

*Supporting Information*

**Thermodynamics of N-H Bond Formation in  
Bis(Phosphine) Molybdenum(II) Diazenides and the  
Influence of the *Trans* Ligand**

*Máté J. Bezdek and Paul J. Chirik\**

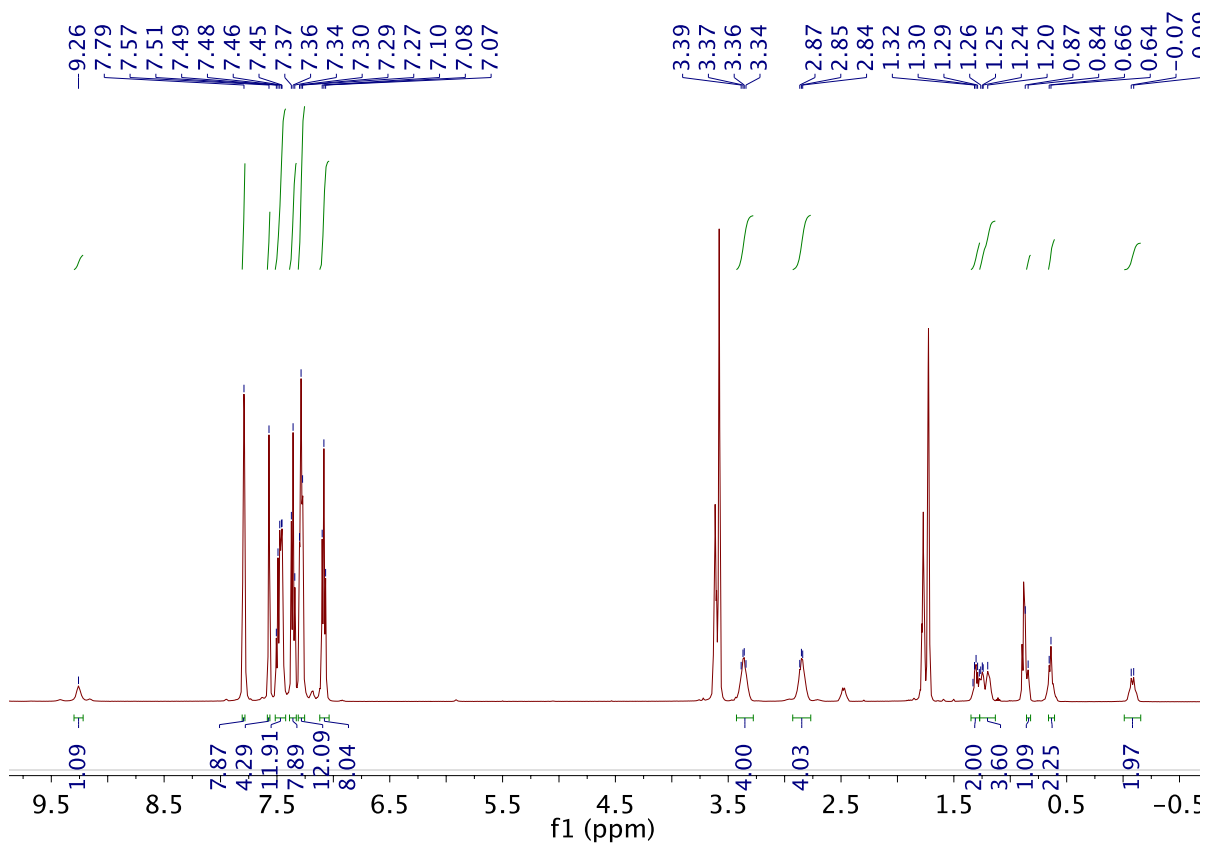
*Department of Chemistry, Princeton University, Princeton, New Jersey 08540*

*pchirik@princeton.edu*

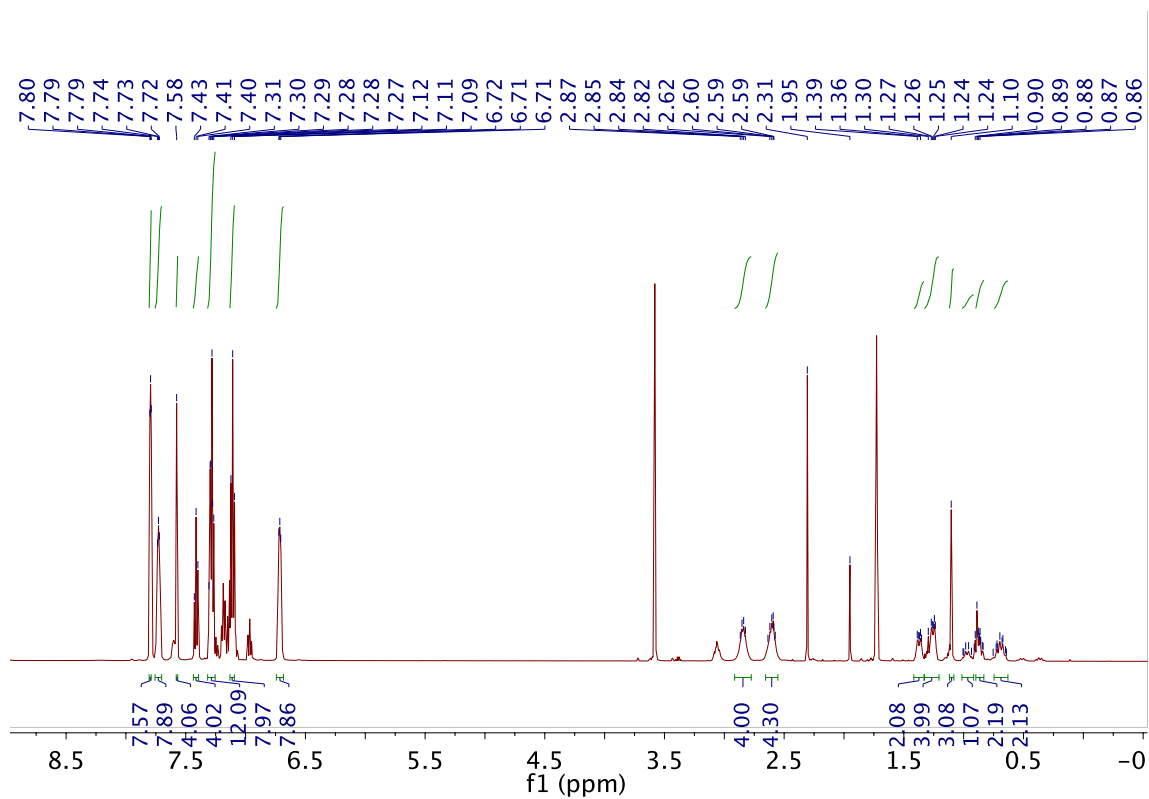
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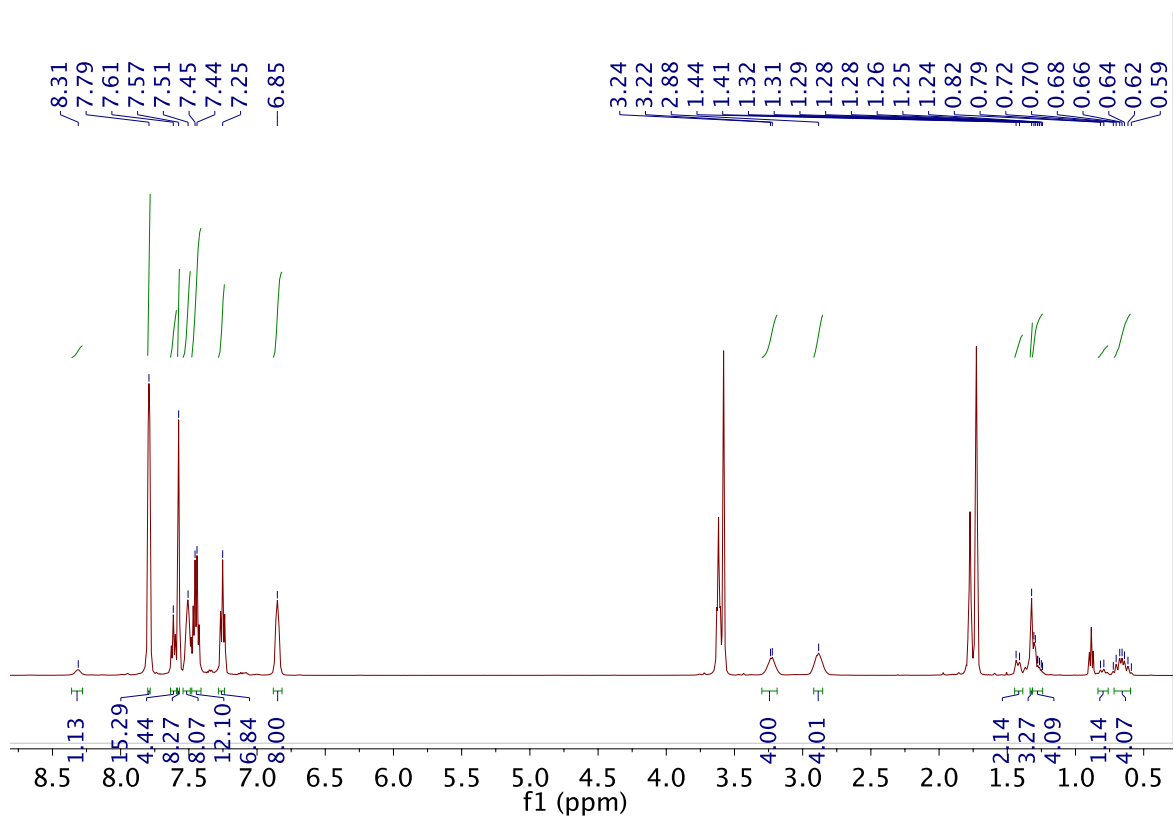
## I. Additional NMR Spectroscopic Data



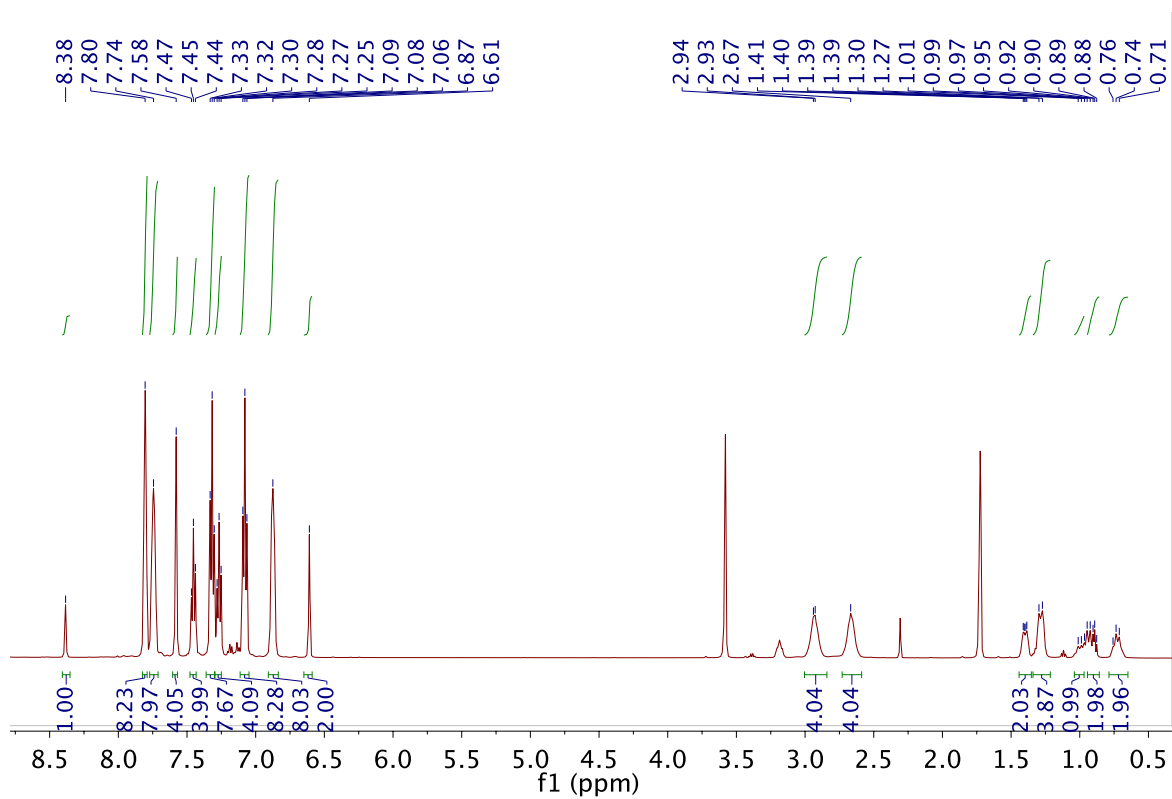
**Figure S1.**  $\text{THF-}d_8$   $^1\text{H}$  NMR spectrum of  $[(\text{dppe})_2\text{Mo}(\text{NNHC}_6\text{H}_{11})(\text{I})][\text{BARF}_{24}]$  (**[1-H]<sup>+</sup>**) at 295 K.



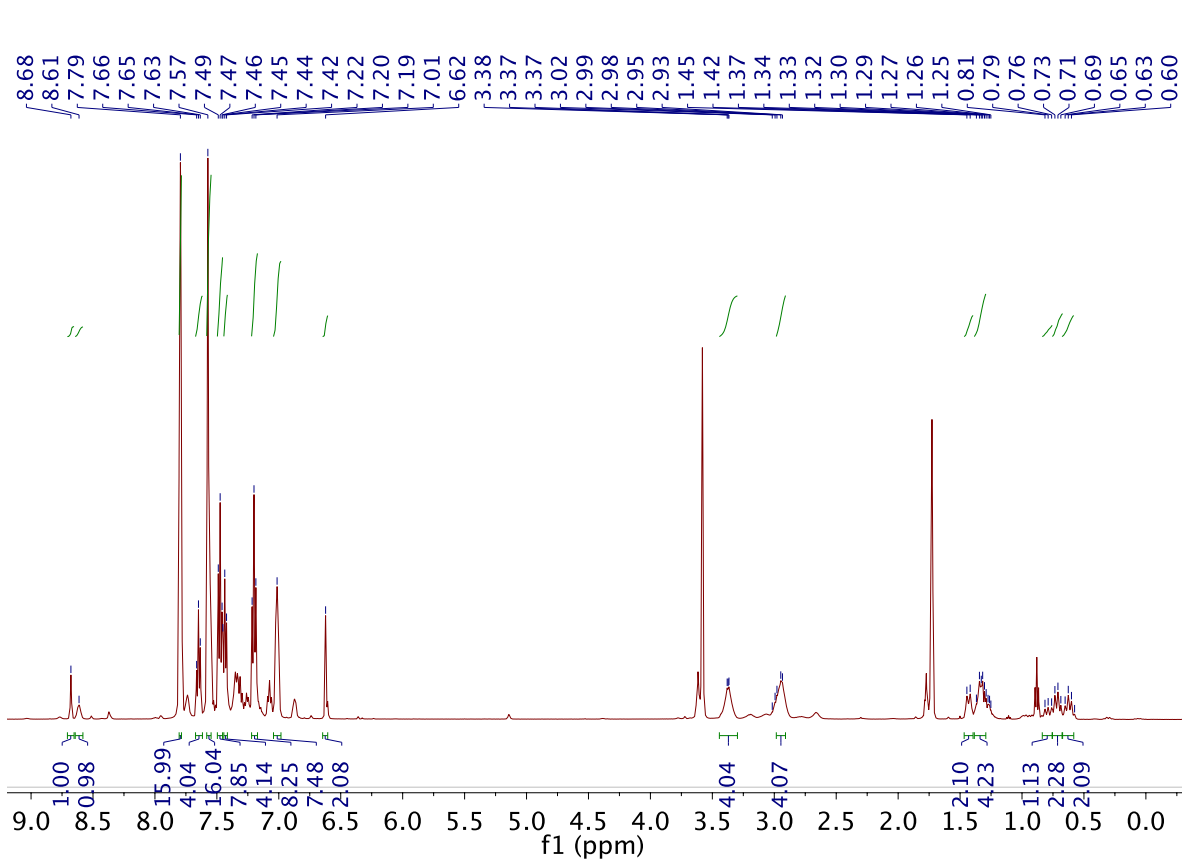
**Figure S2.** THF- $d_8$   $^1\text{H}$  NMR spectrum of  $[(\text{dppe})_2(\text{CH}_3\text{CN})\text{Mo}(\text{NNC}_6\text{H}_{11})][\text{BarF}_{24}]$  ( $[2]^+$ ) at 295 K.



**Figure S3.** THF- $d_8$   $^1\text{H}$  NMR spectrum of  $[(\text{dppe})_2(\text{CH}_3\text{CN})\text{Mo}(\text{NNHC}_6\text{H}_{11})][\text{BARF}_{24}]_2$  ( $[2\text{-H}]^{2+}$ ) at 295 K.

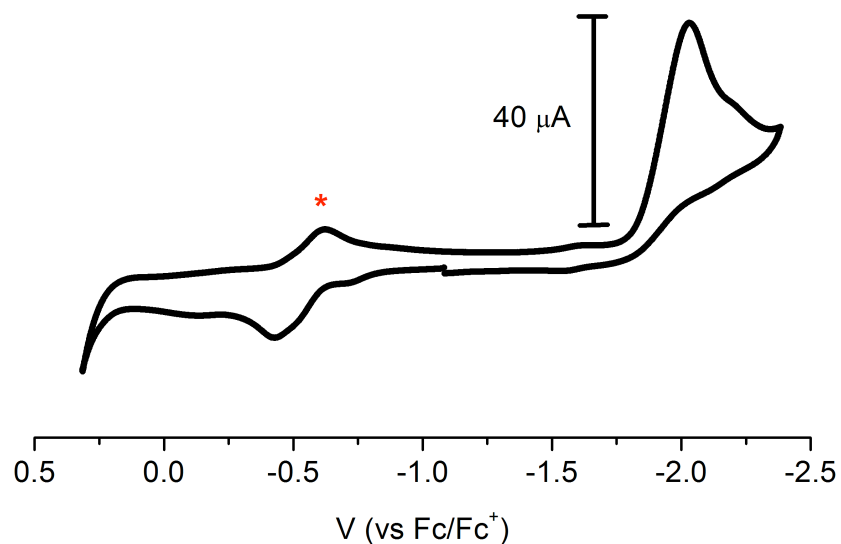


**Figure S4.**  $\text{THF-}d_8$   $^1\text{H}$  NMR spectrum of  $[(\text{dppe})_2(3,5\text{-}(\text{CF}_3)_2\text{C}_6\text{H}_3\text{CN})\text{Mo}(\text{NNC}_6\text{H}_{11})][\text{BARF}_{24}]$  ( $[\mathbf{3}]^+$ ) at 295 K.

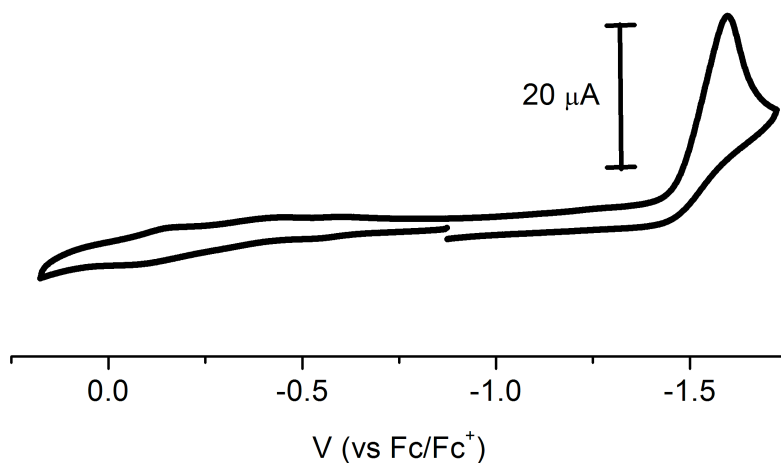


**Figure S5.** THF- $d_8$   $^1\text{H}$  NMR spectrum of  $[(\text{dppe})_2(3,5\text{-(CF}_3)_2\text{C}_6\text{H}_3\text{CN)Mo(NNHC}_6\text{H}_{11})][\text{BArF}_{24}]_2$  ( $[\mathbf{3-H}]^{2+}$ ) at 295 K.

## II. Additional Electrochemical Data



**Figure S6.** Cyclic voltammogram of **[1-H]<sup>+</sup>** using a glassy carbon working electrode, platinum wire counter electrode, silver wire reference electrode, 0.1 M [<sup>n</sup>Bu<sub>4</sub>N][PF<sub>6</sub>], scan rate 100 mV/sec in THF at 295 K versus Cp<sub>2</sub>Fe/Cp<sub>2</sub>Fe<sup>+</sup>. \*Denotes minor impurity.



**Figure S7.** Cyclic voltammogram of **[2-H]<sup>+</sup>** using a glassy carbon working electrode, platinum wire counter electrode, silver wire reference electrode, 0.1 M [<sup>n</sup>Bu<sub>4</sub>N][PF<sub>6</sub>], scan rate 100 mV/sec in THF at 295 K versus Cp<sub>2</sub>Fe/Cp<sub>2</sub>Fe<sup>+</sup>.

### III. DFT Input Examples

#### Geometry Optimizations: $[(\text{Me}_2\text{PCH}_2\text{CH}_2\text{PMe}_2)_2\text{Mo}(\text{NNC}_6\text{H}_{11})](\text{I})$

```
! RKS B3LYP RIJCOSX def2-SVP def2-SVP/J Normalprint SlowConv TightSCF  
Opt Pal8 UCO
```

```
%basis NewGTO 42 "def2-TZVP(-f)" end  
NewGTO 7 "def2-TZVP(-f)" end  
NewGTO 15 "def2-TZVP(-f)" end  
NewGTO 53 "def2-TZVP(-f)" end  
NewAuxGTO 42 "def2-TZVP/J" end  
NewAuxGTO 7 "def2-TZVP/J" end  
NewAuxGTO 15 "def2-TZVP/J" end  
NewAuxGTO 53 "def2-TZVP/J" end  
end
```

```
%SCF MaxIter 500  
TolE 1e-7  
TolErr 1e-6  
end
```

```
* xyz 0 1
```

```
XYZ Coordinates
```

```
*
```



**Numerical Frequency Calculations: [(Me<sub>2</sub>PCH<sub>2</sub>CH<sub>2</sub>PMe<sub>2</sub>)<sub>2</sub>Mo(NNC<sub>6</sub>H<sub>11</sub>)(I)]**

! RKS B3LYP RIJCOSX SLOWCONV TIGHTSCF DEF2-SVP DEF2-SVP/J  
NORMALPRINT NUMFREQ GRID4 NOFINALGRID PAL8 ZORA

```
%basis NewGTO 42 "def2-TZVP(-f)" end
      NewGTO 7 "def2-TZVP(-f)" end
      NewGTO 15 "def2-TZVP(-f)" end
      NewGTO 53 "def2-TZVP(-f)" end
      NewAuxGTO 42 "def2-TZVP/J" end
      NewAuxGTO 7 "def2-TZVP/J" end
      NewAuxGTO 15 "def2-TZVP/J" end
      NewAuxGTO 53 "def2-TZVP/J" end
end
```

```
%SCF MaxIter 500
      TolE 1e-7
      TolErr 1e-6
end
```

```
%FREQ RESTART TRUE
CENTRALDIFF TRUE
INCREMENT 0.01
END
```

```
* xyz 0 1
```

XYZ Coordinates from Geometry Optimization

\*

#### IV. Coordinates from Geometry Optimizations

$[(\text{Me}_2\text{PCH}_2\text{CH}_2\text{PMe}_2)_2\text{Mo}(\text{NNC}_6\text{H}_{11})(\text{I})]$

C	-2.72614909235340	2.08398042386782	-0.59475529529315
C	-0.69060819502678	-0.70476748710821	3.91264135590640
C	-1.42429333369685	0.26819297870990	4.85480761194865
C	-0.47691616449512	0.96055168336717	5.84173702209409
C	0.34076835839944	-0.06011724518236	6.64412991421693
C	0.14526983413084	-1.71092969231317	4.72713097874870
C	1.09421406629549	-1.02415400718947	5.71762757525275
C	-1.76077757961125	2.98797532040245	0.17583391311848
C	2.01732568671048	-3.13553051376642	-0.01900540107636
C	2.99106276468145	-2.11553330144151	-0.61459079939943
C	-3.48730722716575	-0.51162698654273	-1.49132328125782
C	-3.41700793055368	0.04091549977140	1.29564969565753
C	0.59721540290695	3.41497184986324	-1.41050891227820
C	0.80720495311896	3.21698875768044	1.43316325163438
C	-0.59269824601170	-3.71503059405596	0.95409968291286
C	-0.17853433264487	-3.45907264373366	-1.83938365919751
C	3.36781478748622	-0.26886189426309	1.55802004310760
C	3.68410149763970	0.61082234609835	-1.13744335988436
N	0.06950790051799	-0.09344876512508	1.78671936671548
N	0.19622767421871	0.06333334732186	2.99658714032821
P	-2.41241139865865	0.28208353504942	-0.23132511099670
P	0.00284590063291	2.39998539139564	-0.00122658382988
P	0.23802413086033	-2.61177775201435	-0.26115670663568
P	2.55378065537000	-0.38494121172264	-0.08604019558095
Mo	0.06681213970423	-0.10162688811457	-0.04005094733542
I	0.16884557926202	0.06173217095198	-3.06447299843804
H	-3.77629857221263	2.33847025307409	-0.36770254912947
H	-2.58257047769667	2.20700827830382	-1.68156760789307
H	-1.42990802100011	-1.25599716869496	3.30479912025007
H	-2.18111000884578	-0.30871818037641	5.41895315593118
H	-1.97707543174792	1.01459419171371	4.26043491543566
H	0.21092484106303	1.61703624435279	5.28105469702952
H	-1.05387323798167	1.61142261025454	6.52171988002473
H	-0.33835185456799	-0.64110494463426	7.29827744250372
H	1.04748716601083	0.45984782207961	7.31395832092616
H	-0.55358025247178	-2.36797749725936	5.27933615856828
H	0.71228820988640	-2.36033644013438	4.03805185121237
H	1.85507379528492	-0.46163954919682	5.14987175888442
H	1.63436678417173	-1.78286850095595	6.30965765588423
H	-1.99419924382116	2.96666073322144	1.25405092692939

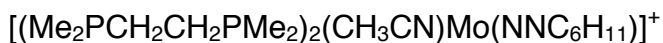
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H	2.17764266662136	-4.14004716409718	-0.44723160794211
H	2.93192523621432	-2.12512465184769	-1.71587302048261
H	4.03360301300023	-2.34545647415173	-0.33398184337163
H	3.32225948351501	0.77025206264546	1.91707077757666
H	4.41904885730799	-0.59816006554571	1.52173707873548
H	2.81557799527482	-0.87923329432797	2.28618269237169
H	3.69780756218773	1.64989464428747	-0.77390831094851
H	3.30316721834547	0.61144671320090	-2.16918826716399
H	4.71289272504770	0.21521204346619	-1.12006777954879
H	-1.68117165089887	-3.69094473833663	0.78969173225533
H	-0.39348842595385	-3.35256608675639	1.97336576907502
H	-0.24121555058000	-4.75671974519112	0.86642829779628
H	-1.24542738864378	-3.31003888065667	-2.06405681065342
H	0.03946265284215	-4.53851587302508	-1.78327084806529
H	0.38864474313305	-3.00198460496115	-2.66096310713855
H	-4.49004348468426	-0.05457737274809	-1.51772102064971
H	-3.59167252713692	-1.58354462305156	-1.26228533608494
H	-3.00863849721758	-0.41434825868735	-2.47696312783253
H	-2.96782135756799	0.60289358441733	2.12645235854470
H	-3.41374670815392	-1.02361317480180	1.57410525489791
H	-4.45889916290165	0.37361521107899	1.15739398426624
H	0.45266773346522	4.49176264172047	-1.22139799661936
H	0.06126102767031	3.11694316777651	-2.32230896842923
H	1.66452143638761	3.21230543302112	-1.58369343383560
H	0.53416505559487	4.28247343611211	1.50918851520552
H	1.90055828257476	3.13433445594527	1.33201744718395
H	0.51461425662483	2.69002652063931	2.35397208260193

[(Me<sub>2</sub>PCH<sub>2</sub>CH<sub>2</sub>PMe<sub>2</sub>)<sub>2</sub>Mo(NNHC<sub>6</sub>H<sub>11</sub>)(I)]

C	1.40054452622826	2.98327192916155	-0.82035363273763
C	-0.59407845220580	0.94146670011956	4.15421931840566
C	0.29978230596215	1.60554635792061	5.21701080018690
C	1.31188950864591	0.63552418702047	5.85001010574781
C	0.61489907581928	-0.60767771814050	6.42064500147308
C	-1.25075600691680	-0.33208675598291	4.70994485595503
C	-0.24326017237622	-1.29793180700134	5.35090392243072
C	2.45050368124116	2.35646646506007	0.10249007299668
C	-2.72615571861044	-2.53919602098054	0.01220841506150
C	-1.48894209628458	-3.30073527396398	-0.48079072663811
C	-1.27412052608073	3.05089936049828	-1.81234978443339
C	-0.82420268377544	3.39091072366325	0.97301859792247

C	3.43069994931950	0.10087358272053	-1.29914440310694
C	3.32148463531302	-0.01017258755870	1.52600760121453
C	-3.81296152039577	-0.00723840006274	0.84023895667073
C	-3.37900953208446	-0.54863812573399	-1.92053324489892
C	0.09600236744747	-3.20104652996725	1.91523754387178
C	1.35226442466125	-3.55211977277735	-0.62061166758307
N	-0.33773808327083	0.12726290041230	1.87743930858110
N	0.23092793028995	0.65291361794802	2.96587263598125
P	-0.29832116636015	2.32191196604187	-0.43619374204954
P	2.28261461052332	0.49225487016665	0.08742107732077
P	-2.53442854635591	-0.70218381894312	-0.29165818693381
P	0.06287798408995	-2.53585284308111	0.20144888630973
Mo	-0.12753526642759	-0.07912818324979	0.04720274463478
I	0.20277763952670	-0.45992973802861	-2.79997350202492
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H	-0.35231270760745	2.01621709436585	6.00207236338292
H	0.82182926587598	2.46876016656390	4.77525694940872
H	2.04387712516892	0.32006838581657	5.09182314902425
H	1.88004316453697	1.15429720193215	6.63562069885303
H	-0.02272124682958	-0.31020143628963	7.26898258904374
H	1.35939635813578	-1.30921277924988	6.82355634275834
H	-1.99638187845106	-0.02232521655713	5.45835649599552
H	-1.80028821548858	-0.83036021452255	3.90126539061871
H	0.41423830666598	-1.69963378353138	4.56745087679890
H	-0.77645251688997	-2.15626798354092	5.78410247985840
H	2.30160927792188	2.69746530146123	1.13800745105994
H	3.46691071748817	2.65832628339320	-0.18953606448625
H	-2.85225851798405	-2.67583265011157	1.09596120544463
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H	-1.40809141930658	-3.24417482159764	-1.57536844660291
H	-1.54375101039153	-4.36432918163114	-0.20492774977166
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H	-0.04510079198407	-4.29015925289883	1.94672956155119
H	-0.68440651112894	-2.70549873066227	2.50078286333458
H	2.33289014833298	-3.31593064138038	-0.18863463607627
H	1.37695564203465	-3.29860989321636	-1.68662868460847
H	1.16319268964577	-4.62760282226850	-0.50175014334350
H	-4.07690839633526	1.00616241845319	0.51394184637687
H	-3.38650021539715	0.06276262859910	1.84689331454569
H	-4.72493993032360	-0.61873908637084	0.86201128486964
H	-3.28519089011625	0.47840887451691	-2.29040718055461
H	-4.43979155659979	-0.81949690371295	-1.83545794443209

H	-2.89096875990503	-1.20278369101390	-2.64884658055308
H	-1.08118123148366	4.12712762177865	-1.91702473495954
H	-2.34414185292788	2.89853570703948	-1.62267653016442
H	-1.01346886055447	2.53596620767047	-2.74365698421416
H	-0.18679986249389	3.20107382585674	1.84322900288630
H	-1.84881390412186	3.12462977016128	1.25801316752149
H	-0.77820388316700	4.45917846380499	0.72277330593041
H	4.45223100810746	0.41274995281359	-1.04453024514942
H	3.10367037933405	0.61826091815411	-2.20559538385912
H	3.41149115899265	-0.97343403995839	-1.51002772765585
H	4.21009100503412	0.62510999034155	1.63678737746912
H	3.65114200768740	-1.04609504746279	1.37739094566997
H	2.72328653471349	0.01837028932922	2.44350601636105
H	0.89778737598218	1.40585770715324	2.78357052368907



C	-2.83780967211001	2.08872701036099	-0.41427403373805
C	-0.63656362550471	-0.72219321753984	3.89679846614777
C	-1.37406313005126	0.15234419743176	4.92303946886065
C	-0.41926663345878	0.87776533265022	5.87995942137803
C	0.52942601156377	-0.10400654281782	6.57833383147073
C	0.35261285404636	-1.67420885724907	4.59278671894076
C	1.30077901171578	-0.95564273713996	5.56163406071107
C	-1.78955102337288	2.97952089356689	0.25729382755930
C	1.75350432980981	-3.17307067758264	0.39834873368170
C	2.91073264896383	-2.30037328100821	-0.09871281448487
C	-3.49821739401560	-0.47185068147867	-1.49288186469398
C	-3.37228255225403	-0.12623945769668	1.33899923970370
C	0.21142007578930	3.29526198784753	-1.77074528643208
C	0.95054974453050	3.41773264913323	0.99487921503030
C	-1.07327192479673	-3.70729784977946	0.50329095110772
C	0.20525856222182	-3.27190410526935	-2.00535388818190
C	3.26807438393572	-0.06914533919908	1.68101823339992
C	3.76134000753020	0.22561341278986	-1.11068191903934
N	0.00903089456114	-0.01831444098105	1.74800310673716
N	0.09418712762746	0.16733464121932	2.93839604449789
P	-2.43963810337906	0.27792241020159	-0.19162396903710
P	-0.06188487458039	2.43130796113700	-0.16881286117911
P	0.13515948593977	-2.58504885931772	-0.29916675518869
P	2.52315209833826	-0.47618025156917	0.05306062577600
Mo	0.03516224012768	-0.07829460128195	-0.10249431977104
N	0.11773168811935	0.02752791452241	-2.34838795847399
C	0.13133964738680	0.16140113729679	-3.49373663703586

C	0.12573299818964	0.36735845053445	-4.93480681855036
H	-3.84958757844102	2.30493871531894	-0.03241719465200
H	-2.86195560313544	2.27871911764715	-1.50075257056154
H	-1.36222342346706	-1.31585488401067	3.31370066797842
H	-2.04397584174174	-0.50783098577082	5.50413826861225
H	-2.02317778926817	0.87205866671569	4.39644819574328
H	0.17390631952317	1.61674861264674	5.31312014497404
H	-1.00236435086172	1.44664188514017	6.62317334698978
H	-0.05381463051218	-0.76984239024397	7.24254885272749
H	1.23222419289221	0.44274790284979	7.22912510601631
H	-0.24948226605256	-2.41579702881308	5.14932563282865
H	0.92160146413690	-2.24169948063227	3.83586458588849
H	1.98525105572482	-0.30704923812198	4.98657703081455
H	1.93230737100938	-1.69593242124723	6.08080228721825
H	-1.87414354146561	2.91624082305552	1.35554112744684
H	-1.92958049182537	4.03839588691119	-0.01991824447190
H	1.66541162216022	-3.11308284141060	1.49648124873687
H	1.91528526522601	-4.23445189242152	0.14339428769754
H	3.11056197982661	-2.50194209779195	-1.16446390636817
H	3.84364645362785	-2.53070396913061	0.44213848307209
H	3.18213158957725	1.01087566339504	1.87102646645638
H	4.32841874453462	-0.36433991109692	1.72289077171543
H	2.71719103193149	-0.58386513474093	2.47940957698746
H	3.82241720734679	1.31647584274493	-0.97550290363205
H	3.45510999810776	0.02393239161227	-2.14895953760644
H	4.76149286842511	-0.20792481546454	-0.94686401139407
H	-2.06460498228200	-3.56254927995316	0.04637856851572
H	-1.15183556618803	-3.45671419916826	1.57195455577636
H	-0.78673061684047	-4.76680492158314	0.40104947121279
H	-0.76574448517472	-3.13761120450479	-2.50543470672197
H	0.45731957674593	-4.34482861678699	-1.99652264889136
H	0.96386473422235	-2.73621281891445	-2.59287175163022
H	-4.52615583681902	-0.07579646717438	-1.46569649437314
H	-3.53578314647512	-1.56377533985903	-1.35919199552825
H	-3.06436816107797	-0.26399828367744	-2.48309075553121
H	-2.93092631292892	0.41663559564094	2.18632071919107
H	-3.29017604296198	-1.20287434460686	1.54994752730412
H	-4.43661763781521	0.14559733160059	1.25319301039168
H	0.03310392952642	4.37871381654729	-1.67822618777303
H	-0.47130568968113	2.89304508726086	-2.53309747216060
H	1.24364690354748	3.13003553808329	-2.11548503692105
H	0.64722801542016	4.47711906267447	1.01139425225884
H	2.01019232434396	3.35447747160815	0.70259095794200
H	0.84750638124878	2.99356205456793	2.00543288919837

H	-0.62261248850044	1.12749315879931	-5.20827447179083
H	-0.12203254665915	-0.57142302020410	-5.45411835730755
H	1.11506303819601	0.71080110272797	-5.27614034857604

$[(\text{Me}_2\text{PCH}_2\text{CH}_2\text{PMe}_2)_2(\text{CH}_3\text{CN})\text{Mo}(\text{NNHC}_6\text{H}_{11})]^+$

C	-2.47820199287073	2.30310389448328	-0.31329417734630
C	0.42800508039487	-1.00337194289910	4.15580685729583
C	-0.47662947069303	-1.54086482272545	5.27743180797088
C	-1.34745697144653	-0.45556588992714	5.93332905404904
C	-0.49716196207322	0.72291988970067	6.42551223379880
C	1.22185145075601	0.23370589727534	4.61600438051073
C	0.34801679877603	1.30522274286739	5.28346026552435
C	-1.36273005315453	3.04608653947086	0.42645643772049
C	1.48095773974446	-3.46317214564962	-0.09709446248334
C	2.68379604557553	-2.65268848203587	-0.59091627862203
C	-3.56588926076567	-0.13128776356326	-1.31888733713457
C	-3.30646493535585	0.23005023637417	1.48706203411073
C	0.87657664829716	3.19712243286744	-1.36968037959678
C	1.31472175819778	3.02159244578419	1.43976991446173
C	-1.36062319086396	-3.68926400298272	0.26107479734294
C	-0.28562404610982	-3.14762630973242	-2.32244936971288
C	3.44698678378829	-0.78920223127406	1.46102525694740
C	3.75765217648757	-0.09695435787181	-1.27961619664113
N	0.05952178397106	-0.50776322681282	1.78987772821138
N	-0.40572867389181	-0.72517397182508	2.96091285129417
P	-2.34235389864853	0.45355659859193	-0.07289828703114
P	0.30324855973421	2.26087805636054	0.11248516583048
P	-0.11277296953682	-2.62339608946753	-0.56351643443920
P	2.52555568889404	-0.84297475603962	-0.13197922994031
Mo	0.07083444931582	-0.20190830520163	-0.07472239195735
N	0.05075281003123	0.12499239946444	-2.22355303156974
C	-0.04086299887256	0.33594475506735	-3.36091651388005
C	-0.19339593041212	0.63494552633375	-4.77805386082765
H	-3.46914026133532	2.65609679829096	0.00562751202847
H	-2.40856794028499	2.49006362529115	-1.39461464606635
H	1.13968818238026	-1.78823610212264	3.86305789860668
H	0.17183109281614	-1.98891202635573	6.04347006039474
H	-1.09887690082420	-2.36018731274270	4.88884305160083
H	-2.09882712596009	-0.08037448766884	5.21858422012641
H	-1.91724133396611	-0.89631481839054	6.76244416669396
H	0.16797779454728	0.37984116422408	7.23346320585391
H	-1.13770844369092	1.50064698404992	6.86255656771110
H	1.98795960093447	-0.11126715970928	5.32678965042026

H	1.76185842273167	0.65121504004464	3.75657997859728
H	-0.32056061773558	1.75545420698769	4.53163027030177
H	0.98423454318368	2.11978172105999	5.65529998800873
H	-1.53066643646363	3.00414232026725	1.51220112404104
H	-1.34129237063627	4.10912922869612	0.14694198165840
H	1.48952001479799	-3.53842409767609	0.99933316702173
H	1.50133975433196	-4.48841900574388	-0.49256001556438
H	2.75092239305185	-2.70423847568302	-1.68711235286364
H	3.62665342163180	-3.05766204062309	-0.19804807579886
H	3.55134052016174	0.24767058978123	1.79792051815693
H	4.44384775778287	-1.23505209436843	1.35745374089735
H	2.88340442093071	-1.33331657857020	2.22488594772036
H	3.97769922562436	0.93152945637452	-0.97017823265344
H	3.35143246559418	-0.06982260443748	-2.29738617407294
H	4.69497736294410	-0.66785162266152	-1.28645888672807
H	-2.36187657354934	-3.41824605953065	-0.09562748445128
H	-1.32658725350351	-3.52019663440765	1.34415144429081
H	-1.19192033047900	-4.75566432721697	0.06009042688567
H	-1.27644472316169	-2.86505482693091	-2.697063477113474
H	-0.16021763125387	-4.23280834747260	-2.42806637967784
H	0.46359992744976	-2.64341725539118	-2.94164473033938
H	-4.50838412837902	0.42637157205532	-1.24856467560435
H	-3.77431297803302	-1.19646748585189	-1.16523146086443
H	-3.15519265931624	-0.00504465614761	-2.32757166473910
H	-2.80658278788991	0.75055481015304	2.31076786984583
H	-3.37810824534571	-0.83529056068853	1.73719865704970
H	-4.32164891582926	0.63421736957018	1.38689506382578
H	0.90444024973644	4.27659024107924	-1.17462114001941
H	0.20123996361974	3.01188212829973	-2.21133895058284
H	1.87922304326524	2.85963684758419	-1.65659110404571
H	1.19357461286243	4.11268656288002	1.46398474446689
H	2.37330768693705	2.78474094029819	1.27772818547374
H	1.01629163487750	2.60350896574498	2.40761003516986
H	-0.97160257225079	1.39476845023300	-4.92918044511516
H	-0.48597209022319	-0.26774036017340	-5.32910232104685
H	0.74542061052783	1.01343480098154	-5.20353532868369
H	-1.41328443387814	-0.82365780601534	3.08777131731773

$[(\text{Me}_2\text{PCH}_2\text{CH}_2\text{PMe}_2)_2(3,5\text{-(CF}_3)_2\text{C}_6\text{H}_3\text{CN})\text{Mo}(\text{NNC}_6\text{H}_{11})]^+$

C	-2.57079609458288	2.26858065360035	-0.36399987551141
C	-0.69557264176694	-0.68340020232502	4.08783915457051
C	-1.34131487124169	0.27989694895093	5.09620532066853
C	-0.31471652955158	0.94911711710914	6.01836497344655



C	0.56669423488677	-0.08702197820737	6.72716096493936
C	0.22423557660395	-1.69612240893930	4.79482085810985
C	1.24613481165456	-1.02852340059855	5.72453720242028
C	-1.51396345640554	3.06993783035276	0.39860314555817
C	1.66521887021106	-3.32925033315730	0.38369631797965
C	2.85639143598086	-2.47131964086373	-0.05722902034162
C	-3.41815932743455	-0.22470649510877	-1.45426901852990
C	-3.39606227345022	0.12911877998273	1.37125110049019
C	0.71946691300024	3.29888311296895	-1.39979744391312
C	1.15801377045283	3.19964677346029	1.43544909644212
C	-1.18292502776791	-3.72327443048398	0.50704232186270
C	0.08434614596831	-3.20766979990533	-1.99585772748734
C	3.24037715479778	-0.45387237356559	1.95395304120614
C	3.86051118903727	0.10943354396673	-0.76587400676965
N	0.02469062195596	-0.08809722787826	1.92604436951176
N	0.10527053149835	0.11824269873412	3.11086136896031
P	-2.35306131959783	0.43406511050012	-0.10993826456761
P	0.19477552558138	2.38786913499128	0.10882680623508
P	0.06948580119844	-2.62050397985623	-0.25187593853386
P	2.54958688853545	-0.65882219931345	0.26724984564021
Mo	0.09292494137258	-0.11900527055621	0.06949048873674
N	0.18348526993545	0.07028675237736	-2.11502795294671
C	0.13889503923617	0.25733118293692	-3.25698560671204
C	-0.00057894022692	0.53291978553903	-4.64764530294404
C	-1.16730743714469	0.10017350739802	-5.31330999449212
C	0.97225235678406	1.28045706792752	-5.33418874157432
C	0.76184071376806	1.61426499928547	-6.67247147569358
C	-1.35564220917529	0.43504231057661	-6.64913538623755
C	-0.39766855376189	1.19773648359045	-7.33412369572519
C	1.79861361240313	2.46684878702380	-7.37818654306102
C	-2.62279932502255	0.01584342023155	-7.36799007853658
F	1.66045848506183	2.41848550827225	-8.70706714843806
F	1.70016255709869	3.74958959195099	-6.99956817336371
F	3.03753940501319	2.05711818714017	-7.06305286483421
F	-3.34786345748373	1.09836748502552	-7.69305181054736
F	-3.38690372135091	-0.77950324062609	-6.60215148519470
F	-2.34919523947556	-0.64780666814885	-8.49451245913869
H	-3.58924882824429	2.57393408225547	-0.07078695788164
H	-2.48412459610434	2.45414840755044	-1.44865616417616
H	-1.47549677620797	-1.22552188738736	3.52504258381239
H	-2.05597633419251	-0.30363528728704	5.70410637683077
H	-1.93536038963896	1.03685698921316	4.55635582531507
H	0.32544920063277	1.62623630227660	5.42608091947879
H	-0.83839866502210	1.58021234228778	6.75531397060598

H	-0.05360582618368	-0.68567089911154	7.42045234301268
H	1.32318577010085	0.42050585540485	7.34831520670456
H	-0.42579859229823	-2.37232696262486	5.37965821820836
H	0.73115419734496	-2.32647790300094	4.04324143169150
H	1.96938707415027	-0.45596703143017	5.11800387348520
H	1.82580665617523	-1.80218887675807	6.25484365072525
H	-1.69389981767038	3.01030880535356	1.48558196240726
H	-1.55022930252194	4.13820369726778	0.12356330079304
H	1.58746627541894	-3.34944688113729	1.48390282764188
H	1.77802766469794	-4.37400221621183	0.04808774974672
H	3.02917469313623	-2.58200802069400	-1.14085751526539
H	3.78503893680425	-2.79033909463262	0.44331264249673
H	3.16459650289355	0.59879037899408	2.26326432130644
H	4.29398025605219	-0.77232103644412	1.99642578004062
H	2.65692857041906	-1.04562676205303	2.67118708341163
H	3.95202456483535	1.17804717798296	-0.51770846379903
H	3.59636755636880	0.02567287238759	-1.83149897377708
H	4.83757689266654	-0.37392388756031	-0.60436626065568
H	-2.17082151666927	-3.50574285095782	0.07224572857637
H	-1.23649200215627	-3.52446686937592	1.58817393122552
H	-0.95007683236295	-4.78852626988488	0.34546326451679
H	-0.88275545316729	-2.99248395312119	-2.47482848289038
H	0.27706987942899	-4.29126283309273	-2.05417018774434
H	0.86333219063132	-2.67975525577682	-2.56311578868587
H	-4.41253478757504	0.24931920170404	-1.45580823564007
H	-3.54692481869633	-1.31064927037264	-1.33147026565450
H	-2.93990431626762	-0.03943098352632	-2.42781603930204
H	-2.95423653659006	0.63646992445283	2.24081391424517
H	-3.42629332391967	-0.94825387200234	1.59006285290058
H	-4.42412091134563	0.49682977338669	1.22614936684241
H	0.65380193707981	4.38958927793775	-1.25589332486315
H	0.07695849929446	3.01951760513309	-2.24788279904949
H	1.75806890711252	3.03469588787137	-1.65319887595758
H	0.93856937222708	4.27773634756257	1.50069140504653
H	2.23474160864091	3.06532125054972	1.24649900491948
H	0.91750003588212	2.71664556851210	2.39485867096566
H	1.87697080665377	1.61329689454443	-4.82185190686727
H	-1.91856780451728	-0.48681093536003	-4.78352964037772
H	-0.55050832689180	1.47023341281602	-8.37954099504929

$[(\text{Me}_2\text{PCH}_2\text{CH}_2\text{PMe}_2)_2(3,5\text{-(CF}_3)_2\text{C}_6\text{H}_3\text{CN})\text{Mo}(\text{NNHC}_6\text{H}_{11})]^+$

C	-3.14192284328805	1.82879340759245	-0.36361116870786
C	-0.63638042592112	-1.03405437175683	4.07718389909297

C	-1.36366798423644	0.02134263986973	4.93231664102626
C	-0.44367173586662	0.69660161684801	5.95840754386625
C	0.27578608190986	-0.33418636872245	6.83798073077185
C	0.12430133111255	-2.03600702998389	4.96365742754975
C	1.04419628383327	-1.35262201870004	5.98684305835246
C	-2.42787276280735	2.80940989912358	0.56957422628088
C	2.56625829744780	-2.27273296117270	0.12691573401165
C	3.38210069076201	-1.05225360781077	-0.31809713807519
C	-3.28342815037162	-0.75050793621389	-1.58550101542089
C	-3.41661504378787	-0.52535341164771	1.27569415169185
C	-0.19607910447461	3.92145211419551	-0.86498721717701
C	-0.03386260363473	3.50879636442240	1.96383185005095
C	0.01634443912894	-3.53610086489129	0.51988283366305
C	0.82398081195778	-2.78187503243115	-2.09458934902348
C	3.27401784429949	0.84661075027925	1.85148055237912
C	3.42320817195169	1.78119807994379	-0.83690029557881
N	-0.01270621141432	-0.14402760748527	1.89288494496176
N	0.29634982707020	-0.42208017437187	3.10231624461432
P	-2.47880223639000	0.10043624114500	-0.17400323017694
P	-0.57463328935874	2.66667239742000	0.42458295138308
P	0.77384123379944	-2.12416894909678	-0.37729760436126
P	2.54774548641921	0.53537136503061	0.18346114824867
Mo	0.04950648068982	0.25179363646892	0.06289859689206
N	0.04954716116762	0.51531002935085	-2.09710117564642
C	0.03323303880625	0.51377638270602	-3.26751359436501
C	-0.03228405807199	0.41601048675886	-4.68200502608814
C	0.17636146602909	1.54283692084363	-5.51622343085401
C	-0.31664545126086	-0.83979840795116	-5.27896035874644
C	-0.39825237739348	-0.95590635015152	-6.66406199819530
C	0.10403614013846	1.40377708061045	-6.89946045498455
C	-0.19166006184434	0.16215679127356	-7.48467327287459
C	-0.69934575214604	-2.30389869775296	-7.29836635310956
C	0.39119979375011	2.58416605644896	-7.80867009822163
F	-1.63679485076061	-2.19373188482758	-8.25045280177483
F	0.39312975411799	-2.83354658946004	-7.87137411219862
F	-1.14385192509543	-3.18762923846471	-6.38656819552004
F	1.54045480939926	2.39722605950218	-8.47764658703536
F	0.50509734692363	3.73145724513471	-7.11902184664458
F	-0.57888001692737	2.74470525568522	-8.72052010368587
H	-4.23215041167179	1.84226390308618	-0.19210409567991
H	-2.97869190999738	2.11419683565880	-1.41744934901059
H	-1.37112809237176	-1.57123291961756	3.45961127011791
H	-2.18769246092118	-0.49035438749188	5.46142491739690
H	-1.83355886370410	0.77029612497299	4.27229171592477

H	0.30834793799502	1.31593975572733	5.43355333527047
H	-1.02914369516130	1.39252735803899	6.58158966924190
H	-0.46731823557985	-0.87077045360489	7.45685167600520
H	0.95786347524112	0.17227009096708	7.54076983676596
H	-0.62559343289837	-2.64070595310111	5.50324431207175
H	0.69285050991460	-2.73608550425861	4.32802094341486
H	1.87871646608565	-0.84006533466183	5.46923789600244
H	1.51866503721082	-2.11558685292458	6.62516088801884
H	-2.68455919491639	2.59290488747969	1.62069275080370
H	-2.74523934700477	3.84726633634824	0.37337016321414
H	2.58249325481816	-2.36578852362483	1.22664028628374
H	2.99613156596467	-3.20464990981742	-0.27644915355150
H	3.46795170891515	-1.02782686799396	-1.41773658608968
H	4.41048776002394	-1.09233977291625	0.07792792982974
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