Journal Name

ARTICLE TYPE

Cite this: DOI: 10.1039/xxxxxxxxxx

Electronic Supplementary Information (ESI): Scrutinizing Substituent Effect on Mo–Based Electrocatalysts for Molecular Hydrogen Release through an Axial–Equatorial Decomposition: A DFT Study†

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Received Date
Accepted Date

DOI: 10.1039/xxxxxxxxxx

www.rsc.org/journalname

Input Gaussian 09 commands, energy profiles of reactions (IRCs) with no substituent groups and including the most electron–withdrawing and electron–donor substituent groups ($-$CN and $-NH_2$, respectively); pictures of transition states of systems without including substituent groups (with 0, 1, 2 and 3 water molecules); linear correlations between relative energies and Hammett/Swain–Lupton sigma constants and sets of cartesian coordinates of all stationary points found during this research (reactant complexes, product complexes along with transitions states) are included here.

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† Electronic Supplementary Information (ESI) available: [details of any supplementary information available should be included here]. See DOI: 10.1039/b000000x/

‡ These authors contributed equally to this work.

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1 Gaussian commands used for the Molecular Hydrogen Release (MHR) process.

1.1 To find transition states

1.1.1 Intramolecular MHR process: No water molecule.

#p UBP86/GenECP NoSymm SCF=(maxcyc=100,NoVarAcc,XQC)
Int=(Grid=Ultrafine,acc2e=11) Guess=Huckel
Opt=(CalcFC,noeigen,notrust,ts,maxcycle=200) freq
CPHF(MaxInv=10000) SCRF=(Solvent=Water,PCM)

Geometrical optimization of the transition state

1 2
Input geometry

F O N C H 0
6-31+G(d,p)
****
Mo 0
MWB28
****

Mo 0
MWB28

1.1.2 Water–assisted MHR process: Three water molecules

UBP86/GenECP Guess=Huckel Int=(Grid=Ultrafine,acc2e=12)
SCF=(NoVarAcc,VeryTight,XQC,MaxCyc=200)
SCRF=(Solvent=Water,PCM) NoSymm
Opt=(CalcAll,NoEigenTest,NoTrust,QST3,MaxStep=50
,MaxCycles=80)

Reactant-like

1 2
Mo -0.20470200 -0.25460300 -0.95295300
O 0.43894500 0.68992000 -2.59856400
H 0.01665200 0.30341400 -3.43815100
H -0.93221900 -1.10259800 -2.19043200
O -0.29243400 -0.11071800 -5.22518900
H -2.50910000 -1.31394400 -2.74966800
H -0.52447900 0.69232400 -5.72800100
N -1.63874700 -1.84028900 -0.27102500
N 1.47112000 -1.57612300 -0.86514200
N 1.53287800 1.22428500 -0.34564300
N -1.87430100 1.06480400 -0.78434400
C -2.70536200 -1.55130600 0.53810500
N -0.18519300 -0.24493200 1.34560200
C -2.71626900 -0.16129900 1.22648100
C -2.85286800 0.97912200 0.17780900
C 2.31481100 -1.67246900 0.21585400
C -2.47485200 -4.11688200 -0.52406800
H -2.32631400 -5.11262400 -0.95264700
C -3.70349300 -2.51952900 0.78554700
H -4.57138700 -2.28167300 1.39697300
C 2.55247200 0.80864900 0.45226400
C 3.49144300 -0.72182500 2.22590400
H 3.30379200 -1.60356400 2.85666100
H 3.63497400 0.15519900 2.86887600
H 4.42068800 -0.88150700 1.66460600
C -3.93686900 1.88403900 0.17397900
H -4.72394100 1.80580300 0.92574200
C -3.90232700 -0.10903800 2.21507900
H -3.92667400 0.83686200 2.77157700
H -3.84155000 -0.93434800 2.93706800
H -4.85820200 -0.20357600 1.67891800
C 3.75033100 1.54433600 0.53836700
H 4.59472700 1.20472900 1.12509200
C 1.03356900 -0.12132500 3.43065700
H 1.96104800 -0.10725600 4.00150100
C -1.36639000 0.14872000 3.40810900
H -2.29142700 0.34313000 3.93741800
C 1.00295400 -0.30239200 2.03539200
C 1.67661200 -2.40745300 -1.92370500
H 0.97674100 -2.22914200 -2.74268300
C 2.33170600 -0.50339900 1.24239500
C -1.37447800 -0.06453600 2.01692300
C -4.04262600 2.88237800 -0.80952200
H -4.91417000 3.54792600 -0.84829300
C 3.23239100 -2.73735900 0.29575900
H 3.83217100 -2.88293400 1.18723600
C 1.67362700 2.39707800 -1.02371500
H 0.86432400 2.66241400 -1.70599800
C -0.15948800 0.13386000 4.11365900
H -0.15428800 0.31374400 5.19314800
C 3.88430300 2.75353100 -0.14797500
H 4.81869800 3.32090400 -0.07423400
C 2.81037000 3.20377200 -0.92556500
H 2.86051000 4.15736600 -1.45778200
C 2.66422900 -3.38643700 -1.96020500
H 2.81709600 -3.97388900 -2.87028500
C -1.99294200 2.04691600 -1.74366900
H -1.20080200 2.03360500 -2.49318300
C -3.03495300 2.95880300 -1.78619900
H -3.06024800 3.69422500 -2.59518300
C 3.42526400 -3.59507300 -0.79811200
H 4.17714300 -4.38241500 -0.74660900
C -3.59410300 -3.81323700 0.26371400
H -4.36546900 -4.56243700 0.46895100
C -1.55045500 -3.10629300 -0.78684400
H -0.71231100 -3.29204900 -1.46253400
O -2.15643100 -2.02690900 -5.62221700
H -2.78237700 -1.95975400 -6.36798700
H -1.01357400 -0.76745100 -5.46018700
H -2.69689600 -1.91314200 -4.78945800
O -3.31708000 -1.52981900 -3.27627200
H -3.80818400 -2.20668500 -2.77126600

Product-like

1 2
Mo -0.35416400 -0.16073500 -1.03878800

O 0.07441000 0.61885000 -2.61105600
H -0.05790100 0.37651600 -4.21928400
H -1.12294100 -1.31243400 -2.38266400
O -0.11187700 0.24959100 -5.21333400
H -1.72037800 -0.78489400 -2.24336500
H -0.76094400 0.87734100 -5.54453800
N -1.79414800 -1.77473800 -0.16973900
N 1.29741500 -1.55421500 -1.03849200
N 1.29042700 1.28751300 -0.41333700
N -2.00282400 1.22429200 -0.68638700
C -2.81501900 -1.43478300 0.66743300
N -0.22773700 -0.20251600 1.30452700
C -2.73569900 -0.04740900 1.36552900
C -2.84195800 1.16262300 0.39612300
C 2.15222800 -1.64677200 0.03847500
C -2.66243200 -4.03792100 -0.31838700
H -2.53612100 -5.05316400 -0.70356600
C -3.82172000 -2.37088100 0.97940200
H -4.66128900 -2.09089600 1.61287700
C 2.38034300 0.88416200 0.29224700
C 3.49631000 -0.64401000 1.93837100
H 3.41113600 -1.52991000 2.57979300
H 3.62876800 0.22728100 2.59634000
H 4.40605000 -0.75015000 1.32435100
C -3.75174500 2.20702400 0.64029800
H -4.43171300 2.16998900 1.49477300
C -3.86659000 0.03415800 2.41842800
H -3.79089700 0.94491600 3.02578900
H -3.82522500 -0.82620500 3.10094700
H -4.85411700 0.03780600 1.92861100
C 3.54846900 1.67491900 0.35092100
H 4.41257500 1.36296600 0.93236000
C 1.08831700 -0.32554800 3.31700800
H 2.05097900 -0.45322200 3.80363000
C -1.27890100 0.03429000 3.47436500
H -2.14536100 0.24357200 4.12281800
C 0.98195400 -0.34553300 1.91467200
C 1.38804700 -2.53029700 -2.00885500
H 0.73959500 -2.37653500 -2.86944500
C 2.24883200 -0.45819700 1.04453400
C -1.34383300 -0.04464300 2.08435500
C -3.81546400 3.28804400 -0.23736700
H -4.49366900 4.17557000 0.01825700
C 2.93023300 -2.80154100 0.22598000
H 3.54504000 -2.90889700 1.11854500
C 1.32971100 2.49789400 -1.03209900
H 0.43845900 2.78129800 -1.59123300
C -0.04007200 -0.11821300 4.10578200
H 0.03599200 -0.07198200 5.19659600
C 3.59435500 2.90010100 -0.32487600
H 4.50783400 3.50436300 -0.31639600
C 2.44893200 3.33060600 -1.01002700
H 2.41582200 4.28867600 -1.53316700
C 2.18565800 -3.65873100 -1.90103500
H 2.19460200 -4.39564800 -2.71302300
C -2.12092300 2.28241400 -1.55032800
H -1.46874800 2.23157300 -2.42683500
C -2.99771800 3.33653000 -1.34805000
H -3.05839400 4.15766000 -2.06696900
C 2.93966500 -3.82907100 -0.72796200
H 3.53217600 -4.72978500 -0.56016300
C -3.75070300 -3.68311000 0.48921800
H -4.52127500 -4.41519300 0.75112200
C -1.72404300 -3.05241000 -0.63461800
H -0.86692800 -3.28504500 -1.27263200
O -0.58282300 -2.30235900 -5.92731600
H -0.71967200 -2.31437100 -6.89007600
H -0.38142500 -1.32426000 -5.69542900
H -1.98495500 -2.71942300 -5.02042900
O -2.81186500 -2.86418400 -4.47354900
H -2.69887900 -3.74370900 -4.06787600

Suggested transition state

1 2
Mo -0.20470200 -0.25460300 -0.95295300
O 0.43894500 0.68992000 -2.59856400
H -0.09138900 0.15865400 -4.06281200
H -1.05089200 -1.10966900 -2.21280500
O -0.29243400 -0.11071800 -5.22518900
H -1.94361000 -1.16285700 -2.38110800
H -0.52447900 0.69232400 -5.72800100
N -1.63874700 -1.84028900 -0.27102500
N 1.47112000 -1.57612300 -0.86514200
N 1.53287800 1.22428500 -0.34564300
N -1.87430100 1.06480400 -0.78434400
C -2.70536200 -1.55130600 0.53810500
N -0.18519300 -0.24493200 1.34560200
C -2.71626900 -0.16129900 1.22648100
C -2.85286800 0.97912200 0.17780900
C 2.31481100 -1.67246900 0.21585400
C -2.47485200 -4.11688200 -0.52406800
H -2.32631400 -5.11262400 -0.95264700
C -3.70349300 -2.51952900 0.78554700
H -4.57138700 -2.28167300 1.39697300
C 2.55247200 0.80864900 0.45226400
C 3.49144300 -0.72182500 2.22590400
H 3.30379200 -1.60356400 2.85666100
H 3.63497400 0.15519900 2.86887600
H 4.42068800 -0.88150700 1.66460600
C -3.93686900 1.88403900 0.17397900
H -4.72394100 1.80580300 0.92574200
C -3.90232700 -0.10903800 2.21507900
H -3.92667400 0.83686200 2.77157700
H -3.84155000 -0.93434800 2.93706800
H -4.85820200 -0.20357600 1.67891800
C 3.75033100 1.54433600 0.53836700
H 4.59472700 1.20472900 1.12509200
C 1.03356900 -0.12132500 3.43065700
H 1.96104800 -0.10725600 4.00150100
C -1.36639000 0.14872000 3.40810900
H -2.29142700 0.34313000 3.93741800

C 1.00295400 -0.30239200 2.03539200
C 1.67661200 -2.40745300 -1.92370500
H 0.97674100 -2.22914200 -2.74268300
C 2.33170600 -0.50339900 1.24239500
C -1.37447800 -0.06453600 2.01692300
C -4.04262600 2.88237800 -0.80952200
H -4.91417000 3.54792600 -0.84829300
C 3.23239100 -2.73735900 0.29575900
H 3.83217100 -2.88293400 1.18723600
C 1.67362700 2.39707800 -1.02371500
H 0.86432400 2.66241400 -1.70599800
C -0.15948800 0.13386000 4.11365900
H -0.15428800 0.31374400 5.19314800
C 3.88430300 2.75353100 -0.14797500
H 4.81869800 3.32090400 -0.07423400
C 2.81037000 3.20377200 -0.92556500
H 2.86051000 4.15736600 -1.45778200
C 2.66422900 -3.38643700 -1.96020500
H 2.81709600 -3.97388900 -2.87028500
C -1.99294200 2.04691600 -1.74366900
H -1.20080200 2.03360500 -2.49318300
C -3.03495300 2.95880300 -1.78619900
H -3.06024800 3.69422500 -2.59518300
C 3.42526400 -3.59507300 -0.79811200
H 4.17714300 -4.38241500 -0.74660900
C -3.59410300 -3.81323700 0.26371400
H -4.36546900 -4.56243700 0.46895100
C -1.55045500 -3.10629300 -0.78684400
H -0.71231100 -3.29204900 -1.46253400
O -2.15643100 -2.02690900 -5.62221700
H -2.78237700 -1.95975400 -6.36798700
H -1.26998100 -1.00095700 -5.54374200
H -2.91363800 -1.86751800 -4.45549800
O -3.31708000 -1.52981900 -3.27627200
H -3.80818400 -2.20668500 -2.77126600

O N C H 0
6-31+G(d,p)
****
Mo 0
MWB28
****

Mo 0
MWB28

1.2 IRCs calculations

1.2.1 Forward and reverse branches

# UBP86/GenECP Int=(acc2e=11,Grid=Ultrafine)
# SCF=(NoVarAcc,Tight,XQC,MaxCyc=200) NoSymm Guess=read
# geom=check IRC=(rcfc,Phase=(1,62),MaxPoints=1000,
StepSize=10,maxcycle=1000,Report=cartesian)

1.2.2 Forward branch

# UBP86/GenECP Int=(acc2e=11,Grid=Ultrafine)
# SCF=(NoVarAcc,Tight,XQC,MaxCyc=200)
# SCRF=(Solvent=Water,PCM)
# CPHF(MaxInv=10000) Guess=read geom=check nosymm
# IRC=(forward,rcfc,MaxPoints=1000,StepSize=10,
maxcycle=1000,Report=cartesian)

1.2.3 Reverse branch

# UBP86/GenECP Int=(acc2e=11,Grid=Ultrafine)
# SCF=(NoVarAcc,Tight,XQC,MaxCyc=200)
# SCRF=(Solvent=Water,PCM)
# CPHF(MaxInv=10000) Guess=read geom=check nosymm
# IRC=(reverse,rcfc,MaxPoints=1000,
StepSize=10,maxcycle=1000,Report=cartesian)

1.3 To optimize geometries of reactant and product complexes coming from IRCs

UBP86/GenECP Int=(Grid=Ultrafine)
SCF=(NoVarAcc,Tight,XQC,MaxCyc=200)
SCRF=(Solvent=Water,PCM) guess=huckel
nosymm opt=(maxcycle=200) freq

2 Relative energy profiles coming from IRCs

Energy profiles of reactions without including substituent groups involving both substituent groups: that one having the most electron–donating behavior ($\mathbf{G_{ax}} = \mathbf{G_{eq}} = NH_2$; $\mathbf{G_{ax}} = NH_2$ and $\mathbf{G_{eq}} = NH_2$) and the one presenting the substituent group having the most electron–withdrawing ($\mathbf{G_{ax}} = \mathbf{G_{eq}} = CN$; $\mathbf{G_{ax}} = CN$ and $\mathbf{G_{eq}} = CN$) behavior are included here.

2.1 Intramolecular MHR processes

2.1.1 With no substituents

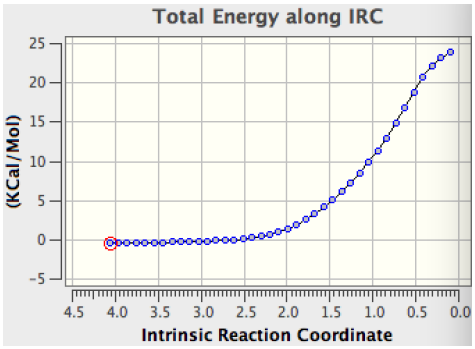

Fig. 1 Reverse branch.

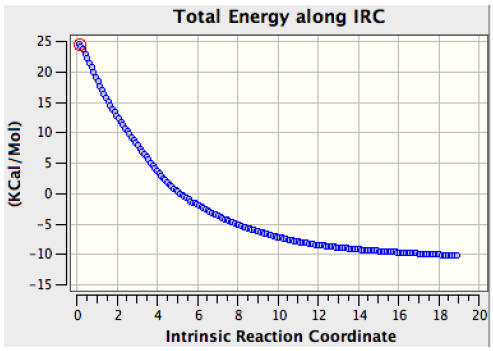

Fig. 2 Forward branch.

2.1.2 With $-NH_2$ substituent at the axial *para*–position

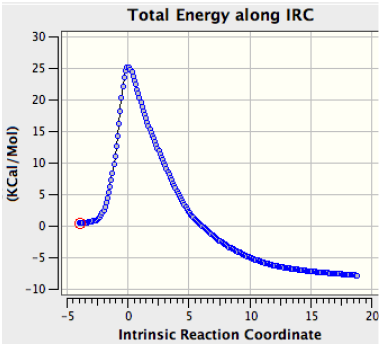

Fig. 3 Forward and reverse branches.

2.1.3 With $-$CN substituent at the axial *para*–position

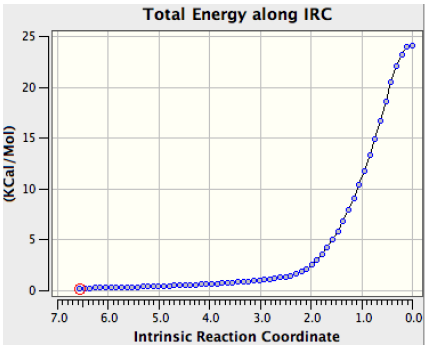

Fig. 4 Reverse branch.

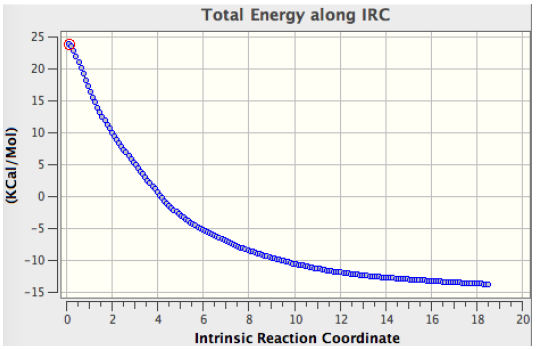

Fig. 5 Forward branch.

2.1.4 With $-NH_2$ substituent at the equatorial *para*–position

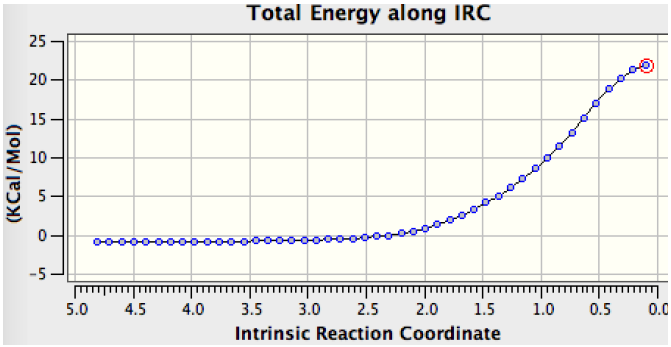

Fig. 6 Reverse branch.

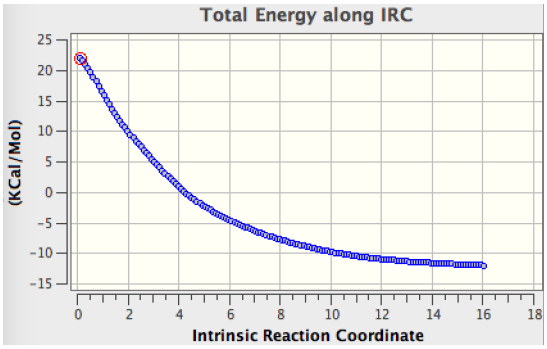

Fig. 7 Forward branch.

2.1.5 With $-CN$ substituent at the equatorial *para*–position

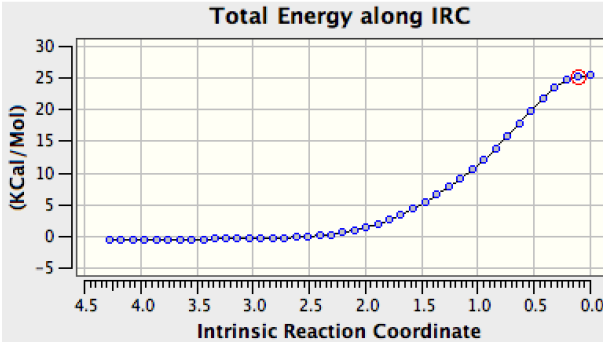

Fig. 8 Reverse branch.

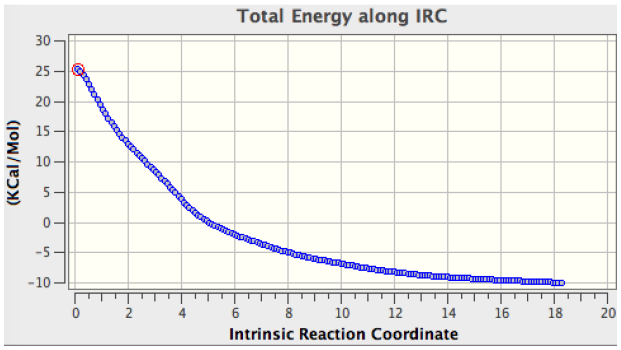

Fig. 9 Forward branch.

2.1.6 With $-NH_2$ substituent at the global *para*–position

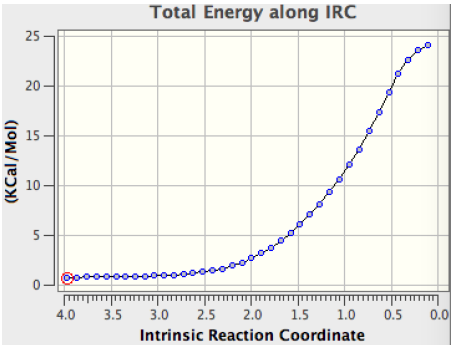

Fig. 10 Reverse branch.

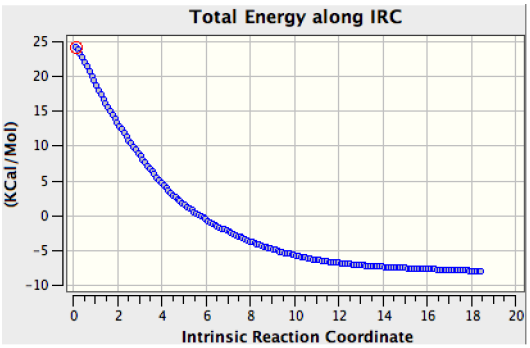

Fig. 11 Forward branch.

2.1.7 With −CN substituent at the global *para*–position

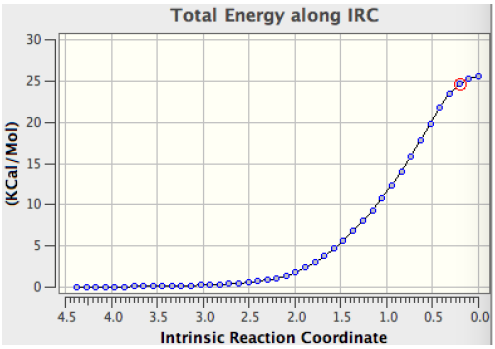

Fig. 12 Reverse branch.

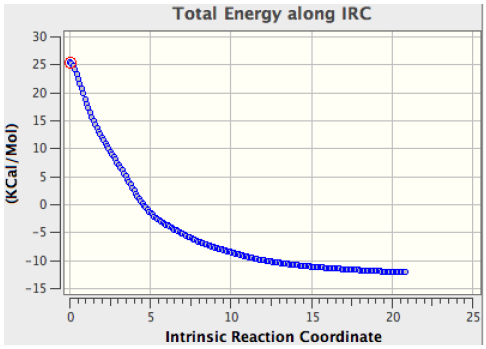

Fig. 13 Forward branch.

2.2 Water–Assisted MHR processes: One water molecule

2.2.1 With no substituents

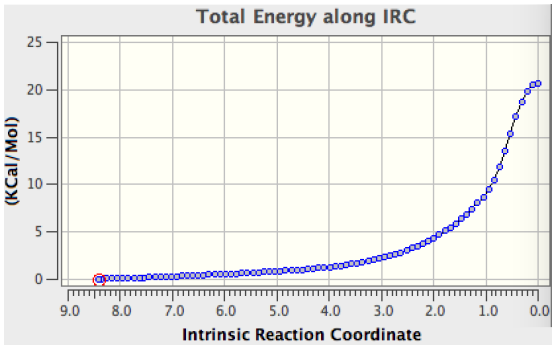

Fig. 14 Reverse branch.

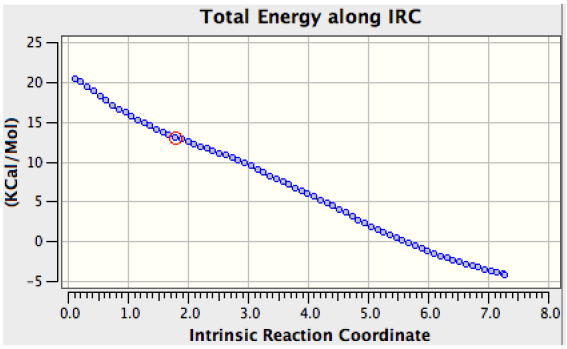

Fig. 15 Forward branch.

2.2.2 With $-NH_2$ substituent at the axial *para*–position

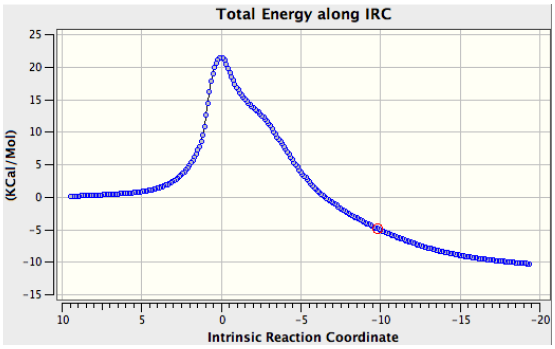

Fig. 16 Forward and reverse branches.

2.2.3 With −CN substituent at the axial *para*–position

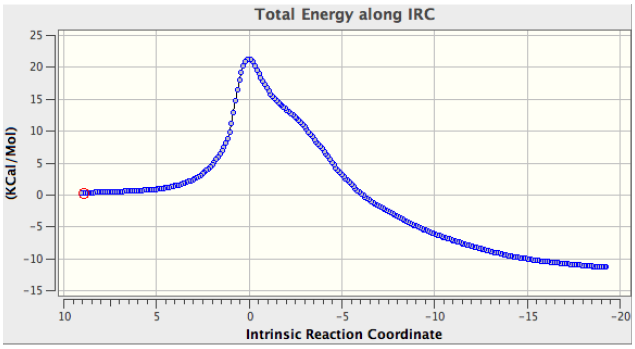

Fig. 17 Forward and reverse branches.

2.2.4 With $-NH_2$ substituent at the equatorial *para*–position

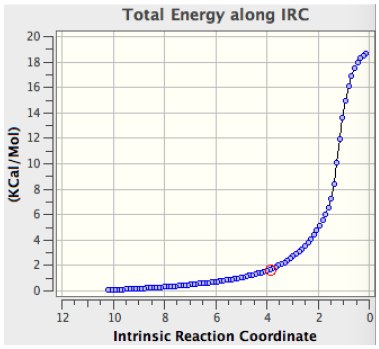

Fig. 18 Reverse branch.

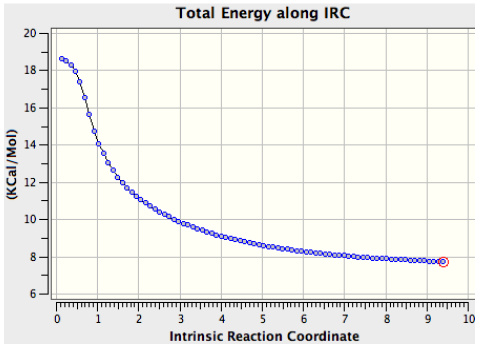

Fig. 19 Forward branch.

2.2.5 With −CN substituent at the equatorial *para*–position

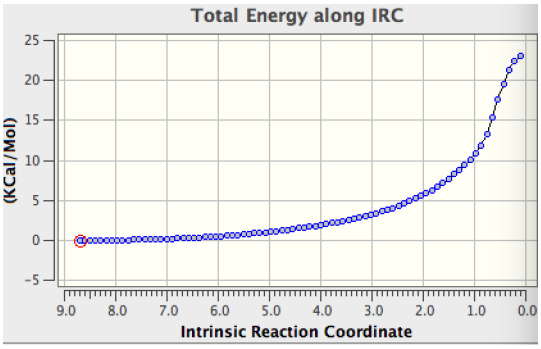

Fig. 20 Reverse branch.

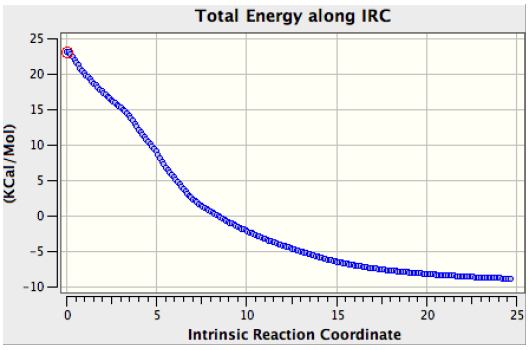

Fig. 21 Forward branch.

2.2.6 With $-NH_2$ substituent at the global *para*–position

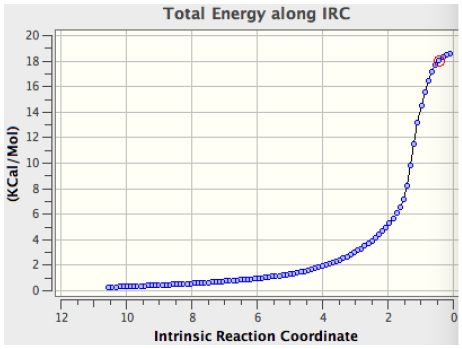

Fig. 22 Reverse branch.

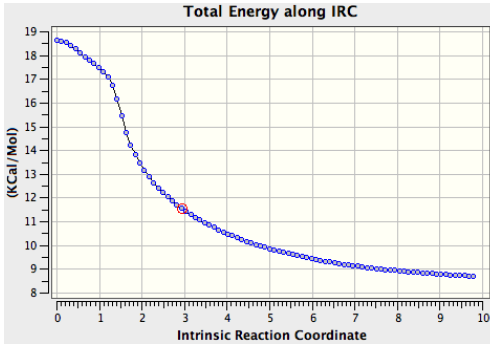

Fig. 23 Forward branch.

2.2.7 With $-CN$ substituent at the global *para*–position

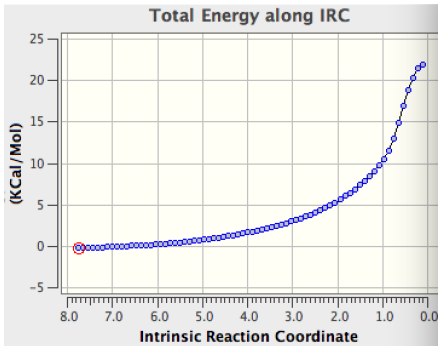

Fig. 24 Reverse branch.

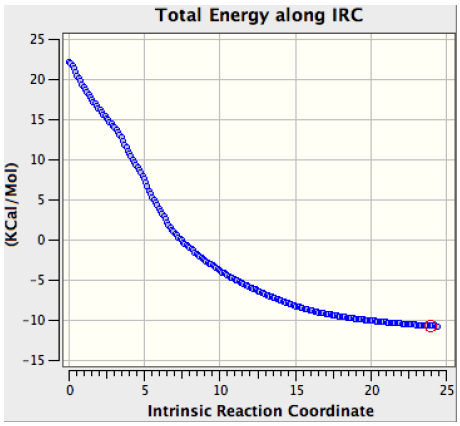

Fig. 25 Forward branch.

3 Linear Correlations (Figure 6 of the main article)

3.1 Axial *para*–substitution. $\Delta E^{\ddagger}$ *versus* σ_p.

3.1.1 Intramolecular MHR processes:

$$\begin{aligned} \Delta E^{\ddagger} &= a + b \cdot \sigma_p \\ a &= 24.5212 \pm 0.0375 \\ b &= -0.64471 \pm 0.08405 \\ \text{Pearson's r} &= -0.96762 \\ \text{R} - \text{Square} &= 0.93629 \\ \text{Adj. R} - \text{Square} &= 0.92036 \end{aligned}$$

3.1.2 Water–assisted MHR processes:

$$\begin{aligned} \Delta E^{\ddagger} &= a + b \cdot \sigma_p \\ a &= 21.30051 \pm 0.0213 \\ b &= -0.49546 \pm 0.0479 \\ \text{Pearson's r} &= -0.9818 \\ \text{R} - \text{Square} &= 0.96393 \\ \text{Adj. R} - \text{Square} &= 0.95491 \end{aligned}$$

3.2 Equatorial *para*–substitution. $\Delta E^{\ddagger}$ *versus* σ_p.

3.2.1 Intramolecular MHR processes:

$$\begin{aligned} \Delta E^{\ddagger} &= a + b \cdot \sigma_p \\ a &= 24.5845 \pm 0.0314 \\ b &= 2.19298 \pm 0.0704 \\ \text{Pearson's r} &= 0.99794 \\ \text{R} - \text{Square} &= 0.99589 \\ \text{Adj. R} - \text{Square} &= 0.99486 \end{aligned}$$

3.2.2 Water–assisted MHR processes:

$$\begin{aligned} \Delta E^{\ddagger} &= a + b \cdot \sigma_p \\ a &= 21.27072 \pm 0.0443 \\ b &= 3.43185 \pm 0.09928 \\ \text{Pearson's r} &= 0.99833 \\ \text{R} - \text{Square} &= 0.99666 \\ \text{Adj. R} - \text{Square} &= 0.99583 \end{aligned}$$

3.3 Axial *para*–substitution. ΔE° *versus* σ_p.

3.3.1 Intramolecular MHR processes:

$$\begin{aligned} \Delta E^{\circ} &= a + b \cdot \sigma_p \\ a &= -10.9547 \pm 0.2003 \\ b &= -4.21349 \pm 0.4489 \\ \text{Pearson's r} &= -0.97804 \\ \text{R} - \text{Square} &= 0.95657 \\ \text{Adj. R} - \text{Square} &= 0.94571 \end{aligned}$$

3.3.2 Water–assisted MHR processes:

$$\begin{aligned} \Delta E^{\circ} &= a + b \cdot \sigma_p \\ a &= -12.49779 \pm 0.1497 \\ b &= -2.91463 \pm 0.33547 \\ \text{Pearson's r} &= -0.97451 \\ \text{R} - \text{Square} &= 0.94968 \\ \text{Adj. R} - \text{Square} &= 0.9371 \end{aligned}$$

3.4 Equatorial *para*–substitution. ΔE° *versus* σ_p.

3.4.1 Intramolecular MHR processes:

$$\begin{aligned} \Delta E^{\circ} &= a + b \cdot \sigma_p \\ a &= -10.67078 \pm 0.156 \\ b &= 1.61552 \pm 0.3497 \\ \text{Pearson's r} &= 0.91768 \\ \text{R} - \text{Square} &= 0.84213 \\ \text{Adj. R} - \text{Square} &= 0.80266 \end{aligned}$$

3.4.2 Water–assisted MHR processes:

$$\begin{aligned}
\Delta E^{\circ} &= a + b \cdot \sigma_{\mathrm{p}} \\
a &= -11.72479 \pm 0.2102 \\
b &= 3.60165 \pm 0.47114 \\
\text{Pearson's r} &= 0.96744 \\
\mathrm{R-Square} &= 0.93594 \\
\mathrm{Adj.\,R-Square} &= 0.91992
\end{aligned}$$

All energy values are given in $\mathrm{kcal\,mol^{-1}}$.

4 Optimized geometries of reactants, transition states and products from MHRs simulated through IRCs calculations.

4.1 Transition States: structures with no substituent groups

4.1.1 Intramolecular MHR process: No water molecule

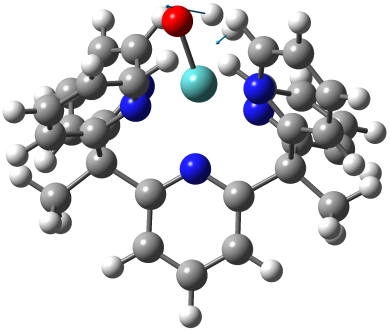

Fig. 26 Vibrational modes of transition state without including a water molecule.

4.1.2 Water–assisted MHR process: One water molecule.

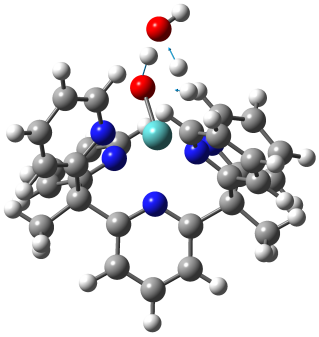

Fig. 27 Vibrational modes of transition state including one water molecule.

4.1.3 Water–assisted MHR process: Two water molecules.

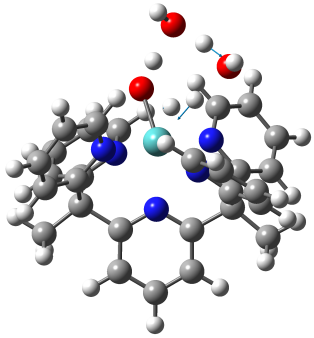

Fig. 28 Vibrational modes of transition state including two water molecules.

4.1.4 Water–assisted MHR process: Three water molecules.

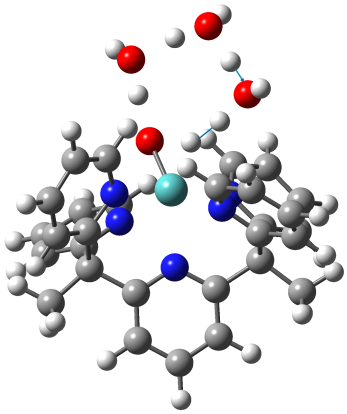

Fig. 29 Vibrational modes of transition state including three water molecules.

4.2 Intramolecular MHR Processes:

4.2.1 Structures with no substituent groups: hydrogen atoms at all positions

Reactant complex: $[PY_5Me_2Mo(H)(OH)]^+$

Mo 0.033395 0.012739 -0.928595
O -0.586456 0.875254 -2.699347
N -1.629182 -1.350706 -0.887302
N 1.531880 -1.541446 -0.410573
N 1.710886 1.340187 -0.826023
N -1.569852 1.511330 -0.398558
C -2.514711 -1.364729 0.164229
N 0.034491 -0.024593 1.302217
C -2.473705 -0.187563 1.185543
C -2.599087 1.163070 0.426117
C 2.573648 -1.266500 0.430602
C -2.784423 -3.251820 -1.878718
H -2.870646 -3.942955 -2.721486
C -3.478871 -2.386451 0.262555
H -4.147710 -2.437104 1.121031
C 2.653391 1.262414 0.176149
C 3.737192 0.146355 2.169784
H 3.708478 -0.693622 2.879318
H 3.728326 1.082079 2.747531
H 4.692526 0.099058 1.627349
C -3.703894 2.019513 0.595427
H -4.538063 1.732740 1.235137
C -3.663144 -0.333100 2.164406
H -3.724060 0.526245 2.847274
H -3.566587 -1.244638 2.772852
H -4.613955 -0.390719 1.615050
C 3.696637 2.205461 0.253774
H 4.428389 2.151061 1.059142
C 1.222798 0.229888 3.385716
H 2.154329 0.377556 3.928919
C -1.166594 -0.049850 3.393250
H -2.100697 -0.140518 3.944240
C 1.212962 0.118637 1.986290
C 1.489287 -2.771456 -1.008514
H 0.630915 -2.951741 -1.655468
C 2.545250 0.086393 1.186225
C -1.147546 -0.109185 1.990191
C -3.743728 3.256927 -0.062168
H -4.600546 3.923399 0.073740
C 3.610367 -2.203553 0.619313
H 4.453450 -1.968118 1.267643
C 1.863665 2.328579 -1.773491
H 1.111526 2.307520 -2.566870
C 0.024777 0.136088 4.097547
C 3.820785 3.226910 -0.697234
H 4.632315 3.956085 -0.623838
C 2.882977 3.272532 -1.744003
H 2.934027 4.029464 -2.531926
C 2.466986 -3.745454 -0.832911
H 2.363349 -4.707902 -1.340557
C -1.611884 2.716075 -1.029744
H -0.768219 2.934880 -1.683948
C -2.665519 3.618786 -0.882361
H -2.632363 4.579661 -1.402639
C 3.568756 -3.450422 -0.014181
H 4.373330 -4.175279 0.138925
C -3.613394 -3.348704 -0.749425
H -4.363513 -4.139569 -0.660683
C -1.811739 -2.256004 -1.902094
H -1.124346 -2.147350 -2.744699
H -0.176634 0.440682 -3.467679
H 0.708395 -0.803618 -2.253249
H 0.020502 0.200921 5.189342

Transition state: $[PY_5Me_2MoO\cdots H\cdots H]^{+\ \ddagger}$

Mo 0.00408900 -0.01817500 -0.99276400
O -0.55872600 0.80570900 -2.61222300
N -1.67672100 -1.37440600 -0.91602000
N 1.50283300 -1.58253900 -0.39348100
N 1.70051300 1.30153400 -0.88679200
N -1.54244900 1.52102400 -0.32273800
C -2.55969100 -1.38327000 0.13873900
N -0.01781800 -0.03072700 1.24891500
C -2.52300600 -0.20274700 1.15410200
C -2.62271200 1.15590100 0.41347700
C 2.56388000 -1.27729600 0.40808000
C -2.79747800 -3.32642900 -1.85530700
H -2.87107400 -4.03898800 -2.68125900
C -3.50554500 -2.41809800 0.26232100
H -4.17312000 -2.45704300 1.12232800
C 2.61446500 1.25132200 0.13856000
C 3.69521100 0.15580600 2.14344700
H 3.68557900 -0.69485600 2.84040100
H 3.66420200 1.08335100 2.73345400
H 4.65216400 0.13703800 1.60201400
C -3.74268100 2.00454700 0.51790100
H -4.62736500 1.69523100 1.07445200
C -3.71782600 -0.33176600 2.12818700
H -3.77239700 0.53665500 2.80081300
H -3.63651300 -1.23799900 2.74622300
H -4.66606700 -0.38671600 1.57380600
C 3.63250500 2.21985800 0.23699200
H 4.34131300 2.19196300 1.06374600
C 1.17677700 0.15500400 3.34178800
H 2.11067900 0.28269400 3.88555100
C -1.20854400 -0.12790800 3.35216600
H -2.14248300 -0.23761000 3.90017300
C 1.16575100 0.09292600 1.93989200
C 1.45879200 -2.81174000 -0.98583900
H 0.57345100 -3.02063700 -1.58844700
C 2.50865600 0.07915100 1.15429600
C -1.19413600 -0.14273800 1.94923600
C -3.72341600 3.26288200 -0.09844400
H -4.58809500 3.92792300 -0.01527500
C 3.62788500 -2.18641500 0.56306900
H 4.48814500 -1.93056900 1.18082700
C 1.85681600 2.27818000 -1.84251600

H 1.12438000 2.22956600 -2.65358600
C -0.01633100 0.03951400 4.05922000
C 3.75975200 3.23303700 -0.72231400
H 4.55163300 3.98188300 -0.63339900
C 2.85569700 3.24466800 -1.79727600
H 2.91496100 3.99190200 -2.59370000
C 2.46855900 -3.76136000 -0.84833800
H 2.36900500 -4.73044000 -1.34374900
C -1.52337400 2.74310300 -0.91388400
H -0.63368300 2.97130600 -1.50219600
C -2.57811800 3.65087300 -0.81041300
H -2.50015800 4.63108300 -1.28795000
C 3.59118600 -3.43476800 -0.07216200
H 4.41806600 -4.13987500 0.05154700
C -3.62574600 -3.40836700 -0.72502800
H -4.36477300 -4.20711000 -0.61710400
C -1.84611800 -2.31118600 -1.90593700
H -1.17041000 -2.21568400 -2.75938500
H 0.28030100 -0.26777600 -2.83633100
H 0.79675900 -0.95832300 -2.48446200
H -0.01498100 0.07306100 5.15224300

Product complex: $[PY_5Me_2MoO)]^+ + H_2$
Mo -0.08201200 -0.05118100 -0.87352100
O -0.13120500 -0.07469200 -2.62785800
N -1.71567900 -1.43460700 -0.58072400
N 1.51355500 -1.49100100 -0.63856300
N 1.56303400 1.33928600 -0.70732900
N -1.66275300 1.39694400 -0.59138700
C -2.62404700 -1.27431500 0.43887200
N -0.02316700 -0.02101600 1.38566200
C -2.52429700 0.00472400 1.32205300
C -2.58966000 1.26927100 0.41605600
C 2.49279700 -1.33497700 0.31400600
C -2.87311700 -3.44571400 -1.30509400
H -2.94660000 -4.25697600 -2.03409400
C -3.62413300 -2.24272300 0.64603800
H -4.32745200 -2.14040000 1.47140900
C 2.52139000 1.20828500 0.26993800
C 3.71134500 -0.04527800 2.11299700
H 3.71379100 -0.92407000 2.77396900
H 3.72632700 0.84915300 2.75232000
H 4.63967200 -0.05861000 1.52266400
C -3.57315900 2.26009700 0.59428700
H -4.29317300 2.18137000 1.40782300
C -3.71443600 0.02934100 2.30899400
H -3.68054400 0.92386000 2.94765800
H -3.69885700 -0.84925700 2.97003900
H -4.67208000 0.03205200 1.76728600
C 3.52666300 2.18445200 0.40183100
H 4.26973800 2.10672800 1.19458100
C 1.23734800 -0.00815000 3.45169300
H 2.19401000 -0.01047300 3.97236700
C -1.17190300 0.01580800 3.51559700
H -2.09937500 0.03139800 4.08638500
C 1.18162600 -0.02400800 2.05230000
C 1.58808000 -2.56157000 -1.48952700
H 0.82634600 -2.59913500 -2.26935700
C 2.47118800 -0.04774100 1.18966100
C -1.19075500 -0.00095600 2.11526300
C -3.66296400 3.35179200 -0.28149900
H -4.43554500 4.11187700 -0.13592200
C 3.48845500 -2.31824900 0.46435000
H 4.25091100 -2.21662200 1.23562700
C 1.67895300 2.36413400 -1.60891300
H 0.94140900 2.36853900 -2.41332600
C 0.05175400 0.01201600 4.19854200
C 3.60866600 3.25968900 -0.49508100
H 4.39709300 4.00934200 -0.38461900
C 2.67764400 3.33117300 -1.54305900
H 2.71343900 4.12180700 -2.29714500
C 2.57411700 -3.54002000 -1.40338900
H 2.57659800 -4.36714100 -2.11808000
C -1.78058100 2.44517200 -1.46484600
H -1.06155300 2.45945300 -2.28485300
C -2.75816000 3.42932300 -1.35146700
H -2.79724100 4.23753500 -2.08643300
C 3.53516100 -3.43220700 -0.38636100
H 4.31747300 -4.18625200 -0.26302200
C -3.75243800 -3.34170000 -0.21604000
H -4.53645300 -4.08508700 -0.04723700
C -1.87699200 -2.48412500 -1.44602900
H -1.17928600 -2.51376100 -2.28455400
H 3.15446400 -0.32087100 -6.59762900
H 3.89251900 -0.24118400 -6.48163000
H 0.08087000 0.02476100 5.29147700

4.2.2 Structures with substituent groups at axial position only

Reactant complex: $[PY_4(p{-}\mathbf{NH_2}PY)Me_2Mo(H)(OH)]^+$
Mo 0.03052400 -0.00861300 -1.07895000
O -0.55933300 0.87851600 -2.85734000
N -1.63923600 -1.36323200 -1.01997700
N 1.55233700 -1.53722500 -0.57128600
N 1.70570900 1.32582200 -0.98271300
N -1.56251600 1.50612800 -0.55083800
C -2.53441100 -1.36117800 0.02528500
N 0.02645700 -0.04325500 1.14482800
C -2.48131300 -0.18300800 1.04271100
C -2.58996900 1.16825200 0.28026300
C 2.58193800 -1.25780600 0.28726600
C -2.80355500 -3.27071100 -1.99587100
H -2.88656600 -3.97172000 -2.83092400
C -3.51014900 -2.37170000 0.12536500
H -4.18736000 -2.40408200 0.97816100
C 2.63768500 1.26399800 0.03133900
C 3.72781100 0.16715900 2.02864800
H 3.71240500 -0.67413500 2.73660500
H 3.70467500 1.10155100 2.60844100
H 4.68360900 0.13451500 1.48582400
C -3.68546700 2.03714000 0.45095600

H -4.52050300 1.76072000 1.09389900
C -3.67558600 -0.31041800 2.01802300
H -3.72279000 0.54841600 2.70273500
H -3.59608100 -1.22481300 2.62445500
H -4.62640400 -0.35156300 1.46699200
C 3.67221400 2.21723400 0.11059000
H 4.39444600 2.17796000 0.92535300
C 1.21811300 0.18793600 3.23481800
H 2.15320900 0.32466300 3.77579800
C -1.17902200 -0.09224800 3.23826600
H -2.11720300 -0.18062600 3.78387900
C 1.19833300 0.10154800 1.84468600
C 1.53127700 -2.77037800 -1.16904500
H 0.68279900 -2.95893500 -1.82661700
C 2.53544400 0.09185100 1.04663900
C -1.15019500 -0.12933300 1.84596400
C -3.71481500 3.27479500 -0.20670000
H -4.56395400 3.95034900 -0.06688400
C 3.62400700 -2.18725200 0.48719400
H 4.45597100 -1.94502200 1.14737300
C 1.86385400 2.30478300 -1.93944700
H 1.11982200 2.26691300 -2.74020600
C 0.01661200 0.08185800 3.97602900
C 3.79860700 3.23172700 -0.84742200
H 4.60104800 3.97051800 -0.76911200
C 2.87427500 3.25801300 -1.90705800
H 2.92852000 4.00761500 -2.70185800
C 2.51405300 -3.73590000 -0.98131000
H 2.42374100 -4.69885700 -1.49082700
C -1.59473200 2.70963500 -1.18355700
H -0.75233800 2.91639000 -1.84355600
C -2.63697900 3.62507100 -1.03200700
H -2.59599300 4.58504200 -1.55346200
C 3.60378200 -3.43350800 -0.14771000
H 4.41264300 -4.15140700 0.01529100
C -3.64603300 -3.34594600 -0.87471200
H -4.40554700 -4.12754100 -0.78382000
C -1.82366200 -2.28272800 -2.02421300
H -1.13011000 -2.19144900 -2.86332600
H -0.19776100 0.39786100 -3.62245100
H 0.60417600 -0.89703600 -2.40497500
N 0.01059500 0.13357600 5.33515300
H 0.86385300 0.30735600 5.85963600
H -0.86098700 0.10257200 5.85742100

Transition state: $[PY_4(p\text{–}\mathbf{NH_2}PY)Me_2MoO\cdots H\cdots H]^{+\ \ddagger}$
Mo 0.00233600 -0.01963700 -0.99747500
O -0.53259100 0.81779100 -2.62568600
N -1.67299000 -1.36785900 -0.91142100
N 1.50422500 -1.58185700 -0.39387100
N 1.70071700 1.30010000 -0.88714000
N -1.54922600 1.51873400 -0.34025500
C -2.55917000 -1.37565800 0.14373900
N -0.01733900 -0.02415900 1.24095400
C -2.51969700 -0.19600300 1.15986600
C -2.62003300 1.16002000 0.41430000
C 2.56132500 -1.27357100 0.41252300
C -2.79815200 -3.32182400 -1.84837800
H -2.87155200 -4.03519700 -2.67386000
C -3.50769700 -2.40779400 0.26545500
H -4.17691100 -2.44325400 1.12444100
C 2.61404100 1.25277000 0.13980000
C 3.69530800 0.16127500 2.14472900
H 3.68745800 -0.68877600 2.84235500
H 3.66471300 1.08937300 2.73400600
H 4.65158400 0.14305900 1.60195900
C -3.73724100 2.01216200 0.52700600
H -4.61507800 1.70802900 1.09706300
C -3.71575700 -0.32388600 2.13227300
H -3.77054500 0.54417500 2.80525900
H -3.63480200 -1.23045500 2.74997600
H -4.66396000 -0.37846400 1.57767500
C 3.63199900 2.22176700 0.23732600
H 4.33994900 2.19503800 1.06490800
C 1.18202600 0.16407000 3.33471100
H 2.12062600 0.27960300 3.87411500
C -1.21150300 -0.11561300 3.34605400
H -2.14852400 -0.21759200 3.89145100
C 1.15999300 0.10211000 1.94325500
C 1.46431300 -2.81245400 -0.98338000
H 0.58028500 -3.02364600 -1.58768700
C 2.50625500 0.08386900 1.15868100
C -1.18697700 -0.13554200 1.95354500
C -3.72492100 3.26688700 -0.09635100
H -4.58700300 3.93422000 -0.00431100
C 3.62696000 -2.18099900 0.56983800
H 4.48545900 -1.92320900 1.18921100
C 1.85880000 2.27683400 -1.84328700
H 1.12657800 2.22431800 -2.65466300
C -0.01533200 0.05493400 4.08152300
C 3.75971400 3.23518200 -0.72185700
H 4.55027100 3.98539900 -0.63192300
C 2.85597700 3.24492300 -1.79747300
H 2.91467500 3.99200600 -2.59425200
C 2.47460700 -3.76094400 -0.84149900
H 2.37748000 -4.73153200 -1.33459100
C -1.53893900 2.73620500 -0.94147300
H -0.65904200 2.95484200 -1.54800700
C -2.58936900 3.64751800 -0.82816100
H -2.51649300 4.62412300 -1.31399600
C 3.59463800 -3.43073100 -0.06305000
H 4.42240400 -4.13413400 0.06482200
C -3.62824100 -3.40220400 -0.71852300
H -4.36736400 -4.20058900 -0.60894100
C -1.84759900 -2.30666500 -1.90177500
H -1.17452700 -2.21176900 -2.75727500
H 0.29436300 -0.28563100 -2.84035200
H 0.78645800 -0.98368400 -2.49240400
N -0.01385600 0.09249400 5.44155400
H 0.84141800 0.26598900 5.96278800
H -0.88271000 0.05644100 5.96792900

Product complex: $[PY_4(p-\mathbf{NH_2}PY)Me_2MoO]^+ + H_2$

Mo -0.07192500 -0.03115000 -1.02523800
O -0.10742600 -0.04366900 -2.79128700
N -1.72956900 -1.37871400 -0.79094100
N 1.48551400 -1.49897800 -0.71462100
N 1.59454800 1.31865600 -0.87811800
N -1.61741000 1.44036100 -0.67469600
C -2.61114200 -1.26765700 0.26231900
N -0.02620300 -0.01453800 1.25118500
C -2.52125900 -0.00461000 1.17348900
C -2.58424900 1.27172000 0.28680200
C 2.48892300 -1.31751600 0.20618600
C -2.86984400 -3.39835700 -1.53083000
H -2.95400300 -4.18926500 -2.28134200
C -3.57831200 -2.26559500 0.47818300
H -4.25452500 -2.20200000 1.33007300
C 2.51934100 1.22113900 0.13883200
C 3.70069300 -0.01809900 2.00075400
H 3.71035300 -0.90242200 2.65470000
H 3.70503800 0.87183000 2.64634700
H 4.63120500 -0.01526800 1.41375500
C -3.60394800 2.23056000 0.43189300
H -4.36086000 2.11556000 1.20672600
C -3.72062100 -0.00072100 2.14942800
H -3.70930400 0.89530900 2.78717300
H -3.69547400 -0.87863300 2.81097200
H -4.67340900 -0.01787000 1.59952700
C 3.49738900 2.21904200 0.29842800
H 4.20895400 2.16622200 1.12188700
C 1.22413500 0.00805400 3.32146200
H 2.17941600 0.00991600 3.84583200
C -1.19229300 0.01594000 3.37000900
H -2.12587500 0.02558500 3.93190200
C 1.16636100 -0.00666700 1.92915900
C 1.54283600 -2.58294600 -1.54882900
H 0.74195500 -2.65801600 -2.28468800
C 2.46367100 -0.02655600 1.07337700
C -1.19053600 -0.00643100 1.97657500
C -3.67979900 3.33679000 -0.42671700
H -4.48042900 4.07211000 -0.30735000
C 3.51128500 -2.27686300 0.32745200
H 4.29756300 -2.15211000 1.07093900
C 1.73591000 2.33236200 -1.79369800
H 1.04109800 2.29703900 -2.63609200
C 0.03074400 0.02331800 4.08387700
C 3.59245500 3.29019700 -0.60527700
H 4.35560200 4.06119600 -0.46797300
C 2.70705200 3.32393900 -1.69544200
H 2.76102700 4.10352000 -2.46045200
C 2.55238500 -3.53991000 -1.48973900
H 2.53960100 -4.38019000 -2.18865100
C -1.70976500 2.51076600 -1.52318500
H -0.93825300 2.57566500 -2.29072700
C -2.71884100 3.46645800 -1.44047100
H -2.73516500 4.29550600 -2.15258900
C 3.55178500 -3.39673500 -0.51576500
H 4.35485700 -4.13223300 -0.41535800
C -3.70813700 -3.35056800 -0.40454900
H -4.46219900 -4.12147600 -0.22352300
C -1.90669300 -2.40610200 -1.68481400
H -1.24849100 -2.38144600 -2.55649800
H 2.93087800 -0.42658200 -6.96563200
H 3.66733200 -0.52143500 -6.85095700
N 0.05848800 0.00604700 5.45258400
H 0.93121300 0.19547100 5.94033800
H -0.79292700 0.19783400 5.97573400

Reactant complex: $[PY_4(p-\mathbf{CH_3}PY)Me_2Mo(H)(OH)]^+$

Mo 0.03248100 0.00093900 -1.07297700
O -0.57706700 0.87391900 -2.84418900
N -1.63506400 -1.35662000 -1.02548900
N 1.53530100 -1.54696000 -0.55622300
N 1.71139900 1.32737600 -0.96972100
N -1.56428400 1.50792700 -0.53996100
C -2.52388900 -1.36438700 0.02391900
N 0.02963700 -0.03814800 1.15666100
C -2.47643000 -0.18802600 1.04523300
C -2.59388500 1.16381600 0.28593400
C 2.57242500 -1.27285600 0.29230300
C -2.79661800 -3.25714600 -2.01298300
H -2.88295900 -3.95091600 -2.85361500
C -3.49375600 -2.38065400 0.12223800
H -4.16548800 -2.42453200 0.97885100
C 2.64890700 1.25321900 0.03782600
C 3.73022500 0.14132700 2.03428200
H 3.70288900 -0.69878700 2.74359600
H 3.71801500 1.07674300 2.61252500
H 4.68632600 0.09650200 1.49292700
C -3.69439500 2.02578900 0.45605500
H -4.52944600 1.74319200 1.09642100
C -3.66718200 -0.32616800 2.02344400
H -3.72135800 0.53239200 2.70789500
H -3.57781300 -1.23941600 2.63034800
H -4.61835900 -0.37585200 1.47387200
C 3.69076500 2.19782000 0.11755600
H 4.41820800 2.14697800 0.92704800
C 1.21115400 0.20899300 3.24365700
H 2.14623700 0.35545000 3.78321200
C -1.16507200 -0.06958100 3.25011200
H -2.10360700 -0.15987000 3.79523700
C 1.20436500 0.10484300 1.84734700
C 1.49833100 -2.77770200 -1.15485000
H 0.64346000 -2.95905300 -1.80611000
C 2.53933400 0.07870300 1.04968800
C -1.14766400 -0.12156100 1.84790800
C -3.72875700 3.26380200 -0.20079100
H -4.58212400 3.93441700 -0.06339700
C 3.60886500 -2.20943300 0.48581000
H 4.44759800 -1.97369300 1.13969100
C 1.86881900 2.31265700 -1.91983700
H 1.12042200 2.28757500 -2.71675400
C 0.01825900 0.11255600 3.97959900

C 3.81853200 3.21705800 -0.83532800
H 4.62809900 3.94814500 -0.75895500
C 2.88664400 3.25809400 -1.88763900
H 2.94097800 4.01278900 -2.67751700
C 2.47603200 -3.75049100 -0.97481000
H 2.37590900 -4.71257100 -1.48394300
C -1.60101400 2.71272600 -1.17077000
H -0.75694900 2.92704000 -1.82606100
C -2.64982300 3.62095000 -1.02192000
H -2.61249700 4.58188200 -1.54182300
C 3.57314000 -3.45552000 -0.14928200
H 4.37763300 -4.17962000 0.00775500
C -3.63053700 -3.34583500 -0.88657800
H -4.38538100 -4.13218000 -0.79777200
C -1.81956200 -2.26583100 -2.03724100
H -1.12950600 -2.16399100 -2.87836700
H -0.18465800 0.42356500 -3.61249600
H 0.67369400 -0.84024700 -2.39896900
C 0.02085900 0.19509500 5.48509500
H 0.61544200 -0.62807800 5.91899100
H 0.48397000 1.13854200 5.82299900
H -0.99899600 0.13974100 5.89513800

Transition state: $[PY_4(p\text{–}\mathbf{CH_3}PY)Me_2MoO\cdots H\cdots H]^{+\,\ddagger}$
Mo 0.00323100 -0.01783800 -1.00524000
O -0.54971100 0.80958800 -2.62795400
N -1.67815800 -1.36891600 -0.92328200
N 1.49867400 -1.58379400 -0.40053000
N 1.70315500 1.29832000 -0.89677500
N -1.54245400 1.52374500 -0.33919200
C -2.56054300 -1.37571500 0.13295500
N -0.01943400 -0.02654400 1.23592400
C -2.52160700 -0.19418900 1.14715000
C -2.62024800 1.16282000 0.40316200
C 2.55806000 -1.27944800 0.40388300
C -2.80220500 -3.32233100 -1.85763200
H -2.87734900 -4.03610800 -2.68245100
C -3.50703900 -2.40952600 0.25896400
H -4.17366100 -2.44623200 1.11985400
C 2.61601900 1.24776200 0.12984900
C 3.69180900 0.15342100 2.13783600
H 3.67856100 -0.69530700 2.83710000
H 3.66348200 1.08253600 2.72549000
H 4.64916700 0.13022000 1.59722400
C -3.73828900 2.01396500 0.50935800
H -4.62110300 1.70794700 1.07068600
C -3.71633700 -0.32029100 2.12156800
H -3.76994500 0.54917000 2.79288200
H -3.63539700 -1.22543100 2.74126100
H -4.66482100 -0.37541600 1.56754800
C 3.63626200 2.21408900 0.22785000
H 4.34424500 2.18544700 1.05530400
C 1.16900700 0.16689300 3.32989200
H 2.10686900 0.29490200 3.86888700
C -1.20342300 -0.11250600 3.34194700
H -2.14138700 -0.21784700 3.88559600
C 1.16060200 0.09840400 1.93180200
C 1.45398800 -2.81367000 -0.99138600
H 0.56952700 -3.02159300 -1.59576400
C 2.50552800 0.07837300 1.14832700
C -1.19063400 -0.13422900 1.93987500
C -3.71977100 3.27033100 -0.11092200
H -4.58280300 3.93726900 -0.02570300
C 3.61987300 -2.19070500 0.56227100
H 4.47909300 -1.93600900 1.18193700
C 1.86261800 2.27408500 -1.85306600
H 1.13058400 2.22559200 -2.66460700
C -0.01929800 0.05780800 4.07176800
C 3.76660900 3.22625900 -0.73216700
H 4.55986200 3.97366500 -0.64312000
C 2.86316800 3.23882600 -1.80772400
H 2.92431600 3.98544800 -2.60462300
C 2.46149100 -3.76519200 -0.85038000
H 2.36128800 -4.73471100 -1.34484000
C -1.52467900 2.74355000 -0.93516300
H -0.63770000 2.96713400 -1.52935300
C -2.57710800 3.65372300 -0.82971900
H -2.49958600 4.63211700 -1.31108100
C 3.58261300 -3.43980000 -0.07155300
H 4.40779900 -4.14633700 0.05539300
C -3.62921800 -3.40213000 -0.72602800
H -4.36836400 -4.20039100 -0.61549000
C -1.85081700 -2.30750300 -1.91181500
H -1.17704400 -2.21344700 -2.76695200
H 0.28464500 -0.27355200 -2.84798200
H 0.79324000 -0.96670700 -2.49611200
C -0.00941900 0.11425800 5.57831900
H 0.61355900 -0.69605600 5.99621500
H 0.42479900 1.06672500 5.92985500
H -1.02475300 0.02079200 5.99291400

Product complex: $[PY_4(p\text{–}\mathbf{CH_3}PY)Me_2MoO]^+ + H_2$
Mo -0.07658800 -0.04494600 -1.02048900
O -0.11638400 -0.06792600 -2.77687200
N -1.71345300 -1.42329900 -0.73624600
N 1.51203000 -1.48842800 -0.76905500
N 1.57040400 1.34015100 -0.84669100
N -1.65196400 1.40688900 -0.73764500
C -2.62181200 -1.26617100 0.28473100
N -0.02861700 -0.01377100 1.24091200
C -2.52559200 0.01236900 1.16957000
C -2.58426700 1.27866400 0.26537900
C 2.48753800 -1.33200200 0.18774900
C -2.86715500 -3.43687300 -1.46132900
H -2.94007900 -4.24715600 -2.19155600
C -3.61840000 -2.23791400 0.49231200
H -4.32110000 -2.13823400 1.31858600
C 2.51983700 1.21193000 0.14029700
C 3.70017600 -0.04131700 1.99006900
H 3.69963900 -0.92009500 2.65107600
H 3.71257700 0.85286800 2.62978800
H 4.63099000 -0.05465600 1.40357700

C -3.56596300 2.27151600 0.44144700
H -4.29040300 2.19197700 1.25100500
C -3.72052700 0.03722000 2.15051100
H -3.68937900 0.93150100 2.78965200
H -3.70837500 -0.84122500 2.81179200
H -4.67550100 0.04008900 1.60400500
C 3.52159200 2.19027300 0.28093600
H 4.25714400 2.11472600 1.08090000
C 1.21610100 -0.00319300 3.31420400
H 2.17390100 -0.00839300 3.83501300
C -1.17999000 0.02163800 3.36759100
H -2.11365000 0.03514000 3.93002700
C 1.16887500 -0.01772400 1.91706400
C 1.58773100 -2.56210800 -1.61636100
H 0.82869000 -2.60079200 -2.39869300
C 2.46403500 -0.04338700 1.06151100
C -1.19434600 0.00597700 1.96747900
C -3.64891400 3.36629300 -0.43141700
H -4.42055400 4.12765000 -0.28748900
C 3.48059500 -2.31673200 0.34450200
H 4.24024000 -2.21430200 1.11844800
C 1.69442400 2.36389400 -1.74902600
H 0.96600300 2.36419700 -2.56190100
C 0.03298200 0.01824800 4.07816400
C 3.61036800 3.26539200 -0.61597900
H 4.39582200 4.01701200 -0.49799500
C 2.69002300 3.33342800 -1.67367400
H 2.73211800 4.12310600 -2.42851000
C 2.57122200 -3.54247500 -1.52307100
H 2.57446800 -4.37201600 -2.23498000
C -1.76260000 2.45873700 -1.60816800
H -1.03909200 2.47406800 -2.42422100
C -2.73806900 3.44509500 -1.49628800
H -2.77110300 4.25594900 -2.22867400
C 3.52878600 -3.43340500 -0.50287700
H 4.30921700 -4.18852000 -0.37427100
C -3.74482500 -3.33701100 -0.37031000
H -4.52626200 -4.08293100 -0.20075000
C -1.87433800 -2.47212300 -1.60326300
H -1.17916000 -2.49706400 -2.44426500
H 3.05105500 -0.39992300 -6.83932700
H 3.78664600 -0.49646800 -6.72054500
C 0.07377600 0.05169100 5.58589500
H 0.77033600 -0.70684100 5.98269300
H 0.42912800 1.03471800 5.94598400
H -0.92247200 -0.12726800 6.01988000

Reactant complex: $[PY_4(p-\mathbf{F}PY)Me_2Mo(H)(OH)]^+$
Mo 0.03334000 0.01141100 -0.93147300
O -0.57860300 0.88082500 -2.69953300
N -1.63121200 -1.35001800 -0.88588700
N 1.53583200 -1.53864500 -0.41731300
N 1.71220100 1.33813000 -0.82661200
N -1.56956200 1.51279700 -0.39806500
C -2.51569900 -1.36452100 0.16656900
N 0.03364800 -0.02821000 1.30178500
C -2.47591200 -0.18602700 1.18623000
C -2.59908500 1.16524000 0.42620300
C 2.57438500 -1.26679100 0.42962100
C -2.78656100 -3.25392500 -1.87255200
H -2.87338600 -3.94607100 -2.71441000
C -3.47853000 -2.38692800 0.26851100
H -4.14565500 -2.43725300 1.12832200
C 2.65223700 1.26230400 0.17791700
C 3.73516600 0.14593700 2.17318500
H 3.70775600 -0.69575000 2.88079300
H 3.72388100 1.08135400 2.75158800
H 4.69138800 0.10131900 1.63253600
C -3.70446500 2.02083800 0.59457900
H -4.53892800 1.73463000 1.23410200
C -3.66334600 -0.33009500 2.16737200
H -3.72456500 0.53128900 2.84779000
H -3.56579600 -1.24090200 2.77683700
H -4.61482500 -0.38921800 1.61976300
C 3.69450000 2.20621200 0.25842200
H 4.42383700 2.15348200 1.06603800
C 1.23345600 0.22358200 3.38272600
H 2.15238600 0.36368100 3.94816600
C -1.17956200 -0.04700900 3.38966500
H -2.10159700 -0.12612500 3.96159400
C 1.21217300 0.11462300 1.98494600
C 1.49761200 -2.76779100 -1.01862600
H 0.64221400 -2.94751200 -1.66956100
C 2.54559400 0.08525200 1.18709900
C -1.14886100 -0.10905300 1.98838500
C -3.74421300 3.25760000 -0.06428500
H -4.60143400 3.92372900 0.07049800
C 3.61047700 -2.20373700 0.62127900
H 4.44990300 -1.97001300 1.27489800
C 1.86693700 2.32609300 -1.77429400
H 1.11667400 2.30396800 -2.56937300
C 0.02363500 0.13292400 4.06169000
C 3.82017500 3.22695100 -0.69284500
H 4.63042300 3.95728600 -0.61728200
C 2.88529100 3.27088200 -1.74233800
H 2.93776200 4.02754600 -2.53039000
C 2.47528700 -3.74120600 -0.84140500
H 2.37442200 -4.70217300 -1.35238900
C -1.61139600 2.71703100 -1.02982400
H -0.76732600 2.93559200 -1.68362300
C -2.66551700 3.61948200 -0.88363200
H -2.63232200 4.58013700 -1.40424700
C 3.57313700 -3.44844700 -0.01638900
H 4.37732100 -4.17327800 0.13849800
C -3.61378400 -3.35050800 -0.74194000
H -4.36301600 -4.14190800 -0.65104700
C -1.81494800 -2.25726500 -1.89908100
H -1.12920900 -2.14961800 -2.74301900
H -0.18051800 0.44074000 -3.47088000
H 0.68620200 -0.81846100 -2.25685900
F 0.01849800 0.21460400 5.41593300

Transition state: $[PY_4(p{-}\mathbf{F}PY)Me_2MoO\cdots H\cdots H]^{+\,\ddagger}$

Mo 0.00377200 -0.01721400 -0.99587200
O -0.55258600 0.81104300 -2.61477400
N -1.67717500 -1.37119100 -0.91677500
N 1.50191700 -1.58318800 -0.39477000
N 1.70257400 1.30032700 -0.88557100
N -1.54454600 1.52203400 -0.32438600
C -2.55741100 -1.38304200 0.14059000
N -0.01706600 -0.03037300 1.24896300
C -2.52344300 -0.20130400 1.15504500
C -2.62379800 1.15733300 0.41345700
C 2.56291900 -1.27988300 0.40748300
C -2.79708600 -3.32550000 -1.85281400
H -2.87196200 -4.03771200 -2.67894000
C -3.50004300 -2.42009000 0.26763900
H -4.16445000 -2.46116300 1.12998800
C 2.61509300 1.25034000 0.14096900
C 3.69481400 0.15142000 2.14631500
H 3.68536000 -0.70140600 2.84072800
H 3.66295400 1.07824100 2.73758000
H 4.65246800 0.13443700 1.60651000
C -3.74520800 2.00373000 0.51779000
H -4.62872000 1.69432000 1.07611000
C -3.71577900 -0.33134000 2.13165000
H -3.77272200 0.53921300 2.80142600
H -3.63100200 -1.23628200 2.75125600
H -4.66462300 -0.39050200 1.57916500
C 3.63238100 2.21916200 0.24290400
H 4.33957700 2.19114400 1.07100600
C 1.18932300 0.15273900 3.33874500
H 2.11090500 0.27010900 3.90468100
C -1.22021500 -0.11816800 3.34924800
H -2.14213500 -0.21585600 3.91862500
C 1.16675800 0.09130600 1.93852200
C 1.45814200 -2.81151100 -0.98887300
H 0.57283000 -3.01966300 -1.59180500
C 2.51025500 0.07647000 1.15498800
C -1.19397200 -0.13855700 1.94779000
C -3.72874400 3.26054900 -0.10175700
H -4.59442900 3.92428400 -0.01914000
C 3.62705700 -2.18868000 0.56162500
H 4.48700100 -1.93412800 1.18030000
C 1.86023200 2.27813400 -1.83992400
H 1.12904200 2.23015200 -2.65213000
C -0.01603200 0.04397100 4.02290800
C 3.76076200 3.23306900 -0.71532000
H 4.55191400 3.98237200 -0.62420400
C 2.85853600 3.24503500 -1.79181500
H 2.91877800 3.99309700 -2.58736400
C 2.46816000 -3.76110400 -0.85284600
H 2.36871700 -4.72942200 -1.34972300
C -1.52852600 2.74273500 -0.91847700
H -0.63998200 2.97086900 -1.50856500
C -2.58491400 3.64869700 -0.81594600
H -2.50922000 4.62792600 -1.29580300
C 3.59066400 -3.43577900 -0.07608700
H 4.41758500 -4.14095800 0.04658600
C -3.62105800 -3.41043300 -0.71953000
H -4.35734900 -4.21129300 -0.60911400
C -1.84850700 -2.30794400 -1.90674000
H -1.17629900 -2.21054200 -2.76268000
H 0.28181300 -0.26643800 -2.83800000
H 0.79363400 -0.95968900 -2.48455800
F -0.01416600 0.08910000 5.37969800

Product complex: $[PY_4(p{-}\mathbf{F}PY)Me_2MoO]^+ + H_2$

Mo -0.08358600 -0.04996500 -0.87974000
O -0.13146300 -0.07276000 -2.63354800
N -1.71890100 -1.42991800 -0.58816400
N 1.50847200 -1.49215400 -0.63572400
N 1.56332000 1.33750400 -0.71358800
N -1.66052000 1.39934800 -0.58721300
C -2.62189500 -1.27605200 0.43752200
N -0.02272800 -0.02082100 1.38504400
C -2.52435900 0.00269800 1.32234700
C -2.58838200 1.26971100 0.41925400
C 2.49025900 -1.33490200 0.31406300
C -2.87620400 -3.44152500 -1.31188100
H -2.95299800 -4.24991700 -2.04373000
C -3.61690500 -2.24833200 0.64920600
H -4.31475800 -2.15130600 1.47983200
C 2.51881500 1.21097100 0.26733000
C 3.71083100 -0.04229600 2.11170600
H 3.71423100 -0.92194500 2.77167700
H 3.72503600 0.85236000 2.75082100
H 4.63945400 -0.05424500 1.52219700
C -3.57246600 2.25923600 0.59942700
H -4.29306300 2.17840400 1.41220900
C -3.71213200 0.02509900 2.31189900
H -3.67931500 0.92017300 2.95001900
H -3.69442700 -0.85401600 2.97234600
H -4.67061500 0.02600100 1.77209000
C 3.52001700 2.19038500 0.40332600
H 4.26004200 2.11601500 1.19923300
C 1.24997500 -0.00695600 3.44681400
H 2.19396100 -0.00786200 3.98899300
C -1.18152300 0.01507900 3.51269600
H -2.09469100 0.02989400 4.10505700
C 1.18256000 -0.02261800 2.04846900
C 1.57938000 -2.56624800 -1.48266400
H 0.81433400 -2.60745100 -2.25888800
C 2.47189300 -0.04566700 1.18713100
C -1.19019700 -0.00217900 2.11278100
C -3.66227100 3.35266900 -0.27419900
H -4.43558900 4.11177700 -0.12778000
C 3.48598300 -2.31766700 0.46491500
H 4.25051000 -2.21433000 1.23387800
C 1.68038400 2.36182900 -1.61597100
H 0.94683200 2.36228600 -2.42412500
C 0.05273100 0.01196500 4.15931900
C 3.60219000 3.26520600 -0.49421900
H 4.38750200 4.01763200 -0.38093200

C 2.67554100 3.33218100 -1.54642600
H 2.71225600 4.12198200 -2.30134600
C 2.56540300 -3.54466600 -1.39623900
H 2.56483700 -4.37443900 -2.10781300
C -1.77766800 2.45026600 -1.45775800
H -1.05730900 2.46802300 -2.27645000
C -2.75604500 3.43337400 -1.34270600
H -2.79449000 4.24359500 -2.07545500
C 3.53014300 -3.43378600 -0.38310500
H 4.31285400 -4.18742000 -0.26016000
C -3.74754500 -3.34497400 -0.21565000
H -4.52754100 -4.09175100 -0.04354300
C -1.88415800 -2.47641900 -1.45685600
H -1.19351500 -2.49945800 -2.30158800
H 3.18185400 -0.33594000 -6.59766400
H 3.91932300 -0.25548200 -6.47851500
F 0.08999000 0.02810700 5.52169300

Reactant complex: $[PY_4(p-\mathbf{CF_3}PY)Me_2Mo(H)(OH)]^+$
Mo 0.03820900 0.02463300 -1.57003800
O -0.60279300 0.83469700 -3.35359000
N -1.61453800 -1.35624000 -1.56063800
N 1.50138400 -1.58017700 -1.06171600
N 1.72000900 1.34943100 -1.43125700
N -1.60795200 1.48000300 -1.07499300
C -2.47838700 -1.39602000 -0.49469300
N 0.04990400 -0.01955300 0.62523500
C -2.46138100 -0.21653400 0.52897600
C -2.62355500 1.12569900 -0.23481300
C 2.55741200 -1.32107500 -0.23776500
C -2.74938000 -3.25530400 -2.56664800
H -2.84122100 -3.93323800 -3.41921800
C -3.41858000 -2.44007800 -0.39462700
H -4.06929400 -2.52147400 0.47524100
C 2.67953800 1.22905500 -0.45353400
C 3.75826400 0.05054500 1.50753700
H 3.70913800 -0.79481300 2.20989700
H 3.77701300 0.98157600 2.09227800
H 4.71066100 -0.01504000 0.96175400
C -3.73691400 1.96810400 -0.05257500
H -4.55677300 1.67268000 0.60180900
C -3.64299100 -0.39531400 1.51141500
H -3.73778800 0.46768400 2.18554300
H -3.51216600 -1.29725100 2.12803800
H -4.59163800 -0.48950600 0.96343300
C 3.73162500 2.16068400 -0.36274700
H 4.48183200 2.06945800 0.42205500
C 1.24450200 0.24699300 2.71093300
H 2.18039000 0.37705800 3.25049500
C -1.15820600 0.03449700 2.71835400
H -2.09544200 -0.02229200 3.26761800
C 1.23280900 0.10024500 1.31968400
C 1.42444600 -2.80030500 -1.66615700
H 0.55956100 -2.95632300 -2.31084400
C 2.56369200 0.02933200 0.52632700
C -1.13586900 -0.08298300 1.32347400
C -3.80488200 3.19859600 -0.71948900
H -4.66928400 3.85379700 -0.57765500
C 3.57816400 -2.27842500 -0.06561700
H 4.43713700 -2.06192800 0.56807200
C 1.85446800 2.37017500 -2.34328700
H 1.08889800 2.38475300 -3.12330400
C 0.03837500 0.21796000 3.42112700
C 3.84320000 3.21217400 -1.28178200
H 4.66588400 3.92834800 -1.20528300
C 2.88225800 3.30521900 -2.30327100
H 2.92269700 4.08979400 -3.06399800
C 2.38374300 -3.79675400 -1.50439400
H 2.25697500 -4.75471600 -2.01485900
C -1.67881300 2.68003500 -1.71553100
H -0.85034600 2.90647200 -2.38567400
C -2.74383600 3.56701100 -1.55979700
H -2.73301900 4.52242100 -2.09090600
C 3.49955300 -3.52344400 -0.70015600
H 4.29256800 -4.26369500 -0.56070600
C -3.55000600 -3.38721700 -1.42126900
H -4.28021000 -4.19635400 -1.33051800
C -1.79557500 -2.24021700 -2.58949000
H -1.12620200 -2.09971200 -3.44261000
H -0.10580200 0.48680000 -4.11446100
H 0.90793700 -0.63051600 -2.86684300
C 0.03782200 0.30005300 4.92789800
F 1.06408600 1.06876500 5.40407800
F 0.18008700 -0.94161100 5.50705000
F -1.12508800 0.82518900 5.41937600

Transition state: $[PY_4(p-\mathbf{CF_3}PY)Me_2MoO\cdots H\cdots H]^{+\ \ddagger}$
Mo 0.00708100 -0.01524700 -0.99456900
O -0.58035900 0.78455600 -2.60832800
N -1.67958300 -1.38131500 -0.91298100
N 1.51265600 -1.57630300 -0.40063100
N 1.70156400 1.30631300 -0.89602800
N -1.54513000 1.52938400 -0.33406200
C -2.55886700 -1.38130700 0.14166800
N -0.01750100 -0.02359500 1.22582800
C -2.52729400 -0.18944200 1.14438300
C -2.62941600 1.16442900 0.39509500
C 2.57224600 -1.27189500 0.40242900
C -2.79452100 -3.33963100 -1.83758000
H -2.86801600 -4.05867900 -2.65762300
C -3.50128200 -2.41862500 0.27594200
H -4.16705700 -2.45450800 1.13732700
C 2.61505500 1.25820700 0.12875900
C 3.69906000 0.16783600 2.13496200
H 3.69269900 -0.68200500 2.83295100
H 3.66614700 1.09690600 2.72254800
H 4.65586100 0.15012600 1.59345200
C -3.75141500 2.01089300 0.49068300
H -4.63953200 1.70164300 1.04174800
C -3.72154900 -0.31344000 2.11959800
H -3.78108600 0.56233800 2.78223100
H -3.63819000 -1.21330000 2.74659700

H -4.66888400 -0.37721700 1.56481700
C 3.63043700 2.22958600 0.22552300
H 4.33952900 2.20548800 1.05202100
C 1.18163500 0.15967200 3.32149400
H 2.11635900 0.28391800 3.86357000
C -1.21438200 -0.09152300 3.33176200
H -2.15089500 -0.18367200 3.87765100
C 1.16884900 0.09427800 1.92416700
C 1.46692700 -2.80661300 -0.99005200
H 0.58446900 -3.01476400 -1.59649900
C 2.51402200 0.08544600 1.14493800
C -1.19704400 -0.12018500 1.93354300
C -3.72944400 3.26750100 -0.12927600
H -4.59607500 3.93093500 -0.05480700
C 3.63286700 -2.18341800 0.56510900
H 4.49160400 -1.92802600 1.18513200
C 1.85473800 2.27936700 -1.85477100
H 1.12388600 2.23049200 -2.66671700
C -0.01738800 0.06849600 4.03915500
C 3.75548200 3.23955800 -0.73704800
H 4.54641600 3.98958800 -0.65053800
C 2.85265300 3.24710700 -1.81246800
H 2.91140200 3.99164300 -2.61121900
C 2.47364900 -3.75843200 -0.84598200
H 2.37345200 -4.72805100 -1.34001800
C -1.52225700 2.75026900 -0.92645400
H -0.62799500 2.98150600 -1.50655400
C -2.57958900 3.65641000 -0.83272200
H -2.49981600 4.63578300 -1.31150300
C 3.59434500 -3.43305000 -0.06682100
H 4.41883500 -4.14013000 0.06109600
C -3.62038500 -3.41338700 -0.70589400
H -4.35849700 -4.21221900 -0.59218000
C -1.84276600 -2.32440500 -1.89408100
H -1.16424300 -2.23597300 -2.74610600
H 0.26362200 -0.25935600 -2.83967100
H 0.80266100 -0.94223400 -2.47856600
C -0.01198500 0.07676000 5.54697300
F 1.02598200 0.80602200 6.05831400
F 0.11313000 -1.19441300 6.06414800
F -1.16687200 0.59253300 6.06808000

Product complex: $[PY_4(p-\mathbf{CF_3}PY)Me_2MoO]^+ + H_2$
Mo -0.07426600 -0.04976500 -1.53074000
O -0.11252900 -0.08126300 -3.27690300
N -1.71536200 -1.43380800 -1.24252200
N 1.52759400 -1.48790900 -1.28137400
N 1.57456600 1.34381100 -1.35970200
N -1.66379000 1.39911200 -1.26448000
C -2.63235500 -1.26692800 -0.23412200
N -0.02934900 -0.01245000 0.71231300
C -2.53446500 0.01295500 0.64782400
C -2.59762800 1.27235100 -0.26541500
C 2.50278400 -1.32423900 -0.32815700
C -2.87859200 -3.43429700 -1.98182600
H -2.94910700 -4.24512700 -2.71134800
C -3.64331900 -2.22697600 -0.03898400
H -4.35462700 -2.12032900 0.77881400
C 2.52833100 1.21491500 -0.38008000
C 3.70382700 -0.02848300 1.47902100
H 3.70407700 -0.90622600 2.14144500
H 3.71301700 0.86845700 2.11504200
H 4.63658200 -0.04155000 0.89606500
C -3.58974300 2.25766300 -0.10293800
H -4.31621200 2.18065300 0.70487900
C -3.72846800 0.04101300 1.62986100
H -3.69767300 0.93806400 2.26518900
H -3.71728200 -0.83656200 2.29242100
H -4.68369000 0.04281500 1.08429400
C 3.53970000 2.18595300 -0.25349700
H 4.27979800 2.11117100 0.54216900
C 1.22327400 0.00550000 2.78769900
H 2.17673200 0.00741200 3.31255600
C -1.19571300 0.02792400 2.83694600
H -2.12680600 0.04632400 3.40040200
C 1.17332600 -0.01281800 1.39371000
C 1.60769100 -2.55902500 -2.12899300
H 0.84413200 -2.60673100 -2.90629400
C 2.47113100 -0.03596900 0.54579200
C -1.20309400 0.00882700 1.44230100
C -3.67752100 3.34168800 -0.98726700
H -4.45611200 4.09790800 -0.85422200
C 3.50651000 -2.29937400 -0.17610600
H 4.26697800 -2.19206800 0.59618500
C 1.69601600 2.36025700 -2.26800500
H 0.95753200 2.36651200 -3.07133100
C 0.02872100 0.03071300 3.53013900
C 3.62955900 3.25175800 -1.15956400
H 4.42206400 3.99775000 -1.05372500
C 2.70145200 3.32097000 -2.20960600
H 2.74288700 4.10553700 -2.96947600
C 2.60143100 -3.52988000 -2.04237600
H 2.60910000 -4.35875000 -2.75477100
C -1.77717500 2.44086000 -2.14425500
H -1.04760300 2.45806500 -2.95466700
C -2.76285100 3.41900000 -2.04815900
H -2.79898700 4.22276000 -2.78792300
C 3.56137600 -3.41265500 -1.02607500
H 4.34905900 -4.16089000 -0.90166500
C -3.76971600 -3.32294900 -0.90382900
H -4.56140100 -4.06035200 -0.74494200
C -1.87220100 -2.48128300 -2.10897900
H -1.16231100 -2.51986700 -2.93666200
H 3.14662100 -0.66077000 -7.33861200
H 3.84511600 -0.69299100 -7.06352300
C 0.05676400 -0.00860000 5.02970200
F 1.19108900 0.55722200 5.55016100
F 0.01712300 -1.30138300 5.52276300
F -1.01272900 0.63910900 5.59250000

Reactant complex: $[PY_4(p-\mathbf{CN}PY)Me_2Mo(H)(OH)]^+$
Mo 0.03933200 0.04730500 -0.89754100

O -0.61163800 0.80204500 -2.70321800
N -1.61392200 -1.34166400 -0.89304500
N 1.49217300 -1.57334700 -0.40247800
N 1.72164100 1.38282100 -0.75243200
N -1.62818000 1.48878300 -0.44281500
C -2.47172700 -1.37828500 0.17565200
N 0.05684900 0.01681400 1.26807100
C -2.45953900 -0.18983800 1.18914600
C -2.63379800 1.14290500 0.41266800
C 2.55437900 -1.31585500 0.41386600
C -2.73845500 -3.24759300 -1.88994000
H -2.83009800 -3.92917100 -2.73943300
C -3.40703800 -2.42628900 0.28148800
H -4.05602000 -2.50772500 1.15253500
C 2.69100700 1.24373200 0.20900300
C 3.77274200 0.04597700 2.15380200
H 3.71838700 -0.79891500 2.85618100
H 3.80136800 0.97637400 2.73895600
H 4.72259300 -0.02705600 1.60428500
C -3.74540300 1.98692300 0.59850500
H -4.55711400 1.69807300 1.26580600
C -3.63830200 -0.36984700 2.17444200
H -3.73904600 0.49739700 2.84191000
H -3.49865700 -1.26537800 2.79832000
H -4.58705500 -0.47491800 1.62841400
C 3.74763500 2.17064700 0.29687700
H 4.51080700 2.06572400 1.06724700
C 1.26139700 0.28208400 3.35527400
H 2.19873300 0.39577700 3.89584000
C -1.15492100 0.10485400 3.36427300
H -2.09024300 0.05825600 3.91757300
C 1.24472400 0.12282000 1.97065500
C 1.40103400 -2.79328900 -1.00144700
H 0.53466300 -2.94358900 -1.64544800
C 2.57423800 0.03543600 1.17737100
C -1.13200300 -0.03443500 1.97736600
C -3.82257000 3.20886700 -0.08244600
H -4.68617200 3.86471000 0.06117500
C 3.56735800 -2.28185000 0.58460100
H 4.43297200 -2.06972100 1.21057100
C 1.84027100 2.41288700 -1.65178500
H 1.06606700 2.43803000 -2.42276800
C 0.05005500 0.28083800 4.07934200
C 3.84644600 3.23350400 -0.61039000
H 4.67372100 3.94493300 -0.53857500
C 2.87096600 3.34593900 -1.61487100
H 2.90296100 4.14103100 -2.36471200
C 2.35123800 -3.79874300 -0.83819700
H 2.21418400 -4.75767200 -1.34397200
C -1.70913900 2.67950000 -1.09916600
H -0.89182400 2.89684700 -1.78547500
C -2.77338800 3.56702200 -0.94157800
H -2.77185900 4.51395300 -1.48763700
C 3.47308400 -3.52984800 -0.04185600
H 4.26127400 -4.27551900 0.09610100
C -3.53433600 -3.37754900 -0.74180200
H -4.26074300 -4.18963000 -0.64650400
C -1.79039900 -2.22653500 -1.91884900
H -1.12704600 -2.08171900 -2.77613800
H -0.08259300 0.48795100 -3.45729800
H 1.00472300 -0.51492800 -2.16272600
C 0.04436600 0.42297000 5.49930600
N 0.03865700 0.54762000 6.67322600

Transition state: $[PY_4(p-\mathbf{CN}PY)Me_2MoO\cdots H\cdots H]^{+\ \ddagger}$
Mo 0.00891700 -0.01641900 -0.98557900
O -0.59207700 0.77246300 -2.59211100
N -1.68027100 -1.39111700 -0.90448200
N 1.52137600 -1.57661000 -0.40186500
N 1.70250900 1.30774000 -0.88839400
N -1.54736400 1.52926300 -0.32887100
C -2.56331700 -1.38433300 0.14477000
N -0.01681200 -0.02920200 1.22024400
C -2.53067500 -0.19183700 1.14597100
C -2.63275800 1.16226900 0.39717000
C 2.58014900 -1.27265000 0.40161400
C -2.79724100 -3.34246800 -1.83577600
H -2.86917700 -4.06196300 -2.65537000
C -3.51257900 -2.41676200 0.27338300
H -4.18391200 -2.44942900 1.13042300
C 2.61742900 1.25744300 0.13394100
C 3.70488000 0.16534600 2.13582500
H 3.70080000 -0.68562600 2.83228100
H 3.67037600 1.09325400 2.72505600
H 4.66103100 0.15029000 1.59303000
C -3.75424400 2.00930600 0.49324900
H -4.64363500 1.69918500 1.04168000
C -3.72546000 -0.31518400 2.12063700
H -3.78333500 0.55986200 2.78422100
H -3.64363400 -1.21599100 2.74640800
H -4.67279200 -0.37624000 1.56552800
C 3.63250900 2.22928400 0.22932400
H 4.34345100 2.20453100 1.05410000
C 1.18840500 0.14867100 3.31727500
H 2.12257100 0.26677700 3.86136600
C -1.21926800 -0.09689900 3.32710000
H -2.15373900 -0.19279200 3.87538300
C 1.17234000 0.08582800 1.92474400
C 1.47431600 -2.80625800 -0.99144800
H 0.59322900 -3.01336000 -1.59980700
C 2.51907200 0.08214400 1.14694400
C -1.19891800 -0.12262500 1.93381400
C -3.73009500 3.26779900 -0.12281400
H -4.59663600 3.93131900 -0.04829200
C 3.64027300 -2.18485500 0.56436900
H 4.49904000 -1.92983900 1.18442500
C 1.85252500 2.28038700 -1.84715000
H 1.12166600 2.23399800 -2.65883300
C -0.01600900 0.05642800 4.04845300
C 3.75476000 3.23979700 -0.73274500
H 4.54572600 3.98989400 -0.64741400
C 2.85060600 3.24817400 -1.80650000

H 2.90779300 3.99285200 -2.60506500
C 2.47974400 -3.75933500 -0.84605300
H 2.37899200 -4.72871200 -1.34031500
C -1.52187200 2.75188500 -0.91669300
H -0.62605500 2.98614000 -1.49320000
C -2.57882000 3.65858700 -0.82241700
H -2.49750600 4.63932600 -1.29803000
C 3.60026600 -3.43452500 -0.06686800
H 4.42408400 -4.14233100 0.06130400
C -3.63063900 -3.40945800 -0.70984100
H -4.37460700 -4.20361300 -0.60120700
C -1.83829100 -2.33330600 -1.88482300
H -1.15193800 -2.25026700 -2.73105600
H 0.25125000 -0.24883800 -2.83323100
H 0.80491900 -0.92996000 -2.46636900
C -0.01565500 0.10880100 5.47394400
N -0.01555500 0.15163700 6.65388900

Product complex: $[PY_4(p-\mathbf{CN}PY)Me_2MoO]^+ + H_2$
Mo -0.08171700 -0.05068700 -0.85902400
O -0.13087400 -0.07455300 -2.59881500
N -1.72399100 -1.43643200 -0.56295700
N 1.52414700 -1.49110400 -0.62402200
N 1.57216800 1.34226900 -0.69058800
N -1.67263600 1.39796500 -0.57546300
C -2.63620800 -1.27088000 0.44856500
N -0.02294800 -0.02100000 1.37968900
C -2.53097700 0.00418200 1.33583200
C -2.60249700 1.26457000 0.42500200
C 2.50630600 -1.32969900 0.32091700
C -2.89771900 -3.42665800 -1.31090100
H -2.97337900 -4.23319000 -2.04451000
C -3.65181800 -2.22693800 0.64058200
H -4.36013500 -2.12190000 1.46107500
C 2.53427900 1.20558000 0.27825800
C 3.71786100 -0.04414300 2.12733900
H 3.72019700 -0.92394300 2.78693400
H 3.73261900 0.85109000 2.76554200
H 4.64698100 -0.05737300 1.53872600
C -3.60068900 2.24352500 0.59009100
H -4.32506200 2.16145200 1.39916200
C -3.71915400 0.02871600 2.32509700
H -3.68496400 0.92410900 2.96247800
H -3.70322600 -0.85087200 2.98478800
H -4.67768700 0.03145000 1.78547200
C 3.55448300 2.16891500 0.39438700
H 4.30257600 2.08812000 1.18183400
C 1.24850300 -0.00796100 3.44603000
H 2.20391600 -0.00960400 3.96708700
C -1.18165100 0.01473700 3.51099400
H -2.10746100 0.02948700 4.08280600
C 1.18535900 -0.02366400 2.05721400
C 1.59906800 -2.55600700 -1.47878400
H 0.82738900 -2.60372600 -2.24786800
C 2.47919900 -0.04658600 1.20199200
C -1.19319500 -0.00122800 2.12082900
C -3.69546700 3.32796800 -0.29244800
H -4.47785200 4.07981900 -0.15689400
C 3.51586500 -2.30148100 0.45661400
H 4.28282500 -2.19669600 1.22272200
C 1.68892200 2.35916400 -1.59786700
H 0.94056700 2.37412600 -2.39169200
C 0.05303700 0.01146400 4.21012500
C 3.64112200 3.23487400 -0.51119600
H 4.43974400 3.97539100 -0.41313700
C 2.70185400 3.31274800 -1.55011400
H 2.73940000 4.09862600 -2.30869100
C 2.59775700 -3.52331400 -1.40881700
H 2.60147300 -4.34763600 -2.12636600
C -1.79161700 2.44039200 -1.45249100
H -1.06233100 2.46516000 -2.26280200
C -2.78287900 3.41284000 -1.35400700
H -2.82381900 4.21809700 -2.09175200
C 3.56658100 -3.40841500 -0.40125700
H 4.35807700 -4.15455300 -0.28900100
C -3.78526800 -3.31677200 -0.23030000
H -4.57982100 -4.05153000 -0.07347300
C -1.88667700 -2.47793700 -1.43433000
H -1.17807700 -2.51744100 -2.26285400
H 3.15045200 -0.32374700 -6.56968400
H 3.88863900 -0.24441000 -6.45423800
C 0.09073600 0.02750900 5.63126900
N 0.12203700 0.04086000 6.81387500

4.2.3 Structures with substituent groups at equatorial position only

Reactant complex: $[(p-\mathbf{NH_2}PY)_4PYMe_2Mo(H)(OH)]^+$
Mo 0.02475500 0.07027900 -0.91472400
O -0.61824400 0.95356600 -2.69036700
N -1.63934200 -1.30430500 -0.89245800
N 1.47667500 -1.53960600 -0.38338300
N 1.73300300 1.37742400 -0.77822100
N -1.60164300 1.53343000 -0.38198900
C -2.48455500 -1.35262900 0.19014500
N 0.04913600 0.03562300 1.28682500
C -2.46696600 -0.16304500 1.20512100
C -2.63579500 1.17511500 0.43536700
C 2.55091400 -1.29103100 0.42334100
C -2.74701700 -3.26344600 -1.82909600
H -2.83508500 -3.96264300 -2.66581900
C -3.39428700 -2.40779400 0.33923800
H -4.03051600 -2.47725300 1.22179000
C 2.70004400 1.25423900 0.19187600
C 3.76185100 0.07979500 2.16695500
H 3.70006100 -0.75846400 2.87677000
H 3.78980200 1.01526200 2.74438100
H 4.71541000 -0.00177300 1.62481200
C -3.75509400 1.99861300 0.61186600
H -4.57932700 1.68825000 1.25525500
C -3.64026600 -0.33732100 2.19894200
H -3.73567400 0.53488100 2.86097600

H -3.49704100 -1.22715400 2.83046500
H -4.59249200 -0.44883400 1.65987100
C 3.76535900 2.16507300 0.28080300
H 4.52107200 2.05698300 1.05942700
C 1.24882100 0.31920400 3.36924500
H 2.18792200 0.44277800 3.90617100
C -1.14776100 0.12634000 3.38799400
H -2.08324800 0.08009500 3.94291800
C 1.23668000 0.15539500 1.97695100
C 1.40532600 -2.76738900 -0.97718600
H 0.52944500 -2.93629800 -1.60418300
C 2.56969300 0.06361500 1.18278500
C -1.13480900 -0.01689000 1.99256200
C -3.84101200 3.25393600 -0.04031700
C 3.56904700 -2.23799700 0.59354500
H 4.42848200 -2.02030400 1.22783300
C 1.88082100 2.40816300 -1.67651700
H 1.10660700 2.44548500 -2.44868200
C 0.04883500 0.30988200 4.08861300
C 3.90004200 3.23439500 -0.63310200
C 2.91259200 3.33160500 -1.64655100
H 2.95111900 4.12088000 -2.40387000
C 2.35899900 -3.76172900 -0.83647400
H 2.22244600 -4.71905500 -1.34742800
C -1.67914800 2.74823800 -0.99770500
H -0.84225700 2.99597600 -1.65080700
C -2.74195400 3.62830600 -0.85561800
H -2.72097600 4.59226200 -1.37275300
C 3.50568600 -3.50438200 -0.04117200
C -3.53545800 -3.40721000 -0.65843000
C -1.82996600 -2.22519100 -1.88751600
H -1.18496100 -2.09491900 -2.76135700
H -0.12932200 0.56680000 -3.43739900
H 0.82798400 -0.63528900 -2.24738900
N -4.91396900 4.09093700 0.15692800
H -5.05483200 4.86516200 -0.48881500
H -5.76562200 3.71056700 0.56521600
N 4.98315200 4.09854000 -0.58501700
H 5.48608900 4.16605800 0.29914100
H 4.88125100 4.99427800 -1.06061700
N 4.51472800 -4.42053900 0.08682600
H 4.36458000 -5.37968800 -0.21736500
H 5.23615100 -4.28441500 0.79124700
N -4.44649200 -4.42652200 -0.52142200
H -4.38232000 -5.22935200 -1.14369500
H -4.83786000 -4.62007800 0.39826500
H 0.04847200 0.41883100 5.17679200

Transition state: $[(p\text{–}\mathbf{NH_2}\text{PY})_4\text{PYMe}_2\text{MoO}\cdots\text{H}\cdots\text{H}]^{+\ \ddagger}$
Mo -0.00359400 0.00276200 -1.00088200
O -0.56864000 0.83134400 -2.63008100
N -1.69565500 -1.35079600 -0.92130100
N 1.47963300 -1.57283900 -0.40747200
N 1.71560600 1.31248900 -0.88291400
N -1.53337700 1.53311400 -0.31926700
C -2.56383000 -1.36649200 0.14554700
N -0.00926400 -0.02002000 1.23020100
C -2.52232600 -0.17894400 1.15669500
C -2.62521400 1.17644300 0.40817400
C 2.56298400 -1.28858300 0.37509800
C -2.81049200 -3.32937900 -1.82139400
H -2.88698300 -4.05092000 -2.64008200
C -3.49428800 -2.40183400 0.30145100
H -4.15232300 -2.43253400 1.17007800
C 2.63884700 1.24670000 0.13118700
C 3.71334200 0.11844400 2.12474900
H 3.69330000 -0.73677200 2.81608300
H 3.69514600 1.04234000 2.72124900
H 4.66990300 0.09179200 1.58258100
C -3.74542100 2.01045600 0.51332000
H -4.62489100 1.69744300 1.07767500
C -3.70898000 -0.30473400 2.14115100
H -3.76336600 0.57000000 2.80546300
H -3.61857200 -1.20399000 2.76850200
H -4.66118800 -0.36968300 1.59437800
C 3.66469100 2.19813800 0.24328500
H 4.38238700 2.14509100 1.06219500
C 1.19687100 0.15830700 3.32263000
H 2.13580300 0.26965300 3.86179400
C -1.19385200 -0.06980400 3.34435300
H -2.12797100 -0.15535200 3.89689100
C 1.18163600 0.08813300 1.92206900
C 1.43004700 -2.80582600 -0.99466600
H 0.53412200 -3.01686900 -1.58117500
C 2.52610600 0.06296000 1.13537100
C -1.18641500 -0.10890400 1.94265800
C -3.75362400 3.28433700 -0.11032800
C 3.61838600 -2.19514200 0.51941000
H 4.48221600 -1.94682200 1.13670300
C 1.87802600 2.30897100 -1.81412000
H 1.13810100 2.28819100 -2.62053800
C 0.00411700 0.07952200 4.04916300
C 3.80815200 3.24322600 -0.69897900
C 2.87868100 3.26614900 -1.76908700
H 2.93493600 4.02585800 -2.55494000
C 2.42668200 -3.76151800 -0.88531000
H 2.30851500 -4.72749400 -1.38436100
C -1.53180500 2.76043700 -0.90669600
H -0.64213400 3.00204400 -1.49008700
C -2.58315500 3.66151200 -0.81958300
H -2.50415100 4.63942500 -1.30357900
C 3.58663900 -3.46004700 -0.12381200
C -3.63149700 -3.42691600 -0.66963900
C -1.87964400 -2.30450500 -1.89002200
H -1.22043900 -2.21649400 -2.75807500
H 0.28067800 -0.23567200 -2.85308100
H 0.80688700 -0.92605400 -2.51828800
N -4.82513900 4.13371100 0.01522900
H -4.89293800 4.93682100 -0.60639000
H -5.71365000 3.76482800 0.34800000
N 4.84731400 4.15219200 -0.61733900
H 5.31225600 4.25964500 0.28307500

H 4.75058600 5.02338900 -1.13673600
N 4.63237200 -4.33721600 -0.02747400
H 4.51488300 -5.29814900 -0.34030700
H 5.36939600 -4.17701800 0.65537800
N -4.56863700 -4.42390900 -0.52903300
H -4.49511900 -5.24829000 -1.12182400
H -4.97359000 -4.59035800 0.39029800
H 0.01034500 0.12454700 5.14177800

Product complex: $[(p\text{−}\mathbf{NH_2}\text{PY})_4\text{PYMe}_2\text{MoO}]^+ + \text{H}_2$
Mo -0.09076000 -0.05473900 -1.00173700
O -0.14047600 -0.08334900 -2.76247100
N -1.72408200 -1.44726900 -0.69376100
N 1.52092700 -1.48648700 -0.76680600
N 1.55623400 1.34492300 -0.83130600
N -1.68823600 1.38581100 -0.72438400
C -2.65031000 -1.28045800 0.30929800
N -0.03111600 -0.01815800 1.23385700
C -2.54640300 0.00093900 1.19020600
C -2.62712200 1.25768500 0.27274900
C 2.51053600 -1.32723500 0.17535200
C -2.88616700 -3.46731700 -1.40605400
H -2.94892900 -4.28776500 -2.12671100
C -3.66116500 -2.22754600 0.51657200
H -4.37640600 -2.10341400 1.32967500
C 2.53360800 1.21084100 0.12733500
C 3.70907900 -0.03426100 1.98909900
H 3.70592500 -0.91093300 2.65318200
H 3.71827400 0.86347000 2.62428200
H 4.64329500 -0.05001400 1.40827800
C -3.62683100 2.22317500 0.44477900
H -4.35310800 2.12924200 1.25223100
C -3.72537900 0.02599700 2.19009600
H -3.68752900 0.92396300 2.82398300
H -3.70007700 -0.85054600 2.85388200
H -4.68940700 0.02368200 1.65998300
C 3.55279400 2.16370100 0.24984600
H 4.30926100 2.06807600 1.02898600
C 1.23106700 0.00609000 3.30594700
H 2.18794900 0.00745800 3.82672800
C -1.17872000 0.02655900 3.37121000
H -2.10568700 0.04315700 3.94329600
C 1.17914100 -0.01636100 1.90849300
C 1.61128300 -2.56741500 -1.60319400
H 0.84739100 -2.62501000 -2.38068300
C 2.47794500 -0.04090800 1.05410000
C -1.20298800 0.00317300 1.97299000
C -3.74226200 3.33306300 -0.42951800
C 3.51779000 -2.28835900 0.32668400
H 4.28529500 -2.16952200 1.09159100
C 1.67580700 2.38349200 -1.71635700
H 0.92481500 2.41315900 -2.50828400
C 0.04577400 0.02818500 4.05936200
C 3.64950700 3.26238500 -0.64050400
C 2.67948000 3.33714600 -1.67248600
H 2.70518900 4.13162200 -2.42400900
C 2.60075300 -3.53383300 -1.52879500
H 2.60266400 -4.36310400 -2.24213000
C -1.82262100 2.43996100 -1.58846500
H -1.09879300 2.47335200 -2.40459100
C -2.80865400 3.40821900 -1.49455500
H -2.84809700 4.21441700 -2.23280400
C 3.58715600 -3.42668700 -0.51528100
C -3.80246000 -3.35637600 -0.32916100
C -1.88757500 -2.51610100 -1.53451900
H -1.17792800 -2.57428000 -2.36198200
H 3.76844500 -0.38582500 -6.79414800
H 3.67046500 0.35495700 -6.71575600
N -4.69360000 4.30565000 -0.22994300
H -4.90632200 4.94383100 -0.99423600
H -5.47417900 4.10664800 0.39295200
N 4.54612400 -4.39487200 -0.33239000
H 4.71834900 -5.05948900 -1.08416900
H 5.35649700 -4.17933700 0.24525100
N 4.62036600 4.22476900 -0.48711700
H 5.42259100 4.01874100 0.10539100
H 4.81409400 4.84867500 -1.26810700
N -4.76244300 -4.31297200 -0.09365100
H -5.53304500 -4.08876000 0.53318100
H -4.99464900 -4.96348100 -0.84187000
H 0.07550300 0.04611200 5.15215300

Reactant complex: $[(p\text{−}\mathbf{CH_3}\text{PY})_4\text{PYMe}_2\text{Mo(H)(OH)}]^+$
Mo 0.03110700 0.01208600 -1.07174600
O -0.58561100 0.88481500 -2.84283700
N -1.63335100 -1.34995800 -1.02830300
N 1.52492600 -1.54508400 -0.55018700
N 1.71480100 1.33299400 -0.95832800
N -1.56975200 1.50732100 -0.53934200
C -2.51995300 -1.36351900 0.02006800
N 0.03185900 -0.02630200 1.15869200
C -2.47865700 -0.18622800 1.04263100
C -2.60114300 1.16454800 0.28260700
C 2.56689200 -1.27927600 0.29070800
C -2.79714200 -3.25113700 -2.00808500
H -2.88250100 -3.94210900 -2.85261900
C -3.48687500 -2.38222700 0.11810900
H -4.15582500 -2.42308400 0.97817600
C 2.65909800 1.25017800 0.03865500
C 3.73486600 0.12700900 2.03455600
H 3.69910100 -0.71220800 2.74479700
H 3.73094800 1.06353000 2.61114100
H 4.69127200 0.07323600 1.49459000
C -3.70290600 2.02339700 0.45415600
H -4.53373000 1.73171000 1.09760100
C -3.66693100 -0.33096300 2.02289700
H -3.72729800 0.52895500 2.70509000
H -3.57007600 -1.24227900 2.63180200
H -4.61839400 -0.38814300 1.47466800
C 3.70780700 2.18777500 0.11678200
H 4.43942600 2.12041500 0.92265500
C 1.21864200 0.23240800 3.24329400

H 2.15021300 0.37885000 3.78683600
C -1.17140100 -0.03920300 3.24950200
H -2.10622100 -0.12566900 3.80001600
C 1.21064500 0.11423000 1.84446500
C 1.48675100 -2.77603300 -1.14710700
H 0.63054300 -2.95814300 -1.79671900
C 2.54545400 0.07345800 1.04782300
C -1.15155200 -0.10582800 1.84662700
C -3.76470100 3.27074200 -0.19393000
C 3.59823400 -2.22107300 0.48068500
H 4.43750000 -1.98457500 1.13507300
C 1.87527500 2.32888600 -1.89633300
H 1.12310300 2.32120500 -2.69023100
C 0.01954400 0.14641000 3.95472000
C 3.85475300 3.22408200 -0.82096400
C 2.89939400 3.26354700 -1.86204300
H 2.94947500 4.02368400 -2.64869300
C 2.46114600 -3.74871900 -0.96964600
H 2.35231000 -4.70977000 -1.48149600
C -1.61795900 2.71623200 -1.16443200
H -0.77590600 2.94123900 -1.81891100
C -2.66977100 3.61513900 -1.01315000
H -2.63137000 4.57737100 -1.53322200
C 3.57610200 -3.47708500 -0.14728000
C -3.64057000 -3.36168500 -0.88165800
C -1.82244900 -2.26124100 -2.03596700
H -1.13750600 -2.16026600 -2.88183100
H -0.16916900 0.44942700 -3.60701200
H 0.71022700 -0.80116300 -2.39978200
C -4.94145300 4.19817200 -0.01623800
H -5.68337100 3.78366700 0.68380100
H -4.61202600 5.18030000 0.36626600
H -5.44248300 4.38298000 -0.98305000
C 4.97127900 4.23532400 -0.72707600
H 4.57056300 5.25518000 -0.58275000
H 5.64895900 4.01307200 0.11248100
H 5.56792000 4.25560200 -1.65654700
C 4.67609500 -4.48900700 0.05426400
H 5.45634100 -4.11098900 0.73291400
H 4.27324300 -5.42716600 0.47540800
H 5.14960600 -4.74848500 -0.90920500
C -4.66044200 -4.46679800 -0.76021400
H -5.34533500 -4.29542100 0.08506800
H -5.25850300 -4.55793800 -1.68343200
H -4.16320500 -5.44143000 -0.60259300
H 0.01433400 0.21557700 5.04629700

Transition state: $[(p\text{–}\mathbf{CH_3}\text{PY})_4\text{PYMe}_2\text{MoO}\cdots\text{H}\cdots\text{H}]^{+\ \ddagger}$

Mo 0.00271400 -0.01646800 -1.00181000
O -0.55854900 0.80521300 -2.62600700
N -1.68039700 -1.37099000 -0.91917000
N 1.49981300 -1.57803500 -0.40100000
N 1.70309200 1.29956000 -0.89090000
N -1.53793600 1.52116200 -0.33428400
C -2.56628700 -1.37497200 0.13094200
N -0.01884900 -0.02798800 1.23875400
C -2.52648800 -0.19271300 1.14531500
C -2.61987300 1.16524400 0.40164600
C 2.56114200 -1.27963100 0.40046900
C -2.81319600 -3.32169800 -1.84465900
H -2.88637800 -4.03564500 -2.67101000
C -3.51862300 -2.40333400 0.25411900
H -4.18913300 -2.42785800 1.11354400
C 2.61780400 1.24909300 0.13073900
C 3.69485100 0.15180400 2.13855000
H 3.68206600 -0.69816800 2.83635400
H 3.66532200 1.08017600 2.72746500
H 4.65268800 0.12996000 1.59877700
C -3.73520700 2.01834200 0.50740000
H -4.61613800 1.70742700 1.07072700
C -3.72034300 -0.31608300 2.12110900
H -3.77034000 0.55315200 2.79306300
H -3.64213100 -1.22235800 2.73963400
H -4.66968400 -0.36714800 1.56827400
C 3.63917800 2.21448400 0.22777100
H 4.34729000 2.17775800 1.05604600
C 1.17537300 0.15682100 3.33295900
H 2.10947700 0.28274100 3.87689500
C -1.21074000 -0.11809600 3.34270600
H -2.14526300 -0.22441100 3.89048200
C 1.16540500 0.09341300 1.93119600
C 1.46240100 -2.81013300 -0.98937400
H 0.57969400 -3.02383400 -1.59442000
C 2.51004900 0.07706400 1.14740500
C -1.19636500 -0.13525800 1.93983700
C -3.73820400 3.28418800 -0.10610600
C 3.62078600 -2.19188300 0.55903800
H 4.47653300 -1.93231900 1.18305100
C 1.86681200 2.27969800 -1.84128000
H 1.13587600 2.23898900 -2.65440700
C -0.01832600 0.04608000 4.05078100
C 3.78784600 3.24066300 -0.72132300
C 2.86859400 3.23917900 -1.79310100
H 2.92718900 3.98601400 -2.59167600
C 2.46972600 -3.75687200 -0.84726900
H 2.36527400 -4.72613400 -1.34405400
C -1.52474400 2.74497000 -0.92449300
H -0.63661300 2.97667400 -1.51401400
C -2.57685200 3.65041700 -0.81928400
H -2.49303800 4.62993300 -1.30017200
C 3.60641900 -3.45052800 -0.06873100
C -3.65874800 -3.41229600 -0.71890600
C -1.85659500 -2.31530800 -1.89978800
H -1.18095700 -2.23153100 -2.75489300
H 0.27973500 -0.27071200 -2.84665600
H 0.79532500 -0.96215400 -2.49739900
C -4.66626900 -4.52490400 -0.56944000
H -4.15946800 -5.48289200 -0.35104500
H -5.37451300 -4.32331800 0.24954600
H -5.23890900 -4.67030700 -1.50161200
C 4.87346300 4.28270100 -0.60632900
H 4.43952800 5.28973400 -0.46927300

H 5.54126000 4.07974800 0.24570900
H 5.48495000 4.32060400 -1.52515900
C -4.92516600 4.21022800 -0.00467400
H -5.71169000 3.79342200 0.64325700
H -4.62285800 5.19218000 0.39934900
H -5.36103900 4.39487700 -1.00265000
C 4.74009900 -4.43156400 0.09295500
H 5.52142000 -4.04271500 0.76397600
H 4.37354500 -5.38967600 0.50161400
H 5.20246400 -4.65678400 -0.88450200
H -0.01732700 0.08087000 5.14369100

Product complex: $[(p\text{-}\mathbf{CH_3}\text{PY})_4\text{PYMe}_2\text{MoO}]^+ + \text{H}_2$
Mo -0.08492100 -0.05290200 -1.01938800
O -0.13432200 -0.08087700 -2.77538600
N -1.71852500 -1.43556900 -0.71359400
N 1.51358100 -1.48940200 -0.78391700
N 1.55963500 1.33829900 -0.84618500
N -1.66796700 1.39474000 -0.74450900
C -2.63543600 -1.26592100 0.29442900
N -0.02819400 -0.01741600 1.23438500
C -2.53292000 0.01586000 1.17357400
C -2.59571200 1.27622300 0.26091500
C 2.49239200 -1.33687500 0.16727200
C -2.88690500 -3.44575400 -1.42207100
H -2.95539200 -4.26225500 -2.14749200
C -3.64451700 -2.22493000 0.49817100
H -4.35383500 -2.10363800 1.31704800
C 2.52280300 1.20501300 0.12370200
C 3.70703700 -0.04895700 1.97220800
H 3.70590200 -0.92732100 2.63384400
H 3.72165100 0.84645900 2.61027900
H 4.63740100 -0.06477700 1.38520200
C -3.57853100 2.26801700 0.43377100
H -4.29707900 2.18640000 1.24959500
C -3.72076800 0.04747200 2.16276900
H -3.68197200 0.94351700 2.79908800
H -3.70772800 -0.83016100 2.82523700
H -4.67958800 0.05320400 1.62324900
C 3.53374800 2.17519900 0.25094800
H 4.27956700 2.08466000 1.04105200
C 1.23088200 -0.00634100 3.30308500
H 2.18716500 -0.01130500 3.82456500
C -1.17836000 0.02547900 3.36518300
H -2.10621800 0.04491400 3.93536100
C 1.17739100 -0.02327700 1.90400800
C 1.59844900 -2.56149900 -1.63187900
H 0.84140200 -2.60371100 -2.41661700
C 2.47018100 -0.05026400 1.04471100
C -1.19744100 0.00758500 1.96523100
C -3.68781300 3.36924900 -0.43624100
C 3.48906800 -2.31854200 0.31683200
H 4.24919100 -2.20951400 1.09073400
C 1.68143400 2.36904700 -1.73985900
H 0.94116300 2.38667200 -2.54180400
C 0.04480900 0.01815900 4.05039200
C 3.63638700 3.26546700 -0.63373300
C 2.68545600 3.32652100 -1.67444500
H 2.71856300 4.11741300 -2.43010300
C 2.58615000 -3.53394700 -1.54302000
H 2.58959600 -4.35790800 -2.26318000
C -1.79253500 2.44204800 -1.61800800
H -1.07682600 2.45710700 -2.44138300
C -2.76986300 3.42260600 -1.50644600
H -2.80736500 4.22516200 -2.24946100
C 3.55875200 -3.44481300 -0.52470700
C -3.79203600 -3.34293800 -0.34444800
C -1.88296300 -2.49653200 -1.56387900
H -1.17780000 -2.54694800 -2.39526700
H 3.22969800 -0.25464900 -6.40080700
H 3.91333600 -0.40054200 -6.67625100
C -4.86855700 -4.37401800 -0.11337400
H -4.42534900 -5.33351900 0.21003700
H -5.58029000 -4.05022600 0.66204000
H -5.42914500 -4.57686200 -1.04225300
C -4.73759800 4.43447900 -0.24006700
H -5.46430400 4.14962200 0.53672200
H -4.27093700 5.38939500 0.06320700
H -5.28465800 4.62896800 -1.17872400
C 4.71318500 4.31097800 -0.48277200
H 4.27899300 5.27032200 -0.14656400
H 5.47345200 4.00679900 0.25358800
H 5.21466100 4.50607400 -1.44627800
C 4.62295800 -4.49972500 -0.35185500
H 5.39377000 -4.18399700 0.36845200
H 4.17929700 -5.44302800 0.01566900
H 5.11331100 -4.72937800 -1.31354300
H 0.07315000 0.03168000 5.14334800

Reactant complex: $[(p\text{-}\mathbf{F}\text{PY})_4\text{PYMe}_2\text{Mo(H)(OH)}]^+$
Mo 0.03226700 0.01308200 -0.92903800
O -0.57645700 0.89121100 -2.69314100
N -1.63447700 -1.34735400 -0.89109700
N 1.53508200 -1.53941600 -0.41164100
N 1.71750900 1.33837200 -0.82407500
N -1.57546800 1.51090200 -0.39765000
C -2.51501800 -1.36210700 0.16435300
N 0.03387300 -0.02494100 1.30345500
C -2.47555500 -0.18872800 1.18916400
C -2.60262800 1.15961100 0.42775700
C 2.57416500 -1.26547900 0.43319600
C -2.78540300 -3.25339200 -1.88964500
H -2.88884800 -3.95481400 -2.72000100
C -3.48013000 -2.38007000 0.27365200
H -4.16007900 -2.45217900 1.12110400
C 2.65785300 1.25613800 0.17846300
C 3.73844600 0.14410100 2.17500000
H 3.70646300 -0.69271200 2.88791500
H 3.73215400 1.08137500 2.75004700
H 4.69382200 0.09174800 1.63283500
C -3.71139200 2.00624400 0.60683800
H -4.55303600 1.74347600 1.24617500

C -3.66532000 -0.33786000 2.16645300
H -3.72802700 0.51946100 2.85135600
H -3.56653900 -1.24957800 2.77408700
H -4.61576300 -0.39596300 1.61630400
C 3.70911800 2.18901800 0.26242300
H 4.45394100 2.15355400 1.05596500
C 1.22106300 0.23843000 3.38726000
H 2.15203300 0.38878300 3.93058700
C -1.16815200 -0.04103300 3.39497400
H -2.10214400 -0.12972500 3.94637500
C 1.21114000 0.12067300 1.98876600
C 1.49773600 -2.76613000 -1.01555400
H 0.64318800 -2.95038400 -1.66565900
C 2.54671800 0.08495200 1.19172400
C -1.14751800 -0.10689500 1.99257200
C -3.72699700 3.22847500 -0.06493200
C 3.61372900 -2.19470200 0.63051800
H 4.46122400 -1.98736100 1.28182000
C 1.87258100 2.32473800 -1.77131700
H 1.12140400 2.30865000 -2.56555300
C 0.02274700 0.14815800 4.09906800
C 3.80717200 3.18981200 -0.70051900
C 2.89132200 3.26936500 -1.75389600
H 2.96357300 4.03353400 -2.53093900
C 2.47108600 -3.74532700 -0.85076000
H 2.39174600 -4.71013000 -1.35533500
C -1.62429800 2.71329100 -1.03220400
H -0.78541600 2.93698700 -1.69026200
C -2.67485600 3.61945900 -0.89393700
H -2.66714500 4.58228700 -1.40859700
C 3.54810600 -3.42294100 -0.02145600
C -3.58998300 -3.32153600 -0.74997000
C -1.81957500 -2.25116800 -1.90550500
H -1.13976400 -2.14227200 -2.75365100
H -0.18019900 0.45560500 -3.46804200
H 0.69585200 -0.80745700 -2.25614400
H 0.01796300 0.21789800 5.19041800
F -4.79214500 4.05632500 0.10565400
F 4.82222700 4.09857000 -0.61313400
F 4.54569800 -4.32642600 0.16882700
F -4.51918200 -4.31059900 -0.63719800

Transition state: $[(p\text{−}\mathbf{F}\text{PY})_4\text{PYMe}_2\text{MoO}\cdots\text{H}\cdots\text{H}]^{+\,\ddagger}$
Mo 0.00444200 -0.01665600 -0.99278600
O -0.55239300 0.81581800 -2.60919200
N -1.68165100 -1.36920300 -0.92043200
N 1.50401400 -1.58426900 -0.39120000
N 1.70687500 1.30160300 -0.88450700
N -1.54853300 1.52052000 -0.32312600
C -2.55953300 -1.37890900 0.13837500
N -0.01694700 -0.02956500 1.24929300
C -2.52370200 -0.20272600 1.15834200
C -2.62612200 1.15371300 0.41559800
C 2.56530500 -1.27742600 0.40931200
C -2.79975400 -3.32385500 -1.86936000
H -2.89144100 -4.04548900 -2.68361800
C -3.50755600 -2.40851900 0.27116800
H -4.18669000 -2.46964200 1.12008500
C 2.61913700 1.24670100 0.14078400
C 3.69873200 0.15320500 2.14626800
H 3.68723200 -0.69525800 2.84558200
H 3.66947500 1.08165600 2.73474000
H 4.65555200 0.13115700 1.60444000
C -3.75106100 1.99149900 0.52936600
H -4.64145000 1.70740200 1.08902100
C -3.71814500 -0.33622000 2.13155200
H -3.77407700 0.52964700 2.80697700
H -3.63424700 -1.24328100 2.74785200
H -4.66639100 -0.39122200 1.57695600
C 3.64382200 2.20590500 0.24655600
H 4.36709500 2.19609100 1.06032700
C 1.17796500 0.15813100 3.34290400
H 2.11180600 0.28524000 3.88681200
C -1.20761600 -0.12061100 3.35393200
H -2.14129700 -0.22828000 3.90268100
C 1.16607000 0.09358500 1.94154900
C 1.46247200 -2.81173500 -0.98552800
H 0.57884800 -3.02606200 -1.58807100
C 2.51176400 0.07741200 1.15813700
C -1.19241300 -0.13962300 1.95146400
C -3.70894700 3.23360200 -0.10342800
C 3.63289900 -2.17766000 0.57119800
H 4.50092900 -1.94768200 1.18736000
C 1.86386600 2.27733900 -1.83895200
H 1.13292900 2.23293500 -2.65156600
C -0.01527000 0.04673200 4.06077700
C 3.74409100 3.20055000 -0.72360100
C 2.86066500 3.24624000 -1.80449900
H 2.93908500 4.00248600 -2.58861000
C 2.46776700 -3.76646200 -0.85920900
H 2.39065000 -4.73925300 -1.34838400
C -1.53853500 2.73832600 -0.92270700
H -0.65385500 2.97161100 -1.51568800
C -2.59064200 3.64864000 -0.82975800
H -2.54111300 4.62862300 -1.30839300
C 3.56917000 -3.41062300 -0.07760900
C -3.60380300 -3.37716000 -0.72941500
C -1.85454500 -2.30265900 -1.91139000
H -1.18650500 -2.20652800 -2.77025100
H 0.28783600 -0.25941000 -2.83496100
H 0.79991300 -0.95195000 -2.48199600
F 4.73271300 4.13310200 -0.61530300
F 4.59539700 -4.28625800 0.07403100
F -4.52055000 -4.37415200 -0.59365100
F -4.78361200 4.05924800 0.00104900
H -0.01384600 0.08274600 5.15343600

Product complex: $[(p\text{−}\mathbf{F}\text{PY})_4\text{PYMe}_2\text{MoO}]^+ + \text{H}_2$
Mo -0.08279800 -0.05421100 -0.87026300
O -0.12961100 -0.08048600 -2.62512000
N -1.72487500 -1.43240600 -0.58648300
N 1.51523900 -1.49567800 -0.63115900

N 1.56761800 1.33509800 -0.71487500
N -1.66412100 1.39639700 -0.58823100
C -2.62884900 -1.27154500 0.43655400
N -0.02172000 -0.02251200 1.38432700
C -2.52516700 0.00196100 1.32628600
C -2.59025100 1.26486900 0.41924000
C 2.49929300 -1.32898500 0.31427800
C -2.88995300 -3.43888400 -1.32694900
H -2.98744900 -4.25315600 -2.04760300
C -3.63499000 -2.22988900 0.65031400
H -4.34879900 -2.14942200 1.46842800
C 2.52211600 1.20801700 0.26616000
C 3.71586800 -0.03644700 2.11294600
H 3.72208500 -0.91525200 2.77369200
H 3.72646800 0.85678000 2.75388700
H 4.64412800 -0.04488200 1.52238000
C -3.57768000 2.24756600 0.60716100
H -4.31011900 2.18799200 1.41052500
C -3.71497500 0.02653900 2.31325200
H -3.67883600 0.91921200 2.95422300
H -3.69976100 -0.85259000 2.97345100
H -4.67299300 0.03155200 1.77212700
C 3.52785000 2.18026200 0.40658800
H 4.28117600 2.12773700 1.19103100
C 1.23994300 -0.01349200 3.45108100
H 2.19662600 -0.01557400 3.97163100
C -1.16923300 0.00705100 3.51635000
H -2.09604700 0.01981300 4.08818200
C 1.18321200 -0.02469700 2.05232400
C 1.58778800 -2.57146600 -1.47396900
H 0.82202400 -2.62339800 -2.24827900
C 2.47509500 -0.04354600 1.19093300
C -1.18859500 -0.00565400 2.11663800
C -3.64139000 3.32319700 -0.27884400
C 3.50581600 -2.29805200 0.46882000
H 4.28601600 -2.20931600 1.22307200
C 1.68563900 2.35562100 -1.61959400
H 0.95571200 2.35695100 -2.43053900
C 0.05480100 0.00235900 4.19903500
C 3.58254000 3.23538800 -0.50457300
C 2.67651100 3.33064900 -1.56280600
H 2.73164900 4.12655600 -2.30811000
C 2.57423500 -3.54976900 -1.39943900
H 2.59236400 -4.38968800 -2.09659700
C -1.78334100 2.44549900 -1.45897400
H -1.06800000 2.46562400 -2.28152700
C -2.75692700 3.43376600 -1.35354500
H -2.81401300 4.25143000 -2.07463600
C 3.52415900 -3.39924700 -0.38729500
C -3.74316300 -3.30733100 -0.22938600
C -1.89492000 -2.47518400 -1.45683200
H -1.20577000 -2.50413500 -2.30218000
H 3.17342400 -0.33074500 -6.57753700
H 3.91016100 -0.24280200 -6.45910100
H 0.08449200 0.01157100 5.29180600
F -4.60114200 4.26925900 -0.09632700
F 4.55812700 4.17343800 -0.36641100
F 4.50256400 -4.33182400 -0.23776200
F -4.71912000 -4.23168500 -0.02004900

Reactant complex: $[(p\text{-}\mathbf{CF_3}\text{PY})_4\text{PYMe}_2\text{Mo(H)(OH)}]^+$
Mo .03423500 -0.01928000 -1.57235000
O -0.54223900 0.86787500 -3.32635800
N -1.63230800 -1.36918900 -1.53298500
N 1.54174100 -1.55896000 -1.08357500
N 1.71000600 1.30257300 -1.47050700
N -1.56990500 1.48698100 -1.04116800
C -2.52385700 -1.38339300 -0.48641900
N 0.02811000 -0.06892000 0.66270800
C -2.48077300 -0.21457700 0.54115800
C -2.59625300 1.13703600 -0.21780400
C 2.57275700 -1.29189400 -0.22552500
C -2.78858200 -3.26330200 -2.53607200
H -2.87527900 -3.94970600 -3.38157000
C -3.49306700 -2.39645100 -0.39091400
H -4.16808200 -2.44300600 0.46144100
C 2.64522600 1.22580800 -0.46207300
C 3.73014700 0.10874400 1.53071700
H 3.70492700 -0.73518900 2.23525900
H 3.71439300 1.03967400 2.11573500
H 4.68690700 0.06998300 0.99016200
C -3.70509100 1.98736600 -0.05162000
H -4.54241700 1.70040900 0.58159400
C -3.67321100 -0.35552600 1.51664900
H -3.72629300 0.49970600 2.20527900
H -3.58464500 -1.27064200 2.12035900
H -4.62449100 -0.40280900 0.96704000
C 3.68790300 2.16433100 -0.37561600
H 4.41426500 2.11214300 0.43295400
C 1.21557100 0.15794800 2.74766900
H 2.14555600 0.30098900 3.29432200
C -1.17391600 -0.12503300 2.75041200
H -2.10774700 -0.22212700 3.30037800
C 1.20497300 0.06820500 1.34678700
C 1.51318100 -2.78572000 -1.69448900
H 0.66566900 -2.97081500 -2.35303800
C 2.53861400 0.04987500 0.54656700
C -1.15338500 -0.15816800 1.34705500
C -3.73909300 3.22116800 -0.71308800
C 3.61330600 -2.22214900 -0.03546900
H 4.44859300 -1.99013400 0.62209600
C 1.87140600 2.28731900 -2.42137700
H 1.12978600 2.26540900 -3.22347100
C 0.01769100 0.04980500 3.45638200
C 3.81339400 3.18324500 -1.32866600
C 2.88480500 3.23138300 -2.38771700
H 2.94215400 3.98561400 -3.17654500
C 2.48781200 -3.75699800 -1.51929700
H 2.39125900 -4.71496900 -2.03516500
C -1.61120800 2.68827600 -1.67657100
H -0.77109700 2.90965700 -2.33348600
C -2.66181100 3.59146800 -1.53332000

H -2.62956400 4.55060200 -2.05523100
C 3.57982000 -3.45999000 -0.68319400
C -3.62262900 -3.35517800 -1.40670300
C -1.81836800 -2.27033300 -2.55321400
H -1.13849600 -2.16226500 -3.40065500
H -0.18333000 0.42521700 -4.11581800
H 0.61731000 -0.88954900 -2.89346800
C -4.90634700 4.16832600 -0.53318200
C 4.90319800 4.21692900 -1.23187600
C 4.68937000 -4.46963300 -0.50420600
C -4.62784500 -4.47422700 -1.29714900
F -5.31841600 -4.65734600 -2.46740000
F -5.55055000 -4.26353200 -0.31305700
F -4.01992600 -5.67772300 -1.01834200
F -5.39517100 4.59886800 -1.73814800
F -5.94543100 3.60353900 0.14573000
F -4.53546600 5.29247200 0.16160900
F 5.60295700 4.33591200 -2.40854000
F 4.39954500 5.47111800 -0.96430800
F 5.81351600 3.94240600 -0.25149100
F 5.60255200 -4.09174000 0.43576100
F 5.37866300 -4.67203400 -1.67500400
F 4.20225800 -5.69490100 -0.12684400
H 0.01292300 0.09928900 4.54878900

Transition state: $[(p\text{–}\mathbf{CF_3}\text{PY})_4\text{PYMe}_2\text{MoO}\cdots\text{H}\cdots\text{H}]^{+\ \ddagger}$
Mo 0.01054000 0.00302900 -0.99400400
O -0.51926500 0.86669800 -2.59215200
N -1.66425400 -1.34425100 -0.93606800
N 1.50211200 -1.56991700 -0.40488300
N 1.70876100 1.30863600 -0.86646400
N -1.54765500 1.53716600 -0.32298600
C -2.55497500 -1.36647800 0.11343500
N -0.02473500 -0.02616000 1.25277100
C -2.52977100 -0.19785300 1.14063600
C -2.62742800 1.16280300 0.40551100
C 2.55369500 -1.27469300 0.41086900
C -2.77366600 -3.28845000 -1.90426200
H -2.84447200 -3.98904600 -2.73954200
C -3.49771800 -2.40077700 0.22575800
H -4.17137600 -2.44798000 1.07916700
C 2.61724300 1.24771500 0.16253000
C 3.68345700 0.13647500 2.16779200
H 3.66512200 -0.71809800 2.85958900
H 3.65279400 1.05945200 2.76454500
H 4.64418700 0.11736400 1.63304900
C -3.75538700 2.00007800 0.50747600
H -4.64206800 1.68419300 1.05456400
C -3.73002400 -0.33709300 2.10624800
H -3.79037700 0.52565500 2.78547600
H -3.64843100 -1.24666900 2.71892900
H -4.67551700 -0.39146200 1.54707000
C 3.63927600 2.20612800 0.27692100
H 4.34308500 2.16931000 1.10596200
C 1.15741600 0.14716900 3.35109100
H 2.08730100 0.27181700 3.90197500
C -1.22751100 -0.14022700 3.34560300
H -2.16377900 -0.25472900 3.88816800
C 1.15343500 0.09088700 1.94900400
C 1.46419100 -2.79169100 -1.01324200
H 0.58842300 -2.99869500 -1.62922500
C 2.50180100 0.07303900 1.17188600
C -1.20389300 -0.14386900 1.94276500
C -3.73232700 3.25932900 -0.10265400
C 3.61828300 -2.18126500 0.56543500
H 4.47474600 -1.93185200 1.18888800
C 1.87748500 2.29017100 -1.81688900
H 1.15594400 2.25295500 -2.63724000
C -0.03984800 0.02589100 4.05883200
C 3.77292300 3.22297500 -0.67692000
C 2.87615900 3.25051800 -1.76148900
H 2.94500000 4.00003900 -2.55383600
C 2.46745600 -3.74407400 -0.87797900
H 2.37122600 -4.70647600 -1.38563900
C -1.53143800 2.76071400 -0.91072800
H -0.64279100 3.00069500 -1.49480500
C -2.58636600 3.66382200 -0.80857300
H -2.50900600 4.64750200 -1.27735800
C 3.58258600 -3.41956900 -0.08618100
C -3.60626400 -3.38126700 -0.77374000
C -1.83135900 -2.26995000 -1.93986900
H -1.16408900 -2.16277200 -2.79747000
H 0.28969200 -0.22223200 -2.83496800
H 0.77758600 -0.93443400 -2.47854500
C -4.58435900 -4.52034400 -0.64324700
C -4.92325700 4.19048200 -0.01589700
C 4.70484700 -4.42109100 0.08054300
C 4.84183200 4.27796900 -0.55190800
F 5.14609500 -4.88704200 -1.12959000
F 4.29421900 -5.51878400 0.79505000
F 5.78350300 -3.90036400 0.73171500
F 5.74552700 4.00528400 0.43460400
F 5.55062000 4.42780000 -1.71804600
F 4.30785400 5.51510500 -0.26979500
F -4.56773300 5.41225900 0.49337400
F -5.92248500 3.70057400 0.77156800
F -5.46476000 4.42648300 -1.25396000
F -5.24775400 -4.76366300 -1.81838200
F -5.53088100 -4.29859800 0.31605600
F -3.95325500 -5.69866800 -0.30963100
H -0.04508400 0.05332200 5.15185600

Product complex: $[(p\text{–}\mathbf{CF_3}\text{PY})_4\text{PYMe}_2\text{MoO}]^+ + \text{H}_2$
Mo -0.07018600 -0.05008000 -1.56271400
O -0.10278400 -0.08144000 -3.30813600
N -1.70169300 -1.42382600 -1.27447100
N 1.51095600 -1.49001100 -1.29153000
N 1.56868200 1.33430800 -1.38504100
N -1.64013300 1.39966400 -1.28303000
C -2.60801100 -1.26832800 -0.25240300
N -0.02634800 -0.01021500 0.71956100
C -2.52227500 0.01279500 0.62872900

C -2.57250700 1.27539400 -0.28038000
C 2.48271300 -1.32856100 -0.33268900
C -2.84895400 -3.43842300 -2.00152300
H -2.92546800 -4.24489000 -2.73423100
C -3.59877700 -2.24010400 -0.03716000
H -4.30100900 -2.14135800 0.78813300
C 2.51250600 1.21564200 -0.39236100
C 3.70143300 -0.02749700 1.46076600
H 3.70194800 -0.90210400 2.12702100
H 3.71205700 0.86811400 2.09813900
H 4.63242200 -0.04155300 0.87451900
C -3.55273700 2.26588300 -0.10474000
H -4.27987300 2.18824900 0.70111000
C -3.72345800 0.03965600 1.60205800
H -3.69702400 0.93545800 2.23899200
H -3.71286300 -0.83464200 2.26857900
H -4.67560100 0.03835500 1.05061000
C 3.50614300 2.19723300 -0.24563500
H 4.23846400 2.12880600 0.55647400
C 1.21885800 0.01430800 2.79007900
H 2.17102000 0.01644400 3.31843400
C -1.19097400 0.03358200 2.83607100
H -2.12201000 0.04977100 3.40050300
C 1.17021000 -0.00820900 1.38959300
C 1.58780300 -2.56903400 -2.13232100
H 0.83882400 -2.61463000 -2.92279500
C 2.46426800 -0.03543000 0.53354200
C -1.19627600 0.01077400 1.43480900
C -3.63123700 3.35503900 -0.98532600
C 3.47214100 -2.31085600 -0.16120300
H 4.23108000 -2.20311800 0.61109300
C 1.69522000 2.35126800 -2.29524500
H 0.98179200 2.34284800 -3.12038300
C 0.02761600 0.03534500 3.52417500
C 3.59131100 3.26596000 -1.15113100
C 2.67988500 3.32712700 -2.21997200
H 2.72602700 4.10895500 -2.98142700
C 2.56359200 -3.55139100 -2.02944000
H 2.56950300 -4.38341400 -2.73709900
C -1.75125200 2.44642900 -2.15992800
H -1.03600300 2.45975800 -2.98223100
C -2.72118800 3.43437400 -2.05360700
H -2.75587600 4.23941200 -2.79102800
C 3.51696200 -3.43158300 -1.00340100
C -3.72035000 -3.33796600 -0.90268100
C -1.86473200 -2.46981600 -2.14509900
H -1.18258600 -2.49114100 -2.99602300
H 3.04377100 -0.53600400 -7.26989300
H 3.73377700 -0.80596100 -7.14508100
C -4.66320100 4.43889300 -0.78467500
C 4.63320600 4.34418900 -0.97811800
C 4.55941000 -4.50669000 -0.80958000
C -4.75824900 -4.40558400 -0.65589600
F -5.34333700 -4.82927200 -1.81943400
F -5.76000300 -3.98551400 0.17161700
F -4.20584700 -5.52290300 -0.07202100
F 5.17248000 4.73166600 -2.17587200
F 5.66697600 3.95406400 -0.17569100
F 4.09847500 5.47810800 -0.41006900
F -5.21185800 4.84730500 -1.97098600
F -5.69099900 4.04435700 0.02270800
F -4.11286200 5.55940500 -0.20634200
F 5.09322200 -4.91983100 -2.00159400
F 5.59635300 -4.09992700 -0.02077900
F 4.02485900 -5.62694100 -0.21656900
H 0.04863200 0.05309700 4.61716300

Reactant complex: $[(p\text{-}\mathbf{CN}\text{PY})_4\text{PYMe}_2\text{Mo(H)(OH)}]^+$
Mo 0.03534700 0.00973900 -0.92200200
O -0.52533600 0.89291900 -2.67285900
N -1.62769500 -1.33863900 -0.87465400
N 1.54037200 -1.52746500 -0.43560900
N 1.71144900 1.33136600 -0.82957400
N -1.56996500 1.51835200 -0.39778700
C -2.51810400 -1.35215600 0.17581400
N 0.03138800 -0.03055400 1.31409700
C -2.47749400 -0.17719200 1.19634300
C -2.59585900 1.17008300 0.42966800
C 2.57170400 -1.25976600 0.42614000
C -2.77009000 -3.24810200 -1.86778800
H -2.85616900 -3.94260400 -2.70593200
C -3.47841900 -2.36649800 0.28229900
H -4.15335200 -2.41338400 1.13490200
C 2.64796500 1.25805100 0.18039300
C 3.73435400 0.14679700 2.17574200
H 3.70833800 -0.69377800 2.88408800
H 3.72007000 1.08006900 2.75682400
H 4.69049300 0.10448200 1.63447200
C -3.70422200 2.01578700 0.59302000
H -4.54226100 1.73380700 1.22774300
C -3.66872900 -0.31495700 2.17375500
H -3.72268300 0.54407900 2.85744900
H -3.57703700 -1.22601400 2.78284800
H -4.62041800 -0.36803000 1.62543800
C 3.68734700 2.19344500 0.26565500
H 4.41626000 2.14623800 1.07252800
C 1.22179400 0.20626900 3.39548600
H 2.15230400 0.35138200 3.94049600
C -1.16792900 -0.07605500 3.40277700
H -2.10086200 -0.16937200 3.95475800
C 1.20907800 0.10942800 1.99519000
C 1.51061500 -2.75660300 -1.04289100
H 0.66658400 -2.94191800 -1.70566400
C 2.54134900 0.08547700 1.19334500
C -1.14912400 -0.11612200 1.99974300
C -3.74075400 3.25724600 -0.07549800
C 3.60666700 -2.18821900 0.62398100
H 4.44286500 -1.95760000 1.28105100
C 1.87084200 2.31289800 -1.78424300
H 1.12960400 2.28760100 -2.58626700
C 0.02470600 0.10251600 4.10580100
C 3.81340300 3.22138100 -0.69430500

C 2.87925200 3.26058100 -1.75733200
H 2.93791600 4.01470100 -2.54512300
C 2.47710100 -3.73342900 -0.86257200
H 2.38331400 -4.69320800 -1.37412200
C -1.61118800 2.71594400 -1.03951500
H -0.77196300 2.93477900 -1.69838800
C -2.65833300 3.62300000 -0.90139700
H -2.63013100 4.58170000 -1.42271300
C 3.57428600 -3.43944000 -0.02138700
C -3.60438300 -3.34527500 -0.73007000
C -1.81185600 -2.24619800 -1.89107600
H -1.13876200 -2.13651000 -2.74352400
H -0.17664700 0.45208500 -3.46826900
H 0.58965200 -0.88137800 -2.23577300
H 0.02129700 0.15843900 5.19783100
C 4.86558100 4.18332200 -0.59420900
N 5.73227500 4.97943400 -0.51582000
C 4.62612200 -4.39002000 0.18363000
N 5.48941100 -5.17456400 0.34782000
C -4.86514100 4.13318200 0.09381900
N -5.78618600 4.85357200 0.22922400
C -4.57613000 -4.38806500 -0.61173300
N -5.37542100 -5.24950500 -0.51680600

Transition state: $[(p\text{−}\mathbf{CN}\text{PY})_4\text{PYMe}_2\text{MoO}\cdots\text{H}\cdots\text{H}]^{+\,\ddagger}$

Mo 0.00418900 -0.00766100 -0.99819300
O -0.52290200 0.84662800 -2.59550600
N -1.66248200 -1.35545400 -0.91354800
N 1.49456200 -1.57436800 -0.40062100
N 1.70408000 1.29680000 -0.89722500
N -1.55458300 1.53150500 -0.33799100
C -2.54785700 -1.37067800 0.14365100
N -0.01644600 -0.00798100 1.25095900
C -2.52169000 -0.18902700 1.15605100
C -2.62941100 1.16142900 0.40373800
C 2.55144200 -1.27173400 0.40927000
C -2.76223300 -3.31949000 -1.85610500
H -2.83597100 -4.03237900 -2.67992200
C -3.48171800 -2.40444800 0.27655500
H -4.15144900 -2.44721600 1.13346800
C 2.62092600 1.24747500 0.12768200
C 3.69643300 0.15953500 2.14106200
H 3.67817800 -0.68481800 2.84520600
H 3.67230700 1.09089700 2.72465600
H 4.65404600 0.12928900 1.60139000
C -3.75821300 1.99176600 0.50304200
H -4.64201300 1.68210700 1.05864500
C -3.71523100 -0.32105000 2.13093900
H -3.77543600 0.55008600 2.79922100
H -3.62496300 -1.22199900 2.75478300
H -4.66385100 -0.38752600 1.57854200
C 3.64143700 2.20281600 0.22648900
H 4.35245800 2.17759000 1.05010300
C 1.17766500 0.20237800 3.33785000
H 2.11024300 0.33850600 3.88124300
C -1.20621200 -0.09377800 3.35121000
H -2.13838300 -0.20309700 3.90164500
C 1.16536000 0.12105900 1.93705400
C 1.45021300 -2.80305300 -0.99495700
H 0.57220900 -3.01505100 -1.60584200
C 2.50880800 0.08650100 1.15294700
C -1.19102200 -0.11911600 1.94841300
C -3.74642500 3.25219700 -0.12777100
C 3.61132700 -2.17637500 0.57340200
H 4.47101100 -1.92616100 1.19225500
C 1.86614800 2.26758600 -1.86049400
H 1.14037800 2.22189500 -2.67634800
C -0.01511500 0.08939800 4.05379600
C 3.77039600 3.22028300 -0.74330900
C 2.86120200 3.23055400 -1.82628900
H 2.92658800 3.97346100 -2.62412800
C 2.44626300 -3.76039300 -0.85330100
H 2.34864900 -4.72994300 -1.34509900
C -1.54590800 2.74655700 -0.94293700
H -0.66231400 2.98195200 -1.53654100
C -2.60022000 3.65032000 -0.84896200
H -2.53502600 4.62786400 -1.33045300
C 3.57088100 -3.43339800 -0.06460000
C -3.59124700 -3.41101100 -0.71306200
C -1.83122800 -2.29433500 -1.90695200
H -1.17368100 -2.19153100 -2.77242700
H 0.26909000 -0.24617400 -2.83745100
H 0.74806400 -0.96459000 -2.47046700
C 4.64917700 -4.36345300 0.10273800
C -4.53930400 -4.47002000 -0.56829700
C -4.88725100 4.11794700 -0.02746300
C 4.80513500 4.20154100 -0.63316600
N 5.65615300 5.01258400 -0.54589900
N 5.53345300 -5.12924000 0.23691000
N -5.32045600 -5.34601000 -0.45123600
N -5.82093900 4.83005800 0.05216400
H -0.01410700 0.13532500 5.14614100

Product complex: $[(p\text{−}\mathbf{CN}\text{PY})_4\text{PYMe}_2\text{MoO}]^+ + \text{H}_2$

Mo 0.00000000 0.00000000 0.00000000
O 0.00000000 0.00000000 1.73776388
N 2.13599463 0.00000000 -0.23985945
N -0.28972840 -2.11551839 -0.28313787
N -2.13536839 0.02524979 -0.24450446
N 0.26780077 2.11316664 -0.29820722
C 2.75824140 0.70478198 -1.24536027
N 0.00167610 -0.01402911 -2.30129285
C 1.88912888 1.61198555 -2.16615278
C 1.07305962 2.61328099 -1.29650734
C -1.13410541 -2.61566206 -1.24831182
C 4.29000703 -0.78506970 0.56911483
H 4.84960081 -1.34603148 1.32033299
C 4.14584813 0.61626927 -1.41218361
H 4.64579632 1.14599256 -2.22041361
C -2.76008585 -0.65422215 -1.26568067
C -2.84776557 -2.39557287 -3.09705438
H -2.27985674 -3.09355078 -3.72858226

H -3.38934431 -1.71507241 -3.76934891
H -3.58861913 -2.97399146 -2.52514596
C 1.16128249 3.99582307 -1.50246153
H 1.77146789 4.40291149 -2.30636913
C 2.81443302 2.40373345 -3.11888805
H 2.23102858 3.05025793 -3.78992139
H 3.40444387 1.72592463 -3.75206898
H 3.51250643 3.03692656 -2.55116479
C -4.13569213 -0.49829493 -1.47638963
H -4.63525405 -1.00101929 -2.30238216
C -0.88119968 -0.84610672 -4.38804637
H -1.59127868 -1.46708616 -4.93178040
C 0.95958397 0.71017093 -4.39507301
H 1.68780439 1.30440169 -4.94454796
C -0.89121239 -0.79176316 -2.98698042
C 0.32606964 -2.99080437 0.57341416
H 0.93418160 -2.54599723 1.36061461
C -1.90893953 -1.61160976 -2.15124439
C 0.91391495 0.73462137 -2.99391929
C 0.47916405 4.89479858 -0.65081122
C -1.29065863 -3.99941294 -1.39875906
H -1.94176610 -4.40674029 -2.16954695
C -2.90397111 0.73934719 0.63928226
H -2.37615413 1.16781731 1.49224212
C 0.05506210 -0.08997095 -5.10043726
C -4.91144830 0.29661135 -0.60076832
C -4.27460632 0.90005328 0.50772423
H -4.83048703 1.48098156 1.24632065
C 0.19002262 -4.36857955 0.49304502
H 0.70576979 -5.01158554 1.20879451
C -0.35022853 2.99156169 0.55406338
H -0.90807857 2.54794756 1.37839335
C -0.27316121 4.36987644 0.42404337
H -0.78800885 5.01565426 1.13802455
C -0.62494940 -4.89673421 -0.53322018
C 4.93140002 -0.14291323 -0.51469469
C 2.91010934 -0.68704987 0.66035446
H 2.37807738 -1.14545460 1.49490118
H -2.86683873 -1.50374662 5.72884443
H -3.56726167 -1.71756134 5.56078142
H 0.07766624 -0.12163376 -6.19310386
C -6.31603115 0.45531350 -0.82098412
N -7.47325574 0.58950207 -1.00104790
C -0.79400259 -6.30947232 -0.68819686
N -0.93057541 -7.47327181 -0.81399526
C 6.34850180 -0.23004093 -0.69129923
N 7.51605941 -0.30512321 -0.83473509
C 0.57509611 6.30654191 -0.86403345
N 0.65125579 7.46976731 -1.03795193

4.2.4 Structures with substituent groups at global position

Reactant complex: $[(p\text{–}\mathbf{NH_2}\text{PY})_5\text{Me}_2\text{Mo(H)(OH)}]^+$
Mo 0.02450000 -0.00430100 -1.09810100
O -0.57089700 0.91897100 -2.87570900
N -1.64527900 -1.37036800 -1.03379800
N 1.55477000 -1.52597200 -0.57797400
N 1.70589000 1.33468700 -0.97433500
N -1.55927800 1.49832200 -0.54417500
C -2.53617700 -1.37891400 0.01532000
N 0.02247400 -0.05002900 1.13388300
C -2.48998600 -0.19592800 1.03070100
C -2.60351000 1.15620900 0.26731900
C 2.59112800 -1.25456900 0.27577400
C -2.79282900 -3.30962500 -1.97949200
H -2.86939500 -4.01999800 -2.80813100
C -3.49668900 -2.39345800 0.13913600
H -4.17027700 -2.42171300 0.99595800
C 2.63999500 1.27243800 0.03680900
C 3.72233200 0.16429500 2.03622400
H 3.70204700 -0.67940900 2.74148800
H 3.69666600 1.09700300 2.61888400
H 4.68183700 0.13334000 1.49970000
C -3.70405700 2.00528000 0.43983900
H -4.53826400 1.71499500 1.07915400
C -3.67943500 -0.32872200 2.01148800
H -3.73192800 0.53309200 2.69211900
H -3.59119600 -1.23932400 2.62281800
H -4.63161800 -0.38036100 1.46361300
C 3.67253600 2.22128700 0.13385200
H 4.39358700 2.17210200 0.95038300
C 1.20872900 0.19363000 3.22604300
H 2.14218600 0.33255300 3.76968000
C -1.18639200 -0.08219300 3.22672600
H -2.12516400 -0.16632000 3.77222200
C 1.19362400 0.09789200 1.83475000
C 1.55157600 -2.75948900 -1.17589900
H 0.69889100 -2.96170100 -1.82448500
C 2.53822700 0.09167300 1.04432200
C -1.15583000 -0.13241500 1.83279300
C -3.76003500 3.26444500 -0.21045600
C 3.63640800 -2.16949300 0.47638900
H 4.45948400 -1.92762500 1.14908700
C 1.87041500 2.33204300 -1.90963300
H 1.12926300 2.30871500 -2.71485500
C 0.00646500 0.09600400 3.96436500
C 3.81340500 3.26172400 -0.81026300
C 2.87345100 3.28582300 -1.87230300
H 2.92461700 4.04451500 -2.65991600
C 2.53866800 -3.71561400 -1.01100700
H 2.45272400 -4.67442300 -1.53063000
C -1.60561600 2.71576800 -1.15492500
H -0.75504600 2.94901900 -1.79607000
C -2.64978600 3.61894500 -1.01802000
H -2.60609600 4.58458900 -1.53046700
C 3.64761100 -3.42544900 -0.17393300
C -3.64133000 -3.39974100 -0.84717600
C -1.83316800 -2.31035600 -2.01706500
H -1.15043500 -2.22401600 -2.86623900
H -0.20272900 0.42364000 -3.62812400
H 0.59595600 -0.88827300 -2.44409300
N 0.00060600 0.13707200 5.33005300

H 0.83755200 0.41561900 5.83662200
H -0.87977800 0.21583700 5.83343400
N 4.78544300 4.24416300 -0.67157600
H 5.59264500 4.01377100 -0.09250300
H 5.03477800 4.76171600 -1.51389600
N 4.69458200 -4.30750600 -0.02982700
H 4.55040700 -5.27808800 -0.30202000
H 5.34425900 -4.17329100 0.74272900
N -4.54063400 -4.43473700 -0.69161300
H -5.29046000 -4.31907100 -0.01157000
H -4.80551500 -4.96435300 -1.52059200
N -4.85603500 4.08414500 -0.08867800
H -4.77492700 5.05655300 -0.37889200
H -5.52511500 3.90922200 0.65836700

Transition state: $[(p\text{–}\mathbf{NH_2}\text{PY})_5\text{Me}_2\text{MoO}\cdots\text{H}\cdots\text{H}]^{+\,\ddagger}$
Mo -0.00326800 -0.01748200 -1.00221700
O -0.52869200 0.80895900 -2.65543100
N -1.68170300 -1.37266200 -0.91251000
N 1.48581600 -1.57510800 -0.37225500
N 1.70344600 1.30758600 -0.87487600
N -1.55115000 1.50231000 -0.35022600
C -2.56040500 -1.38707300 0.14841300
N -0.02254300 -0.01557600 1.24212500
C -2.52761000 -0.19734100 1.15769000
C -2.63231400 1.15266400 0.39805800
C 2.55822900 -1.26963200 0.41807500
C -2.79790100 -3.35131000 -1.81860300
H -2.86973700 -4.07283400 -2.63799400
C -3.49657300 -2.41959800 0.29514400
H -4.16030500 -2.44924400 1.15964400
C 2.61626400 1.26399800 0.15086600
C 3.68868500 0.16402500 2.16025600
H 3.67425900 -0.68629300 2.85772200
H 3.65840800 1.09224000 2.74968200
H 4.64823600 0.14377000 1.62317800
C -3.75138600 1.98876000 0.50990100
H -4.62127400 1.68218500 1.09221800
C -3.72077300 -0.32425100 2.13379500
H -3.78010400 0.54940000 2.79912500
H -3.63360800 -1.22445500 2.76034400
H -4.66959300 -0.38960700 1.58127000
C 3.63321700 2.22597700 0.26199300
H 4.34115600 2.19105200 1.09047800
C 1.17142200 0.18761500 3.33837200
H 2.10815000 0.30719100 3.88078600
C -1.22094100 -0.08223800 3.34701400
H -2.15921600 -0.17937300 3.89160400
C 1.15444700 0.11287700 1.94556300
C 1.45765900 -2.81360500 -0.94881100
H 0.56899200 -3.04008100 -1.54138700
C 2.50617700 0.08994900 1.16632400
C -1.19437300 -0.11931400 1.95262400
C -3.77186100 3.25386900 -0.12970300
C 3.62606800 -2.16032500 0.57343400
H 4.48280100 -1.89747900 1.19448600
C 1.86940400 2.29528400 -1.81592600
H 1.14042400 2.25127700 -2.63203400
C -0.02708600 0.09182400 4.08183800
C 3.77726600 3.26170300 -0.68950600
C 2.85959200 3.26355900 -1.76976800
H 2.91673200 4.01539700 -2.56341700
C 2.46730100 -3.75476500 -0.82657600
H 2.36548500 -4.72664900 -1.31791400
C -1.56328200 2.72088000 -0.95603500
H -0.68224700 2.95332700 -1.55618300
C -2.61465800 3.62153400 -0.86513200
H -2.54559000 4.59236700 -1.36495300
C 3.61750000 -3.42972700 -0.06087900
C -3.62939400 -3.44483300 -0.67486400
C -1.86446700 -2.32801300 -1.88286300
H -1.20311000 -2.23942600 -2.74912100
H 0.32019700 -0.28939000 -2.84780100
H 0.82047900 -0.98195800 -2.50807800
N -0.03181200 0.19194000 5.44731700
H 0.84496500 0.12765000 5.95952000
H -0.86950900 -0.05919000 5.96737100
N -4.87690300 4.06878300 -0.06967300
H -4.78160700 5.04466800 -0.34322800
H -5.59047300 3.88421500 0.63251400
N 4.73518800 4.25182600 -0.54225300
H 5.52809800 4.04756200 0.06495800
H 4.98898200 4.77900700 -1.37680500
N 4.64541000 -4.31915100 0.11208900
H 4.70481400 -5.13882300 -0.48782200
H 5.52531500 -3.99804600 0.50995300
N -4.50306900 -4.49768700 -0.49160700
H -4.76563900 -5.04587200 -1.30928400
H -5.24985000 -4.38517600 0.19241400

Product complex: $[(p\text{–}\mathbf{NH_2}\text{PY})_5\text{Me}_2\text{MoO})]^+ + \text{H}_2$
Mo -0.07490900 -0.02991400 -1.01312600
O -0.11210600 -0.04052300 -2.79125300
N -1.74811100 -1.37441800 -0.79044300
N 1.47656900 -1.50176200 -0.67945700
N 1.60735400 1.31499100 -0.87822200
N -1.61280800 1.44514500 -0.63282400
C -2.62763700 -1.27621600 0.26472300
N -0.02803900 -0.01635000 1.25214800
C -2.53368300 -0.01816000 1.18478300
C -2.60583500 1.26074900 0.30075800
C 2.50428700 -1.30908600 0.21409300
C -2.90529300 -3.38798000 -1.53746100
H -2.99348600 -4.17303900 -2.29475700
C -3.59841300 -2.26331700 0.48377400
H -4.27115900 -2.19768700 1.33938700
C 2.53251400 1.22689300 0.13821300
C 3.70149100 -0.00288600 2.01829400
H 3.71041200 -0.88846300 2.67085400
H 3.69747000 0.88686500 2.66461500
H 4.63676700 0.00461400 1.43911900
C -3.64011200 2.19252800 0.44269000

H -4.41292900 2.04918700 1.19811800
C -3.72315600 -0.02165100 2.17251900
H -3.71170900 0.87562700 2.80884400
H -3.68698400 -0.89939300 2.83420100
H -4.68122700 -0.04510300 1.63230000
C 3.51767200 2.21098600 0.29887300
H 4.22780900 2.15442700 1.12449500
C 1.22253200 0.00708500 3.32511400
H 2.17715700 0.01186100 3.85122900
C -1.19150600 0.01269200 3.37522500
H -2.12359200 0.01942700 3.94012000
C 1.16800600 -0.00480300 1.93120300
C 1.53180400 -2.61181400 -1.48053100
H 0.71289500 -2.72046500 -2.19294700
C 2.47245400 -0.01652100 1.08064100
C -1.19491400 -0.01207300 1.98032600
C -3.72769500 3.33390000 -0.39465000
C 3.53838000 -2.24450400 0.33139300
H 4.33918500 -2.09534100 1.05593300
C 1.76802600 2.32650200 -1.79113500
H 1.07606700 2.29784500 -2.63718500
C 0.03075100 0.02087700 4.08736500
C 3.63801400 3.29284200 -0.60844900
C 2.74072800 3.31068600 -1.70554100
H 2.79929800 4.08412800 -2.47753700
C 2.54421800 -3.55645400 -1.43748100
H 2.51553700 -4.41154700 -2.11894000
C -1.70165300 2.54496400 -1.44487800
H -0.90919400 2.64842300 -2.18732200
C -2.71660900 3.48544100 -1.37765600
H -2.71634900 4.33212700 -2.07005900
C 3.58974600 -3.39797600 -0.49226700
C -3.75221900 -3.35946300 -0.40122300
C -1.94364500 -2.39967600 -1.68092200
H -1.29060300 -2.37933300 -2.55760000
H 2.99555300 -0.41183500 -7.00804700
H 3.73225700 -0.50221700 -6.89141700
N 0.05978100 -0.01301300 5.46643900
H 0.92624600 0.25050300 5.93292300
H -0.78452100 0.25432600 5.96986100
N -4.72065600 4.26859000 -0.22752800
H -4.88948000 4.94337900 -0.97074000
H -5.53641700 4.02706200 0.33170400
N 4.58270500 -4.33606600 -0.34628700
H 4.72218500 -5.02327200 -1.08410600
H 5.41756000 -4.09265600 0.18310500
N 4.56409800 4.30057100 -0.40746000
H 5.34816600 4.10267300 0.21293000
H 4.81278600 4.87575200 -1.21120700
N -4.66092900 -4.37017200 -0.14393300
H -5.41706900 -4.16947700 0.50931500
H -4.94148000 -4.95927100 -0.92685000

Reactant complex: $[(p\text{-}\mathbf{CH_3}\text{PY})_5\text{Me}_2\text{Mo(H)(OH)}]^+$
Mo 0.03093300 0.00035600 -1.07781800
O -0.57608700 0.88198300 -2.85010300
N -1.63720700 -1.35759200 -1.02459000
N 1.53574500 -1.54362100 -0.55838600
N 1.71240500 1.32505300 -0.96659300
N -1.56306700 1.50415400 -0.54231800
C -2.52883300 -1.36293500 0.02026500
N 0.02800000 -0.03891700 1.15299100
C -2.48017500 -0.18617100 1.04220300
C -2.59369400 1.16618100 0.28247800
C 2.57218500 -1.27470600 0.28999200
C -2.80717100 -3.25926800 -1.99894000
H -2.89151500 -3.95446100 -2.84016000
C -3.50292700 -2.37481300 0.11802600
H -4.17662000 -2.40651200 0.97480000
C 2.65049900 1.25125200 0.03746600
C 3.72849700 0.13796100 2.03679300
H 3.69901100 -0.70218500 2.74607600
H 3.71625900 1.07363900 2.61473600
H 4.68575000 0.09214300 1.49756500
C -3.69031600 2.03133700 0.45610500
H -4.52124500 1.74481800 1.10162900
C -3.66959500 -0.32207900 2.02223400
H -3.72073900 0.53624900 2.70724200
H -3.58190600 -1.23611000 2.62833700
H -4.62177500 -0.36859100 1.47417300
C 3.69395400 2.19476600 0.11755000
H 4.41979700 2.13610600 0.92930200
C 1.20850600 0.20866900 3.24096400
H 2.14328900 0.35560600 3.78099000
C -1.16757200 -0.06860400 3.24653500
H -2.10629800 -0.15827000 3.79150800
C 1.20288200 0.10326700 1.84454800
C 1.50833000 -2.77587500 -1.15559100
H 0.65595000 -2.96298900 -1.80878800
C 2.54010500 0.07625100 1.04935100
C -1.15008100 -0.12102000 1.84407500
C -3.74690500 3.27917000 -0.19168300
C 3.60754100 -2.21155100 0.48418200
H 4.44151000 -1.97127400 1.14400600
C 1.87588200 2.31583300 -1.90962300
H 1.12889200 2.29919000 -2.70841000
C 0.01543700 0.11248900 3.97661500
C 3.84219700 3.22736100 -0.82405400
C 2.89509100 3.25573600 -1.87305700
H 2.94739600 4.01164300 -2.66367100
C 2.48708900 -3.74298200 -0.97414800
H 2.38569600 -4.70420400 -1.48730800
C -1.60647700 2.71258000 -1.16796400
H -0.76498100 2.93210700 -1.82513100
C -2.65282500 3.61757900 -1.01423200
H -2.61079000 4.57941700 -1.53476700
C 3.59670800 -3.46649900 -0.14557400
C -3.65829600 -3.35840200 -0.87722900
C -1.82721200 -2.27481100 -2.02767200
H -1.13808900 -2.18294300 -2.87096700
H -0.18111100 0.42726600 -3.61445200
H 0.66706000 -0.84464500 -2.40712000

C 0.01772300 0.19127200 5.48256700
H 0.58367700 -0.65276300 5.91516600
H 0.51050100 1.11766600 5.82525900
H -1.00429600 0.16672500 5.89044500
C -4.91795800 4.21305900 -0.01007900
H -5.66112200 3.80142200 0.69033200
H -4.58217400 5.19242700 0.37398000
H -5.41941600 4.40285300 -0.97568100
C 4.95110300 4.24653400 -0.72545400
H 4.54262500 5.26394400 -0.58530400
H 5.62531100 4.03053800 0.11854000
H 5.55308200 4.26942700 -1.65141000
C 4.70161700 -4.47234000 0.06005900
H 5.47454100 -4.09177100 0.74573200
H 4.30225100 -5.41482500 0.47494100
H 5.18415500 -4.72518800 -0.90075700
C -4.68639700 -4.45592000 -0.75587600
H -5.37614400 -4.27434100 0.08335400
H -5.27864600 -4.54928700 -1.68263900
H -4.19714700 -5.43294700 -0.58813700

Transition state: $[(p\text{–}\mathbf{CH_3}\text{PY})_5\text{Me}_2\text{MoO}\cdots\text{H}\cdots\text{H}]^{+\,\ddagger}$
Mo 0.00199200 -0.01620200 -1.00738900
O -0.55039500 0.81183100 -2.63329300
N -1.67942200 -1.36831700 -0.92164200
N 1.49853000 -1.57806100 -0.40442100
N 1.70390200 1.29859300 -0.89174400
N -1.54033400 1.51980200 -0.34028900
C -2.56430200 -1.37397800 0.13033500
N -0.01979400 -0.02848700 1.23361100
C -2.52398700 -0.19273400 1.14599500
C -2.61880000 1.16492400 0.40172900
C 2.55774100 -1.28031800 0.40042500
C -2.81302700 -3.32009900 -1.84597500
H -2.88705400 -4.03355800 -2.67273800
C -3.51555000 -2.40318900 0.25413600
H -4.18461100 -2.42857200 1.11471800
C 2.61756600 1.24757300 0.13113400
C 3.69184300 0.14937900 2.13972100
H 3.67704300 -0.69999800 2.83822800
H 3.66371000 1.07815600 2.72804900
H 4.64994700 0.12573700 1.60043400
C -3.73361100 2.01844100 0.51131800
H -4.61177300 1.70851300 1.07949900
C -3.71726700 -0.31727100 2.12219900
H -3.76765500 0.55151600 2.79465400
H -3.63768800 -1.22357400 2.74052100
H -4.66692200 -0.36901400 1.56990400
C 3.63971400 2.21211800 0.22926100
H 4.34702200 2.17451300 1.05821500
C 1.16839600 0.16269800 3.32875100
H 2.10622700 0.28992500 3.86809700
C -1.20421300 -0.11354100 3.34026800
H -2.14230300 -0.21821200 3.88394700
C 1.16075600 0.09505800 1.93053500
C 1.46276200 -2.80964300 -0.99401200
H 0.58125200 -3.02261300 -1.60122200
C 2.50718600 0.07622100 1.14837900
C -1.19176600 -0.13476900 1.93802500
C -3.73982800 3.28334400 -0.10390100
C 3.61696000 -2.19302500 0.56019300
H 4.47123700 -1.93445000 1.18660800
C 1.86945600 2.27947900 -1.84121600
H 1.13895900 2.23897900 -2.65486400
C -0.02007100 0.05445000 4.07069500
C 3.78993100 3.23895900 -0.71890200
C 2.87134600 3.23875000 -1.79132400
H 2.93075100 3.98633800 -2.58918700
C 2.46965000 -3.75670000 -0.85059800
H 2.36636200 -4.72555200 -1.34846600
C -1.53096100 2.74234900 -0.93337800
H -0.64623000 2.97180000 -1.52891500
C -2.58239400 3.64809500 -0.82426700
H -2.50119600 4.62667000 -1.30756200
C 3.60425800 -3.45109200 -0.06879600
C -3.65649800 -3.41242000 -0.71862100
C -1.85791400 -2.31253300 -1.90286900
H -1.18484700 -2.22719500 -2.75983800
H 0.28424000 -0.27319400 -2.85187300
H 0.79305600 -0.96693800 -2.50431300
C -0.01019300 0.10877900 5.57761300
H 0.60525100 -0.70758200 5.99517700
H 0.43161900 1.05688700 5.93156900
H -1.02657300 0.02306200 5.99158500
C -4.66188700 -4.52678400 -0.56702700
H -4.15384500 -5.48344300 -0.34538700
H -5.37121800 -4.32431400 0.25088900
H -5.23379600 -4.67592900 -1.49909400
C 4.87562900 4.28075600 -0.60177900
H 4.44194100 5.28750900 -0.46158800
H 5.54392400 4.07549200 0.24935700
H 5.48671000 4.32127700 -1.52078500
C -4.92603900 4.20982300 0.00278300
H -5.70830400 3.79489000 0.65708200
H -4.62109300 5.19293000 0.40201900
H -5.36866600 4.39169000 -0.99275400
C 4.73767500 -4.43219400 0.09483300
H 5.51559500 -4.04532500 0.77096600
H 4.36983200 -5.39206500 0.49817200
H 5.20500100 -4.65351500 -0.88118600

Product complex: $[(p\text{–}\mathbf{CH_3}\text{PY})_5\text{Me}_2\text{MoO})]^+ + \text{H}_2$
Mo -0.09902200 -0.05689200 -1.02864300
O -0.15381400 -0.08680500 -2.78650100
N -1.73127900 -1.43662600 -0.71384400
N 1.49699100 -1.49420500 -0.79133500
N 1.54679100 1.33145900 -0.86109100
N -1.67678400 1.39271000 -0.74501500
C -2.64205100 -1.26718000 0.30062000
N -0.03557400 -0.01738800 1.22680600
C -2.53662700 0.01586900 1.17794200
C -2.60032000 1.27632900 0.26521200

C 2.47794700 -1.34121400 0.15823400
C -2.90023400 -3.45123100 -1.41025600
H -2.97223500 -4.26902800 -2.13394700
C -3.64703600 -2.22848500 0.51306300
H -4.35117300 -2.10724700 1.33645500
C 2.50981400 1.20127000 0.11005100
C 3.69961600 -0.05057700 1.95657300
H 3.70080700 -0.92820900 2.61916400
H 3.71623500 0.84531500 2.59392300
H 4.62792100 -0.06684200 1.36625800
C -3.57900600 2.27119800 0.44328900
H -4.29400500 2.19115500 1.26241800
C -3.72138300 0.04923800 2.17062300
H -3.67988200 0.94569500 2.80618700
H -3.70686100 -0.82755000 2.83414700
H -4.68183800 0.05500800 1.63391000
C 3.51883300 2.17342100 0.23630500
H 4.26438500 2.08545300 1.02699700
C 1.22414600 -0.00751700 3.29261500
H 2.18553600 -0.01511100 3.80688400
C -1.17131700 0.02506700 3.36343200
H -2.10067600 0.04269400 3.93302400
C 1.16799500 -0.02385500 1.89605900
C 1.57925900 -2.56819000 -1.63748200
H 0.82126700 -2.61023300 -2.42137000
C 2.45958900 -0.05283400 1.03353600
C -1.19716200 0.00781200 1.96366200
C -3.68936300 3.37351500 -0.42542900
C 3.47318300 -2.32409100 0.30791800
H 4.23515500 -2.21440100 1.07994500
C 1.66854100 2.36057000 -1.75707700
H 0.92964400 2.37415200 -2.56050900
C 0.04666500 0.01835600 4.06604200
C 3.62040500 3.26284000 -0.64995900
C 2.67061000 3.32018900 -1.69192600
H 2.70335400 4.10968500 -2.44912300
C 2.56541600 -3.54225700 -1.54779600
H 2.56657400 -4.36763300 -2.26638400
C -1.80264600 2.44131800 -1.61726800
H -1.09101100 2.45445800 -2.44425200
C -2.77627400 3.42485500 -1.50000600
H -2.81492900 4.22809600 -2.24227000
C 3.53965600 -3.45271200 -0.53115700
C -3.79790700 -3.34876100 -0.32623800
C -1.89988100 -2.49967100 -1.56130200
H -1.20125800 -2.54875500 -2.39838600
H 3.70395900 -0.21969300 -6.84919700
H 4.12591600 -0.25454100 -6.22854800
C 0.09852800 0.05325700 5.57367000
H 0.79417100 -0.70813400 5.96706200
H 0.45997900 1.03483900 5.93209800
H -0.89551600 -0.12160700 6.01471400
C -4.86997700 -4.38224800 -0.08489900
H -4.42280900 -5.33714900 0.24682700
H -5.58201100 -4.05450000 0.68865200
H -5.43112300 -4.59575900 -1.01105100
C -4.73518500 4.44165100 -0.22346800
H -5.45876100 4.15836100 0.55685800
H -4.26469400 5.39530700 0.07795900
H -5.28670000 4.63811700 -1.15914900
C 4.69483200 4.31089000 -0.49888700
H 4.25945900 5.26808500 -0.15793100
H 5.45814100 4.00631900 0.23423300
H 5.19308000 4.51060800 -1.46312900
C 4.60119200 -4.50995200 -0.35570900
H 5.38882200 -4.18203600 0.34068000
H 4.16003000 -5.44103300 0.04493000
H 5.06952900 -4.76647300 -1.32143000

Reactant complex: $[(p\text{-}\mathbf{F}\text{PY})_5\text{Me}_2\text{Mo(H)(OH)}]^+$
Mo 0.03197300 0.01054500 -0.93178600
O -0.56804800 0.89605300 -2.69352200
N -1.63755000 -1.34762200 -0.88838500
N 1.54107000 -1.53579100 -0.41987800
N 1.71794700 1.33556100 -0.82549000
N -1.57357000 1.51260300 -0.39690000
C -2.51807600 -1.36118900 0.16716700
N 0.03222100 -0.03018100 1.30368200
C -2.47866700 -0.18633000 1.18987700
C -2.60146300 1.16297700 0.42802200
C 2.57601000 -1.26453800 0.43196300
C -2.78911300 -3.25674200 -1.88123200
H -2.89276500 -3.96002300 -2.70998400
C -3.48307600 -2.37865600 0.27998700
H -4.16258400 -2.44883000 1.12793600
C 2.65505200 1.25667700 0.18038600
C 3.73552100 0.14577800 2.17884300
H 3.70621800 -0.69306200 2.88951500
H 3.72530300 1.08248000 2.75498700
H 4.69186000 0.09766000 1.63844500
C -3.70985800 2.00992800 0.60594500
H -4.55213800 1.74889400 1.24509600
C -3.66682100 -0.33203700 2.16927700
H -3.72809600 0.52717000 2.85211500
H -3.56908700 -1.24344000 2.77760700
H -4.61797000 -0.38970000 1.62071300
C 3.70441200 2.19143000 0.26734700
H 4.44585800 2.15947300 1.06414400
C 1.23095400 0.22728400 3.38514200
H 2.14922900 0.36997200 3.95097900
C -1.18185300 -0.04380300 3.39186900
H -2.10387900 -0.12172700 3.96395800
C 1.20948800 0.11475100 1.98814100
C 1.51033000 -2.76140500 -1.02800000
H 0.65954400 -2.94577900 -1.68289000
C 2.54623300 0.08453100 1.19301100
C -1.14960500 -0.10905700 1.99123500
C -3.72437200 3.23156900 -0.06730700
C 3.61564900 -2.19284200 0.63269400
H 4.45851500 -1.98695800 1.29038900
C 1.87557500 2.32036100 -1.77404700
H 1.12707600 2.30155200 -2.57076000

C 0.02096400 0.13787300 4.06446900
C 3.80452700 3.19060900 -0.69692100
C 2.89273500 3.26643400 -1.75423200
H 2.96689300 4.02929200 -2.53236800
C 2.48465800 -3.73892400 -0.86152400
H 2.40964600 -4.70189600 -1.37024200
C -1.62103000 2.71447100 -1.03216900
H -0.78135500 2.93721400 -1.68957500
C -2.67123000 3.62134500 -0.89549400
H -2.66255700 4.58383700 -1.41073900
C 3.55656900 -3.41841100 -0.02453600
C -3.59352800 -3.32256100 -0.74124800
C -1.82357000 -2.25449600 -1.90026800
H -1.14466300 -2.14808000 -2.74928900
H -0.18653400 0.45169800 -3.47089600
H 0.66697100 -0.82736800 -2.25992900
F -4.78898500 4.05957600 0.10171000
F 4.81662800 4.10176900 -0.60644000
F 4.55429500 -4.32100000 0.16829900
F -4.52275700 -4.31087000 -0.62598700
F 0.01536000 0.22274900 5.41716000

Transition state: $[(p\text{–}\mathbf{F}\text{PY})_5\text{Me}_2\text{MoO}\cdots\text{H}\cdots\text{H}]^{+\,\ddagger}$
Mo 0.00403700 -0.01561700 -0.99523000
O -0.54659300 0.82166400 -2.61076800
N -1.68221100 -1.36604800 -0.92071400
N 1.50336700 -1.58466200 -0.39236400
N 1.70895300 1.30023300 -0.88282000
N -1.55072600 1.52156100 -0.32372500
C -2.55739500 -1.37888100 0.14060100
N -0.01638900 -0.02948600 1.25000300
C -2.52435300 -0.20158700 1.15976400
C -2.62753000 1.15490800 0.41615900
C 2.56433400 -1.27998300 0.40931800
C -2.79948100 -3.32272700 -1.86695300
H -2.89241700 -4.04385400 -2.68152400
C -3.50221300 -2.41079200 0.27658000
H -4.17814400 -2.47435800 1.12786600
C 2.61994000 1.24545800 0.14350600
C 3.69815400 0.14891500 2.14981100
H 3.68666100 -0.70148200 2.84688400
H 3.66827500 1.07687300 2.73919900
H 4.65569900 0.12823900 1.60965700
C -3.75392200 1.99040500 0.52974700
H -4.64335500 1.70605200 1.09078400
C -3.71640000 -0.33633100 2.13537400
H -3.77496500 0.53162900 2.80797900
H -3.62897400 -1.24211600 2.75321000
H -4.66518200 -0.39563300 1.58256100
C 3.64437400 2.20449800 0.25220900
H 4.36617200 2.19459500 1.06726500
C 1.19016500 0.15686200 3.34038000
H 2.11162300 0.27433100 3.90647100
C -1.21962200 -0.11026400 3.35153600
H -2.14131000 -0.20580200 3.92162200
C 1.16685000 0.09220200 1.94084700
C 1.46247800 -2.81112000 -0.98892100
H 0.57912800 -3.02457300 -1.59219300
C 2.51320700 0.07473700 1.15946000
C -1.19250200 -0.13555100 1.95066700
C -3.71450900 3.23126400 -0.10583400
C 3.63198300 -2.17997400 0.57052600
H 4.49937200 -1.95158300 1.18814400
C 1.86751200 2.27689100 -1.83621300
H 1.13753400 2.23323900 -2.64971900
C -0.01536000 0.05236800 4.02536600
C 3.74614400 3.19957200 -0.71726300
C 2.86419500 3.24568700 -1.79942400
H 2.94373300 4.00252200 -2.58285300
C 2.46799500 -3.76573300 -0.86408100
H 2.39125900 -4.73757300 -1.35520200
C -1.54356000 2.73827000 -0.92571800
H -0.65978000 2.97167800 -1.52002000
C -2.59734600 3.64664500 -0.83379500
H -2.54994400 4.62576700 -1.31439400
C 3.56902000 -3.41149800 -0.08121500
C -3.59935100 -3.37924400 -0.72410300
C -1.85701200 -2.29930500 -1.91194700
H -1.19244400 -2.20107500 -2.77320300
H 0.28866200 -0.25782100 -2.83612900
H 0.79593800 -0.95336300 -2.48205000
F -0.01344400 0.10139800 5.38073600
F 4.73413600 4.13211700 -0.60679300
F 4.59501200 -4.28701700 0.06931500
F -4.51258300 -4.37882000 -0.58556100
F -4.79027500 4.05499400 -0.00221500

Product complex: $[(p\text{–}\mathbf{F}\text{PY})_5\text{Me}_2\text{MoO})]^+ + \text{H}_2$
Mo -0.08369500 -0.05410200 -0.87667800
O -0.12945400 -0.08040600 -2.63106900
N -1.72714500 -1.42903700 -0.59235100
N 1.51145600 -1.49708000 -0.62896400
N 1.56805300 1.33261100 -0.72058800
N -1.66150600 1.39769400 -0.58592300
C -2.62693600 -1.27289300 0.43537300
N -0.02129500 -0.02256600 1.38387800
C -2.52522100 0.00080300 1.32594700
C -2.58819300 1.26569600 0.42107700
C 2.49725000 -1.32964100 0.31455300
C -2.89184500 -3.43663400 -1.33097000
H -2.99172900 -4.24923600 -2.05319900
C -3.62906400 -2.23420400 0.65326500
H -4.33864000 -2.15762300 1.47540700
C 2.51964600 1.20988500 0.26404700
C 3.71523100 -0.03424400 2.11228500
H 3.72238400 -0.91388300 2.77204700
H 3.72494400 0.85920900 2.75302300
H 4.64386200 -0.04130600 1.52266700
C -3.57515200 2.24818900 0.61077900
H -4.30766500 2.18798900 1.41400800
C -3.71296900 0.02433700 2.31515300
H -3.67747400 0.91772500 2.95534900

H -3.69656300 -0.85513600 2.97501400
H -4.67164600 0.02815000 1.77559500
C 3.52116200 2.18554900 0.40870500
H 4.27142200 2.13646200 1.19629300
C 1.25216500 -0.01350900 3.44649000
H 2.19608700 -0.01476200 3.98874900
C -1.17934600 0.00631400 3.51324400
H -2.09199700 0.01868400 4.10640800
C 1.18401700 -0.02414200 2.04878900
C 1.58170200 -2.57542900 -1.46894600
H 0.81391700 -2.62979100 -2.24097400
C 2.47581800 -0.04231600 1.18882600
C -1.18821100 -0.00663900 2.11396400
C -3.63850800 3.32497000 -0.27396100
C 3.50358200 -2.29842000 0.46999700
H 4.28498800 -2.20868000 1.22286100
C 1.68693400 2.35293600 -1.62585400
H 0.96089100 2.35048100 -2.44034800
C 0.05518600 0.00159100 4.16006200
C 3.57589400 3.24043300 -0.50291900
C 2.67406000 3.33141400 -1.56519500
H 2.72987800 4.12682400 -2.31099600
C 2.56799200 -3.55372500 -1.39384900
H 2.58420500 -4.39548800 -2.08881400
C -1.77992400 2.44866200 -1.45485500
H -1.06392800 2.47056900 -2.27674000
C -2.75334700 3.43679500 -1.34803600
H -2.80976600 4.25571900 -2.06773600
C 3.52029800 -3.40123800 -0.38417600
C -3.73909700 -3.31024600 -0.22809100
C -1.90010400 -2.47018800 -1.46459700
H -1.21632800 -2.49450600 -2.31455000
H 3.18713500 -0.33614200 -6.57322100
H 3.92365900 -0.24996900 -6.45217200
F -4.59795900 4.27072600 -0.09052400
F 4.54734100 4.18204900 -0.36103500
F 4.49875100 -4.33331600 -0.23476600
F -4.71110400 -4.23777000 -0.01510300
F 0.09286800 0.01299500 5.52156600

Reactant complex: $[(p\text{–}\mathbf{CF_3}\text{PY})_5\text{Me}_2\text{Mo(H)(OH)}]^+$
Mo 0.03466200 0.00299300 -1.57093700
O -0.56356800 0.86610300 -3.32288500
N -1.62660100 -1.35309400 -1.53635300
N 1.52537700 -1.55763200 -1.07407200
N 1.71468100 1.31629300 -1.46171600
N -1.58133000 1.49681800 -1.04573800
C -2.50455000 -1.37871500 -0.47985800
N 0.03442500 -0.04483700 0.65629500
C -2.47516700 -0.20303900 0.54303800
C -2.60654500 1.14320600 -0.22222400
C 2.56229600 -1.29770800 -0.22401800
C -2.77276700 -3.25169400 -2.53627100
H -2.86408600 -3.93409000 -3.38441800
C -3.45760700 -2.40622600 -0.37482100
H -4.12003200 -2.46758000 0.48646100
C 2.65701200 1.22688900 -0.46164900
C 3.73867900 0.09379800 1.52677300
H 3.70388300 -0.74849100 2.23335300
H 3.73862400 1.02716900 2.10806900
H 4.69361900 0.04100900 0.98444400
C -3.72287800 1.98348600 -0.05907300
H -4.55786800 1.69137800 0.57505100
C -3.66372000 -0.35626600 1.52117300
H -3.73571900 0.50558900 2.19973000
H -3.55771400 -1.26346000 2.13422500
H -4.61360800 -0.42671700 0.97192600
C 3.70623100 2.15775200 -0.37560800
H 4.43913900 2.09438700 0.42625800
C 1.22702400 0.20595300 2.73703500
H 2.15871300 0.35121900 3.27942900
C -1.17164200 -0.04770700 2.74390200
H -2.10743700 -0.12077300 3.29345900
C 1.21289100 0.08817100 1.34037500
C 1.48001000 -2.78109800 -1.68619400
H 0.62877600 -2.95588700 -2.34272000
C 2.54606800 0.04790100 0.54357400
C -1.14788700 -0.11747400 1.34351000
C -3.76794000 3.21328800 -0.72725500
C 3.59386500 -2.23835900 -0.03646300
H 4.43490100 -2.01530600 0.61681900
C 1.87292400 2.30827600 -2.40512600
H 1.12542600 2.30035100 -3.20166200
C 0.02378000 0.13241000 3.44324100
C 3.83148600 3.18124400 -1.32357600
C 2.89354900 3.24466500 -2.37322500
H 2.94935100 4.00440900 -3.15678000
C 2.44603600 -3.76274000 -1.51504900
H 2.33863900 -4.71947700 -2.03094600
C -1.63319700 2.69568700 -1.68605200
H -0.79447900 2.92325200 -2.34239600
C -2.69262100 3.58905500 -1.54788200
H -2.66843700 4.54598300 -2.07424200
C 3.54307400 -3.47599200 -0.68365400
C -3.58722700 -3.36072500 -1.39458700
C -1.81349000 -2.24756300 -2.55994000
H -1.14417200 -2.12626400 -3.41435800
H -0.16558100 0.45896800 -4.11274700
H 0.70448000 -0.80924100 -2.88897400
C 0.02297000 0.18814600 4.95843000
F 1.04593200 0.95079600 5.44249700
F 0.16800000 -1.06475300 5.49916800
F -1.14070100 0.70134800 5.45295000
C -4.94454300 4.15010900 -0.55484000
C 4.93256500 4.20419500 -1.23188300
C 4.64510100 -4.49699500 -0.51003000
C -4.57385000 -4.49665300 -1.27438200
F -5.26461500 -4.69791400 -2.44057500
F -5.49580500 -4.29434300 -0.28817400
F -3.94338600 -5.68630200 -0.98962300
F -5.44000900 4.56280400 -1.76335700
F -5.97620100 3.58141700 0.13192400

F -4.58390500 5.28511800 0.12727400
F 5.62487500 4.31834400 -2.41306500
F 4.44246000 5.46170700 -0.95802300
F 5.84640500 3.91761000 -0.25853400
F 5.55360700 -4.13701100 0.44081900
F 5.33969800 -4.68684800 -1.67887500
F 4.14544100 -5.72188400 -0.15221600

Transition state: $[(p\text{–}\mathbf{CF_3}\text{PY})_5\text{Me}_2\text{MoO}\cdots\text{H}\cdots\text{H}]^{+\ \ddagger}$
Mo 0.01180100 0.00593500 -0.99072900
O -0.53603000 0.85939100 -2.58302700
N -1.67170600 -1.34403800 -0.93453200
N 1.50133200 -1.57184500 -0.41098600
N 1.71240200 1.30566200 -0.86314400
N -1.54658000 1.54445100 -0.31670400
C -2.55331200 -1.36671500 0.11991000
N -0.02448200 -0.02845700 1.24395200
C -2.53209300 -0.19194600 1.14086000
C -2.63065800 1.16763600 0.40299600
C 2.55251300 -1.28689400 0.40852600
C -2.77886300 -3.29061800 -1.89424400
H -2.85355700 -3.99185600 -2.72853600
C -3.48881400 -2.40738500 0.24265700
H -4.15450000 -2.45907300 1.10203400
C 2.62047000 1.23878000 0.16517300
C 3.68675300 0.11954700 2.16689800
H 3.66865800 -0.73651300 2.85693000
H 3.65995200 1.04223700 2.76443300
H 4.64650700 0.09833200 1.63075800
C -3.76178100 2.00096800 0.49691500
H -4.65241500 1.68248700 1.03600900
C -3.73172900 -0.32939800 2.10737400
H -3.79705900 0.53855000 2.77961300
H -3.64845000 -1.23471900 2.72609300
H -4.67621800 -0.39099300 1.54747300
C 3.64434900 2.19499800 0.28205500
H 4.34839600 2.15527400 1.11069500
C 1.16301400 0.13242900 3.34290600
H 2.09584100 0.24282900 3.89132300
C -1.23183100 -0.12122100 3.33848700
H -2.16897400 -0.22549800 3.88049400
C 1.15598100 0.07761400 1.94391100
C 1.45696600 -2.79165300 -1.02304900
H 0.58276900 -2.99124400 -1.64325200
C 2.50525800 0.05973900 1.17087000
C -1.20524400 -0.13302400 1.93805500
C -3.73827900 3.25869800 -0.11632800
C 3.60838000 -2.20256800 0.56864100
H 4.46183400 -1.96313800 1.20010900
C 1.88229100 2.28795300 -1.81175200
H 1.16105600 2.25657300 -2.63232200
C -0.03932100 0.02842600 4.04925800
C 3.78022800 3.21256300 -0.67027200
C 2.88403700 3.24516800 -1.75466900
H 2.95496300 3.99598300 -2.54550400
C 2.45245000 -3.75155000 -0.88504700
H 2.35083300 -4.71279400 -1.39350100
C -1.52783500 2.76828400 -0.90315700
H -0.63459400 3.01284600 -1.47822000
C -2.58744000 3.66741100 -0.81120300
H -2.51053700 4.65015600 -1.28203900
C 3.56475100 -3.43940200 -0.08471600
C -3.60040000 -3.38606600 -0.75691600
C -1.83869700 -2.26938800 -1.93555400
H -1.17447400 -2.16188200 -2.79558200
H 0.27712100 -0.21036200 -2.83353700
H 0.78098800 -0.91839600 -2.47388200
C -4.57524900 -4.52995500 -0.62031600
C -4.92893100 4.19096700 -0.02883900
C 4.69338700 -4.43821500 0.05622900
C 4.85350900 4.26429500 -0.54414600
F 5.35895700 -4.60891800 -1.13142400
F 4.22813900 -5.67301900 0.42355000
F 5.61838700 -4.06080500 0.98350800
F 5.75385700 3.98841500 0.44403900
F 5.56406200 4.40939900 -1.70920100
F 4.32239700 5.50230900 -0.26406600
F -4.60729000 5.35037200 0.62891500
F -5.98725600 3.63660500 0.62742000
F -5.37039400 4.55719000 -1.27329700
F -5.25624900 -4.76199300 -1.78662000
F -5.50544600 -4.31790800 0.35591800
F -3.93364600 -5.70667200 -0.30821700
C -0.04449600 0.11797500 5.56042400
F -0.02924000 1.42506500 5.98187300
F -1.15059800 -0.46290900 6.10857400
F 1.05087000 -0.48490700 6.11224200

Product complex: $[(p\text{–}\mathbf{CF_3}\text{PY})_5\text{Me}_2\text{MoO})]^+ + \text{H}_2$
Mo -0.07254900 -0.05074800 -1.54932300
O -0.10622700 -0.08417700 -3.29060300
N -1.70888200 -1.42657800 -1.26066400
N 1.51862700 -1.48781700 -1.28709300
N 1.56956600 1.33776800 -1.37541400
N -1.65047400 1.39722200 -1.27600600
C -2.61761500 -1.26635400 -0.24359100
N -0.02671300 -0.01219100 0.71467800
C -2.52673200 0.01315200 0.63931100
C -2.57977100 1.27416200 -0.27201900
C 2.49159900 -1.32396000 -0.33170900
C -2.86791600 -3.42859100 -1.99929400
H -2.94619800 -4.23325600 -2.73366700
C -3.61877300 -2.23004900 -0.03611200
H -4.32399000 -2.12840000 0.78624100
C 2.51547300 1.21751500 -0.38706100
C 3.70408500 -0.02392400 1.46755700
H 3.70778300 -0.90062200 2.13108000
H 3.71262800 0.87119800 2.10582800
H 4.63544800 -0.03435000 0.88220700
C -3.56344600 2.26230300 -0.09854400
H -4.28823100 2.18693000 0.70961900
C -3.72465600 0.04149200 1.61653000

H -3.69521500 0.93699100 2.25389400
H -3.71584500 -0.83469700 2.28068700
H -4.67812400 0.04364900 1.06773900
C 3.51462500 2.19536100 -0.24667000
H 4.24918900 2.12703800 0.55336900
C 1.22440900 0.00271200 2.78571100
H 2.17726500 0.00521500 3.31148100
C -1.19284600 0.02305600 2.83432500
H -2.12357000 0.04049700 3.39822800
C 1.17213300 -0.01240700 1.38942000
C 1.59753200 -2.56275600 -2.13112800
H 0.84387400 -2.61242200 -2.91687700
C 2.46821300 -0.03352900 0.53868400
C -1.19736800 0.00714600 1.43732400
C -3.64644600 3.34589100 -0.98420300
C 3.48919800 -2.29995200 -0.16767900
H 4.24992000 -2.19094200 0.60267100
C 1.69464000 2.35098300 -2.28794500
H 0.97479100 2.34687300 -3.10734600
C 0.03043000 0.02285200 3.52179600
C 3.60003700 3.25938000 -1.15592500
C 2.68511900 3.32210200 -2.22082700
H 2.73071900 4.10211800 -2.98406000
C 2.58080600 -3.53890800 -2.03653600
H 2.58866900 -4.36878300 -2.74660500
C -1.76529600 2.43883300 -2.15685500
H -1.04983600 2.45244200 -2.97894000
C -2.73916600 3.42372100 -2.05425600
H -2.77761300 4.22541300 -2.79504100
C 3.53735200 -3.41586800 -1.01455200
C -3.74426700 -3.32269900 -0.90578800
C -1.87344600 -2.46858500 -2.13359800
H -1.18357700 -2.49718100 -2.97786300
H 3.10162600 -0.58023500 -7.23313700
H 3.78416600 -0.86072400 -7.09158900
C 0.05822000 -0.01563700 5.02898500
F 1.19294100 0.54844100 5.54264200
F 0.01418000 -1.30714300 5.50744800
F -1.00822600 0.63735300 5.58396700
C -4.68252200 4.42830000 -0.78677400
C 4.64888200 4.33459300 -0.99116600
C 4.58863000 -4.48584100 -0.82944800
C -4.79444400 -4.38296500 -0.66887200
F -5.38009500 -4.79005600 -1.83713400
F -5.79282100 -3.95851700 0.15940400
F -4.25189700 -5.50771300 -0.09315100
F 5.18801000 4.70889200 -2.19228500
F 5.68041000 3.94403500 -0.18716500
F 4.11804600 5.47280900 -0.43125900
F -5.23339200 4.82795400 -1.97425400
F -5.70710400 4.03341100 0.02372400
F -4.13313500 5.55127700 -0.21475100
F 5.12410600 -4.88387700 -2.02511700
F 5.62211500 -4.07729300 -0.03792600
F 4.06050100 -5.61277300 -0.24581900

Reactant complex: $[(p-\mathbf{CN}\text{PY})_5\text{Me}_2\text{Mo(H)(OH)}]^+$

Mo 0.03605000 0.02619500 -0.91373000
O -0.55616500 0.87841000 -2.66113400
N -1.62122800 -1.33015300 -0.87644300
N 1.52439800 -1.53413200 -0.41948400
N 1.71390900 1.34001700 -0.81274400
N -1.58186500 1.52035600 -0.39531800
C -2.49937000 -1.35633500 0.18211900
N 0.03805300 -0.01547200 1.31080000
C -2.47314600 -0.17680500 1.20075600
C -2.60691400 1.16713300 0.43133200
C 2.56347800 -1.27348200 0.43110700
C -2.75518200 -3.23652500 -1.87688500
H -2.84566700 -3.92399100 -2.72024000
C -3.44616900 -2.38344200 0.29225400
H -4.11044100 -2.44738700 1.15205600
C 2.65791100 1.25313500 0.18844300
C 3.74555100 0.12252900 2.17530600
H 3.71324500 -0.71888600 2.88286900
H 3.74584100 1.05631700 2.75568900
H 4.69897200 0.07000400 1.63042000
C -3.72221900 2.00291400 0.59389400
H -4.55788600 1.71499300 1.22922500
C -3.66130500 -0.32953300 2.17941600
H -3.73405000 0.53351000 2.85624700
H -3.55385500 -1.23517700 2.79425100
H -4.61096400 -0.40264200 1.63024000
C 3.70192600 2.18292500 0.27518900
H 4.43717700 2.12478000 1.07556000
C 1.23847800 0.23402000 3.38845100
H 2.16929300 0.37494800 3.93297400
C -1.17101000 -0.01928900 3.39754000
H -2.10316500 -0.09700100 3.95199000
C 1.21859100 0.11587800 1.99413400
C 1.47602100 -2.75857900 -1.02955500
H 0.62646500 -2.93290500 -1.68820200
C 2.55035400 0.07444100 1.19522900
C -1.14510700 -0.08736600 1.99957500
C -3.76987300 3.24145700 -0.07936200
C 3.59083700 -2.21197800 0.62280900
H 4.43474100 -1.99076900 1.27315500
C 1.86866200 2.33015000 -1.75868300
H 1.12187700 2.31953300 -2.55548100
C 0.03072700 0.15996600 4.10296700
C 3.82632500 3.21684900 -0.67822200
C 2.88310700 3.27150300 -1.73211200
H 2.93953000 4.03207400 -2.51374200
C 2.43499100 -3.74560100 -0.85707800
H 2.32974400 -4.70362600 -1.36955200
C -1.63345600 2.71670800 -1.03969800
H -0.79544400 2.94324000 -1.69723700
C -2.68944600 3.61374200 -0.90527400
H -2.66929100 4.57094500 -1.42967900
C 3.53891200 -3.46201000 -0.02319800
C -3.57235500 -3.35238100 -0.72908600
C -1.80453700 -2.22641200 -1.89985400

H -1.13818700 -2.10268800 -2.75615500
H -0.16039900 0.48107300 -3.45751400
H 0.70396000 -0.78959500 -2.22581900
C 4.88697600 4.17020900 -0.58111800
N 5.75996900 4.95927600 -0.50503500
C 4.58287000 -4.42438300 0.17436700
N 5.43865300 -5.21757900 0.33257600
C -4.90255100 4.10730700 0.08498800
N -5.83041600 4.81962100 0.21633100
C -4.53109500 -4.40806800 -0.60835200
N -5.31913500 -5.27903900 -0.51175800
C 0.02440600 0.25749200 5.53480700
N 0.01882000 0.33907700 6.70876700

Transition state: $[(p\text{−}\mathbf{CN}\text{PY})_5\text{Me}_2\text{MoO}\cdots\text{H}\cdots\text{H}]^{+\ ‡}$
Mo 0.00401800 -0.00754800 -0.98098500
O -0.55726700 0.83401600 -2.56704300
N -1.67315600 -1.36212600 -0.90102000
N 1.50015100 -1.57641000 -0.40657100
N 1.70094200 1.29639900 -0.88367800
N -1.55321800 1.53326400 -0.30749300
C -2.54792200 -1.37918500 0.16102900
N -0.01230600 -0.02463500 1.24985100
C -2.52252500 -0.19595000 1.17222900
C -2.63116200 1.15824500 0.42576500
C 2.55972300 -1.28261200 0.40250800
C -2.77610800 -3.31954300 -1.84473100
H -2.85569100 -4.02953700 -2.67029900
C -3.47773100 -2.41769400 0.29982700
H -4.13901400 -2.46779800 1.16281000
C 2.61877500 1.24208000 0.13921700
C 3.70867500 0.14103900 2.13799200
H 3.69986000 -0.70983800 2.83437700
H 3.68447800 1.06782100 2.72895100
H 4.66283800 0.11916800 1.59214500
C -3.76022400 1.98766900 0.52709300
H -4.64672000 1.67488900 1.07658200
C -3.71374500 -0.32999100 2.14956300
H -3.77565700 0.54199900 2.81669700
H -3.62303100 -1.23095700 2.77327200
H -4.66243300 -0.39751600 1.59762600
C 3.63540100 2.20143900 0.24252600
H 4.34730200 2.17555900 1.06528000
C 1.19872000 0.15614800 3.33531300
H 2.13310700 0.27853000 3.87770800
C -1.20550000 -0.10797700 3.35366600
H -2.13592200 -0.20976900 3.90726300
C 1.17519200 0.08927300 1.93932000
C 1.45120500 -2.80119800 -1.00870600
H 0.57291700 -3.00700700 -1.62075800
C 2.51743200 0.07010000 1.15442600
C -1.18823500 -0.12763000 1.95634600
C -3.74487100 3.25185300 -0.09616000
C 3.61665000 -2.19126600 0.56173300
H 4.47742900 -1.94726300 1.18154800
C 1.85827100 2.26997500 -1.84368600
H 1.13266600 2.22848800 -2.65959500
C -0.00187100 0.05525600 4.06085700
C 3.75986500 3.22246100 -0.72344700
C 2.85145700 3.23510800 -1.80631200
H 2.91481800 3.98120300 -2.60120300
C 2.44525300 -3.76166900 -0.87434800
H 2.34480100 -4.72709900 -1.37354800
C -1.53951100 2.75286300 -0.90203400
H -0.65182000 2.99541900 -1.48649800
C -2.59522600 3.65546500 -0.80789400
H -2.52787600 4.63622400 -1.28242700
C 3.57166700 -3.44342600 -0.08479500
C -3.59394300 -3.41489600 -0.69594600
C -1.84276500 -2.29472300 -1.89539200
H -1.18558900 -2.19116100 -2.76119400
H 0.24508800 -0.22911200 -2.82491000
H 0.75070800 -0.94046500 -2.45791400
C -4.88684100 4.11668900 0.00312200
N -5.82115800 4.82784500 0.08199000
C 4.79242100 4.20665200 -0.61013100
N 5.64071500 5.01984100 -0.52019000
C -4.54216700 -4.47628100 -0.54963400
N -5.32147300 -5.35263700 -0.43166400
C 4.64764600 -4.37782200 0.07453400
N 5.52969900 -5.14714300 0.20219500
C 0.00268700 0.10864600 5.49269200
N 0.00620700 0.15273500 6.66947000

Product complex: $[(p\text{−}\mathbf{CN}\text{PY})_5\text{Me}_2\text{MoO})]^+ + \text{H}_2$
Mo -0.05244100 -0.13276900 -0.86879800
O -0.07671400 -0.20918700 -2.60141500
N -1.70520700 -1.48118800 -0.55410000
N 1.53355500 -1.56556700 -0.55983400
N 1.58919400 1.25641000 -0.71650300
N -1.61140200 1.33777100 -0.62946900
C -2.62391800 -1.28225100 0.44867200
N -0.01376900 -0.04575800 1.40093100
C -2.51257400 0.00755600 1.31432600
C -2.53521000 1.25711600 0.38554200
C 2.51613000 -1.37093900 0.38173200
C -2.89277000 -3.47322100 -1.27741400
H -2.97913500 -4.29218100 -1.99416500
C -3.64963500 -2.21394600 0.65870300
H -4.36611400 -2.08387500 1.46705200
C 2.51997500 1.17013000 0.29103000
C 3.71551300 -0.03477000 2.16493500
H 3.73162900 -0.90766200 2.83307900
H 3.70866600 0.86354500 2.79858700
H 4.64776100 -0.03368800 1.58105300
C -3.48573900 2.27321100 0.55413300
H -4.20269300 2.23853300 1.37213300
C -3.71475200 0.07387000 2.28433600
H -3.66459700 0.97227700 2.91600700
H -3.73242000 -0.79758700 2.95429200
H -4.66443600 0.09722700 1.72970000
C 3.49621500 2.16552300 0.43432800

H 4.21569400 2.13070700 1.25019400
C 1.23435300 -0.03904400 3.47366800
H 2.18332000 -0.04410100 4.00589400
C -1.19366300 -0.00525000 3.51280000
H -2.12451500 0.01468000 4.07574100
C 1.18262100 -0.04911100 2.07994200
C 1.60788200 -2.66163600 -1.37694800
H 0.84077300 -2.74214800 -2.14666000
C 2.48156600 -0.06846400 1.23387500
C -1.18730400 -0.01586300 2.11817700
C -3.54747000 3.35352100 -0.35334500
C 3.52886300 -2.32492200 0.55112300
H 4.30134900 -2.19179000 1.30569300
C 1.71725000 2.24851900 -1.65209900
H 1.01632300 2.21246100 -2.48685400
C 0.03198400 -0.02063600 4.21336300
C 3.58092400 3.22359500 -0.49749100
C 2.68581000 3.23952100 -1.58996300
H 2.73665100 4.00456500 -2.36704000
C 2.60001400 -3.62658700 -1.27870900
H 2.60580000 -4.47714200 -1.96288100
C -1.70884700 2.36180700 -1.53331500
H -1.00473700 2.33770100 -2.36468600
C -2.64984400 3.37708700 -1.44320800
H -2.67700600 4.16592000 -2.19731000
C 3.57982500 -3.46922100 -0.27430200
C -3.78872200 -3.33005000 -0.19495000
C -1.87864100 -2.53608700 -1.41037300
H -1.17708200 -2.59726400 -2.24307100
H 2.64856300 0.43858800 -6.89007800
H 3.32761900 0.72558200 -6.74494500
C 4.57773400 4.24103300 -0.34688800
N 5.39515100 5.08046200 -0.22473500
C 4.62059200 -4.43830000 -0.10102300
N 5.47470000 -5.23718900 0.03931200
C -4.83798200 -4.27996000 0.02509100
N -5.69880900 -5.06391200 0.20397700
C -4.52164100 4.38899000 -0.17863000
N -5.32086800 5.24268500 -0.03705800
C 0.05473100 -0.01334300 5.64254400
N 0.07337700 -0.00787900 6.82160800

4.3 Water–Assisted MHR Processes: One water molecule

4.3.1 Structures with no substituent groups: hydrogen atoms at all positions

Reactant complex: $[PY_5Me_2Mo(H)(OH)\cdots H_2O]^+$

Mo 0.01532700 -0.01833300 -0.80107100
O 0.66078900 0.77877200 -2.56870700
H 0.23774400 0.38242200 -3.36007900
H -0.67137900 -0.90727000 -2.09218500
O -1.08739100 -0.65781900 -4.55419200
H -1.20369300 -0.91846000 -3.60472600
H -1.82930000 -0.04767500 -4.72955200
N -1.46827400 -1.56203600 -0.19900800
N 1.68811200 -1.37042500 -0.68293200
N 1.60134400 1.51586800 -0.29197600
N -1.66903500 1.30530200 -0.76707600
C -2.52570400 -1.24802300 0.60657500
N 0.00006800 0.04868400 1.43257200
C -2.51206100 0.14090300 1.29403000
C -2.61803000 1.26888300 0.23086600
C 2.56102800 -1.33893300 0.37788400
C -2.37904200 -3.79209800 -0.51615400
H -2.25907200 -4.78084400 -0.96628300
C -3.56114500 -2.17941500 0.82512100
H -4.41867500 -1.91473400 1.44252400
C 2.63331700 1.19997200 0.54013200
C 3.69006500 -0.22156000 2.34332000
H 3.59082000 -1.10627300 2.98967100
H 3.74368900 0.66672000 2.98877300
H 4.64547800 -0.30044900 1.80465400
C -3.66315500 2.21237200 0.26190700
H -4.40080200 2.18966700 1.06332400
C -3.71157800 0.23937300 2.26535900
H -3.71181600 1.20041500 2.80002500
H -3.68403700 -0.56758400 3.01228400
H -4.66267300 0.16279700 1.71875500
C 3.73572500 2.06516100 0.67778400
H 4.57430700 1.80037300 1.32122500
C 1.18081700 0.10636600 3.53552000
H 2.10960800 0.03577200 4.09831400
C -1.20732900 0.38816100 3.49350900
H -2.14405200 0.55730400 4.02115300
C 1.17485900 -0.01013900 2.13610700
C 1.88218400 -2.31770800 -1.65573800
H 1.20463700 -2.24641700 -2.50988000
C 2.50859600 -0.12074500 1.34934800
C -1.18504600 0.21751800 2.10030500
C -3.78186900 3.19382100 -0.73095000
H -4.59568900 3.92318200 -0.69408800
C 3.52455000 -2.35471600 0.53059700
H 4.18318200 -2.36864100 1.39823800
C 1.63176500 2.70199200 -0.95693100
H 0.78485500 2.89600300 -1.61465300
C -0.01642400 0.32410500 4.22029500
H -0.02253700 0.43442500 5.30838600
C 3.76549200 3.28248200 -0.01653700
H 4.62005500 3.95655500 0.09359900
C 2.67985200 3.61556900 -0.83912600
H 2.63789500 4.56146400 -1.38551700
C 2.85515300 -3.31082800 -1.57965900
H 2.95117500 -4.03694000 -2.39134600
C -1.81449500 2.25622000 -1.75309600
H -1.05495600 2.20808900 -2.53771400
C -2.83490500 3.19946500 -1.76997500
H -2.87915500 3.92463900 -2.58759600
C 3.67114400 -3.35858500 -0.43823500
H 4.42073300 -4.14410600 -0.30757500
C -3.49921000 -3.45875800 0.26114400
H -4.30311100 -4.17916500 0.43708800

C -1.40359700 -2.82209500 -0.72604500
H -0.53079900 -3.03204000 -1.34421900

Transition state: $[PY_5Me_2MoO\cdots H\cdots H\cdots H_2O]^{+}$ ‡
Mo -0.00753500 -0.08416200 -0.95350000
O 0.56922900 0.63931000 -2.60066700
H 0.33380300 -0.00954300 -3.57109600
H -1.09996300 -1.02510900 -2.28946400
O -0.06055800 -0.88132200 -4.36480900
H -0.75315900 -1.08775500 -3.07790100
H -0.73459800 -0.48412700 -4.95097400
N -1.46807800 -1.64980400 -0.24641900
N 1.65886200 -1.45167000 -0.85941500
N 1.53227400 1.43331100 -0.34999900
N -1.69873500 1.23843600 -0.86342100
C -2.52710200 -1.31629500 0.54673000
N 0.02306100 -0.04069400 1.31069600
C -2.49447600 0.07967100 1.22164700
C -2.61328100 1.21163800 0.16195000
C 2.53170400 -1.45473800 0.20174200
C -2.36812800 -3.88470800 -0.52363800
H -2.24417800 -4.88415600 -0.94794200
C -3.56170100 -2.24259000 0.77847600
H -4.42431500 -1.96791200 1.38459600
C 2.60891200 1.09099400 0.40854800
C 3.72430700 -0.36217800 2.14601300
H 3.63846700 -1.24922100 2.79076300
H 3.79863000 0.52196900 2.79542400
H 4.66390100 -0.44437300 1.58010000
C -3.64232700 2.17123300 0.22415500
H -4.35446600 2.16323400 1.04836000
C -3.67665500 0.18656100 2.21319200
H -3.65596500 1.14315700 2.75524900
H -3.64710100 -0.62593500 2.95375600
H -4.63722900 0.12509500 1.68124000
C 3.71637000 1.95441000 0.51216000
H 4.59321600 1.66497400 1.09098500
C 1.23377300 -0.05399600 3.40232000
H 2.17060700 -0.15701100 3.94710300
C -1.14752800 0.27869800 3.39846200
H -2.07366200 0.45440700 3.94260100
C 1.20283300 -0.13892200 2.00177000
C 1.81915600 -2.40016200 -1.83771400
H 1.15532800 -2.29943700 -2.70142100
C 2.51636200 -0.24738600 1.18680100
C -1.14986100 0.13586900 2.00229600
C -3.77918500 3.14869300 -0.77065300
H -4.58155400 3.88913500 -0.71027900
C 3.45685000 -2.50517900 0.35097400
H 4.11538100 -2.54407700 1.21799100
C 1.51233300 2.64733000 -0.96217100
H 0.62623800 2.86529800 -1.55824400
C 0.05153700 0.17732100 4.10907000
H 0.06190900 0.26846500 5.19877400
C 3.69909600 3.19877000 -0.13200700
H 4.55790500 3.87140400 -0.05072500
C 2.56111400 3.56208300 -0.86675100
H 2.48188700 4.52989400 -1.36852400
C 2.75376300 -3.43037900 -1.76264200
H 2.82531200 -4.15567000 -2.57760700
C -1.86279200 2.17905700 -1.85266300
H -1.13018100 2.11032900 -2.66180000
C -2.87227000 3.13567300 -1.84280000
H -2.93811500 3.85460300 -2.66427200
C 3.56661600 -3.51136500 -0.62124400
H 4.28838500 -4.32295800 -0.49364600
C -3.49319100 -3.53298100 0.23602100
H -4.29910600 -4.24952400 0.41852100
C -1.39004400 -2.91720100 -0.74456900
H -0.50790400 -3.14155400 -1.34621400

Product complex: $[PY_5Me_2MoO\cdots H_2O]^{+} + H_2$
Mo 0.11043000 -0.07623300 -0.70257800
O 0.12991500 -0.16799200 -2.47106000
H -0.14274700 0.05106800 -4.20889700
H -6.22114400 -1.27817700 -4.58880600
O -0.27927200 0.14097400 -5.18989800
H -5.71659400 -1.44102000 -5.12108800
H -0.89305700 0.89217100 -5.28426300
N -1.47426000 -1.51578700 -0.38244600
N 1.75533500 -1.44092800 -0.41019800
N 1.68324100 1.38523300 -0.45794200
N -1.54381300 1.31083400 -0.60770500
C -2.46997500 -1.30483500 0.53944300
N 0.05762600 0.02949900 1.54417600
C -2.43876700 0.01564400 1.36080000
C -2.48929100 1.23147900 0.38715900
C 2.65409300 -1.26921600 0.61584600
C -2.54025100 -3.58625300 -1.07342100
H -2.53324400 -4.44912800 -1.74423800
C -3.48625400 -2.26356900 0.70790600
H -4.26568900 -2.11495000 1.45405600
C 2.63440200 1.26685900 0.52633300
C 3.75377900 0.07580800 2.45244100
H 3.72879700 -0.77863800 3.14414800
H 3.73332200 0.99386300 3.05750000
H 4.70995400 0.04573100 1.90922900
C -3.48627800 2.21947300 0.48909500
H -4.21818000 2.18376100 1.29520500
C -3.67334300 0.06148100 2.29033100
H -3.67697800 0.97749400 2.89838600
H -3.68049000 -0.79511900 2.98000200
H -4.60493200 0.03766400 1.70567600
C 3.64592600 2.23763500 0.64619700
H 4.38788200 2.16467500 1.44038500
C 1.21685800 0.13659300 3.66432300
H 2.14672100 0.16488700 4.23046600
C -1.19226600 0.13008600 3.61271200
H -2.14604900 0.15592000 4.13774400
C 1.22944800 0.06543000 2.26527600
C 1.92351800 -2.50143300 -1.26055400
H 1.23907000 -2.53372000 -2.11056200

C 2.56130200 0.03171800 1.46919300
C -1.14370600 0.06227300 2.21433900
C -3.57337300 3.25396900 -0.45421000
H -4.35425000 4.01437200 -0.36583600
C 3.64478300 -2.24065800 0.85129800
H 4.33805500 -2.13051000 1.68416300
C 1.79178200 2.40923400 -1.35997100
H 1.04299900 2.42484500 -2.15238100
C -0.00311000 0.16872700 4.35160200
H -0.02662100 0.22283400 5.44340000
C 3.73277500 3.30119400 -0.26325600
H 4.52677900 4.04646500 -0.16367100
C 2.79467500 3.37293900 -1.30404100
H 2.82551500 4.16252900 -2.05918400
C 2.91125300 -3.46739100 -1.09193700
H 2.99060400 -4.28871400 -1.80898900
C -1.66741500 2.29307300 -1.55391400
H -0.94242100 2.25338100 -2.36910800
C -2.65817100 3.27019000 -1.51804500
H -2.70002000 4.02568700 -2.30705600
C 3.77496200 -3.35452100 0.00870300
H 4.54979800 -4.10194000 0.20042300
C -3.52850200 -3.41374900 -0.09280700
H -4.32644300 -4.14914000 0.04264100
C -1.53707500 -2.62678300 -1.17890700
H -0.75032700 -2.71861300 -1.92805100

4.3.2 Structures with substituent groups at axial position only

Reactant complex: $[PY_4(p{-}\mathbf{NH_2}PY)Me_2Mo(H)(OH)\cdots H_2O]^+$
Mo 0.02198800 -0.03908300 -0.94915700
O 0.64615400 0.78365500 -2.72508300
H 0.24474000 0.35957900 -3.51160900
H -0.57821100 -0.98713700 -2.24267000
O -1.14815300 -0.75652000 -4.66541900
H -1.16830900 -0.97743400 -3.69710500
H -1.90622800 -0.15385800 -4.78982900
N -1.48174800 -1.56381000 -0.36018200
N 1.69942100 -1.38253900 -0.81875400
N 1.59746500 1.50846900 -0.44159200
N -1.66145800 1.28865300 -0.91956800
C -2.52846500 -1.24757800 0.46164200
N 0.00925300 0.02602600 1.27621200
C -2.50133000 0.13829400 1.15361000
C -2.60357700 1.26287000 0.08629200
C 2.57873700 -1.34077700 0.23798200
C -2.41154000 -3.79029400 -0.66883100
H -2.30149900 -4.77911800 -1.12159500
C -3.56685000 -2.17413000 0.68937500
H -4.41487100 -1.90540400 1.31815700
C 2.62820600 1.19900800 0.39502100
C 3.70273100 -0.20976500 2.19630700
H 3.61589500 -1.09631500 2.84183200
H 3.74707300 0.67831600 2.84275100
H 4.65783800 -0.27743200 1.65535300
C -3.64423600 2.21191900 0.11693500
H -4.37559600 2.19938900 0.92427200
C -3.70198600 0.24742600 2.12238800
H -3.69201500 1.20748600 2.65894000
H -3.68457200 -0.56073900 2.86799700
H -4.65322300 0.18153200 1.57453500
C 3.72392900 2.07313500 0.53363500
H 4.56347000 1.81506900 1.17840600
C 1.19465400 0.07253200 3.38193900
H 2.12776600 0.00868500 3.93942600
C -1.20187700 0.35025000 3.34293300
H -2.14239400 0.50668200 3.86885300
C 1.17854100 -0.03096500 1.99292400
C 1.89604800 -2.33897100 -1.78440900
H 1.21540700 -2.27916900 -2.63657500
C 2.51682600 -0.12229600 1.20648900
C -1.16975700 0.19784600 1.95895200
C -3.76549500 3.18824100 -0.88059700
H -4.57389900 3.92354800 -0.84066500
C 3.54978900 -2.34918300 0.39204800
H 4.21358500 -2.35082500 1.25588000
C 1.62077500 2.69472100 -1.10566200
H 0.77488600 2.88034100 -1.76726600
C -0.00701000 0.28445900 4.09942600
C 3.74604200 3.29170400 -0.15880600
H 4.59515300 3.97216600 -0.04516700
C 2.66039400 3.61764400 -0.98384100
H 2.61245300 4.56372900 -1.52947600
C 2.87358600 -3.32671600 -1.70446100
H 2.96798000 -4.05890300 -2.51100000
C -1.81178700 2.23267700 -1.91185800
H -1.05710100 2.17412200 -2.70068000
C -2.82709000 3.18131800 -1.92753000
H -2.87378500 3.90115200 -2.74981400
C 3.69783500 -3.36090400 -0.56822100
H 4.45334800 -4.14042500 -0.43580100
C -3.52156200 -3.45242900 0.12222400
H -4.32788400 -4.16805800 0.30644200
C -1.43314200 -2.82617300 -0.88801200
H -0.56774400 -3.04228700 -1.51448700
N -0.01355600 0.40386200 5.45415500
H 0.85355100 0.40105300 5.98487300
H -0.87080600 0.60945600 5.96047800

Transition state: $[PY_4(p{-}\mathbf{NH_2}PY)Me_2MoO\cdots H\cdots H\cdots H_2O]^{+\ddagger}$
Mo -0.01146400 -0.08369800 -0.95558400
O 0.55191000 0.65160900 -2.61609300
H 0.36757900 -0.02310900 -3.55542700
H -1.11927100 -1.02481000 -2.30156100
O 0.02951400 -0.93917100 -4.36455900
H -0.72572100 -1.11678700 -3.04859700
H -0.64055600 -0.58172200 -4.97984600
N -1.47756400 -1.64232200 -0.25211700
N 1.65363300 -1.44447000 -0.85873300
N 1.52556300 1.43627500 -0.36207300
N -1.70138500 1.24035900 -0.86306400

C -2.52966700 -1.30674000 0.55033500
N 0.02258000 -0.03910700 1.30094100
C -2.49225200 0.08829000 1.22823100
C -2.61222300 1.21833800 0.16627400
C 2.52942200 -1.44644000 0.20151500
C -2.38733300 -3.87399200 -0.52901800
H -2.26942000 -4.87300800 -0.95617100
C -3.56567000 -2.23079300 0.78544600
H -4.42337400 -1.95535400 1.39814100
C 2.59933500 1.09797100 0.40367500
C 3.72518700 -0.34961300 2.13960400
H 3.64347100 -1.23635400 2.78536100
H 3.80025300 0.53507900 2.78810700
H 4.66295700 -0.43076800 1.57036900
C -3.63978000 2.17976600 0.22862100
H -4.34866000 2.17585300 1.05570800
C -3.67552900 0.19778100 2.21799900
H -3.65161600 1.15397000 2.76078500
H -3.64958100 -0.61526000 2.95794300
H -4.63609200 0.14045200 1.68543700
C 3.70447300 1.96480300 0.50782200
H 4.57985200 1.67901600 1.09060200
C 1.24060100 -0.04757100 3.39214800
H 2.18217800 -0.14110900 3.93155500
C -1.14935300 0.27927900 3.39221000
H -2.07977400 0.44021600 3.93469900
C 1.19721200 -0.13480300 2.00258800
C 1.81590000 -2.39427700 -1.83733900
H 1.15596800 -2.29181800 -2.70425100
C 2.51262200 -0.23899800 1.18599700
C -1.14298000 0.14142900 2.00603200
C -3.77850600 3.15539900 -0.76792700
H -4.57830200 3.89854100 -0.70564300
C 3.45584000 -2.49579000 0.34979300
H 4.11634100 -2.53196000 1.21551400
C 1.50699800 2.64823900 -0.97843200
H 0.62416200 2.86064300 -1.58128800
C 0.05580900 0.18581200 4.12997400
C 3.68764500 3.20779500 -0.13887000
H 4.54457600 3.88255400 -0.05481700
C 2.55243800 3.56646300 -0.88010800
H 2.47323700 4.53258500 -1.38522400
C 2.74906400 -3.42544900 -1.75981000
H 2.81958500 -4.15179200 -2.57408200
C -1.86907200 2.17758100 -1.85521500
H -1.13942100 2.10209800 -2.66686400
C -2.87606600 3.13680600 -1.84400200
H -2.94369000 3.85352100 -2.66737400
C 3.56345900 -3.50565700 -0.61910200
H 4.28437400 -4.31782000 -0.49021900
C -3.50559400 -3.52027600 0.23945000
H -4.31240100 -4.23462900 0.42672800
C -1.40732100 -2.90904200 -0.75336400
H -0.52874100 -3.13533400 -1.35988600
N 0.07121800 0.29116200 5.48670600
H 0.94767300 0.28031300 6.00170700
H -0.77129400 0.52527400 6.00521500

Product complex: $[PY_4(p-\mathbf{NH_2}PY)Me_2MoO\cdots H_2O]^+ + H_2$
Mo -0.00890100 -0.08624100 -0.83804200
O -0.02669800 -0.16109000 -2.62630100
H 0.57700300 -0.46427200 -4.21442500
H -5.29114100 -0.91623000 -5.48349400
O 0.93061700 -0.63161300 -5.13477100
H -5.39484400 -0.17775600 -5.57505800
H 0.29244100 -0.19186300 -5.72568000
N -1.55118300 -1.53509500 -0.38834400
N 1.66852400 -1.41136800 -0.62968500
N 1.54458100 1.40379600 -0.59763900
N -1.68259600 1.25662800 -0.72564100
C -2.54007300 -1.28960000 0.53045900
N 0.02848800 0.04022300 1.42268900
C -2.47103900 0.03795100 1.33542000
C -2.56604200 1.22663500 0.32994200
C 2.58774500 -1.26381000 0.38536500
C -2.66702100 -3.58503400 -1.05920300
H -2.67438000 -4.46075000 -1.71299100
C -3.58898700 -2.21269000 0.69722600
H -4.36658600 -2.03416500 1.43879800
C 2.56247500 1.25994900 0.31045500
C 3.75240300 0.07014200 2.19362200
H 3.74528800 -0.77802800 2.89344700
H 3.76415100 0.99534000 2.78844700
H 4.68778600 0.02291100 1.61678200
C -3.54561700 2.22785700 0.46022400
H -4.22340000 2.22832300 1.31350300
C -3.67045300 0.10172000 2.30898800
H -3.64264100 1.02142000 2.91087900
H -3.66351500 -0.75297700 3.00145500
H -4.62289200 0.08824500 1.75898400
C 3.61271100 2.19610100 0.34340700
H 4.41475900 2.09832400 1.07408200
C 1.27069800 0.15352800 3.49188700
H 2.22236700 0.18053600 4.02163100
C -1.14843100 0.16780000 3.52885200
H -2.08312100 0.20192300 4.08751600
C 1.21856500 0.06852400 2.10256100
C 1.82279800 -2.46378100 -1.49818600
H 1.13011400 -2.47366100 -2.34304000
C 2.52294500 0.02840100 1.25690800
C -1.14008000 0.09042300 2.13817200
C -3.67945900 3.23634300 -0.50732600
H -4.43821000 4.01506900 -0.39066000
C 3.57587300 -2.24344000 0.59179500
H 4.28225400 -2.14815700 1.41586600
C 1.59675500 2.43727900 -1.49203000
H 0.77150600 2.49386400 -2.20209500
C 0.07267600 0.20605600 4.24701900
C 3.65440300 3.25999400 -0.56841100
H 4.47587400 3.98116300 -0.53438300
C 2.62907500 3.37158300 -1.51886400
H 2.61196600 4.17200300 -2.26285800

C 2.80108000 -3.44236100 -1.35244200
H 2.86336700 -4.25520800 -2.08126000
C -1.86606100 2.20493700 -1.70149700
H -1.20336700 2.11271400 -2.56549800
C -2.83755800 3.19859300 -1.63153200
H -2.92524900 3.92534300 -2.44394400
C 3.68179400 -3.35341600 -0.26155900
H 4.44820100 -4.11326900 -0.08570700
C -3.66117400 -3.36777000 -0.09404600
H -4.48145500 -4.07795100 0.04306100
C -1.63246800 -2.65884100 -1.16414200
H -0.82869900 -2.79743700 -1.88742400
N 0.09396900 0.26583000 5.60883600
H 0.96941800 0.40744000 6.10654100
H -0.76275600 0.42395400 6.13348700

Reactant complex: $[PY_4(p-\mathbf{CH_3}PY)Me_2Mo(H)(OH)\cdots H_2O]^+$
Mo 0.01716900 -0.03554500 -0.94377100
O 0.65275100 0.76929900 -2.71430800
H 0.23742700 0.36255500 -3.50398800
H -0.64088100 -0.94820900 -2.23392000
O -1.10269900 -0.70679000 -4.68433700
H -1.18787200 -0.95574600 -3.72774100
H -1.85346600 -0.10319500 -4.84390300
N -1.46668700 -1.57669900 -0.34001000
N 1.69796400 -1.37705300 -0.81994300
N 1.59180200 1.51122400 -0.43525800
N -1.67110800 1.28339000 -0.90948300
C -2.52091200 -1.26396600 0.47130600
N 0.00516600 0.03474500 1.28824000
C -2.50507400 0.12436700 1.15968900
C -2.61450400 1.25011600 0.09431500
C 2.57566700 -1.33556900 0.23710000
C -2.37826800 -3.80810800 -0.65190500
H -2.25926600 -4.79706200 -1.10191400
C -3.55491500 -2.19602000 0.69426300
H -4.40958400 -1.93145900 1.31572800
C 2.62458100 1.20387700 0.39923700
C 3.69660000 -0.20746800 2.20078000
H 3.60956500 -1.09554000 2.84418900
H 3.73900000 0.67918400 2.84935400
H 4.65243800 -0.27278400 1.66097400
C -3.65943700 2.19390400 0.12774300
H -4.39193500 2.17464500 0.93395500
C -3.70327000 0.22392600 2.13249100
H -3.70036400 1.18414600 2.66869600
H -3.67661000 -0.58390400 2.87838600
H -4.65526400 0.14974600 1.58707400
C 3.71902200 2.07910200 0.53822200
H 4.55872800 1.82224400 1.18332500
C 1.18113800 0.07725700 3.39299700
H 2.11427800 0.00073300 3.94989700
C -1.19421500 0.35538800 3.35557100
H -2.13482300 0.51548300 3.88078700
C 1.17706200 -0.02370800 1.99562100
C 1.89594000 -2.32727000 -1.78980900
H 1.21388900 -2.26560200 -2.64098900
C 2.51282900 -0.11836400 1.20860700
C -1.17485300 0.19795400 1.96238200
C -3.78428200 3.17186300 -0.86778500
H -4.59731500 3.90197400 -0.82801500
C 3.54984100 -2.34145900 0.38758200
H 4.21328800 -2.34570100 1.25164900
C 1.61345200 2.69692500 -1.10093100
H 0.76638700 2.88256400 -1.76093800
C -0.01024900 0.29018400 4.10488500
C 3.73961900 3.29651600 -0.15631200
H 4.58800000 3.97807600 -0.04430100
C 2.65317900 3.61988200 -0.98153400
H 2.60428700 4.56501800 -1.52867700
C 2.87770200 -3.31160600 -1.71484900
H 2.97537900 -4.04001700 -2.52431000
C -1.82367900 2.22993900 -1.89881900
H -1.06850000 2.17869800 -2.68750900
C -2.84423000 3.17302200 -1.91314900
H -2.89377000 3.89479900 -2.73349400
C 3.70112200 -3.34744200 -0.57827800
H 4.45913300 -4.12509900 -0.44919900
C -3.49563500 -3.47531100 0.13008100
H -4.29845800 -4.19600100 0.30973400
C -1.40419600 -2.83794800 -0.86607700
H -0.53338000 -3.04839700 -1.48689000
C -0.00903000 0.45203100 5.60376300
H 0.34613700 1.46208900 5.87833500
H -1.01768200 0.32282600 6.02555200
H 0.67248400 -0.27166500 6.08074600

Transition state: $[PY_4(p-\mathbf{CH_3}PY)Me_2MoO\cdots H\cdots H\cdots H_2O]^{+\ddagger}$
Mo -0.01033500 -0.08390300 -0.95742700
O 0.56009100 0.64154000 -2.60968500
H 0.34081300 -0.01802500 -3.56987900
H -1.10531400 -1.03028400 -2.29319400
O -0.03585700 -0.90552300 -4.36537700
H -0.74470900 -1.10224900 -3.07029400
H -0.70973500 -0.52285800 -4.96123600
N -1.46465500 -1.65229800 -0.24624500
N 1.66218400 -1.44177500 -0.85893000
N 1.52162100 1.44157400 -0.35806100
N -1.70640100 1.23215500 -0.86615300
C -2.52303600 -1.32106800 0.54909700
N 0.02141500 -0.03427300 1.30472800
C -2.49386400 0.07543500 1.22366200
C -2.61774400 1.20548400 0.16232200
C 2.53613300 -1.43830400 0.20182800
C -2.35929200 -3.88985200 -0.52080100
H -2.23335500 -4.88925000 -0.94467000
C -3.55461200 -2.25021000 0.78285500
H -4.41686400 -1.97763200 1.39045500
C 2.59799200 1.10727500 0.40492100
C 3.72262200 -0.33624800 2.14439500
H 3.64377800 -1.22417000 2.78878500
H 3.79019400 0.54805800 2.79435600

H 4.66263600 -0.41134900 1.57812700
C -3.64846400 2.16323800 0.22585700
H -4.35772500 2.15562300 1.05257500
C -3.67584000 0.17952100 2.21565000
H -3.65657800 1.13598500 2.75802600
H -3.64419100 -0.63292200 2.95613300
H -4.63663100 0.11616600 1.68423400
C 3.70000600 1.97769800 0.50899700
H 4.57679000 1.69507600 1.09123700
C 1.22652100 -0.05020300 3.39805500
H 2.16737800 -0.15531600 3.93766000
C -1.14259800 0.27370200 3.39639600
H -2.07355100 0.43951100 3.93707500
C 1.19789200 -0.12929600 2.00004300
C 1.82774900 -2.39135300 -1.83581200
H 1.16404800 -2.29518100 -2.70025300
C 2.51343200 -0.23025400 1.18595000
C -1.14697600 0.13647100 2.00122300
C -3.79060400 3.13854400 -0.77039400
H -4.59395600 3.87782100 -0.70860300
C 3.46777500 -2.48286300 0.35172700
H 4.12757800 -2.51591300 1.21804900
C 1.49705600 2.65358300 -0.97412300
H 0.61180600 2.86427200 -1.57404600
C 0.05023000 0.17871400 4.12983200
C 3.67779500 3.22015100 -0.13867200
H 4.53246500 3.89793200 -0.05639300
C 2.54022500 3.57467000 -0.87828300
H 2.45708300 4.54040200 -1.38344700
C 2.76758000 -3.41663000 -1.75887200
H 2.84235600 -4.14316100 -2.57248300
C -1.87620100 2.17006600 -1.85710300
H -1.14601600 2.10049100 -2.66848500
C -2.88745600 3.12479000 -1.84578600
H -2.95762700 3.84175800 -2.66864200
C 3.58214700 -3.49086300 -0.61815800
H 4.30841800 -4.29826000 -0.48946000
C -3.48380000 -3.54073200 0.24082000
H -4.28739600 -4.25935700 0.42539900
C -1.38409100 -2.91982600 -0.74369700
H -0.50202300 -3.14217700 -1.34631700
C 0.07361600 0.32518500 5.63019300
H 0.41584800 1.33837100 5.91025700
H -0.92624500 0.17611100 6.06654900
H 0.77360100 -0.39222100 6.08936100

Product complex: $[PY_4(p{-}\mathbf{CH_3}PY)Me_2MoO\cdots H_2O]^+ + H_2$
Mo 0.11261500 -0.08628900 -0.87441300
O 0.13313500 -0.20114200 -2.64582600
H -0.23295800 -0.03573200 -4.36094600
H -5.97302500 -1.47525300 -4.76363500
O -0.41783000 0.02594700 -5.33741500
H -6.39487600 -0.85510500 -4.72058100
H -1.16182400 0.65164100 -5.40737000
N -1.45516500 -1.53371800 -0.51135400
N 1.76944000 -1.43209100 -0.58110000
N 1.66762500 1.39046100 -0.61277400
N -1.55258000 1.28397200 -0.80847500
C -2.46484500 -1.30377300 0.39011700
N 0.05496200 0.04184200 1.37642300
C -2.43728600 0.02771900 1.19218100
C -2.48783000 1.22842500 0.19872100
C 2.65344400 -1.26381900 0.45908600
C -2.51335900 -3.61491700 -1.18061500
H -2.49458700 -4.49235600 -1.83198000
C -3.48912600 -2.25428000 0.55554400
H -4.28148500 -2.08871600 1.28436100
C 2.62949800 1.26943500 0.36034300
C 3.74731400 0.09005800 2.29383400
H 3.71866000 -0.75724600 2.99408100
H 3.72872100 1.01448900 2.88931600
H 4.70427200 0.05072500 1.75258900
C -3.47633200 2.22512300 0.29558600
H -4.19826500 2.20877400 1.11137600
C -3.67371200 0.08552800 2.11844700
H -3.67565900 1.00651100 2.71890400
H -3.68522300 -0.76544100 2.81510900
H -4.60408700 0.06062700 1.53187600
C 3.65041600 2.23209900 0.46248100
H 4.40261500 2.15561700 1.24668200
C 1.20502900 0.16464100 3.49767600
H 2.13758700 0.19405900 4.06139100
C -1.19114600 0.16251700 3.44345800
H -2.14896800 0.19305900 3.96259200
C 1.22137000 0.08109200 2.10202600
C 1.95069300 -2.49147000 -1.43126900
H 1.28242100 -2.51574900 -2.29490500
C 2.55619300 0.03988600 1.30940200
C -1.14190900 0.08331900 2.04582300
C -3.56779800 3.24481700 -0.66399200
H -4.34102600 4.01327300 -0.57808800
C 3.63609900 -2.23915200 0.71048600
H 4.31580900 -2.13206900 1.55496200
C 1.76692500 2.41471600 -1.51548200
H 1.00179000 2.44010000 -2.29161700
C -0.01152700 0.20735000 4.20539900
C 3.73260200 3.29225200 -0.45147000
H 4.53399200 4.03133600 -0.36572000
C 2.77801200 3.37089900 -1.47641800
H 2.80099500 4.16114600 -2.23111300
C 2.93081400 -3.46209800 -1.24577800
H 3.02014700 -4.28267200 -1.96267000
C -1.68436600 2.24895500 -1.77234700
H -0.97191000 2.18534500 -2.59760100
C -2.66710800 3.23419600 -1.74065100
H -2.71497500 3.97503200 -2.54324200
C 3.77514400 -3.35463200 -0.12932900
H 4.54213600 -4.10637500 0.07650800
C -3.52176700 -3.41815200 -0.22559400
H -4.32613300 -4.14708500 -0.09310200
C -1.50385300 -2.66171800 -1.28437300
H -0.69845600 -2.77568100 -2.01008700

C -0.03745200 0.30585400 5.71032600
H 0.37466900 1.27480200 6.04571600
H -1.06221400 0.21617500 6.10294700
H 0.58342300 -0.48303900 6.16949000

Reactant complex: $[PY_4(p\text{–}\mathbf{F}PY)Me_2Mo(H)(OH)\cdots H_2O]^+$
Mo 0.01490100 -0.01952700 -0.80343100
O 0.65339800 0.78299500 -2.56919600
H 0.23544800 0.38351000 -3.36203200
H -0.65388800 -0.91890300 -2.09471100
O -1.07331400 -0.65492800 -4.55953700
H -1.19949200 -0.92638800 -3.61502700
H -1.81778000 -0.04885100 -4.73821300
N -1.47248300 -1.55993800 -0.20457800
N 1.68927800 -1.36967300 -0.68153700
N 1.60064300 1.51756200 -0.29232100
N -1.67062400 1.30329100 -0.76638200
C -2.52693100 -1.24852800 0.60659100
N 0.00063100 0.04586500 1.43271200
C -2.51270900 0.13963700 1.29608500
C -2.61722300 1.26877700 0.23392100
C 2.56131600 -1.33830500 0.38012700
C -2.38773800 -3.78842700 -0.52434700
H -2.27046800 -4.77587700 -0.97799600
C -3.56212300 -2.17941100 0.82749900
H -4.41639500 -1.91605000 1.44991800
C 2.63279700 1.20266000 0.53973100
C 3.69020000 -0.21761800 2.34553800
H 3.59010900 -1.10131600 2.99321600
H 3.74428200 0.67269500 2.98830800
H 4.64610800 -0.29814300 1.80841400
C -3.66117400 2.21343700 0.26814500
H -4.39634900 2.19239900 1.07182500
C -3.70964100 0.23885200 2.27019700
H -3.70691900 1.19932000 2.80611300
H -3.68344800 -0.57036500 3.01479900
H -4.66183100 0.16560500 1.72549600
C 3.73570700 2.06705100 0.67656200
H 4.57438500 1.80301500 1.32012500
C 1.19407600 0.10925700 3.53220500
H 2.11079600 0.05108100 4.11512300
C -1.21787900 0.38088600 3.49158600
H -2.14209500 0.54214000 4.04244600
C 1.17611100 -0.00942300 2.13454900
C 1.88416000 -2.31901200 -1.65243500
H 1.20822000 -2.24873400 -2.50781100
C 2.51045400 -0.11856200 1.34966600
C -1.18447200 0.21335600 2.10000000
C -3.78144000 3.19447300 -0.72466300
H -4.59392500 3.92514500 -0.68538100
C 3.52338600 -2.35467500 0.53648700
H 4.18062600 -2.36804000 1.40516300
C 1.63147100 2.70273400 -0.95866400
H 0.78460300 2.89601400 -1.61666400
C -0.01466300 0.31900100 4.18527200
C 3.76576200 3.28335300 -0.01957200
H 4.62068000 3.95709400 0.08948700
C 2.68007900 3.61596600 -0.84211100
H 2.63842600 4.56126800 -1.38949400
C 2.85595600 -3.31292700 -1.57311100
H 2.95235300 -4.04028300 -2.38362100
C -1.81814700 2.25408300 -1.75234000
H -1.06054900 2.20509900 -2.53872000
C -2.83743100 3.19845600 -1.76642500
H -2.88313400 3.92344000 -2.58410300
C 3.67036800 -3.36010600 -0.43054100
H 4.41894200 -4.14615800 -0.29765100
C -3.50441300 -3.45676600 0.25884900
H -4.30821900 -4.17687700 0.43612200
C -1.41194800 -2.81922100 -0.73517100
H -0.54166300 -3.02892900 -1.35686200
F -0.02226800 0.45630200 5.53494400

Transition state: $[PY_4(p\text{–}\mathbf{F}PY)Me_2MoO\cdots H\cdots H\cdots H_2O]^{+\ \ddagger}$
Mo -0.00628000 -0.08465600 -0.95745300
O 0.56450100 0.64282800 -2.60246700
H 0.32513400 -0.00326800 -3.58082900
H -1.08779200 -1.03461700 -2.29101400
O -0.07202500 -0.86847400 -4.36937200
H -0.75001800 -1.08748400 -3.08705400
H -0.75141200 -0.46976500 -4.94835700
N -1.46739900 -1.65175700 -0.24720200
N 1.66006600 -1.44968800 -0.85890900
N 1.53422700 1.43424100 -0.35089500
N -1.69975500 1.23558900 -0.86336300
C -2.52655600 -1.31947600 0.54613300
N 0.02269000 -0.04142300 1.31077700
C -2.49567000 0.07659200 1.22206400
C -2.61264700 1.21010800 0.16357000
C 2.53051600 -1.45454600 0.20469400
C -2.36882500 -3.88588100 -0.52697000
H -2.24510300 -4.88500600 -0.95206900
C -3.56200900 -2.24483800 0.77669900
H -4.42455600 -1.97066300 1.38310700
C 2.61021200 1.09263500 0.40881100
C 3.72286800 -0.36060300 2.15021400
H 3.63394100 -1.24614400 2.79674300
H 3.79922800 0.52579700 2.79644100
H 4.66310600 -0.44664900 1.58635800
C -3.64013900 2.17101600 0.22925600
H -4.35035400 2.16383100 1.05509900
C -3.67616100 0.18287800 2.21535800
H -3.65381900 1.13861000 2.75906600
H -3.64803000 -0.63222400 2.95321400
H -4.63727100 0.12439700 1.68448500
C 3.71903700 1.95405900 0.51182200
H 4.59507300 1.66474800 1.09190900
C 1.24563700 -0.04464200 3.39925500
H 2.17099500 -0.13291300 3.96494200
C -1.16024300 0.27457600 3.39574200
H -2.07427900 0.43963900 3.96242900
C 1.20302900 -0.13512900 2.00055700

C 1.82235100 -2.39925400 -1.83629600
H 1.16124300 -2.29817700 -2.70190300
C 2.51738500 -0.24564000 1.18827800
C -1.15067600 0.13293000 2.00101800
C -3.77779100 3.14912100 -0.76465300
H -4.57882400 3.89076400 -0.70195900
C 3.45293200 -2.50651200 0.35777600
H 4.10860300 -2.54638700 1.22691100
C 1.51675700 2.64697000 -0.96568400
H 0.63150400 2.86471900 -1.56311200
C 0.05074200 0.17886000 4.07314500
C 3.70400400 3.19691900 -0.13532700
H 4.56373900 3.86842100 -0.05495400
C 2.56696600 3.56022600 -0.87148900
H 2.48950600 4.52712300 -1.37526400
C 2.75465400 -3.43111400 -1.75756100
H 2.82739900 -4.15677900 -2.57208200
C -1.86494700 2.17739800 -1.85147000
H -1.13377900 2.10875100 -2.66187400
C -2.87308400 3.13529600 -1.83868500
H -2.93960100 3.85488700 -2.65950800
C 3.56375600 -3.51355600 -0.61349200
H 4.28330400 -4.32660300 -0.48308700
C -3.49420400 -3.53444200 0.23224100
H -4.30067800 -4.25063200 0.41344400
C -1.38998900 -2.91874700 -0.74639600
H -0.50761100 -3.14309300 -1.34768900
F 0.06302800 0.29515500 5.42571700

Product complex: $[PY_4(p{-}\mathbf{F}PY)Me_2MoO\cdots H_2O]^+ + H_2$
Mo 0.11981200 -0.06972600 -0.71288100
O 0.14930900 -0.15843100 -2.48230300
H -0.14617900 0.04629900 -4.21631200
H -6.32566200 -1.31882500 -4.46577900
O -0.29094800 0.12799600 -5.19701900
H -5.83384600 -1.47488400 -5.01182700
H -0.96169300 0.82918600 -5.28847600
N -1.45408300 -1.51716500 -0.37756900
N 1.77211300 -1.42500900 -0.42794000
N 1.67965100 1.39956800 -0.43197700
N -1.54314300 1.30441100 -0.63117700
C -2.46277100 -1.30099800 0.52831400
N 0.05842300 0.02971200 1.54230800
C -2.43754400 0.02086800 1.34703100
C -2.48298800 1.23549500 0.37031400
C 2.65574500 -1.26994700 0.61411200
C -2.51411100 -3.58778600 -1.07585200
H -2.49721500 -4.45495600 -1.74083800
C -3.48603900 -2.25408900 0.68316000
H -4.27664900 -2.10007600 1.41634600
C 2.63830700 1.26719400 0.54263600
C 3.74938300 0.06232200 2.46673000
H 3.71684700 -0.79339100 3.15668400
H 3.73136600 0.98050900 3.07193200
H 4.70818600 0.02713800 1.92894200
C -3.47320600 2.22947400 0.47598800
H -4.19872100 2.20232800 1.28822700
C -3.67421700 0.06755600 2.27337900
H -3.67793400 0.98228100 2.88344500
H -3.68635500 -0.79190900 2.95963200
H -4.60394700 0.04870100 1.68602900
C 3.65895600 2.22803700 0.66111000
H 4.40804000 2.14210400 1.44723300
C 1.22019500 0.13194200 3.66387800
H 2.13364400 0.15850800 4.25526900
C -1.21125600 0.13081300 3.60127000
H -2.15420000 0.15960800 4.14429200
C 1.22721200 0.06074800 2.26532700
C 1.95112400 -2.47598600 -1.28852200
H 1.28277700 -2.49157300 -2.15211100
C 2.56255700 0.02590000 1.47659100
C -1.14560900 0.06510200 2.20407200
C -3.56153400 3.26031000 -0.47153000
H -4.33636300 4.02642600 -0.37994900
C 3.63601000 -2.24973200 0.85696600
H 4.31515400 -2.15322600 1.70310000
C 1.78281900 2.43447400 -1.32190700
H 1.02135700 2.46909300 -2.10125500
C -0.01305700 0.16478200 4.31064000
C 3.74474300 3.29876100 -0.23995300
H 4.54604000 4.03643200 -0.14257900
C 2.79401300 3.38972000 -1.26743100
H 2.82032100 4.18869900 -2.01272000
C 2.92983900 -3.44983200 -1.11298500
H 3.01812300 -4.26289900 -1.83841300
C -1.67102200 2.28141400 -1.58299400
H -0.95416500 2.23051800 -2.40514600
C -2.65577700 3.26436200 -1.54378600
H -2.70079300 4.01518100 -2.33712900
C 3.77368400 -3.35573700 0.00490000
H 4.53952000 -4.11072900 0.20274000
C -3.51978100 -3.40625900 -0.11501500
H -4.32325700 -4.13759700 0.00889600
C -1.50495200 -2.63307900 -1.16786900
H -0.70220900 -2.73533100 -1.89822400
F -0.04826900 0.23157000 5.66979400

Reactant complex: $[PY_4(p{-}\mathbf{CF_3}PY)Me_2Mo(H)(OH)\cdots H_2O]^+$
Mo -0.01955200 -0.06436800 -1.40918500
O 0.59368000 0.66056500 -3.20781400
H 0.11560800 0.28477700 -3.98417300
H -0.87436900 -0.81030900 -2.66654300
O -0.71413900 -0.35899300 -5.55288000
H -1.51614500 -0.84769600 -5.28674700
H -1.04634400 0.37862100 -6.09922700
N -1.47110600 -1.64612300 -0.80524600
N 1.64221900 -1.43182700 -1.32435300
N 1.62410600 1.43168300 -0.98006500
N -1.70861300 1.25383900 -1.32994000
C -2.52392700 -1.35200100 0.01150200
N -0.01841800 0.00731700 0.79188300
C -2.53402300 0.03666500 0.70244200

C -2.66146600 1.18128100 -0.33992000
C 2.50872000 -1.41268100 -0.25911600
C -2.34194100 -3.88918300 -1.12473400
H -2.21156300 -4.87179100 -1.58507600
C -3.53736100 -2.30544100 0.24021300
H -4.39387700 -2.06103800 0.86709200
C 2.64710500 1.12231800 -0.13313800
C 3.67969300 -0.30146600 1.68467700
H 3.55478500 -1.16835800 2.35069900
H 3.77476100 0.59750700 2.31004200
H 4.62624200 -0.42304000 1.13835900
C -3.71666700 2.11263700 -0.29077200
H -4.46125300 2.05977300 0.50288200
C -3.72432400 0.10443500 1.68681500
H -3.74602500 1.06594600 2.21998400
H -3.66672600 -0.70087100 2.43413300
H -4.67900300 0.00346700 1.15034400
C 3.76081700 1.97462700 -0.00377600
H 4.58878500 1.71236600 0.65454500
C 1.19645700 0.17838800 2.87651600
H 2.13585100 0.15592800 3.42442000
C -1.20748900 0.37361700 2.86649400
H -2.14280100 0.52466300 3.40179500
C 1.16952900 -0.01145200 1.48962800
C 1.82303600 -2.37225700 -2.30287600
H 1.15359900 -2.27790200 -3.16214900
C 2.49332000 -0.17970300 0.69906400
C -1.19979000 0.15536500 1.48505800
C -3.83917200 3.11523000 -1.26166400
H -4.66422400 3.83134500 -1.21609800
C 3.44744300 -2.45093500 -0.10163700
H 4.09894700 -2.48378700 0.77089000
C 1.68382000 2.59855900 -1.67863400
H 0.84886500 2.78623400 -2.35296400
C 0.00153600 0.39100300 3.57372300
C 3.81717700 3.17203000 -0.72936200
H 4.68078600 3.83590200 -0.62862100
C 2.74592700 3.49687400 -1.57497400
H 2.72628400 4.42617700 -2.15041400
C 2.77605500 -3.38512200 -2.22414300
H 2.86715700 -4.10903800 -3.03822500
C -1.85344400 2.22735600 -2.29181000
H -1.09168200 2.20353200 -3.07526600
C -2.88456700 3.15930100 -2.29267400
H -2.93256700 3.90398100 -3.09220200
C 3.57751600 -3.45449100 -1.07360200
H 4.30710300 -4.25795400 -0.93847600
C -3.45496100 -3.58160100 -0.32847200
H -4.24221400 -4.31849600 -0.14537600
C -1.39068100 -2.89660200 -1.34515400
H -0.52882800 -3.08074500 -1.98648800
C 0.00014300 0.55715700 5.07281700
F -0.25148000 -0.63278900 5.72041600
F -0.96377600 1.43415800 5.49321100
F 1.19760300 1.01224600 5.54918900

Transition state: $[PY_4(p\text{–}\mathbf{CF_3}PY)Me_2MoO\cdots H\cdots H\cdots H_2O]^{+\ ‡}$
Mo -0.00143300 -0.08620200 -0.95475000
O 0.58904700 0.61873400 -2.58603200
H 0.27470700 0.01513300 -3.60213000
H -1.05846100 -1.04169100 -2.27626100
O -0.19421600 -0.78910700 -4.37223000
H -0.78887300 -1.05288200 -3.12065000
H -0.88512600 -0.33976600 -4.89858700
N -1.46775200 -1.65428500 -0.24354600
N 1.66678200 -1.46177200 -0.84477900
N 1.55101900 1.43767200 -0.35771500
N -1.69427900 1.23565100 -0.87131000
C -2.52835900 -1.32040800 0.54629900
N 0.02581400 -0.03199400 1.29105600
C -2.49719300 0.07868700 1.21285800
C -2.61191900 1.20880300 0.15078400
C 2.53669000 -1.45403900 0.21711700
C -2.35815000 -3.89487200 -0.50357500
H -2.22980700 -4.89665300 -0.92091900
C -3.55979800 -2.24868300 0.78513000
H -4.42401900 -1.97253200 1.38828300
C 2.62702600 1.09656900 0.40041200
C 3.72873800 -0.34722800 2.15355500
H 3.63640200 -1.22702400 2.80738500
H 3.80799600 0.54428400 2.79227500
H 4.66935200 -0.44046800 1.59129900
C -3.64061000 2.16904100 0.20904300
H -4.35583100 2.16173000 1.03044200
C -3.67933900 0.19061800 2.20361100
H -3.66036400 1.15012500 2.74066900
H -3.65145000 -0.61913900 2.94731200
H -4.63914800 0.12618700 1.67084600
C 3.73782200 1.95631200 0.49898200
H 4.61502200 1.66699600 1.07737500
C 1.23858500 -0.01013100 3.38728500
H 2.17688800 -0.09384700 3.93160100
C -1.15382400 0.28922600 3.37917900
H -2.08250200 0.46167800 3.91900900
C 1.20745600 -0.11326200 1.99213700
C 1.82355000 -2.41970800 -1.81180900
H 1.15454000 -2.33064800 -2.67217800
C 2.52532300 -0.23529900 1.18846700
C -1.15150400 0.13724200 1.98849400
C -3.77429000 3.14491200 -0.78726500
H -4.57782900 3.88432100 -0.73096800
C 3.45951900 -2.50514600 0.37821100
H 4.11614200 -2.53833200 1.24676900
C 1.53290300 2.64817000 -0.97546200
H 0.64680300 2.86622000 -1.57167100
C 0.05028800 0.21639000 4.09166800
C 3.72257800 3.19732500 -0.15152000
H 4.58368900 3.86761800 -0.07574900
C 2.58424800 3.56082200 -0.88551200
H 2.50708300 4.52662200 -1.39139400
C 2.75975600 -3.44794900 -1.72947700
H 2.83187000 -4.18067300 -2.53749600

C -1.85324900 2.17648600 -1.86068400
H -1.11809600 2.11219000 -2.66717000
C -2.86346900 3.13224700 -1.85564200
H -2.92621700 3.85054000 -2.67774400
C 3.57097500 -3.51762400 -0.58662500
H 4.29341300 -4.32744200 -0.45183100
C -3.48554100 -3.54239700 0.25248400
H -4.28892100 -4.26073800 0.43884500
C -1.38489500 -2.92463900 -0.73271700
H -0.50366400 -3.14949700 -1.33492400
C 0.05327900 0.31105000 5.59667300
F -0.15407300 -0.91693500 6.18658900
F -0.93334500 1.13507100 6.06552000
F 1.24090100 0.77917400 6.08694800

Product complex: $[PY_4(p-\mathbf{CF_3}PY)Me_2MoO\cdots H_2O]^+ + H_2$
Mo 0.07986100 -0.13167100 -1.30007200
O 0.10646100 -0.23171400 -3.05756700
H 0.25003200 0.07820600 -4.82627000
H -5.79264700 -1.36822200 -5.56510700
O 0.33252000 0.21342400 -5.80543400
H -5.19762300 -1.41168400 -6.02174200
H 0.42023700 1.17833000 -5.91220400
N -1.53969900 -1.53120600 -0.97350400
N 1.70162400 -1.53411500 -0.99038000
N 1.69850100 1.29834400 -1.11277000
N -1.54512200 1.29347700 -1.18218800
C -2.50416100 -1.30785800 -0.02223100
N 0.06620300 -0.00207200 0.92807700
C -2.43872800 0.01625700 0.79354600
C -2.49041400 1.22351800 -0.18886500
C 2.63192000 -1.34958500 0.00196400
C -2.65632500 -3.58344800 -1.63698500
H -2.68379700 -4.44288700 -2.31155600
C -3.52607600 -2.25459800 0.17807500
H -4.27886900 -2.09858500 0.94945500
C 2.65155400 1.18462600 -0.13118100
C 3.77610000 0.00672900 1.80171300
H 3.75113500 -0.84136900 2.50137000
H 3.77391700 0.93137200 2.39687000
H 4.72507400 -0.03854500 1.24738900
C -3.48985300 2.21062600 -0.09962400
H -4.22328700 2.18249900 0.70523800
C -3.65682500 0.08591800 1.74294100
H -3.64345500 1.01170500 2.33610000
H -3.66095800 -0.76096500 2.44449300
H -4.59779000 0.06094100 1.17394100
C 3.67530800 2.14516900 -0.03088500
H 4.41942500 2.07760400 0.76164300
C 1.25939000 0.11690700 3.03372800
H 2.19742700 0.14213000 3.58499600
C -1.15860100 0.14389000 3.01340900
H -2.10483100 0.19233500 3.54907300
C 1.24928000 0.02842700 1.64089300
C 1.82994300 -2.61291700 -1.82172300
H 1.11275700 -2.66493300 -2.64250800
C 2.57140700 -0.03413900 0.83361900
C -1.12802000 0.05516300 1.62123500
C -3.57576700 3.23314100 -1.05457300
H -4.35873500 3.99258200 -0.97736100
C 3.62584200 -2.32169000 0.22236700
H 4.34701000 -2.20050600 1.02941500
C 1.81606800 2.30405700 -2.03221500
H 1.06587400 2.31350100 -2.82345500
C 0.04527500 0.18059400 3.73832900
C 3.77045400 3.19186900 -0.95825200
H 4.57340500 3.92936200 -0.87380400
C 2.83028400 3.25706400 -1.99708200
H 2.86838700 4.03256700 -2.76626100
C 2.81900900 -3.58067500 -1.67013300
H 2.86729400 -4.41729600 -2.37176800
C -1.66301900 2.26711100 -2.13631800
H -0.93277100 2.22598000 -2.94612200
C -2.65661300 3.24171300 -2.11446700
H -2.69580700 3.98992700 -2.91023600
C 3.72173200 -3.44974800 -0.60431000
H 4.50004100 -4.19697700 -0.42643800
C -3.60786400 -3.40237400 -0.62239600
H -4.40907400 -4.12893700 -0.46139700
C -1.64435000 -2.63715300 -1.77181000
H -0.88570900 -2.73528500 -2.54886400
C 0.02948400 0.22106100 5.24008200
F -0.04877000 -1.04245600 5.79536500
F -1.04373800 0.91637100 5.73328800
F 1.15772600 0.79531400 5.76190200

Reactant complex: $[PY_4(p-\mathbf{CN}PY)Me_2Mo(H)(OH)\cdots H_2O]^+$
Mo -0.01471700 -0.01026500 -0.73450200
O 0.61164200 0.66083600 -2.54931500
H 0.10529600 0.30953600 -3.31971100
H -0.96186000 -0.66853400 -1.96778700
O -0.76493000 -0.30464200 -4.86816300
H -1.64448700 -0.65353500 -4.62860000
H -0.95133000 0.43032300 -5.48299800
N -1.45392200 -1.61054200 -0.14363000
N 1.64958600 -1.38262000 -0.64906400
N 1.64688500 1.47301900 -0.34033800
N -1.70725200 1.31485000 -0.65614700
C -2.51603500 -1.31953600 0.66157200
N -0.02593100 0.07471600 1.43704100
C -2.54442100 0.07066400 1.35010800
C -2.67201000 1.22272200 0.31666900
C 2.50817100 -1.35799200 0.42020200
C -2.29589400 -3.86366000 -0.45644200
H -2.15197800 -4.84710000 -0.91070500
C -3.52053400 -2.28328100 0.88721700
H -4.38605700 -2.04463000 1.50371500
C 2.65761500 1.17505000 0.52523500
C 3.67239600 -0.23865500 2.36086300
H 3.53898400 -1.10030700 3.03198700
H 3.76894000 0.66352800 2.98098700
H 4.62115100 -0.36747100 1.81988100

C -3.73355100 2.14733300 0.35924600
H -4.49235600 2.08036800 1.13814500
C -3.74164300 0.12631200 2.32658700
H -3.77647200 1.08756700 2.85923000
H -3.67978800 -0.67769200 3.07482600
H -4.69183800 0.01558400 1.78380200
C 3.76729500 2.03147900 0.66237100
H 4.58505300 1.77838600 1.33680400
C 1.18609900 0.27922800 3.52618300
H 2.12216900 0.26742300 4.08016800
C -1.23133600 0.43857100 3.50993000
H -2.16907400 0.57412200 4.04473400
C 1.16317100 0.06985200 2.14841000
C 1.83179900 -2.32147400 -1.62571700
H 1.16888100 -2.22528200 -2.49004600
C 2.49161900 -0.11744200 1.36886500
C -1.21406500 0.20833200 2.13548600
C -3.84370900 3.15928500 -0.60327300
H -4.67487900 3.86880600 -0.56526400
C 3.44637300 -2.39603600 0.58363300
H 4.09455600 -2.42751400 1.45856000
C 1.71727900 2.62980900 -1.05449500
H 0.89543500 2.80627800 -1.74740100
C -0.01976000 0.48363400 4.23317800
C 3.83335500 3.21954300 -0.07714500
H 4.69432100 3.88602400 0.02867200
C 2.77666300 3.53064600 -0.94564300
H 2.76665800 4.45049000 -1.53621600
C 2.78408100 -3.33524500 -1.54097300
H 2.87990500 -4.06068100 -2.35295700
C -1.83663700 2.29581000 -1.60859500
H -1.06422600 2.28357600 -2.38160400
C -2.87302000 3.22295000 -1.61694200
H -2.91273300 3.97662000 -2.40818100
C 3.57888700 -3.40101700 -0.38635200
H 4.30801000 -4.20415800 -0.24658900
C -3.41802200 -3.56226100 0.32827100
H -4.19953000 -4.30599700 0.50834400
C -1.35481900 -2.86071700 -0.67652800
H -0.48896700 -3.03800500 -1.31437500
C -0.01466000 0.69895600 5.64326800
N -0.00951700 0.88354100 6.80958500

Transition state: $[PY_4(p-\mathbf{CN}PY)Me_2MoO\cdots H\cdots H\cdots H_2O]^{+\ddagger}$
Mo 0.00138500 -0.09249000 -0.95136800
O 0.60378400 0.60895900 -2.56383600
H 0.24365500 0.03865700 -3.61520800
H -1.02406300 -1.04840500 -2.26743600
O -0.26668700 -0.72499700 -4.36323900
H -0.80444500 -1.02529100 -3.14879500
H -0.96473000 -0.24837200 -4.85564900
N -1.47408700 -1.66486100 -0.24994800
N 1.67161900 -1.47654300 -0.83279900
N 1.55996600 1.43629000 -0.34696200
N -1.69217100 1.22987100 -0.86510600
C -2.53580200 -1.33294400 0.53813200
N 0.02529000 -0.04567400 1.28241900
C -2.50269600 0.06244700 1.20984900
C -2.61325100 1.19720000 0.15308800
C 2.54469000 -1.46152900 0.22472000
C -2.36134200 -3.90598600 -0.51329200
H -2.23097000 -4.90720300 -0.93129300
C -3.56819100 -2.26183800 0.77249600
H -4.43434500 -1.98629900 1.37312000
C 2.63560800 1.09048700 0.40821300
C 3.73216000 -0.35441000 2.16169800
H 3.63982200 -1.23537500 2.81386100
H 3.80816900 0.53629100 2.80179300
H 4.67423200 -0.44479500 1.60136000
C -3.64181100 2.15780300 0.21145800
H -4.36025500 2.14647500 1.02986300
C -3.68745900 0.17299300 2.19758800
H -3.66748000 1.12986700 2.73917200
H -3.66349800 -0.64018200 2.93751200
H -4.64578000 0.11283500 1.66157400
C 3.74770900 1.94866300 0.50881800
H 4.62603000 1.65597900 1.08377500
C 1.23987000 -0.02549200 3.38278100
H 2.17573900 -0.11061900 3.93075600
C -1.16533700 0.25891900 3.37265600
H -2.09501500 0.41938400 3.91402600
C 1.20858900 -0.12244200 1.99274600
C 1.82495000 -2.43531600 -1.79748500
H 1.14758000 -2.35380700 -2.65164500
C 2.53059300 -0.24240200 1.19419900
C -1.15644200 0.11506700 1.98612300
C -3.77112000 3.13854400 -0.78021100
H -4.57484500 3.87769400 -0.72355400
C 3.47389200 -2.50828000 0.38221400
H 4.13467600 -2.53781400 1.24759300
C 1.54099400 2.64930200 -0.95806300
H 0.65438800 2.87137000 -1.55227900
C 0.04318000 0.18949700 4.10135200
C 3.73169800 3.19315400 -0.13492400
H 4.59361100 3.86225100 -0.05754500
C 2.59241400 3.56182800 -0.86455200
H 2.51500400 4.53047700 -1.36487700
C 2.76893600 -3.45690400 -1.72143900
H 2.84054600 -4.19030300 -2.52870200
C -1.84602200 2.17586200 -1.84998200
H -1.10877600 2.11917500 -2.65452800
C -2.85627500 3.13152400 -1.84470900
H -2.91507000 3.85381500 -2.66345800
C 3.58652900 -3.51927600 -0.58317900
H 4.31509500 -4.32422900 -0.45198300
C -3.49128000 -3.55486000 0.23952000
H -4.29476600 -4.27392300 0.42265800
C -1.38926800 -2.93415900 -0.74046800
H -0.50821500 -3.15753200 -1.34303800
C 0.05300300 0.31970000 5.52135600
N 0.06151900 0.42754800 6.69743000

Product complex: $[PY_4(p-\mathbf{CN}PY)Me_2MoO\cdots H_2O]^+ + H_2$
Mo 0.03593800 -0.09635200 -0.68076200
O 0.04636900 -0.18748500 -2.43194500
H 0.15665600 0.06326300 -4.23259700
H -5.87188200 -1.07667700 -4.76376900
O 0.21977600 0.16280600 -5.21578900
H -5.35359800 -1.24939000 -5.27954700
H 0.29507000 1.12392900 -5.35984700
N -1.55863000 -1.52685700 -0.34379700
N 1.68889300 -1.46978000 -0.38823500
N 1.63189200 1.36384000 -0.50152700
N -1.61596400 1.29997200 -0.54039400
C -2.52137900 -1.32125700 0.61195600
N 0.03878900 0.02483500 1.54296000
C -2.46982400 -0.00157300 1.43538000
C -2.55244100 1.20744200 0.45791000
C 2.62730400 -1.26821300 0.59175700
C -2.64934500 -3.59003800 -1.01422100
H -2.66692200 -4.44682300 -1.69236600
C -3.53114000 -2.28168200 0.80973600
H -4.28308400 -2.13973300 1.58455400
C 2.59580900 1.26295800 0.46960000
C 3.75857900 0.10107300 2.38890100
H 3.75690400 -0.75096500 3.08406900
H 3.74268200 1.02260300 2.98859700
H 4.70322600 0.07782400 1.82600500
C -3.57292900 2.17228100 0.55489200
H -4.30031500 2.12699400 1.36430900
C -3.68106800 0.04305200 2.39514900
H -3.67720000 0.96555400 2.99347300
H -3.66612100 -0.80800500 3.09139400
H -4.62633200 0.00646500 1.83402600
C 3.60555200 2.23927400 0.56112500
H 4.35869900 2.18232600 1.34584000
C 1.25412700 0.15050200 3.63797200
H 2.19490900 0.18674400 4.18363900
C -1.17563400 0.13320500 3.63939200
H -2.11603300 0.15765200 4.18639100
C 1.22900500 0.07292300 2.24944700
C 1.82993000 -2.54050000 -1.22693300
H 1.10116400 -2.60801800 -2.03611300
C 2.54624100 0.04042700 1.43140000
C -1.15149500 0.05590900 2.25077300
C -3.68607100 3.19404800 -0.39750300
H -4.48452400 3.93651700 -0.31413900
C 3.64841600 -2.21651800 0.79165600
H 4.37773000 -2.08246000 1.58918100
C 1.72244500 2.37325800 -1.41905100
H 0.96301800 2.37461800 -2.20137100
C 0.03939500 0.18220600 4.36741400
C 3.67378900 3.28912900 -0.36461600
H 4.46549600 4.03937800 -0.28650900
C 2.72195500 3.34215100 -1.39299100
H 2.73889500 4.12018000 -2.16027600
C 2.84483300 -3.48430100 -1.09618600
H 2.90257800 -4.31589100 -1.80291900
C -1.75909100 2.27242100 -1.49132700
H -1.03200700 2.25059400 -2.30453600
C -2.77385000 3.22490000 -1.46251900
H -2.83353300 3.97379400 -2.25624500
C 3.75951300 -3.33667100 -0.04321800
H 4.55821400 -4.06574100 0.11893400
C -3.60040700 -3.42561500 0.00313600
H -4.39182000 -4.16319100 0.16249900
C -1.64961500 -2.63020300 -1.14618700
H -0.89064600 -2.71723500 -1.92409800
C 0.03963000 0.26097100 5.78835700
N 0.03984900 0.32655800 6.96889500

4.3.3 Structures with substituent groups at equatorial position

Reactant complex: $[(p-\mathbf{NH_2}PY)_4PYMe_2Mo(H)(OH)\cdots H_2O]^+$
Mo 0.02819500 0.00653300 -0.95449200
O 0.68362700 0.82900100 -2.73338500
H 0.21863100 0.45414200 -3.50752300
H -0.75161700 -0.81750500 -2.25484200
O -1.28434800 -0.68306700 -4.64825800
H -1.22271800 -0.83594300 -3.66152800
H -2.03383900 -0.06521500 -4.74662600
N -1.40775800 -1.58172900 -0.32497900
N 1.70501100 -1.35147000 -0.85195600
N 1.62745000 1.51423700 -0.44720800
N -1.68899700 1.31098800 -0.89827700
C -2.49554000 -1.29081600 0.44845300
N -0.00339400 0.08487600 1.25332500
C -2.52526300 0.10399900 1.13094900
C -2.65582200 1.23879400 0.07658100
C 2.54525800 -1.34495700 0.23520100
C -2.27110800 -3.83183400 -0.65611000
H -2.12067600 -4.81799600 -1.10439300
C -3.51293100 -2.22941900 0.65732400
H -4.38291700 -1.97775800 1.26391800
C 2.66890100 1.19510400 0.37499100
C 3.68162900 -0.23109200 2.20371200
H 3.54624900 -1.09520800 2.87156200
H 3.76253600 0.66986100 2.82821700
H 4.63800100 -0.35416900 1.67467100
C -3.72254400 2.15101400 0.11619200
H -4.47795500 2.08462300 0.89960400
C -3.72282800 0.16823400 2.10676500
H -3.75490100 1.13176000 2.63595100
H -3.66462100 -0.63329900 2.85794800
H -4.67324100 0.05802900 1.56412900
C 3.78173200 2.03339600 0.51491000
H 4.61342400 1.75224600 1.16200400
C 1.17621100 0.24253600 3.35945500
H 2.10668400 0.20954800 3.92354900
C -1.21835700 0.45091800 3.31268100
H -2.16071600 0.60091100 3.83676200
C 1.17382700 0.05466800 1.96901000
C 1.90828100 -2.31476000 -1.80363800

H 1.26796000 -2.22915200 -2.68614900
C 2.51227300 -0.11277600 1.19718100
C -1.19585100 0.23474300 1.92734000
C -3.85894500 3.16982300 -0.85384900
C 3.46546200 -2.38247900 0.43408700
H 4.09749800 -2.40640900 1.32201000
C 1.68477100 2.70983900 -1.10043000
H 0.83979400 2.92848600 -1.75337200
C -0.02482100 0.45903400 4.04176100
C 3.84968100 3.26757600 -0.17945200
C 2.73855900 3.60559800 -0.99450300
H 2.70205100 4.55296800 -1.54046400
C 2.83570100 -3.33953800 -1.69625200
H 2.93463000 -4.07307900 -2.50173400
C -1.83711700 2.29311800 -1.84914400
H -1.05992100 2.29363000 -2.61896600
C -2.87055500 3.21506700 -1.86964100
H -2.90891700 3.96341700 -2.66737300
C 3.62178300 -3.42302700 -0.51829700
C -3.43329800 -3.53229700 0.10143500
C -1.31936100 -2.84307200 -0.84107900
H -0.43278000 -3.04523900 -1.44278900
N -4.94282500 4.03286500 -0.85214300
H -5.45180200 4.14249200 0.02420300
H -4.84466800 4.90192100 -1.37546500
N 4.91652100 4.11841800 -0.02147300
H 5.04149400 4.87973900 -0.68535500
H 5.77349900 3.76431400 0.39873400
N 4.47878600 -4.47234100 -0.29323200
H 4.73689900 -5.07268800 -1.07376900
H 5.17852400 -4.39115300 0.44186600
N -4.40664100 -4.46581700 0.32731200
H -5.29678200 -4.18759800 0.73367900
H -4.40541000 -5.33675200 -0.19814900
H -0.03309600 0.60792100 5.12516000

Transition state: $[(p\text{–}\mathbf{NH_2}\text{PY})_4\text{PYMe}_2\text{MoO}\cdots\text{H}\cdots\text{H}\cdots\text{H}_2\text{O}]^{+\,\ddagger}$
Mo -0.02046900 -0.06284000 -0.94608500
O 0.56787400 0.69993300 -2.62904700
H 0.45647900 -0.00916900 -3.45306400
H -1.21254300 -0.83186600 -2.26514000
O 0.20267600 -1.11983300 -4.27885900
H -0.66393700 -1.10731500 -2.82808800
H -0.49764100 -0.91367200 -4.92850000
N -1.45872800 -1.62917100 -0.25300200
N 1.66297100 -1.43564200 -0.87258900
N 1.51069900 1.44136000 -0.33939700
N -1.72086800 1.27497100 -0.82609600
C -2.54071700 -1.31127900 0.52066700
N 0.01422300 -0.03484500 1.30120400
C -2.51264300 0.07252800 1.22614800
C -2.63807800 1.23000800 0.19219100
C 2.52321700 -1.45130100 0.19745700
C -2.37374200 -3.85455400 -0.59504700
H -2.24498700 -4.84553400 -1.03884000
C -3.58032200 -2.22158300 0.72219600
H -4.44335400 -1.95236000 1.33131400
C 2.60836400 1.09783800 0.39192700
C 3.71880300 -0.35108200 2.14170400
H 3.62589200 -1.23019500 2.79666200
H 3.79933000 0.53989300 2.78095900
H 4.65854600 -0.44669300 1.57813700
C -3.66904100 2.17653600 0.28240800
H -4.38657500 2.14029800 1.10223500
C -3.68775100 0.15395100 2.22801300
H -3.67209400 1.10155700 2.78591400
H -3.64726800 -0.67154300 2.95371400
H -4.65128300 0.09580100 1.70089400
C 3.72192300 1.93890500 0.48324900
H 4.60039000 1.63900900 1.05567700
C 1.23206000 -0.01299700 3.39071800
H 2.17212400 -0.09776900 3.93322600
C -1.15366300 0.27905700 3.39322800
H -2.08066300 0.44142300 3.94013000
C 1.19858300 -0.11719500 1.99144800
C 1.83011400 -2.40014900 -1.83300400
H 1.19231400 -2.29139700 -2.71936600
C 2.51396700 -0.23723000 1.17829300
C -1.16065000 0.13040100 1.99781200
C -3.81807200 3.19814300 -0.68621100
C 3.43209600 -2.50160900 0.37496000
H 4.08421800 -2.53383400 1.24785200
C 1.50190000 2.66643400 -0.93570300
H 0.60596400 2.90990400 -1.50684200
C 0.04928800 0.20415100 4.10152100
C 3.72846600 3.20309500 -0.16190700
C 2.55306200 3.56829500 -0.86817800
H 2.46754000 4.53886000 -1.36511100
C 2.74053800 -3.44230300 -1.74101100
H 2.81204400 -4.17422300 -2.55108900
C -1.88918500 2.24268900 -1.78396400
H -1.15984300 2.19661600 -2.59904700
C -2.89174900 3.19889800 -1.75941600
H -2.95348200 3.93779900 -2.56424200
C 3.55062500 -3.54321700 -0.58147300
C -3.53516500 -3.52286700 0.15098000
C -1.39075300 -2.89352600 -0.76473500
H -0.49604500 -3.12373700 -1.34618000
N 4.39754500 -4.60379900 -0.37860100
H 4.62636000 -5.21001900 -1.16365200
H 5.11045600 -4.53970000 0.34539000
N -4.56189500 -4.40455800 0.31347900
H -5.33794500 -4.19307000 0.93558900
H -4.47180200 -5.36791900 0.00091800
N -4.79230400 4.16754000 -0.56471100
H -5.03586600 4.70459200 -1.39523600
H -5.57602400 3.98391900 0.05970100
N 4.80014700 4.04983500 -0.05774900
H 4.85904900 4.86026500 -0.67015200
H 5.68631300 3.69824500 0.29818500
H 0.06179700 0.30197900 5.19068600

Product complex: $[(p\text{–}\mathbf{NH_2}\text{PY})_4\text{PYMe}_2\text{MoO}\cdots\text{H}_2\text{O}]^+ + \text{H}_2$

Mo 0.07052800 -0.12483700 -0.85271900
O 0.09666400 -0.24872900 -2.62646300
H 0.06310500 0.09159400 -4.32151500
H -6.06666200 -1.08199300 -4.68613600
O 0.04982200 0.24992300 -5.30836800
H -5.95273100 -0.39507500 -4.96829300
H -0.06956800 1.21273600 -5.40076300
N -1.52611800 -1.54666200 -0.49952700
N 1.71315000 -1.49958900 -0.52734000
N 1.66542600 1.32963100 -0.65480000
N -1.58225300 1.27479900 -0.76514500
C -2.51955500 -1.32164400 0.42375700
N 0.03889100 0.03020800 1.36830100
C -2.47398700 0.01488400 1.22117500
C -2.54227400 1.20589400 0.21738400
C 2.63647800 -1.30514200 0.47281600
C -2.60983000 -3.63495500 -1.13007200
H -2.60898000 -4.51188300 -1.78365300
C -3.53607800 -2.26164100 0.62904400
H -4.30703200 -2.08716800 1.37954500
C 2.63894200 1.22490100 0.31075400
C 3.74482100 0.08085700 2.27695900
H 3.71065900 -0.75374200 2.99250900
H 3.73122400 1.01665200 2.85462000
H 4.70245900 0.02722500 1.73828300
C -3.55957600 2.16508000 0.29487300
H -4.30277200 2.12271400 1.09134500
C -3.69108900 0.08141900 2.17188000
H -3.68873100 1.01512600 2.75287800
H -3.68168600 -0.75581600 2.88515000
H -4.63333900 0.03627600 1.60600400
C 3.66897200 2.16830500 0.39765400
H 4.42509400 2.09277500 1.17932900
C 1.21399700 0.20375800 3.48172600
H 2.14794100 0.24914700 4.04044300
C -1.19560100 0.19615700 3.44822800
H -2.14504700 0.23813900 3.98045400
C 1.22035000 0.08641100 2.08741600
C 1.87260500 -2.59679000 -1.33115300
H 1.17276800 -2.66990800 -2.16638700
C 2.55490100 0.01899000 1.29208100
C -1.16244000 0.08409400 2.05387400
C -3.67203500 3.20285600 -0.66426600
C 3.63207400 -2.25732600 0.72523300
H 4.34334300 -2.11152000 1.53822100
C 1.78278500 2.34617800 -1.56488500
H 1.02136500 2.36967000 -2.34594500
C -0.00094100 0.25993000 4.18170300
C 3.77561700 3.23401200 -0.53176300
C 2.79533300 3.29111200 -1.55539800
H 2.81937700 4.06639200 -2.32659100
C 2.85709500 -3.55578700 -1.15877400
H 2.91765600 -4.40097300 -1.85040700
C -1.71928300 2.25120300 -1.71557500
H -0.98390300 2.22513300 -2.52244000
C -2.72165900 3.20738800 -1.71694800
H -2.76147500 3.94975600 -2.51942400
C 3.76252100 -3.42016200 -0.07540100
C -3.60806400 -3.45176000 -0.13891400
C -1.61218800 -2.68319600 -1.25870900
H -0.83726700 -2.80295600 -2.01723200
H 5.55954400 3.99645000 0.18478300
H 4.95012500 4.79310500 -1.21217100
H -4.84807400 4.74703300 -1.37149200
H -5.42883300 4.00972800 0.06619400
H -5.38906200 -4.14598700 0.65487900
H -4.73820000 -5.11852400 -0.60592900
H 5.47103100 -4.14976700 0.83332800
H 4.93142800 -5.06571000 -0.51447700
N 4.70374200 -4.38273500 0.20568800
N 4.76179800 4.18266300 -0.41972500
N -4.57826300 -4.39502100 0.09199100
N -4.63976400 4.17384500 -0.55622700
H -0.01639200 0.34977600 5.27124700

Reactant complex: $[(p\text{–}\mathbf{CH_3}\text{PY})_4\text{PYMe}_2\text{Mo(H)(OH)}\cdots\text{H}_2\text{O}]^+$

Mo 0.02024300 -0.02463000 -0.94391100
O 0.66077700 0.78633900 -2.71271100
H 0.23569900 0.38838200 -3.50080200
H -0.66155200 -0.91920700 -2.23831100
O -1.14442800 -0.69219500 -4.67091700
H -1.18892800 -0.92015700 -3.70424400
H -1.89544300 -0.08363000 -4.80878100
N -1.45571400 -1.57333400 -0.33814800
N 1.69827600 -1.37100900 -0.82418000
N 1.59765100 1.51129500 -0.43206700
N -1.67378400 1.28913300 -0.90095200
C -2.51381100 -1.27040100 0.46788100
N 0.00520100 0.04201200 1.28893600
C -2.50994400 0.11889400 1.15585700
C -2.62399900 1.24633100 0.09234000
C 2.57271900 -1.33625200 0.23295800
C -2.36247200 -3.80549500 -0.64973200
H -2.23492900 -4.79315600 -1.10311600
C -3.54113600 -2.20877200 0.68990500
H -4.39480900 -1.94413300 1.31418200
C 2.63338900 1.20339600 0.39607600
C 3.69713200 -0.21398000 2.20075800
H 3.60089500 -1.09893800 2.84738200
H 3.74690500 0.67487600 2.84572500
H 4.65338300 -0.28891700 1.66306800
C -3.67701800 2.18166600 0.12302100
H -4.41419900 2.14537600 0.92572300
C -3.70697300 0.20971100 2.13073700
H -3.71361200 1.17188200 2.66343800
H -3.67090900 -0.59573000 2.87900500
H -4.65906900 0.12458900 1.58710800
C 3.73005900 2.07430000 0.53557100
H 4.56645600 1.80686100 1.18231200
C 1.18791700 0.11187900 3.39113000
H 2.11755900 0.04665100 3.95321600

C -1.20140200 0.38173300 3.35089200
H -2.13841900 0.54767700 3.87910700
C 1.18143300 -0.01013100 1.99204000
C 1.90059100 -2.32420300 -1.78893700
H 1.22447800 -2.26339000 -2.64538300
C 2.51634500 -0.11805600 1.20559400
C -1.18058700 0.20584500 1.95834700
C -3.82144000 3.17669200 -0.85881000
C 3.54239700 -2.34574200 0.38484900
H 4.20207100 -2.34707100 1.25291800
C 1.62964700 2.70261600 -1.08989000
H 0.78273900 2.90123300 -1.74650900
C -0.00936900 0.32647100 4.07690800
C 3.77745700 3.30262100 -0.14895900
C 2.67332200 3.61557000 -0.96839900
H 2.62241100 4.56331200 -1.51335200
C 2.87851700 -3.30818500 -1.70892800
H 2.97480100 -4.03448800 -2.52201100
C -1.82956200 2.24609200 -1.87911900
H -1.07001100 2.21220600 -2.66481700
C -2.85717100 3.17765700 -1.89184900
H -2.90264400 3.90494000 -2.70919800
C 3.71061900 -3.36617400 -0.57056800
C -3.49613400 -3.49762000 0.13267000
C -1.39283300 -2.83481700 -0.86301000
H -0.52175900 -3.04568500 -1.48358600
C 4.94852400 4.24336500 -0.00784900
H 4.61347900 5.23643800 0.33971300
H 5.69523000 3.85918800 0.70424300
H 5.44557400 4.39621600 -0.98227000
C 4.73499000 -4.45918100 -0.39222400
H 5.34985300 -4.57813500 -1.30115000
H 5.40364100 -4.25368400 0.45838300
H 4.24076700 -5.43091800 -0.20985000
C -4.94390100 4.18475500 -0.81704500
H -5.62691500 3.99512300 0.02609500
H -4.54943300 5.21196200 -0.71391700
H -5.53322200 4.16152900 -1.75106900
C -4.59271800 -4.50583500 0.36739600
H -4.18938500 -5.42151800 0.83469500
H -5.38324200 -4.10221900 1.01874400
H -5.05298900 -4.81101300 -0.58907700
H -0.01481700 0.43996900 5.16472300

Transition state: $[(p\text{–}\mathbf{CH_3}\text{PY})_4\text{PYMe}_2\text{MoO}\cdots\text{H}\cdots\text{H}\cdots\text{H}_2\text{O}]^{+\,\ddagger}$
Mo -0.01016600 -0.07930800 -0.95283000
O 0.56705500 0.64561200 -2.60910400
H 0.37129800 -0.02373800 -3.54454900
H -1.13231000 -0.99722800 -2.29549400
O 0.01331300 -0.94094700 -4.35295900
H -0.73986900 -1.10032100 -3.04562000
H -0.64832300 -0.57356000 -4.97157900
N -1.46923300 -1.64057400 -0.25206300
N 1.65806100 -1.44854200 -0.86184800
N 1.52636400 1.43080100 -0.35125900
N -1.70250300 1.24385300 -0.85347600
C -2.52761900 -1.31537600 0.54326800
N 0.02278600 -0.04154600 1.30820600
C -2.49713600 0.07832600 1.22426600
C -2.61763100 1.21407400 0.16782800
C 2.53256400 -1.45262800 0.19523800
C -2.37711800 -3.87191500 -0.53115200
H -2.25038000 -4.86946400 -0.96212200
C -3.55855000 -2.24386400 0.77526400
H -4.41560800 -1.96657900 1.38953900
C 2.60536700 1.09357000 0.40407800
C 3.72547200 -0.35943300 2.14156300
H 3.64111900 -1.24733900 2.78544200
H 3.79838200 0.52432400 2.79165700
H 4.66532500 -0.43929800 1.57577700
C -3.64925800 2.17081000 0.23200000
H -4.36056400 2.15190600 1.05802600
C -3.67654600 0.18091400 2.21923000
H -3.65667900 1.13675900 2.76274300
H -3.64352600 -0.63295100 2.95819800
H -4.63835000 0.11849800 1.68960700
C 3.70926000 1.95958100 0.51004700
H 4.58257700 1.66556600 1.09353300
C 1.23636000 -0.05178700 3.39866000
H 2.17405900 -0.15363700 3.94222700
C -1.14523500 0.27742500 3.39792400
H -2.07086700 0.45229500 3.94324700
C 1.20404200 -0.13814200 1.99816900
C 1.82340900 -2.40104100 -1.83435600
H 1.16321100 -2.30508400 -2.70209000
C 2.51766600 -0.24572800 1.18226500
C -1.15000000 0.13404400 2.00184400
C -3.80669100 3.16461700 -0.75016000
C 3.46110500 -2.49984700 0.34206400
H 4.12168400 -2.52918000 1.20901300
C 1.51276000 2.64871600 -0.95827600
H 0.62747100 2.87383500 -1.55305400
C 0.05487900 0.17795300 4.10734400
H 0.06655800 0.26917100 5.19706600
C 3.71491400 3.21382000 -0.12710300
C 2.56054200 3.55912400 -0.86013800
H 2.47609800 4.52771100 -1.36228600
C 2.75998500 -3.42575200 -1.75641400
H 2.83008400 -4.14972300 -2.57424600
C -1.87312600 2.19056800 -1.83493200
H -1.14281100 2.13084000 -2.64722900
C -2.88468600 3.14108600 -1.81888500
H -2.94942600 3.86205900 -2.64028900
C 3.58749800 -3.52274300 -0.61802300
C -3.51457500 -3.54238200 0.23471000
C -1.39953600 -2.90859000 -0.75185100
H -0.52012800 -3.13680600 -1.35634500
C -4.62033100 -4.53888600 0.47411900
H -4.22551200 -5.45380700 0.94970500
H -5.40996700 -4.12341900 1.11875300
H -5.07844300 -4.84759500 -0.48219500
C 4.89454300 4.14859300 -0.02608700

H 4.58349400 5.12935400 0.37434600
H 5.68247500 3.74010600 0.62529400
H 5.33076700 4.33372800 -1.02371400
C -4.90587900 4.19558700 -0.67179100
H -5.57255300 4.01280300 0.18555400
H -4.48469800 5.21192300 -0.56816000
H -5.51577900 4.19461100 -1.59238600
C 4.56662200 -4.65683300 -0.44336700
H 5.15174700 -4.82142000 -1.36445700
H 5.26463200 -4.46604100 0.38681300
H 4.03339900 -5.60104200 -0.22843700

Product complex: $[(p\text{-}\mathbf{CH_3}\text{PY})_4\text{PYMe}_2\text{MoO}\cdots\text{H}_2\text{O}]^+ + \text{H}_2$
Mo 0.06111100 -0.12095500 -0.86350200
O 0.07893500 -0.24067500 -2.63185500
H 0.06495900 0.10928300 -4.35814900
H -5.75606600 -1.23235500 -5.01722900
O 0.06401300 0.26919100 -5.34102800
H -6.03732100 -0.54804600 -4.88657900
H -0.05418500 1.23238200 -5.43208500
N -1.52375100 -1.54836900 -0.50892800
N 1.70896500 -1.48286100 -0.55122600
N 1.64153100 1.34348800 -0.67701300
N -1.58801100 1.27085900 -0.75866000
C -2.50156600 -1.33092000 0.42887700
N 0.04439800 0.02702600 1.37490000
C -2.45920000 0.00136400 1.23225000
C -2.52793200 1.20089700 0.23983200
C 2.63405600 -1.27994800 0.44256500
C -2.61036700 -3.62611400 -1.14446600
H -2.61574500 -4.49493000 -1.80962000
C -3.51154700 -2.28877500 0.63075800
H -4.27338400 -2.12447300 1.39295100
C 2.60349000 1.25448000 0.29773700
C 3.75297500 0.10890600 2.23611200
H 3.74249200 -0.73383700 2.94251200
H 3.73267000 1.03741300 2.82497700
H 4.70298600 0.07669700 1.68239000
C -3.53433200 2.17958100 0.33131000
H -4.26108900 2.14051500 1.14318100
C -3.67723300 0.05972900 2.18240800
H -3.67389500 0.98736800 2.77276700
H -3.66932800 -0.78412900 2.88764700
H -4.61881900 0.02114200 1.61488900
C 3.60915300 2.23369100 0.38846500
H 4.35758400 2.17463800 1.17908900
C 1.23288400 0.17565900 3.47818800
H 2.17066900 0.21820900 4.03035700
C -1.17653500 0.15759100 3.46071200
H -2.12274800 0.18785500 3.99914500
C 1.22699300 0.08127200 2.08086700
C 1.86730500 -2.56992300 -1.36841800
H 1.16033600 -2.64118600 -2.19735200
C 2.54946500 0.03899700 1.26838600
C -1.14913200 0.06621100 2.06341000
C -3.65569500 3.21388900 -0.61608800
C 3.64101200 -2.23451800 0.67436700
H 4.35603000 -2.08721800 1.48396900
C 1.74363700 2.35261200 -1.59618900
H 0.99253000 2.35032100 -2.38708700
C 0.02263400 0.21393700 4.18328500
C 3.70118700 3.29377100 -0.53299100
C 2.74012100 3.31984500 -1.56527400
H 2.75804700 4.09173300 -2.34064900
C 2.86898800 -3.51746300 -1.19937400
H 2.93287400 -4.35714100 -1.89825800
C -1.73047400 2.24368900 -1.71157400
H -1.01065900 2.20749800 -2.53154200
C -2.73077100 3.20704500 -1.68143000
H -2.78123900 3.94971500 -2.48361500
C 3.77819600 -3.38256200 -0.12896900
C -3.59038800 -3.46188200 -0.14309100
C -1.61121600 -2.67159200 -1.28648200
H -0.84597500 -2.77505300 -2.05679300
C 4.77513000 4.34711200 -0.42555600
H 4.33687500 5.31983200 -0.13695000
H 5.53279300 4.07884700 0.32702200
H 5.27982400 4.49789900 -1.39529200
C -4.72553500 4.27118800 -0.50336900
H -5.47409500 4.01094800 0.26120500
H -4.28143600 5.24486100 -0.22651700
H -5.24249100 4.41673200 -1.46735000
C -4.67014400 -4.49013300 0.08364900
H -4.24054500 -5.41771100 0.50385400
H -5.43851300 -4.12421400 0.78234900
H -5.16014400 -4.76524100 -0.86615700
C 4.84865700 -4.41175400 0.13596500
H 5.58823300 -4.04854800 0.86660700
H 4.40320600 -5.34064300 0.53685400
H 5.37650200 -4.68416700 -0.79402000
H 0.01414400 0.28634200 5.27424600

Reactant complex: $[(p\text{-}\mathbf{F}\text{PY})_4\text{PYMe}_2\text{Mo(H)(OH)}\cdots\text{H}_2\text{O}]^+$
Mo 0.01389500 -0.01781300 -0.80033300
O 0.64425000 0.79215100 -2.56401400
H 0.22566000 0.39546300 -3.35902700
H -0.66791300 -0.90677500 -2.09220500
O -1.03723400 -0.61854900 -4.57565300
H -1.21141000 -0.91915200 -3.64936100
H -1.78021900 -0.01870900 -4.77980100
N -1.47090700 -1.56270000 -0.19683400
N 1.69063000 -1.36686700 -0.68637400
N 1.60672600 1.51504200 -0.29450600
N -1.67875900 1.30289900 -0.76104200
C -2.52631300 -1.25031600 0.61201500
N -0.00070800 0.04980700 1.43477700
C -2.51513300 0.13641500 1.30267700
C -2.62540100 1.26039800 0.23770700
C 2.55741000 -1.33638500 0.37951500
C -2.37938400 -3.79693000 -0.52976100
H -2.28251500 -4.78814500 -0.97669600
C -3.56395500 -2.17427600 0.83838500

H -4.42665300 -1.93812300 1.45926000
C 2.63663100 1.19679200 0.53885500
C 3.69155500 -0.22414800 2.34424400
H 3.58895300 -1.10713200 2.99224300
H 3.74948900 0.66367000 2.98962700
H 4.64588200 -0.30695300 1.80397800
C -3.67853500 2.19381600 0.27727000
H -4.42910400 2.18807200 1.06609400
C -3.71385100 0.23204700 2.27463400
H -3.71756000 1.19427300 2.80690100
H -3.68123100 -0.57183100 3.02448800
H -4.66538300 0.14938500 1.72936100
C 3.74435700 2.05117500 0.68428200
H 4.58995700 1.81074800 1.32718000
C 1.18274300 0.12295500 3.53690300
H 2.11221000 0.05771700 4.09915700
C -1.20610100 0.39692800 3.49667700
H -2.14237000 0.56583700 4.02511500
C 1.17409400 -0.00331600 2.13875900
C 1.88696900 -2.31381600 -1.65779000
H 1.21901500 -2.24130300 -2.51882300
C 2.50897600 -0.11978900 1.35249800
C -1.18447300 0.21881500 2.10482600
C -3.77127700 3.15625600 -0.72465200
C 3.51875100 -2.35020700 0.54577800
H 4.18753800 -2.38662900 1.40429600
C 1.64603400 2.69697800 -0.96605400
H 0.80401500 2.89523100 -1.62810300
C -0.01399400 0.34147800 4.22229500
C 3.75182300 3.25102000 -0.02671700
C 2.69245300 3.61230500 -0.86010200
H 2.67754200 4.55898500 -1.40373800
C 2.85049300 -3.31604800 -1.58622400
H 2.96352700 -4.05303000 -2.38384800
C -1.82678100 2.25367800 -1.74495200
H -1.06846800 2.21175500 -2.53094800
C -2.84642400 3.19730200 -1.77196400
H -2.91195500 3.93148800 -2.57796600
C 3.63976200 -3.33575300 -0.43432400
C -3.47622500 -3.43642600 0.25620300
C -1.40984300 -2.81995000 -0.72950900
H -0.54052400 -3.03307500 -1.35071100
F 4.81540300 4.08694500 0.10951100
F -4.78944600 4.06431700 -0.68116900
F 4.56504500 -4.32006800 -0.26625700
F -4.47195200 -4.33451600 0.47464600
H -0.01892700 0.45811700 5.30958700

Transition state: $[(p\text{−}\mathbf{F}\text{PY})_4\text{PYMe}_2\text{MoO}\cdots\text{H}\cdots\text{H}\cdots\text{H}_2\text{O}]^{+\,\ddagger}$
Mo -0.00964000 -0.08106300 -0.95562000
O 0.55667400 0.65869400 -2.59635900
H 0.33516300 -0.00481400 -3.57670900
H -1.08922100 -1.02388600 -2.28572100
O -0.04252800 -0.88524700 -4.34568000
H -0.73665800 -1.08819700 -3.07798800
H -0.71268400 -0.50717200 -4.94874400
N -1.46973400 -1.65200800 -0.24284500
N 1.66247500 -1.44488500 -0.86733100
N 1.53679500 1.43636900 -0.34922200
N -1.70783500 1.23915800 -0.86015000
C -2.53020000 -1.31707400 0.54744100
N 0.02112500 -0.03930800 1.30975000
C -2.49903800 0.07697100 1.22598400
C -2.62017300 1.20678000 0.16586600
C 2.52907900 -1.44987100 0.19921700
C -2.36743300 -3.89153600 -0.53344200
H -2.26503100 -4.89499500 -0.95061900
C -3.56945800 -2.23349200 0.78339100
H -4.44029500 -1.98452600 1.38803600
C 2.61223000 1.08985200 0.40837000
C 3.72406000 -0.36594600 2.14663400
H 3.63493900 -1.25276300 2.79109900
H 3.80106400 0.51650000 2.79771600
H 4.66328700 -0.44996100 1.58019800
C -3.65514400 2.15771700 0.23794000
H -4.38134000 2.16621900 1.04906100
C -3.68081200 0.18167700 2.21767400
H -3.66177800 1.13848300 2.75919000
H -3.64842100 -0.62934200 2.95953700
H -4.64172900 0.11720400 1.68641800
C 3.72670000 1.94030400 0.51884000
H 4.61076000 1.67348300 1.09648700
C 1.23330600 -0.04277100 3.40178800
H 2.17043600 -0.14182500 3.94669900
C -1.14879900 0.28233800 3.39872600
H -2.07477400 0.45645400 3.94354600
C 1.20067500 -0.13374100 2.00203600
C 1.82663500 -2.39170400 -1.84574000
H 1.17275200 -2.29018800 -2.71658700
C 2.51611400 -0.24629400 1.18856800
C -1.15100200 0.13609600 2.00333700
C -3.76512600 3.11849800 -0.76521500
C 3.45373500 -2.49696000 0.35992000
H 4.12198800 -2.55896700 1.21743000
C 1.52580500 2.64718600 -0.96737700
H 0.64344900 2.87212800 -1.56563900
C 0.05110400 0.18756100 4.10890100
H 0.06201600 0.28222500 5.19815000
C 3.68649600 3.16932200 -0.13917200
C 2.57320600 3.56301300 -0.88352800
H 2.52177400 4.53230400 -1.38312500
C 2.75282300 -3.42960900 -1.77672400
H 2.84193200 -4.16487500 -2.57902700
C -1.87309800 2.18079600 -1.84639700
H -1.14217100 2.11733000 -2.65740700
C -2.87990600 3.14004700 -1.84515100
H -2.96492600 3.86953300 -2.65350200
C 3.54002700 -3.48251000 -0.62499200
C -3.47396000 -3.50928200 0.22660900
C -1.39353200 -2.91829400 -0.74207000
H -0.51127300 -3.14857200 -1.34063700
F -4.76625800 4.04042600 -0.69018000

F 4.75530700 4.00201400 -0.03918200
F 4.43229100 -4.49723300 -0.46215600
F -4.47482100 -4.39785600 0.44885100

Product complex: $[(p\text{–}\mathbf{F}\text{PY})_4\text{PYMe}_2\text{MoO}\cdots\text{H}_2\text{O}]^+ + \text{H}_2$
Mo 0.10164700 -0.10836900 -0.70892000
O 0.13004900 -0.21570600 -2.47608100
H -0.03702100 0.01109100 -4.23312200
H -6.22445700 -0.85965500 -4.27745100
O -0.11898200 0.09887400 -5.21965200
H -5.79310900 -1.15952600 -4.81457600
H -0.50724600 0.98241100 -5.35589000
N -1.48213800 -1.55118000 -0.38649200
N 1.75929800 -1.45937100 -0.39943200
N 1.66931700 1.36577400 -0.48551800
N -1.56109600 1.27268500 -0.62802200
C -2.47865500 -1.33483600 0.53358900
N 0.04693300 0.01756600 1.53266800
C -2.45195400 -0.01208900 1.35066900
C -2.50594200 1.19419700 0.36700800
C 2.66042200 -1.26151600 0.61928500
C -2.53886300 -3.63420800 -1.07163700
H -2.54814700 -4.50849900 -1.72520900
C -3.49667500 -2.28654800 0.71501300
H -4.28894800 -2.15596700 1.45031800
C 2.61332200 1.26766900 0.50794100
C 3.74345100 0.10850800 2.44726700
H 3.72954500 -0.74222200 3.14373100
H 3.70860000 1.02850200 3.04849800
H 4.70046900 0.08978000 1.90493400
C -3.51135500 2.17118500 0.46936400
H -4.25694200 2.15740800 1.26286000
C -3.68769500 0.03581100 2.27799500
H -3.69308300 0.95461200 2.88169900
H -3.69327800 -0.81634200 2.97297100
H -4.61880500 0.00663700 1.69271300
C 3.61340000 2.24660500 0.63603000
H 4.36147700 2.21229400 1.42648100
C 1.20283800 0.13945500 3.65518500
H 2.13151500 0.17718600 4.22261700
C -1.20594600 0.11318000 3.60098800
H -2.16014500 0.13277000 4.12543500
C 1.21709000 0.06610100 2.25692200
C 1.93731300 -2.52709900 -1.23691700
H 1.25098200 -2.58381600 -2.08348300
C 2.55240600 0.04262700 1.46412600
C -1.15516700 0.04365100 2.20336900
C -3.57548800 3.18052300 -0.49194100
C 3.67159300 -2.20651800 0.86518900
H 4.38324300 -2.09663800 1.68180100
C 1.77538900 2.38021200 -1.39730800
H 1.03967600 2.37905400 -2.20158900
C -0.01804500 0.16202800 4.34154700
H -0.04321600 0.21747200 5.43306000
C 3.66759000 3.28498100 -0.29397100
C 2.75971100 3.36243400 -1.35174100
H 2.80601100 4.15216800 -2.10404000
C 2.93673500 -3.48144900 -1.07425700
H 3.04031000 -4.31739500 -1.76878000
C -1.68953200 2.24655700 -1.58078300
H -0.96788100 2.20729400 -2.39832500
C -2.68035000 3.22342500 -1.56255000
H -2.74321400 3.98154900 -2.34571500
C 3.78647300 -3.31117100 0.02059500
C -3.50845500 -3.42659900 -0.08891800
C -1.54321700 -2.66764800 -1.17420200
H -0.76018200 -2.76628700 -1.92593300
F 4.76552800 -4.22395600 0.26200900
F 4.63854300 4.22753300 -0.17017800
F -4.54954200 4.12420600 -0.38962000
F -4.49711400 -4.34235100 0.08477200

Reactant complex: $[(p\text{–}\mathbf{CF_3}\text{PY})_4\text{PYMe}_2\text{Mo(H)(OH)}\cdots\text{H}_2\text{O}]^+$
Mo -0.02772400 -0.08535600 -1.40510400
O 0.52067100 0.72873700 -3.17166200
H 0.17062300 0.27287900 -3.97651800
H -0.60385400 -1.01985100 -2.68354500
O -0.40373400 -0.49549300 -5.55481100
H -1.25736300 -0.95152800 -5.42759300
H -0.58641800 0.18498500 -6.23067000
N -1.51838600 -1.61602900 -0.84271600
N 1.64580400 -1.42126300 -1.30515500
N 1.57757400 1.45426000 -0.92910400
N -1.71342700 1.22544900 -1.34496600
C -2.54920700 -1.32386800 0.00820400
N -0.01308000 -0.03887300 0.83676400
C -2.52568900 0.04882000 0.72365200
C -2.64652500 1.18108700 -0.33166900
C 2.53521100 -1.39210200 -0.25587800
C -2.44544600 -3.83955300 -1.18346900
H -2.34093900 -4.81733400 -1.65910200
C -3.58133300 -2.25456900 0.23837200
H -4.41764400 -2.00293000 0.88743600
C 2.60867300 1.13945400 -0.09906200
C 3.69111300 -0.27518900 1.69548800
H 3.60278800 -1.16018900 2.34249900
H 3.74845300 0.61148400 2.34277500
H 4.64052100 -0.35062000 1.14563400
C -3.69583900 2.11444200 -0.27840800
H -4.42104400 2.08621300 0.53242100
C -3.71433200 0.13641200 1.70937000
H -3.70724200 1.09160500 2.25412000
H -3.67642100 -0.67650300 2.44916200
H -4.67295800 0.06417400 1.17549400
C 3.71988700 1.99461100 0.02295500
H 4.56261400 1.73213600 0.65964300
C 1.19389800 0.01567200 2.92279500
H 2.13000000 -0.04575000 3.47415400
C -1.19802900 0.27373400 2.91277900
H -2.12835800 0.43193200 3.45458500
C 1.17008700 -0.08658900 1.52272000
C 1.83418500 -2.36702900 -2.28511600

H 1.16098900 -2.28991200 -3.14111200
C 2.49584300 -0.17791400 0.71789600
C -1.18960600 0.11744100 1.51764900
C -3.82965300 3.09805800 -1.26700500
C 3.49773700 -2.40537700 -0.11056200
H 4.16874500 -2.41700800 0.74619900
C 1.61410700 2.62727000 -1.61453700
H 0.77134200 2.81643800 -2.27834300
C 0.00248800 0.21362200 3.62292000
C 3.74814200 3.20069600 -0.68790500
C 2.66396500 3.53732400 -1.51406100
H 2.62746800 4.47453700 -2.07423100
C 2.79872200 -3.36297000 -2.21880800
H 2.88743000 -4.08535800 -3.03368400
C -1.88208800 2.17667600 -2.32927200
H -1.14088400 2.12901500 -3.13055800
C -2.90070700 3.11522900 -2.32730100
H -2.96307100 3.84120700 -3.14192900
C 3.62680500 -3.41005500 -1.08160300
C -3.53893500 -3.51789700 -0.35776900
C -1.48103100 -2.86732300 -1.40224000
H -0.63394800 -3.07117000 -2.05583600
C -4.92542700 4.12687500 -1.20565800
C 4.91589500 4.15436900 -0.55334600
C 4.62607300 -4.52665000 -0.91944900
C -4.63949800 -4.52796700 -0.13595200
F 5.37851300 4.56085100 -1.77683500
F 5.97090600 3.60701900 0.11572900
F 4.55689500 5.29248200 0.12557100
F -5.33048000 -4.78303900 -1.29594400
F -5.55391000 -4.12055300 0.79064000
F -4.14239500 -5.73406200 0.28847200
F 5.53635800 -4.28510000 0.06950500
F 5.33293400 -4.75290300 -2.07317600
F 4.01201900 -5.71970100 -0.60818100
F -5.62303600 4.20582900 -2.38740900
F -5.83734300 3.87788500 -0.21953100
F -4.43117800 5.39291200 -0.97578900
H 0.00917800 0.31674000 4.71158200

Transition state: $[(p\text{–}\mathbf{CF_3}\text{PY})_4\text{PYMe}_2\text{MoO}\cdots\text{H}\cdots\text{H}\cdots\text{H}_2\text{O}]^{+\,\ddagger}$
Mo 0.00867000 -0.08509800 -0.97381400
O 0.54983600 0.67668500 -2.57826900
H 0.17128500 0.10158500 -3.68465400
H -0.94304800 -1.11469100 -2.27896600
O -0.31949800 -0.65588800 -4.38474100
H -0.77892900 -1.02796400 -3.17510200
H -1.06427800 -0.21033600 -4.83653900
N -1.44661200 -1.67029300 -0.24531100
N 1.66432200 -1.43727300 -0.84900500
N 1.55891500 1.44694900 -0.35066600
N -1.69314500 1.21382700 -0.87536400
C -2.50847000 -1.33940000 0.54123900
N 0.02593800 -0.03285100 1.31035900
C -2.49176500 0.05760800 1.21251300
C -2.61259000 1.18124400 0.14721700
C 2.53605000 -1.43993900 0.21856800
C -2.32640200 -3.91436300 -0.50976400
H -2.19062200 -4.91737000 -0.92014400
C -3.54448600 -2.26412100 0.77123300
H -4.41390900 -1.98949400 1.36552100
C 2.62596200 1.10077400 0.41446900
C 3.72473100 -0.34660700 2.16667000
H 3.63003500 -1.22872600 2.81653800
H 3.79873700 0.54010700 2.81248400
H 4.66802400 -0.43660500 1.60809700
C -3.64585800 2.13174900 0.21384400
H -4.36080900 2.11528300 1.03380200
C -3.67830200 0.15749800 2.19980900
H -3.66676300 1.11500000 2.74013000
H -3.64276300 -0.65179400 2.94353400
H -4.63787200 0.08654500 1.66708600
C 3.74526600 1.94869300 0.51594500
H 4.61958300 1.65418300 1.09373700
C 1.22811600 -0.02998600 3.40566300
H 2.16257800 -0.12393800 3.95571400
C -1.15494300 0.28701000 3.39132100
H -2.08390700 0.45733400 3.93193000
C 1.20239300 -0.12091700 2.00530100
C 1.83223800 -2.39691700 -1.82109900
H 1.18335300 -2.30122300 -2.69446200
C 2.52298200 -0.23142100 1.19975200
C -1.14910700 0.13474400 1.99612200
C -3.78059000 3.11394700 -0.77594500
C 3.45167300 -2.49000000 0.38319900
H 4.10855600 -2.52215100 1.25058700
C 1.55399700 2.65415900 -0.97522600
H 0.67751300 2.87642900 -1.58317100
C 0.04213000 0.19897300 4.10548800
H 0.04811400 0.29743300 5.19446200
C 3.73547500 3.18645700 -0.13690500
C 2.60487600 3.56241300 -0.88119700
H 2.53646100 4.52711200 -1.38925300
C 2.75213900 -3.43286600 -1.73308800
H 2.82691800 -4.16101300 -2.54397600
C -1.85934200 2.16587200 -1.85729100
H -1.12753400 2.11457000 -2.66665700
C -2.86715200 3.11746600 -1.84696700
H -2.93073500 3.84098300 -2.66359100
C 3.55920700 -3.50669500 -0.58243700
C -3.46015400 -3.55579200 0.23837200
C -1.35914700 -2.94104900 -0.73299000
H -0.47487000 -3.17055300 -1.32850300
C -4.57139100 -4.56167500 0.44924800
C 4.91323300 4.13188000 -0.03293400
C -4.86426600 4.15729100 -0.70134900
C 4.50204800 -4.66252500 -0.37771900
F 5.35459800 4.52321200 -1.26964200
F 5.97667900 3.58190900 0.61951300
F 4.57564700 5.27829600 0.64152900
F 5.03513500 -5.11047100 -1.55701700
F 3.86925000 -5.74714700 0.19381900

F 5.54816200 -4.34994300 0.44650400
F -5.23752400 -4.82116600 -0.72257700
F -4.08611600 -5.76201600 0.89561600
F -5.50122300 -4.13900900 1.35228700
F -5.78023800 3.90418200 0.27933100
F -5.55682400 4.26187400 -1.88253900
F -4.35159200 5.41066500 -0.45031700

Product complex: $[(p\text{−}\mathbf{CF_3}\text{PY})_4\text{PYMe}_2\text{MoO}\cdots\text{H}_2\text{O}]^+ + \text{H}_2$
Mo 0.08959300 -0.14729000 -1.33237200
O 0.11647500 -0.25544600 -3.08924700
H 0.21455600 0.02421100 -4.88741600
H -5.85468000 -1.17296000 -5.41138500
O 0.27536900 0.13489100 -5.86936700
H -5.39222900 -1.58862800 -5.83312700
H 0.31734700 1.09935500 -6.00445300
N -1.51130000 -1.54931900 -0.98408200
N 1.71037600 -1.52792500 -1.01761800
N 1.68041500 1.29337000 -1.12426800
N -1.52751600 1.26821200 -1.22583000
C -2.48688500 -1.31507300 -0.04561100
N 0.06364800 -0.00962000 0.93206100
C -2.43085200 0.01183800 0.76460100
C -2.45974000 1.22062400 -0.21680900
C 2.62607500 -1.34652000 -0.00904000
C -2.61366300 -3.61323400 -1.63543200
H -2.63254300 -4.48039400 -2.29895900
C -3.51116200 -2.25479600 0.15426000
H -4.27755400 -2.08576500 0.90802000
C 2.62384700 1.19078700 -0.13104100
C 3.76700200 0.01385500 1.79256700
H 3.74915800 -0.83511200 2.49094800
H 3.75477000 0.93376200 2.39457000
H 4.71626600 -0.02051000 1.23735000
C -3.42611000 2.23316800 -0.10304600
H -4.14750800 2.22232100 0.71183600
C -3.65926300 0.08868200 1.70010900
H -3.64036900 1.00807900 2.30239500
H -3.67842200 -0.76051300 2.39833400
H -4.59476000 0.07861900 1.12115100
C 3.62677800 2.16675400 -0.00963200
H 4.36396700 2.10698100 0.78870300
C 1.24301700 0.08904100 3.03814600
H 2.17780800 0.10763000 3.59616900
C -1.16644400 0.11576900 3.00757300
H -2.11452700 0.15679900 3.54144700
C 1.23902300 0.01534800 1.63868000
C 1.85620700 -2.60368600 -1.85347500
H 1.16657100 -2.64645400 -2.69779200
C 2.56062600 -0.03379700 0.82681000
C -1.12865000 0.04249000 1.60856000
C -3.49677100 3.26010100 -1.05680300
C 3.61070600 -2.31895900 0.23096100
H 4.32023800 -2.19932000 1.04717500
C 1.79775500 2.30043900 -2.04423600
H 1.06913200 2.29668200 -2.85456700
C 0.02966000 0.13879100 3.73298700
C 3.71237000 3.21738800 -0.93453600
C 2.78872800 3.27232500 -1.99183800
H 2.82698900 4.04698500 -2.76088200
C 2.83303800 -3.57610500 -1.68514800
H 2.89622900 -4.40765300 -2.39058300
C -1.64353300 2.24172800 -2.18300700
H -0.94385900 2.17361300 -3.01720900
C -2.60190000 3.24573200 -2.14079000
H -2.64066700 3.99094900 -2.93844700
C 3.71432600 -3.44631300 -0.59763000
C -3.57971500 -3.41179600 -0.63565800
C -1.60621300 -2.66607400 -1.77014300
H -0.84490900 -2.77611700 -2.54199800
C -4.50553600 4.37474700 -0.91706800
C 4.76727700 4.28989000 -0.79081200
C 4.74539500 -4.51508100 -0.32510100
C -4.65946300 -4.44182400 -0.39640900
F -5.09288500 -5.00895900 -1.56303700
F -5.75270900 -3.91750000 0.23188100
F -4.20555200 -5.47194900 0.39389200
F 5.74383300 -4.08565700 0.50106900
F 4.18252800 -5.61854200 0.27377100
F 5.33532300 -4.96142600 -1.47762000
F 5.30147800 4.64435000 -2.00010200
F 5.80130000 3.90577700 0.01302700
F 4.24489900 5.43847200 -0.24435700
F -5.54733000 4.04201100 -0.09927300
F -5.03690800 4.73844600 -2.12518300
F -3.93464800 5.50941800 -0.38740000
H 0.01643000 0.19580700 4.82471200

Reactant complex: $[(p\text{−}\mathbf{CN}\text{PY})_4\text{PYMe}_2\text{Mo(H)(OH)}\cdots\text{H}_2\text{O}]^+$
Mo -0.03235600 0.00020700 -0.77466500
O 0.49270300 0.80020100 -2.54200300
H 0.15167900 0.33958500 -3.35067300
H -0.59259400 -0.95697000 -2.03724600
O -0.38147900 -0.44203100 -4.90395800
H -1.30986200 -0.74105200 -4.86314500
H -0.36122900 0.20018400 -5.63916100
N -1.52625300 -1.51627200 -0.19834000
N 1.62848900 -1.34460600 -0.67305200
N 1.58932200 1.53133400 -0.32002000
N -1.70987800 1.32153900 -0.71723200
C -2.55021600 -1.21363700 0.66147200
N -0.00545800 0.06385600 1.46840300
C -2.51767900 0.16507500 1.36617700
C -2.63845100 1.29023100 0.30301300
C 2.52296700 -1.31900000 0.37509900
C -2.45809200 -3.74358300 -0.51374900
H -2.36469600 -4.72574900 -0.98097500
C -3.58064900 -2.13503900 0.90965800
H -4.41252200 -1.87693400 1.56211800
C 2.62230900 1.21344600 0.50927400
C 3.70078500 -0.19648500 2.31079300
H 3.60609100 -1.07426700 2.96645600

H 3.77021800 0.69519400 2.94983400
H 4.64659700 -0.28703200 1.75709300
C -3.67855500 2.22674100 0.35786500
H -4.40165800 2.21066900 1.17116600
C -3.70063500 0.26623100 2.35756400
H -3.68602000 1.22598400 2.89385900
H -3.66136000 -0.53989800 3.10450200
H -4.66267600 0.19351900 1.83004700
C 3.73975400 2.05632700 0.62008800
H 4.58486100 1.79516900 1.25436200
C 1.21205800 0.12770900 3.54704400
H 2.15013000 0.06450300 4.09464500
C -1.17803700 0.40403200 3.54614100
H -2.10422800 0.57369400 4.09133300
C 1.18047500 0.01316500 2.14821400
C 1.80227800 -2.30036100 -1.64785600
H 1.13226100 -2.21813700 -2.50577000
C 2.50153900 -0.09590400 1.33832700
C -1.17738200 0.23434500 2.15259900
C -3.81308100 3.21633200 -0.64078700
C 3.46880900 -2.34034200 0.52886500
H 4.14407800 -2.35583000 1.38248600
C 1.63082500 2.69747700 -1.01631900
H 0.78684400 2.88769600 -1.67829100
C 0.02557900 0.34197000 4.25040500
C 3.77527200 3.26706200 -0.10232100
C 2.68429400 3.60369000 -0.92997600
H 2.65582100 4.53872900 -1.49270200
C 2.74710700 -3.31210600 -1.57775100
H 2.82520800 -4.04450400 -2.38390200
C -1.87647500 2.26709400 -1.70760800
H -1.14069900 2.20855700 -2.51284100
C -2.88462600 3.21487000 -1.71024300
H -2.94884500 3.93800400 -2.52625400
C 3.58076000 -3.36870800 -0.43594600
C -3.55001800 -3.41474300 0.32217100
C -1.49801700 -2.77252200 -0.74847900
H -0.65960800 -2.98434500 -1.41051100
C -4.59700100 -4.35767000 0.57826200
C 4.53812500 -4.41720000 -0.26967900
C 4.90775800 4.14117600 0.01364600
C -4.86587900 4.17949500 -0.57149200
N -5.45664900 -5.13662000 0.78415800
N 5.32637300 -5.28408800 -0.13556800
N 5.83548200 4.85997200 0.10542200
N -5.73391100 4.97662100 -0.51888100
H 0.03843900 0.45611600 5.33783500

Transition state: $[(p\text{−}\mathbf{CN}\text{PY})_4\text{PYMe}_2\text{MoO}\cdots\text{H}\cdots\text{H}\cdots\text{H}_2\text{O}]^{+\,\ddagger}$

Mo 0.01303400 -0.08313300 -0.98659300
O 0.54156100 0.69183100 -2.56893500
H 0.12536300 0.12636200 -3.73484900
H -0.89035800 -1.13160900 -2.27617300
O -0.38172800 -0.62077600 -4.37728100
H -0.78017700 -1.01578900 -3.20565400
H -1.14515700 -0.18301300 -4.80638300
N -1.44120100 -1.67454400 -0.24960700
N 1.65854200 -1.43864100 -0.84602900
N 1.57038200 1.44995700 -0.34795200
N -1.68938800 1.21202900 -0.88290300
C -2.50659600 -1.34288000 0.53503400
N 0.02337500 -0.03042600 1.30777600
C -2.49378900 0.05515500 1.20464500
C -2.61349400 1.17825200 0.13919000
C 2.52970200 -1.44610100 0.22573500
C -2.31350000 -3.92337100 -0.51432800
H -2.17978400 -4.92746800 -0.92105400
C -3.54236900 -2.26294500 0.76332500
H -4.41631700 -1.98961000 1.35169700
C 2.63654000 1.09436600 0.41684100
C 3.71862300 -0.35631000 2.17658400
H 3.61475600 -1.23557400 2.82875700
H 3.79663200 0.53201600 2.81962000
H 4.66331300 -0.45539900 1.62212900
C -3.64230500 2.12662100 0.20955100
H -4.36076500 2.10944100 1.02667300
C -3.68190500 0.15364300 2.19041600
H -3.67276200 1.11122700 2.73039900
H -3.64530100 -0.65528400 2.93440900
H -4.64077200 0.08105900 1.65675300
C 3.76275500 1.92784700 0.51539300
H 4.63759000 1.62858900 1.09037000
C 1.22063800 -0.02227000 3.40469100
H 2.15338100 -0.11491600 3.95762000
C -1.16185200 0.29706300 3.38415000
H -2.09172300 0.46898200 3.92244100
C 1.19803300 -0.11796700 2.00434600
C 1.82113500 -2.40627300 -1.81515800
H 1.17748400 -2.30785400 -2.69164900
C 2.52144400 -0.23560200 1.20443600
C -1.15255300 0.13850500 1.98954200
C -3.77516400 3.12609000 -0.77895000
C 3.43467300 -2.49813300 0.39810700
H 4.09112500 -2.53459700 1.26562100
C 1.57259600 2.65661200 -0.97257700
H 0.69655400 2.88608100 -1.57881200
C 0.03364400 0.21137000 4.10041300
C 3.76314700 3.17590400 -0.13980900
C 2.62671800 3.56052900 -0.88271000
H 2.56832900 4.52802900 -1.38494700
C 2.72740900 -3.44933000 -1.72482900
H 2.79916300 -4.18250400 -2.53102600
C -1.84934300 2.17387600 -1.85841400
H -1.11535200 2.13020200 -2.66556200
C -2.85095600 3.12923900 -1.84974300
H -2.91101700 3.86038400 -2.65884400
C 3.53680000 -3.53378700 -0.56493500
C -3.45789100 -3.56604200 0.23096300
C -1.35139800 -2.94603500 -0.73530500
H -0.46696100 -3.17575400 -1.33037800
C -4.51229100 -4.51035100 0.46020100
C 4.45627400 -4.60895300 -0.37975700

C 4.90405300 4.04114100 -0.04137800
C -4.82303000 4.09456900 -0.69725800
N -5.37654600 -5.28839900 0.64535900
N 5.21598200 -5.49995900 -0.22968600
N 5.83859100 4.75260400 0.03667700
N -5.68600800 4.89581600 -0.63331800
H 0.03752100 0.31454400 5.18893200

Product complex: $[(p\text{−}\mathbf{CN}\text{PY})_4\text{PYMe}_2\text{MoO}\cdots\text{H}_2\text{O}]^+ + \text{H}_2$
Mo 0.08054400 -0.13815400 -0.73616200
O 0.10539300 -0.25495100 -2.48392400
H 0.09793700 -0.02083600 -4.32371700
H -6.21384500 -0.66131900 -4.23238200
O 0.09984400 0.06208800 -5.30791500
H -5.73702800 -1.01280100 -4.69456800
H 0.00776400 1.01855700 -5.47238100
N -1.49681900 -1.56230300 -0.38120000
N 1.72498900 -1.47959400 -0.39901400
N 1.63222400 1.33620500 -0.52066800
N -1.55320800 1.25396500 -0.62604300
C -2.48627800 -1.33781600 0.54738700
N 0.03992500 0.00503100 1.54387500
C -2.45082400 -0.01239900 1.36211900
C -2.48258600 1.20194800 0.38757400
C 2.63910900 -1.26890100 0.60791700
C -2.56014400 -3.64452100 -1.04262000
H -2.56133700 -4.51640000 -1.69945900
C -3.50199800 -2.28377200 0.73739400
H -4.28080500 -2.12498300 1.48046400
C 2.56286900 1.27018700 0.49031800
C 3.73686000 0.12234000 2.41356600
H 3.74620200 -0.73163100 3.10578000
H 3.69196900 1.03630300 3.02284100
H 4.68732900 0.12429400 1.85949900
C -3.44474100 2.21175300 0.51345200
H -4.16229500 2.20203700 1.33183700
C -3.68590900 0.04919900 2.29007000
H -3.67525000 0.96237500 2.90180400
H -3.70528100 -0.80646800 2.98016900
H -4.61750100 0.04030300 1.70485200
C 3.52049300 2.28279900 0.63236800
H 4.24426500 2.25766000 1.44482200
C 1.20911000 0.09619500 3.65363800
H 2.14098200 0.12572200 4.21572000
C -1.20040000 0.07652900 3.61349900
H -2.15103000 0.09177700 4.14395300
C 1.21061300 0.04578000 2.25265100
C 1.89549900 -2.55691600 -1.23003900
H 1.20467000 -2.62394100 -2.07153100
C 2.53482400 0.04092500 1.44477200
C -1.15428100 0.02618100 2.21322400
C -3.51967500 3.25438600 -0.43885300
C 3.65030300 -2.20745800 0.84868000
H 4.36165300 -2.06650600 1.65980900
C 1.72973100 2.34328100 -1.44463100
H 1.02142500 2.30649500 -2.27179800
C -0.00767200 0.10920100 4.34263000
C 3.58238700 3.34676200 -0.29555100
C 2.67609000 3.35509400 -1.37886600
H 2.70186200 4.12977100 -2.14760900
C 2.89500100 -3.50367200 -1.06429100
H 2.97882600 -4.33907800 -1.76226900
C -1.67447200 2.22945700 -1.58206700
H -0.98171500 2.16238300 -2.42185300
C -2.62769100 3.23523800 -1.53497500
H -2.67252800 3.98408800 -2.32818500
C 3.78351800 -3.34751800 0.02367200
C -3.54889200 -3.45418800 -0.05233400
C -1.56632500 -2.68425200 -1.16409800
H -0.79389900 -2.78917700 -1.92531200
H -0.02619600 0.14728000 5.43511900
C 4.56336000 4.37910300 -0.14750500
N 5.36858800 5.23084700 -0.02730700
C 4.81784100 -4.30391400 0.27580000
N 5.66776400 -5.09402500 0.48151900
C -4.59284100 -4.41492200 0.14172300
N -5.45020300 -5.20747100 0.29946600
C -4.50138300 4.28687700 -0.30522900
N -5.30763900 5.13971600 -0.19676400

4.3.4 Structures with substituent groups at global position only

Reactant complex: $[(p\text{−}\mathbf{NH_2}\text{PY})_5\text{Me}_2\text{Mo(H)(OH)}\cdots\text{H}_2\text{O}]^+$
Mo 0.08865700 -0.04557800 -0.99852700
O 0.74099500 0.82121300 -2.77424600
H 0.41532700 0.30876400 -3.53524600
H -0.44406500 -0.99874000 -2.33252900
O -2.50846600 -0.56668300 -3.78274600
H -1.77109400 -0.65525800 -3.11393000
H -2.85583800 0.33083100 -3.61759600
N -1.41825100 -1.57680800 -0.42943300
N 1.77409800 -1.39044400 -0.83688700
N 1.63088000 1.50052500 -0.44299100
N -1.61176100 1.27308400 -0.97713300
C -2.48462700 -1.28260300 0.37705500
N 0.03125600 0.00850900 1.23064700
C -2.48430700 0.10627600 1.06851400
C -2.58360500 1.23024300 -0.00188200
C 2.62447500 -1.35456600 0.24316600
C -2.32932600 -3.81410900 -0.75701800
H -2.20312500 -4.79886700 -1.21627700
C -3.51071800 -2.21089200 0.60265100
H -4.35868200 -1.95299300 1.23726000
C 2.66692600 1.19281800 0.39148700
C 3.70843200 -0.21106000 2.22179700
H 3.60448200 -1.09025900 2.87521500
H 3.74295200 0.68347100 2.85991100
H 4.67465500 -0.28810300 1.70217600
C -3.64415000 2.15200300 0.01145400
H -4.39706100 2.11529900 0.79917300
C -3.69517000 0.20397100 2.02544200

H -3.70837100 1.16917000 2.55303600
H -3.67150200 -0.59702800 2.77874300
H -4.63956400 0.11639900 1.46860300
C 3.76077700 2.05223200 0.54746800
H 4.59025800 1.78669000 1.20351600
C 1.18159300 0.09813800 3.35465000
H 2.10526200 0.04699000 3.92906800
C -1.21374100 0.36177500 3.27197900
H -2.16237100 0.52368000 3.78190300
C 1.18951400 -0.03122400 1.96570800
C 1.99743500 -2.36724000 -1.77430200
H 1.34658400 -2.31624800 -2.65106100
C 2.54492800 -0.12872900 1.20490500
C -1.16049800 0.18363600 1.89020800
C -3.77559300 3.14633500 -0.98307800
C 3.57795200 -2.36236700 0.44507800
H 4.21755400 -2.35517900 1.32788100
C 1.67315100 2.70046500 -1.08727500
H 0.83025900 2.90859400 -1.74662500
C -0.03151500 0.31566500 4.04730600
C 3.81442400 3.29281100 -0.13896300
C 2.70821800 3.61625100 -0.96527800
H 2.66081100 4.56609400 -1.50607700
C 2.95484000 -3.36302400 -1.66198300
H 3.06330600 -4.10465500 -2.45896700
C -1.75658500 2.23433300 -1.95359400
H -0.97538300 2.20820900 -2.72009800
C -2.78780000 3.15792400 -2.00077100
H -2.82177400 3.88485100 -2.81853900
C 3.75811700 -3.40848300 -0.49425300
C -3.46841300 -3.50556000 0.03127000
C -1.36427200 -2.84119200 -0.95329200
H -0.49112100 -3.05590900 -1.56993200
N -0.06503100 0.43775800 5.40718300
H 0.79945200 0.54705400 5.93197700
H -0.91849900 0.73786800 5.87211700
N -4.85271700 4.02096700 -1.00143400
H -5.35554900 4.15447800 -0.12460900
H -4.73456300 4.88410500 -1.53088000
N 4.86376600 4.15961700 0.03849600
H 4.97920600 4.93621600 -0.60897500
H 5.72043600 3.82134300 0.47181300
N 4.64840400 -4.43337700 -0.26425300
H 4.93055300 -5.01492500 -1.05116100
H 5.36453300 -4.30541700 0.44853400
N -4.44764800 -4.43583500 0.28273700
H -5.33836700 -4.12430200 0.66492700
H -4.49545100 -5.26793100 -0.30156200

Transition state: $[(p\text{–}\mathbf{NH_2}\text{PY})_5\text{Me}_2\text{MoO}\cdots\text{H}\cdots\text{H}\cdots\text{H}_2\text{O}]^{+\ \ddagger}$
Mo -0.02605000 -0.07869200 -0.94975100
O 0.56998300 0.72118600 -2.65135700
H 0.46890300 0.01357600 -3.42965200
H -1.18466300 -0.77441400 -2.24850300
O 0.23105000 -1.23107000 -4.25107400
H -0.57784000 -1.13336800 -2.71168700
H -0.52791900 -1.12234000 -4.85722600
N -1.47086000 -1.63595000 -0.26429000
N 1.66806100 -1.44338400 -0.86676400
N 1.49963500 1.44124400 -0.34509200
N -1.71982200 1.26784000 -0.81505900
C -2.54334100 -1.31718400 0.52278500
N 0.01680200 -0.05690900 1.29762900
C -2.50655900 0.06215700 1.23799800
C -2.63082800 1.22438300 0.20850800
C 2.53341900 -1.44929000 0.19947000
C -2.40805100 -3.85016100 -0.62336600
H -2.29138700 -4.83705800 -1.07966100
C -3.58773700 -2.22277400 0.72329300
H -4.44302300 -1.95404800 1.34337400
C 2.59574900 1.10207300 0.39118900
C 3.72427900 -0.33679500 2.13784300
H 3.64351400 -1.21825300 2.79116200
H 3.79645500 0.55378700 2.77863500
H 4.66352300 -0.42153400 1.57164200
C -3.65785800 2.17512400 0.30602500
H -4.37004900 2.14119000 1.13061100
C -3.68176800 0.14386500 2.23966300
H -3.65984400 1.08763700 2.80390500
H -3.64716000 -0.68667700 2.95975000
H -4.64567500 0.09584700 1.71216800
C 3.70510500 1.94906200 0.48424800
H 4.58427200 1.65431500 1.05809800
C 1.24173000 -0.04483900 3.38477300
H 2.18619700 -0.12337000 3.92154600
C -1.15075000 0.24298600 3.39413500
H -2.08060800 0.39034600 3.94147200
C 1.19622300 -0.13681400 1.99409700
C 1.83879600 -2.41268700 -1.82278600
H 1.19922300 -2.30903300 -2.71031800
C 2.51483100 -0.23509100 1.17884200
C -1.14957200 0.10863300 2.00636300
C -3.80793600 3.19974600 -0.65891900
C 3.45195700 -2.49176000 0.37757000
H 4.10849100 -2.51410500 1.24745800
C 1.48770400 2.66601900 -0.94041000
H 0.59346600 2.90426900 -1.51629800
C 0.05727100 0.16791200 4.12631100
C 3.70748200 3.21421700 -0.15909100
C 2.53317500 3.57472100 -0.86831300
H 2.44434300 4.54525300 -1.36482000
C 2.75629700 -3.44873500 -1.72759900
H 2.82880500 -4.18457100 -2.53419600
C -1.88976800 2.23818500 -1.76966800
H -1.16532400 2.18833000 -2.58937800
C -2.88785800 3.19910300 -1.73728500
H -2.95090800 3.94017800 -2.54007300
C 3.57263900 -3.53834200 -0.57214400
C -3.55791500 -3.51842300 0.13913700
C -1.41814100 -2.89504400 -0.79068400
H -0.53017200 -3.12533200 -1.38262800
N 4.42634300 -4.59445900 -0.36572900

H 4.66031300 -5.19718100 -1.15213600
H 5.14726500 -4.51523900 0.34894600
N -4.56754800 -4.41273300 0.34654700
H -5.43323100 -4.12237700 0.79435400
H -4.59040800 -5.29105800 -0.16532700
N -4.77638300 4.17484500 -0.52809300
H -5.02256000 4.71329400 -1.35703700
H -5.55991500 3.98903400 0.09605800
N 4.77521300 4.06626100 -0.04883400
H 4.83372100 4.87489400 -0.66376300
H 5.66284100 3.71473700 0.30371600
N 0.07313100 0.25487200 5.48929600
H 0.95757700 0.34090400 5.98422600
H -0.75817300 0.55593000 5.99229700

Product complex: $[(p\text{–}\mathbf{NH_2}\text{PY})_5\text{Me}_2\text{MoO}\cdots\text{H}_2\text{O}]^+ + \text{H}_2$
Mo -0.01474300 -0.07419500 -0.84778200
O -0.03253600 -0.13732700 -2.64927700
H 0.60955400 -0.52538300 -4.14470200
H -5.29116500 -0.91073600 -5.53598300
O 0.99583000 -0.74469800 -5.04955100
H -5.40081600 -0.17251700 -5.62256700
H 0.39012800 -0.32000300 -5.68393200
N -1.54624600 -1.52286500 -0.37064800
N 1.67071000 -1.40536700 -0.64968400
N 1.52833300 1.41588100 -0.56870500
N -1.69655500 1.27308400 -0.73733900
C -2.56228400 -1.26633000 0.51852100
N 0.02040900 0.04290300 1.41080500
C -2.48669200 0.06190300 1.32501400
C -2.57646500 1.25403600 0.32048200
C 2.58579300 -1.27385500 0.37057500
C -2.65659000 -3.59145700 -1.01700300
H -2.64442000 -4.48473300 -1.64772500
C -3.61861800 -2.16751000 0.68342200
H -4.40994400 -1.96454600 1.40522000
C 2.56727300 1.25509600 0.31602100
C 3.74446300 0.04488000 2.19857700
H 3.72907600 -0.80614500 2.89514600
H 3.75664500 0.96782000 2.79715400
H 4.68372500 -0.00439500 1.62828100
C -3.55036700 2.25203600 0.46462500
H -4.22358500 2.25069500 1.32256300
C -3.67986900 0.13166900 2.30557500
H -3.64116900 1.04755400 2.91318900
H -3.67762600 -0.72756400 2.99265100
H -4.63526900 0.13018500 1.76057200
C 3.62252700 2.17175600 0.36031500
H 4.43416100 2.04848600 1.07780900
C 1.25925300 0.13448500 3.48495000
H 2.20982600 0.15074500 4.01762100
C -1.15692000 0.16033000 3.51910100
H -2.09158400 0.19773800 4.07807400
C 1.21153000 0.05885800 2.09300400
C 1.84139200 -2.45632200 -1.51477300
H 1.15719400 -2.46790900 -2.36755900
C 2.52228700 0.01398100 1.25222500
C -1.15057300 0.09594900 2.12583300
C -3.70335900 3.27884600 -0.49962900
C 3.57062800 -2.24818800 0.58425300
H 4.27205200 -2.15388900 1.41373600
C 1.58097000 2.48432300 -1.42400100
H 0.74380800 2.57609400 -2.11721000
C 0.06197300 0.18528900 4.23795100
C 3.67932700 3.27572200 -0.52913100
C 2.61232700 3.40861400 -1.45436400
H 2.58189800 4.22935800 -2.17669200
C 2.81239200 -3.43602400 -1.37604600
H 2.87733000 -4.24341600 -2.11176000
C -1.89333100 2.22687700 -1.70311100
H -1.23848900 2.13895000 -2.57457300
C -2.85609900 3.22205700 -1.63491400
H -2.94515700 3.94798500 -2.44889800
C 3.69851900 -3.37027100 -0.27158600
C -3.70160500 -3.35696400 -0.08671700
C -1.62115400 -2.67582200 -1.10622100
H -0.79663900 -2.84950100 -1.79887200
N 0.08194600 0.21160900 5.61056200
H 0.95174600 0.44013100 6.08739400
H -0.76797000 0.45984800 6.11287300
H 5.53600200 3.96523700 0.06853600
H 4.82858000 4.84585100 -1.23031300
H -4.88879000 4.83848900 -1.14230900
H -5.36711200 4.15625500 0.34835000
H -5.38725700 -4.13083800 0.83711300
H -4.70359800 -5.14352100 -0.37763400
H 5.39487800 -4.14994000 0.60756900
H 4.87233400 -4.98506200 -0.78726200
N 4.61900700 -4.36943400 -0.01566300
N 4.69667700 4.19357300 -0.46029100
N -4.76225200 -4.21671900 0.03857300
N -4.61154300 4.30555900 -0.31908500

Reactant complex: $[(p\text{–}\mathbf{CH_3}\text{PY})_5\text{Me}_2\text{Mo(H)(OH)}\cdots\text{H}_2\text{O}]^+$
Mo 0.02107500 -0.03523900 -0.94902000
O 0.65612100 0.78107300 -2.72042200
H 0.24085500 0.37144700 -3.50728500
H -0.62804400 -0.95439100 -2.24322400
O -1.15616300 -0.73620400 -4.66504400
H -1.17442200 -0.95099300 -3.69398500
H -1.91315800 -0.13254700 -4.79117500
N -1.46587200 -1.57175400 -0.34484200
N 1.70144500 -1.37794800 -0.82020100
N 1.59175400 1.50752400 -0.43549900
N -1.66961400 1.28323900 -0.90823200
C -2.51977500 -1.26420500 0.46620200
N 0.00726900 0.03399200 1.28340700
C -2.50529600 0.12370200 1.15649500
C -2.61460300 1.24990900 0.09089500
C 2.58173100 -1.33500500 0.23233100
C -2.38735700 -3.79944000 -0.65338300
H -2.26635100 -4.78792900 -1.10684400

C -3.55207000 -2.19674600 0.69056000
H -4.40186200 -1.92732600 1.31816400
C 2.62530700 1.20503900 0.39755700
C 3.69849400 -0.20638100 2.20065500
H 3.61259400 -1.09600400 2.84221200
H 3.73715000 0.67933000 2.85077200
H 4.65580000 -0.26781100 1.66307400
C -3.66165200 2.19206500 0.12336600
H -4.39372700 2.16459300 0.93106400
C -3.70173800 0.22278100 2.13125300
H -3.69904800 1.18337200 2.66692700
H -3.67361300 -0.58488300 2.87732300
H -4.65446800 0.14764100 1.58725200
C 3.71573600 2.08322100 0.54149000
H 4.55087700 1.82172200 1.19216200
C 1.18246800 0.07458900 3.38905800
H 2.11512400 -0.00381500 3.94654500
C -1.19235300 0.35500300 3.35090100
H -2.13286900 0.51613300 3.87605400
C 1.17930000 -0.02531600 1.99129000
C 1.90484800 -2.33512000 -1.78168200
H 1.22340400 -2.28332700 -2.63431400
C 2.51695200 -0.11854100 1.20585800
C -1.17337200 0.19721100 1.95762100
C -3.80613700 3.18373800 -0.86179600
C 3.56077800 -2.33594300 0.38086100
H 4.22627300 -2.32837300 1.24444400
C 1.61996700 2.69827000 -1.09405200
H 0.77512700 2.89062800 -1.75525900
C -0.00875600 0.28822300 4.10071300
C 3.75890200 3.31183800 -0.14290700
C 2.65745100 3.61777700 -0.96831200
H 2.60372800 4.56474500 -1.51436300
C 2.88995800 -3.31188100 -1.70369900
H 2.98540200 -4.04108100 -2.51433100
C -1.82690600 2.23585400 -1.89059400
H -1.07199100 2.19333100 -2.68039700
C -2.84903000 3.17339900 -1.90148600
H -2.89556600 3.89678500 -2.72225900
C 3.73134700 -3.35852000 -0.57165000
C -3.51739500 -3.48523500 0.13222000
C -1.41256200 -2.83476800 -0.86907200
H -0.54380500 -3.05156700 -1.49088200
C -0.00815400 0.44954500 5.59989400
H 0.33326200 1.46429600 5.87487700
H -1.01473600 0.30698800 6.02256400
H 0.68310900 -0.26512900 6.07641600
C 4.92342800 4.25976600 0.00432800
H 4.58051400 5.25086800 0.34978900
H 5.66864300 3.88027400 0.72048600
H 5.42476600 4.41537300 -0.96745700
C 4.76641200 -4.44202900 -0.39678000
H 5.37677400 -4.55805600 -1.30915500
H 5.43859200 -4.22817100 0.44901000
H 4.28231300 -5.41776100 -0.20860400
C -4.92095800 4.20010700 -0.81624600
H -5.60060900 4.01747300 0.03117000
H -4.51861600 5.22474200 -0.71775000
H -5.51571500 4.17901800 -1.74687300
C -4.61987100 -4.48663000 0.36899000
H -4.22097200 -5.40768500 0.82950100
H -5.40344400 -4.08011800 1.02699000
H -5.08864700 -4.78374500 -0.58597000

Transition state: $[(p\text{–}\mathbf{CH_3}\text{PY})_5\text{Me}_2\text{MoO}\cdots\text{H}\cdots\text{H}\cdots\text{H}_2\text{O}]^{+\ ‡}$
Mo -0.00808800 -0.07790200 -0.95694000
O 0.56373300 0.66499200 -2.61135100
H 0.39510000 -0.01047500 -3.54050500
H -1.12056600 -0.99920700 -2.31018400
O 0.06790800 -0.94324800 -4.35699900
H -0.70873000 -1.10547100 -3.04503000
H -0.59343400 -0.59399400 -4.98627600
N -1.45467100 -1.65478900 -0.26833700
N 1.67492700 -1.42758900 -0.86456600
N 1.50795300 1.44662800 -0.34328900
N -1.71365900 1.22744800 -0.85290000
C -2.51637900 -1.34377400 0.52866000
N 0.01897100 -0.05013600 1.30323700
C -2.49927900 0.04551700 1.21962100
C -2.62802900 1.18598300 0.16892500
C 2.54761400 -1.42588600 0.19450400
C -2.34414900 -3.89164400 -0.56392500
H -2.20880800 -4.88516900 -1.00157600
C -3.53967800 -2.28252700 0.75300800
H -4.39932600 -2.01661500 1.36868800
C 2.58652000 1.11926900 0.41743900
C 3.72035800 -0.32819700 2.15044200
H 3.64745500 -1.22197500 2.78749700
H 3.77793200 0.55159400 2.80746100
H 4.66294100 -0.39020200 1.58690300
C -3.66680300 2.13471200 0.23787700
H -4.37710800 2.10704100 1.06454900
C -3.68248100 0.13161000 2.21154300
H -3.67100300 1.08327400 2.76262000
H -3.64573700 -0.68759100 2.94435900
H -4.64226200 0.06622900 1.67853200
C 3.67873400 1.99882800 0.53335500
H 4.55216200 1.71345400 1.12089800
C 1.21983400 -0.07081000 3.39924900
H 2.16020000 -0.17296500 3.94011600
C -1.15150600 0.23475200 3.39495000
H -2.08469900 0.38962800 3.93522800
C 1.19476900 -0.14079700 1.99980000
C 1.85453900 -2.37407700 -1.84090000
H 1.19624900 -2.28185700 -2.71064000
C 2.51375100 -0.22529100 1.18862700
C -1.15296100 0.10774300 1.99943900
C -3.83247500 3.13175900 -0.73968500
C 3.48966400 -2.46142500 0.33794600
H 4.14942000 -2.48557000 1.20572000
C 1.48316300 2.66678600 -0.94546500
H 0.59883500 2.88301400 -1.54493500

C 0.04138800 0.14322300 4.13032400
C 3.67280700 3.25575900 -0.09843100
C 2.51894300 3.58974800 -0.83736500
H 2.42561800 4.55922100 -1.33625000
C 2.80346200 -3.38755000 -1.76502200
H 2.88399700 -4.10715700 -2.58578700
C -1.89301000 2.17647100 -1.83064400
H -1.16277300 2.12504000 -2.64372900
C -2.91161000 3.11936100 -1.80963800
H -2.98268300 3.84318500 -2.62804000
C 3.63070100 -3.47879200 -0.62596600
C -3.48472000 -3.57688000 0.20344300
C -1.37416800 -2.91883600 -0.77670000
H -0.49194200 -3.13574800 -1.38136600
C -4.58218300 -4.58429800 0.43555700
H -4.17997600 -5.49901200 0.90533900
H -5.37563300 -4.17982900 1.08251800
H -5.03729800 -4.89052300 -0.52298100
C 4.84013900 4.20460000 0.01403800
H 4.51433700 5.18023900 0.41524900
H 5.62835000 3.80362000 0.66975800
H 5.28128800 4.39820400 -0.97982500
C -4.93853800 4.15493900 -0.65517900
H -5.60288200 3.96368600 0.20215900
H -4.52423200 5.17367700 -0.54730400
H -5.54969600 4.15414900 -1.57495700
C 4.62357300 -4.60137700 -0.45407400
H 4.10237900 -5.55125000 -0.23438800
H 5.20608700 -4.76124000 -1.37762600
H 5.32340200 -4.40107900 0.37238100
C 0.05670000 0.28276800 5.63161800
H -0.88654800 -0.06988600 6.07853900
H 0.89455300 -0.27622100 6.07814300
H 0.17941400 1.34458600 5.91484100

Product complex: $[(p\text{–}\mathbf{CH_3}\text{PY})_5\text{Me}_2\text{MoO}\cdots\text{H}_2\text{O}]^+ + \text{H}_2$
Mo 0.11763400 -0.10537200 -0.88028500
O 0.14117500 -0.23008700 -2.65331000
H -0.23141300 -0.05753500 -4.35364000
H -6.04259000 -1.06379800 -4.77746800
O -0.42263700 0.00855500 -5.32999600
H -6.49093200 -0.76936600 -4.25141300
H -1.17108000 0.62966500 -5.39238800
N -1.44984200 -1.55127700 -0.51198200
N 1.77798900 -1.44543100 -0.57127000
N 1.66970100 1.37467500 -0.62443300
N -1.55040700 1.26335800 -0.81912000
C -2.46395700 -1.32128900 0.38203100
N 0.05620200 0.03458100 1.36467100
C -2.43953800 0.01297800 1.18028900
C -2.49130000 1.20900500 0.18064100
C 2.66594100 -1.26525700 0.46134000
C -2.51307900 -3.63417800 -1.16758500
H -2.48906400 -4.51401500 -1.81755300
C -3.48854500 -2.27037900 0.54737500
H -4.28191000 -2.09389700 1.27393100
C 2.63132200 1.26626100 0.34813900
C 3.74742200 0.10380400 2.29470100
H 3.72115000 -0.74109300 2.99802000
H 3.72079000 1.03085000 2.88587800
H 4.70694400 0.06834800 1.75786100
C -3.48673500 2.19907400 0.26780900
H -4.21249000 2.17309900 1.08122000
C -3.67474000 0.07247600 2.10785200
H -3.67774000 0.99622800 2.70418300
H -3.68417200 -0.77599600 2.80763000
H -4.60587000 0.04320200 1.52277400
C 3.64822300 2.23268500 0.44626700
H 4.39715800 2.15672000 1.23496400
C 1.20243100 0.16781800 3.48857400
H 2.13382600 0.20250200 4.05396600
C -1.19344700 0.15577500 3.43089600
H -2.15200900 0.18435500 3.94888600
C 1.22238600 0.08102600 2.09332900
C 1.96938900 -2.51462800 -1.40624600
H 1.29868500 -2.55987900 -2.26735100
C 2.56111300 0.04243200 1.30540400
C -1.14305200 0.07384400 2.03348200
C -3.59839500 3.22997600 -0.68518100
C 3.65893200 -2.22899800 0.71425900
H 4.34121400 -2.10129500 1.55499300
C 1.77488100 2.39733500 -1.52860900
H 1.01437700 2.42047000 -2.30979000
C -0.01534400 0.20654300 4.19518400
C 3.74965900 3.30128500 -0.46426000
C 2.78274500 3.35244800 -1.49013000
H 2.80253300 4.13656100 -2.25301700
C 2.95936400 -3.47028700 -1.21530700
H 3.05016600 -4.29498400 -1.92912600
C -1.68837100 2.22941600 -1.78048400
H -0.97273200 2.17511500 -2.60388600
C -2.67771500 3.20436600 -1.75410700
H -2.72381800 3.94110900 -2.56218000
C 3.82283100 -3.36316500 -0.10425200
C -3.53995700 -3.45043500 -0.21808300
C -1.50285600 -2.68653900 -1.27449800
H -0.69712600 -2.80998200 -1.99877800
C -0.04364800 0.30533300 5.70033200
H 0.38587500 1.26552900 6.03907100
H -1.07120000 0.23425700 6.08978100
H 0.55992800 -0.49609600 6.16145900
C 4.83792900 4.33914100 -0.35152800
H 4.40998100 5.32408000 -0.09090300
H 5.57524700 4.07180100 0.42123200
H 5.36568700 4.46350300 -1.31290700
C -4.65381500 4.30211200 -0.57356700
H -5.41409100 4.04558800 0.18083200
H -4.19926200 5.26671500 -0.28176500
H -5.15893700 4.46484700 -1.54106300
C -4.63767800 -4.46799500 -0.03390700
H -4.23022800 -5.40793000 0.38040800
H -5.41875400 -4.10303800 0.65094500

H -5.10733100 -4.72093900 -1.00017600
C 4.87459800 -4.40507800 0.18622600
H 5.58324800 -4.06162200 0.95616200
H 4.40767400 -5.33960700 0.54779500
H 5.44243800 -4.66162100 -0.72465500

Reactant complex: $[(p\text{–}\mathbf{F}\text{PY})_5\text{Me}_2\text{Mo(H)(OH)}\cdots\text{H}_2\text{O}]^+$
Mo 0.01308300 -0.01950100 -0.80170900
O 0.63390200 0.79579600 -2.56433000
H 0.22132700 0.39386400 -3.36032800
H -0.64837400 -0.92033300 -2.09341000
O -1.01272800 -0.61760900 -4.58735100
H -1.20867900 -0.93699900 -3.67297900
H -1.75827200 -0.02487800 -4.80268300
N -1.47658100 -1.56019000 -0.20170400
N 1.69141300 -1.36624500 -0.68328000
N 1.60528900 1.51658100 -0.29485100
N -1.68047200 1.30074500 -0.75910700
C -2.52870200 -1.24999100 0.61302800
N -0.00008300 0.04612500 1.43651100
C -2.51571800 0.13554600 1.30643800
C -2.62409200 1.26100700 0.24269900
C 2.55853800 -1.33492200 0.38253200
C -2.39144200 -3.79206200 -0.53799000
H -2.29803900 -4.78193400 -0.98861400
C -3.56689300 -2.17271500 0.84136400
H -4.42613900 -1.93752400 1.46733100
C 2.63526800 1.20027000 0.53906300
C 3.69212800 -0.21864100 2.34698300
H 3.58995000 -1.10115200 2.99575400
H 3.74953700 0.67089200 2.99022900
H 4.64695700 -0.30163600 1.80804800
C -3.67518800 2.19653900 0.28614400
H -4.42260300 2.19348600 1.07793400
C -3.71173800 0.23238700 2.28126800
H -3.71164400 1.19370300 2.81541500
H -3.68122100 -0.57429500 3.02828100
H -4.66445300 0.15427900 1.73784700
C 3.74277400 2.05471900 0.68382700
H 4.58828400 1.81614300 1.32747500
C 1.19639500 0.12283700 3.53492000
H 2.11387700 0.06930300 4.11706100
C -1.21627100 0.38720300 3.49670600
H -2.13983800 0.54841100 4.04863300
C 1.17551600 -0.00372200 2.13847000
C 1.88859100 -2.31546600 -1.65276000
H 1.22146000 -2.24472800 -2.51444900
C 2.51098800 -0.11690500 1.35358800
C -1.18366200 0.21364500 2.10634600
C -3.76967800 3.15849200 -0.71594800
C 3.51964400 -2.34826700 0.55152900
H 4.18813300 -2.38324900 1.41032000
C 1.64486000 2.69720800 -0.96852900
H 0.80311500 2.89378800 -1.63146600
C -0.01181600 0.33258200 4.18939400
C 3.75037900 3.25327700 -0.02962600
C 2.69118700 3.61280300 -0.86396900
H 2.67640600 4.55846600 -1.40934500
C 2.85191700 -3.31751200 -1.57876900
H 2.96515900 -4.05574800 -2.37519400
C -1.83081600 2.25117000 -1.74319100
H -1.07514300 2.20731900 -2.53160600
C -2.84857700 3.19668700 -1.76686300
H -2.91568800 3.93045200 -2.57310300
C 3.64107900 -3.33561700 -0.42666700
C -3.48465400 -3.43265000 0.25384900
C -1.42071500 -2.81667800 -0.73817000
H -0.55397900 -3.03016000 -1.36275600
F -0.01783000 0.47605100 5.53717700
F 4.81354200 4.08917700 0.10552900
F -4.78492100 4.06906700 -0.66870600
F 4.56621300 -4.31935700 -0.25669900
F -4.48096000 -4.32956100 0.47330900

Transition state: $[(p\text{–}\mathbf{F}\text{PY})_5\text{Me}_2\text{MoO}\cdots\text{H}\cdots\text{H}\cdots\text{H}_2\text{O}]^{+\,\ddagger}$
Mo -0.00814500 -0.08162000 -0.95929500
O 0.55222900 0.66225000 -2.59770500
H 0.32604700 0.00216100 -3.58714500
H -1.07594200 -1.03425700 -2.28752000
O -0.05548500 -0.87051900 -4.35166700
H -0.73378200 -1.08750300 -3.08831900
H -0.73150600 -0.48967500 -4.94646000
N -1.46922600 -1.65382900 -0.24366700
N 1.66396300 -1.44289400 -0.86654600
N 1.53891200 1.43725000 -0.34966600
N -1.70881100 1.23592600 -0.86009600
C -2.52959800 -1.32025700 0.54713900
N 0.02098400 -0.04028100 1.31022500
C -2.50003100 0.07389000 1.22666600
C -2.61959600 1.20491000 0.16738800
C 2.52817600 -1.44972300 0.20238900
C -2.36855600 -3.89245000 -0.53720900
H -2.26658300 -4.89546600 -0.95556000
C -3.56965100 -2.23577900 0.78206200
H -4.44015100 -1.98749100 1.38744600
C 2.61374600 1.09139700 0.40896800
C 3.72292100 -0.36453400 2.15106900
H 3.63080200 -1.24987900 2.79726400
H 3.80205000 0.52012700 2.79902500
H 4.66274200 -0.45235400 1.58660200
C -3.65334700 2.15686500 0.24246100
H -4.37768900 2.16633700 1.05520200
C -3.68011300 0.17815300 2.22010600
H -3.65959100 1.13429500 2.76294200
H -3.64903100 -0.63523800 2.95953700
H -4.64157800 0.11634400 1.68997200
C 3.72953000 1.93990400 0.51882500
H 4.61283600 1.67324300 1.09768900
C 1.24534800 -0.03362000 3.39900600
H 2.17094600 -0.11837600 3.96479200
C -1.16121300 0.27881000 3.39617300
H -2.07500200 0.44299400 3.96346900

C 1.20108100 -0.13024500 2.00123500
C 1.83008300 -2.39068700 -1.84417600
H 1.17891000 -2.28869100 -2.71682400
C 2.51736200 -0.24468200 1.19035200
C -1.15157500 0.13333000 2.00237100
C -3.76442900 3.11791800 -0.76022100
C 3.45004400 -2.49843800 0.36680000
H 4.11539400 -2.56163400 1.22647800
C 1.53032300 2.64682900 -0.97038300
H 0.64871600 2.87151900 -1.56987500
C 0.05053500 0.18941300 4.07354100
C 3.69159400 3.16750200 -0.14214200
C 2.57913900 3.56109000 -0.88787900
H 2.52943800 4.52942500 -1.38949700
C 2.75390500 -3.43024200 -1.77167800
H 2.84415100 -4.16580900 -2.57358100
C -1.87538100 2.17843300 -1.84555100
H -1.14571500 2.11501200 -2.65766300
C -2.88113800 3.13860400 -1.84185800
H -2.96689900 3.86849000 -2.64977200
C 3.53743600 -3.48470400 -0.61736300
C -3.47520500 -3.51070200 0.22293100
C -1.39391600 -2.91966000 -0.74428000
H -0.51154800 -3.14987800 -1.34269900
F -4.76401200 4.04093300 -0.68280200
F 4.76132000 3.99860500 -0.04332500
F 4.42675700 -4.50127600 -0.45120100
F -4.47652200 -4.39864600 0.44368200
F 0.06340200 0.31036900 5.42452100

Product complex: $[(p\text{–}\mathbf{F}\text{PY})_5\text{Me}_2\text{MoO}\cdots\text{H}_2\text{O}]^+ + \text{H}_2$
Mo 0.12826400 -0.08730300 -0.72062800
O 0.16927600 -0.18592700 -2.48937000
H -0.10953200 -0.01590000 -4.23564400
H -6.39972900 -0.86662300 -4.08194000
O -0.24646200 0.04507100 -5.21833400
H -5.95631700 -1.14632400 -4.62011100
H -0.88239800 0.77475800 -5.33275600
N -1.44415200 -1.54065900 -0.38952200
N 1.79180600 -1.43010800 -0.42279100
N 1.68014000 1.39329600 -0.43880200
N -1.54539200 1.27841700 -0.66079200
C -2.46106900 -1.31910100 0.50591400
N 0.05261900 0.02215400 1.53068100
C -2.44438100 0.00331100 1.32286300
C -2.48724200 1.21064500 0.33829800
C 2.66812600 -1.26140600 0.62273300
C -2.48982600 -3.62289600 -1.09185200
H -2.48379200 -4.50146200 -1.73965800
C -3.48854400 -2.26419400 0.66387300
H -4.29791700 -2.12824800 1.37935700
C 2.63189700 1.26889600 0.54367900
C 3.73983800 0.08164700 2.48057100
H 3.71025300 -0.77238500 3.17262600
H 3.70953400 1.00026000 3.08447600
H 4.70224200 0.05395300 1.94867500
C -3.48423100 2.19571700 0.44338900
H -4.22539900 2.19122900 1.24115800
C -3.68733500 0.05052800 2.24022100
H -3.69542500 0.96604100 2.84892100
H -3.70254800 -0.80676000 2.92893200
H -4.61331300 0.02926600 1.64694900
C 3.64785800 2.23014500 0.67559800
H 4.40369900 2.17255800 1.45722000
C 1.20038200 0.13073500 3.66056500
H 2.10958500 0.16235600 4.25817300
C -1.23059800 0.11613000 3.58265500
H -2.17680400 0.14009500 4.12018100
C 1.21617400 0.06005000 2.26271600
C 1.98563000 -2.48100800 -1.27875000
H 1.32490400 -2.50863900 -2.14742900
C 2.55915100 0.03299500 1.48408000
C -1.15541500 0.05215100 2.18649300
C -3.54527000 3.20263500 -0.52098500
C 3.66137800 -2.22218400 0.87937600
H 4.35016200 -2.13674500 1.71823000
C 1.78416700 2.42608100 -1.32994300
H 1.03225100 2.45700300 -2.11815000
C -0.03713200 0.15585900 4.30023900
C 3.70645500 3.28209100 -0.23891000
C 2.78332800 3.39299000 -1.28033300
H 2.82789400 4.19804000 -2.01623800
C 2.96988400 -3.44934200 -1.10651100
H 3.08651300 -4.27122700 -1.81568500
C -1.67449200 2.24785900 -1.61882200
H -0.95966800 2.19571300 -2.44223100
C -2.65732500 3.23271700 -1.59819600
H -2.72026000 3.98721100 -2.38492500
C 3.78781700 -3.31205100 0.01703900
C -3.48583500 -3.40581300 -0.13812200
C -1.48659400 -2.66201000 -1.17129800
H -0.67966000 -2.77270100 -1.89527000
F 4.74792800 -4.24208100 0.26981900
F 4.69299400 4.20687800 -0.11326900
F -4.50987400 4.15591500 -0.41517400
F -4.48347200 -4.31488200 0.01127300
F -0.08127300 0.22133500 5.65810000

Reactant complex: $[(p\text{–}\mathbf{CF_3}\text{PY})_5\text{Me}_2\text{Mo(H)(OH)}\cdots\text{H}_2\text{O}]^+$
Mo -0.02374900 -0.06757700 -1.40515600
O 0.54571600 0.72290900 -3.16707300
H 0.16730300 0.29222500 -3.97414600
H -0.67393000 -0.95682600 -2.68164900
O -0.45116800 -0.43964100 -5.53582000
H -1.30982700 -0.88276100 -5.39703400
H -0.63478800 0.25137400 -6.20071300
N -1.50148400 -1.61411000 -0.83262600
N 1.64648600 -1.40917800 -1.30656500
N 1.59108800 1.46335500 -0.93278200
N -1.71296100 1.23552000 -1.34294900
C -2.53770300 -1.32635000 0.01035400
N -0.01410400 -0.01737600 0.82808000

C -2.52808900 0.05049600 0.71950000
C -2.65107000 1.18361300 -0.33536200
C 2.52374600 -1.38772100 -0.24847300
C -2.40851200 -3.84331600 -1.17478700
H -2.29536000 -4.82071000 -1.64910800
C -3.56297700 -2.26461800 0.23994900
H -4.40420900 -2.01899600 0.88489600
C 2.62160100 1.14593000 -0.10316700
C 3.68750200 -0.27263300 1.70034900
H 3.58507900 -1.14981400 2.35604900
H 3.76068200 0.62013500 2.33766500
H 4.63575900 -0.36787500 1.15185300
C -3.70509700 2.11169400 -0.28389100
H -4.43411100 2.07796200 0.52329100
C -3.71758100 0.13055400 1.70445800
H -3.72259100 1.08856600 2.24435100
H -3.67296600 -0.67969100 2.44710500
H -4.67455200 0.04677900 1.16954500
C 3.73872700 1.99306200 0.01629800
H 4.57992500 1.72687000 0.65360800
C 1.19554100 0.08021400 2.91315200
H 2.13254800 0.03699500 3.46352900
C -1.20491600 0.31347100 2.89939500
H -2.13765600 0.47263900 3.43640200
C 1.16920600 -0.05131400 1.51696200
C 1.83463300 -2.35107300 -2.28786000
H 1.16951400 -2.26484700 -3.14966800
C 2.49577800 -0.16662700 0.71946600
C -1.19269600 0.13508800 1.50972300
C -3.83903400 3.09585900 -1.27145000
C 3.47188500 -2.41324100 -0.09241100
H 4.13151700 -2.43638800 0.77292100
C 1.63529000 2.63396800 -1.62240300
H 0.79300300 2.82828800 -2.28518100
C 0.00069600 0.28263600 3.60660600
C 3.77514300 3.19554500 -0.70024000
C 2.69216200 3.53623100 -1.52644800
H 2.66176600 4.47140500 -2.09033700
C 2.78994300 -3.35599900 -2.21428700
H 2.88234700 -4.07660800 -3.03024300
C -1.87955500 2.18957100 -2.32459700
H -1.13362400 2.15172700 -3.12167600
C -2.90453100 3.12108100 -2.32653100
H -2.96593100 3.84911100 -3.13939800
C 3.60083600 -3.41547500 -1.06571400
C -3.50647000 -3.52848800 -0.35393800
C -1.45043600 -2.86339500 -1.39142200
H -0.60024800 -3.06022900 -2.04308700
C -0.00491400 0.41311600 5.11658500
F -0.30730300 -0.78306300 5.71792000
F -0.93648600 1.31653400 5.54451300
F 1.20444400 0.81000200 5.60642400
C -4.95648500 4.10302400 -1.23086300
C 4.94988700 4.14147400 -0.57110700
C 4.58518700 -4.54549900 -0.89415200
C -4.60109500 -4.54770300 -0.13507300
F 5.41249700 4.54093200 -1.79672500
F 6.00216900 3.58839600 0.09738100
F 4.60002200 5.28379700 0.10523900
F -5.29043400 -4.80019200 -1.29566700
F -5.51626800 -4.14953800 0.79417100
F -4.09437200 -5.75086300 0.28328300
F 5.47795400 -4.32241400 0.11426300
F 5.31112700 -4.76814100 -2.03597900
F 3.95034100 -5.73242800 -0.60599500
F -5.75347000 4.03030900 -2.35039400
F -5.77633000 3.94772500 -0.15003300
F -4.48244000 5.39431300 -1.19046500

Transition state: $[(p\text{–}\mathbf{CF_3}\text{PY})_5\text{Me}_2\text{MoO}\cdots\text{H}\cdots\text{H}\cdots\text{H}_2\text{O}]^{+\,\ddagger}$
Mo 0.00943800 -0.07252600 -0.97832700
O 0.56492500 0.69124000 -2.56659100
H 0.18241800 0.12234300 -3.69833600
H -0.93094900 -1.08652600 -2.28580500
O -0.31614100 -0.62761800 -4.38032200
H -0.77215300 -0.99855700 -3.19858800
H -1.05446200 -0.17732400 -4.83856000
N -1.44207600 -1.67202600 -0.26616000
N 1.67771100 -1.42319400 -0.85409300
N 1.55581000 1.46688700 -0.33762200
N -1.69828100 1.21686000 -0.87502000
C -2.50804000 -1.35487200 0.52024700
N 0.02105700 -0.03804400 1.29472400
C -2.50013200 0.03757600 1.19997300
C -2.61911400 1.17180200 0.14525600
C 2.54039700 -1.42575900 0.21851400
C -2.30555500 -3.92066600 -0.54602600
H -2.16293100 -4.91855900 -0.96679200
C -3.53742700 -2.28812900 0.74409300
H -4.41120200 -2.02215600 1.33591600
C 2.62459000 1.11913100 0.42292500
C 3.72079600 -0.33303000 2.17252000
H 3.62661400 -1.21641500 2.82077000
H 3.79265300 0.55374800 2.81863000
H 4.66567600 -0.42038100 1.61644000
C -3.65383500 2.12040300 0.21947200
H -4.36995200 2.09579800 1.03817200
C -3.68931500 0.12598700 2.18499000
H -3.68354100 1.07907300 2.73326000
H -3.65553100 -0.69061200 2.92088700
H -4.64640100 0.05685300 1.64781900
C 3.74148400 1.96935300 0.53006400
H 4.61772800 1.67404600 1.10454700
C 1.22136700 -0.02825600 3.39497000
H 2.15672400 -0.10725600 3.94482400
C -1.17238700 0.25198300 3.37640400
H -2.10486300 0.41096900 3.91359800
C 1.19754400 -0.11518000 1.99714800
C 1.85128500 -2.37796700 -1.82694000
H 1.20372600 -2.28365800 -2.70139800
C 2.52282400 -0.21791600 1.20101400
C -1.15882500 0.11076700 1.98331500

C -3.78933900 3.10991800 -0.76233200
C 3.45598700 -2.47611500 0.38782300
H 4.10546500 -2.51166200 1.26058800
C 1.54486300 2.67831700 -0.95277400
H 0.66623200 2.90334000 -1.55671200
C 0.02786600 0.18158100 4.09142400
C 3.72641700 3.21117000 -0.11496700
C 2.59339500 3.58913000 -0.85418200
H 2.52131300 4.55723200 -1.35518100
C 2.77619300 -3.41021100 -1.73875800
H 2.85903600 -4.13494000 -2.55179200
C -1.86448800 2.17641900 -1.84904700
H -1.13181000 2.13634700 -2.65792000
C -2.87519900 3.12494200 -1.83221400
H -2.93961200 3.85503300 -2.64281500
C 3.57381000 -3.48566600 -0.58262000
C -3.44403500 -3.57485700 0.20148300
C -1.34538400 -2.93894300 -0.76243500
H -0.46092400 -3.15771800 -1.36126200
C -4.52984400 -4.60256000 0.43886100
C 4.90232400 4.15935300 -0.00811800
C -4.87695200 4.14988400 -0.68098600
C 4.52168800 -4.63989700 -0.37738000
C 0.02219500 0.26591000 5.60162100
F 5.34404700 4.55252100 -1.24387500
F 5.96571100 3.61058400 0.64501400
F 4.56061300 5.30360200 0.66709300
F 5.06558800 -5.07592000 -1.55529700
F 3.88670600 -5.72801400 0.18126700
F 5.55865500 -4.32668900 0.45682000
F -4.94101800 -5.17832700 -0.73397800
F -4.08445500 -5.62355500 1.24031400
F -5.63372700 -4.07405400 1.03913200
F -4.36702500 5.40222800 -0.42307900
F -5.56982400 4.25799800 -1.86114600
F -5.79098100 3.88758600 0.29862700
F 1.20315100 0.73960900 6.09725500
F -0.17926800 -0.96826200 6.17223200
F -0.97229400 1.07959900 6.06623000

Product complex: $[(p\text{−}\mathbf{CF_3}\text{PY})_5\text{Me}_2\text{MoO}\cdots\text{H}_2\text{O}]^+ + \text{H}_2$
Mo 0.08627700 -0.13419200 -1.31696100
O 0.10572700 -0.23872400 -3.06869600
H 0.19538800 -0.06383000 -4.89835400
H -5.76369000 -1.29955200 -5.52435400
O 0.24925200 -0.00917300 -5.88399800
H -5.27489900 -1.69966800 -5.93116800
H 0.27396100 0.94648000 -6.07472200
N -1.52809700 -1.52945000 -0.98002500
N 1.70648300 -1.52376900 -1.00406300
N 1.69101400 1.29726000 -1.12077300
N -1.52899100 1.29095500 -1.20102200
C -2.49820900 -1.29672800 -0.03672600
N 0.06427700 -0.00356200 0.93069900
C -2.43454100 0.02612200 0.78040500
C -2.46369100 1.23775700 -0.19686700
C 2.62960200 -1.34009100 -0.00479500
C -2.64137500 -3.58456600 -1.63843500
H -2.66665500 -4.44775700 -2.30683500
C -3.52579900 -2.23327900 0.16281000
H -4.28780900 -2.06622100 0.92138500
C 2.63104500 1.19510100 -0.12535400
C 3.77093900 0.01599900 1.79983800
H 3.75523700 -0.83644700 2.49416000
H 3.75914800 0.93433200 2.40431700
H 4.71991200 -0.01509700 1.24430200
C -3.43657300 2.24532900 -0.08652800
H -4.16112200 2.23109300 0.72544200
C -3.65869700 0.10339700 1.72128100
H -3.63667400 1.02230600 2.32440600
H -3.67821600 -0.74795600 2.41688100
H -4.59613800 0.09602000 1.14579300
C 3.63534500 2.16980400 -0.00234100
H 4.36932300 2.11158000 0.79902900
C 1.25128000 0.08650300 3.03658500
H 2.18751900 0.10497800 3.59097000
C -1.16521200 0.11644700 3.01060300
H -2.11244100 0.16019200 3.54465700
C 1.24238200 0.01861200 1.64074100
C 1.84791300 -2.59548700 -1.84373700
H 1.14671600 -2.64422200 -2.67783900
C 2.56513200 -0.02913300 0.83332200
C -1.12813700 0.04852500 1.61541100
C -3.50766900 3.27056100 -1.04040100
C 3.62373200 -2.30685000 0.22196000
H 4.34033100 -2.18606600 1.03173500
C 1.81261400 2.30112300 -2.04256700
H 1.08615900 2.29692600 -2.85483100
C 0.03602000 0.13711100 3.73401900
C 3.72490600 3.21752400 -0.92932000
C 2.80564300 3.27114900 -1.99010100
H 2.84809200 4.04339100 -2.76128800
C 2.83409600 -3.56141100 -1.69030800
H 2.89435100 -4.39067400 -2.39852300
C -1.64314200 2.26403100 -2.15695800
H -0.93629000 2.20401400 -2.98545600
C -2.60818500 3.26230000 -2.11984000
H -2.64603200 4.00835000 -2.91665800
C 3.72561400 -3.42876900 -0.61239400
C -3.60168800 -3.38488300 -0.63332100
C -1.63017700 -2.64083000 -1.77133300
H -0.87206000 -2.75039300 -2.54638600
C 0.01809500 0.15719700 5.24269000
F -0.04083600 -1.11482000 5.76702100
F -1.06416200 0.83070200 5.73812500
F 1.13685100 0.74178600 5.76726900
C -4.52578900 4.37991000 -0.90730300
C 4.78158800 4.28941100 -0.78435700
C 4.76853100 -4.49241800 -0.35598000
C -4.68510400 -4.41265900 -0.39483500
F -5.12469000 -4.97125100 -1.56272200
F -5.77321700 -3.88677400 0.24026200

F -4.23059500 -5.44705100 0.38818200
F 5.76932100 -4.06060000 0.46498500
F 4.21690700 -5.60247200 0.23821100
F 5.35137200 -4.92333100 -1.51703000
F 5.31899800 4.64004000 -1.99278600
F 5.81227400 3.90463600 0.02289800
F 4.25807200 5.43827400 -0.24134400
F -5.55933600 4.04766100 -0.08020500
F -5.06578600 4.72330400 -2.11680600
F -3.95853100 5.52261700 -0.39485400

Reactant complex: $[(p\text{–}\mathbf{CN}\text{PY})_5\text{Me}_2\text{Mo(H)(OH)}\cdots\text{H}_2\text{O}]^+$
Mo -0.03270300 -0.01443500 -0.99652000
O 0.52456900 0.75497100 -2.75620900
H 0.14926100 0.32667500 -3.56933200
H -0.68848800 -0.91308200 -2.25885900
O -0.43565000 -0.39944900 -5.10739200
H -1.36737100 -0.68537400 -5.05108100
H -0.42175900 0.25810100 -5.82912700
N -1.51209100 -1.55055600 -0.41026300
N 1.62824600 -1.36343100 -0.89830600
N 1.59443800 1.51146800 -0.54312100
N -1.71223300 1.29802000 -0.93819800
C -2.54497900 -1.25269600 0.43673400
N -0.01228600 0.05102600 1.23393100
C -2.52709300 0.12917400 1.13644600
C -2.64579400 1.25880800 0.07668600
C 2.51204000 -1.34275900 0.15663800
C -2.42083700 -3.78348700 -0.73208200
H -2.31653000 -4.76513100 -1.19794300
C -3.56970300 -2.18209200 0.67963500
H -4.40987900 -1.93049700 1.32385400
C 2.62806500 1.19222100 0.28436500
C 3.69457000 -0.22199200 2.09125000
H 3.59078700 -1.09502700 2.75201600
H 3.77575300 0.67356600 2.72354700
H 4.63920900 -0.32555400 1.53817300
C -3.68728900 2.19356100 0.13252700
H -4.41408400 2.17243700 0.94238800
C -3.71317100 0.22192400 2.12453700
H -3.70959700 1.18213200 2.66025600
H -3.67174700 -0.58495100 2.87083900
H -4.67214400 0.14231300 1.59270200
C 3.74905700 2.02991400 0.39389000
H 4.59363800 1.76630300 1.02792500
C 1.21190400 0.14417700 3.31135800
H 2.14841900 0.09222600 3.86147200
C -1.19789900 0.39150000 3.30829700
H -2.12506600 0.55414700 3.85282600
C 1.17570500 0.01293400 1.91847800
C 1.80273100 -2.31125100 -1.87714300
H 1.13572000 -2.22273900 -2.73721800
C 2.49827100 -0.11455300 1.11606000
C -1.18808100 0.21001700 1.92090500
C -3.82057100 3.18519200 -0.86389500
C 3.45010700 -2.37122100 0.31566200
H 4.11637000 -2.39721600 1.17605800
C 1.63972300 2.67662600 -1.24121300
H 0.79500000 2.87183200 -1.90059000
H -4.41805300 -2.00294500 1.36376900
C 2.64087000 1.10120900 0.41554600
C 3.72436300 -0.34890200 2.17388100
H 3.62249900 -1.22582100 2.82951700
H 3.80550200 0.54251900 2.81233100
H 4.66750400 -0.45019200 1.61739800
C -3.64155500 2.12854600 0.22161700
H -4.35815100 2.11283900 1.04029500
C -3.68784000 0.14840800 2.19424200
H -3.67728100 1.10478500 2.73642800
H -3.65603500 -0.66334600 2.93539300
H -4.64588700 0.07966000 1.65885900
C 3.76755500 1.93448800 0.51092100
H 4.64665400 1.63440700 1.07890300
C 1.23160800 -0.01631200 3.39177800
H 2.16479300 -0.10039300 3.94396300
C -1.17122200 0.27480800 3.37613200
H -2.10061700 0.43693000 3.91702100
C 1.20139300 -0.11118100 1.99774100
C 1.82521500 -2.40964100 -1.80735100
H 1.17613700 -2.31758300 -2.68049900
C 2.52626700 -0.22994400 1.20267700
C -1.15658300 0.12250700 1.98695500
C -3.77471400 3.12751300 -0.76636700
C 3.43389100 -2.50029400 0.40939100
H 4.08543000 -2.53874500 1.28042100
C 1.56557100 2.66789100 -0.95873500
H 0.68427200 2.90104500 -1.55609000
C 0.03512100 0.20429200 4.09832600
C 3.76232600 3.18412500 -0.14115500
C 2.62069900 3.57170100 -0.87383100
H 2.55905800 4.54077800 -1.37258200
C 2.73761000 -3.44914000 -1.71807900
H 2.81287700 -4.18284300 -2.52322800
C -1.85419400 2.17369500 -1.85174300
H -1.12319300 2.13182400 -2.66133500
C -2.85507500 3.13014700 -1.84022000
H -2.91673500 3.86141000 -2.64895400
C 3.54160400 -3.52984100 -0.55633700
C -3.45908600 -3.57395800 0.23582700
C -1.35849900 -2.94473500 -0.73872600
H -0.47724200 -3.17061000 -1.33934700
C 0.04325700 0.34033400 5.52372400
N 0.05037300 0.45240100 6.69651200
C -4.50936200 -4.52240600 0.46666500
C 4.46554700 -4.60398100 -0.36999000
C 4.90454700 4.04896100 -0.04940900
C -4.82146900 4.09808400 -0.68156500
N -5.36999200 -5.30408200 0.65311800
N 5.22663900 -5.49232300 -0.21947800
N 5.83969900 4.75987100 0.02334500
N -5.68236600 4.90075300 -0.61494400

Transition state: $[(p\text{-}\mathbf{CN}\text{PY})_5Me_2MoO\cdots H\cdots H\cdots H_2O]^{+\ddagger}$

Mo 0.00751200 -0.08061200 -0.98100900
O 0.55603800 0.67780400 -2.55188700
H 0.14184300 0.10574200 -3.74671700
H -0.90005800 -1.10987000 -2.26445800
O -0.37317200 -0.64164400 -4.35990100
H -0.78376600 -1.01236400 -3.21592100
H -1.12231800 -0.20282200 -4.81324700
N -1.45052500 -1.67405900 -0.25059600
N 1.66462700 -1.44357300 -0.84149200
N 1.57012700 1.45926200 -0.33971000
N -1.69409300 1.21302000 -0.87631600
C -2.51484300 -1.34849200 0.53782100
N 0.02245200 -0.03390400 1.29490100
C -2.50037700 0.04816100 1.20807900
C -2.61538500 1.17692500 0.14723000
C 2.53026900 -1.44592100 0.23080500
C -2.31633400 -3.92537900 -0.51519000
H -2.18138600 -4.92772200 -0.92575100
C -3.54575600 -2.27251300 0.77118800
H -4.41805300 -2.00294500 1.36376900
C 2.64087000 1.10120900 0.41554600
C 3.72436300 -0.34890200 2.17388100
H 3.62249900 -1.22582100 2.82951700
H 3.80550200 0.54251900 2.81233100
H 4.66750400 -0.45019200 1.61739800
C -3.64155500 2.12854600 0.22161700
H -4.35815100 2.11283900 1.04029500
C -3.68784000 0.14840800 2.19424200
H -3.67728100 1.10478500 2.73642800
H -3.65603500 -0.66334600 2.93539300
H -4.64588700 0.07966000 1.65885900
C 3.76755500 1.93448800 0.51092100
H 4.64665400 1.63440700 1.07890300
C 1.23160800 -0.01631200 3.39177800
H 2.16479300 -0.10039300 3.94396300
C -1.17122200 0.27480800 3.37613200
H -2.10061700 0.43693000 3.91702100
C 1.20139300 -0.11118100 1.99774100
C 1.82521500 -2.40964100 -1.80735100
H 1.17613700 -2.31758300 -2.68049900
C 2.52626700 -0.22994400 1.20267700
C -1.15658300 0.12250700 1.98695500
C -3.77471400 3.12751300 -0.76636700
C 3.43389100 -2.50029400 0.40939100
H 4.08543000 -2.53874500 1.28042100
C 1.56557100 2.66789100 -0.95873500
H 0.68427200 2.90104500 -1.55609000
C 0.03512100 0.20429200 4.09832600
C 3.76232600 3.18412500 -0.14115500
C 2.62069900 3.57170100 -0.87383100
H 2.55905800 4.54077800 -1.37258200
C 2.73761000 -3.44914000 -1.71807900
H 2.81287700 -4.18284300 -2.52322800
C -1.85419400 2.17369500 -1.85174300
H -1.12319300 2.13182400 -2.66133500
C -2.85507500 3.13014700 -1.84022000
H -2.91673500 3.86141000 -2.64895400
C 3.54160400 -3.52984100 -0.55633700
C -3.45908600 -3.57395800 0.23582700
C -1.35849900 -2.94473500 -0.73872600
H -0.47724200 -3.17061000 -1.33934700
C 0.04325700 0.34033400 5.52372400
N 0.05037300 0.45240100 6.69651200
C -4.50936200 -4.52240600 0.46666500
C 4.46554700 -4.60398100 -0.36999000
C 4.90454700 4.04896100 -0.04940900
C -4.82146900 4.09808400 -0.68156500
N -5.36999200 -5.30408200 0.65311800
N 5.22663900 -5.49232300 -0.21947800
N 5.83969900 4.75987100 0.02334500
N -5.68236600 4.90075300 -0.61494400

Product complex: $[(p\text{-}\mathbf{CN}\text{PY})_5Me_2MoO\cdots H_2O]^{+} + H_2$

Mo 0.07047200 -0.13546200 -0.70978700
O 0.09207800 -0.25120500 -2.45266100
H 0.13823600 -0.03783300 -4.31407600
H -6.14592500 -0.69716700 -4.28562900
O 0.16774000 0.03198800 -5.29763900
H -5.69121800 -0.99446500 -4.80463500
H 0.13784200 0.99013400 -5.47514200
N -1.52055200 -1.55445600 -0.36667000
N 1.72021600 -1.48365800 -0.37937900
N 1.63826600 1.33292700 -0.51758800
N -1.56608300 1.26353800 -0.59959300
C -2.50413300 -1.32900100 0.56607100
N 0.03854400 0.00647100 1.54292700
C -2.45976400 -0.00609100 1.38499900
C -2.49696800 1.20669500 0.40941300
C 2.64374300 -1.26570900 0.61439600
C -2.59804100 -3.62588300 -1.03527600
H -2.60670900 -4.49449100 -1.69627900
C -3.52545000 -2.26996800 0.75553000
H -4.29973100 -2.11166100 1.50333300
C 2.56845500 1.26938000 0.49205000
C 3.74258700 0.12610900 2.41838700
H 3.75614000 -0.72953000 3.10860400
H 3.69847100 1.04012100 3.02767200
H 4.69166000 0.13070200 1.86237500
C -3.47170600 2.20718000 0.52561700
H -4.19158100 2.19597800 1.34190500
C -3.68938000 0.05731000 2.31999400
H -3.67575000 0.97191700 2.92972000
H -3.70736700 -0.79862000 3.00982000
H -4.62370400 0.04827200 1.73959500
C 3.53032300 2.27978900 0.62801500
H 4.25351600 2.25850000 1.44107100
C 1.22364600 0.09714700 3.65008800
H 2.15599400 0.12574500 4.21005700
C -1.20373700 0.07843000 3.61770300
H -2.15119800 0.09458900 4.15229100
C 1.21458700 0.04853800 2.25622300

C 1.88682800 -2.55618700 -1.21408200
H 1.18075600 -2.63333000 -2.04163900
C 2.53938300 0.04356400 1.45119100
C -1.15673400 0.02905800 2.22456400
C -3.55319500 3.23974300 -0.43434600
C 3.66934300 -2.19423900 0.83880000
H 4.38993100 -2.04886300 1.64085300
C 1.73747000 2.33258300 -1.44732900
H 1.02669300 2.29440900 -2.27236100
C 0.00017000 0.10930300 4.35321000
C 3.59423500 3.33607600 -0.30673300
C 2.68842800 3.34124100 -1.38955400
H 2.71636500 4.11119500 -2.16286000
C 2.90020500 -3.49235500 -1.06659900
H 2.98128300 -4.32655100 -1.76615100
C -1.69065700 2.23070300 -1.56074800
H -0.98895700 2.17117100 -2.39338800
C -2.65712600 3.22532600 -1.52565100
H -2.70526100 3.97006200 -2.32235300
C 3.80181300 -3.32777800 0.00769200
C -3.58119300 -3.43431900 -0.04063000
C -1.59811700 -2.67099700 -1.15437500
H -0.82777700 -2.77775500 -1.91748600
C 4.57870100 4.36749000 -0.16535600
N 5.38586800 5.21753600 -0.05114100
C 4.85108100 -4.27476400 0.24194300
N 5.71172900 -5.05591200 0.43255500
C -4.63061300 -4.39079100 0.15222900
N -5.49164200 -5.17896500 0.30843900
C -4.54789100 4.26343500 -0.31190300
N -5.36323900 5.10769400 -0.21295000
C -0.01896900 0.15659300 5.78214100
N -0.03463500 0.19520700 6.96036200

4.4 Water–Assisted MHR Processes: Two water molecules

4.4.1 Structures with no substituent groups: hydrogen atoms at all positions

Reactant complex: $[PY_5Me_2Mo(H)(OH)\cdots H_2O\cdots H_2O]^+$
Mo 0.04537800 -0.02006900 -0.68057100
O 0.65393800 0.73352900 -2.46077800
H 0.30921800 0.30209700 -3.28070400
H -0.59988100 -0.98015500 -1.94127500
O -0.39316000 -0.21856400 -4.96043800
H -1.97607600 -0.84226300 -2.68618000
H 0.04176400 -1.02046900 -5.30607300
N -1.42632800 -1.54036300 0.00320600
N 1.72524700 -1.36497700 -0.54897500
N 1.63570200 1.54025800 -0.22579500
N -1.63347000 1.31033500 -0.65060000
C -2.46897500 -1.19907600 0.81827300
N 0.07635300 0.11199800 1.55621700
C -2.43857800 0.21012200 1.46147400
C -2.56042600 1.30819300 0.36890600
C 2.62007900 -1.30040500 0.49199000
C -2.33611000 -3.78432300 -0.20867000
H -2.22045700 -4.79026100 -0.62029400
C -3.49899300 -2.12258200 1.08869000
H -4.34639400 -1.83564200 1.71025300
C 2.68684800 1.24472000 0.58765900
C 3.78334400 -0.12696000 2.40476500
H 3.70076300 -0.99485800 3.07575900
H 3.84495200 0.77815900 3.02573000
H 4.72886300 -0.21613200 1.85043200
C -3.59727300 2.26098300 0.39728900
H -4.31833700 2.26463100 1.21392400
C -3.61914700 0.34213300 2.45191000
H -3.60486000 1.31776400 2.95930000
H -3.58134000 -0.44309100 3.22116100
H -4.58055200 0.25471900 1.92526900
C 3.79179200 2.11333300 0.67782500
H 4.64701900 1.86375200 1.30525900
C 1.29506600 0.21486700 3.63581100
H 2.23384300 0.15446000 4.18294900
C -1.09246800 0.50451400 3.63003000
H -2.01859700 0.69053600 4.17027900
C 1.26342000 0.06870700 2.23931500
C 1.90084900 -2.34248600 -1.49572800
H 1.20437800 -2.29793500 -2.33662200
C 2.58280100 -0.05660300 1.43103500
C -1.09567200 0.30154600 2.24074400
C -3.72797200 3.21945500 -0.61622300
H -4.53446000 3.95699200 -0.58015600
C 3.58938100 -2.30911800 0.65481600
H 4.26633900 -2.29504300 1.50818700
C 1.64688700 2.70951000 -0.91890800
H 0.78478800 2.88558100 -1.56192400
C 0.11104300 0.45159900 4.33674500
H 0.12483000 0.58686400 5.42197700
C 3.80111500 3.31496300 -0.04382800
H 4.65685800 3.99259100 0.02967400
C 2.69476600 3.62841600 -0.84619000
H 2.63762800 4.56196000 -1.41207600
C 2.87745800 -3.33107900 -1.40982600
H 2.95784800 -4.08185500 -2.20058400
C -1.79110600 2.23906200 -1.65633000
H -1.05018300 2.16042100 -2.45627600
C -2.80221900 3.19192800 -1.67393200
H -2.85714500 3.89755700 -2.50784500
C 3.71855400 -3.34177000 -0.28584200
H 4.47357100 -4.12078900 -0.14768400
C -3.44500500 -3.42234200 0.57236000
H -4.24489200 -4.13609800 0.78877800
C -1.36670100 -2.82183100 -0.47311100
H -0.50319700 -3.05442700 -1.09644700
O -2.60019200 -0.84323500 -3.46620000
H -2.94865500 -1.75421000 -3.50710200
H -1.26748100 -0.53082800 -4.59377300

Transition state: $[PY_5Me_2MoO\cdots H\cdots H\cdots H_2O\cdots H_2O]^{+\ddagger}$
Mo -0.19892800 -0.50140300 -1.01562700

O 0.40331600 0.21506900 -2.70923600
H -0.01045600 -0.07816600 -3.66115000
H -0.72500600 -1.68174000 -2.26962900
O -0.67927300 -0.36921800 -4.89431900
H -1.47817100 -1.26043700 -2.48626400
H -0.22211000 -1.09624300 -5.35728300
N -1.65684600 -2.01038000 -0.21521000
N 1.50947700 -1.83294400 -0.85070800
N 1.33554100 1.09753400 -0.48757000
N -1.88347200 0.85909300 -0.98187800
C -2.72542500 -1.62140400 0.53846300
N -0.15861900 -0.31953000 1.24091500
C -2.67757900 -0.19917100 1.15309400
C -2.78718600 0.88926700 0.04887300
C 2.39639400 -1.74743800 0.19363000
C -2.58343300 -4.24585100 -0.38620800
H -2.46320000 -5.26968000 -0.74879200
C -3.77999000 -2.51768200 0.79397600
H -4.65003400 -2.19799800 1.36641100
C 2.41528300 0.80559000 0.28290100
C 3.54883000 -0.53785700 2.09293800
H 3.48868800 -1.40209800 2.77059700
H 3.59092700 0.37336100 2.70679400
H 4.49434900 -0.61191300 1.53630600
C -3.79947900 1.86852100 0.08466000
H -4.50567000 1.90282100 0.91299600
C -3.85581800 -0.04031400 2.14294900
H -3.81965200 0.93388600 2.65176100
H -3.83756100 -0.82773800 2.91039800
H -4.81813500 -0.10501800 1.61478800
C 3.51234100 1.68657400 0.34511700
H 4.39521600 1.43639700 0.93266800
C 1.05355700 -0.27742300 3.32785300
H 1.98996200 -0.36423300 3.87549300
C -1.32680100 0.05594500 3.31898200
H -2.25143300 0.24825200 3.85952800
C 1.02359900 -0.39017700 1.92860100
C 1.69377400 -2.83165900 -1.77261500
H 1.01008700 -2.81280100 -2.62471600
C 2.34418600 -0.49784400 1.12252400
C -1.32970200 -0.12315000 1.92642200
C -3.92145500 2.81451100 -0.94096700
H -4.70808200 3.57311500 -0.90099800
C 3.37037100 -2.74738200 0.38067900
H 4.04348700 -2.71154900 1.23601200
C 1.29631300 2.28017000 -1.15274000
H 0.40988400 2.45492000 -1.76182100
C -0.12815300 -0.03292600 4.02929400
H -0.11637000 0.08226700 5.11672300
C 3.47324900 2.90217700 -0.35079300
H 4.32189300 3.59062100 -0.30006200
C 2.32902600 3.21733900 -1.09653400
H 2.23361900 4.16232500 -1.63734200
C 2.67126100 -3.81731700 -1.66164400
H 2.75577800 -4.58409800 -2.43611600
C -2.03192600 1.76984900 -1.99695500
H -1.30926400 1.66499700 -2.80927500
C -3.02018200 2.74916200 -2.01416600
H -3.07347300 3.44263300 -2.85788800
C 3.50819500 -3.79917500 -0.53647400
H 4.26716100 -4.57060000 -0.37929800
C -3.72135500 -3.83585700 0.32216300
H -4.54314200 -4.52884000 0.52346500
C -1.58488500 -3.30644300 -0.63589800
H -0.68837800 -3.58016200 -1.19472400
O -2.60016400 -1.14086200 -3.59793500
H -2.84051900 -2.06567200 -3.80146500
H -1.74306200 -0.83335300 -4.32010300

Product complex: $[PY_5Me_2MoO\cdots H_2O\cdots H_2O]^+ + H_2$
Mo -0.09127900 -0.01542600 -0.70591500
O 0.33805000 0.66035200 -2.32780700
H 0.53301300 0.22519900 -3.86242300
H -0.82064600 -1.30521700 -1.97400600
O 0.60235100 -0.01398900 -4.84881400
H -1.43186500 -0.77197500 -1.87342100
H 1.40332800 -0.56386500 -4.92853800
N -1.52125300 -1.57112300 0.27596300
N 1.59141800 -1.37015700 -0.60395100
N 1.46543300 1.55817200 -0.19048800
N -1.79143300 1.34127600 -0.51146400
C -2.54885400 -1.16394600 1.07130800
N 0.06901700 0.13275100 1.60007100
C -2.45149300 0.26545200 1.67053800
C -2.62022800 1.36277700 0.57948500
C 2.52575900 -1.31176100 0.40799300
C -2.46616700 -3.80190200 0.17794000
H -2.37037000 -4.83211300 -0.17407900
C -3.59826100 -2.04740100 1.38837300
H -4.44195600 -1.71461500 1.99236800
C 2.59009100 1.24804000 0.50383800
C 3.82029200 -0.11885800 2.22548900
H 3.78915800 -0.97842200 2.91079900
H 3.91481500 0.79327500 2.83247600
H 4.72725100 -0.21121400 1.60992300
C -3.61898800 2.35213800 0.68910200
H -4.26679900 2.38819500 1.56359700
C -3.56720800 0.43404300 2.72993900
H -3.48983100 1.40413000 3.24207400
H -3.51215300 -0.35822400 3.49053000
H -4.56045900 0.38188400 2.26058300
C 3.69623700 2.12092000 0.50314900
H 4.61500700 1.85572300 1.02562900
C 1.40564200 0.15861500 3.61553500
H 2.37424500 0.06783000 4.10362100
C -0.97073700 0.49308800 3.75185300
H -1.86095300 0.68065900 4.34869300
C 1.28878000 0.05490000 2.22015900
C 1.69816500 -2.39901400 -1.51266900
H 0.98906400 -2.36314900 -2.34310200
C 2.55706000 -0.06081100 1.33357900
C -1.05711600 0.32806300 2.36008700

C -3.80570100 3.30427300 -0.32071400
H -4.58330000 4.06674100 -0.22140100
C 3.45473200 -2.35470600 0.57594800
H 4.16207500 -2.33298900 1.40391700
C 1.39041600 2.75098000 -0.83411700
H 0.46794300 2.93939100 -1.38389600
C 0.26912600 0.40031700 4.39011500
H 0.34619500 0.51155300 5.47552600
C 3.61999200 3.34719700 -0.17011500
H 4.47566700 4.02887100 -0.16745200
C 2.43040700 3.68167800 -0.83220700
H 2.30659900 4.63433700 -1.35354200
C 2.62857400 -3.42897300 -1.41571200
H 2.64683500 -4.21141200 -2.17923400
C -1.99997800 2.25871100 -1.50907600
H -1.33172700 2.14920200 -2.36800000
C -2.98327400 3.24184600 -1.45543700
H -3.09263300 3.94027500 -2.28949500
C 3.51024600 -3.43209700 -0.32288400
H 4.23846500 -4.23479600 -0.17854400
C -3.56796100 -3.37286700 0.93115900
H -4.38573700 -4.05668100 1.17643700
C -1.47603000 -2.86873500 -0.13157500
H -0.60812300 -3.15459900 -0.73138100
O -1.64587800 -1.26131100 -5.78252200
H -1.68833100 -2.13389600 -5.35097800
H -0.81271800 -0.83876900 -5.42070700

4.5 Water–Assisted MHR Processes: Three water molecules

4.5.1 Structures with no substituent groups: hydrogen atoms at all positions

Reactant complex: $[PY_5Me_2Mo(H)(OH)\cdots H_2O\cdots H_2O\cdots H_2O]^+$
Mo 0.18376300 0.01629800 0.49439400
O 0.19233700 -0.03557400 2.51217700
O 2.47131900 0.33462700 4.14069000
N 1.37135100 0.99881800 -1.10523400
N 1.20928400 -1.87503300 0.32211500
N -1.56046500 -1.31392700 1.12071400
N -0.90180300 1.86066800 0.52355300
C 0.79429700 1.87933100 -1.97767400
N -0.88453500 -0.48627700 -1.41589000
C -0.75227100 1.96439800 -1.98365900
C -1.26902500 2.52141300 -0.62791800
C 0.64168100 -2.94939800 -0.32022400
C 3.55394200 1.51047500 -2.04649700
C 1.58855500 2.63802200 -2.86106800
C -1.70642500 -2.55979700 0.59374100
C -1.31695300 -4.26665000 -1.22744800
C -2.06672500 3.68059100 -0.56521100
C -1.20544000 2.90282400 -3.12665500
C -2.60792500 -3.47974100 1.16364600
C -1.94520200 -2.09262200 -2.87016800
C -2.03277900 0.25020500 -3.40563900
C -1.22312200 -1.78143500 -1.70626900
C 2.47911300 -2.01686100 0.82297800
C -0.87425500 -2.88974400 -0.67706100
C -1.26151900 0.52159400 -2.26439100
C -2.48747500 4.20382200 0.66454100
C 1.40793700 -4.10087400 -0.58583200
C -2.33286800 -0.94905400 2.17735800
C -2.36895000 -1.06863200 -3.71923000
C -3.39767700 -3.10110100 2.25813500
C -3.27164100 -1.79928900 2.76369400
C 3.25912000 -3.15471700 0.63433300
C -1.29318300 2.40416700 1.72780300
C -2.07324700 3.54864500 1.83769400
C 2.72789100 -4.20978100 -0.12401300
C 2.97700600 2.46565700 -2.89895300
C 2.72646200 0.81414400 -1.17089500
O 3.48173100 2.83421500 3.85035800
O 2.26179300 3.15064500 1.46870400
H 2.12851900 0.20406400 5.04423500
H 4.62810900 1.30838700 -2.04507100
H 1.12753100 3.36373800 -3.53005700
H -0.81150300 -4.49758300 -2.17700600
H -2.40178100 -4.29209900 -1.40422900
H -1.07682700 -5.06737300 -0.51304900
H -2.36943100 4.18982300 -1.47949100
H -2.30231300 2.95238500 -3.18882400
H -0.82387300 2.55730100 -4.09863000

H -0.83470400 3.92476800 -2.96054500
H -2.70295500 -4.48886400 0.76345900
H -2.19013000 -3.12386800 -3.11710800
H -2.36425300 1.05358600 -4.06059600
H 2.84918500 -1.15733200 1.38694800
H -3.11200900 5.10070400 0.69996800
H 0.98127500 -4.93425500 -1.14267100
H -2.16538600 0.05728300 2.56140700
H -2.95059000 -1.29569100 -4.61723500
H -4.10271400 -3.81273000 2.69789700
H -3.88014000 -1.44298800 3.59902500
H 4.26519400 -3.19649600 1.06023700
H -0.92611400 1.85733800 2.60104500
H -2.34710300 3.91591000 2.83097400
H 3.31358800 -5.10820900 -0.33809100
H 3.58806500 3.05428900 -3.58899300
H 3.13759800 0.08189000 -0.47584800
H 3.13971400 3.50046600 4.47504400
H 2.88993100 3.32711800 0.74229900
H 1.04101600 0.17854100 2.97739300
H 1.64969300 0.70692100 1.06019000
H 1.88296100 2.24624800 1.26542400
H 2.84785900 1.26561900 4.13091000
H 3.04981200 3.04205600 2.96632700

Transition state: $[PY_5Me_2MoO\cdots H\cdots H\cdots H_2O\cdots H_2O\cdots H_2O]^{+\,\ddagger}$
Mo -0.297806 -0.409138 -1.010885
O 0.187434 0.357268 -2.611569
H 0.396900 -0.006751 -3.960124
H -1.002757 -1.526878 -2.218918
O 0.506406 -0.279684 -4.995516
H -1.910332 -1.320463 -2.780550
H 0.939354 0.475767 -5.435851
N -1.728411 -1.984514 -0.137782
N 1.390368 -1.745141 -0.890144
N 1.294214 1.204801 -0.428466
N -2.005791 0.880198 -0.865507
C -2.760378 -1.631164 0.679015
N -0.180633 -0.289170 1.275835
C -2.706972 -0.211383 1.294963
C -2.879211 0.879625 0.201150
C 2.302321 -1.704056 0.145132
C -2.621503 -4.237306 -0.288023
H -2.502129 -5.254209 -0.671110
C -3.786842 -2.549893 0.979198
H -4.632955 -2.252609 1.598310
C 2.409459 0.853104 0.257040
C 3.556453 -0.543785 2.011178
H 3.482755 -1.397169 2.701569
H 3.660474 0.371977 2.611324
H 4.478422 -0.664150 1.423628
C -3.906103 1.840845 0.284620
H -4.584690 1.845643 1.136767
C -3.846150 -0.074922 2.332898
H -3.811802 0.900250 2.840052
H -3.778564 -0.860825 3.099487
H -4.828210 -0.162213 1.845363
C 3.554488 1.676159 0.244847
H 4.468162 1.371247 0.755750
C 1.110663 -0.174843 3.320786
H 2.070553 -0.226773 3.831556
C -1.275190 0.094909 3.399287
H -2.183503 0.270677 3.972549
C 1.028817 -0.327385 1.927453
C 1.521585 -2.753386 -1.820003
H 0.823556 -2.695993 -2.658478
C 2.321997 -0.459516 1.080884
C -1.328314 -0.108347 2.011738
C -4.083353 2.806523 -0.715133
H -4.883046 3.547955 -0.634356
C 3.221989 -2.754516 0.319352
H 3.906189 -2.752172 1.167340
C 1.262097 2.396742 -1.075394
H 0.341971 2.613505 -1.621801
C -0.047062 0.058607 4.066519
H 0.004425 0.201800 5.149563
C 3.519876 2.905264 -0.427690
H 4.401883 3.552771 -0.433966
C 2.336723 3.287787 -1.079736
H 2.247720 4.247767 -1.595500
C 2.450858 -3.783672 -1.719540
H 2.492075 -4.549848 -2.498966
C -2.206822 1.820273 -1.854925
H -1.502501 1.742674 -2.687336
C -3.210279 2.780095 -1.816756
H -3.300769 3.491934 -2.642575
C 3.300891 -3.813596 -0.600403
H 4.023090 -4.621293 -0.452562
C -3.727771 -3.861535 0.490966
H -4.522994 -4.574404 0.727669
C -1.662654 -3.271584 -0.585917
H -0.803303 -3.511376 -1.214973
O -1.852531 -0.753212 -5.703189
H -2.273060 0.029636 -6.108040
H -0.837696 -0.499594 -5.482037
H -2.400265 -1.034479 -4.550001
O -2.806493 -1.277452 -3.509665
H -3.194077 -2.176408 -3.528613

Product complex: $[PY_5Me_2MoO\cdots H_2O\cdots H_2O\cdots H_2O]^{+} + H_2$
Mo 0.25133300 0.04378400 0.56752000
O 0.27650600 0.03159300 2.38018300
O 2.01308200 0.17563300 4.31217800
N 1.38351900 0.95957500 -1.24806200
N 1.25316400 -1.86228400 0.34625600
N -1.55170100 -1.24627400 1.09172500
N -0.87374800 1.91099700 0.52363400
C 0.78561300 1.88704900 -2.04596300
N -0.87428700 -0.48223900 -1.38440400
C -0.76385500 1.96580300 -1.99391600
C -1.26805700 2.52968100 -0.63362200
C 0.67601700 -2.92622900 -0.31309200

C 3.52921900 1.45549600 -2.26335600
C 1.55305300 2.66859200 -2.93061200
C -1.67392000 -2.51540900 0.62669100
C -1.30272000 -4.26285700 -1.14857800
C -2.09877500 3.66774600 -0.57970500
C -1.25114600 2.89207400 -3.13413600
C -2.56401000 -3.42031000 1.23859300
C -1.90125600 -2.11544900 -2.84351700
C -2.01089300 0.22018900 -3.39838300
C -1.19776800 -1.78234900 -1.67512500
C 2.55297700 -2.00754200 0.77600900
C -0.84605000 -2.87694000 -0.63342500
C -1.25810500 0.51182900 -2.24994300
C -2.50998700 4.20393800 0.64686400
C 1.44874200 -4.04974800 -0.65925800
C -2.34819900 -0.83242800 2.10954800
C -2.33087100 -1.10481300 -3.70625200
C -3.37735100 -2.99397800 2.29678400
C -3.28764400 -1.66176400 2.72405600
C 3.34373100 -3.11849100 0.50029900
C -1.25709100 2.45953800 1.72060900
C -2.06199000 3.58967300 1.82563500
C 2.79393300 -4.15523600 -0.27073500
C 2.93627500 2.46392200 -3.03582700
C 2.71993000 0.73861800 -1.38152800
O 3.31502000 2.50091500 4.09854400
O 2.60904400 3.61815900 1.69978200
H 1.50703100 0.07620500 5.13999000
H 4.59585600 1.22649500 -2.32895100
H 1.08340900 3.43738500 -3.54346400
H -0.82242300 -4.51480200 -2.10517100
H -2.39158900 -4.28610600 -1.30100500
H -1.04527600 -5.05045800 -0.42510200
H -2.43205900 4.15147600 -1.49645200
H -2.34925000 2.91682800 -3.18838200
H -0.86920800 2.55322500 -4.10800000
H -0.90079900 3.92231800 -2.97455600
H -2.63209500 -4.45241700 0.89553700
H -2.13096200 -3.15262300 -3.08117500
H -2.34213100 1.01356700 -4.06550300
H 2.94413200 -1.17571100 1.36687200
H -3.15615500 5.08582700 0.67342500
H 1.00618700 -4.86917900 -1.22419900
H -2.19724900 0.19352300 2.44625800
H -2.90348100 -1.34497800 -4.60646500
H -4.07341700 -3.69297500 2.76978400
H -3.91592000 -1.26868600 3.52739000
H 4.36935800 -3.15605800 0.87728800
H -0.86623000 1.93879600 2.59926100
H -2.32757300 3.97141300 2.81523200
H 3.38131700 -5.03518100 -0.54678300
H 3.53080400 3.07385700 -3.72206300
H 3.14376900 -0.04513800 -0.74863300
H 3.05676100 3.07350500 4.84414000
H 3.39632800 3.54177400 1.13065800
H 1.32301000 0.10218100 3.56114400
H 2.01021000 0.69058800 1.01056300
H 1.57805300 1.38786500 1.00644300
H 2.80145100 1.63900700 4.22635300
H 2.88428400 3.21585100 2.57422500