
H	-0.814671	-4.544291	1.355361
H	-0.894499	-3.233910	2.547355
C	-0.262912	0.591069	3.301364
H	-0.225308	-0.316337	3.916228
H	0.018646	1.438526	3.938070
H	-1.303425	0.735314	2.991576
C	0.860092	2.052622	0.841006
H	-0.121873	2.242043	0.392279

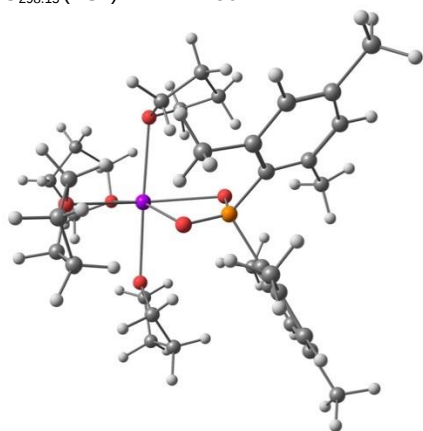
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K-OOPMes₂(THF)₄

E (BS1) = -2721.176007

E (BS2) = -2721.893680

G_{298.15} (BS2) = -2721.156442



O	-0.481379	-0.258927	-1.412861
K	1.959172	-0.293531	-0.323209
P	-1.211531	0.060555	-0.109455
O	-0.321038	0.117565	1.136169
C	-1.809648	2.610815	-1.270657
C	-2.074916	1.693986	-0.222262
C	-2.469339	3.847598	-1.283572
C	-3.375574	4.223095	-0.291113
C	-3.597532	3.327656	0.756306
C	-2.962992	2.082172	0.812754
H	-2.257746	4.541242	-2.094277
C	-3.474162	-1.342147	-1.034955
C	-4.452616	-2.335866	-1.003185
C	-2.563518	-1.204540	0.053412
C	-2.686368	-2.092200	1.147065
C	-3.684504	-3.082053	1.128371
C	-4.575974	-3.224677	0.071036
H	-5.137377	-2.423394	-1.844121
H	-3.758292	-3.756686	1.979294
O	1.699484	-2.995189	-0.831933
C	0.645669	-3.458736	0.044733
C	1.288929	-3.159796	-2.207078
C	-0.351077	-4.204436	-0.839888
H	1.095518	-4.083189	0.823359
H	0.172684	-2.591603	0.516810
C	-0.209673	-3.450107	-2.168443
H	1.529093	-2.243208	-2.756718
H	1.857572	-3.989640	-2.649734
H	-1.364413	-4.169531	-0.433224
H	-0.054685	-5.253519	-0.954132
H	-0.753325	-2.503570	-2.117890
H	-0.546094	-4.026545	-3.034688
O	2.277847	2.386832	-0.086682
C	2.854901	3.273714	-1.066889
C	1.365699	3.119845	0.767236
C	2.483468	4.689436	-0.624682
H	3.934415	3.097685	-1.105622
H	2.429964	3.039597	-2.051993
C	1.136476	4.460716	0.075847
H	0.466318	2.514657	0.894952
H	1.838787	3.259945	1.748836
H	2.425670	5.385010	-1.466037
H	3.222604	5.071929	0.088255
H	0.328312	4.379438	-0.656565
H	0.876831	5.251657	0.784479
C	5.267199	0.216306	-0.726368
O	4.310332	-0.075497	-1.757573
C	4.729291	-1.327192	-2.319070
C	5.128200	-2.185794	-1.112460
C	5.615942	-1.139037	-0.074021

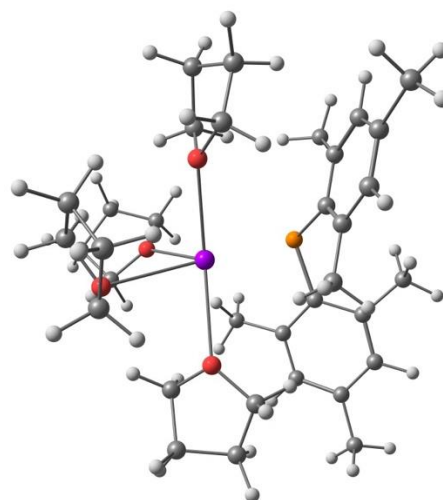
H	5.584325	-1.163124	-2.992682
H	4.253880	-2.726271	-0.739107
H	5.898241	-2.917465	-1.370743
H	5.088274	-1.255886	0.874963
H	6.689757	-1.214931	0.116022
H	4.807578	0.934598	-0.042608
H	6.156483	0.682749	-1.174609
H	3.896384	-1.728412	-2.901314
C	3.134660	0.598025	2.781564
O	3.075460	-0.702620	2.160706
C	2.191828	-1.557298	2.926545
C	1.693711	-0.723462	4.112171
C	1.844514	0.711238	3.586029
H	2.742537	-2.454177	3.231266
H	0.665036	-0.975646	4.382852
H	2.329709	-0.880648	4.990350
H	1.011376	0.945311	2.917630
H	1.906450	1.461319	4.379481
H	3.232695	1.343846	1.988166
H	4.020292	0.655966	3.432007
H	1.360996	-1.853789	2.280934
H	-4.275403	3.606890	1.560096
C	-4.096682	5.545489	-0.352586
H	-3.520743	6.290008	-0.910733
H	-5.067486	5.441448	-0.854225
H	-4.291828	5.941714	0.648944
C	-3.249944	1.205004	2.009791
H	-3.923100	0.380391	1.754634
H	-2.330143	0.764102	2.398965
H	-3.724003	1.789322	2.803600
C	-0.815779	2.356831	-2.382523
H	-1.085020	1.484790	-2.980888
H	-0.757429	3.234281	-3.034209
H	0.180669	2.149337	-1.986945
C	-5.636725	-4.295747	0.068284
H	-5.495622	-4.991222	-0.767777
H	-5.620814	-4.876335	0.994991
H	-6.637785	-3.862991	-0.043426
C	-3.436716	-0.444554	-2.251117
H	-2.429487	-0.399088	-2.669023
H	-4.129862	-0.808629	-3.014498
H	-3.723828	0.581738	-1.999484
C	-1.822922	-2.063681	2.392669
H	-2.441838	-1.825891	3.267321
H	-1.391532	-3.055395	2.574235
H	-1.024504	-1.330359	2.317352

K-PMes₂(THF)₄

E (BS1) = -2570.611956

E (BS2) = -2571.238723

G_{298.15} (BS2) = -2570.509983



K	0.479237	0.874353	0.254813
P	-0.719676	-1.599171	-1.720683

C	-3.191464	-2.515936	-0.515090
C	-2.441243	-1.448921	-1.091675
C	-4.492545	-2.288769	-0.047062
C	-5.132395	-1.053711	-0.175595
C	-4.437322	-0.043484	-0.850313
C	-3.129496	-0.216555	-1.309813
H	-5.032350	-3.117372	0.409426
C	1.294591	-3.434245	-1.090947
C	2.136076	-4.185053	-0.268699
C	0.230306	-2.651527	-0.536443
C	0.109617	-2.658287	0.886356
C	0.978461	-3.431243	1.671685
C	1.997993	-4.209238	1.124669
H	2.923513	-4.777826	-0.731591
H	0.852034	-3.411478	2.753634
O	0.755185	2.386288	-1.884736
C	0.312792	3.741824	-2.039148
C	1.078947	1.934343	-3.206353
C	1.223056	4.351422	-3.124380
H	-0.738845	3.745001	-2.360530
H	0.386779	4.223701	-1.063264
C	1.829479	3.112445	-3.838363
H	1.662439	1.016653	-3.114133
H	0.153884	1.707131	-3.754669
H	2.007689	4.968323	-2.678560
H	0.649117	4.983229	-3.806998
H	2.900059	3.034331	-3.627488
H	1.700393	3.141802	-4.923137
O	-1.716533	1.744202	1.541356
C	-2.824015	1.101088	2.219031
C	-2.133917	3.038395	1.062332
C	-3.991153	2.094896	2.183447
H	-3.062789	0.164542	1.709722
H	-2.503085	0.876964	3.243231
C	-3.285063	3.442466	1.975189
H	-1.267339	3.701970	1.103292
H	-2.469876	2.957280	0.019497
H	-4.594596	2.056027	3.093845
H	-4.641412	1.875920	1.330850
H	-2.896644	3.827846	2.924700
H	-3.929488	4.204128	1.528192
C	1.246804	3.289740	2.649973
O	1.231814	3.343652	1.216979
C	2.580007	3.640568	0.814911
C	3.502021	2.962362	1.853872
C	2.535488	2.534810	2.987343
H	2.725551	4.729907	0.806145
H	4.002279	2.094410	1.422046
H	4.262364	3.661069	2.212126
H	2.357963	1.455053	2.951688
H	2.910501	2.780066	3.984229
H	0.327396	2.792690	2.968912
H	1.264500	4.309549	3.063504
H	2.702984	3.262220	-0.202230
C	3.686884	-0.849705	1.419337
O	2.978159	-0.010949	0.477532
C	3.490860	-0.233307	-0.852935
C	4.891787	-0.798587	-0.650943
C	4.691946	-1.666531	0.600030
H	3.469256	0.722837	-1.384571
H	5.241522	-1.365726	-1.517406
H	5.603169	0.011121	-0.453128
H	4.250578	-2.626618	0.320312
H	5.617835	-1.853707	1.149841
H	2.964574	-1.479742	1.946837
H	4.185625	-0.194641	2.144295
H	2.845592	-0.949309	-1.378480
H	-4.928671	0.912623	-1.023349
C	2.948550	-4.994714	1.992453
H	2.524735	-5.179642	2.984628
H	3.195599	-5.963877	1.544948
H	3.897329	-4.460248	2.138251
C	1.542276	-3.475419	-2.579194
H	2.348128	-4.176239	-2.820187
H	0.639327	-3.771343	-3.125469

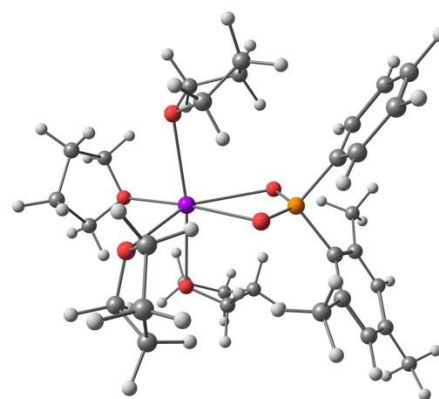
H	1.825130	-2.491646	-2.974504
C	-0.912226	-1.829082	1.627885
H	-1.223840	-0.956938	1.055354
H	-1.838904	-2.382483	1.820395
H	-0.520319	-1.506203	2.598918
C	-6.510206	-0.815558	0.389723
H	-7.053035	-0.054693	-0.181211
H	-7.110347	-1.731859	0.387350
H	-6.465223	-0.465227	1.430259
C	-2.491860	0.916697	-2.077204
H	-2.283665	0.625805	-3.114921
H	-3.154535	1.787488	-2.105261
H	-1.529075	1.225720	-1.661750
C	-2.655206	-3.924176	-0.457817
H	-1.900325	-4.072933	0.320346
H	-3.466436	-4.636763	-0.277026
H	-2.165375	-4.181632	-1.404741

K-OOP(Mes)Ph(THF)₄

E (BS1) = -2603.203832

E (BS2) = -2603.887887

G_{298.15} (BS2) = -2603.226129



O	0.720290	0.592271	-1.490655
K	-1.729028	-0.088884	-0.400412
P	1.406178	0.619071	-0.122487
O	0.497505	0.379032	1.080630
C	3.595313	-0.811171	-1.250917
C	2.806403	-0.598972	-0.089035
C	4.578979	-1.805890	-1.252452
C	4.832617	-2.600453	-0.133358
C	4.087674	-2.350043	1.018520
C	3.091179	-1.365149	1.071461
H	5.165664	-1.958794	-2.155679
C	2.539021	3.065464	-0.983315
C	3.118551	4.320255	-0.785614
C	2.209127	2.251570	0.108859
C	2.463480	2.721510	1.405667
C	3.046249	3.973354	1.606929
C	3.375927	4.774941	0.510035
H	3.362696	4.945573	-1.640039
H	3.235670	4.328502	2.616257
O	-2.451932	2.532293	-0.125540
C	-1.553354	3.145639	0.839173
C	-2.317937	3.204761	-1.391239
C	-0.815458	4.266506	0.096120
H	-2.144429	3.512320	1.685948
H	-0.860843	2.374046	1.190032
C	-0.924276	3.819192	-1.368160
H	-2.457286	2.467024	-2.188151
H	-3.099654	3.972451	-1.491255
H	0.217157	4.370153	0.435297
H	-1.324531	5.226277	0.238014
H	-0.184047	3.044005	-1.585386
H	-0.808276	4.638802	-2.082680
O	-1.379177	-2.810768	-0.579752
C	-1.607936	-3.373201	-1.892589
C	0.011607	-2.973286	-0.234132

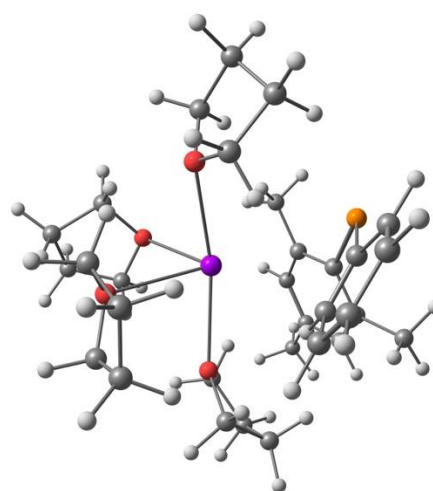
C	-0.226241	-3.737516	-2.465242
H	-2.264046	-4.247416	-1.802354
H	-2.126792	-2.616995	-2.491176
C	0.740540	-2.945379	-1.571312
H	0.281646	-2.155837	0.437344
H	0.160038	-3.930174	0.288539
H	-0.139769	-3.478326	-3.523698
H	-0.043465	-4.812464	-2.364081
H	0.831332	-1.908022	-1.906256
H	1.740467	-3.382068	-1.517765
C	-4.744172	-1.567037	-0.916513
O	-4.003481	-0.768854	-1.854525
C	-4.860642	0.342460	-2.151441
C	-5.448133	0.760821	-0.796693
C	-5.455419	-0.564264	0.014706
H	-5.651962	0.022274	-2.846361
H	-4.798613	1.500328	-0.320371
H	-6.444269	1.197801	-0.905087
H	-4.900476	-0.450302	0.948567
H	-6.467770	-0.900577	0.253402
H	-4.036231	-2.225179	-0.408817
H	-5.470647	-2.187633	-1.461364
H	-4.257791	1.111820	-2.639030
C	-2.765070	-2.157914	2.391768
O	-2.735325	-0.756906	2.055212
C	-2.021454	-0.021320	3.083656
C	-1.687123	-1.035701	4.181864
C	-1.639006	-2.356633	3.401464
H	-2.661245	0.795640	3.435512
H	-0.746844	-0.798018	4.686657
H	-2.481862	-1.072006	4.935223
H	-0.680819	-2.458523	2.880583
H	-1.788026	-3.239149	4.029661
H	-2.628816	-2.730498	1.471361
H	-3.741156	-2.408417	2.833166
H	-1.113812	0.389446	2.632507
H	4.289113	-2.935151	1.912907
H	2.315217	2.718919	-1.986150
H	3.825303	5.751789	0.665221
H	2.178510	2.107995	2.254617
C	2.399653	-1.184084	2.406203
H	2.857812	-1.841931	3.150973
H	2.480210	-0.154180	2.763966
H	1.331550	-1.394675	2.347937
C	3.455269	0.015669	-2.508363
H	2.409875	0.138625	-2.791775
H	3.861949	1.021871	-2.351024
H	4.016012	-0.439919	-3.329446
C	5.868824	-3.694465	-0.174621
H	5.473198	-4.592672	-0.665784
H	6.755128	-3.384862	-0.738147
H	6.185571	-3.983681	0.831787

K-P(Mes)Ph(THF)₄

E (BS1) = -2452.643453

E (BS2) = -2453.234388

G_{298.15} (BS2) = -2452.577857



K	0.522203	0.452977	-0.199461
P	-0.801255	-2.778311	-1.479610
C	-3.257823	-1.709980	-0.366575
C	-2.177293	-1.556817	-1.284485
C	-4.301113	-0.772965	-0.341562
C	-4.352818	0.315510	-1.213582
C	-3.316160	0.443316	-2.144920
C	-2.252892	-0.462656	-2.203385
H	-5.114034	-0.918871	0.367270
C	0.823850	-4.073733	0.358933
C	1.539719	-4.248203	1.537332
C	-0.106081	-3.012086	0.184999
C	-0.294814	-2.170500	1.313118
C	0.421626	-2.350913	2.499393
C	1.356957	-3.381125	2.624945
H	2.245226	-5.072455	1.614760
H	0.241569	-1.682055	3.337824
O	0.686822	2.684981	-1.682539
C	0.056849	3.782484	-0.987042
C	2.072992	3.007305	-1.946738
C	0.991374	4.976862	-1.160962
H	-0.938653	3.932138	-1.415838
H	-0.053845	3.524308	0.074579
C	2.364732	4.291777	-1.172394
H	2.695997	2.167425	-1.626669
H	2.197439	3.144856	-3.028851
H	0.879439	5.712204	-0.359728
H	0.801123	5.475004	-2.118081
H	2.669041	4.040528	-0.152179
H	3.147587	4.892566	-1.642510
O	-1.273189	1.482031	1.579073
C	-1.529569	0.989971	2.904704
C	-2.457957	2.180707	1.123216
C	-3.005951	0.621328	2.890152
H	-0.855593	0.152129	3.085809
H	-1.322616	1.775639	3.647312
C	-3.603988	1.779553	2.074043
H	-2.270511	3.260675	1.144271
H	-2.638029	1.872811	0.091026
H	-3.432438	0.536875	3.893077
H	-3.144686	-0.329498	2.366620
H	-3.862897	2.614618	2.732211
H	-4.501669	1.484936	1.528645
C	1.860935	2.276653	2.602507
O	2.294472	1.950636	1.273823
C	3.572424	1.318864	1.444139
C	3.382698	0.377703	2.642202
C	2.266288	1.070507	3.471538
H	4.332300	2.084919	1.660190
H	3.051556	-0.608931	2.305174
H	4.309906	0.246108	3.205735
H	1.420555	0.394063	3.618625
H	2.613905	1.391188	4.456901
H	0.787519	2.463330	2.558851

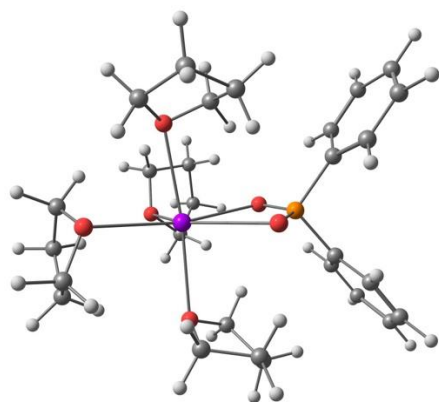
H	2.372008	3.191396	2.937016
H	3.819471	0.820942	0.506243
C	3.272982	-1.699247	-0.603408
O	2.835452	-0.476789	-1.241930
C	3.045220	-0.572675	-2.671514
C	3.802520	-1.881206	-2.905477
C	3.340092	-2.735344	-1.717705
H	3.595764	0.312589	-3.005372
H	3.565662	-2.324509	-3.875932
H	4.884056	-1.712415	-2.857222
H	2.340805	-3.139141	-1.905964
H	4.017311	-3.560262	-1.482065
H	2.559756	-1.952996	0.183402
H	4.259545	-1.534797	-0.147770
H	2.066865	-0.584355	-3.166251
H	-3.337144	1.271650	-2.851378
H	0.987213	-4.764986	-0.465049
H	1.911963	-3.519689	3.547781
H	-1.021571	-1.364668	1.258048
C	-5.471608	1.324905	-1.156730
H	-5.893725	1.513894	-2.150376
H	-6.282910	0.985518	-0.505785
H	-5.121164	2.291415	-0.771454
C	-3.364843	-2.902105	0.548734
H	-4.383067	-3.002481	0.936818
H	-3.095620	-3.820386	0.014102
H	-2.685307	-2.840098	1.405357
C	-1.217426	-0.262545	-3.286273
H	-1.328941	-1.006182	-4.085706
H	-1.308533	0.729614	-3.738414
H	-0.197626	-0.395427	-2.911772

K-OOPPh₂(THF)₄

E (BS1) = -2485.233662

E (BS2) = -2485.884535

G_{298.15} (BS2) = -2485.301868



O	-1.029332	-0.037157	-1.511033
K	1.475300	-0.024045	-0.322522
P	-1.721704	0.057270	-0.151363
O	-0.848001	0.138589	1.100985
C	-3.433684	1.939392	-1.360542
C	-2.842829	1.505850	-0.165717
C	-4.273517	3.053611	-1.371622
C	-4.529351	3.747517	-0.185288
C	-3.944592	3.322609	1.010437
C	-3.107231	2.205592	1.019018
H	-4.723166	3.386006	-2.303300
H	-2.638138	1.873987	1.940236
C	-3.519466	-1.914459	-1.068408
C	-4.359348	-3.018526	-0.918358
C	-2.848950	-1.374966	0.038187
C	-3.037261	-1.956069	1.299082
C	-3.875592	-3.062077	1.452216
C	-4.537668	-3.594820	0.342959
H	-4.870073	-3.434038	-1.782680
H	-4.010624	-3.510332	2.432848
O	1.461999	-2.746756	-0.545620

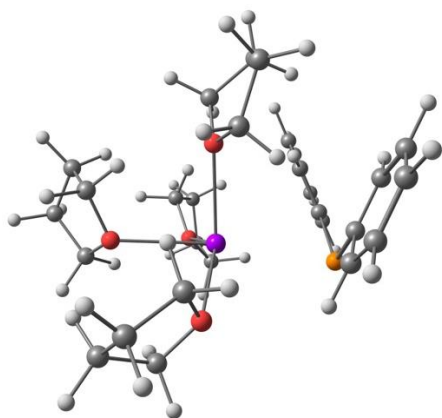
C	0.402522	-3.276813	0.292151
C	1.199604	-3.089381	-1.921715
C	-0.518392	-4.080749	-0.628861
H	0.854043	-3.879877	1.087131
H	-0.129386	-2.435158	0.747687
C	-0.291636	-3.398609	-1.984703
H	1.494423	-2.242665	-2.550939
H	1.809812	-3.959049	-2.205469
H	-1.558401	-4.045254	-0.298697
H	-0.202144	-5.129104	-0.670436
H	-0.851295	-2.460258	-2.034653
H	-0.556238	-4.028582	-2.838417
O	1.771405	2.700821	-0.229819
C	2.289565	3.328666	-1.422284
C	0.453024	3.225613	0.016158
C	1.080409	3.937963	-2.167049
H	3.021356	4.097367	-1.141810
H	2.806232	2.555063	-1.997408
C	-0.133613	3.412678	-1.377860
H	-0.078905	2.498571	0.632947
H	0.522834	4.181897	0.557356
H	1.055716	3.640875	-3.218768
H	1.121661	5.030868	-2.128177
H	-0.463187	2.441622	-1.758557
H	-0.985979	4.096600	-1.390833
C	4.797530	0.679122	-0.500892
O	3.935989	0.236783	-1.563971
C	4.492725	-1.010827	-2.002098
C	4.863225	-1.747415	-0.709430
C	5.200046	-0.593534	0.273997
H	5.381723	-0.821225	-2.622822
H	4.003443	-2.321925	-0.353345
H	5.698455	-2.436800	-0.858419
H	4.616722	-0.680678	1.192883
H	6.261027	-0.570849	0.536306
H	4.242285	1.407061	0.095071
H	5.677298	1.178848	-0.931388
H	3.741597	-1.518711	-2.611340
C	2.463270	1.264453	2.763178
O	2.491738	-0.077067	2.230128
C	1.634778	-0.929868	3.030346
C	1.126919	-0.067237	4.188889
C	1.178318	1.340747	3.580209
H	2.212958	-1.801105	3.356789
H	0.124078	-0.363050	4.508217
H	1.799133	-0.136846	5.051593
H	0.323586	1.480974	2.911865
H	1.198758	2.140306	4.325994
H	2.495915	1.964319	1.924277
H	3.348973	1.424701	3.396014
H	0.799449	-1.257367	2.405460
H	-4.139063	3.863256	1.932790
H	-5.180222	4.617367	-0.193701
H	-3.212144	1.411642	-2.283080
H	-3.365593	-1.476275	-2.049742
H	-5.189190	-4.456271	0.459767
H	-2.506067	-1.540587	2.149769

K-PPh₂(THF)₄

E (BS1) = -2334.669690

E (BS2) = -2335.227231

G_{298.15} (BS2) = -2334.653942



K	-0.521761	0.337873	-0.641483
P	1.727835	-1.623961	-2.170463
C	1.416234	-3.615475	-0.087505
C	0.846765	-2.881042	-1.156340
C	0.714132	-4.627187	0.565821
C	-0.587319	-4.964256	0.175763
C	-1.171941	-4.260239	-0.881804
C	-0.476127	-3.235248	-1.524575
H	1.194233	-5.168664	1.377834
H	-0.966439	-2.685681	-2.325288
C	4.086076	-0.249127	-1.559597
C	5.008895	0.427898	-0.764011
C	2.935550	-0.869403	-1.012477
C	2.772684	-0.755971	0.390555
C	3.702357	-0.090346	1.188717
C	4.833992	0.507423	0.622277
H	5.880782	0.883706	-1.227406
H	3.539250	-0.035958	2.263011
O	-2.804345	-0.537154	-1.781188
C	-3.633269	-1.127788	-0.758289
C	-3.535646	0.510665	-2.455962
C	-5.055797	-0.655610	-1.049227
H	-3.506072	-2.212956	-0.797536
H	-3.301709	-0.775078	0.228197
C	-4.802611	0.740725	-1.634187
H	-2.900336	1.400937	-2.519607
H	-3.766858	0.176121	-3.475764
H	-5.681821	-0.644585	-0.153038
H	-5.528615	-1.304790	-1.794420
H	-4.592385	1.452592	-0.830758
H	-5.630697	1.116937	-2.240322
O	-0.546827	-0.567250	1.870838
C	0.271953	-0.234073	3.003294
C	-1.164075	-1.860062	2.093935
C	0.736166	-1.578011	3.553157
H	1.080171	0.411293	2.650151
H	-0.322127	0.316479	3.748157
C	-0.521092	-2.442569	3.363514
H	-2.246497	-1.725972	2.204050
H	-0.973304	-2.471982	1.210613
H	1.062735	-1.517425	4.594569
H	1.563368	-1.964769	2.949845
H	-1.191799	-2.327338	4.220865
H	-0.293232	-3.504416	3.248357
C	-2.701961	1.981441	1.699693
O	-2.394068	2.075499	0.299188
C	-2.234929	3.469845	-0.052080
C	-2.184891	4.256680	1.272843
C	-1.966510	3.158965	2.327827
H	-3.074875	3.782332	-0.684158
H	-1.395096	5.012070	1.272088
H	-3.137107	4.765673	1.452198
H	-0.902218	2.919369	2.425193
H	-2.354747	3.427453	3.313923
H	-2.358424	1.004486	2.045103
H	-3.788478	2.063306	1.854670
H	-1.307450	3.554991	-0.624971

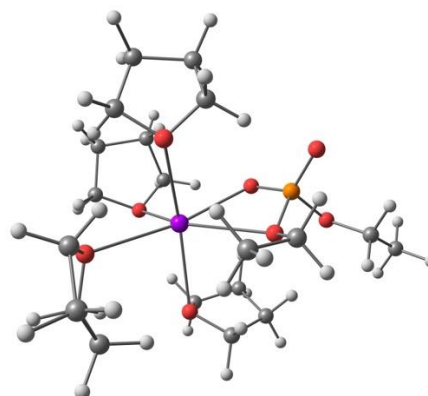
C	1.492273	3.095562	0.498657
O	0.943101	2.562614	-0.727006
C	1.865141	2.792339	-1.815705
C	2.751928	3.942480	-1.352134
C	2.877611	3.648596	0.149616
H	1.276753	3.017577	-2.710022
H	3.715346	3.957792	-1.868198
H	2.250793	4.902558	-1.519209
H	3.640137	2.883371	0.317790
H	3.130652	4.530274	0.744233
H	1.536974	2.297148	1.247849
H	0.816978	3.879292	0.862043
H	2.452661	1.883576	-1.992574
H	-2.182399	-4.502439	-1.203294
H	-1.130306	-5.756356	0.682898
H	2.434388	-3.401019	0.221678
H	4.258922	-0.314824	-2.631808
H	5.562340	1.018507	1.244915
H	1.896037	-1.190718	0.857962

K-OOP(OEt)₂(THF)₄

E (BS1) = -2330.832606

E (BS2) = -2331.454679

G_{298.15} (BS2) = -2330.908536



O	2.364706	-2.583869	-1.031672
K	-0.580465	0.344363	0.170737
O	0.481197	2.758441	0.905095
C	0.773524	2.648989	2.308188
C	2.087617	1.870940	2.357990
H	0.884273	3.654226	2.744522
H	-0.071368	2.143037	2.781230
C	2.838072	2.379703	1.104060
H	2.639821	2.044582	3.285781
H	1.892624	0.798857	2.261376
C	1.731962	3.040301	0.250849
H	3.611717	3.108369	1.362721
H	3.302471	1.546378	0.576730
H	1.869893	4.128816	0.185789
H	1.671394	2.631211	-0.760081
P	2.246913	-1.387563	-0.128386
O	1.310150	-1.339122	1.054135
O	3.719901	-0.933834	0.445835
C	4.796314	-0.793178	-0.491730
H	4.818158	-1.661798	-1.160022
H	4.630040	0.102562	-1.105656
H	6.067591	0.196464	0.951125
H	6.269917	-1.565788	0.885731
H	6.935976	-0.546629	-0.408202
C	1.977761	-0.048834	-2.476034
H	2.849247	0.569013	-2.727788
O	1.822497	-0.059007	-1.049314
H	2.165076	-1.067417	-2.825815
C	6.094378	-0.669808	0.281941
C	0.722497	0.526504	-3.111953
H	-0.145829	-0.107025	-2.906138
H	0.519991	1.534132	-2.731571
H	0.846349	0.596060	-4.198359

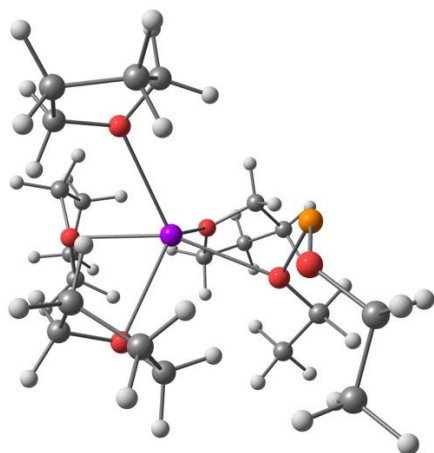
C	-0.974103	-2.749628	-1.814413
O	-1.680525	-1.574396	-1.379434
C	-3.035189	-1.975954	-1.108672
C	-2.984831	-3.471999	-0.718142
C	-1.497844	-3.852429	-0.899504
H	-3.649933	-1.820672	-2.005665
H	-3.324226	-3.636475	0.307400
H	-3.627133	-4.059420	-1.380005
H	-0.964840	-3.810603	0.055075
H	-1.362269	-4.850401	-1.324287
H	0.097318	-2.566363	-1.713323
H	-1.216185	-2.956349	-2.868789
H	-3.417804	-1.327139	-0.316440
C	-1.193962	-0.949152	3.236362
O	-1.702180	0.258994	2.640408
C	-3.139866	0.154633	2.567650
C	-3.486768	-1.346108	2.703344
C	-2.111058	-2.039663	2.694308
H	-3.447386	0.585469	1.609513
H	-4.003935	-1.533096	3.648919
H	-4.134224	-1.692994	1.893930
H	-2.087594	-2.953409	3.293807
H	-1.806893	-2.294982	1.674860
H	-1.253494	-0.881949	4.333123
H	-0.152199	-1.057616	2.927204
H	-3.591545	0.746895	3.373729
C	-2.561036	3.129867	-0.533294
O	-2.757497	1.718735	-0.716087
C	-3.068571	1.505862	-2.108618
C	-2.479876	2.707225	-2.886030
C	-1.814602	3.565734	-1.789936
H	-4.157560	1.443276	-2.233943
H	-1.765093	2.387784	-3.648400
H	-3.276085	3.265047	-3.386717
H	-0.753796	3.314936	-1.686508
H	-1.894496	4.639268	-1.980135
H	-1.992843	3.272678	0.387900
H	-3.533469	3.638378	-0.447254
H	-2.629021	0.547687	-2.393525

K-P(OEt)₂(THF)₄

E (BS1) = -2180.224660

E (BS2) = -2180.749425

G_{298.15} (BS2) = -2180.212521



K	-0.361408	0.174126	-0.089325
O	-2.265055	-1.681524	-0.621755
C	-1.771026	-2.432032	-1.757384
C	-2.141959	-3.887949	-1.487081
H	-2.256070	-2.057293	-2.668762
H	-0.692416	-2.269002	-1.833857
C	-3.450487	-3.738410	-0.699588
H	-2.251979	-4.465917	-2.408096
H	-1.375819	-4.366353	-0.868339
C	-3.169996	-2.499145	0.150489
H	-4.285587	-3.549626	-1.383190

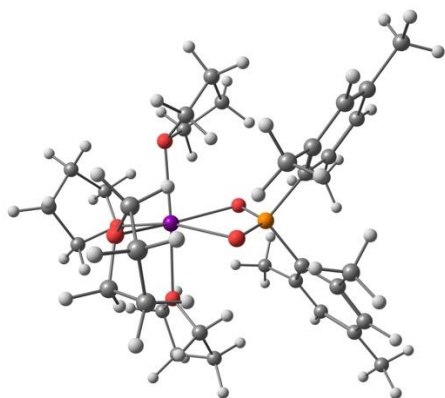
H	-3.694911	-4.612432	-0.090508
H	-4.068210	-1.915373	0.370053
H	-2.688004	-2.766047	1.100152
P	2.297692	-1.214851	-1.541417
O	3.648531	-0.561774	-0.697521
C	4.764598	-1.386213	-0.371713
H	4.733178	-2.308568	-0.970756
H	5.678603	-0.839742	-0.650264
H	4.868261	-0.810921	1.718371
H	3.923795	-2.280953	1.418640
H	5.696452	-2.332694	1.339299
C	1.414250	-3.217900	0.137194
H	1.078265	-3.858451	-0.692029
O	1.309388	-1.846639	-0.235703
H	2.460335	-3.482423	0.341705
C	4.813681	-1.721966	1.113764
C	0.557435	-3.457833	1.370690
H	0.918617	-2.864145	2.217279
H	-0.481411	-3.174501	1.175958
H	0.578220	-4.515555	1.657401
C	1.977511	0.245048	2.402199
O	0.603773	0.689181	2.414081
C	0.633080	2.109287	2.604547
C	1.799212	2.581370	1.735336
C	2.820377	1.428060	1.872524
H	0.811629	2.345215	3.665622
H	1.473566	2.680717	0.695478
H	2.196367	3.549171	2.053606
H	3.277342	1.165195	0.916444
H	3.614589	1.685117	2.579361
H	2.025761	-0.628279	1.750766
H	2.275140	-0.040258	3.420924
H	-0.343312	2.500850	2.309837
C	0.377561	2.246698	-2.896485
O	-0.520049	2.306407	-1.775911
C	-0.472405	3.650942	-1.259078
C	0.888270	4.247125	-1.691152
C	1.566526	3.095741	-2.462812
H	-0.598291	3.587004	-0.175182
H	0.733746	5.113292	-2.340806
H	1.482061	4.574099	-0.834099
H	2.169448	3.443136	-3.305890
H	2.205449	2.499855	-1.802732
H	-0.110598	2.658766	-3.793151
H	0.628248	1.195832	-3.062808
H	-1.309900	4.231008	-1.668604
C	-3.351568	2.122121	0.067553
O	-2.361677	1.683456	1.018847
C	-2.997738	0.875047	2.035018
C	-4.479452	0.764742	1.646579
C	-4.460039	1.079234	0.143168
H	-2.849956	1.344305	3.013727
H	-4.892647	-0.220100	1.878629
H	-5.070851	1.516125	2.180208
H	-4.171625	0.195741	-0.434956
H	-5.417116	1.450820	-0.232326
H	-2.867157	2.186732	-0.908895
H	-3.721207	3.119071	0.349322
H	-2.506896	-0.105720	2.051966

Na-OOPMe₂(THF)₄

E (BS1) = -2283.577256

E (BS2) = -2284.263292

G_{298.15} (BS2) = -2283.519083



O	-0.271167	-0.191402	-1.346329
Na	1.810974	-0.197646	-0.197332
P	-1.047139	0.078159	-0.058127
O	-0.161326	0.129618	1.192125
C	-1.792668	2.584219	-1.242733
C	-1.969524	1.681067	-0.164010
C	-2.502893	3.793185	-1.248207
C	-3.378505	4.152639	-0.223511
C	-3.520809	3.268405	0.847173
C	-2.834724	2.050743	0.897880
H	-2.355436	4.478175	-2.080155
C	-3.231547	-1.408834	-1.042904
C	-4.172729	-2.438269	-1.036666
C	-2.365188	-1.227762	0.075027
C	-2.502344	-2.103638	1.177449
C	-3.460199	-3.131621	1.131190
C	-4.302654	-3.320905	0.041630
H	-4.820914	-2.559920	-1.901880
H	-3.542953	-3.797891	1.987716
O	1.658794	-2.622560	-0.799145
C	0.809202	-3.361507	0.105896
C	1.171139	-2.783193	-2.152373
C	-0.032089	-4.295509	-0.759327
H	1.445848	-3.885169	0.825452
H	0.172606	-2.653949	0.642996
C	-0.188232	-3.468441	-2.041289
H	1.094047	-1.794231	-2.607447
H	1.891838	-3.396842	-2.709736
H	-0.987230	-4.540027	-0.287496
H	0.507981	-5.227828	-0.960490
H	-0.963057	-2.711849	-1.904912
H	-0.424869	-4.071320	-2.922473
O	2.149911	2.202344	-0.100167
C	2.756958	3.019139	-1.124512
C	1.360767	3.031257	0.785138
C	2.462491	4.471963	-0.742880
H	3.825858	2.794985	-1.169607
H	2.309050	2.757868	-2.090515
C	1.149026	4.344525	0.040862
H	0.449750	2.481964	1.021295
H	1.923957	3.198919	1.714247
H	2.387746	5.121747	-1.618880
H	3.253815	4.863151	-0.093435
H	0.296286	4.265075	-0.638744
H	0.967868	5.181019	0.721284
C	4.957400	0.214136	-0.698930
O	3.821828	0.000916	-1.552819
C	4.226203	-1.069220	-2.418916
C	4.921030	-2.080452	-1.497690
C	5.475458	-1.192173	-0.349485
H	4.922981	-0.678124	-3.176081
H	4.183974	-2.787776	-1.111614
H	5.703117	-2.636473	-2.021544
H	5.070042	-1.505961	0.614303
H	6.567154	-1.211152	-0.292862
H	4.624368	0.795818	0.159962
H	5.716404	0.791767	-1.247308
H	3.337604	-1.447925	-2.922887

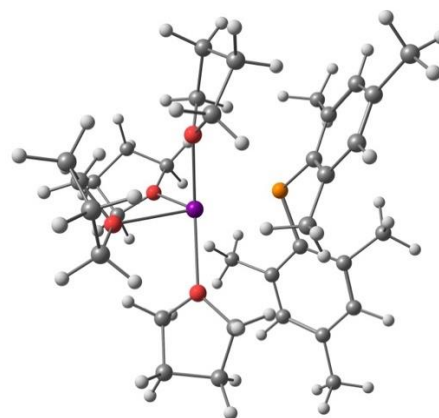
C	3.265691	0.605048	2.593948
O	3.011575	-0.611058	1.864325
C	2.274061	-1.522067	2.718069
C	1.992277	-0.773261	4.027871
C	2.129565	0.696131	3.604297
H	2.868407	-2.430817	2.866065
H	1.003755	-1.014576	4.427641
H	2.739620	-1.023752	4.788651
H	1.218168	1.021823	3.096231
H	2.352649	1.370311	4.435968
H	3.289190	1.421369	1.870814
H	4.243060	0.539340	3.096030
H	1.347250	-1.774554	2.204252
H	-4.177186	3.534282	1.672958
C	-4.152044	5.445435	-0.274696
H	-3.640923	6.193505	-0.888277
H	-5.147849	5.291208	-0.709930
H	-4.298964	5.863529	0.726243
C	-3.044614	1.181004	2.115340
H	-3.671345	0.313457	1.884771
H	-2.093253	0.800883	2.491641
H	-3.539113	1.748563	2.908598
C	-0.853206	2.344164	-2.403538
H	-1.199205	1.526752	-3.041209
H	-0.780372	3.250379	-3.012897
H	0.140379	2.056062	-2.063076
C	-5.320283	-4.432409	0.010664
H	-5.131537	-5.119168	-0.823068
H	-5.305087	-5.014248	0.936575
H	-6.334284	-4.038220	-0.125019
C	-3.174875	-0.529405	-2.270557
H	-2.159233	-0.485701	-2.667891
H	-3.850916	-0.907691	-3.042102
H	-3.470408	0.499144	-2.039501
C	-1.702426	-2.022003	2.462488
H	-2.363250	-1.740413	3.292266
H	-1.288383	-3.006009	2.711413
H	-0.897838	-1.295001	2.396115

Na-PMes₂(THF)₄

E (BS1) = -2133.012427

E (BS2) = -2133.609883

G_{298.15} (BS2) = -2132.875739



Na	0.052271	1.159226	-0.051781
P	-0.042184	-1.384836	1.482841
C	1.821932	-3.363330	0.396198
C	1.575520	-2.074763	0.958726
C	3.118176	-3.719285	-0.007609
C	4.224539	-2.891613	0.183497
C	4.002503	-1.691384	0.870329
C	2.729134	-1.280951	1.263251
H	3.265463	-4.698680	-0.461072
C	-2.550231	-2.636193	1.217053
C	-3.619458	-3.223074	0.534153
C	-1.383914	-2.211081	0.513708
C	-1.398079	-2.350186	-0.901891

C	-2.486410	-2.954293	-1.546786
C	-3.607494	-3.409554	-0.852345
H	-4.485438	-3.555118	1.104363
H	-2.457201	-3.059910	-2.629929
O	0.283832	2.505673	1.803868
C	1.121348	3.662326	1.935765
C	-0.180797	2.220805	3.131462
C	0.396388	4.571455	2.943792
H	2.104844	3.353848	2.319307
H	1.244867	4.092729	0.942297
C	-0.526283	3.594445	3.723466
H	-1.021210	1.531114	3.052082
H	0.621463	1.730930	3.700073
H	-0.193563	5.332025	2.425507
H	1.107466	5.085849	3.595009
H	-1.578374	3.833975	3.545178
H	-0.354651	3.620516	4.802434
O	2.094849	0.975178	-1.189371
C	2.671239	-0.077369	-2.002819
C	3.093350	1.979177	-0.917908
C	4.138256	0.303520	-2.219338
H	2.555444	-1.027859	-1.481841
H	2.115857	-0.113800	-2.947844
C	4.122200	1.826727	-2.031585
H	2.590949	2.947948	-0.896184
H	3.546046	1.789447	0.063804
H	4.506274	-0.011677	-3.199029
H	4.761601	-0.163141	-1.450399
H	3.772737	2.326258	-2.942372
H	5.096953	2.241259	-1.761053
C	0.319384	3.362437	-2.570381
O	0.112677	3.277703	-1.154893
C	-0.959141	4.183797	-0.845605
C	-1.887025	4.200377	-2.079961
C	-1.090068	3.427468	-3.159574
H	-0.541745	5.181983	-0.652370
H	-2.839969	3.712996	-1.864651
H	-2.096579	5.226890	-2.392365
H	-1.486695	2.415689	-3.279554
H	-1.108971	3.918518	-4.135962
H	0.897691	2.486147	-2.867017
H	0.893069	4.271252	-2.809003
H	-1.438406	3.818441	0.062754
C	-3.074345	0.732224	-1.515146
O	-2.239487	1.232441	-0.446479
C	-2.965811	1.191856	0.802380
C	-4.433824	1.040413	0.418027
C	-4.332808	0.179642	-0.847997
H	-2.746267	2.111939	1.351812
H	-5.022068	0.572210	1.211441
H	-4.873052	2.018155	0.189447
H	-4.186521	-0.868137	-0.578314
H	-5.209681	0.255094	-1.496553
H	-2.517208	-0.026308	-2.070266
H	-3.310434	1.563941	-2.189753
H	-2.614189	0.334526	1.387268
H	4.851659	-1.053520	1.111360
C	-4.783995	-4.025508	-1.567225
H	-4.517019	-4.335288	-2.582342
H	-5.163762	-4.904578	-1.034454
H	-5.619564	-3.317699	-1.649858
C	-2.668767	-2.487542	2.715367
H	-3.598012	-2.939165	3.077654
H	-1.822581	-2.953935	3.231302
H	-2.666592	-1.435089	3.023304
C	-0.273832	-1.842371	-1.763770
H	-0.059123	-0.791025	-1.548910
H	0.663753	-2.377632	-1.593687
H	-0.525897	-1.925596	-2.825491
C	5.596797	-3.271348	-0.313020
H	6.383124	-2.908114	0.357986
H	5.705316	-4.357451	-0.402502
H	5.802186	-2.845432	-1.305079
C	2.612302	-0.011549	2.068761
H	2.184549	-0.212700	3.059779

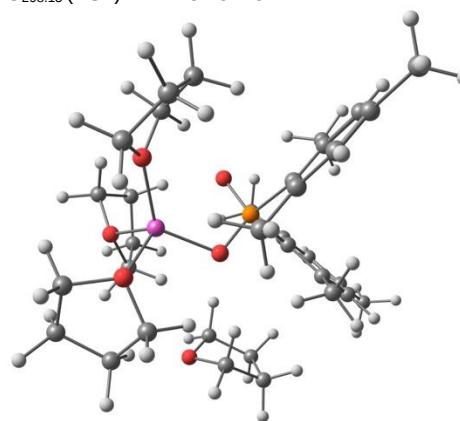
H	3.596020	0.444646	2.217974
H	1.956047	0.728391	1.605355
C	0.755055	-4.427180	0.298075
H	0.071707	-4.293881	-0.546123
H	1.218077	-5.413968	0.195058
H	0.129374	-4.432508	1.197095

Li-OOPMes₂(THF)₄

E (BS1) = - 2128.824799

E (BS2) = -2129.501062

G_{298.15} (BS2) = -2128.754152



O	0.050464	-0.452407	-0.480745
Li	1.232574	-1.789903	0.120204
P	0.062086	0.764700	0.460049
O	0.428729	0.469918	1.906488
C	2.118395	1.819608	-1.272067
C	1.265646	2.032677	-0.160013
C	3.062312	2.801405	-1.611807
C	3.201068	3.988885	-0.896418
C	2.355149	4.187708	0.197299
C	1.399369	3.241358	0.576365
H	3.710800	2.623291	-2.466343
C	-2.030448	2.113297	-0.902397
C	-3.262011	2.768913	-0.990269
C	-1.600293	1.575654	0.338718
C	-2.465890	1.677332	1.456587
C	-3.694585	2.339459	1.317223
C	-4.109370	2.902789	0.111276
H	-3.569430	3.177851	-1.950346
H	-4.347407	2.411038	2.184020
O	-3.268640	-2.446492	-0.972652
C	-3.983592	-1.712030	0.023229
C	-2.908895	-1.465730	-1.954988
C	-4.858018	-0.698127	-0.744225
H	-4.551648	-2.426722	0.625566
H	-3.278576	-1.181271	0.679477
C	-4.169237	-0.605542	-2.130940
H	-2.062844	-0.872863	-1.584902
H	-2.606619	-1.996119	-2.862267
H	-4.880668	0.264546	-0.229724
H	-5.886545	-1.056902	-0.840902
H	-3.925677	0.422299	-2.408103
H	-4.812521	-1.025727	-2.909901
O	3.064970	-1.406227	0.729926
C	4.267758	-1.617262	-0.026789
C	3.425348	-0.529838	1.817935
C	4.997855	-0.263615	-0.021009
H	4.869300	-2.394703	0.465228
H	3.974297	-1.967608	-1.017008
C	4.403557	0.480252	1.204552
H	2.497810	-0.091282	2.188134
H	3.913006	-1.125313	2.603515
H	4.794091	0.291498	-0.939356
H	6.079408	-0.402435	0.055164
H	3.870205	1.377118	0.884465
H	5.169408	0.778554	1.925270
C	1.958678	-4.245752	-1.346731

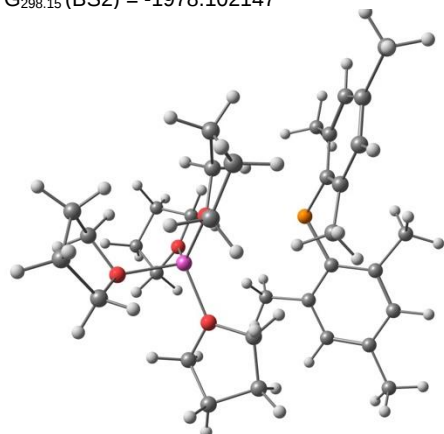
O	1.606721	-2.860561	-1.497098
C	0.588413	-2.815749	-2.515130
C	-0.293120	-4.045652	-2.254033
C	0.642314	-5.025476	-1.494934
H	1.069468	-2.868268	-3.501919
H	-1.152288	-3.773767	-1.637464
H	-0.670440	-4.468292	-3.189080
H	0.230795	-5.265489	-0.512456
H	0.797477	-5.961982	-2.036791
H	2.435892	-4.360288	-0.372108
H	2.676229	-4.518721	-2.132900
H	0.075940	-1.861732	-2.403250
C	0.891887	-3.130688	2.729462
O	0.489249	-3.136011	1.345575
C	-0.964583	-3.138604	1.278581
C	-1.466677	-2.904921	2.713397
C	-0.220788	-2.377045	3.444289
H	-1.297346	-4.099036	0.873234
H	-2.303558	-2.202850	2.739659
H	-1.803464	-3.846464	3.160004
H	-0.096109	-1.306842	3.258302
H	-0.240377	-2.571912	4.520317
H	1.871293	-2.652295	2.782835
H	0.980033	-4.166413	3.089018
H	-1.252706	-2.346521	0.587651
H	2.442581	5.104242	0.776845
C	4.220815	5.028545	-1.285661
H	4.863084	4.674240	-2.096922
H	3.735482	5.953127	-1.621208
H	4.860841	5.294767	-0.436730
C	0.545843	3.561933	1.782092
H	-0.500232	3.721884	1.501474
H	0.561105	2.736670	2.496519
H	0.904061	4.471279	2.272256
C	2.106057	0.582058	-2.141371
H	1.126328	0.397943	-2.582717
H	2.835427	0.693070	-2.949646
H	2.355594	-0.314506	-1.576244
C	-5.442728	3.593755	-0.017472
H	-6.135904	2.999869	-0.626020
H	-5.908041	3.750250	0.959808
H	-5.341353	4.568301	-0.507709
C	-1.219050	1.994435	-2.170269
H	-0.841897	0.978557	-2.297391
H	-1.830707	2.252341	-3.039047
H	-0.352024	2.661849	-2.161693
C	-2.162535	1.095088	2.818145
H	-1.275586	1.546108	3.266827
H	-3.016231	1.248159	3.485268
H	-1.952574	0.026211	2.760213

Li-PMes₂(THF)₄

E (BS1) = -1978.254535

E (BS2) = -1978.841478

G_{298.15} (BS2) = -1978.102147



Li	2.224352	-0.066576	-0.041369
P	-2.019214	-0.062404	1.622890

C	-3.687776	-1.909664	0.121329
C	-2.446502	-1.635043	0.769576
C	-3.922564	-3.165228	-0.456930
C	-3.000380	-4.210032	-0.389068
C	-1.815797	-3.967079	0.316213
C	-1.525756	-2.724475	0.883921
H	-4.874967	-3.335178	-0.957214
C	-3.147498	2.491111	1.317596
C	-3.583008	3.619601	0.619890
C	-2.680933	1.332759	0.620055
C	-2.630626	1.420171	-0.803352
C	-3.106057	2.562277	-1.462264
C	-3.595378	3.676540	-0.778657
H	-3.937900	4.478749	1.187330
H	-3.068936	2.585884	-2.550560
O	2.293165	-0.160465	1.882162
C	3.223179	-1.084309	2.480359
C	1.614636	0.472462	2.983877
C	3.759981	-0.368620	3.734329
H	2.686595	-2.004275	2.744455
H	3.984336	-1.310811	1.733297
C	2.731327	0.765871	3.988314
H	1.096578	1.350302	2.600719
H	0.870437	-0.221016	3.391549
H	4.757807	0.040117	3.556557
H	3.827187	-1.061590	4.576431
H	3.178336	1.742727	3.782392
H	2.356390	0.776218	5.014456
O	1.930327	-1.718774	-0.973275
C	0.788371	-2.093205	-1.793646
C	2.777334	-2.868743	-0.761099
C	0.979303	-3.574199	-2.132850
H	-0.126904	-1.906407	-1.231062
H	0.801174	-1.458121	-2.685201
C	2.488930	-3.781866	-1.944861
H	3.809148	-2.516349	-0.703361
H	2.507818	-3.348416	0.188358
H	0.632567	-3.809502	-3.141896
H	0.418272	-4.193938	-1.427431
H	3.041206	-3.440358	-2.827404
H	2.760395	-4.821487	-1.745265
C	4.628242	0.133038	-1.725795
O	4.159363	0.174692	-0.352627
C	4.731144	1.336750	0.282947
C	4.780299	2.381576	-0.823404
C	5.178233	1.535946	-2.047914
H	5.736134	1.094515	0.654928
H	3.787129	2.818834	-0.958971
H	5.489661	3.185592	-0.612786
H	4.769964	1.932890	-2.980322
H	6.266670	1.497751	-2.147717
H	3.766471	-0.148520	-2.343468
H	5.390444	-0.642286	-1.819519
H	4.089267	1.592402	1.127396
C	1.296199	1.730070	-2.244450
O	1.320912	1.415311	-0.831338
C	0.804867	2.532163	-0.056372
C	0.724349	3.704196	-1.030047
C	0.463970	3.003320	-2.370387
H	1.491221	2.711036	0.775833
H	-0.069013	4.402904	-0.754870
H	1.674433	4.248964	-1.057855
H	-0.596417	2.759433	-2.461539
H	0.761667	3.602021	-3.234920
H	0.870130	0.876779	-2.777533
H	2.325233	1.887172	-2.586959
H	-0.175462	2.249126	0.334181
H	-1.090668	-4.772236	0.426412
C	-4.123531	4.884862	-1.511102
H	-3.734199	4.934217	-2.533403
H	-5.219716	4.870008	-1.582768
H	-3.851717	5.816178	-1.001591
C	-3.175773	2.532950	2.825883
H	-3.626119	3.464492	3.183851
H	-3.737536	1.686059	3.236820

H	-2.168225	2.461649	3.255283
C	-1.987641	0.343812	-1.636223
H	-1.017004	0.080332	-1.203960
H	-2.569473	-0.582209	-1.672080
H	-1.837200	0.686296	-2.664985
C	-3.260866	-5.542111	-1.046943
H	-2.951790	-6.376906	-0.407349
H	-4.322906	-5.671922	-1.278760
H	-2.707628	-5.643548	-1.990846
C	-0.221136	-2.571431	1.627972
H	-0.386080	-2.357325	2.691556
H	0.370600	-3.490583	1.564224
H	0.372142	-1.739750	1.237884
C	-4.807826	-0.902184	0.080648
H	-4.633031	-0.096042	-0.639554
H	-5.753244	-1.387454	-0.182621
H	-4.921226	-0.414465	1.055957

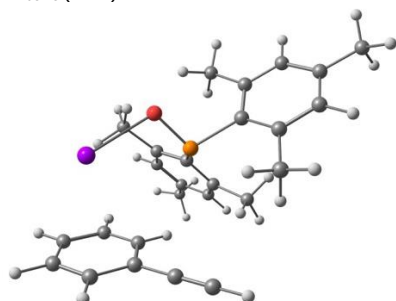
Modes of Interaction

K-OPMe₂ + phenylacetylene

E (BS1) = -2024.309379

E (BS2) = -2024.768771

G_{298.15} (BS2) = -2024.375413



6	-2.175248	-2.371092	-2.070408
6	-1.408437	-2.986015	-2.777498
19	-2.090335	-1.797695	2.240336
1	-0.728644	-3.524898	-3.400682
6	-2.864874	-0.259974	-1.016985
6	-3.067949	-1.639067	-1.227717
6	-4.133868	-2.289483	-0.570203
6	-4.972324	-1.569937	0.285747
6	-4.758314	-0.200673	0.496940
6	-3.705638	0.449720	-0.159077
1	-2.040688	0.238273	-1.510793
1	-4.294216	-3.350419	-0.733809
1	-5.792984	-2.076550	0.784989
1	-5.411243	0.354945	1.163431
1	-3.527489	1.507819	0.001192
15	0.416067	-0.597432	0.492142
8	0.171327	-0.827096	2.040710
6	3.121439	0.299099	1.020148
6	2.286880	-0.585586	0.294904
6	4.510346	0.236029	0.862260
6	5.116222	-0.693104	0.011989
6	4.289563	-1.594036	-0.661744
6	2.894375	-1.561865	-0.529940
1	5.135217	0.927900	1.424399
1	4.739971	-2.348091	-1.304430
6	0.275745	1.590852	-1.300178
6	-0.140991	2.841759	-1.761139
6	0.039875	1.198538	0.048264
6	-0.668194	2.103321	0.876635
6	-1.070157	3.351138	0.372545
6	-0.812707	3.750471	-0.936716
1	0.057359	3.110298	-2.797243
1	-1.600365	4.030682	1.038617
6	-1.222590	5.109660	-1.445248
1	-1.623425	5.053263	-2.462978
1	-1.984251	5.563642	-0.804256
1	-0.367907	5.797515	-1.476413
6	-1.067111	1.811169	2.310845
1	-0.900940	2.691508	2.941516

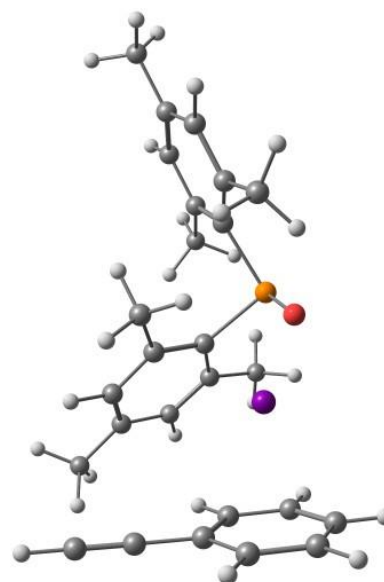
1	-2.144693	1.591285	2.364333
1	-0.524502	0.958980	2.713109
6	0.929951	0.662577	-2.294440
1	0.450300	-0.322731	-2.279523
1	0.848744	1.065030	-3.308380
1	1.989668	0.502172	-2.076529
6	2.553366	1.310821	1.985595
1	2.126065	2.171281	1.460298
1	1.751186	0.856831	2.571380
1	3.331099	1.681306	2.660662
6	2.094737	-2.588791	-1.303154
1	1.291859	-3.022366	-0.702781
1	1.617372	-2.149286	-2.185589
1	2.746853	-3.396763	-1.649452
6	6.612248	-0.714402	-0.178431
1	6.916577	-0.041326	-0.990757
1	7.136274	-0.386549	0.725013
1	6.969490	-1.716080	-0.437488

Na-OPMe₂ + phenylacetylene

E (BS1) = -1586.708673

E (BS2) = -1587.135416

G_{298.15} (BS2) = -1586.738537



11	-1.439578	-1.830864	-0.099243
15	1.056283	-0.330218	-1.379813
6	0.101892	0.769676	-0.159014
6	0.050326	0.522383	1.238491
6	-0.723932	1.794652	-0.688425
6	-0.780095	1.299685	2.058170
6	-1.532442	2.554865	0.165758
6	-1.569007	2.331250	1.544222
1	-0.807203	1.091494	3.126214
1	-2.162556	3.331492	-0.261075
6	2.750419	-0.325663	-0.556528
6	3.447647	0.915841	-0.551275
6	3.455487	-1.480383	-0.139563
6	4.767473	0.985900	-0.102785
6	4.788095	-1.365556	0.289619
6	5.463693	-0.148669	0.327869
1	5.270113	1.951632	-0.101618
1	5.307462	-2.268228	0.607566
8	0.366643	-1.750014	-1.179034
6	-4.311171	1.606915	-2.228640
6	-4.254783	0.672529	-1.461653
1	-4.363363	2.431339	-2.906065
6	-4.184644	-0.429868	-0.555399
6	-3.936171	-0.209341	0.816231
6	-4.348787	-1.752565	-1.023031
6	-3.849592	-1.289767	1.697107
6	-4.266565	-2.827178	-0.133247
6	-4.015392	-2.600643	1.228153

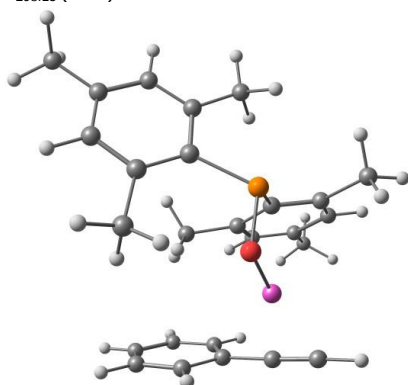
1	-3.799884	0.803372	1.174439
1	-4.538564	-1.924788	-2.077164
1	-3.652683	-1.107962	2.748970
1	-4.399461	-3.89731	-0.501339
1	-3.954007	-3.437671	1.916637
6	-0.775885	2.104698	-2.168468
1	0.193402	2.442176	-2.547400
1	-1.057181	1.227488	-2.758274
1	-1.507546	2.893328	-2.364805
6	0.860098	-0.573540	1.897483
1	0.416870	-0.853896	2.858427
1	0.929040	-1.461017	1.265899
1	1.888012	-0.248211	2.088056
6	-2.436655	3.172762	2.445708
1	-3.328605	3.530836	1.922146
1	-2.757529	2.612835	3.329669
1	-1.893596	4.057490	2.802084
6	2.798563	2.193143	-1.029455
1	3.542031	2.988545	-1.134311
1	2.313307	2.050697	-2.001692
1	2.024104	2.544644	-0.340410
6	2.851907	-2.868316	-0.079268
1	2.010664	-2.976868	-0.761788
1	3.616671	-3.623108	-0.292768
1	2.472516	-3.079331	0.930421
6	6.894897	-0.050353	0.793578
1	6.999742	0.666228	1.617020
1	7.268807	-1.018116	1.140674
1	7.555150	0.293486	-0.012202

Li-OPMe₂ + phenylacetylene

E (BS1) = -1431.957660

E (BS2) = -1432.371280

G_{298.15} (BS2) = -1431.971496



15	-1.172907	1.066108	1.557219
6	0.103419	1.540112	0.231303
6	0.690127	2.831165	0.335381
6	0.609956	0.646801	-0.750152
6	1.734046	3.196523	-0.520309
6	1.653593	1.059380	-1.592070
6	2.228083	2.326570	-1.497890
1	2.171789	4.187710	-0.422605
1	2.029486	0.360714	-2.335206
6	-2.424273	0.118120	0.539516
6	-3.159513	0.881354	-0.408285
6	-2.820165	-1.220063	0.774160
6	-4.215069	0.300400	-1.113895
6	-3.896467	-1.757775	0.052010
6	-4.603814	-1.025827	-0.900345
1	-4.753428	0.903446	-1.842890
1	-4.182998	-2.790423	0.243454
8	-0.294742	0.046485	2.432127
3	1.362405	0.167517	1.867670
6	3.669918	0.456452	2.086305
6	3.515924	-0.514216	1.371943
1	3.861913	1.300743	2.715588
6	3.267616	-1.639263	0.523796
6	3.741897	-1.639784	-0.800991

6	2.509697	-2.726887	0.998586
6	3.458274	-2.717088	-1.634952
6	2.224147	-3.793977	0.150790
6	2.696605	-3.790994	-1.163691
1	4.319439	-0.795688	-1.160774
1	2.146949	-2.722486	2.021954
1	3.825644	-2.716979	-2.656246
1	1.632775	-4.626896	0.516956
1	2.471551	-4.624665	-1.821569
6	0.217715	3.847399	1.352451
1	-0.826769	4.128873	1.184749
1	0.277492	3.464851	2.376136
1	0.826152	4.754579	1.293829
6	0.089552	-0.760834	-0.930995
1	0.809246	-1.360636	-1.492718
1	-0.094866	-1.253387	0.024023
1	-0.857944	-0.766165	-1.478526
6	3.336855	2.753429	-2.425461
1	4.125134	3.289073	-1.886220
1	3.788668	1.894325	-2.929703
1	2.960318	3.431789	-3.201335
6	-2.116048	-2.153299	1.735734
1	-2.809726	-2.923061	2.089657
1	-1.288293	-2.675061	1.235916
1	-1.680794	-1.625181	2.581878
6	-2.822210	2.325878	-0.696687
1	-1.891275	2.421915	-1.265260
1	-3.619660	2.800275	-1.275689
1	-2.685867	2.899312	0.227835
6	-5.766299	-1.624732	-1.651701
1	-6.722786	-1.226180	-1.290001
1	-5.711007	-1.397659	-2.722236
1	-5.798218	-2.712259	-1.536601

Intermediates, transition states, and products in the Gibbs energy profiles

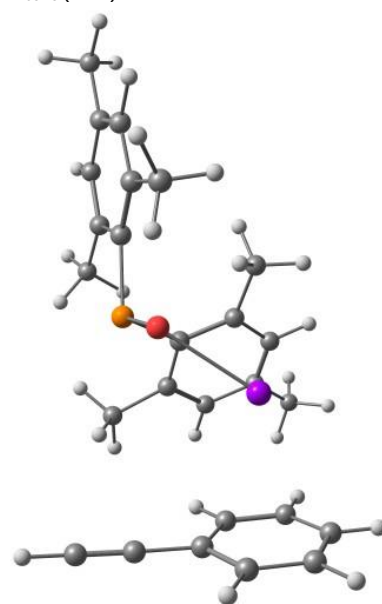
Hydrophosphorylation catalyzed by K-OPMe₂

Int-TS-1-Mes-K

E (BS1) = -2024.310337

E (BS2) = -2024.768574

G_{298.15} (BS2) = -2024.374780



6	-3.717662	-1.729829	2.103690
6	-3.313519	-2.217754	3.135314
19	-1.586600	-1.218935	-1.498438

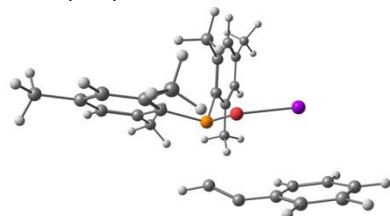
1	-2.955074	-2.649444	4.044620
6	-4.743587	-1.939225	-0.131691
6	-4.166081	-1.141914	0.880114
6	-3.995881	0.240495	0.655398
6	-4.382712	0.807666	-0.559919
6	-4.951035	0.010886	-1.561692
6	-5.133420	-1.361228	-1.341970
1	-4.876444	-3.002543	0.039317
1	-3.544265	0.852282	1.426596
1	-4.232852	1.869709	-0.725544
1	-5.252719	0.455186	-2.505299
1	-5.579714	-1.981404	-2.113427
15	1.055104	-0.926128	0.809188
8	0.394472	-1.950384	-0.200014
6	0.309751	1.218626	-1.035169
6	0.252755	0.722464	0.294208
6	-0.456371	2.331264	-1.408588
6	-1.277410	3.000283	-0.495001
6	-1.330926	2.508277	0.809879
6	-0.600758	1.380805	1.212987
1	-0.404352	2.684898	-2.437180
1	-1.976185	3.001731	1.533622
6	3.537339	0.417224	1.037908
6	4.900814	0.631940	0.831978
6	2.838033	-0.574641	0.292548
6	3.585341	-1.358337	-0.619955
6	4.959915	-1.118405	-0.784793
6	5.639402	-0.126447	-0.083237
1	5.403170	1.404988	1.411169
1	5.509732	-1.734482	-1.494881
6	2.989916	-2.447420	-1.488860
1	3.704695	-3.269342	-1.609722
1	2.048618	-2.817026	-1.084146
1	2.778994	-2.061943	-2.496389
6	2.841965	1.261231	2.078976
1	2.133111	1.965297	1.632131
1	2.268938	0.635684	2.772688
1	3.568377	1.836328	2.660511
6	7.114674	0.117402	-0.281327
1	7.674696	-0.036040	0.649264
1	7.532040	-0.554706	-1.036971
1	7.310746	1.147477	-0.603097
6	1.166487	0.563438	-2.096806
1	2.210874	0.881221	-2.015013
1	1.165686	-0.522670	-1.988429
1	0.815643	0.831264	-3.099224
6	-0.786677	0.895448	2.633692
1	-1.525140	1.513749	3.153440
1	-1.131518	-0.142143	2.665368
1	0.144664	0.935828	3.205802
6	-2.077258	4.209770	-0.909400
1	-2.869412	4.431353	-0.188177
1	-1.439971	5.100129	-0.981063
1	-2.537819	4.067263	-1.893062

TS-1-Mes-K

E (BS1) = -2024.295269

E (BS2) = -2024.754333

G_{298.15} (BS2) = -2024.359203



6	-1.722775	-2.280945	1.673361
6	-0.524493	-1.940060	1.844568
19	-2.639565	0.149383	-1.596666
1	0.348410	-2.105250	2.452476
6	-3.348107	-2.942248	-0.081520
6	-2.947852	-2.095583	0.990044
6	-3.831601	-1.039003	1.352949

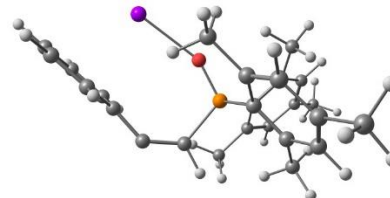
6	-5.031107	-0.836383	0.668546
6	-5.398337	-1.666757	-0.400947
6	-4.542645	-2.721802	-0.762361
1	-2.694718	-3.757263	-0.376914
1	-3.558065	-0.385019	2.175039
1	-5.683057	-0.020248	0.970399
1	-6.333588	-1.508175	-0.928761
1	-4.813653	-3.379356	-1.584445
15	0.372317	-0.424142	0.134572
8	-0.415882	-0.860426	-1.135167
6	0.689321	2.170331	-1.043691
6	0.258980	1.453481	0.108421
6	0.420684	3.537239	-1.150050
6	-0.274070	4.237753	-0.156097
6	-0.704886	3.524365	0.960295
6	-0.452317	2.150789	1.112752
1	0.759277	4.070488	-2.036276
1	-1.254279	4.043453	1.742944
6	3.000480	-0.350309	1.094641
6	4.350199	-0.700145	1.138335
6	2.190121	-0.761149	0.000202
6	2.775017	-1.568903	-1.005904
6	4.134538	-1.904160	-0.912354
6	4.944036	-1.478435	0.138899
1	4.951251	-0.365562	1.981660
1	4.569010	-2.521114	-1.696517
6	2.033663	-2.071100	-2.225081
1	2.507523	-2.982073	-2.604528
1	0.979739	-2.253102	-2.020836
1	2.071074	-1.327371	-3.031561
6	2.442153	0.473392	2.230434
1	2.234178	1.502785	1.921404
1	1.499451	0.060600	2.603665
1	3.148256	0.507623	3.064639
6	6.403668	-1.849066	0.212258
1	6.628283	-2.406137	1.129712
1	6.701305	-2.468751	-0.638459
1	7.041249	-0.956752	0.218067
6	1.424967	1.497048	-2.177418
1	2.436964	1.206661	-1.877489
1	0.906608	0.584511	-2.479950
1	1.506222	2.168262	-3.037104
6	-0.942835	1.501414	2.386751
1	-1.852840	1.994477	2.743450
1	-1.142451	0.437667	2.266671
1	-0.193260	1.598010	3.182209
6	-0.530166	5.717285	-0.290447
1	-1.299445	6.055369	0.409762
1	0.380738	6.293308	-0.084307
1	-0.849973	5.977939	-1.305067

Z-1I-Mes-K

E (BS1) = -2024.324769

E (BS2) = -2024.786595

G_{298.15} (BS2) = -2024.384312



15	-0.104040	-0.104626	-0.204831
6	-1.449274	-1.347023	0.010354
6	-2.245045	-1.231344	1.182652
6	-1.662980	-2.439397	-0.861896
6	-3.250461	-2.170097	1.424786
6	-2.683015	-3.355519	-0.569705
6	-3.495449	-3.236842	0.556317
1	-3.855580	-2.066169	2.322592
1	-2.839937	-4.189654	-1.248798
6	-0.931401	1.545258	-0.171689
6	-2.111347	1.776840	-0.919070

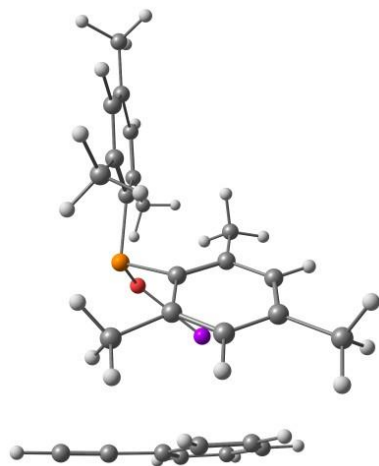
6	-0.336904	2.626911	0.530761
6	-2.695785	3.050028	-0.903852
6	-0.960821	3.877363	0.512041
6	-2.147302	4.111714	-0.187566
1	-3.605123	3.211094	-1.477738
1	-0.498200	4.696765	1.057676
8	0.876705	-0.305890	0.945492
19	3.121221	-0.513109	1.916163
6	0.700435	-0.098728	-1.839770
6	2.013728	-0.160549	-2.059718
1	-0.009708	0.057503	-2.656886
6	3.157355	-0.331245	-1.256037
6	3.939208	0.785346	-0.804244
6	3.704117	-1.626967	-0.968014
6	5.152106	0.613499	-0.145264
6	4.919600	-1.779897	-0.309379
6	5.667091	-0.668279	0.122689
1	3.576263	1.788382	-1.009894
1	3.153807	-2.506205	-1.291480
1	5.707420	1.494068	0.171440
1	5.291141	-2.784766	-0.118934
1	6.622204	-0.795350	0.621681
6	-4.600818	-4.222014	0.835942
1	-4.546991	-4.598917	1.863196
1	-5.584732	-3.751520	0.718872
1	-4.556477	-5.076717	0.155349
6	-2.075327	-0.121987	2.197722
1	-1.022202	0.084121	2.397962
1	-2.532767	0.810207	1.851125
1	-2.559547	-0.399147	3.138166
6	-0.867453	-2.690191	-2.121548
1	-1.074163	-1.937106	-2.889111
1	0.209330	-2.670546	-1.946090
1	-1.130015	-3.666160	-2.538416
6	-2.793725	5.473073	-0.176679
1	-3.075230	5.768836	0.840888
1	-2.107666	6.240297	-0.553869
1	-3.695409	5.492185	-0.794917
6	-2.816574	0.719702	-1.741782
1	-3.435319	0.068747	-1.116523
1	-3.473148	1.199874	-2.472470
1	-2.129237	0.076569	-2.293809
6	0.958938	2.521218	1.305578
1	1.767622	2.127348	0.683750
1	1.255416	3.510677	1.664687
1	0.858632	1.855936	2.167186

Int-TS-1M-Mes-K

E (BS1) = -2024.310285

E (BS2) = -2024.768582

G_{298.15} (BS2) = -2024.374569



15	-1.055463	-0.926320	0.815480
6	-0.253013	0.720530	0.294843
6	-0.310257	1.212768	-1.035933
6	0.599776	1.382312	1.211782
6	0.454361	2.325479	-1.412269

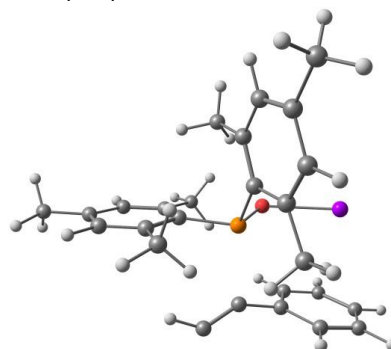
6	1.328227	2.509842	0.805851
6	1.273986	2.998390	-0.500321
1	0.402131	2.676135	-2.441873
1	1.972669	3.006161	1.528373
6	-2.837921	-0.575715	0.296389
6	-3.537064	0.419617	1.037232
6	-3.584889	-1.361859	-0.614268
6	-4.899815	0.635777	0.828017
6	-4.958768	-1.120350	-0.782474
6	-5.637904	-0.124639	-0.085910
1	-5.402027	1.411611	1.403600
1	-5.508320	-1.738254	-1.491183
8	-0.394837	-1.954170	-0.190106
19	1.583831	-1.226609	-1.493918
6	3.329522	-2.203109	3.142039
6	3.728035	-1.718656	2.106606
1	2.975926	-2.631753	4.054689
6	4.170374	-1.134745	0.878914
6	4.746562	-1.934674	-0.131576
6	3.995857	0.246285	0.649137
6	5.130985	-1.360581	-1.345437
6	4.377372	0.809550	-0.569670
6	4.944485	0.010186	-1.570067
1	4.882744	-2.996944	0.043289
1	3.545201	0.860059	1.419320
1	5.576337	-1.982787	-2.115805
1	4.224397	1.870561	-0.738988
1	5.242141	0.451502	-2.516358
6	-1.165677	0.553393	-2.096075
1	-1.166402	-0.532162	-1.982554
1	-2.209839	0.872858	-2.017948
1	-0.812581	0.816016	-3.099117
6	2.071677	4.208285	-0.917700
1	2.864855	4.431765	-0.198181
1	2.530623	4.065146	-1.902014
1	1.433195	5.097802	-0.989267
6	0.786526	0.900503	2.633522
1	-0.144578	0.941869	3.205955
1	1.131858	-0.136852	2.667674
1	1.524910	1.520420	3.151472
6	-2.842259	1.266300	2.076524
1	-3.569006	1.843104	2.655946
1	-2.269785	0.642608	2.772337
1	-2.133031	1.969069	1.628213
6	-2.989767	-2.455445	-1.477720
1	-2.049636	-2.824744	-1.070056
1	-3.705613	-3.276785	-1.596194
1	-2.776734	-2.074560	-2.486556
6	-7.112362	0.121022	-0.287817
1	-7.305965	1.150136	-0.614132
1	-7.529473	-0.553382	-1.041559
1	-7.674446	-0.027672	0.642299

TS-1M-Mes-K

E (BS1) = -2024.299940

E (BS2) = -2024.763797

G_{298.15} (BS2) = -2024.361533



15	0.007407	-0.255452	-0.122548
6	-0.171651	1.609010	-0.012213
6	-0.940190	2.315221	-0.971866
6	0.571993	2.340994	0.940919

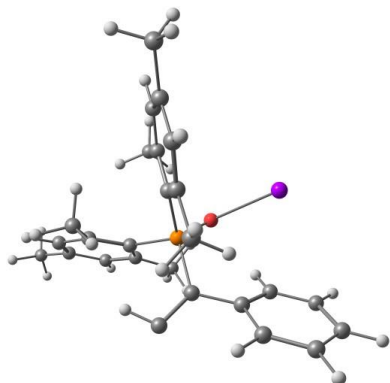
6	-0.985580	3.713030	-0.923415
6	0.498725	3.740088	0.954110
6	-0.284469	4.446007	0.038668
1	-1.583775	4.243122	-1.661871
1	1.069179	4.289097	1.700069
6	-1.744147	-0.842753	-0.085506
6	-2.552614	-0.497254	1.024015
6	-2.248380	-1.772147	-1.032352
6	-3.848311	-1.020145	1.132772
6	-3.548998	-2.262787	-0.883965
6	-4.373515	-1.894830	0.183978
1	-4.455045	-0.737116	1.990237
1	-3.927631	-2.963517	-1.625371
8	0.685330	-0.488941	-1.507014
19	2.989582	0.446593	-1.697780
6	0.104440	-2.397301	2.285950
6	0.882749	-1.822496	1.453703
1	-0.945339	-2.195948	2.477797
6	2.254617	-1.923940	0.955498
6	2.529740	-2.650406	-0.221257
6	3.324768	-1.278929	1.605814
6	3.828488	-2.722725	-0.732284
6	4.621286	-1.337646	1.086411
6	4.879757	-2.055558	-0.088238
1	1.714629	-3.152612	-0.729603
1	3.133025	-0.738913	2.526648
1	4.020634	-3.298003	-1.634084
1	5.432219	-0.835395	1.606505
1	5.888946	-2.110027	-0.486249
6	-1.712755	1.611463	-2.061789
1	-1.108978	0.818858	-2.509671
1	-2.622861	1.145977	-1.670730
1	-2.006432	2.319762	-2.842002
6	-0.386287	5.949163	0.094246
1	0.483539	6.391965	0.588635
1	-0.470993	6.382354	-0.907500
1	-1.275815	6.260830	0.656575
6	1.471952	1.668099	1.951692
1	0.943384	0.927864	2.557237
1	2.296447	1.132800	1.470363
1	1.912915	2.407919	2.625971
6	-2.085502	0.438764	2.115340
1	-2.719382	0.331906	3.000265
1	-1.057630	0.228068	2.418072
1	-2.125501	1.485803	1.799229
6	-1.447217	-2.277863	-2.211146
1	-0.526228	-2.771371	-1.889151
1	-2.042279	-2.994973	-2.784836
1	-1.135207	-1.467715	-2.872817
6	-5.778238	-2.430278	0.297980
1	-6.440382	-1.967809	-0.445058
1	-5.809451	-3.511507	0.124242
1	-6.201766	-2.232059	1.286856

ZM-1I-Mes-K

E (BS1) = -2024.280915

E (BS2) = -2024.741865

G_{298.15} (BS2) = -2024.345254



15	-0.112740	-0.391752	-0.157770
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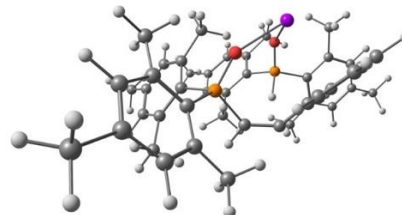
6	0.039070	1.449852	0.074944
6	-0.671302	2.261361	-0.860321
6	0.908935	2.080256	0.999111
6	-0.492427	3.647147	-0.846018
6	1.050330	3.476906	0.966601
6	0.362623	4.280401	0.060300
1	-1.042454	4.249361	-1.565580
1	1.721108	3.944049	1.683251
6	-1.894039	-0.811440	0.055333
6	-2.775083	-0.097132	0.902151
6	-2.385441	-1.925257	-0.673609
6	-4.129253	-0.454523	0.932262
6	-3.745975	-2.238824	-0.608696
6	-4.641989	-1.503565	0.169963
1	-4.797244	0.099166	1.587702
1	-4.110261	-3.094271	-1.172587
8	0.366227	-0.592565	-1.609814
19	2.620287	0.464907	-2.113463
6	0.217292	-1.775768	2.254635
6	0.771967	-1.420062	1.061859
1	-0.818988	-1.390528	2.315701
6	2.178199	-1.811895	0.727114
6	2.576896	-2.271215	-0.546648
6	3.163303	-1.772508	1.733398
6	3.904488	-2.632150	-0.807973
6	4.485566	-2.132459	1.476424
6	4.870123	-2.551354	0.198958
1	1.828034	-2.363524	-1.325076
1	2.857445	-1.465099	2.727802
1	4.175723	-2.998219	-1.795766
1	5.220286	-2.084483	2.276117
1	5.900646	-2.829578	-0.002617
6	-1.657310	1.711713	-1.869142
1	-1.272311	0.821301	-2.367417
1	-2.599451	1.433626	-1.385509
1	-1.883845	2.471190	-2.622385
6	0.513335	5.779545	0.064991
1	1.383227	6.092361	0.649203
1	0.620866	6.172956	-0.951456
1	-0.370833	6.259557	0.502447
6	1.715437	1.352566	2.048850
1	1.092174	0.725970	2.689303
1	2.464181	0.688629	1.609834
1	2.242193	2.076451	2.676254
6	-2.354505	1.030345	1.819411
1	-3.087581	1.136883	2.623874
1	-1.381843	0.849700	2.279292
1	-2.298276	1.989169	1.295506
6	-1.496759	-2.833862	-1.492441
1	-0.665514	-3.213957	-0.889277
1	-2.071457	-3.690660	-1.854445
1	-1.051783	-2.311855	-2.341212
6	-6.110672	-1.839733	0.190613
1	-6.630492	-1.375472	-0.657271
1	-6.274279	-2.919521	0.117254
1	-6.590301	-1.479720	1.105510

Int-TS-2-Mes-K

E (BS1) = -3140.883407

E (BS2) = -3141.650673

G_{298.15} (BS2) = -3140.913617



15	2.434863	-0.295043	-0.032150
6	4.251939	-0.595751	0.164878
6	5.084380	-0.138635	-0.894787
6	4.842825	-1.294755	1.246217
6	6.461449	-0.366138	-0.839629

6	6.230613	-1.499210	1.247760
6	7.059251	-1.044787	0.224333
1	7.082985	-0.002897	-1.654959
1	6.673090	-2.032959	2.084999
6	2.245304	1.551281	-0.098408
6	2.777395	2.359626	0.941468
6	1.437570	2.166272	-1.091659
6	2.448603	3.718517	0.999916
6	1.140676	3.530522	-0.984081
6	1.616448	4.323737	0.057976
1	2.852629	4.316677	1.813197
1	0.500691	3.979663	-1.739393
8	1.988580	-0.991450	-1.312689
19	-0.023651	-2.058979	-2.338088
6	1.429892	-0.743005	1.426164
6	0.589195	-1.778972	1.605334
1	1.553358	-0.001073	2.220020
6	0.374505	-2.911615	0.738324
6	-0.951264	-3.306818	0.394008
6	1.416258	-3.776916	0.294204
6	-1.211097	-4.431096	-0.387074
6	1.149889	-4.915862	-0.463228
6	-0.162517	-5.252831	-0.830551
1	-1.781376	-2.718646	0.770994
1	2.445016	-3.526330	0.530849
1	-2.240943	-4.680597	-0.632055
1	1.978079	-5.542059	-0.788553
1	-0.363625	-6.141502	-1.421317
15	-2.390928	-0.023429	-0.192315
6	-2.684548	1.771521	-0.079906
6	-3.650025	2.369657	-0.928068
6	-1.882205	2.583280	0.757235
6	-3.802985	3.756357	-0.913042
6	-2.076117	3.970090	0.734910
6	-3.023116	4.576240	-0.089970
1	-4.544646	4.208444	-1.567111
1	-1.456914	4.590626	1.376676
6	-3.895377	-0.945356	0.286596
6	-4.362848	-0.817528	1.620391
6	-4.563805	-1.816121	-0.608233
6	-5.499656	-1.522307	2.018460
6	-5.702858	-2.496103	-0.157079
6	-6.192052	-2.361648	1.141852
1	-5.848200	-1.415506	3.042710
1	-6.217197	-3.158662	-0.848427
8	-1.825143	-0.430585	-1.544723
1	-1.513734	-0.292677	0.870042
6	4.094038	-1.834685	2.443493
1	3.309667	-2.539256	2.168113
1	4.792041	-2.347010	3.110997
1	3.606283	-1.043404	3.018997
6	4.555579	0.604456	-2.100838
1	5.342803	0.714188	-2.851162
1	3.711533	0.076881	-2.549111
1	4.205475	1.606382	-1.833484
6	8.545129	-1.294235	0.247245
1	8.823643	-2.073408	-0.473185
1	9.104300	-0.392439	-0.024247
1	8.880326	-1.621433	1.235468
6	-0.813008	2.038499	1.671831
1	-1.232301	1.433094	2.480644
1	-0.097707	1.411910	1.139640
1	-0.254694	2.859592	2.124603
6	-4.506893	1.554735	-1.864877
1	-3.887202	0.963358	-2.545087
1	-5.151354	0.856953	-1.321279
1	-5.146404	2.205247	-2.466135
6	-3.184064	6.073865	-0.120053
1	-4.240040	6.361800	-0.082057
1	-2.667663	6.548077	0.718909
1	-2.771007	6.491845	-1.046438
6	3.721770	1.849124	2.006919
1	3.362080	0.946073	2.501138
1	4.705750	1.616581	1.589656
1	3.857054	2.610140	2.779750

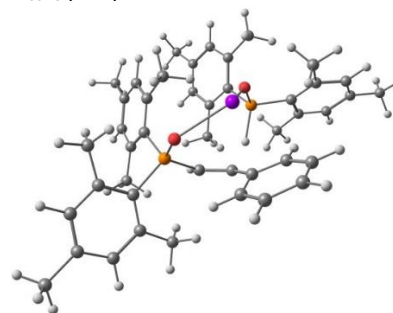
6	0.836311	1.451497	-2.281229
1	1.561189	0.812375	-2.784472
1	-0.011309	0.828627	-1.981959
1	0.460181	2.190723	-2.994957
6	1.259372	5.784877	0.148471
1	1.991472	6.404976	-0.384596
1	0.279671	5.981222	-0.297302
1	1.240380	6.127174	1.187749
6	-3.656277	0.033669	2.646535
1	-4.182465	-0.008652	3.602878
1	-2.631675	-0.316674	2.816804
1	-3.600618	1.082532	2.341243
6	-4.111378	-2.107044	-2.021802
1	-3.200835	-2.714698	-2.015391
1	-4.886070	-2.672532	-2.546850
1	-3.884842	-1.207100	-2.591355
6	-7.429046	-3.093555	1.592753
1	-8.258475	-2.395157	1.757904
1	-7.752430	-3.827946	0.850229
1	-7.256632	-3.615670	2.540076

TS-2-Mes-K

E (BS1) = -3140.872301

E (BS2) = -3141.633891

G_{298.15} (BS2) = -3140.895102



15	-2.374936	-0.383538	0.194538
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6	-5.108000	-0.308044	0.720700
6	-4.559886	-1.411715	-1.393844
6	-6.458792	-0.575746	0.487014
6	-5.928112	-1.657319	-1.576194
6	-6.893035	-1.251644	-0.655599
1	-7.190882	-0.245371	1.220300
1	-6.245106	-2.181379	-2.474321
6	-2.207931	1.464041	0.313597
6	-2.710291	2.295335	-0.724653
6	-1.439262	2.056854	1.346999
6	-2.428787	3.664842	-0.711218
6	-1.187286	3.434783	1.310263
6	-1.663113	4.258005	0.293963
1	-2.815834	4.282790	-1.518049
1	-0.579668	3.868591	2.100121
8	-2.065490	-1.113880	1.497905
19	0.083554	-2.038874	2.480542
6	-1.170034	-0.668923	-1.128696
6	-0.148446	-1.553316	-1.245685
1	-1.149481	0.214329	-1.766124
6	-0.069059	-2.840863	-0.547255
6	1.204084	-3.411047	-0.290533
6	-1.194558	-3.616828	-0.173187
6	1.347140	-4.630034	0.370608
6	-1.054998	-4.848221	0.467763
6	0.215636	-5.357192	0.763686
1	2.091736	-2.880326	-0.617337
1	-2.189851	-3.236616	-0.365675
1	2.342145	-5.021611	0.565060
1	-1.943052	-5.409768	0.747043
1	0.322325	-6.312805	1.268683
15	2.237581	-0.126042	-0.018607
6	2.365249	1.717894	-0.119421
6	3.077481	2.407642	0.902201
6	1.659370	2.465545	-1.084266

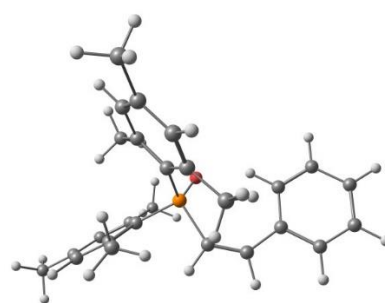
6	3.065198	3.800928	0.926494
6	1.675601	3.868551	-1.017221
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1	3.615719	4.315850	1.710908
1	1.123917	4.429138	-1.768255
6	3.930123	-0.792388	-0.350609
6	4.496726	-0.573791	-1.633715
6	4.631011	-1.605694	0.575823
6	5.751060	-1.103345	-1.941540
6	5.887664	-2.115427	0.217468
6	6.472538	-1.871674	-1.024255
1	6.169734	-0.917383	-2.928083
1	6.421724	-2.729129	0.939085
8	1.755419	-0.498155	1.395642
1	1.225704	-0.775620	-1.072306
6	-3.639596	-1.891924	-2.493414
1	-2.940315	-2.656712	-2.149880
1	-4.231226	-2.324836	-3.304532
1	-3.034369	-1.085841	-2.913902
6	-4.752996	0.445255	1.983044
1	-5.616088	0.488923	2.652416
1	-3.922386	-0.029420	2.509160
1	-4.450161	1.473595	1.759864
6	-8.354334	-1.549902	-0.870272
1	-8.676030	-2.397277	-0.251817
1	-8.980213	-0.694946	-0.594103
1	-8.561145	-1.805340	-1.913402
6	0.876960	1.868667	-2.230507
1	1.314886	2.178400	-3.186551
1	0.842978	0.782766	-2.219919
1	-0.151679	2.242057	-2.211220
6	3.851816	1.680986	1.974089
1	3.193526	1.014083	2.535498
1	4.642879	1.059386	1.542419
1	4.316972	2.391855	2.661992
6	2.379392	6.061272	0.030101
1	3.396454	6.452039	-0.094809
1	1.752968	6.496482	-0.752855
1	2.016255	6.424742	0.998111
6	-3.554563	1.796059	-1.876292
1	-3.122442	0.925904	-2.373296
1	-4.559281	1.514158	-1.550022
1	-3.655644	2.582660	-2.628497
6	-0.814880	1.299841	2.497215
1	-1.515923	0.602948	2.956722
1	0.058218	0.738701	2.145485
1	-0.466842	2.007943	3.255049
6	-1.371559	5.735810	0.277266
1	-2.269050	6.317546	0.522192
1	-0.597030	5.997108	1.002630
1	-1.038722	6.063784	-0.713028
6	3.777663	0.212009	-2.702965
1	4.321701	0.156003	-3.649316
1	2.769399	-0.176808	-2.876393
1	3.679207	1.267544	-2.433813
6	4.107488	-1.997734	1.941024
1	3.226391	-2.639689	1.850363
1	4.877420	-2.554759	2.483058
1	3.807641	-1.136876	2.536890
6	7.832110	-2.419511	-1.374427
1	8.565624	-1.611982	-1.488359
1	8.200462	-3.098977	-0.600766
1	7.808356	-2.965209	-2.324392

Z-isomer-Mes

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E (BS2) = -1425.436013

G_{298.15} (BS2) = -1425.017937



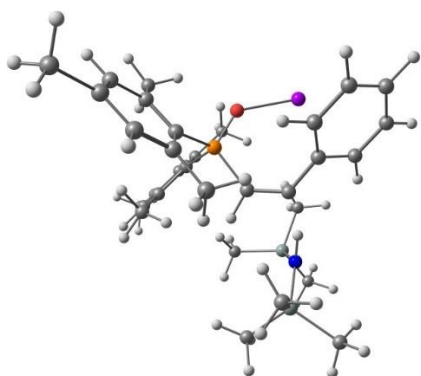
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6	0.765724	2.144551	0.718943
6	-1.001527	3.463384	-1.002002
6	0.649720	3.540683	0.721612
6	-0.228950	4.221313	-0.119710
1	-1.681598	3.969458	-1.683129
1	1.274128	4.111042	1.404403
6	-1.755017	-0.998441	-0.009675
6	-2.490798	-0.489086	1.090961
6	-2.352659	-1.962971	-0.857811
6	-3.806341	-0.917678	1.291763
6	-3.675241	-2.353633	-0.612626
6	-4.423566	-1.841454	0.446696
1	-4.361531	-0.516600	2.136519
1	-4.129161	-3.087980	-1.273326
8	0.523223	-0.828977	-1.677425
6	0.792021	-1.311012	1.057413
6	2.048307	-1.773194	1.226903
1	0.075114	-1.623517	1.812661
6	3.303976	-1.568078	0.499493
6	4.472882	-2.080884	1.097893
6	3.429245	-0.873078	-0.720093
6	5.723333	-1.899992	0.512729
6	4.681919	-0.695792	-1.302563
6	5.832685	-1.201999	-0.691594
1	4.391267	-2.621078	2.037387
1	2.541560	-0.514513	-1.227859
1	6.609433	-2.302282	0.994824
1	4.759680	-0.161728	-2.245273
1	6.805184	-1.057722	-1.153225
1	2.184118	-2.388626	2.116719
6	1.773562	1.546376	1.669465
1	2.531319	0.962944	1.141365
1	2.288730	2.343232	2.211989
1	1.311936	0.885271	2.407212
6	-1.812229	1.363142	-2.050204
1	-2.143989	2.070400	-2.814890
1	-1.288918	0.542759	-2.544704
1	-2.705488	0.946958	-1.573796
6	-0.321064	5.725009	-0.107209
1	0.162435	6.154044	-0.993587
1	-1.363835	6.059444	-0.117688
1	0.167034	6.148227	0.775031
6	-1.945528	0.519231	2.078713
1	-0.915186	0.313709	2.376680
1	-1.965055	1.533666	1.670188
1	-2.555745	0.514196	2.985824
6	-1.652342	-2.616457	-2.027920
1	-1.398966	-1.894558	-2.807308
1	-0.709504	-3.081658	-1.731659
1	-2.299404	-3.385554	-2.458953
6	-5.838272	-2.295185	0.698382
1	-6.485506	-1.452328	0.962189
1	-6.260596	-2.791799	-0.179606
1	-5.879173	-3.005859	1.533336

Int-TS-2H-Mes-K

E (BS1) = -2898.371270

E (BS2) = -2898.994519

G_{298.15} (BS2) = -2898.374389



15	1.367528	-0.059263	-0.414159
6	2.840339	-0.203131	0.685127
6	4.083171	0.212926	0.134664
6	2.810398	-0.750029	1.993008
6	5.249948	0.079862	0.890906
6	4.013657	-0.864790	2.703833
6	5.240039	-0.460088	2.178905
1	6.192310	0.408637	0.458853
1	3.983056	-1.281551	3.707264
6	1.165784	1.744720	-0.792119
6	1.201965	2.709242	0.250482
6	0.857550	2.178621	-2.106753
6	0.951465	4.053170	-0.040972
6	0.614073	3.537832	-2.343435
6	0.656800	4.494227	-1.331110
1	0.978151	4.774382	0.772319
1	0.383794	3.853591	-3.357936
8	1.631364	-0.897547	-1.664496
19	0.248296	-2.149694	-3.295649
6	-0.205682	-0.450225	0.379857
6	-1.017652	-1.511643	0.225466
1	-0.580864	0.396330	0.963569
6	-0.705443	-2.773488	-0.414265
6	-1.686430	-3.392425	-1.239905
6	0.496896	-3.501064	-0.203440
6	-1.453143	-4.615904	-1.870535
6	0.716677	-4.735723	-0.812709
6	-0.245103	-5.299292	-1.665003
1	-2.638577	-2.886785	-1.375028
1	1.271181	-3.067785	0.420123
1	-2.222645	-5.049897	-2.504395
1	1.655777	-5.256160	-0.640468
1	-0.066431	-6.259220	-2.140100
7	-3.325912	-0.196961	0.818607
14	-3.668980	0.929326	-0.465564
14	-3.646222	-0.091397	2.514073
1	-2.480447	-0.876262	0.595611
6	1.562263	-1.204602	2.719277
1	1.070876	-2.042276	2.222679
1	1.821966	-1.522235	3.732716
1	0.815240	-0.412654	2.803028
6	4.212281	0.825896	-1.242173
1	5.265114	0.889060	-1.529396
1	3.677770	0.238837	-1.991494
1	3.798468	1.839410	-1.266599
6	6.517296	-0.616665	2.962679
1	7.094009	-1.478089	2.603011
1	7.158637	0.264831	2.859535
1	6.316586	-0.774365	4.026155
6	1.507418	2.380558	1.694786
1	0.924576	1.536569	2.067183
1	2.562845	2.135730	1.841250
1	1.272622	3.240682	2.326924
6	0.754300	1.270920	-3.314443
1	1.606855	0.597429	-3.393399
1	-0.160649	0.666060	-3.272219
1	0.690175	1.873508	-4.224431
6	0.403244	5.952062	-1.614428
1	1.334839	6.529736	-1.570026
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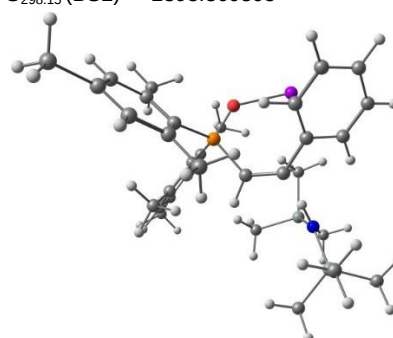
1	-0.279260	6.385992	-0.876009
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1	-2.532131	-2.062998	3.702871
1	-1.353466	-0.927934	3.030975
1	-2.269850	-0.521441	4.505980
6	-5.340642	-0.882274	2.840327
1	-5.832340	-1.096220	1.882636
1	-5.267228	-1.827723	3.389662
1	-6.010873	-0.218800	3.405467
6	-2.747162	2.556919	-0.266128
1	-3.138931	3.196719	0.527317
1	-1.690326	2.316022	0.002236
1	-2.732396	3.155625	-1.188831
6	-3.732276	1.653220	3.204078
1	-4.481860	2.265881	2.686191
1	-4.076186	1.525666	4.243315
1	-2.781812	2.196744	3.229077
6	-3.242226	0.220224	-2.159751
1	-2.165780	0.073508	-2.308605
1	-3.769288	-0.720768	-2.341208
1	-3.564971	0.970551	-2.903807
6	-5.558636	1.080200	-0.496009
1	-5.896000	1.228034	-1.534721
1	-5.984822	0.145133	-0.124470
1	-5.996106	1.901350	0.086671

TS-2H-Mes-K

E (BS1) = -2898.365595

E (BS2) = -2898.987350

G_{298.15} (BS2) = -2898.369395



15	1.465661	-0.044053	-0.309159
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6	4.236647	-0.132954	-0.079483
6	3.076613	-1.183037	1.804691
6	5.456718	-0.470736	0.508962
6	4.330859	-1.498683	2.347451
6	5.528828	-1.155363	1.724371
1	6.376254	-0.190377	0.000534
1	4.364883	-2.031065	3.294371
6	1.429036	1.803384	-0.440456
6	1.574713	2.596610	0.728623
6	1.131716	2.448240	-1.669146
6	1.382618	3.979869	0.653844
6	0.956764	3.837307	-1.687505
6	1.058953	4.622639	-0.540452
1	1.490286	4.568889	1.561113
1	0.729348	4.317068	-2.636426
8	1.467062	-0.735528	-1.670787
19	-0.213740	-1.650002	-3.275834
6	-0.060346	-0.349550	0.613929
6	-0.990512	-1.311817	0.449949
1	-0.323674	0.499260	1.249052
6	-0.866649	-2.542756	-0.324985
6	-2.007796	-3.003753	-1.030324
6	0.291833	-3.356133	-0.373301
6	-1.972567	-4.170250	-1.796822
6	0.319695	-4.533334	-1.121482
6	-0.803772	-4.942156	-1.852884
1	-2.920391	-2.419587	-0.964369
1	1.183317	-3.044946	0.158361
1	-2.860782	-4.486490	-2.337718

1	1.227574	-5.130551	-1.146088
1	-0.775315	-5.856110	-2.438711
7	-3.387245	-0.125830	0.673648
14	-3.409524	1.117864	-0.503479
14	-4.295965	-0.282819	2.117814
1	-2.316326	-0.769332	0.691700
6	1.874999	-1.614295	2.615850
1	1.248233	-2.334557	2.088253
1	2.211393	-2.083787	3.543884
1	1.225532	-0.778445	2.883732
6	4.280647	0.611084	-1.394919
1	5.305686	0.651702	-1.771666
1	3.649408	0.128111	-2.143599
1	3.923319	1.639964	-1.285449
6	6.860328	-1.521020	2.327042
1	7.352565	-2.307914	1.742456
1	7.538996	-0.661298	2.341444
1	6.748559	-1.886886	3.351346
6	1.961717	2.040633	2.079824
1	1.340292	1.198119	2.385886
1	2.999667	1.696495	2.089456
1	1.857551	2.814815	2.843909
6	0.979481	1.747332	-3.002769
1	1.760882	1.009539	-3.176939
1	0.012281	1.238331	-3.060565
1	0.999603	2.486261	-3.808433
6	0.805563	6.106691	-0.584731
1	1.062620	6.528106	-1.561221
1	-0.255059	6.323077	-0.404359
1	1.380208	6.634167	0.182508
6	-3.485778	-1.625264	3.180958
1	-3.444721	-2.581704	2.646116
1	-2.455791	-1.357200	3.443850
1	-4.037964	-1.788518	4.114716
6	-6.096132	-0.801937	1.813292
1	-6.143337	-1.739150	1.245145
1	-6.639850	-0.955550	2.754641
1	-6.640963	-0.043318	1.238751
6	-2.455231	2.680547	-0.001506
1	-2.909759	3.155757	0.876341
1	-1.418289	2.439838	0.255413
1	-2.432833	3.425321	-0.807372
6	-4.363149	1.311091	3.149381
1	-4.872660	2.117895	2.608114
1	-4.900635	1.162577	4.095128
1	-3.353951	1.665038	3.392314
6	-2.559812	0.487516	-2.085958
1	-1.535214	0.225761	-1.806953
1	-3.071082	-0.395506	-2.486989
1	-2.526361	1.259007	-2.863683
6	-5.167206	1.660517	-0.962749
1	-5.157062	2.408137	-1.766539
1	-5.769643	0.810649	-1.304593
1	-5.685724	2.109668	-0.107221

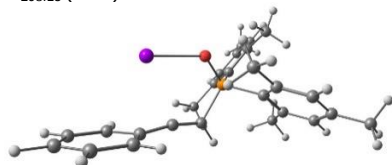
Z-E isomerisation

TS-3-Mes-K

E (BS1) = -2024.313674

E (BS2) = -2024.776381

G_{298.15} (BS2) = -2024.376838



15	-0.250736	-0.123563	0.149071
6	-1.607773	-1.365118	0.128266
6	-2.665440	-1.184711	1.058612
6	-1.602436	-2.510697	-0.700152
6	-3.706011	-2.115932	1.099821
6	-2.668682	-3.415496	-0.617419

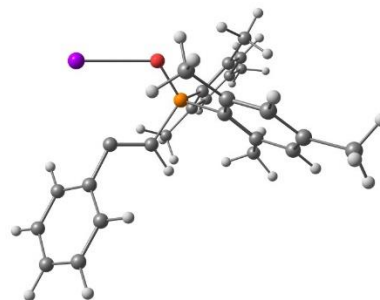
6	-3.735591	-3.233518	0.261982
1	-4.512797	-1.964933	1.813397
1	-2.657523	-4.291866	-1.260620
6	-1.044587	1.517323	-0.118755
6	-2.030764	1.682239	-1.120720
6	-0.613015	2.651327	0.618860
6	-2.612767	2.942635	-1.309791
6	-1.228544	3.885063	0.393178
6	-2.241578	4.053310	-0.554919
1	-3.375383	3.053576	-2.076869
1	-0.897961	4.744744	0.971712
8	0.468077	-0.249348	1.490409
19	2.952286	-0.316597	1.970238
6	0.938726	-0.192951	-1.244920
6	2.208739	-0.319614	-0.949064
1	0.512399	-0.009089	-2.242198
6	3.570151	-0.390614	-0.890743
6	4.385414	0.774213	-0.590549
6	4.290803	-1.649534	-0.947259
6	5.746025	0.660292	-0.335125
6	5.648858	-1.715825	-0.681907
6	6.409954	-0.576467	-0.358940
1	3.906626	1.750497	-0.571168
1	3.736180	-2.553386	-1.185228
1	6.306251	1.567768	-0.114620
1	6.136800	-2.688046	-0.733191
1	7.474049	-0.648705	-0.160453
6	-4.886588	-4.204718	0.309891
1	-5.159138	-4.448639	1.342113
1	-5.778669	-3.778013	-0.165352
1	-4.646451	-5.135543	-0.211295
6	-2.737124	-0.016050	2.016079
1	-1.761976	0.206632	2.453830
1	-3.087314	0.891687	1.514200
1	-3.437312	-0.238729	2.825755
6	-0.508372	-2.828603	-1.692118
1	-0.474067	-2.101910	-2.510232
1	0.481257	-2.829920	-1.230545
1	-0.680843	-3.813950	-2.132787
6	-2.883032	5.400311	-0.767141
1	-3.308333	5.787424	0.165922
1	-2.148985	6.137491	-1.113581
1	-3.684233	5.348481	-1.509426
6	-2.522334	0.566480	-2.018333
1	-3.273606	-0.053353	-1.519454
1	-2.984529	0.992463	-2.913001
1	-1.723840	-0.100060	-2.350156
6	0.515567	2.618805	1.626429
1	1.455347	2.331160	1.140979
1	0.656779	3.612990	2.058799
1	0.332653	1.901895	2.428023

E-1l-Mes-K

E (BS1) = -2024.328784

E (BS2) = -2024.790265

G_{298.15} (BS2) = -2024.389711



15	-0.308326	-0.126936	0.618643
6	-1.629801	-1.292381	0.081255
6	-2.945868	-1.027380	0.548290
6	-1.391241	-2.456956	-0.684788

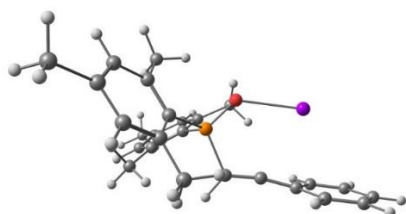
6	-3.983804	-1.895965	0.204314
6	-2.468610	-3.297654	-0.998329
6	-3.770463	-3.035273	-0.576087
1	-4.987539	-1.676853	0.561583
1	-2.275695	-4.187661	-1.591997
6	-0.827465	1.548174	0.033044
6	-1.396583	1.738038	-1.249896
6	-0.578966	2.680601	0.850534
6	-1.778405	3.025581	-1.646963
6	-0.982791	3.944439	0.408259
6	-1.603529	4.139785	-0.827147
1	-2.217921	3.156570	-2.632955
1	-0.792902	4.804007	1.046838
8	-0.217089	-0.230981	2.140607
19	1.972164	-0.735003	3.282455
6	1.269502	-0.330729	-0.218135
6	2.408116	-0.591771	0.465259
1	1.227034	-0.138343	-1.301379
6	3.650036	-0.565099	-0.316288
6	4.036721	0.564250	-1.074903
6	4.536131	-1.666118	-0.307216
6	5.241048	0.590183	-1.778565
6	5.722415	-1.652030	-1.037204
6	6.090636	-0.519459	-1.772643
1	3.379400	1.429923	-1.092268
1	4.271234	-2.542547	0.280589
1	5.513240	1.478435	-2.344154
1	6.372265	-2.523924	-1.023512
1	7.026185	-0.501043	-2.324279
6	-4.912289	-3.953393	-0.928459
1	-5.352073	-4.399705	-0.028618
1	-5.714649	-3.408606	-1.439056
1	-4.584626	-4.766414	-1.582053
6	-3.299593	0.175543	1.395242
1	-2.551272	0.356739	2.168938
1	-3.371464	1.083825	0.788122
1	-4.268844	0.021392	1.877288
6	-0.036856	-2.864706	-1.217825
1	0.331587	-2.163958	-1.973882
1	0.724296	-2.904824	-0.436778
1	-0.104871	-3.850991	-1.684902
6	-2.064797	5.508092	-1.258072
1	-3.064022	5.727382	-0.860484
1	-1.392775	6.290482	-0.891672
1	-2.122793	5.585638	-2.347772
6	-1.623556	0.625600	-2.251199
1	-2.532416	0.058019	-2.030833
1	-1.732875	1.051091	-3.252600
1	-0.797442	-0.087268	-2.286307
6	0.150277	2.613908	2.174655
1	1.152893	2.192044	2.041420
1	0.261682	3.619827	2.588711
1	-0.366738	1.982037	2.898074

TS-4-Mes-K

E (BS1) = -2024.313674

E (BS2) = -2024.776381

G_{298.15} (BS2) = -2024.376838



15	-0.250736	-0.123563	0.149071
6	-1.607773	-1.365118	0.128266
6	-2.665440	-1.184711	1.058612
6	-1.602436	-2.510697	-0.700152
6	-3.706011	-2.115932	1.099821
6	-2.668682	-3.415496	-0.617419

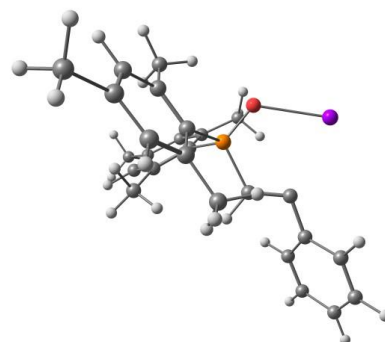
6	-3.735591	-3.233518	0.261982
1	-4.512797	-1.964933	1.813397
1	-2.657523	-4.291866	-1.260620
6	-1.044587	1.517323	-0.118755
6	-2.030764	1.682239	-1.120720
6	-0.613015	2.651327	0.618860
6	-2.612767	2.942635	-1.309791
6	-1.228544	3.885063	0.393178
6	-2.241578	4.053310	-0.554919
1	-3.375383	3.053576	-2.076869
1	-0.897961	4.744744	0.971712
8	0.468077	-0.249348	1.490409
19	2.952286	-0.316597	1.970238
6	0.938726	-0.192951	-1.244920
6	2.208739	-0.319614	-0.949064
1	0.512399	-0.009089	-2.242198
6	3.570151	-0.390614	-0.890743
6	4.385414	0.774213	-0.590549
6	4.290803	-1.649534	-0.947259
6	5.746025	0.660292	-0.335125
6	5.648858	-1.715825	-0.681907
6	6.409954	-0.576467	-0.358940
1	3.906626	1.750497	-0.571168
1	3.736180	-2.553386	-1.185228
1	6.306251	1.567768	-0.114620
1	6.136800	-2.688046	-0.733191
1	7.474049	-0.648705	-0.160453
6	-4.886588	-4.204718	0.309891
1	-5.159138	-4.448639	1.342113
1	-5.778669	-3.778013	-0.165352
1	-4.646451	-5.135543	-0.211295
6	-2.737124	-0.016050	2.016079
1	-1.761976	0.206632	2.453830
1	-3.087314	0.891687	1.514200
1	-3.437312	-0.238729	2.825755
6	-0.508372	-2.828603	-1.692118
1	-0.474067	-2.101910	-2.510232
1	0.481257	-2.829920	-1.230545
1	-0.680843	-3.813950	-2.132787
6	-2.883032	5.400311	-0.767141
1	-3.308333	5.787424	0.165922
1	-2.148985	6.137491	-1.113581
1	-3.684233	5.348481	-1.509426
6	-2.522334	0.566480	-2.018333
1	-3.273606	-0.053353	-1.519454
1	-2.984529	0.992463	-2.913001
1	-1.723840	-0.100060	-2.350156
6	0.515567	2.618805	1.626429
1	1.455347	2.331160	1.140979
1	0.656779	3.612990	2.058799
1	0.332653	1.901895	2.428023

E-1l-Mes-K

E (BS1) = -2024.328784

E (BS2) = -2024.790265

G_{298.15} (BS2) = -2024.389711



15	-0.308326	-0.126936	0.618643
6	-1.629801	-1.292381	0.081255
6	-2.945868	-1.027380	0.548290
6	-1.391241	-2.456956	-0.684788

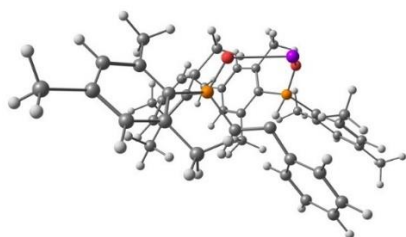
6	-3.983804	-1.895965	0.204314
6	-2.468610	-3.297654	-0.998329
6	-3.770463	-0.035273	-0.576087
1	-4.987539	-1.676853	0.561583
1	-2.275695	-4.187661	-1.591997
6	-0.827465	1.548174	0.033044
6	-1.396583	1.738038	-1.249896
6	-0.578966	2.680601	0.850534
6	-1.778405	3.025581	-1.646963
6	-0.982791	3.944439	0.408259
6	-1.603529	4.139785	-0.827147
1	-2.217921	3.156570	-2.632955
1	-0.792902	4.804007	1.046838
8	-0.217089	-0.230981	2.140607
19	1.972164	-0.735003	3.282455
6	1.269502	-0.330729	-0.218135
6	2.408116	-0.591771	0.465259
1	1.227034	-0.138343	-1.301379
6	3.650036	-0.565099	-0.316288
6	4.036721	0.564250	-1.074903
6	4.536131	-1.666118	-0.307216
6	5.241048	0.590183	-1.778565
6	5.722415	-1.652030	-1.037204
6	6.090636	-0.519459	-1.772643
1	3.379400	1.429923	-1.092268
1	4.271234	-2.542547	0.280589
1	5.513240	1.478435	-2.344154
1	6.372265	-2.523924	-1.023512
1	7.026185	-0.501043	-2.324279
6	-4.912289	-3.953393	-0.928459
1	-5.352073	-4.399705	-0.028618
1	-5.714649	-3.408606	-1.439056
1	-4.584626	-4.766414	-1.582053
6	-3.299593	0.175543	1.395242
1	-2.551272	0.356739	2.168938
1	-3.371464	1.083825	0.788122
1	-4.268844	0.021392	1.877288
6	-0.036856	-2.864706	-1.217825
1	0.331587	-2.163958	-1.973882
1	0.724296	-2.904824	-0.436778
1	-0.104871	-3.850991	-1.684902
6	-2.064797	5.508092	-1.258072
1	-3.064022	5.727382	-0.860484
1	-1.392775	6.290482	-0.891672
1	-2.122793	5.585638	-2.347772
6	-1.623556	0.625600	-2.251199
1	-2.532416	0.058019	-2.030833
1	-1.732875	1.051091	-3.252600
1	-0.797442	-0.087268	-2.286307
6	0.150277	2.613908	2.174655
1	1.152893	2.192044	2.041420
1	0.261682	3.619827	2.588711
1	-0.366738	1.982037	2.898074

Int-TS-5-Mes-K

E (BS1) = -3140.889327

E (BS2) = -3141.656684

G_{298.15} (BS2) = -3140.917225



15	-2.541565	-0.485650	0.519267
6	-4.347956	-0.807761	0.300620
6	-4.879610	-1.978646	-0.292149
6	-5.242497	0.159512	0.834200
6	-6.270797	-2.123967	-0.385841

6	-6.620858	-0.034227	0.713358
6	-7.159710	-1.163363	0.093401
1	-6.667279	-3.025636	-0.845874
1	-7.290838	0.717518	1.124524
6	-2.251469	1.174318	-0.244178
6	-2.717046	1.444936	-1.556453
6	-1.526241	2.177556	0.450123
6	-2.449893	2.689175	-2.138898
6	-1.298053	3.407756	-0.176252
6	-1.744390	3.687044	-1.467505
1	-2.814748	2.881967	-3.145212
1	-0.741641	4.166910	0.365514
8	-2.232355	-0.521348	2.011876
19	-0.082752	-1.589545	2.892219
6	-1.489798	-1.578152	-0.455502
6	-0.609432	-2.411170	0.143695
1	-1.619156	-1.499251	-1.544517
6	0.255195	-3.214924	-0.725448
6	0.388454	-4.606677	-0.512440
6	1.071796	-2.642865	-1.728418
6	1.275651	-5.377662	-1.258547
6	1.992091	-3.407651	-2.446242
6	2.100889	-4.781558	-2.220838
1	-0.212801	-5.071960	0.265598
1	0.995956	-1.578158	-1.917545
1	1.343205	-6.447470	-1.075220
1	2.623702	-2.927413	-3.190191
1	2.816344	-5.378352	-2.779218
15	2.352297	0.211481	0.918845
6	2.220039	1.934277	0.356650
6	2.454016	3.003470	1.253743
6	1.900182	2.199913	-0.993240
6	2.376572	4.312093	0.773435
6	1.856395	3.527570	-1.430472
6	2.091627	4.596867	-0.566368
1	2.562661	5.132394	1.462384
1	1.626915	3.725985	-2.473697
6	3.967695	-0.529905	0.475842
6	5.086098	0.166550	-0.044779
6	4.041507	-1.941365	0.640151
6	6.211571	-0.570025	-0.440057
6	5.183824	-2.624038	0.222752
6	6.277796	-1.958482	-0.335329
1	7.065291	-0.031439	-0.842749
1	5.218327	-3.703975	0.342221
8	1.950618	-0.008545	2.370188
1	1.478995	-0.457752	0.043976
6	-3.555327	0.486231	-2.375593
1	-3.233451	-0.552241	-2.298739
1	-4.605127	0.519598	-2.066589
1	-3.511638	0.765552	-3.431894
6	-0.981495	2.028570	1.853893
1	-0.519209	2.968702	2.165508
1	-1.760711	1.760282	2.568612
1	-0.215842	1.253589	1.918134
6	-1.445932	5.007916	-2.127137
1	-1.326279	5.805548	-1.388213
1	-0.514365	4.954994	-2.703516
1	-2.241625	5.297431	-2.820589
6	-4.047892	-3.113565	-0.845341
1	-3.474151	-2.812217	-1.726962
1	-3.324934	-3.489844	-0.119758
1	-4.701741	-3.938779	-1.140800
6	-4.783474	1.414583	1.542814
1	-5.605902	1.833407	2.129047
1	-3.948628	1.211268	2.215680
1	-4.456771	2.181615	0.833826
6	-8.650395	-1.331991	-0.048643
1	-9.048542	-0.665045	-0.823576
1	-8.912453	-2.356691	-0.326692
1	-9.169911	-1.085473	0.883490
6	2.950515	-2.747776	1.303747
1	1.953685	-2.488649	0.946478
1	3.092498	-3.812052	1.105667
1	2.974444	-2.593023	2.388333

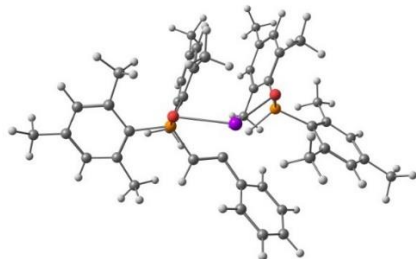
6	5.181070	1.668113	-0.190121
1	6.204574	1.943825	-0.456295
1	4.519197	2.056418	-0.968088
1	4.927798	2.186895	0.736063
6	7.487268	-2.723861	-0.804026
1	7.250402	-3.317555	-1.695309
1	8.312571	-2.053168	-1.057640
1	7.835774	-3.423784	-0.036919
6	1.607161	1.108770	-1.994171
1	2.394655	0.349422	-2.029501
1	0.665509	0.602271	-1.755309
1	1.508084	1.531806	-2.996468
6	2.820909	2.790360	2.702429
1	2.027640	2.270100	3.242979
1	3.719110	2.171372	2.803210
1	3.016350	3.750545	3.186673
6	2.018111	6.021963	-1.048147
1	2.869494	6.607434	-0.685150
1	2.004644	6.075456	-2.139907
1	1.110121	6.513181	-0.678443

TS-5-Mes-K

E (BS1) = -3140.876410

E (BS2) = -3141.636915

G_{298.15} (BS2) = -3140.896692



15	2.499702	-0.925318	-0.563640
6	4.287192	-1.102870	-0.102324
6	4.804530	-1.994086	0.872293
6	5.201761	-0.280207	-0.823762
6	6.187313	-2.024977	1.108884
6	6.568678	-0.356924	-0.548380
6	7.087716	-1.219128	0.418467
1	6.565421	-2.709390	1.863795
1	7.247334	0.280148	-1.110567
6	2.098583	0.818721	-0.104667
6	2.363507	1.250267	1.224202
6	1.694595	1.782495	-1.065394
6	2.300665	2.609463	1.536170
6	1.651096	3.133978	-0.697195
6	1.978118	3.575163	0.581553
1	2.511818	2.919188	2.556840
1	1.345354	3.861628	-1.443883
8	2.354240	-1.217077	-2.062627
19	-0.086628	-1.692288	-2.807008
6	1.410468	-2.050547	0.321559
6	0.106162	-1.763899	0.522764
1	1.820821	-3.055309	0.455147
6	-0.808287	-2.856746	0.891394
6	-0.738971	-4.138721	0.300492
6	-1.900144	-2.594033	1.745935
6	-1.713252	-5.104723	0.548150
6	-2.866601	-3.563618	2.005019
6	-2.784796	-4.821152	1.400127
1	0.079207	-4.362422	-0.380310
1	-1.986398	-1.610545	2.196788
1	-1.641360	-6.079044	0.071157
1	-3.700176	-3.330222	2.661729
1	-3.550884	-5.568696	1.584378
15	-2.078894	0.280317	-0.636585
6	-1.874462	2.026791	-0.121059
6	-2.236193	3.090822	-0.981271
6	-1.340191	2.307746	1.154099
6	-2.052604	4.405842	-0.547484
6	-1.197761	3.640543	1.556341

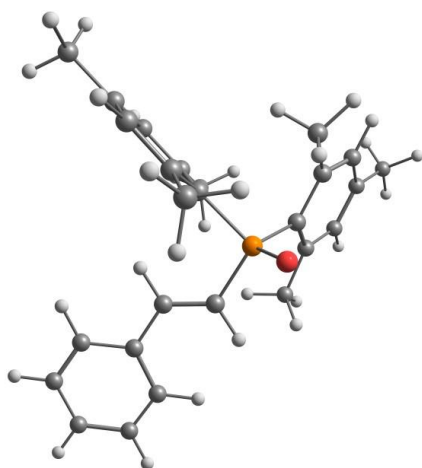
6	-1.548442	4.703166	0.723474
1	-2.336219	5.220906	-1.210012
1	-0.800875	3.849159	2.546424
6	-3.823534	-0.257672	-0.272777
6	-4.769891	0.429571	0.533032
6	-4.184456	-1.539736	-0.781963
6	-6.006403	-0.176177	0.808766
6	-5.429504	-2.092481	-0.481075
6	-6.360407	-1.430771	0.321538
1	-6.717462	0.364331	1.428568
1	-5.673123	-3.074689	-0.879423
8	-1.777288	0.119954	-2.147540
1	-1.001378	-0.577531	0.115069
6	2.704727	0.306671	2.351956
1	2.047903	-0.565246	2.357210
1	3.735236	-0.053661	2.283228
1	2.597292	0.818439	3.311783
6	1.261629	1.472368	-2.480437
1	1.280698	2.385722	-3.081703
1	1.888786	0.718807	-2.953351
1	0.225199	1.112251	-2.474112
6	1.988044	5.040018	0.926961
1	1.445884	5.628765	0.183222
1	1.537247	5.222386	1.906961
1	3.016219	5.421496	0.968915
6	3.986282	-2.954521	1.706485
1	3.122782	-2.483642	2.176119
1	3.616358	-3.792569	1.106221
1	4.610888	-3.375700	2.498203
6	4.784088	0.704182	-1.892712
1	5.661306	1.044116	-2.449066
1	4.075465	0.258377	-2.591526
1	4.304153	1.586253	-1.458085
6	8.567472	-1.270811	0.696274
1	8.942111	-0.293189	1.021378
1	8.802424	-1.999964	1.476411
1	9.128991	-1.544307	-0.204599
6	-3.269725	-2.376595	-1.648348
1	-2.308018	-2.539111	-1.156237
1	-3.711128	-3.361190	-1.819745
1	-3.093749	-1.893048	-2.612123
6	-4.576697	1.803997	1.136275
1	-5.483735	2.096123	1.672069
1	-3.750850	1.838410	1.848714
1	-4.376685	2.566058	0.381303
6	-7.691549	-2.058693	0.643907
1	-7.561607	-3.004100	1.184037
1	-8.305665	-1.398655	1.262811
1	-8.253963	-2.288043	-0.268777
6	-0.986031	1.217897	2.138399
1	-1.886003	0.699774	2.494032
1	-0.330489	0.459312	1.703993
1	-0.485676	1.640579	3.013322
6	-2.887864	2.855017	-2.322041
1	-2.274233	2.215488	-2.958114
1	-3.844636	2.332349	-2.199557
1	-3.085366	3.805113	-2.826093
6	-1.414020	6.134342	1.177474
1	-2.398632	6.607884	1.275006
1	-0.913452	6.202190	2.146845
1	-0.844008	6.730642	0.456862

E-isomer-Mes

E (BS1) = -1425.023411

E (BS2) = -1425.444144

G_{298.15} (BS2) = -1425.025574



15	-0.412645	-0.160375	1.185655
6	-1.809311	-1.074986	0.412866
6	-1.711077	-2.359110	-0.171559
6	-3.080021	-0.442136	0.485353
6	-2.861299	-2.953382	-0.706822
6	-4.195166	-1.079442	-0.063203
6	-4.108622	-2.331519	-0.675973
1	-2.773630	-3.938234	-1.158270
1	-5.160612	-0.582655	-0.002141
6	-0.329400	1.457096	0.307307
6	-0.478708	1.538533	-1.101480
6	-0.094936	2.641448	1.049534
6	-0.451054	2.792342	-1.719759
6	-0.082871	3.871144	0.379912
6	-0.270173	3.973625	-0.998181
1	-0.569036	2.842396	-2.799671
1	0.086584	4.775542	0.958841
8	-0.623446	-0.074495	2.682255
6	1.189390	-0.921519	0.848765
6	2.173977	-0.345474	0.138356
1	1.365754	-1.844173	1.393971
6	3.529671	-0.869373	-0.058721
6	3.938492	-2.133842	0.404574
6	4.460842	-0.076879	-0.752554
6	5.237585	-2.581606	0.186304
6	5.762676	-0.525163	-0.969723
6	6.155788	-1.779387	-0.499885
1	3.234945	-2.770545	0.931675
1	4.153089	0.898973	-1.118701
1	5.537301	-3.560410	0.549166
1	6.468405	0.102853	-1.505399
1	7.168644	-2.133002	-0.668234
1	1.976838	0.601811	-0.358434
6	-0.660959	0.339019	-2.005947
1	-0.040774	-0.508984	-1.710940
1	-1.699377	-0.004163	-2.019452
1	-0.387245	0.607688	-3.029936
6	0.163786	2.667269	2.539088
1	0.383358	3.690385	2.856602
1	-0.686924	2.291602	3.110231
1	1.012153	2.033364	2.811151
6	-0.235623	5.308463	-1.696462
1	-0.331378	6.133622	-0.985366
1	0.709252	5.443530	-2.237451
1	-1.041791	5.393061	-2.432691
6	-0.432105	-3.158689	-0.262200
1	0.356360	-2.628368	-0.802510
1	-0.038456	-3.406108	0.728610
1	-0.618870	-4.100850	-0.783671
6	-3.299810	0.911479	1.125015
1	-4.360611	1.048387	1.351049
1	-2.734034	1.016866	2.052836
1	-2.995420	1.724248	0.457852
6	-5.326106	-2.982241	-1.279595
1	-5.646918	-2.450989	-2.184068

1	-5.129004	-4.021839	-1.555197
1	-6.171142	-2.966449	-0.582789

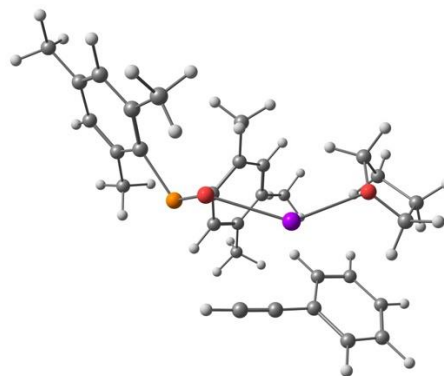
Influence of explicit THF solvent molecules in the nucleophilic addition and protonation steps

Int-TS-1-Mes-K-1THF

E (BS1) = -2256.822151

E (BS2) = -2257.362046

G_{298.15} (BS2) = -2256.857250



C	2.305997	0.645574	-2.581793
C	1.260161	0.590826	-3.193274
K	0.993199	-1.880015	-1.230096
H	0.327375	0.572031	-3.715830
C	4.749362	0.343454	-2.398501
C	3.516856	0.703304	-1.820333
C	3.475419	1.114692	-0.473246
C	4.652975	1.189047	0.267357
C	5.874981	0.840192	-0.313891
C	5.918581	0.411658	-1.643582
H	4.779521	0.021955	-3.434731
H	2.522211	1.373906	-0.027036
H	4.615475	1.515993	1.301451
H	6.790263	0.899373	0.267382
H	6.866104	0.133971	-2.095426
P	-2.062636	0.022679	-1.441670
O	-1.423825	-1.407052	-1.637324
C	-0.838868	0.127437	1.224663
C	-1.080190	0.771419	-0.011247
C	0.048948	0.720826	2.133244
C	0.693292	1.937444	1.880448
C	0.446001	2.591796	0.656914
C	-0.417060	1.982153	-0.260484
H	0.241379	0.218729	3.079830
H	-0.583148	2.473507	-1.217490
C	-4.428571	1.086380	-0.314038
C	-5.736481	1.068469	0.173098
C	-3.740018	-0.131130	-0.586505
C	-4.439937	-1.343996	-0.375579
C	-5.759861	-1.314421	0.105982
C	-6.427746	-0.127635	0.395032
H	-6.233411	2.015854	0.376150
H	-6.274784	-2.261733	0.259492
O	2.665402	-2.496844	0.696790
C	4.107242	-2.409129	0.577654
C	2.292214	-2.272486	2.069877
C	4.632900	-1.938130	1.943546
H	4.504300	-3.390416	0.294673
H	4.332787	-1.695798	-0.220377
C	3.379914	-1.360378	2.619321
H	1.295528	-1.827779	2.078722
H	2.259596	-3.229652	2.610200
H	5.438501	-1.208876	1.838441
H	5.012732	-2.787229	2.520218
H	3.198356	-0.332039	2.290244
H	3.433093	-1.375568	3.710881

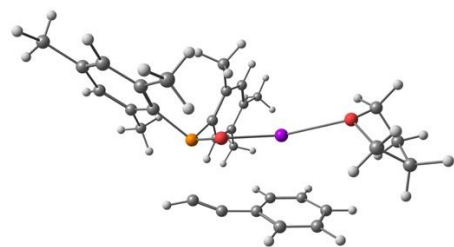
C	-1.511917	-1.175990	1.580224
H	-2.557785	-1.011965	1.863366
H	-1.524403	-1.844351	0.715735
H	-1.010192	-1.667806	2.419702
C	1.647583	2.521021	2.890514
H	2.648555	2.662984	2.464582
H	1.315916	3.507571	3.236999
H	1.742016	1.872421	3.765619
C	1.119788	3.899365	0.326528
H	2.212746	3.805393	0.333365
H	0.821866	4.252604	-0.664337
H	0.866529	4.680678	1.053543
C	-3.782399	2.434671	-0.530887
H	-3.258533	2.480035	-1.492452
H	-4.533473	3.229903	-0.509806
H	-3.035979	2.656550	0.238350
C	-3.841538	-2.716530	-0.603719
H	-4.604123	-3.405370	-0.984733
H	-2.990470	-2.673418	-1.282394
H	-3.478495	-3.137836	0.343636
C	-7.842785	-0.119346	0.917855
H	-8.506095	0.465332	0.268682
H	-8.248801	-1.133119	0.987004
H	-7.898078	0.332080	1.916421

TS-1-Mes-K-1THF

E (BS1) = -2256.803172

E (BS2) = -2257.342830

G_{298.15} (BS2) = -2256.838088



C	-0.538147	0.620789	3.118995
C	0.706684	0.563988	3.094618
K	-1.666137	-0.558077	-0.421116
H	1.623034	0.718822	3.630221
C	-2.648411	-0.639209	2.856616
C	-1.871042	0.536606	2.661684
C	-2.484195	1.626762	1.981750
C	-3.793324	1.531127	1.512075
C	-4.542735	0.361635	1.704085
C	-3.955638	-0.717214	2.382463
H	-2.201973	-1.483033	3.373234
H	-1.914100	2.536162	1.824485
H	-4.233347	2.378166	0.991885
H	-5.563576	0.295034	1.342734
H	-4.524068	-1.629241	2.542780
P	1.534066	-0.310650	0.895637
O	0.510913	-1.445564	0.580345
C	0.948158	0.831217	-1.702672
C	1.081149	1.052997	-0.311118
C	0.371309	1.837897	-2.490394
C	-0.069148	3.057658	-1.962320
C	0.080391	3.288851	-0.580343
C	0.646033	2.281688	0.208452
H	0.261948	1.663532	-3.559486
H	0.733499	2.450828	1.277360
C	4.266215	0.229245	0.524067
C	5.604747	-0.072955	0.264215
C	3.259346	-0.756372	0.332121
C	3.658745	-2.052808	-0.081430
C	5.016346	-2.312164	-0.318538
C	6.006009	-1.341559	-0.164336
H	6.355407	0.700761	0.413531
H	5.303121	-3.313305	-0.636199
O	-3.541534	-2.043051	-1.514451

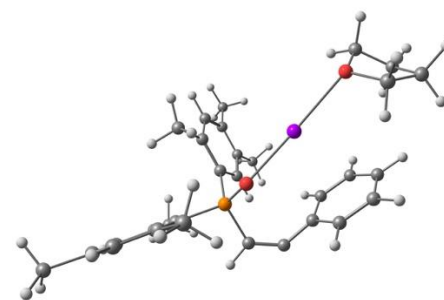
C	-4.230583	-2.957050	-0.634820
C	-4.520727	-1.530110	-2.431673
C	-5.707342	-2.500438	-0.591995
H	-4.136027	-3.977393	-1.026988
H	-3.734769	-2.912855	0.338912
C	-5.757456	-1.303736	-1.567575
H	-4.112370	-0.623047	-2.886046
H	-4.713787	-2.266987	-3.225275
H	-6.013895	-2.213901	0.416241
H	-6.364565	-3.307403	-0.925727
H	-5.656601	-0.359561	-1.023901
H	-6.679570	-1.269450	-2.153251
C	1.394099	-0.454618	-2.357699
H	2.486729	-0.505777	-2.417415
H	1.072440	-1.321171	-1.774601
H	0.996641	-0.534505	-3.374001
C	-0.692932	4.097810	-2.856414
H	-1.709634	4.350492	-2.531071
H	-0.119947	5.032969	-2.843843
H	-0.745641	3.749677	-3.891486
C	-0.383674	4.579379	0.045687
H	-1.462417	4.728908	-0.088967
H	-0.172996	4.592570	1.118447
H	0.110749	5.448499	-0.405010
C	3.938519	1.625413	1.000335
H	3.221343	1.616175	1.828170
H	4.843205	2.137477	1.340470
H	3.488794	2.230210	0.206080
C	2.695948	-3.193192	-0.332725
H	3.189322	-4.152605	-0.144539
H	1.792654	-3.106505	0.268899
H	2.374810	-3.198420	-1.383058
C	7.453253	-1.644229	-0.460820
H	8.123334	-1.027997	0.147424
H	7.689344	-2.696577	-0.270756
H	7.693916	-1.442839	-1.513524

Z-1I-Mes-K-1THF

E (BS1) = -2256.835867

E (BS2) = -2257.380124

G_{298.15} (BS2) = -2256.873432



C	0.148411	-0.723779	3.003682
C	1.281841	-0.613227	2.292406
K	-1.953815	-0.455863	-0.773076
H	2.265350	-0.601264	2.772769
C	-1.852031	-2.039960	2.310675
C	-1.209187	-0.788097	2.578146
C	-2.053572	0.367094	2.531673
C	-3.417280	0.269750	2.252982
C	-4.023766	-0.971284	2.001375
C	-3.212800	-2.121507	2.034578
H	-1.250271	-2.944349	2.329413
H	-1.621018	1.341132	2.739254
H	-4.016309	1.178457	2.233413
H	-5.087586	-1.043621	1.800655
H	-3.653395	-3.097180	1.839107
P	1.379915	-0.498562	0.483922
O	0.371894	-1.372736	-0.262547
C	1.104524	1.607146	-1.400527
C	1.043726	1.233705	-0.037725
C	0.660390	2.888939	-1.749500

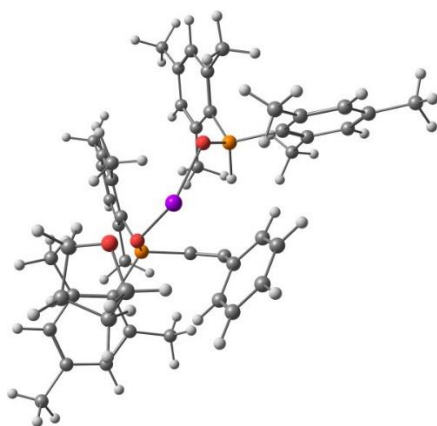
C	0.168323	3.806156	-0.813443
C	0.119522	3.432167	0.544616
C	0.557904	2.154071	0.900694
H	0.702322	3.185096	-2.795547
H	0.524851	1.860647	1.944718
C	4.154676	0.054637	0.385512
C	5.480345	-0.246404	0.054797
C	3.127906	0.862421	0.045241
C	3.472230	-2.086163	-0.582926
C	4.813708	-2.335292	-0.894707
C	5.832198	-1.428489	-0.597712
H	6.258508	0.464664	0.322030
H	5.067875	-3.275462	-1.378269
O	-4.182674	-1.048890	-2.057614
C	-4.887890	-2.204518	-1.545028
C	-5.151421	-0.011450	-2.290251
C	-6.252922	-1.700933	-1.027448
H	-5.001502	-2.944120	-2.346373
H	-4.270953	-2.642631	-0.754341
C	-6.148222	-0.168732	-1.148594
H	-4.622293	0.946273	-2.302724
H	-5.633503	-0.158302	-3.267824
H	-6.444011	-2.024835	-0.001799
H	-7.061889	-2.080711	-1.657847
H	-5.731158	0.623765	-0.233549
H	-7.108424	0.310551	-1.355249
C	1.641568	0.689045	-2.473632
H	2.732913	0.610440	-2.413447
H	1.243555	-0.323660	-2.370094
H	1.388097	1.066667	-3.468158
C	-0.298549	5.168525	-1.254286
H	-1.349695	5.336797	-0.990031
H	0.277061	5.964659	-0.766906
H	-0.196703	5.292106	-2.335636
C	-0.402729	4.378732	1.594487
H	-1.450457	4.646743	1.409693
H	-0.339729	3.932849	2.590540
H	0.163632	5.317640	1.608652
C	3.905362	1.372433	1.086365
H	3.185157	1.290307	1.902768
H	4.841098	1.751399	1.506122
H	3.521403	2.128665	0.394537
C	2.472939	-3.166965	-0.931196
H	2.999048	-4.042512	-1.322300
H	1.886838	-3.474684	-0.061808
H	1.750055	-2.827750	-1.676296
C	7.262547	-1.711529	-0.978204
H	7.961830	-1.267640	-0.263022
H	7.457159	-2.786943	-1.029269
H	7.495621	-1.290268	-1.964581

Z-2I-Mes-K-1THF

E (BS1) = -3373.388880

E (BS2) = -3374.236757

G_{298.15} (BS2) = -3373.387576



P	-2.061337	0.439544	-0.521630
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C	-3.882871	0.435337	-0.865326
C	-4.726885	0.840644	0.204210
C	-4.475959	-0.039980	-2.061977
C	-6.114773	0.744666	0.066492
C	-5.873376	-0.116228	-2.145783
C	-6.712158	0.259937	-1.097693
H	-6.743525	1.060678	0.895625
H	-6.316314	-0.482116	-3.068739
C	-1.631315	2.200528	-0.126646
C	-1.967771	3.235331	-1.037072
C	-0.833706	2.520820	1.004749
C	-1.471451	4.528583	-0.831663
C	-0.366150	3.830274	1.162269
C	-0.656319	4.847379	0.253564
H	-1.728317	5.304721	-1.548589
H	0.261543	4.054006	2.021195
O	-1.828123	-0.511462	0.645744
K	-0.181830	-2.080590	1.723089
C	-1.005322	0.084175	-1.968410
C	-0.305619	-1.027496	-2.262994
H	-0.941529	0.957259	-2.624131
C	-0.345692	-2.309921	-1.605475
C	0.863058	-2.960949	-1.220436
C	-1.539205	-3.070102	-1.436585
C	0.874087	-4.235895	-0.658526
C	-1.520117	-4.358344	-0.906466
C	-0.319933	-4.955435	-0.492107
H	1.804668	-2.451747	-1.395526
H	-2.489242	-2.625571	-1.712257
H	1.824274	-4.681108	-0.371938
H	-2.457662	-4.898082	-0.793404
H	-0.312433	-5.958680	-0.076518
P	2.692310	-0.157395	0.124728
C	3.253974	1.562399	0.354569
C	4.206764	1.847699	1.364726
C	2.666504	2.622245	-0.377938
C	4.562085	3.174387	1.611383
C	3.056991	3.936016	-0.089951
C	3.995381	4.235419	0.897156
H	5.294139	3.384567	2.387325
H	2.602093	4.746263	-0.653037
C	4.080325	-1.214608	-0.424141
C	4.673012	-0.946075	-1.684713
C	4.533096	-2.318206	0.340275
C	5.724124	-1.748042	-2.132948
C	5.593822	-3.087306	-0.155262
C	6.208731	-2.818801	-1.378190
H	6.169920	-1.531473	-3.100533
H	5.941928	-3.930044	0.436540
O	1.960004	-0.691675	1.345452
H	1.882285	-0.097010	-1.020277
C	-3.713777	-0.449748	-3.301721
H	-3.024229	-1.274112	-3.123570
H	-4.417385	-0.757516	-4.079829
H	-3.111962	0.369558	-3.703976
C	-4.203814	1.412287	1.502714
H	-4.998434	1.433974	2.253136
H	-3.372478	0.825577	1.893004
H	-3.845718	2.437857	1.367268
C	-8.208913	0.126854	-1.208869
H	-8.543314	-0.849930	-0.836443
H	-8.723127	0.892020	-0.619220
H	-8.541684	0.209881	-2.247846
C	1.632432	2.422709	-1.458474
H	2.058385	1.955183	-2.351379
H	0.805897	1.793441	-1.132025
H	1.211561	3.385126	-1.754814
C	4.835935	0.761464	2.201438
H	4.071947	0.197095	2.744085
H	5.393519	0.047744	1.587279
H	5.526706	1.189197	2.931886
C	4.363711	5.662055	1.211644
H	5.438728	5.766826	1.390589
H	4.081834	6.335995	0.397893
H	3.851492	6.004946	2.119422

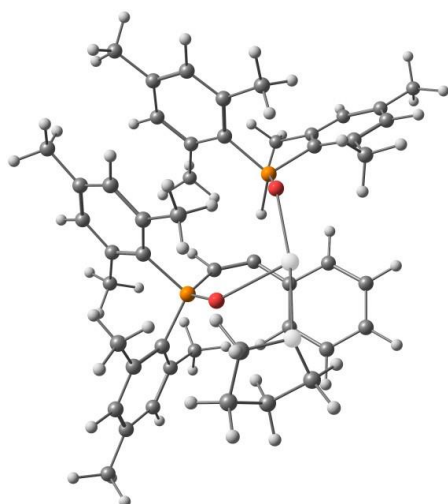
C	-2.872001	3.040354	-2.233604
H	-2.584858	2.188135	-2.850648
H	-3.909925	2.879788	-1.927506
H	-2.844490	3.927470	-2.871634
C	-0.417663	1.534863	2.072783
H	-1.268737	0.986205	2.478364
H	0.294872	0.800823	1.690725
H	0.073846	2.071347	2.889905
C	-0.115950	6.239700	0.453748
H	-0.718106	6.797318	1.182324
H	0.909623	6.213548	0.836174
H	-0.120941	6.808846	-0.480472
C	4.187900	0.161525	-2.587072
H	4.780982	0.191904	-3.503880
H	3.140846	0.010989	-2.875095
H	4.262280	1.142014	-2.107996
C	3.920643	-2.763286	1.649338
H	2.921180	-3.177733	1.485644
H	4.539710	-3.545205	2.097496
H	3.808511	-1.950003	2.364868
C	7.365765	-3.648725	-1.869540
H	8.315217	-3.118079	-1.725201
H	7.432763	-4.598966	-1.332649
H	7.275908	-3.861841	-2.939589
O	-2.277196	-2.970212	3.201694
C	-2.968576	-3.965538	2.420254
H	-2.228579	-4.490157	1.809167
C	-3.998871	-3.183667	1.616326
H	-3.511676	-2.681862	0.775507
H	-4.809448	-3.813072	1.239355
C	-4.461440	-2.148611	2.650964
H	-4.883993	-1.253262	2.191791
H	-5.215860	-2.584279	3.314870
C	-3.170739	-1.849024	3.427372
H	-2.677933	-0.948697	3.048588
H	-3.339393	-1.738389	4.504527
H	-3.450495	-4.695570	3.087549

TS-2-Mes-K-1THF

E (BS1) = -3373.377207

E (BS2) = -3374.219691

G_{298.15} (BS2) = -3373.37162



P	-2.015545	0.375632	-0.382297
C	-3.763902	0.429309	-0.971244
C	-4.742844	0.784173	-0.003815
C	-4.181943	0.049829	-2.269587
C	-6.096725	0.730745	-0.342680
C	-5.554363	0.012536	-2.555735
C	-6.527320	0.338798	-1.612516
H	-6.834118	1.006700	0.407657
H	-5.866915	-0.278559	-3.555431
C	-1.572545	2.102658	0.141058

C	-1.833887	3.200856	-0.722386
C	-0.836351	2.333202	1.330600
C	-1.356968	4.472051	-0.389209
C	-0.379960	3.627599	1.614572
C	-0.619406	4.709333	0.772014
H	-1.565533	5.299022	-1.064022
H	0.196246	3.782927	2.522941
O	-1.963966	-0.641098	0.752182
K	-0.186664	-2.143533	1.801366
C	-0.748067	0.135858	-1.650989
C	0.112282	-0.891299	-1.863470
H	-0.503332	1.103960	-2.086234
C	-0.122055	-2.279646	-1.455747
C	0.985671	-3.125967	-1.190925
C	-1.403539	-2.883388	-1.402639
C	-1.822374	-4.459212	-0.818101
C	-1.566458	-4.225959	-1.062140
C	-0.458873	-5.021768	-0.746589
H	1.988616	-2.723413	-1.282373
H	-2.281689	-2.285350	-1.609912
H	1.697602	-5.067072	-0.603629
H	-2.566263	-4.650694	-1.028042
H	-0.589386	-6.064608	-0.472530
P	2.533838	-0.222470	-0.162958
C	2.963721	1.553690	0.135518
C	3.636811	1.895817	1.342244
C	2.521918	2.586606	-0.716719
C	3.846372	3.237708	1.654903
C	2.756277	3.924382	-0.358387
C	3.411320	4.273183	0.817110
H	4.366536	3.485360	2.577767
H	2.409317	4.708069	-1.028010
C	4.130114	-1.106484	-0.468539
C	4.892042	-0.747599	-1.610615
C	4.563430	-2.199881	0.324854
C	6.078360	-1.424944	-1.899618
C	5.760988	-2.848722	-0.008789
C	6.540305	-2.475295	-1.103179
H	6.649690	-1.128837	-2.776565
H	6.089029	-3.679665	0.611334
O	1.829070	-0.765386	1.091702
H	1.565775	-0.452418	-1.416679
C	-3.249588	-0.294874	-3.409792
H	-2.674850	-1.204174	-3.225950
H	-3.829730	-0.449001	-4.323613
H	-2.521910	0.495504	-3.605778
C	-4.389460	1.263334	1.386621
H	-5.279092	1.272057	2.021850
H	-3.633100	0.628843	1.850148
H	-3.989132	2.282427	1.360712
C	-7.995528	0.259629	-1.941947
H	-8.444069	-0.646856	-1.516317
H	-8.543270	1.113097	-1.528987
H	-8.161924	0.233979	-3.022600
C	1.814737	2.371990	-2.034497
H	2.423885	2.765873	-2.856453
H	1.599567	1.329704	-2.253663
H	0.869444	2.923716	-2.041256
C	4.140707	0.850445	2.306700
H	3.319025	0.216410	2.647273
H	4.875343	0.192114	1.831692
H	4.616766	1.321423	3.170713
C	3.643889	5.713495	1.194830
H	4.696763	5.893488	1.439975
H	3.363393	6.390446	0.383383
H	3.058192	5.988582	2.079864
C	-2.618284	3.091989	-2.010489
H	-2.255856	2.290288	-2.656263
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H	-2.537261	4.024700	-2.574604
C	-0.463185	1.262726	2.329903
H	-1.323053	0.658517	2.621524
H	0.300299	0.600855	1.908004
H	-0.039003	1.729694	3.223727
C	-0.085572	6.083265	1.081892

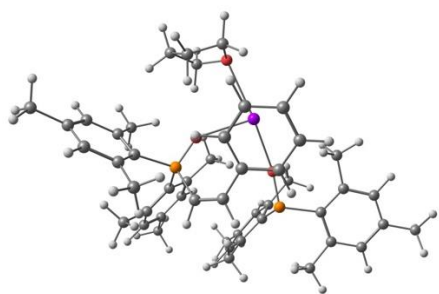
H	-0.869124	6.844367	0.996049
H	0.328596	6.131942	2.092486
H	0.710028	6.360678	0.380881
C	4.456563	0.349054	-2.551201
H	5.103778	0.376766	-3.431536
H	3.430296	0.194851	-2.898271
H	4.495934	1.332212	-2.073603
C	3.807059	-2.748075	1.516194
H	2.832110	-3.139633	1.214569
H	4.377931	-3.563898	1.969528
H	3.617003	-1.987890	2.273533
C	7.837623	-3.174632	-1.417971
H	8.697595	-2.554094	-1.135949
H	7.922615	-4.121929	-0.877906
H	7.929678	-3.381088	-2.489605
O	-2.320313	-3.140027	3.161525
C	-2.976429	-4.091213	2.299473
H	-2.217653	-4.547399	1.656725
C	-4.022765	-3.280085	1.546862
H	-3.542267	-2.698960	0.755146
H	-4.811870	-3.902136	1.115803
C	-4.522708	-2.340336	2.652884
H	-4.966383	-1.423327	2.260401
H	-5.269468	-2.845553	3.274831
C	-3.246623	-2.064013	3.461462
H	-2.777415	-1.124130	3.155623
H	-3.426197	-2.039663	4.542237
H	-3.441520	-4.884129	2.904089

Z-isomer-Mes-1THF

E (BS1) = -3373.433618

E (BS2) = -3374.273409

G_{298.15} (BS2) = -3373.421976



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C	-4.720568	0.839110	0.337110
C	-4.625445	0.041320	-1.976000
C	-6.114819	0.831572	0.259340
C	-6.026825	0.053553	-1.997444
C	-6.791494	0.437515	-0.897126
H	-6.686026	1.146049	1.129558
H	-6.532537	-0.247074	-2.911277
C	-1.571940	2.036939	-0.077835
C	-1.991101	3.152115	-0.850081
C	-0.695151	2.241666	1.018813
C	-1.537671	4.430187	-0.509561
C	-0.284774	3.545412	1.319486
C	-0.685962	4.651399	0.573069
H	-1.864429	5.275321	-1.110611
H	0.393622	3.689960	2.154902
O	-1.873417	-0.714944	0.527513
K	-0.039554	-2.247189	1.500924
C	-1.196563	0.087354	-2.052705
C	-0.530509	-1.009509	-2.456883
H	-0.988792	1.007373	-2.591021
C	-0.592257	-2.392311	-1.963058
C	0.592212	-3.154560	-1.968511
C	-1.776743	-2.992287	-1.497912
C	0.604757	-4.458527	-1.473920
C	-1.768738	-4.306381	-1.026552
C	-0.577017	-5.039442	-0.998763

H	1.509428	-2.697380	-2.326281
H	-2.703459	-2.432474	-1.499149
H	1.532782	-5.022391	-1.463791
H	-2.693309	-4.756892	-0.679560
H	-0.572637	-6.059226	-0.624975
P	2.693387	-0.311848	-0.652838
C	2.957272	1.427159	0.047848
C	3.461572	1.645477	1.354772
C	2.560546	2.550980	-0.710162
C	3.621855	2.948059	1.836090
C	2.751555	3.844518	-0.200989
C	3.292995	4.067561	1.063283
H	4.015636	3.093013	2.841163
H	2.451479	4.696528	-0.807493
C	4.458729	-0.965929	-0.493142
C	5.479678	-0.340152	-1.255720
C	4.789598	-2.168867	0.185828
C	6.779589	-0.856817	-1.270990
C	6.104632	-2.654313	0.140464
C	7.122928	-2.010324	-0.564138
H	7.539739	-0.346115	-1.859912
H	6.336944	-3.573313	0.676199
O	1.812943	-1.034695	0.431331
H	0.183419	-0.861769	-3.266133
C	-3.938574	-0.374522	-3.256308
H	-3.344382	-1.282276	-3.139120
H	-4.687919	-0.566899	-4.028275
H	-3.265506	0.398795	-3.635180
C	-4.103098	1.321911	1.630953
H	-4.850759	1.314200	2.427998
H	-3.263108	0.700460	1.942358
H	-3.734010	2.347880	1.531812
C	-8.296942	0.413901	-0.942456
H	-8.690988	-0.444690	-0.384595
H	-8.722751	1.314566	-0.488074
H	-8.664670	0.339080	-1.969499
C	1.926335	2.431983	-2.078169
H	2.680732	2.347995	-2.870360
H	1.290951	1.548596	-2.150766
H	1.321994	3.318583	-2.294396
C	3.818144	0.493667	2.263310
H	3.098428	-0.315948	2.124042
H	4.811191	0.092811	2.031685
H	3.822183	0.812435	3.310865
C	3.476761	5.462456	1.607295
H	4.486918	5.604423	2.008364
H	3.311333	6.218172	0.834063
H	2.777650	5.667507	2.427430
C	-2.940546	3.064739	-2.024793
H	-2.714029	2.242620	-2.705684
H	-3.974921	2.931107	-1.694626
H	-2.894051	3.988954	-2.606358
C	-0.142136	1.143537	1.896343
H	-0.940704	0.568398	2.371132
H	0.487489	0.456988	1.319768
H	0.480703	1.584573	2.678917
C	-0.180789	6.033210	0.893224
H	-0.946782	6.792847	0.707530
H	0.137870	6.110741	1.936373
H	0.684001	6.282954	0.266718
C	5.205271	0.888861	-2.088921
H	6.016126	1.059977	-2.803477
H	4.270726	0.782901	-2.650669
H	5.100856	1.787876	-1.474170
C	3.796766	-2.997515	0.978025
H	2.883157	-3.182161	0.411605
H	4.250498	-3.956507	1.251051
H	3.490769	-2.493111	1.899008
C	8.536975	-2.535214	-0.556964
H	9.137178	-2.055376	0.227535
H	8.563366	-3.613502	-0.369900
H	9.041617	-2.342390	-1.509528
O	-2.032300	-3.074620	3.175770
C	-2.813204	-4.060578	2.474066
H	-2.147707	-4.595297	1.789655

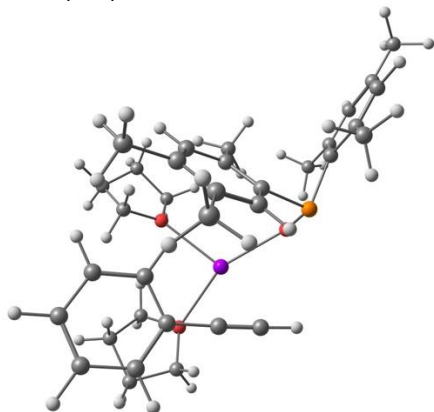
C	-3.913983	-3.265709	1.784196
H	-3.510443	-2.761045	0.902054
H	-4.765832	-3.885126	1.490855
C	-4.256353	-2.231522	2.865944
H	-4.707791	-1.326093	2.456365
H	-4.949281	-2.660261	3.597545
C	-2.891066	-1.956161	3.515314
H	-2.430451	-1.048702	3.113823
H	-2.951817	-1.870052	4.606079
H	-3.230567	-4.786675	3.187567

Int-TS-1-Mes-K-2THF

E (BS1) = -2489.32699

E (BS2) = -2489.947173

G_{298.15} (BS2) = -2489.332362



C	-2.030606	1.571283	2.041188
C	-1.225718	1.385831	2.928933
K	-0.981730	-1.406445	1.220421
H	-0.491706	1.250159	3.694122
C	-4.271053	2.195141	1.217910
C	-2.956576	1.758262	0.967102
C	-2.554552	1.497203	-0.357858
C	-3.454178	1.675002	-1.407189
C	-4.757604	2.109422	-1.151863
C	-5.162084	2.367444	0.161080
H	-4.579891	2.396074	2.238279
H	-1.538566	1.178613	-0.558894
H	-3.133616	1.475672	-2.424561
H	-5.455535	2.247204	-1.971968
H	-6.174101	2.704740	0.362364
P	2.251508	0.232905	1.610747
O	1.435876	-1.105640	1.775197
C	1.332117	0.476300	-1.172539
C	1.511539	1.080508	0.091688
C	0.701369	1.209302	-2.188512
C	0.234919	2.515485	-2.004680
C	0.391785	3.115831	-0.739806
C	1.020032	2.382179	0.271275
H	0.571697	0.743295	-3.164210
H	1.130845	2.843813	1.250748
C	4.824781	0.964819	0.679792
C	6.151079	0.769510	0.290472
C	3.960341	-0.147428	0.894142
C	4.506051	-1.444291	0.729770
C	5.849918	-1.594167	0.347012
C	6.690537	-0.509275	0.114082
H	6.783693	1.640950	0.128992
H	6.242914	-2.602782	0.226567
O	-3.473838	-2.170803	1.832638
C	-4.342617	-1.374669	2.674380
C	-4.214068	-2.590893	0.670610
C	-5.623310	-1.108644	1.862181
H	-4.546427	-1.920906	3.602699
H	-3.806837	-0.453827	2.925438
C	-5.205240	-1.460759	0.425808
H	-3.495502	-2.749952	-0.137137
H	-4.734115	-3.538016	0.878584

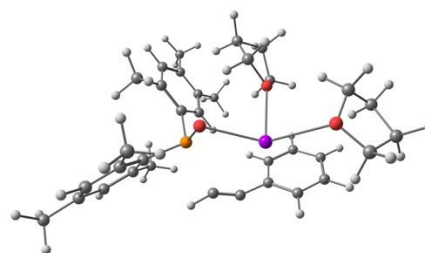
H	-5.966270	-0.076994	1.962988
H	-6.429179	-1.771093	2.193647
H	-4.697851	-0.613929	-0.046043
H	-6.045870	-1.761145	-0.205287
O	-1.407862	-2.247657	-1.258013
C	-0.795240	-3.465503	-1.743510
C	-2.011677	-1.526598	-2.354542
C	-0.825337	-3.371840	-3.268428
H	0.216966	-3.533376	-1.334029
H	-1.381640	-4.319996	-1.381451
C	-2.077400	-2.518190	-3.512857
H	-2.991491	-1.167578	-2.028647
H	-1.383541	-0.661311	-2.598021
H	-0.870251	-4.355475	-3.742311
H	0.065803	-2.852240	-3.636015
H	-2.980349	-3.134103	-3.436524
H	-2.079842	-2.020648	-4.485938
C	1.814462	-0.923870	-1.456835
H	2.891954	-0.933889	-1.656958
H	1.647104	-1.564122	-0.589052
H	1.306556	-1.345726	-2.328208
C	-0.461461	3.244677	-3.124022
H	-1.485529	3.520815	-2.844072
H	0.054367	4.177481	-3.382912
H	-0.512395	2.628213	-4.026073
C	-0.145711	4.496820	-0.466430
H	-1.234521	4.534150	-0.598051
H	0.077720	4.807858	0.557751
H	0.280095	5.244192	-1.147067
C	4.351483	2.389423	0.851480
H	3.751790	2.507378	1.760884
H	5.202938	3.074382	0.907679
H	3.716434	2.710167	0.019574
C	3.715225	-2.724264	0.905178
H	4.352087	-3.509277	1.329014
H	2.834153	-2.565943	1.526251
H	3.361871	-3.092833	-0.067677
C	8.130778	-0.694440	-0.294426
H	8.351494	-0.172105	-1.233114
H	8.816522	-0.291639	0.461281
H	8.372959	-1.752210	-0.433931

TS-1-Mes-K-2THF

E (BS1) = -2489.307277

E (BS2) = -2489.927341

G_{298.15} (BS2) = -2489.314731



C	-0.426308	-1.997523	2.360195
C	0.717733	-2.000478	1.851854
K	-1.641864	-1.417370	-0.641877
H	1.707640	-2.416844	1.918838
C	-2.873664	-2.321260	2.169191
C	-1.753380	-1.501790	2.468210
C	-2.000601	-0.157429	2.849161
C	-3.299779	0.339524	2.902385
C	-4.392177	-0.473462	2.578897
C	-4.166733	-1.805984	2.213714
H	-2.708920	-3.362070	1.903355
H	-1.158911	0.480065	3.098639
H	-3.461302	1.374558	3.191180
H	-5.402696	-0.079698	2.621413
H	-5.005868	-2.450573	1.968855
P	1.495930	-0.621446	-0.180937
O	0.748785	-0.931002	-1.516354

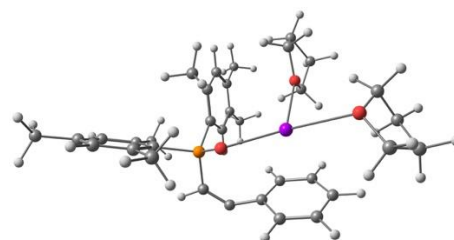
C	2.383167	2.003431	-1.017787
C	1.687314	1.224613	-0.071099
C	2.404678	3.393227	-0.844931
C	1.751659	4.037501	0.212416
C	1.031120	3.259856	1.140307
C	1.017162	1.872403	0.973665
H	2.944282	4.000598	-1.569227
H	0.466871	1.266904	1.689686
C	4.038378	-0.983448	0.963488
C	5.302409	-1.570105	1.087090
C	3.253477	-1.220115	-0.198149
C	3.781124	-2.070841	-1.205473
C	5.050107	-2.637926	-1.032656
C	5.829617	-2.406725	0.102288
H	5.887274	-1.366678	1.981877
H	5.441639	-3.280052	-1.819365
O	-4.015859	-1.822714	-1.791364
C	-4.938529	-2.815342	-1.291993
C	-4.756791	-0.623935	-2.084524
C	-6.232886	-2.069271	-0.903320
H	-5.119548	-3.569243	-2.067898
H	-4.462260	-3.307629	-0.438169
C	-5.842162	-0.584633	-1.016093
H	-4.057424	0.213292	-2.037961
H	-5.189322	-0.686744	-3.094326
H	-6.574990	-2.337588	0.099292
H	-7.035075	-2.307979	-1.607864
H	-5.415787	-0.225187	-0.074493
H	-6.682717	0.059052	-1.288566
O	-2.122357	1.149398	-0.989218
C	-1.435934	1.605875	-2.183611
C	-2.457909	2.272098	-0.150020
C	-1.159917	3.092082	-1.965797
H	-0.531055	1.003541	-2.304331
H	-2.100236	1.440947	-3.043300
C	-2.308792	3.506925	-1.035458
H	-3.472334	2.122490	0.231553
H	-1.764324	2.303996	0.697798
H	-1.143060	3.650301	-2.905680
H	-0.199002	3.227421	-1.465885
H	-3.226852	3.677926	-1.609036
H	-2.091230	4.408572	-0.456557
C	3.084011	1.377720	-2.196957
H	4.013211	0.883312	-1.892452
H	2.448581	0.614508	-2.653864
H	3.334099	2.130613	-2.950185
C	1.794947	5.538589	0.334698
H	0.789733	5.974147	0.273369
H	2.213972	5.853430	1.298145
H	2.402220	5.982918	-0.458396
C	0.276707	3.903002	2.276004
H	-0.493877	4.593401	1.910904
H	-0.215078	3.148653	2.896481
H	0.939746	4.489302	2.923956
C	3.581469	-0.074877	2.082414
H	2.536531	-0.244623	2.357691
H	4.196040	-0.231428	2.973573
H	3.661665	0.979725	1.799730
C	3.071501	-2.367256	-2.507959
H	3.535975	-3.226492	-3.001911
H	2.006236	-2.546239	-2.366752
H	3.144304	-1.513879	-3.192695
C	7.176426	-3.063253	0.271642
H	7.836605	-2.463949	0.906414
H	7.080193	-4.049978	0.743249
H	7.672307	-3.213691	-0.692632

Z-1l-Mes-K-2THF

E (BS1) = -2489.344008

E (BS2) = -2489.968518

G_{298.15} (BS2) = -2489.349779



C	0.769140	-1.745348	2.875237
C	1.834141	-1.373877	2.147353
K	-1.663973	-1.082013	-0.731304
H	2.846598	-1.389577	2.563519
C	-1.205207	-3.045826	2.095393
C	-0.611469	-1.817433	2.531758
C	-1.517366	-0.729918	2.745129
C	-2.891399	-0.871502	2.553629
C	-3.449105	-2.090122	2.135402
C	-2.577789	-3.171354	1.907136
H	-0.556507	-3.900150	1.920569
H	-1.122436	0.224159	3.080362
H	-3.538256	-0.014796	2.733771
H	-4.520206	-2.198857	2.002032
H	-2.979719	-4.127840	1.578654
P	1.797112	-0.809962	0.421836
O	0.810516	-1.554007	-0.474567
C	1.362993	1.701948	-0.827236
C	1.356871	0.973546	0.382031
C	0.978666	3.047355	-0.784590
C	0.580298	3.688227	0.393265
C	0.552726	2.949800	1.592854
C	0.946633	1.610498	1.559816
H	0.990323	3.620096	-1.709240
H	0.954655	1.044455	2.485324
C	4.532749	-0.060875	0.349009
C	5.850054	-0.171300	-0.112971
C	3.536678	-0.922469	-0.175506
C	3.907049	-1.905563	-1.130557
C	5.237022	-1.970214	-1.559163
C	6.224484	-1.112029	-1.070945
H	6.602553	0.499704	0.294418
H	5.508930	-2.722658	-2.295832
O	-3.983928	-1.751569	-1.905007
C	-4.648881	-2.938882	-1.416714
C	-4.932991	-0.670409	-1.895100
C	-5.943001	-2.471698	-0.716412
H	-4.858983	-3.610898	-2.257616
H	-3.959402	-3.444611	-0.733760
C	-5.795010	-0.940253	-0.667779
H	-4.366170	0.261796	-1.849461
H	-5.533655	-0.686814	-2.816973
H	-6.053277	-2.915031	0.276105
H	-6.818874	-2.750734	-1.309584
H	-5.256130	-0.633589	0.234639
H	-6.753633	-0.415775	-0.697438
O	-2.382661	1.419889	-1.111548
C	-2.205293	2.239849	-2.288779
C	-2.839361	2.230944	-0.008350
C	-2.529999	3.676512	-1.868351
H	-1.178288	2.124993	-2.648293
H	-2.892271	1.875340	-3.062841
C	-3.445711	3.473317	-0.651872
H	-3.554461	1.638405	0.569744
H	-1.987053	2.481721	0.633419
H	-3.003205	4.243878	-2.673554
H	-1.617395	4.198049	-1.569787
H	-4.473622	3.271369	-0.972916
H	-3.458144	4.330573	0.026111
C	1.785228	1.091929	-2.142327
H	2.871331	0.951956	-2.183458
H	1.333528	0.106926	-2.285912
H	1.501076	1.737266	-2.978225
C	0.176888	5.139231	0.375320
H	-0.859657	5.272183	0.708242

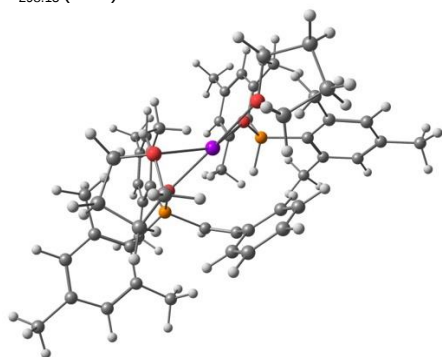
H	0.800155	5.735091	1.052943
H	0.268727	5.564533	-0.627352
C	0.102698	3.581568	2.884818
H	-0.933559	3.936154	2.818911
H	0.161775	2.868188	3.710976
H	0.716267	4.452128	3.146140
C	4.264625	1.011875	1.382624
H	3.587366	0.683810	2.172603
H	5.203924	1.312336	1.854873
H	3.821002	1.903735	0.928986
C	2.947269	-2.912810	-1.724949
H	3.495795	-3.609665	-2.365262
H	2.427593	-3.485311	-0.953218
H	2.166925	-2.429883	-2.317102
C	7.652534	-1.229203	-1.538117
H	8.221533	-0.321855	-1.315977
H	8.159660	-2.066704	-1.042636
H	7.705571	-1.413996	-2.616018

Z-2I-Mes-K-2THF

E (BS1) = -3605.890274

E (BS2) = -3606.818776

G_{298.15} (BS2) = -3605.862949



P	2.400955	0.499463	0.508874
C	4.206135	0.188947	0.799706
C	5.038938	0.173059	-0.352613
C	4.775542	-0.127256	2.058203
C	6.387591	-0.171354	-0.229242
C	6.134585	-0.468225	2.124679
C	6.957444	-0.505153	1.000717
H	7.007821	-0.176856	-1.122702
H	6.559682	-0.709541	3.095687
C	2.309599	2.178264	-0.278034
C	2.918722	3.293764	0.352604
C	1.502675	2.401434	-1.425848
C	2.672248	4.584387	-0.131584
C	1.289982	3.712178	-1.867658
C	1.847955	4.820260	-1.231090
H	3.135880	5.427476	0.375000
H	0.649794	3.867934	-2.732439
O	1.891714	-0.615907	-0.394466
K	-0.134277	-1.974841	-1.154883
C	1.414842	0.724741	2.027848
C	0.517965	-0.099744	2.603071
H	1.589503	1.716866	2.454300
C	0.234394	-1.476418	2.269255
C	-1.114089	-1.917725	2.132633
C	1.229039	-2.494005	2.210770
C	-1.438024	-3.252276	1.900442
C	0.898294	-3.834365	2.022958
C	-0.434978	-4.233096	1.850656
H	-1.910798	-1.188836	2.233451
H	2.273086	-2.215565	2.302249
H	-2.482433	-3.532998	1.784629
H	1.692334	-4.577040	1.989881
H	-0.686866	-5.279601	1.706815
P	-2.393409	0.837220	0.197356
C	-2.645568	2.556001	-0.365688
C	-3.635418	2.823788	-1.344831

C	-1.787953	3.596124	0.067002
C	-3.756496	4.115094	-1.858737
C	-1.949424	4.874859	-0.482327
C	-2.919081	5.156319	-1.443595
H	-4.518536	4.310595	-2.609329
H	-1.286357	5.668625	-0.149232
C	-3.877991	0.230490	1.079570
C	-4.227245	0.847266	2.308828
C	-4.629538	-0.876904	0.615363
C	-5.331861	0.378854	3.022288
C	-5.729755	-1.304429	1.370637
C	-6.104154	-0.692178	2.566377
H	-5.588705	0.860888	3.962354
H	-6.306781	-2.151734	1.009084
O	-1.924007	-0.074719	-0.924006
H	-1.458845	0.959236	1.237607
C	4.036212	-0.091119	3.376730
H	3.191717	-0.778630	3.411056
H	4.720528	-0.353690	4.188007
H	3.630709	0.900980	3.592455
C	4.549117	0.546076	-1.733648
H	5.261980	0.209323	-2.491041
H	3.578104	0.101490	-1.949204
H	4.443264	1.631062	-1.835268
C	8.406156	-0.907110	1.101545
H	8.548817	-1.944047	0.772081
H	9.039652	-0.278513	0.467101
H	8.770346	-0.835191	2.130335
C	-0.695340	3.411295	1.090639
H	-1.097680	3.238143	2.093023
H	-0.047131	2.568490	0.857400
H	-0.067749	4.303113	1.132374
C	-4.551979	1.746699	-1.868931
H	-3.975827	0.933496	-2.319664
H	-5.161999	1.311352	-1.071428
H	-5.226833	2.149297	-2.628098
C	-3.046642	6.532976	-2.042255
H	-4.090778	6.863100	-2.063048
H	-2.464881	7.268496	-1.480011
H	-2.686763	6.542847	-3.078474
C	3.865401	3.183141	1.527299
H	3.479773	2.555345	2.331257
H	4.827959	2.760270	1.224297
H	4.053228	4.173793	1.949522
C	0.815624	1.313688	-2.220297
H	1.501612	0.512388	-2.497496
H	-0.007419	0.864536	-1.659883
H	0.392217	1.743704	-3.133070
C	1.575908	6.216344	-1.728721
H	2.227518	6.469891	-2.574628
H	0.542548	6.316869	-2.076033
H	1.750277	6.960473	-0.945970
C	-3.423916	1.977367	2.903299
H	-3.873075	2.310283	3.841782
H	-2.395939	1.663246	3.121133
H	-3.373946	2.839861	2.232739
C	-4.308941	-1.665995	-0.632541
H	-3.357056	-2.192773	-0.542593
H	-5.094792	-2.405416	-0.807758
H	-4.227183	-1.034717	-1.517240
C	-7.306621	-1.161903	3.342784
H	-8.136799	-0.451380	3.245102
H	-7.657441	-2.134495	2.986860
H	-7.081127	-1.246702	4.411000
O	1.763336	-3.566388	-2.373597
C	2.200379	-4.438179	-1.313918
H	1.361362	-4.587758	-0.627896
C	3.394857	-3.728988	-0.688333
H	3.047060	-2.917741	-0.043234
H	4.035561	-4.402570	-0.112672
C	4.080229	-3.148224	-1.932621
H	4.714039	-2.289757	-1.703630
H	4.696491	-3.911189	-2.420931
C	2.887352	-2.770515	-2.822144
H	2.618669	-1.716648	-2.703900

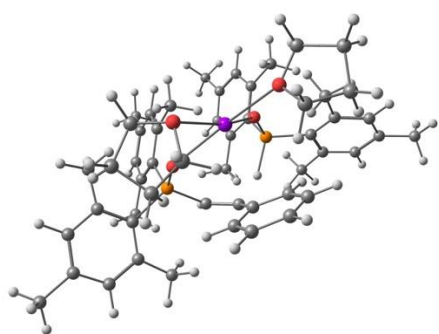
H	3.068522	-2.974736	-3.883842
H	2.486404	-5.416978	-1.728197
O	-1.896113	-3.774394	-2.048766
C	-2.058665	-5.097972	-1.526186
H	-1.542175	-5.825521	-2.171775
C	-3.569445	-5.319145	-1.539908
H	-3.838982	-6.378398	-1.536125
H	-4.017520	-4.845900	-0.661203
C	-4.003950	-4.591443	-2.833021
H	-4.144344	-5.298511	-3.655091
H	-4.941410	-4.047451	-2.696569
C	-2.824071	-3.637198	-3.137670
H	-2.326145	-3.909709	-4.078280
H	-3.113918	-2.585102	-3.188366
H	-1.605845	-5.119748	-0.533034

TS-2-Mes-K-2THF

E (BS1) = -3605.878735

E (BS2) = -3606.802070

G_{298.15} (BS2) = -3605.847548



P	2.346891	0.416318	0.409993
C	4.104590	0.153026	0.911130
C	5.059387	0.102231	-0.140154
C	4.526296	-0.099361	2.238558
C	6.386313	-0.224186	0.149238
C	5.870752	-0.422061	2.473516
C	6.813759	-0.501191	1.450066
H	7.105224	-0.258729	-0.666234
H	6.186050	-0.613514	3.496207
C	2.265790	2.079540	-0.413978
C	2.846713	3.217231	0.207617
C	1.486024	2.266570	-1.583315
C	2.631503	4.488195	-0.334971
C	1.302461	3.562336	-2.084063
C	1.853020	4.687479	-1.476440
H	3.081969	5.346758	0.157653
H	0.689545	3.689050	-2.972657
O	1.973835	-0.740235	-0.508088
K	-0.149573	-1.986403	-1.301889
C	1.162155	0.723596	1.742666
C	0.097672	-0.003361	2.168599
H	1.184121	1.785191	1.987111
C	-0.029633	-1.459802	2.050352
C	-1.320538	-2.048259	2.040109
C	1.070123	-2.353748	2.056917
C	-1.500738	-3.428247	1.977356
C	0.891327	-3.736630	2.026945
C	-0.394009	-4.287304	1.972903
H	-2.191831	-1.404462	2.089683
H	2.076567	-1.956026	2.072539
H	-2.507601	-3.836762	1.953616
H	1.760971	-4.388485	2.036157
H	-0.531894	-5.364390	1.948680
P	-2.243322	0.829553	0.420904
C	-2.351224	2.552697	-0.255987
C	-3.088602	2.768874	-1.454175
C	-1.607253	3.619962	0.287524
C	-3.058971	4.022006	-2.064190
C	-1.614974	4.867093	-0.358312
C	-2.321808	5.089317	-1.534323

H	-3.628149	4.172551	-2.978984
H	-1.038471	5.679133	0.078691
C	-3.927848	0.410115	1.062001
C	-4.419359	1.139538	2.176461
C	-4.683163	-0.687914	0.578859
C	-5.656139	0.812474	2.734628
C	-5.918343	-0.979073	1.177463
C	-6.430597	-0.242148	2.243838
H	-6.016807	1.390123	3.582934
H	-6.494114	-1.817827	0.793103
O	-1.815894	-0.110840	-0.717429
H	-1.229273	0.661785	1.654209
C	3.632729	-0.017725	3.456237
H	2.884566	-0.812873	3.482865
H	4.238904	-0.105920	4.361939
H	3.084162	0.924520	3.509806
C	4.719178	0.430450	-1.576713
H	5.523347	0.103460	-2.241142
H	3.790526	-0.047126	-1.890346
H	4.593503	1.509964	-1.712250
C	8.243718	-0.885056	1.730108
H	8.423821	-1.936839	1.474167
H	8.941328	-0.285868	1.135848
H	8.492896	-0.756157	2.787255
C	-0.784242	3.538769	1.551336
H	-1.154826	4.259697	2.289266
H	-0.790677	2.557151	2.015660
H	0.254740	3.804489	1.333671
C	-3.912070	1.680427	-2.096709
H	-3.286919	0.814641	-2.326949
H	-4.703714	1.333262	-1.424714
H	-4.381896	2.042830	-3.014872
C	-2.282950	6.422547	-2.235843
H	-3.284252	6.738407	-2.548347
H	-1.863875	7.201084	-1.592321
H	-1.665981	6.371464	-3.141414
C	3.708387	3.151318	1.448728
H	3.241523	2.583144	2.255595
H	4.677477	2.686992	1.247451
H	3.892202	4.160528	1.826287
C	0.790901	1.156016	-2.337291
H	1.466439	0.328282	-2.557550
H	-0.052475	0.767194	-1.757379
H	0.391579	1.547721	-3.277599
C	1.593247	6.072877	-2.008044
H	2.507355	6.676135	-2.018405
H	1.191160	6.041377	-3.024468
H	0.865455	6.601084	-1.380504
C	-3.633608	2.264381	2.804560
H	-4.137638	2.627406	3.703893
H	-2.630772	1.935664	3.095182
H	-3.516677	3.109493	2.120475
C	-4.244602	-1.596176	-0.547572
H	-3.289705	-2.077303	-0.333741
H	-4.999391	-2.371313	-0.706345
H	-4.107668	-1.052206	-1.483055
C	-7.766893	-0.571409	2.858242
H	-8.483852	0.244561	2.706245
H	-8.194484	-1.478619	2.422185
H	-7.680550	-0.722242	3.940364
O	1.789688	-3.624771	-2.398030
C	2.175213	-4.490553	-1.314804
H	1.319238	-4.597518	-0.641367
C	3.382256	-3.814307	-0.676565
H	3.050384	-2.983853	-0.048482
H	3.990258	-4.503152	-0.083622
C	4.108589	-3.268810	-1.913726
H	4.760705	-2.424402	-1.682132
H	4.713916	-4.054073	-2.379836
C	2.945880	-2.868418	-2.832914
H	2.706531	-1.805919	-2.732465
H	3.142825	-3.093845	-3.887503
H	2.432354	-5.487108	-1.705120
O	-1.870109	-3.893289	-2.051377
C	-1.964698	-5.156752	-1.382422

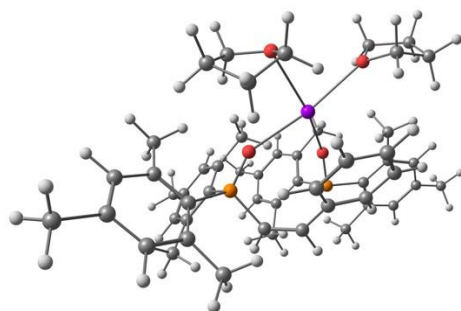
H	-1.565028	-5.957656	-2.023983
C	-3.459973	-5.334749	-1.139613
H	-3.739093	-6.376488	-0.961584
H	-3.762030	-4.740542	-0.271788
C	-4.071324	-4.759551	-2.434879
H	-4.271399	-5.556442	-3.156677
H	-5.010210	-4.233387	-2.248069
C	-2.973305	-3.810617	-2.971946
H	-2.638063	-4.114636	-3.972565
H	-3.286172	-2.764599	-3.012463
H	-1.364697	-5.098164	-0.472030

Z-isomer-Mes-2THF

E (BS1) = -3605.934087

E (BS2) = -3606.854743

G_{298.15} (BS2) = -3605.895858



P	2.432837	0.467110	0.561155
C	4.235668	0.253724	0.856425
C	5.059718	0.302953	-0.301585
C	4.818015	-0.059637	2.107745
C	6.422445	0.022227	-0.185660
C	6.192332	-0.331334	2.165465
C	7.011348	-0.304080	1.038328
H	7.040118	0.062846	-1.079654
H	6.632166	-0.570256	3.130195
C	2.195580	2.129742	-0.200761
C	2.847085	3.265422	0.345926
C	1.339118	2.292786	-1.320871
C	2.639656	4.520848	-0.236006
C	1.184043	3.569707	-1.870915
C	1.815593	4.696582	-1.347648
H	3.142495	5.382946	0.195324
H	0.522028	3.684450	-2.724085
O	1.960746	-0.689228	-0.299506
K	-0.180178	-2.008502	-1.038488
C	1.473701	0.675393	2.080700
C	0.609311	-0.180971	2.655535
H	1.452507	1.700619	2.438686
C	0.400872	-1.617872	2.428115
C	-0.900186	-2.135937	2.579486
C	1.441376	-2.503210	2.091872
C	-1.161493	-3.488135	2.362822
C	1.183566	-3.861247	1.897508
C	-0.118257	-4.357668	2.024833
H	-1.708385	-1.458331	2.835570
H	2.451812	-2.132294	1.979366
H	-2.175323	-3.864090	2.462602
H	2.000518	-4.531631	1.649381
H	-0.315137	-5.415425	1.876925
P	-2.361870	0.762554	0.819355
C	-2.416057	2.350309	-0.211792
C	-3.021815	2.386687	-1.495399
C	-1.736021	3.504167	0.235341
C	-2.974586	3.554290	-2.261163
C	-1.728391	4.666080	-0.552530
C	-2.342440	4.716094	-1.800850
H	-3.445648	3.559585	-3.243074
H	-1.206865	5.546206	-0.181420
C	-4.216331	0.474642	1.036688
C	-4.954350	1.424668	1.794531

C	-4.870755	-0.735272	0.687307
C	-6.293872	1.194605	2.119927
C	-6.215178	-0.928616	1.041816
C	-6.954976	0.023066	1.742766
H	-6.830515	1.948297	2.694146
H	-6.696852	-1.862393	0.755573
O	-1.796829	-0.317199	-0.172889
H	-0.054268	0.245422	3.406093
C	4.070270	-0.101445	3.420831
H	3.324124	-0.897898	3.453834
H	4.774703	-0.275222	4.238293
H	3.545312	0.833984	3.628946
C	4.546835	0.687415	-1.671697
H	5.265928	0.389586	-2.438995
H	3.589262	0.218917	-1.899186
H	4.408656	1.770832	-1.748878
C	8.480980	-0.622678	1.127218
H	8.703014	-1.583328	0.646641
H	9.083115	0.136971	0.617086
H	8.814679	-0.683845	2.166589
C	-0.990964	3.568162	1.550073
H	-1.591159	4.061335	2.325481
H	-0.741566	2.572432	1.916290
H	-0.068757	4.146840	1.435362
C	-3.714006	1.174763	-2.070077
H	-3.125492	0.281614	-1.845652
H	-4.703690	1.032544	-1.621547
H	-3.846441	1.276598	-3.152128
C	-2.283997	5.957582	-2.655722
H	-3.243901	6.152157	-3.146597
H	-2.020606	6.839063	-2.063474
H	-1.533230	5.859062	-3.450268
C	3.796564	3.218532	1.523153
H	3.435754	2.601548	2.347807
H	4.775278	2.824616	1.233547
H	3.947147	4.227819	1.914848
C	0.548364	1.181021	-1.969478
H	1.200951	0.383226	-2.332463
H	-0.174427	0.745203	-1.271670
H	-0.013923	1.583599	-2.816123
C	1.572797	6.062788	-1.932597
H	2.425144	6.728524	-1.766572
H	1.379843	6.008373	-3.008148
H	0.695541	6.530163	-1.468711
C	-4.322589	2.702545	2.292011
H	-4.950063	3.172344	3.055527
H	-3.336716	2.509767	2.729044
H	-4.170668	3.426590	1.486061
C	-4.209566	-1.864931	-0.073793
H	-3.205563	-2.075851	0.290280
H	-4.825392	-2.767317	-0.004524
H	-4.095844	-1.618528	-1.133799
C	-8.408344	-0.197810	2.080799
H	-9.065264	0.391569	1.427763
H	-8.690108	-1.248981	1.965347
H	-8.632057	0.102008	3.110756
O	1.711217	-3.382730	-2.538931
C	2.218337	-4.361937	-1.616285
H	1.424681	-4.598790	-0.900717
C	3.448963	-3.715139	-0.992043
H	3.141897	-2.984295	-0.239474
H	4.128277	-4.442512	-0.539085
C	4.050978	-2.989608	-2.203439
H	4.686114	-2.148475	-1.919352
H	4.647995	-3.682794	-2.805844
C	2.803134	-2.540254	-2.978594
H	2.537004	-1.504915	-2.748010
H	2.921081	-2.643832	-4.063567
H	2.481065	-5.285898	-2.153759
O	-1.778259	-3.999172	-1.846554
C	-1.909680	-5.294688	-1.253991
H	-1.504973	-6.064467	-1.930163
C	-3.414410	-5.463831	-1.058292
H	-3.713133	-6.511812	-0.972232
H	-3.725406	-4.939046	-0.150320

C	-3.994910	-4.772163	-2.313003
H	-4.261132	-5.504912	-3.079673
H	-4.889929	-4.192281	-2.077652
C	-2.839399	-3.869316	-2.807496
H	-2.479683	-4.190413	-3.794815
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H	-1.331684	-5.298002	-0.327473

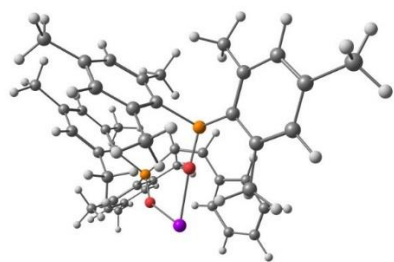
Bishydrophosphorylation with Mes₂P(O)H

Int-TS-1-Mes-DA

E (BS1) = -3140.929252

E (BS2) = -3141.688110

G_{298.15} (BS2) = -3140.945896



15	-2.447168	-0.315247	0.034490
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6	-5.040578	-0.006879	0.948247
6	-4.917517	-1.205253	-1.185141
6	-6.427396	-0.164724	0.931967
6	-6.312831	-1.336200	-1.146590
6	-7.087356	-0.825092	-0.107134
1	-7.007357	0.240371	1.757824
1	-6.805528	-1.856817	-1.963457
6	-2.116145	1.498214	0.098160
6	-2.735888	2.368347	-0.836925
6	-1.220025	2.036605	1.057917
6	-2.458518	3.738096	-0.785690
6	-0.993366	3.417250	1.070787
6	-1.593600	4.286051	0.161662
1	-2.938086	4.392652	-1.509372
1	-0.301100	3.817315	1.805627
8	-1.982237	-1.077787	1.262779
19	0.113008	-2.140794	2.283907
6	-1.541699	-0.747248	-1.471937
6	-0.767073	-1.819662	-1.716483
1	-1.479600	0.071124	-2.183231
6	-0.627511	-3.074311	-0.965425
6	0.629668	-3.709723	-0.960485
6	-1.683246	-3.665422	-0.246223
6	0.842016	-4.867918	-0.213116
6	-1.474791	-4.834117	0.489152
6	-0.209189	-5.432256	0.519446
1	1.447888	-3.260093	-1.514272
1	-2.663074	-3.204973	-0.248259
1	1.824499	-5.330317	-0.202889
1	-2.300633	-5.278218	1.037435
1	-0.048209	-6.338878	1.095445
15	2.380919	-0.409696	-0.433709
6	2.440185	1.458384	-0.135610
6	2.998621	2.012694	1.045475
6	1.830547	2.335784	-1.059178
6	2.993663	3.395998	1.240783
6	1.856824	3.721478	-0.835344
6	2.444559	4.274760	0.299259
1	3.433012	3.800377	2.151590
1	1.390652	4.379137	-1.566317
6	4.229398	-0.786089	-0.352331
6	5.074649	-0.218770	-1.341970
6	4.792439	-1.762231	0.512198
6	6.429058	-0.562439	-1.407566

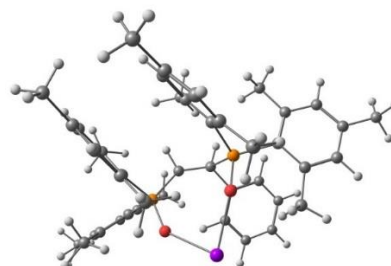
6	6.154579	-2.079503	0.409645
6	6.999555	-1.484191	-0.528475
1	7.049778	-0.102260	-2.174600
1	6.566059	-2.824186	1.089050
8	1.713595	-0.980912	0.871759
1	-0.122389	-1.754039	-2.591506
6	-4.224856	-1.801652	-2.389600
1	-3.532096	-2.601447	-2.120870
1	-4.970766	-2.224867	-3.067065
1	-3.652004	-1.060037	-2.951713
6	-4.440616	0.738361	2.120195
1	-5.175681	0.824965	2.924353
1	-3.556688	0.231525	2.511879
1	-4.138132	1.751054	1.834866
6	-8.585248	-0.984321	-0.090746
1	-8.904706	-1.606811	0.753512
1	-9.084337	-0.015135	0.020350
1	-8.948024	-1.451688	-1.010051
6	1.141548	1.858786	-2.318376
1	1.825781	1.865189	-3.176549
1	0.770110	0.839695	-2.212703
1	0.303850	2.518829	-2.565637
6	3.593947	1.137246	2.121517
1	2.980162	0.241949	2.243180
1	4.603437	0.805731	1.854119
1	3.659100	1.678228	3.071145
6	2.454648	5.764175	0.537102
1	3.456631	6.117988	0.805896
1	2.129728	6.313311	-0.351287
1	1.787521	6.042006	1.362320
6	-3.720614	1.922791	-1.895764
1	-3.410801	1.020374	-2.424946
1	-4.706572	1.720653	-1.467299
1	-3.838226	2.711934	-2.642791
6	-0.457250	1.220497	2.075189
1	-1.131392	0.647763	2.717004
1	0.232729	0.526278	1.583397
1	0.138529	1.888528	2.702532
6	-1.283087	5.759285	0.169247
1	-2.154128	6.353908	-0.123505
1	-0.951871	6.093251	1.156557
1	-0.478781	5.987331	-0.540463
6	4.549532	0.756710	-2.368122
1	5.260146	0.869095	-3.192555
1	3.594530	0.416762	-2.783550
1	4.369574	1.747005	-1.939242
6	4.006330	-2.515612	1.567659
1	3.093972	-2.951170	1.157321
1	4.625710	-3.315062	1.988529
1	3.693413	-1.861117	2.385646
6	8.469302	-1.818176	-0.585798
1	9.061931	-1.119188	0.019276
1	8.666977	-2.824542	-0.202902
1	8.853734	-1.761707	-1.609574

TS-1-Mes-DA

E (BS1) = -3140.904412

E (BS2) = -3141.665253

G_{298.15} (BS2) = -3140.920046



15	-2.026998	-0.590864	0.226541
6	-3.661293	-1.394563	-0.151218
6	-4.770352	-1.029153	0.658164

6	-3.843245	-2.384088	-1.147641
6	-6.023569	-1.599654	0.417359
6	-5.121442	-2.924967	-1.349724
6	-6.228190	-2.538891	-0.595448
1	-6.860930	-1.305207	1.046691
1	-5.248519	-3.679277	-2.122781
6	-2.397384	1.233862	0.170057
6	-3.110304	1.798661	-0.919076
6	-1.846723	2.101947	1.146335
6	-3.258819	3.188352	-1.001381
6	-2.034968	3.483500	1.023555
6	-2.731057	4.052389	-0.041598
1	-3.804839	3.604234	-1.845470
1	-1.604230	4.133440	1.781150
8	-1.671021	-1.109410	1.622763
19	0.296079	-1.516996	3.106706
6	-0.849924	-0.726544	-1.046804
6	0.484358	-1.220089	-1.154436
1	-1.109405	-0.021948	-1.828373
6	0.957330	-2.534239	-0.614591
6	2.170159	-3.065530	-1.086202
6	0.246934	-3.270658	0.347299
6	2.675307	-4.267535	-0.592911
6	0.751840	-4.475334	0.845899
6	1.972996	-4.975387	0.386009
1	2.728692	-2.520246	-1.840481
1	-0.699959	-2.890290	0.712476
1	3.618815	-4.649295	-0.972237
1	0.181145	-5.028953	1.587935
1	2.364402	-5.911607	0.773503
15	1.922717	0.069196	-0.033286
6	1.758885	1.926314	-0.188474
6	2.271586	2.709292	0.887974
6	1.020917	2.575543	-1.199880
6	1.996568	4.076184	0.936788
6	0.764280	3.952466	-1.101418
6	1.224400	4.718653	-0.037975
1	2.398886	4.659825	1.762088
1	0.183380	4.427118	-1.888928
6	3.721254	-0.330495	-0.275744
6	4.381083	0.064705	-1.468722
6	4.418423	-1.175422	0.631782
6	5.702343	-0.326988	-1.703177
6	5.739245	-1.543570	0.348148
6	6.408272	-1.126253	-0.802962
1	6.187186	-0.004385	-2.621904
1	6.259404	-2.186613	1.054596
8	1.522405	-0.226798	1.420890
1	0.882770	-1.087689	-2.160629
6	-2.740574	-2.928194	-2.028957
1	-1.924733	-3.362451	-1.446362
1	-3.144783	-3.708716	-2.681148
1	-2.286515	-2.153701	-2.651226
6	-4.679152	-0.032527	1.794287
1	-5.515833	-0.177489	2.484057
1	-3.747023	-0.143618	2.350760
1	-4.725665	0.998490	1.429808
6	-7.597730	-3.109799	-0.860924
1	-8.123567	-3.338112	0.072210
1	-8.221132	-2.395760	-1.414023
1	-7.540868	-4.026197	-1.455524
6	0.504590	1.916452	-2.456135
1	0.959753	2.388763	-3.334884
1	0.722419	0.856345	-2.504640
1	-0.577824	2.051949	-2.539271
6	3.124698	2.136167	1.995905
1	2.538793	1.467266	2.628982
1	3.953750	1.543358	1.598935
1	3.542877	2.941990	2.605515
6	0.896182	6.184405	0.079078
1	1.766666	6.764816	0.403247
1	0.546517	6.593827	-0.872942
1	0.105195	6.349391	0.820900
6	-3.757331	0.990425	-2.026080
1	-3.137551	0.164417	-2.376797

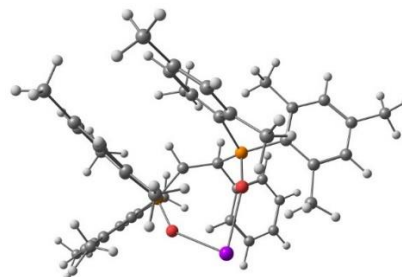
1	-4.709632	0.558290	-1.703038
1	-3.961369	1.637476	-2.883940
6	-1.033169	1.630128	2.330001
1	-1.620448	0.978083	2.983354
1	-0.152764	1.073082	1.999379
1	-0.695924	2.493328	2.911363
6	-2.868808	5.546696	-0.180090
1	-3.849412	5.823758	-0.581071
1	-2.737220	6.051485	0.781577
1	-2.113994	5.948529	-0.867412
6	3.701366	0.886545	-2.535649
1	4.346173	0.981957	-3.413154
1	2.766633	0.422697	-2.863071
1	3.455417	1.892291	-2.185039
6	3.825135	-1.741372	1.904532
1	2.943744	-2.349746	1.689601
1	4.564139	-2.375831	2.403038
1	3.517194	-0.951647	2.591971
6	7.842153	-1.513477	-1.057596
1	8.531475	-0.760247	-0.654297
1	8.089391	-2.467210	-0.581246
1	8.049332	-1.600102	-2.128838

DA-I-Mes-K

E (BS1) = -3140.908434

E (BS2) = -3141.672347

G_{298.15} (BS2) = -3140.923532



15	-1.864329	-0.595750	0.268141
6	-3.392285	-1.611628	-0.121077
6	-4.559415	-1.378248	0.654779
6	-3.438976	-2.611578	-1.122546
6	-5.731068	-2.093674	0.388043
6	-4.638655	-3.301023	-1.354995
6	-5.799971	-3.051941	-0.625558
1	-6.612514	-1.899874	0.996503
1	-4.657792	-4.060907	-2.133345
6	-2.494428	1.158305	0.150176
6	-3.250145	1.605133	-0.963340
6	-2.078356	2.113392	1.110690
6	-3.585034	2.960624	-1.075345
6	-2.453316	3.453859	0.964054
6	-3.204867	3.904392	-0.120588
1	-4.161125	3.284701	-1.939812
1	-2.127316	4.168797	1.715993
8	-1.543972	-1.051382	1.702162
19	0.314438	-1.156154	3.333646
6	-0.620352	-0.553552	-0.901015
6	0.796093	-1.004317	-1.000320
1	-0.895062	0.152463	-1.671083
6	1.209805	-2.404648	-0.584411
6	2.355457	-2.980507	-1.155779
6	0.515829	-3.137124	0.390266
6	2.808265	-4.238115	-0.755355
6	0.966664	-4.397730	0.792493
6	2.118324	-4.951560	0.227508
1	2.902586	-2.432933	-1.917172
1	-0.373369	-2.710023	0.841422
1	3.698239	-4.660133	-1.213649
1	0.410965	-4.949419	1.546806
1	2.467219	-5.931471	0.540709
15	1.901677	0.166036	0.045789
6	1.579201	1.970068	-0.256774

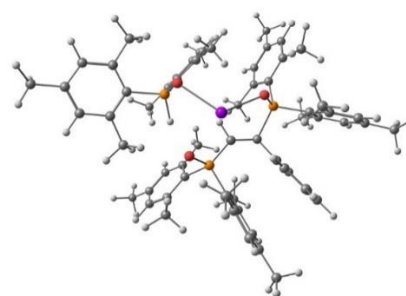
6	1.999999	2.824037	0.806881
6	0.829383	2.535242	-1.314947
6	1.580164	4.154776	0.830204
6	0.416957	3.873400	-1.227688
6	0.750991	4.693412	-0.156837
1	1.910820	4.789305	1.649379
1	-0.183273	4.278181	-2.039012
6	3.696609	-0.195545	-0.238827
6	4.370148	0.266635	-1.398266
6	4.404339	-1.031910	0.669821
6	5.713390	-0.064460	-1.603928
6	5.746891	-1.333687	0.414616
6	6.427648	-0.856013	-0.705388
1	6.209263	0.303037	-2.499109
1	6.274559	-1.974552	1.116841
8	1.558317	-0.071329	1.508920
1	1.142506	-0.883988	-2.031869
6	-2.258415	-3.014507	-1.977821
1	-1.472915	-3.491201	-1.384129
1	-2.580148	-3.728294	-2.742922
1	-1.784083	-2.155377	-2.456110
6	-4.616439	-0.371835	1.785122
1	-5.445523	-0.611808	2.457976
1	-3.687829	-0.367980	2.358145
1	-4.778455	0.644283	1.411049
6	-7.086044	-3.781042	-0.922071
1	-7.629772	-4.023632	-0.002920
1	-7.755554	-3.167415	-1.538606
1	-6.901948	-4.712066	-1.466519
6	0.482467	1.876463	-2.631251
1	0.991731	2.414743	-3.439799
1	0.769841	0.835472	-2.709348
1	-0.591605	1.952205	-2.824027
6	2.907970	2.389326	1.938762
1	2.351647	1.854392	2.711218
1	3.703081	1.721382	1.600744
1	3.375701	3.270273	2.387942
6	0.239558	6.106034	-0.056742
1	1.006113	6.783660	0.333436
1	-0.091037	6.482636	-1.028941
1	-0.617010	6.158430	0.626227
6	-3.737449	0.696986	-2.074626
1	-2.990644	-0.037574	-2.378544
1	-4.632152	0.140525	-1.778201
1	-3.995059	1.294100	-2.954434
6	-1.207695	1.773638	2.299615
1	-1.728297	1.108640	2.995908
1	-0.291082	1.273553	1.978237
1	-0.934231	2.689202	2.832291
6	-3.550462	5.362583	-0.286175
1	-4.560437	5.492106	-0.689416
1	-3.492324	5.898442	0.666073
1	-2.860303	5.855248	-0.982599
6	3.698727	1.092525	-2.466732
1	4.378609	1.249335	-3.307773
1	2.807220	0.595426	-2.855213
1	3.388946	2.072279	-2.095107
6	3.807372	-1.661250	1.910480
1	2.906539	-2.230765	1.676000
1	4.536238	-2.341125	2.360789
1	3.532333	-0.903699	2.647954
6	7.882999	-1.174689	-0.928582
1	8.525984	-0.431766	-0.439304
1	8.145862	-2.153227	-0.515193
1	8.134284	-1.170752	-1.993504

Int-TS-2-Mes-DA

E (BS1) = -4257.480275

E (BS2) = -4258.547717

G_{298.15} (BS2) = -4257.463682



15	-0.345588	2.135524	-0.106938
6	0.855881	3.545427	-0.089735
6	1.451675	3.951304	1.129304
6	1.191728	4.240744	-1.275263
6	2.348581	5.022057	1.140792
6	2.068802	5.330415	-1.209375
6	2.665323	5.735283	-0.016650
1	2.815353	5.302579	2.082498
1	2.311096	5.859408	-2.128627
6	-1.586169	2.685629	1.208888
6	-1.961937	1.880213	2.307521
6	-2.259084	3.926885	1.030009
6	-2.969975	2.311979	3.184185
6	-3.249690	4.321175	1.934976
6	-3.625872	3.529616	3.022666
1	-3.244378	1.669269	4.017691
1	-3.752755	5.272826	1.774648
8	-1.264012	2.112320	-1.352532
19	-0.076300	0.282405	-2.873730
6	0.500480	0.647145	0.015524
6	1.843043	0.210968	0.534532
1	-0.219382	-0.168736	-0.065779
6	2.984912	1.196990	0.389395
6	3.257695	1.820418	-0.832476
6	3.834881	1.454425	1.470232
6	4.350728	2.670398	-0.977624
6	4.926592	2.313781	1.337366
6	5.192436	2.921276	0.109335
1	2.590293	1.637959	-1.665692
1	3.634703	0.980060	2.426505
1	4.541136	3.145833	-1.935424
1	5.569504	2.506089	2.191807
1	6.043030	3.588083	0.000260
15	2.349203	-1.360671	-0.490849
6	1.967206	-3.019405	0.253728
6	1.240775	-3.239257	1.444161
6	2.478392	-4.148059	-0.450866
6	1.122964	-4.538629	1.954012
6	2.313424	-5.425898	0.089171
6	1.659935	-5.645626	1.304668
1	0.569843	-4.680884	2.878247
1	2.709965	-6.275977	-0.461147
6	4.197407	-1.342786	-0.522937
6	4.926424	-1.606283	0.662347
6	4.905706	-1.023918	-1.710438
6	6.323643	-1.556062	0.639877
6	6.304481	-0.987809	-1.677007
6	7.035828	-1.246284	-0.517675
1	6.866287	-1.757470	1.560474
1	6.837315	-0.743149	-2.592684
8	1.733808	-1.288113	-1.882014
1	1.853322	-0.110676	1.583611
15	-3.065124	-0.792009	-1.140560
6	-4.846552	-0.515662	-1.376578
6	-5.400070	0.770946	-1.181546
6	-5.659877	-1.578655	-1.838707
6	-6.767950	0.952939	-1.421388
6	-7.017824	-1.345471	-2.059579
6	-7.593632	-0.087657	-1.848997
1	-7.195561	1.941099	-1.271238
1	-7.640300	-2.163794	-2.413723
6	-2.833406	-2.187705	0.017662

6	-3.483262	-2.136450	1.278015
6	-2.011927	-3.295092	-0.304714
6	-3.315806	-3.192188	2.176729
6	-1.901354	-4.337294	0.623971
6	-2.538845	-4.310556	1.863234
1	-3.811222	-3.138788	3.143417
1	-1.273806	-5.186205	0.372520
8	-2.322339	-0.933643	-2.457586
1	-2.653743	0.313799	-0.384591
6	4.257084	-0.720564	-3.042440
1	3.571779	0.125759	-2.976951
1	5.030133	-0.480877	-3.778114
1	3.671552	-1.563754	-3.413102
6	4.286607	-1.957857	1.986554
1	4.986702	-1.753340	2.800999
1	3.380344	-1.387725	2.188862
1	4.021271	-3.018614	2.033444
6	8.539513	-1.153058	-0.507847
1	8.963208	-1.414171	-1.482404
1	8.864635	-0.130986	-0.274810
1	8.976662	-1.813692	0.247005
6	0.541922	-2.151819	2.212669
1	1.224621	-1.617356	2.883496
1	0.088632	-1.422843	1.547572
1	-0.253011	-2.578546	2.828031
6	3.193075	-4.056950	-1.779969
1	2.695753	-3.353279	-2.448683
1	4.227093	-3.719892	-1.659099
1	3.217426	-5.040378	-2.256606
6	1.489233	-7.037787	1.854929
1	2.420026	-7.610803	1.786819
1	1.174778	-7.017409	2.902095
1	0.729956	-7.592537	1.289469
6	0.719618	3.839363	-2.655150
1	-0.307129	3.477509	-2.650012
1	0.820354	4.677843	-3.350805
1	1.355538	3.030466	-3.044970
6	1.179253	3.268462	2.448768
1	2.018754	3.424839	3.131380
1	0.278688	3.667335	2.926425
1	1.038276	2.194091	2.332928
6	3.663099	6.863592	0.019959
1	4.685805	6.472833	0.098906
1	3.611679	7.474795	-0.885774
1	3.501442	7.516144	0.884506
6	-1.347464	0.534328	2.605833
1	-0.260494	0.584749	2.682319
1	-1.739560	0.141217	3.548635
1	-1.573445	-0.193854	1.827172
6	-1.980701	4.867579	-0.120954
1	-2.790656	5.596915	-0.214662
1	-1.048934	5.422366	0.026618
1	-1.889392	4.314904	-1.056814
6	-4.701440	3.981602	3.977497
1	-4.937941	3.203761	4.709251
1	-4.392695	4.877938	4.529219
1	-5.624492	4.237968	3.444844
6	-4.598402	1.957289	-0.697476
1	-4.407185	1.890883	0.379501
1	-3.621498	2.057031	-1.179474
1	-5.159788	2.880443	-0.865145
6	-5.108624	-2.961256	-2.096934
1	-4.162270	-2.923858	-2.643283
1	-4.924260	-3.500887	-1.162260
1	-5.816159	-3.548719	-2.687760
6	-9.067408	0.128616	-2.077201
1	-9.660469	-0.361091	-1.294929
1	-9.321275	1.192108	-2.071079
1	-9.387830	-0.295820	-3.034700
6	-4.370679	-0.988036	1.699163
1	-4.512124	-1.001522	2.782780
1	-3.955971	-0.012592	1.438044
1	-5.358291	-1.054649	1.231773
6	-1.209786	-3.427185	-1.579862
1	-1.823343	-3.299741	-2.472926

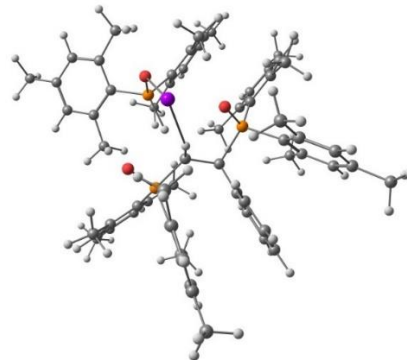
1	-0.415538	-2.677002	-1.632305
1	-0.735417	-4.411639	-1.610487
6	-2.378884	-5.440503	2.847216
1	-1.724138	-6.222257	2.453832
1	-1.953565	-5.083880	3.792422
1	-3.346626	-5.896893	3.086156

TS-2-Mes-DA

E (BS1) = -4257.445696

E (BS2) = -4258.508072

G_{298.15} (BS2) = -4257.421311



15	0.891007	2.393443	-0.361736
6	2.713981	2.755234	-0.575458
6	3.559645	3.153610	0.492478
6	3.287540	2.625852	-1.868400
6	4.896287	3.478373	0.233676
6	4.629441	2.961673	-2.074978
6	5.453272	3.405448	-1.041605
1	5.525110	3.782405	1.067555
1	5.042992	2.860820	-3.075943
6	0.388317	3.574100	0.973911
6	-0.114606	3.190769	2.237135
6	0.476969	4.958802	0.667629
6	-0.515382	4.168712	3.153593
6	0.064550	5.899671	1.617652
6	-0.438035	5.530975	2.866589
1	-0.901345	3.849734	4.118903
1	0.140099	6.955664	1.368534
8	0.139478	2.784867	-1.641879
19	-0.093601	0.033433	-3.541946
6	0.485712	0.667414	-0.142408
6	1.251287	-0.406792	0.649017
1	0.585600	0.397163	-1.191554
6	2.748999	-0.227838	0.836008
6	3.631241	-0.155633	-0.249753
6	3.286485	-0.176949	2.126817
6	5.005509	-0.068043	-0.056828
6	4.664393	-0.066050	2.331077
6	5.529969	-0.020740	1.238531
1	3.231567	-0.178418	-1.255557
1	2.618977	-0.229254	2.982659
1	5.667748	-0.024161	-0.916011
1	5.057857	-0.022551	3.342816
1	6.602526	0.055698	1.391777
15	0.928127	-2.053880	-0.289219
6	-0.253121	-3.229011	0.514439
6	-0.991190	-2.987181	1.696132
6	-0.351854	-4.509025	-0.102772
6	-1.707390	-4.036128	2.285470
6	-1.097156	-5.513184	0.517964
6	-1.755387	-5.312156	1.732465
1	-2.259681	-3.832957	3.198605
1	-1.161539	-6.484670	0.033426
6	2.527250	-2.974324	-0.250099
6	3.017732	-3.470799	0.982281
6	3.303067	-3.149682	-1.424776
6	4.259124	-4.110314	1.023791
6	4.534592	-3.808818	-1.327577
6	5.038344	-4.288443	-0.118933

1	4.625789	-4.474078	1.980627
1	5.124020	-3.939421	-2.231590
8	0.497919	-1.741894	-1.717777
1	0.841419	-0.522390	1.646311
15	-2.639979	0.299822	-1.045480
6	-4.084170	1.480684	-1.011694
6	-3.954033	2.777918	-0.473731
6	-5.307129	1.114241	-1.628673
6	-5.041994	3.658721	-0.504671
6	-6.369459	2.025204	-1.637663
6	-6.265339	3.298031	-1.070536
1	-4.922335	4.652861	-0.079723
1	-7.303255	1.731263	-2.112861
6	-3.400331	-1.196707	-0.247485
6	-4.015267	-1.055678	1.020971
6	-3.405862	-2.469518	-0.869101
6	-4.687636	-2.137278	1.594715
6	-4.096508	-3.523640	-0.256930
6	-4.763587	-3.377836	0.958510
1	-5.157972	-2.005694	2.567368
1	-4.100202	-4.494323	-0.746667
8	-2.344273	0.045544	-2.540097
1	-1.186124	0.612723	-0.297388
6	2.916357	-2.664102	-2.805520
1	2.790512	-1.578855	-2.835801
1	3.701393	-2.932651	-3.517877
1	1.974178	-3.095852	-3.146013
6	2.263922	-3.368433	2.287697
1	2.961507	-3.444667	3.125734
1	1.725871	-2.428798	2.400820
1	1.531678	-4.176277	2.385272
6	6.391285	-4.946157	-0.040399
1	6.725910	-5.292650	-1.022307
1	7.143749	-4.241878	0.336267
1	6.380781	-5.801701	0.642606
6	-1.081548	-1.653044	2.389865
1	-0.210880	-1.459763	3.026857
1	-1.181096	-0.837015	1.677421
1	-1.960836	-1.634198	3.035803
6	0.302823	-4.867983	-1.418149
1	0.264885	-4.040929	-2.126360
1	1.354207	-5.140168	-1.282149
1	-0.206857	-5.728293	-1.859837
6	-2.517681	-6.431768	2.390810
1	-1.850408	-7.263660	2.645635
1	-3.006251	-6.097481	3.309607
1	-3.287090	-6.832863	1.722201
6	2.550447	2.057603	-3.061284
1	1.580417	2.536538	-3.194729
1	3.153878	2.158600	-3.967214
1	2.386666	0.982699	-2.900817
6	3.141574	3.235119	1.944292
1	4.025628	3.136173	2.579963
1	2.663683	4.189689	2.182582
1	2.453447	2.440998	2.223854
6	6.905547	3.731380	-1.276777
1	7.549311	2.903661	-0.952638
1	7.109020	3.911873	-2.336329
1	7.213388	4.617585	-0.712148
6	-0.224826	1.754744	2.675888
1	-0.707098	1.147940	1.912368
1	0.762862	1.316828	2.858722
1	-0.795564	1.677581	3.604785
6	1.029830	5.498038	-0.632835
1	0.794150	6.561351	-0.729883
1	2.119637	5.393053	-0.669299
1	0.626426	4.953611	-1.487358
6	-0.909747	6.567519	3.853333
1	-0.869712	6.190335	4.879579
1	-0.304977	7.478075	3.796558
1	-1.949095	6.856242	3.650997
6	-2.663574	3.245077	0.138276
1	-2.414208	2.671385	1.033386
1	-1.826815	3.137035	-0.557203
1	-2.725358	4.296069	0.433178

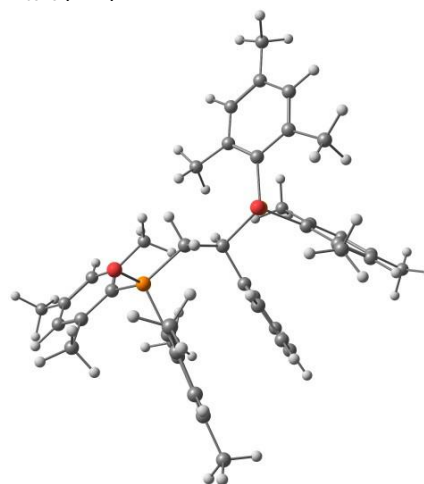
6	-5.526979	-0.222466	-2.298002
1	-4.642189	-0.525469	-2.860406
1	-5.738842	-1.009348	-1.567239
1	-6.378867	-0.165254	-2.982181
6	-7.439698	4.243597	-1.065269
1	-8.126768	4.014228	-0.240508
1	-7.116462	5.281606	-0.942514
1	-8.016360	4.171129	-1.993191
6	-3.967187	0.232879	1.809302
1	-4.124259	0.030566	2.872785
1	-3.003439	0.737921	1.709252
1	-4.736855	0.940263	1.487159
6	-2.699920	-2.775231	-2.170753
1	-3.164578	-2.259444	-3.014610
1	-1.657602	-2.454686	-2.139126
1	-2.730764	-3.852915	-2.359457
6	-5.514602	-4.523325	1.586973
1	-5.398742	-5.442986	1.007167
1	-5.164877	-4.718717	2.606671
1	-6.587218	-4.303764	1.654830

P-DA-Mes

E (BS1) = -2541.574704

E (BS2) = -2542.298629

G_{298.15} (BS2) = -2541.535804



15	2.400375	-0.867673	1.153418
6	2.891050	0.889271	0.892435
6	3.256727	1.392557	-0.380810
6	2.920942	1.756420	2.014125
6	3.688985	2.716858	-0.493253
6	3.359997	3.073999	1.844520
6	3.757977	3.573902	0.604897
1	3.958599	3.093095	-1.477196
1	3.378551	3.730852	2.710703
6	3.463598	-1.833614	-0.009158
6	3.008394	-2.692972	-1.030592
6	4.863534	-1.724255	0.222827
6	3.932531	-3.390235	-1.816272
6	5.746359	-2.439561	-0.592221
6	5.307916	-3.275246	-1.620784
1	3.559616	-4.040870	-2.603323
1	6.813812	-2.338625	-0.411003
8	2.678779	-1.384409	2.551603
6	0.541005	-0.934524	1.038860
6	-0.408284	-0.364005	-0.031174
1	0.325013	-0.421273	1.981856
6	-0.090172	1.038746	-0.505110
6	0.089380	2.090516	0.403606
6	-0.075522	1.326570	-1.874036
6	0.265788	3.396909	-0.044637
6	0.112974	2.632544	-2.328386
6	0.278471	3.673609	-1.413581
1	0.074053	1.885334	1.466408
1	-0.223130	0.522558	-2.589152

1	0.399862	4.197321	0.676240
1	0.121380	2.836039	-3.395306
1	0.417327	4.692169	-1.764149
15	-2.151546	-0.238236	0.773654
6	-3.301080	-1.690324	0.665475
6	-3.005723	-2.964265	0.130770
6	-4.596661	-1.463655	1.215139
6	-3.997619	-3.953433	0.108847
6	-5.547769	-2.485857	1.170074
6	-5.277937	-3.736559	0.611751
1	-3.750402	-4.924428	-0.312267
1	-6.531388	-2.294942	1.592552
6	-2.999993	1.058286	-0.238944
6	-3.359208	0.782085	-1.584445
6	-3.253998	2.349150	0.287816
6	-3.956605	1.779874	-2.357645
6	-3.849035	3.314495	-0.535797
6	-4.207648	3.058174	-1.856280
1	-4.222041	1.551965	-3.387095
1	-4.031323	4.302642	-0.120258
8	-1.925676	0.126450	2.227464
1	-0.457874	-1.018832	-0.895874
1	0.304516	-1.981003	1.243213
6	-2.969236	2.781854	1.708607
1	-2.102344	2.290891	2.139699
1	-2.834583	3.866724	1.741511
1	-3.820553	2.538100	2.356158
6	-3.125603	-0.547931	-2.262005
1	-3.303972	-0.455033	-3.336109
1	-2.101875	-0.905283	-2.137891
1	-3.791764	-1.324901	-1.878305
6	-4.807456	4.130321	-2.728123
1	-5.289769	4.909005	-2.130200
1	-4.033109	4.615211	-3.336167
1	-5.548569	3.716012	-3.418942
6	-1.662370	-3.346307	-0.427793
1	-1.421079	-2.801465	-1.344137
1	-0.869805	-3.159254	0.295139
1	-1.638367	-4.411584	-0.668196
6	-5.027012	-0.164787	1.858706
1	-4.250928	0.234613	2.512713
1	-5.249730	0.597817	1.105962
1	-5.933779	-0.325520	2.447109
6	-6.331683	-4.812435	0.579308
1	-7.234457	-4.465214	0.064011
1	-5.971797	-5.709542	0.068434
1	-6.632925	-5.098669	1.593853
6	2.454866	1.361804	3.397487
1	3.015582	0.515454	3.794581
1	2.546818	2.213753	4.076542
1	1.403784	1.052954	3.392853
6	3.190001	0.601243	-1.667711
1	3.085915	1.289501	-2.510242
1	4.094964	0.008077	-1.828767
1	2.338853	-0.077174	-1.699071
6	4.183945	5.009119	0.438415
1	3.372882	5.603864	-0.000828
1	4.446184	5.463948	1.397779
1	5.045364	5.095926	-0.231863
6	1.550364	-2.891187	-1.339834
1	1.013555	-3.279145	-0.474179
1	1.071808	-1.957094	-1.643678
1	1.422195	-3.606344	-2.155828
6	5.481454	-0.849375	1.291909
1	6.520095	-1.146208	1.459605
1	5.480987	0.203986	0.993710
1	4.936671	-0.924414	2.233976
6	6.287387	-4.049995	-2.463343
1	5.837998	-4.366932	-3.408852
1	7.178884	-3.455348	-2.686853
1	6.624861	-4.953108	-1.939341

**Cyclization of
hydrophosphorylated alkene**

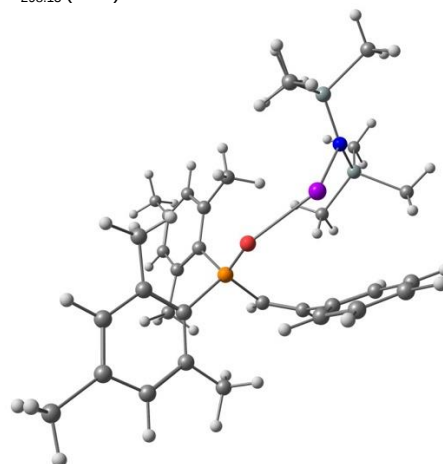
Z-mono-

CYC-I1-Mes

E (BS1) = -2898.410348

E (BS2) = -2899.034557

G_{298.15} (BS2) = -2898.411902



P	1.664253	0.022086	-0.252285
C	3.364994	0.367741	0.347602
C	3.704676	-0.225358	1.596153
C	4.303915	1.207509	-0.300531
C	4.961389	0.020827	2.151102
C	5.549864	1.419506	0.306133
C	5.903331	0.838367	1.522142
H	5.208716	-0.440058	3.104301
H	6.266542	2.063160	-0.196729
C	1.528084	-1.795531	-0.524976
C	2.512026	-2.476994	-1.288747
C	0.420032	-2.523132	-0.014977
C	2.360509	-3.844348	-1.539428
C	0.323405	-3.891111	-0.296846
C	1.271196	-4.571627	-1.060387
H	3.122267	-4.352314	-2.125294
H	-0.527057	-4.439537	0.099843
O	0.655290	0.566891	0.742879
C	1.356296	0.636991	-1.929838
C	0.637323	1.714644	-2.291960
H	1.639137	-0.054250	-2.718566
C	0.113266	2.815912	-1.469117
C	-1.138883	3.363568	-1.811113
C	0.797086	3.343708	-0.357311
C	-1.716715	4.369274	-1.034283
C	0.227840	4.363271	0.407305
C	-1.035785	4.871004	0.080684
H	-1.672470	2.971172	-2.671826
H	1.768636	2.953582	-0.081771
H	-2.692897	4.762321	-1.300567
H	0.770525	4.761076	1.259892
H	-1.478648	5.660256	0.680777
H	0.371253	1.783461	-3.346671
C	4.081900	1.903523	-1.624182
H	3.278143	2.641197	-1.579807
H	4.994235	2.429040	-1.917137
H	3.831461	1.207614	-2.428019
C	2.769832	-1.131572	2.365422
H	3.173027	-1.327698	3.361750
H	1.778662	-0.686490	2.473643
H	2.641319	-2.094955	1.862021
C	7.256780	1.072474	2.140122
H	7.164615	1.409278	3.178525
H	7.845767	0.147566	2.154839
H	7.824877	1.824141	1.585579
C	3.763757	-1.826611	-1.833475
H	3.571624	-0.887628	-2.355075
H	4.480415	-1.609404	-1.036279
H	4.249735	-2.497990	-2.545545
C	-0.683525	-1.940754	0.838829
H	-1.329684	-2.745687	1.196163
H	-0.289052	-1.405726	1.703346

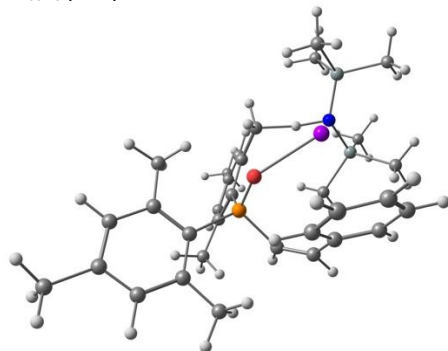
H	-1.316267	-1.247427	0.279652
C	1.111498	-6.036014	-1.374230
H	0.532940	-6.174428	-2.296360
H	2.080780	-6.521550	-1.521344
H	0.578583	-6.559500	-0.574916
N	-3.875095	0.130145	0.452068
Si	-4.108592	0.103112	-1.213706
Si	-4.475148	-0.746118	1.752628
C	-5.368184	-1.168529	-1.873424
H	-5.046991	-2.194586	-1.656512
H	-6.357199	-1.031741	-1.418130
H	-5.494551	-1.088396	-2.961589
C	-4.690299	1.795480	-1.874969
H	-4.737550	1.828942	-2.971724
H	-5.690291	2.039317	-1.493016
H	-4.016271	2.595878	-1.546602
C	-2.491906	-0.276665	-2.156297
H	-2.175444	-1.313800	-1.987343
H	-2.599888	-0.139213	-3.240881
H	-1.666012	0.364245	-1.829803
C	-6.196836	-0.200617	2.366900
H	-6.954104	-0.336011	1.583970
H	-6.528132	-0.767835	3.247217
H	-6.198569	0.863347	2.637858
C	-3.342093	-0.523920	3.283692
H	-3.297170	0.525717	3.610599
H	-3.721836	-1.094112	4.141238
H	-2.317585	-0.876121	3.102964
C	-4.615527	-2.631204	1.496646
H	-4.875811	-3.156272	2.425458
H	-5.391823	-2.868724	0.759100
H	-3.674550	-3.055677	1.126234
K	-1.698262	1.427453	1.256766

TS-1-Mes-CYC

E (BS1) = -2898.380870

E (BS2) = -2899.002502

G_{298.15} (BS2) = -2898.381800



P	1.635834	0.042834	-0.107718
C	3.428745	-0.006012	0.302083
C	3.765681	-0.712306	1.487724
C	4.449424	0.658396	-0.421878
C	5.098856	-0.755626	1.904881
C	5.768566	0.580800	0.041787
C	6.119514	-0.123295	1.193837
H	5.341660	-1.299027	2.814905
H	6.545346	1.094183	-0.519140
C	1.031180	-1.668221	-0.298865
C	1.700237	-2.536876	-1.213333
C	-0.138521	-2.127933	0.401175
C	1.178428	-3.796562	-1.489153
C	-0.612715	-3.428296	0.057532
C	0.000720	-4.250889	-0.866220
H	1.700492	-4.445682	-2.187528
H	-1.509313	-3.778967	0.564547
O	0.912491	0.872465	0.942881
C	1.324950	0.690422	-1.782869
C	0.747300	1.847841	-2.156246
H	1.445876	-0.051022	-2.566335
C	0.411183	3.044258	-1.368945

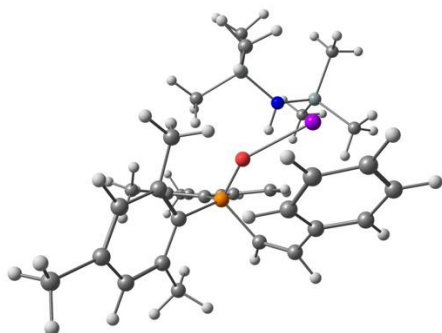
C	-0.762559	3.748357	-1.708261
C	1.185274	3.510132	-0.289356
C	-1.190888	4.837916	-0.947542
C	0.766356	4.611479	0.458401
C	-0.429520	5.268759	0.144905
H	-1.351798	3.414383	-2.557697
H	2.100188	2.998223	-0.022088
H	-2.109752	5.353201	-1.210994
H	1.373359	4.956008	1.290516
H	-0.754426	6.120561	0.734834
H	0.435688	1.909772	-3.199266
C	4.227774	1.458929	-1.684668
H	3.555716	2.305838	-1.530061
H	5.182692	1.854311	-2.040417
H	3.801775	0.855049	-2.490277
C	2.750390	-1.449033	2.331655
H	3.165940	-1.651785	3.322322
H	1.826096	-0.882324	2.458333
H	2.481009	-2.408065	1.877929
C	7.554016	-0.215138	1.644788
H	7.627174	-0.261492	2.735636
H	8.029790	-1.121337	1.248789
H	8.138891	0.640479	1.294742
C	3.027801	-2.206764	-1.865711
H	3.070930	-1.217647	-2.324059
H	3.843730	-2.249386	-1.137188
H	3.245436	-2.934688	-2.651622
C	-0.927797	-1.400413	1.377511
H	-1.455746	-2.083327	2.050870
H	-0.391328	-0.640717	1.939698
H	-2.137367	-0.795944	0.753719
C	-0.553886	-5.613394	-1.196254
H	-0.816705	-5.684835	-2.258686
H	0.183537	-6.400822	-0.998750
H	-1.451014	-5.834132	-0.611036
N	-3.213182	-0.255028	0.388177
Si	-3.570489	-0.325226	-1.299732
Si	-4.373703	-0.315077	1.662724
C	-4.974763	-1.521539	-1.739657
H	-4.730836	-2.540810	-1.417375
H	-5.923435	-1.242094	-1.267374
H	-5.144644	-1.550123	-2.823687
C	-4.057861	1.388268	-1.958128
H	-4.278633	1.362422	-3.033237
H	-4.945621	1.778275	-1.446972
H	-3.246346	2.112387	-1.810352
C	-2.042915	-0.879849	-2.259835
H	-1.772677	-1.913680	-2.023722
H	-2.226970	-0.817243	-3.340186
H	-1.172804	-0.256498	-2.035465
C	-5.909262	0.734105	1.306677
H	-6.463922	0.374132	0.433251
H	-6.598162	0.719246	2.161050
H	-5.637682	1.780201	1.120038
C	-3.591145	0.401353	3.244126
H	-3.507721	1.497305	3.207919
H	-4.216180	0.176560	4.117042
H	-2.599548	-0.022173	3.445564
C	-4.937658	-2.075717	2.066414
H	-5.629278	-2.103085	2.917785
H	-5.446239	-2.529500	1.207940
H	-4.079081	-2.712174	2.312135
K	-1.477157	1.746019	1.129898

CYC-I2-Mes

E (BS1) = -2898.393081

E (BS2) = -2899.017566

G_{298.15} (BS2) = -2898.393106



P	-1.216040	0.302848	-0.473126
C	-2.933883	0.369418	0.192688
C	-3.213425	-0.112566	1.497448
C	-3.995178	0.867876	-0.602478
C	-4.540569	-0.129903	1.942730
C	-5.302120	0.832588	-0.106335
C	-5.600989	0.326832	1.159113
H	-4.746720	-0.503428	2.942886
H	-6.106057	1.221032	-0.727125
C	-0.503932	1.921239	-0.705772
C	-0.935496	3.111330	-0.047143
C	0.697524	1.948509	-1.546170
C	-0.317789	4.322857	-0.322480
C	1.226489	3.262194	-1.838484
C	0.750125	4.408354	-1.256981
H	-0.655199	5.222365	0.185683
H	2.068884	3.320104	-2.526078
O	-0.353076	-0.646533	0.356633
C	-1.413913	-0.362145	-2.170594
C	-1.506622	-1.645613	-2.567509
H	-1.393285	0.392675	-2.950102
C	-1.450145	-2.870305	-1.749929
C	-0.657990	-3.942967	-2.209730
C	-2.098084	-3.003216	-0.508369
C	-0.462226	-5.080634	-1.422217
C	-1.913113	-4.145260	0.272478
C	-1.082166	-5.181080	-0.170375
H	-0.173398	-3.865552	-3.179785
H	-2.744905	-2.209782	-0.156463
H	0.164940	-5.888888	-1.787438
H	-2.419999	-4.227069	1.229671
H	-0.937165	-6.066287	0.441765
H	-1.520529	-1.824666	-3.643398
C	-3.798115	1.480121	-1.970717
H	-3.760705	0.712453	-2.750441
H	-4.633422	2.145981	-2.203905
H	-2.874232	2.059554	-2.034662
C	-2.162707	-0.590522	2.475939
H	-2.621024	-0.744974	3.457111
H	-1.702740	-1.525167	2.148357
H	-1.346417	0.127296	2.582833
C	-7.014123	0.323084	1.682289
H	-7.163929	-0.468441	2.422561
H	-7.252383	1.276579	2.170688
H	-7.738787	0.182628	0.874527
C	-2.039303	3.140920	0.988558
H	-3.033319	3.005951	0.553704
H	-1.915308	2.361336	1.745162
H	-2.032146	4.106043	1.502808
C	1.362222	0.835418	-2.053788
H	2.155352	0.974466	-2.783315
H	1.023372	-0.178212	-1.898627
H	2.439606	0.356475	-0.157006
C	1.351976	5.755477	-1.570351
H	0.605511	6.432203	-2.005514
H	1.724954	6.243278	-0.660974
H	2.184577	5.672586	-2.275290
N	3.097147	-0.093475	0.502760
Si	4.559993	-0.514868	-0.358965
Si	2.786679	0.375679	2.166338
C	5.337354	0.992728	-1.174879

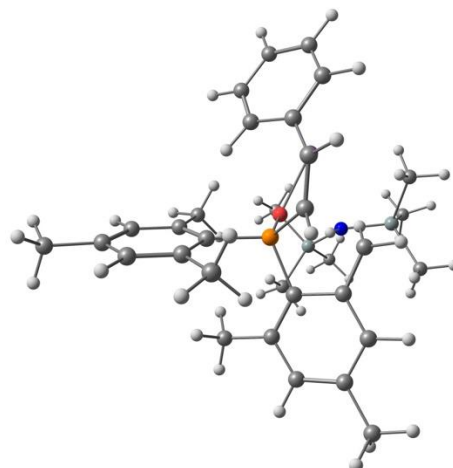
H	4.616246	1.482167	-1.839124
H	5.644077	1.727878	-0.421758
H	6.221007	0.728668	-1.768319
C	5.793499	-1.345560	0.796828
H	6.571022	-1.844165	0.205041
H	6.291897	-0.632455	1.459448
H	5.314995	-2.110586	1.419870
C	4.111282	-1.772886	-1.705874
H	3.232930	-1.463418	-2.284074
H	4.939495	-1.884549	-2.416155
H	3.931629	-2.774667	-1.290582
C	4.367788	0.836128	3.085000
H	4.953430	1.582529	2.536842
H	4.109307	1.270631	4.058784
H	5.011096	-0.028553	3.274809
C	1.983333	-1.063828	3.104944
H	2.573400	-1.987868	3.035497
H	1.896371	-0.825684	4.172224
H	0.965851	-1.250356	2.741042
C	1.585555	1.814985	2.169168
H	1.300998	2.088870	3.192396
H	2.007643	2.702431	1.685722
H	0.683104	1.536474	1.620256
K	1.416852	-2.379831	0.185246

TS-2-Mes-CYC

E (BS1) = -2898.379452

E (BS2) = -2899.001707

G_{298.15} (BS2) = -2898.376181



P	-1.072650	0.240199	-0.448063
C	-2.735727	-0.001220	0.305975
C	-2.881537	-0.608103	1.582002
C	-3.895266	0.456352	-0.373580
C	-4.164646	-0.754029	2.123451
C	-5.151372	0.289809	0.217649
C	-5.312251	-0.315105	1.464253
H	-4.264969	-1.222064	3.099565
H	-6.028724	0.646832	-0.315997
C	-0.691019	1.990772	-0.584024
C	-1.207193	3.078631	0.153943
C	0.205927	2.202513	-1.678590
C	-0.911078	4.368486	-0.286425
C	0.397617	3.526389	-2.134300
C	-0.144323	4.605855	-1.447451
H	-1.298026	5.217631	0.272472
H	1.026307	3.699303	-3.005167
O	-0.005156	-0.550891	0.316312
C	-1.062341	-0.194580	-2.221952
C	-1.056457	-1.489385	-2.759457
H	-1.518014	0.572231	-2.836162
C	-0.804281	-2.752850	-2.110615
C	-0.043162	-3.764166	-2.767587
C	-1.313910	-3.099398	-0.825563
C	0.239364	-4.987420	-2.164297

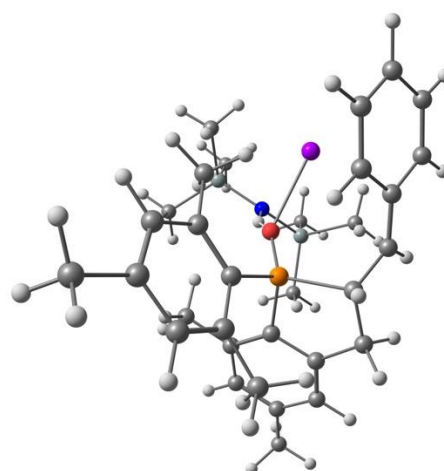
C	-1.030748	-4.325876	-0.225292
C	-0.236614	-5.283080	-0.875580
H	0.346451	-3.555625	-3.761494
H	-1.971951	-2.407705	-0.316360
H	0.839161	-5.719693	-2.699767
H	-1.452862	-4.546173	0.752850
H	-0.023841	-6.240267	-0.409353
H	-1.027355	-1.527049	-3.849483
C	-3.869742	1.131270	-1.725758
H	-3.677244	0.405051	-2.521722
H	-4.838061	1.596188	-1.927015
H	-3.102258	1.905574	-1.792362
C	-1.737057	-1.114684	2.432171
H	-2.119083	-1.437676	3.404707
H	-1.231771	-1.960372	1.959908
H	-0.973429	-0.352986	2.592458
C	-6.674880	-0.454276	2.091505
H	-6.706429	-1.289499	2.797271
H	-6.943582	0.453838	2.646127
H	-7.448596	-0.611833	1.333898
C	-2.079206	2.905506	1.374759
H	-3.106616	2.640295	1.104909
H	-1.707816	2.116110	2.033225
H	-2.115294	3.836057	1.948454
C	0.748281	1.022947	-2.304800
H	1.118316	1.103271	-3.326435
H	1.318371	0.340896	-1.689496
H	1.940486	0.163108	0.343486
C	0.104161	6.022683	-1.901533
H	-0.838171	6.541159	-2.115844
H	0.616486	6.604124	-1.125390
H	0.719036	6.051890	-2.805461
N	2.858692	0.008569	0.773641
Si	4.187040	0.147430	-0.357354
Si	2.666022	0.299241	2.494962
C	4.279859	1.866893	-1.116451
H	3.338600	2.119842	-1.616977
H	4.458569	2.622332	-0.342084
H	5.088173	1.942308	-1.853964
C	5.815729	-0.276534	0.484364
H	6.593573	-0.401371	-0.279040
H	6.152096	0.505200	1.170852
H	5.750868	-1.216840	1.043722
C	3.927795	-1.129266	-1.735743
H	2.936602	-1.076442	-2.200961
H	4.656256	-0.964022	-2.539036
H	4.099619	-2.152802	-1.374291
C	4.274887	0.837159	3.308023
H	4.687890	1.736437	2.838597
H	4.082576	1.074538	4.361715
H	5.040660	0.055949	3.282653
C	2.089048	-1.297125	3.335222
H	2.808856	-2.112804	3.184733
H	1.987107	-1.156537	4.418389
H	1.106604	-1.614944	2.966912
C	1.341887	1.615845	2.715566
H	1.052174	1.739724	3.765665
H	1.678194	2.587917	2.337410
H	0.457359	1.327086	2.142377

CYC-I3-Mes

E (BS1) = -2898.430538

E (BS2) = -2899.052010

G_{298.15} (BS2) = -2898.426450



P	-1.177255	0.287007	-0.350258
C	-2.669157	-0.124684	0.636145
C	-2.650329	-1.183500	1.586482
C	-3.884856	0.582540	0.422949
C	-3.818769	-1.481724	2.297077
C	-5.020224	0.239021	1.162642
C	-5.011973	-0.784935	2.109975
H	-3.790402	-2.293820	3.019310
H	-5.940280	0.790850	0.986922
C	-0.949619	2.072936	-0.425477
C	-0.621901	2.932506	0.641129
C	-1.004378	2.533270	-1.744863
C	-0.370228	4.269873	0.341292
C	-0.740201	3.879603	-2.015641
C	-0.421726	4.758378	-0.977531
H	-0.115423	4.953859	1.147679
H	-0.779364	4.245560	-3.038863
O	0.073365	-0.401227	0.193877
C	-1.467993	0.074991	-2.230085
C	-0.506129	-0.867632	-2.867096
H	-2.507643	-0.276425	-2.301114
C	-0.480792	-2.238987	-2.624140
C	0.529405	-3.105659	-3.200325
C	-1.411427	-2.910795	-1.740005
C	0.634142	-4.446808	-2.866767
C	-1.283970	-4.258435	-1.421100
C	-0.252223	-5.056027	-1.949476
H	1.235939	-2.671440	-3.905686
H	-2.224674	-2.342715	-1.297722
H	1.421891	-5.041785	-3.327050
H	-2.006332	-4.701472	-0.736681
H	-0.169142	-6.109328	-1.701580
H	0.280379	-0.430937	-3.476495
C	-4.039754	1.720642	-0.560293
H	-3.696465	1.459895	-1.562968
H	-5.093938	1.996606	-0.641577
H	-3.485055	2.608867	-0.246181
C	-1.448512	-2.052740	1.880117
H	-1.689942	-2.759328	2.678776
H	-1.164690	-2.627631	0.992704
H	-0.582149	-1.461786	2.176515
C	-6.241290	-1.111750	2.916757
H	-6.264609	-2.168577	3.199124
H	-6.266684	-0.525878	3.844560
H	-7.155841	-0.881611	2.362012
C	-0.530665	2.412244	2.051018
H	-1.497063	2.026299	2.394962
H	0.181325	1.583578	2.105387
H	-0.206732	3.193203	2.743506
C	-1.361546	1.516567	-2.808662
H	-2.307960	1.804716	-3.281286
H	-0.607412	1.539832	-3.601954
H	1.805977	0.024746	0.777071
C	-0.112572	6.207539	-1.254260
H	-0.714816	6.869499	-0.622186
H	0.939636	6.429859	-1.039540

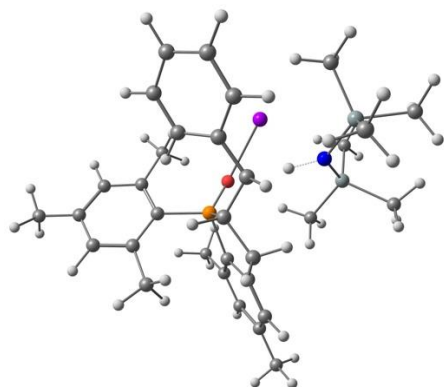
H	-0.303624	6.465414	-2.299331
N	2.828336	-0.058562	0.865591
Si	3.565731	0.806884	-0.468077
Si	3.281373	-0.558114	2.475500
C	2.807951	2.523911	-0.629370
H	1.743233	2.456424	-0.870812
H	2.904810	3.094874	0.300869
H	3.293679	3.097299	-1.428592
C	5.429865	0.951926	-0.263869
H	5.848317	1.432174	-1.157034
H	5.706542	1.566168	0.598933
H	5.916019	-0.022903	-0.156398
C	3.199042	-0.132626	-2.066545
H	2.119066	-0.269269	-2.206008
H	3.563420	0.423931	-2.938910
H	3.691802	-1.113879	-2.088496
C	5.147647	-0.630804	2.686413
H	5.615175	0.356205	2.624916
H	5.380571	-1.045754	3.674713
H	5.619721	-1.276604	1.938574
C	2.597336	-2.298508	2.790186
H	3.078568	-3.049906	2.149414
H	2.793432	-2.602726	3.825717
H	1.510205	-2.352299	2.652398
C	2.535487	0.584490	3.777261
H	2.854581	0.298056	4.786958
H	2.837178	1.625257	3.611826
H	1.440115	0.549425	3.755987
K	1.511523	-2.446506	-0.358220

TS-3-Mes-CYC

E (BS1) = -2898.40780101

E (BS2) = -2899.025525

G_{298.15} (BS2) = -2898.402173



P	-1.325812	0.190677	0.178237
C	-2.932409	-0.716267	0.190324
C	-3.211491	-1.678961	1.199039
C	-3.918814	-0.454184	-0.802190
C	-4.444520	-2.343517	1.183376
C	-5.128789	-1.153737	-0.766765
C	-5.417264	-2.100478	0.216275
H	-4.643113	-3.080295	1.957317
H	-5.869591	-0.947840	-1.535254
C	-1.690405	1.936230	-0.091729
C	-2.456427	2.787773	0.724869
C	-1.054308	2.405614	-1.244997
C	-2.576855	4.121098	0.333778
C	-1.195346	3.745198	-1.614872
C	-1.958451	4.614348	-0.829795
H	-3.165663	4.800524	0.946059
H	-0.705241	4.116839	-2.511456
O	-0.505460	-0.090411	1.430673
C	-0.420055	-0.038817	-1.444832
C	0.904022	-0.805333	-1.387158
H	-1.143720	-0.555845	-2.091951
C	0.810613	-2.262937	-1.205402
C	1.909873	-3.111693	-1.512107

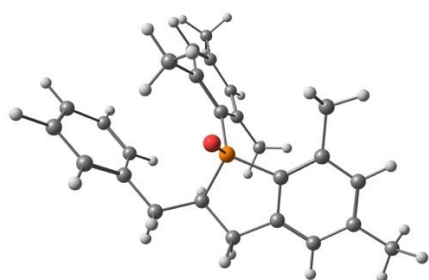
C	-0.328202	-2.914561	-0.664195
C	1.896397	-4.474244	-1.230149
C	-0.337502	-4.281461	-0.374344
C	0.777955	-5.077887	-0.638954
H	2.790830	-2.681130	-1.973397
H	-1.236267	-2.354764	-0.485839
H	2.768078	-5.075002	-1.479336
H	-1.238304	-4.723795	0.045236
H	0.770204	-6.141205	-0.419193
H	1.453743	-0.587501	-2.311147
C	-3.781372	0.571501	-1.907333
H	-2.835557	0.504452	-2.445881
H	-4.582093	0.430747	-2.637492
H	-3.860514	1.590670	-1.519219
C	-2.261481	-2.077753	2.308470
H	-2.754806	-2.797407	2.967424
H	-1.361753	-2.552405	1.906863
H	-1.932111	-1.221421	2.896706
C	-6.743221	-2.814609	0.239876
H	-6.697257	-3.723722	0.846010
H	-7.524395	-2.172154	0.665320
H	-7.065869	-3.088061	-0.769812
C	-3.134029	2.271844	1.967658
H	-3.947248	1.581884	1.714693
H	-2.429482	1.718250	2.596749
H	-3.555299	3.090327	2.556952
C	-0.204408	1.400143	-1.988418
H	-0.409510	1.435182	-3.064025
H	0.850726	1.669963	-1.862600
H	1.979547	-0.112238	-0.574006
C	-2.116912	6.064913	-1.208002
H	-3.174518	6.333952	-1.309904
H	-1.693496	6.720047	-0.437598
H	-1.616127	6.288512	-2.153692
N	3.030291	0.381174	-0.020606
Si	3.074192	1.787841	0.991146
Si	4.478738	-0.442480	-0.496063
C	3.640225	1.325531	2.755273
H	4.533042	0.689697	2.753426
H	3.876708	2.221908	3.343200
H	2.852058	0.796372	3.310977
C	4.210048	3.185072	0.388571
H	4.005494	4.096250	0.965701
H	5.275427	2.965275	0.492163
H	4.016990	3.415997	-0.666331
C	1.390908	2.602164	1.208510
H	0.631616	1.894980	1.547276
H	1.481033	3.396306	1.961459
H	1.032741	3.068758	0.286548
C	6.106121	0.424910	-0.049504
H	6.191109	0.664195	1.015819
H	6.936927	-0.248312	-0.298661
H	6.255150	1.347873	-0.617511
C	4.571060	-0.672306	-2.375145
H	4.798024	0.295829	-2.839398
H	5.373009	-1.366239	-2.656654
H	3.642556	-1.031757	-2.825626
C	4.640769	-2.127734	0.382446
H	5.526845	-2.666188	0.022714
H	4.785287	-1.973449	1.461213
H	3.789523	-2.799137	0.231617
K	1.659405	-1.419696	1.658592

3-Mes

E (BS1) = -1425.0591694

E (BS2) = -1425.476307

G_{298.15} (BS2) = -1425.053306



P	0.409291	-0.540855	0.586590
C	-0.558606	0.971697	0.196445
C	-1.731573	1.262111	0.941353
C	-0.189791	1.829449	-0.875928
C	-2.491164	2.388190	0.602418
C	-0.988926	2.939845	-1.168254
C	-2.141095	3.242292	-0.441733
H	-3.392357	2.594979	1.173868
H	-0.699195	3.585307	-1.993829
C	2.180149	-0.234338	0.378433
C	2.975114	0.728946	1.024089
C	2.741085	-1.178878	-0.491146
C	4.342145	0.734801	0.743564
C	4.112478	-1.150211	-0.752924
C	4.924903	-0.190470	-0.140809
H	4.976142	1.478911	1.220559
H	4.552462	-1.874032	-1.434699
O	0.064119	-1.184220	1.909609
C	0.326152	-1.683454	-0.876585
C	-0.706793	-2.803606	-0.706271
H	0.059078	-1.072008	-1.742065
C	-2.131947	-2.327756	-0.509388
C	-2.940086	-2.926500	0.466857
C	-2.679602	-1.291472	-1.277999
C	-4.253734	-2.503800	0.674158
C	-3.987743	-0.855002	-1.064599
C	-4.780825	-1.458757	-0.087222
H	-2.527002	-3.724268	1.078282
H	-2.080054	-0.805044	-2.040714
H	-4.858815	-2.980017	1.440490
H	-4.383713	-0.036833	-1.659302
H	-5.797834	-1.116673	0.081057
H	-0.651870	-3.452593	-1.591629
C	1.035840	1.645718	-1.745747
H	1.136382	0.634911	-2.144774
H	0.984892	2.329399	-2.596739
H	1.958174	1.862835	-1.200353
C	-2.249869	0.416577	2.081805
H	-3.210385	0.812162	2.423221
H	-2.385499	-0.623740	1.786738
H	-1.554151	0.404982	2.923656
C	-2.965559	4.461264	-0.763986
H	-4.001401	4.341455	-0.433422
H	-2.561768	5.349411	-0.261453
H	-2.966822	4.670272	-1.838286
C	2.361605	1.745167	1.952212
H	1.726151	2.447753	1.400794
H	1.726152	1.262232	2.701775
H	3.131080	2.321234	2.472612
C	1.773713	-2.193853	-1.069904
H	1.983767	-2.386059	-2.127408
H	1.902123	-3.150520	-0.546758
H	-0.420290	-3.421436	0.150124
C	6.408208	-0.146403	-0.406862
H	6.729876	0.860650	-0.694640
H	6.976114	-0.419066	0.490875
H	6.691998	-0.836958	-1.205547

Influence of the metal cation in the hydrophosphorylation reaction

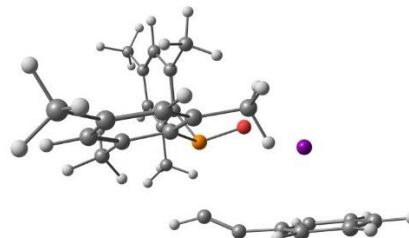
Hydrophosphorylation catalyzed by Na-OPMes₂

Int-TS-1-Mes-Na

E (BS1) = -1586.702288

E (BS2) = -1587.131107

G_{298.15} (BS2) = -1586.734857



6	2.416784	-0.918291	1.908238
6	1.203608	-0.734231	2.172782
11	2.653269	-1.195805	-1.520344
1	0.508082	-0.619906	2.984971
6	4.203266	0.068625	0.517378
6	3.513658	-1.067035	1.040497
6	3.974247	-2.355214	0.631048
6	5.030412	-2.487659	-0.269053
6	5.678376	-1.357637	-0.795756
6	5.257876	-0.083919	-0.381952
1	3.884669	1.059905	0.823208
1	3.477970	-3.236970	1.024100
1	5.349989	-3.482740	-0.566966
1	6.501451	-1.468249	-1.493937
1	5.753552	0.801875	-0.770119
15	-0.207376	-0.412788	0.189813
8	0.640050	-0.951767	-1.000597
6	-2.676882	-0.645713	-1.250190
6	-1.941426	-1.025426	-0.101894
6	-3.961157	-1.165088	-1.444188
6	-4.540307	-2.064119	-0.543957
6	-3.785747	-2.461105	0.561843
6	-2.497583	-1.964011	0.795106
1	-4.520254	-0.864123	-2.327863
1	-4.205414	-3.181704	1.260174
6	-1.235086	2.056398	1.059887
6	-1.331016	3.448793	1.111602
6	-0.383101	1.433930	0.108805
6	0.401796	2.263169	-0.732079
6	0.273989	3.656131	-0.640888
6	-0.591138	4.274094	0.261437
1	-1.997913	3.899535	1.843741
1	0.875672	4.275755	-1.302397
6	1.409135	1.746928	-1.737454
1	1.744723	2.563193	-2.383626
1	2.299749	1.358151	-1.225478
1	1.002037	0.949876	-2.359213
6	-2.064227	1.262302	2.041823
1	-2.931942	0.797618	1.563891
1	-1.485834	0.456501	2.502525
1	-2.428510	1.910157	2.843834
6	-0.733681	5.773873	0.313533
1	-0.784114	6.135271	1.346176
1	0.104414	6.272424	-0.182304
1	-1.654344	6.101687	-0.186100
6	-2.120085	0.299758	-2.287101
1	-2.143044	1.337403	-1.939094
1	-1.079699	0.056255	-2.513667
1	-2.703705	0.242503	-3.210374
6	-1.752419	-2.458843	2.014218
1	-2.294686	-3.285570	2.481851
1	-0.745522	-2.807313	1.768222
1	-1.638720	-1.672609	2.768563
6	-5.940341	-2.580663	-0.758655
1	-6.100514	-3.530360	-0.239680
1	-6.684207	-1.869401	-0.377182

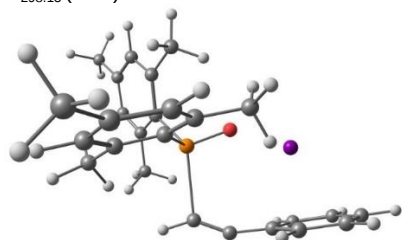
1 -6.153311 -2.729626 -1.822071

TS-1-Mes-Na

E (BS1) = -1586.691687

E (BS2) = -1587.121384

G_{298.15} (BS2) = -1586.722896



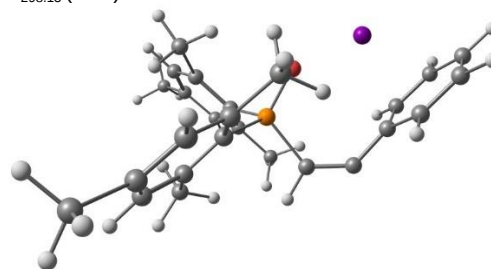
6	2.416784	-0.918291	1.908238
6	1.203608	-0.734231	2.172782
11	2.653269	-1.195805	-1.520344
1	0.508082	-0.619906	2.984971
6	4.203266	0.068625	0.517378
6	3.513658	-1.067035	1.040497
6	3.974247	-2.355214	0.631048
6	5.030412	-2.487659	-0.269053
6	5.678376	-1.357637	-0.795756
6	5.257876	-0.083919	-0.381952
1	3.884669	1.059905	0.823208
1	3.477970	-3.236970	1.024100
1	5.349989	-3.482740	-0.566966
1	6.501451	-1.468249	-1.493937
1	5.753552	0.801875	-0.770119
15	-0.207376	-0.412788	0.189813
8	0.640050	-0.951767	-1.000597
6	-2.676882	-0.645713	-1.250190
6	-1.941426	-1.025426	-0.101894
6	-3.961157	-1.165088	-1.444188
6	-4.540307	-2.064119	-0.543957
6	-3.785747	-2.461105	0.561843
6	-2.497583	-1.964011	0.795106
1	-4.520254	-0.864123	-2.327863
1	-4.205414	-3.181704	1.260174
6	-1.235086	2.056398	1.059887
6	-1.331016	3.448793	1.111602
6	-0.383101	1.433930	0.108805
6	0.401796	2.263169	-0.732079
6	0.273989	3.656131	-0.640888
6	-0.591138	4.274094	0.261437
1	-1.997913	3.899535	1.843741
1	0.875672	4.275755	-1.302397
6	1.409135	1.746928	-1.737454
1	1.744723	2.563193	-2.383626
1	2.299749	1.358151	-1.225478
1	1.002037	0.949876	-2.359213
6	-2.064227	1.262302	2.041823
1	-2.931942	0.797618	1.563891
1	-1.485834	0.456501	2.502525
1	-2.428510	1.910157	2.843834
6	-0.733681	5.773873	0.313533
1	-0.784114	6.135271	1.346176
1	0.104414	6.272424	-0.182304
1	-1.654344	6.101687	-0.186100
6	-2.120085	0.299758	-2.287101
1	-2.143044	1.337403	-1.939094
1	-1.079699	0.056255	-2.513667
1	-2.703705	0.242503	-3.210374
6	-1.752419	-2.458843	2.014218
1	-2.294686	-3.285570	2.481851
1	-0.745522	-2.807313	1.768222
1	-1.638720	-1.672609	2.768563
6	-5.940341	-2.580663	-0.758655
1	-6.100514	-3.530360	-0.239680
1	-6.684207	-1.869401	-0.377182
1	-6.153311	-2.729626	-1.822071

Z-1I-Mes-Na

E (BS1) = -1586.718417

E (BS2) = -1587.150678

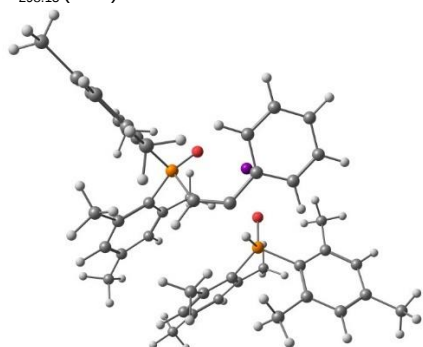
G_{298.15} (BS2) = -1586.748921



6	2.240313	0.020676	1.904836
6	0.918828	0.028213	1.727294
11	3.019895	-0.290040	-1.631037
1	0.227458	0.178874	2.561850
6	4.071264	0.966854	0.508904
6	3.338757	-0.149306	1.039794
6	3.865913	-1.447203	0.721950
6	5.008995	-1.603438	-0.058322
6	5.697823	-0.493324	-0.582435
6	5.209872	0.790632	-0.274179
1	3.724829	1.970423	0.737192
1	3.354525	-2.324040	1.108613
1	5.364387	-2.608534	-0.274130
1	6.593330	-0.622256	-1.180890
1	5.724961	1.668873	-0.656830
15	0.048850	-0.047524	0.127043
8	0.991602	-0.139184	-1.074720
6	-2.013197	-1.375695	-1.198279
6	-1.166685	-1.418999	-0.057688
6	-2.926191	-2.411331	-1.412216
6	-3.029069	-3.501990	-0.545728
6	-2.167247	-3.544580	0.549317
6	-1.235809	-2.531701	0.812940
1	-3.571488	-2.364230	-2.286335
1	-2.213122	-4.395010	1.224788
6	-2.121628	1.610076	0.913765
6	-2.830712	2.817167	0.926084
6	-0.935986	1.510632	0.144374
6	-0.459715	2.657482	-0.542522
6	-1.207857	3.838030	-0.496793
6	-2.404114	3.938625	0.216002
1	-3.741261	2.878631	1.517088
1	-0.835522	4.709208	-1.030478
6	0.837563	2.698842	-1.320060
1	1.028481	3.719170	-1.664076
1	1.685728	2.382881	-0.705615
1	0.811725	2.037582	-2.189411
6	-2.700161	0.478237	1.736293
1	-3.259975	-0.227175	1.114833
1	-1.942002	-0.096191	2.271387
1	-3.389596	0.882641	2.482399
6	-3.205250	5.214730	0.213001
1	-3.863131	5.275630	1.084799
1	-2.554626	6.094969	0.209482
1	-3.838342	5.277076	-0.681333
6	-1.999990	-0.246319	-2.205191
1	-2.540813	0.628392	-1.829863
1	-0.984146	0.073614	-2.443592
1	-2.488127	-0.565920	-3.129867
6	-0.370847	-2.705639	2.038868
1	-0.544953	-3.690954	2.479009
1	0.693164	-2.614354	1.813672
1	-0.594163	-1.956443	2.804878
6	-4.044507	-4.588816	-0.786234
1	-3.801186	-5.494924	-0.224272
1	-5.045282	-4.264530	-0.474233
1	-4.107430	-4.847766	-1.848181

Int-TS-2-Mes-Na

E (BS1) = -2703.282717
 E (BS2) = -2704.019484
 G_{298.15} (BS2) = -2703.278933

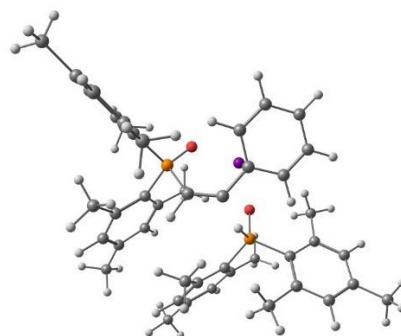


15	2.413021	-0.341094	-0.050590
6	4.230998	-0.665438	0.058564
6	5.022292	-0.188977	-1.024824
6	4.859252	-1.395944	1.097322
6	6.396882	-0.433775	-1.035212
6	6.243519	-1.615402	1.032414
6	7.031946	-1.145115	-0.014750
1	6.986756	-0.058578	-1.868332
1	6.715465	-2.175088	1.835797
6	2.228366	1.504137	-0.054603
6	2.791403	2.273633	0.999511
6	1.411499	2.157519	-1.014361
6	2.484326	3.633705	1.103400
6	1.140387	3.523772	-0.862489
6	1.646494	4.278778	0.192139
1	2.913385	4.202454	1.924972
1	0.496030	4.004508	-1.593706
8	1.907146	-0.992151	-1.338606
11	-0.017930	-1.871134	-1.697723
6	1.459136	-0.849960	1.423436
6	0.644408	-1.908246	1.594106
1	1.596752	-0.134518	2.238478
6	0.416138	-3.008312	0.690094
6	-0.917215	-3.392039	0.355848
6	1.452758	-3.835327	0.166293
6	-1.186903	-4.459328	-0.500442
6	1.173280	-4.922038	-0.658291
6	-0.144136	-5.238155	-1.021014
1	-1.741764	-2.837953	0.793375
1	2.485054	-3.593795	0.395909
1	-2.219983	-4.698088	-0.740530
1	1.995930	-5.521398	-1.041658
1	-0.353059	-6.084332	-1.668234
15	-2.401672	-0.110430	-0.186752
6	-2.620636	1.694924	-0.130029
6	-3.505034	2.315141	-1.048284
6	-1.849182	2.486798	0.753742
6	-3.615124	3.705452	-1.051014
6	-2.002149	3.878113	0.713560
6	-2.872306	4.506474	-0.176246
1	-4.292898	4.175620	-1.759258
1	-1.408064	4.484494	1.391232
6	-3.964062	-0.972754	0.194706
6	-4.520847	-0.804234	1.489481
6	-4.591014	-1.841195	-0.732357
6	-5.700611	-1.472822	1.818122
6	-5.774812	-2.485242	-0.348696
6	-6.349368	-2.314012	0.910297
1	-6.119121	-1.335792	2.812091
1	-6.257320	-3.147483	-1.062545
8	-1.751851	-0.571499	-1.486765
1	-1.609317	-0.390940	0.936811
6	4.159307	-1.957981	2.313903
1	3.356752	-2.649072	2.058180
1	4.881809	-2.491892	2.936735
1	3.706702	-1.176188	2.929595
6	4.450659	0.588579	-2.188374

1	5.213211	0.730596	-2.958215
1	3.598188	0.068657	-2.629271
1	4.100343	1.577473	-1.877116
6	8.516234	-1.400321	-0.059141
1	8.864238	-1.894999	0.851733
1	8.780791	-2.037988	-0.911150
1	9.075488	-0.464978	-0.174772
6	-0.854214	1.918101	1.735573
1	-1.343924	1.359813	2.539519
1	-0.144150	1.241883	1.259241
1	-0.279073	2.725219	2.192755
6	-4.315158	1.518778	-2.040489
1	-3.665281	0.910549	-2.676436
1	-5.012674	0.839106	-1.541216
1	-4.895886	2.182690	-2.685043
6	-2.988854	6.007698	-0.220959
1	-4.037021	6.325541	-0.218300
1	-2.486404	6.472797	0.631330
1	-2.535776	6.406846	-1.136723
6	3.751757	1.717873	2.027001
1	3.389530	0.805606	2.501886
1	4.722215	1.484144	1.579689
1	3.916427	2.452458	2.819359
6	0.780366	1.491399	-2.216110
1	1.486964	0.867001	-2.761645
1	-0.061886	0.856427	-1.929469
1	0.393021	2.259571	-2.891921
6	1.315834	5.741841	0.335653
1	2.154051	6.370851	0.010335
1	0.444945	6.013071	-0.267523
1	1.106830	6.001851	1.378676
6	-3.871692	0.056232	2.545895
1	-4.472257	0.054816	3.458244
1	-2.874109	-0.315622	2.807002
1	-3.760790	1.094325	2.219832
6	-4.059725	-2.150783	-2.113730
1	-3.112107	-2.693334	-2.059652
1	-4.779340	-2.773647	-2.651686
1	-3.870880	-1.253012	-2.702734
6	-7.630505	-3.010378	1.287852
1	-7.942466	-3.720036	0.517019
1	-7.520434	-3.555315	2.231814
1	-8.442399	-2.286777	1.428619

TS-2-Mes-Na

E (BS1) = -2703.271142
 E (BS2) = -2704.002299
 G_{298.15} (BS2) = -2703.262339



15	2.357040	-0.401468	-0.248518
6	4.115553	-0.797237	0.125127
6	5.076714	-0.369769	-0.831617
6	4.542820	-1.531285	1.257638
6	6.424181	-0.676309	-0.633945
6	5.908671	-1.814002	1.403408
6	6.864252	-1.399362	0.477814
1	7.149414	-0.340288	-1.371410
1	6.230745	-2.376221	2.276104
6	2.215404	1.448062	-0.307439
6	2.725992	2.230012	0.765281

6	1.461254	2.090943	-1.321070
6	2.458873	3.600952	0.808505
6	1.223545	3.469076	-1.225937
6	1.699348	4.242677	-0.171914
1	2.853931	4.181755	1.638644
1	0.630079	3.943785	-2.002897
8	2.003082	-1.081418	-1.574001
11	-0.029429	-1.682931	-2.034662
6	1.154688	-0.726796	1.068486
6	0.137954	-1.620893	1.161158
1	1.128245	0.138470	1.729638
6	0.057334	-2.890320	0.424534
6	-1.218949	-3.457401	0.169541
6	1.181060	-3.648417	0.006209
6	-1.364883	-4.657916	-0.522917
6	1.034256	-4.864540	-0.660655
6	-0.237733	-5.371431	-0.946110
1	-2.103279	-2.941163	0.527489
1	2.178343	-3.270696	0.192514
1	-2.360858	-5.048906	-0.712345
1	1.919508	-5.417167	-0.964667
1	-0.348708	-6.316224	-1.469852
15	-2.242870	-0.166986	-0.043106
6	-2.369979	1.670782	0.097586
6	-3.068937	2.385107	-0.916237
6	-1.677551	2.392192	1.091953
6	-3.052193	3.778365	-0.907409
6	-1.690457	3.796085	1.057597
6	-2.364242	4.507649	0.071670
1	-3.591605	4.313217	-1.685987
1	-1.151267	4.337632	1.831276
6	-3.930045	-0.860788	0.232348
6	-4.518911	-0.686817	1.512278
6	-4.603168	-1.654632	-0.730821
6	-5.769634	-1.243272	1.783979
6	-5.856836	-2.193479	-0.406289
6	-6.464119	-1.995338	0.832876
1	-6.206724	-1.092529	2.768474
1	-6.370391	-2.793572	-1.153573
8	-1.727292	-0.498048	-1.461015
1	-1.243279	-0.839762	1.002550
6	3.633270	-2.028257	2.358742
1	2.912756	-2.768286	2.005219
1	4.231117	-2.498341	3.144052
1	3.052744	-1.224665	2.817011
6	4.714175	0.431044	-2.061947
1	5.569349	0.488737	-2.740076
1	3.872943	-0.015459	-2.595713
1	4.425609	1.454147	-1.799632
6	8.324705	-1.723072	0.657812
1	8.511367	-2.206620	1.620523
1	8.678240	-2.396819	-0.131902
1	8.940343	-0.818108	0.604692
6	-0.914837	1.766100	2.235995
1	-1.370331	2.050820	3.191560
1	-0.878779	0.680724	2.199130
1	0.113499	2.140852	2.244858
6	-3.833277	1.685048	-2.012506
1	-3.171691	1.031452	-2.585433
1	-4.629287	1.054845	-1.603082
1	-4.290939	2.412543	-2.687654
6	-2.354930	6.014144	0.039559
1	-3.373498	6.415069	-0.013544
1	-1.871020	6.430617	0.926966
1	-1.819362	6.385777	-0.841957
6	3.568703	1.671845	1.890043
1	3.118371	0.796792	2.361771
1	4.562097	1.375331	1.543025
1	3.697454	2.429014	2.667596
6	0.844679	1.397645	-2.515446
1	1.524228	0.682772	-2.977999
1	-0.066435	0.866530	-2.216841
1	0.553485	2.144173	-3.259949
6	1.399825	5.715687	-0.077165
1	2.320290	6.303551	0.014747

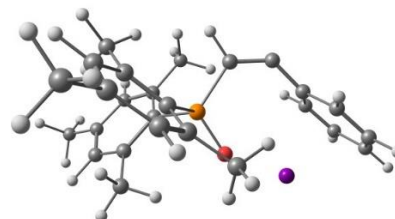
1	0.856432	6.069280	-0.957165
1	0.789623	5.935531	0.806178
6	-3.826654	0.076472	2.615019
1	-4.393198	-0.000031	3.546516
1	-2.822551	-0.316156	2.804735
1	-3.722655	1.137654	2.371294
6	-4.055729	-1.989575	-2.101183
1	-3.131370	-2.568542	-2.028741
1	-4.789962	-2.583295	-2.653424
1	-3.817701	-1.099333	-2.683222
6	-7.820021	-2.574039	1.145345
1	-8.164449	-3.238290	0.347906
1	-7.802923	-3.144133	2.080973
1	-8.568120	-1.781321	1.268027

Z-1l-Mes-Na

E (BS1) = -1586.718417

E (BS2) = -1587.150678

G_{298.15} (BS2) = -1586.748918



15	-0.048790	-0.047526	0.126987
6	1.166752	-1.419000	-0.057700
6	2.013331	-1.375686	-1.198240
6	1.235811	-2.531718	0.812913
6	2.926316	-2.411336	-1.412151
6	2.167245	-3.544610	0.549320
6	3.029123	-3.502016	-0.545680
1	3.571663	-2.364228	-2.286232
1	2.213070	-4.395052	1.224779
6	0.936003	1.510657	0.144415
6	2.121594	1.610115	0.913870
6	0.459708	2.657529	-0.542442
6	2.830601	2.817259	0.926324
6	1.207767	3.838116	-0.496580
6	2.403963	3.938745	0.216326
1	3.741119	2.878733	1.517372
1	0.835416	4.709306	-1.030237
8	-0.991475	-0.139176	-1.074831
11	-3.019741	-0.289865	-1.631282
6	-0.918870	0.028167	1.727189
6	-2.240363	0.020584	1.904656
1	-0.227548	0.178848	2.561784
6	-3.338784	-0.149420	1.039591
6	-4.071331	0.966722	0.508716
6	-3.865886	-1.447332	0.721712
6	-5.209949	0.790470	-0.274350
6	-5.008979	-1.603596	-0.058541
6	-5.697864	-0.493496	-0.582612
1	-3.724934	1.970301	0.737020
1	-3.354461	-2.324156	1.108353
1	-5.725077	1.668701	-0.656975
1	-5.364333	-2.608702	-0.274364
1	-6.593379	-0.622451	-1.181051
6	4.044548	-4.588862	-0.786157
1	4.107481	-4.847830	-1.848098
1	5.045323	-4.264586	-0.474148
1	3.801205	-5.494958	-0.224185
6	2.000210	-0.246277	-2.205115
1	0.984384	0.073653	-2.443600
1	2.540987	0.628427	-1.829705
1	2.488437	-0.565840	-3.129756
6	0.370784	-2.705660	2.038795
1	0.594040	-1.956455	2.804812
1	-0.693217	-2.614395	1.813539
1	0.544882	-3.690970	2.478952

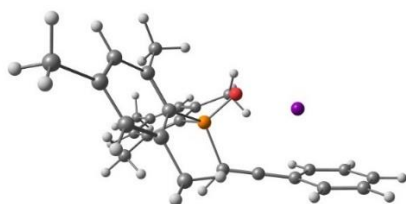
6	3.204856	5.215007	0.213638
1	3.836370	5.278730	-0.681705
1	2.554016	6.095102	0.212421
1	3.864168	5.274913	1.084419
6	2.700165	0.478246	1.736330
1	3.259987	-0.227120	1.114827
1	3.389597	0.882622	2.482455
1	1.942021	-0.096229	2.271397
6	-0.837523	2.698858	-1.320061
1	-1.685716	2.382903	-0.705648
1	-1.028437	3.719177	-1.664104
1	-0.811631	2.037580	-2.189396

TS-3-Mes-Na

E (BS1) = -1586.704042

E (BS2) = -1587.136657

G_{298.15} (BS2) = -1586.734067



15	-0.133684	-0.099984	0.144603
6	-1.451018	-1.385260	0.159915
6	-2.490552	-1.244837	1.116373
6	-1.424103	-2.525777	-0.676506
6	-3.495540	-2.217581	1.178087
6	-2.453795	-3.471628	-0.569822
6	-3.503072	-3.331690	0.337032
1	-4.288438	-2.098568	1.912793
1	-2.425385	-4.342818	-1.219058
6	-0.951443	1.528098	-0.098647
6	-1.983133	1.688150	-1.054354
6	-0.488303	2.660773	0.618853
6	-2.578656	2.945653	-1.213858
6	-1.117400	3.891820	0.424980
6	-2.177594	4.055364	-0.472422
1	-3.374399	3.053452	-1.945322
1	-0.764155	4.750719	0.988754
8	0.628223	-0.213354	1.465438
11	2.972360	-0.210508	1.682147
6	1.034690	-0.160163	-1.277064
6	2.314259	-0.263563	-1.023012
1	0.586955	0.014068	-2.265295
6	3.644206	-0.373779	-0.756607
6	4.455183	0.769118	-0.348862
6	4.329304	-1.658200	-0.718269
6	5.770895	0.606973	0.076402
6	5.640593	-1.767196	-0.287367
6	6.392838	-0.650775	0.129505
1	4.013014	1.761428	-0.398989
1	3.782469	-2.543812	-1.033870
1	6.328845	1.495425	0.363625
1	6.098661	-2.754050	-0.279589
1	7.421454	-0.756900	0.458208
6	-4.612894	-4.349028	0.409392
1	-4.850160	-4.608980	1.446468
1	-5.533676	-3.955180	-0.038971
1	-4.351777	-5.266214	-0.125856
6	-2.581567	-0.080703	2.074610
1	-1.605374	0.176303	2.491727
1	-2.974613	0.814575	1.582122
1	-3.255120	-0.328791	2.899386
6	-0.346320	-2.798382	-1.698620
1	-0.362526	-2.067961	-2.514072
1	0.653500	-2.769337	-1.265652
1	-0.496909	-3.787652	-2.142134
6	-2.836625	5.396795	-0.648400
1	-3.241468	5.764621	0.302459
1	-2.120864	6.147525	-1.001798

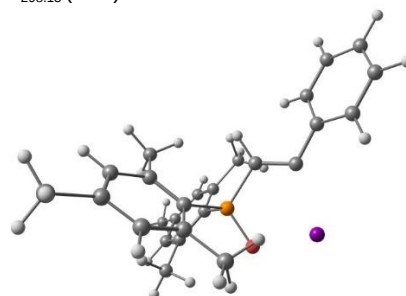
1	-3.658427	5.348562	-1.370307
6	-2.505649	0.572407	-1.937147
1	-3.228888	-0.057990	-1.409059
1	-3.011525	1.000904	-2.806549
1	-1.717568	-0.084184	-2.309417
6	0.690891	2.623857	1.567417
1	1.602939	2.319202	1.042523
1	0.865444	3.619283	1.986212
1	0.540346	1.915859	2.385852

E-1I-Mes-Na

E (BS1) = -1586.730397

E (BS2) = -1587.160513

G_{298.15} (BS2) = -1586.757092



15	-0.244704	-0.042542	0.746649
6	-1.490831	-1.317063	0.291312
6	-2.834388	-1.065304	0.678202
6	-1.171581	-2.538190	-0.347390
6	-3.820881	-2.007265	0.376103
6	-2.199205	-3.448984	-0.624459
6	-3.528604	-3.203475	-0.282882
1	-4.847316	-1.799278	0.669135
1	-1.945515	-4.381235	-1.122722
6	-0.828289	1.540437	0.001370
6	-1.321568	1.575297	-1.325767
6	-0.716272	2.751961	0.730750
6	-1.751671	2.794390	-1.863892
6	-1.164286	3.940972	0.147043
6	-1.701560	3.985457	-1.141095
1	-2.130505	2.807845	-2.882990
1	-1.079902	4.863229	0.716848
8	-0.180404	-0.007166	2.278064
11	1.829072	-0.269602	3.059878
6	1.377276	-0.252072	-0.010255
6	2.491014	-0.387588	0.747464
1	1.384672	-0.158109	-1.104941
6	3.771083	-0.502287	0.030105
6	4.900530	0.231755	0.450438
6	3.940083	-1.372271	-1.070267
6	6.120350	0.135803	-0.215945
6	5.170479	-1.495260	-1.716249
6	6.266651	-0.735292	-1.300789
1	4.802513	0.891280	1.310137
1	3.094763	-1.966934	-1.404844
1	6.966309	0.730037	0.120377
1	5.272488	-2.182527	-2.552697
1	7.223379	-0.826968	-1.806924
6	-4.611613	-4.208494	-0.578379
1	-4.890907	-4.760894	0.327557
1	-5.518507	-3.718952	-0.948256
1	-4.285934	-4.939167	-1.324036
6	-3.274017	0.193242	1.393809
1	-2.561385	0.492141	2.164543
1	-3.379321	1.032168	0.698371
1	-4.246176	0.031776	1.867428
6	0.222824	-2.935464	-0.773536
1	0.602910	-2.290761	-1.572184
1	0.939614	-2.874247	0.047435
1	0.217265	-3.962078	-1.149168
6	-2.210197	5.277827	-1.725459
1	-3.234925	5.482032	-1.389792
1	-1.593665	6.126987	-1.414131

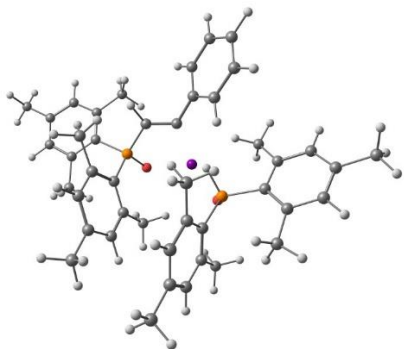
1	-2.224204	5.244234	-2.818714
6	-1.429197	0.363096	-2.226582
1	-2.331900	-0.217908	-2.014579
1	-1.480559	0.685921	-3.270004
1	-0.580333	-0.317010	-2.136321
6	-0.102398	2.850958	2.109705
1	0.934740	2.497980	2.103649
1	-0.100013	3.893192	2.440220
1	-0.635990	2.245215	2.843578

Int-TS-3-Mes-Na

E (BS1) = -2703.292013

E (BS2) = -2704.027133

G_{298.15} (BS2) = -2703.285904



15	-2.513777	-0.410010	0.632697
6	-4.344328	-0.620562	0.543691
6	-4.897244	-1.924952	0.447977
6	-5.224603	0.488081	0.655509
6	-6.284132	-2.075281	0.338059
6	-6.603207	0.280655	0.540125
6	-7.155229	-0.986184	0.348341
1	-6.692336	-3.080007	0.259411
1	-7.265079	1.139456	0.620913
6	-2.092866	1.203454	-0.158963
6	-2.436875	1.421798	-1.518298
6	-1.438070	2.235151	0.561213
6	-2.146843	2.652802	-2.112951
6	-1.168453	3.446892	-0.086495
6	-1.514597	3.682496	-1.415383
1	-2.433167	2.810272	-3.150387
1	-0.670290	4.232108	0.474360
8	-2.050290	-0.486864	2.088575
11	-0.029799	-1.343608	2.281469
6	-1.702469	-1.643438	-0.413617
6	-0.531948	-2.186655	-0.020415
1	-2.207068	-1.884411	-1.354659
6	0.066605	-3.204911	-0.886728
6	-0.501053	-4.496059	-0.987457
6	1.267873	-2.976465	-1.595746
6	0.100927	-5.498372	-1.747661
6	1.859463	-3.975486	-2.366030
6	1.286212	-5.248476	-2.445526
1	-1.420399	-4.707340	-0.447509
1	1.737532	-2.000071	-1.537312
1	-0.363215	-6.480499	-1.801168
1	2.779871	-3.759338	-2.903370
1	1.754225	-6.029486	-3.037664
15	2.333977	0.121500	0.920664
6	2.244205	1.813786	0.280083
6	2.448701	2.921395	1.136485
6	1.995422	2.011867	-1.096730
6	2.424838	4.204136	0.588407
6	1.996534	3.317715	-1.598585
6	2.218533	4.424017	-0.778089
1	2.592449	5.055439	1.243588
1	1.821037	3.468622	-2.660018
6	3.975385	-0.644151	0.662809
6	5.142690	0.026588	0.222974
6	4.019444	-2.048641	0.891872

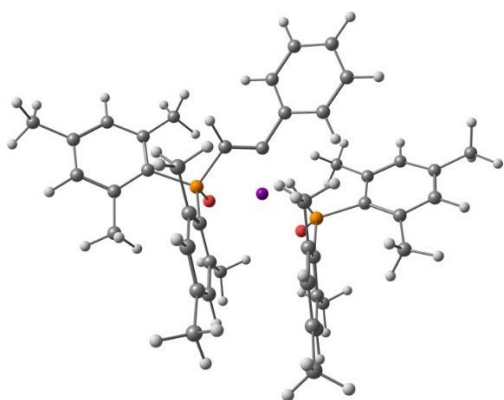
6	6.300988	-0.727346	-0.012675
6	5.198763	-2.747741	0.636630
6	6.351361	-2.107615	0.173546
1	7.193949	-0.209867	-0.352771
1	5.216608	-3.820961	0.808669
8	1.796529	-0.047216	2.341354
1	1.523221	-0.589541	0.020620
6	-3.115848	0.395281	-2.398977
1	-2.379681	-0.279682	-2.847921
1	-3.843332	-0.219448	-1.867310
1	-3.641740	0.896425	-3.216103
6	-1.017574	2.146527	2.011845
1	-0.689505	3.131382	2.355102
1	-1.823266	1.795341	2.657486
1	-0.182484	1.455026	2.147976
6	-1.209556	4.995241	-2.087204
1	-0.936460	5.763192	-1.359030
1	-0.374919	4.890872	-2.789953
1	-2.069782	5.356538	-2.660959
6	-4.084522	-3.200915	0.505444
1	-3.646120	-3.454919	-0.463686
1	-3.263511	-3.138487	1.221394
1	-4.732758	-4.030214	0.802679
6	-4.780772	1.906421	0.940204
1	-5.625653	2.476782	1.336041
1	-3.978488	1.948213	1.678884
1	-4.425572	2.419514	0.042529
6	-8.640217	-1.172073	0.177144
1	-9.203836	-0.395851	0.703486
1	-8.919577	-1.115394	-0.882736
1	-8.966663	-2.148533	0.547403
6	2.849894	-2.829005	1.446749
1	1.908063	-2.604136	0.941140
1	3.024652	-3.901417	1.334311
1	2.719723	-2.614652	2.513263
6	5.250866	1.517336	-0.001818
1	6.288916	1.779324	-0.220825
1	4.637257	1.859461	-0.838767
1	4.943509	2.087282	0.876729
6	7.605261	-2.892397	-0.109356
1	8.438313	-2.235305	-0.372611
1	7.901325	-3.490245	0.759798
1	7.449771	-3.591258	-0.939857
6	1.752142	0.872958	-2.059314
1	2.574171	0.148944	-2.058616
1	0.832981	0.328953	-1.816950
1	1.651260	1.256252	-3.077335
6	2.734808	2.769484	2.610835
1	1.896035	2.308496	3.136224
1	3.602719	2.125341	2.789521
1	2.942351	3.745079	3.057706
6	2.239065	5.823037	-1.335863
1	1.477395	6.449539	-0.858768
1	3.207633	6.302364	-1.151915
1	2.057401	5.828471	-2.413402

TS-3-Mes-Na

E (BS1) = -2703.282256

E (BS2) = -2704.011765

G_{298.15} (BS2) = -2703.270527



15	-2.385464	-0.463612	0.643067
6	-4.184715	-0.806165	0.437131
6	-4.603104	-2.163446	0.433848
6	-5.171963	0.213146	0.369306
6	-5.952944	-2.467038	0.227340
6	-6.507707	-0.147905	0.161666
6	-6.918763	-1.477075	0.053271
1	-6.255120	-3.511529	0.222438
1	-7.253547	0.640937	0.103552
6	-2.003537	1.209414	-0.008514
6	-2.233573	1.477605	-1.383617
6	-1.545367	2.251243	0.835789
6	-2.054750	2.774394	-1.867771
6	-1.387792	3.534144	0.296610
6	-1.651466	3.823914	-1.039489
1	-2.248918	2.970797	-2.919539
1	-1.043450	4.330396	0.950044
8	-1.991309	-0.633912	2.112524
11	0.016346	-1.383028	2.454346
6	-1.493082	-1.618132	-0.429089
6	-0.186283	-1.879286	-0.212825
1	-2.076927	-2.095376	-1.221132
6	0.463277	-2.941583	-0.991987
6	-0.119678	-4.223377	-1.104668
6	1.736082	-2.755341	-1.573267
6	0.533527	-5.260597	-1.768873
6	2.383103	-3.789949	-2.245532
6	1.788397	-5.050694	-2.347805
1	-1.086051	-4.402035	-0.642381
1	2.223236	-1.792090	-1.488637
1	0.061245	-6.237539	-1.835302
1	3.361880	-3.612242	-2.683373
1	2.297658	-5.859155	-2.864266
15	2.051303	0.122136	0.894892
6	1.965366	1.838793	0.267688
6	2.270161	2.944929	1.097349
6	1.606018	2.052604	-1.080863
6	2.236764	4.228994	0.549148
6	1.608991	3.355604	-1.591126
6	1.934626	4.455715	-0.797911
1	2.486494	5.075170	1.185521
1	1.352861	3.508982	-2.636112
6	3.747652	-0.570065	0.602983
6	4.835477	0.070233	-0.042103
6	3.906160	-1.924647	1.016781
6	6.015218	-0.656481	-0.273835
6	5.101848	-2.596726	0.769962
6	6.172985	-1.983607	0.113717
1	6.839425	-0.154768	-0.774492
1	5.196253	-3.631140	1.091837
8	1.688268	0.049750	2.403255
1	0.940063	-0.822493	0.226969
6	-2.679753	0.430908	-2.379082
1	-1.848577	-0.223282	-2.659970
1	-3.480725	-0.206892	-1.997509
1	-3.046972	0.913384	-3.288537
6	-1.210532	2.091090	2.301402
1	-0.999175	3.072479	2.734893

1	-2.017873	1.620700	2.864566
1	-0.322423	1.466920	2.436320
6	-1.511658	5.220190	-1.584247
1	-1.115916	5.905581	-0.831112
1	-0.843385	5.241909	-2.451149
1	-2.481737	5.608181	-1.917669
6	-3.686184	-3.340874	0.695401
1	-3.271859	-3.748352	-0.231834
1	-2.850739	-3.086412	1.348451
1	-4.256794	-4.141367	1.175500
6	-4.902570	1.689844	0.561335
1	-5.841032	2.199047	0.796529
1	-4.207627	1.879605	1.380910
1	-4.485268	2.160697	-0.332278
6	-8.357931	-1.827515	-0.219345
1	-9.038462	-1.086242	0.210446
1	-8.552024	-1.859436	-1.299075
1	-8.614230	-2.810349	0.187119
6	2.820317	-2.699438	1.733167
1	1.871474	-2.656808	1.192552
1	3.095469	-3.754361	1.807507
1	2.666159	-2.310882	2.744639
6	4.850259	1.510044	-0.504704
1	5.844150	1.761367	-0.884193
1	4.132129	1.702204	-1.304942
1	4.616648	2.205107	0.303234
6	7.446335	-2.740915	-0.159675
1	8.192144	-2.106975	-0.646990
1	7.883476	-3.128828	0.767719
1	7.259584	-3.604205	-0.809426
6	1.274913	0.914584	-2.015899
1	2.149967	0.280726	-2.202369
1	0.487138	0.272488	-1.616611
1	0.938657	1.299628	-2.981920
6	2.707266	2.790161	2.533638
1	1.948603	2.287215	3.134884
1	3.609684	2.172206	2.605431
1	2.931341	3.767838	2.969070
6	1.978556	5.851009	-1.365834
1	1.348343	6.537129	-0.789943
1	2.998742	6.252396	-1.333753
1	1.643248	5.872165	-2.405878

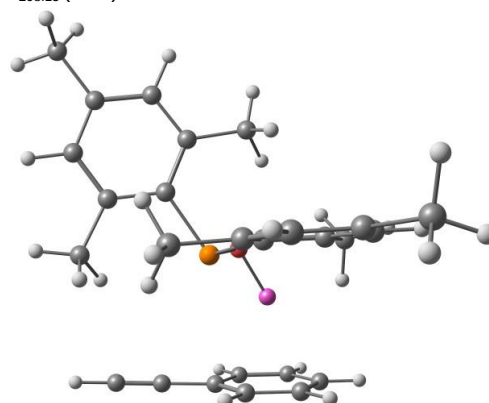
Hydrophosphorylation catalyzed by Li-OPMes₂

Int-TS-1-Mes-Li

E (BS1) = -1431.946931

E (BS2) = -1432.363408

G_{298.15} (BS2) = -1431.966078



6	2.558370	-3.185103	1.271228
6	1.908833	-4.001775	1.884195
3	2.301110	-1.031719	-1.714247
1	1.336437	-4.721301	2.428361
6	3.384126	-0.882220	0.993045
6	3.317919	-2.218488	0.545694

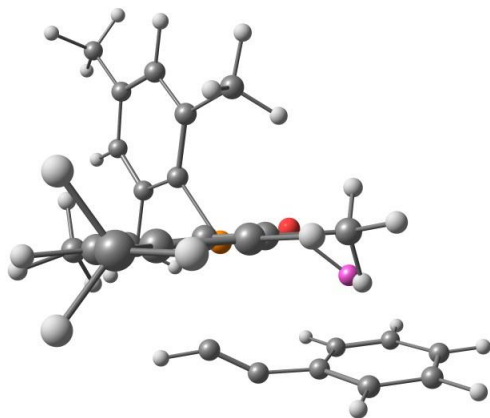
6	3.972835	-2.576551	-0.653143
6	4.678272	-1.613450	-1.384843
6	4.738593	-0.286852	-0.931365
6	4.090122	0.070991	0.257947
1	2.863897	-0.600936	1.900636
1	3.921373	-3.601945	-1.003086
1	5.183612	-1.900473	-2.301683
1	5.281664	0.459006	-1.502582
1	4.119579	1.098534	0.604712
15	-0.001336	-0.439163	-0.039103
8	0.607216	-0.803086	-1.471538
6	-2.638918	-0.168765	-1.231106
6	-1.835112	-0.785110	-0.241326
6	-3.992483	-0.505069	-1.337799
6	-4.588490	-1.449687	-0.497350
6	-3.779610	-2.082074	0.447667
6	-2.418642	-1.775053	0.584386
1	-4.595137	-0.020316	-2.103726
1	-4.214545	-2.842458	1.092917
6	-0.595153	1.957537	1.320073
6	-0.516535	3.322393	1.610828
6	-0.007682	1.433647	0.136248
6	0.693544	2.335647	-0.705790
6	0.750392	3.697146	-0.371934
6	0.148008	4.219324	0.772444
1	-0.983659	3.690517	2.522364
1	1.283249	4.372002	-1.039236
6	1.417245	1.935711	-1.976449
1	1.672689	2.827989	-2.556415
1	2.364270	1.427332	-1.751520
1	0.830729	1.264971	-2.600052
6	-1.310788	1.071161	2.311032
1	-2.265731	0.705942	1.921083
1	-0.710866	0.186560	2.553009
1	-1.509596	1.612545	3.240395
6	0.194643	5.694048	1.083966
1	0.318389	5.873233	2.157340
1	1.017766	6.188284	0.558868
1	-0.734101	6.194588	0.780499
6	-2.073262	0.834656	-2.205310
1	-1.885722	1.800737	-1.726441
1	-1.119410	0.478533	-2.599238
1	-2.764560	0.998524	-3.037318
6	-1.628168	-2.541849	1.623522
1	-2.239146	-3.346283	2.044806
1	-0.721408	-2.985702	1.203419
1	-1.306317	-1.901591	2.451127
6	-6.058077	-1.768864	-0.609748
1	-6.299305	-2.719558	-0.125009
1	-6.668802	-0.991846	-0.132246
1	-6.376270	-1.827684	-1.656062

TS-1-Mes-Li

E (BS1) = -1431.937450

E (BS2) = -1432.354528

G_{298.15} (BS2) = -1431.951976



6	2.618855	-0.820476	1.894304
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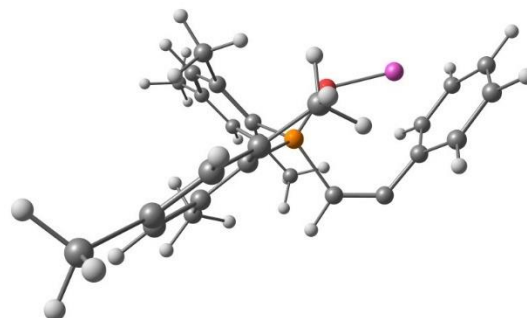
6	1.421055	-0.584475	2.187443
3	2.626616	-1.041802	-1.089198
1	0.744544	-0.408994	3.004181
6	4.317305	0.025680	0.308811
6	3.624538	-1.054073	0.932902
6	3.936551	-2.373179	0.487000
6	4.858360	-2.585336	-0.537260
6	5.515159	-1.508720	-1.153647
6	5.239486	-0.206998	-0.713046
1	4.100947	1.039449	0.628810
1	3.421101	-3.213248	0.940880
1	5.057749	-3.601332	-0.865837
1	6.227638	-1.681816	-1.952931
1	5.736137	0.639714	-1.178238
15	-0.018925	-0.325170	0.210211
8	0.907245	-0.791363	-0.965363
6	-2.418587	-0.807466	-1.280070
6	-1.668918	-1.112423	-0.118250
6	-3.641937	-1.451075	-1.492700
6	-4.145970	-2.399385	-0.597878
6	-3.376695	-2.715841	0.523292
6	-2.147307	-2.095284	0.776630
1	-4.212543	-1.208727	-2.386812
1	-3.737325	-3.469974	1.218939
6	-1.267724	2.041828	1.034973
6	-1.489047	3.419621	1.070333
6	-0.352207	1.491608	0.098208
6	0.363112	2.375308	-0.748405
6	0.108188	3.752213	-0.671834
6	-0.815991	4.298663	0.217601
1	-2.202180	3.816035	1.790221
1	0.655802	4.416715	-1.336485
6	1.410468	1.937301	-1.748612
1	1.720896	2.791416	-2.357360
1	2.305899	1.551899	-1.246189
1	1.052071	1.148145	-2.409702
6	-2.032477	1.181551	2.013310
1	-2.843896	0.631658	1.526731
1	-1.387095	0.438003	2.490948
1	-2.469813	1.798791	2.802722
6	-1.080843	5.781785	0.267607
1	-0.941968	6.177605	1.280323
1	-0.413485	6.329265	-0.403955
1	-2.112809	6.010889	-0.025046
6	-1.943348	0.187051	-2.311356
1	-2.070978	1.217496	-1.964798
1	-0.882602	0.047167	-2.529590
1	-2.508577	0.073383	-3.240638
6	-1.383327	-2.509847	2.013851
1	-1.854806	-3.381869	2.475789
1	-0.343106	-2.762793	1.791746
1	-1.361473	-1.711941	2.764236
6	-5.484070	-3.051829	-0.835201
1	-5.572741	-3.994043	-0.286553
1	-6.302608	-2.400171	-0.503660
1	-5.646479	-3.256055	-1.898438

Z-1I-Mes-Li

E (BS1) = -1431.964039

E (BS2) = -1432.384395

G_{298.15} (BS2) = -1431.978614



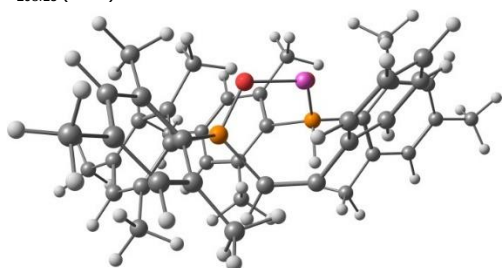
6	2.370843	0.341231	1.930565
6	1.050472	0.235876	1.750964
3	2.944284	0.013795	-1.231590
1	0.339752	0.349876	2.574150
6	4.005987	1.349326	0.347832
6	3.407378	0.209498	0.978928
6	3.928187	-1.068287	0.590350
6	4.899886	-1.190010	-0.401246
6	5.421059	-0.059411	-1.056488
6	4.971094	1.209912	-0.647060
1	3.654509	2.338332	0.623661
1	3.511836	-1.960186	1.048043
1	5.233385	-2.182354	-0.692893
1	6.168229	-0.161478	-1.835315
1	5.362743	2.101310	-1.129687
15	0.209113	0.032750	0.145270
8	1.177237	0.061119	-1.050422
6	-1.596991	-1.587513	-1.223967
6	-0.790087	-1.498404	-0.056553
6	-2.337480	-2.748686	-1.454575
6	-2.305283	-3.837194	-0.579062
6	-1.492675	-3.739698	0.548750
6	-0.730819	-2.597746	0.831199
1	-2.955717	-2.802629	-2.347644
1	-1.443661	-4.578298	1.238520
6	-2.172323	1.384230	0.872220
6	-3.037937	2.483315	0.862474
6	-0.971194	1.442678	0.121919
6	-0.642432	2.636436	-0.569941
6	-1.545722	3.704521	-0.546799
6	-2.755222	3.647014	0.147078
1	-3.957212	2.425891	1.440339
1	-1.286735	4.613887	-1.083580
6	0.649590	2.846884	-1.327314
1	0.706359	3.880707	-1.678531
1	1.523033	2.652532	-0.698289
1	0.730624	2.181518	-2.189812
6	-2.601464	0.189691	1.696657
1	-3.039081	-0.595574	1.073118
1	-1.780719	-0.262816	2.256238
1	-3.358944	0.498538	2.421866
6	-3.724426	4.800167	0.120664
1	-4.309012	4.851756	1.044147
1	-3.206691	5.754487	-0.014743
1	-4.435026	4.694208	-0.709050
6	-1.726201	-0.472025	-2.237794
1	-2.384697	0.322590	-1.872595
1	-0.761909	-0.017175	-2.470450
1	-2.157179	-0.859817	-3.164553
6	0.091578	-2.627646	2.097706
1	0.019048	-3.614265	2.562326
1	1.145485	-2.412244	1.914576
1	-0.257619	-1.890565	2.827657
6	-3.111689	-5.078026	-0.861464
1	-3.038601	-5.797223	-0.041272
1	-4.170009	-4.836451	-1.011136
1	-2.764397	-5.572949	-1.776257

Int-TS-2-Mes-Li

E (BS1) = -2548.532029

E (BS2) = -2549.256262

G_{298.15} (BS2) = -2548.511526



15	2.307898	-0.319988	0.007923
6	4.125237	-0.648822	0.001228
6	4.841028	-0.225260	-1.154077
6	4.821520	-1.332791	1.029722
6	6.208844	-0.487194	-1.251922
6	6.195349	-1.570980	0.874426
6	6.908833	-1.162067	-0.249585
1	6.741086	-0.153415	-2.139501
1	6.720545	-2.095102	1.668587
6	2.103935	1.519314	-0.008685
6	2.694526	2.300760	1.019923
6	1.283460	2.164857	-0.973834
6	2.421050	3.670764	1.092303
6	1.051167	3.540318	-0.854198
6	1.589442	4.311213	0.173966
1	2.878035	4.250641	1.890316
1	0.414979	4.018824	-1.593697
8	1.706357	-0.986459	-1.238602
3	0.056482	-1.730129	-1.060742
6	1.428082	-0.879502	1.509277
6	0.698097	-2.000984	1.665102
1	1.521774	-0.165673	2.330550
6	0.562373	-3.104581	0.740068
6	-0.729743	-3.571159	0.358495
6	1.669092	-3.851781	0.240208
6	-0.896061	-4.654955	-0.504236
6	1.490737	-4.957681	-0.582951
6	0.209977	-5.365274	-0.980755
1	-1.604919	-3.075626	0.768050
1	2.674581	-3.536119	0.495367
1	-1.901678	-4.961916	-0.779936
1	2.364124	-5.498541	-0.939727
1	0.079069	-6.225276	-1.630150
15	-2.351431	-0.246011	-0.016820
6	-2.507803	1.561821	-0.107331
6	-3.244101	2.142269	-1.168912
6	-1.848907	2.388792	0.834547
6	-3.330122	3.532938	-1.252621
6	-1.982075	3.775523	0.714592
6	-2.710999	4.367862	-0.317174
1	-3.892082	3.974279	-2.071799
1	-1.480905	4.409142	1.440806
6	-3.983212	-1.034070	0.164950
6	-4.732327	-0.743396	1.334162
6	-4.488506	-1.954529	-0.787533
6	-5.977134	-1.349244	1.514261
6	-5.742730	-2.531267	-0.553819
6	-6.505635	-2.240594	0.577989
1	-6.543705	-1.120825	2.413342
1	-6.130827	-3.236494	-1.283996
8	-1.525786	-0.815320	-1.169291
1	-1.739616	-0.476652	1.223719
6	4.211258	-1.825454	2.322557
1	3.432216	-2.571167	2.164445
1	4.989572	-2.276634	2.943344
1	3.753143	-1.020440	2.900510
6	4.193274	0.510809	-2.303674
1	4.915360	0.664087	-3.109253
1	3.340607	-0.045377	-2.697499
1	3.823383	1.492820	-1.993559
6	8.381595	-1.445313	-0.392320
1	8.934139	-0.541758	-0.672420
1	8.806426	-1.832229	0.537941
1	8.563268	-2.188279	-1.178463
6	-0.984205	1.857745	1.951852
1	-1.566289	1.322310	2.708658
1	-0.218897	1.172609	1.582965
1	-0.471341	2.683468	2.449120
6	-3.918674	1.305986	-2.227284
1	-3.204711	0.632205	-2.709721
1	-4.719236	0.689106	-1.807059
1	-4.356137	1.943243	-2.999061
6	-2.780973	5.866463	-0.449472
1	-3.723869	6.185215	-0.903733
1	-2.679432	6.358432	0.522168

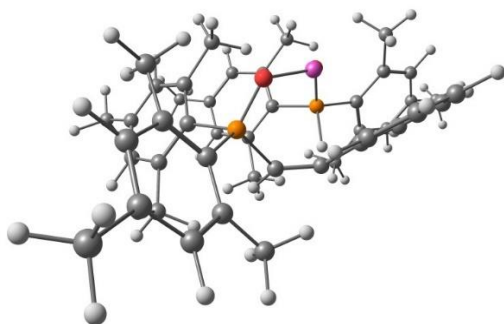
1	-1.969546	6.235216	-1.089616
6	3.647622	1.745293	2.052740
1	3.226527	0.902910	2.604075
1	4.579319	1.400052	1.596545
1	3.897919	2.517175	2.784519
6	0.631086	1.486366	-2.156525
1	1.356995	0.961129	-2.778982
1	-0.113025	0.751345	-1.849596
1	0.127626	2.238929	-2.769991
6	1.257647	5.774568	0.301904
1	2.051567	6.323399	0.817242
1	1.098426	6.235406	-0.677811
1	0.334968	5.913495	0.879281
6	-4.230511	0.186213	2.412368
1	-4.952187	0.242275	3.230231
1	-3.280978	-0.161250	2.834460
1	-4.069687	1.201191	2.037231
6	-3.760492	-2.375481	-2.043655
1	-2.804518	-2.850347	-1.814829
1	-4.376342	-3.084564	-2.602927
1	-3.537374	-1.528935	-2.696050
6	-7.865786	-2.855845	0.777616
1	-8.653337	-2.180584	0.419819
1	-7.964157	-3.795507	0.226796
1	-8.063270	-3.051497	1.835971

TS-2-Mes-Li

E (BS1) = -2548.521101

E (BS2) = -2549.239984

G_{298.15} (BS2) = -2548.496001



15	2.245212	-0.410080	-0.199742
6	4.002191	-0.895998	0.033106
6	4.906415	-0.518691	-0.997170
6	4.478387	-1.644247	1.138151
6	6.248495	-0.890798	-0.900047
6	5.835955	-1.991437	1.181136
6	6.736241	-1.629944	0.180229
1	6.930556	-0.593729	-1.693019
1	6.197356	-2.562800	2.032128
6	2.179796	1.438434	-0.236292
6	2.761350	2.179241	0.828253
6	1.453986	2.131603	-1.239278
6	2.595035	3.565816	0.874999
6	1.326807	3.524088	-1.144347
6	1.875530	4.260799	-0.098293
1	3.044547	4.116209	1.697999
1	0.764329	4.042325	-1.916044
8	1.747241	-1.050685	-1.506451
3	-0.022258	-1.514010	-1.504539
6	1.101666	-0.755006	1.161921
6	0.100960	-1.668719	1.253091
1	1.079968	0.096611	1.840353
6	0.016850	-2.925175	0.488582
6	-1.259945	-3.502021	0.263748
6	1.134495	-3.666679	0.027048
6	-1.415017	-4.701877	-0.425002
6	0.980189	-4.882907	-0.636746
6	-0.293954	-5.402965	-0.881188
1	-2.138809	-2.995833	0.648872
1	2.134416	-3.283017	0.183400

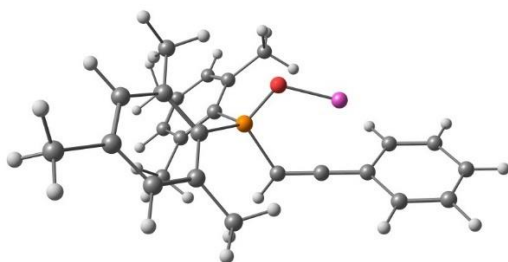
1	-2.412231	-5.101246	-0.587480
1	1.861478	-5.424503	-0.969988
1	-0.410982	-6.348026	-1.403132
15	-2.222062	-0.238018	0.002928
6	-2.249070	1.602186	0.084650
6	-2.814544	2.323068	-1.004624
6	-1.616910	2.311218	1.127334
6	-2.730667	3.713541	-1.019726
6	-1.559906	3.712887	1.065647
6	-2.104841	4.431727	0.007884
1	-3.167860	4.255104	-1.855497
1	-1.068148	4.246615	1.875426
6	-3.952177	-0.848754	0.135768
6	-4.647390	-0.603596	1.347450
6	-4.568607	-1.644586	-0.865436
6	-5.942582	-1.097835	1.517331
6	-5.868209	-2.118105	-0.642374
6	-6.578559	-1.850945	0.528820
1	-6.461092	-0.895681	2.451527
1	-6.336804	-2.722305	-1.415466
8	-1.596758	-0.639148	-1.358583
1	-1.297714	-0.907953	1.106535
6	3.633115	-2.095930	2.308101
1	2.857045	-2.805332	2.014973
1	4.267834	-2.588818	3.049108
1	3.125026	-1.267068	2.804678
6	4.488889	0.288703	-2.204980
1	5.308939	0.341059	-2.925304
1	3.618564	-0.149991	-2.697193
1	4.221053	1.313153	-1.927133
6	8.185200	-2.037103	0.245912
1	8.844160	-1.207772	-0.031700
1	8.460652	-2.375303	1.248649
1	8.391844	-2.858899	-0.450931
6	-1.000909	1.678646	2.353933
1	-1.564931	1.967800	3.248362
1	-0.967512	0.592509	2.323757
1	0.021353	2.046721	2.486397
6	-3.505906	1.634660	-2.155323
1	-2.821948	0.956267	-2.670056
1	-4.352683	1.033592	-1.809228
1	-3.883610	2.369435	-2.870662
6	-2.023965	5.935047	-0.050263
1	-3.015445	6.378380	-0.196807
1	-1.598225	6.349301	0.867368
1	-1.400227	6.263015	-0.889859
6	3.582356	1.557654	1.934589
1	3.073375	0.721072	2.416331
1	4.541582	1.183988	1.566374
1	3.786991	2.300790	2.709120
6	0.777992	1.483132	-2.425866
1	1.448563	0.820336	-2.973823
1	-0.086240	0.890291	-2.113853
1	0.417268	2.259485	-3.106289
6	1.686959	5.751839	-0.001465
1	2.634540	6.260181	0.207581
1	1.274132	6.163545	-0.926170
1	0.999562	6.006007	0.813811
6	-4.028530	0.171591	2.484578
1	-4.671961	0.134120	3.367099
1	-3.053813	-0.238377	2.766935
1	-3.877533	1.223147	2.223487
6	-3.916329	-2.037949	-2.172311
1	-2.994288	-2.599531	-2.008459
1	-4.604692	-2.660105	-2.751326
1	-3.644964	-1.169817	-2.774800
6	-7.988804	-2.347814	0.714803
1	-8.714952	-1.606209	0.357785
1	-8.165012	-3.270934	0.154511
1	-8.210038	-2.536441	1.769737

TS-3-Mes-Li

E (BS1) = -1431.949088

E (BS2) = -1432.369804

G_{298.15} (BS2) = -1431.965497



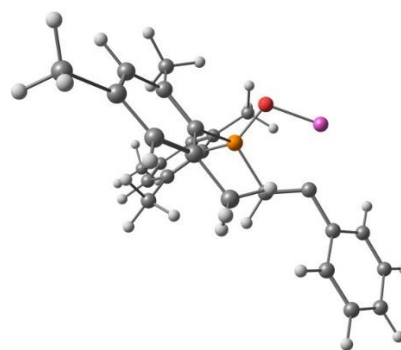
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6	-1.235712	-1.445444	0.235389
6	-2.342903	-1.353511	1.118506
6	-1.081528	-2.593580	-0.574638
6	-3.286673	-2.382868	1.136049
6	-2.056210	-3.597223	-0.517340
6	-3.170847	-3.508782	0.316805
1	-4.132641	-2.302944	1.814585
1	-1.932983	-4.476555	-1.144216
6	-0.955586	1.490454	-0.049472
6	-1.858296	1.558474	-1.136545
6	-0.717213	2.651250	0.733951
6	-2.538884	2.755964	-1.388211
6	-1.423741	3.819952	0.438514
6	-2.346855	3.894961	-0.608655
1	-3.232948	2.794103	-2.224180
1	-1.244194	4.702261	1.048290
8	0.700155	-0.099414	1.603561
3	2.551361	0.093592	1.457245
6	1.238695	-0.039358	-1.092086
6	2.509421	-0.122313	-0.787573
1	0.850797	0.185040	-2.092525
6	3.836741	-0.208961	-0.469506
6	4.550685	0.882533	0.178180
6	4.623388	-1.407252	-0.701600
6	5.901343	0.769984	0.505816
6	5.960084	-1.469614	-0.355113
6	6.635497	-0.391176	0.249611
1	4.030031	1.825206	0.329656
1	4.146292	-2.249383	-1.193480
1	6.394043	1.631251	0.952596
1	6.505367	-2.384516	-0.578701
1	7.687372	-0.458645	0.503817
6	-4.220954	-4.588678	0.336876
1	-4.508029	-4.845256	1.361997
1	-5.131337	-4.257907	-0.178346
1	-3.869971	-5.497320	-0.159933
6	-2.564863	-0.180350	2.046681
1	-1.636727	0.144370	2.522234
1	-2.978054	0.680548	1.511321
1	-3.273855	-0.454418	2.832148
6	0.078826	-2.810259	-1.516860
1	0.080344	-2.086043	-2.338118
1	1.042467	-2.717929	-1.011789
1	0.019827	-3.809025	-1.956628
6	-3.089860	5.175206	-0.889703
1	-3.639565	5.515374	-0.004665
1	-2.398627	5.980444	-1.165340
1	-3.805442	5.050648	-1.706960
6	-2.149423	0.395817	-2.061031
1	-2.869914	-0.300196	-1.619864
1	-2.576149	0.767146	-2.996542
1	-1.258636	-0.182240	-2.315706
6	0.266561	2.711804	1.881333
1	1.285996	2.487883	1.550291
1	0.263126	3.714606	2.316959
1	0.036434	1.983767	2.660323

E-1I-Mes-Li

E (BS1) = -1431.979534

E (BS2) = -1432.398620

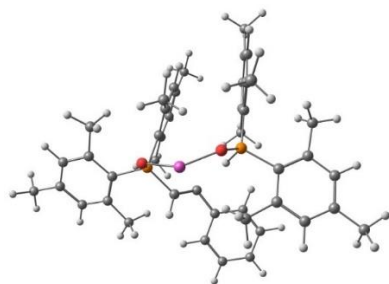
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6	-2.749060	-1.102144	0.775215
6	-1.087942	-2.554252	-0.286671
6	-3.728519	-2.058442	0.495701
6	-2.108732	-3.478309	-0.540925
6	-3.434568	-3.248414	-0.173387
1	-4.749690	-1.867659	0.816828
1	-1.852480	-4.409658	-1.039303
6	-0.787012	1.527448	0.064377
6	-1.258045	1.558457	-1.269961
6	-0.726862	2.733244	0.810762
6	-1.709480	2.770673	-1.807148
6	-1.194278	3.913486	0.226773
6	-1.700675	3.956042	-1.074914
1	-2.073932	2.781751	-2.831327
1	-1.153594	4.831572	0.808108
8	-0.050414	-0.023827	2.318242
3	1.701719	-0.196596	2.790846
6	1.456344	-0.252930	0.046943
6	2.522982	-0.351546	0.880619
1	1.512846	-0.188747	-1.046234
6	3.852641	-0.475907	0.255226
6	4.959117	0.212929	0.793552
6	4.087695	-1.303677	-0.864243
6	6.225099	0.117719	0.218612
6	5.360670	-1.425570	-1.421232
6	6.435438	-0.707793	-0.890313
1	4.806954	0.837888	1.670712
1	3.259971	-1.867410	-1.285369
1	7.054580	0.676185	0.644727
1	5.514392	-2.079816	-2.275810
1	7.426023	-0.799122	-1.326578
6	-4.518005	-4.245148	-0.493168
1	-5.245666	-4.318149	0.321272
1	-5.069745	-3.945823	-1.393274
1	-4.104058	-5.240630	-0.676870
6	-3.186190	0.147617	1.506986
1	-2.464472	0.448688	2.268620
1	-3.311628	0.990083	0.819352
1	-4.147848	-0.025687	1.997241
6	0.304413	-2.933680	-0.734774
1	0.666724	-2.281866	-1.536009
1	1.031486	-2.870258	0.077027
1	0.304314	-3.958227	-1.115748
6	-2.193211	5.251106	-1.667089
1	-2.962172	5.707941	-1.033879
1	-1.377949	5.979060	-1.755238
1	-2.618313	5.099504	-2.662907
6	-1.326030	0.346946	-2.174985
1	-2.219009	-0.253453	-1.975772
1	-1.369884	0.670314	-3.218444
1	-0.464077	-0.315484	-2.074865
6	-0.162612	2.833545	2.210257
1	0.884483	2.513769	2.240165
1	-0.206831	3.870805	2.552717
1	-0.701967	2.203780	2.919729

Int-TS-4-Mes-Li

E (BS1) = -2548.527941
 E (BS2) = -2549.250960
 G_{298.15} (BS2) = -2548.505667

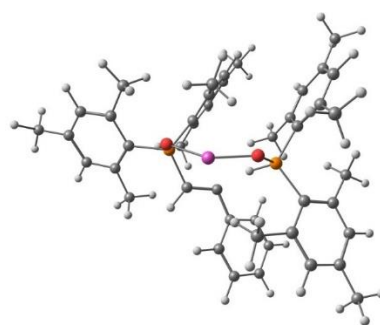


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6	4.672080	-2.013736	-0.087925
6	5.028751	0.155380	-1.158841
6	6.063410	-2.186846	-0.059992
6	6.405687	-0.070426	-1.106047
6	6.948751	-1.233181	-0.555876
1	6.460954	-3.104113	0.366376
1	7.072241	0.687276	-1.510994
6	2.046776	1.081696	0.234284
6	2.397939	1.102306	1.612411
6	1.492448	2.249661	-0.352218
6	2.156208	2.252905	2.366177
6	1.282186	3.376664	0.453529
6	1.589975	3.401193	1.810100
1	2.417261	2.246244	3.421637
1	0.844075	4.259118	-0.002825
8	1.993100	-0.279804	-2.245298
3	0.240368	-0.484167	-2.643662
6	1.257011	-1.750836	-0.121065
6	0.426723	-1.647525	0.943706
1	1.324348	-2.634739	-0.781073
6	-0.373601	-2.832632	1.270183
6	0.160955	-4.143809	1.245511
6	-1.722131	-2.703533	1.675517
6	-0.614048	-5.253575	1.581250
6	-2.507705	-3.814147	1.970284
6	-1.959059	-5.100624	1.929971
1	1.201087	-4.282041	0.966320
1	-2.155711	-1.711589	1.734261
1	-0.169725	-6.246080	1.558910
1	-3.550528	-3.675613	2.243998
1	-2.565493	-5.966664	2.179585
15	-2.053034	0.235215	-0.890009
6	-2.160708	1.948518	-0.312587
6	-2.426117	2.998750	-1.223401
6	-1.927616	2.227986	1.053241
6	-2.424033	4.311634	-0.750845
6	-1.954116	3.560452	1.477892
6	-2.185603	4.614518	0.594743
1	-2.626533	5.119098	-1.450215
1	-1.779160	3.775352	2.528157
6	-3.609481	-0.705277	-0.779507
6	-4.849488	-0.191830	-0.327943
6	-3.496582	-2.083492	-1.114687
6	-5.933800	-1.070943	-0.207981
6	-4.609262	-2.912187	-0.970523
6	-5.837471	-2.428237	-0.513339
1	-6.884323	-0.674852	0.138954
1	-4.508856	-3.966230	-1.216447
8	-1.425255	0.125579	-2.290369
1	-1.210211	-0.371545	0.064204
6	3.008289	-0.074890	2.331318
1	2.324033	-0.927059	2.288589
1	3.963002	-0.376170	1.893339
1	3.184050	0.174037	3.380864
6	1.091906	2.405778	-1.803838
1	0.848524	3.453104	-2.000216
1	1.875628	2.094291	-2.492159

1	0.199561	1.822540	-2.039634
6	1.318388	4.618625	2.654450
1	0.869996	5.422181	2.064415
1	0.635227	4.380547	3.477725
1	2.240646	5.002222	3.106403
6	3.850000	-3.146341	0.481250
1	3.167039	-2.811738	1.262934
1	3.241278	-3.628912	-0.288485
1	4.511967	-3.905641	0.905496
6	4.569141	1.446087	-1.794261
1	5.419572	1.973982	-2.232616
1	3.834482	1.257199	-2.579136
1	4.101754	2.112854	-1.064084
6	8.439621	-1.445926	-0.516335
1	8.698125	-2.368113	0.011073
1	8.854954	-1.508346	-1.529257
1	8.944753	-0.612695	-0.014843
6	-2.226594	-2.708115	-1.647353
1	-1.331140	-2.362667	-1.129389
1	-2.267906	-3.793155	-1.529443
1	-2.102954	-2.482451	-2.712139
6	-5.102662	1.253863	0.032392
1	-6.158746	1.389048	0.278204
1	-4.516325	1.577390	0.895718
1	-4.862750	1.931300	-0.789805
6	-7.014489	-3.353734	-0.350735
1	-7.221360	-3.896754	-1.279636
1	-6.815385	-4.105880	0.421827
1	-7.917265	-2.807226	-0.065419
6	-1.689160	1.150737	2.082232
1	-2.541192	0.462883	2.142437
1	-0.801143	0.543898	1.863480
1	-1.557571	1.597017	3.070709
6	-2.737053	2.755764	-2.680590
1	-1.845770	2.448346	-3.233935
1	-3.477581	1.960775	-2.813567
1	-3.132734	3.666662	-3.136981
6	-2.168338	6.044679	1.066972
1	-3.068092	6.580455	0.744994
1	-2.104471	6.105217	2.156479
1	-1.309659	6.583327	0.648319

TS-4-Mes-Li

E (BS1) = -2548.523875
 E (BS2) = -2549.243326
 G_{298.15} (BS2) = -2548.500484



15	2.417751	-0.595364	-0.640286
6	4.221099	-0.981667	-0.504841
6	4.758514	-2.114704	0.158827
6	5.118097	-0.070656	-1.135281
6	6.149474	-2.297240	0.180703
6	6.493023	-0.305778	-1.082787
6	7.035136	-1.413317	-0.428317
1	6.545860	-3.167709	0.696722
1	7.159492	0.401868	-1.569743
6	2.160545	0.999730	0.254896
6	2.488281	1.068154	1.638486
6	1.676425	2.167192	-0.391709
6	2.320167	2.268904	2.330105

6	1.528386	3.344429	0.356075
6	1.835975	3.422304	1.710106
1	2.564987	2.296918	3.389021
1	1.143630	4.226624	-0.147331
8	2.075816	-0.486681	-2.146199
3	0.303679	-0.488431	-2.533518
6	1.351988	-1.841653	0.076943
6	0.204538	-1.506005	0.713657
1	1.657788	-2.861181	-0.179858
6	-0.736362	-2.587018	1.101589
6	-0.767284	-3.878578	0.533409
6	-1.732263	-2.281012	2.050225
6	-1.743257	-4.806544	0.888575
6	-2.705811	-3.208448	2.420013
6	-2.720461	-4.475022	1.833058
1	-0.030660	-4.148063	-0.218424
1	-1.731101	-1.288038	2.490124
1	-1.750947	-5.789062	0.423313
1	-3.464344	-2.937235	3.149139
1	-3.488342	-5.195173	2.101468
15	-1.951289	0.267900	-0.788414
6	-2.247527	2.019835	-0.383795
6	-2.835683	2.876533	-1.344426
6	-1.788385	2.540883	0.845464
6	-2.924422	4.242016	-1.066823
6	-1.902920	3.915695	1.079459
6	-2.451508	4.783699	0.133995
1	-3.378463	4.899119	-1.804815
1	-1.550366	4.314984	2.026789
6	-3.464949	-0.767167	-0.679271
6	-4.599735	-0.432537	0.102094
6	-3.395225	-2.058276	-1.276670
6	-5.615769	-1.382278	0.270702
6	-4.436622	-2.964825	-1.070690
6	-5.554310	-2.654055	-0.294415
1	-6.479824	-1.113772	0.873111
1	-4.364394	-3.949691	-1.524995
8	-1.331636	0.188700	-2.209804
1	-0.948985	-0.301775	0.175220
6	2.987875	-0.112796	2.433016
1	2.262853	-0.929908	2.406075
1	3.936856	-0.494849	2.048663
1	3.142520	0.174004	3.475944
6	1.268244	2.273742	-1.845469
1	1.177755	3.328073	-2.120027
1	1.974107	1.796331	-2.521544
1	0.287052	1.818346	-2.011823
6	1.647904	4.700626	2.484303
1	1.115031	5.449798	1.892642
1	1.082364	4.525244	3.406076
1	2.613157	5.129911	2.779617
6	3.954511	-3.185358	0.862095
1	3.185110	-2.779485	1.518217
1	3.454548	-3.845623	0.145557
1	4.621687	-3.806812	1.464583
6	4.667855	1.164072	-1.879573
1	5.524614	1.652404	-2.349939
1	3.939139	0.915357	-2.652750
1	4.197229	1.889186	-1.209577
6	8.524363	-1.635838	-0.389088
1	8.779977	-2.533154	0.180867
1	8.932091	-1.748634	-1.400463
1	9.038596	-0.783256	0.069252
6	-2.245733	-2.534412	-2.139568
1	-1.279778	-2.401565	-1.648573
1	-2.359979	-3.600942	-2.347703
1	-2.211551	-1.995252	-3.089657
6	-4.804917	0.898314	0.789578
1	-5.752698	0.887597	1.333828
1	-4.015527	1.118696	1.511347
1	-4.834708	1.730505	0.082832
6	-6.631495	-3.677369	-0.048613
1	-6.903097	-4.202418	-0.970488
1	-6.286111	-4.437005	0.664065
1	-7.533950	-3.219124	0.365558

6	-1.231317	1.667432	1.943231
1	-2.005563	1.003029	2.346094
1	-0.413182	1.025226	1.608103
1	-0.864981	2.281479	2.768451
6	-3.395971	2.354162	-2.644614
1	-2.600008	1.995023	-3.301734
1	-4.067654	1.505130	-2.476918
1	-3.958953	3.135491	-3.161556
6	-2.517192	6.267176	0.389252
1	-3.434437	6.703527	-0.018675
1	-2.473664	6.491108	1.458997

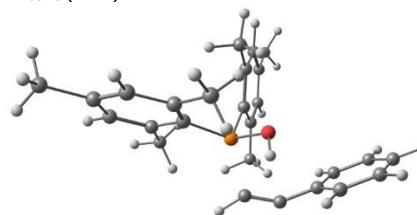
Mes₂P(O)H as a nucleophile

Int-TS-1-Mes-H

E (BS1) = -1424.953705

E (BS2) = -1425.341267

G_{298.15} (BS2) = -1424.928639



15	-0.434338	-0.841977	0.278075
6	-1.850212	0.290663	0.542141
6	-1.791804	1.706434	0.521150
6	-3.061052	-0.352028	0.911383
6	-2.946996	2.426802	0.853474
6	-4.183783	0.414618	1.224425
6	-4.148518	1.811120	1.203072
1	-2.8967837	3.512544	0.840763
1	-5.104095	-0.093366	1.502017
6	-0.693125	-1.741998	-1.296895
6	-1.012045	-1.097227	-2.517181
6	-0.568493	-3.150629	-1.259797
6	-1.226492	-1.878383	-3.656489
6	-0.790630	-3.888097	-2.426664
6	-1.131006	-3.272588	-3.632815
1	-1.468497	-1.379273	-4.591651
1	-0.690221	-4.969754	-2.390075
8	0.893456	0.056052	-0.076639
6	0.568249	-1.795105	1.846569
6	1.803367	-1.977932	1.604394
1	-0.126554	-2.011669	2.642808
6	2.895297	-1.778976	0.718967
6	3.240987	-2.748246	-0.257995
6	3.698883	-0.612966	0.803149
6	4.317136	-2.541729	-1.119539
6	4.769726	-0.424094	-0.061200
6	5.090346	-1.381500	-1.032395
1	2.657829	-3.663209	-0.324583
1	3.449426	0.144116	1.539410
1	4.551691	-3.297213	-1.864743
1	5.357941	0.486528	0.016247
1	5.927460	-1.224832	-1.705408
1	1.290540	0.400248	0.740789
6	-1.097374	0.400591	-2.651890
1	-1.891348	0.819969	-2.028479
1	-0.159369	0.871892	-2.347566
1	-1.296639	0.680739	-3.689019
6	-0.195699	-3.895937	0.923145
1	-0.953996	-3.778250	0.781697
1	-0.098893	-4.964879	-0.204985
1	0.757710	-3.549641	0.412611
6	-1.403563	-4.086453	-4.870719
1	-2.476935	-4.290995	-4.972611
1	-1.087900	-3.556113	-5.774298
1	-0.888387	-5.050718	-4.836447
6	-0.563122	2.519850	0.186018
1	0.214379	2.408716	0.944767
1	-0.124605	2.241919	-0.772043

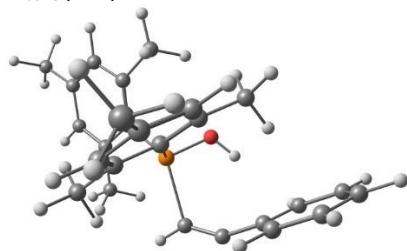
1	-0.826996	3.579522	0.145759
6	-3.173459	-1.856108	0.994533
1	-4.172036	-2.147016	1.330135
1	-2.993560	-2.336339	0.027588
1	-2.452889	-2.270328	1.708918
6	-5.375852	2.621441	1.529507
1	-6.063855	2.651394	0.675147
1	-5.926650	2.188405	2.370751
1	-5.117662	3.653853	1.781428

TS-1-Mes-H

E (BS1) = -1424.923062

E (BS2) = -1425.341063

G_{298.15} (BS2) = -1424.926472



15	-0.503010	-0.778250	0.269889
6	0.347470	0.842193	0.128606
6	1.321689	1.188247	-0.840622
6	0.063076	1.746540	1.185395
6	1.963266	2.429042	-0.728171
6	0.725776	2.972784	1.243908
6	1.684406	3.335369	0.294446
1	2.713257	2.688749	-1.470858
1	0.493881	3.655161	2.057951
6	-2.281957	-0.523564	-0.142399
6	-2.731468	0.158184	-1.299853
6	-3.224423	-1.043347	0.775607
6	-4.105828	0.327199	-1.491645
6	-4.588724	-0.850289	0.538559
6	-5.050281	-0.158777	-0.583174
1	-4.446638	0.848789	-2.382711
1	-5.306245	-1.255192	1.247516
8	-0.028176	-1.717699	-0.999000
6	0.568249	-1.795105	1.846569
6	1.803367	-1.977932	1.604394
1	-0.126554	-2.011669	2.642808
6	2.895297	-1.778976	0.718967
6	3.240987	-2.748246	-0.257995
6	3.698883	-0.612966	0.803149
6	4.317136	-2.541729	-1.119539
6	4.769726	-0.424094	-0.061200
6	5.090346	-1.381500	-1.032395
1	2.657829	-3.663209	-0.324583
1	3.449426	0.144116	1.539410
1	4.551691	-3.297213	-1.864743
1	5.357941	0.486528	0.016247
1	5.927460	-1.224832	-1.705408
1	0.827856	-2.129769	-0.794686
6	-1.793395	0.681773	-2.355675
1	-1.123102	1.448906	-1.959279
1	-1.170103	-0.122509	-2.754710
1	-2.355662	1.118030	-3.184748
6	-2.811444	-1.810892	2.010192
1	-2.235584	-1.187938	2.702136
1	-3.693542	-2.169282	2.546723
1	-2.197130	-2.682376	1.762134
6	-6.522623	0.072076	-0.802229
1	-6.827243	1.046349	-0.399307
1	-6.772585	0.069878	-1.867533
1	-7.125530	-0.691725	-0.302732
6	1.750621	0.309443	-1.992724
1	2.279971	-0.580803	-1.646588
1	0.910072	-0.027210	-2.598997
1	2.436581	0.863363	-2.638314
6	-0.932677	1.416605	2.272329
1	-0.978773	2.224550	3.006845

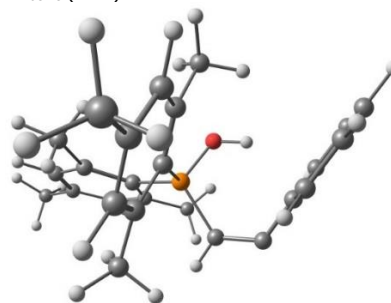
1	-1.941824	1.269137	1.875033
1	-0.650477	0.502259	2.806631
6	2.378293	4.670632	0.366029
1	1.731722	5.469006	-0.019614
1	2.631762	4.932717	1.398335
1	3.297498	4.675517	-0.226456

Z-1I-Mes-H

E (BS1) = -1424.933159

E (BS2) = -1425.354540

G_{298.15} (BS2) = -1424.938298



15	-0.420909	-0.553197	0.128058
6	0.647681	0.916367	0.012910
6	1.500326	1.174211	-1.087979
6	0.659947	1.781662	1.136081
6	2.376481	2.261610	-1.008529
6	1.549571	2.856499	1.155885
6	2.433090	3.103420	0.102805
1	3.032665	2.457623	-1.852289
1	1.545471	3.520100	2.016864
6	-2.189996	-0.226640	-0.131966
6	-2.712718	1.021888	-0.560879
6	-3.078940	-1.306136	0.142807
6	-4.101993	1.177245	-0.628544
6	-4.454079	-1.089257	0.046311
6	-4.989707	0.149219	-0.313374
1	-4.498417	2.133971	-0.957162
1	-5.125495	-1.919136	0.250757
8	-0.056836	-1.568454	-1.083621
6	-0.049998	-1.381590	1.693366
6	1.136724	-1.976871	1.898766
1	-0.845789	-1.322941	2.436051
6	2.196709	-2.045607	0.927985
6	2.298006	-3.128205	0.006747
6	3.227844	-1.067739	0.877098
6	3.346739	-3.203222	-0.914275
6	4.259785	-1.153549	-0.047620
6	4.334075	-2.217669	-0.959134
1	1.557338	-3.923387	0.048145
1	3.183492	-0.227412	1.563124
1	3.384126	-4.043151	-1.603804
1	5.014911	-0.371407	-0.068725
1	5.145647	-2.276566	-1.677460
1	0.795940	-2.030457	-0.919235
6	-1.883371	2.207530	-0.996055
1	-1.401031	2.710873	-0.154329
1	-1.096381	1.927822	-1.698215
1	-2.529484	2.937136	-1.489937
6	-2.629637	-2.703961	0.510854
1	-2.359391	-2.779191	1.567968
1	-3.445731	-3.407754	0.329625
1	-1.766612	-3.031807	-0.070295
6	-6.479128	0.360063	-0.365451
1	-6.882763	0.511476	0.643468
1	-6.738529	1.239248	-0.961373
1	-6.989196	-0.510810	-0.788999
6	1.540190	0.365202	-2.364026
1	2.075854	-0.578738	-2.222715
1	0.546519	0.124910	-2.744586
1	2.074883	0.929451	-3.132092
6	-0.263722	1.620728	2.321988
1	-0.396133	2.584686	2.820126

1	-1.257001	1.256428	2.045257
1	0.151260	0.918330	3.050789
6	3.417406	4.240700	0.167957
1	2.992728	5.107330	0.683836
1	4.316131	3.941882	0.721995
1	3.735598	4.551717	-0.831050

Influence of the P-bound group R in the hydrophosphorylation reaction catalyzed by K-OPR₂

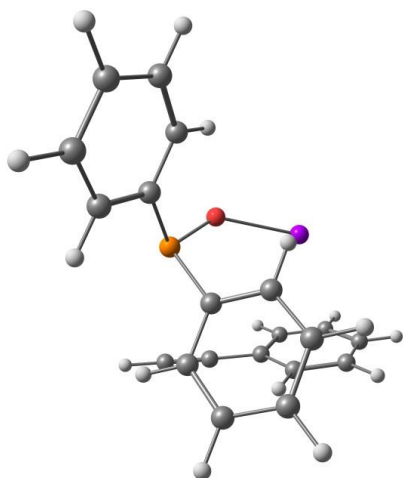
R = Ph

Int-TS-1-Ph-K

E (BS1) = -1788.367299

E (BS2) = -1788.760449

G_{298.15} (BS2) = -1788.519310



15	-1.254103	-0.464267	1.162397
6	-0.698533	0.979598	0.090913
6	-0.536452	0.828186	-1.296341
6	-0.386788	2.218319	0.663477
6	-0.069701	1.877153	-2.088070
6	0.067948	3.281527	-0.125206
6	0.235124	3.111439	-1.501309
1	-0.803293	-0.123225	-1.754774
1	-0.490478	2.350166	1.737799
1	0.047077	1.742107	-3.160796
1	0.302930	4.237334	0.335858
1	0.596650	3.932658	-2.113721
6	-2.992369	-0.477634	0.472894
6	-3.896872	0.563395	0.733407
6	-3.431267	-1.575775	-0.276395
6	-5.201630	0.514527	0.243337
6	-4.739380	-1.631789	-0.766355
6	-5.628549	-0.586128	-0.508937
1	-3.572776	1.424231	1.315943
1	-2.722858	-2.378172	-0.467257
1	-5.888938	1.332304	0.445589
1	-5.066479	-2.490326	-1.348642
1	-6.646639	-0.627285	-0.886353
8	-0.575130	-1.731401	0.519435
19	1.361933	-2.223407	-0.855350
6	1.837346	0.726575	3.206156
6	2.463963	0.465197	2.204042
1	1.276759	0.957213	4.085679
6	3.173699	0.142258	1.006708
6	4.072635	-0.945869	0.978934
6	2.947053	0.880931	-0.173886
6	4.723696	-1.287759	-0.208401
6	3.601764	0.529476	-1.355466
6	4.488724	-0.554422	-1.379367

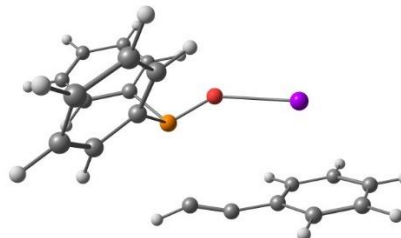
1	4.247111	-1.514858	1.886383
1	2.249269	1.709623	-0.157298
1	5.415121	-2.124955	-0.219453
1	3.412893	1.100930	-2.259101
1	4.997043	-0.823045	-2.300453

TS-1-Ph-K

E (BS1) = -1788.349493

E (BS2) = -1788.742682

G_{298.15} (BS2) = -1788.503452



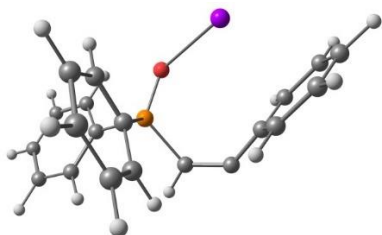
15	-0.807713	-0.224410	0.294072
6	-1.572363	1.442043	0.049980
6	-1.470714	2.083420	-1.193093
6	-2.192087	2.118787	1.111038
6	-2.001396	3.360097	-1.381418
6	-2.728972	3.394132	0.924055
6	-2.635171	4.018146	-0.322972
1	-0.978436	1.561747	-2.010126
1	-2.250007	1.650494	2.090765
1	-1.925203	3.842855	-2.352794
1	-3.211327	3.905462	1.752854
1	-3.047187	5.012890	-0.467087
6	-2.301443	-1.291630	0.058149
6	-3.455382	-1.156394	0.847810
6	-2.233820	-2.349694	-0.860723
6	-4.519962	-2.045543	0.707596
6	-3.299146	-3.241677	-1.222
6	-4.445865	-3.093616	-0.216584
1	-3.526935	-0.346214	1.569157
1	-1.338746	-2.453229	-1.467598
1	-5.410206	-1.922755	1.319103
1	-3.235931	-4.051655	-1.722974
1	-5.274559	-3.788039	-0.322077
8	0.125840	-0.487252	-0.921906
19	2.318500	0.123206	-1.798647
6	0.716868	-0.084537	2.290034
6	1.921490	-0.124745	1.984919
1	-0.015703	-0.006443	3.069565
6	3.110155	-0.257123	1.237968
6	3.571881	-1.539079	0.824487
6	3.886379	0.876424	0.864785
6	4.731429	-1.669185	0.063964
6	5.047653	0.728745	0.104534
6	5.479315	-0.540364	-0.309662
1	2.994200	-2.416487	1.099514
1	3.563852	1.863825	1.182708
1	5.054070	-2.660072	-0.245832
1	5.621624	1.611717	-0.166070
1	6.384880	-0.650090	-0.898522

Z-1l-Ph-K

E (BS1) = -1788.385384

E (BS2) = -1788.779016

G_{298.15} (BS2) = -1788.532465



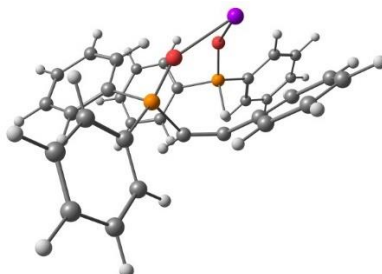
15	-0.779131	-0.499906	0.068675
6	-0.554350	1.318758	0.015441
6	-0.613273	1.967281	-1.230443
6	-0.305679	2.072988	1.169457
6	-0.410897	3.345022	-1.318364
6	-0.112253	3.453390	1.080441
6	-0.159299	4.089381	-0.161664
1	-0.816779	1.388882	-2.128190
1	-0.245067	1.574792	2.131433
1	-0.454040	3.838336	-2.285154
1	0.082735	4.029512	1.980214
1	-0.002596	5.161889	-0.229735
6	-2.581979	-0.741475	0.014003
6	-3.425307	-0.120170	0.946946
6	-3.126253	-1.593152	-0.954602
6	-4.799477	-0.353241	0.910077
6	-4.502768	-1.821855	-0.991451
6	-5.339092	-1.204265	-0.058992
1	-3.009789	0.551174	1.693572
1	-2.464541	-2.068158	-1.672246
1	-5.449814	0.129770	1.633494
1	-4.921905	-2.481413	-1.745901
1	-6.409928	-1.383590	-0.087122
8	-0.105059	-1.117308	-1.155873
19	2.203246	-0.364015	-1.876180
6	-0.226139	-1.078983	1.691377
6	1.058832	-1.243672	2.042544
1	-1.052251	-1.267148	2.384216
6	2.237111	-1.034446	1.272312
6	2.926630	-2.120992	0.645961
6	2.873001	0.244075	1.181299
6	4.146587	-1.940825	0.002136
6	4.099100	0.408442	0.539373
6	4.756695	-0.674574	-0.066567
1	2.481943	-3.111156	0.690025
1	2.387939	1.101882	1.636393
1	4.631976	-2.798772	-0.457865
1	4.544142	1.400450	0.500889
1	5.716605	-0.543238	-0.555439

Int-TS-2-Ph-K

E (BS1) = -2668.975902

E (BS2) = -2669.609581

G_{298.15} (BS2) = -2669.185324



15	-2.229861	-0.051944	0.219145
6	-3.937936	-0.236665	-0.387507
6	-5.009872	0.006325	0.486185
6	-4.197830	-0.643044	-1.702299
6	-6.322414	-0.157954	0.047858
6	-5.513955	-0.808948	-2.139368
6	-6.575188	-0.566882	-1.265668

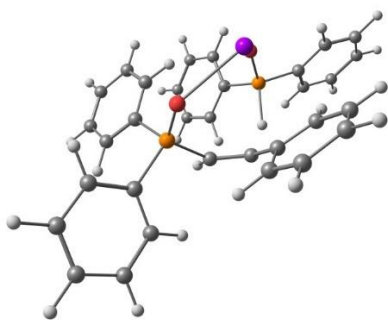
1	-4.815261	0.326659	1.505884
1	-3.367950	-0.829711	-2.377649
1	-7.148154	0.032386	0.727337
1	-5.708917	-1.126361	-3.159603
1	-7.598772	-0.695043	-1.605650
6	-2.038547	1.727160	0.590832
6	-2.853634	2.715314	0.023116
6	-0.947899	2.107091	1.390373
6	-2.588748	4.065999	0.260615
6	-0.690481	3.455336	1.631089
6	-1.509477	4.436821	1.065294
1	-3.693860	2.433602	-0.604291
1	-0.284319	1.349401	1.797333
1	-3.225005	4.826671	-0.183601
1	0.160280	3.740605	2.241792
1	-1.301420	5.487423	1.245827
8	-1.985173	-0.891680	1.467516
19	0.136173	-1.948817	2.348933
6	-1.067569	-0.250686	-1.149081
6	-0.134515	-1.210187	-1.376768
1	-0.986323	0.698455	-1.687099
6	-0.190519	-2.544610	-0.780258
6	1.003326	-3.216271	-0.409389
6	-1.401136	-3.265336	-0.628251
6	0.980665	-4.491012	0.157004
6	-1.421816	-4.544391	-0.075225
6	-0.235871	-5.161481	0.341864
1	1.959343	-2.728599	-0.571599
1	-2.330507	-2.804288	-0.946375
1	1.915134	-4.967664	0.442507
1	-2.370781	-5.062442	0.039190
1	-0.256044	-6.156025	0.777556
15	2.249928	0.062910	-0.037489
6	2.163021	1.870037	-0.278507
6	2.762557	2.740878	0.644257
6	1.444447	2.398636	-1.358215
6	2.643000	4.120368	0.486148
6	1.321026	3.780890	-1.512790
6	1.917189	4.641265	-0.590206
1	3.318595	2.336406	1.485389
1	0.978067	1.730118	-2.074822
1	3.110045	4.790885	1.201932
1	0.753765	4.183504	-2.346674
1	1.816504	5.716419	-0.706609
6	4.000161	-0.348654	-0.338589
6	4.707893	0.194822	-1.422242
6	4.618237	-1.309799	0.474037
6	6.016185	-0.210899	-1.679796
6	5.928712	-1.714519	0.213959
6	6.629004	-1.166757	-0.862838
1	4.237972	0.942319	-2.055689
1	4.067615	-1.721776	1.314462
1	6.560873	0.219911	-2.515082
1	6.403825	-2.454326	0.852314
1	7.648701	-1.480934	-1.065617
8	1.860477	-0.336870	1.396696
1	1.277754	-0.573256	-1.133224

TS-2-Ph-K

E (BS1) = -2668.970333

E (BS2) = -2669.600351

G_{298.15} (BS2) = -2669.179191



15	-2.229861	-0.051944	0.219145
6	-3.937936	-0.236665	-0.387507
6	-5.009872	0.006325	0.486185
6	-4.197830	-0.643044	-1.702299
6	-6.322414	-0.157954	0.047858
6	-5.513955	-0.808948	-2.139368
6	-6.575188	-0.566882	-1.265668
1	-4.815261	0.326659	1.505884
1	-3.367950	-0.829711	-2.377649
1	-7.148154	0.032386	0.727337
1	-5.708917	-1.126361	-3.159603
1	-7.598772	-0.695043	-1.605650
6	-2.038547	1.727160	0.590832
6	-2.853634	2.715314	0.023116
6	-0.947899	2.107091	1.390373
6	-2.588748	4.065999	0.260615
6	-0.690481	3.455336	1.631089
6	-1.509477	4.436821	1.065294
1	-3.693860	2.433602	-0.604291
1	-0.284319	1.349401	1.797333
1	-3.225005	4.826671	-0.183601
1	0.160280	3.740605	2.241792
1	-1.301420	5.487423	1.245827
8	-1.985173	-0.891680	1.467516
19	0.136173	-1.948817	2.348933
6	-1.067569	-0.250686	-1.149081
6	-0.134515	-1.210187	-1.376768
1	-0.986323	0.698455	-1.687099
6	-0.190519	-2.544610	-0.780258
6	1.003326	-3.216271	-0.409389
6	-1.401136	-3.265336	-0.628251
6	0.980665	-4.491012	0.157004
6	-1.421816	-4.544391	-0.075225
6	-0.235871	-5.161481	0.341864
1	1.959343	-2.728599	-0.571599
1	-2.330507	-2.804288	-0.946375
1	1.915134	-4.967664	0.442507
1	-2.370781	-5.062442	0.039190
1	-0.256044	-6.156025	0.777556
15	2.249928	0.062910	-0.037489
6	2.163021	1.870037	-0.278507
6	2.762557	2.740878	0.644257
6	1.444447	2.398636	-1.358215
6	2.643000	4.120368	0.486148
6	1.321026	3.780890	-1.512790
6	1.917189	4.641265	-0.590206
1	3.318595	2.336406	1.485389
1	0.978067	1.730118	-2.074822
1	3.110045	4.790885	1.201932
1	0.753765	4.183504	-2.346674
1	1.816504	5.716419	-0.706609
6	4.000161	-0.348654	-0.338589
6	4.707893	0.194822	-1.422242
6	4.618237	-1.309799	0.474037
6	6.016185	-0.210899	-1.679796
6	5.928712	-1.714519	0.213959
6	6.629004	-1.166757	-0.862838
1	4.237972	0.942319	-2.055689
1	4.067615	-1.721776	1.314462
1	6.560873	0.219911	-2.515082
1	6.403825	-2.454326	0.852314

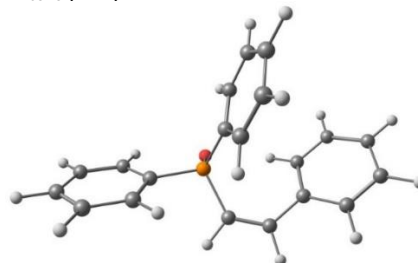
1	7.648701	-1.480934	-1.065617
8	1.860477	-0.336870	1.396696
1	1.277754	-0.573256	-1.133224

Z-P-Ph

E (BS1) = -1189.080110

E (BS2) = -1189.432181

G_{298.15} (BS2) = -1189.169259



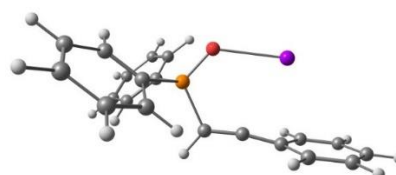
15	-0.815497	-0.582006	-0.653929
6	0.027072	0.946939	-0.126240
6	0.350132	1.884189	-1.114684
6	0.347152	1.209916	1.212161
6	0.991303	3.073918	-0.768747
6	0.989134	2.398899	1.554960
6	1.312454	3.331326	0.565469
1	0.114351	1.663331	-2.150781
1	0.117114	0.479635	1.981182
1	1.246209	3.794800	-1.539950
1	1.244419	2.595044	2.592133
1	1.817851	4.254265	0.834432
6	-2.549479	-0.396046	-0.126373
6	-2.912228	-0.311809	1.225514
6	-3.535223	-0.313662	-1.116635
6	-4.250604	-0.149034	1.580374
6	-4.874519	-0.150002	-0.758521
6	-5.232346	-0.067678	0.588402
1	-2.152676	-0.372610	1.999649
1	-3.242485	-0.384386	-2.159313
1	-4.528519	-0.085842	2.628293
1	-5.636930	-0.088490	-1.529518
1	-6.274475	0.059096	0.866754
8	-0.704500	-0.808416	-2.145210
6	-0.207020	-1.909362	0.415688
6	1.066083	-2.195890	0.750994
1	-0.994020	-2.536372	0.829008
6	2.302943	-1.535502	0.318001
6	2.448665	-0.945403	-0.950186
6	3.387982	-1.493656	1.212131
6	3.631169	-0.292361	-1.290348
6	4.566052	-0.833480	0.872005
6	4.688524	-0.225204	-0.380050
1	1.643931	-1.016053	-1.674463
1	3.291110	-1.966822	2.185623
1	3.728919	0.160689	-2.272383
1	5.389145	-0.796346	1.579497
1	5.607785	0.286588	-0.649308
1	1.213250	-3.005685	1.466268

TS-3-Ph-K

E (BS1) = -1788.371448

E (BS2) = -1788.767021

G_{298.15} (BS2) = -1788.523335

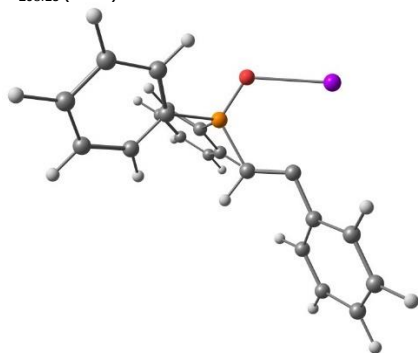


15	0.849347	-0.036060	0.212720
6	1.816856	1.502869	0.095144

6	3.114758	1.576292	0.624422
6	1.237303	2.649197	-0.467906
6	3.819931	2.778517	0.590925
6	1.944748	3.851648	-0.499242
6	3.235581	3.917050	0.029142
1	3.574749	0.692109	1.055351
1	0.236644	2.595755	-0.885977
1	4.824959	2.827522	0.999560
1	1.490926	4.734226	-0.940366
1	3.787522	4.852000	0.000632
6	2.043199	-1.371256	-0.084623
6	2.896969	-1.349673	-1.198699
6	2.051210	-2.479540	0.772325
6	3.749493	-2.424653	-1.446621
6	2.907568	-3.552721	0.522752
6	3.755997	-3.526673	-0.586428
1	2.904709	-0.489882	-1.862444
1	1.389174	-2.486043	1.632706
1	4.411067	-2.402413	-2.307635
1	2.915084	-4.406716	1.193971
1	4.422849	-4.361684	-0.780310
8	0.165681	-0.198183	1.566977
19	-2.349396	-0.365067	1.962510
6	-0.319266	-0.041016	-1.187405
6	-1.604424	-0.025238	-0.924454
1	0.154503	-0.067260	-2.182884
6	-2.968915	-0.029737	-0.887568
6	-3.726615	-1.258013	-0.726377
6	-3.750513	1.191377	-0.828990
6	-5.094820	-1.238110	-0.488756
6	-5.114112	1.162900	-0.584670
6	-5.820181	-0.039655	-0.397355
1	-3.198537	-2.206102	-0.795521
1	-3.238741	2.140796	-0.962179
1	-5.611265	-2.189929	-0.374529
1	-5.649992	2.109983	-0.544520
1	-6.889380	-0.041112	-0.213859

E-1I-Ph-K

E (BS1) = -1788.387500
E (BS2) = -1788.781705
G_{298.15} (BS2) = -1788.537137

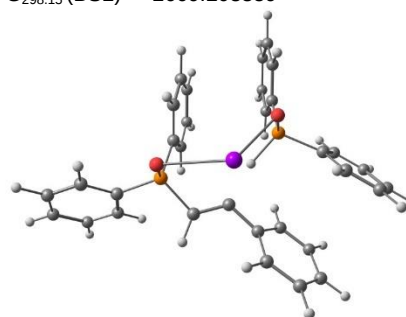


6	-1.880082	-0.140359	-0.497749
6	-0.735386	-0.095090	0.225025
19	-1.323777	-0.442617	-3.285798
1	-0.689965	-0.060829	1.326715
6	-4.155805	-1.032485	0.058027
6	-3.137043	-0.074350	0.258789
6	-3.405561	0.964672	1.179669
6	-4.622863	1.040375	1.857097
6	-5.605297	0.066502	1.660412
6	-5.357090	-0.976594	0.760845
1	-3.983792	-1.834000	-0.657465
1	-2.645733	1.723515	1.347652
1	-4.801451	1.858614	2.550917
1	-6.551186	0.122185	2.191486
1	-6.111942	-1.742025	0.597261
15	0.882135	-0.089969	-0.550418
8	0.895486	-0.310966	-2.061015
6	3.083009	1.581545	-0.019499
6	1.685025	1.483672	-0.089203

6	3.689250	2.807093	0.253990
6	2.904755	3.945303	0.459698
6	1.512939	3.856144	0.389952
6	0.904734	2.630058	0.117030
1	3.695639	0.697958	-0.171787
1	4.771793	2.874620	0.310010
1	3.378172	4.898503	0.676603
1	0.901511	4.738945	0.552919
1	-0.177336	2.555916	0.067767
6	2.144085	-1.302554	1.664881
6	2.861949	-2.323515	2.286300
6	1.872692	-1.368675	0.289955
6	2.328184	-2.464591	-0.452430
6	3.048074	-3.485335	0.171387
6	3.314211	-3.415966	1.540185
1	1.805280	-0.450012	2.246654
1	3.071692	-2.266916	3.350434
1	2.117507	-2.503453	-1.516645
1	3.402249	-4.331735	-0.410073
1	3.874728	-4.209409	2.025939

Int-TS-4-Ph-K

E (BS1) = -2668.996051
E (BS2) = -2669.629188
G_{298.15} (BS2) = -2669.203359



15	-2.651802	-0.558433	0.490190
6	-4.340387	-0.745891	-0.161557
6	-4.570991	-1.041021	-1.512949
6	-5.426598	-0.564829	0.704041
6	-5.876820	-1.148016	-1.991897
6	-6.731636	-0.672703	0.222563
6	-6.957109	-0.962487	-1.125200
1	-3.733792	-1.192557	-2.187859
1	-5.238653	-0.349116	1.751169
1	-6.051694	-1.379313	-3.038506
1	-7.571080	-0.533037	0.897432
1	-7.973112	-1.047353	-1.499640
6	-2.102021	1.110599	0.003848
6	-1.879203	1.457864	-1.336265
6	-1.955315	2.080585	1.002956
6	-1.527700	2.764046	-1.669437
6	-1.592804	3.386894	0.666556
6	-1.387872	3.730920	-0.669058
1	-1.975723	0.707028	-2.114022
1	-2.127301	1.802576	2.038013
1	-1.352190	3.028481	-2.707929
1	-1.467113	4.131758	1.446500
1	-1.099364	4.743609	-0.930736
8	-2.640430	-0.676627	2.014920
19	-0.214986	-1.133487	2.836226
6	-1.617309	-1.752335	-0.354867
6	-0.285923	-1.541739	-0.351766
1	-2.119070	-2.669284	-0.698834
6	0.679873	-2.568574	-0.715323
6	0.727250	-3.806430	-0.032740
6	1.709491	-2.296756	-1.645161
6	1.761965	-4.714594	-0.256479
6	2.724891	-3.217228	-1.885566
6	2.766984	-4.427286	-1.183903
1	-0.053507	-4.038803	0.688298
1	1.706817	-1.345176	-2.168656

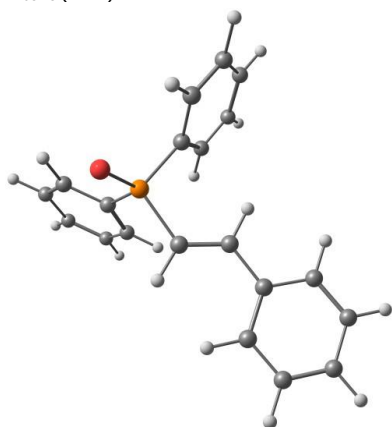
1	1.779494	-5.654385	0.290202
1	3.504267	-2.979851	-2.604181
1	3.574373	-5.133023	-1.355331
15	1.795376	0.692082	0.655092
6	1.914540	2.409279	0.068065
6	1.977003	3.448991	1.004479
6	1.888688	2.713193	-1.301117
6	2.044092	4.775417	0.577003
6	1.971072	4.038878	-1.726961
6	2.050309	5.071278	-0.788561
1	1.965847	3.206091	2.062555
1	1.792115	1.917011	-2.033812
1	2.093087	5.577983	1.307497
1	1.958004	4.267418	-2.788682
1	2.106771	6.103747	-1.120978
6	3.410428	-0.073924	0.259999
6	4.206393	0.301009	-0.832147
6	3.798218	-1.177494	1.036357
6	5.354133	-0.425333	-1.150622
6	4.944114	-1.903485	0.716075
6	5.722851	-1.532316	-0.382609
1	3.937326	1.162420	-1.433555
1	3.196105	-1.464583	1.892887
1	5.964090	-0.123583	-1.997480
1	5.228103	-2.759761	1.321095
1	6.613653	-2.099515	-0.636210
8	1.534806	0.612898	2.169104
1	0.715030	-0.136504	-0.045477

E-P-Ph

E (BS1) = -1189.081995

E (BS2) = -1189.435446

G_{298.15} (BS2) = -1189.174120



15	-1.016664	-0.040657	1.103053
6	-2.056702	-1.224720	0.190825
6	-1.597648	-1.896671	-0.951071
6	-3.362591	-1.447792	0.648456
6	-2.442175	-2.772870	-1.634070
6	-4.203722	-2.325240	-0.035428
6	-3.745115	-2.985696	-1.178067
1	-0.581249	-1.741747	-1.300786
1	-3.706821	-0.940428	1.544294
1	-2.082120	-3.292493	-2.517097
1	-5.214325	-2.496232	0.323501
1	-4.400552	-3.669765	-1.709138
6	-1.164866	1.545492	0.217487
6	-1.167943	1.631742	-1.182261
6	-1.268659	2.712707	0.984639
6	-1.264889	2.875445	-1.804797
6	-1.367930	3.956198	0.358569
6	-1.363868	4.038136	-1.035064
1	-1.100587	0.731334	-1.784690
1	-1.278097	2.634394	2.067046
1	-1.267775	2.938197	-2.888938
1	-1.449702	4.858396	0.957489
1	-1.442284	5.005494	-1.522519

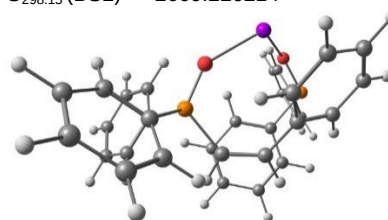
8	-1.408352	0.080230	2.556381
6	0.666711	-0.620426	0.830523
6	1.647396	0.121887	0.287885
1	0.854986	-1.628409	1.196485
6	3.046426	-0.272483	0.091912
6	3.551710	-1.528273	0.477153
6	3.922210	0.646308	-0.512255
6	4.888248	-1.848716	0.262400
6	5.261427	0.324864	-0.727012
6	5.748715	-0.924494	-0.340390
1	2.896832	-2.255030	0.947225
1	3.541793	1.618887	-0.812750
1	5.263565	-2.821577	0.565901
1	5.922910	1.048205	-1.194416
1	6.791437	-1.178900	-0.505487
1	1.408357	1.125296	-0.059574

Int-TS-5-Ph-DA

E (BS1) = -2669.043167

E (BS2) = -2669.653345

G_{298.15} (BS2) = -2669.226214



15	-2.329159	0.308148	0.241180
6	-4.133522	0.155082	0.076323
6	-4.946015	0.654289	1.107238
6	-4.723694	-0.462761	-1.033961
6	-6.330680	0.524616	1.029907
6	-6.112219	-0.588424	-1.108738
6	-6.914605	-0.097310	-0.078153
1	-4.496267	1.147101	1.964612
1	-4.099702	-0.842898	-1.836580
1	-6.955327	0.911159	1.829501
1	-6.564795	-1.067865	-1.971441
1	-7.994489	-0.194928	-0.137752
6	-2.014040	2.086627	0.436686
6	-2.489093	3.021681	-0.493013
6	-1.247516	2.511775	1.527275
6	-2.180411	4.372181	-0.339803
6	-0.945198	3.865569	1.681224
6	-1.405907	4.794049	0.745519
1	-3.096609	2.697051	-1.333277
1	-0.884798	1.778848	2.240369
1	-2.543856	5.095729	-1.063175
1	-0.345948	4.193446	2.525318
1	-1.165108	5.846509	0.861890
8	-1.765197	-0.466629	1.417976
19	0.322329	-1.719820	2.184816
6	-1.631961	-0.073051	-1.381704
6	-1.009795	-1.193527	-1.787765
1	-1.629268	0.776307	-2.059775
6	-0.857782	-2.470633	-1.071643
6	0.377664	-3.141552	-1.148753
6	-1.887998	-3.036823	-0.298385
6	0.599503	-4.311382	-0.420595
6	-1.670541	-4.216080	0.416202
6	-0.422609	-4.849825	0.369345
1	1.178105	-2.715490	-1.744316
1	-2.860433	-2.560149	-0.261453
1	1.569714	-4.796145	-0.466917
1	-2.475884	-4.641974	1.007473
1	-0.253670	-5.763609	0.931342
15	3.280666	-1.170328	0.031353
6	2.367968	0.112792	-0.989330
6	1.689469	1.167612	-0.361493
6	2.346964	0.042368	-2.388250
6	1.039583	2.148214	-1.110578

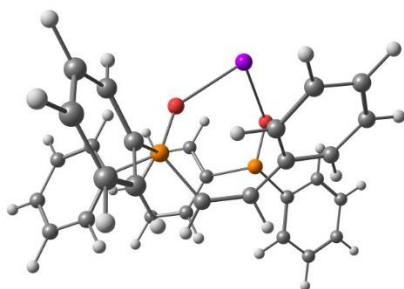
6	1.686527	1.015529	-3.145881
6	1.035652	2.073532	-2.507779
1	1.691069	1.210244	0.725239
1	2.853185	-0.779557	-2.891283
1	0.534745	2.969220	-0.612092
1	1.680945	0.947952	-4.231002
1	0.524324	2.834154	-3.091560
6	4.811225	-0.110647	0.226803
6	5.675306	0.156177	-0.845670
6	5.140719	0.385826	1.493769
6	6.832539	0.912440	-0.658606
6	6.301054	1.140176	1.687403
6	7.151085	1.406445	0.611416
1	5.436737	-0.223824	-1.837521
1	4.463038	0.169914	2.315971
1	7.489192	1.117502	-1.500604
1	6.543421	1.521661	2.676785
1	8.055532	1.990345	0.758999
8	2.598907	-1.137381	1.447283
1	-0.510444	-1.149158	-2.754373

TS-5-Ph-DA

E (BS1) = -2669.026095

E (BS2) = -2669.653272

G_{298.15} (BS2) = -2669.222888



15	-1.793408	-0.031863	-0.059526
6	-3.305168	-0.996680	-0.446482
6	-4.192227	-1.321513	0.589340
6	-3.604493	-1.388616	-1.757129
6	-5.363453	-2.028118	0.316448
6	-4.777828	-2.093867	-2.030737
6	-5.658270	-2.413487	-0.994585
1	-3.951972	-1.026758	1.606421
1	-2.901607	-1.157812	-2.552821
1	-6.044950	-2.280889	1.123878
1	-5.001477	-2.399044	-3.048986
1	-6.569853	-2.964753	-1.206752
6	-2.388583	1.691207	-0.156469
6	-2.782604	2.278098	-1.368002
6	-2.467585	2.432522	1.026749
6	-3.234789	3.596459	-1.392951
6	-2.929395	3.749893	1.001156
6	-3.311045	4.333984	-0.207153
1	-2.740404	1.705943	-2.290349
1	-2.149248	1.973318	1.956780
1	-3.534125	4.047561	-2.334659
1	-2.981556	4.321866	1.923065
1	-3.666829	5.359999	-0.227979
8	-1.355554	-0.372394	1.363582
19	0.329748	-1.705825	2.681214
6	-0.604384	-0.199368	-1.346186
6	0.572741	-0.956964	-1.267127
1	-0.586824	0.650134	-2.021262
6	0.668515	-2.340652	-0.712966
6	1.926178	-2.950495	-0.533074
6	-0.471669	-3.080117	-0.353412
6	2.042275	-4.217177	0.033434
6	-0.358357	-4.348114	0.228105
6	0.899077	-4.918517	0.437548
1	2.823804	-2.410284	-0.818449
1	-1.457179	-2.673775	-0.536745

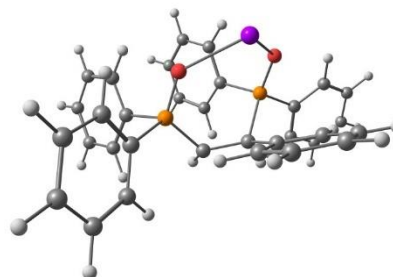
1	3.026726	-4.656191	0.168133
1	-1.258614	-4.890173	0.504776
1	0.989348	-5.901867	0.889646
15	2.157006	0.088197	0.305421
6	1.538808	1.804161	0.474669
6	1.393202	2.346130	1.760843
6	1.110441	2.556747	-0.630182
6	0.871717	3.626962	1.936903
6	0.584610	3.837697	-0.453817
6	0.466451	4.376228	0.828302
1	1.704722	1.749	2.613073
1	1.184541	2.146969	-1.631530
1	0.776468	4.041464	2.937138
1	0.249914	4.407310	-1.315786
1	0.047553	5.368783	0.964274
6	3.822236	0.310747	-0.446706
6	4.020785	0.939856	-1.687276
6	4.915952	-0.304951	0.181629
6	5.287175	0.972981	-2.269796
6	6.182733	-0.273647	-0.403933
6	6.373065	0.365497	-1.631143
1	3.188712	1.413947	-2.199025
1	4.754806	-0.798820	1.135226
1	5.428334	1.471730	-3.224918
1	7.022473	-0.746853	0.098427
1	7.357682	0.388476	-2.089209
8	2.347669	-0.515958	1.720339
1	1.276775	-0.788122	-2.081225

DA-I-Ph-K

E (BS1) = -2669.034722

E (BS2) = -2669.663980

G_{298.15} (BS2) = -2669.231172



15	-1.663722	-0.013123	-0.053114
6	-3.132875	-1.092565	-0.374521
6	-3.967833	-1.467665	0.687786
6	-3.446977	-1.524076	-1.669205
6	-5.092595	-2.262255	0.460160
6	-4.572873	-2.316855	-1.901344
6	-5.397514	-2.687519	-0.836196
1	-3.718706	-1.139478	1.692496
1	-2.781115	-1.254978	-2.485301
1	-5.730128	-2.552766	1.291113
1	-4.803769	-2.650057	-2.909572
1	-6.272089	-3.306923	-1.014464
6	-2.406490	1.652820	-0.231806
6	-2.764272	2.195344	-1.475560
6	-2.591203	2.417459	0.925177
6	-3.281755	3.487579	-1.557509
6	-3.114905	3.709373	0.843618
6	-3.458706	4.248009	-0.397034
1	-2.638392	1.608465	-2.380696
1	-2.300368	1.995583	1.881775
1	-3.552275	3.901232	-2.525153
1	-3.246685	4.297516	1.747727
1	-3.863243	5.254090	-0.462383
8	-1.281735	-0.278804	1.412041
19	0.176387	-1.976156	2.539471
6	-0.455256	-0.163497	-1.273089
6	0.895105	-0.754256	-1.016509
1	-0.435792	0.696840	-1.934544
6	0.984482	-2.240022	-0.670940

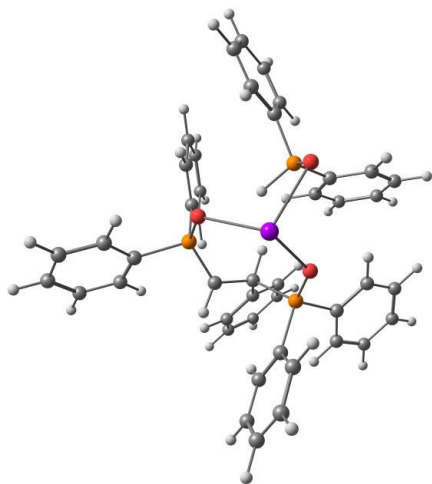
6	2.229548	-2.857033	-0.450215
6	-0.168211	-3.024800	-0.529643
6	2.313547	-4.193332	-0.061162
6	-0.089798	-4.366128	-0.136108
6	1.151809	-4.954033	0.113277
1	3.144414	-2.285915	-0.572283
1	-1.132882	-2.584620	-0.742188
1	3.288454	-4.642537	0.106705
1	-1.002741	-4.946210	-0.030745
1	1.217539	-5.993282	0.422100
15	1.950916	0.168792	0.314559
6	1.295143	1.858313	0.481393
6	1.081386	2.342317	1.776971
6	1.016599	2.682676	-0.617407
6	0.601650	3.637981	1.973879
6	0.528361	3.972805	-0.419551
6	0.321610	4.452950	0.876069
1	1.290656	1.692589	2.620094
1	1.169251	2.321058	-1.627603
1	0.437696	4.006446	2.982509
1	0.297566	4.599173	-1.275772
1	-0.065668	5.456153	1.026861
6	3.623441	0.384253	-0.398553
6	3.835917	0.836800	-1.709636
6	4.726067	0.052267	0.400527
6	5.132455	0.961981	-2.207898
6	6.022446	0.177402	-0.100322
6	6.227559	0.632752	-1.404531
1	2.994632	1.092707	-2.346321
1	4.551686	-0.307597	1.409550
1	5.288141	1.313349	-3.223719
1	6.871558	-0.080595	0.526194
1	7.236237	0.728650	-1.795556
8	2.070947	-0.496447	1.682979
1	1.507865	-0.599243	-1.913314

Int-TS-6-Ph-DA

E (BS1) = -3549.631274

E (BS2) = -3550.499054

G_{298.15} (BS2) = -3549.885681



15	0.670574	-2.296545	-0.139209
6	0.605631	-4.106055	0.169457
6	-0.107953	-4.650572	1.246404
6	1.315980	-4.965042	-0.679423
6	-0.118291	-6.028864	1.464549
6	1.308081	-6.344259	-0.462671
6	0.589801	-6.878239	0.609816
1	-0.657629	-3.986455	1.905624
1	1.863803	-4.532450	-1.510673
1	-0.677408	-6.441079	2.300126
1	1.859031	-7.002078	-1.129516
1	0.582105	-7.951285	0.779993
6	1.830437	-1.624595	1.124924

6	1.392606	-1.202922	2.388420
6	3.196328	-1.539020	0.818549
6	2.297804	-0.679048	3.314383
6	4.105436	-1.035621	1.748799
6	3.655936	-0.595043	2.995907
1	0.340063	-1.278459	2.637661
1	3.528066	-1.845320	-0.167510
1	1.942924	-0.339723	4.283794
1	5.157371	-0.962380	1.491272
1	4.360458	-0.186625	3.715058
8	1.394326	-2.107601	-1.491582
19	0.502066	-0.649982	-3.357344
6	-0.894440	-1.722668	0.223212
6	-1.219595	-0.301353	0.574967
1	-1.712236	-2.394141	-0.017930
6	-1.932760	-0.058196	1.900620
6	-2.618988	-1.085783	2.558744
6	-1.899217	1.209620	2.499625
6	-3.275698	-0.849040	3.768811
6	-2.543414	1.448441	3.713028
6	-3.242196	0.419926	4.350497
1	-2.614989	-2.078320	2.121029
1	-1.369978	2.017065	2.004911
1	-3.806329	-1.659603	4.260982
1	-2.500610	2.438077	4.159562
1	-3.747812	0.603911	5.294154
15	-2.073663	0.511750	-0.882066
6	-2.904936	2.059055	-0.390322
6	-2.254518	3.267093	-0.678431
6	-4.116486	2.079044	0.316685
6	-2.807963	4.478422	-0.261965
6	-4.666008	3.290611	0.731605
6	-4.011799	4.492191	0.445066
1	-1.318181	3.248956	-1.224994
1	-4.631901	1.152841	0.546061
1	-2.296732	5.408686	-0.488871
1	-5.603632	3.297635	1.279603
1	-4.441657	5.435361	0.769854
6	-3.398717	-0.603231	-1.451654
6	-4.265105	-1.281228	-0.581232
6	-3.544308	-0.774460	-2.835291
6	-5.255415	-2.121003	-1.090943
6	-4.536259	-1.614538	-3.342972
6	-5.391903	-2.290611	-2.470957
1	-4.162902	-1.165406	0.491397
1	-2.877596	-0.242656	-3.507253
1	-5.918435	-2.645721	-0.409405
1	-4.640552	-1.741440	-4.416716
1	-6.162743	-2.946692	-2.864441
8	-1.092337	0.800618	-2.008428
1	-0.299624	0.296891	0.596107
15	2.288051	1.437965	-1.278038
6	4.031525	1.396539	-0.764785
6	4.896537	0.558880	-1.484427
6	4.520276	2.125043	0.326517
6	6.233564	0.443295	-1.106910
6	5.860293	2.011471	0.698061
6	6.716320	1.169259	-0.014516
1	4.519596	0.002795	-2.337189
1	3.860198	2.776758	0.888560
1	6.898427	-0.209368	-1.664792
1	6.234836	2.580031	1.543964
1	7.758511	1.080855	0.277843
6	1.554808	2.902525	-0.512252
6	1.143812	2.849585	0.827733
6	1.428390	4.092199	-1.238706
6	0.625984	3.990426	1.440910
6	0.903505	5.228928	-0.622511
6	0.507637	5.179087	0.716532
1	1.233451	1.924356	1.390868
1	1.734534	4.121945	-2.279912
1	0.308243	3.949192	2.478149
1	0.802461	6.151660	-1.185810
1	0.098980	6.064487	1.193885
8	2.145033	1.328885	-2.783396

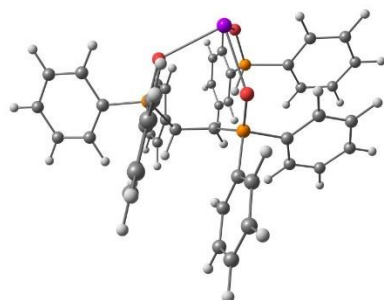
1 1.679696 0.393117 -0.562109

TS-6-Ph-DA

E (BS1) = -3549.628962

E (BS2) = -3550.492709

G_{298.15} (BS2) = -3549.879831



15	-0.123400	-1.888000	-0.105100
6	1.463600	-2.603500	-0.684100
6	2.274500	-3.250000	0.256500
6	1.869500	-2.562800	-2.025700
6	3.469100	-3.854400	-0.136300
6	3.067500	-3.159900	-2.417200
6	3.866900	-3.809900	-1.473200
1	1.952300	-3.272800	1.291300
1	1.245900	-2.074900	-2.768800
1	4.095700	-4.345200	0.601800
1	3.376000	-3.122000	-3.458100
1	4.800100	-4.274000	-1.778500
6	-1.356800	-2.988800	-0.918900
6	-1.762700	-2.732800	-2.236200
6	-1.869300	-4.104200	-0.250000
6	-2.659600	-3.585800	-2.879000
6	-2.766100	-4.961000	-0.889800
6	-3.159900	-4.703100	-2.204900
1	-1.375800	-1.856800	-2.750900
1	-1.565300	-4.285700	0.776300
1	-2.971200	-3.381000	-3.899500
1	-3.161800	-5.823800	-0.363500
1	-3.859800	-5.369200	-2.701400
8	-0.244900	-2.079800	1.411000
19	0.282100	-0.285900	3.170300
6	-0.102300	-0.268800	-0.705300
6	-1.291100	0.683600	-0.738100
1	0.449200	-0.210400	-1.649700
6	-0.821900	2.099300	-1.053700
6	-0.993100	2.616000	-2.343500
6	-0.204400	2.904200	-0.084300
6	-0.560700	3.905200	-2.662300
6	0.210500	4.198300	-0.395100
6	0.037300	4.703200	-1.685300
1	-1.470600	2.700000	-3.102100
1	-0.057600	2.513100	0.916600
1	-0.696900	4.286500	-3.670600
1	0.689300	4.804000	0.366300
1	0.373800	5.706600	-1.928700
15	-2.365400	0.741600	0.771800
6	-3.407100	-0.753100	0.777100
6	-3.514500	-1.471900	1.973700
6	-4.146900	-1.161700	-0.342200
6	-4.353200	-2.583400	2.052800
6	-4.987400	-2.269400	-0.260000
6	-5.092200	-2.981100	0.937600
1	-2.941800	-1.150400	2.836100
1	-4.067700	-0.624500	-1.280900
1	-4.428200	-3.138700	2.983300
1	-5.549500	-2.585200	-1.132900
1	-5.743600	-3.847900	0.997500
6	-3.515800	2.124500	0.457400
6	-4.161900	2.322600	-0.771400
6	-3.746100	3.019000	1.509500
6	-5.030000	3.399900	-0.939800

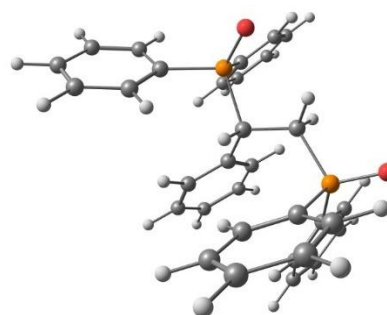
6	-4.617200	4.096100	1.339000
6	-5.260400	4.287100	0.115200
1	-3.982000	1.649700	-1.602500
1	-3.230100	2.866600	2.451800
1	-5.523000	3.550400	-1.895600
1	-4.789200	4.786800	2.159300
1	-5.936500	5.126300	-0.019300
8	-1.674900	0.939500	2.108400
1	-2.026200	0.416800	-1.519800
15	2.560500	0.903500	0.888800
6	3.088600	2.353100	-0.073700
6	3.540800	3.501200	0.588800
6	2.999500	2.347300	-1.471000
6	3.909000	4.628700	-0.142600
6	3.375700	3.475000	-2.201100
6	3.829000	4.618300	-1.537900
1	3.581700	3.507400	1.674100
1	2.613800	1.472700	-1.989800
1	4.254500	5.520100	0.373600
1	3.296600	3.469400	-3.284300
1	4.110100	5.498100	-2.106200
6	4.020700	-0.198300	0.845700
6	4.771600	-0.426100	-0.316900
6	4.397000	-0.832900	2.036500
6	5.880600	-1.272800	-0.282600
6	5.502600	-1.683900	2.068400
6	6.249400	-1.903100	0.909200
1	4.500400	0.061900	-1.247700
1	3.827100	-0.637800	2.939600
1	6.456400	-1.442500	-1.187900
1	5.785500	-2.167200	2.998600
1	7.112500	-2.559900	0.932000
8	2.213400	1.239500	2.339900
1	1.493200	0.343700	0.181400

DA-P-Ph

E (BS1) = -3549.670729

E (BS2) = -3550.529724

G_{298.15} (BS2) = -3549.913186



15	-2.490147	0.176303	-1.345908
6	-2.865768	1.398518	-0.046062
6	-3.287809	1.080884	1.249808
6	-2.711468	2.747662	-0.406093
6	-3.514810	2.094202	2.182481
6	-2.943054	3.757511	0.524584
6	-3.336714	3.431059	1.825141
1	-3.439673	0.048677	1.540349
1	-2.409312	3.005255	-1.416870
1	-3.832146	1.836503	3.188431
1	-2.816204	4.797116	0.237422
1	-3.510817	4.216995	2.554098
6	-2.966320	-1.480206	-0.750616
6	-2.524421	-2.057553	0.451414
6	-3.800438	-2.221308	-1.599730
6	-2.910452	-3.354257	0.791114
6	-4.184731	-3.518008	-1.256716
6	-3.738899	-4.086684	-0.062359
1	-1.890709	-1.501205	1.131429
1	-4.138348	-1.768973	-2.526380
1	-2.565095	-3.790445	1.723795

1	-4.830710	-4.083371	-1.921832
1	-4.036580	-5.096526	0.204274
8	-3.164024	0.520546	-2.653120
6	-0.663036	0.158493	-1.564852
6	0.220096	-0.428366	-0.453703
1	-0.377239	1.187453	-1.806708
6	0.218923	0.314623	0.863482
6	0.164874	1.714230	0.920283
6	0.294272	-0.398063	2.068645
6	0.162017	2.379831	2.144515
6	0.298472	0.265575	3.296531
6	0.228211	1.658784	3.338576
1	0.113596	2.291236	0.005600
1	0.349232	-1.481802	2.043948
1	0.104591	3.463694	2.163611
1	0.351757	-0.307660	4.217491
1	0.222356	2.178337	4.292167
15	1.929350	-0.661009	-1.175278
6	2.834135	-1.693251	0.021763
6	2.231810	-2.867432	0.503998
6	4.159950	-1.411266	0.380228
6	2.931316	-3.722691	1.353148
6	4.858634	-2.269603	1.230427
6	4.244454	-3.421559	1.723135
1	1.216826	-3.122267	0.215333
1	4.650246	-0.523300	-0.002463
1	2.452752	-4.623993	1.724117
1	5.883239	-2.037511	1.504966
1	4.788212	-4.086864	2.387196
6	2.700903	0.985092	-1.177442
6	3.113701	1.651228	-0.012374
6	2.808827	1.629878	-2.417632
6	3.629367	2.944018	-0.093401
6	3.319998	2.926013	-2.493728
6	3.729497	3.583260	-1.331897
1	3.033458	1.165201	0.952901
1	2.493630	1.104870	-3.313611
1	3.948053	3.453596	0.810910
1	3.400681	3.419837	-3.457443
1	4.128422	4.591735	-1.390564
8	1.855941	-1.261429	-2.560344
1	-0.109285	-1.455997	-0.274882
1	-0.513532	-0.426595	-2.477784

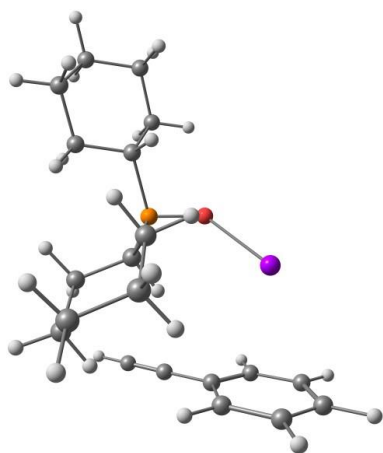
R = Cy

Int-TS-1-Cy

E (BS1) = -1795.638674

E (BS2) = -1796.015867

G_{298.15} (BS2) = -1795.637637



15	-1.261667	-0.601704	0.942070
8	-0.546839	-1.867599	0.305409
19	1.410279	-1.892556	-1.126141
6	2.267125	1.206068	2.987280

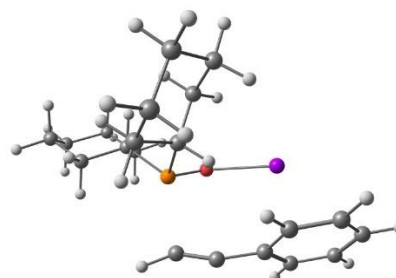
6	2.871826	0.650343	2.097985
1	1.733168	1.692375	3.774293
6	3.567483	-0.004302	1.035571
6	4.018773	-1.332594	1.187642
6	3.787823	0.662476	-0.188530
6	4.675626	-1.975219	0.135865
6	4.441722	0.010516	-1.235580
6	4.888152	-1.308165	-1.078202
1	3.846326	-1.848153	2.126580
1	3.440083	1.682758	-0.307419
1	5.022804	-2.995975	0.264176
1	4.605539	0.532596	-2.173441
1	5.401240	-1.810477	-1.892579
6	-0.354534	0.861009	0.114012
6	-0.503017	2.214873	0.822763
6	0.476667	3.250574	0.249595
6	0.326283	3.395144	-1.271833
6	0.439540	2.041262	-1.987324
6	-0.554595	1.030792	-1.397926
1	0.694085	0.560947	0.278214
1	-0.336002	2.091145	1.899285
1	-1.528270	2.588916	0.707362
1	0.332999	4.224638	0.734534
1	1.501167	2.931680	0.485394
1	1.072422	4.097591	-1.663612
1	-0.659263	3.828513	-1.494263
1	0.270955	2.166698	-3.065039
1	1.462244	1.653638	-1.869080
1	-0.478780	0.063917	-1.916703
1	-1.574748	1.385840	-1.592633
6	-2.926086	-0.537595	0.041962
6	-3.762816	0.704019	0.380509
6	-5.150973	0.670034	-0.277942
6	-5.911076	-0.617187	0.063633
6	-5.084766	-1.857639	-0.298657
6	-3.706606	-1.820410	0.374019
1	-2.719954	-0.545371	-1.039663
1	-3.239554	1.615112	0.072845
1	-3.882868	0.769332	1.472148
1	-5.735389	1.548799	0.024189
1	-5.029782	0.734529	-1.369023
1	-6.880443	-0.636251	-0.450129
1	-6.125678	-0.632445	1.141915
1	-5.624292	-2.770440	-0.014313
1	-4.954272	-1.896543	-1.390013
1	-3.106769	-2.690063	0.085111
1	-3.841851	-1.882400	1.465174

TS-1-Cy

E (BS1) = -1795.628637

E (BS2) = -1796.003573

G_{298.15} (BS2) = -1795.625153

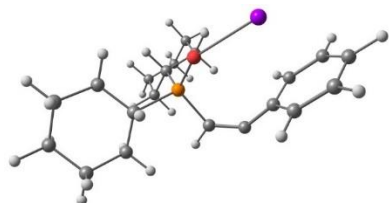


15	0.898271	0.623453	0.259338
8	0.226871	1.386019	-0.937493
19	-2.041217	0.960566	-1.785519
6	-0.584522	0.976690	2.347977
6	-1.781829	0.927697	2.026147
1	0.161453	1.071314	3.109858
6	-2.967110	0.832144	1.266891
6	-3.631157	1.997863	0.791888
6	-3.530531	-0.431184	0.931591
6	-4.781921	1.897233	0.011242

6	-4.677371	-0.514395	0.144485
6	-5.313094	0.643645	-0.327780
1	-3.224965	2.972301	1.044787
1	-3.048133	-1.333772	1.292568
1	-5.267357	2.804549	-0.338153
1	-5.080859	-1.492594	-0.103129
1	-6.209003	0.571415	-0.936001
6	0.298818	-1.152607	0.046449
6	0.786592	-2.153631	1.100925
6	0.053899	-3.497110	0.960514
6	0.190850	-4.069636	-0.457577
6	-0.252706	-3.058647	-1.524781
6	0.495309	-1.728184	-1.362668
1	-0.784931	-1.036101	0.207179
1	0.642400	-1.746026	2.108561
1	1.864288	-2.321737	0.975399
1	0.432702	-4.217796	1.695909
1	-1.011133	-3.346063	1.188335
1	-0.383578	-4.999467	-0.549760
1	1.243439	-4.331756	-0.636070
1	-0.091129	-3.472108	-2.528582
1	-1.333599	-2.877607	-1.425825
1	0.177133	-1.000529	-2.120163
1	1.565247	-1.899717	-1.541551
6	2.746564	0.471934	-0.135906
6	3.567862	0.168847	1.128221
6	5.071008	0.089605	0.824259
6	5.571883	1.370526	0.144894
6	4.750155	1.693311	-1.110135
6	3.249510	1.763704	-0.796354
1	2.885213	-0.352047	-0.851735
1	3.231662	-0.761526	1.598214
1	3.389907	0.967268	1.863158
1	5.635194	-0.096972	1.746843
1	5.258735	-0.767770	0.162142
1	6.635764	1.278961	-0.106714
1	5.486813	2.207188	0.853056
1	5.090254	2.638155	-1.553299
1	4.923055	0.912160	-1.864439
1	2.667778	1.963627	-1.701306
1	3.064485	2.609101	-0.116216

Z-1I-Cy

E (BS1) = -1795.670173
E (BS2) = -1796.048476
G_{298.15} (BS2) = -1795.663951

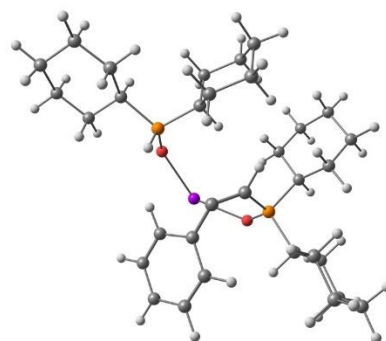


1			
5	-0.527365	0.206809	-0.034299
8	0.457386	0.552444	-1.153768
19	2.803793	0.608795	-1.877095
6	0.158235	0.215549	1.646169
6	1.443638	0.311581	2.004447
1	-0.624121	0.090053	2.402337
6	2.643078	0.463619	1.275767
6	3.443139	-0.663469	0.889021
6	3.216798	1.751594	1.008922
6	4.701940	-0.507962	0.316586
6	4.475906	1.888809	0.434382
6	5.244200	0.766684	0.071668
1	3.056227	-1.661856	1.073217
1	2.650383	2.637483	1.283001
1	5.270309	-1.395930	0.046994
1	4.866588	2.888660	0.256541
1	6.232697	0.881160	-0.360965
6	-1.929999	1.413866	-0.086076
6	-2.700812	1.631595	1.228921

6	-3.747678	2.743587	1.069623
6	-4.701450	2.465566	-0.098450
6	-3.928172	2.251314	-1.405191
6	-2.888544	1.132546	-1.258490
1	-1.392143	2.347693	-0.309308
1	-2.004482	1.888942	2.032385
1	-3.203518	0.703801	1.527557
1	-4.310641	2.858800	2.003503
1	-3.230386	3.697065	0.893104
1	-5.416700	3.289182	-0.209580
1	-5.289999	1.563836	0.122944
1	-4.618308	2.014331	-2.223892
1	-3.416752	3.183954	-1.681335
1	-2.321638	1.016344	-2.189000
1	-3.411318	0.184020	-1.080496
6	-1.195538	-1.490780	-0.327532
6	-2.206829	-1.973026	0.727160
6	-2.694892	-3.395507	0.418193
6	-1.524393	-4.377609	0.292261
6	-0.514034	-3.900284	-0.757749
6	-0.021236	-2.479752	-0.456113
1	-1.702588	-1.436521	-1.300974
1	-3.061413	-1.291489	0.778238
1	-1.729865	-1.962172	1.715222
1	-3.389324	-3.726997	1.199375
1	-3.260993	-3.383986	-0.523906
1	-1.892972	-5.378884	0.039349
1	-1.019346	-4.461920	1.264703
1	0.339503	-4.587405	-0.806181
1	-0.988955	-3.914404	-1.748959
1	0.663412	-2.138563	-1.239945
1	0.545530	-2.481508	0.484388

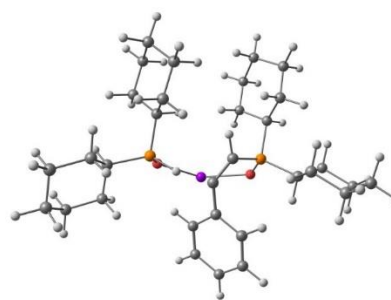
Int-TS-2-Cy

E (BS1) = -2683.562950
E (BS2) = -2684.164424
G_{298.15} (BS2) = -2683.461450



15	-2.408166	-0.009132	0.474350
8	-2.133874	-0.755229	1.786569
19	0.167808	-1.456793	2.512202
6	-1.101768	-0.135462	-0.785338
6	-0.428939	-1.233685	-1.192365
1	-0.896964	0.833100	-1.252800
6	-0.665120	-2.576369	-0.718694
6	0.320291	-3.282498	0.031162
6	-1.826489	-3.317616	-1.073200
6	0.119191	-4.593946	0.458296
6	-2.007063	-4.636135	-0.663632
6	-1.048939	-5.288739	0.120879
1	1.259896	-2.785731	0.259297
1	-2.582813	-2.840664	-1.688611
1	0.894765	-5.085991	1.042231
1	-2.914765	-5.160597	-0.954889
1	-1.197729	-6.315422	0.441436
6	-4.000863	-0.628178	-0.233292
6	-4.211520	-0.390191	-1.737853
6	-5.486394	-1.095286	-2.220608
6	-6.713593	-0.653412	-1.412695
6	-6.498784	-0.866902	0.091062

6	-5.223103	-0.166749	0.580061
1	-3.886730	-1.710962	-0.083042
1	-3.340752	-0.742036	-2.298667
1	-4.299348	0.683995	-1.938628
1	-5.641645	-0.898178	-3.288137
1	-5.356291	-2.181604	-2.115132
1	-7.606249	-1.194094	-1.749321
1	-6.901519	0.413405	-1.600638
1	-7.365879	-0.503174	0.655659
1	-6.415849	-1.943269	0.295878
1	-5.064990	-0.366868	1.645455
1	-5.347055	0.918622	0.470740
6	-2.592716	1.794374	0.846312
6	-2.952484	2.693542	-0.349845
6	-3.068132	4.165067	0.073561
6	-1.792614	4.657276	0.766053
6	-1.443115	3.770820	1.967112
6	-1.321446	2.298805	1.556295
1	-3.419476	1.838717	1.569233
1	-3.893925	2.367364	-0.800290
1	-2.182732	2.602839	-1.126473
1	-3.291551	4.785391	-0.802562
1	-3.917376	4.273429	0.762779
1	-1.908689	5.700471	1.082994
1	-0.960842	4.635888	0.048054
1	-0.506753	4.105490	2.430027
1	-2.227305	3.869541	2.730566
1	-1.118266	1.674888	2.433427
1	-0.466247	2.188959	0.879260
15	2.926796	-0.285936	0.166748
8	2.414328	-0.805603	1.506446
6	2.214180	1.347272	-0.257444
6	2.036891	1.593577	-1.765950
6	1.304053	2.921808	-1.999778
6	2.023054	4.092539	-1.316990
6	2.212818	3.835618	0.183404
6	2.941976	2.509917	0.440526
1	1.209478	1.261190	0.175286
1	1.477566	0.762854	-2.208585
1	3.014206	1.629132	-2.260920
1	1.206238	3.108002	-3.075521
1	0.284432	2.839989	-1.599690
1	1.464473	5.023235	-1.472135
1	3.007144	4.233573	-1.785990
1	2.768160	4.660510	0.645033
1	1.230466	3.802820	0.671036
1	3.013515	2.320876	1.518036
1	3.968016	2.582314	0.058578
6	4.757634	-0.257842	0.105254
6	5.313029	0.171887	-1.264653
6	6.846966	0.105866	-1.287508
6	7.363537	-1.280519	-0.887424
6	6.816948	-1.696630	0.483062
6	5.284699	-1.649472	0.511931
1	5.072360	0.472011	0.863871
1	4.986221	1.186886	-1.507753
1	4.907641	-0.489605	-2.042224
1	7.210727	0.377693	-2.285198
1	7.245987	0.855359	-0.589987
1	8.459780	-1.288719	-0.879168
1	7.046586	-2.015500	-1.640460
1	7.160233	-2.704792	0.742993
1	7.211841	-1.018661	1.252510
1	4.907387	-1.911831	1.504723
1	4.887388	-2.397487	-0.189175
1	2.572696	-1.114023	-0.921738



15	-2.403263	-0.078970	0.466559
8	-2.218270	-0.742224	1.835855
19	0.098684	-0.868008	2.888732
6	-0.929404	-0.128244	-0.585853
6	-0.066045	-1.153552	-0.759193
1	-0.698577	0.840585	-1.037985
6	-0.252354	-2.507402	-0.274662
6	0.657725	-3.088785	0.650144
6	-1.267047	-3.353588	-0.789414
6	0.518461	-4.411635	1.070432
6	-1.386394	-4.678235	-0.377507
6	-0.504648	-5.219785	0.565096
1	1.474197	-2.486936	1.039676
1	-1.953475	-2.956533	-1.530541
1	1.225174	-4.816602	1.791451
1	-2.180989	-5.294266	-0.792012
1	-0.605395	-6.251799	0.887506
6	-3.826693	-0.865508	-0.406747
6	-3.845125	-0.708599	-1.936787
6	-4.983627	-1.536815	-2.547816
6	-6.340441	-1.164292	-1.936091
6	-6.319545	-1.296800	-0.408044
6	-5.180993	-0.473884	0.210737
1	-3.648720	-1.927351	-0.184459
1	-2.881147	-1.010600	-2.357061
1	-3.986791	0.345201	-2.203675
1	-5.004528	-1.397711	-3.635285
1	-4.786664	-2.603159	-2.368639
1	-7.134067	-1.790579	-2.360631
1	-6.581257	-0.125450	-2.203283
1	-7.281074	-0.982403	0.015347
1	-6.183997	-2.353102	-0.137581
1	-5.156784	-0.616208	1.296655
1	-5.369951	0.592267	0.029340
6	-2.759626	1.719599	0.711607
6	-3.013263	2.526760	-0.574104
6	-3.259296	4.010650	-0.265087
6	-2.109172	4.618083	0.545063
6	-1.874541	3.829659	1.838203
6	-1.626601	2.343855	1.552203
1	-3.676424	1.740366	1.317089
1	-3.872338	2.117280	-1.112731
1	-2.149438	2.439437	-1.244671
1	-3.402231	4.563210	-1.201198
1	-4.193372	4.107946	0.305787
1	-2.316994	5.670165	0.772959
1	-1.191746	4.600909	-0.060228
1	-1.024080	4.245578	2.392058
1	-2.755870	3.929363	2.486932
1	-1.529163	1.794655	2.495177
1	-0.675684	2.235661	1.015018
15	2.570375	0.004215	0.250543
8	2.280256	-0.256538	1.749373
6	2.292550	1.801043	-0.101679
6	2.025316	2.131199	-1.580276
6	1.601477	3.598376	-1.735187
6	2.640504	4.549764	-1.126689
6	2.929177	4.205749	0.340829
6	3.350328	2.737839	0.500390
1	1.351661	1.974168	0.442261
1	1.255364	1.465940	-1.985800
1	2.931635	1.958069	-2.172016

TS-2-Cy

E (BS1) = -2683.554452

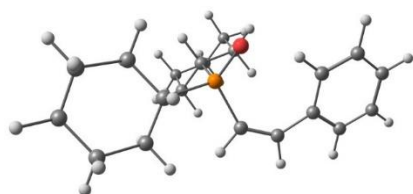
E (BS2) = -2684.151106

G_{298.15} (BS2) = -2683.452865

1	1.442289	3.835422	-2.793975
1	0.636680	3.746552	-1.230056
1	2.300138	5.588667	-1.212727
1	3.574144	4.475228	-1.702161
1	3.706234	4.868428	0.740924
1	2.023581	4.383279	0.938384
1	3.505745	2.497504	1.558316
1	4.310594	2.580188	-0.008789
6	4.343300	-0.410846	-0.098411
6	4.742714	-0.225359	-1.571712
6	6.187029	-0.681148	-1.827822
6	6.418877	-2.124478	-1.366710
6	6.042116	-2.295797	0.109354
6	4.596280	-1.857680	0.369233
1	4.949573	0.264088	0.523350
1	4.634227	0.822785	-1.866093
1	4.059590	-0.805477	-2.207358
1	6.424686	-0.576476	-2.893320
1	6.872790	-0.015538	-1.284800
1	7.464019	-2.412846	-1.531418
1	5.803580	-2.801411	-1.976058
1	6.177394	-3.338799	0.420517
1	6.719401	-1.690445	0.728331
1	4.349340	-1.944788	1.431763
1	3.912844	-2.529711	-0.170008
1	1.452087	-0.692037	-0.649529

Z-P-Cy

(BS1) = -1196.363198
E (BS2) = -1196.698773
G_{298.15} (BS2) = -1196.296344



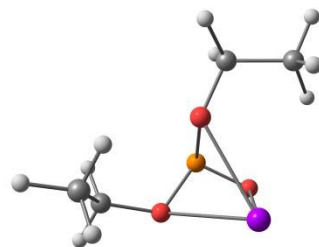
15	-0.488911	0.494467	-0.431220
8	0.103860	1.011609	-1.728956
6	0.368231	0.949235	1.103127
6	1.667460	1.146435	1.413312
1	-0.311104	1.009435	1.949817
6	2.912709	1.121099	0.635230
6	4.115791	1.138118	1.368886
6	2.987408	1.080295	-0.770718
6	5.352423	1.095488	0.729523
6	4.226851	1.043857	-1.405573
6	5.412183	1.046277	-0.664463
1	4.072300	1.178025	2.454162
1	2.072332	1.091116	-1.354948
1	6.265834	1.103602	1.317072
1	4.268139	1.016268	-2.490957
1	6.373287	1.016114	-1.169613
6	-2.214881	1.144213	-0.245149
6	-2.806978	1.280378	1.169464
6	-4.208938	1.906977	1.119305
6	-5.151565	1.133165	0.191212
6	-4.558197	1.013841	-1.216843
6	-3.167853	0.368084	-1.178289
1	-2.102118	2.158357	-0.655008
1	-2.159612	1.904170	1.792530
1	-2.866775	0.297147	1.650839
1	-4.624262	1.957607	2.132742
1	-4.122300	2.942196	0.761188
1	-6.131781	1.622711	0.152657
1	-5.316388	0.125947	0.599524
1	-5.220829	0.427451	-1.864307
1	-4.479621	2.013933	-1.664829
1	-2.745620	0.316634	-2.187571
1	-3.267329	-0.663599	-0.817959
6	-0.525946	-1.350523	-0.399545

6	-1.112512	-1.965479	0.883035
6	-1.098427	-3.499354	0.817143
6	0.308831	-4.040339	0.539489
6	0.893123	-3.426554	-0.738125
6	0.889476	-1.894196	-0.676282
1	-1.168332	-1.625452	-1.247492
1	-2.135389	-1.612807	1.045193
1	-0.518835	-1.634340	1.744831
1	-1.489937	-3.912877	1.754185
1	-1.777008	-3.829231	0.018135
1	0.287135	-5.133890	0.462710
1	0.962907	-3.795269	1.388158
1	1.915339	-3.787343	-0.902916
1	0.298703	-3.754014	-1.602479
1	1.273176	-1.470635	-1.608675
1	1.562582	-1.563487	0.124866
1	1.853137	1.346252	2.469633

R = OEt

Int-TS-1-OEt

E (BS1) = -1633.983391
E (BS2) = -1634.340953
G_{298.15} (BS2) = -1634.137092



15	-2.232119	0.437099	1.190290
8	-1.722510	-0.941384	1.634684
19	-0.258189	-1.137448	-0.572047
6	2.913482	2.993156	-0.084401
6	2.940689	1.783652	-0.036352
1	2.893052	4.060543	-0.124215
6	2.957736	0.355540	0.014019
6	2.711463	-0.318509	1.228220
6	3.199594	-0.395435	-1.155760
6	2.710933	-1.713511	1.267839
6	3.196793	-1.791059	-1.106361
6	2.953293	-2.454088	0.103698
1	2.510632	0.257449	2.124997
1	3.388665	0.122119	-2.090651
1	2.516297	-2.222763	2.206587
1	3.389348	-2.360627	-2.010563
1	2.954509	-3.539268	0.139468
8	-0.748940	1.194303	0.745783
6	-0.804232	2.524171	0.223140
1	-0.018198	3.104679	0.720494
1	-1.766777	2.992257	0.475865
6	-0.597264	2.547601	-1.285170
1	-1.392495	1.985990	-1.782217
1	0.371544	2.109134	-1.549152
1	-0.606805	3.579525	-1.656289
8	-2.655645	0.210354	-0.503887
6	-3.951477	-0.342459	-0.729787
1	-4.639786	-0.037883	0.074458
1	-4.337860	0.089402	-1.661553
6	-3.918725	-1.863992	-0.824638
1	-4.924883	-2.264858	-0.995525
1	-3.284328	-2.189413	-1.658983

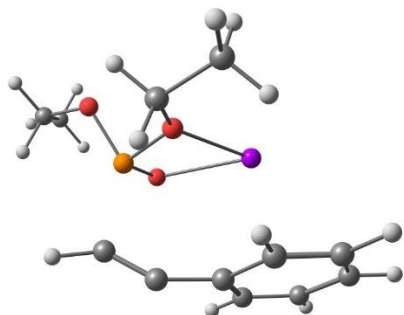
1 -3.522492 -2.287848 0.102521

TS-1-OEt

E (BS1) = -1633.959793

E (BS2) = -1634.317959

G_{298.15} (BS2) = -1634.112005



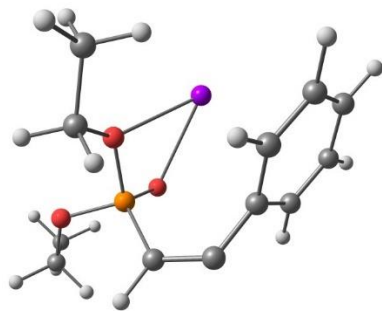
15	-1.541705	-0.243476	0.320716
8	-1.107366	-1.369335	-0.620850
19	0.830190	-0.319999	-1.970010
6	-0.400764	-0.369555	2.367389
6	0.839756	-0.421591	2.175687
1	-1.160141	-0.373118	3.126779
6	1.946492	-0.449751	1.292399
6	2.418923	-1.674069	0.747349
6	2.607598	0.745369	0.901897
6	3.484130	-1.692181	-0.153423
6	3.666021	0.713552	-0.004612
6	4.115034	-0.501581	-0.543765
1	1.930519	-2.599805	1.034458
1	2.267917	1.691243	1.310830
1	3.822709	-2.643133	-0.556436
1	4.147352	1.644578	-0.292599
1	4.945677	-0.521141	-1.242462
8	-0.674695	1.067715	-0.314335
6	-0.771503	2.343424	0.328262
1	-0.411601	2.262060	1.361877
1	-1.821442	2.657735	0.358687
6	0.061882	3.343261	-0.451966
1	-0.302260	3.431241	-1.481387
1	1.112987	3.037857	-0.478171
1	0.004748	4.331734	0.016746
8	-3.051715	0.372971	-0.142633
6	-4.201274	-0.319802	0.360874
1	-3.992017	-0.726040	1.362311
1	-4.995055	0.427369	0.473529
6	-4.643531	-1.435948	-0.573701
1	-3.852511	-2.184539	-0.673854
1	-5.545814	-1.924255	-0.187425
1	-4.865477	-1.037230	-1.569233

Z-1i-OEt

E (BS1) = -1633.988705

E (BS2) = -1634.353343

G_{298.15} (BS2) = -1634.144131



15 -1.341607 -0.128899 0.140848

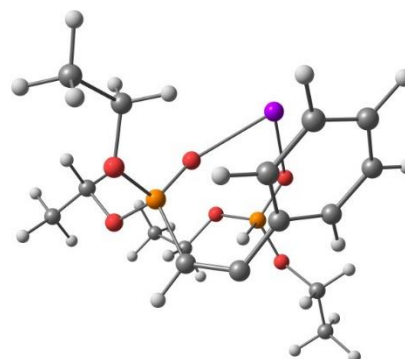
8	-0.975765	-1.107364	-0.945372
19	1.091726	0.054166	-2.059251
6	-0.846903	-0.503911	1.820611
6	0.428695	-0.728335	2.193806
1	-1.677601	-0.507255	2.532107
6	1.564974	-0.706482	1.319948
6	2.026332	-1.875357	0.644140
6	2.350700	0.473265	1.151264
6	3.175413	-1.856326	-0.144752
6	3.495674	0.482059	0.355665
6	3.926194	-0.679046	-0.308735
1	1.458404	-2.795444	0.747909
1	2.043310	1.381868	1.661234
1	3.488438	-2.770291	-0.645086
1	4.060910	1.405929	0.251569
1	4.827114	-0.672806	-0.914527
8	-0.665775	1.286219	-0.331134
6	-0.702846	2.465728	0.508012
1	-0.400645	2.188463	1.522649
1	-1.731559	2.838621	0.538965
6	0.238405	3.491452	-0.087252
1	-0.059295	3.748285	-1.109300
1	1.265697	3.113789	-0.100435
1	0.218509	4.405695	0.514823
8	-2.909884	0.296240	0.184059
6	-3.897908	-0.737263	0.440381
1	-3.469162	-1.513316	1.085201
1	-4.698256	-0.244033	0.998260
6	-4.410117	-1.331134	-0.857949
1	-3.597041	-1.820435	-1.400447
1	-5.188867	-2.071859	-0.645672
1	-4.838931	-0.551548	-1.495460

Int-TS-2-OEt

E (BS1) = -2360.188025

E (BS2) = -2360.765878

G_{298.15} (BS2) = -2360.415248



15	-1.173621	1.173990	-0.576139
8	-0.829518	0.578934	0.766441
19	-0.721497	-1.510110	2.172021
6	-0.618055	0.334111	-2.056339
6	-0.586596	-1.000725	-2.250860
1	-0.314864	1.043736	-2.831804
6	-1.079946	-1.969629	-1.309264
6	-0.223552	-2.948410	-0.727112
6	-2.466148	-2.076886	-0.993742
6	-0.712813	-3.934508	0.126945
6	-2.950597	-3.077306	-0.152033
6	-2.083342	-4.015043	0.429643
1	0.835702	-2.923039	-0.964640
1	-3.154148	-1.361264	-1.434155
1	-0.021294	-4.657824	0.553851
1	-4.016513	-3.122014	0.061022
1	-2.463637	-4.798706	1.077791
15	2.260207	-0.327268	0.644786
8	1.834427	-1.193031	1.787833
1	1.362528	-0.264925	-0.424464
8	-0.551579	2.659152	-0.798607

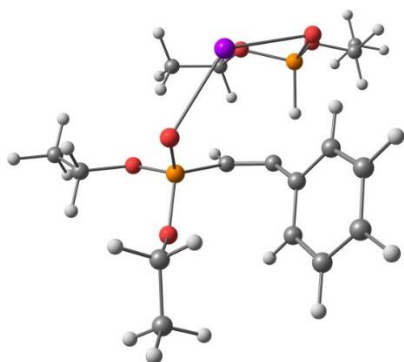
6	-0.792254	3.668629	0.210563
1	-0.269914	3.380452	1.128531
1	-1.866748	3.713857	0.422146
6	-0.294194	4.995234	-0.321767
1	-0.838650	5.276899	-1.228140
1	0.772501	4.946529	-0.558461
1	-0.444732	5.776759	0.430245
8	-2.781709	1.447139	-0.677220
6	-3.663430	1.053719	0.399302
1	-3.405021	1.612072	1.305172
1	-3.531613	-0.013562	0.605332
6	-5.083473	1.346802	-0.037274
1	-5.338706	0.779271	-0.937514
1	-5.214328	2.412085	-0.251166
1	-5.780975	1.065710	0.759013
8	2.549610	1.175287	1.111577
6	2.802392	2.191261	0.097061
1	1.940628	2.239142	-0.576167
1	3.688384	1.901156	-0.475763
6	3.016711	3.508196	0.809372
1	3.872455	3.446998	1.488602
1	2.131327	3.789742	1.386494
1	3.216268	4.293982	0.074049
8	3.651786	-0.740215	-0.059809
6	3.636940	-1.856291	-0.993619
1	2.794371	-1.734849	-1.685129
1	3.495301	-2.784030	-0.429142
6	4.953287	-1.860148	-1.738566
1	5.792063	-1.972930	-1.045164
1	5.083405	-0.929805	-2.299530
1	4.972148	-2.696361	-2.444700

TS-2-OEt

E (BS1) = -2360.180643

E (BS2) = -2360.751991

G_{298.15} (BS2) = -2360.404602



15	-1.889277	0.799148	-0.185676
8	-1.809522	0.512545	1.295763
19	0.495243	0.190500	2.401095
6	-0.441817	0.379512	-1.148532
6	0.185373	-0.819206	-1.180494
1	-0.006062	1.259650	-1.626887
6	-0.416391	-2.025450	-0.621265
6	0.214004	-2.773182	0.405710
6	-1.613683	-2.556012	-1.160990
6	-0.356866	-3.946421	0.897264
6	-2.161304	-3.745505	-0.683846
6	-1.547380	-4.446229	0.358721
1	1.158097	-2.424268	0.815968
1	-2.106373	-2.015974	-1.962529
1	0.143282	-4.484959	1.699005
1	-3.081453	-4.122679	-1.123685
1	-1.979761	-5.368615	0.734985
15	2.877245	-0.098377	0.176661
8	2.791777	-0.895601	1.456118
1	1.891271	-0.564410	-0.880331
8	-2.027734	2.381830	-0.528800
6	-3.125044	3.125600	0.052142

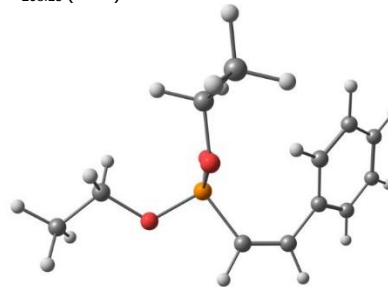
1	-3.154941	2.938445	1.131172
1	-4.061975	2.767018	-0.388454
6	-2.906311	4.594426	-0.242130
1	-2.860438	4.771410	-1.321052
1	-1.973389	4.946884	0.208728
1	-3.733276	5.182232	0.169527
8	-3.241022	0.172174	-0.832356
6	-4.152564	-0.614114	-0.023851
1	-4.615785	0.034888	0.726321
1	-3.592869	-1.396415	0.494516
6	-5.191578	-1.207953	-0.950383
1	-4.723701	-1.862553	-1.691520
1	-5.740381	-0.422166	-1.478975
1	-5.907760	-1.799125	-0.369977
8	2.364877	1.406772	0.568919
6	2.359821	2.459031	-0.427434
1	2.081716	2.042898	-1.402417
1	3.375160	2.859496	-0.504099
6	1.373475	3.521960	0.008175
1	1.641297	3.914783	0.994789
1	0.356043	3.123601	0.044764
1	1.387589	4.352849	-0.705123
8	4.383534	0.228397	-0.349348
6	5.135858	-0.857993	-0.952942
1	4.477372	-1.436235	-1.613263
1	5.491237	-1.520161	-0.156463
6	6.288773	-0.258434	-1.728236
1	6.936264	0.327339	-1.068485
1	5.921623	0.393134	-2.527001
1	6.886615	-1.057250	-2.178916

Z-P-OEt

E (BS1) = -1034.677712

E (BS2) = -1035.001173

G_{298.15} (BS2) = -1034.776654



15	1.108032	-0.385715	0.115834
8	0.684650	-0.277425	1.541900
6	0.196595	-1.480780	-0.970654
6	-1.136547	-1.633801	-1.077270
1	0.834227	-2.157904	-1.533114
6	-2.221044	-0.863820	-0.456750
6	-3.442617	-1.511958	-0.200966
6	-2.102838	0.499451	-0.136641
6	-4.498062	-0.831005	0.401516
6	-3.162574	1.182615	0.453962
6	-4.359615	0.518671	0.734589
1	-3.552489	-2.559996	-0.465885
1	-1.194809	1.029870	-0.390096
1	-5.429983	-1.350092	0.604884
1	-3.056917	2.237898	0.687801
1	-5.183942	1.053135	1.197315
1	-1.476801	-2.459609	-1.701928
8	2.584486	-1.006466	-0.124784
6	3.724852	-0.323976	0.454732
1	3.505025	-0.073656	1.497886
1	3.891704	0.605757	-0.100964
6	4.923081	-1.243217	0.355379
1	5.129442	-1.501165	-0.687916
1	4.750297	-2.166575	0.916337
1	5.805920	-0.745576	0.769559
8	1.149092	1.046459	-0.654132
6	1.187274	2.284993	0.105005

1	2.205509	2.435779	0.479788
1	0.517241	2.198343	0.964646
6	0.772282	3.409693	-0.818883
1	-0.250568	3.263857	-1.180110
1	1.439873	3.471998	-1.683666
1	0.815247	4.361924	-0.280032