

Making Endo-Dig Cyclizations Favorable Again: Conceptually New Synthetic Approach to Benzotriazoles via Azide Group Directed Lithiation/Cyclization of 2-Azidoaryl Bromides

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Supporting information
Theoretical part

Table of contents

Ph-N ₃ -Li(THF) ₃	6
R _{N3}	6
TS _{1-5-N3}	8
P _{1-5-N3}	10
TS _{1-4-N3}	12
P _{1-4-N3}	14
Ph-N ₃ -anion.....	16
R _{N3-a}	16
TS _{1-5-N3-a}	17
P _{1-5-N3-a}	18
Ph-N ₃ + Ph-Li(THF) ₃	19
Ph-N ₃	19
Ph-Li(THF) ₃	20
TS _{N3-inter}	22
P _{N3-inter}	24
Ph-C(Me)=N ₂ -Li(THF) ₃	26
R _{CN2}	26
TS _{1-5-CN2}	28
P _{1-5-CN2}	30
Ph-C(Me)=N ₂ -anion	32
R _{CN2-a}	32
TS _{1-5-CN2-a}	33
P _{1-5-CN2-a}	34
Ph-CH ₂ -NC-Li(THF) ₃	35
R _{CNC}	35
TS _{1-5-CNC-C}	37
P _{1-5-CNC-C}	39
TS _{1-5-CNC-CN}	41
P _{1-5-CNC-CN}	43
TS _{1-5-CNC-N}	45

P ₁₋₅ -CNC-N	47
Ph-CH ₂ -NC-anion	49
R _{CNC-a}	49
TS ₁₋₅ -CNC-C-a.....	50
R _{CNC-C-a}	51
TS ₁₋₅ -CNC-CN-a.....	52
R _{CNC-CN-a}	53
TS ₁₋₅ -CNC-N-a	54
R _{CNC-N-a}	55
Ph-NCO-Li(THF) ₃	56
R _{NCO}	56
P ₁₋₅ -NCO.....	58
TS ₁₋₄ -NCO	60
P ₁₋₄ -NCO.....	62
Ph-NCO-anion.....	64
R _{NCO-a}	64
P ₁₋₅ -NCO-a	65
TS ₁₋₄ -NCO-a	66
P ₁₋₄ -NCO-a	67
Ph-NCS-Li(THF) ₃	68
R _{NCS}	68
TS ₁₋₅ -NCS.....	70
P ₁₋₅ -NCS	72
TS ₁₋₄ -NCS.....	74
P ₁₋₄ -NCS	76
Ph-NCS-anion	78
R _{NCS-a}	78
P ₁₋₅ -NCS-a	79
TS ₁₋₄ -NCS-a	80
P ₁₋₄ -NCS-a	81
Ph-OCN-Li(THF) ₃	82

R _{OCN}	82
TS _{1-5-OCN}	84
P _{1-5-OCN}	86
TS _{1-4-OCN}	88
P _{1-4-OCN}	90
Ph-OCN-anion.....	92
R _{OCN-a}	92
TS _{1-5-OCN-a}	93
P _{1-5-OCN-a}	94
TS _{1-4-OCN-a}	95
P _{1-4-OCN-a}	96
Ph-SCN-Li(THF) ₃	97
R _{SCN}	97
TS _{1-5-SCN}	99
P _{1-5-SCN}	101
TS _{1-4-SCN}	103
P _{1-4-SCN}	105
Ph-SCN-anion	107
R _{SCN-a}	107
TS _{1-5-SCN-a}	108
P _{1-5-SCN-a}	109
TS _{1-4-SCN-a}	110
P _{1-4-SCN-a}	111
Ph-CH ₂ -CN-Li(THF) ₃	112
R _{CCN}	112
TS _{1-5-CCN-C}	114
P _{1-5-CCN-C}	116
TS _{1-5-CCN-N}	118
P _{1-5-CCN-N}	120
TS _{1-4-CCN}	122
P _{1-4-CCN}	124
TS _{1-4-CCN-B}	126

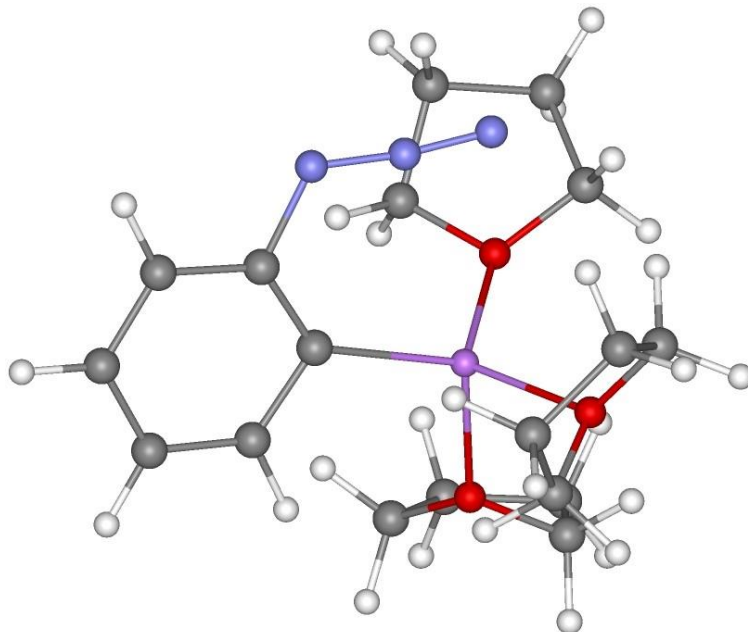
P ₁₋₄ -CCN-B	128
Ph-CH ₂ -CN-anion	130
R _{CCN} -a.....	130
TS ₁₋₅ -CCN-C-a.....	131
P ₁₋₅ -CCN-C-a.....	132
TS ₁₋₅ -CCN-N-a	133
P ₁₋₅ -CCN-N-a.....	134
TS ₁₋₄ -CCN-a	135
P ₁₋₄ -CCN-a.....	136
TS ₁₋₄ -CCN-B-a.....	137
P ₁₋₄ -CCN-B-a	138
Ph-CH ₂ -C≡CMe-Li(THF) ₃	139
R _{CCC}	139
TS ₁₋₅ -CCC-sigma	141
P ₁₋₅ -CCC-sigma.....	143
TS ₁₋₅ -CCC-pi	145
P ₁₋₅ -CCC-pi.....	147
TS ₁₋₄ -CCC	149
P ₁₋₄ -CCC.....	151
Ph-CH ₂ -C≡CMe-anion	153
R _{CCC} -a.....	153
TS ₁₋₅ -CCC-sigma-a	154
P ₁₋₅ -CCC-sigma-a.....	155
TS ₁₋₅ -CCC-pi-a	156
P ₁₋₅ -CCC-pi-a.....	157
TS ₁₋₄ -CCC-a	158
P ₁₋₄ -CCC-a.....	159

Ph-N₃-Li(THF)₃

R_{N3}

E = -196.913159 E⁰ = -196.478974

No. of Negative Frequencies = 0



Atomic Coordinates:

6	-0.05495702	-2.34192963	-4.35831009
6	-0.13030722	-2.99358144	-3.12165082
6	0.16007356	-0.96160943	-4.38401574
6	-0.00587216	-2.24854617	-1.93499988
1	-0.06744069	-2.81488382	-0.99444390
6	0.19901797	-0.84587719	-1.87834387
3	0.20279448	-0.09677914	0.15951623
6	0.28849092	-0.27073785	-3.16550217
7	0.53690509	1.14901927	-3.34484251
1	0.23754841	-0.42106718	-5.33030942
1	-0.15512684	-2.89793382	-5.29261724
1	-0.28689285	-4.07560629	-3.08266666
7	0.80119482	1.84829130	-2.37710177
7	1.07024919	2.61831144	-1.55965357
8	-1.22110349	1.35796298	0.60725463
8	-0.47402439	-1.53891850	1.52409314
8	2.06243163	0.05768047	1.06793185
6	-1.04050414	2.67075046	1.20616811
6	-2.31309714	1.41153374	-0.35690571
6	-2.54930179	2.89603327	-0.62648806
1	-2.00284245	0.82433544	-1.23382466
1	-3.20416840	0.93897844	0.09518906
6	-2.23325852	3.51544171	0.74652450
1	-0.98368087	2.54489499	2.29826784
1	-0.08962359	3.08933797	0.83962881

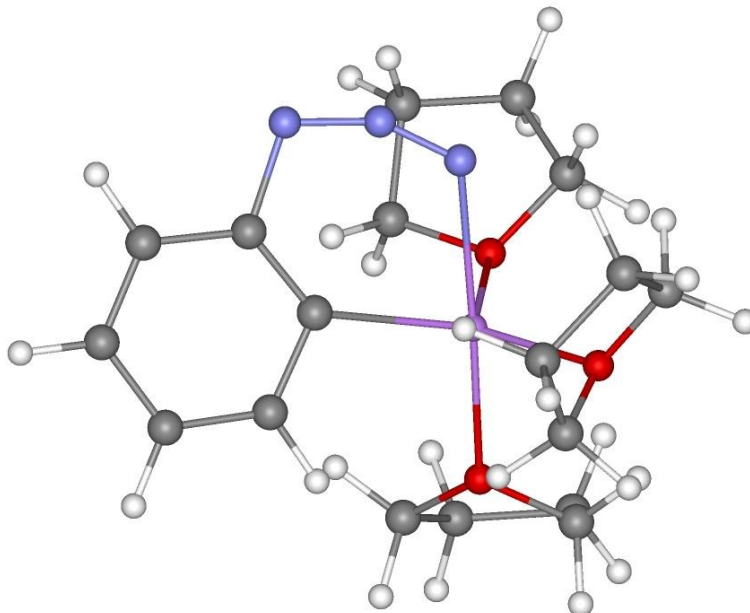
1	-3.57222078	3.10230401	-0.96880191
1	-1.84379072	3.26609068	-1.38442138
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1	-3.08731275	3.39088064	1.43020936
6	2.95657014	1.19713245	1.00734173
6	2.86611247	-1.09270834	0.70883225
6	3.72460874	-0.60175702	-0.45627704
1	3.47947766	-1.39201446	1.58007809
1	2.17675310	-1.90664111	0.44891053
6	4.00958054	0.87655884	-0.08235176
1	2.34479343	2.07807408	0.77613772
1	3.42528267	1.32860075	1.99847401
1	3.13261915	-0.66087402	-1.37995404
1	4.64055295	-1.19482250	-0.58241815
1	5.02693481	1.00797826	0.31190348
1	3.89596872	1.53621766	-0.95212183
6	-0.31476746	-1.37439203	2.94581617
6	-1.73680666	-2.21833303	1.36260556
6	-2.67700099	-1.61725255	2.43177398
1	-2.06190585	-2.06431955	0.32593451
1	-1.58271116	-3.29984134	1.53155312
6	-1.70588545	-0.96304695	3.45703678
1	0.00604593	-2.33680912	3.38781789
1	0.47347394	-0.62680694	3.10068442
1	-3.30425202	-2.39503883	2.88774971
1	-3.34411732	-0.86424358	1.99246191
1	-1.80746548	0.13009369	3.43805333
1	-1.88015668	-1.30439648	4.48638828

TS_{1-5-N3}

E = -196.903476 E0 = -196.470003

No. of Negative Frequencies = 1

freq = - 205.42



Atomic Coordinates:

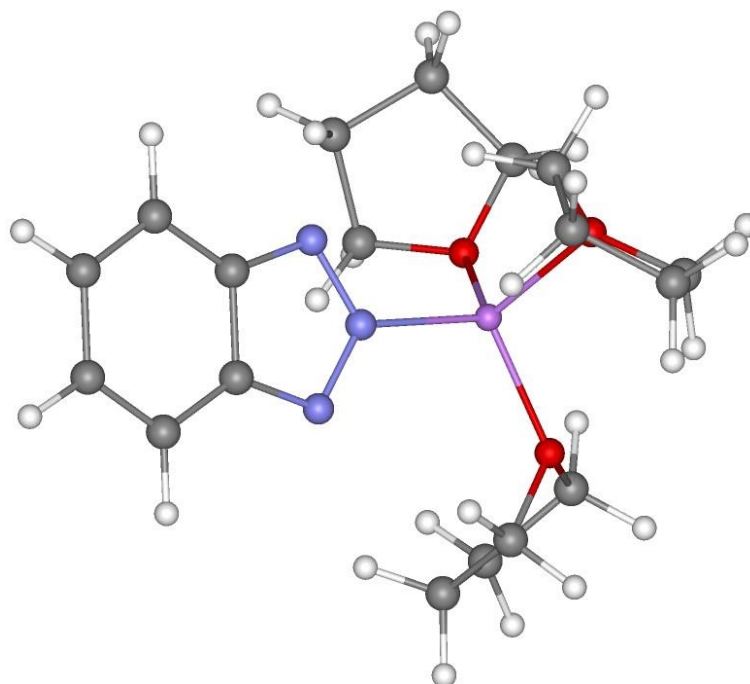
6	-0.36164692	-2.28996166	-4.27789845
6	-0.21231260	-2.91029038	-3.02998129
6	-0.18550008	-0.90825525	-4.38630513
6	0.09340266	-2.13434080	-1.89730283
1	0.19435320	-2.66022382	-0.93911000
6	0.26909050	-0.73463280	-1.96408915
3	0.31275319	0.08466785	0.15853855
6	0.14225896	-0.18014723	-3.22966391
7	0.36148225	1.26875643	-3.48300469
1	-0.28145252	-0.39260451	-5.34482195
1	-0.60361541	-2.87839229	-5.16533042
1	-0.33359819	-3.99339664	-2.93864671
7	0.75381542	1.79911154	-2.43035820
7	1.05923190	1.79086906	-1.30280387
8	-1.29916244	1.38039975	0.67929057
8	-0.41116698	-1.48607548	1.43488808
8	2.14426195	0.05800536	1.17938599
6	-1.09559008	2.74693795	1.13190247
6	-2.34412921	1.36081194	-0.33872259
6	-2.56644547	2.81913041	-0.73854863
1	-1.99738552	0.71807094	-1.16170828
1	-3.25443979	0.92150559	0.10692527
6	-2.27300831	3.55500025	0.58070884
1	-1.03998122	2.73478290	2.23087516
1	-0.13671866	3.10773601	0.72403511
1	-3.58154099	2.99843782	-1.11725911

1	-1.84759356	3.11739451	-1.51541146
1	-2.01983338	4.61425274	0.43916349
1	-3.13973024	3.49371159	1.25708235
6	3.07498607	1.16766924	1.20420442
6	2.92912562	-1.09366555	0.78687133
6	3.83093151	-0.57352175	-0.33392587
1	3.51352787	-1.44640943	1.65809792
1	2.22806887	-1.87968700	0.47802343
6	4.12083772	0.88940529	0.09740149
1	2.49288326	2.08229194	1.03928760
1	3.54415942	1.20826978	2.20337659
1	3.27305435	-0.59040682	-1.27964531
1	4.74351664	-1.17420222	-0.44799375
1	5.14093772	1.00751638	0.48885987
1	3.99545226	1.57760313	-0.74748810
6	-0.25975146	-1.40623359	2.86567243
6	-1.67136206	-2.16023800	1.22876461
6	-2.61572827	-1.64769679	2.34096900
1	-2.00051644	-1.93701901	0.20641476
1	-1.50911103	-3.25002740	1.31792599
6	-1.65211203	-1.02056349	3.38855902
1	0.05417714	-2.39473635	3.25245028
1	0.52922819	-0.67171149	3.06914046
1	-3.20919273	-2.47091887	2.76127861
1	-3.31472851	-0.89510222	1.95402667
1	-1.75774865	0.07217965	3.39914962
1	-1.82643393	-1.39405722	4.40674973

P_{1-5-N3}

E = -197.018855 E0 = -196.580795

No. of Negative Frequencies = 0



Atomic Coordinates:

6	-0.54458004	-1.59285492	-5.34096617
6	-1.81943479	-2.01083979	-4.86509826
6	0.38540265	-0.99272917	-4.50021605
6	-2.19387451	-1.83844396	-3.53765086
1	-3.17203074	-2.16018926	-3.17514270
6	-1.25900174	-1.22963141	-2.67175799
3	0.23244034	0.32236279	0.83298409
6	0.01835400	-0.81098137	-3.14894420
7	0.69452796	-0.26366740	-2.09428831
1	1.36270963	-0.67296101	-4.86646743
1	-0.29732320	-1.75061625	-6.39278066
1	-2.51555233	-2.47790723	-5.56485618
7	-0.13883178	-0.35274071	-1.04401054
7	-1.32308888	-0.92506080	-1.34058276
8	-1.15430863	1.69292928	1.36545375
8	0.13375394	-1.17288066	2.19417696
8	2.05517136	1.16380281	1.03195516
6	-0.79501793	3.07754484	1.59841582
6	-2.36041362	1.71650983	0.55743208
6	-2.09776919	2.83058095	-0.45491283
1	-2.47336241	0.72068617	0.10696742
1	-3.22389685	1.94667309	1.20913903
6	-1.30624111	3.87732042	0.37237290
1	-1.27822569	3.41652181	2.53122853
1	0.29495549	3.10586839	1.73040511

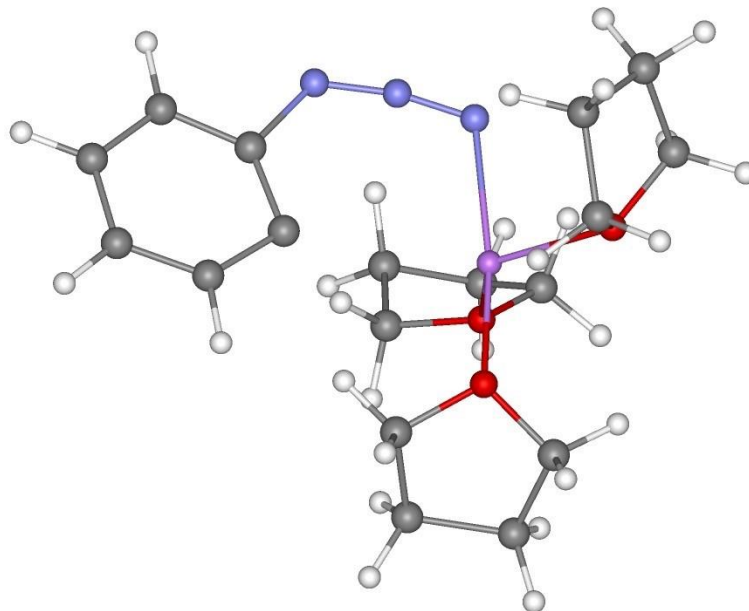
1	-3.02362406	3.23809450	-0.88222902
1	-1.48251800	2.43353905	-1.27411766
1	-0.47846258	4.30431394	-0.20865253
1	-1.95167189	4.70605725	0.69534194
6	2.83196238	1.42943920	-0.16710766
6	3.01431901	0.72682784	2.01896236
6	4.01686379	-0.16096500	1.25523046
1	3.51107189	1.61518749	2.45034391
1	2.45654406	0.20595576	2.80808255
6	3.86659121	0.29518814	-0.22612059
1	2.13748972	1.41855979	-1.01726832
1	3.30939714	2.42064398	-0.06114829
1	3.75464353	-1.22210362	1.36201748
1	5.03788875	-0.02625466	1.63770805
1	4.81624037	0.63643831	-0.65967148
1	3.47596854	-0.51889906	-0.85051603
6	-0.84520271	-1.16838843	3.26356499
6	0.12833406	-2.51745087	1.65147084
6	-1.35253125	-2.89405492	1.60660653
1	0.60839879	-2.47202434	0.66548308
1	0.70999639	-3.17828402	2.32111676
6	-1.92774511	-2.20651401	2.87357815
1	-0.34047094	-1.44656235	4.20519573
1	-1.21814147	-0.13897744	3.34754489
1	-1.50846011	-3.98129629	1.60558890
1	-1.79529138	-2.46832812	0.69489025
1	-2.89125574	-1.72568491	2.65990703
1	-2.08469633	-2.92375365	3.69134177

*TS*_{I-4-N3}

E = -196.887484 E0 = -196.454427

No. of Negative Frequencies = 1

freq = - 101.70



Atomic Coordinates:

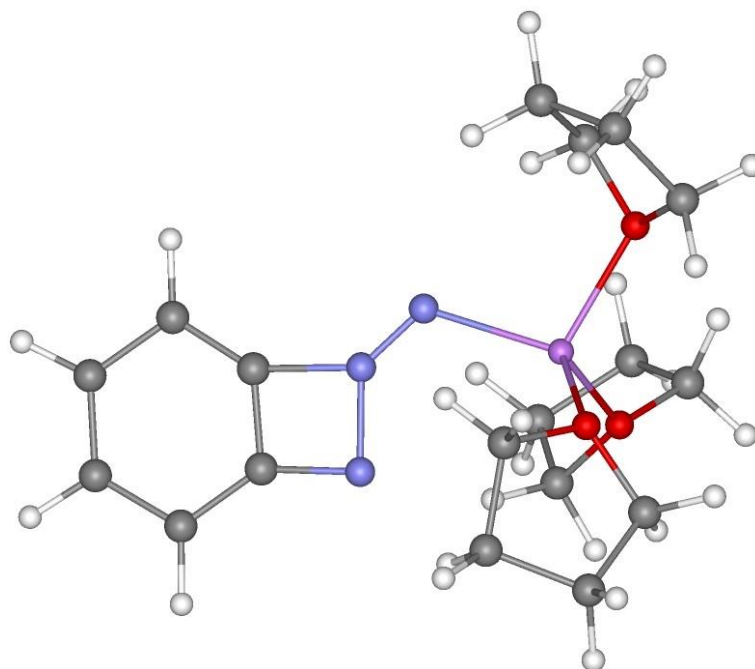
6	-1.07428254	-2.08420608	-4.82999213
6	-1.31007691	-2.90508152	-3.72243477
6	-0.48636472	-0.82857773	-4.63684435
6	-0.96911170	-2.46073820	-2.42796460
1	-1.17630961	-3.16087219	-1.60594738
6	-0.39248929	-1.20519925	-2.15172894
3	0.56141547	0.39988653	0.57767966
6	-0.16260614	-0.43977923	-3.32784853
7	0.46319475	0.83699914	-3.17040183
1	-0.27512156	-0.17179364	-5.48398830
1	-1.33708758	-2.41544637	-5.83654309
1	-1.75959611	-3.89253930	-3.86379706
7	0.81015578	1.09530501	-2.01670070
7	1.24518038	1.60298132	-1.06619102
8	-1.23269647	1.48865847	0.80837120
8	-0.05642066	-1.28093430	1.60916988
8	2.37494237	0.37252067	1.59565002
6	-1.11211437	2.91959125	1.05220412
6	-2.23707548	1.26248904	-0.23214958
6	-2.41826072	2.61103791	-0.92203162
1	-1.85989954	0.45505885	-0.88368550
1	-3.17380060	0.93809242	0.25537946
6	-2.23438045	3.58954945	0.25169947
1	-1.18112697	3.09018172	2.13728746
1	-0.12027548	3.24792346	0.69716220
1	-3.39918161	2.70020481	-1.40734873

1	-1.63958085	2.76520487	-1.68400716
1	-1.96513635	4.60604805	-0.06563250
1	-3.15703234	3.64770604	0.84931628
6	3.31354692	1.47085298	1.49417391
6	3.17451577	-0.81992049	1.40014041
6	4.12421211	-0.46735467	0.24858811
1	3.72886426	-1.03293561	2.33307456
1	2.48223793	-1.64424007	1.18923543
6	4.33340721	1.06589474	0.40635211
1	2.73894860	2.37312423	1.25057856
1	3.79966630	1.60507091	2.47686016
1	3.64548302	-0.69516556	-0.71315228
1	5.06395541	-1.03268962	0.30756649
1	5.35712253	1.31671032	0.71563105
1	4.12322046	1.58468777	-0.53692886
6	-0.20267201	-1.29316035	3.04264341
6	-1.08718965	-2.16620619	1.11128329
6	-2.31902387	-1.88630497	1.99170467
1	-1.19581406	-1.92968721	0.04443178
1	-0.73842647	-3.20872610	1.22947092
6	-1.72215552	-1.28798246	3.30019696
1	0.26499727	-2.21210352	3.44382512
1	0.33247975	-0.42003349	3.43923006
1	-2.89800495	-2.80180212	2.17272889
1	-2.98378566	-1.16040758	1.50609702
1	-2.08313979	-0.26303246	3.45702896
1	-1.97730622	-1.87885966	4.19055731

P_{1-4-N3}

E = -196.892805 E0 = -196.457785

No. of Negative Frequencies = 0



Atomic Coordinates:

6	-0.30203444	-1.03446446	-5.75703680
6	-0.49759197	-2.32733122	-5.25736875
6	-0.11526941	0.10869617	-4.93300079
6	-0.52025440	-2.57329895	-3.84947853
1	-0.67092304	-3.57183782	-3.43724911
6	-0.33682563	-1.44749146	-3.09394247
3	0.05437504	0.12117163	0.98283524
6	-0.13920783	-0.13799506	-3.56163693
7	-0.02968680	0.48358585	-2.29392428
1	0.03399367	1.09714162	-5.36889637
1	-0.29258360	-0.89595599	-6.84117189
1	-0.63502218	-3.15936626	-5.94895214
7	-0.22538489	-0.83064967	-1.68454719
7	-0.26503014	-1.20333317	-0.53860748
8	-1.24585559	1.65806163	1.17086553
8	-0.13322019	-1.01966293	2.67136367
8	1.92614466	0.88000502	1.00627230
6	-0.75183293	3.01504693	1.38615213
6	-2.33260809	1.70567000	0.20351503
6	-2.01362442	2.91256973	-0.66912805
1	-2.32622917	0.75105036	-0.33918051
1	-3.29044220	1.82074059	0.74334399
6	-1.47833901	3.91652554	0.36971031
1	-0.95639130	3.30060349	2.43041282
1	0.33712067	2.98990316	1.23266752
1	-2.89236498	3.28822491	-1.21079413

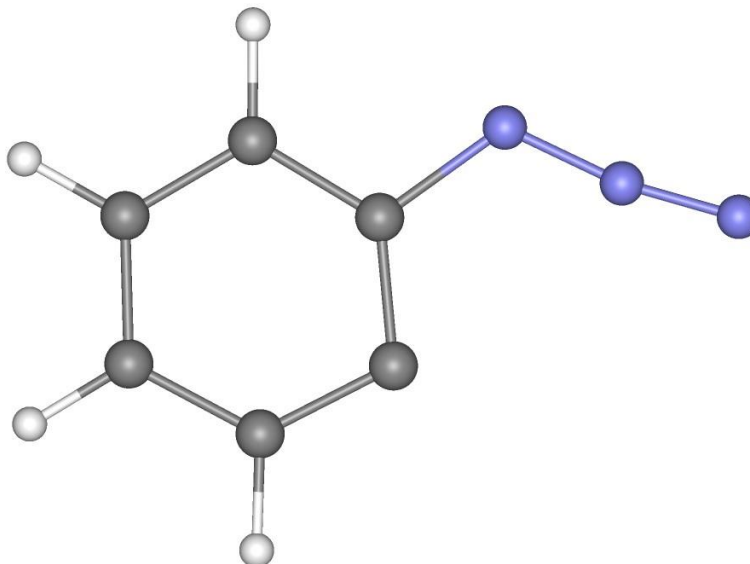
1	-1.23719352	2.62464773	-1.39366776
1	-0.80265146	4.66184126	-0.07053448
1	-2.30860808	4.45413439	0.85239589
6	2.61365548	1.04578541	-0.26300648
6	2.93860583	0.43796373	1.93681033
6	3.87820292	-0.49079603	1.13211685
1	3.48026842	1.32270950	2.31728162
1	2.42063819	-0.05111353	2.77240243
6	3.53461461	-0.17668802	-0.35320263
1	1.84528667	1.09933493	-1.05039580
1	3.19140448	1.98820332	-0.22721694
1	3.68753571	-1.54714429	1.36368636
1	4.93066564	-0.28128163	1.36765075
1	4.42674788	0.02491558	-0.96089301
1	2.99304715	-1.01528978	-0.81079065
6	-1.17787082	-0.74944509	3.63510052
6	-0.15915242	-2.45284030	2.46252259
6	-1.64916230	-2.79767950	2.38553342
1	0.38608517	-2.65807549	1.53325323
1	0.33784422	-2.94833324	3.31721050
6	-2.31129003	-1.76025809	3.33560591
1	-0.76876811	-0.89353993	4.65074309
1	-1.46728158	0.30172990	3.50878997
1	-1.85083046	-3.83554590	2.68264822
1	-1.99308696	-2.65682948	1.35203825
1	-3.16478749	-1.27059660	2.84856871
1	-2.67483094	-2.22341852	4.26312599

Ph-N₃-anion

R_{N3-a}

E = -66.162860 E0 = -66.077709

No. of Negative Frequencies = 0



Atomic Coordinates:

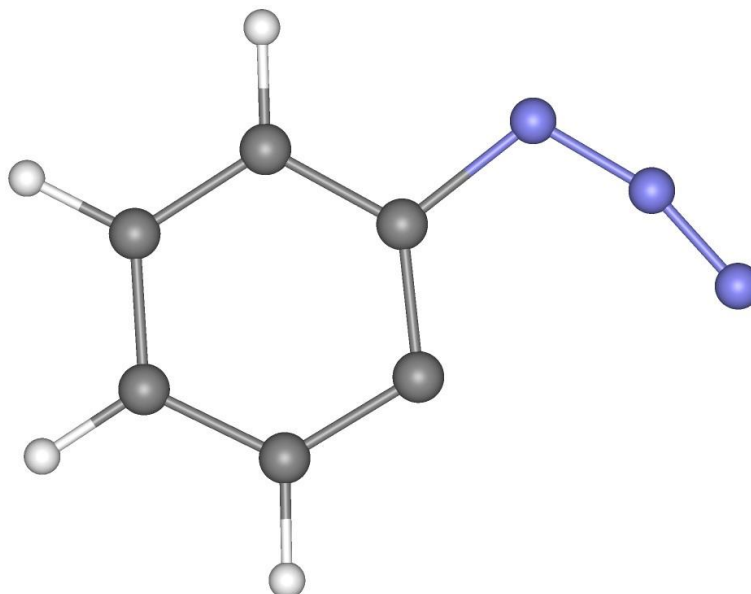
6	-0.27275169	-1.24805923	-1.22336699
6	-0.35157610	-1.88984683	0.02149263
6	-0.01726763	0.12919128	-1.25833373
6	-0.17343388	-1.14264407	1.20441122
1	-0.24599534	-1.70090696	2.15290129
6	0.08764677	0.24874155	1.25409327
6	0.15019876	0.81307069	-0.03838988
7	0.41035349	2.23836115	-0.20760956
1	0.05036953	0.66099544	-2.21526907
1	-0.40733588	-1.80606979	-2.15447526
1	-0.55146968	-2.96960873	0.06434743
7	0.57298662	2.93478450	0.79311981
7	0.74827503	3.73199099	1.60707885

*TS*_{1-5-N3-a}

E = -66.159480 E0 = -66.074559

No. of Negative Frequencies = 1

freq = - 160.05



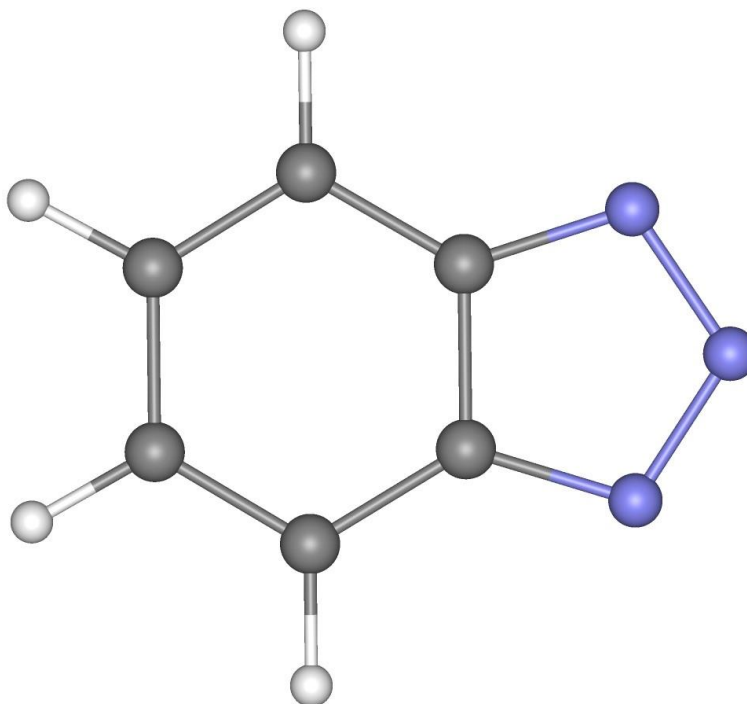
Atomic Coordinates:

6	-0.27020285	-1.23768087	-1.20339964
6	-0.34070719	-1.83905470	0.06325197
6	-0.01699855	0.13736630	-1.29752100
6	-0.15587704	-1.05087883	1.21838725
1	-0.21928885	-1.56250766	2.19226730
6	0.10018022	0.33231387	1.16471052
6	0.15813444	0.86765527	-0.10943830
7	0.42227441	2.32741724	-0.35175859
1	0.04412439	0.63707534	-2.27256551
1	-0.41060828	-1.83098956	-2.11175705
1	-0.53874509	-2.91605330	0.14566638
7	0.57178419	2.94142473	0.71613437
7	0.65593020	3.19391216	1.84602230

$P_{1-5-N3-a}$

E = -66.271858 E0 = -66.182388

No. of Negative Frequencies = 0



Atomic Coordinates:

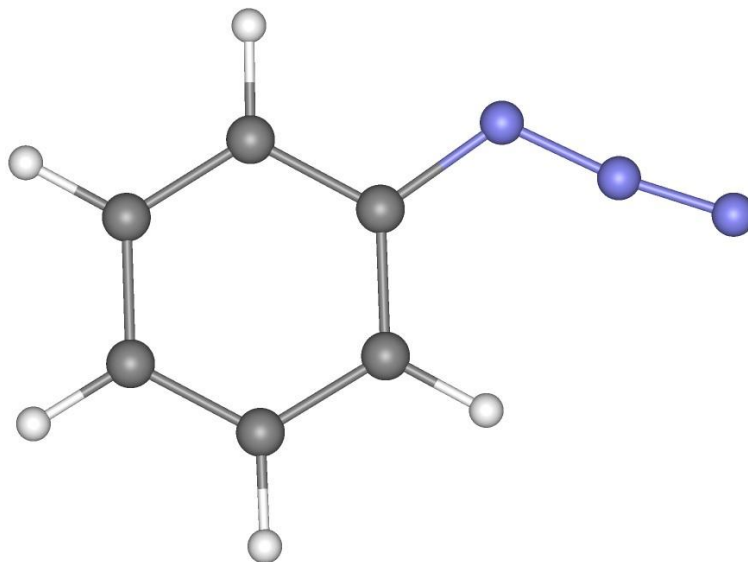
6	0.28372154	-0.28233261	-1.61478300
6	-0.98989903	-0.69990838	-1.13925740
6	1.21192350	0.31972555	-0.76423503
6	-1.35780699	-0.52277378	0.19518097
1	-2.33775608	-0.84453460	0.55951882
6	-0.42856613	0.08471262	1.06543352
6	0.85234103	0.50462223	0.58718921
7	1.52544894	1.05142589	1.64577905
1	2.19120734	0.64034268	-1.13135983
1	0.53503125	-0.43875076	-2.66798996
1	-1.69015827	-1.16830747	-1.83719008
7	0.69326365	0.96468816	2.70393963
7	-0.48875075	0.39109045	2.39777411

Ph-N₃ + Ph-Li(THF)₃

Ph-N₃

E = -66.785434 E0 = -66.684814

No. of Negative Frequencies = 0



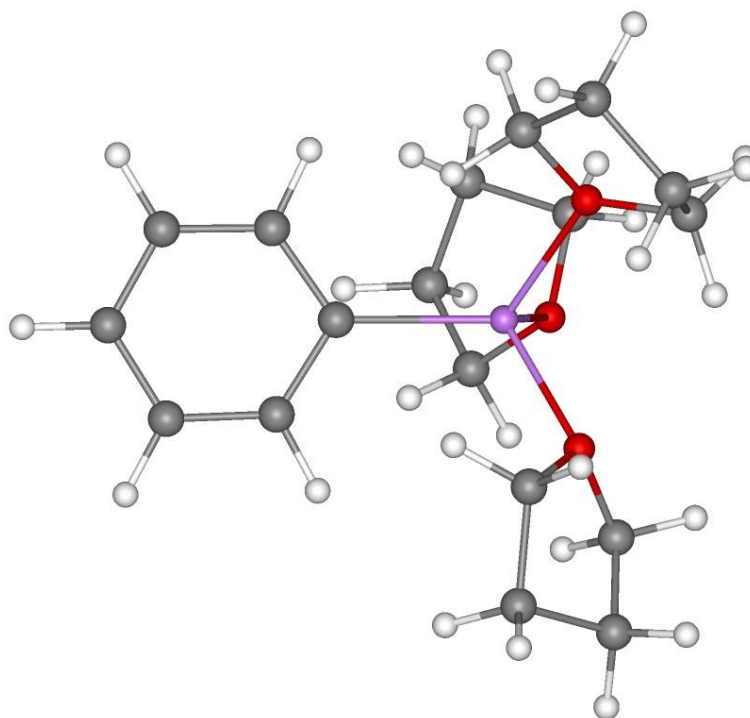
Atomic Coordinates:

6	-0.47496861	-1.28080063	-1.31408188
6	-0.85029103	-1.79637248	-0.06660170
6	0.13314483	-0.02712601	-1.40860103
6	-0.61218460	-1.04563666	1.09149715
1	-0.90087271	-1.43806942	2.06799855
6	-0.00453321	0.21069477	1.01240327
1	0.17724212	0.78889120	1.92056146
6	0.36930883	0.72071455	-0.24326982
7	0.99203029	1.98598446	-0.42302791
1	0.43050961	0.38668644	-2.37251793
1	-0.65630338	-1.85761887	-2.22237630
1	-1.32494666	-2.77575062	0.00303189
7	1.22400464	2.68789255	0.56743478
7	1.49785989	3.44051072	1.38754946

Ph-Li(THF)₃

E = -167.742860 E0 = -167.312040

No. of Negative Frequencies = 0



Atomic Coordinates:

6	1.14241965	0.74347661	-4.54385990
6	1.58365433	-0.42744298	-3.91406504
6	0.38857554	1.66142296	-3.80218733
6	1.26094112	-0.66254315	-2.56619874
1	1.64323400	-1.59875975	-2.13040306
6	0.49534399	0.22163816	-1.75832753
3	0.10467272	-0.06156898	0.33674438
6	0.08759468	1.39135431	-2.45547640
1	0.03970450	2.58611674	-4.27467410
1	1.38427988	0.93819629	-5.59154412
1	2.17937453	-1.15484402	-4.47624068
8	-1.62299836	0.83706367	1.01651615
8	-0.20808588	-1.98914642	0.98778235
8	1.59778462	0.69391720	1.54225385
6	-1.65204821	2.08843303	1.75065923
6	-2.69139068	0.82794924	0.02132960
6	-3.24544937	2.25386269	-0.00695223
1	-2.25242338	0.49549715	-0.93127291
1	-3.45845277	0.10399195	0.34825745
6	-3.01224439	2.71735731	1.44204867
1	-1.49200645	1.86120065	2.81428099
1	-0.82589657	2.72937274	1.39690397
1	-4.30085771	2.28576811	-0.30876631
1	-2.66683529	2.87500250	-0.70685083
1	-3.00235938	3.80997338	1.55331994

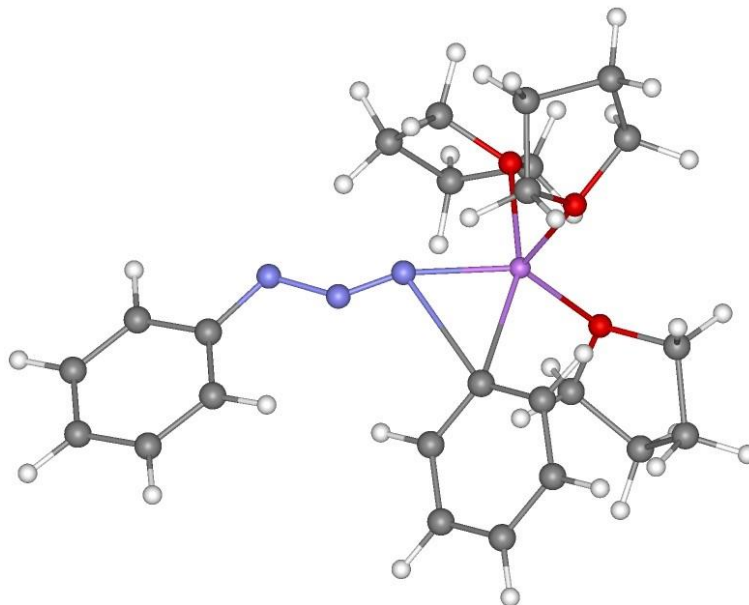
1	-3.78761555	2.30788751	2.10799948
6	2.25559847	1.83092876	0.89891624
6	2.61580578	-0.25132908	1.94290135
6	3.72054496	-0.09064994	0.90154312
1	2.97630748	-0.00131248	2.95883446
1	2.14690554	-1.24496750	1.96037575
6	3.73378259	1.43713945	0.69966011
1	1.73691139	1.99372639	-0.05774713
1	2.14026543	2.71500122	1.54672017
1	3.42783931	-0.59708062	-0.02977518
1	4.68775823	-0.48874696	1.23837092
1	4.37250042	1.91865538	1.45535436
1	4.09901908	1.72653962	-0.29387000
6	-1.15849095	-2.34701711	2.01815049
6	-0.24282825	-2.99487546	-0.07407090
6	-1.28673088	-4.03735473	0.35512895
1	-0.50982509	-2.47213575	-1.00496266
1	0.76741945	-3.41724526	-0.18247714
6	-2.18255421	-3.24199858	1.32224505
1	-0.63680699	-2.89102729	2.82715499
1	-1.57183542	-1.41212022	2.42063866
1	-0.80929061	-4.87566406	0.88500181
1	-1.83596883	-4.44584568	-0.50328955
1	-2.90442521	-2.62763738	0.76302506
1	-2.73579688	-3.88076713	2.02412624
1	-0.49502038	2.16060752	-1.92323206

$TS_{N3-inter}$

E = -234.522035 E0 = -233.990278

No. of Negative Frequencies = 1

freq = - 96.86



Atomic Coordinates:

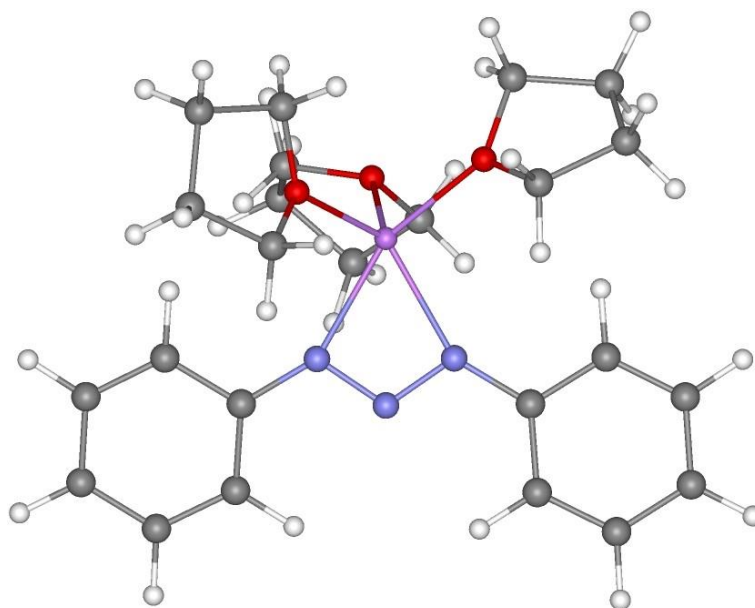
6	1.42991570	-2.84861690	-3.34101395
6	1.73583539	-3.25899170	-2.03732307
6	0.84208655	-1.59309505	-3.54972781
6	1.43876610	-2.42143971	-0.94469272
1	1.67384568	-2.78361803	0.06345985
6	0.84868726	-1.16229392	-1.14466395
3	-0.17146482	-0.59688518	0.90673499
6	0.57633426	-0.76124374	-2.44896415
7	0.65539272	3.07215385	-1.08618945
1	0.59983221	-1.26372532	-4.56452147
1	1.65628724	-3.49806467	-4.18923750
1	2.20992461	-4.23116080	-1.86854845
7	0.71905809	1.80171286	-0.87688504
7	0.62042752	0.98276115	-0.03314781
8	-1.23882712	0.66444827	2.43374840
8	-1.82989553	-1.84504865	0.62609777
8	1.17792883	-1.35709795	2.26536478
6	-0.80220174	2.02908247	2.62711710
6	-2.67558994	0.72896761	2.52749936
6	-3.06829138	1.98455828	1.72984475
1	-3.06961279	-0.21654171	2.13513954
1	-2.96487817	0.82788818	3.59156087
6	-1.81924989	2.90470497	1.86472393
1	-0.81000454	2.25315857	3.71035886
1	0.22305244	2.10329343	2.24462506
1	-3.98408554	2.44695366	2.12287132

1	-3.24264757	1.72924422	0.67545112
1	-1.42637797	3.18520933	0.87837836
1	-2.03951005	3.82846407	2.41683325
6	2.54453823	-0.87901849	2.12655104
6	0.89286794	-1.59484619	3.67329114
6	2.17280161	-1.23228815	4.44444397
1	0.04002361	-0.95492573	3.94684719
1	0.60401853	-2.65009893	3.79948465
6	2.88216705	-0.26301768	3.48127493
1	3.20685597	-1.73310561	1.89801595
1	2.55859759	-0.17758974	1.28182059
1	2.79502353	-2.12508521	4.60786763
1	1.95298711	-0.78753786	5.42409829
1	2.45207706	0.74711294	3.55637956
1	3.96422962	-0.19661635	3.65691465
6	-1.65236292	-3.26587830	0.88145976
6	-2.62907901	-1.66725978	-0.58307282
6	-3.16512436	-3.05518975	-0.94270202
1	-3.42182905	-0.93648654	-0.36171802
1	-1.97135411	-1.26352713	-1.36871421
6	-2.05192532	-3.97514298	-0.41184055
1	-0.60296348	-3.42900435	1.16608942
1	-2.30386682	-3.55262228	1.72619106
1	-3.33367393	-3.16404203	-2.02200777
1	-4.11454203	-3.25530747	-0.42189804
1	-2.38958289	-5.00584214	-0.23797092
1	-1.20349801	-3.99408082	-1.11103341
1	0.15076538	0.23805524	-2.63493604
6	0.99915051	3.50139441	-2.38650110
6	0.63074207	4.82014529	-2.72161941
6	1.72432032	2.73689732	-3.32514340
6	2.04714436	3.27901042	-4.57200036
1	2.04215909	1.72562849	-3.06545010
1	2.61051510	2.67472092	-5.28638636
6	1.66839733	4.58654846	-4.90577108
1	1.92822416	5.00485047	-5.87932876
6	0.96172564	5.35341900	-3.96925472
1	0.66394637	6.37545960	-4.21235223
1	0.08178624	5.41049338	-1.98592246

$P_{N3-inter}$

E = -234.624141 E0 = -234.089200

No. of Negative Frequencies = 0



Atomic Coordinates:

6	-0.88352449	-2.98459596	-5.00243492
6	0.11013126	-1.99919458	-5.11198011
6	-1.58679686	-3.10852169	-3.79676646
6	0.40396846	-1.14972513	-4.04429558
1	1.18703909	-0.39701813	-4.12961910
6	-0.30664358	-1.26240617	-2.82442531
3	-0.18284061	-0.21093583	0.48005079
6	-1.30210451	-2.26162970	-2.72266574
7	0.84731141	1.26836206	-0.80016651
1	-2.36716324	-3.86628484	-3.69480301
1	-1.10158645	-3.64640850	-5.84197920
1	0.67209976	-1.89867606	-6.04359583
7	0.61894451	0.61635792	-1.91582562
7	-0.08102993	-0.47170132	-1.68972230
8	-1.93080009	0.80215391	0.99786745
8	-0.80476799	-2.15002957	1.09264309
8	1.27789950	-0.10384823	2.03846448
6	-1.73338841	2.09213394	1.65026370
6	-2.83773494	0.97431760	-0.12878127
6	-2.76292923	2.45689944	-0.48103427
1	-2.49259411	0.30554968	-0.92920486
1	-3.85651164	0.68228571	0.18537606
6	-2.62699877	3.09814400	0.91152936
1	-1.99074932	1.98411063	2.71542456
1	-0.66736612	2.35146248	1.55913203
1	-3.64784378	2.80526149	-1.03063907
1	-1.86805044	2.65440215	-1.08815082
1	-2.17846934	4.09980846	0.88156267

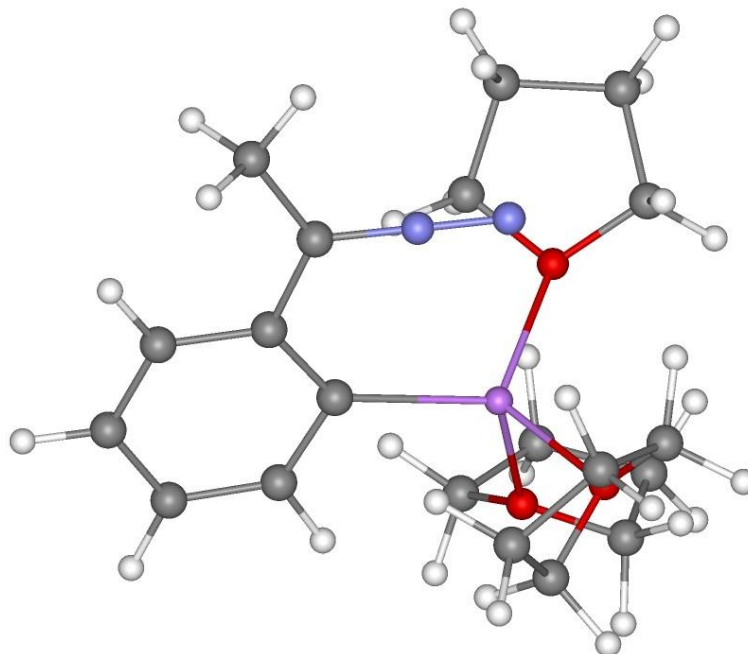
1	-3.61234329	3.17595203	1.39648092
6	2.67428680	-0.24528132	1.70027886
6	1.18556963	-0.50311635	3.41674036
6	2.44843133	0.07003433	4.09933782
1	0.23968491	-0.11075709	3.81310733
1	1.16644458	-1.60770137	3.47937153
6	3.42689868	0.32106169	2.91430359
1	2.90274700	-1.31799848	1.54955391
1	2.83522842	0.29136531	0.75769388
1	2.85462835	-0.63542957	4.83684146
1	2.22202128	1.00808714	4.62311723
1	3.60708055	1.39602019	2.78064206
1	4.39970983	-0.16825991	3.05643792
6	-1.90672652	-2.53616668	1.93039549
6	-0.17565080	-3.37280732	0.64912653
6	-1.29737501	-4.44113978	0.58177834
1	0.29582886	-3.15685757	-0.31841486
1	0.60685822	-3.66118919	1.37458669
6	-2.53014520	-3.73198351	1.20337211
1	-1.53371454	-2.82680239	2.93271224
1	-2.56134918	-1.66055022	2.02979565
1	-1.01727478	-5.33510377	1.15578732
1	-1.49322603	-4.75608335	-0.45108186
1	-3.20816986	-3.37300142	0.41637437
1	-3.10271353	-4.38405510	1.87687967
1	-1.85770102	-2.33967380	-1.78528036
6	1.52702811	2.48275767	-0.96108056
6	1.90668564	3.16095771	0.22143720
6	1.84438723	3.08409975	-2.20452439
6	2.52029083	4.30420449	-2.24526617
1	1.54667320	2.58184217	-3.12429020
1	2.75407511	4.75126204	-3.21451907
6	2.89649910	4.96635384	-1.06575797
1	3.42140100	5.92178216	-1.11038627
6	2.58145640	4.38336959	0.16868497
1	2.86273238	4.88441919	1.09782058
1	1.66224214	2.70011515	1.18171948

Ph-C(Me)=N₂-Li(THF)₃

R_{CN2}

E = -200.117692 E0 = -199.645786

No. of Negative Frequencies = 0



Atomic Coordinates:

6	-0.13359687	-2.57545290	-3.94135034
6	-0.16012317	-3.18023372	-2.68211898
6	0.06177049	-1.19300902	-4.03065743
6	-0.00972848	-2.38030423	-1.53292653
1	-0.03683159	-2.90907118	-0.56818924
6	0.17297408	-0.97680308	-1.53991084
3	0.17807364	-0.23687636	0.49552657
6	0.22097692	-0.41732347	-2.85678029
6	0.45963292	1.02998102	-3.05470526
1	0.09644802	-0.73220948	-5.02161580
1	-0.25558044	-3.16815692	-4.85080757
1	-0.30014328	-4.26215687	-2.59494280
7	0.77265790	1.76972046	-2.03035663
7	1.05965134	2.43338733	-1.12526562
8	-1.27211594	1.20402172	0.94684618
8	-0.50300951	-1.67663160	1.86794784
8	2.03892848	-0.09544038	1.42270356
6	-1.12342373	2.50070516	1.58524824
6	-2.30943986	1.28225130	-0.07484827
6	-2.53397279	2.77336682	-0.31703172
1	-1.94862353	0.71675871	-0.94683708
1	-3.22331091	0.79776478	0.31530981
6	-2.29215849	3.35693590	1.08659050
1	-1.12131192	2.34909414	2.67565641
1	-0.15589653	2.92903349	1.27734284

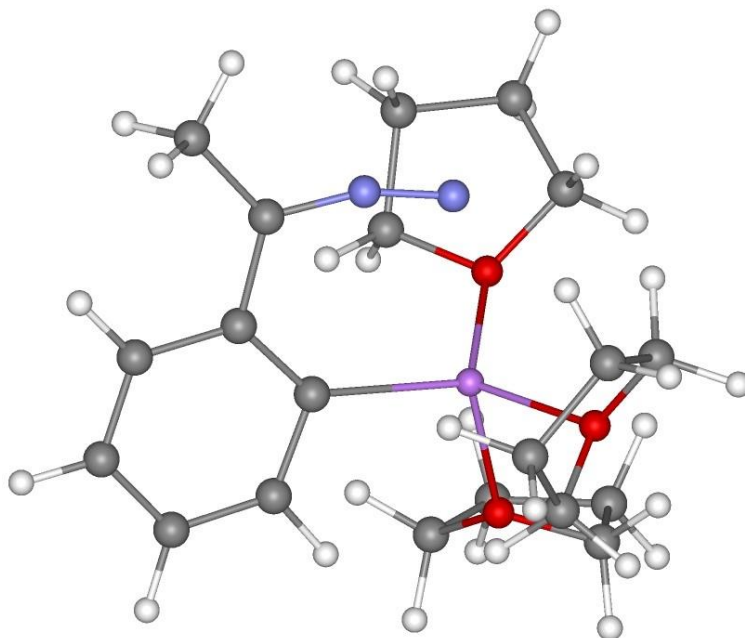
1	-3.53788116	2.98822145	-0.70735048
1	-1.78854923	3.16289889	-1.02531948
1	-2.04585230	4.42716905	1.07565724
1	-3.18069919	3.21317036	1.72085433
6	2.93619889	1.04158947	1.40971040
6	2.84204480	-1.22818127	1.00903378
6	3.69017520	-0.68715508	-0.14212128
1	3.46232644	-1.56157902	1.86290762
1	2.15293323	-2.03184444	0.71864791
6	3.96062092	0.78221635	0.27825245
1	2.32437555	1.93795400	1.24833390
1	3.42986615	1.11063029	2.39548479
1	3.09313796	-0.72217757	-1.06387792
1	4.61183138	-1.26595453	-0.29153102
1	4.98739793	0.92171785	0.64455540
1	3.80158542	1.46992977	-0.56223200
6	-0.32623925	-1.54472944	3.29070793
6	-1.78688342	-2.31266123	1.70702945
6	-2.70185831	-1.65857236	2.76163485
1	-2.09991872	-2.16264128	0.66603237
1	-1.67466336	-3.39695651	1.89398372
6	-1.70769825	-1.13448407	3.83922668
1	-0.00668367	-2.51944436	3.70520175
1	0.47034008	-0.80747283	3.45179631
1	-3.42376031	-2.37968286	3.16808241
1	-3.26677863	-0.82667485	2.32137389
1	-1.77787156	-0.04252989	3.93022088
1	-1.89139917	-1.56877435	4.83134486
6	0.44700180	1.73022083	-4.39627844
1	0.60698013	2.81050816	-4.28269994
1	1.23641468	1.33699155	-5.05831912
1	-0.51834077	1.57894632	-4.90517076

*TS*_{1-5-CN2}

E = -200.116682 E0 = -199.645053

No. of Negative Frequencies = 1

freq = - 115.29



Atomic Coordinates:

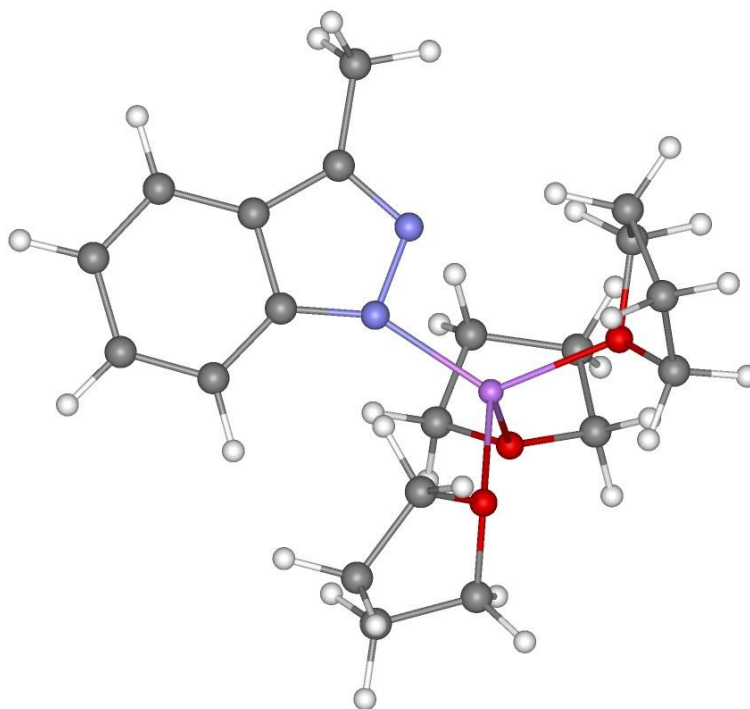
6	-0.19366442	-2.55746979	-3.91329458
6	-0.18813420	-3.14014842	-2.64353717
6	0.00699054	-1.17911935	-4.03756389
6	-0.00202190	-2.31897929	-1.51520369
1	-0.01045205	-2.82185464	-0.53750649
6	0.19464785	-0.92078682	-1.57118442
3	0.20816342	-0.15409980	0.49418856
6	0.21218741	-0.37855427	-2.88552331
6	0.46105701	1.06891150	-3.14573388
1	0.01096377	-0.73757732	-5.03722105
1	-0.34526919	-3.16541252	-4.80810477
1	-0.33017712	-4.21917273	-2.53104392
7	0.78393753	1.77358147	-2.10241302
7	1.02877797	2.08222793	-1.00762020
8	-1.34661435	1.19320802	0.98410107
8	-0.49034206	-1.65693188	1.83702023
8	2.06349025	-0.10975840	1.45763318
6	-1.18656100	2.50920123	1.57783176
6	-2.34420465	1.25907326	-0.07826835
6	-2.55688637	2.74664177	-0.35495166
1	-1.95246291	0.684444189	-0.93104903
1	-3.27196847	0.78119886	0.28551290
6	-2.34108299	3.35963366	1.04019448
1	-1.19402857	2.39300053	2.67237671
1	-0.21165518	2.91526675	1.26208709
1	-3.55141262	2.95730287	-0.77077242

1	-1.79586756	3.11685226	-1.05693447
1	-2.09069679	4.42867206	1.01130760
1	-3.24227613	3.23214937	1.66001134
6	2.97965085	1.01015848	1.50921947
6	2.85496821	-1.23671207	1.00863849
6	3.73473147	-0.66238646	-0.10279866
1	3.45379287	-1.61773136	1.85793313
1	2.15846476	-2.01532421	0.67177707
6	4.00869070	0.78922950	0.37456122
1	2.38369170	1.92287205	1.38819623
1	3.46657489	1.01954667	2.50091367
1	3.16103462	-0.65734041	-1.03954948
1	4.65425777	-1.24506360	-0.25058227
1	5.03429726	0.91233017	0.75003688
1	3.85214833	1.50553787	-0.44169496
6	-0.28081085	-1.59542105	3.26021780
6	-1.79573684	-2.24786914	1.67783895
6	-2.66910510	-1.61947290	2.78264211
1	-2.12801221	-2.04245912	0.65247941
1	-1.71128450	-3.34258052	1.81166276
6	-1.63619719	-1.16481549	3.85505466
1	0.01269078	-2.59829850	3.62415553
1	0.54323889	-0.89298258	3.43705435
1	-3.39651693	-2.34211264	3.17648971
1	-3.22488652	-0.75675850	2.39350176
1	-1.67005291	-0.07506794	3.98501463
1	-1.81109931	-1.62852903	4.83542915
6	0.43161663	1.72923038	-4.49912697
1	0.62268209	2.80682282	-4.41002514
1	1.19386509	1.30607934	-5.17488191
1	-0.54713177	1.59762004	-4.98849623

$P_{1-5-CN2}$

E = -200.234401 E0 = -199.758839

No. of Negative Frequencies = 0



Atomic Coordinates:

6	0.89011142	-2.11502276	-4.69677661
6	1.79540986	-2.29878032	-3.61776150
6	-0.27135191	-1.36520011	-4.53451692
6	1.55865217	-1.73617215	-2.36713137
1	2.25723759	-1.89683255	-1.54178179
6	0.38561027	-0.96535294	-2.18812963
3	0.08661058	0.17377023	0.85437796
6	-0.53437676	-0.78423103	-3.27447205
6	-1.56968313	0.01567069	-2.71359681
1	-0.96409684	-1.23251454	-5.36968033
1	1.11255726	-2.57315614	-5.66247219
1	2.69430953	-2.89912051	-3.77633903
7	-1.27912509	0.27615580	-1.42544627
7	-0.07998515	-0.31337939	-1.08005784
8	-0.80287767	1.83668515	1.67101457
8	-0.63212838	-1.36466117	2.01412626
8	2.04129598	0.45578655	1.41369979
6	-0.06859360	2.93245804	2.25736432
6	-1.90016820	2.45612277	0.95197813
6	-1.26745635	3.67381302	0.26467871
1	-2.27825305	1.70599946	0.24436648
1	-2.67813666	2.75240872	1.68022719
6	-0.08384285	4.05865013	1.20022736
1	-0.58222685	3.24889183	3.18379964
1	0.93048882	2.55560713	2.51064589

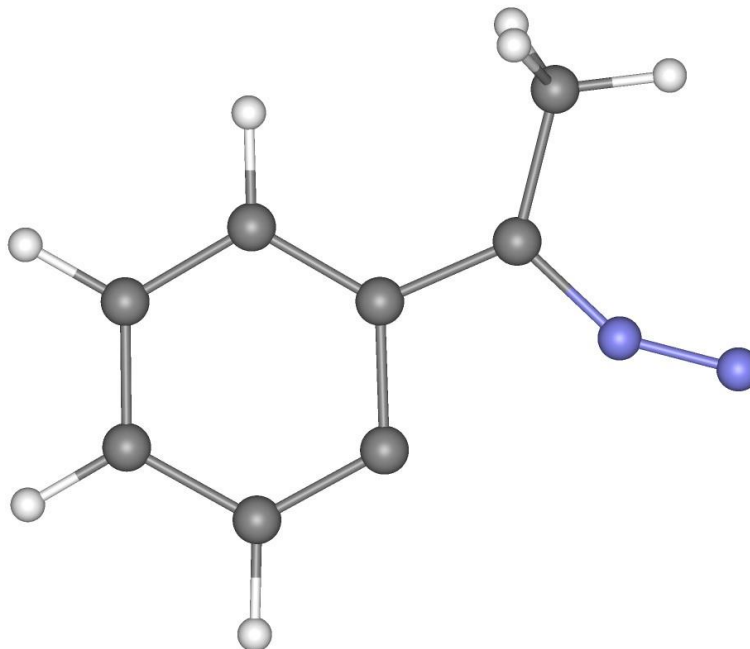
1	-1.98822132	4.49230498	0.13452386
1	-0.89878529	3.37690605	-0.72642072
1	0.86087593	4.08723898	0.64086643
1	-0.22425128	5.04079334	1.67231102
6	2.95312708	0.85616882	0.34591370
6	2.73265723	-0.46787807	2.28280261
6	3.67357826	-1.23214105	1.35437871
1	3.29340533	0.09403302	3.05360929
1	1.96718325	-1.08706813	2.76985259
6	4.15033995	-0.11915908	0.39750217
1	2.38217262	0.80008603	-0.59182640
1	3.26282968	1.89980529	0.51845857
1	3.10904250	-2.00290724	0.80949860
1	4.50090418	-1.71780388	1.88945256
1	5.04050010	0.37999397	0.80745074
1	4.40801525	-0.50226478	-0.59821013
6	-1.65929132	-1.14608463	3.00996824
6	-1.07048153	-2.51846073	1.25318411
6	-2.56614563	-2.27453077	1.04040397
1	-0.48304144	-2.53714391	0.32716162
1	-0.87822617	-3.43244307	1.84595395
6	-2.99897434	-1.55946382	2.35021315
1	-1.43670630	-1.77286511	3.89168542
1	-1.60617302	-0.08814740	3.29720523
1	-3.12050212	-3.20523751	0.85957110
1	-2.69987169	-1.61123813	0.17476487
1	-3.62779279	-0.68596492	2.13345019
1	-3.56759664	-2.22597065	3.01355973
6	-2.81698790	0.53587911	-3.36117737
1	-3.41569121	1.09590426	-2.62889352
1	-2.59271501	1.20937152	-4.20522306
1	-3.44315735	-0.27930840	-3.76033518

Ph-C(Me)=N²-anion

*R*_{CN2-a}

E = -69.366226 E0 = -69.243805

No. of Negative Frequencies = 0



Atomic Coordinates:

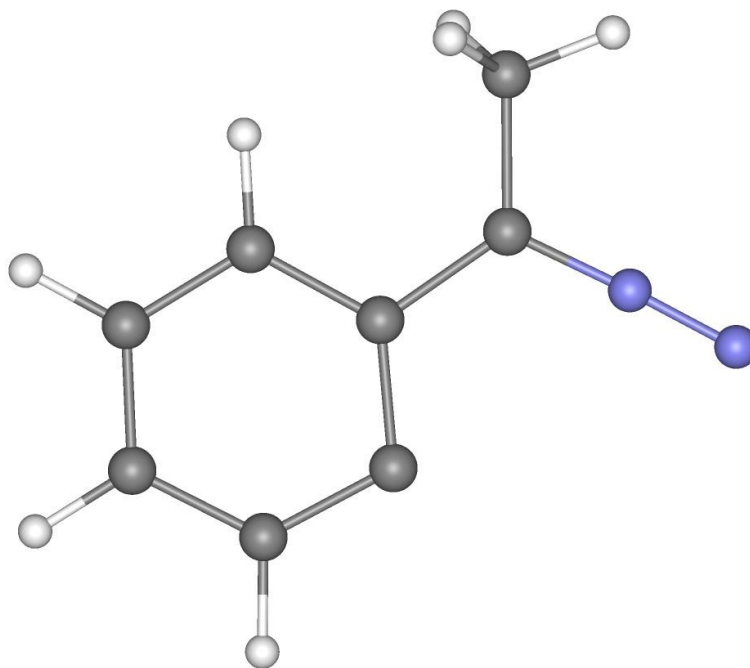
6	-0.41511831	-2.13990399	-0.72319273
6	-0.39109803	-2.65084461	0.57799596
6	-0.20666166	-0.76548043	-0.94993951
6	-0.15414044	-1.77369453	1.67221452
1	-0.14106690	-2.20710783	2.68344851
6	0.05695876	-0.40829438	1.49208485
6	0.02596738	0.08790548	0.15249173
6	0.25351493	1.50413393	0.09319242
1	-0.22664392	-0.37861712	-1.97690789
1	-0.59598158	-2.80726003	-1.57188099
1	-0.55380544	-3.72258580	0.74855165
7	0.45255441	2.04962230	1.30829406
7	0.66828435	2.97623600	1.99266811
6	0.29976198	2.38396138	-1.12726156
1	0.41437906	3.43991814	-0.84429782
1	1.13942342	2.12080471	-1.80091987
1	-0.62632798	2.29120679	-1.72654143

*TS*_{1-5-CN2-a}

E = -69.360917 E0 = -69.238843

No. of Negative Frequencies = 1

freq = - 399.60



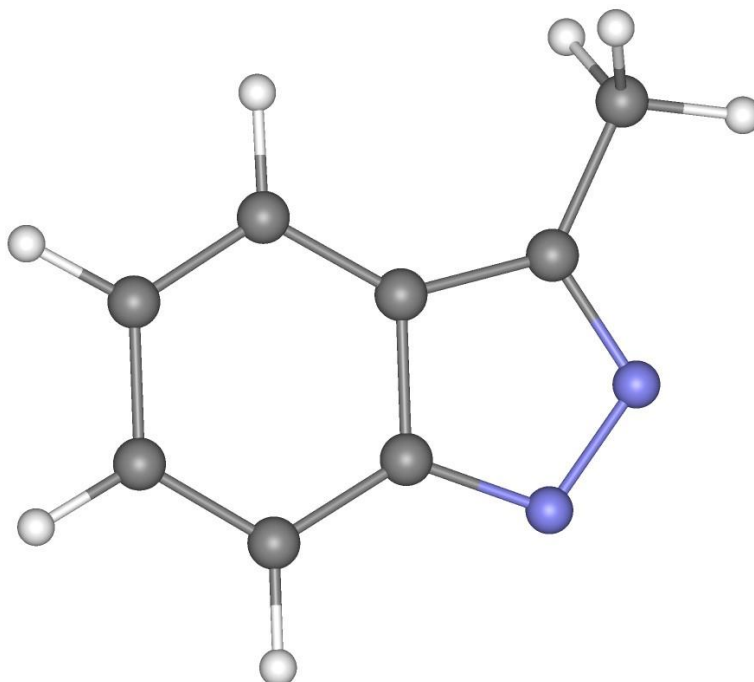
Atomic Coordinates:

6	1.14807251	-1.17268397	-1.47112491
6	2.18855338	-1.50165120	-0.59329399
6	0.08555858	-0.38430383	-1.00412226
6	2.14434330	-1.03370482	0.73744673
1	2.98942117	-1.32220793	1.38621019
6	1.11226557	-0.23713782	1.28378815
6	0.08080913	0.06510470	0.34159678
6	-1.08131049	0.89560913	0.75646776
1	-0.72412771	-0.13376965	-1.70367762
1	1.15517041	-1.52113729	-2.50841002
1	3.02700186	-2.11916010	-0.94791923
7	-1.14635774	1.34050105	1.98034368
7	-1.16307941	1.71339573	3.07410578
6	-2.22823138	1.27891099	-0.14959836
1	-2.96638371	1.89578063	0.38306226
1	-1.87370213	1.85132770	-1.02565235
1	-2.74800336	0.38512668	-0.53922259

*P*_{1-5-CN2-a}

E = -69.484373 E0 = -69.357449

No. of Negative Frequencies = 0



Atomic Coordinates:

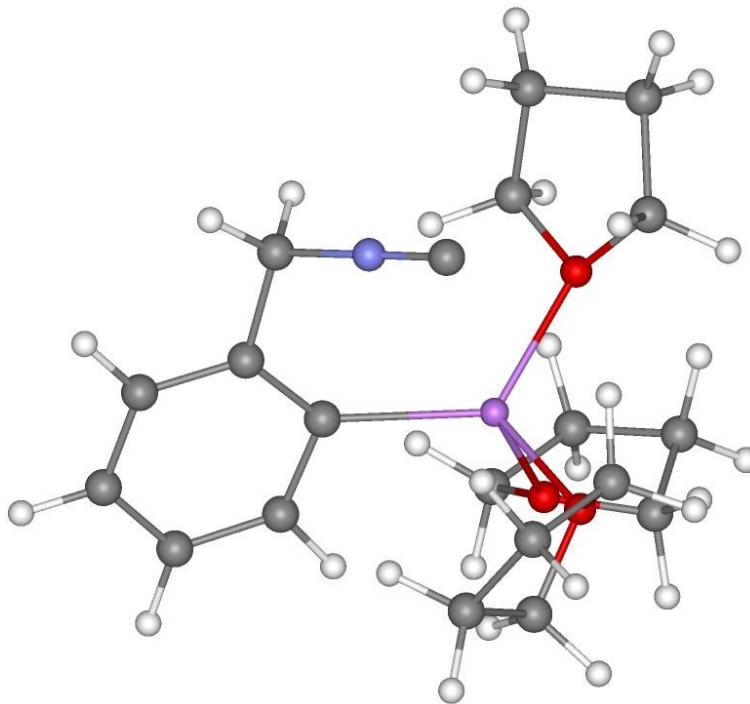
6	1.27312904	-1.22315342	-1.39655191
6	2.17429299	-1.39875767	-0.30876297
6	0.10430977	-0.47610397	-1.24295933
6	1.91950835	-0.83248820	0.93931779
1	2.61272356	-0.96785422	1.77499342
6	0.74071921	-0.07169988	1.11554748
6	-0.17721768	0.10850631	0.01259531
6	-1.20162073	0.90850129	0.58016206
1	-0.57944556	-0.34931937	-2.08998885
1	1.50461997	-1.68127662	-2.36279740
1	3.08253085	-1.99012791	-0.46076891
7	-0.90216982	1.16265467	1.88004650
7	0.27895285	0.57344408	2.22641264
6	-2.45293819	1.44743300	-0.04635316
1	-3.01167168	2.02596555	0.70553250
1	-2.24678210	2.11565580	-0.90343501
1	-3.11894080	0.64862057	-0.42299017

Ph-CH₂-NC-Li(THF)₃

R_{CNC}

E = -189.582049 E0 = -189.125058

No. of Negative Frequencies = 0



Atomic Coordinates:

6	0.51795640	-2.45313864	-4.17405535
6	0.45819407	-3.09073788	-2.93132496
6	0.33399170	-1.06602352	-4.22512688
6	0.22298631	-2.33274050	-1.77031116
1	0.19792539	-2.89109055	-0.82229816
6	0.02913931	-0.92735657	-1.75264876
3	0.09763646	-0.12191677	0.25729096
6	0.08963575	-0.34310320	-3.04355370
6	-0.17438770	1.15538329	-3.21838848
1	0.38285764	-0.55359730	-5.19268974
1	0.70815040	-3.01982951	-5.08793469
1	0.59891438	-4.17448484	-2.86728245
7	0.63793452	1.99135643	-2.38021805
6	1.29362254	2.66857700	-1.67379326
8	-1.12521711	1.44448881	0.87583643
8	-0.57870722	-1.56971850	1.60304985
8	1.96943937	0.00638210	1.15816009
6	-0.72794019	2.79095638	1.26538681
6	-2.37587829	1.50377225	0.13656656
6	-2.56953748	2.97416470	-0.23435815
1	-2.28246649	0.82116894	-0.72227589
1	-3.19147866	1.14612842	0.79115840
6	-1.93544551	3.68600646	0.97411939

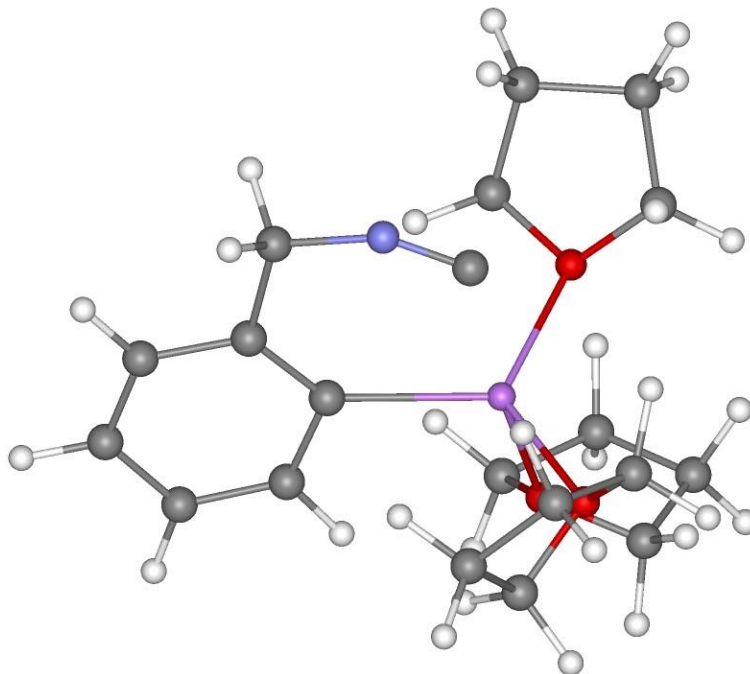
1	-0.44065784	2.76419803	2.32682217
1	0.14314835	3.08431618	0.65663024
1	-3.62606656	3.23308859	-0.38598476
1	-2.01309218	3.21732493	-1.15178456
1	-1.63929786	4.72122384	0.75906723
1	-2.63381048	3.69414944	1.82529961
6	2.90825081	1.10562366	1.03184081
6	2.74292714	-1.19499547	0.92903482
6	3.65179429	-0.83818861	-0.24709881
1	3.32331648	-1.43188954	1.84162468
1	2.03460586	-2.00865830	0.72705417
6	3.98320444	0.65483331	0.01257232
1	2.34224137	1.98338197	0.69545136
1	3.34729059	1.30674607	2.02505330
1	3.08867281	-0.95262136	-1.18319459
1	4.54727235	-1.47291114	-0.29308697
1	4.99187328	0.78113135	0.43040851
1	3.92061555	1.24368792	-0.91143593
6	-0.54681327	-1.35405951	3.02510668
6	-1.75875413	-2.36504310	1.35643958
6	-2.81806156	-1.88776332	2.38154940
1	-2.03336569	-2.21160481	0.30485360
1	-1.50865330	-3.43005634	1.51118469
6	-2.00191672	-1.04094385	3.39902616
1	-0.19029470	-2.27369058	3.52781163
1	0.16507982	-0.54076877	3.21563841
1	-3.30944188	-2.74478991	2.86202453
1	-3.59914791	-1.28417040	1.90062275
1	-2.19555939	0.03035551	3.25299062
1	-2.22773933	-1.29405583	4.44381661
1	-1.22403106	1.39244637	-2.97505391
1	-0.00091490	1.46905666	-4.25959318

*TS*_{I-5-CNC-C}

E = -189.578449 E0 = -189.122244

No. of Negative Frequencies = 1

freq = - 119.20



Atomic Coordinates:

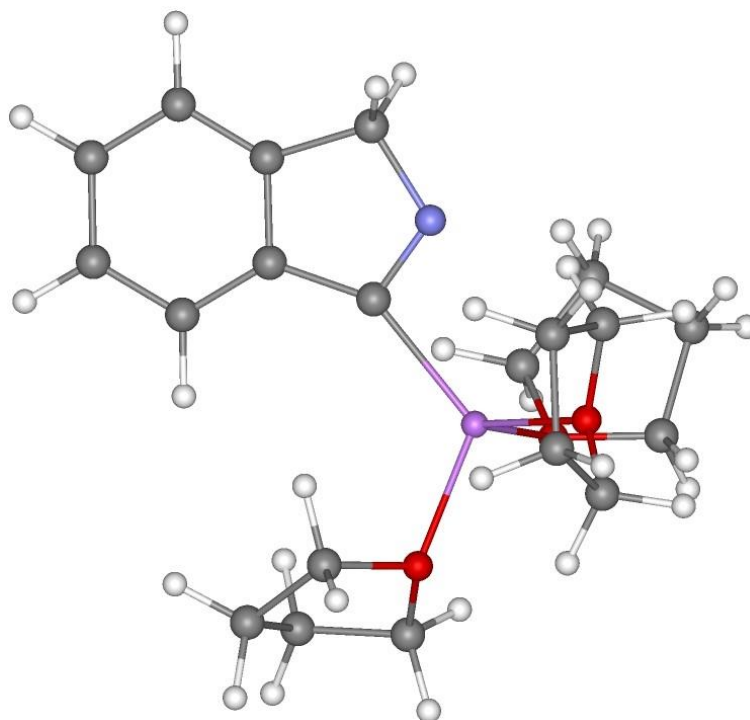
6	-0.04863396	-2.53756268	-4.14217665
6	-0.09536627	-3.07474098	-2.85069335
6	0.11864594	-1.15781491	-4.28978329
6	0.01154382	-2.21959484	-1.74225627
1	-0.02665338	-2.69330161	-0.75153434
6	0.17421989	-0.81109307	-1.83244573
3	0.23892811	0.04023674	0.22700312
6	0.23083342	-0.33043742	-3.15478013
6	0.41900062	1.16506882	-3.49871098
1	0.16968632	-0.72993989	-5.29852023
1	-0.12885400	-3.18033539	-5.02133878
1	-0.21033107	-4.15413439	-2.71063436
7	0.77977176	1.94266754	-2.35695406
6	0.97013140	2.02214998	-1.18875159
8	-1.38405661	1.31085718	0.80844481
8	-0.48572469	-1.52785919	1.57612205
8	2.09436717	-0.05810430	1.23067968
6	-1.21014783	2.61316574	1.42895266
6	-2.40671023	1.39830744	-0.22428730
6	-2.62637442	2.89181485	-0.46627227
1	-2.03690329	0.84177090	-1.09872431
1	-3.32655020	0.91294278	0.15031371
6	-2.37478110	3.47670485	0.93512071
1	-1.19679326	2.47159898	2.52052644
1	-0.23887198	3.02051074	1.10307276

1	-3.63091947	3.11142527	-0.85260557
1	-1.88211532	3.27559428	-1.17903407
1	-2.12209606	4.54542397	0.91975293
1	-3.26160624	3.34050698	1.57354547
6	3.03196487	1.04086958	1.32658029
6	2.86301785	-1.18736147	0.75410659
6	3.76328160	-0.59704349	-0.33228013
1	3.44987115	-1.60784502	1.59345268
1	2.15235288	-1.94033651	0.39027880
6	4.08136780	0.82254600	0.20872492
1	2.45425176	1.96547382	1.20832847
1	3.49846886	1.01911654	2.32788064
1	3.19268513	-0.53432276	-1.26884955
1	4.66433588	-1.20145347	-0.50463896
1	5.10079339	0.88642964	0.61485891
1	3.98084733	1.57719435	-0.58160623
6	-0.24634129	-1.51942864	2.99514591
6	-1.80255274	-2.09207700	1.42410481
6	-2.64405909	-1.49667353	2.57197850
1	-2.15462841	-1.84164821	0.41546303
1	-1.73414847	-3.19279064	1.51259908
6	-1.58139203	-1.08751101	3.63313549
1	0.03700141	-2.53891114	3.31995460
1	0.59241866	-0.83671097	3.17838408
1	-3.36652925	-2.22837824	2.95837511
1	-3.20342480	-0.61725884	2.22808557
1	-1.59602999	-0.00142933	3.79413521
1	-1.74128861	-1.57606925	4.60403287
1	-0.50714645	1.59197880	-3.92130460
1	1.20124348	1.28781239	-4.26495716

*P*_{1-5-CNC-C}

E = -189.634632 E0 = -189.175552

No. of Negative Frequencies = 0



Atomic Coordinates:

6	0.59126534	-1.92584208	-5.12333840
6	1.64094136	-1.86540247	-4.19173059
6	-0.69769260	-1.48569670	-4.77852439
6	1.41991872	-1.36193436	-2.90228942
1	2.23656054	-1.32244095	-2.17540043
6	0.13710307	-0.91627540	-2.55019749
3	0.03110310	0.17927290	0.78386481
6	-0.91274257	-0.98605119	-3.49296416
6	-2.13213791	-0.44995532	-2.79765750
1	-1.50657785	-1.54099461	-5.51226702
1	0.77989100	-2.32075395	-6.12405705
1	2.63460429	-2.21690980	-4.47956113
7	-1.67342396	-0.09257848	-1.42733458
6	-0.38071434	-0.34277218	-1.26740386
8	-0.95330548	1.81205140	1.53839395
8	-0.54739649	-1.32576250	2.08117350
8	1.97849006	0.61397911	1.33831525
6	-0.31813147	2.98757504	2.07848590
6	-2.06380466	2.30408156	0.74371587
6	-1.49940976	3.53304836	0.01398455
1	-2.35847413	1.48480089	0.06795130
1	-2.88993250	2.57984486	1.42599871
6	-0.36207352	4.04006899	0.94953567
1	-0.88961346	3.32885651	2.96184645
1	0.69195763	2.69613054	2.39440761

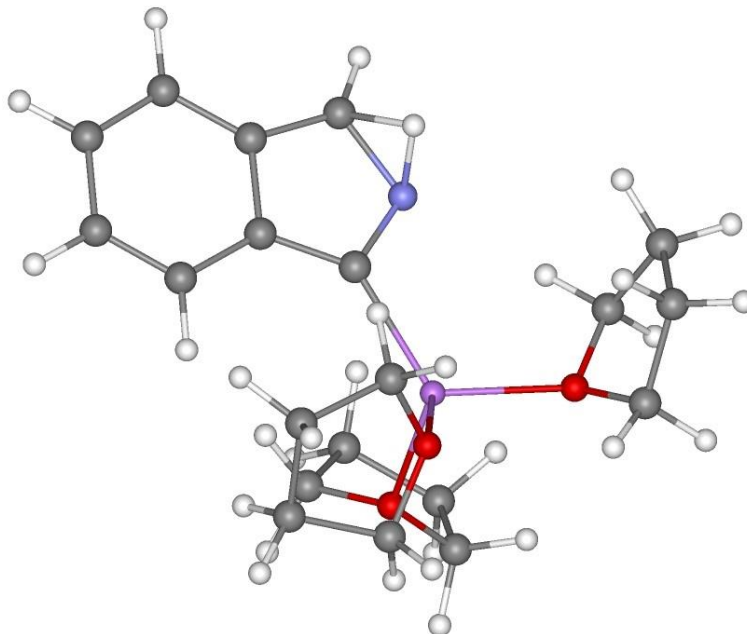
1	-2.27207507	4.29383853	-0.16164079
1	-1.09259596	3.22625664	-0.95878362
1	0.59501450	4.07897204	0.41188625
1	-0.56259214	5.04325621	1.35044970
6	2.78824439	1.10262572	0.22625244
6	2.74733601	-0.36657228	2.07104139
6	3.63168301	-1.02472400	1.01464845
1	3.35286950	0.13916539	2.84673353
1	2.02948037	-1.04341307	2.55366932
6	4.02570372	0.18406653	0.14228907
1	2.15131338	1.05040242	-0.66973481
1	3.06086763	2.15251377	0.42094377
1	3.03793196	-1.74662595	0.43460434
1	4.49923777	-1.54371599	1.44468524
1	4.91115416	0.68403751	0.56212845
1	4.25739940	-0.09751760	-0.89337836
6	-1.49725044	-1.07502461	3.14401404
6	-1.02843255	-2.51091629	1.40061981
6	-2.53806898	-2.28860477	1.29617589
1	-0.51417479	-2.55316408	0.43181192
1	-0.77605197	-3.40214519	2.00622251
6	-2.87697794	-1.54257438	2.61543572
1	-1.19255959	-1.65234151	4.03501866
1	-1.44485944	-0.00298013	3.37209878
1	-3.09508546	-3.22858850	1.18258256
1	-2.73629157	-1.64513813	0.42673095
1	-3.54552756	-0.69226255	2.42698394
1	-3.36789921	-2.20123661	3.34561201
1	-2.95298643	-1.18734267	-2.73928191
1	-2.55121111	0.44341341	-3.29476678

*TS*_{1-5-CNC-CN}

E = -189.571858 E0 = -189.117316

No. of Negative Frequencies = 1

freq = - 1444.01



Atomic Coordinates:

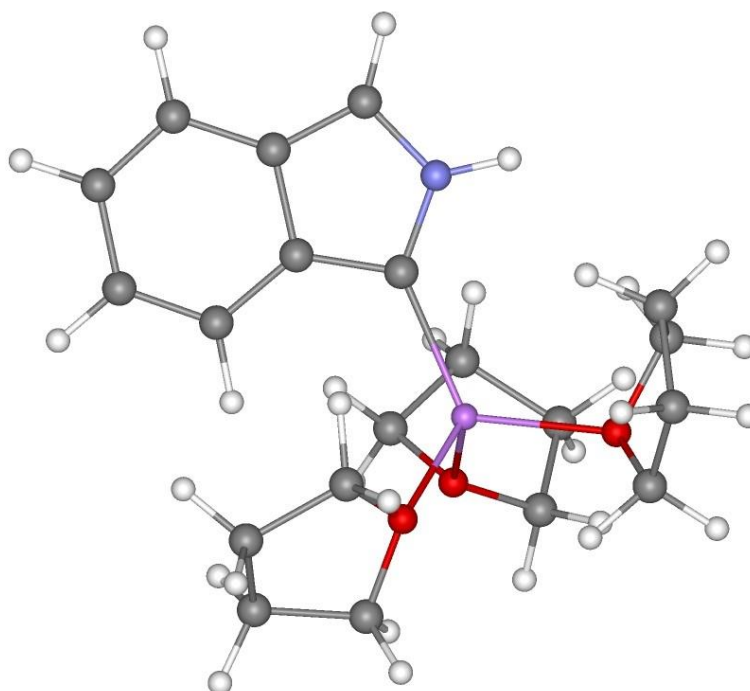
6	0.56081697	-2.39357114	-4.77430317
6	1.33731750	-2.59059487	-3.59626191
6	-0.49554207	-1.49620977	-4.79339449
6	1.05531186	-1.89158468	-2.43282420
1	1.65896709	-2.04731899	-1.53315429
6	-0.02546848	-0.96751654	-2.40507209
3	-0.00918420	0.27145036	0.70710369
6	-0.80208802	-0.77643573	-3.60985870
6	-1.79075072	0.17756043	-3.28928080
1	-1.08187428	-1.35219859	-5.70430480
1	0.80764031	-2.96063186	-5.67465169
1	2.16537153	-3.30288122	-3.62094087
7	-1.62005222	0.53242236	-1.84702378
6	-0.49859065	-0.11846113	-1.34663479
8	-1.03063952	1.80595824	1.61046674
8	-0.41333520	-1.32565413	1.96771102
8	1.94866577	0.74326312	1.12573796
6	-0.39738596	2.97705067	2.16007853
6	-2.22241780	2.28104631	0.92693514
6	-1.86559792	3.67992092	0.37098680
1	-2.45409754	1.55087882	0.13911772
1	-3.04664409	2.33713329	1.66040104
6	-0.51379146	4.03048670	1.05249109
1	-0.93745443	3.29133372	3.07373734
1	0.63192194	2.69998286	2.42221669
1	-2.64715462	4.41177965	0.61720249

1	-1.76186551	3.64867497	-0.72110807
1	0.31568598	3.91265609	0.34135138
1	-0.48571556	5.05519233	1.44772256
6	2.73273346	1.10224495	-0.04878534
6	2.79244784	-0.04937644	1.98502533
6	3.61198697	-0.90651089	1.02102641
1	3.44122082	0.61482231	2.58758207
1	2.13126401	-0.61784217	2.65246428
6	3.88647872	0.07323807	-0.14404303
1	2.03869643	1.06849346	-0.90079618
1	3.11216252	2.13003341	0.07967526
1	3.00372853	-1.75685880	0.68042046
1	4.53225398	-1.29809737	1.47562232
1	4.85924167	0.56855778	-0.01416131
1	3.89646552	-0.43655676	-1.11588592
6	-1.38038346	-1.20843036	3.03592285
6	-0.78249795	-2.52862427	1.24979329
6	-2.30898719	-2.45592977	1.15098101
1	-0.27438793	-2.49622646	0.27820748
1	-0.44503297	-3.40932454	1.82791937
6	-2.72087927	-1.72831331	2.46186241
1	-1.04445841	-1.82580752	3.88850417
1	-1.39862526	-0.15352733	3.33765298
1	-2.76733816	-3.44903567	1.05196503
1	-2.58060610	-1.85491008	0.27236068
1	-3.41237615	-0.90198814	2.25056749
1	-3.21319181	-2.40515448	3.17387995
1	-2.73286347	0.41361129	-3.78191126
1	-1.35910104	1.32778089	-2.73029634

*P*_{1-5-CNC-CN}

E = -189.639743 E0 = -189.179402

No. of Negative Frequencies = 0



Atomic Coordinates:

6	0.78793334	-2.41930465	-4.46507144
6	1.40289439	-2.50415682	-3.17865253
6	-0.28271739	-1.57216577	-4.69368989
6	0.94325691	-1.73508901	-2.12035913
1	1.42114165	-1.81520245	-1.13799999
6	-0.15150865	-0.84645709	-2.30167575
3	-0.15790856	0.25353738	0.64195020
6	-0.77351829	-0.77355537	-3.62394172
6	-1.80857016	0.15721330	-3.51021174
1	-0.74398468	-1.52138291	-5.68358759
1	1.17235222	-3.03815811	-5.27907969
1	2.24178955	-3.18908408	-3.03454435
7	-1.78192277	0.59391032	-2.19561384
6	-0.80220987	0.03655075	-1.38211141
8	-0.98773619	1.81411249	1.77112832
8	-0.49840980	-1.38297289	1.85672124
8	1.84497102	0.58934838	0.85212924
6	-0.17763582	2.93885428	2.19285625
6	-2.15094443	2.38314518	1.13311384
6	-1.58613634	3.52372180	0.28388092
1	-2.62837293	1.57667943	0.56028027
1	-2.85170499	2.75397915	1.90528717
6	-0.44572441	4.07971444	1.17656558
1	-0.47962534	3.23068892	3.21363334
1	0.86225366	2.58924004	2.20970807
1	-2.34071232	4.28182591	0.03390308

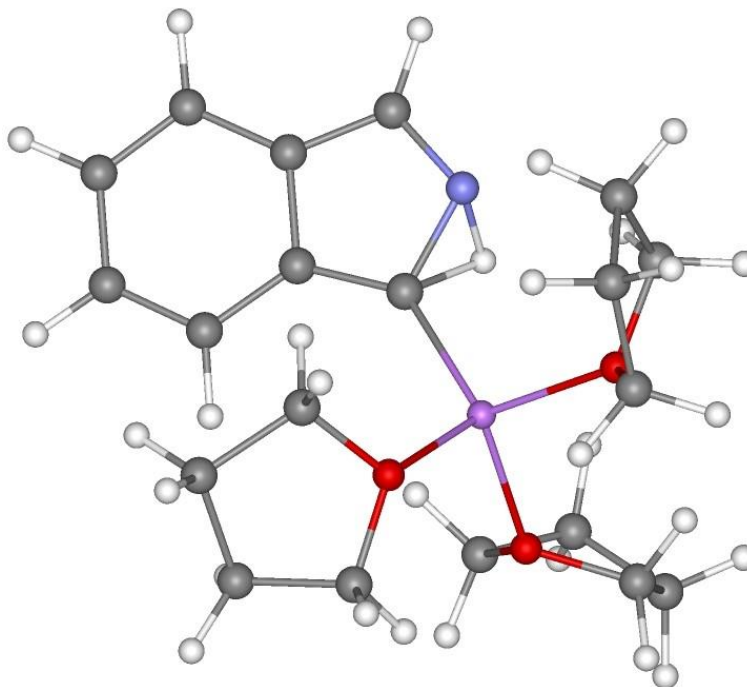
1	-1.17331028	3.10725059	-0.64627521
1	0.44684325	4.31292075	0.58173435
1	-0.75259925	4.99746256	1.69708129
6	2.59851429	1.06959031	-0.29706584
6	2.77082680	-0.10085897	1.71401713
6	3.70537664	-0.84023907	0.75564172
1	3.32331380	0.63385852	2.33118686
1	2.17772680	-0.75267473	2.36930376
6	3.83527809	0.14707876	-0.43114158
1	1.91233287	1.02973765	-1.15380130
1	2.89334756	2.11729466	-0.11188831
1	3.23410486	-1.77812201	0.42973937
1	4.67309506	-1.08435540	1.21470955
1	4.76376683	0.73058550	-0.35821511
1	3.84133150	-0.37910401	-1.39377046
6	-1.34709627	-1.29872520	3.02372984
6	-0.95270237	-2.55717947	1.13742892
6	-2.47937353	-2.46618376	1.20020490
1	-0.54644375	-2.49774005	0.12047831
1	-0.56933688	-3.45989405	1.64870548
6	-2.74415310	-1.79756305	2.57830608
1	-0.92711704	-1.94437825	3.81589601
1	-1.32688836	-0.25444647	3.36114301
1	-2.96055170	-3.44848010	1.10246682
1	-2.82723791	-1.82291961	0.38004763
1	-3.45590284	-0.96633867	2.48450391
1	-3.15501264	-2.50803706	3.30894848
1	-2.53376340	0.52844626	-4.22850617
1	-2.45161883	1.27802174	-1.85922788

*TS*_{I-5-CNC-N}

E = -189.587254 E0 = -189.132800

No. of Negative Frequencies = 1

freq = - 1314.43



Atomic Coordinates:

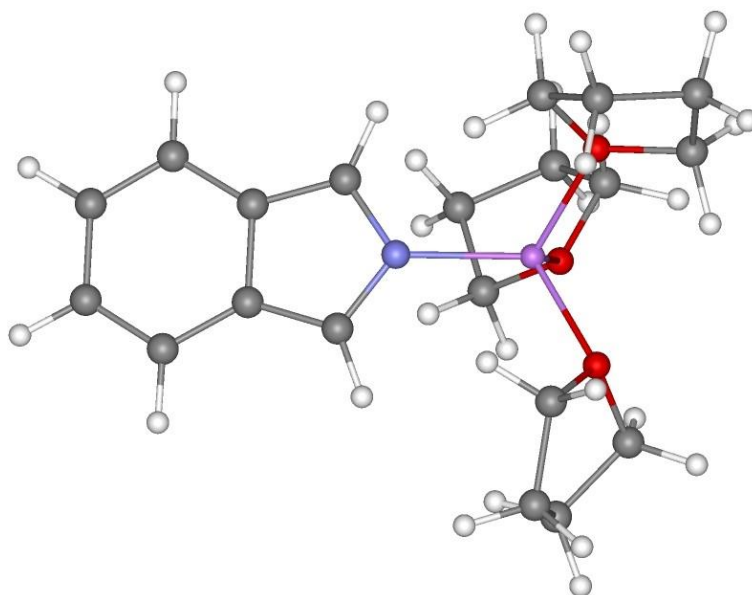
6	0.91050105	-1.82428449	-4.93518846
6	1.49861434	-2.26958192	-3.71408174
6	-0.17588045	-0.96634027	-4.94008962
6	1.00161794	-1.84392687	-2.49158469
1	1.45559587	-2.19138664	-1.55813299
6	-0.10924264	-0.96010440	-2.45255762
3	-0.23813803	0.17697586	0.68151010
6	-0.71436302	-0.53039879	-3.69619899
6	-1.80660745	0.28252967	-3.34789768
1	-0.61667577	-0.63733015	-5.88440753
1	1.32847589	-2.17445698	-5.88191665
1	2.34839027	-2.95492227	-3.75299823
7	-1.85914009	0.45235748	-1.98766372
6	-0.76810887	-0.33224899	-1.34585690
8	-1.11258740	1.88445239	1.40678948
8	-0.63635346	-1.26504939	2.08689238
8	1.76026602	0.56669093	0.95160492
6	-0.37320410	2.93934602	2.05709071
6	-2.10347148	2.55927830	0.58875232
6	-1.34803455	3.74109453	-0.03295143
1	-2.46473855	1.83595781	-0.15484319
1	-2.92899993	2.89715758	1.24258432
6	-0.24035587	4.06805152	1.01044721
1	-0.94154821	3.28062605	2.94182750
1	0.58340385	2.51275559	2.38483266

1	-2.01177884	4.59423521	-0.22737783
1	-0.90540873	3.42769234	-0.98786897
1	0.75265734	4.05621473	0.54159575
1	-0.37989894	5.05399295	1.47479483
6	2.52087187	0.95586734	-0.22991417
6	2.63957158	-0.18993468	1.80778768
6	3.49813441	-1.00400994	0.84120887
1	3.25816837	0.50049819	2.41295043
1	2.00461785	-0.78793893	2.47520516
6	3.73328425	-0.00336783	-0.31352794
1	1.83451694	0.87248709	-1.08355041
1	2.83786594	2.00607959	-0.11637229
1	2.92944912	-1.87737168	0.49051722
1	4.43320435	-1.35874805	1.29580395
1	4.67342100	0.54638544	-0.16333214
1	3.78699683	-0.50391820	-1.28845794
6	-1.54697051	-1.01215494	3.19566311
6	-0.94898856	-2.56292668	1.51712321
6	-2.44908928	-2.71946817	1.73842814
1	-0.65356377	-2.52484071	0.45971279
1	-0.37384486	-3.34528832	2.04591377
6	-2.62347805	-2.11757777	3.14677805
1	-0.97391933	-1.02693520	4.13678329
1	-1.95981963	-0.00362053	3.04676418
1	-2.78445509	-3.76316403	1.67343620
1	-2.99102324	-2.12679328	0.98615205
1	-3.63179787	-1.71746758	3.31667806
1	-2.42942303	-2.88196790	3.91373264
1	-2.55183416	0.74070489	-3.99693589
1	-2.13688131	-0.47390592	-1.28565394

*P*_{1-5-CNC-N}

E = -189.688177 E0 = -189.228476

No. of Negative Frequencies = 0



Atomic Coordinates:

6	-2.13065132	-1.98808853	-4.93978001
6	-0.78418632	-2.40227198	-5.16170792
6	-2.47160148	-1.21740045	-3.83766016
6	0.22941568	-2.04832381	-4.28301077
1	1.25758274	-2.37181153	-4.46783090
6	-0.08636271	-1.26338252	-3.14403387
3	0.15123086	0.34370734	0.73116522
6	-1.45887224	-0.84123808	-2.91781105
6	-1.43313926	-0.08937659	-1.72199243
1	-3.50807122	-0.90510372	-3.68181985
1	-2.90169824	-2.28414660	-5.65476074
1	-0.55312564	-3.00682882	-6.04174949
7	-0.15862635	-0.02893189	-1.21485016
6	0.65705965	-0.73173697	-2.06648227
8	-0.72263688	2.05596613	1.36887510
8	-0.51299067	-1.25100409	1.79898021
8	2.10036446	0.64930671	1.23394089
6	-0.24335570	2.82037804	2.51150346
6	-1.18310590	2.97065764	0.33260789
6	-0.46702955	4.28610161	0.62552681
1	-0.93471519	2.51507224	-0.63583384
1	-2.27892774	3.08117140	0.41556099
6	-0.46395508	4.30065837	2.16489696
1	-0.80024656	2.50078031	3.40584828
1	0.82198942	2.57650727	2.65146583
1	-0.98026597	5.15230425	0.18734333
1	0.56065146	4.25364548	0.23283657
1	0.31498040	4.94582802	2.59244868

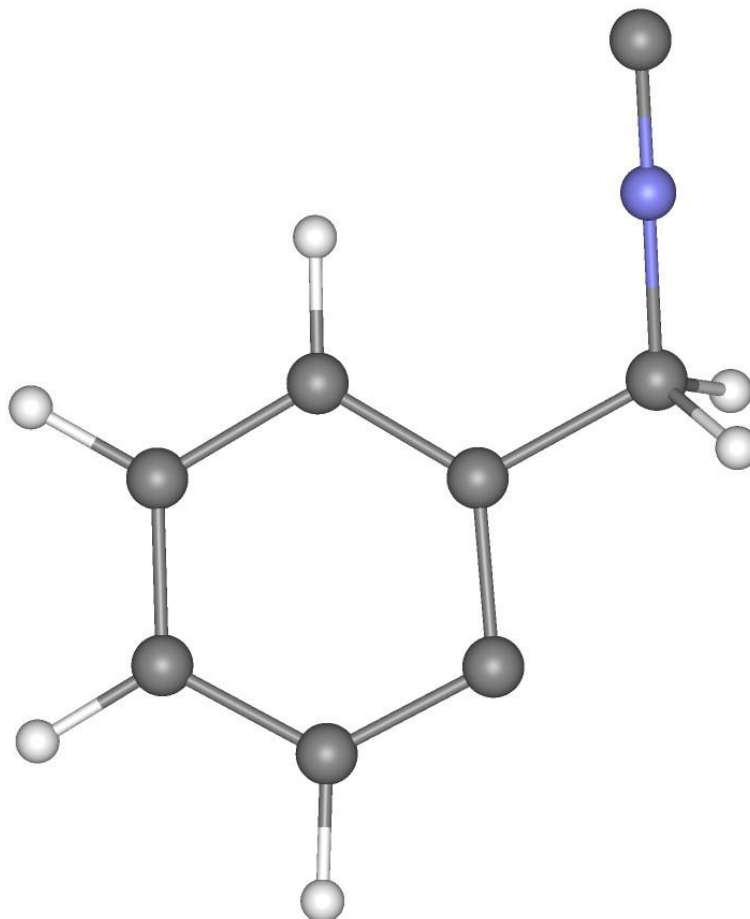
1	-1.43807471	4.64680989	2.54206051
6	2.92177970	1.22630661	0.17377409
6	2.87327006	-0.37770923	1.89580296
6	3.72781448	-0.98129324	0.78438731
1	3.49878742	0.07945181	2.68538118
1	2.15797043	-1.07147329	2.35779539
6	4.12183168	0.27240022	-0.02506830
1	2.28024000	1.30688437	-0.71572590
1	3.24175568	2.23442876	0.48380236
1	3.11563114	-1.66271035	0.17565641
1	4.59764773	-1.53388154	1.16459612
1	5.04183877	0.71666291	0.38194124
1	4.29526089	0.04946961	-1.08561356
6	-1.66297421	-1.08202622	2.67848627
6	-0.67306550	-2.48392041	1.03033349
6	-2.17164021	-2.76273965	1.04512674
1	-0.26031454	-2.30036168	0.02906813
1	-0.10464477	-3.28678036	1.53307667
6	-2.55825457	-2.31172775	2.46524736
1	-1.29821987	-0.98537008	3.71292838
1	-2.17123407	-0.14727827	2.39014787
1	-2.40556448	-3.81765693	0.84962409
1	-2.66819906	-2.14467094	0.28286097
1	-3.62394792	-2.06663964	2.56661106
1	-2.31708698	-3.09858065	3.19634052
1	-2.26564041	0.39301090	-1.20874707
1	1.72532267	-0.83304408	-1.87357106

Ph-CH₂-NC-anion

R_{CNC-a}

E = -58.832656 E0 = -58.724583

No. of Negative Frequencies = 0



Atomic Coordinates:

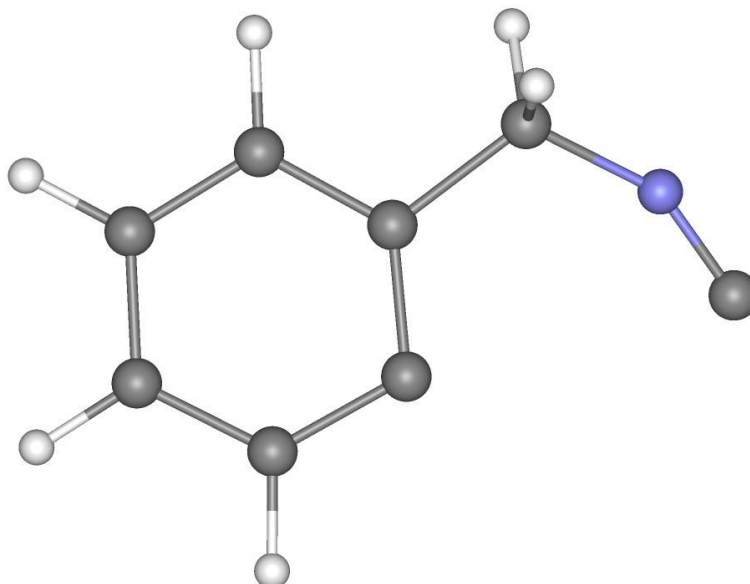
6	0.75768331	-1.46445638	-0.87186054
6	0.11787325	-2.29972873	0.05379794
6	0.56183810	-0.07690283	-0.78153823
6	-0.70522322	-1.74007874	1.05119938
1	-1.18453105	-2.44601689	1.74946553
6	-0.93935795	-0.35102714	1.21006561
6	-0.25925054	0.43086536	0.23935859
6	-0.53021065	1.93712627	0.35413182
1	1.05967504	0.58542205	-1.50071587
1	1.40221375	-1.87976263	-1.65211055
1	0.26704603	-3.38756026	-0.00424983
7	0.38191647	2.80901346	-0.34140472
6	1.13604600	3.51687400	-0.90746854
1	-0.52396582	2.20023138	1.42260546
1	-1.54175273	2.16600107	-0.02127603

TS_{1-5-CNC-C-a}

E = -58.822081 E0 = -58.714750

No. of Negative Frequencies = 1

freq = - 121.30



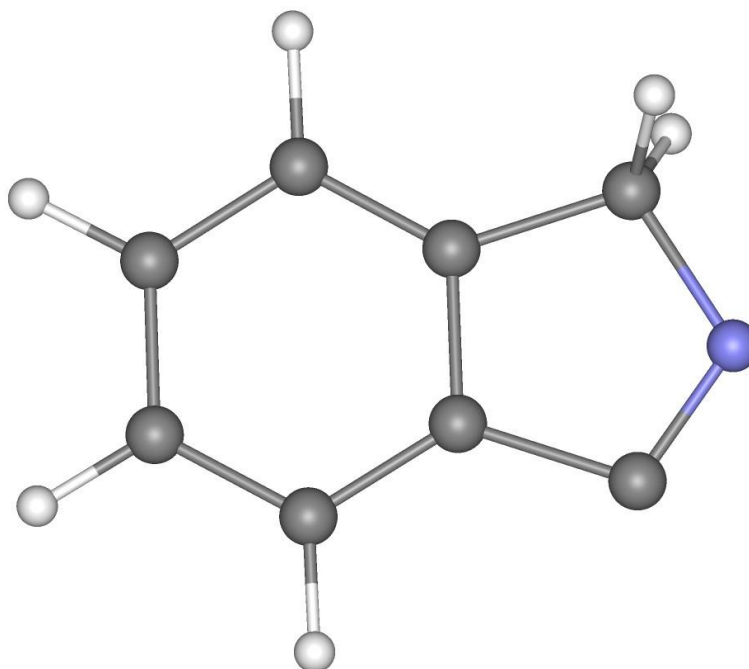
Atomic Coordinates:

6	0.75769495	-0.88369808	-1.60986810
6	1.93959008	-0.78608718	-0.86032289
6	-0.42698838	-0.36891457	-1.06492953
6	1.90821052	-0.17863783	0.40883119
1	2.86420364	-0.12606469	0.95609106
6	0.74083585	0.35627939	1.00751124
6	-0.41013004	0.23175407	0.20989500
6	-1.77492138	0.80948733	0.66725734
1	-1.36023719	-0.44723196	-1.64637367
1	0.75305445	-1.36102562	-2.59413947
1	2.87690200	-1.19192438	-1.26775071
7	-1.89699677	0.94901841	2.08423134
6	-1.44221233	1.00723329	3.18360592
1	-2.60155067	0.17733949	0.29879086
1	-1.92745475	1.81247232	0.22717042

$R_{CNC-C-a}$

E = -58.868731 E0 = -58.758731

No. of Negative Frequencies = 0



Atomic Coordinates:

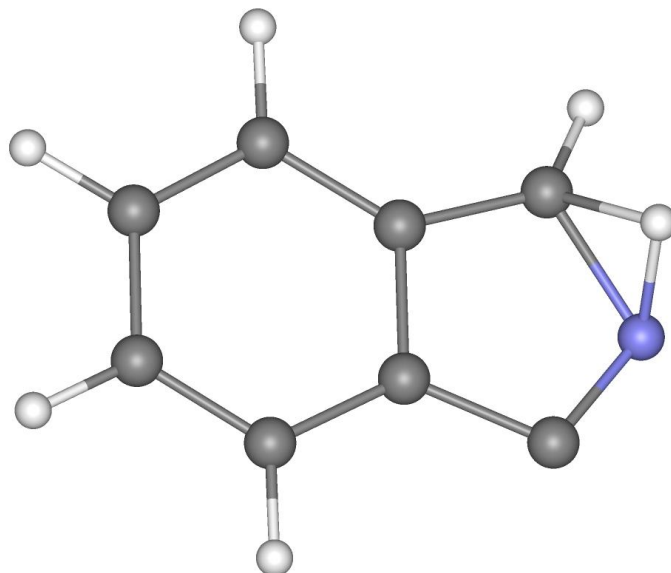
6	0.81909180	-0.75953343	-1.60859138
6	1.86515262	-0.69498589	-0.67144133
6	-0.47316784	-0.31898588	-1.26158573
6	1.63710967	-0.19225367	0.61871054
1	2.44176453	-0.13550420	1.36014436
6	0.35373403	0.24878106	0.97310785
6	-0.69393838	0.18042969	0.02388138
6	-1.90703276	0.72616778	0.73154647
1	-1.27817729	-0.37605947	-2.00415767
1	1.01030759	-1.15383300	-2.61179927
1	2.86355936	-1.04204658	-0.95855083
7	-1.43617229	1.08648163	2.11073578
6	-0.14781107	0.82583089	2.28148166
1	-2.72967875	-0.01348973	0.79064051
1	-2.32474122	1.61900079	0.22587766

*TS*_{1-5-CNC-CN-a}

E = -58.811586 E0 = -58.706210

No. of Negative Frequencies = 1

freq = - 1444.68



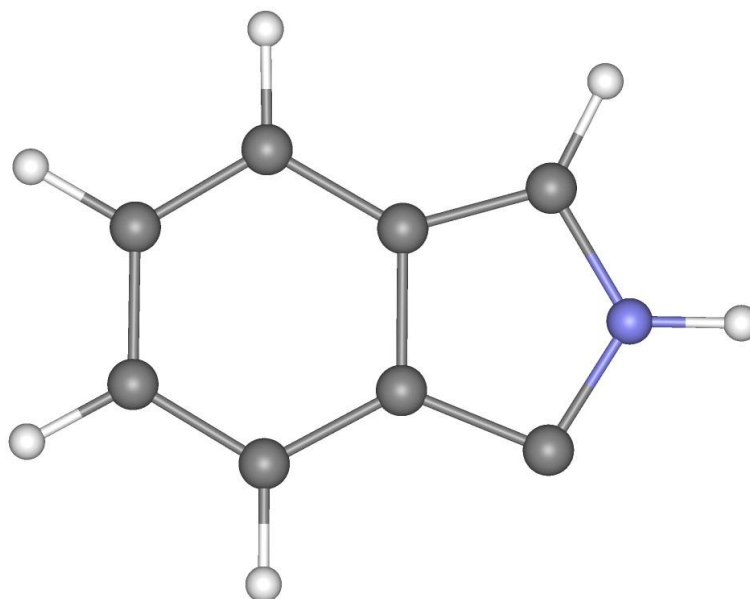
Atomic Coordinates:

6	0.82818446	-0.84140651	-1.60326158
6	1.88405812	-0.65242576	-0.66497137
6	-0.47723275	-0.47388428	-1.29941844
6	1.62679474	-0.09521913	0.58260341
1	2.42837685	0.06314795	1.31137075
6	0.30850321	0.28212220	0.93832442
6	-0.76166559	0.08497562	-0.02430283
6	-1.94225887	0.54175248	0.59516896
1	-1.27135747	-0.62214393	-2.03944112
1	1.05396673	-1.27805502	-2.58167520
1	2.90109901	-0.94850980	-0.93948303
7	-1.54024879	0.98673773	2.02601610
6	-0.16794859	0.89313560	2.15699260
1	-2.98538141	0.29943426	0.38075617
1	-1.88488965	1.76033859	1.16132117

$R_{CNC-CN-a}$

E = -58.884677 E0 = -58.773407

No. of Negative Frequencies = 0



Atomic Coordinates:

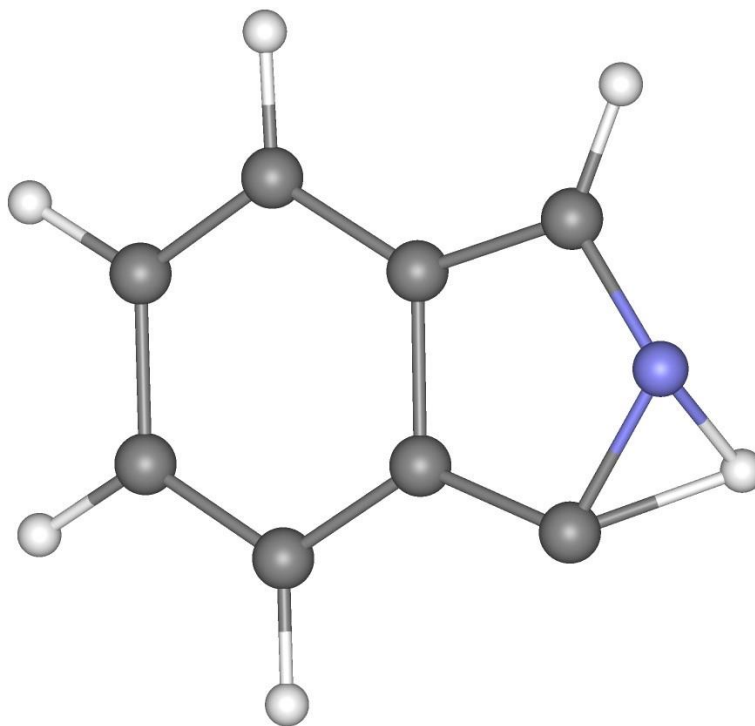
6	1.01519768	-1.30332555	-1.21952436
6	1.62900724	-1.38512422	0.06822236
6	-0.05902189	-0.45631194	-1.45680814
6	1.15629813	-0.60876855	1.12300873
1	1.62026977	-0.66387164	2.11405846
6	0.06514012	0.27046374	0.93733847
6	-0.56009742	0.34808632	-0.39321431
6	-1.59121356	1.28169789	-0.27238190
1	-0.51047916	-0.41403744	-2.45493009
1	1.40267915	-1.92306126	-2.03514335
1	2.47402311	-2.06403338	0.21678124
7	-1.54651706	1.70836660	1.06311480
6	-0.57520744	1.15140882	1.87745017
1	-2.31886909	1.66181951	-0.98768116
1	-2.20120957	2.39669110	1.41970907

*TS*_{I-5-CNC-N-a}

E = -58.836714 E0 = -58.730749

No. of Negative Frequencies = 1

freq = - 1372.14



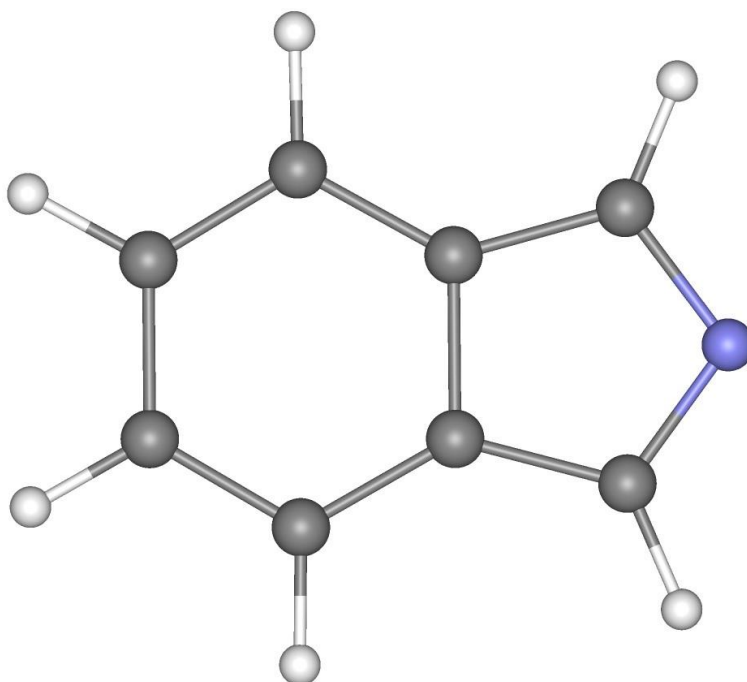
Atomic Coordinates:

6	0.97407827	-1.32420557	-1.17154226
6	1.57013734	-1.36184038	0.12543370
6	-0.06605713	-0.45432749	-1.46597065
6	1.12310885	-0.50627604	1.12768727
1	1.58575005	-0.51198084	2.12038825
6	0.06333359	0.39392216	0.87103201
6	-0.56630055	0.40506097	-0.44288777
6	-1.60229558	1.34722433	-0.37501996
1	-0.50206768	-0.44318417	-2.47096170
1	1.35236274	-1.99598157	-1.94927660
1	2.38617998	-2.06406641	0.31933050
7	-1.57041575	1.98438703	0.85766067
6	-0.52419540	1.40200996	1.71078795
1	-2.32876060	1.62632337	-1.14021676
1	-1.89485815	1.50293466	1.88355535

$R_{CNC-N-a}$

E = -58.946251 E0 = -58.834969

No. of Negative Frequencies = 0



Atomic Coordinates:

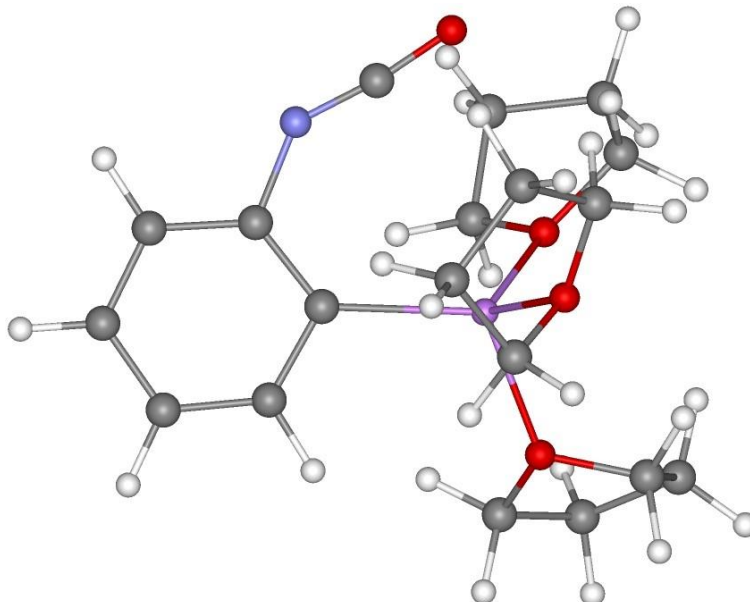
6	-1.20799336	-0.68352390	-1.46827788
6	0.13852797	-1.09758138	-1.69068719
6	-1.54355647	0.08736791	-0.35706967
6	1.15103169	-0.74118522	-0.80215798
1	2.18087745	-1.06756353	-0.98754609
6	0.84363183	0.04192464	0.33749005
6	-0.53804037	0.46669659	0.56575936
6	-0.49761306	1.21817005	1.76584771
1	-2.58323718	0.39728393	-0.20057931
1	-1.98322017	-0.97806745	-2.18258879
1	0.37355920	-1.70275416	-2.57187807
7	0.76925730	1.28135529	2.27177883
6	1.57734531	0.58026418	1.42304624
1	-1.32816958	1.70994755	2.27686210
1	2.64759945	0.48766550	1.62000069

Ph-NCO-Li(THF)₃

R_{NCO}

E = -198.796352 E0 = -198.361927

No. of Negative Frequencies = 0



Atomic Coordinates:

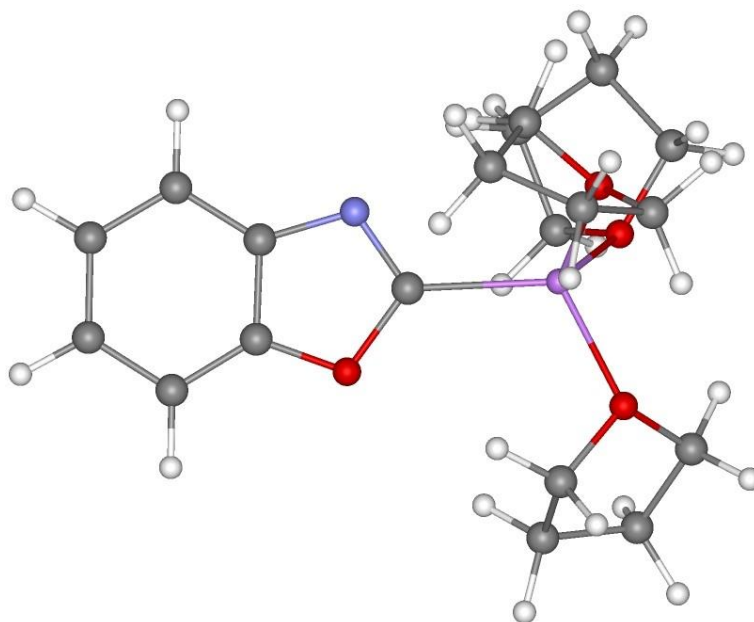
6	-0.03684251	-2.24111749	-4.42101009
6	-0.18992067	-2.98296459	-3.24460285
6	0.21920004	-0.86982937	-4.32852247
6	-0.09667886	-2.33648198	-1.99884301
1	-0.21552104	-2.96976705	-1.10787642
6	0.15011599	-0.95130752	-1.82309947
3	0.18368284	-0.19468148	0.20426654
6	0.31205993	-0.27442962	-3.05745097
7	0.60382929	1.12524123	-3.06870867
1	0.35330666	-0.26379755	-5.22764434
1	-0.10983411	-2.71975289	-5.39962458
1	-0.38132590	-4.05886152	-3.29807779
6	0.86625561	2.00698139	-2.28856151
8	1.13870330	2.96378789	-1.62719697
8	-1.15326245	1.34759088	0.57963699
8	-0.47548904	-1.56809103	1.61003564
8	2.05258922	0.04766654	1.04827985
6	-0.95720752	2.68176771	1.12677416
6	-2.29887634	1.35651412	-0.32120158
6	-2.55398603	2.82767174	-0.64075952
1	-2.03563980	0.73160512	-1.18708150
1	-3.16177315	0.90457881	0.20153996
6	-2.17341331	3.50454918	0.68804427
1	-0.85627931	2.59424032	2.21943779
1	-0.02470492	3.09195575	0.70830407
1	-3.59340861	3.01751471	-0.94028224

1	-1.88983447	3.16695809	-1.44882527
1	-1.93227197	4.57010022	0.57817502
1	-2.99390469	3.40883986	1.41603692
6	2.90808154	1.21502421	0.92987347
6	2.86933846	-1.09763728	0.70170201
6	3.70932180	-0.61146882	-0.47631569
1	3.49410436	-1.37721459	1.57131988
1	2.18731876	-1.92312395	0.45813150
6	4.01927942	0.85524303	-0.08908410
1	2.27487977	2.04972770	0.60266648
1	3.32678073	1.44730530	1.92407728
1	3.09664399	-0.65468828	-1.38767562
1	4.61557129	-1.21338806	-0.62795515
1	5.01158459	0.94446443	0.37524845
1	3.99673920	1.51884809	-0.96303172
6	-0.35985015	-1.31615612	3.02268564
6	-1.71472050	-2.29203857	1.44698923
6	-2.69067580	-1.71503293	2.50216564
1	-2.03528198	-2.15646236	0.40616412
1	-1.52444906	-3.36549618	1.62560800
6	-1.77221986	-0.90239310	3.45815327
1	-0.03559218	-2.24279684	3.53368854
1	0.40997358	-0.54490052	3.15401841
1	-3.21979630	-2.52198422	3.02687550
1	-3.44663295	-1.06821871	2.03805021
1	-1.90941230	0.17532396	3.29722059
1	-1.96055457	-1.11941764	4.51826208

*P*_{1-5-NCO}

E = -198.813409 E0 = -198.376533

No. of Negative Frequencies = 0



Atomic Coordinates:

6	-0.54397465	-1.45162278	-5.55532494
6	0.31546168	-2.48492476	-5.13133253
6	-0.99325349	-0.46441991	-4.66461736
6	0.75567858	-2.56803105	-3.80367690
1	1.42170759	-3.36750546	-3.47406808
6	0.31324716	-1.58772273	-2.90449420
3	-0.02584473	0.39754183	0.87452678
6	-0.54545673	-0.56341657	-3.34804753
8	-0.81787956	0.24773414	-2.28248678
1	-1.65841710	0.33777431	-4.98738965
1	-0.86714147	-1.41733181	-6.59750089
1	0.64315880	-3.23412789	-5.85461537
6	-0.09431586	-0.31182863	-1.14791248
7	0.56358350	-1.38978011	-1.54242586
8	-1.30794810	1.91150167	1.30257178
8	-0.40693674	-1.10693843	2.18372520
8	1.83868282	1.06299351	1.38720248
6	-0.83829340	3.20564226	1.74715100
6	-2.29933919	2.18394966	0.28170135
6	-1.69208066	3.32288257	-0.54214327
1	-2.44769215	1.25654907	-0.28529646
1	-3.24422430	2.48460818	0.77166633
6	-0.86999563	4.12738684	0.50365020
1	-1.51453831	3.57524571	2.53838830
1	0.16313522	3.05434961	2.17054694
1	-2.46073346	3.93150250	-1.03704221
1	-1.03704406	2.89731441	-1.31375438
1	0.14254544	4.33389983	0.13280370

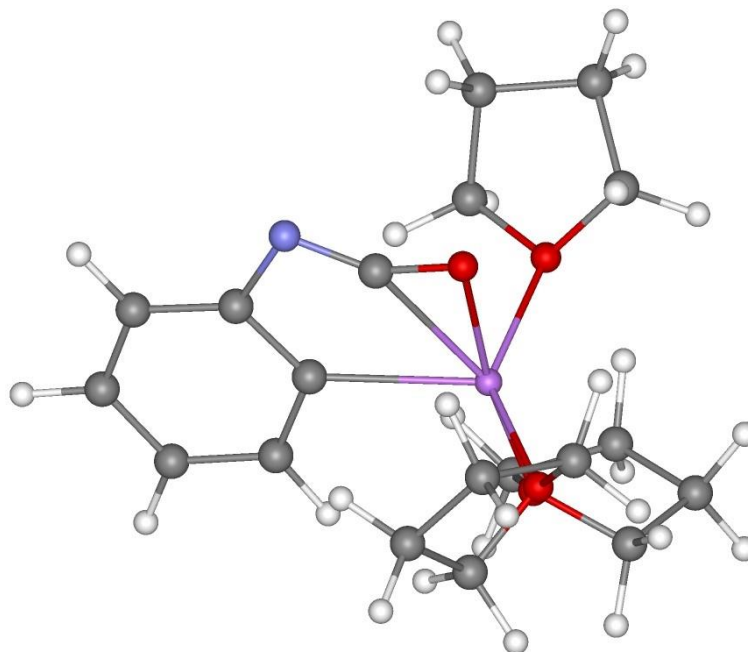
1	-1.34113077	5.08996150	0.74571127
6	2.74949810	1.21146308	0.26915986
6	2.60708617	0.40729174	2.42432124
6	3.57806778	-0.55623156	1.69953352
1	3.15686062	1.17624438	2.99577976
1	1.88873723	-0.09106998	3.08780592
6	3.49385146	-0.12490173	0.20837173
1	2.13950814	1.42116704	-0.61871960
1	3.42856491	2.06099459	0.47136927
1	3.26945829	-1.60279437	1.82168142
1	4.59533761	-0.45667799	2.10300577
1	4.48156625	-0.02854771	-0.26234026
1	2.89302628	-0.84084819	-0.37005717
6	-1.54421983	-1.08695138	3.07982800
6	-0.34930862	-2.44450999	1.62305753
6	-1.81244211	-2.78492259	1.34280145
1	0.27556461	-2.39645299	0.72028519
1	0.09681740	-3.12843502	2.36941977
6	-2.56358611	-2.11384349	2.52226559
1	-1.20444987	-1.36691323	4.09240223
1	-1.91437895	-0.05299338	3.10155446
1	-1.98996982	-3.86715988	1.28584782
1	-2.10428532	-2.33308765	0.38460208
1	-3.48834832	-1.62742740	2.18508669
1	-2.83391634	-2.84657977	3.29542130

TS_{1-4-NCO}

E = -198.782033 E0 = -198.347731

No. of Negative Frequencies = 1

freq = - 173.01



Atomic Coordinates:

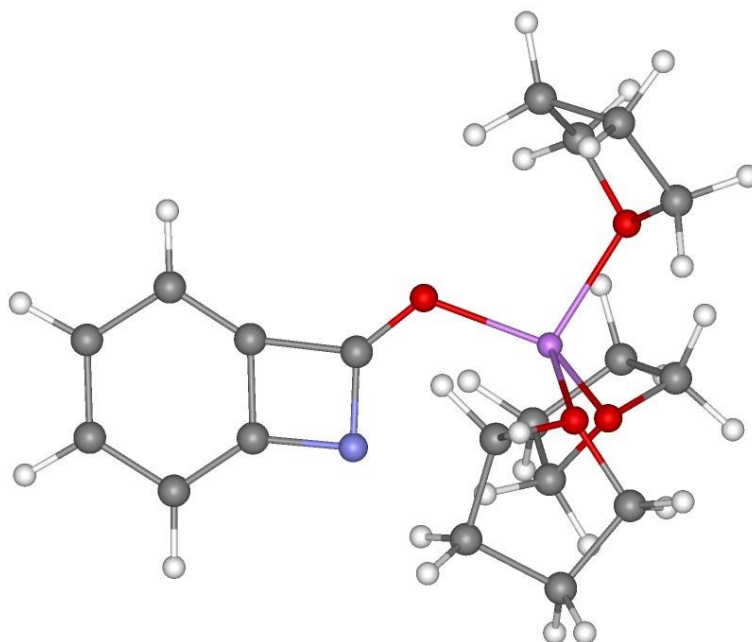
6	-0.24365859	-2.12945064	-4.30812786
6	-0.24944610	-2.76216044	-3.06295744
6	0.03065104	-0.75065177	-4.41840984
6	0.00950005	-2.02374596	-1.88019290
1	0.00289309	-2.55533781	-0.92182596
6	0.25958462	-0.65008871	-1.95391602
3	0.29389239	0.21192871	0.23524730
6	0.28001332	-0.05198973	-3.23944599
7	0.61833873	1.32509709	-3.09930429
1	0.05740663	-0.25549670	-5.39066408
1	-0.44608417	-2.70968544	-5.21110389
1	-0.45629613	-3.83351619	-2.99996608
6	0.79421689	1.39997213	-1.83142019
8	1.08123933	2.04903403	-0.85184754
8	-1.51655033	1.32453676	0.54198061
8	-0.40182131	-1.38534981	1.50183100
8	2.20335855	-0.03178596	1.09843168
6	-1.47395028	2.68384971	1.06619972
6	-2.48480254	1.26197225	-0.54526905
6	-2.67694903	2.70560318	-1.00115863
1	-2.07190319	0.59481493	-1.31554332
1	-3.42787336	0.83433423	-0.15733385
6	-2.57241457	3.46492006	0.33344860
1	-1.62490876	2.63816636	2.15596003
1	-0.47465510	3.09452073	0.85423297

1	-3.63737469	2.86050995	-1.51082054
1	-1.86660643	2.99971783	-1.68395013
1	-2.31126964	4.52418885	0.20872855
1	-3.52535587	3.40786241	0.88203237
6	3.20713968	1.00501571	1.21197329
6	2.92080007	-1.19717290	0.62701566
6	3.87147031	-0.65905642	-0.44830065
1	3.47310960	-1.64548501	1.47474752
1	2.17887885	-1.91522200	0.25609193
6	4.18483863	0.78528669	0.03582565
1	2.68617925	1.96857063	1.18021054
1	3.71674422	0.89229145	2.18617595
1	3.35656885	-0.63790200	-1.41781478
1	4.77194294	-1.28007980	-0.54831973
1	5.22666596	0.89580017	0.36692641
1	4.00248055	1.51235889	-0.76503196
6	-0.09385633	-1.46904142	2.90863365
6	-1.73436298	-1.92618587	1.38670962
6	-2.50855269	-1.35879201	2.59047983
1	-2.12943065	-1.63475254	0.40609094
1	-1.67644616	-3.02982550	1.43275772
6	-1.39363814	-1.07318960	3.63912097
1	0.19609516	-2.50885979	3.14964698
1	0.75922617	-0.80555406	3.09486139
1	-3.26226471	-2.06908807	2.95593886
1	-3.02023385	-0.42934221	2.30999959
1	-1.37795126	-0.00871629	3.90849237
1	-1.52457804	-1.65282810	4.56293301

$P_{1-4-NCO}$

E = -198.812474 E0 = -198.376339

No. of Negative Frequencies = 0



Atomic Coordinates:

6	-1.97735960	-2.10117467	-5.08208877
6	-0.63092209	-1.93518094	-5.40396193
6	-2.50961066	-1.80102895	-3.79136156
6	0.30382470	-1.44580911	-4.43781549
1	1.35815481	-1.31626767	-4.69191342
6	-0.22109244	-1.16111057	-3.20036059
3	0.39915585	0.33536497	0.80942034
6	-1.58665061	-1.33046019	-2.87749807
7	-1.46715419	-0.87451443	-1.49848923
1	-3.56877517	-1.94212950	-3.57044907
1	-2.65675674	-2.47813038	-5.85065896
1	-0.28516771	-2.18281770	-6.40888513
6	-0.13450763	-0.68033341	-1.72971755
8	0.77637671	-0.26061477	-0.97812462
8	-0.94668969	1.81508533	1.09609181
8	-0.06970229	-1.12697423	2.13014473
8	2.20347906	1.12191284	1.39406056
6	-0.57214227	3.18227738	1.37040949
6	-2.10901636	1.90288705	0.22726037
6	-1.76910254	3.03472662	-0.75284170
1	-2.23433483	0.91944974	-0.25210235
1	-2.98974104	2.15194511	0.84762767
6	-0.79589401	3.94883336	0.04892208
1	-1.22219306	3.57344586	2.17432527
1	0.46762274	3.17134334	1.72286561
1	-2.66939087	3.56694117	-1.08773453
1	-1.27066544	2.62011061	-1.63918167

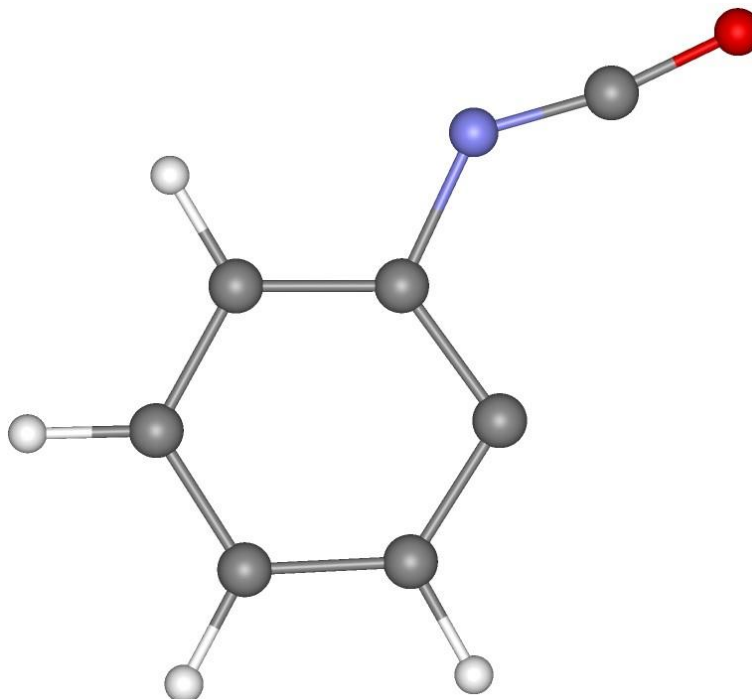
1	0.14983341	4.08112183	-0.49345384
1	-1.21680614	4.94591093	0.23766269
6	3.15151238	1.36974464	0.32784428
6	2.95697903	0.51206622	2.47188600
6	4.12646091	-0.26124586	1.80955811
1	3.32698479	1.30823606	3.14066450
1	2.25689139	-0.12623658	3.02680142
6	4.02280906	0.11411309	0.30804020
1	2.57509484	1.52388023	-0.59227116
1	3.73781640	2.27667917	0.56729583
1	4.03246456	-1.34481130	1.95833974
1	5.08820427	0.05364335	2.23776729
1	5.00327355	0.28875710	-0.15498928
1	3.50020398	-0.66886416	-0.25782820
6	-1.13705792	-0.96728179	3.09923223
6	-0.18295092	-2.48352717	1.62862582
6	-1.68696627	-2.69219778	1.45586741
1	0.38925282	-2.53164425	0.69327248
1	0.25790970	-3.17705179	2.36917469
6	-2.29113042	-1.89348989	2.64095836
1	-0.75617893	-1.25848307	4.09380873
1	-1.39503973	0.09989598	3.11306202
1	-1.96691721	-3.75423027	1.47345133
1	-1.99191979	-2.25298058	0.49435419
1	-3.16858150	-1.31710468	2.31996377
1	-2.60388686	-2.55267629	3.46296812

Ph-NCO-anion

$R_{\text{NCO-a}}$

E = -68.045087 E0 = -67.959275

No. of Negative Frequencies = 0



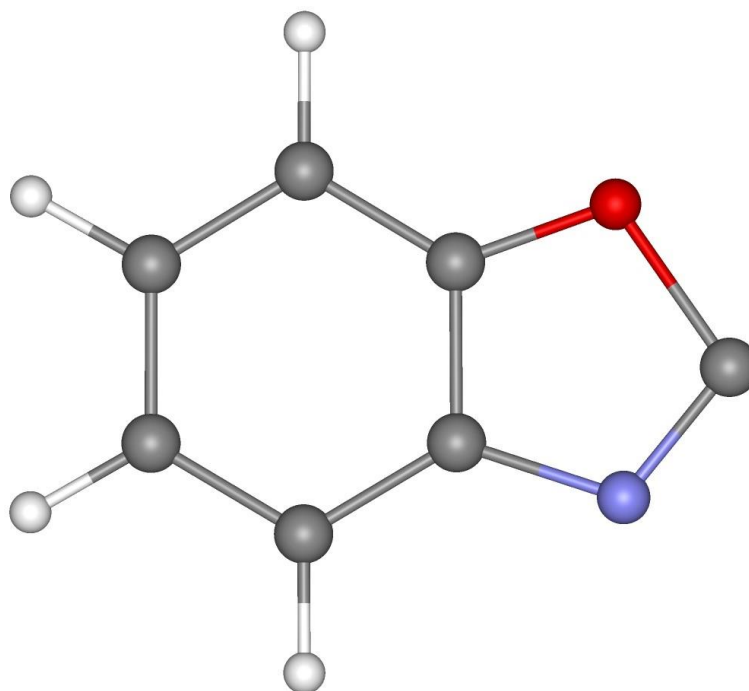
Atomic Coordinates:

6	-0.25207947	-1.20530596	-1.28212845
6	-0.40484847	-1.91577114	-0.08357207
6	0.03744488	0.16528120	-1.22194006
6	-0.26541324	-1.24378066	1.14868933
1	-0.39593299	-1.85296074	2.05826772
6	0.02581278	0.13533384	1.29460133
6	0.16443338	0.77876629	0.03892297
7	0.46231485	2.18706334	0.00776921
1	0.16248968	0.74744552	-2.14271881
1	-0.35528311	-1.70372880	-2.25026673
1	-0.63198760	-2.99061095	-0.11395663
6	0.62998175	2.98896183	0.90711385
8	0.82306758	3.90930622	1.63921834

*P*_{1-5-NCO-a}

E = -68.060534 E0 = -67.973099

No. of Negative Frequencies = 0



Atomic Coordinates:

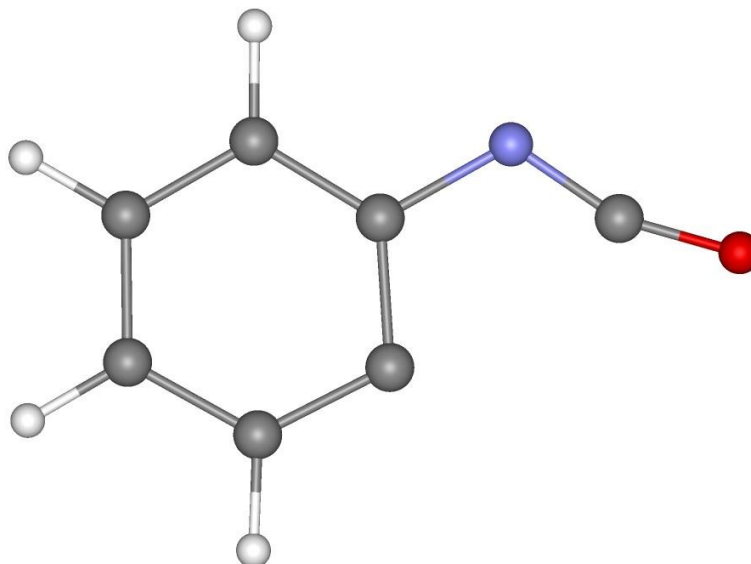
6	-0.42723690	-0.05264996	-1.62056603
6	0.43112788	-1.08340433	-1.19408986
6	-0.87628689	0.93584737	-0.72504133
6	0.86434597	-1.15357298	0.14189910
1	1.53102736	-1.95096326	0.48067640
6	0.42458992	-0.17548171	1.04404031
6	-0.44183334	0.86094272	0.60373741
8	-0.72077207	1.66706056	1.63734636
1	-1.54272416	1.73687166	-1.05451028
1	-0.75119206	-0.01817801	-2.66482278
1	0.76389183	-1.83777172	-1.91246702
6	0.05981726	1.06675912	2.86363219
7	0.68524520	0.00454052	2.40016554

TS_{1-4-NCO-a}

E = -68.044465 E0 = -67.958865

No. of Negative Frequencies = 1

freq = - 106.15



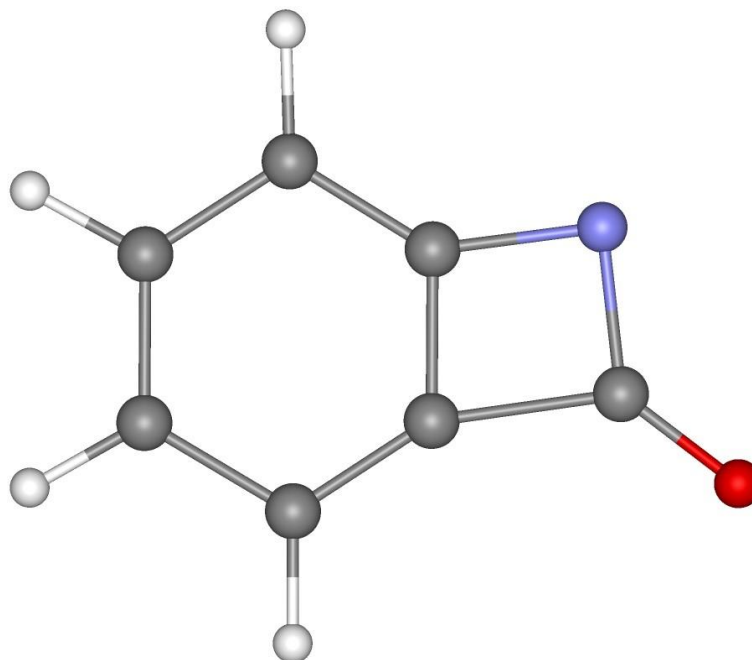
Atomic Coordinates:

6	-0.25358949	-1.21231434	-1.27996750
6	-0.39317715	-1.86035253	-0.04706818
6	0.03721875	0.16305751	-1.30679373
6	-0.24099020	-1.12849899	1.15383076
1	-0.36037743	-1.68386345	2.09707855
6	0.05021184	0.24946800	1.20062581
6	0.17876423	0.84475747	-0.08731360
7	0.47376540	2.24011076	-0.09931695
1	0.15028802	0.68842390	-2.26118551
1	-0.36843175	-1.76488966	-2.21721929
1	-0.62027675	-2.93436819	-0.02132717
6	0.58691352	2.78643359	1.01503767
8	0.75968102	3.61203594	1.85361917

*P*_{1-4-NCO-a}

E = -68.067318 E0 = -67.979927

No. of Negative Frequencies = 0



Atomic Coordinates:

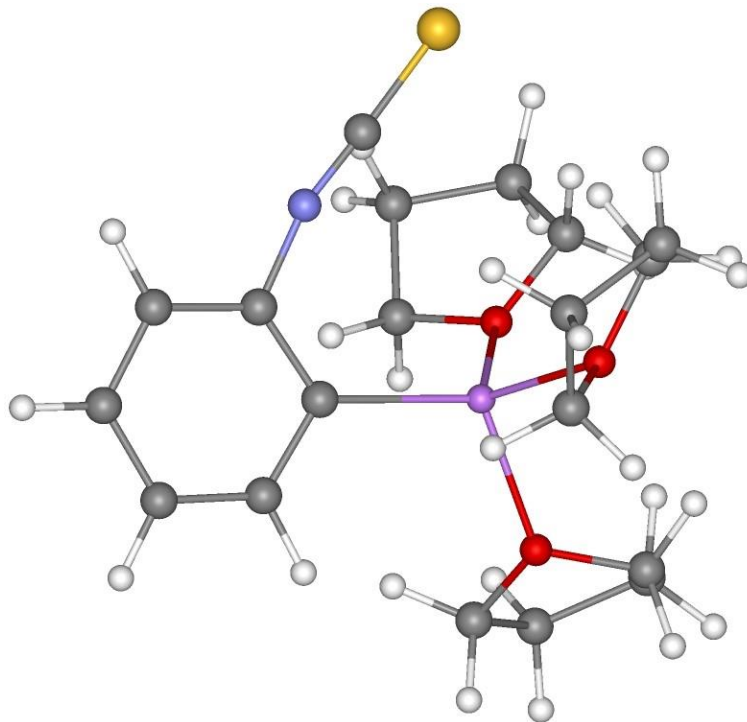
6	-1.00934474	-0.60157256	-1.27416338
6	0.33651751	-0.43908951	-1.60825050
6	-1.53157357	-0.29914605	0.01708260
6	1.27243067	0.05299871	-0.63551929
1	2.32854088	0.18156648	-0.89396277
6	0.76321334	0.34249575	0.60680563
6	-0.60640906	0.17740384	0.94680967
7	-0.52264024	0.61812962	2.29438944
1	-2.59218328	-0.43937062	0.24162012
1	-1.69613525	-0.97907610	-2.03953920
1	0.67815645	-0.68838433	-2.61622288
6	0.84113229	0.83281537	2.11535148
8	1.73829500	1.24122941	2.84559909

Ph-NCS-Li(THF)₃

R_{NCS}

E = -192.929536 E0 = -192.497684

No. of Negative Frequencies = 0



Atomic Coordinates:

6	-0.17411303	-2.23949437	-4.49752275
6	-0.42276112	-3.02425604	-3.36364301
6	0.16410376	-0.89619017	-4.32938794
6	-0.33603902	-2.45131480	-2.08337387
1	-0.52831343	-3.11772371	-1.23112841
6	-0.00832021	-1.09633164	-1.82480843
3	0.10836257	-0.29194977	0.18273188
6	0.23989411	-0.37372460	-3.02049911
7	0.59809909	0.98001091	-2.92518947
1	0.37067086	-0.25679967	-5.19086097
1	-0.23850745	-2.66682463	-5.49988096
1	-0.68195659	-4.08066433	-3.48078256
6	0.91029293	2.06682694	-2.55997249
16	1.34109942	3.56529275	-2.11218068
8	-1.19112568	1.27305377	0.56429729
8	-0.49486073	-1.63102278	1.63400826
8	2.01708130	0.00469636	0.88016388
6	-0.91831865	2.62224044	1.03947455
6	-2.36085780	1.29389910	-0.30481760
6	-2.56703463	2.76026008	-0.67780293
1	-2.14769987	0.62798953	-1.15363952
1	-3.22497960	0.89682708	0.25883457
6	-2.11497386	3.47554790	0.60764132

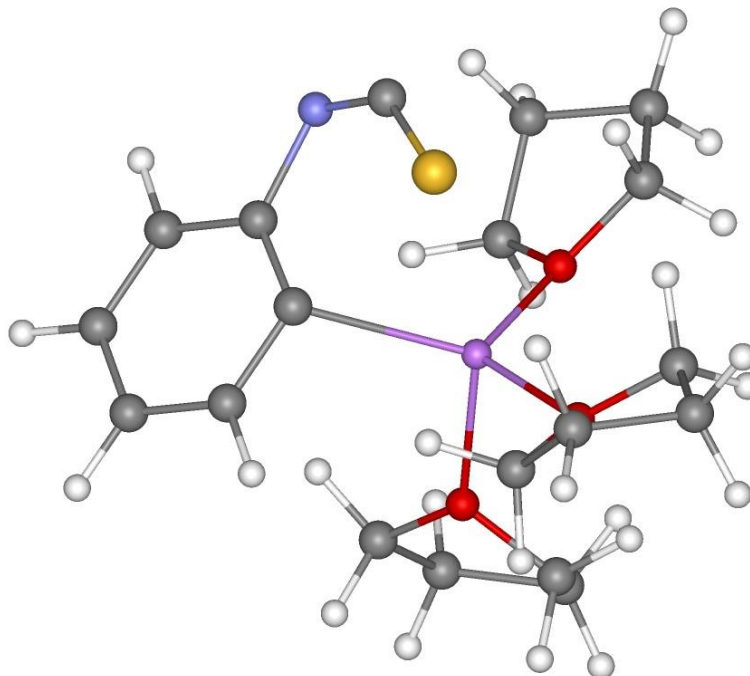
1	-0.77781242	2.57985134	2.13045905
1	0.01130815	2.97537443	0.56466782
1	-3.60750721	2.98053604	-0.95203441
1	-1.91455856	3.03871531	-1.51812860
1	-1.83260974	4.52344220	0.44087440
1	-2.91220094	3.44639357	1.36661677
6	2.77265326	1.25280281	0.89913015
6	2.87021729	-1.06637601	0.38111059
6	3.98937140	-0.36205708	-0.37939219
1	3.25794816	-1.64228135	1.24034661
1	2.24291753	-1.71493405	-0.24763173
6	4.20451060	0.89729353	0.47861683
1	2.30540529	1.94982283	0.18519009
1	2.71069234	1.67790464	1.91274838
1	3.64387816	-0.09041958	-1.38789084
1	4.89155219	-0.98169034	-0.47159069
1	4.82451466	0.66058532	1.35700652
1	4.68432772	1.71805879	-0.07068133
6	-0.28574852	-1.38450605	3.03617041
6	-1.76720500	-2.30708354	1.54600064
6	-2.65634613	-1.69719023	2.65846937
1	-2.14596214	-2.15587163	0.52691128
1	-1.60778470	-3.38775372	1.71111685
6	-1.65290600	-0.91666015	3.55361120
1	0.03276076	-2.32283904	3.52918844
1	0.51931072	-0.64321031	3.12048806
1	-3.17871729	-2.48582493	3.21675132
1	-3.41707765	-1.02478436	2.24098566
1	-1.75897155	0.16495373	3.39492593
1	-1.78570271	-1.12260052	4.62430237

*TS*_{I-5-NCS}

E = -192.884081 E0 = -192.453262

No. of Negative Frequencies = 1

freq = - 169.56



Atomic Coordinates:

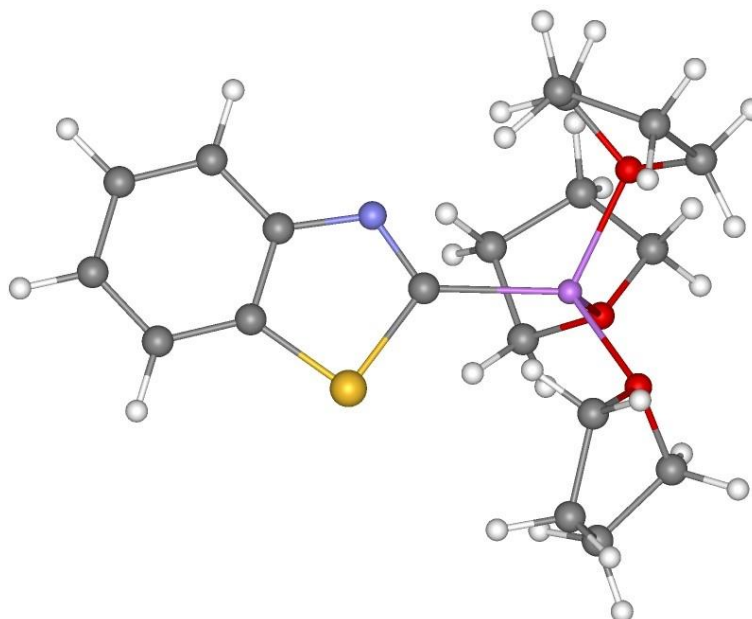
6	-1.52614004	-2.41959369	-3.54658575
6	-0.48695286	-3.03531628	-2.83302492
6	-1.59152653	-1.02417945	-3.62318233
6	0.46827784	-2.24096192	-2.17162075
1	1.23926417	-2.74678050	-1.57689499
6	0.41023273	-0.84172673	-2.24580023
3	0.44799307	0.06521264	-0.11338824
6	-0.58609986	-0.25657981	-3.00821779
7	-0.65558929	1.20881542	-3.26672465
1	-2.38059783	-0.51730988	-4.18601111
1	-2.27535532	-3.02651043	-4.05957643
1	-0.42589910	-4.12637197	-2.78370820
6	0.38039752	1.82010938	-2.89748841
16	1.79073324	1.43202305	-2.19824569
8	-0.90095074	1.54720666	0.34282016
8	-0.40149266	-1.43059296	1.07301636
8	2.21440915	0.15913729	0.95727451
6	-0.56967829	2.96477962	0.43361461
6	-2.27575249	1.40170027	-0.11661508
6	-2.66938537	2.76507814	-0.68109391
1	-2.30187521	0.59740965	-0.86473374
1	-2.90500872	1.12087821	0.74736521
6	-1.88621767	3.72121708	0.23509700
1	-0.10926972	3.14040581	1.41795482
1	0.15888816	3.19636529	-0.35936165

1	-3.75477308	2.93093310	-0.65064417
1	-2.32353497	2.84969592	-1.72092289
1	-1.72646265	4.71123982	-0.21204821
1	-2.40924537	3.85405600	1.19510856
6	2.87365322	1.38173283	1.38739217
6	3.21726045	-0.80156532	0.50601169
6	4.53940106	-0.03289121	0.45246680
1	3.24798220	-1.62908378	1.23437681
1	2.89787200	-1.18923150	-0.47246311
6	4.34812329	1.01665068	1.56133675
1	2.73641825	2.14801883	0.60550628
1	2.38619973	1.71762380	2.31442014
1	4.65543103	0.45980427	-0.52426131
1	5.40754838	-0.68478818	0.61705788
1	4.52402458	0.56993049	2.55210821
1	5.00780073	1.88748720	1.45121477
6	-0.31575002	-1.41914563	2.50911470
6	-1.46127684	-2.36266998	0.76410756
6	-2.53554043	-2.14924846	1.85519474
1	-1.79500702	-2.15702728	-0.25962002
1	-1.05223391	-3.38839023	0.80100217
6	-1.77508491	-1.40489516	2.99086451
1	0.20938883	-2.33237344	2.84903495
1	0.27286133	-0.53992255	2.79861131
1	-2.94998973	-3.10885517	2.19214865
1	-3.36819446	-1.54178121	1.47693664
1	-2.13028811	-0.36942017	3.08149628
1	-1.88898772	-1.89029858	3.96957934

*P*_{1-5-NCS}

E = -192.963483 E0 = -192.529407

No. of Negative Frequencies = 0



Atomic Coordinates:

6	-1.67376967	-2.29359277	-5.02981630
6	-0.36592725	-2.70915534	-5.34860582
6	-1.93352158	-1.60923189	-3.84135630
6	0.69970650	-2.44615024	-4.48254321
1	1.71046983	-2.77073312	-4.73434275
6	0.44272220	-1.75840082	-3.28628066
3	0.20233824	0.35005185	0.92300317
6	-0.87596737	-1.33275295	-2.95514043
7	-0.99823460	-0.66279138	-1.74088926
1	-2.94268483	-1.28279618	-3.58348758
1	-2.49127226	-2.51009207	-5.72011406
1	-0.18007190	-3.24359220	-6.28234433
6	0.11072398	-0.49983593	-1.05147806
16	1.52878689	-1.27670745	-1.99686032
8	-1.21353348	1.77699949	1.19730842
8	-0.16558086	-1.07425422	2.34292365
8	1.96691061	1.22922855	1.41744637
6	-0.91346130	3.13382391	1.59068247
6	-2.19730975	1.88759849	0.13457968
6	-1.69519303	3.05425033	-0.72349687
1	-2.21695423	0.92701009	-0.39952893
1	-3.18267301	2.10450432	0.58750472
6	-0.96072340	3.97486161	0.29326049
1	-1.67819374	3.47213442	2.31321882
1	0.06592415	3.11758604	2.08687956
1	-2.51567403	3.56656464	-1.24355114
1	-0.99615882	2.67121933	-1.47904771
1	0.04965983	4.22150494	-0.05935006

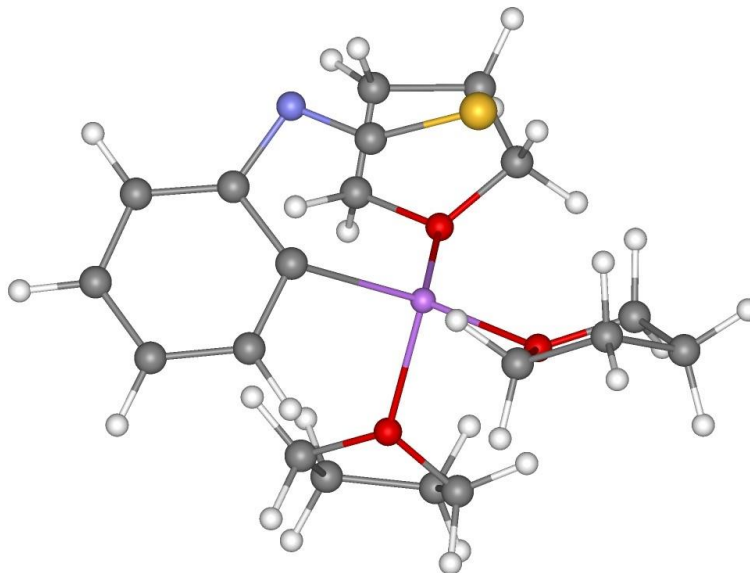
1	-1.49610413	4.91974467	0.45977172
6	2.73974757	1.72262597	0.28319706
6	2.88562527	0.56183362	2.31119805
6	3.87467188	-0.13356174	1.37795628
1	3.38839058	1.31014230	2.95245302
1	2.29025081	-0.11447431	2.93909408
6	4.06010847	0.91516929	0.25765346
1	2.12000221	1.56553471	-0.61079025
1	2.92033826	2.80156472	0.42151920
1	3.42173418	-1.05153641	0.97641526
1	4.81782138	-0.39711652	1.87573352
1	4.91722822	1.56847410	0.47481961
1	4.22833260	0.44585794	-0.71995785
6	-1.29552922	-0.93530531	3.23804088
6	-0.23930160	-2.42957121	1.83285886
6	-1.72543691	-2.63412080	1.53277564
1	0.40645323	-2.48001455	0.94697429
1	0.12831259	-3.12531691	2.61012098
6	-2.42882593	-1.81036939	2.64662520
1	-0.99696333	-1.28743841	4.24113728
1	-1.53474780	0.13471281	3.28756378
1	-2.01121156	-3.69445500	1.54271342
1	-1.95081272	-2.21890707	0.54070995
1	-3.23689671	-1.19451834	2.23072308
1	-2.86352445	-2.45620560	3.42211992

TS_{1-4-NCS}

E = -192.901665 E0 = -192.470076

No. of Negative Frequencies = 1

freq = - 196.17



Atomic Coordinates:

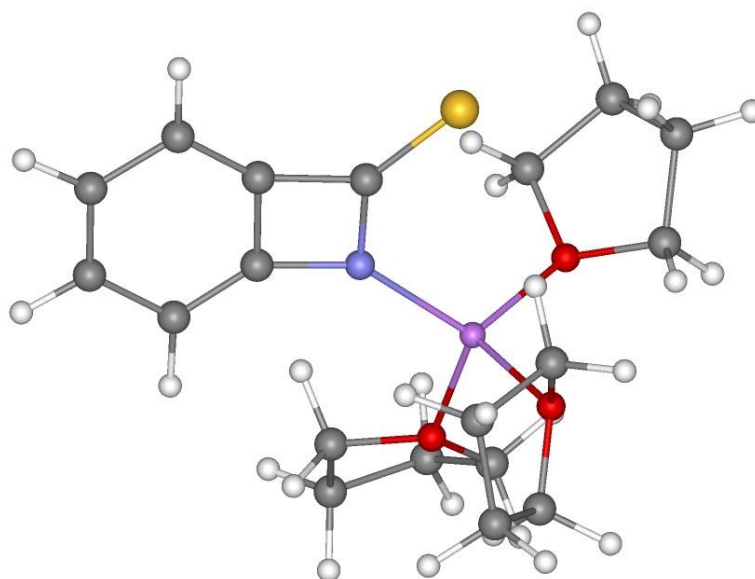
6	-1.43918812	-2.52145389	-3.67456031
6	-0.52623873	-3.07676768	-2.77257322
6	-1.49176846	-1.12919117	-3.89394689
6	0.35443961	-2.24690989	-2.03139991
1	1.05566468	-2.71288108	-1.33085017
6	0.27134467	-0.86256995	-2.17732217
3	0.37354000	0.03228553	-0.05248120
6	-0.62113870	-0.33633130	-3.14710832
7	-0.37176884	1.05291897	-3.24625707
1	-2.15949108	-0.69801341	-4.64189638
1	-2.10818927	-3.17767941	-4.23561553
1	-0.49528186	-4.16045595	-2.63364428
6	0.64717357	1.18975141	-2.47016997
16	1.82058857	2.21591652	-1.95708267
8	-1.04949492	1.44476161	0.39343042
8	-0.36330791	-1.53299801	1.14456374
8	2.20473553	0.11036527	0.84732588
6	-0.73627214	2.84367987	0.67618178
6	-2.33258293	1.37209791	-0.29070275
6	-2.55904471	2.76422519	-0.87187884
1	-2.26452412	0.58144648	-1.05046311
1	-3.11295743	1.10687464	0.44604852
6	-1.95596038	3.65715945	0.22693959
1	-0.52358390	2.93353650	1.75263997
1	0.16442967	3.10324567	0.09684120
1	-3.62098347	2.97210820	-1.06039844
1	-2.00163775	2.86787592	-1.81395608

1	-1.66992091	4.65237937	-0.13811424
1	-2.67030166	3.78474390	1.05513047
6	2.81113380	1.23969180	1.52526688
6	3.22658427	-0.58564583	0.06167970
6	4.52141314	0.21472660	0.24126011
1	3.30534001	-1.60864235	0.46405646
1	2.88714911	-0.62425117	-0.98399513
6	4.30125355	0.91312571	1.59525129
1	2.62833882	2.15260123	0.93258013
1	2.32524418	1.33741246	2.50738276
1	4.61511447	0.96110504	-0.56031845
1	5.41184505	-0.42765522	0.22649345
1	4.50754753	0.22505352	2.42968718
1	4.92058973	1.81109809	1.72259355
6	-0.20144586	-1.52810860	2.57445713
6	-1.56018926	-2.30680520	0.90380001
6	-2.52464315	-1.97256631	2.06821383
1	-1.93063070	-2.04051395	-0.09313640
1	-1.29316176	-3.37857957	0.90260454
6	-1.61376838	-1.27932251	3.12069062
1	0.19043039	-2.51059397	2.90039705
1	0.53299687	-0.75181000	2.82199989
1	-2.98991806	-2.88560452	2.46361389
1	-3.33092285	-1.30277616	1.74201988
1	-1.81256560	-0.19937391	3.15095739
1	-1.74601430	-1.68268586	4.13376423

*P*_{1-4-NCS}

E = -192.943514 E0 = -192.510256

No. of Negative Frequencies = 0



Atomic Coordinates:

6	-2.15779394	-1.17909267	-4.41177983
6	-1.28654875	-2.10949218	-4.97721411
6	-1.93194022	-0.58403314	-3.13233209
6	-0.10234775	-2.52737834	-4.29457970
1	0.57596941	-3.26220446	-4.73213443
6	0.10434188	-1.94186649	-3.07034212
3	0.17236193	0.07384066	0.52036022
6	-0.77478487	-0.99535275	-2.50002871
7	0.01434396	-0.83292672	-1.28261311
1	-2.64530627	0.12992847	-2.71678999
1	-3.05417683	-0.89340977	-4.96733023
1	-1.51604059	-2.52799357	-5.95845599
6	0.90476740	-1.76139008	-1.77887837
16	2.30721569	-2.42667063	-1.14081814
8	-1.02230868	1.74538310	0.68710010
8	-0.38573855	-1.16409499	2.03901261
8	1.96940007	0.89009204	1.02227397
6	-0.66315390	2.86940689	1.53545663
6	-1.73932479	2.23002230	-0.48654980
6	-2.01020990	3.71574456	-0.23113085
1	-1.09926457	2.07173716	-1.36929670
1	-2.65305786	1.62881796	-0.59854376
6	-0.81779269	4.11083295	0.65738708
1	-1.35220877	2.89822613	2.39808130
1	0.36024620	2.69733047	1.89567382
1	-2.95548269	3.85104663	0.31641501
1	-2.06748432	4.29207100	-1.16380292
1	0.08443120	4.26127869	0.04513998
1	-0.99610146	5.02188402	1.24408729

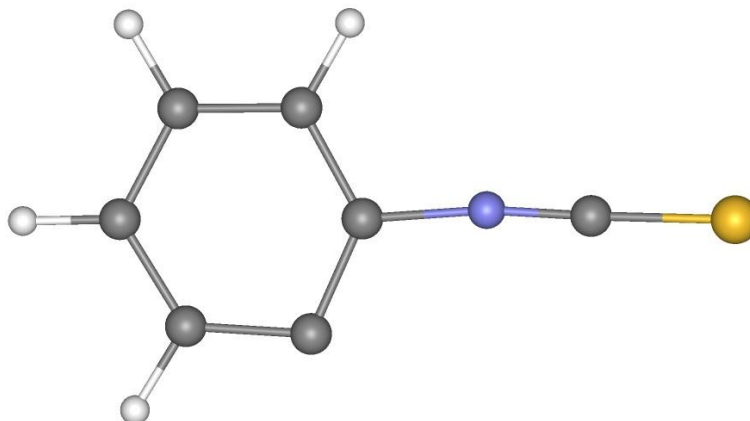
6	2.85057758	1.22469321	-0.09771483
6	2.76551339	0.36415188	2.11938384
6	4.09381515	-0.05253305	1.49367592
1	2.90153488	1.16103466	2.87327028
1	2.20120704	-0.46265603	2.57250471
6	4.28137947	1.02798482	0.41379838
1	2.61553180	0.53632101	-0.92365617
1	2.63256924	2.25910114	-0.40390886
1	3.98850659	-1.04048343	1.02286207
1	4.91370773	-0.08124311	2.22428913
1	4.67414114	1.95624352	0.85765250
1	4.95998306	0.71381161	-0.38987978
6	-1.69985490	-1.04053001	2.64364577
6	-0.14847317	-2.57869810	1.81352415
6	-1.50790789	-3.10932018	1.37024377
1	0.64741406	-2.66172871	1.05872922
1	0.18360402	-3.04584018	2.75982193
6	-2.47911907	-2.33345051	2.28993542
1	-1.58160077	-0.91980994	3.73376872
1	-2.15504955	-0.12845970	2.23227648
1	-1.59602375	-4.19838684	1.48013682
1	-1.67084295	-2.84779884	0.31521738
1	-3.43293675	-2.11447526	1.79212633
1	-2.69968668	-2.90966520	3.19992966

Ph-NCS-anion

R_{NCS-a}

E = -62.179727 E0 = -62.096130

No. of Negative Frequencies = 0



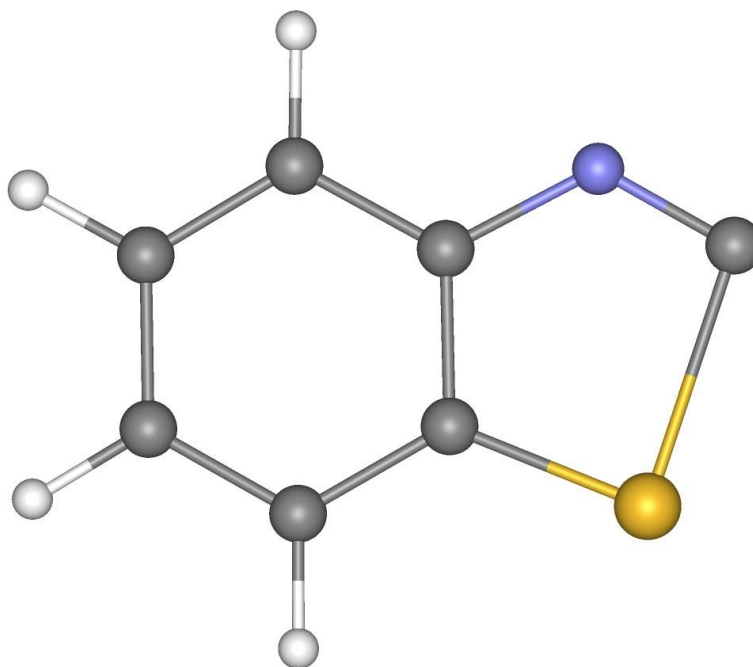
Atomic Coordinates:

6	-0.26619937	-1.17103297	-1.25634098
6	-0.52758402	-1.98170176	-0.13926450
6	0.08466295	0.16511140	-1.04821914
6	-0.43297780	-1.44252346	1.15648189
1	-0.65007571	-2.12961016	1.99047634
6	-0.08388227	-0.09966038	1.46200190
6	0.16133530	0.64190239	0.28162852
7	0.52221895	2.00123027	0.40602367
1	0.29507455	0.82658431	-1.89687808
1	-0.33418276	-1.57089761	-2.27138661
1	-0.80463296	-3.03437610	-0.28922479
6	0.81460715	3.12156843	0.65495157
16	1.22163598	4.67340566	0.94975021

*P*_{1-5-NCS-a}

E = -62.216662 E0 = -62.131528

No. of Negative Frequencies = 0



Atomic Coordinates:

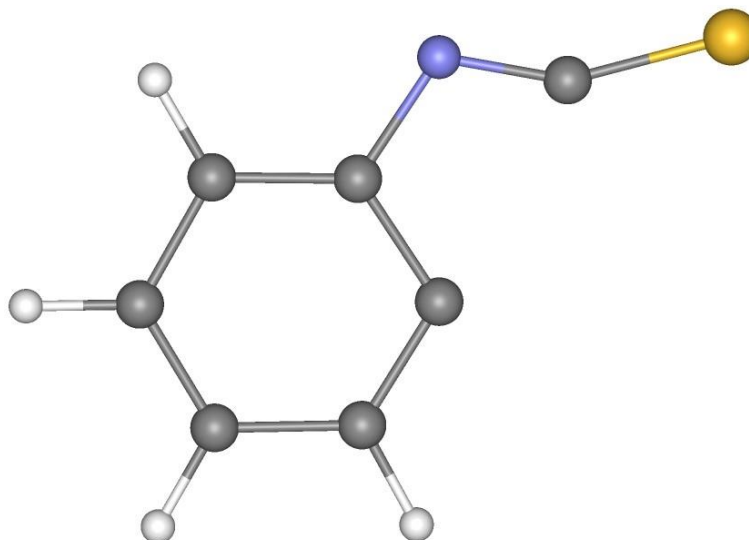
6	-0.56250675	-0.09820684	-1.63249920
6	0.18792722	-1.20186706	-1.18846006
6	-0.81468614	0.98481677	-0.78166069
6	0.68882573	-1.21836302	0.11922425
1	1.27460238	-2.06229192	0.49055825
6	0.44562454	-0.14084262	0.98601161
6	-0.32020287	0.99107671	0.54090063
16	-0.51468655	2.22158158	1.75232741
1	-1.39878838	1.83569785	-1.13845708
1	-0.95525818	-0.08228304	-2.65343829
1	0.37971972	-2.04276355	-1.85955786
6	0.68063967	0.89798732	3.06935124
7	0.90878959	-0.08454218	2.29569978

TS_{1-4-NCS-a}

E = -62.170511 E0 = -62.086927

No. of Negative Frequencies = 1

freq = - 133.25



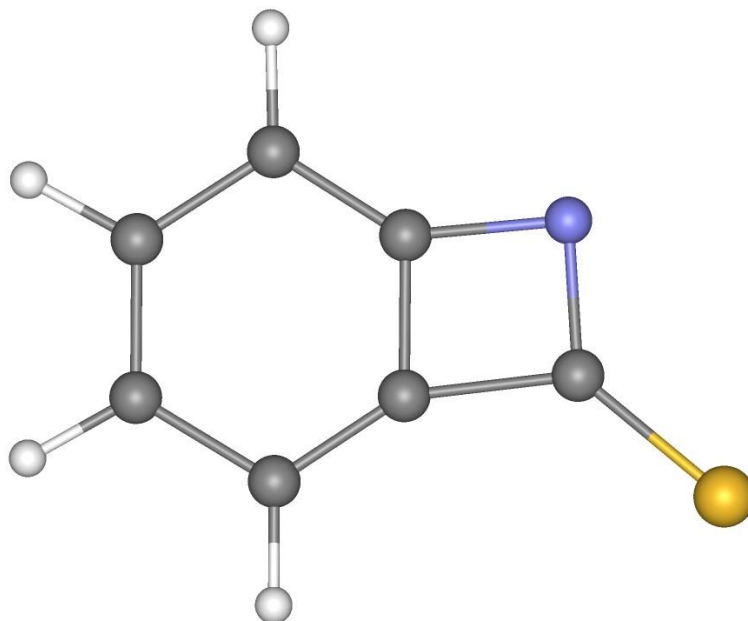
Atomic Coordinates:

6	-1.46388856	0.45367159	-0.96905428
6	-0.72154763	-0.48595658	-1.69340116
6	-1.01334026	0.87746144	0.29454125
6	0.48033591	-1.00980581	-1.15714884
1	1.03159927	-1.74552504	-1.76007252
6	0.97687537	-0.62427969	0.09575214
6	0.18122061	0.33665013	0.79299557
7	0.71388430	0.69721077	2.04621604
1	-1.58218313	1.61130204	0.87327405
1	-2.39232854	0.86003074	-1.38040297
1	-1.07713597	-0.81322073	-2.67832895
6	1.78796307	0.10408292	2.31130197
16	3.07854556	-0.26162179	3.22432770

*P*_{1-4-NCS-a}

E = -62.200968 E0 = -62.115535

No. of Negative Frequencies = 0



Atomic Coordinates:

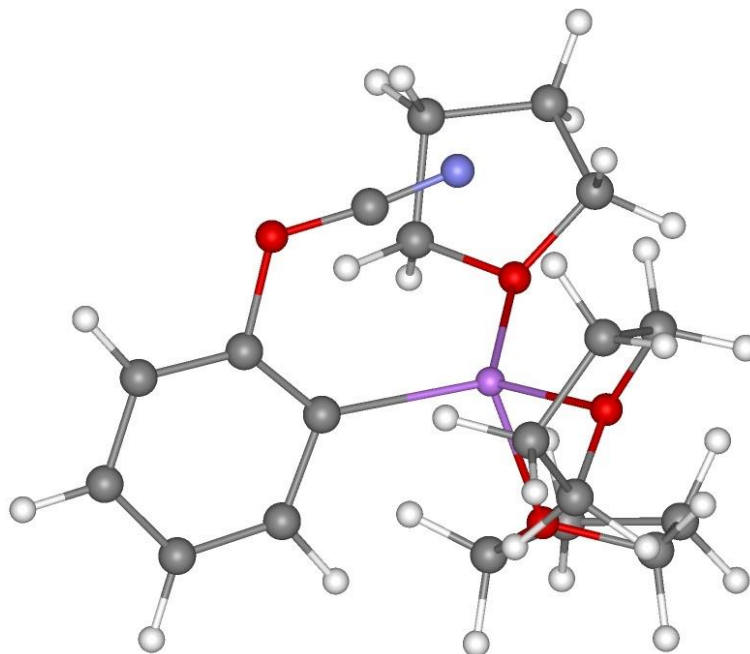
6	-1.42210804	0.43198112	-0.95630946
6	-0.55697072	-0.50258830	-1.52560248
6	-1.19274637	1.02076033	0.32593357
6	0.62999305	-0.92725678	-0.83715160
1	1.31024246	-1.65968514	-1.28050995
6	0.83703000	-0.35444234	0.39125718
6	-0.04087339	0.59463517	0.97006025
7	0.72804896	0.76615942	2.18128083
1	-1.88964503	1.75055869	0.74532527
1	-2.31552017	0.72800274	-1.51526593
1	-0.78723150	-0.91705133	-2.51028924
6	1.63316198	-0.14482455	1.70015366
16	3.06661877	-0.78624903	2.31111790

Ph-OCN-Li(THF)₃

R_{OCN}

E = -198.758962 E0 = -198.325483

No. of Negative Frequencies = 0



Atomic Coordinates:

6	0.04578816	-2.42607684	-4.38728115
6	-0.16859927	-3.05353066	-3.15302019
6	0.31837528	-1.05282826	-4.41564816
6	-0.11945779	-2.30478502	-1.96463483
1	-0.28458529	-2.84869025	-1.02536918
6	0.14062541	-0.90809328	-1.91725648
3	0.16964030	0.02010965	0.08444782
6	0.34948337	-0.40030665	-3.18452048
8	0.66733635	1.05428739	-3.33954824
1	0.50131066	-0.52265315	-5.35205739
1	0.00817743	-2.99280818	-5.31930725
1	-0.37328638	-4.12715610	-3.11941143
6	0.82391426	1.72063332	-2.25882533
7	0.99338847	2.42846396	-1.33573926
8	-1.38988228	1.32605765	0.59426533
8	-0.48821579	-1.49465462	1.46321199
8	2.04286107	0.06496020	0.98056339
6	-1.18471543	2.61560013	1.23875473
6	-2.42310163	1.45516469	-0.42409600
6	-2.60925902	2.95649756	-0.63834171
1	-2.08174707	0.90600556	-1.31382673
1	-3.34853672	0.98365786	-0.04556591
6	-2.33782178	3.50844696	0.77238891
1	-1.16453910	2.45091646	2.32687115
1	-0.21287837	3.01303411	0.90691471

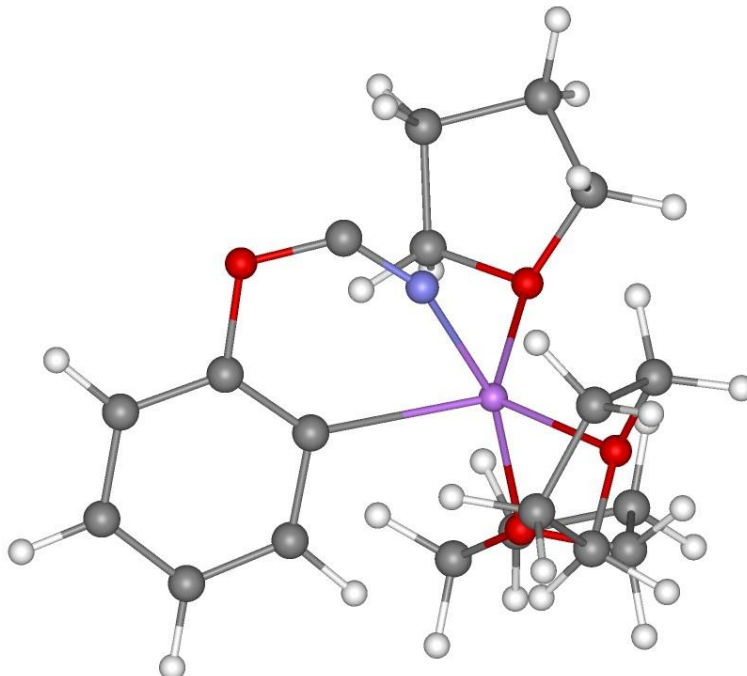
1	-3.61017498	3.20559436	-1.01592660
1	-1.85704248	3.33519013	-1.34487294
1	-2.06394737	4.57190285	0.77461007
1	-3.22208079	3.37668323	1.41547032
6	2.95521682	1.19024982	1.03879460
6	2.84506984	-1.07615783	0.59804155
6	3.78052717	-0.53478995	-0.48392746
1	3.40508465	-1.43970229	1.48109377
1	2.15872641	-1.85933997	0.25075706
6	4.05415355	0.92001297	-0.01782242
1	2.36706119	2.09145437	0.82931075
1	3.37761420	1.24604282	2.05782837
1	3.25458664	-0.54031982	-1.44820689
1	4.69715677	-1.13236910	-0.58142001
1	5.05435640	1.02382176	0.42566441
1	3.97761199	1.62550108	-0.85463386
6	-0.20372329	-1.46609041	2.87478022
6	-1.81152945	-2.05406182	1.36024421
6	-2.61476080	-1.41819302	2.51081249
1	-2.19039033	-1.82659751	0.35570081
1	-1.74848430	-3.15248122	1.47802407
6	-1.52335627	-1.04728274	3.55689761
1	0.10764167	-2.47688455	3.19926786
1	0.62932601	-0.76764574	3.02262638
1	-3.36582808	-2.11313444	2.90996281
1	-3.13456136	-0.51661271	2.16229618
1	-1.53091172	0.03210437	3.75807176
1	-1.66161690	-1.56914714	4.51358656

*TS*_{1-5-OCN}

E = -198.736308 E0 = -198.302976

No. of Negative Frequencies = 1

freq = - 220.63



Atomic Coordinates:

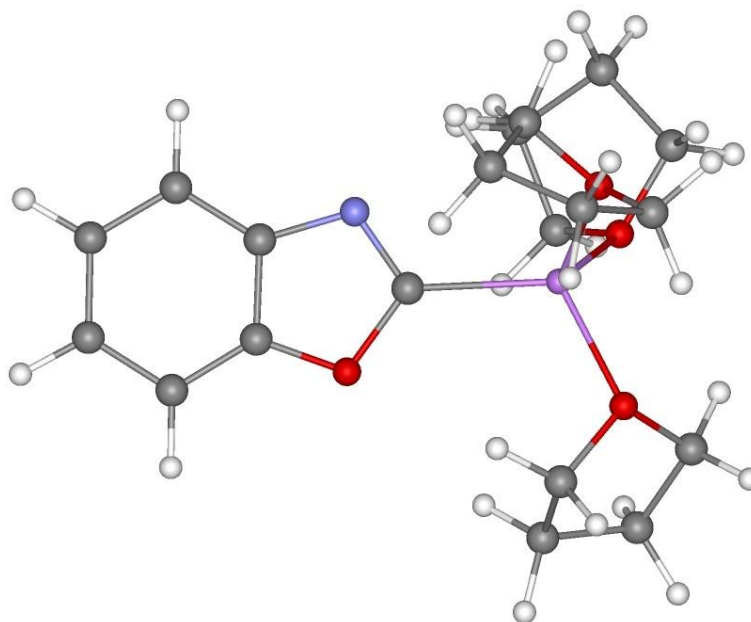
6	-0.15487239	-2.43186947	-4.30668003
6	-0.01128533	-2.97867767	-3.02443959
6	-0.06120945	-1.04651623	-4.48809281
6	0.20854113	-2.13633834	-1.91872655
1	0.31581322	-2.59964803	-0.93144471
6	0.29238359	-0.73909932	-2.07251599
3	0.27741879	0.19168586	0.19153362
6	0.17538971	-0.26433150	-3.35578772
8	0.32767366	1.16904628	-3.61234246
1	-0.15402792	-0.59194316	-5.47661006
1	-0.32771910	-3.08007973	-5.16778299
1	-0.06845851	-4.06139930	-2.88381643
6	0.61861976	1.80074700	-2.48398066
7	0.76896904	1.42895282	-1.34176239
8	-1.30877346	1.47240105	0.89225857
8	-0.46519164	-1.46489776	1.34421664
8	2.10468889	0.11774313	1.22171459
6	-0.93608140	2.84211554	1.20796298
6	-2.40193488	1.48758575	-0.07448591
6	-2.57942993	2.94763999	-0.49881025
1	-2.13196597	0.82566980	-0.91141608
1	-3.30392489	1.09447240	0.42615826
6	-2.11219710	3.70683475	0.75543403
1	-0.73116997	2.88844005	2.28756301

1	-0.02083745	3.09403456	0.64601130
1	-3.61515590	3.17619707	-0.78387589
1	-1.91913418	3.17586720	-1.34774443
1	-1.81139033	4.74188109	0.54466581
1	-2.90386548	3.72228715	1.52085392
6	2.99307317	1.25586492	1.08554833
6	2.91384187	-1.04195159	0.91922972
6	3.75420926	-0.61708742	-0.28717273
1	3.54498406	-1.28350914	1.79596004
1	2.22854035	-1.87795507	0.72693700
6	4.00883282	0.89131922	-0.02364289
1	2.36910223	2.12189821	0.83419673
1	3.49194378	1.42756139	2.05576973
1	3.16530923	-0.74732790	-1.20476443
1	4.68211972	-1.19861302	-0.37474084
1	5.03745140	1.08103012	0.31371022
1	3.82737233	1.48064952	-0.93062993
6	-0.35231515	-1.40843927	2.78124623
6	-1.69165805	-2.18550060	1.08403182
6	-2.66928801	-1.80864604	2.22546145
1	-2.03055231	-1.90253228	0.07968741
1	-1.47442199	-3.26869562	1.08993085
6	-1.77028370	-1.08435873	3.26477813
1	-0.01144419	-2.39186350	3.15873011
1	0.40201801	-0.64822842	3.01933960
1	-3.13871202	-2.70868261	2.64555730
1	-3.47217382	-1.15044512	1.86901287
1	-1.93138328	0.00064404	3.21947145
1	-1.94743826	-1.42393206	4.29429404

*P*_{1-5-OCN}

E = -198.813409 E0 = -198.376533

No. of Negative Frequencies = 0



Atomic Coordinates:

6	-0.54397465	-1.45162278	-5.55532494
6	0.31546168	-2.48492476	-5.13133253
6	-0.99325349	-0.46441991	-4.66461736
6	0.75567858	-2.56803105	-3.80367690
1	1.42170759	-3.36750546	-3.47406808
6	0.31324716	-1.58772273	-2.90449420
3	-0.02584473	0.39754183	0.87452678
6	-0.54545673	-0.56341657	-3.34804753
8	-0.81787956	0.24773414	-2.28248678
1	-1.65841710	0.33777431	-4.98738965
1	-0.86714147	-1.41733181	-6.59750089
1	0.64315880	-3.23412789	-5.85461537
6	-0.09431586	-0.31182863	-1.14791248
7	0.56358350	-1.38978011	-1.54242586
8	-1.30794810	1.91150167	1.30257178
8	-0.40693674	-1.10693843	2.18372520
8	1.83868282	1.06299351	1.38720248
6	-0.83829340	3.20564226	1.74715100
6	-2.29933919	2.18394966	0.28170135
6	-1.69208066	3.32288257	-0.54214327
1	-2.44769215	1.25654907	-0.28529646
1	-3.24422430	2.48460818	0.77166633
6	-0.86999563	4.12738684	0.50365020
1	-1.51453831	3.57524571	2.53838830
1	0.16313522	3.05434961	2.17054694
1	-2.46073346	3.93150250	-1.03704221
1	-1.03704406	2.89731441	-1.31375438
1	0.14254544	4.33389983	0.13280370

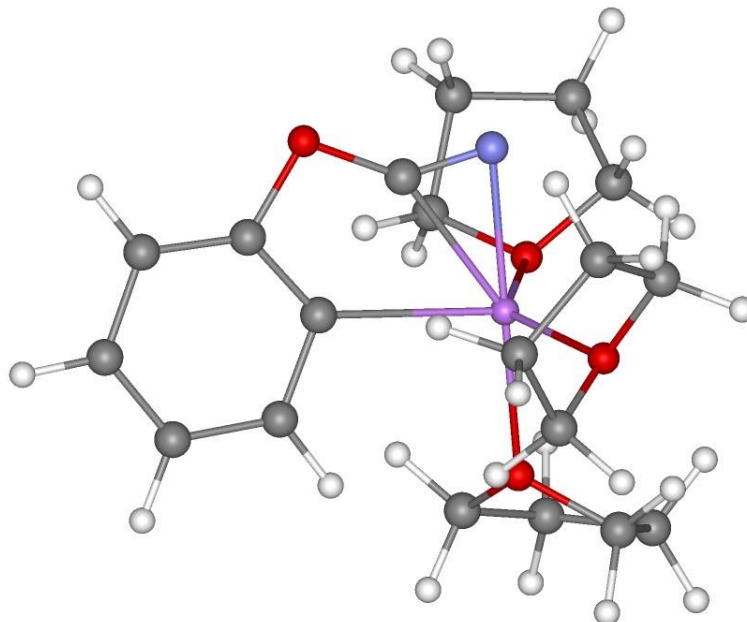
1	-1.34113077	5.08996150	0.74571127
6	2.74949810	1.21146308	0.26915986
6	2.60708617	0.40729174	2.42432124
6	3.57806778	-0.55623156	1.69953352
1	3.15686062	1.17624438	2.99577976
1	1.88873723	-0.09106998	3.08780592
6	3.49385146	-0.12490173	0.20837173
1	2.13950814	1.42116704	-0.61871960
1	3.42856491	2.06099459	0.47136927
1	3.26945829	-1.60279437	1.82168142
1	4.59533761	-0.45667799	2.10300577
1	4.48156625	-0.02854771	-0.26234026
1	2.89302628	-0.84084819	-0.37005717
6	-1.54421983	-1.08695138	3.07982800
6	-0.34930862	-2.44450999	1.62305753
6	-1.81244211	-2.78492259	1.34280145
1	0.27556461	-2.39645299	0.72028519
1	0.09681740	-3.12843502	2.36941977
6	-2.56358611	-2.11384349	2.52226559
1	-1.20444987	-1.36691323	4.09240223
1	-1.91437895	-0.05299338	3.10155446
1	-1.98996982	-3.86715988	1.28584782
1	-2.10428532	-2.33308765	0.38460208
1	-3.48834832	-1.62742740	2.18508669
1	-2.83391634	-2.84657977	3.29542130

TS1-4-OCN

E = -198.750195 E0 = -198.316480

No. of Negative Frequencies = 1

freq = - 182.73



Atomic Coordinates:

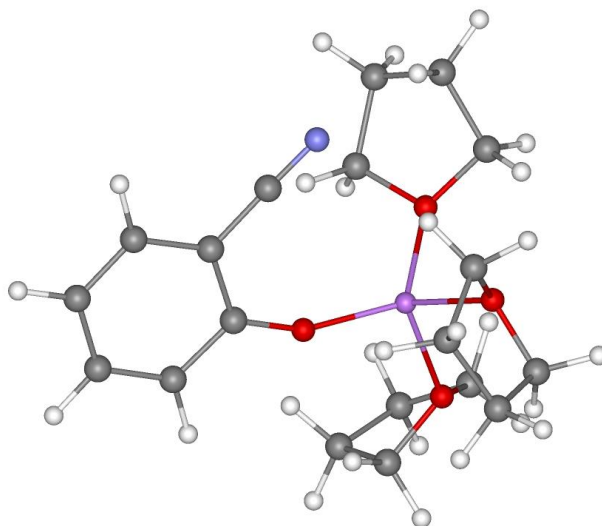
6	0.03139742	-2.39387385	-4.34809171
6	-0.09844922	-2.94405557	-3.06663613
6	0.28464960	-1.01980639	-4.52295906
6	0.01130324	-2.13359167	-1.91437018
1	-0.08686918	-2.59952179	-0.92918997
6	0.24809069	-0.75859338	-2.05593475
3	0.23861791	0.32122025	0.16634206
6	0.38374146	-0.27909174	-3.35353625
8	0.66304903	1.09425813	-3.25856899
1	0.40179375	-0.57776392	-5.51306008
1	-0.05779771	-3.03662470	-5.22597069
1	-0.28611479	-4.01520376	-2.95918777
6	0.67243453	1.23279599	-1.88266529
7	0.82893542	2.03329997	-1.00590844
8	-1.63014827	1.34745403	0.69254428
8	-0.46031581	-1.38326951	1.38786226
8	2.14294513	0.03061660	1.05453723
6	-1.45005919	2.66007014	1.30094727
6	-2.54798317	1.46501309	-0.43111148
6	-2.64276386	2.95838903	-0.73814131
1	-2.14427438	0.86629409	-1.26097266
1	-3.52742676	1.04972222	-0.13010913
6	-2.50399323	3.57186433	0.66606019
1	-1.56322215	2.54707881	2.39009707
1	-0.43065445	3.00452391	1.06602563
1	-3.58345000	3.22618608	-1.23806100

1	-1.79799178	3.26438992	-1.37158977
1	-2.18397231	4.62222245	0.64729016
1	-3.45850126	3.50984247	1.21208569
6	3.09667157	1.12222187	1.06588581
6	2.89928028	-1.13577257	0.66221702
6	3.81510298	-0.64479456	-0.46422701
1	3.48222451	-1.49969802	1.53035997
1	2.18174694	-1.90889565	0.35884518
6	4.09290111	0.83554815	-0.08090287
1	2.52450470	2.04600866	0.92307798
1	3.60112136	1.13443452	2.04895746
1	3.28194525	-0.69996427	-1.42251588
1	4.73147454	-1.24571240	-0.54219552
1	5.12886541	0.98845932	0.25226989
1	3.90465603	1.50063935	-0.93272484
6	-0.12503060	-1.51228779	2.78471871
6	-1.80486027	-1.89488488	1.28448432
6	-2.54436490	-1.37889052	2.53467793
1	-2.22201552	-1.54650681	0.33173420
1	-1.76656015	-3.00053274	1.27264932
6	-1.39777740	-1.10227161	3.55027052
1	0.14270845	-2.56533095	2.99404963
1	0.74686228	-0.87330041	2.96955903
1	-3.26706979	-2.11845784	2.90504311
1	-3.08535059	-0.45295620	2.30389982
1	-1.36162484	-0.03616388	3.81084494
1	-1.50838202	-1.67473598	4.48129412

$P_{1-4-OCN}$

E = -198.860364 E0 = -198.424906

No. of Negative Frequencies = 0



Atomic Coordinates:

6	-0.12250615	-2.92652693	-3.95103884
6	0.30511621	-1.99115010	-4.91646505
6	-0.21425222	-2.59103584	-2.60592559
6	0.64030196	-0.70726596	-4.50175972
1	0.97635993	0.03999602	-5.22329145
6	0.55332691	-0.34564945	-3.13779685
3	0.05955861	0.13326967	0.61650013
6	0.11596039	-1.28388397	-2.12231437
8	0.03112070	-0.96627462	-0.87602519
1	-0.54619459	-3.32655318	-1.86975165
1	-0.38758717	-3.93912680	-4.26649843
1	0.37299602	-2.26787922	-5.96854575
6	0.90044035	0.96500514	-2.72008438
7	1.18522132	2.03767064	-2.34101724
8	-1.11372281	1.79662177	0.69571805
8	-0.75677049	-1.04962332	2.13290536
8	1.87200675	0.69016425	1.41429234
6	-0.61396186	3.08507086	1.13805223
6	-2.04270625	2.00438787	-0.41407564
6	-2.02712199	3.51173833	-0.72290719
1	-1.68431782	1.39481677	-1.25542208
1	-3.03695029	1.64201445	-0.10850956
6	-0.70242484	3.98211179	-0.09242670
1	-1.25053234	3.45790112	1.96249690

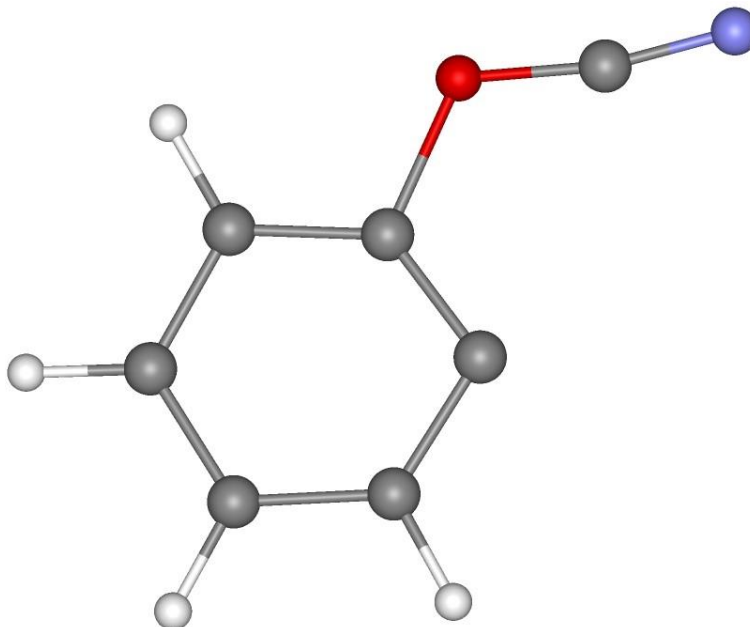
1	0.40455823	2.92401545	1.51686807
1	-2.88251105	4.01560784	-0.24741052
1	-2.07166983	3.70585374	-1.80218802
1	0.13642984	3.77288603	-0.77085059
1	-0.70687128	5.05080141	0.16245444
6	2.95689003	1.02633319	0.51321937
6	2.47716043	-0.15223618	2.42234793
6	3.51650247	-1.02350835	1.67687057
1	2.96354657	0.49388068	3.17519245
1	1.66725908	-0.71671725	2.90131513
6	3.70045007	-0.29870601	0.31223379
1	2.51706539	1.45024343	-0.39812425
1	3.59922627	1.78302907	1.00148886
1	3.14606575	-2.04646537	1.52943772
1	4.45544102	-1.08350326	2.24438036
1	4.75569275	-0.14568571	0.04949829
1	3.22175320	-0.86990136	-0.49426701
6	-1.90863112	-0.63289025	2.90034288
6	-1.00516921	-2.42747322	1.76906019
6	-2.48159689	-2.44609138	1.36423138
1	-0.31729881	-2.66991823	0.94998174
1	-0.81028202	-3.07444386	2.64520231
6	-3.12323508	-1.38897143	2.30488823
1	-1.74863365	-0.90427052	3.95896735
1	-1.97279988	0.45910101	2.81399947
1	-2.93318676	-3.44157911	1.47162390
1	-2.56619103	-2.13470497	0.31410253
1	-3.78538204	-0.71321633	1.74770549
1	-3.71794274	-1.85726834	3.10131862

Ph-OCN-anion

R_{OCN-a}

E = -68.008950 E0 = -67.924255

No. of Negative Frequencies = 0



Atomic Coordinates:

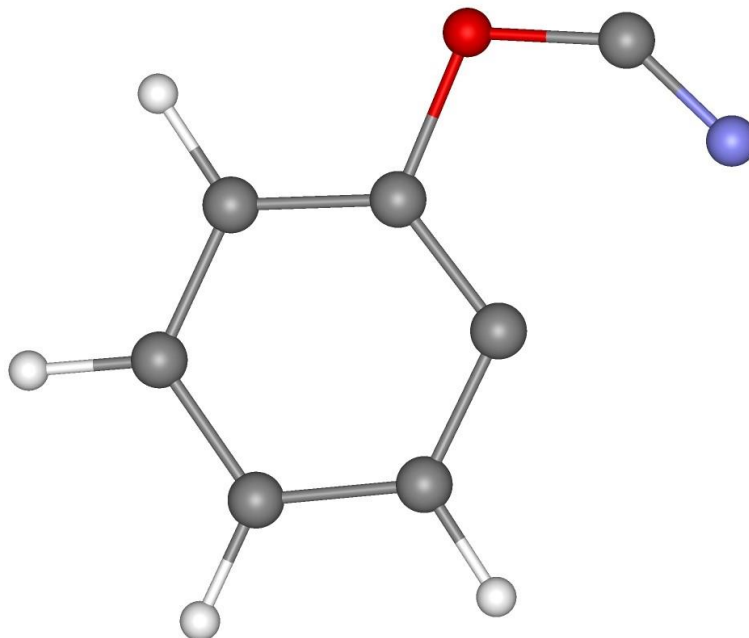
6	-0.19142367	-1.24084550	-1.25706905
6	-0.41047900	-1.87873259	-0.02605883
6	0.11065197	0.13006550	-1.26938732
6	-0.32555601	-1.14281728	1.17313845
1	-0.50679701	-1.69530186	2.10920591
6	-0.02511876	0.24088490	1.23067386
6	0.16949706	0.76061957	-0.02492343
8	0.50104760	2.22633929	-0.17036829
1	0.28816615	0.66408212	-2.20913060
1	-0.25328388	-1.79557613	-2.19718218
1	-0.64726144	-2.95043876	-0.00740809
6	0.58528208	2.93672950	0.90191763
7	0.70527492	3.74499123	1.74659194

*TS*_{1-5-OCN-a}

E = -67.989425 E0 = -67.904972

No. of Negative Frequencies = 1

freq = - 240.75



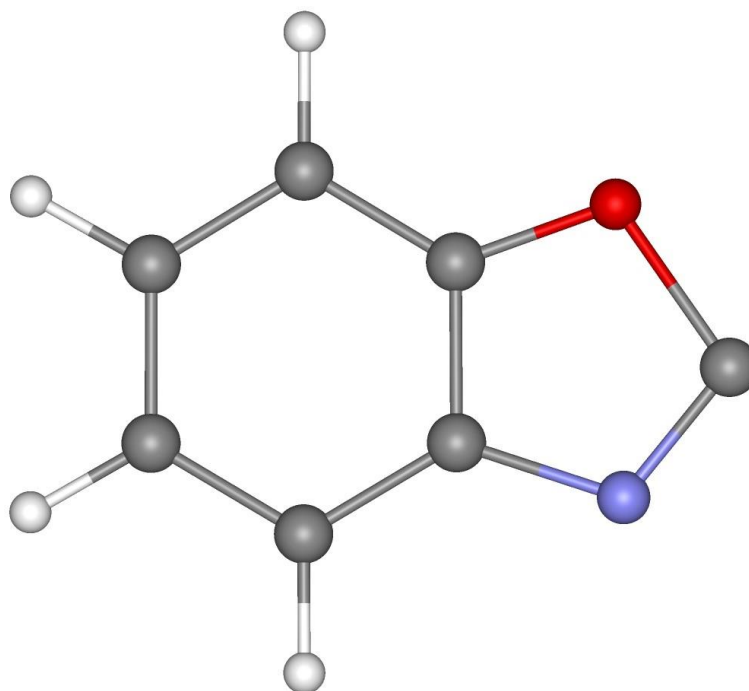
Atomic Coordinates:

6	-0.18744759	-1.21393628	-1.22021830
6	-0.39157322	-1.76958593	0.05259746
6	0.11990568	0.15122199	-1.34233841
6	-0.28702589	-0.95503194	1.19998428
1	-0.45325088	-1.42377770	2.18125290
6	0.01893453	0.41129389	1.10333920
6	0.20613998	0.89206442	-0.16182358
8	0.53363079	2.33007388	-0.34833625
1	0.28355413	0.60778112	-2.32511002
1	-0.26600464	-1.83601061	-2.11633360
1	-0.63158614	-2.83582425	0.14734191
6	0.59247705	2.94534394	0.82967618
7	0.46224620	2.69638748	1.99996824

*P*_{1-5-OCN-a}

E = -68.060534 E0 = -67.973099

No. of Negative Frequencies = 0



Atomic Coordinates:

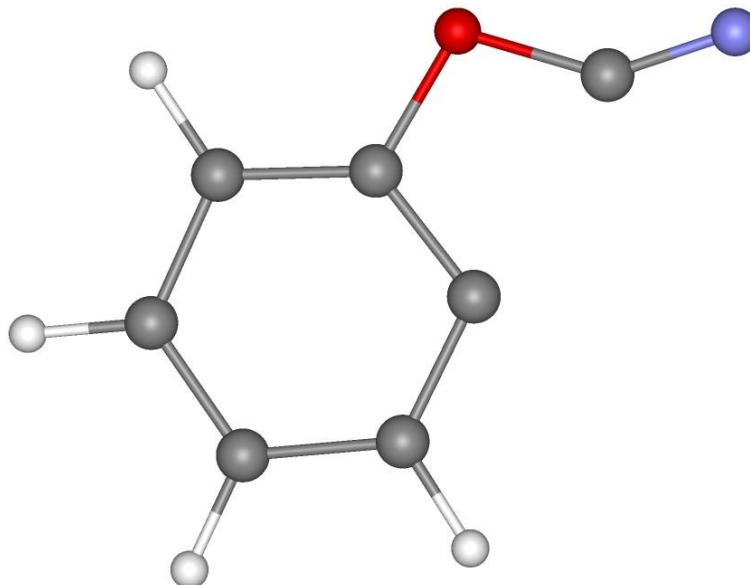
6	-0.42723690	-0.05264996	-1.62056603
6	0.43112788	-1.08340433	-1.19408986
6	-0.87628689	0.93584737	-0.72504133
6	0.86434597	-1.15357298	0.14189910
1	1.53102736	-1.95096326	0.48067640
6	0.42458992	-0.17548171	1.04404031
6	-0.44183334	0.86094272	0.60373741
8	-0.72077207	1.66706056	1.63734636
1	-1.54272416	1.73687166	-1.05451028
1	-0.75119206	-0.01817801	-2.66482278
1	0.76389183	-1.83777172	-1.91246702
6	0.05981726	1.06675912	2.86363219
7	0.68524520	0.00454052	2.40016554

TS_{1-4-OCN-a}

E = -68.006410 E0 = -67.921247

No. of Negative Frequencies = 1

freq = - 126.18



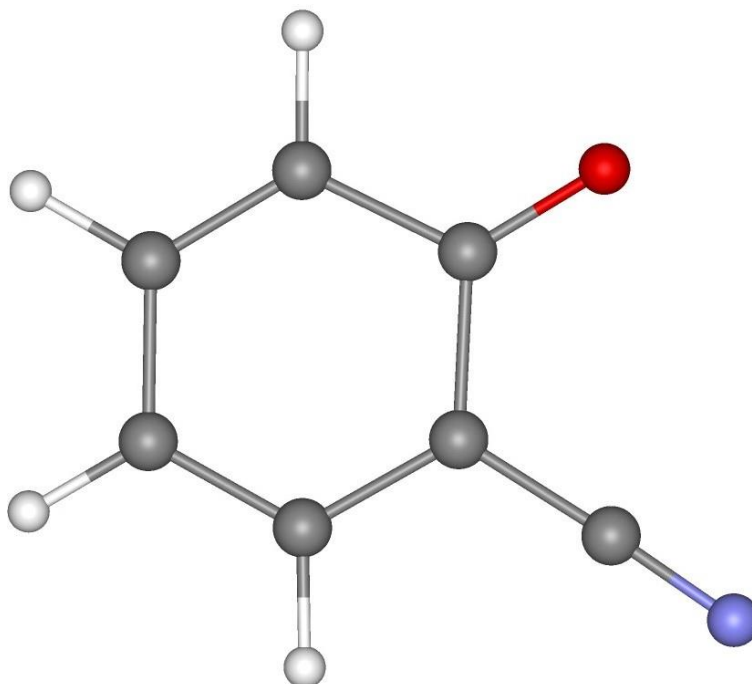
Atomic Coordinates:

6	-0.19131867	-1.24247491	-1.25663683
6	-0.39455047	-1.79569322	0.01489392
6	0.11734488	0.12569713	-1.39282008
6	-0.29147177	-0.98538459	1.17095004
1	-0.45827924	-1.45884324	2.14866919
6	0.01377647	0.38122280	1.08242285
6	0.20151772	0.85777450	-0.20948537
8	0.50199672	2.23321510	-0.19400771
1	0.27916812	0.57439488	-2.37741048
1	-0.27122042	-1.86950541	-2.14908258
1	-0.63408540	-2.86178169	0.10583241
6	0.49246502	2.58109427	1.13657343
7	0.63465703	3.46028438	1.92010123

*P*_{1-4-OCN-a}

E = -68.110842 E0 = -68.024047

No. of Negative Frequencies = 0



Atomic Coordinates:

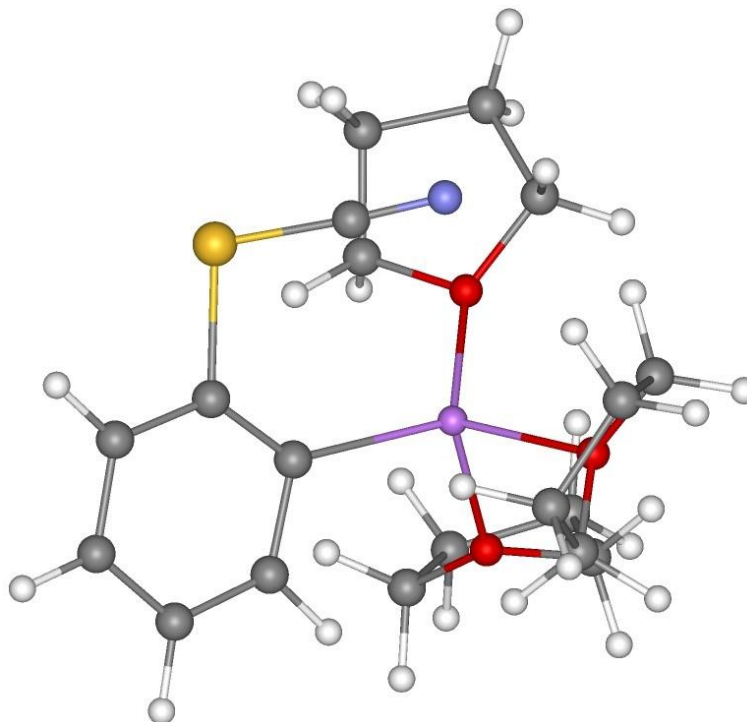
6	-0.41744070	-1.59991714	-0.53209353
6	0.01509641	-0.65122860	-1.49021775
6	-0.51408712	-1.28095429	0.81269950
6	0.34670295	0.62845485	-1.04895914
1	0.68442500	1.38468587	-1.76398342
6	0.25965934	0.98799389	0.31495464
6	-0.18504647	0.03367737	1.34644191
8	-0.27457549	0.31873030	2.57035880
1	-0.84938226	-2.02124562	1.54435774
1	-0.68195196	-2.61104372	-0.86330359
1	0.08794922	-0.91281706	-2.54737907
6	0.61351376	2.31079373	0.69423388
7	0.91513732	3.41287040	0.96289003

Ph-SCN-Li(THF)₃

R_{SCN}

E = -192.907799 E0 = -192.477004

No. of Negative Frequencies = 0



Atomic Coordinates:

6	0.11416103	-2.50045759	-4.33299574
6	0.19042984	-3.10899235	-3.07503838
6	0.03124586	-1.10482762	-4.40529979
6	0.17543076	-2.31967783	-1.91264523
1	0.24731402	-2.85169614	-0.95350257
6	0.06185122	-0.90187865	-1.90447804
3	0.16070653	-0.04276232	0.10394356
6	0.00096907	-0.38658607	-3.19930692
16	-0.23436127	1.44721016	-3.51972192
1	0.00521909	-0.60187790	-5.37558788
1	0.13607108	-3.09436947	-5.24877953
1	0.26695842	-4.19784633	-3.00219312
6	0.73742216	2.13748975	-2.31564185
7	1.37704999	2.67070950	-1.48664269
8	-1.16504232	1.44375398	0.66347817
8	-0.52913778	-1.53789448	1.42206042
8	2.01929953	0.03501237	1.01856942
6	-0.84115420	2.77239379	1.16589300
6	-2.37274534	1.51291057	-0.14802173
6	-2.60933799	2.99885390	-0.41422345
1	-2.19987673	0.91382670	-1.05411032
1	-3.20568747	1.06917692	0.42674257
6	-2.06830073	3.64025288	0.87582072

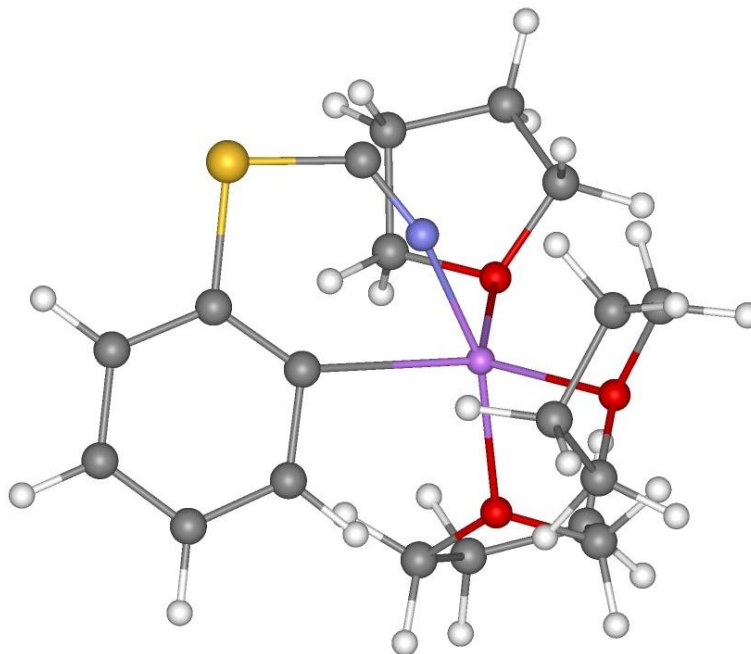
1	-0.60729764	2.67996320	2.23713337
1	0.04694304	3.13698761	0.62546299
1	-3.66735058	3.22710882	-0.60083581
1	-2.02209888	3.32875341	-1.28359868
1	-1.80544055	4.69949113	0.75449702
1	-2.80869601	3.55717770	1.68670667
6	2.93358891	1.16184241	1.05629910
6	2.82908477	-1.11014791	0.66325439
6	3.75023017	-0.58803666	-0.43916090
1	3.39785984	-1.44247559	1.55289435
1	2.14856471	-1.91106600	0.34731951
6	4.03572103	0.86968624	0.00884637
1	2.35085215	2.06119079	0.82577047
1	3.35065440	1.23801629	2.07605343
1	3.20827939	-0.59918552	-1.39478225
1	4.66296333	-1.19026312	-0.54444636
1	5.03425712	0.96802200	0.45740789
1	3.96755225	1.56585002	-0.83616946
6	-0.44201463	-1.36494084	2.84816023
6	-1.75489036	-2.26727972	1.19493905
6	-2.75416579	-1.77817492	2.27383286
1	-2.06161558	-2.06772300	0.16031984
1	-1.55139215	-3.34772976	1.30450681
6	-1.86638921	-0.98885411	3.27631797
1	-0.11859263	-2.31576787	3.31404077
1	0.31710350	-0.59522482	3.03691281
1	-3.25643591	-2.62942203	2.75334747
1	-3.53161187	-1.13471475	1.84144535
1	-2.01402349	0.09225559	3.15107442
1	-2.07012410	-1.24806236	4.32413161

*TS*_{1-5-SCN}

E = -192.892836 E0 = -192.461873

No. of Negative Frequencies = 1

freq = - 169.67



Atomic Coordinates:

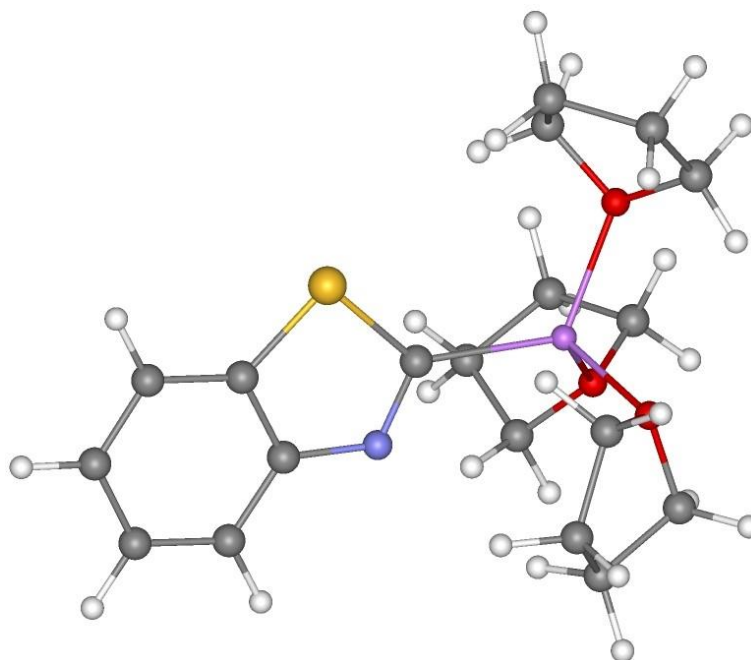
6	-0.31476761	-2.43956242	-4.22990991
6	-0.01699823	-2.91470305	-2.94681318
6	-0.28709497	-1.06383752	-4.48704245
6	0.28251870	-2.00604087	-1.91532955
1	0.50330135	-2.41338521	-0.92182626
6	0.29994248	-0.61795927	-2.14464333
3	0.32067325	0.19088510	0.19734560
6	0.04292566	-0.18845493	-3.43710407
16	0.18734280	1.59815456	-3.84777099
1	-0.50239094	-0.69418283	-5.49306555
1	-0.55386547	-3.13617422	-5.03583089
1	-0.01680020	-3.98984468	-2.74786409
6	0.69055584	2.09017439	-2.28367318
7	0.85088916	1.40721686	-1.28774276
8	-1.30497686	1.44161634	0.85614588
8	-0.43263686	-1.48205223	1.31686669
8	2.13917991	0.08378081	1.26656219
6	-0.96535727	2.80697374	1.22308473
6	-2.36349341	1.46825453	-0.14980383
6	-2.55201374	2.93756055	-0.53516748
1	-2.05258697	0.83632132	-0.99558241
1	-3.27495321	1.04449330	0.30677708
6	-2.13978668	3.66608391	0.75591938
1	-0.79744272	2.82533205	2.30996672
1	-0.03551523	3.09059650	0.70152775
1	-3.58174306	3.15752018	-0.84737369

1	-1.86994861	3.20292193	-1.35564153
1	-1.84934974	4.71150190	0.58578114
1	-2.95633674	3.64626212	1.49469859
6	3.02561095	1.22487535	1.13555797
6	2.95716323	-1.07216798	0.97669631
6	3.80056102	-0.64860627	-0.22814943
1	3.58670510	-1.30319992	1.85745148
1	2.27905889	-1.91529311	0.78953549
6	4.05273283	0.86004065	0.03665068
1	2.40106495	2.08790793	0.87572720
1	3.51469708	1.40018556	2.11002645
1	3.21612838	-0.77905039	-1.14874728
1	4.72919680	-1.22938150	-0.31304241
1	5.07790065	1.04884105	0.38478717
1	3.88122139	1.44896836	-0.87239359
6	-0.35417072	-1.43336902	2.75680320
6	-1.64672677	-2.21190876	1.02372934
6	-2.65434488	-1.84739731	2.14239233
1	-1.96347220	-1.92731333	0.01275887
1	-1.41984237	-3.29304326	1.03037928
6	-1.78594619	-1.12524272	3.20900672
1	-0.01341593	-2.41614409	3.13595287
1	0.38780310	-0.66846625	3.01750650
1	-3.13026345	-2.75221846	2.54446042
1	-3.45062376	-1.19027343	1.76964673
1	-1.95603369	-0.04142895	3.16981610
1	-1.98427502	-1.47576698	4.23095701

*P*_{1-5-SCN}

E = -192.963167 E0 = -192.529185

No. of Negative Frequencies = 0



Atomic Coordinates:

6	-1.66614189	-1.15859566	-5.62675306
6	-0.91413624	-2.26413707	-5.18255626
6	-1.91866591	-0.07715910	-4.77727392
6	-0.40509804	-2.30365172	-3.88344517
1	0.17899245	-3.15499054	-3.52887840
6	-0.64747585	-1.22636749	-3.01081612
3	0.20481687	0.25048721	0.95649554
6	-1.40817872	-0.11320117	-3.47047692
16	-1.52995301	1.05438349	-2.16720804
1	-2.50137421	0.77660038	-5.12652995
1	-2.05689382	-1.14398499	-6.64611360
1	-0.72849721	-3.09760615	-5.86271047
6	-0.53204732	-0.04114701	-1.04279175
7	-0.19742368	-1.13710288	-1.69598237
8	-0.57371808	1.77075886	2.05694462
8	-0.04307257	-1.42824112	2.07617758
8	2.21503172	0.62663996	0.90298278
6	0.22819225	2.83264114	2.61973247
6	-1.77366966	2.41439199	1.56749648
6	-1.28645166	3.72003326	0.91936414
1	-2.25648816	1.71793828	0.86998283
1	-2.44659663	2.61033689	2.42271400
6	0.03064935	4.04469578	1.68412259
1	-0.13586534	3.05035931	3.64030698
1	1.25999221	2.46254851	2.67470530
1	-2.03454935	4.51917442	1.00657647
1	-1.08520510	3.55666244	-0.14756640

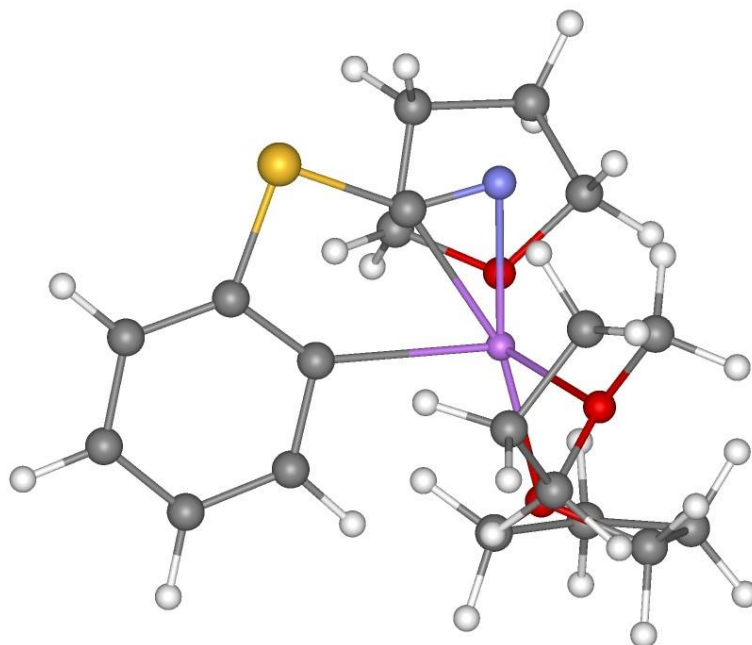
1	0.87121141	4.14107446	0.98436278
1	-0.03740465	4.97920487	2.25733316
6	2.64716144	1.28128054	-0.32682398
6	3.07999361	-0.51785634	1.09627346
6	3.28093554	-1.06988659	-0.31312867
1	4.03360794	-0.18571957	1.54856384
1	2.56505270	-1.19579761	1.78989943
6	3.41559266	0.22085999	-1.15308058
1	1.73827165	1.63827960	-0.83008413
1	3.28726183	2.13948392	-0.06162738
1	2.38566446	-1.62748276	-0.62448689
1	4.15920133	-1.72524729	-0.39293879
1	4.47020065	0.51053794	-1.26658007
1	2.98345825	0.09855769	-2.15389543
6	-0.77576895	-1.43137437	3.32311616
6	-0.48147707	-2.60942542	1.35470615
6	-1.99443217	-2.63281785	1.57734301
1	-0.18464634	-2.48055731	0.30413793
1	0.01219885	-3.49752634	1.79208198
6	-2.15347546	-2.07240264	3.01721683
1	-0.21257553	-2.02544508	4.06445134
1	-0.83015172	-0.38984275	3.66639936
1	-2.41936214	-3.63901617	1.46308860
1	-2.47351021	-1.96889272	0.84451692
1	-2.96397587	-1.33348583	3.06980885
1	-2.37920458	-2.86796940	3.74084678

TS1-4-SCN

E = -192.899369 E0 = -192.468565

No. of Negative Frequencies = 1

freq = - 146.61



Atomic Coordinates:

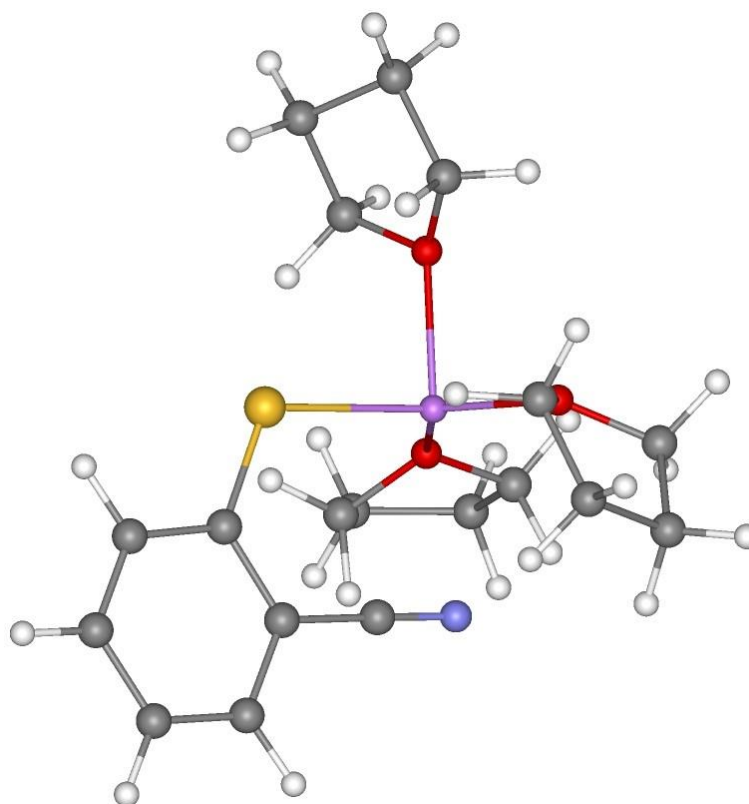
6	0.01868299	-2.30425575	-4.29170833
6	-0.15035767	-2.76954176	-2.98368019
6	0.33840729	-0.95698688	-4.52580621
6	-0.01031753	-1.88952007	-1.88996308
1	-0.14475418	-2.29601362	-0.88143233
6	0.29796895	-0.53026385	-2.07803952
3	0.24756374	0.32502936	0.16342716
6	0.47049116	-0.11930860	-3.41501543
16	0.90336388	1.61939918	-3.45060325
1	0.48063825	-0.59395338	-5.54554162
1	-0.09233185	-2.98710148	-5.13632079
1	-0.39208549	-3.82123175	-2.80923928
6	0.81420719	1.57179386	-1.67258135
7	0.92149903	2.21414982	-0.66986036
8	-1.74197277	1.25050343	0.50596255
8	-0.45955216	-1.32076525	1.46796067
8	2.19715085	-0.09939874	1.00123896
6	-1.73367443	2.49947507	1.25597188
6	-2.55092404	1.41749414	-0.69217647
6	-2.70846808	2.92517867	-0.87848526
1	-2.02974879	0.91381804	-1.51882483
1	-3.52869454	0.92743678	-0.52936742
6	-2.76294432	3.41210105	0.58015078
1	-1.97675756	2.27122681	2.30567528
1	-0.71882765	2.92293690	1.19528918

1	-3.60531813	3.18625514	-1.45646528
1	-1.82484460	3.33662245	-1.38704448
1	-2.50837293	4.47464105	0.69080088
1	-3.76728357	3.25144154	1.00263410
6	3.21285785	0.92769636	1.10270371
6	2.89481200	-1.27295624	0.53168680
6	3.84729198	-0.75405228	-0.55299768
1	3.45006997	-1.72658111	1.37560554
1	2.14268007	-1.98536099	0.17018564
6	4.17691857	0.69071574	-0.08114286
1	2.69549915	1.89285771	1.06228494
1	3.73020943	0.81341124	2.07309728
1	3.32940796	-0.73260344	-1.52084756
1	4.74059505	-1.38589307	-0.65213444
1	5.22357087	0.79577933	0.23674476
1	3.98997543	1.41393297	-0.88470018
6	-0.05357339	-1.47979829	2.84236603
6	-1.81254120	-1.81853072	1.42643727
6	-2.47958923	-1.31372319	2.72121908
1	-2.27609980	-1.44697269	0.50526949
1	-1.78498467	-2.92408304	1.39657728
6	-1.27765713	-1.05733471	3.67697572
1	0.20169414	-2.54146635	3.02186995
1	0.84090460	-0.86341103	2.99026441
1	-3.18638457	-2.05290760	3.12192007
1	-3.02932641	-0.38394185	2.52811128
1	-1.21189087	0.00677008	3.94138570
1	-1.34718284	-1.63270898	4.61016183

*P*_{1-4-SCN}

E = -192.991874 E0 = -192.558956

No. of Negative Frequencies = 0



Atomic Coordinates:

6	0.02964820	-1.94408218	-5.16357092
6	0.77339770	-3.02541028	-4.64982833
6	-0.39327393	-0.90447390	-4.34150855
6	1.08267467	-3.04271603	-3.29468759
1	1.65579839	-3.86543168	-2.86360938
6	0.65589922	-1.98978395	-2.45159600
3	0.00170063	0.29213626	0.44722718
6	-0.09956136	-0.87829477	-2.95189862
16	-0.64445754	0.44835143	-1.94759255
1	-0.96764868	-0.07356934	-4.75358365
1	-0.22091552	-1.91841616	-6.22668599
1	1.10148090	-3.83607553	-5.30073987
6	0.98578437	-2.03992244	-1.06913163
7	1.26254856	-2.09945124	0.06891385
8	-0.98141707	2.07423606	0.94856914
8	-1.23510833	-0.88826079	1.60370753
8	1.90971991	0.97824431	0.83130991
6	-0.40129155	3.34378853	0.54955095
6	-2.42747402	2.13033451	0.78678926
6	-2.72518754	3.46209184	0.08964350
1	-2.74274111	1.25811378	0.19641491
1	-2.88409046	2.07725919	1.78966656
6	-1.55756792	4.34356170	0.56564992

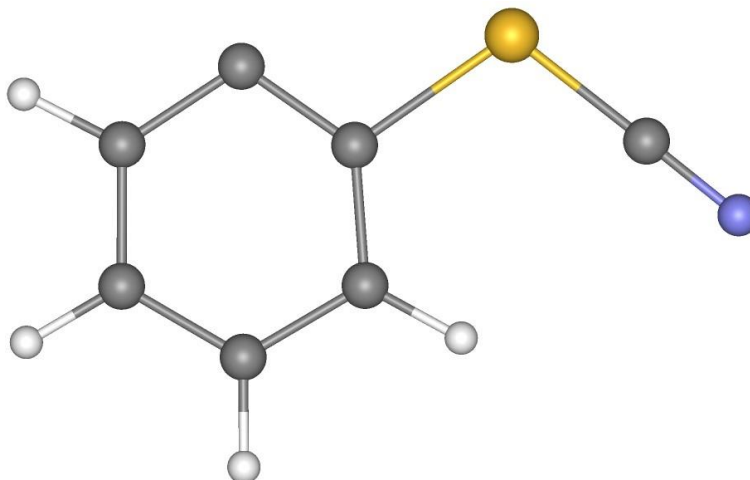
1	0.40620634	3.57639595	1.25769617
1	0.02253306	3.24060981	-0.46470808
1	-3.71230116	3.86195932	0.35822937
1	-2.68430558	3.33317221	-1.00201477
1	-1.37201289	5.20776242	-0.08628800
1	-1.73765214	4.70946692	1.58852967
6	2.72380190	1.41416267	-0.28303561
6	2.83681384	0.54356223	1.84492438
6	3.96725660	-0.17853173	1.09047509
1	3.21271205	1.42922618	2.39104307
1	2.28550803	-0.10037959	2.54263330
6	3.91044619	0.43276556	-0.33928546
1	2.07748772	1.39989320	-1.17210676
1	3.06504685	2.44814542	-0.08902462
1	3.76393600	-1.25552022	1.04995482
1	4.93893544	-0.02351442	1.57918125
1	4.84006933	0.95037579	-0.61248907
1	3.72766520	-0.35232002	-1.08357415
6	-0.90218221	-1.39686992	2.91367840
6	-2.05235596	-1.90877541	0.98703460
6	-3.01184647	-2.32670787	2.10378935
1	-2.51974498	-1.45983603	0.10119733
1	-1.40858175	-2.74761738	0.66853911
6	-2.12628115	-2.22957591	3.37616959
1	0.00268593	-2.02397116	2.83321545
1	-0.68747983	-0.52724791	3.54973511
1	-3.42155392	-3.33347436	1.94699570
1	-3.85125685	-1.61958247	2.16227122
1	-2.66355957	-1.74385029	4.20118771
1	-1.80790756	-3.22195228	3.72303617

Ph-SCN-anion

R_{SCN-a}

E = -62.165705 E0 = -62.083649

No. of Negative Frequencies = 0



Atomic Coordinates:

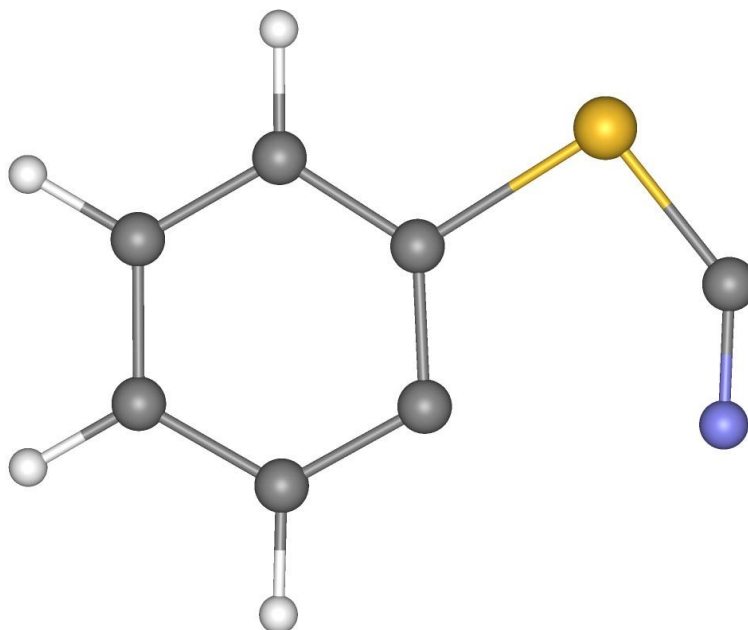
6	0.32666355	-1.06700883	-1.00066072
6	-0.14997556	-2.01496514	-0.08069890
6	0.30573868	0.29520674	-0.65949458
6	-0.64386775	-1.60268769	1.17198260
1	-1.00468185	-2.38887594	1.85398300
6	-0.69257960	-0.24554123	1.57795848
6	-0.20351440	0.60019808	0.60678179
16	-0.29106716	2.40758576	1.20079793
1	0.67041256	1.05502114	-1.35665211
1	0.71169570	-1.37722226	-1.97600421
1	-0.13331242	-3.07969045	-0.34789402
6	0.33511290	3.37934643	-0.05731905
7	0.76937534	4.03863338	-0.93278020

*TS*_{1-5-SCN-a}

E = -62.147566 E0 = -62.065708

No. of Negative Frequencies = 1

freq = - 176.82



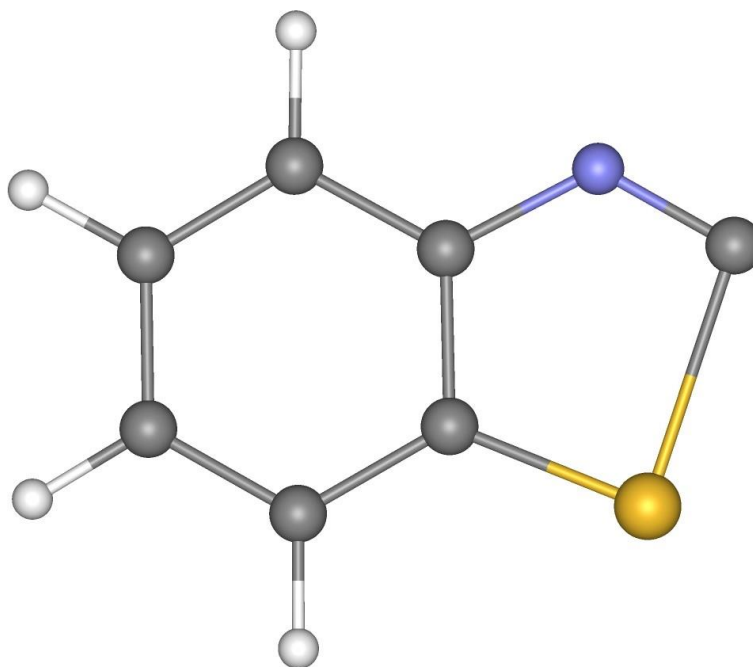
Atomic Coordinates:

6	0.57505047	-0.80791802	-1.50202307
6	0.09831817	-1.75983460	-0.58742285
6	0.54906290	0.55471979	-1.16380239
6	-0.40240856	-1.34197779	0.66222796
1	-0.76866438	-2.11232830	1.35693460
6	-0.43789881	0.01546854	1.02149049
6	0.03832749	0.90487696	0.09532383
16	0.03290472	2.76958750	0.48806119
1	0.92166899	1.29990971	-1.87838044
1	0.96602274	-1.11978160	-2.47481661
1	0.11877338	-2.82450271	-0.85202747
6	-0.64773314	2.63795029	2.04416580
7	-1.04342396	1.78383022	2.79026896

*P*_{1-5-SCN-a}

E = -62.216662 E0 = -62.131528

No. of Negative Frequencies = 0



Atomic Coordinates:

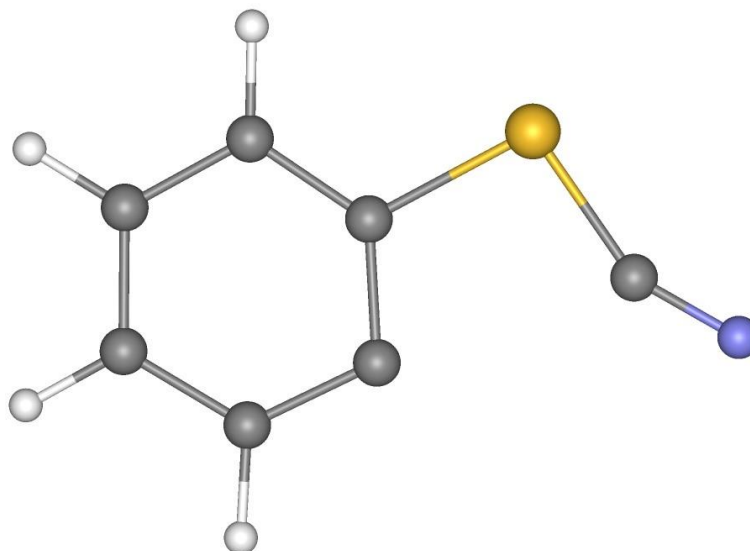
6	-0.56250675	-0.09820684	-1.63249920
6	0.18792722	-1.20186706	-1.18846006
6	-0.81468614	0.98481677	-0.78166069
6	0.68882573	-1.21836302	0.11922425
1	1.27460238	-2.06229192	0.49055825
6	0.44562454	-0.14084262	0.98601161
6	-0.32020287	0.99107671	0.54090063
16	-0.51468655	2.22158158	1.75232741
1	-1.39878838	1.83569785	-1.13845708
1	-0.95525818	-0.08228304	-2.65343829
1	0.37971972	-2.04276355	-1.85955786
6	0.68063967	0.89798732	3.06935124
7	0.90878959	-0.08454218	2.29569978

*TS*_{1-4-SCN-a}

E = -62.155991 E0 = -62.074141

No. of Negative Frequencies = 1

freq = - 103.44



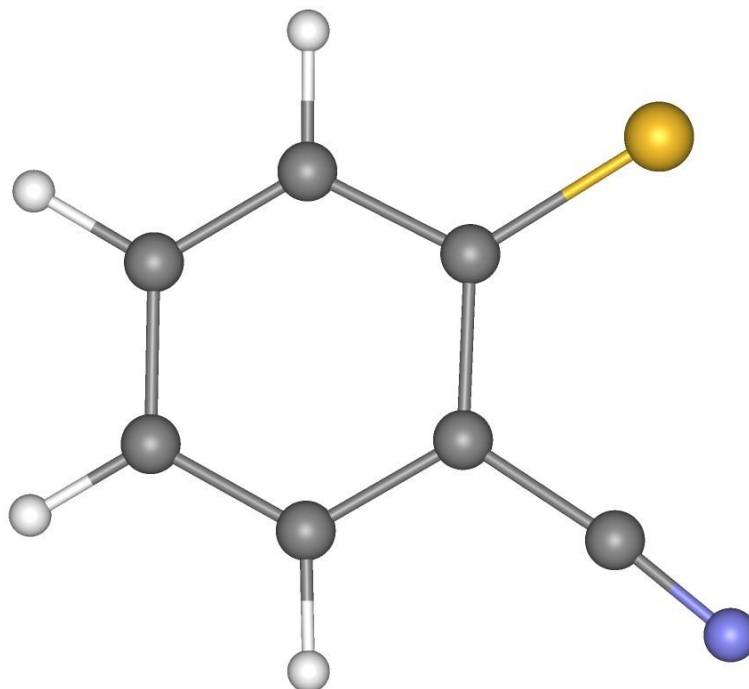
Atomic Coordinates:

6	0.59932471	-0.83529722	-1.56350641
6	0.12661130	-1.80025735	-0.66303641
6	0.56209160	0.52065816	-1.19950558
6	-0.37920600	-1.40531069	0.59279982
1	-0.73816223	-2.20078725	1.26384109
6	-0.44676309	-0.06092955	1.02487752
6	0.04489548	0.83838577	0.06677866
16	-0.01191401	2.59721662	0.55847358
1	0.92959047	1.28231202	-1.89706153
1	0.99423620	-1.12755849	-2.54050444
1	0.15430930	-2.86081481	-0.94447309
6	-0.70843249	2.34943837	2.12805618
7	-1.12658124	2.70294442	3.17326061

*P*_{1-4-SCN-a}

E = -62.256488 E0 = -62.171084

No. of Negative Frequencies = 0



Atomic Coordinates:

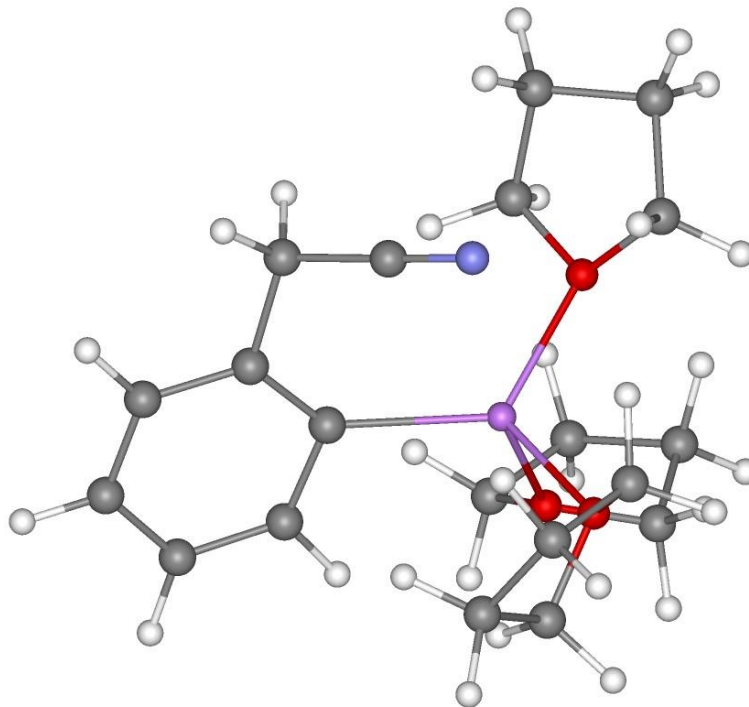
6	-0.36999385	-0.01029101	-1.71170935
6	0.37269693	-1.08896768	-1.18198016
6	-0.79784459	1.03313729	-0.90101019
6	0.66699621	-1.08087206	0.17932037
1	1.23923696	-1.89740366	0.62651585
6	0.23786631	-0.02476483	1.01696296
6	-0.52239234	1.09026899	0.50372874
16	-1.07213653	2.40774130	1.48375591
1	-1.37127930	1.86172575	-1.32182319
1	-0.61404876	0.00638837	-2.77876065
1	0.70881617	-1.90908182	-1.81888792
6	0.58941485	-0.10768580	2.39847943
7	0.93266794	-0.28019485	3.50540819

Ph-CH₂-CN-Li(THF)₃

R_{CCN}

E = -189.620241 E0 = -189.163271

No. of Negative Frequencies = 0



Atomic Coordinates:

6	0.46412139	-2.50350447	-4.16878391
6	0.40435768	-3.11625933	-2.91327815
6	0.32421307	-1.11255519	-4.24494147
6	0.20714626	-2.32995974	-1.76457710
1	0.18080966	-2.86788207	-0.80538387
6	0.05580304	-0.91843578	-1.77168273
3	0.11609554	-0.09589617	0.24006561
6	0.12155696	-0.36113938	-3.07345566
6	-0.07570833	1.15238599	-3.26244595
1	0.37615801	-0.62070090	-5.22272971
1	0.62360863	-3.09249681	-5.07446134
1	0.51683435	-4.20191741	-2.83035486
6	0.63841175	1.96021238	-2.27851726
7	1.21239547	2.63013574	-1.51583639
8	-1.15281749	1.43046347	0.87310832
8	-0.56780102	-1.56155843	1.58672526
8	1.97818586	0.01627583	1.15365318
6	-0.77586511	2.76562894	1.31747595
6	-2.38247768	1.50661954	0.10045730
6	-2.58049385	2.98809279	-0.22095864
1	-2.25846654	0.85655380	-0.77928559
1	-3.21205445	1.11754732	0.71849615
6	-1.98436906	3.66026165	1.02879231

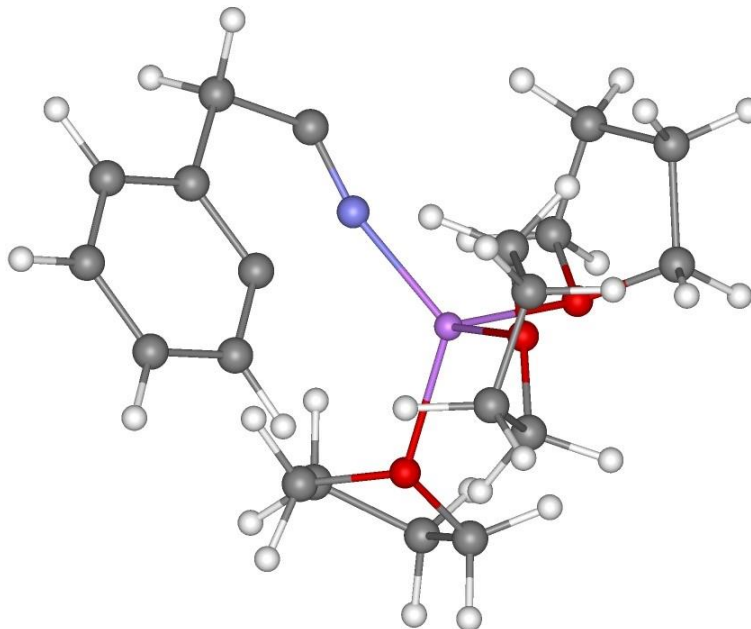
1	-0.51445922	2.70476834	2.38432039
1	0.10562689	3.08475488	0.73924861
1	-3.63540991	3.24326182	-0.38967144
1	-2.00346512	3.27001279	-1.11401279
1	-1.69360628	4.70559116	0.86023678
1	-2.70432605	3.62998243	1.86138031
6	2.91468569	1.11708646	1.02343073
6	2.75149784	-1.18385667	0.91923932
6	3.65339484	-0.82509137	-0.26178039
1	3.33704288	-1.42166278	1.82832178
1	2.04283971	-1.99792118	0.71997973
6	3.98187010	0.66936039	-0.00573296
1	2.34369852	1.99347639	0.69456233
1	3.36218710	1.31381048	2.01377934
1	3.08516802	-0.94195109	-1.19451106
1	4.55026111	-1.45756077	-0.31218075
1	4.99396377	0.79909636	0.40277748
1	3.90866688	1.25653395	-0.92971031
6	-0.52176104	-1.34896108	3.00877806
6	-1.75895429	-2.34251996	1.34885722
6	-2.80406533	-1.85673398	2.38455056
1	-2.04221318	-2.18388325	0.30041008
1	-1.51998604	-3.41092333	1.49825164
6	-1.97002307	-1.02076418	3.39621606
1	-0.17087818	-2.27325961	3.50708593
1	0.20044466	-0.54368106	3.19452277
1	-3.30014773	-2.70976299	2.86734122
1	-3.58307973	-1.24383584	1.91214390
1	-2.15387303	0.05249866	3.25284582
1	-2.18930419	-1.27337999	4.44253464
1	-1.14655362	1.41344155	-3.18180272
1	0.25111388	1.48020169	-4.26349369

*TS*_{1-5-CCN-C}

E = -189.593688 E0 = -189.137119

No. of Negative Frequencies = 1

freq = - 209.88



Atomic Coordinates:

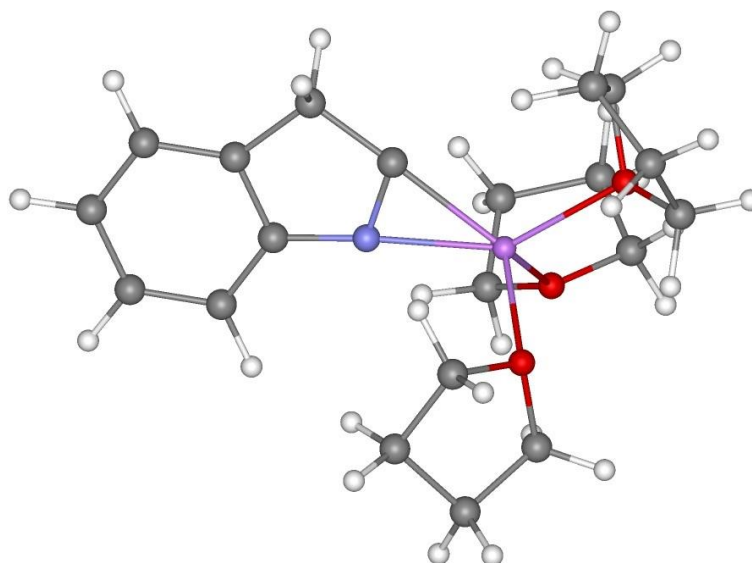
6	1.21539574	-2.53602473	-4.12838403
6	1.52109732	-2.84889624	-2.79781352
6	0.35299379	-1.46715512	-4.41212846
6	0.96670985	-2.08209244	-1.75546328
1	1.20903584	-2.35637489	-0.72066423
6	0.11291994	-1.00577043	-2.03610229
3	-0.22205194	0.19361360	0.47797166
6	-0.19529749	-0.71209821	-3.36257901
6	-1.15987368	0.45649080	-3.61060481
1	0.11157059	-1.23434370	-5.45493803
1	1.64056041	-3.12589108	-4.94321607
1	2.18494401	-3.68958659	-2.57321955
6	-1.52792470	1.00846254	-2.27084198
7	-1.08910344	0.53543428	-1.22876358
8	-1.03817807	1.65347877	1.78884537
8	-0.75333214	-1.50499174	1.47968274
8	1.77023032	0.53590425	0.73374646
6	-0.26997780	2.78555322	2.24449605
6	-2.29261570	2.21321125	1.32769902
6	-1.91834923	3.52211570	0.60839731
1	-2.75566871	1.47333603	0.66363545
1	-2.94080598	2.39687630	2.20478433
6	-0.53529001	3.90010887	1.21478877
1	-0.62373895	3.07951531	3.25077059
1	0.77690726	2.46201100	2.31116703
1	-2.67591460	4.30045077	0.77265156

1	-1.83379680	3.33591389	-0.47038122
1	0.23699849	3.89620166	0.43359725
1	-0.53359318	4.89178480	1.68790099
6	2.47727662	1.18109406	-0.37139421
6	2.65028548	-0.42233649	1.38005642
6	3.82390420	-0.62322437	0.42076963
1	2.98173731	0.00028716	2.34545392
1	2.06873722	-1.33546176	1.57424226
6	3.94359821	0.76795313	-0.22617526
1	2.03007340	0.82182506	-1.31141765
1	2.31516295	2.26578072	-0.28795892
1	3.57202449	-1.37539702	-0.34060246
1	4.73904868	-0.94006092	0.93900383
1	4.48240977	1.45872806	0.44106166
1	4.46242143	0.74744463	-1.19345574
6	-1.22198849	-1.50367899	2.84695113
6	-1.60863552	-2.43573471	0.77106256
6	-3.01184329	-2.13860809	1.30750420
1	-1.47585859	-2.24223632	-0.30111208
1	-1.29006069	-3.46802448	1.00781804
6	-2.75415682	-1.72307945	2.78249664
1	-0.72342548	-2.32332780	3.39446285
1	-0.92881198	-0.54196995	3.28659710
1	-3.68098122	-3.00515380	1.22016656
1	-3.45087929	-1.30743990	0.73893447
1	-3.30143573	-0.80642374	3.03856368
1	-3.06448055	-2.50574366	3.48835496
1	-2.06551453	0.13290322	-4.15249971
1	-0.70245870	1.24464751	-4.23391838

*P*_{1-5-CCN-C}

E = -189.637928 E0 = -189.179585

No. of Negative Frequencies = 0



Atomic Coordinates:

6	-1.94461244	-1.91511852	-4.92863977
6	-2.80266881	-1.98971751	-3.82101029
6	-0.65362339	-1.37114348	-4.79732443
6	-2.39274691	-1.52565036	-2.56128903
1	-3.05879197	-1.58240162	-1.69698912
6	-1.10664849	-0.98586129	-2.43756138
3	0.29360599	0.30472491	0.52839644
6	-0.24005023	-0.90740063	-3.54911713
6	1.02838742	-0.27707725	-3.03272991
1	0.00677591	-1.31745996	-5.66680307
1	-2.28282144	-2.28230990	-5.89967716
1	-3.80143095	-2.41494642	-3.94231887
6	0.74847357	-0.02852215	-1.54018828
7	-0.48508004	-0.45698432	-1.26794984
8	-1.20222101	1.63908632	1.18876858
8	0.18055824	-1.30073484	1.88357888
8	1.94294031	1.31929016	1.50452876
6	-0.92361830	2.92528623	1.78117635
6	-2.30435288	1.87446151	0.28343956
6	-1.95485791	3.19626902	-0.41591970
1	-2.35539266	1.00583682	-0.38358642
1	-3.23833419	1.96143532	0.87074102
6	-1.10686758	3.95744144	0.64501205
1	-1.64410028	3.10397528	2.60073464
1	0.09245027	2.87795365	2.19114389
1	-2.85330562	3.75045990	-0.71955947
1	-1.35641030	2.99139492	-1.31352529
1	-0.13687472	4.25671578	0.22637385
1	-1.61002377	4.86313196	1.01081234

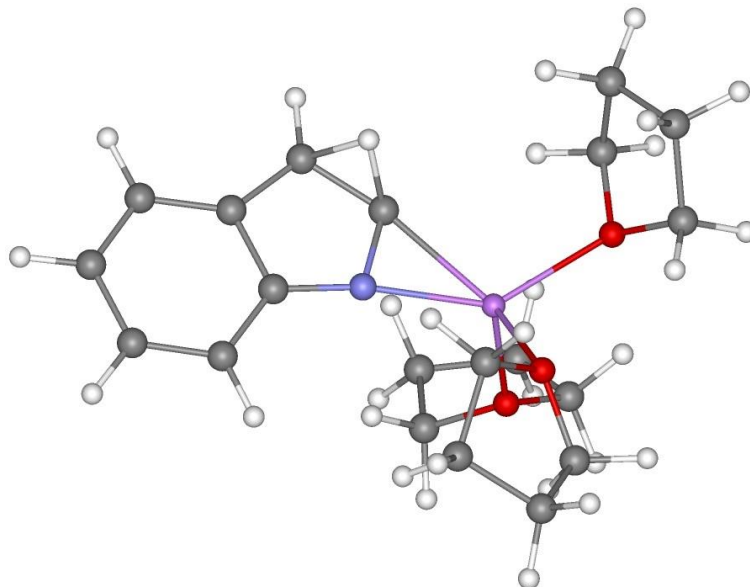
6	2.93013316	1.78013506	0.55352263
6	2.69428707	0.73586537	2.59004317
6	3.93475245	0.06925492	1.94639245
1	2.99271965	1.53694144	3.29114116
1	2.02456178	0.03499495	3.10378503
6	3.96130799	0.64922071	0.50484655
1	2.40350494	1.92415600	-0.39947818
1	3.36855641	2.73006854	0.91480131
1	3.83598360	-1.02448747	1.92920260
1	4.84657528	0.31510371	2.50853863
1	4.95728190	1.00169992	0.20362556
1	3.61349092	-0.10048705	-0.22005424
6	-1.00759931	-1.42619615	2.71669799
6	0.45757799	-2.58471186	1.26996147
6	-0.90696054	-3.25449445	1.14624151
1	0.94860406	-2.38429677	0.30860476
1	1.13744486	-3.16440675	1.92260382
6	-1.57459943	-2.83868012	2.47093562
1	-0.72087183	-1.26390950	3.76835476
1	-1.70144527	-0.62881409	2.41239091
1	-0.83952049	-4.34386885	1.02256032
1	-1.44227217	-2.82758664	0.28626352
1	-2.67131434	-2.83719253	2.41428261
1	-1.27786600	-3.52306215	3.28010235
1	1.27970496	0.67410672	-3.53489521
1	1.91760451	-0.92148791	-3.15098831

*TS*_{1-5-CCN-N}

E = -189.605664 E0 = -189.150890

No. of Negative Frequencies = 1

freq = - 1157.18



Atomic Coordinates:

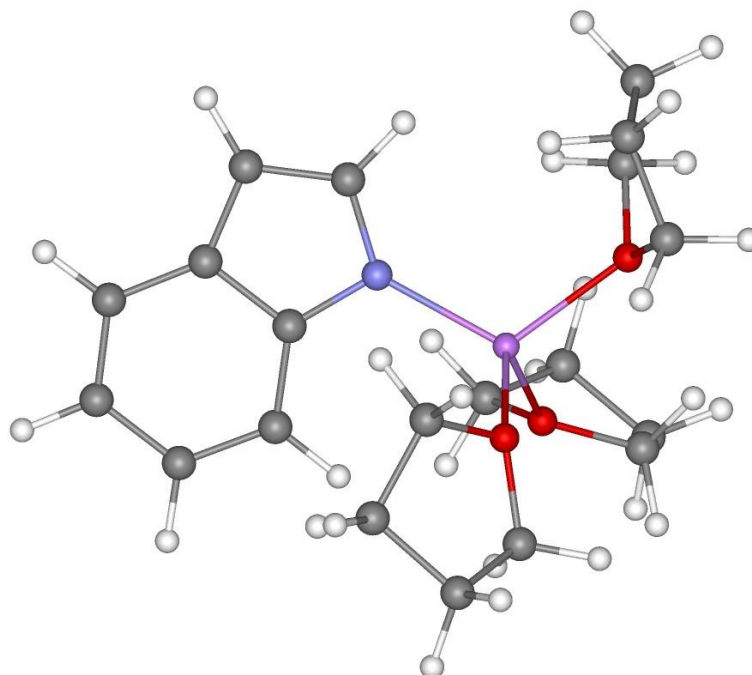
6	-1.78114975	-1.86857586	-5.01749643
6	-2.45724847	-2.28635441	-3.84446191
6	-0.67760606	-1.02118714	-4.93770718
6	-2.05010156	-1.86711200	-2.58097962
1	-2.58064874	-2.19154983	-1.68259229
6	-0.92938153	-1.00854385	-2.47999935
3	0.24075680	0.19749895	0.46708229
6	-0.24957295	-0.58552940	-3.66836870
6	0.79860466	0.27984508	-3.19372440
1	-0.16064456	-0.69823675	-5.84471252
1	-2.13278715	-2.21676028	-5.99055541
1	-3.31706990	-2.95387174	-3.93863187
6	0.69051822	0.36988659	-1.72495380
7	-0.33788308	-0.49303422	-1.34826257
8	-1.25105011	1.53594205	1.12006004
8	0.02650719	-1.41159024	1.82613578
8	1.91567539	1.06134079	1.46633753
6	-0.93548918	2.80185237	1.73912577
6	-2.25112405	1.84029400	0.11959939
6	-1.73741999	3.12115207	-0.54644775
1	-2.30683325	0.97266882	-0.54864522
1	-3.22484771	1.99972101	0.62109494
6	-1.01227685	3.86195444	0.61259498
1	-1.68033838	3.00760915	2.52961181
1	0.05663039	2.69696098	2.19590575
1	-2.54772753	3.71438340	-0.99156783
1	-1.02247544	2.85331677	-1.33613708

1	-0.01118930	4.18943921	0.30252673
1	-1.56732356	4.74893650	0.94865412
6	2.81695881	1.83033532	0.63752360
6	2.74983982	0.39955548	2.44011597
6	4.06857882	0.04859316	1.70926820
1	2.93535875	1.09065650	3.28285865
1	2.19026423	-0.47183594	2.80276465
6	4.01085800	0.89754092	0.40830290
1	2.26562808	2.06983515	-0.28211380
1	3.11144701	2.75072946	1.17729449
1	4.12206193	-1.02345818	1.47731516
1	4.93930445	0.30140092	2.33005081
1	4.94091279	1.44990485	0.21735897
1	3.79981129	0.25811710	-0.46030115
6	-0.96708192	-1.34285617	2.88809567
6	-0.02927872	-2.72046282	1.19391530
6	-1.40582815	-3.27675358	1.54823475
1	0.12871083	-2.56240239	0.11834982
1	0.77953797	-3.35135411	1.60510972
6	-1.59992430	-2.73847931	2.97696905
1	-0.46262639	-1.03651530	3.81786807
1	-1.70064066	-0.56891728	2.61176868
1	-1.44877566	-4.37255511	1.48853028
1	-2.16452161	-2.85659168	0.87092966
1	-2.65304050	-2.69603585	3.28582537
1	-1.05670445	-3.36854466	3.69802445
1	1.46387753	0.90176576	-3.79426407
1	1.65876851	-0.26212867	-2.32328037

*P*_{1-5-CCN-N}

E = -189.699133 E0 = -189.239116

No. of Negative Frequencies = 0



Atomic Coordinates:

6	-2.30259355	-2.13536246	-3.95930912
6	-2.77409659	-1.63540117	-2.72146336
6	-0.96161773	-2.00505252	-4.32136098
6	-1.90929883	-0.99783416	-1.82848478
1	-2.28626678	-0.61188185	-0.87585354
6	-0.54883978	-0.85674445	-2.17516007
3	0.23159081	0.23789101	0.46774257
6	-0.06518829	-1.36569758	-3.43755776
6	1.33098430	-1.06620679	-3.45786261
1	-0.61083785	-2.39656249	-5.27994492
1	-3.00206424	-2.62855955	-4.63784410
1	-3.83005576	-1.74806267	-2.46470512
6	1.59095155	-0.41910305	-2.25071133
7	0.47610267	-0.27554418	-1.44970869
8	-1.18179770	1.66993003	0.71850473
8	-0.19554263	-1.40707281	1.58826670
8	1.85086607	1.12234630	1.35622634
6	-1.25006424	2.57567642	1.85433079
6	-1.62269693	2.36897395	-0.48063848
6	-1.34347439	3.84036511	-0.19013261
1	-1.06130111	1.94397118	-1.32337422
1	-2.70110697	2.18488899	-0.63025470
6	-1.71158745	3.93627877	1.30217850
1	-1.94914176	2.16030232	2.59742943
1	-0.24416506	2.61920143	2.30122815
1	-1.93507312	4.51528770	-0.82287283

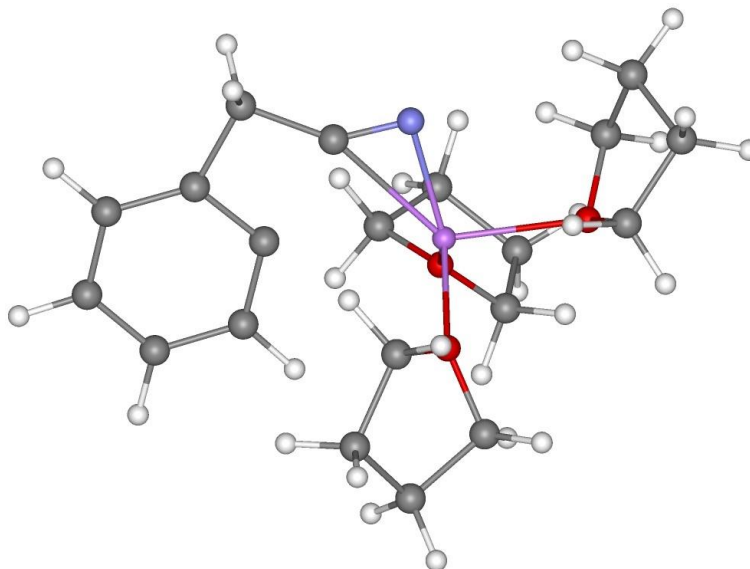
1	-0.27629062	4.06076494	-0.34581657
1	-1.22728304	4.77720061	1.81633749
1	-2.79995259	4.05068411	1.41536145
6	2.64663994	1.98761660	0.49447678
6	2.75881450	0.32928203	2.15401832
6	3.94224551	0.06816880	1.22585671
1	3.06383786	0.90273687	3.04956299
1	2.20960205	-0.56792359	2.46910952
6	4.08977690	1.43081030	0.51597807
1	2.18560065	1.95565635	-0.50301721
1	2.59696702	3.01820859	0.88257111
1	3.67935190	-0.72053544	0.50585101
1	4.85148615	-0.23288181	1.76364405
1	4.75113417	2.09369913	1.09253137
1	4.50743537	1.33418914	-0.49440231
6	-1.43002467	-1.50661044	2.35244599
6	0.09934523	-2.69973290	0.96938872
6	-1.20929190	-3.48246273	1.02798210
1	0.45945867	-2.49811595	-0.04836238
1	0.89492621	-3.19017264	1.55785695
6	-1.81149585	-2.99100850	2.35641205
1	-1.24488907	-1.09721689	3.35729230
1	-2.19519262	-0.89003371	1.85143663
1	-1.04844037	-4.56856023	1.00420727
1	-1.85147820	-3.20522143	0.17936071
1	-2.89801318	-3.13741934	2.42036463
1	-1.34346126	-3.50906287	3.20783086
1	2.04552094	-1.29076748	-4.24633624
1	2.55998564	-0.04731903	-1.91061031

TS_{1-4-CCN}

E = -189.605672 E0 = -189.149286

No. of Negative Frequencies = 1

freq = - 169.23



Atomic Coordinates:

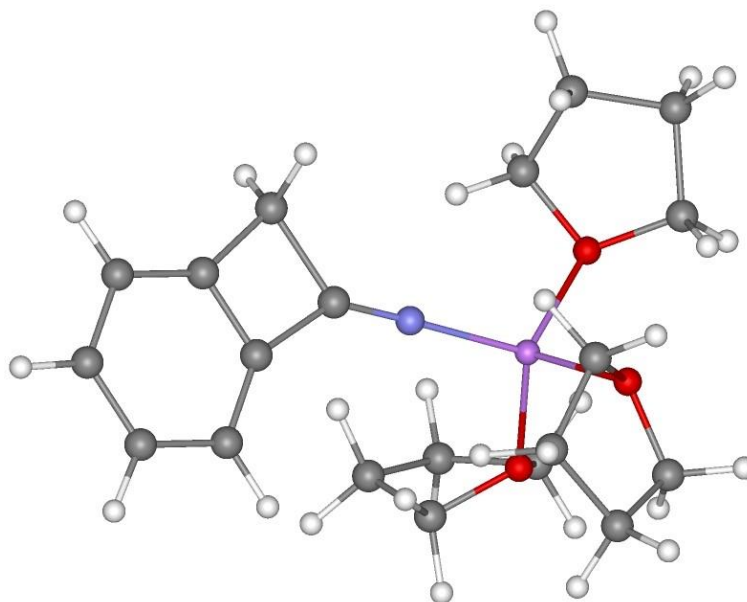
6	1.21003527	-2.93432196	-3.96928746
6	1.45133545	-3.06250915	-2.59253393
6	0.50887443	-1.82410974	-4.46820544
6	0.99959430	-2.08211534	-1.68854909
1	1.19692956	-2.21433191	-0.61846868
6	0.29884784	-0.96027704	-2.16740450
3	-0.21003903	0.47922800	0.11002616
6	0.06927008	-0.86352820	-3.55359115
6	-0.69934700	0.42696843	-3.69250683
1	0.32108916	-1.73150498	-5.54160990
1	1.56823237	-3.70493468	-4.65543275
1	1.99589573	-3.93754495	-2.22462823
6	-0.69212681	0.74712433	-2.19332874
7	-1.04682240	1.55579425	-1.36809925
8	-0.79213367	1.75452932	1.81257800
8	-1.12113241	-1.16527367	0.95984110
8	1.82058446	0.60903341	0.45411976
6	-0.03017577	2.99462231	1.84968396
6	-2.20658158	2.07046961	1.68744538
6	-2.26594200	3.51811231	1.20651882
1	-2.64466030	1.36082470	0.97199868
1	-2.68632834	1.94673936	2.67640251
6	-1.05551196	4.13177274	1.93092798
1	0.64808600	2.95524659	2.71603100
1	0.56639225	3.05702394	0.92543260
1	-3.21710836	4.00698654	1.45854987
1	-2.11754993	3.53733693	0.11762493

1	-0.68737258	5.05095758	1.45544062
1	-1.30300196	4.35944875	2.97976423
6	2.75048151	1.00656064	-0.57979467
6	2.63135096	0.18739115	1.56330664
6	3.78199456	-0.61353299	0.93252800
1	3.01003811	1.07773603	2.10142234
1	1.99110612	-0.39154234	2.24202372
6	3.93126189	0.01724210	-0.48213510
1	2.20496388	0.96572411	-1.53023770
1	3.07447857	2.04542391	-0.38483112
1	3.50792438	-1.67403692	0.85199777
1	4.70139541	-0.54524542	1.52974520
1	4.89225576	0.53475505	-0.60569739
1	3.85809439	-0.75315318	-1.25999256
6	-1.24880758	-1.49348345	2.35770675
6	-2.00500465	-2.06820767	0.26167634
6	-3.27132572	-2.10086504	1.12645470
1	-2.14086499	-1.67200422	-0.75153601
1	-1.53041114	-3.06478960	0.19662616
6	-2.72865412	-1.89881087	2.56973557
1	-0.57081421	-2.33511461	2.59137184
1	-0.93694548	-0.60727605	2.92529666
1	-3.82625963	-3.04123686	1.00887848
1	-3.93806208	-1.27452455	0.84424711
1	-3.28722469	-1.11394934	3.09641111
1	-2.80042422	-2.81717601	3.16818778
1	-1.72964082	0.32759319	-4.07668942
1	-0.20023899	1.22075546	-4.27544183

*P*_{1-4-CCN}

E = -189.623816 E0 = -189.166410

No. of Negative Frequencies = 0



Atomic Coordinates:

6	-0.01845861	-2.67029999	-5.47213392
6	0.66367504	-3.24915399	-4.38595930
6	-0.72247166	-1.45671697	-5.34100732
6	0.67282812	-2.64051114	-3.11818199
1	1.20684479	-3.09754518	-2.28099124
6	-0.02788505	-1.43753894	-2.99564098
3	0.05624419	0.44401541	0.98160217
6	-0.71010851	-0.85864380	-4.08297384
6	-1.21534224	0.34965179	-3.30541218
1	-1.24506588	-1.02547461	-6.19817459
1	0.00137491	-3.17802365	-6.43933550
1	1.19562255	-4.19143795	-4.53913422
6	-0.43477570	-0.30295654	-2.04039071
7	-0.26266280	0.00496667	-0.84747647
8	-1.08884963	1.96456249	1.75467658
8	-0.28360870	-1.13133131	2.25110169
8	1.99492811	1.04737781	1.28668895
6	-0.50949759	3.13644372	2.39531980
6	-2.06472197	2.39018644	0.76000921
6	-1.62993856	3.79950836	0.37307171
1	-2.00087443	1.65930368	-0.06188146
1	-3.07142022	2.38359893	1.21601823
6	-1.14910171	4.36367631	1.72286885
1	-0.71650989	3.08618941	3.47612560
1	0.57998884	3.09155511	2.24098965
1	-2.44305965	4.38798040	-0.07304009
1	-0.80009322	3.74211409	-0.34780910
1	-0.43701354	5.19316459	1.61622143

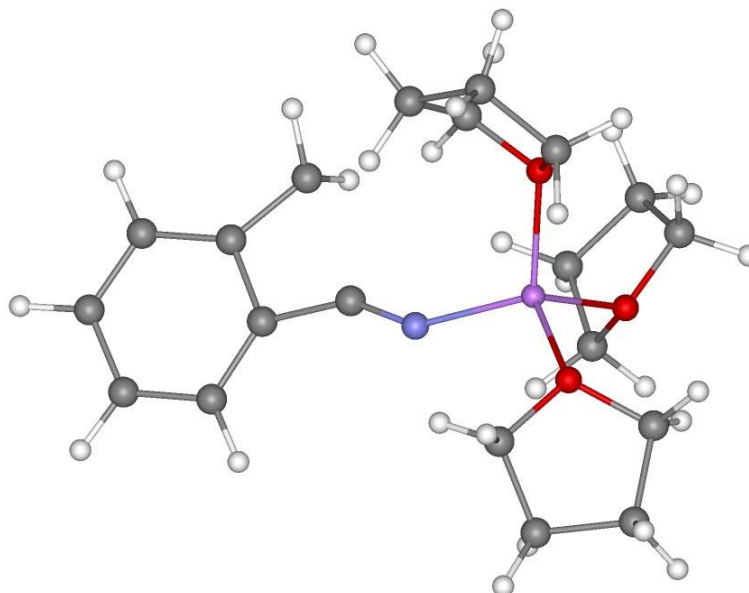
1	-2.00710310	4.72551380	2.30954432
6	2.69431229	1.23658072	0.03261470
6	2.87760596	0.27446707	2.13608158
6	3.76302901	-0.58158615	1.19306088
1	3.48699794	0.96792646	2.74159269
1	2.23713445	-0.31639691	2.80454626
6	3.35350814	-0.11693777	-0.22809964
1	1.94140569	1.51400777	-0.71592948
1	3.43817806	2.04741386	0.14963924
1	3.58469649	-1.65609454	1.33168938
1	4.82814734	-0.39112672	1.38646472
1	4.20668345	-0.04869076	-0.91646193
1	2.59861233	-0.78891731	-0.65952705
6	-1.31655450	-1.12000885	3.26318574
6	-0.44679125	-2.37183445	1.52043937
6	-1.96149838	-2.51166574	1.35902745
1	0.08619104	-2.24571777	0.56827231
1	-0.01264211	-3.20050640	2.11125254
6	-2.51911825	-1.89965837	2.67234242
1	-0.92931765	-1.61050936	4.17375727
1	-1.53277615	-0.06700494	3.48623269
1	-2.27340901	-3.55415428	1.20979915
1	-2.27829163	-1.92282161	0.48737403
1	-3.37114177	-1.23672185	2.47209356
1	-2.85676828	-2.67743770	3.37140166
1	-2.30853448	0.41851224	-3.17948351
1	-0.82260259	1.32870842	-3.62606133

TS1-4-CCN-B

E = -189.611627 E0 = -189.156162

No. of Negative Frequencies = 1

freq = - 297.89



Atomic Coordinates:

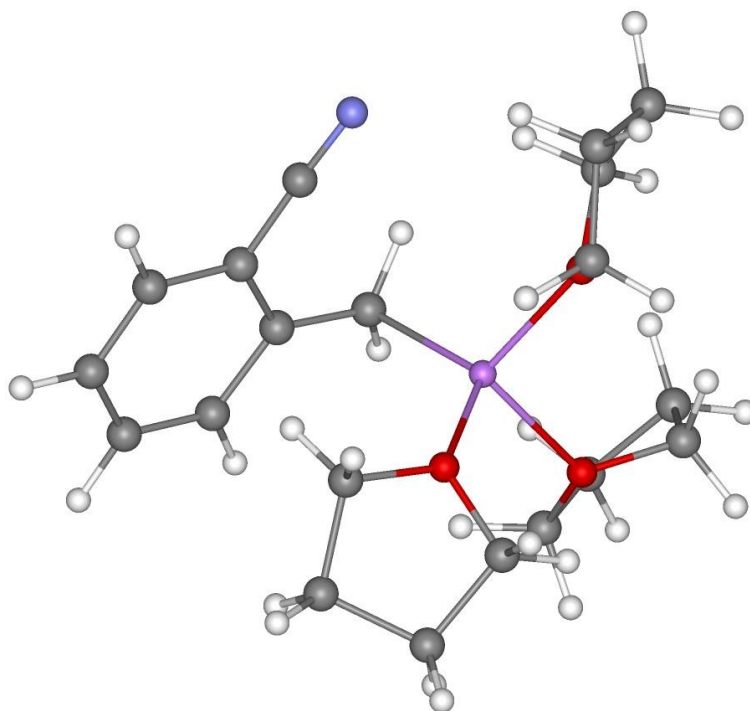
6	-0.91598165	-1.51187650	-5.84116739
6	0.35562576	-1.87911312	-5.35935492
6	-1.90436964	-0.99165838	-4.99155628
6	0.68408506	-1.69353638	-4.00891827
1	1.67948741	-1.93102767	-3.62968848
6	-0.29663161	-1.12149406	-3.18751661
3	0.37912457	0.24597073	1.03479802
6	-1.60317247	-0.82769223	-3.62769423
6	-2.33999446	-0.35889193	-2.43447739
1	-2.89298001	-0.74099397	-5.38320303
1	-1.13806328	-1.64895585	-6.90258879
1	1.09894946	-2.27902012	-6.05169164
6	-0.27177300	-0.63793766	-1.80660231
7	0.37433870	-0.42760753	-0.81034699
8	-0.84214048	1.82317548	1.27405120
8	-0.26006624	-1.20382635	2.31333864
8	2.25679763	0.76037889	1.60653133
6	-0.33929041	3.14097745	1.63598824
6	-1.80201251	1.96842932	0.18433491
6	-1.31571874	3.19660791	-0.57454576
1	-1.78657711	1.04626512	-0.41775242
1	-2.80820616	2.12893733	0.61334234
6	-0.86902727	4.12465446	0.57169033
1	-0.68981321	3.38987494	2.65084530
1	0.75959442	3.07678898	1.64799120
1	-2.09641914	3.64056277	-1.20615770
1	-0.46647251	2.91480399	-1.21459009

1	-0.10264370	4.84855142	0.26386760
1	-1.72963675	4.68855475	0.96141070
6	3.24474394	0.67686181	0.53963482
6	2.84617369	0.28100892	2.84964384
6	4.28804708	-0.13527515	2.51483142
1	2.79505278	1.08845348	3.59644490
1	2.23464188	-0.56544766	3.19999076
6	4.22018861	-0.40181778	0.99973043
1	2.69560870	0.43156431	-0.38051373
1	3.74330174	1.65712726	0.43444191
1	4.60984569	-1.01062678	3.09457770
1	4.98861947	0.68733328	2.72359444
1	5.19856452	-0.32712928	0.50641833
1	3.79849820	-1.39744203	0.79490057
6	-1.41968197	-0.99060888	3.15629660
6	-0.44226055	-2.50173867	1.69582936
6	-1.92515706	-2.53261327	1.32777676
1	0.23413437	-2.54631404	0.83283705
1	-0.17875876	-3.28988066	2.42591226
6	-2.59186936	-1.76249950	2.49789043
1	-1.19925463	-1.37704992	4.16659430
1	-1.57565888	0.09479487	3.21266248
1	-2.31059466	-3.55509386	1.21785663
1	-2.07015830	-1.99990694	0.37791711
1	-3.37231795	-1.08224770	2.13308028
1	-3.05551808	-2.44819494	3.22069803
1	-2.79854834	-1.18360784	-1.86740443
1	-3.07465480	0.44944920	-2.58197975

*P*_{1-4-CCN-B}

E = -189.648044 E0 = -189.191263

No. of Negative Frequencies = 0



Atomic Coordinates:

6	3.83715631	-1.26981447	-1.86470287
6	4.00642495	-0.11550075	-2.66949585
6	2.57998328	-1.74082159	-1.52916269
6	2.86762556	0.53688981	-3.12717653
1	2.95409795	1.42736232	-3.75328299
6	1.57250778	0.07443716	-2.79454741
3	-0.38956247	-0.15781799	0.11101313
6	1.36335743	-1.10369683	-1.96579863
6	0.08746010	-1.56920884	-1.57297003
1	2.48802286	-2.64442196	-0.92018674
1	4.71914287	-1.80924879	-1.50887558
1	5.00042728	0.24280905	-2.93572871
6	0.44587817	0.81162049	-3.23810441
7	-0.50401543	1.42331925	-3.55718871
8	-1.99671261	1.07101548	-0.22541110
8	-1.02098403	-1.23725326	1.79070678
8	1.01491127	1.02656547	1.01895350
6	-1.84387974	2.51594622	-0.08943234
6	-2.99534070	0.78956071	-1.25521328
6	-3.73759264	2.10612531	-1.47825577
1	-2.47393057	0.46979904	-2.16945747
1	-3.63462146	-0.02618456	-0.88614386
6	-2.61257979	3.13239021	-1.25885411
1	-2.26551120	2.81296710	0.88696879
1	-0.76938096	2.74591622	-0.10072461

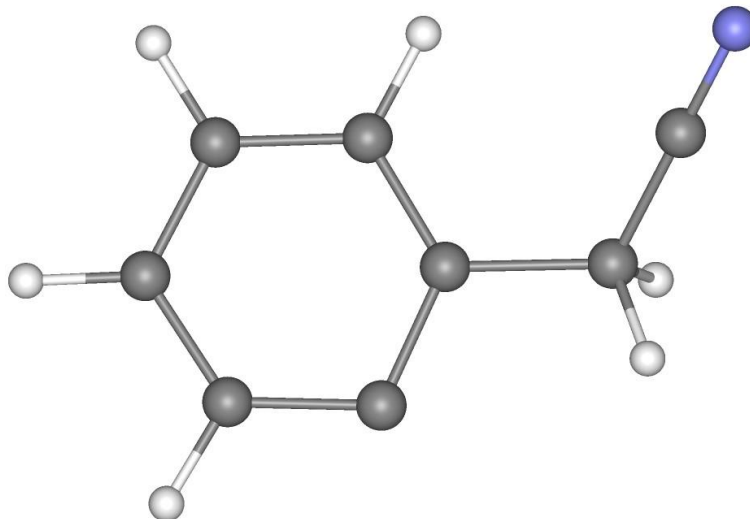
1	-4.54120116	2.23704984	-0.73615079
1	-4.17615426	2.16208270	-2.48305422
1	-1.97036191	3.17578760	-2.14959772
1	-2.98312144	4.14038194	-1.02810837
6	2.31299369	1.43223930	0.51614515
6	1.07441483	1.26857274	2.43988097
6	2.48601525	0.82211008	2.86922306
1	0.92375801	2.34841310	2.62590071
1	0.25525946	0.70407864	2.90244432
6	3.31807675	0.91027267	1.55556047
1	2.43214597	1.00674725	-0.48619586
1	2.33390731	2.53569752	0.45244139
1	2.46812606	-0.20857297	3.24852304
1	2.88329049	1.46609676	3.66560284
1	4.18422707	1.57870646	1.64906135
1	3.68570838	-0.08047056	1.25845716
6	-2.41849413	-1.33108013	2.13788077
6	-0.48455346	-2.56539275	1.99498697
6	-1.60824363	-3.54850956	1.58960027
1	0.42279888	-2.64514111	1.38298400
1	-0.21730113	-2.67939221	3.06079493
6	-2.88035567	-2.65667626	1.51849503
1	-2.51885525	-1.34382452	3.23954724
1	-2.91150433	-0.43534591	1.73914781
1	-1.70970135	-4.35261451	2.33088980
1	-1.39942903	-4.00999886	0.61624165
1	-3.17657935	-2.49865259	0.47253491
1	-3.73501949	-3.08925443	2.05584860
1	0.03603965	-2.58743951	-1.17525730
1	-0.77877039	-1.26862550	-2.17075668

Ph-CH₂-CN-anion

R_{CCN-a}

E = -58.869104 E0 = -58.760976

No. of Negative Frequencies = 0



Atomic Coordinates:

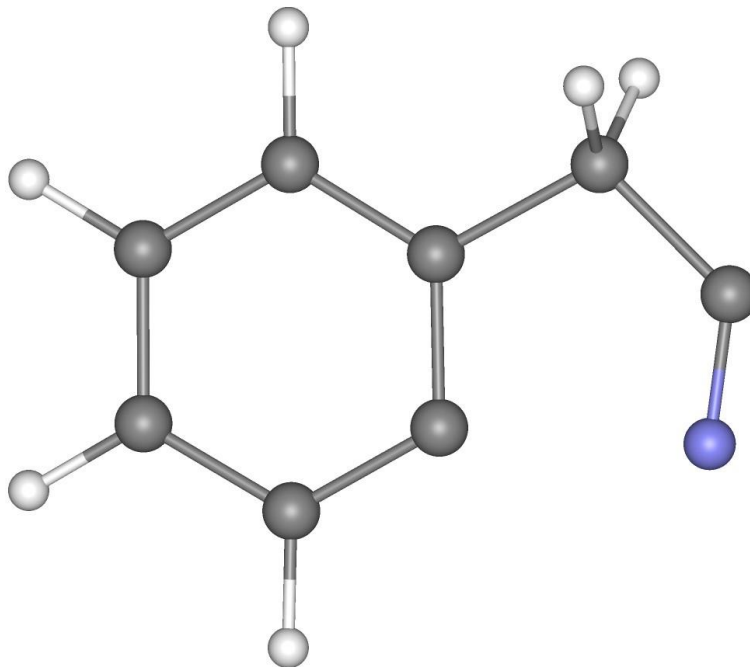
6	0.68708997	-1.49767879	-0.88734676
6	0.07943002	-2.30422238	0.08576097
6	0.50289913	-0.10852173	-0.82412364
6	-0.69515624	-1.71197677	1.10107882
1	-1.14535079	-2.39416087	1.84103942
6	-0.91858009	-0.31597559	1.23107423
6	-0.27964478	0.43572275	0.21153627
6	-0.53031328	1.95890821	0.25222770
1	0.98167926	0.53113589	-1.57747092
1	1.29959487	-1.93775376	-1.67966955
1	0.21919071	-3.39424336	0.05013885
6	0.56188918	2.81635769	-0.19989942
7	1.43891816	3.50136992	-0.55421242
1	-0.78029034	2.20250311	1.29846126
1	-1.42135578	2.21853568	-0.34859482

TS1-5-CCN-C-a

E = -58.852477 E0 = -58.744742

No. of Negative Frequencies = 1

freq = - 175.64



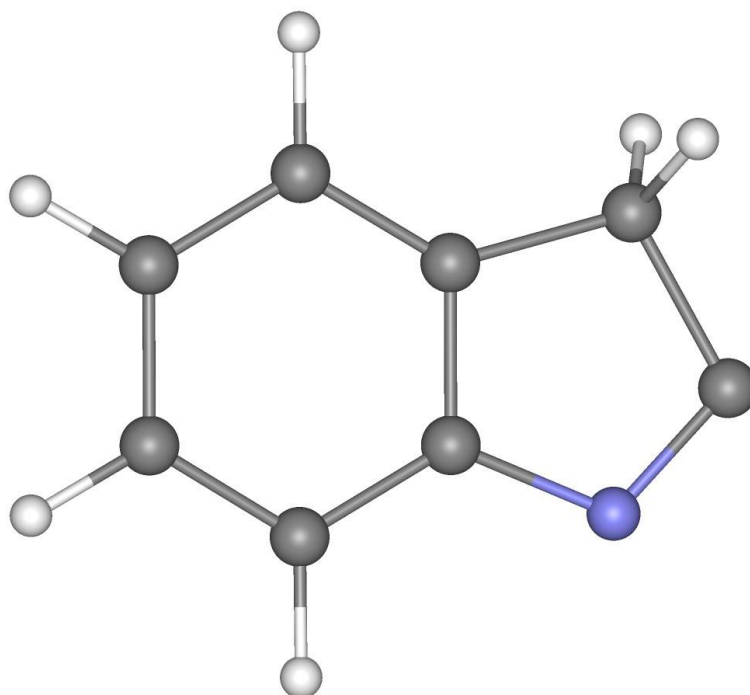
Atomic Coordinates:

6	0.24561838	-1.20944180	-1.64333373
6	0.94577223	-1.83885643	-0.60036959
6	-0.43118258	0.00577297	-1.41832839
6	0.98490307	-1.26867909	0.68817480
1	1.53936233	-1.78135541	1.48517351
6	0.31599389	-0.05824555	0.92963794
6	-0.37921894	0.55290784	-0.13404634
6	-0.92215996	1.78205994	0.56326045
1	-0.97344617	0.48567224	-2.24149598
1	0.22760543	-1.66877267	-2.63656906
1	1.46427523	-2.78500340	-0.80355608
6	-0.26806406	1.38967912	1.93519011
7	-0.17797983	1.80103715	3.06996897
1	-2.02466902	1.84381775	0.62594389
1	-0.54681000	2.74940735	0.18034949

*P*_{1-5-CCN-C-a}

E = -58.875182 E0 = -58.765503

No. of Negative Frequencies = 0



Atomic Coordinates:

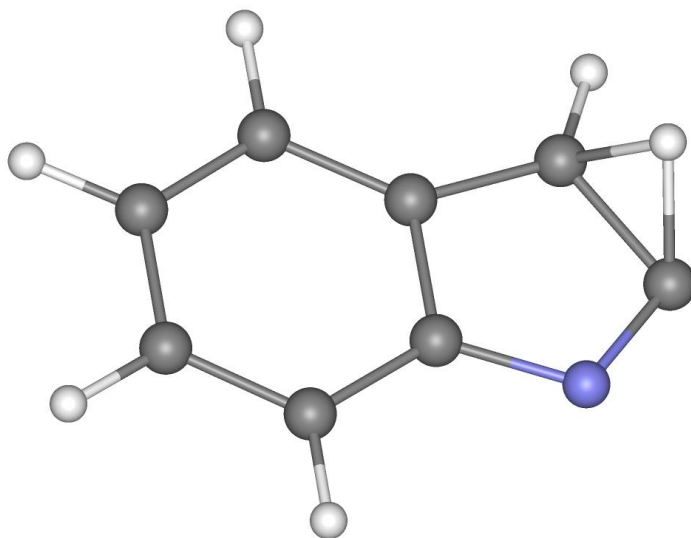
6	-1.03417263	-0.76787159	-1.48460767
6	-1.88321494	-0.83746878	-0.36794543
6	0.26004904	-0.22125438	-1.35123816
6	-1.46411610	-0.36963939	0.88759091
1	-2.11998703	-0.42045684	1.76148472
6	-0.17451081	0.17485040	1.01982785
6	0.68486374	0.24585300	-0.10825362
6	1.94895110	0.87607210	0.41910068
1	0.91665112	-0.17022477	-2.22723056
1	-1.37748635	-1.13723056	-2.45570939
1	-2.88570723	-1.26325925	-0.48164455
6	1.66446818	1.13001433	1.94613652
7	0.42287970	0.69463124	2.19256897
1	2.20083312	1.83603936	-0.06827436
1	2.84049911	0.22994514	0.31819409

*TS*_{1-5-CCN-N-a}

E = -58.847995 E0 = -58.741496

No. of Negative Frequencies = 1

freq = - 1204.90



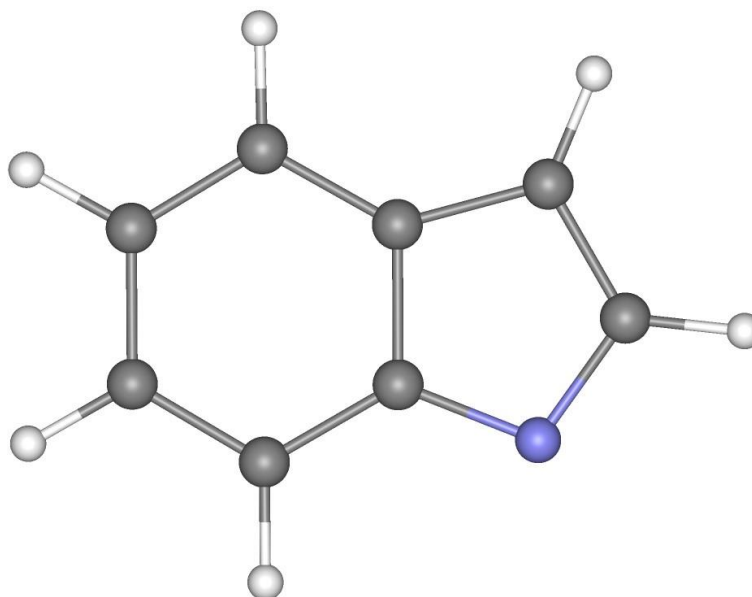
Atomic Coordinates:

6	-1.07983005	-0.71944561	-1.51524456
6	-1.86366010	-0.88457740	-0.34507697
6	0.17833679	-0.11247200	-1.44050997
6	-1.41245510	-0.44739612	0.89922540
1	-2.01847735	-0.57594429	1.80069554
6	-0.13838554	0.16905070	0.99912776
6	0.65393772	0.33343085	-0.19363041
6	1.84688238	0.98874631	0.28391108
1	0.77939171	0.01359028	-2.34798732
1	-1.46408552	-1.07116510	-2.47721467
1	-2.84226333	-1.36899453	-0.42601150
6	1.69367367	1.22519062	1.76196445
7	0.49362403	0.63143847	2.12517013
1	2.63348850	1.44867983	-0.32065241
1	2.53982219	0.36986800	1.19623344

*P*_{1-5-CCN-N-a}

E = -58.955110 E0 = -58.843508

No. of Negative Frequencies = 0



Atomic Coordinates:

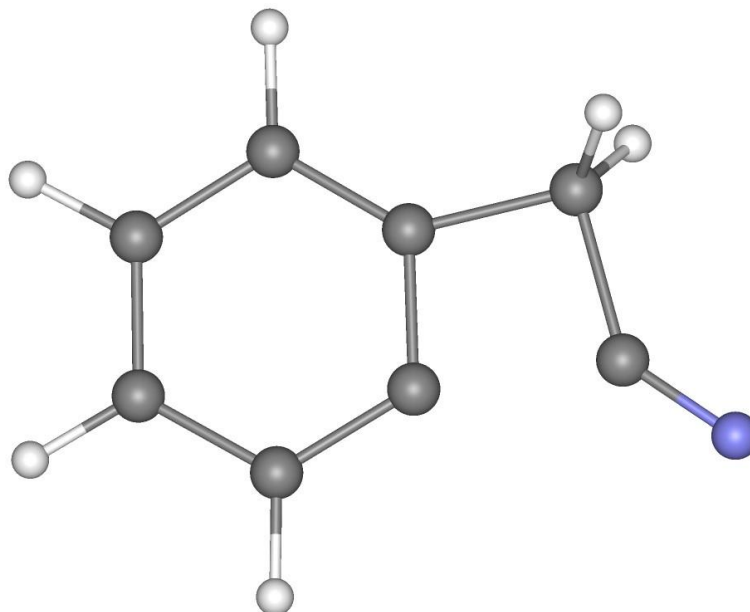
6	-1.62185848	-0.83644849	-0.96169699
6	-2.08794923	-0.33287782	0.28000421
6	-0.27760718	-0.71264544	-1.32689085
6	-1.21441648	0.30026088	1.17013755
1	-1.57063516	0.68983926	2.12913347
6	0.14682278	0.43901087	0.82814735
6	0.62829613	-0.07756309	-0.44749180
6	2.01985550	0.22858286	-0.46107923
1	0.06463698	-1.10767664	-2.29044571
1	-2.32589440	-1.32810851	-1.64044993
1	-3.14486377	-0.44322676	0.54167361
6	2.26085031	0.88241937	0.76240544
7	1.15586840	1.02190911	1.55451091
1	2.74217145	0.00729308	-1.24706736
1	3.22472315	1.26923130	1.10910932

TS_{1-4-CCN-a}

E = -58.852477 E0 = -58.744742

No. of Negative Frequencies = 1

freq = - 175.64



Atomic Coordinates:

6	0.24561838	-1.20944180	-1.64333373
6	0.94577223	-1.83885643	-0.60036959
6	-0.43118258	0.00577297	-1.41832839
6	0.98490307	-1.26867909	0.68817480
1	1.53936233	-1.78135541	1.48517351
6	0.31599389	-0.05824555	0.92963794
6	-0.37921894	0.55290784	-0.13404634
6	-0.92215996	1.78205994	0.56326045
1	-0.97344617	0.48567224	-2.24149598
1	0.22760543	-1.66877267	-2.63656906
1	1.46427523	-2.78500340	-0.80355608
6	-0.26806406	1.38967912	1.93519011
7	-0.17797983	1.80103715	3.06996897
1	-2.02466902	1.84381775	0.62594389
1	-0.54681000	2.74940735	0.18034949

*P*_{1-4-CCN-a}

E = -58.856757 E0 = -58.749271

No. of Negative Frequencies = 0



Atomic Coordinates:

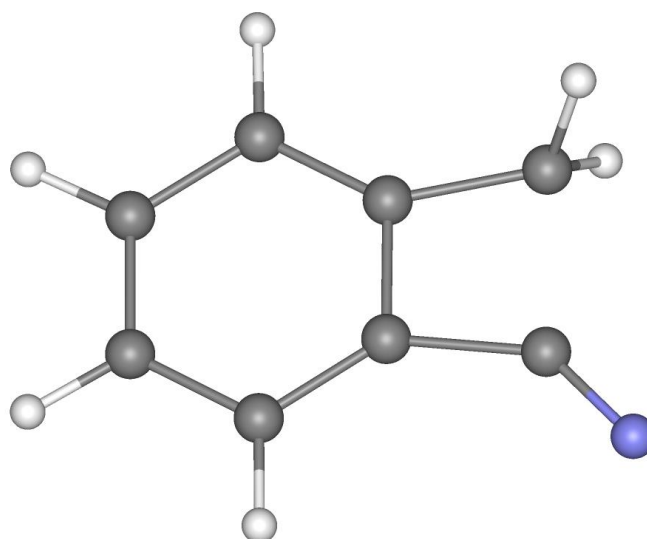
6	0.25137025	-1.20489086	-1.61555894
6	0.93169627	-1.77951523	-0.52649727
6	-0.45231553	0.01144089	-1.47682206
6	0.93554740	-1.16385010	0.73874384
1	1.46379981	-1.60871114	1.58693563
6	0.23527276	0.04130919	0.86571203
6	-0.44989611	0.62426576	-0.22244087
6	-0.97504870	1.84123363	0.50813299
1	-0.97538163	0.44224057	-2.33651929
1	0.27099604	-1.71329724	-2.58492154
1	1.46588860	-2.72425066	-0.67553147
6	-0.12279840	1.12653419	1.88168323
7	0.07010116	1.39490822	3.06464853
1	-2.07162360	1.89833781	0.62192913
1	-0.57760833	2.81424497	0.17050607

TS1-4-CCN-B-a

E= -58.85667939 E0 = -58.74770133

No. of Negative Frequencies = 1

freq = - 15.38



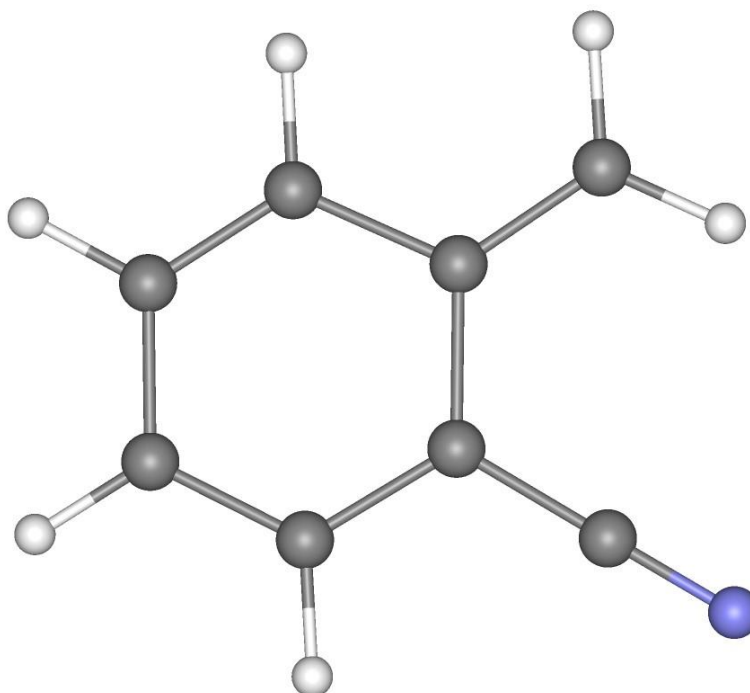
Atomic Coordinates:

6	-0.02474524	-1.73500249	-1.04213212
6	0.20559205	-2.03759083	0.31218268
6	-0.19319759	-0.40155770	-1.47277853
6	0.27564825	-1.02184056	1.28259269
1	0.45413982	-1.25113601	2.33645826
6	0.10572138	0.29683949	0.84265721
6	-0.12533136	0.61286502	-0.51344360
6	-0.22358303	2.11284425	-0.39170042
1	-0.37324573	-0.18608036	-2.53066420
1	-0.07409501	-2.55125743	-1.77004796
1	0.33143977	-3.08442207	0.60791214
6	0.08049196	1.70468651	1.39262744
7	0.19649508	2.30266525	2.45258084
1	-1.21129367	2.55012193	-0.61778293
1	0.57596332	2.68886502	-0.88846152

*P*_{1-4-CCN-B-a}

E = -58.918864 E0 = -58.810556

No. of Negative Frequencies = 0



Atomic Coordinates:

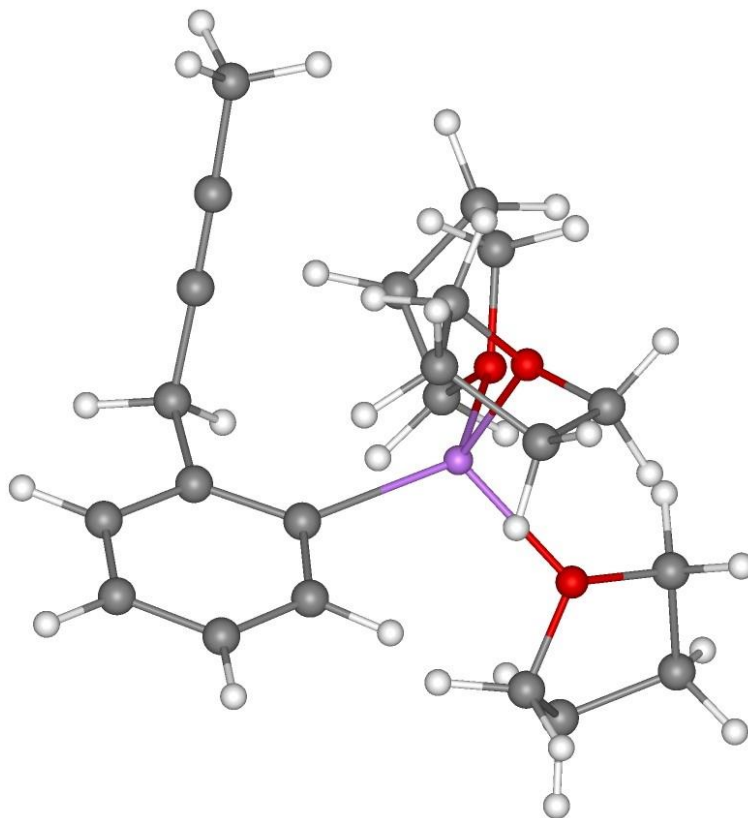
6	0.05290190	-1.65341227	-1.04183924
6	0.16950208	-2.02941425	0.32921616
6	-0.06819884	-0.33551695	-1.42410955
6	0.15757164	-1.01364298	1.28045000
1	0.24479125	-1.25785287	2.34331552
6	0.03487819	0.35035586	0.92764913
6	-0.08797116	0.77328068	-0.48011761
6	-0.21126251	2.08570107	-0.89392691
1	-0.15571945	-0.08565084	-2.48633890
1	0.05956643	-2.43134184	-1.81345623
1	0.26560851	-3.07566475	0.62308133
6	0.03189766	1.31604673	1.96005600
7	0.02888553	2.12465167	2.81640807
1	-0.22517510	2.91221546	-0.18408976
1	-0.29727613	2.32024527	-1.95629801

Ph-CH₂-C≡CMe-Li(THF)₃

R_{CCC}

E = -192.776581 E0 = -192.282446

No. of Negative Frequencies = 0



Atomic Coordinates:

6	0.88102844	-2.12423292	-4.15984262
6	1.05401707	-2.86214379	-2.98472220
6	0.28693908	-0.85832478	-4.07822823
6	0.63499596	-2.31574245	-1.75814544
1	0.79697360	-2.94196200	-0.86632700
6	0.02856166	-1.04132046	-1.60845989
3	-0.10596111	-0.39332468	0.44533834
6	-0.12527474	-0.34304278	-2.83607278
6	-0.77714490	1.04995616	-2.83871904
1	0.14530804	-0.27275854	-4.99361028
1	1.19569991	-2.52588332	-5.12583471
1	1.51001896	-3.85679728	-3.02497746
6	0.13793165	2.13391306	-2.47256110
6	0.91534615	3.03034696	-2.19450827
8	-1.17407528	1.22141450	1.18589692
8	-0.87438665	-1.84071299	1.71756052
8	1.78230476	0.00479396	1.18522170
6	-0.50629227	2.49924377	1.38754675
6	-2.53897804	1.45272660	0.74415948
6	-2.63780503	2.95062023	0.44210064

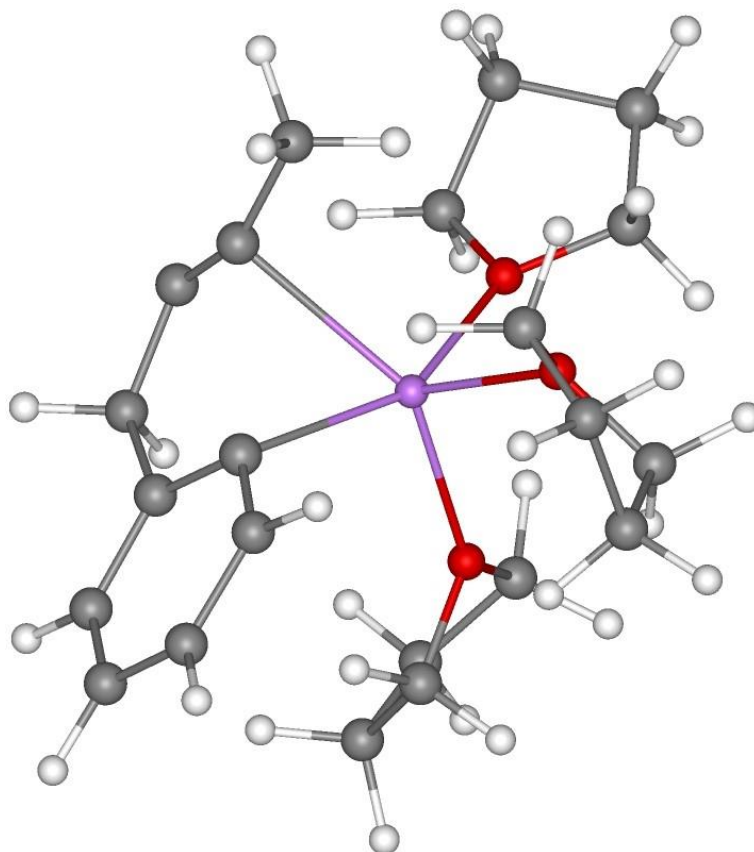
1	-2.72891720	0.80992464	-0.12864675
1	-3.22335310	1.15934873	1.56024756
6	-1.62433782	3.54075612	1.43883010
1	0.08606901	2.42160187	2.30955591
1	0.16572734	2.67948392	0.53230720
1	-3.65730838	3.33666022	0.57558115
1	-2.31534749	3.15599279	-0.58931517
1	-1.27363404	4.54190505	1.15465591
1	-2.06008857	3.59756587	2.44852627
6	2.72701732	0.53271297	0.22091912
6	2.52345390	-0.95427656	1.96413143
6	3.41433826	-1.69406115	0.95331039
1	3.12772167	-0.41748779	2.72017047
1	1.79298954	-1.59639665	2.47383770
6	3.63168283	-0.65092631	-0.17954492
1	2.14289300	0.94324341	-0.61324297
1	3.30687571	1.33999105	0.70626956
1	2.88880681	-2.57451820	0.56048607
1	4.35448825	-2.03167815	1.41087192
1	4.68121354	-0.33622389	-0.25991428
1	3.31730024	-1.06194097	-1.14681928
6	-1.43132551	-1.60099743	3.03730914
6	-1.64500872	-2.88230680	1.06457601
6	-3.05022307	-2.72914713	1.63942231
1	-1.56220510	-2.70189137	-0.01635625
1	-1.21354713	-3.86982698	1.31265835
6	-2.75088195	-2.39915394	3.11506798
1	-0.70464892	-1.92618312	3.80005282
1	-1.57724102	-0.51448905	3.13266633
1	-3.66131716	-3.63372393	1.51839953
1	-3.56496715	-1.89174649	1.14450211
1	-3.55326250	-1.82624156	3.59891541
1	-2.60768518	-3.32696321	3.68837669
1	-1.62502209	1.03920875	-2.13293127
1	-1.19879141	1.27339778	-3.83479515
6	1.86313883	4.09992644	-1.89642552
1	1.42085110	5.09207108	-2.08024310
1	2.19131638	4.07232959	-0.84421315
1	2.76402256	4.01729112	-2.52501500

TS_{1-5-CCC-sigma}

E = -192.750014 E0 = -192.256489

No. of Negative Frequencies = 1

freq = - 173.82



Atomic Coordinates:

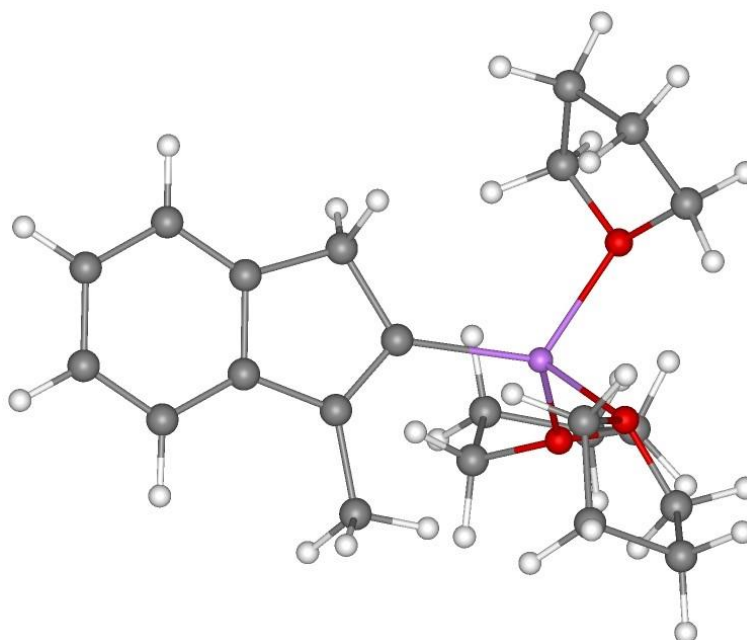
6	0.05261824	-3.11001611	-3.36577012
6	1.32734280	-2.80751641	-2.87093856
6	-0.96745419	-2.15563339	-3.25223252
6	1.54855903	-1.56754434	-2.24408726
1	2.55687734	-1.38601954	-1.84695705
6	0.54394042	-0.58345532	-2.11631129
3	0.05938124	0.34328064	-0.08417364
6	-0.70981961	-0.90334529	-2.66652370
6	-1.84778808	0.15321109	-2.68413638
1	-1.96201915	-2.38336465	-3.65562938
1	-0.14143108	-4.06821571	-3.85308335
1	2.14131892	-3.53214182	-2.97435325
6	-1.30834431	1.48422329	-2.34470622
6	-0.12927281	1.80808137	-2.04452844
8	-0.89259617	1.82953289	1.18672878
8	-0.88442908	-1.29462254	0.89803039
8	1.90941018	0.41230397	0.97042701
6	-0.25667747	2.40803911	2.35926779
6	-2.02698065	2.65531564	0.81504015
6	-1.63653715	4.05934538	1.26400985

1	-2.16248646	2.53489572	-0.26964069
1	-2.92998600	2.30296746	1.35036283
6	-0.93512969	3.77164351	2.60529827
1	-0.37850294	1.71908489	3.21173219
1	0.81635527	2.49632515	2.13563284
1	-2.50003002	4.73029219	1.36711407
1	-0.93660717	4.50123537	0.53922692
1	-0.21110042	4.54727718	2.88857674
1	-1.67945862	3.69448133	3.41188606
6	3.12749946	0.65840712	0.20748017
6	2.21186375	-0.54179547	2.01104166
6	3.28298614	-1.44309218	1.40221754
1	2.59322778	-0.01263568	2.90567930
1	1.27283685	-1.05179022	2.26259538
6	4.14665081	-0.42062492	0.63664158
1	2.84738202	0.59778760	-0.85355020
1	3.48618771	1.67680252	0.42997756
1	2.81437602	-2.15414346	0.70635698
1	3.85082136	-2.00476594	2.15660176
1	4.90965632	0.00891845	1.30270241
1	4.66212398	-0.86330482	-0.22552301
6	-2.00661331	-1.24951902	1.79948405
6	-0.83212255	-2.66573317	0.42892317
6	-2.30224475	-3.10000341	0.25454589
1	-0.24518474	-2.67213513	-0.49656113
1	-0.32420352	-3.27854946	1.19710843
6	-3.10363779	-2.07622927	1.10991822
1	-1.71484756	-1.70351022	2.76664545
1	-2.25722097	-0.19368748	1.95817200
1	-2.45272852	-4.13353914	0.59492878
1	-2.59643209	-3.04685514	-0.80106517
1	-3.71516484	-1.42990673	0.46570947
1	-3.77067186	-2.55750550	1.83823941
1	-2.66604708	-0.13973030	-1.99700586
1	-2.30931065	0.16963583	-3.68670888
6	0.94172428	2.79041838	-1.81538706
1	0.59882364	3.79734123	-2.10491043
1	1.26468509	2.83291488	-0.76149311
1	1.82643268	2.54716958	-2.42302641

*P*_{1-5-CCC-sigma}

E = -192.839381 E0 = -192.342940

No. of Negative Frequencies = 0



Atomic Coordinates:

6	0.01824931	-1.38686210	-5.90942811
6	0.76036979	-0.19666216	-5.93811699
6	-0.45436965	-1.89792046	-4.68578635
6	1.04332660	0.50305099	-4.75475026
1	1.62342857	1.42888135	-4.79214897
6	0.57169342	-0.00499481	-3.53129689
3	-0.07352318	0.04479168	0.88323955
6	-0.17650914	-1.20615516	-3.50847604
6	-0.52868844	-1.48042294	-2.06163842
1	-1.03216621	-2.82670862	-4.66810655
1	-0.19221327	-1.91773434	-6.84032701
1	1.12181739	0.18862294	-6.89468267
6	0.07124373	-0.33253717	-1.22978633
6	0.69726444	0.48672386	-2.14792579
8	-1.07074706	1.77788714	1.39045278
8	-1.06349411	-1.35516754	2.07166987
8	1.72457547	0.14488765	1.87211140
6	-0.45689996	2.82593951	2.18866797
6	-1.82577721	2.37616928	0.29252181
6	-1.35410759	3.82753188	0.21772060
1	-1.61156323	1.77831761	-0.60605177
1	-2.90128330	2.31249556	0.53576657
6	-1.06329067	4.14370714	1.69566082
1	-0.66488377	2.61566146	3.24879006
1	0.63360433	2.78985753	2.02644270
1	-2.10891419	4.49063619	-0.22566055
1	-0.43404736	3.89909153	-0.38070498

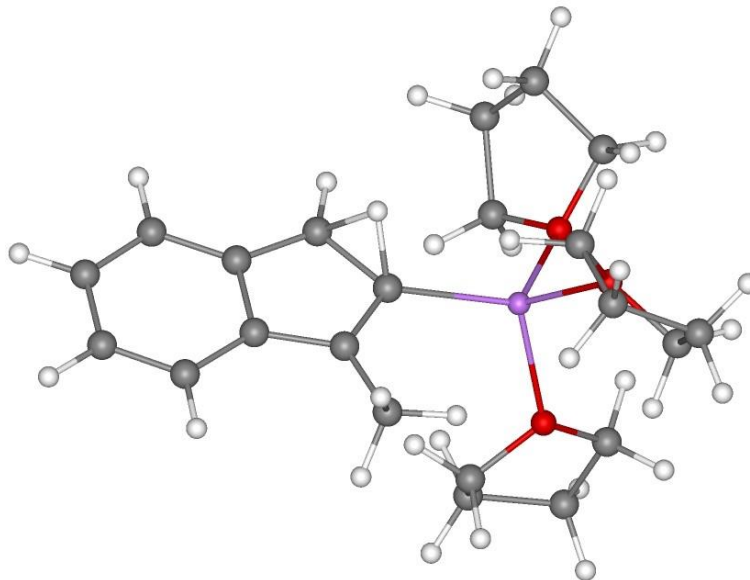
1	-0.37935942	4.99215607	1.83259572
1	-1.99885413	4.36486309	2.23227688
6	2.85752809	-0.28241149	1.06867531
6	1.94191342	-0.25931153	3.25146446
6	3.22093884	-1.12112872	3.26377378
1	2.03882935	0.64233289	3.87800006
1	1.04843371	-0.81779732	3.56983668
6	3.38302927	-1.52256656	1.78508055
1	2.46942054	-0.46119332	0.05511143
1	3.61462753	0.52283737	1.04631490
1	3.13176794	-1.98332425	3.93816317
1	4.08623675	-0.52519506	3.59021070
1	4.42084849	-1.76155597	1.51668069
1	2.74941313	-2.38875885	1.54076598
6	-2.40336768	-1.10808090	2.54462437
6	-1.05008980	-2.70024693	1.52252269
6	-2.50971798	-3.03259085	1.11974641
1	-0.35504091	-2.68399732	0.67247002
1	-0.67296992	-3.39529074	2.29217735
6	-3.29650171	-1.75040990	1.48324048
1	-2.54304847	-1.58421396	3.53405694
1	-2.51442325	-0.02041102	2.64349171
1	-2.88076599	-3.89583226	1.69008963
1	-2.59265717	-3.27278739	0.05226034
1	-3.36769284	-1.08253072	0.61298687
1	-4.31078376	-1.96097466	1.84898965
1	-0.12962894	-2.46228240	-1.73901605
1	-1.62495167	-1.54782270	-1.92018588
6	1.44991088	1.76007638	-1.85087203
1	1.43419119	1.98064783	-0.77238332
1	2.50752719	1.69993700	-2.16683293
1	1.02214264	2.62877621	-2.38447295

*TS*_{1-5-CCC-*pi*}

E = -192.797747 E0 = -192.305607

No. of Negative Frequencies = 1

freq = - 1126.17



Atomic Coordinates:

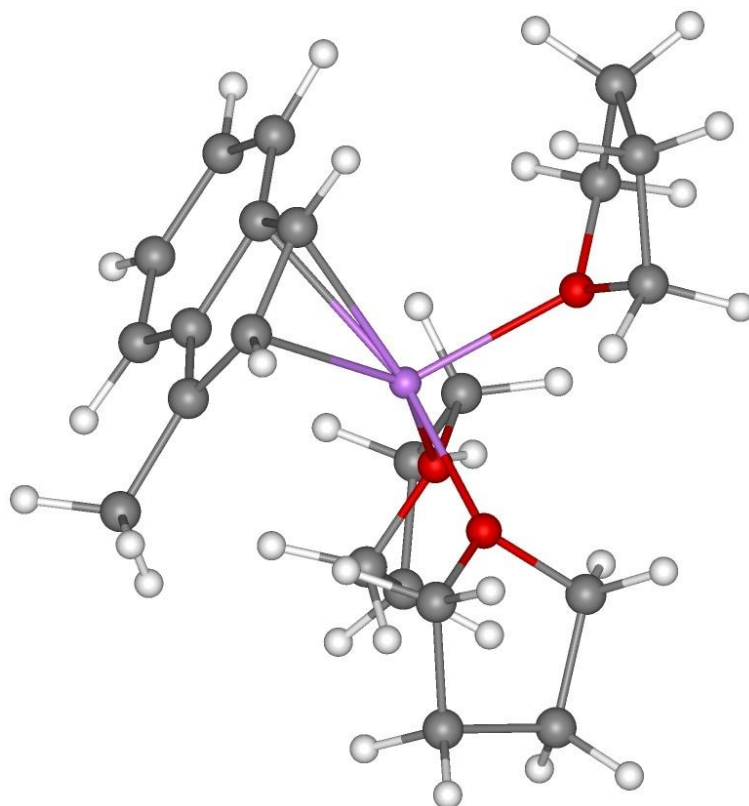
6	0.39752396	-1.76880523	-5.73184746
6	1.22675301	-0.61464057	-5.77390433
6	-0.30445625	-2.09411517	-4.57659687
6	1.36820449	0.21251010	-4.66745076
1	2.00854338	1.09709714	-4.72288073
6	0.67378723	-0.10166732	-3.46648042
3	-0.24720033	0.15184013	0.83703242
6	-0.17626145	-1.26945455	-3.43602995
6	-0.74175448	-1.32886811	-2.12550271
1	-0.94571384	-2.97967608	-4.55077536
1	0.31261778	-2.39956304	-6.61937007
1	1.75862558	-0.37767452	-6.69874913
6	-0.21531214	-0.19317368	-1.29075556
6	0.60167075	0.55168612	-2.20191059
8	-1.14079629	1.89012500	1.45147762
8	-1.14555102	-1.30119173	1.99358831
8	1.62430741	0.14539541	1.66915070
6	-0.48026586	2.81571198	2.35912922
6	-1.87747507	2.64084574	0.43988279
6	-1.32000937	4.06110947	0.50315014
1	-1.71972552	2.12862930	-0.51984199
1	-2.95086624	2.61511326	0.69858931
6	-1.00790186	4.20975406	2.00288298
1	-0.71106467	2.50878034	3.39040140
1	0.60764410	2.73573291	2.19705628
1	-2.03473284	4.80883069	0.13439368
1	-0.39905605	4.13637603	-0.09391593

1	-0.27402039	4.99791405	2.21820316
1	-1.92748853	4.43258809	2.56555093
6	2.72199050	-0.23639130	0.79636034
6	1.93482161	-0.27485790	3.02553974
6	3.20505082	-1.14789873	2.94003507
1	2.08667435	0.61868825	3.65324066
1	1.05877615	-0.82454094	3.40171478
6	3.29324684	-1.49523040	1.44091781
1	2.29357272	-0.38008690	-0.20583369
1	3.46812639	0.57879381	0.77019502
1	3.14074362	-2.03493275	3.58421295
1	4.09044355	-0.57211895	3.24755871
1	4.31790777	-1.71376432	1.11182754
1	2.65695032	-2.35922496	1.19730695
6	-2.52483918	-1.15166232	2.39726875
6	-0.96128288	-2.65408537	1.47806421
6	-2.37219907	-3.25889706	1.30552835
1	-0.41577125	-2.55869409	0.52777100
1	-0.34967523	-3.22637862	2.19435242
6	-3.30355385	-2.03548443	1.42587146
1	-2.64671323	-1.49507769	3.44196421
1	-2.76358179	-0.08113852	2.33895826
1	-2.58569305	-3.98073120	2.10756711
1	-2.48022535	-3.77944623	0.34527209
1	-3.40248814	-1.52355267	0.45742084
1	-4.30590162	-2.29565415	1.79239823
1	-1.35010080	-2.14498611	-1.72976628
1	-1.41946452	-0.22454665	-1.71477676
6	1.27455125	1.86515672	-1.89416277
1	1.17033402	2.11680197	-0.82625188
1	2.35649643	1.85175271	-2.12000790
1	0.85177813	2.70697899	-2.47502425

*P*_{1-5-CCC-*pi*}

E = -192.883617 E0 = -192.386581

No. of Negative Frequencies = 0



Atomic Coordinates:

6	1.31798809	-2.89964247	-2.61758161
6	2.18774988	-1.82892239	-2.96199320
6	-0.00944923	-2.65903659	-2.27066466
6	1.73658427	-0.51149692	-2.94793137
1	2.41037312	0.29785471	-3.24572189
6	0.39626493	-0.22717935	-2.58486027
3	-0.49954728	0.04401314	-0.18199394
6	-0.50646925	-1.33079297	-2.25162697
6	-1.79036326	-0.76738153	-1.98714897
1	-0.67560972	-3.49880374	-2.04945320
1	1.69207991	-3.92547610	-2.65054096
1	3.21519633	-2.04887880	-3.26115139
6	-1.67842531	0.63694473	-2.16789742
6	-0.34639317	0.99297199	-2.50977013
8	-0.99042109	1.75943680	1.04838581
8	-1.37575593	-1.29648374	1.33526704
8	1.45738641	-0.04499511	0.63866959
6	-0.54261481	1.90776190	2.41283505
6	-1.49864557	3.04926939	0.66005667
6	-0.48510290	4.04814771	1.23148235
1	-1.58053014	3.05374194	-0.43299851
1	-2.50336751	3.19805181	1.10084416
6	0.00043344	3.35426597	2.53455056

1	-1.39898347	1.75243390	3.09460382
1	0.20045275	1.12030728	2.59015707
1	-0.92984686	5.03555767	1.41420122
1	0.34717062	4.17607290	0.52549445
1	1.09580325	3.37145411	2.61046026
1	-0.39957980	3.84563892	3.43201790
6	2.45469281	0.94664091	0.29970705
6	2.11818121	-1.33653932	0.80722011
6	3.62871920	-1.07696884	0.67345905
1	1.84036871	-1.71071400	1.80540551
1	1.74605681	-2.02799068	0.03659225
6	3.74530576	0.43594944	0.93524044
1	2.54823805	1.01352259	-0.79755399
1	2.10517066	1.91279592	0.69009476
1	3.96030104	-1.31049499	-0.34813755
1	4.21806630	-1.68231311	1.37504140
1	3.75298656	0.65014461	2.01551344
1	4.64250604	0.88170723	0.48485167
6	-2.65361952	-1.01856718	1.93693191
6	-1.27493405	-2.73582687	1.29614930
6	-2.69859967	-3.26109831	1.00470894
1	-0.54168157	-2.99247687	0.52133778
1	-0.91073140	-3.09519043	2.27678175
6	-3.61980266	-2.05421381	1.33925117
1	-2.57273188	-1.13331467	3.03541329
1	-2.90772601	0.02198577	1.69835015
1	-2.92718395	-4.14224600	1.61949052
1	-2.80165127	-3.54992521	-0.04905530
1	-4.07990860	-1.65525696	0.42582390
1	-4.42330778	-2.31451632	2.04161984
1	-2.70271574	-1.31465257	-1.75849715
1	-2.50470137	1.34461296	-2.07375385
6	0.15364642	2.36596971	-2.87109085
1	-0.64580431	3.11656805	-2.76938689
1	0.99896701	2.70096605	-2.24247260
1	0.50551551	2.41660770	-3.91672748

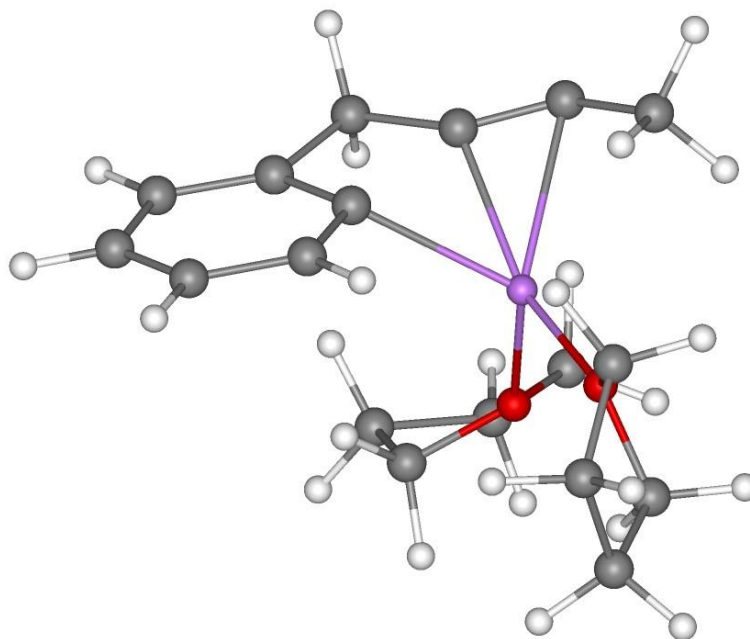
TS1-4-CCC

Note: in this TS Li is coordinated to three atoms of carbon, thus one of three solvating THF molecules is pushed to outer sphere.

E = -149.248887 E0 = -148.870302

No. of Negative Frequencies = 1

freq = - 236.50



Atomic Coordinates:

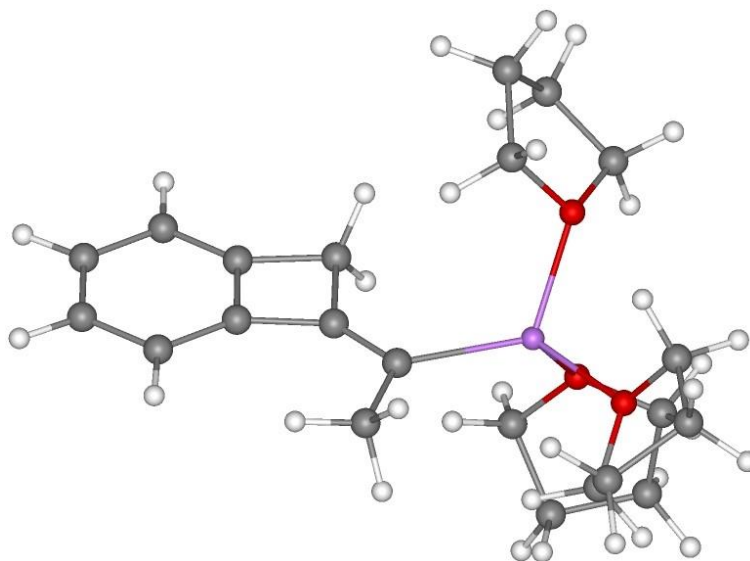
6	-2.15896617	-0.63727026	-3.62020693
6	-0.79063957	-0.92838826	-3.51977244
6	-2.72967981	0.38281209	-2.83902664
6	0.03445727	-0.21783732	-2.62592211
1	1.09913599	-0.47415069	-2.58402315
6	-0.52327288	0.78853901	-1.81332652
3	0.48318809	0.65418181	0.21644770
6	-1.89824646	1.07262189	-1.95568281
6	-2.08409807	2.25648723	-1.03569874
1	-3.79124428	0.62523399	-2.94133395
1	-2.77984035	-1.19847006	-4.32194569
1	-0.36320856	-1.71579537	-4.14756629
6	-0.62349221	2.31870656	-0.61997304
6	0.17192830	3.03310275	0.10930280
8	-0.69203781	-0.21725715	1.62761191
8	2.17899508	-0.41438630	0.45078084
6	3.33580612	-0.48916806	-0.40971743
6	2.44366920	-1.35424915	1.51640649
6	3.10351141	-2.56898464	0.83229993
1	3.12813563	-0.88117287	2.24377885
1	1.48550849	-1.56380966	2.00672053
6	3.65770310	-1.99018211	-0.50311176
1	3.07439757	-0.01622927	-1.36461639

1	4.16566018	0.07567678	0.05254715
1	2.36346500	-3.35560869	0.63583725
1	3.89331756	-2.99935999	1.46235514
1	4.73458338	-2.16496360	-0.62681610
1	3.13966366	-2.43818760	-1.36130484
6	-1.24535430	0.68541737	2.63997698
6	-1.70706922	-1.17950264	1.22623371
6	-3.03856270	-0.56945813	1.65732484
1	-1.61449941	-1.33102985	0.14164822
1	-1.51368648	-2.13555295	1.74521450
6	-2.64814969	0.15483500	2.95854541
1	-0.56925412	0.67406708	3.50800437
1	-1.25739443	1.69925928	2.20601839
1	-3.81897320	-1.32790377	1.80515710
1	-3.38963436	0.14770921	0.90156888
1	-3.34144061	0.96392828	3.22341316
1	-2.61675939	-0.55807297	3.79685634
1	-2.78376419	2.10273345	-0.19399344
1	-2.40151958	3.17611546	-1.55538816
6	1.65734666	2.97242288	0.24022805
1	1.97678834	2.71999475	1.26784415
1	2.15379712	2.26270080	-0.46721269
1	2.09972968	3.96044571	0.03451642

$P_{1-4-CCC}$

E = -192.786774 E0 = -192.292351

No. of Negative Frequencies = 0



Atomic Coordinates:

6	-3.04397769	-1.00113336	-5.49350897
6	-2.25033713	0.13673538	-5.72126135
6	-3.04055841	-1.65550428	-4.24315000
6	-1.41817417	0.68005986	-4.72436778
1	-0.81155162	1.56196054	-4.93757103
6	-1.41734372	0.03181384	-3.47965170
3	0.35635944	0.13194580	0.76805122
6	-2.21848573	-1.11322793	-3.26443013
6	-1.75381477	-1.27764881	-1.82031095
1	-3.65951993	-2.54107425	-4.07706338
1	-3.67126067	-1.38329375	-6.30172762
1	-2.28181784	0.61112610	-6.70527586
6	-0.86754992	-0.00525715	-2.08058461
6	-0.00490307	0.68331863	-1.29411752
8	1.70074492	1.29080131	1.87483236
8	-1.28422954	0.19261044	2.00180421
8	1.23877935	-1.71642976	1.04918201
6	2.76622909	1.93289610	1.12646951
6	1.27966700	2.16246169	2.96147655
6	2.20349959	3.38844867	2.91443604
1	0.22543760	2.43047983	2.78965102
1	1.35012477	1.60205956	3.90611802
6	2.63247757	3.42179219	1.43659663
1	3.73966811	1.53791191	1.47123452
1	2.62270344	1.67844084	0.06793624
1	3.08106869	3.23967669	3.56202018
1	1.69148503	4.30434787	3.23831775
1	1.84380361	3.86678968	0.81161639
1	3.56644340	3.97469146	1.26913151

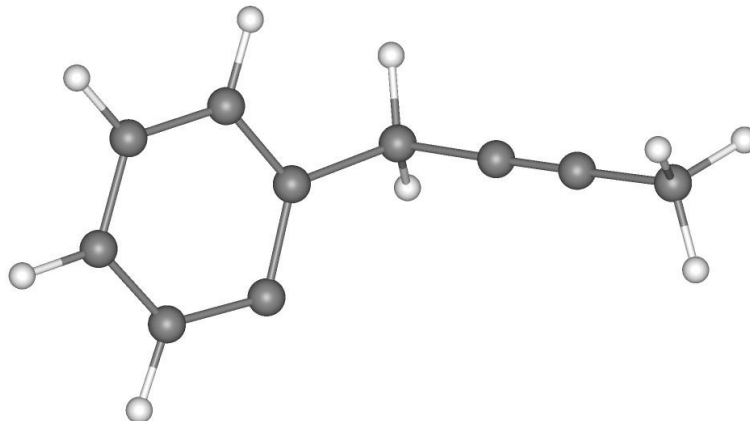
6	2.21587287	-2.04854270	2.07255961
6	1.63226103	-2.34214297	-0.20275490
6	3.15186839	-2.44320939	-0.11523694
1	1.16391702	-3.34085668	-0.27548005
1	1.25670842	-1.69133157	-1.00640869
6	3.35555598	-2.81076189	1.36690288
1	2.55094010	-1.10097685	2.52157848
1	1.72748790	-2.65566814	2.85225576
1	3.60311815	-1.46572428	-0.34406063
1	3.56900781	-3.19011052	-0.80391042
1	3.24014239	-3.89594837	1.50638581
1	4.34378451	-2.52481964	1.75156481
6	-2.42997465	0.92880384	1.47044633
6	-1.76504921	-0.93382973	2.76530424
6	-3.09475428	-1.30843991	2.11446516
1	-0.99873353	-1.71894591	2.70599918
1	-1.90243893	-0.63803590	3.82275207
6	-3.67918217	0.07710153	1.77474761
1	-2.46993234	1.91650034	1.95788984
1	-2.23822619	1.06672485	0.39536325
1	-3.74406092	-1.89597915	2.77792210
1	-2.90943150	-1.88889980	1.19902213
1	-4.36940296	0.04625642	0.92161561
1	-4.22657354	0.48101693	2.63955642
1	-1.20655623	-2.21008033	-1.60053592
1	-2.54773091	-1.14797644	-1.06455935
6	0.64873632	1.89076161	-1.95598923
1	1.73677747	1.72616338	-2.08035051
1	0.25292802	2.16188831	-2.95423674
1	0.55797361	2.79026385	-1.31866119

Ph-CH₂-C≡CMe-anion

R_{CCC-a}

E = -62.019063 E0 = -61.873673

No. of Negative Frequencies = 0



Atomic Coordinates:

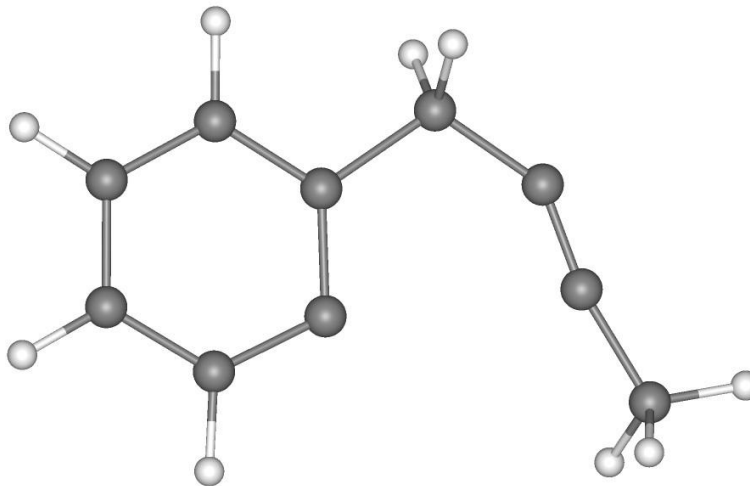
6	0.75255413	-2.12803903	-1.12870459
6	0.24316349	-3.27668303	-0.50722843
6	0.24498163	-0.87421137	-0.75216324
6	-0.75855990	-3.14990837	0.47531159
1	-1.11990670	-4.08610173	0.93412818
6	-1.31246299	-1.91674003	0.90631164
6	-0.75552747	-0.79444089	0.23416248
6	-1.34438569	0.58435853	0.60954286
1	0.64249883	0.03259835	-1.22848532
1	1.53584893	-2.20140440	-1.88969846
1	0.63439598	-4.26610815	-0.78791027
6	-0.47535612	1.75046720	0.45951128
6	0.25781201	2.71723611	0.33779836
1	-1.68767489	0.49183263	1.65427798
1	-2.26315974	0.75493857	0.01575840
6	1.16163087	3.85418364	0.19644031
1	0.76594707	4.60691519	-0.50707055
1	1.32992711	4.36329530	1.16102147
1	2.14827344	3.53781148	-0.18300368

*TS*_{1-5-CCC-sigma-a}

E = -62.006572 E0 = -61.862109

No. of Negative Frequencies = 1

freq = - 114.28



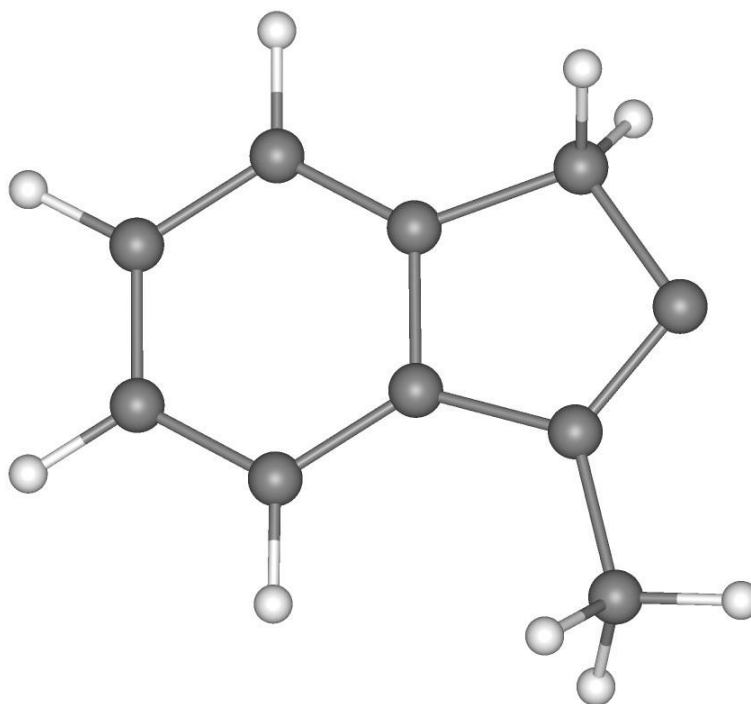
Atomic Coordinates:

6	-0.49259185	-2.75225059	-1.04740192
6	0.68321482	-2.85747601	-0.28966325
6	-1.12205943	-1.50287224	-1.14145077
6	1.19415271	-1.71284597	0.35050094
1	2.12051078	-1.84451378	0.93475157
6	0.59394752	-0.43169249	0.28426830
6	-0.58282099	-0.37701964	-0.48729677
6	-1.39728937	0.94801794	-0.68506450
1	-2.04651109	-1.41645405	-1.73624279
1	-0.91374319	-3.62472741	-1.55654528
1	1.19301272	-3.82824410	-0.20277536
6	-0.79603020	2.08434185	0.01254743
6	0.14136301	2.43264375	0.72920252
1	-2.43689577	0.78731247	-0.34004435
1	-1.48405052	1.15984445	-1.76822751
6	1.13088508	3.10138442	1.56408255
1	2.13792502	3.01539044	1.12480913
1	0.90179167	4.17688853	1.68958886
1	1.17518907	2.64227243	2.56496119

*P*_{1-5-CCC-sigma-a}

E = -62.082208 E0 = -61.934588

No. of Negative Frequencies = 0



Atomic Coordinates:

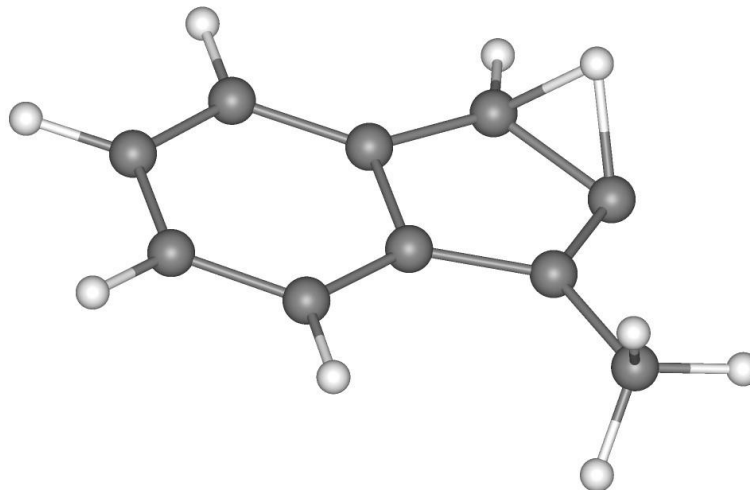
6	-0.41364433	-1.15500514	-2.35963362
6	0.32762015	0.03607906	-2.38714018
6	-0.88306583	-1.65814467	-1.12513010
6	0.61143610	0.73869677	-1.20334746
1	1.19117144	1.66606663	-1.24540323
6	0.14466399	0.24032910	0.03344575
6	-0.60649834	-0.96874525	0.05227269
6	-0.95395343	-1.22826261	1.51056159
1	-1.46228930	-2.58843384	-1.10208799
1	-0.62568363	-1.68948747	-3.29028963
1	0.68916159	0.42188234	-3.34644373
6	-0.35091685	-0.08278363	2.34490720
6	0.27156399	0.72934016	1.40997170
1	-0.56183849	-2.20496834	1.85525298
1	-2.04933599	-1.28244409	1.66469471
6	1.01924913	2.00228077	1.72835539
1	0.98271143	2.16921449	2.81552153
1	2.08312399	1.96355761	1.41861519
1	0.58652439	2.89082810	1.22587722

*TS*_{1-5-CCC-pi-a}

E = -62.052358 E0 = -61.908489

No. of Negative Frequencies = 1

freq = - 1158.14



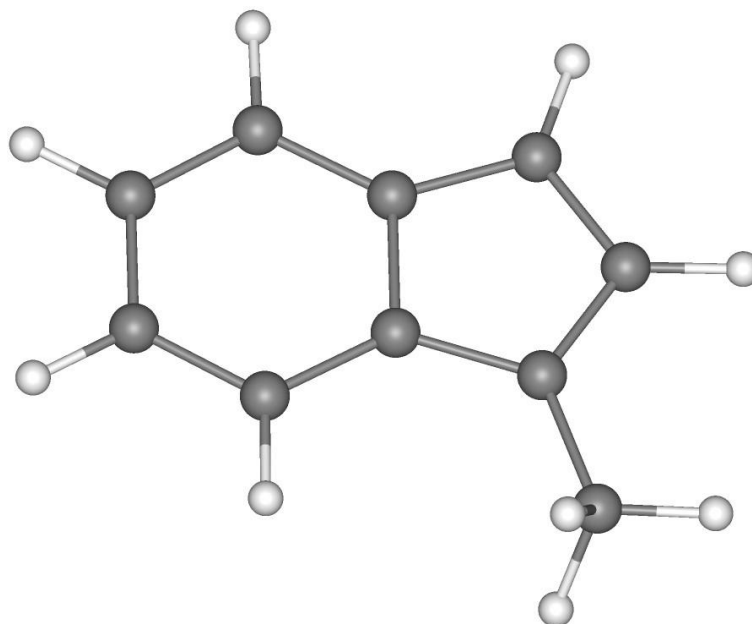
Atomic Coordinates:

6	-0.38441201	-1.18997408	-2.39179818
6	0.31441061	0.04468391	-2.41244429
6	-0.80402982	-1.73754727	-1.17443833
6	0.60634146	0.72967946	-1.23367869
1	1.14607788	1.68143224	-1.27553454
6	0.19778064	0.19239620	0.01907727
6	-0.52447483	-1.06344668	0.02819712
6	-0.81721145	-1.33959242	1.41611381
1	-1.34869881	-2.68834077	-1.15957259
1	-0.59629428	-1.70808530	-3.33158689
1	0.62508565	0.46495825	-3.37482188
6	-0.22611008	-0.27425106	2.29278557
6	0.31458248	0.66030402	1.36369805
1	-1.17757118	-2.29447727	1.80876354
1	-1.52452115	-0.48438830	2.07678895
6	0.92626967	1.98336052	1.75147914
1	0.90350408	2.08298855	2.84764480
1	1.98082664	2.08684879	1.42675487
1	0.38844451	2.85345122	1.32257225

*P*_{1-5-CCC-*pi*-a}

E = -62.149680 E0 = -62.001520

No. of Negative Frequencies = 0



Atomic Coordinates:

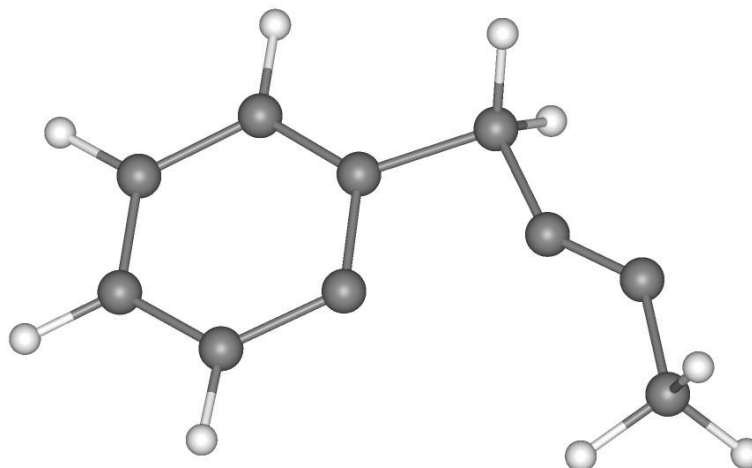
6	1.12200321	-2.52691122	-0.03059148
6	1.99232922	-1.45929124	-0.37995462
6	-0.21270882	-2.27985505	0.30250022
6	1.52849181	-0.14067094	-0.39679220
1	2.21267220	0.67171630	-0.66872513
6	0.18360950	0.14475937	-0.06470882
6	-0.71690724	-0.95891648	0.29644666
6	-1.99075299	-0.39318346	0.57863191
1	-0.87060997	-3.11536131	0.56990759
1	1.50390248	-3.55278394	-0.02301621
1	3.03416940	-1.67459723	-0.63753132
6	-1.87639603	1.00722273	0.39753947
6	-0.56025252	1.35808419	0.00536782
1	-2.88687920	-0.93692792	0.87987685
1	-2.68815411	1.72790152	0.53899624
6	-0.04727914	2.74115483	-0.28259455
1	-0.84676745	3.48878261	-0.14428356
1	0.79136479	3.04007996	0.37813275
1	0.32816485	2.85879727	-1.31920162

TS_{1-4-CCC-a}

E = -62.005581 E0 = -61.861106

No. of Negative Frequencies = 1

freq = - 150.63



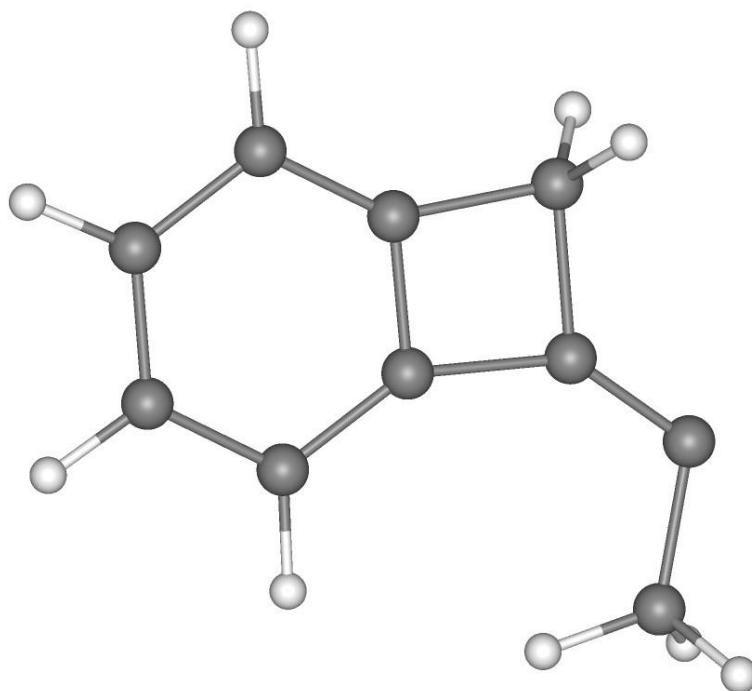
Atomic Coordinates:

6	-0.54190462	-2.86722826	-0.99971965
6	0.53034666	-2.89314677	-0.09389809
6	-1.16746438	-1.64491470	-1.30105490
6	0.98051503	-1.70265695	0.51243085
1	1.82320007	-1.77048280	1.21538931
6	0.37876268	-0.45669921	0.23576520
6	-0.69735697	-0.47830536	-0.68228361
6	-1.19488707	0.94177257	-0.83766877
1	-2.00606461	-1.62504105	-2.00956632
1	-0.88812587	-3.79362096	-1.46807453
1	1.01478346	-3.85152801	0.13723492
6	-0.26539794	1.66880111	0.08856827
6	0.08816000	2.76975296	0.59600315
1	-2.25330216	1.07132547	-0.53559949
1	-1.11557156	1.32335942	-1.87515270
6	1.11679004	3.22911512	1.55608316
1	1.79629030	3.97463738	1.10409951
1	0.66558879	3.72416537	2.43537600
1	1.73563816	2.38069467	1.92206768

*P*_{1-4-CCC-a}

E = -62.031921 E0 = -61.886215

No. of Negative Frequencies = 0



Atomic Coordinates:

6	-1.65625470	-1.01261369	-2.07903466
6	-0.86757303	0.12639050	-2.31815786
6	-1.63109478	-1.65512517	-0.81714018
6	-0.02558015	0.67875936	-1.33176870
1	0.57274527	1.56475881	-1.55474398
6	0.00154598	0.04183627	-0.07520748
6	-0.80152083	-1.10936324	0.15106512
6	-0.31841406	-1.25998696	1.59171839
1	-2.24768383	-2.54229120	-0.63631923
1	-2.29352833	-1.40271756	-2.87742175
1	-0.91174370	0.59758123	-3.30581291
6	0.56212296	0.01483400	1.32010098
6	1.41988491	0.68421096	2.12762609
1	0.24875121	-2.18312756	1.80492693
1	-1.09608823	-1.13491813	2.36559664
6	2.10248609	1.89057271	1.50966605
1	3.20142112	1.76988881	1.56641276
1	1.85181834	2.13799809	0.44486686
1	1.88870578	2.79331277	2.11362693