ELECTRONIC SUPPLEMENTARY INFORMATION

Reactivity of Metal Hydrides with CO_2: Going Beyond Formate with a High-Valent Cationic Pentahydride Mo(VI) Complex

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I. General Information

I.1. Experimental

All reactions were performed in oven-dried glassware with rigorous exclusion of air and moisture, using a nitrogen-filled *Jacomex* glove box (O_2 < 1 ppm, H_2O < 1 ppm) or an argon-filled MBraun glove box (O_2 < 1 ppm, H_2O < 1 ppm), both equipped with vacuum line. Solvents used were pre-dried (tetrahydrofuran and *n*-pentane by passing through a Puresolv MD 7 solvent purification machine; benzene and 1,2-dichlorobenzene by distillation over CaH_2), degassed by freeze-pump-thaw cycles, dried over molecular sieves and stored in the glove box. THF-d_8 (purchased from *Eurisotop*) and *o*-$C_6D_4Cl_2$ (purchased from *Deutero*) were degassed by freeze-pump-thaw cycles, dried over molecular sieves and stored in the glove box.

$[MoH_4(depe)_2]$,[1] $[MoH_5(depe)_2][HB(C_6F_5)_3]$[2] and $[NEt_3H][B(C_6H_5)_4]$[3] were synthesized according to reported procedures and stored in the glove box.

I.2. Nuclear Magnetic Resonance

^1H, ^{11}B, ^{19}F and ^{31}P NMR spectra were recorded in THF-d_8 by using Wilmad quick pressure valve NMR tubes or J. Young high-vacuum valve NMR tubes on a *Bruker* Avance III 400 spectrometer. Chemical shifts are in parts per million (ppm) downfield from tetramethylsilane and are referenced to the residual solvent resonances as the internal standard ($C_6HD_3Cl_2$: δ reported = 7.17 ppm, 6.90 ppm; $C_4HD_7O_2$: δ reported = 3.58, 1.72 for ^1H NMR). ^{11}B, ^{19}F and ^{31}P NMR spectra were calibrated according to the IUPAC recommendation using a unified chemical shift scale based on the proton resonance of tetramethylsilane as primary reference.[4,5] Data are reported as follows: chemical shift, multiplicity (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, sext = sextet; m = multiplet), coupling constant (Hz), and integration.

I.3. Crystallographic data collection and refinement

Data for compounds (**1.BPh$_4$**), (**3.BPh$_4$**), (**4.BPh$_4$**) and (**7.BPh$_4$**) were collected at low temperature (100 K) either on a Bruker Kappa Apex II diffractometer using a Mo-Kα radiation (l = 0.71073Å) micro-source or on a XtaLAB Synergy, Dualflex, HyPix diffractometer using micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray source. The structures have been solved using the new dual-space algorithm program SHELXT[6] and refined by means of least-squares procedures using the SHELXL-2018,[7] program included in the software package WinGX version 1.63[8] or with the aid of the software package Crystal[9]. The Atomic Scattering Factors were taken from International tables for X-Ray Crystallography[10]. Hydrogen atoms were placed geometrically and refined using a riding model. All non-hydrogens atoms were anisotropically refined. Drawing of molecules in the following figures were performed with the program Mercury[11] with 30% probability displacement ellipsoids for non-hydrogen atoms. The crystal structures have been deposited at the Cambridge Crystallographic Data Centre and allocated the deposition numbers CCDC **2365476**, **2365477**, **2365478** and **2365557**.

I.4. Miscellaneous

Infrared (IR) spectra were recorded in a nitrogen filled *Jacomex* glove box (O_2 < 1 ppm, H_2O < 1 ppm) on an *Agilent* Cary 630 FT-IR spectrophotometer equipped with a transmission module and are reported in wavenumbers (cm^{-1}).

II. Syntheses, Characterization Data and Spectra for the New Compounds

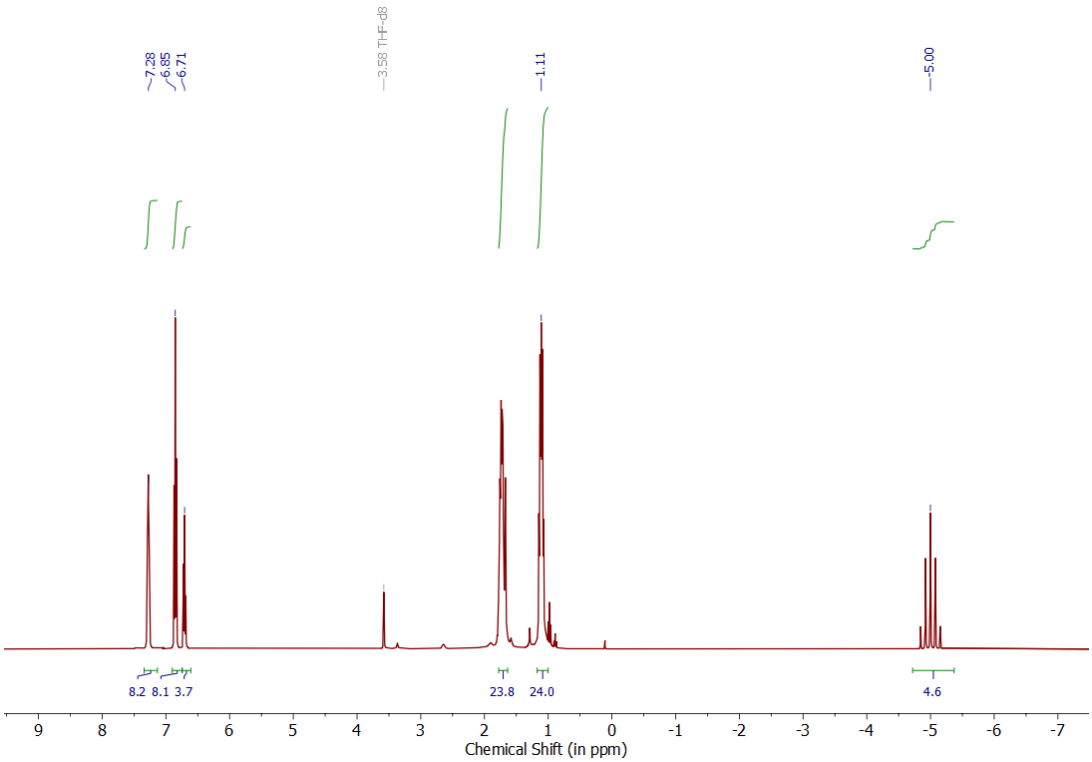
II.1. $[Mo(depe)_2H_5][B(C_6H_5)_4]$ ($1.BPh_4$)

II.1.1. Experimental procedure

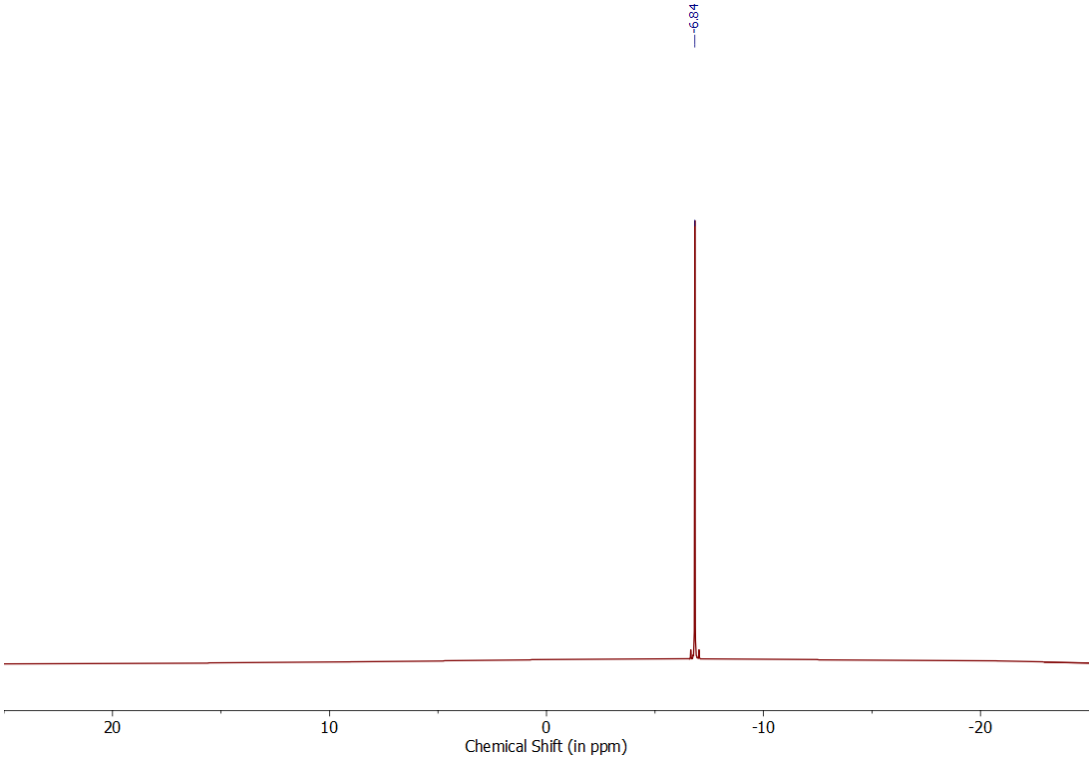
$[MoH_4(depe)_2]$ (60.0 mg, 117 µmol, 1.00 equiv.) was dissolved in THF (1 mL). A solution of $[HNEt_3][B(C_6H_5)_4]$ (50.0 mg, 117 µmol, 1.00 equiv.) in THF (1 mL) was added. The reaction mixture was left at room temperature for 30 min, under continuous stirring. The resulting pale-yellow solution was then dropwise transferred in a large volume (ca. 10 mL) of precooled pentane (-40°C), triggering immediate precipitation of an off-white solid. The solution was decanted off and the solid washed twice with cold pentane (2 x 5 mL). The resulting off-white powder was then dried under an Ar atmosphere at room temperature yielding the desired compound (85.0 mg, 87%). Single crystals suitable for X-ray diffraction were obtained by storing at -40°C a concentrated THF solution of the complex layered by pentane over a few days.

^{1}H-NMR (400 MHz, THF-d_8) δ 7.28 (br. m, 8H, *meta*-C_6H_5), 6.85 (t, $^{3}J_{(H-H)}$ = 7.4 Hz, 8H, *ortho*-C_6H_5), 6.71 (t, $^{3}J_{(H-H)}$ = 7.2 Hz, 4H, *para*-C_6H_5), 1.85 – 1.58 (m, 24H, -CH_2-CH_3 & -CH_2-CH_2-), 1.11 (m, 24H, -CH_2-CH_3), -5.00 (quin, $^{2}J_{(P-H)}$ = 30.8 Hz, 5H, Mo-*H*).
^{11}B-NMR (128 MHz, THF-d_8) δ -6.8.
^{13}C{^{1}H}-NMR (101 MHz, THF-d_8) δ 164.0 (q, $^{2}J_{(B-C)}$ = 50.1 Hz, *ipso*-C_6H_5), 135.9 (br. s, *meta*-C_6H_5), 124.4 (m, *ortho*-C_6H_5), 120.5 (s, *para*-C_6H_5), 25.7 (m, -CH_2-), 25.1 (m, -CH_2-), 7.7 (s, -CH_3).
^{31}P{^{1}H}-NMR (162 MHz, THF-d_8) δ 73.7 (s). **^{31}P{^{1}H}$_{sel}$-NMR** (162 MHz, THF-d_8) δ 73.7 (sext, $^{2}J_{(P-H)}$ = 30.8 Hz).

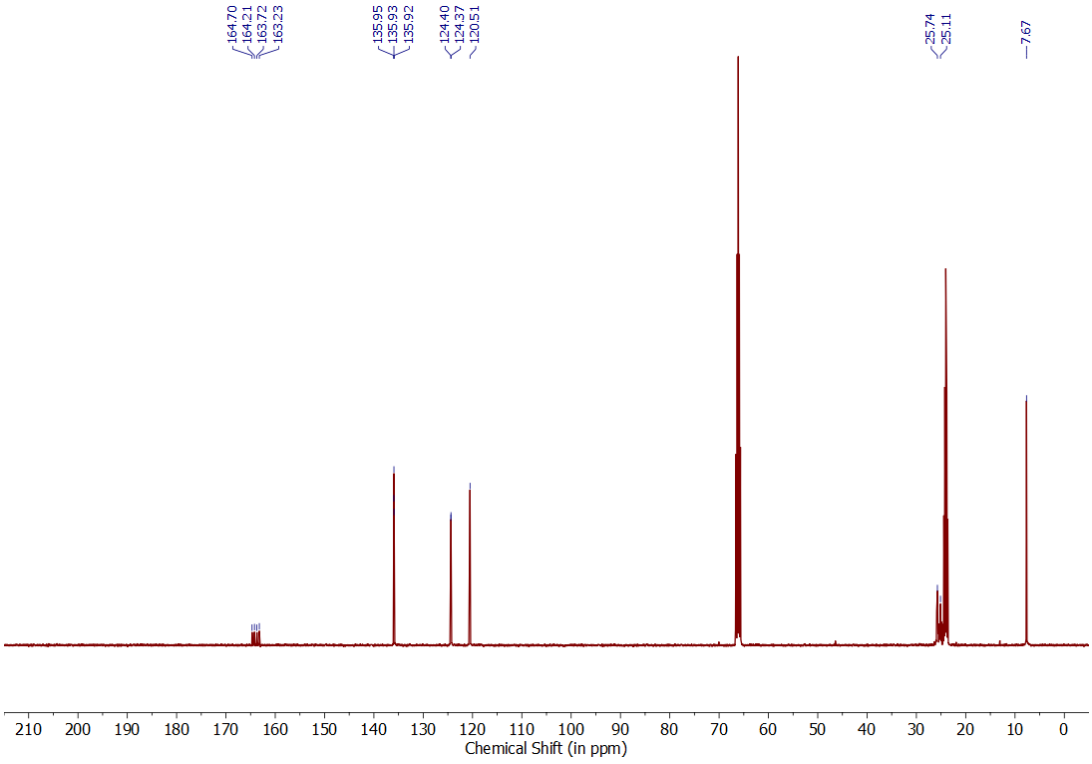
II.1.2. ^{1}H-NMR spectrum (400 MHz, THF-d8)



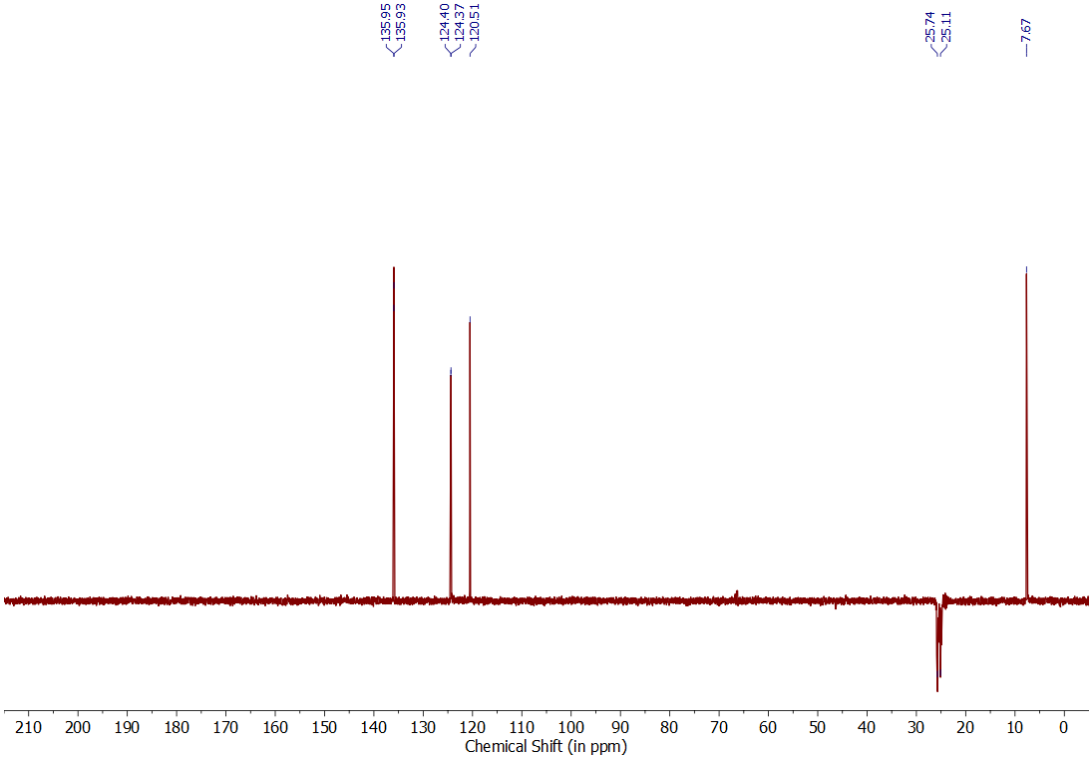
II.1.3. $^{11}B\{^1H\}$-NMR spectrum (128 MHz, THF-d_8)



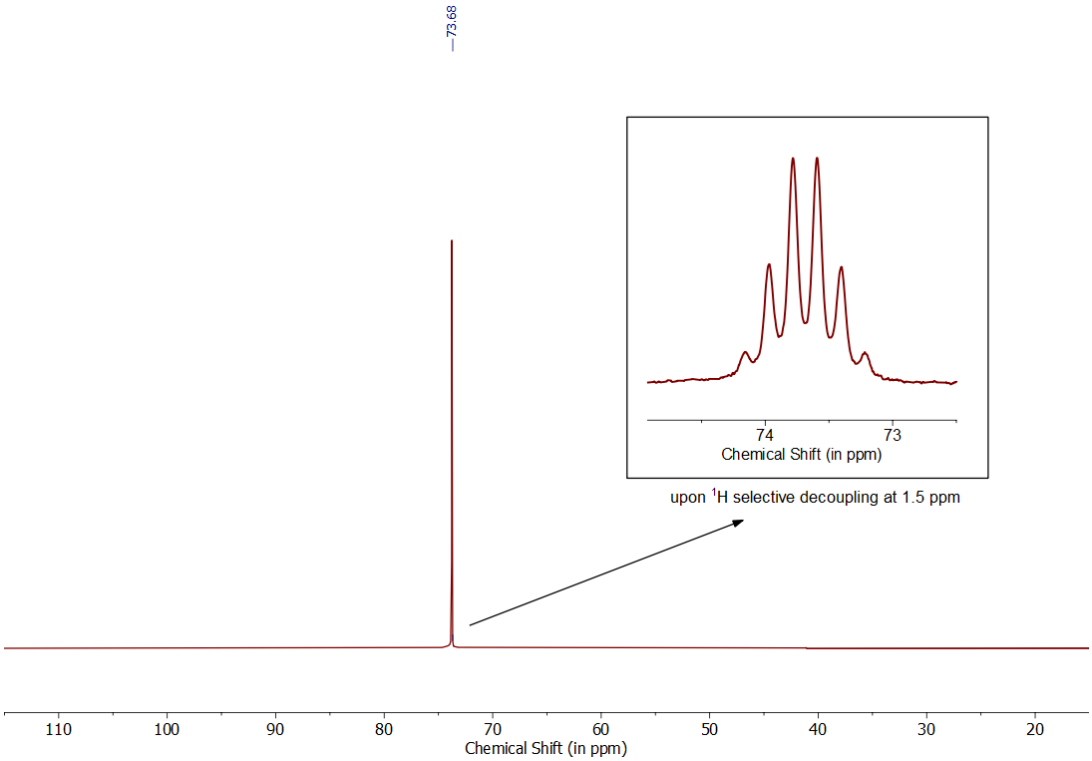
II.1.4. $^{13}C\{^1H\}$-NMR spectrum (101 MHz, THF-d_8)



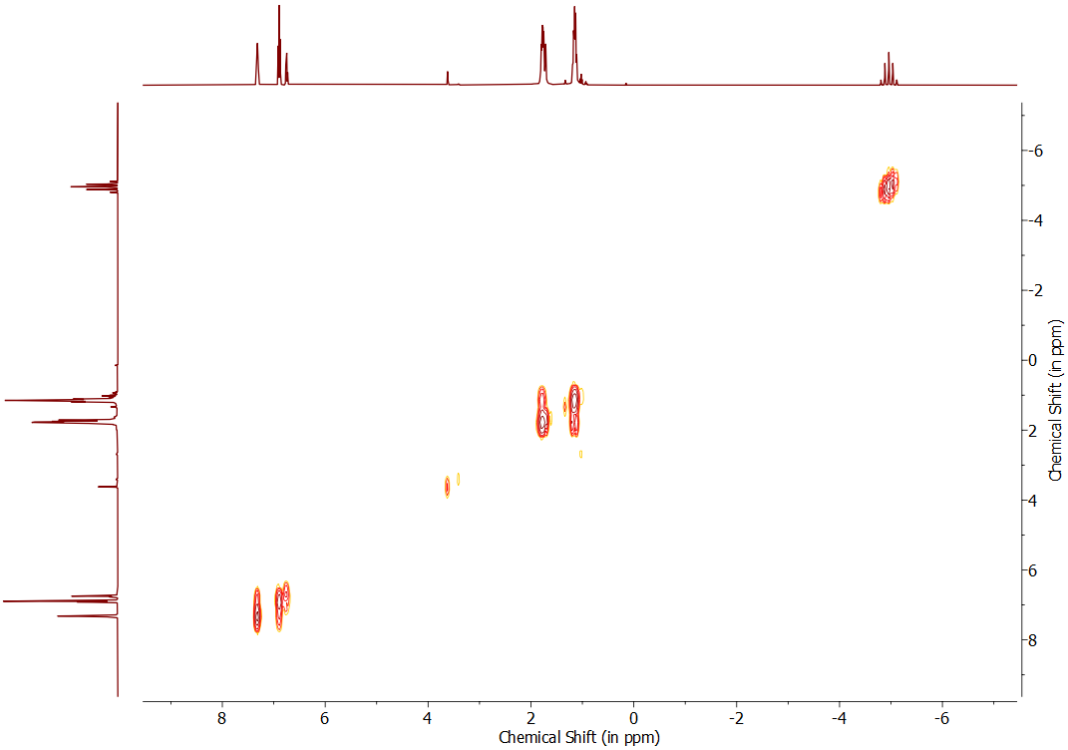
II.1.5. ^{13}C-DEPT NMR spectrum (101 MHz, THF-d_8)



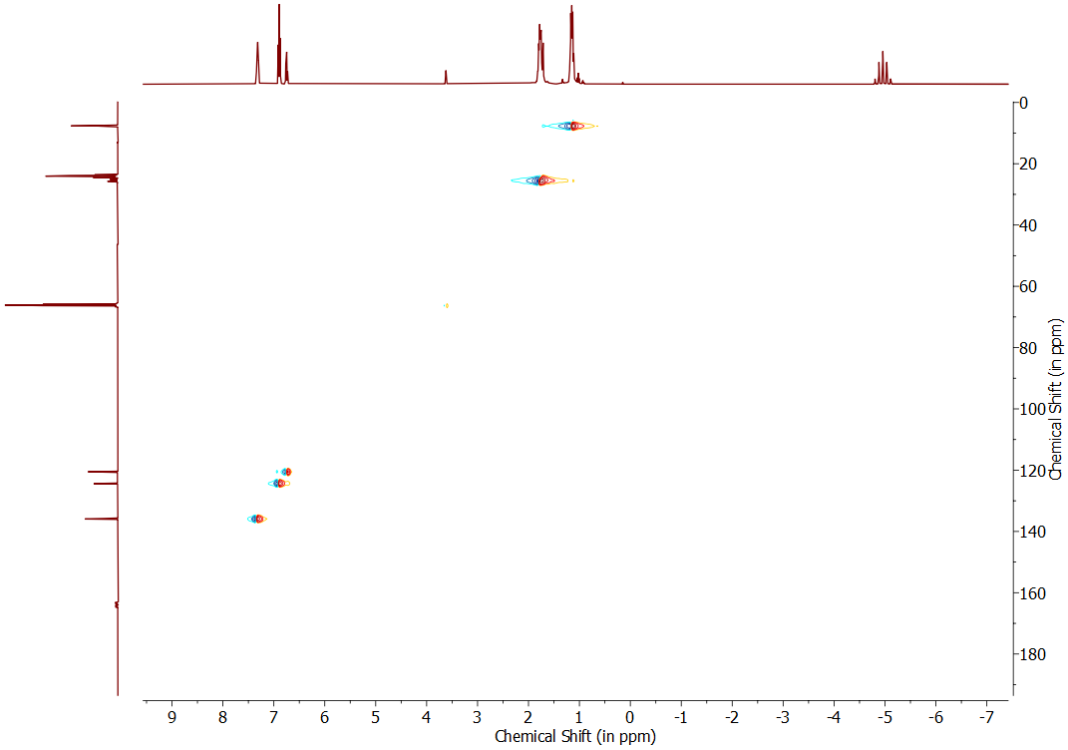
II.1.6. ^{31}P{^{1}H}-NMR spectrum (162 MHz, THF-d_8)



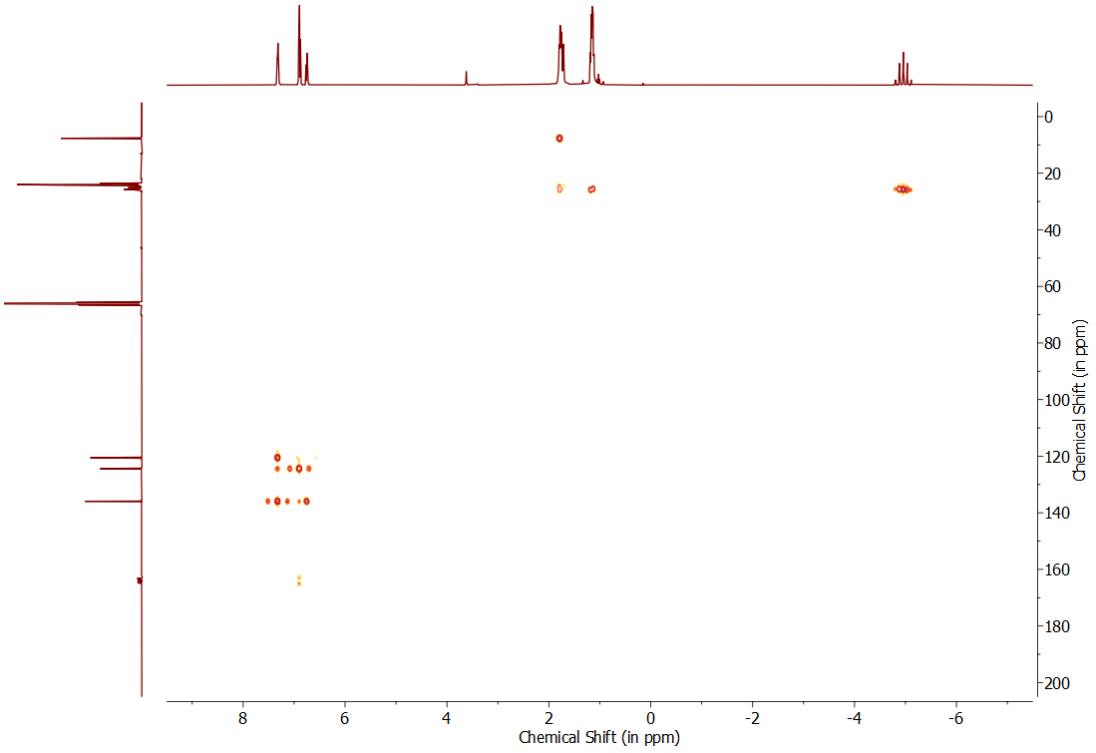
II.1.7. ^{1}H-^{1}H COSY NMR spectrum



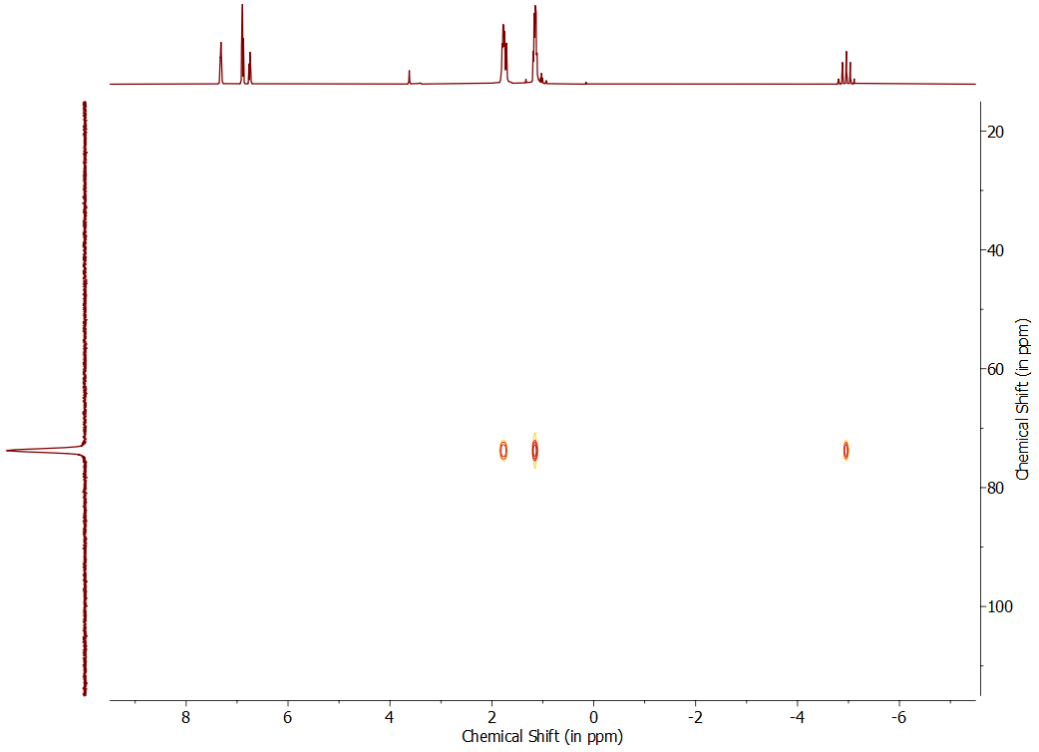
II.1.8. ^{13}C-^{1}H HSQC NMR spectrum



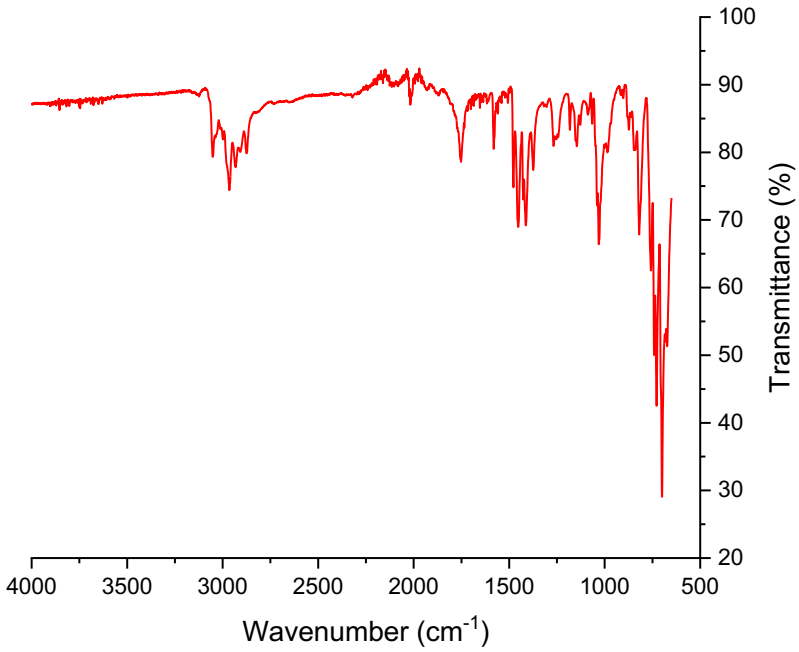
II.1.9. ^{13}C-^{1}H HMBC NMR spectrum



II.1.10. ^{31}P-^{1}H HMQC NMR spectrum



II.1.11. FT-IR spectrum (ATR)



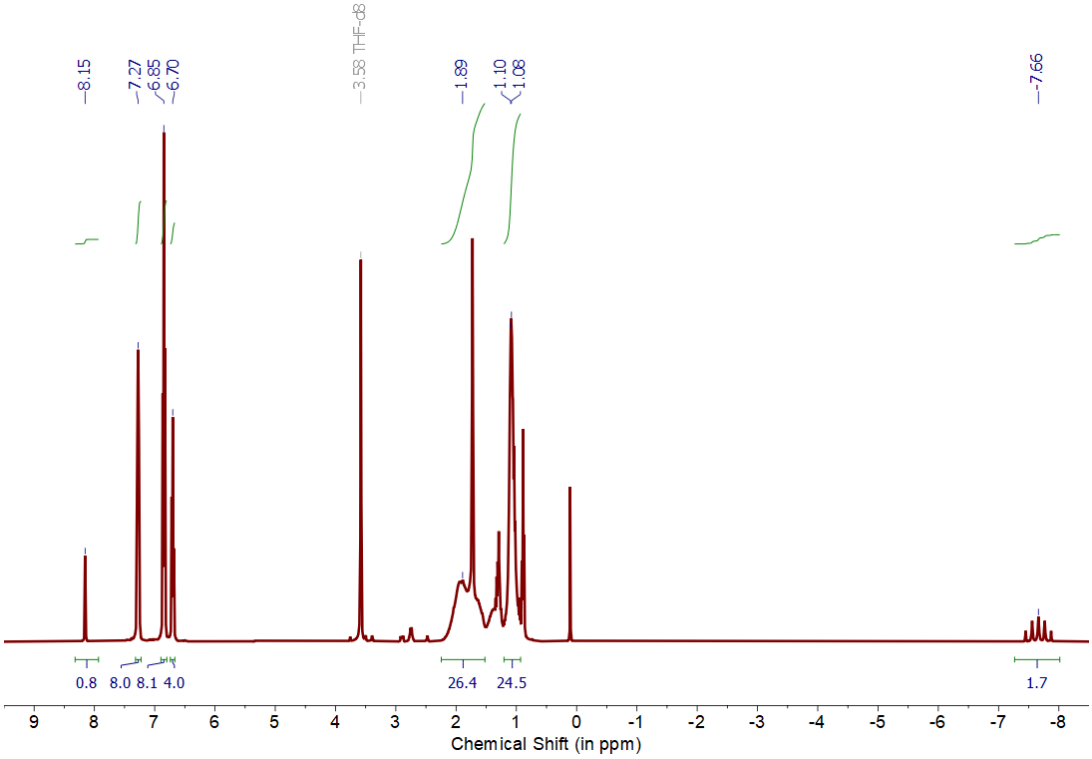
II.2. **[Mo(depe)$_2$(HCOO)H$_2$][B(C$_6$H$_5$)$_4$]** (3.BPh$_4$)

II.2.1. Experimental procedure

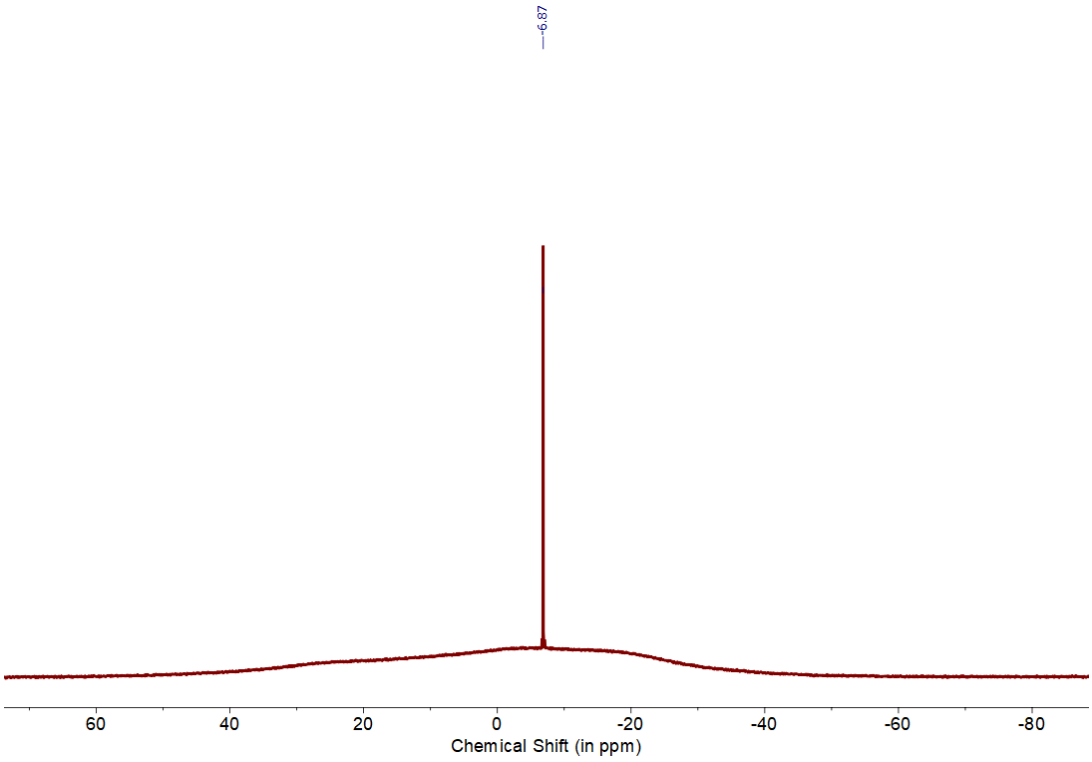
In an Wilmad pressure NMR tube, [Mo(depe)$_2$H$_5$][BPh$_4$] (20.0 mg, 24.0 µmol, 1.00 equiv.) was dissolved in THF (1 mL). The tube was placed at 0°C, evacuated and finally pressurized with carbon dioxide (3 bar). The reaction mixture was left at room temperature for 24h. After pressure was carefully released, the solution was slowly poured in cold pentane (ca. 5 mL), triggering immediate precipitation of a pink solid. The solution was decanted off and the solid washed twice with cold pentane (2 x 5 mL). The solid was then dried under an argon flux at room temperature to yield the desired compound (15.5 mg, 74%). Single crystals suitable for X-ray diffraction were obtained by storing at -40°C a concentrated THF solution of the complex **5.BPh$_4$**, layered by pentane over a few days.

^{1}H-NMR (400 MHz, *THF-d8*) δ 8.15 (s, 1H, *H*COO), 7.27 (br. m, 8H, *meta*-C$_6$*H*$_5$), 6.85 (t, ^{3}J$_{(H-H)}$ = 7.4 Hz, 8H, *ortho*-C$_6$*H*$_5$), 6.69 (t, ^{3}J$_{(H-H)}$ = 7.2 Hz, 4H, *para*-C$_6$*H*$_5$), 2.21-1.52 (m, 24H, C*H*$_2$ and C*H*$_3$ from depe), 1.22-0.94 (m, 24H, C*H*$_2$ and C*H*$_3$ from depe), -7.66 (pseudo-quintet, ^{2}J$_{(P-H),app}$ = 42.6 Hz, 2H).
^{11}B-NMR (128 MHz, *THF-d8*) δ -6.87
^{13}C{^{1}H}-NMR (101 MHz, *THF-d8*) δ 176.9 (m, H*C*OO), 163.9 (q, ^{2}J$_{(B-C)}$ = 50.3 Hz, *ipso*-C$_6$H$_5$), 135.9 (br. s, *meta*-*C*$_6$H$_5$), 124.3 (m, *ortho*-*C*$_6$H$_5$), 120.4 (s, *para*-*C*$_6$H$_5$), 22.85, 20.43, 17.11, 13.41, 7.48, 7.06.
^{31}P{^{1}H}-NMR (162 MHz, *THF-d8*) δ 78.3 (s, 2P), 44.0 (s, 2P). **^{31}P{^{1}H}$_{sel}$-NMR** (162 MHz, THF-d$_8$) δ 78.3 (t,^{2}J$_{(P-H)}$ = 42.6 Hz), 48.3 (t,^{2}J$_{(P-H)}$ = 36.7 Hz).

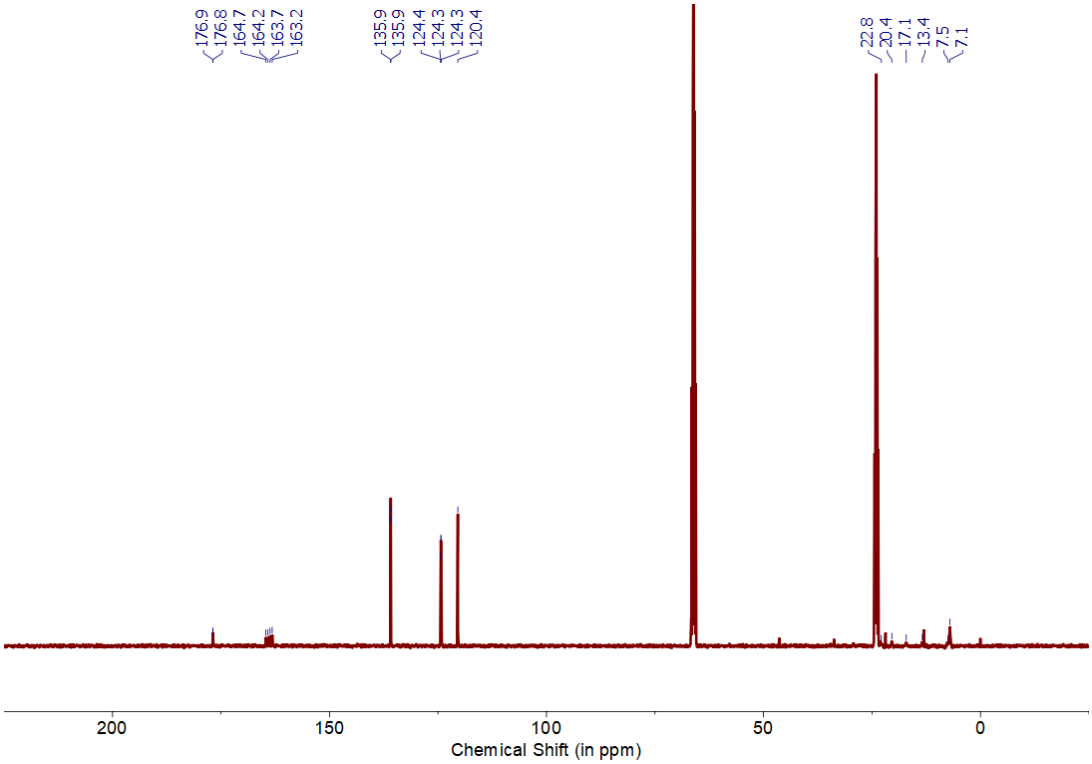
II.2.2. ^{1}H-NMR spectrum (400 MHz, THF-d8)



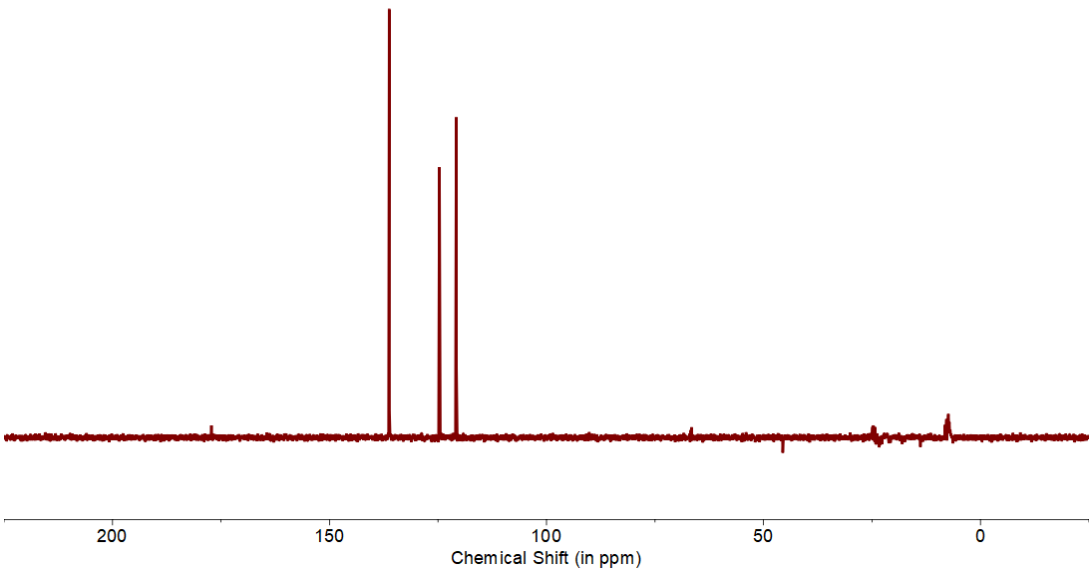
II.2.3. ^{11}B{^{1}H}-NMR spectrum (128 MHz, THF-d8*)*



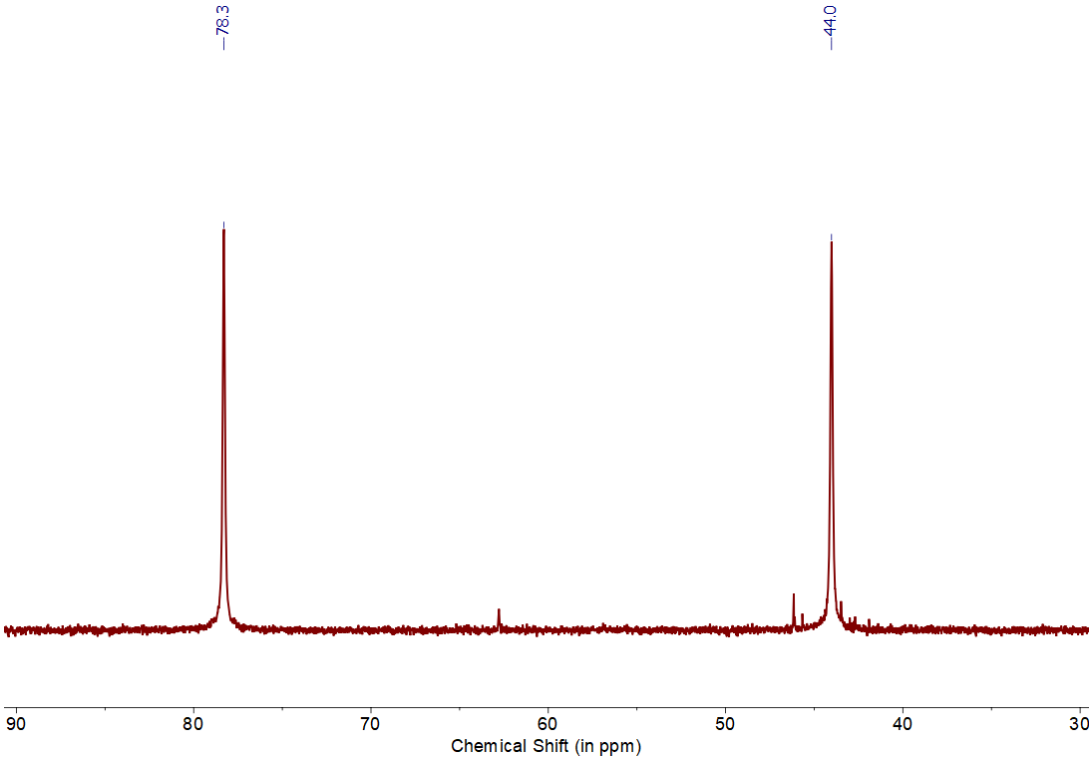
II.2.4. $^{13}C\{^{1}H\}$-NMR spectrum (101 MHz, THF-d8*)*



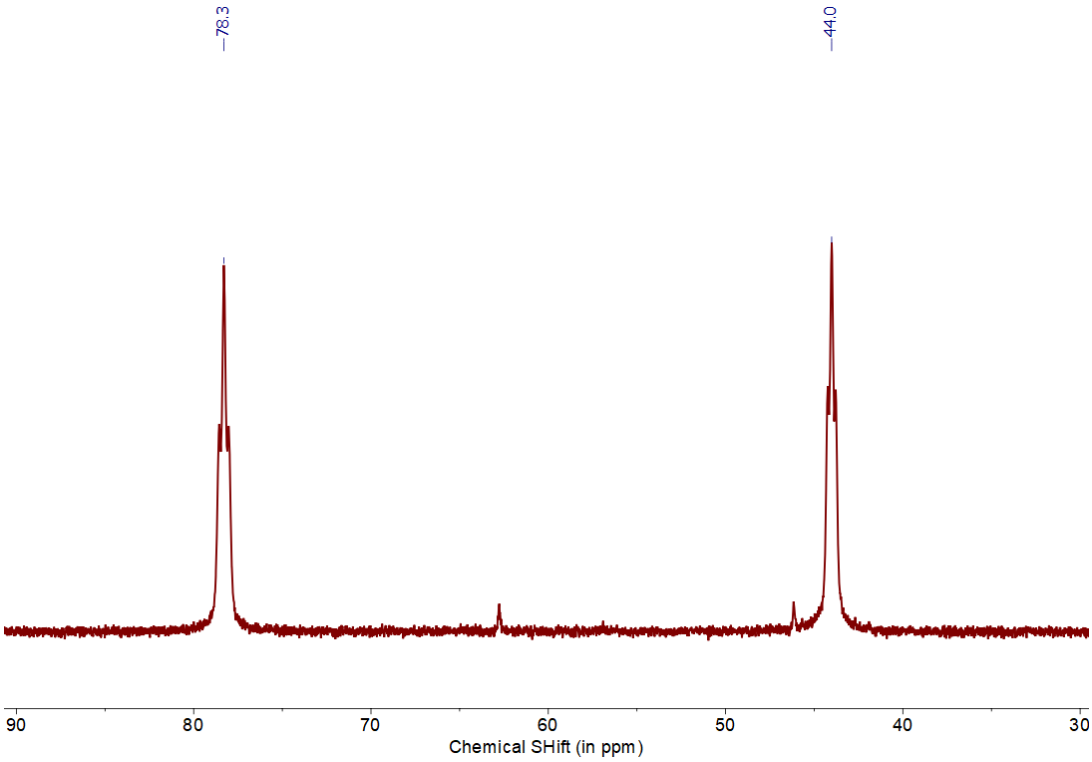
II.2.5. ^{13}C-DEPT NMR spectrum (101 MHz, THF-d8)



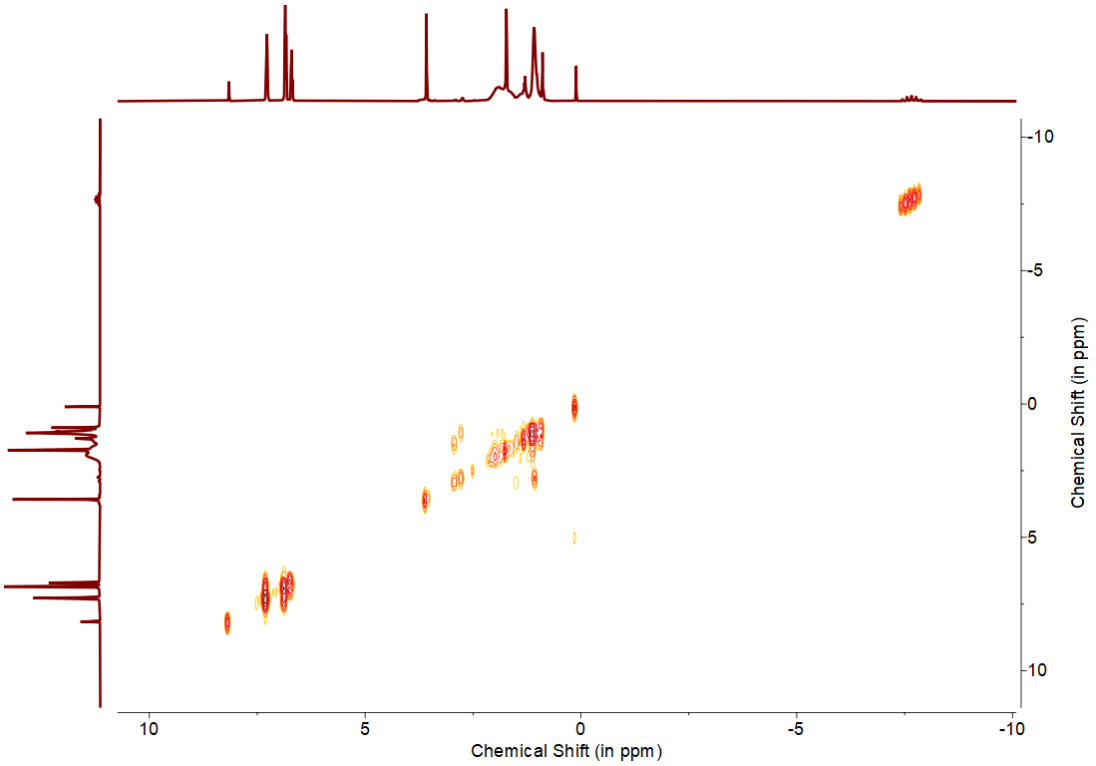
II.2.6. $^{31}P\{^{1}H\}$-NMR spectrum (162 MHz, THF-d8)



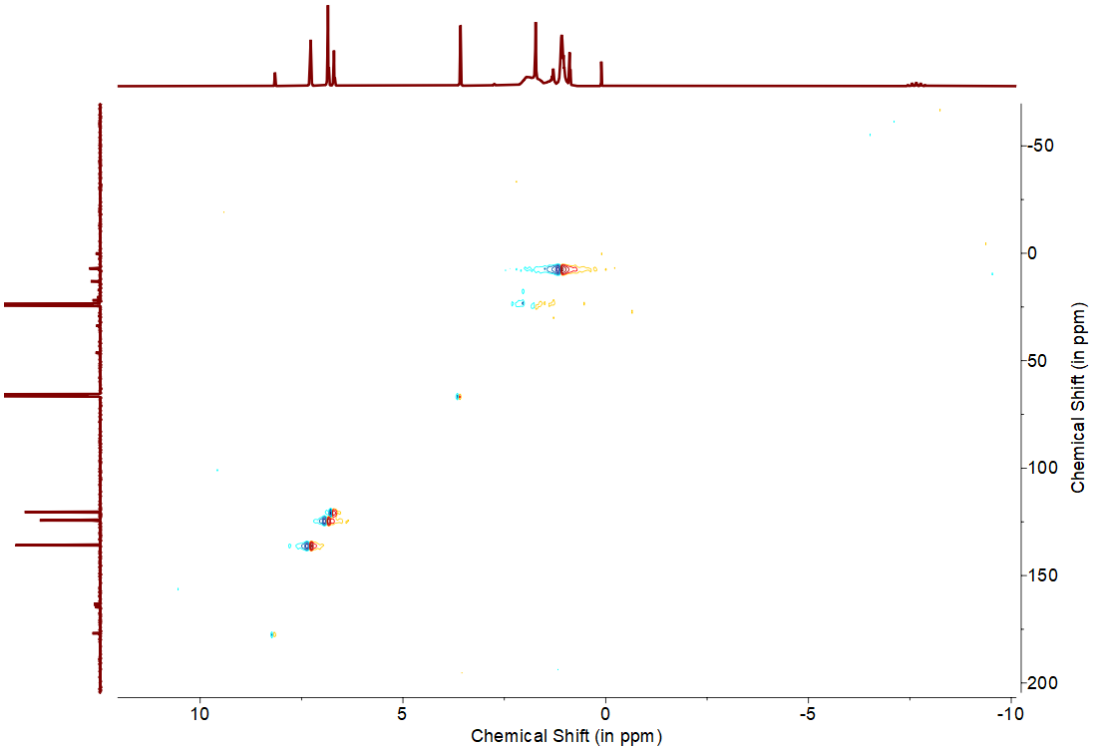
II.2.7. $^{31}P\{^{1}H\}_{sel\ (\delta = 1.5\ ppm)}$-NMR spectrum (162 MHz, THF-d8)



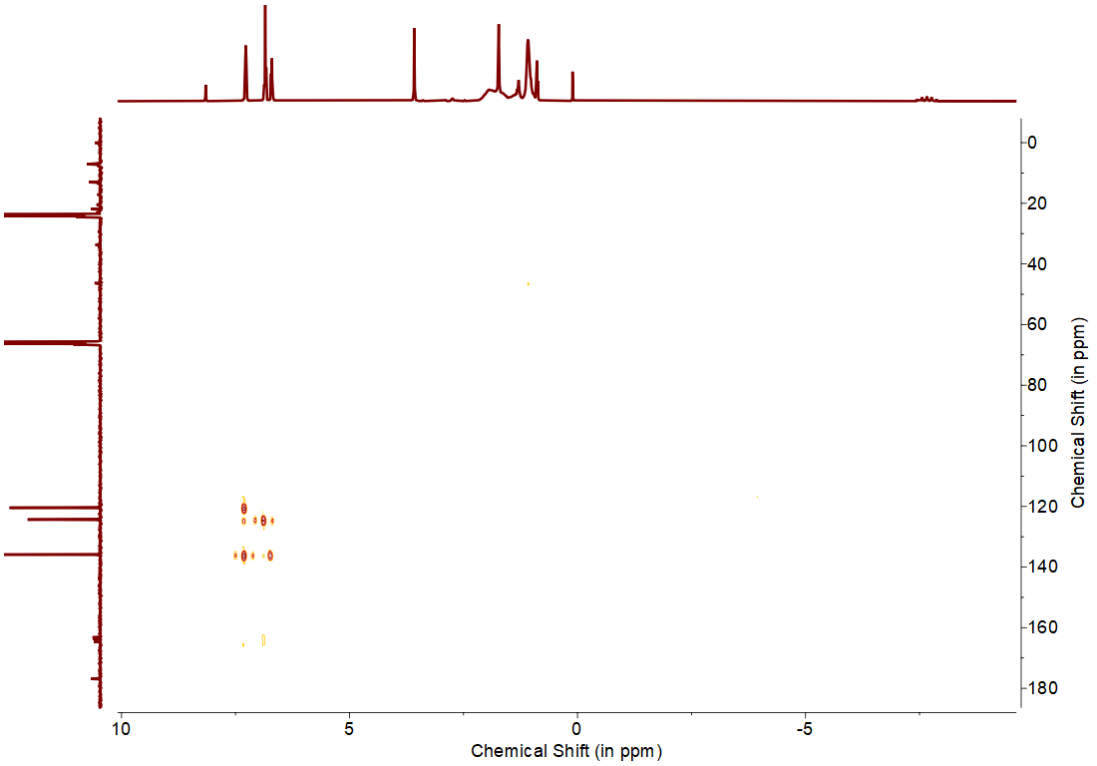
II.2.8. ^{1}H-^{1}H COSY NMR spectrum



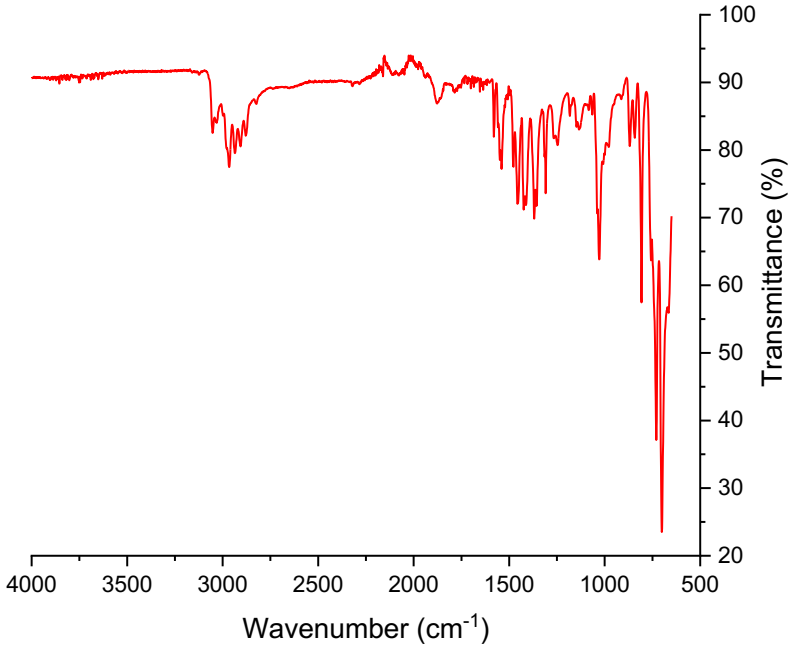
II.2.9. ^{13}C-^{1}H HSQC NMR spectrum



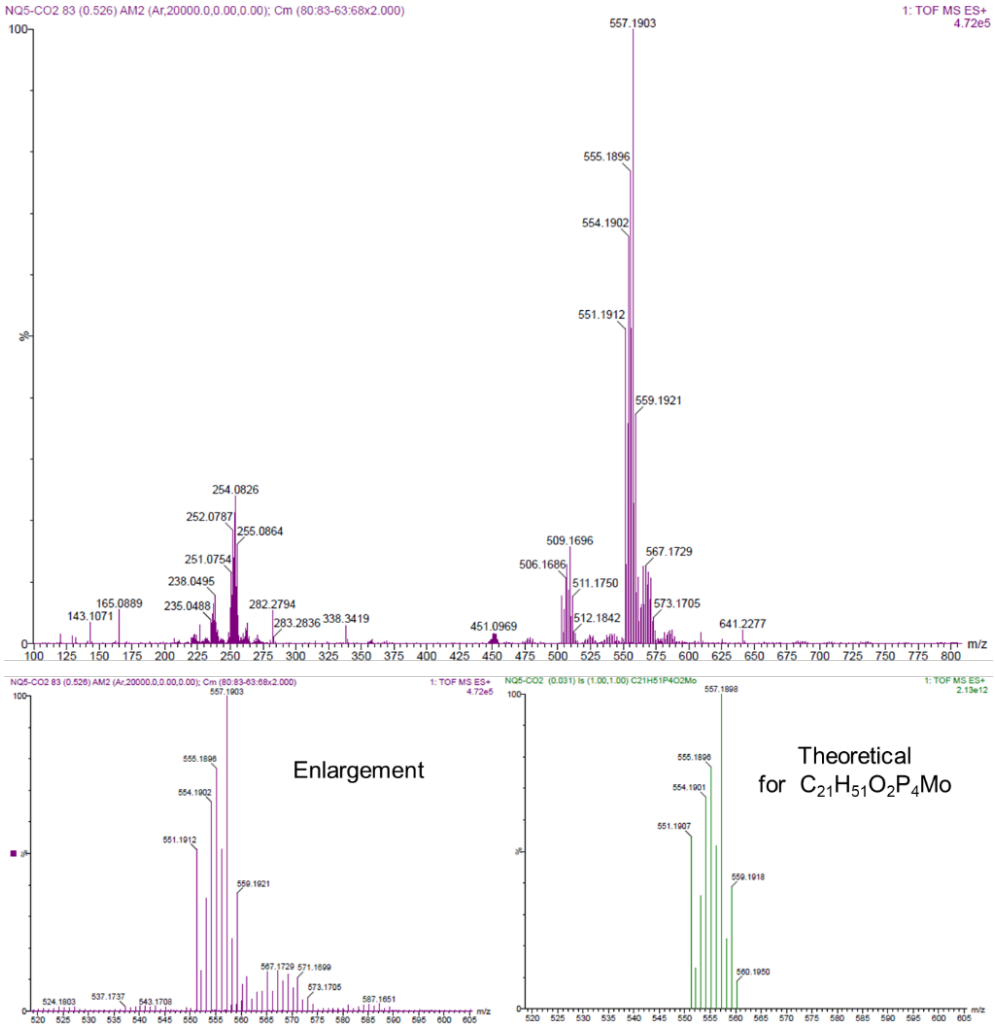
II.2.10. ^{13}C-^{1}H HMBC NMR spectrum



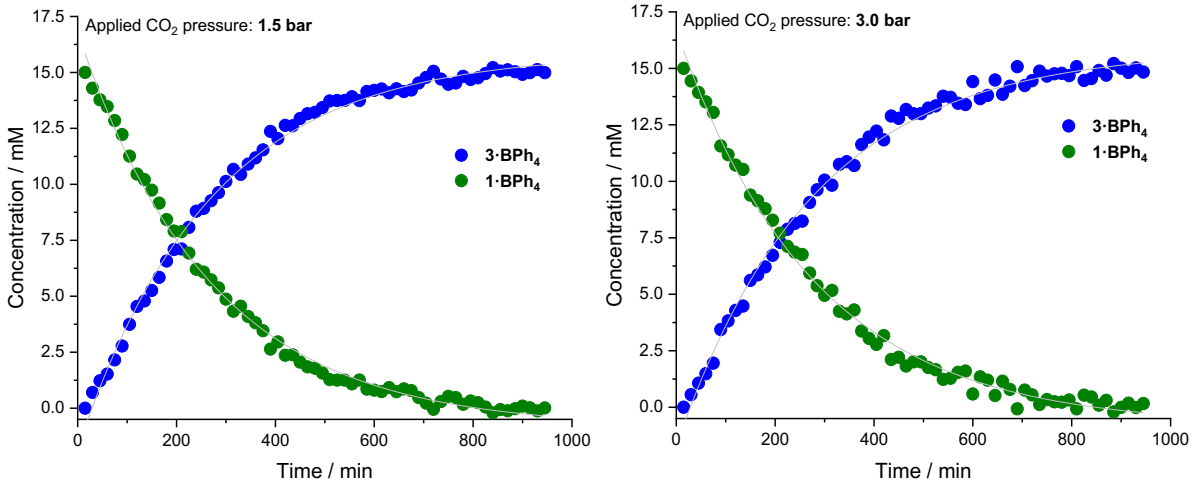
II.2.11. FT-IR spectrum (ATR)



II.2.12. ESI-HRMS spectrum



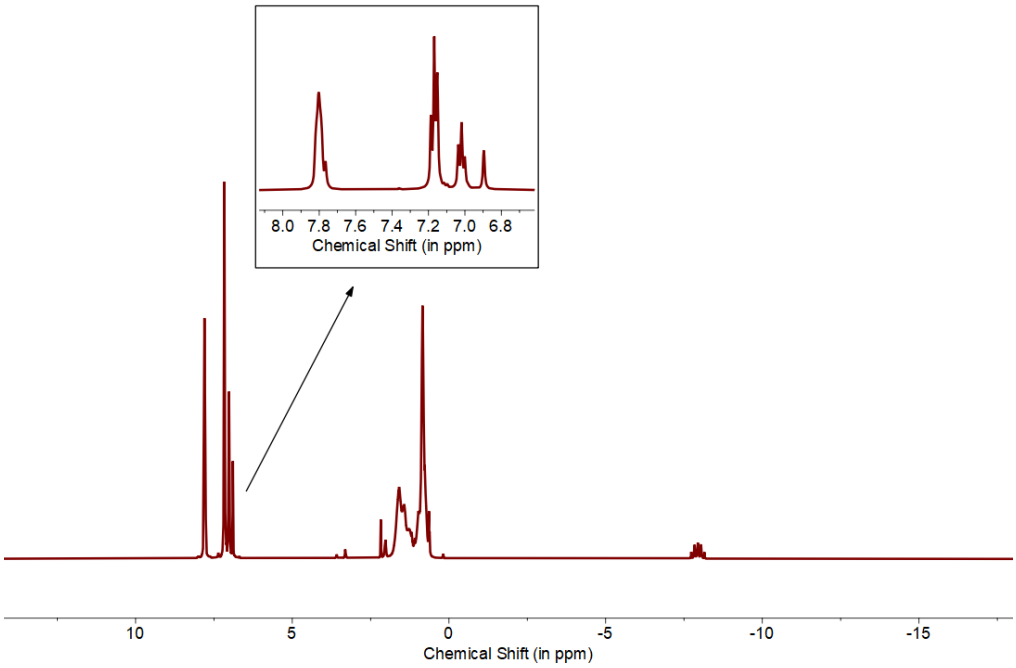
II.2.13. CO_2 pressure effect on reaction kinetics



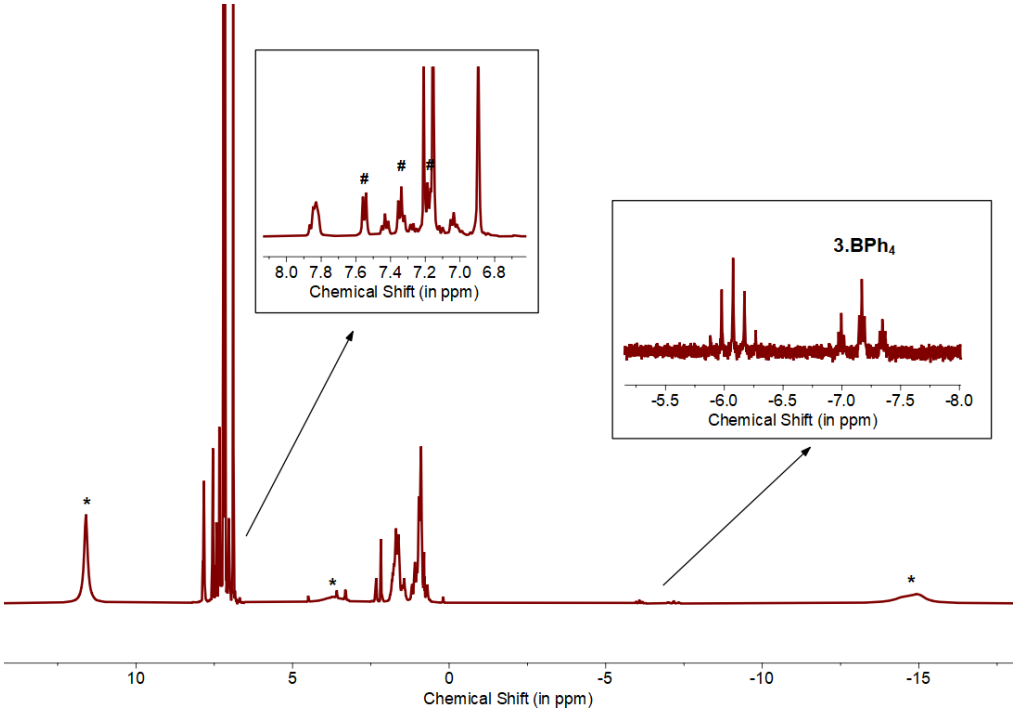
II.2.14. Thermal Stability in $C_6D_4Cl_2$ (100°C, CO_2) – case of the BPh_4^- counter-anion

Further reactivity with CO_2 was investigated at 100°C, in two different solvents (thf-d8 or $C_6D_4Cl_2$). In a typical experiment 30 µmol of **3.BPh$_4$** was dissolved in the desired solvent (ca. 700 µL). The tube was placed at 0°C, evacuated, pressurized with carbon dioxide (1 bar) and finally placed at 100°C. Evolution of the reaction medium was monitored by NMR spectroscopies.

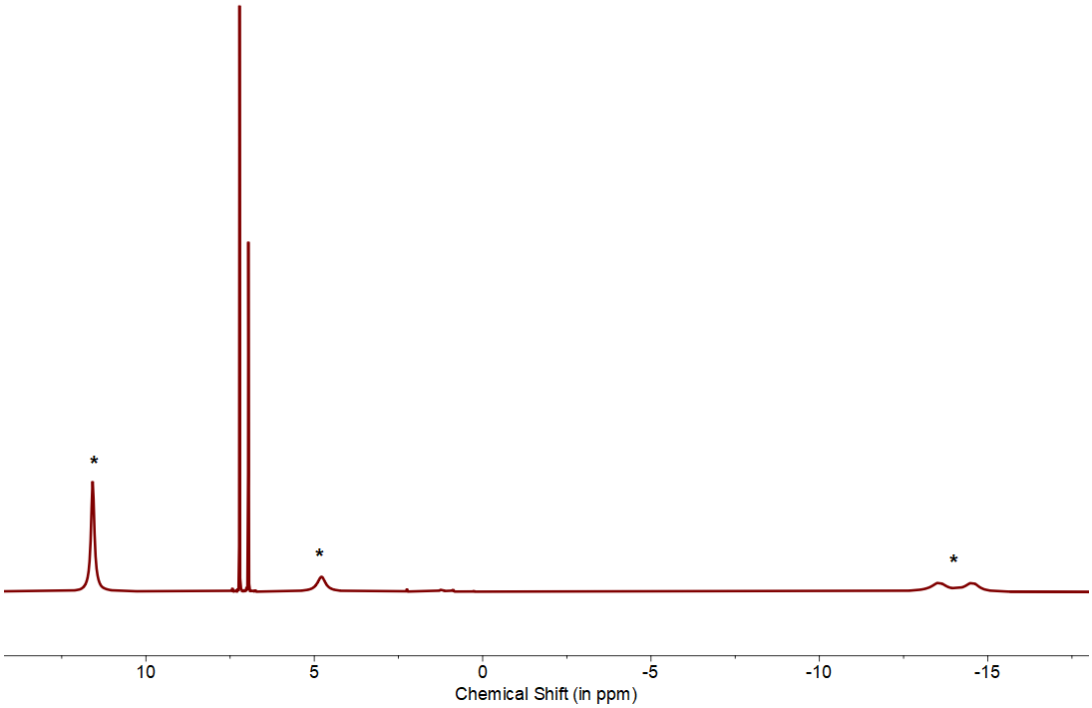
*(A) ^{1}H-NMR spectrum of a solution of **3.BPh$_4$** in $C_6D_4Cl_2$, before heating at 100°C for 24h.*



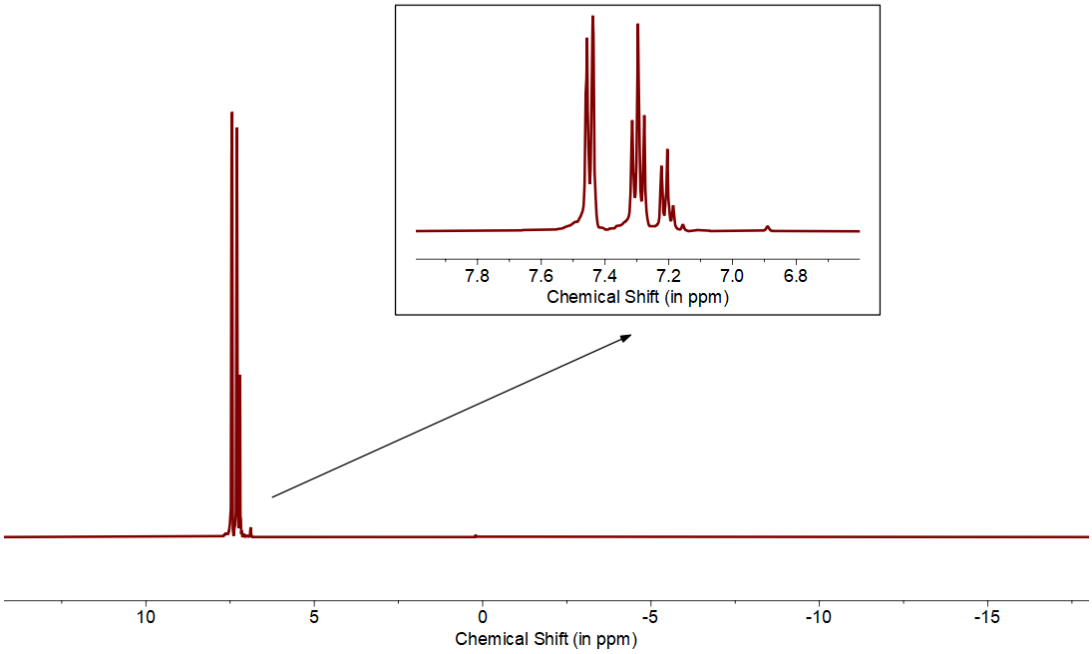
(B) ^{1}H-NMR spectrum of a solution of **3.BPh$_4$** in $C_6D_4Cl_2$, after heating at 100°C for 24h. * indicates the location of signals associated with paramagnetic species (see authentic sample ^{1}H-NMR spectrum on **II.2.12.C**). # indicates the location of paramagnetism-affected signals associated with biphenyl (see authentic sample ^{1}H-NMR spectrum on **II.2.12.D**). Insert boxes display the formation of the characteristic hydride signal of 4.**BPh$_4$** at -7.2 ppm and the formation of new aromatic signals assigned to oxidative degradation of BPh_4^- anion.



(C) ^{1}H-NMR spectrum of a solution of **[Mo(depe)$_2$Cl$_2$]** in $C_6D_4Cl_2$. This complex is paramagnetic and the large, poorly-resolved signals displayed properly match those of the paramagnetic products formed in the thermal decomposition of **3.BPh$_4$** under CO_2.

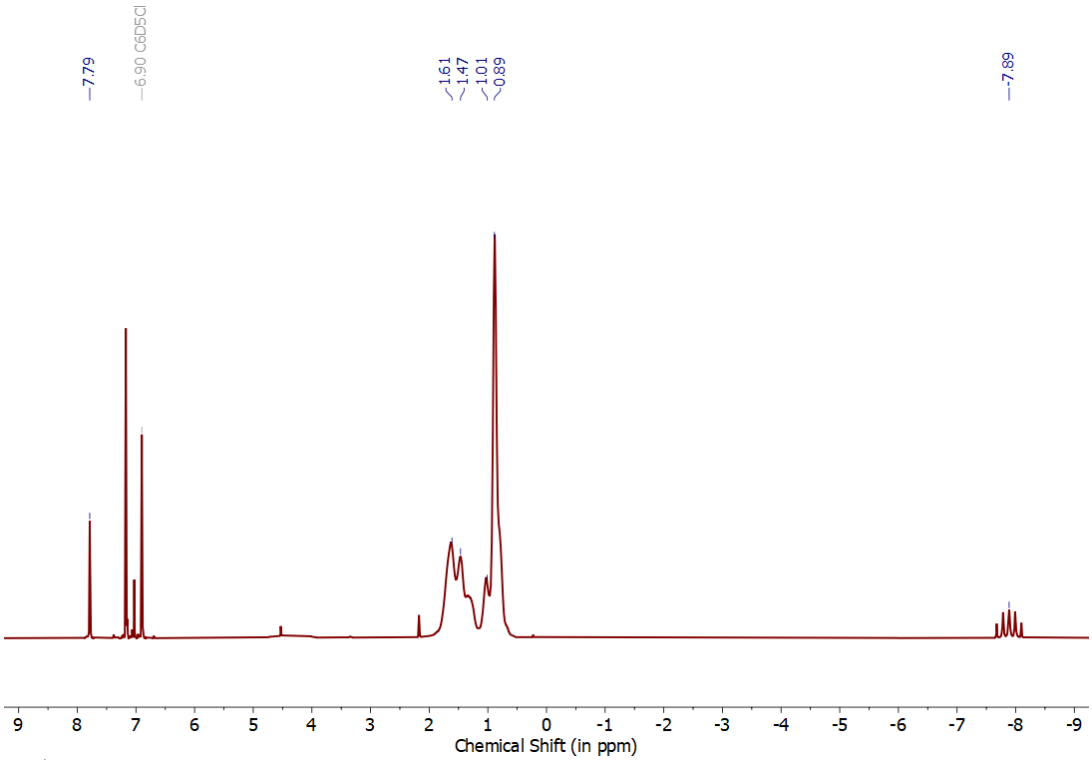


(D) ^{1}H-NMR spectrum of a solution of **[Mo(depe)$_2$Cl$_2$]** in $C_6D_4Cl_2$. This complex is paramagnetic and the large, poorly-resolved signals displayed properly match those of the paramagnetic products formed in the thermal decomposition of **3.BPh$_4$** under CO_2.

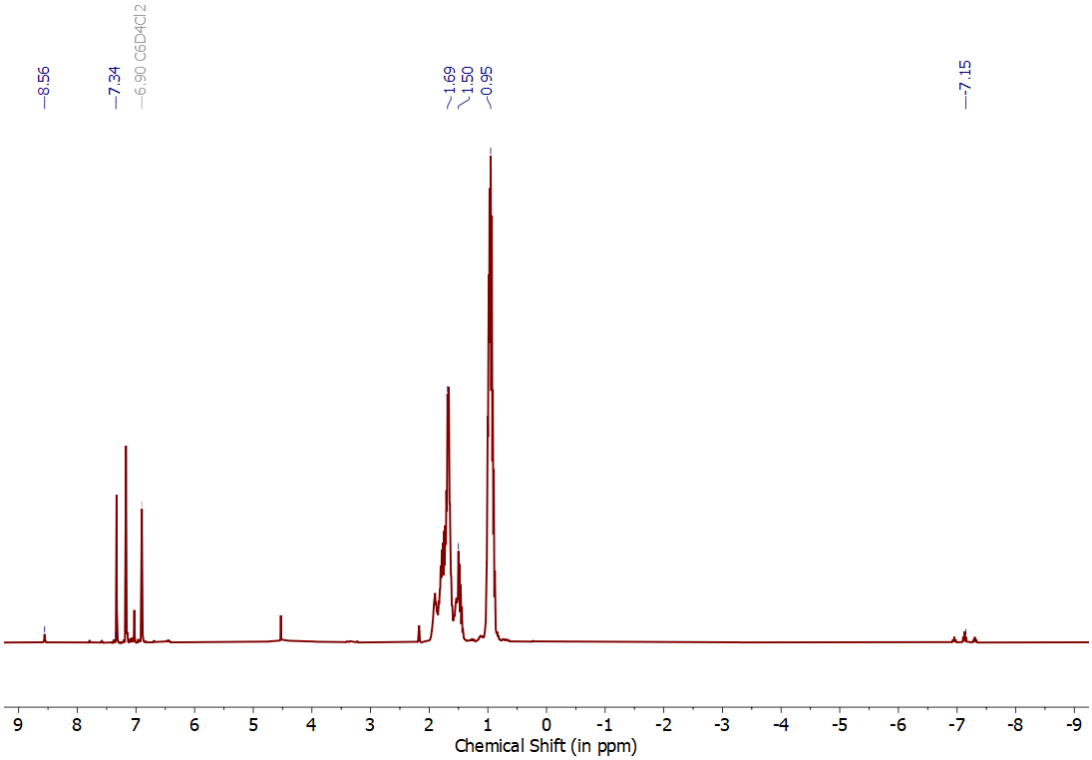


II.2.15. Thermal Stability in $C_6D_4Cl_2$ (100°C, CO_2) – case of the $HB(C_6F_5)_3^-$ counter-anion

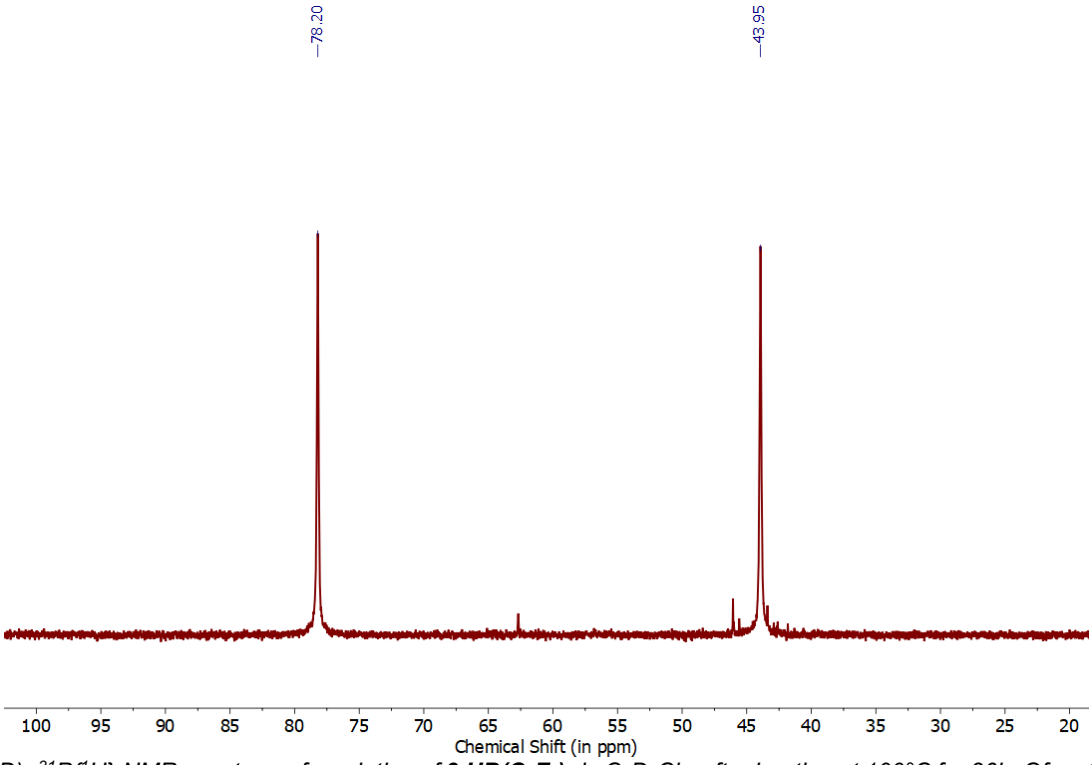
*(A) ^{1}H-NMR spectrum of a solution of **3.HB(C_6F_5)$_3$** in $C_6D_4Cl_2$, before heating at 100°C for 36h.*



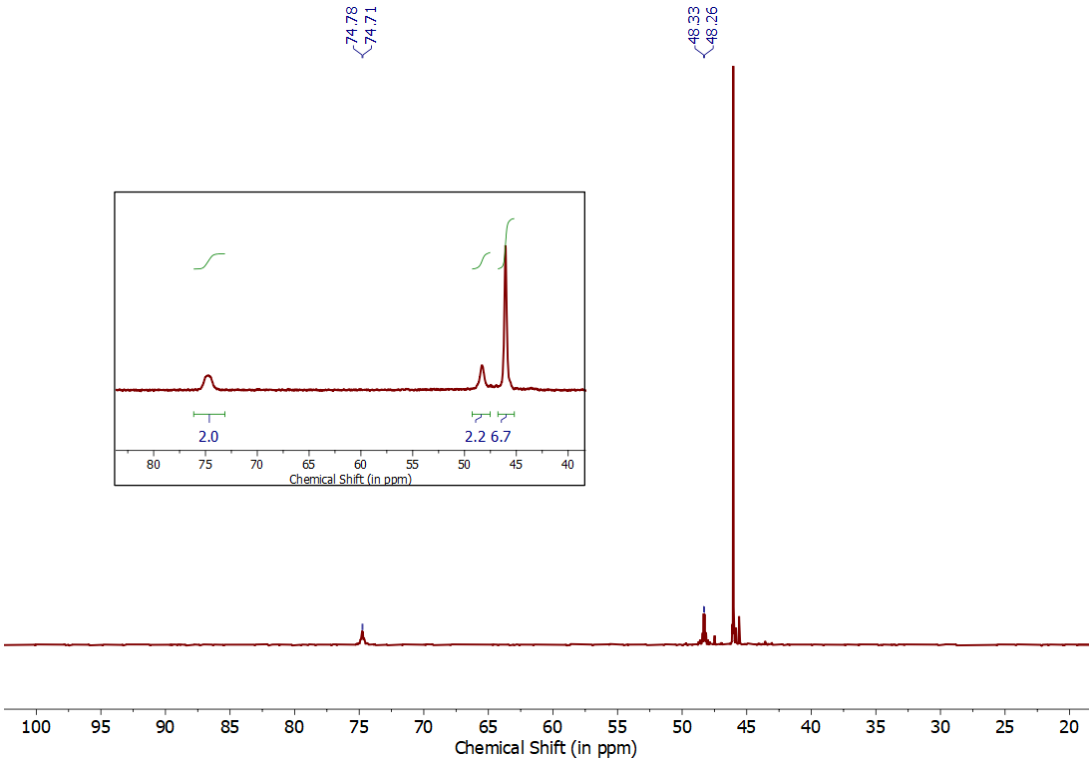
*(B) ^{1}H-NMR spectrum of a solution of **3.HB(C_6F_5)$_3$** in $C_6D_4Cl_2$, after heating at 100°C for 36h. Of particular interest are the free formate anion signal at 8.56 ppm, the new formate-containing species at 7.34 ppm and the characteristic hydride signal of **4.HB(C_6F_5)$_3$** at -7.2 ppm*



*(C) ^{31}P-NMR spectrum of a solution of **3.HB(C_6F_5)$_3$** in $C_6D_4Cl_2$, before heating at 100°C for 36h.*

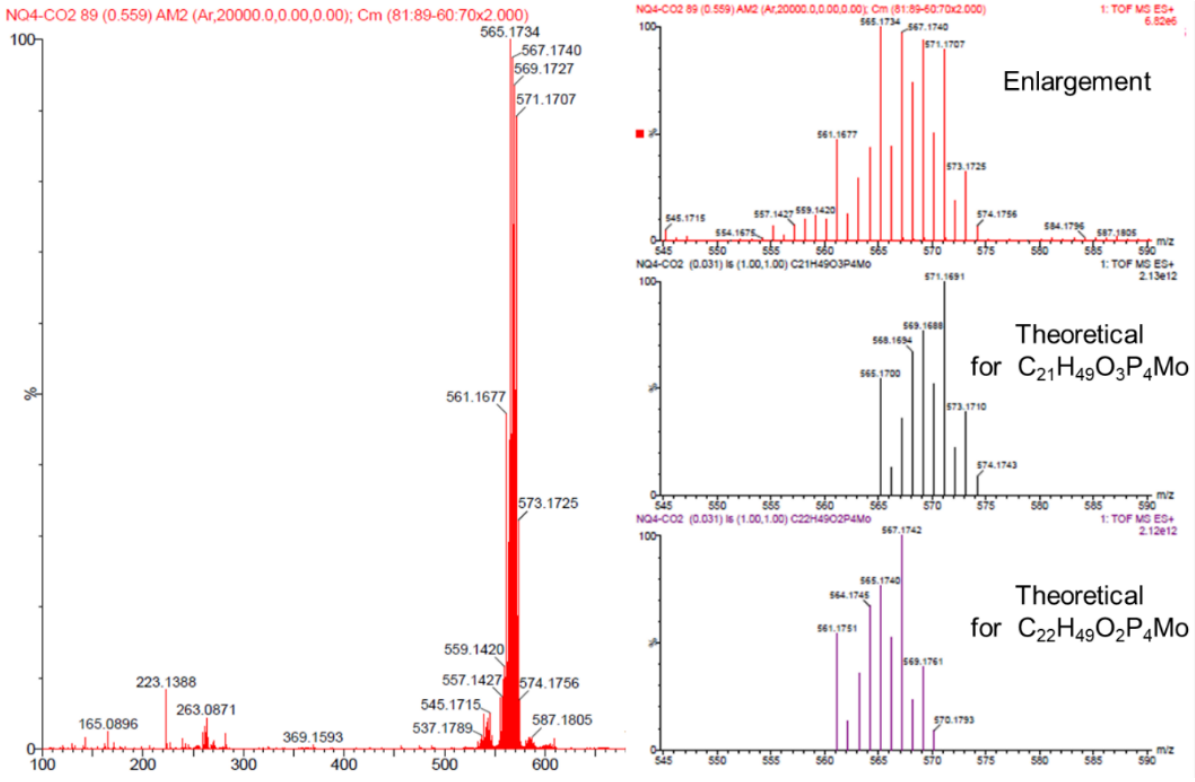


*(D) $^{31}P\{^1H\}$-NMR spectrum of a solution of **3.HB(C_6F_5)$_3$** in $C_6D_4Cl_2$, after heating at 100°C for 36h. Of particular interest are the diagnostic signal of **4.HB(C_6F_5)$_3$** at 74.8 and 48.3 ppm. To better assess the relative proportion of **4.HB(C_6F_5)$_3$** and **5.HB(C_6F_5)$_3$** by the end of the reaction, undecoupled ^{31}P integrations were used (insert).*



II.2.16. HRMS analysis of the thermal decomposition of 3.HB(C_6F_5)$_3$

ESI-HRMS analysis of the thermal decomposition of ***3.HB(C_6F_5)$_3$***: experimental spectrum and enlargement of the main feature (red traces), theoretical isotopic pattern calculated for **5$^+$**, [MoO(depe)$_2$(HCOO)]$^+$ (black traces) and theoretical isotopic pattern calculated for **4$^+$**, [Mo(CO)$_2$(depe)$_2$H]$^+$ (purple traces)



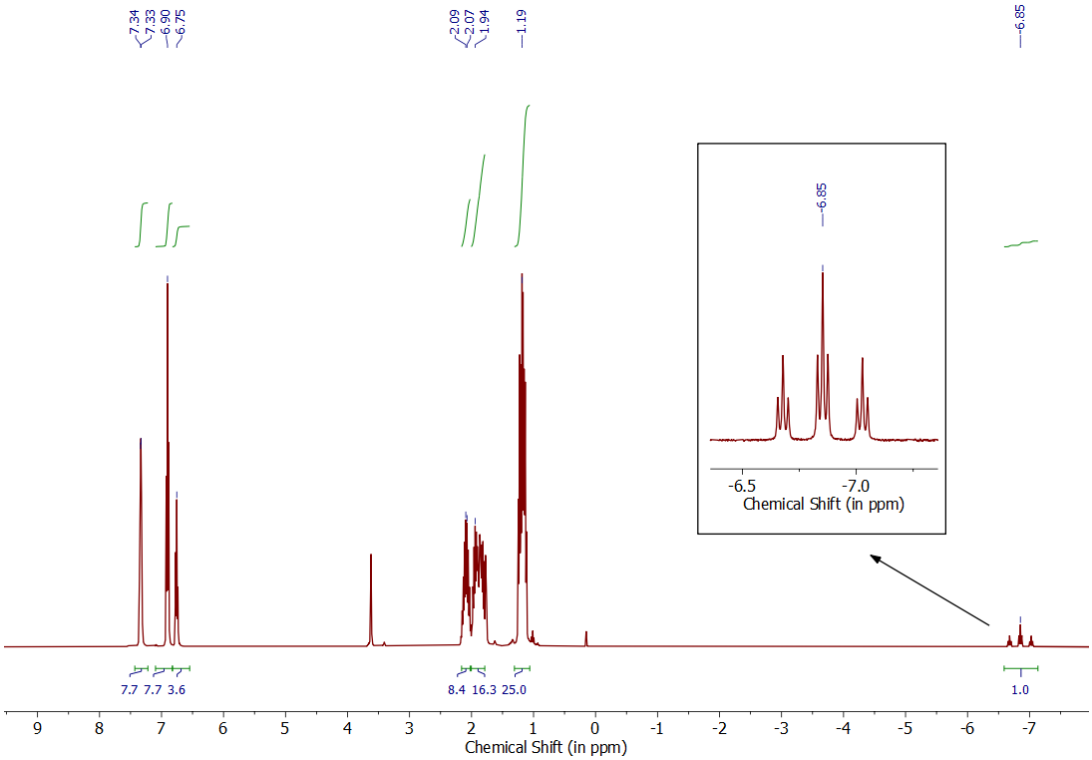
II.3. $[Mo(depe)_2(CO)_2H][B(C_6H_5)_4]$ ($4.BPh_4$)

II.3.1. Experimental procedure

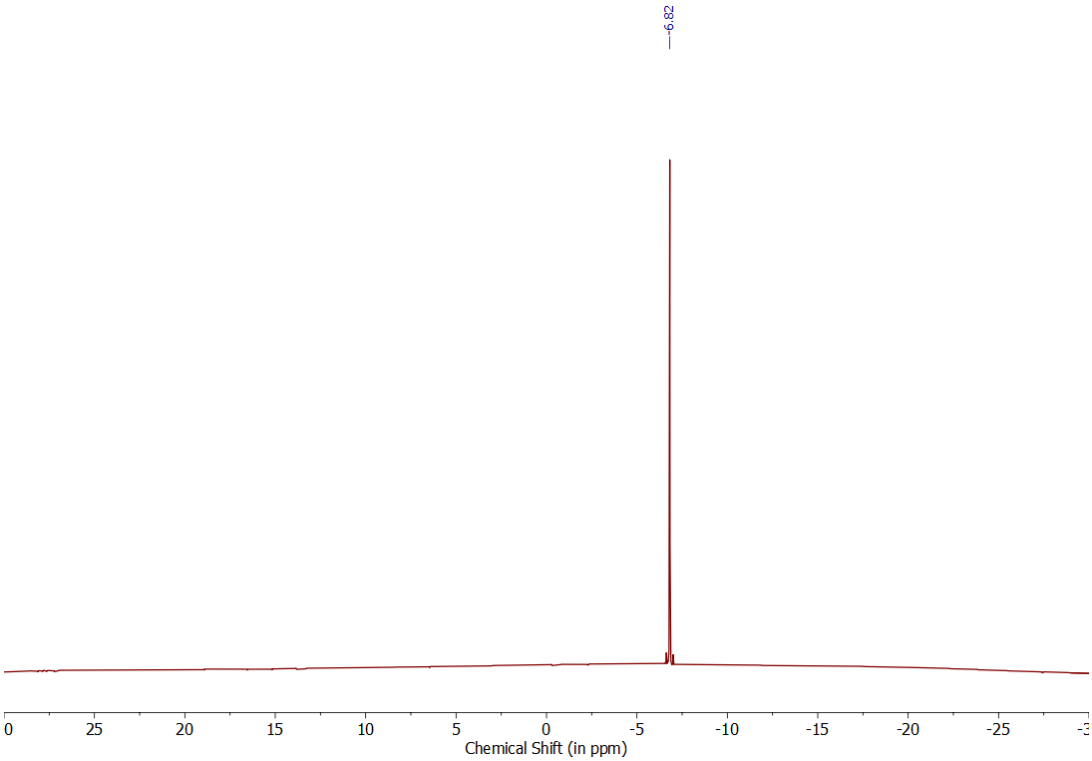
In an Wilmad pressure NMR tube, $[Mo(depe)_2H_5][B(C_6H_5)_4]$ (20.0 mg, 24.0 µmol, 1.00 equiv.) was dissolved in THF (1 mL). The tube was placed at 0°C, evacuated and finally pressurized with carbon monoxide (3 bar). The reaction mixture was left at room temperature for 24h. After pressure was carefully released, the pale-yellow solution was poured in cold pentane (ca. 5 mL), triggering immediate precipitation of an off-white solid. The solution was decanted off and the solid washed twice with cold pentane (2 x 5 mL). The solid was then dried under high vacuum at room temperature to yield the desired compound (15.9 mg, 75%). Single crystals suitable for X-ray diffraction were obtained by storing at -40°C a concentrated THF solution of the complex layered by pentane over a few days.

^{1}H-NMR (400 MHz, THF-d_8) δ 7.33 (br. m, 8H, *meta*-C_6H_5), 6.90 (t, $^{3}J_{(H-H)}$ = 7.3 Hz, 8H, *ortho*-C_6H_5), 6.75 (t, $^{3}J_{(H-H)}$ = 7.3 Hz, 4H, *para*-C_6H_5), 2.10 (m, 8H, -CH_2- CH_2-), 2.02 – 1.79 (m, 16H, -CH_2- CH_3), 1.18 (m, 24H, -CH_2- CH_3), -6.85 (tt, $^{2}J_{(P-H)}$ = 69.8, 9.1 Hz, 1H, Mo-*H*).
^{11}B-NMR (128 MHz, THF-d_8) δ -6.8.
^{13}C{^{1}H}-NMR (101 MHz, THF-d_8) δ 209.8 (s; Mo-*C*O), 163.9 (q, $^{2}J_{(B-C)}$ = 50.3 Hz, *ipso*-C_6H_5), 135.9 (br. s, *meta*-C_6H_5), 124.4 (m, *ortho*-C_6H_5), 120.5 (s, *para*-C_6H_5), 23.3 (m, -CH_2-), 21.6 (m, -CH_2-), 7.5 (br. s, -CH_3), 7.3 (br. s, -CH_3).
^{31}P{^{1}H}-NMR (162 MHz, THF-d_8) δ 74.9 (m), 48.3 (m). **^{31}P{^{1}H}$_{sel}$-NMR** (162 MHz, THF-d_8) δ 74.9 (d,$^{2}J_{(P-H)}$ = 68.9 Hz), 48.3 (br. s).

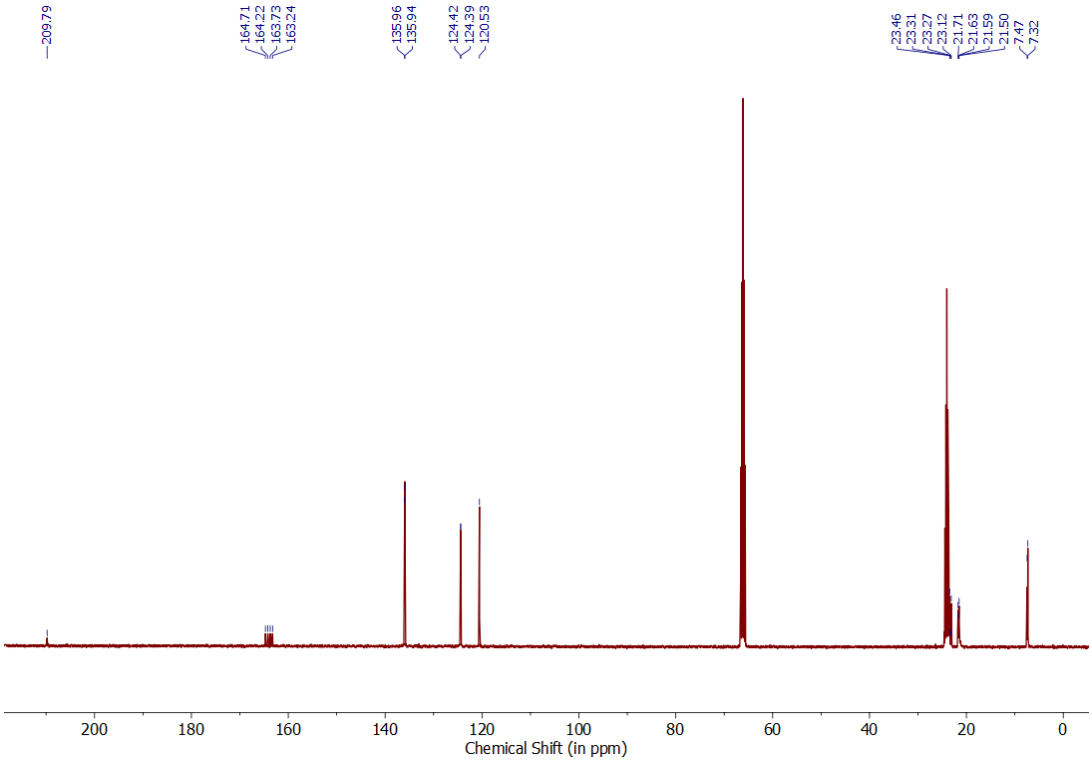
II.3.2. ^{1}H-NMR spectrum (400 MHz, THF-d8)



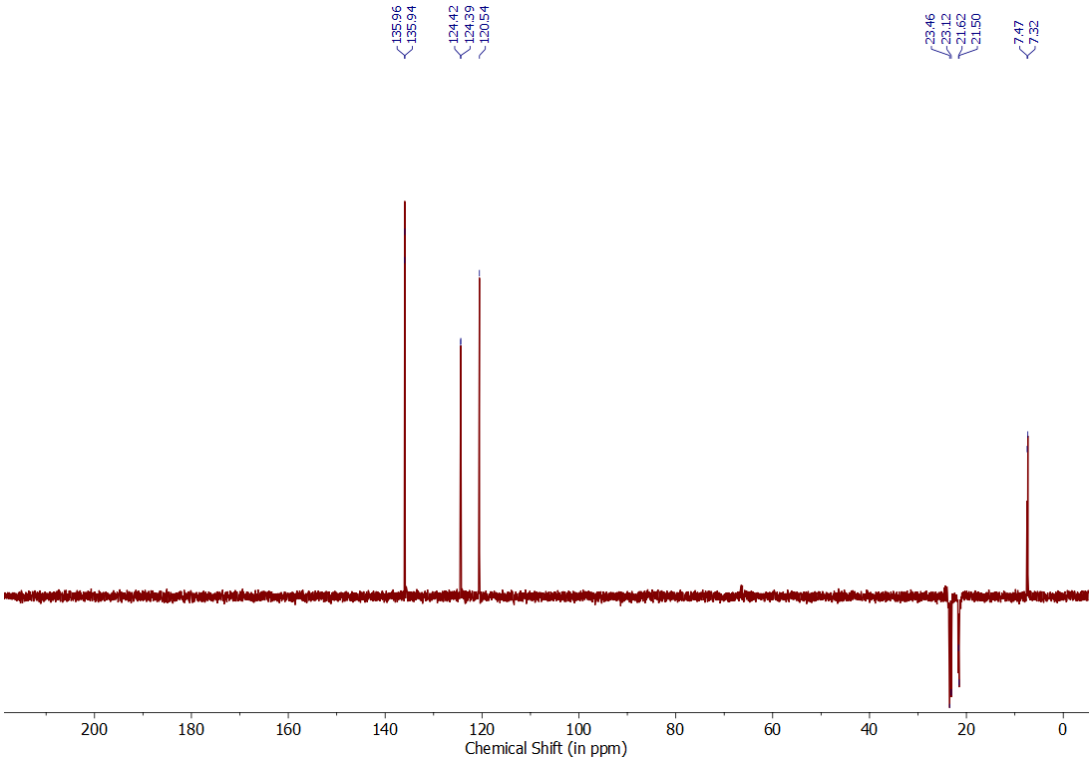
II.3.3. $^{11}B\{^1H\}$-NMR spectrum (128 MHz, THF-d_8)



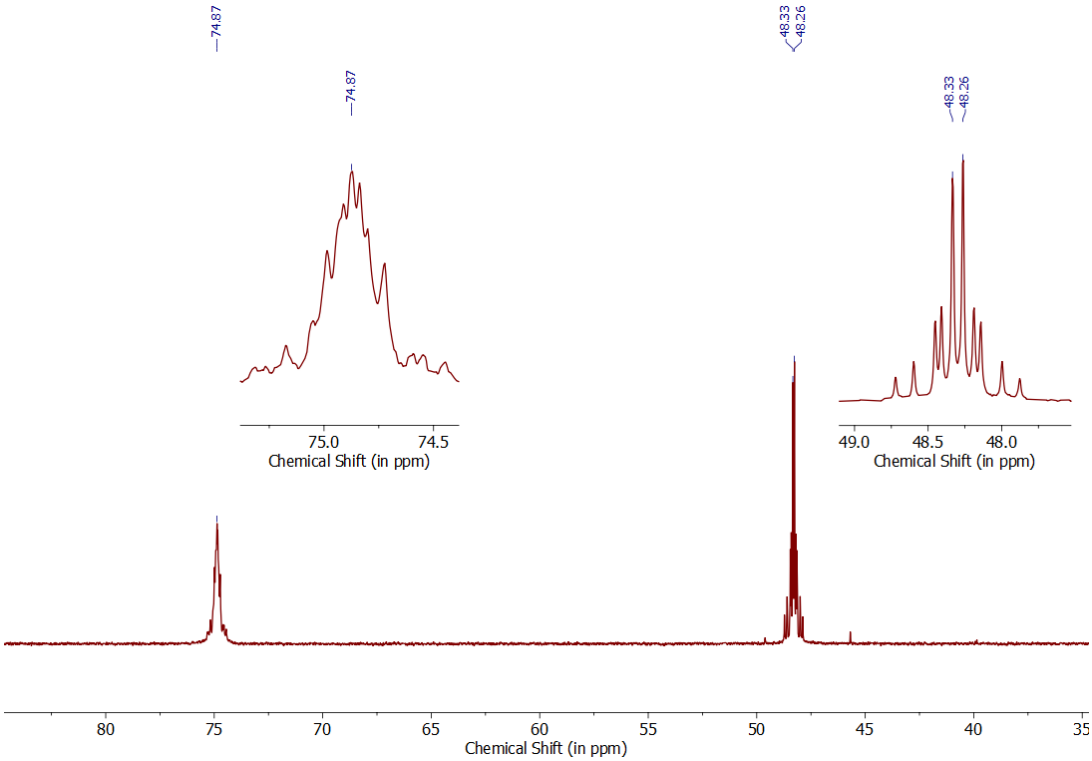
II.3.4. $^{13}C\{^1H\}$-NMR spectrum (101 MHz, THF-d_8)



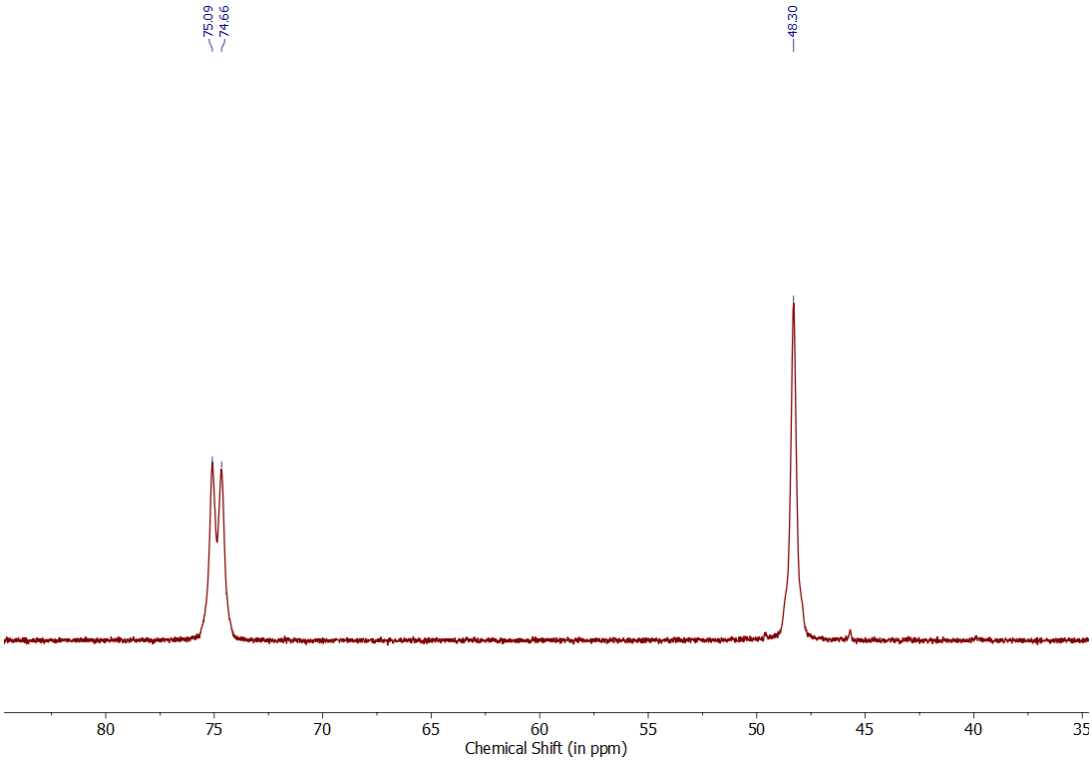
II.3.5. ^{13}C-DEPT NMR spectrum (101 MHz, THF-d_8)



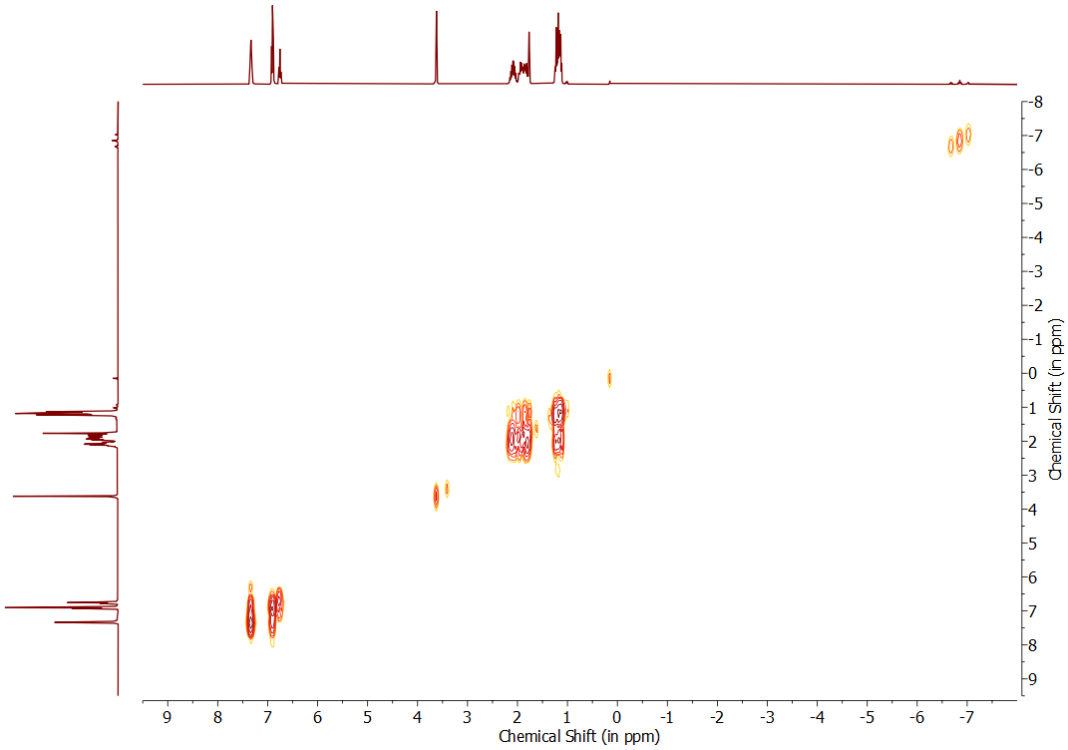
II.3.6. ^{31}P{^{1}H}-NMR spectrum (162 MHz, THF-d_8)



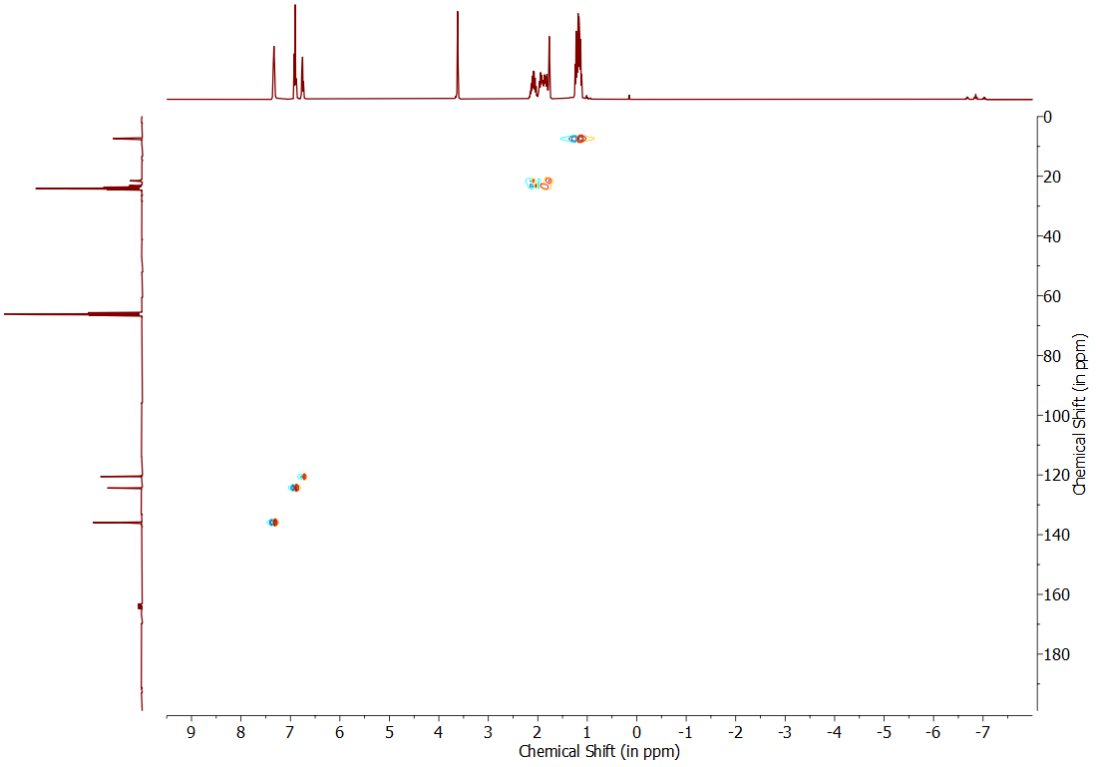
II.3.7. $^{31}P\{^{1}H\}_{sel\ (\delta = 1.5\ ppm)}$-NMR spectrum (162 MHz, THF-d_8)



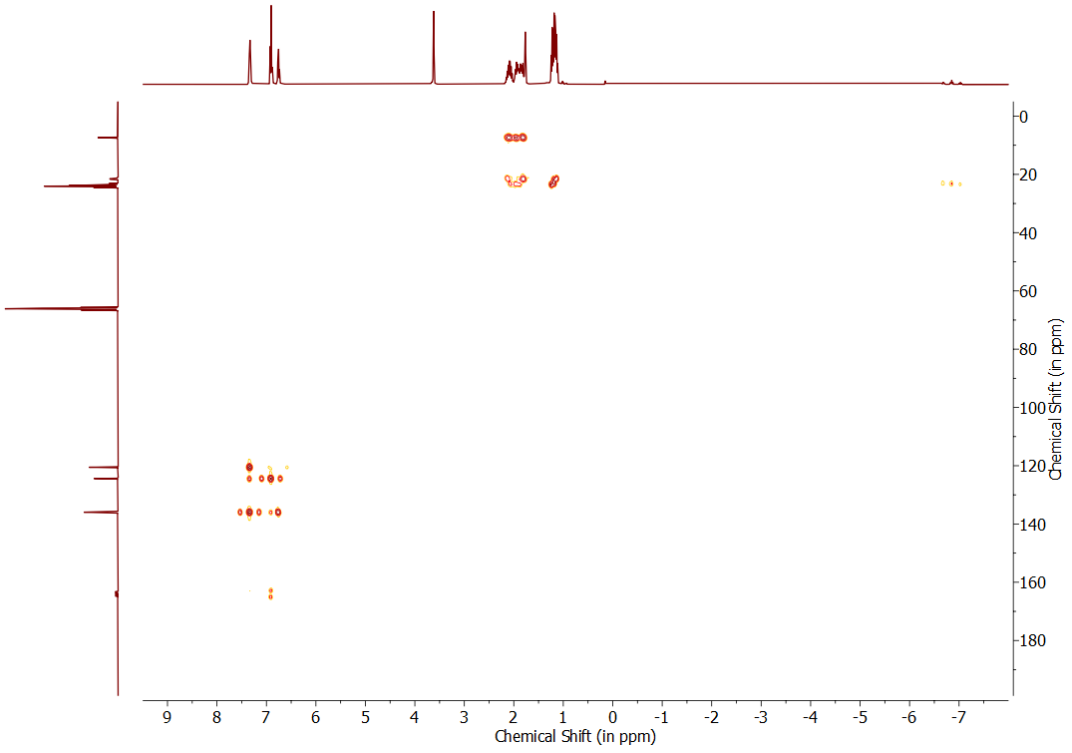
II.3.8. ^{1}H-^{1}H COSY NMR spectrum



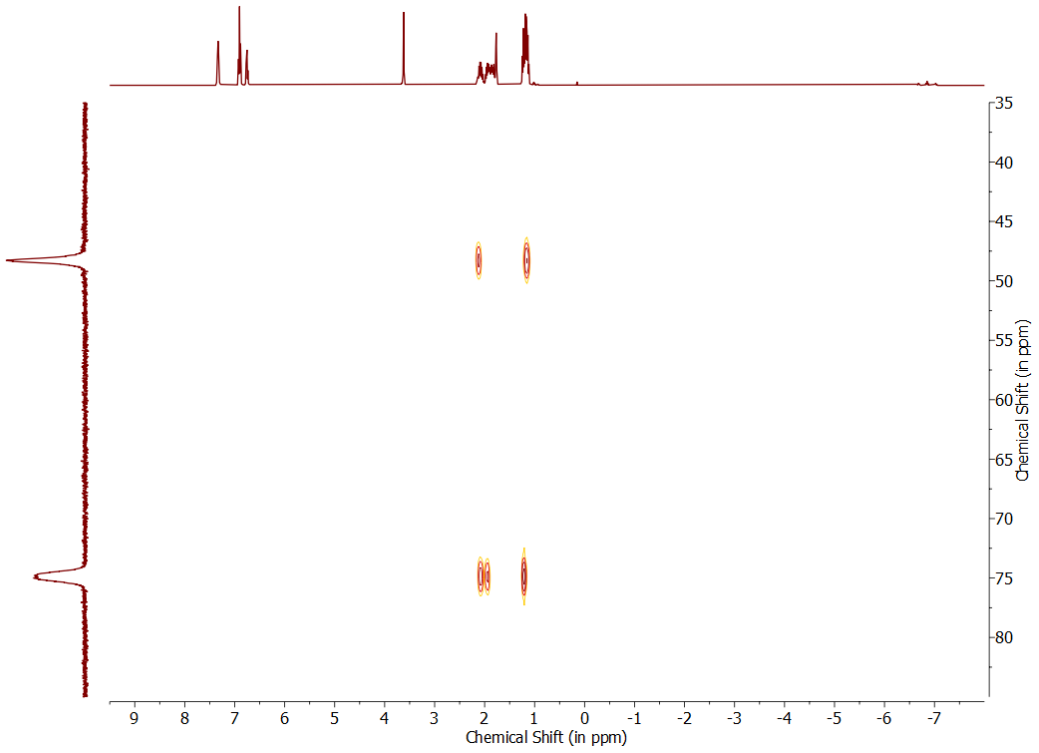
II.3.9. ^{13}C-^{1}H HSQC NMR spectrum



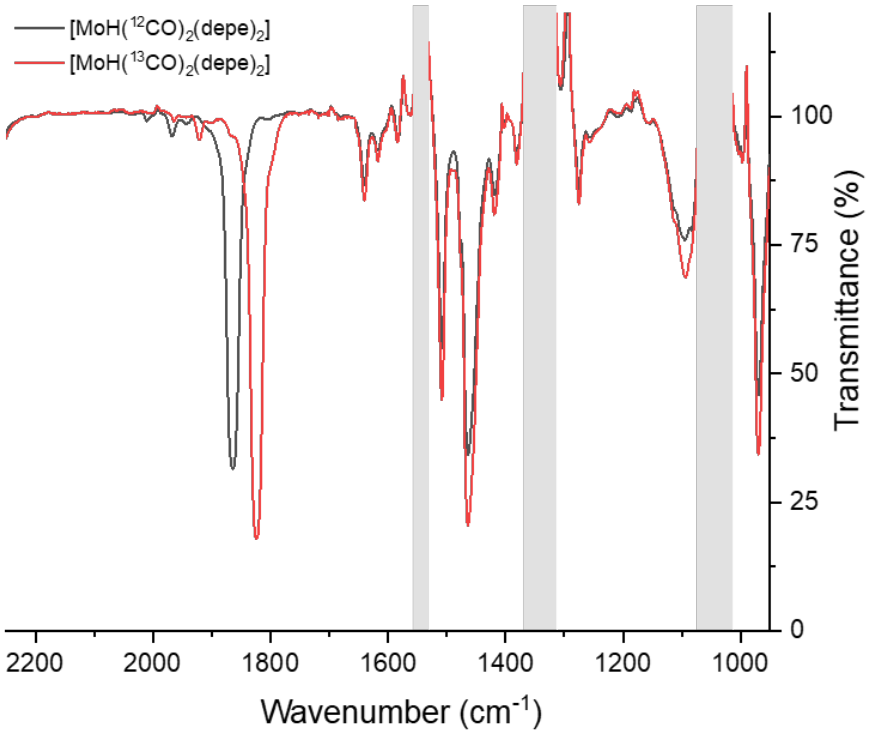
II.3.10. ^{13}C-^{1}H HMBC NMR spectrum



II.3.11. ^{31}P-^{1}H HMQC NMR spectrum

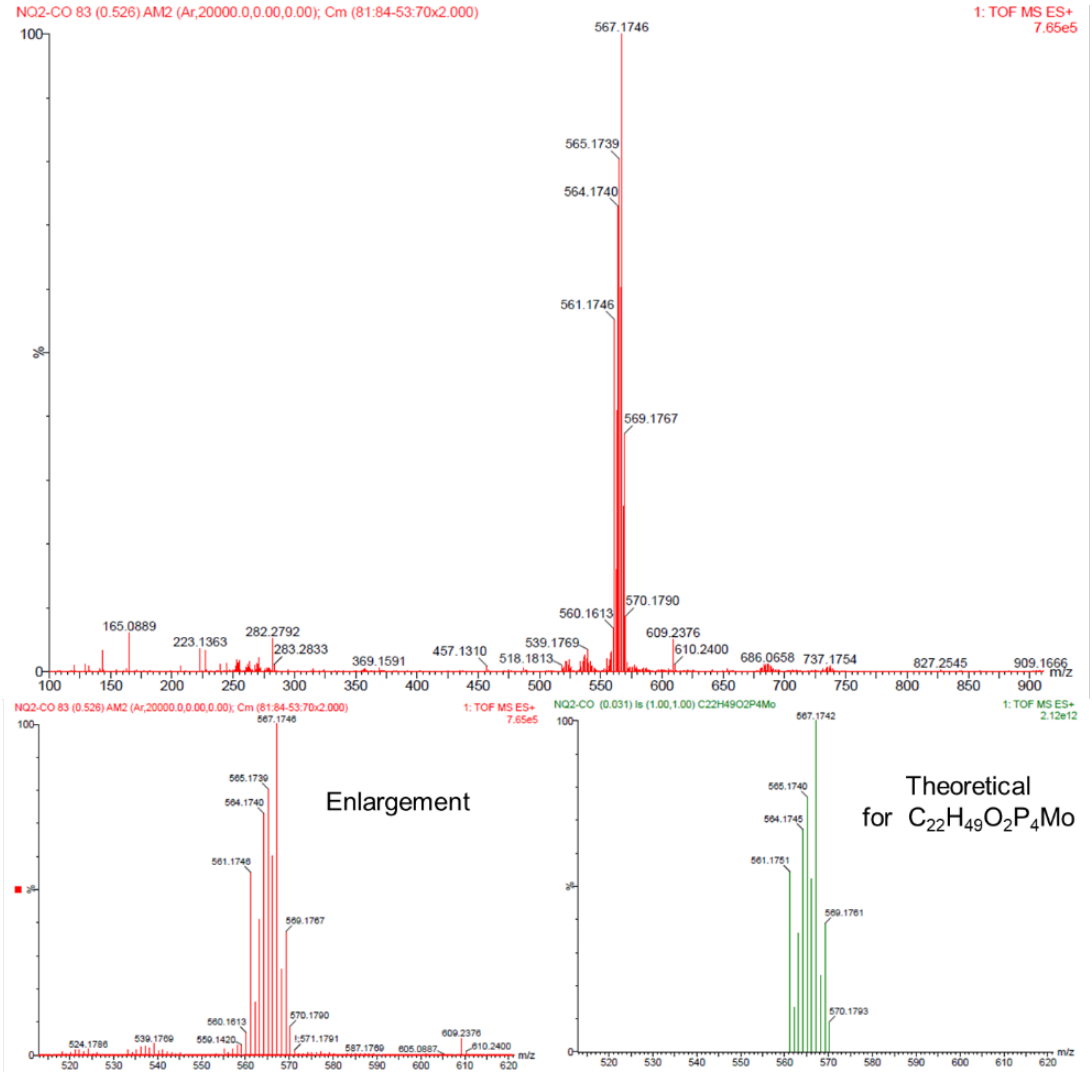


II.3.12. FT-IR spectrum (^{13}CO vs ^{12}CO) – liquid phase



Gray boxes correspond to solvent strong absorption area.

II.3.13. ESI-HRMS spectrum



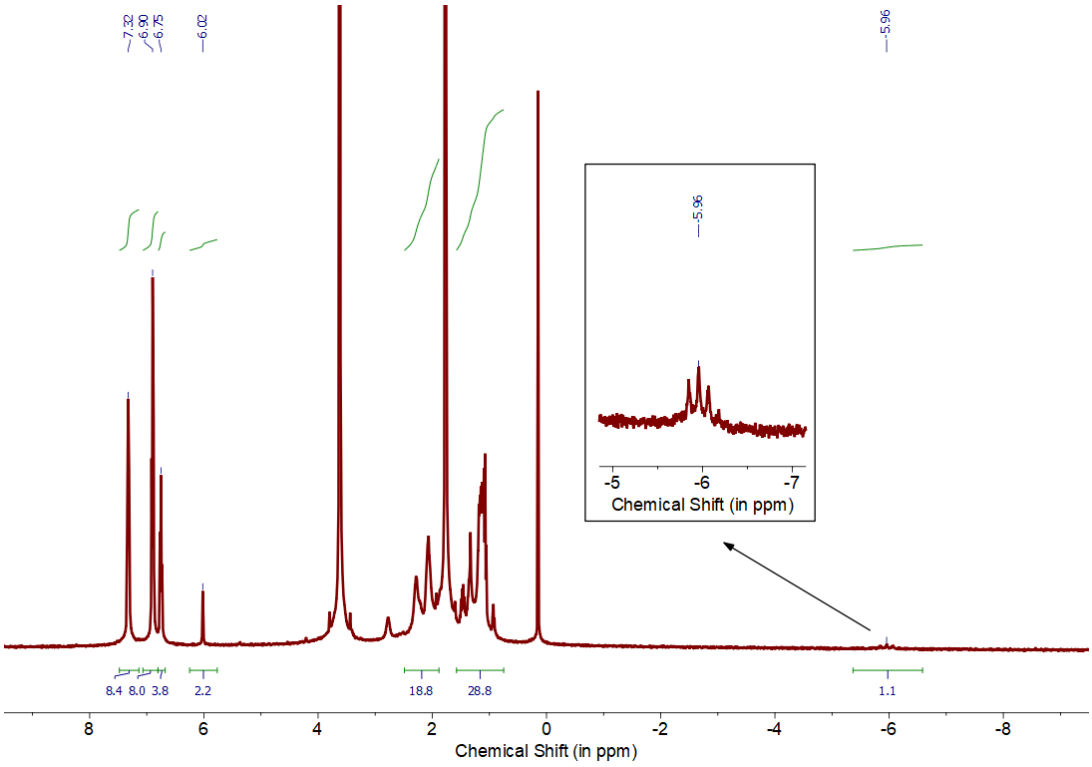
II.4. [Mo(depe)$_2$(CH_2S_2)H] (6.BPh_4)

II.4.1. Experimental procedure

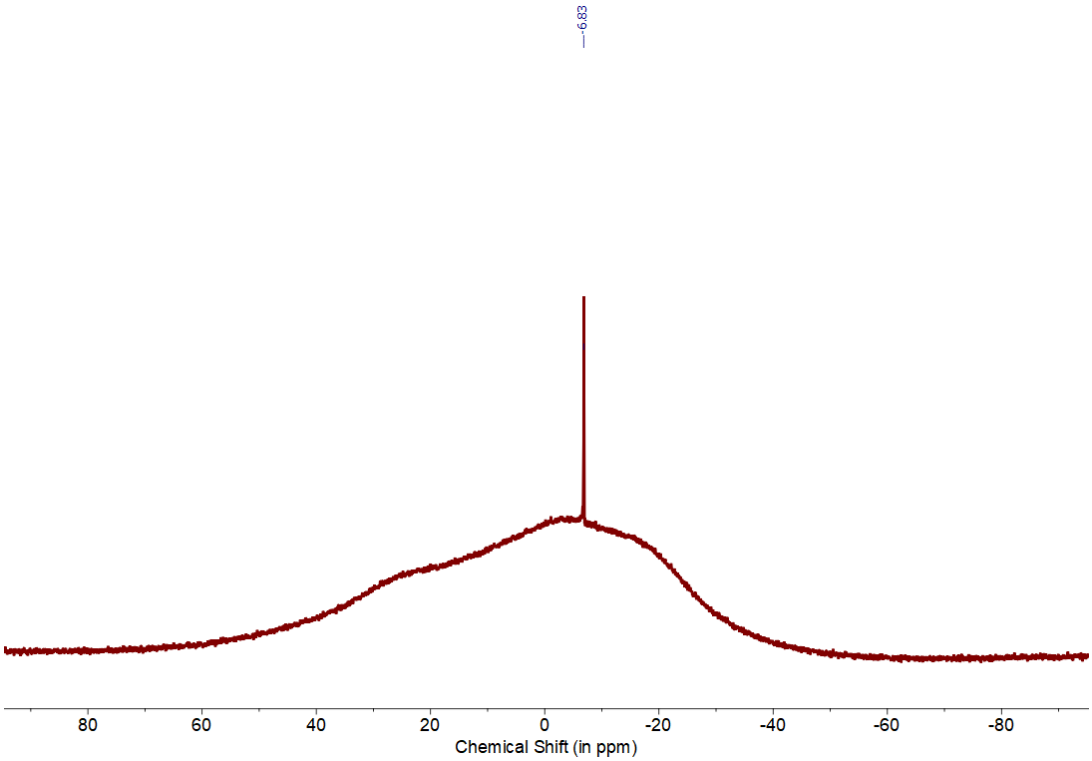
In a Fisher-Porter flask, [Mo(depe)$_2H_4$] (20.0 mg, 39.0 µmol, 1.00 equiv.) was dissolved in THF (1 mL). A solution of [$HNEt_3$][$B(C_6H_5)_4$] (16.4 mg, 39.0 µmol, 1.00 equiv.) and CS_2 (3.0 mg, 39.0 µmol, 1.00 equiv.) in THF (1 mL) was added. The solution immediately turns brown. The reaction mixture was left at room temperature for 24h, under continuous stirring. Pentane (ca. 5 mL) was added to the solution, triggering immediate precipitation of a brown solid. The solution was decanted off and the resulting solid was washed twice with cold pentane (2 x 5 mL). The brown powder was then dried under high vacuum at room temperature to yield the title compound with a purity of *ca.* 92%, based on ^{31}P-NMR spectroscopy (27.5 mg, 78%).

^{1}H-NMR (400 MHz, THF-d_8) δ 7.28 (br. m, 8H, *meta*-C_6H_5), 6.86 (t, $^3J_{(H-H)}$ = 7.3 Hz, 8H, *ortho*-C_6H_5), 6.71 (t, $^3J_{(H-H)}$ = 7.3 Hz, 4H, *para*-C_6H_5), 5.98 (s, 2H, -CH_2S_2-), 2.35-1.85 (m, 18H), 1.50 – 0.79 (m, 30H), -5.99 (quintet, $^2J_{(P-H)}$ = 43.1 Hz, 1H, Mo-*H*).
^{11}B-NMR (128 MHz, THF-d_8) δ -6.8.
^{13}C{^{1}H}-NMR (101 MHz, THF-d_8) δ 163.9 (q, $^2J_{(B-C)}$ = 50.3 Hz, *ipso*-C_6H_5), 135.9 (br. s, *meta*-C_6H_5), 124.4 (m, *ortho*-C_6H_5), 120.5 (s, *para*-C_6H_5), 61.5 (s, -S-CH_2-S-), 21.1 (m, -CH_2-), 8.6 (s, -CH_3), 7.9 (s, -CH_3).
^{31}P{^{1}H}-NMR (162 MHz, THF-d_8) δ 69.0 (s). **^{31}P{^{1}H}$_{sel}$-NMR** (162 MHz, THF-d_8) δ 69.0 (d,$^2J_{(P-H)}$ = 43.1 Hz).

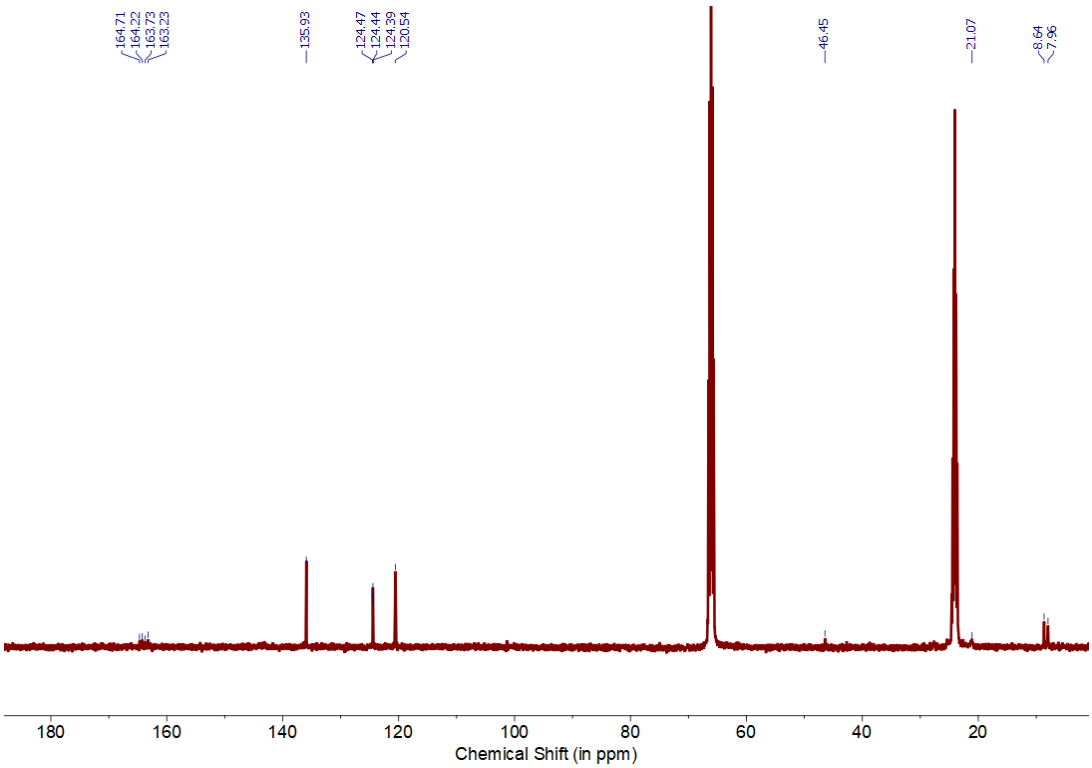
II.4.2. ^{1}H-NMR spectrum (400 MHz, THF-d8)



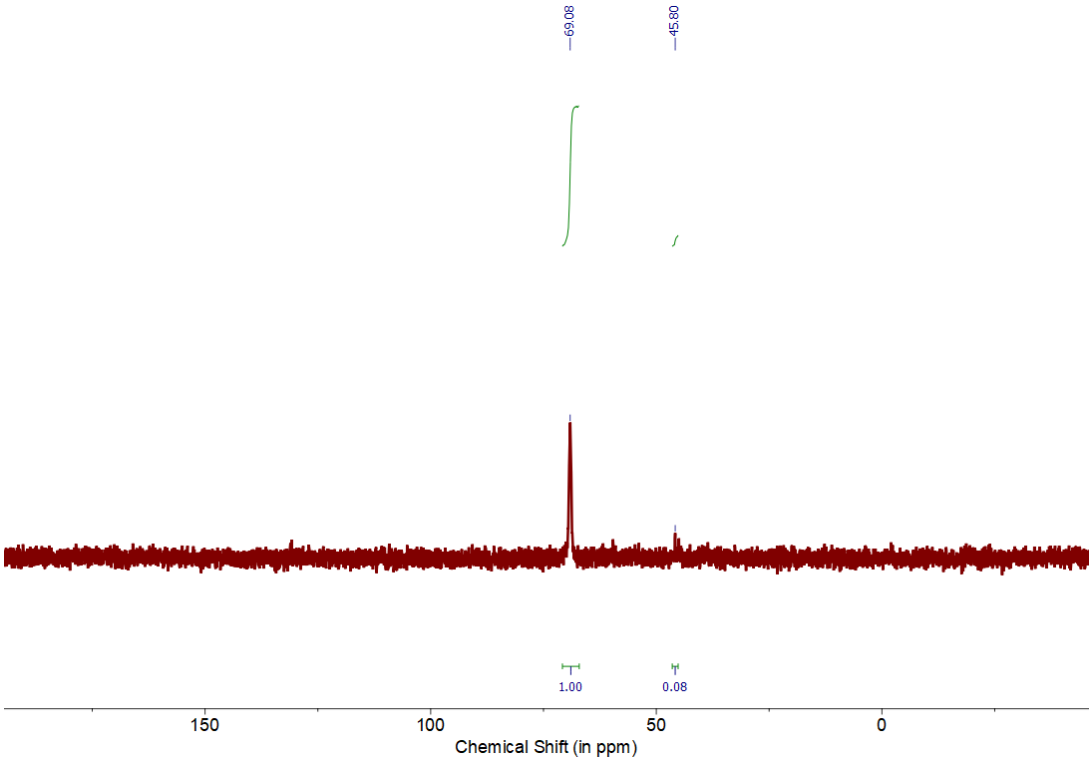
II.4.3. $^{11}B\{^1H\}$-NMR spectrum (128 MHz, THF-d_8)



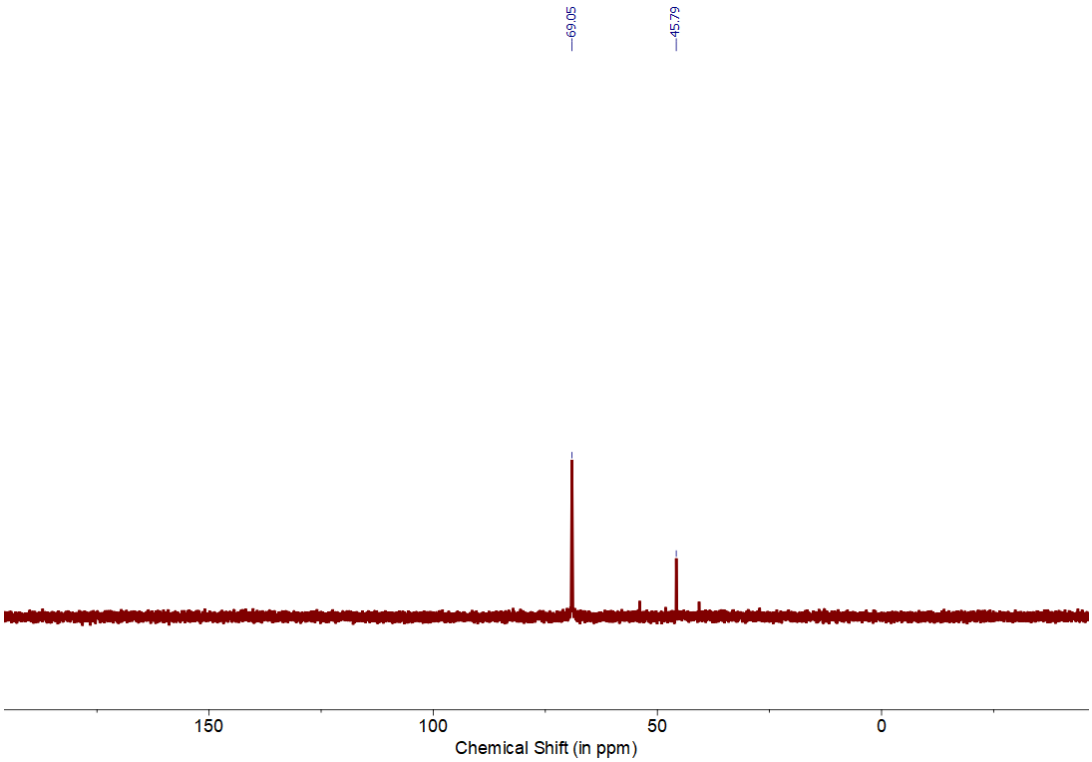
II.4.4. $^{13}C\{^1H\}$-NMR spectrum (101 MHz, THF-d_8)



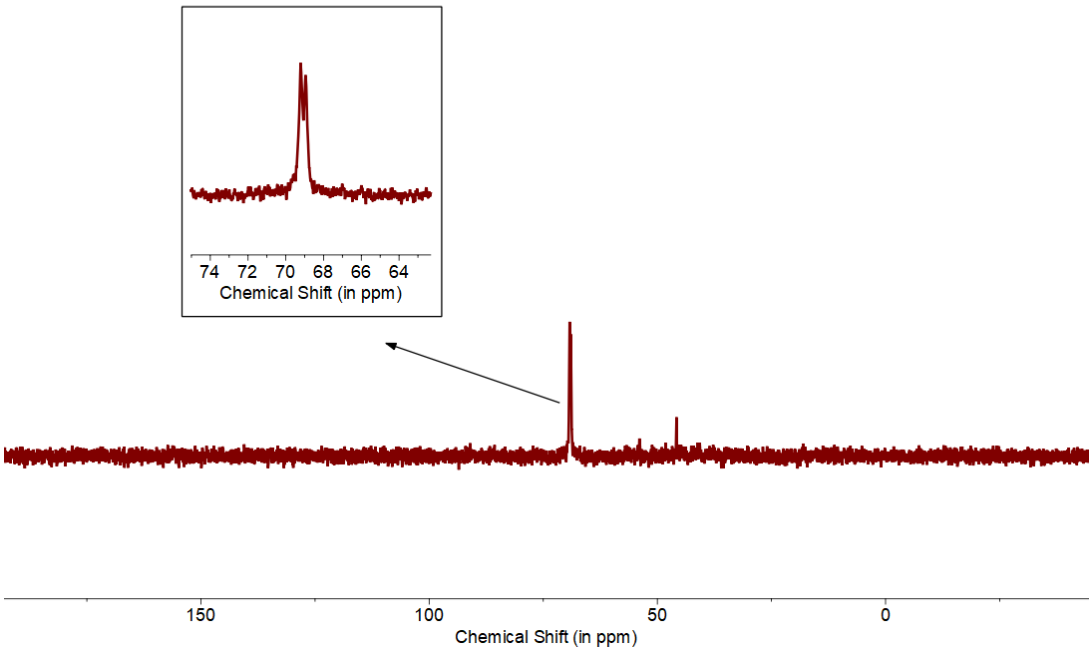
II.4.5. ^{31}P-NMR spectrum (162 MHz, THF-d_8)



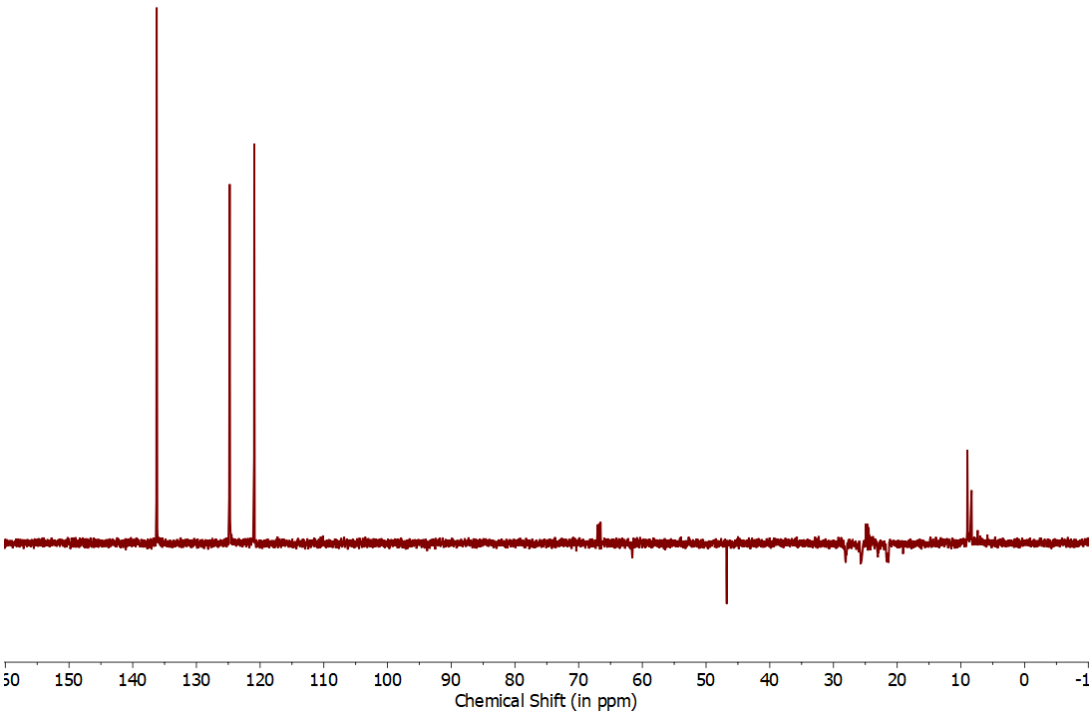
II.4.6. ^{31}P{^{1}H} NMR spectrum (162 MHz, THF-d_8)



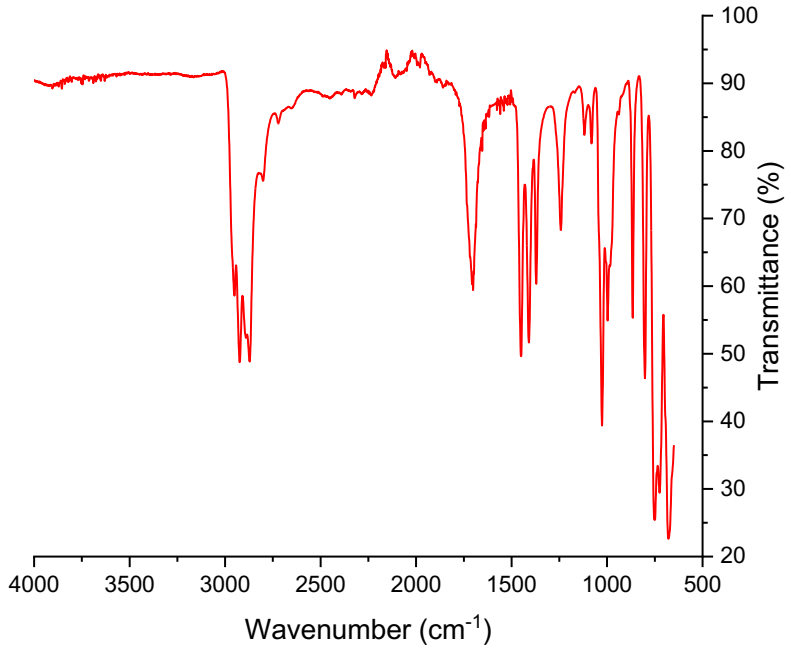
II.4.7. $^{31}P\{^{1}H\}_{sel\ (\delta = 1.5\ ppm)}$-NMR spectrum (162 MHz, THF-d_8)



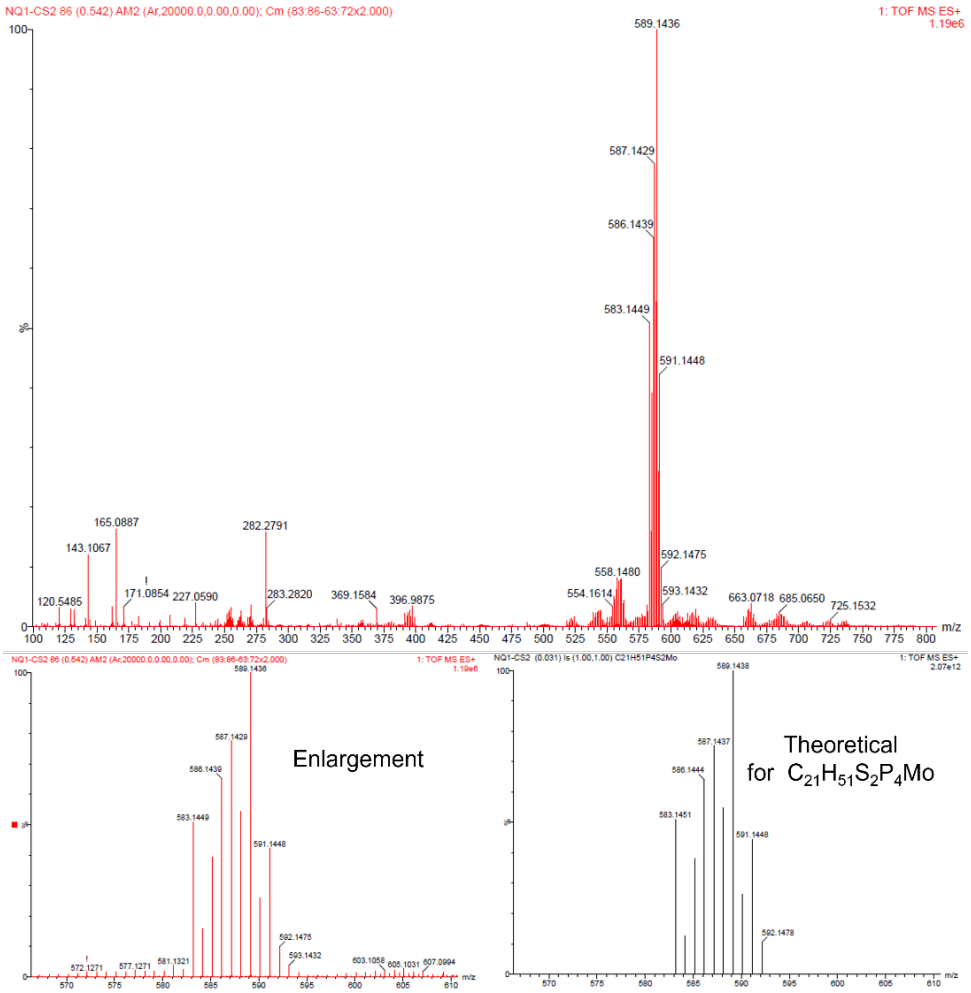
II.4.8. ^{13}C-DEPT NMR spectrum (101 MHz, THF-d_8)



II.4.9. FT-IR spectrum (ATR)



II.4.10. ESI-HRMS spectrum



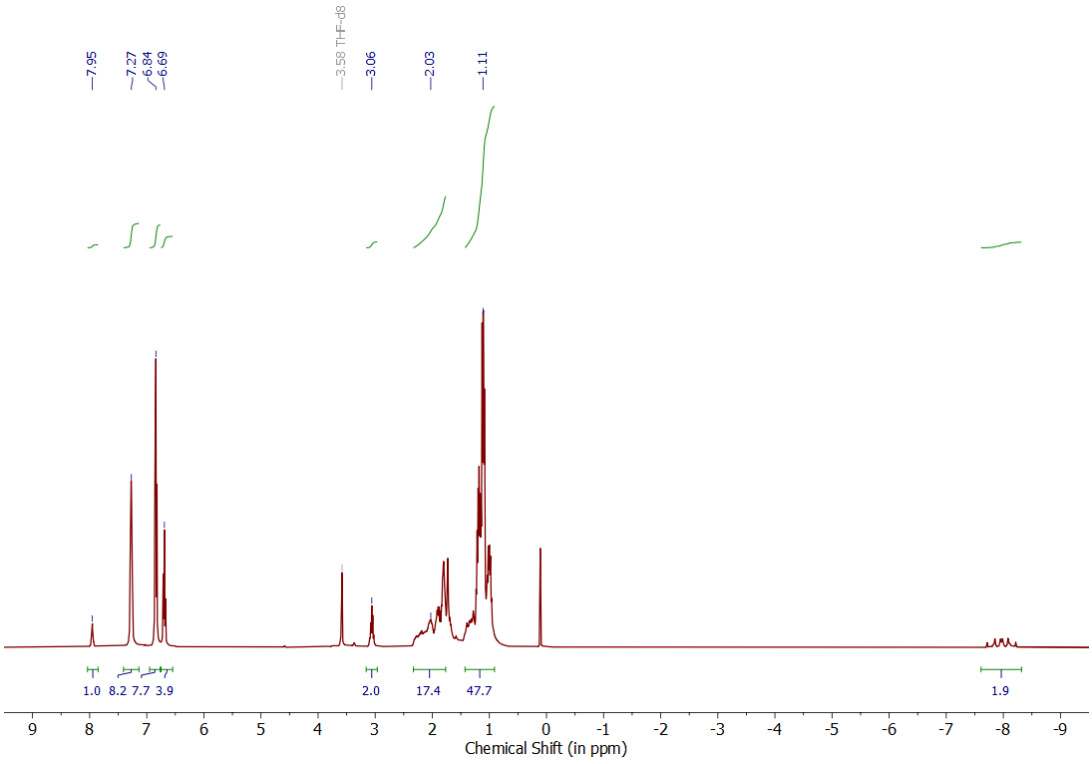
II.5. [Mo(depe)$_2$(^{i}PrNCHN^{i}Pr)H$_2$] (7.BPh$_4$)

II.5.1. Experimental procedure

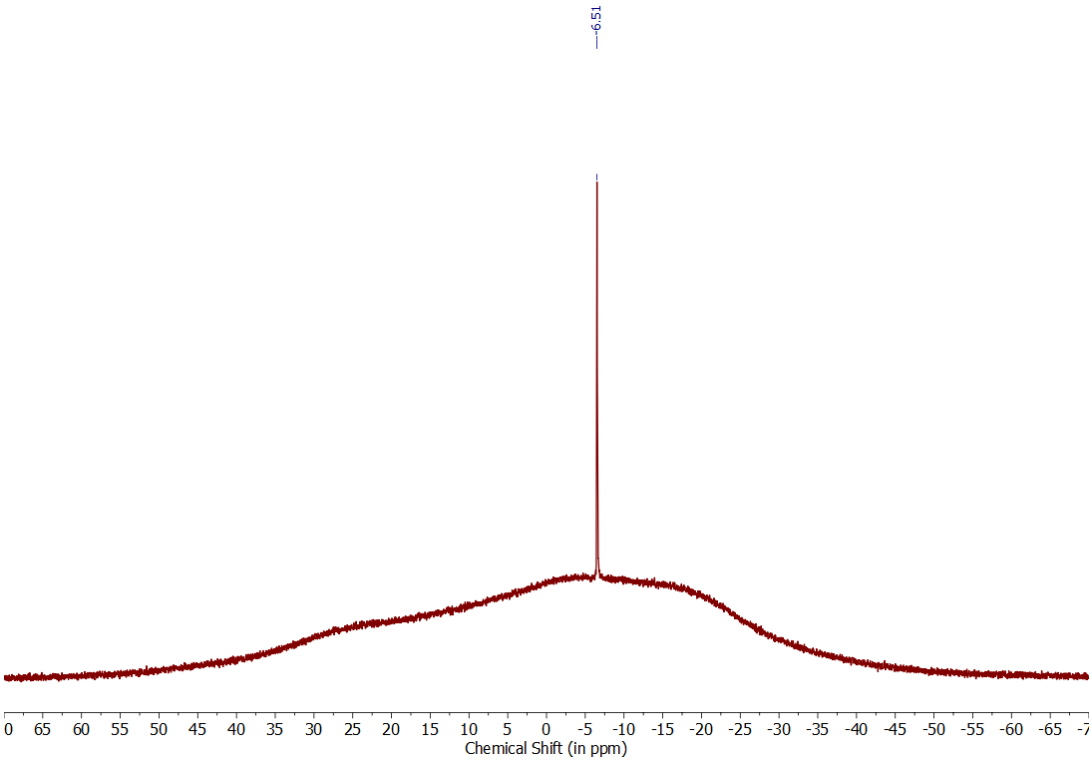
In a Fisher-Porter flask, [Mo(depe)$_2$H$_4$] (20.0 mg, 39.0 µmol, 1.00 equiv.) was dissolved in THF (1 mL). A solution of [HNEt$_3$][B(C$_6$H$_5$)$_4$] (16.4 mg, 39.0 µmol, 1.00 equiv.) and ^{i}PrNCN^{i}Pr (4.9 mg, 39.0 µmol, 1.00 equiv.) in THF (1 mL) was added. The reaction mixture was left at room temperature for 24h, under continuous stirring. Pentane (ca. 10 mL) was added to the orange solution, triggering immediate phase separation of a dark orange oil. The solution was decanted off and the oil triturated twice with cold pentane (2 x 5 mL). The solid was then dried under high vacuum at room temperature to yield the desired compound (12.7 mg, 34%). Single crystals suitable for X-ray diffraction were obtained by storing at -40°C a concentrated THF solution of the complex layered by pentane over a few days.

^{1}H-NMR (400 MHz, THF-d$_8$, 293K) δ 7.95 (m, 1H, ^{i}PrNC*H*N^{i}Pr), 7.27 (br. m, 8H, *meta*-C$_6$*H*$_5$), 6.84 (t, ^{3}J$_{(H-H)}$ = 7.4 Hz, 8H, *ortho*-C$_6$*H*$_5$), 6.69 (t, ^{3}J$_{(H-H)}$ = 7.2 Hz, 4H, *para*-C$_6$*H*$_5$), 3.06 (hept., 2H, -C*H*(CH$_3$)$_2$), 2.33-1.76 (m, 16H, -C*H*$_2$-CH$_3$), 1.11 (m, 44H, -C*H*$_2$-C*H*$_2$- & -CH(C*H*$_3$)$_2$ & -CH$_2$-C*H*$_3$), -7.97 (m, 2H).
^{11}B-NMR (128 MHz, THF-d$_8$) δ -6.5.
^{13}C{^{1}H}-NMR (101 MHz, THF-d$_8$) δ 164.3 (q, ^{2}J$_{(B-C)}$ = 49.5 Hz, *ipso*-*C*$_6$H$_5$), 159.4 (m, ^{i}PrN*C*HN^{i}Pr), 136.2 (br. s, *meta*-*C*$_6$H$_5$), 124.6 (m, *ortho*-*C*$_6$H$_5$), 120.7 (s, *para*-*C*$_6$H$_5$), 49.8 (-*C*H(CH$_3$)$_2$), 27.0 (-*C*H$_2$-), 26.1 (-*C*H$_2$-), 21.9 (-*C*H$_3$), 20.8 (-*C*H$_2$-), 13.6 (-*C*H$_2$-), 8.5 (-*C*H$_3$), 7.8 (-*C*H$_3$), 7.5 (-*C*H$_3$).
^{31}P{^{1}H}-NMR (162 MHz, THF-d$_8$) δ 71.0 (m), 41.5 (m). **^{31}P{^{1}H}$_{sel}$-NMR** (162 MHz, THF-d$_8$) δ 71.0 (t,^{2}J$_{(P-H)}$ = 50.8 Hz), 48.3 (t,^{2}J$_{(P-H)}$ = 43.5 Hz).

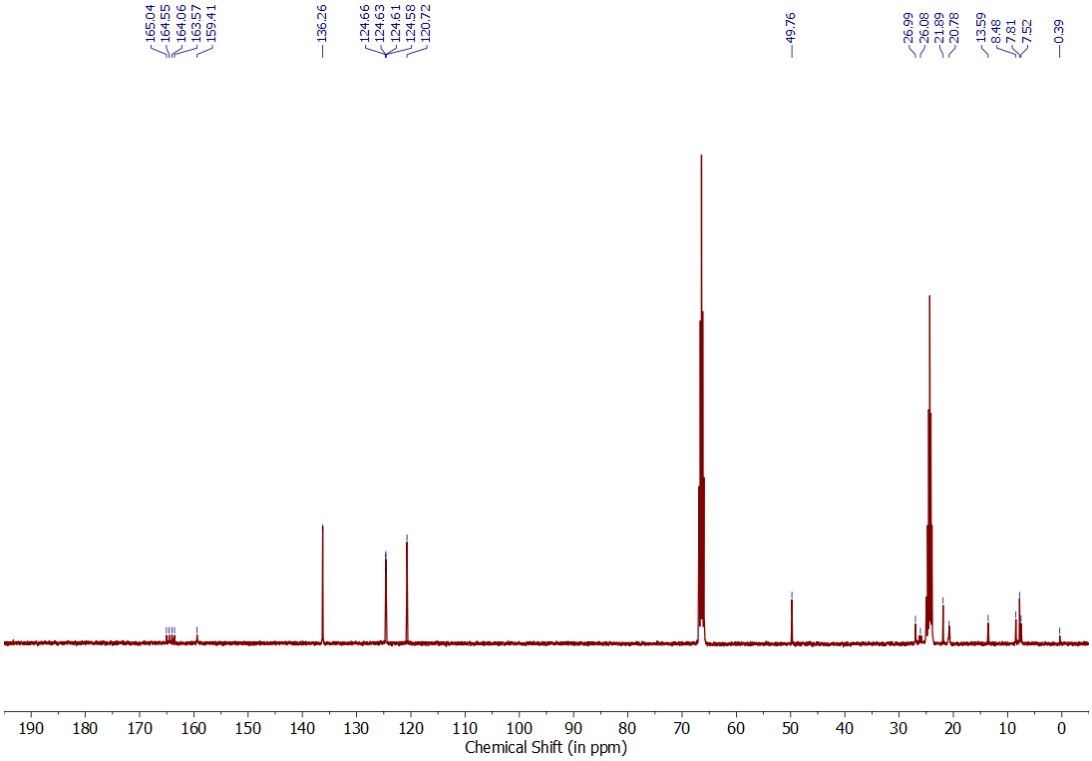
II.5.2. ^{1}H-NMR spectrum (400 MHz, THF-d8)



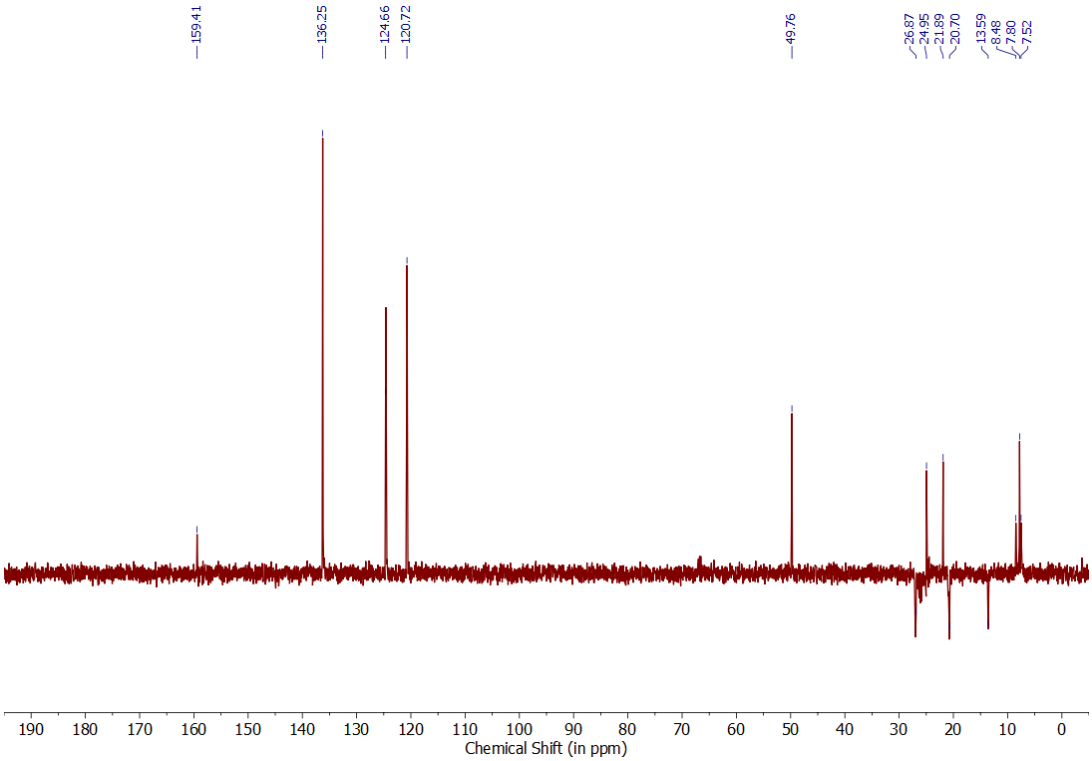
II.5.3. $^{11}B\{^1H\}$-NMR spectrum (128 MHz, THF-d_8)



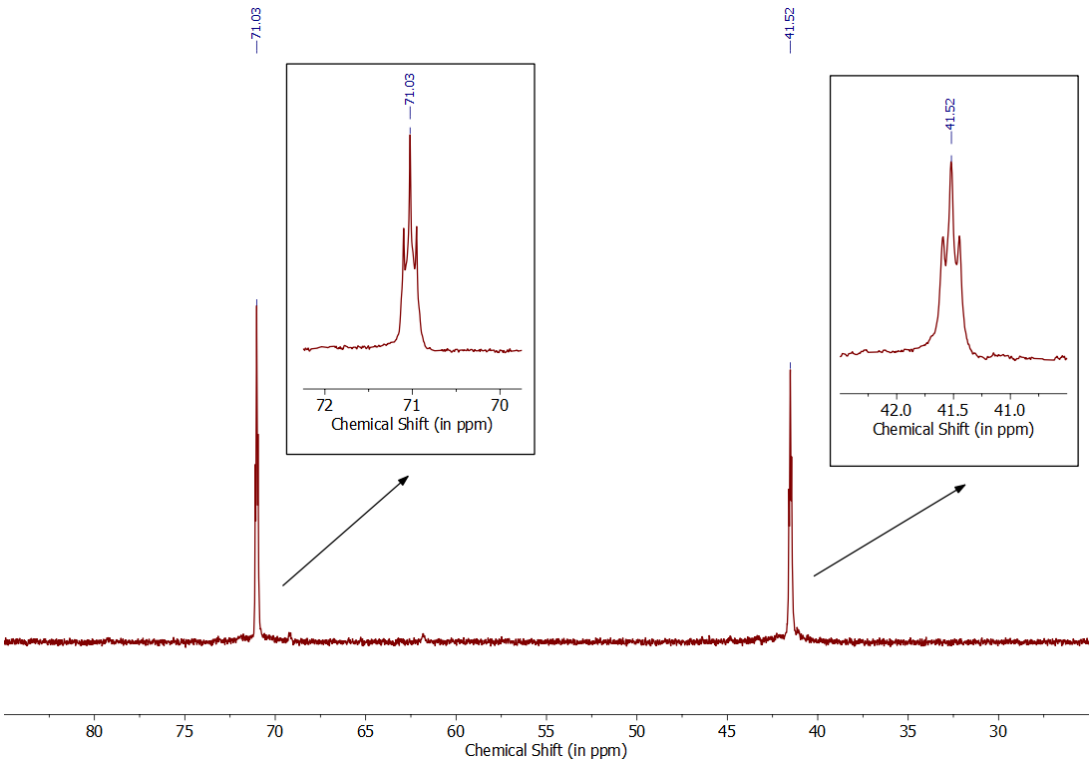
II.5.4. $^{13}C\{^1H\}$-NMR spectrum (101 MHz, THF-d_8)



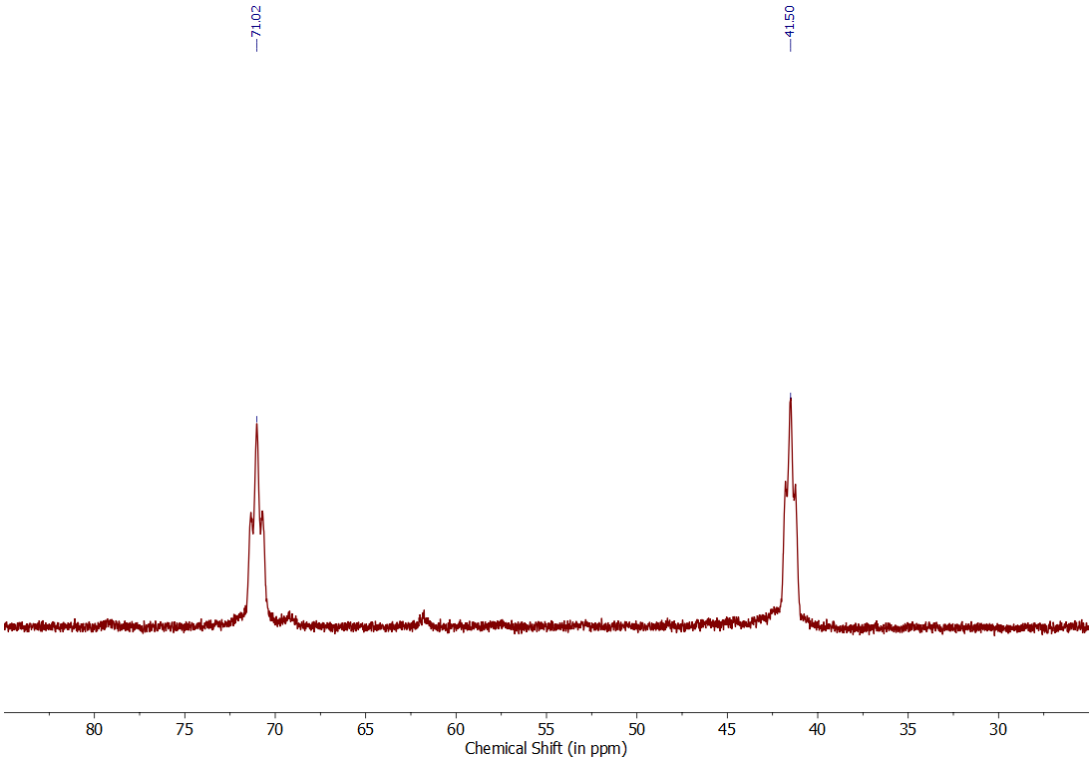
II.5.5. ^{13}C-DEPT NMR spectrum (101 MHz, THF-d_8)



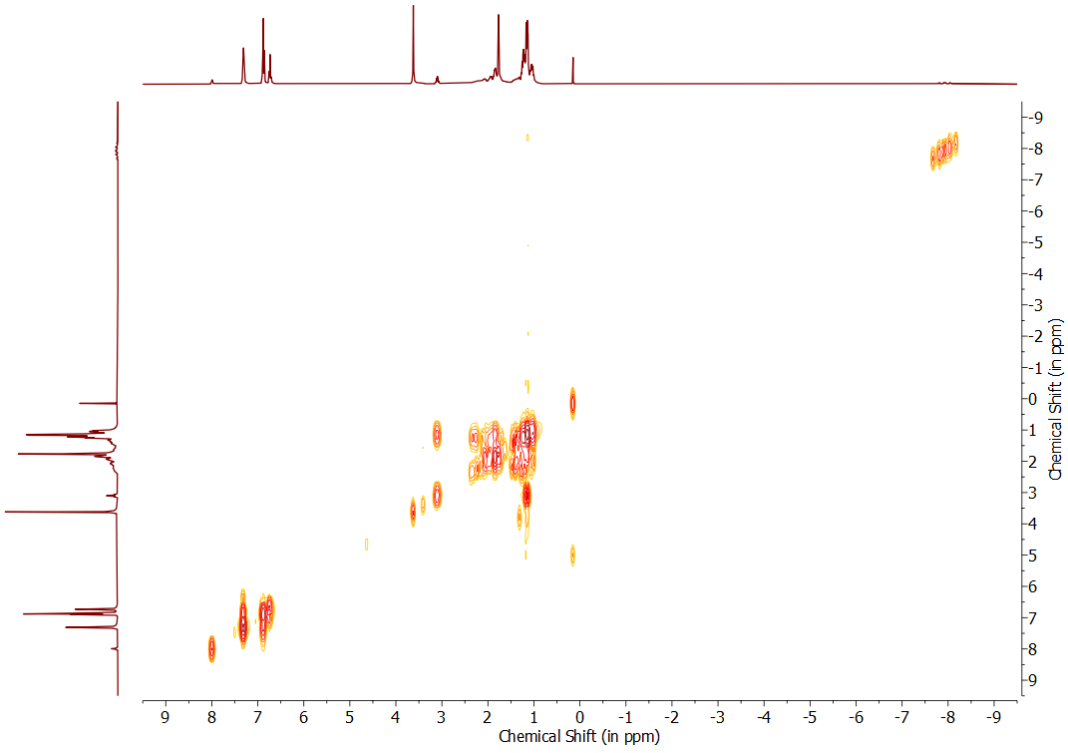
II.5.6. ^{31}P{^{1}H}-NMR spectrum (162 MHz, THF-d_8)



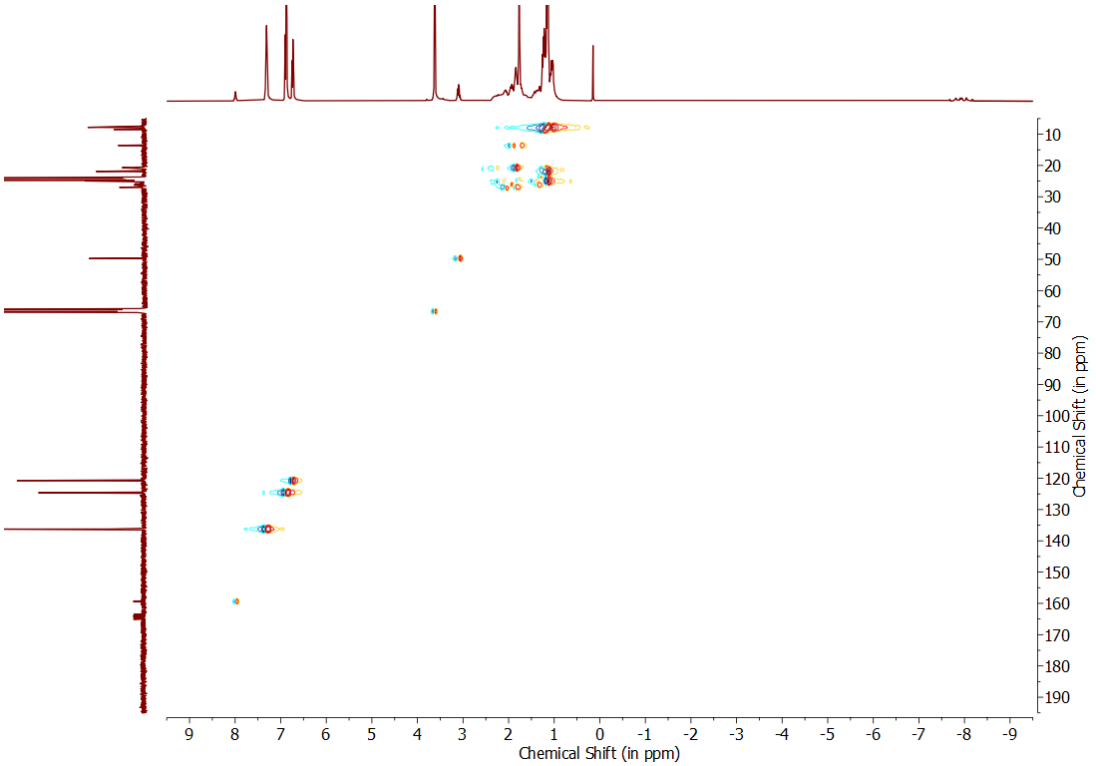
II.5.7. $^{31}P\{^{1}H\}_{sel\ (\delta = 1.5\ ppm)}$-NMR spectrum (162 MHz, THF-d_8)



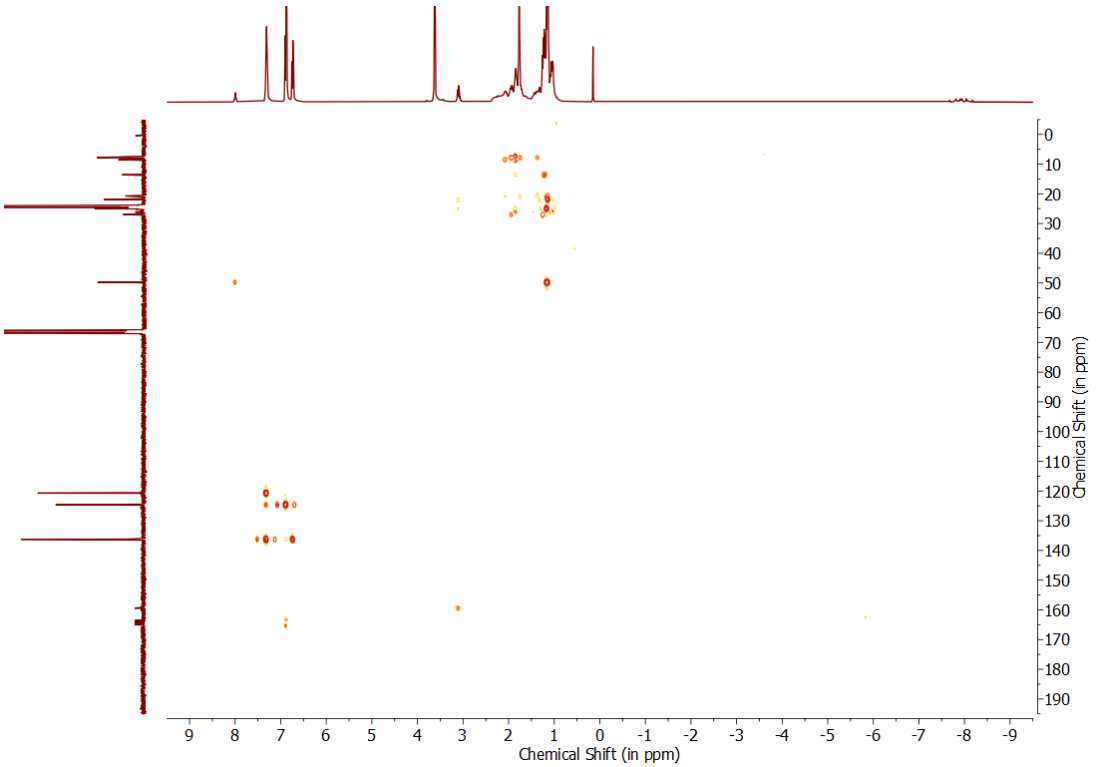
II.5.8. ^{1}H-^{1}H COSY NMR spectrum



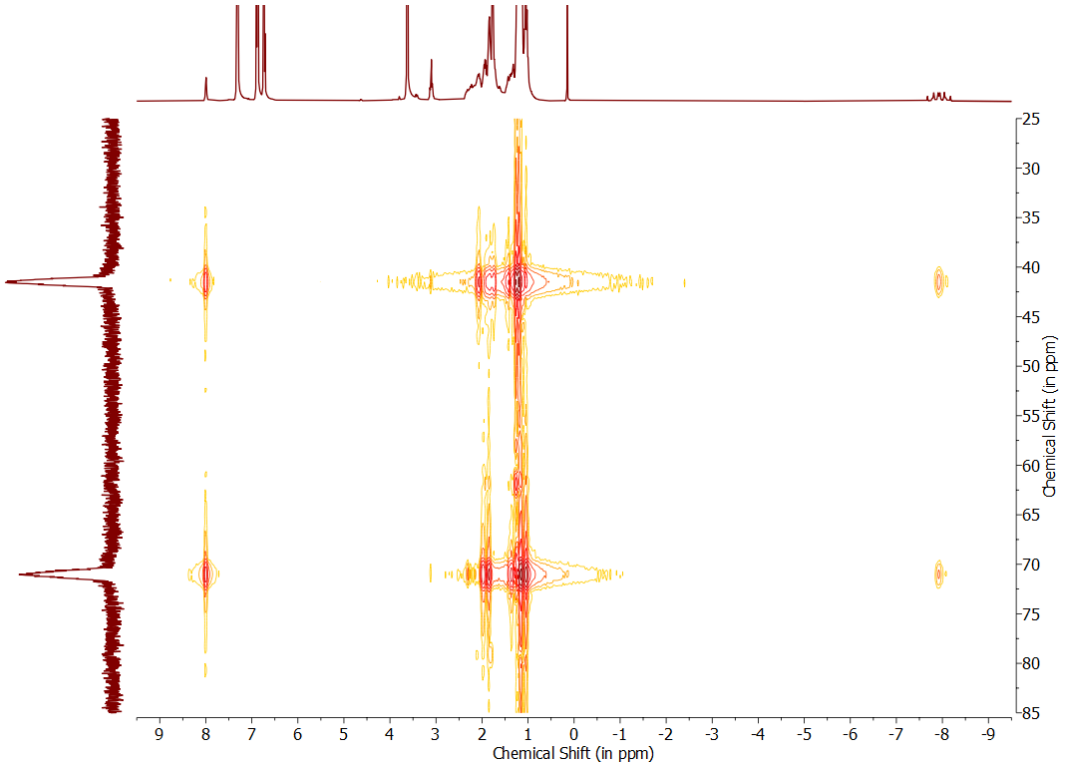
II.5.9. ^{13}C-^{1}H HSQC NMR spectrum



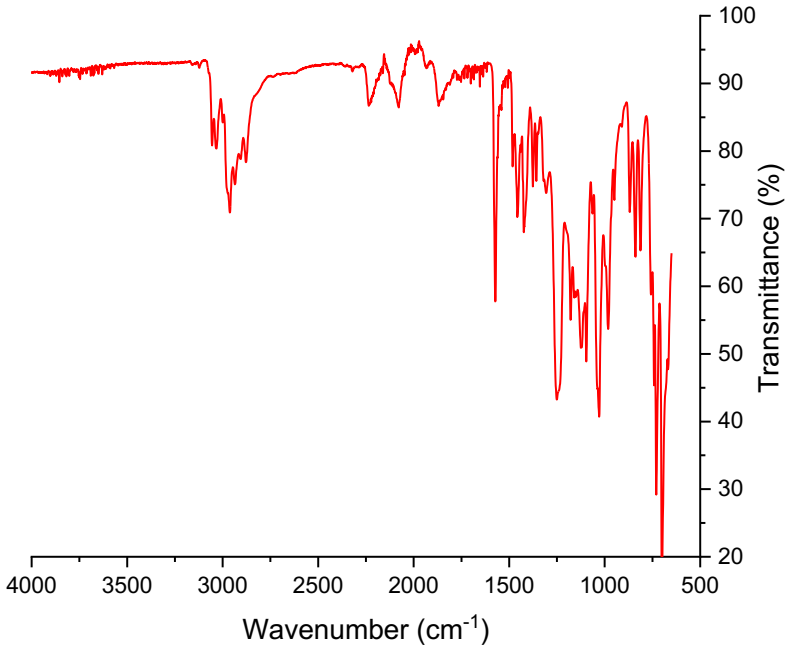
II.5.10. ^{13}C-^{1}H HMBC NMR spectrum



II.5.11. ^{31}P-^{1}H HMQC NMR spectrum



II.5.12. FT-IR spectrum (ATR)



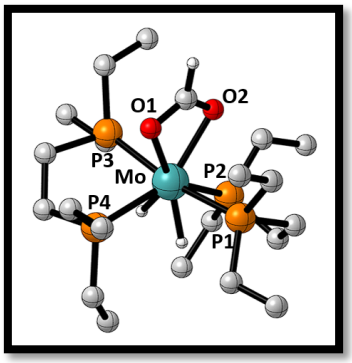
III. Computational Details

III.1. General Information

All geometry optimizations and frequency calculations were carried out without symmetry constraints with the Gaussian16 Revision B.01 suite of programs[12] using the B3LYP[13–15] functional in conjunction with the Grimme D3(BJ) dispersion correction.[16,17] The Molybdenum atom was modelled using the relativistic effective core potential SDD[18–20] basis set, augmented with an f-type polarization function having an exponent of 1.043.[21] The 6-31G(d,p)[22,23] basis set was used for other atoms (H, C, O, P). Therefore, the level of theory of the optimizations can be described as B3LYP-D3(BJ)/SDD+f(Mo), 6-31G** (other atoms). Further energy refinement single-point calculations were performed at the higher M06-L[24]-D3/def2-TZVPP[25,26] level of theory considering solvents (tetrahydrofuran: THF) effects by means of the Polarizable Continuum Model (PCM)[27–29] method. Frequency calculations were performed on minima (reactants, intermediates and products) resulting in positive definite Hessian matrices. Transition states (TS) were identified by a single negative eigenvalue in their diagonalized force constant matrices. To confirm the TSs nature, the eigenvectors associated with the negative eigenvalue were confirmed to correspond to the motion along the reaction coordinate employing the Intrinsic Reaction Coordinate (IRC) method.[30] Molecular structure images were generated utilizing Cylview software.[31] For the thermal evolution of compound $\mathbf{3}^{+}$ into $\mathbf{4}^{+}$ and $\mathbf{5}^{+}$, the GoodVibes package[32] was employed to correct free energy at 373.15 K.

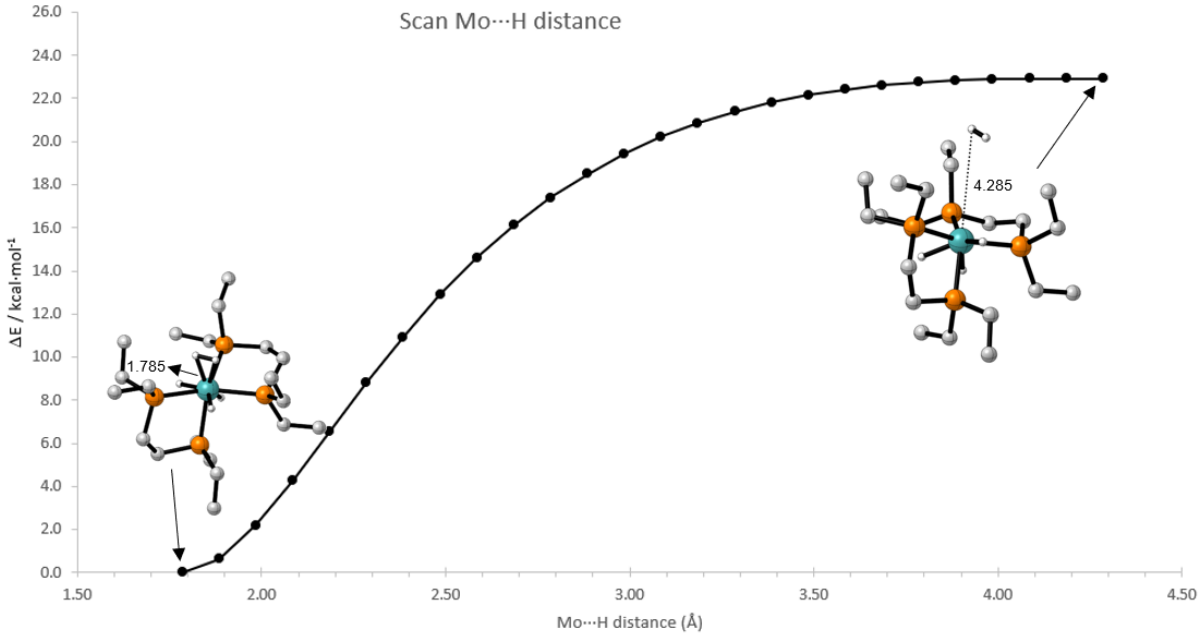
III.2. Detailed Results

Table S1. Comparison of the X-ray diffraction structure of naked cationic $\mathbf{3}^{+}$ *versus* the DFT-computed structure. Distances and bond angles are given in angstroms and º, respectively. The image shows the DFT-optimized geometry at B3LYP-D3(BJ)/SDD+f(Mo), 6-31G** (other atoms) level of theory. Hydrogen atoms in the diphosphine ligands have been omitted for clarity.



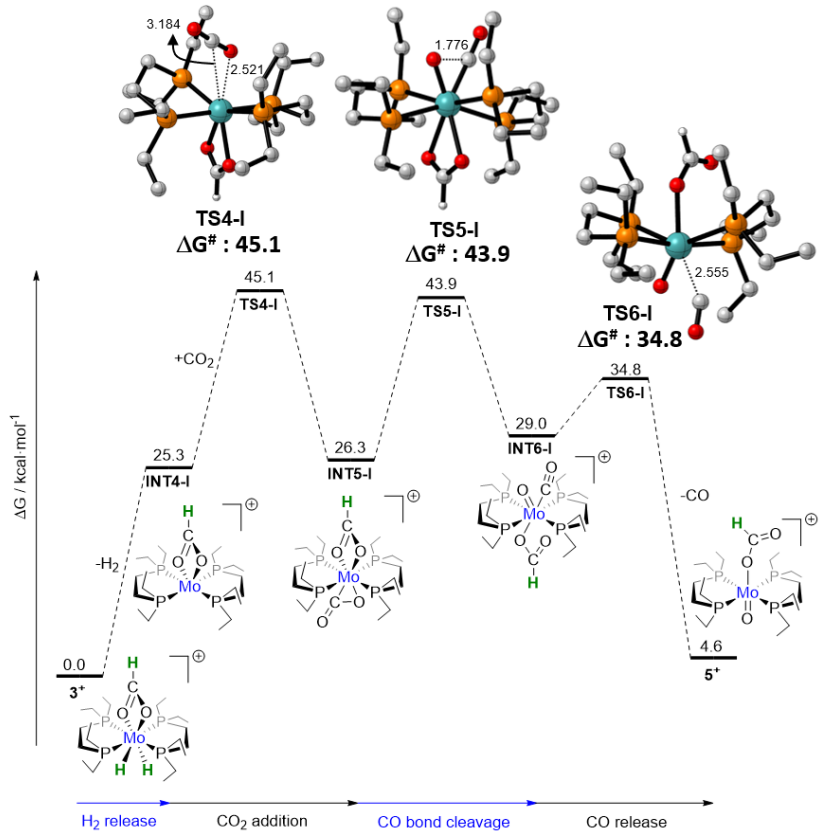
	X-ray value	DFT value	Difference	Relative error (%)
Mo-O1	2.254	2.282	0.028	1.2
Mo-O2	2.274	2.284	0.010	0.4
Mo-P1	2.463	2.499	0.036	1.5
Mo-P2	2.414	2.441	0.027	1.1
Mo-P3	2.485	2.487	0.002	0.1
Mo-P4	2.425	2.441	0.016	0.7
P1-Mo-P2	81.5	81.9	0.4	0.5
P3-Mo-P4	82.2	82.1	-0.1	-0.1

Figure S1. Energy scan of the H_2 release from **INT1**, leading to **INT1´** + H_2. The Mo···H distance has been increased from 1.785 to 4.285 Å by step of 0.100 Å. Energy (ΔE in kcal·mol^{-1}) and distances in angstroms. All data have been computed at the B3LYP-D3(BJ)/SDD+f(Mo), 6-31G** (other atoms) level of theory. Hydrogen atoms in the diphosphine ligands have been omitted for clarity.



This scan shows that the release of H_2 from **INT1** affording **INT1´** + H_2 is barrierless.

Figure S2. **Pathway I**: Energy profile for the thermal evolution of complex **3$^+$** into complex **5$^+$**. All data have been computed at the PCM(o-dichlorobenzene)-M06-L-D3/def2-TZVPP//B3LYP-D3(BJ)/SDD+f(Mo), 6-31G** (other atoms) level of theory. Free energies (ΔG) have been corrected at 373.15 K. All activation barriers are referred to **3$^+$**. Distances and energies are given in Å and kcal·mol^{-1}, respectively.



Scheme S1. Competitive pathways (outer or inner-sphere mechanisms) for the hydride transfer from the Molybdenum hydride intermediate **INT1'** to the CO_2 molecule. Distances are given in Å. Structures of the TS and Gibbs free energy (ΔG in kcal·mol^{-1} from initial reactants) have been computed at the PCM(o-dichlorobenzene)-M06-L-D3/def2-TZVPP//B3LYP-D3(BJ)/SDD+f(Mo), 6-31G** (other atoms) level of theory. Hydrogen atoms in the diphosphine ligands have been omitted for clarity.

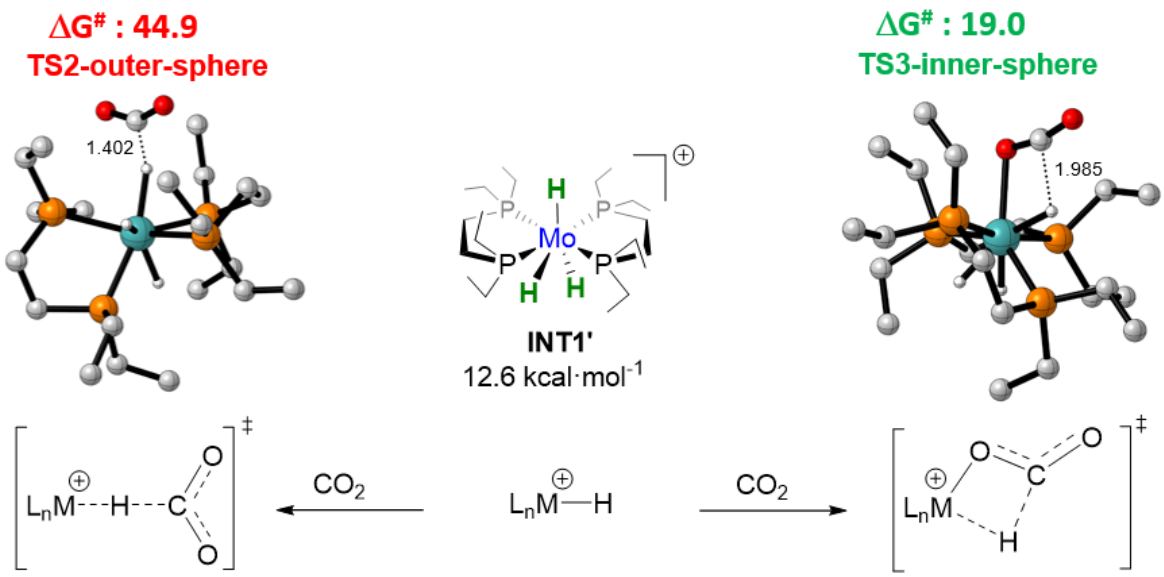
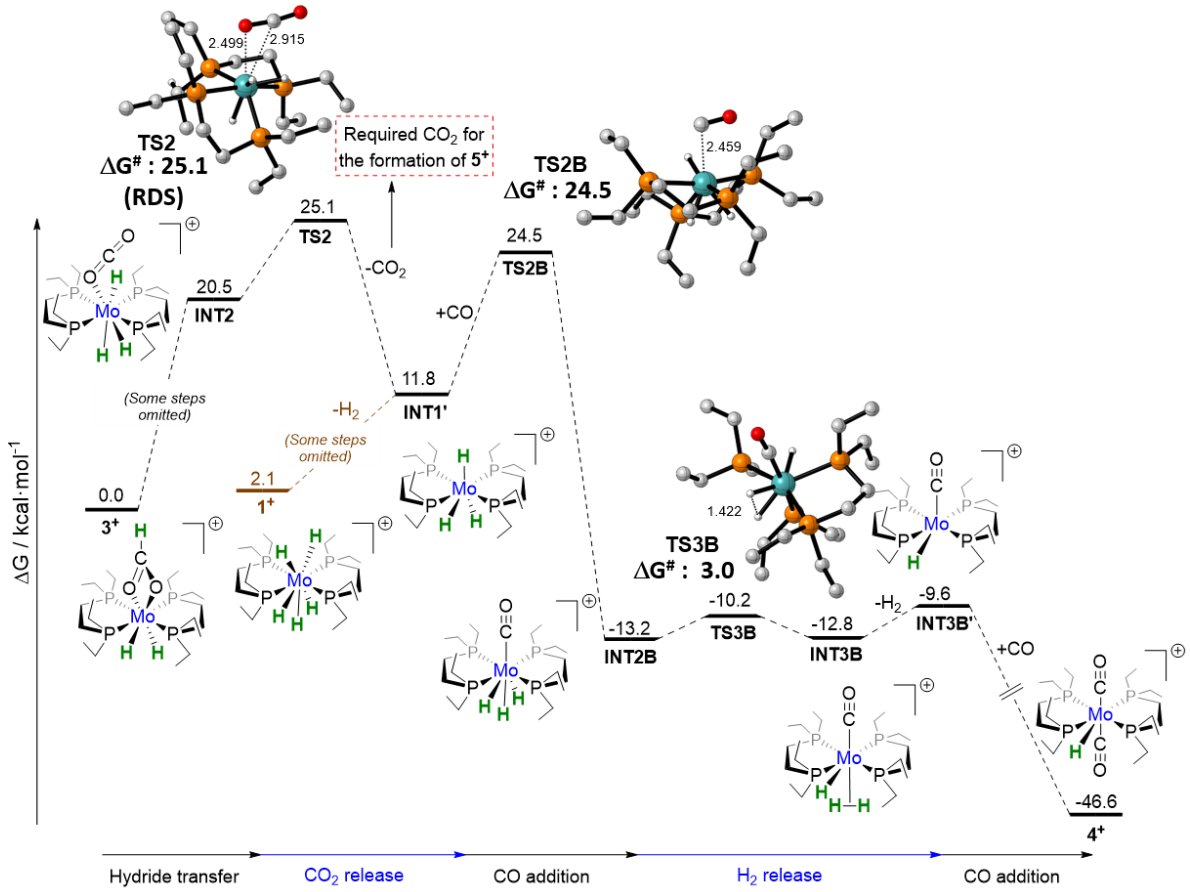
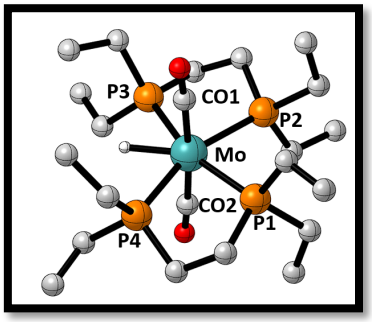


Figure S3. Computed profile for the thermal evolution of complex **3⁺** and its reactivity with carbon monoxide, affording complex **4⁺**. All data have been computed at the PCM(*o*-dichlorobenzene)-M06-L-D3/def2-TZVPP//B3LYP-D3(BJ)/SDD+f(Mo), 6-31G** (other atoms) level of theory. Free energies have been corrected at 373.15 K. All activation barriers are referred to **3⁺**. Distances and energies are given in Å and kcal·mol^{-1}, respectively.



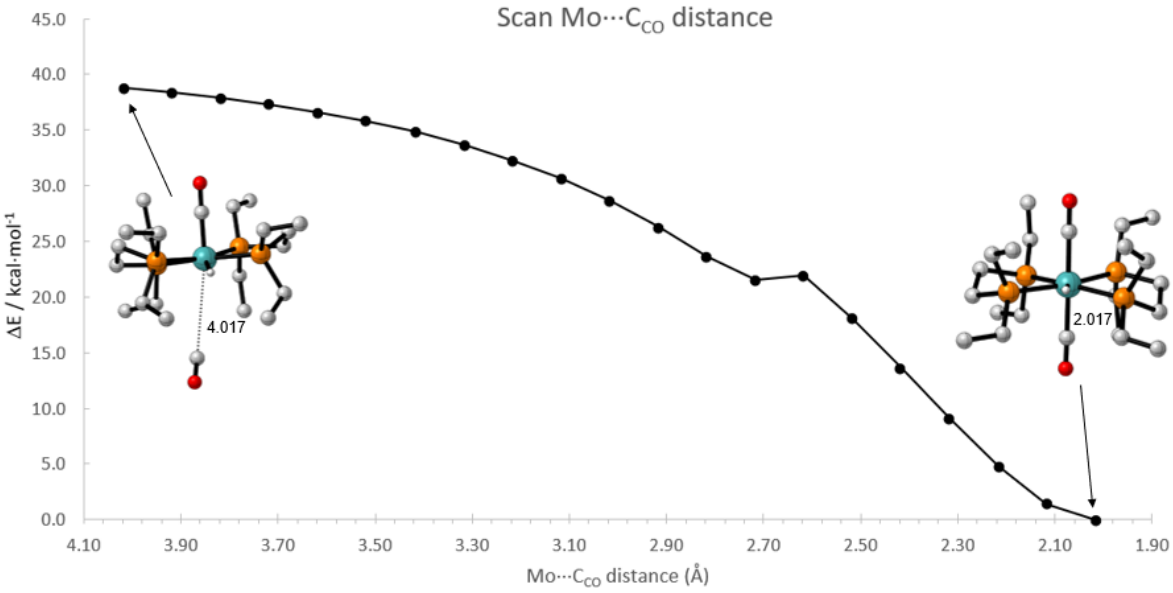
We investigated two processes forming complex **4⁺**: (i) the direct reaction of complex **1⁺** with CO at room temperature (25°C) and (ii) the thermal evolution of complex **3⁺**, when heated at 100 ºC. Note that these two processes involve the same intermediate **INT1'** and share the subsequent steps. In the first process, no transition state associated to the direct addition of CO was found on the potential energy surface due to the high coordination number of **1⁺**. As a result, the initial step involves the release of H_2 forming **INT1'**. This step has been omitted in this profile for clarity and has been described in the Fig. 2 of the manuscript. The second process, associated to the thermal evolution, starts by the formation of **INT2** which has been previously described in the main text in Fig. 3 and has been omitted in this profile for clarity, as well. The transition state from **INT2** to **INT1'**, associated to release of CO_2 (**TS2**), was computed in Fig. 2 but at 25°C. In this new profile, we corrected the energies at 373.15 K using GoodVives software. It lies at 25.1 kcal·mol^{-1} from **3⁺**. It is important to mention that this release of CO_2 is crucial for the last step of the profile computed for the thermal evolution of **3⁺** into **5⁺** (see Fig.3 in the main text). Once **INT1'** is formed, the rest of the profile is shared between the two processes. The subsequent addition of CO occurs through **TS2B**, which lies at 12.7 kcal·mol^{-1} from **INT1'** ($\Delta G^{\#}$: 24.5 kcal·mol^{-1} from the free complex **3⁺**). Remarkably, this addition is highly exergonic, ΔG: -25.0 kcal·mol^{-1}, affording **INT2B**, where CO is coordinated to the metal centre by the carbon atom. Afterwards, in order to add the second molecule of CO in *trans* to the first one, the release of a second molecule of H_2 is required by a new reductive elimination process, giving the Mo(II) intermediate **INT3B'**. This H_2 release is even energetically easier than the first one (**TS3B** with $\Delta G^{\#}$: 3.0 kcal·mol^{-1}). Then, the coordination of the second molecule of CO was found to be barrierless according to an energy scan where the CO was located at 4.0 Å and gradually approached to the Mo centre until forming the final product **4⁺** (Figure S4). In line with experimental observations, the formation of **4⁺** (see Table S2 for geometrical features) from **3⁺** after successive releases of H_2 and additions of CO is strongly exergonic, with an overall ΔG value of up to -46.6 kcal·mol^{-1} (-49.8 kcal·mol^{-1} from complex **1⁺**). The rate-determining step corresponds to CO_2 release with an activation barrier of 25.1 kcal·mol^{-1}, further confirming the feasibility of the reaction.

Table S2. Comparison of the X-ray diffraction structure of naked cationic **4**$^{+}$ *versus* the DFT-computed structure. Distances and bond angles are given in angstroms and º, respectively. The image shows the DFT-optimized geometry at B3LYP-D3(BJ)/SDD+f(Mo), 6-31G** (other atoms) level of theory. Hydrogen atoms in the diphosphine ligands have been omitted for clarity.



	X-ray value	DFT value	Difference	Relative error (%)
Mo-CO1	2.015	2.017	0.002	0.1
Mo-CO2	2.009	2.006	-0.003	-0.1
Mo-P1	2.451	2.468	0.017	0.7
Mo-P2	2.531	2.555	0.024	0.9
Mo-P3	2.451	2.477	0.026	1.1
Mo-P4	2.526	2.551	0.025	1.0
P1-Mo-P2	77.2	77.5	0.3	0.4
P3-Mo-P4	77.5	78.0	0.5	0.6

Figure S4. Energy scan of the CO addition to **INT3B´**. The Mo···C_{CO} distance has been decrease from 4.017 to 2.017 Å by step of 0.100 Å. Energy (ΔE) and distances are given in kcal·mol^{-1} and angstroms. All data have been computed at the B3LYP-D3(BJ)/SDD+f(Mo), 6-31G** (other atoms) level of theory. Hydrogen atoms in the diphosphine ligands have been omitted for clarity.



This scan shows that the addition of CO on Mo centre is barrierless.

III.3. Cartesian Coordinates and E+ZPE and free energies (G) of optimized structures

78

1^+

C	-3.217456	1.206178	0.857417
H	-3.338445	0.631257	1.780648
H	-3.882919	2.071919	0.922112
C	-3.544541	0.337127	-0.358677
H	-3.499656	0.927059	-1.280209
H	-4.552647	-0.081071	-0.290618
C	-2.557665	-1.639238	-2.239516
H	-3.629815	-1.821148	-2.370923
H	-2.279944	-0.813241	-2.901606
C	-1.746438	-2.891329	-2.579625
H	-0.676155	-2.697612	-2.477425
H	-1.943207	-3.201368	-3.609370
H	-2.006416	-3.730757	-1.927378
C	-2.927375	-2.360400	0.581168
H	-2.154790	-3.135189	0.592752
H	-2.931817	-1.934391	1.589920
C	-4.290581	-2.953270	0.219435
H	-5.078831	-2.195256	0.197981
H	-4.581544	-3.702450	0.961051
H	-4.272468	-3.447007	-0.755735
C	-1.518853	3.214247	-0.354383
H	-0.488071	3.484304	-0.599739
H	-1.946800	2.822059	-1.283421
C	-2.289656	4.443872	0.131929
H	-1.805654	4.910703	0.993395
H	-3.317532	4.199671	0.415079
H	-2.341023	5.193565	-0.662673
C	-1.140238	2.491575	2.457040
H	-0.188366	3.029342	2.385094
H	-1.918853	3.238935	2.640863
C	-1.089767	1.477474	3.601851
H	-0.895817	1.991585	4.547223
H	-0.303648	0.738374	3.437245
H	-2.036841	0.940327	3.707997
C	3.509016	-0.522970	0.382185
H	3.616177	0.110446	1.269294
H	4.381836	-1.180820	0.340775
C	3.400318	0.332119	-0.882639
H	3.372388	-0.304499	-1.772239
H	4.258293	1.002513	-0.987431
C	2.253236	2.760976	0.199109
H	1.322402	3.292972	0.413889
H	4.241726	3.223234	-0.595529
H	2.954693	4.251918	-1.236696
C	2.310631	-3.036281	-0.395059
H	2.337353	-2.713985	-1.440529
H	3.316492	-3.380689	-0.132438
C	1.295754	-4.166379	-0.211899
H	1.263691	-4.515824	0.824174
H	1.563196	-5.019416	-0.841352
H	0.290496	-3.844102	-0.492890
C	2.010766	-2.082937	2.360223
H	1.910926	-1.172239	2.959415
H	1.091610	-2.653110	2.526683
C	3.247769	-2.887457	2.768031
H	3.197062	-3.141536	3.830392
H	4.170946	-2.322560	2.609680
H	3.325837	-3.824712	2.210644
Mo	-0.026324	-0.174754	0.004373
H	0.765797	0.506106	1.357972
H	-0.638942	0.611695	-1.385860
H	-0.230567	-1.842747	0.039516
H	-0.700203	-0.712078	1.489221
H	0.499473	-0.920400	-1.447675
P	-1.443201	1.751938	0.789737
P	-2.287055	-1.019411	-0.522825
P	1.955752	-1.519729	0.603655
P	1.815904	1.301253	-0.864216
C	1.702674	1.999166	-2.572787
H	0.919526	2.764722	-2.540233
H	2.645108	2.512506	-2.789537
C	1.390715	0.969215	-3.660646
H	2.166878	0.200841	-3.724438
H	1.334656	1.461636	-4.635349
H	0.440629	0.468470	-3.465834
H	2.569674	2.327973	1.154341
C	3.306303	3.730628	-0.342887
H	3.541063	4.489103	0.409230

Sum of electronic and zero-point Energies= -2227.173063
Sum of electronic and thermal Free Energies= -2227.242084

79

3^+

C	-0.131195	-0.169060	-2.829063
H	-0.195128	-0.206088	-3.924935
C	2.476078	-2.587895	-0.013681
H	2.163895	-3.154356	-0.897864
H	3.509161	-2.875021	0.200645
C	1.556175	-2.904989	1.171507
H	1.914781	-2.405237	2.077411
H	1.532551	-3.980303	1.376075
C	-1.286889	2.849799	1.230662
H	-1.550677	2.370776	2.179515
H	-1.219392	3.925404	1.416784
C	-2.335805	2.536776	0.160677
H	-2.108480	3.086858	-0.759465
H	-3.332255	2.853788	0.481034
C	3.131148	-0.769110	-2.177953
H	4.037403	-1.383889	-2.161039
H	2.421164	-1.274640	-2.840187
C	3.436534	0.645049	-2.684933
H	2.537977	1.266259	-2.682266
H	3.821574	0.607313	-3.707676
H	4.196118	1.135839	-2.069351
C	3.654188	0.035357	0.573865
H	3.599779	1.102370	0.334435
H	3.296863	-0.062059	1.604425
C	5.093497	-0.467772	0.444511
H	5.180878	-1.526922	0.701143
H	5.748794	0.086087	1.122830
H	5.481427	-0.334676	-0.568594
C	-1.062288	-2.588689	2.418769
H	-2.126289	-2.448735	2.206134
H	-0.922050	-3.646861	2.669306
C	-0.640783	-1.693865	3.584498
H	0.420674	-1.807613	3.823394
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H	-0.820955	-0.641508	3.355144
C	-0.825086	-3.605495	-0.282068
H	-0.269463	-3.530062	-1.219815
H	-0.572304	-4.566194	0.181837
C	-2.325534	-3.515625	-0.561140
H	-2.918862	-3.633258	0.350342
H	-2.628244	-4.307099	-1.252266
H	-2.577172	-2.559747	-1.020370
C	-3.579575	-0.037259	0.848831
H	-3.572476	-1.109068	0.628956
H	-3.140977	0.068856	1.847340
C	-5.008278	0.509335	0.816787
H	-5.044162	1.578362	1.043922
H	-5.624038	-0.001963	1.562260
H	-5.479063	0.357348	-0.157757
C	-3.250886	0.829056	-1.934649
H	-4.113729	1.489676	-1.796282
H	-2.569853	1.341125	-2.621784
C	-3.690473	-0.517703	-2.515034

H	-2.835767	-1.173182	-2.693637
H	-4.207759	-0.368091	-3.466888
H	-4.382162	-1.038730	-1.846615
C	1.432348	2.509902	2.195185
H	2.468912	2.402730	1.861172
H	1.289720	3.563831	2.455714
C	1.171518	1.622527	3.412471
H	0.139675	1.710425	3.765035
H	1.827065	1.911592	4.238389
H	1.354573	0.570988	3.181690
C	1.003655	3.332652	-0.557243
H	2.025838	3.000360	-0.770514
H	0.436279	3.135790	-1.469635
C	0.978360	4.821357	-0.199535
H	-0.041305	5.185111	-0.046371
H	1.411617	5.405532	-1.016358
H	1.555497	5.041799	0.702333
O	-0.302202	-1.220355	-2.145050
O	0.111749	0.928106	-2.243331
P	2.374781	-0.785979	-0.488394
P	-0.167132	-2.280107	0.832636
P	-2.353529	0.727261	-0.314127
P	0.364737	2.158725	0.726955
Mo	0.010307	-0.073202	-0.195286
H	0.905283	-0.211920	1.212548
H	-0.788369	0.107410	1.265374

Sum of electronic and zero-point Energies=-2414.607735
Sum of electronic and thermal Free Energies= -2414.677985

78

4^{+}

C	-0.032575	0.242372	2.040087
C	0.206231	0.279767	-1.972385
C	-3.180046	1.153404	-1.066960
H	-4.006943	1.868963	-1.101403
H	-2.904509	0.907669	-2.097460
C	-3.572246	-0.102426	-0.291047
H	-4.339180	-0.678267	-0.816610
H	-3.992727	0.173225	0.681217
C	-2.332529	-2.571442	-1.176014
H	-1.549338	-3.314920	-0.998244
H	-3.284166	-3.058612	-0.942948
C	-2.322389	-2.114603	-2.637140
H	-3.144891	-1.423855	-2.843820
H	-2.446305	-2.973514	-3.302390
H	-1.391826	-1.611518	-2.904641
C	-2.550837	-1.963535	1.669397
H	-1.744546	-2.646243	1.946044
H	-2.507100	-1.143654	2.394425
C	-1.242785	3.313202	-1.393457
H	-0.371234	3.798993	-0.943048
H	-0.887789	2.854487	-2.322119
C	-2.351180	4.331001	-1.673729
H	-3.218669	3.867991	-2.151604
H	-1.982751	5.108200	-2.348923
H	-2.690753	4.825421	-0.759559
C	-2.400809	2.711698	1.231239
H	-3.275427	3.291300	0.916690
H	-2.765239	1.902431	1.872530
C	-1.419804	3.592114	2.007437
H	-0.588492	3.004346	2.399292
H	-1.924105	4.061494	2.856197
H	-1.010586	4.391258	1.382484
C	3.572602	-0.582175	-0.278810
H	3.595376	-0.734443	-1.363360
H	4.593085	-0.352356	0.040246
C	3.033027	-1.820753	0.432176
H	3.086680	-1.689387	1.516923
H	3.610129	-2.716356	0.184339
C	1.351220	-2.823483	-1.706187
H	0.330122	-2.882161	-2.090034
H	1.847811	-2.066923	-2.322800
C	2.052470	-4.177166	-1.841420
H	3.067022	-4.160802	-1.433239
H	2.132030	-4.450294	-2.897403
H	1.499544	-4.974593	-1.338716
C	0.772711	-3.496378	1.081156
H	-0.242238	-3.797392	0.802344
H	1.424460	-4.339057	0.831728
C	0.856010	-3.195112	2.580868
H	1.888078	-3.022759	2.896743
H	0.479802	-4.045151	3.156763
H	0.273936	-2.314896	2.858465
C	2.948904	2.111272	-1.198707
H	2.624730	1.713769	-2.165986
H	2.332134	2.996484	-1.014027
C	4.436081	2.473522	-1.226915
H	4.767823	2.906332	-0.279272
H	4.627543	3.212048	-2.010211
H	5.062655	1.602657	-1.438333
C	3.113104	1.508508	1.662222
H	2.851128	0.774366	2.430848
H	4.205703	1.525014	1.590392
C	2.581094	2.891145	2.044095
H	2.893830	3.653347	1.324661
H	2.961431	3.185745	3.025600
H	1.490977	2.898896	2.089368
C	-3.904307	-2.676424	1.742363
H	-4.096940	-3.004009	2.767781
H	-3.933576	-3.564621	1.106297
H	-4.729784	-2.022784	1.447378
Mo	0.060340	0.187512	0.025991
O	-0.081466	0.326434	3.198658
O	0.320518	0.388776	-3.127565
P	-2.089672	-1.193037	0.044352
P	-1.682463	1.908875	-0.274731
P	1.245229	-2.071395	-0.008893
P	2.445058	0.857405	0.062123
H	0.480407	1.832189	0.194658

Sum of electronic and zero-point Energies= -2451.553012
Sum of electronic and thermal Free Energies= -2451.625804

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C	0.305086	-0.410821	-2.911757
H	0.075691	0.061906	-3.884446
C	1.250784	-3.265513	-0.324971
H	1.144352	-3.277960	-1.411294
H	1.984776	-4.027065	-0.046890
C	-0.091577	-3.522461	0.364519
H	0.038671	-3.587968	1.449849
H	-0.525908	-4.471961	0.036507
C	0.051610	3.609586	0.009700
H	-0.140307	3.818535	1.067220
H	0.498672	4.511117	-0.420394
C	-1.250973	3.243683	-0.707597
H	-1.071172	3.086136	-1.776269
H	-1.990558	4.044699	-0.620167
C	3.437022	-1.460760	-0.931799
H	3.916800	-2.444967	-0.895312
H	3.097239	-1.311058	-1.958437
C	4.423930	-0.375817	-0.498563
H	3.977061	0.618951	-0.549180
H	5.294683	-0.376362	-1.159758
H	4.785231	-0.529860	0.521926
C	2.518421	-1.750235	1.839832
H	2.936830	-0.775132	2.109584
H	1.631248	-1.868758	2.468332
C	3.531390	-2.868476	2.093259
H	3.105500	-3.855879	1.895720

H	3.849503	-2.854549	3.139651
H	4.427253	-2.760265	1.475946
C	-2.647855	-2.486264	1.262817
H	-3.519188	-1.900756	0.955934
H	-2.921430	-3.541962	1.161375
C	-2.277220	-2.158433	2.712377
H	-1.421432	-2.747426	3.055020
H	-3.117378	-2.387979	3.373334
H	-2.016929	-1.104773	2.829826
C	-1.983570	-2.519605	-1.624003
H	-2.520274	-1.627400	-1.957499
H	-1.113224	-2.611663	-2.279300
C	-2.876296	-3.760175	-1.710257
H	-2.364842	-4.659069	-1.353988
H	-3.161619	-3.939801	-2.750387
H	-3.795576	-3.642860	-1.130631
C	-2.755518	2.071184	1.544685
H	-3.230441	1.147531	1.892387
H	-1.936920	2.259909	2.246515
C	-3.753716	3.230860	1.525298
H	-3.272388	4.175550	1.258218
H	-4.199093	3.360293	2.515539
H	-4.568740	3.057327	0.817088
C	-3.328989	1.351337	-1.272372
H	-3.776817	2.321910	-1.511961
H	-2.838828	0.989590	-2.181930
C	-4.405019	0.371171	-0.803351
H	-3.983228	-0.610812	-0.583414
H	-5.160165	0.238147	-1.582570
H	-4.916534	0.726360	0.095204
C	2.545782	2.644467	1.178961
H	3.397452	1.978693	1.011556
H	2.886174	3.662319	0.961289
C	2.062148	2.530434	2.628519
H	1.237855	3.219564	2.834826
H	2.876028	2.782452	3.313585
H	1.713887	1.520947	2.855897
C	2.037680	2.388421	-1.733042
H	2.557395	1.452977	-1.955831
H	1.201592	2.436764	-2.436551
C	2.973306	3.588168	-1.898012
H	2.480137	4.532220	-1.648183
H	3.308464	3.659631	-2.936332
H	3.863254	3.496903	-1.269997
O	0.966727	-1.443618	-2.863698
O	-0.194442	0.226857	-1.895898
P	1.903264	-1.578162	0.093915
P	-1.294213	-2.136822	0.048535
P	-1.958211	1.645570	-0.068267
P	1.256509	2.191278	-0.066220
Mo	-0.039036	0.050802	0.259591
O	-0.058787	0.102976	1.943430

Sum of electronic and zero-point Energies= -2488.709075
Sum of electronic and thermal Free Energies= -2488.783167

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INT1

C	-3.406096	0.429692	0.790225
H	-3.449314	-0.170340	1.705529
H	-4.266315	1.104784	0.806778
C	-3.439209	-0.478951	-0.441860
H	-3.463988	0.119186	-1.359511
H	-4.331470	-1.111161	-0.446526
C	-1.955477	-2.176275	-2.252585
H	-2.967716	-2.552086	-2.436267
H	-1.806343	-1.310988	-2.905964
C	-0.912668	-3.254920	-2.549748
H	0.097569	-2.872688	-2.385224
H	-0.991492	-3.580605	-3.590425
H	-1.050002	-4.136451	-1.916492
C	-2.291994	-2.983564	0.546798
H	-1.377530	-3.583675	0.590585
H	-2.439873	-2.584507	1.556622
C	-3.482814	-3.846667	0.123732
H	-4.412041	-3.272014	0.078807
H	-3.634861	-4.655092	0.844399
H	-3.323019	-4.305598	-0.855304
C	-2.159567	2.825698	-0.264486
H	-1.226995	3.391285	-0.347491
H	-2.334395	2.389557	-1.254277
C	-3.305318	3.760351	0.131835
H	-3.101920	4.272956	1.075250
H	-4.254321	3.227340	0.235839
H	-3.446732	4.527785	-0.634598
C	-1.807864	2.130580	2.543891
H	-1.043198	2.915333	2.532268
H	-2.773819	2.623018	2.695879
C	-1.527658	1.138739	3.674449
H	-1.569287	1.647778	4.641360
H	-0.537861	0.690714	3.563314
H	-2.266369	0.331258	3.697937
C	3.587676	0.236651	-0.020501
H	3.756299	0.917281	0.820785
H	4.538464	-0.259842	-0.234186
C	3.074494	1.004466	-1.238830
H	3.004172	0.340093	-2.105275
H	3.746770	1.824829	-1.507342
C	1.677394	3.151247	0.126272
H	0.706152	3.482494	0.504987
H	3.388619	3.998558	-0.946352
H	1.845159	4.768586	-1.334983
C	2.831241	-2.549347	-0.362133
H	2.707737	-2.334508	-1.428285
H	3.897743	-2.720652	-0.182662
C	2.011155	-3.778204	0.033940
H	2.146995	-4.028086	1.090641
H	2.315904	-4.648507	-0.553469
H	0.946972	-3.605079	-0.141800
C	2.787062	-1.342759	2.296760
H	2.591905	-0.404952	2.826796
H	2.061359	-2.065970	2.683889
C	4.218145	-1.829981	2.538401
H	4.400769	-1.942972	3.610670
H	4.958914	-1.124037	2.152136
H	4.401392	-2.801228	2.071303
Mo	0.039833	-0.146983	0.182230
H	0.748100	0.746141	1.493542
H	-0.707102	0.331316	-1.270236
H	0.002099	-1.556929	1.276740
H	-0.496561	-0.911374	1.711294
H	0.587658	-1.108336	-1.119378
P	-1.804881	1.381543	0.852094
P	-1.898389	-1.520463	-0.527957
P	2.323827	-1.012901	0.533450
P	1.358610	1.643790	-0.912419
C	0.855375	2.323537	-2.559784
H	-0.065012	2.893116	-2.395612
H	1.622044	3.037150	-2.877549
C	0.637433	1.261735	-3.639945
H	1.559379	0.717936	-3.864781
H	0.299407	1.732477	-4.567177
H	-0.113012	0.531370	-3.328679
H	2.215712	2.778153	1.003903
C	2.427069	4.312694	-0.529986
H	2.632484	5.092613	0.208735

Sum of electronic and zero-point Energies= -2227.166127
Sum of electronic and thermal Free Energies= -2227.235301

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INT1'

C	2.236371	-2.784650	-0.200479
H	1.931110	-3.333480	-1.099014
H	3.255973	-3.105563	0.030723
C	1.283402	-3.102661	0.958337
H	1.658829	-2.667650	1.890069
H	1.196167	-4.183961	1.109874
C	-1.014843	3.099773	0.865048
H	-1.411344	2.775367	1.832509
H	-0.794840	4.168533	0.945844
C	-2.032499	2.827853	-0.246146
H	-1.684198	3.259074	-1.190754
H	-2.997885	3.288854	-0.017915
C	2.820798	-1.005359	-2.405927
H	3.710147	-1.643457	-2.448291
H	2.044665	-1.502843	-2.998943
C	3.111613	0.384460	-2.976927
H	2.220276	1.015577	-2.932988
H	3.429181	0.310215	-4.020441
H	3.912459	0.886219	-2.425011
C	3.607420	-0.236058	0.308978
H	3.571983	0.842956	0.129425
H	3.341575	-0.377126	1.362060
C	5.005861	-0.782224	0.014923
H	5.069212	-1.860817	0.182949
H	5.740620	-0.307413	0.671444
H	5.310255	-0.584557	-1.016020
C	-1.360203	-2.779611	2.160055
H	-2.405249	-2.541769	1.940606
H	-1.296065	-3.863488	2.313341
C	-0.903523	-2.019867	3.408061
H	0.136225	-2.243833	3.663839
H	-1.520368	-2.298424	4.266639
H	-0.990111	-0.941248	3.257632
C	-1.081373	-3.477288	-0.673674
H	-0.660510	-3.150903	-1.632927
H	-0.693429	-4.486540	-0.493211
C	-2.611311	-3.493473	-0.745331
H	-3.046208	-3.968165	0.137343
H	-2.946135	-4.054971	-1.621650
H	-3.017823	-2.482561	-0.822117
C	-3.673857	0.504215	0.501737
H	-3.730382	-0.587969	0.445559
H	-3.365559	0.731383	1.528778
C	-5.029065	1.136287	0.178500
H	-4.988418	2.229146	0.204212
H	-5.779352	0.821157	0.909232
H	-5.388532	0.838112	-0.810055
C	-2.890184	0.985090	-2.291070
H	-3.772100	1.631961	-2.343679
H	-2.109850	1.446557	-2.904239
C	-3.213774	-0.417171	-2.811150
H	-2.334319	-1.069529	-2.774612
H	-3.550938	-0.375548	-3.850377
H	-4.006773	-0.892406	-2.226542
C	1.454399	2.353792	2.186858
H	2.493130	2.058529	2.003266
H	1.463730	3.426529	2.405533
C	0.885429	1.576300	3.374240
H	-0.161418	1.832127	3.563677
H	1.450644	1.809226	4.280965
H	0.938017	0.499705	3.203173
C	1.522971	3.182251	-0.595686
H	2.383555	2.580352	-0.902590
H	0.893112	3.267334	-1.486795
C	1.969611	4.559759	-0.099794
H	1.127546	5.165120	0.248303
H	2.450804	5.110407	-0.913187
H	2.691265	4.485360	0.717447
P	2.200796	-0.965861	-0.658892
P	-0.395639	-2.350899	0.644758
P	-2.233125	0.998183	-0.557625
P	0.552548	2.129186	0.585489
Mo	-0.056304	-0.073247	-0.209677
H	0.847043	-0.265052	1.196154
H	-0.877491	0.232981	1.233658
H	0.234378	0.925203	-1.605757

Sum of electronic and zero-point Energies= -2225.967024
Sum of electronic and thermal Free Energies= -2226.036119

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INT2B

C	0.210457	0.989834	-2.145953
H	0.388170	-1.220893	-1.707377
C	2.282915	-2.763636	-0.250438
H	1.986179	-3.184626	-1.216846
H	3.270185	-3.166435	-0.011908
C	1.261509	-3.122457	0.829471
H	1.575374	-2.719824	1.798268
H	1.162386	-4.207046	0.942368
C	-1.061019	2.588310	1.586917
H	-1.168709	1.910804	2.438868
H	-0.942497	3.600253	1.985743
C	-2.268652	2.480192	0.663775
H	-2.200868	3.220035	-0.141190
H	-3.199807	2.680318	1.200483
C	3.272901	-0.733836	-2.069483
H	4.111238	-1.438333	-2.077870
H	2.578495	-1.045259	-2.855473
C	3.767832	0.692468	-2.326690
H	2.947084	1.413297	-2.290183
H	4.223223	0.763433	-3.317825
H	4.523014	0.996103	-1.595863
C	3.619225	-0.394706	0.783259
H	3.747636	0.682419	0.648692
H	3.166566	-0.528923	1.769312
C	4.985391	-1.084427	0.719548
H	4.914186	-2.158240	0.909213
H	5.650266	-0.664729	1.479994
H	5.468401	-0.945185	-0.250838
C	-1.351775	-2.734414	1.990839
H	-2.411366	-2.594950	1.764092
H	-1.215287	-3.801321	2.204142
C	-0.956423	-1.891829	3.202730
H	0.094891	-2.032007	3.470653
H	-1.557728	-2.173177	4.071753
H	-1.105923	-0.826686	3.010320
C	-1.097251	-3.669930	-0.714311
H	-0.453387	-3.665389	-1.599278
H	-0.981899	-4.645399	-0.227473
C	-2.553115	-3.447295	-1.125561
H	-3.228838	-3.494781	-0.266200
H	-2.869915	-4.220284	-1.830926
H	-2.679741	-2.478366	-1.611885
C	-3.542963	-0.154230	0.867417
H	-3.563763	-1.159464	0.437240
H	-3.092306	-0.253063	1.860592
C	-4.963090	0.408810	0.966039
H	-4.978415	1.421220	1.379037
H	-5.571308	-0.219005	1.623506
H	-5.455491	0.436745	-0.009026
C	-3.269133	1.228637	-1.686774
H	-4.129269	1.835144	-1.383415
H	-2.610807	1.879138	-2.272227
C	-3.723919	0.041460	-2.535276
H	-2.869235	-0.530971	-2.904202
H	-4.289169	0.393655	-3.402404
H	-4.372059	-0.636787	-1.972175
C	1.738809	2.210377	2.061894
H	2.727259	2.087476	1.614884

H	1.689035	3.240530	2.428005
C	1.539175	1.238034	3.226328
H	0.625859	1.463008	3.783332
H	2.376010	1.314466	3.925993
H	1.467884	0.204373	2.883148
C	0.893122	3.523846	-0.391360
H	1.793273	3.239961	-0.947678
H	0.090559	3.574616	-1.133837
C	1.083469	4.886058	0.280830
H	0.202947	5.187732	0.854984
H	1.252842	5.652353	-0.480612
H	1.946166	4.896855	0.951084
O	0.331427	1.585354	-3.130498
P	2.352639	-0.918494	-0.473027
P	-0.403519	-2.389436	0.433746
P	-2.321735	0.801640	-0.151012
P	0.488168	2.077821	0.700989
Mo	-0.034336	-0.121849	-0.474577
H	0.071569	-0.224536	1.253118
H	-1.250310	-0.743983	-1.465550

Sum of electronic and zero-point Energies= -2339.349168
Sum of electronic and thermal Free Energies= -2339.418681

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INT2

C	-0.359712	-0.023570	3.444373
H	-0.479267	-1.527610	1.335858
C	-2.021858	-2.797453	-0.840524
H	-1.951052	-3.494021	0.001242
H	-2.911163	-3.077397	-1.410569
C	-0.760655	-2.871263	-1.704190
H	-0.868399	-2.232837	-2.586353
H	-0.575722	-3.892975	-2.052078
C	0.748474	3.315503	-0.328588
H	1.190235	3.354665	-1.329200
H	0.385084	4.321714	-0.102889
C	1.782503	2.841746	0.689240
H	1.378005	2.894551	1.706329
H	2.681838	3.463559	0.662984
C	-3.376255	-1.437452	1.303130
H	-4.202445	-2.059845	0.944018
H	-2.803873	-2.043436	2.013033
C	-3.909692	-0.176052	1.986154
H	-3.093427	0.458611	2.342041
H	-4.534269	-0.435757	2.845204
H	-4.524413	0.421132	1.305228
C	-3.332098	-0.242259	-1.340033
H	-3.483249	0.774533	-0.965953
H	-2.744745	-0.148340	-2.259441
C	-4.690166	-0.887460	-1.629138
H	-4.590474	-1.905778	-2.013234
H	-5.228682	-0.307430	-2.384319
H	-5.318949	-0.926107	-0.736014
C	2.090334	-2.335044	-1.954342
H	2.985771	-1.985906	-1.430552
H	2.253926	-3.394737	-2.182190
C	1.872162	-1.544628	-3.246116
H	1.074736	-1.984639	-3.850937
H	2.781777	-1.545531	-3.853239
H	1.603081	-0.507001	-3.039755
C	1.035588	-3.736051	0.324233
H	0.141382	-3.882720	0.937356
H	1.111744	-4.594042	-0.354449
C	2.267893	-3.658306	1.222120
H	3.184638	-3.523553	0.640294
H	2.377563	-4.582928	1.795798
H	2.181654	-2.830916	1.930248
C	3.150184	1.153132	-1.221320
H	3.499396	0.137693	-1.425784
H	2.422553	1.374679	-2.007471
C	4.317718	2.141467	-1.262298
H	3.981733	3.175419	-1.145420
H	4.836023	2.074239	-2.223282
H	5.052437	1.937931	-0.478676
C	3.486072	0.739877	1.643408
H	4.115205	1.632958	1.719356
H	2.957917	0.635051	2.596794
C	4.343207	-0.496823	1.369369
H	3.723836	-1.386184	1.248016
H	5.029418	-0.677636	2.201063
H	4.947023	-0.374056	0.465734
C	-1.354840	2.491422	-2.103405
H	-2.406026	2.198484	-2.131273
H	-1.327958	3.578870	-2.229087
C	-0.580222	1.805978	-3.229610
H	0.476417	2.091267	-3.226446
H	-0.993880	2.091908	-4.200586
H	-0.625472	0.718760	-3.137057
C	-1.946270	2.928841	0.727845
H	-2.774046	2.220537	0.819918
H	-1.474043	2.967411	1.714432
C	-2.467577	4.309697	0.319192
H	-1.662117	5.040349	0.204581
H	-3.145303	4.692097	1.087593
H	-3.023719	4.271444	-0.620705
O	-0.245935	-0.804790	4.293727
O	-0.492056	0.809831	2.619231
P	-2.222857	-1.090876	-0.108589
P	0.698864	-2.242699	-0.733079
P	2.183394	1.051677	0.363349
P	-0.700464	2.139446	-0.402752
Mo	0.041346	-0.218237	0.372088
H	0.201054	-0.194293	-1.315068
H	1.182852	-0.877598	1.442617

Sum of electronic and zero-point Energies= -2414.556736
Sum of electronic and thermal Free Energies= -2414.630036

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INT3B

C	0.527487	1.387887	-1.828442
H	0.569450	-0.884835	-1.896841
C	3.163888	-1.025540	1.352745
H	3.638727	-1.951773	1.017603
H	3.933951	-0.456039	1.880529
C	1.990636	-1.345523	2.293811
H	1.752642	-0.476889	2.911801
H	2.255692	-2.168059	2.966912
C	-2.772251	1.620074	0.950434
H	-2.848598	0.893164	1.764380
H	-3.326810	2.512416	1.254095
C	-3.314866	1.033951	-0.353217
H	-3.326255	1.795041	-1.139881
H	-4.341237	0.675578	-0.239077
C	3.570531	-0.989714	-1.519250
H	4.615954	-1.088619	-1.207732
H	3.153568	-2.002619	-1.551021
C	3.474093	-0.331449	-2.897644
H	2.439110	-0.267578	-3.243175
H	4.038984	-0.909318	-3.633948
H	3.878711	0.684231	-2.890741
C	3.545202	1.539619	-0.064789
H	3.179824	2.153049	-0.894353
H	3.166476	2.007650	0.850459
C	5.073824	1.477418	-0.061635
H	5.458728	0.835067	0.736222
H	5.488818	2.476974	0.094671
H	5.466229	1.105415	-1.011342
C	-0.693713	-2.478912	2.611687
H	-1.446527	-3.048211	2.058352
H	-0.120072	-3.206236	3.197972

C	-1.376060	-1.467856	3.528040
H	-0.656618	-0.951092	4.166500
H	-2.098207	-1.968041	4.179298
H	-1.911029	-0.710634	2.948638
C	1.032084	-3.380478	0.560983
H	1.903689	-3.141152	-0.054967
H	1.387304	-4.026020	1.372783
C	-0.000143	-4.124279	-0.288101
H	-0.869428	-4.430121	0.300603
H	0.439816	-5.030988	-0.712492
H	-0.354022	-3.511366	-1.123101
C	-3.020761	-1.845288	-0.164598
H	-2.355159	-2.690672	-0.353409
H	-2.982037	-1.663764	0.914871
C	-4.446948	-2.180923	-0.608367
H	-5.137704	-1.348568	-0.447603
H	-4.827568	-3.032992	-0.037783
H	-4.487969	-2.450533	-1.666604
C	-2.670135	-0.486091	-2.731531
H	-3.762256	-0.495877	-2.811462
H	-2.317535	0.438583	-3.199903
C	-2.070015	-1.703411	-3.440328
H	-0.977679	-1.661421	-3.453056
H	-2.407990	-1.741777	-4.479074
H	-2.368646	-2.641456	-2.962174
C	-0.414070	2.772860	2.286053
H	0.562879	3.215254	2.059264
H	-1.092867	3.599237	2.516210
C	-0.308079	1.832243	3.480846
H	-1.285736	1.444228	3.775232
H	0.112279	2.357904	4.342683
H	0.338362	0.983013	3.253229
C	-1.039611	3.513730	-0.397314
H	0.002208	3.810618	-0.554766
H	-1.395637	3.173287	-1.372895
C	-1.871559	4.704651	0.085832
H	-2.921884	4.440250	0.237710
H	-1.843694	5.498115	-0.666408
H	-1.490519	5.128470	1.017795
O	0.796191	2.104699	-2.713501
P	2.653115	-0.078128	-0.186920
P	0.454812	-1.775655	1.327508
P	-2.220265	-0.356308	-0.939303
P	-0.975319	2.009191	0.696159
Mo	0.203103	0.102977	-0.386385
H	1.030510	0.915762	0.857585
H	0.277581	-1.473596	-1.368372

Sum of electronic and zero-point Energies= -2339.343802
Sum of electronic and thermal Free Energies= -2339.413615

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INT3B'

C	0.388203	1.012635	-1.951492
C	3.172245	-0.967034	1.418729
H	3.750647	-1.846655	1.123530
H	3.871474	-0.296962	1.926298
C	2.039643	-1.379272	2.379775
H	1.820953	-0.568176	3.078791
H	2.341254	-2.247368	2.975468
C	-2.662867	1.763778	0.904488
H	-2.742739	1.122232	1.787660
H	-3.162195	2.708467	1.139665
C	-3.288452	1.086049	-0.314033
H	-3.289952	1.768349	-1.170133
H	-4.327631	0.800180	-0.129729
C	3.484300	-1.149420	-1.452595
H	4.544218	-1.179789	-1.177989
H	3.110382	-2.174370	-1.364094
C	3.304034	-0.637095	-2.882873
H	2.255142	-0.655107	-3.187014
H	3.871504	-1.257592	-3.581823
H	3.656099	0.392337	-2.992065
C	3.487005	1.487062	-0.209681
H	3.089174	2.028708	-1.073768
H	3.137359	2.027643	0.676628
C	5.014852	1.428649	-0.252519
H	5.427663	0.846029	0.576727
H	5.430159	2.437788	-0.182103
H	5.377549	0.990554	-1.185633
C	-0.645558	-2.521910	2.742194
H	-1.414109	-3.060701	2.177431
H	-0.063373	-3.274325	3.286679
C	-1.297134	-1.528854	3.704097
H	-0.554252	-1.011222	4.316413
H	-1.985123	-2.042548	4.380845
H	-1.861792	-0.769496	3.155069
C	0.924415	-3.191416	0.389873
H	2.014767	-3.269813	0.379623
H	0.549267	-4.131426	0.806332
C	0.392784	-2.976784	-1.033076
H	-0.689468	-3.086490	-1.080076
H	0.828000	-3.681887	-1.748119
H	0.654363	-1.975520	-1.437589
C	-3.175900	-1.807884	0.034371
H	-2.550433	-2.698385	-0.085019
H	-3.140483	-1.559450	1.101475
C	-4.608876	-2.103779	-0.414323
H	-5.254722	-1.224966	-0.331794
H	-5.046766	-2.889795	0.207488
H	-4.642020	-2.447560	-1.451271
C	-2.737703	-0.578852	-2.605199
H	-3.828468	-0.606059	-2.696194
H	-2.393263	0.345978	-3.079129
C	-2.102534	-1.786578	-3.297622
H	-1.011030	-1.722665	-3.278038
H	-2.411569	-1.828636	-4.345210
H	-2.400644	-2.729972	-2.829389
C	-0.248313	2.803104	2.154794
H	0.746066	3.204429	1.927383
H	-0.893749	3.657378	2.379862
C	-0.182301	1.859291	3.351956
H	-1.174452	1.502086	3.638506
H	0.248410	2.368834	4.218376
H	0.435165	0.988272	3.126167
C	-0.831235	3.488655	-0.572656
H	0.224898	3.665438	-0.802161
H	-1.276182	3.138538	-1.508522
C	-1.508882	4.778452	-0.102754
H	-2.563033	4.623849	0.145202
H	-1.470232	5.526692	-0.899525
H	-1.015385	5.208822	0.771845
O	0.560086	1.573056	-2.968555
P	2.594450	-0.134944	-0.172092
P	0.452783	-1.737926	1.469664
P	-2.294653	-0.406320	-0.815006
P	-0.850613	2.035200	0.582422
Mo	0.148301	0.012394	-0.300701
H	1.033349	0.966434	0.767283

Sum of electronic and zero-point Energies= -2338.161755
Sum of electronic and thermal Free Energies= -2338.231654

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INT3

C	2.422683	-2.656297	0.034435
H	2.133783	-3.211771	-0.864430
H	3.442941	-2.961594	0.282095
C	1.457176	-2.965130	1.183725
H	1.791801	-2.479940	2.106059
H	1.404408	-4.041648	1.376839
C	-1.293147	2.858150	1.298853

H	-1.561287	2.381215	2.247238
H	-1.227258	3.934531	1.482673
C	-2.336979	2.544106	0.223631
H	-2.115275	3.108153	-0.689582
H	-3.335643	2.851066	0.546383
C	3.108818	-0.850827	-2.128170
H	3.986237	-1.506235	-2.122165
H	2.366669	-1.314820	-2.785362
C	3.481169	0.545803	-2.638045
H	2.615635	1.212047	-2.667893
H	3.873275	0.481592	-3.656071
H	4.251115	1.011594	-2.016094
C	3.676057	-0.063843	0.629547
H	3.639702	1.006931	0.401632
H	3.325722	-0.165060	1.662329
C	5.103381	-0.594810	0.479556
H	5.171487	-1.658124	0.724641
H	5.776712	-0.061547	1.156526
H	5.483219	-0.459505	-0.536188
C	-1.216862	-2.670638	2.308877
H	-2.264423	-2.473715	2.065064
H	-1.129413	-3.745666	2.505914
C	-0.802015	-1.856553	3.536263
H	0.238151	-2.044077	3.817733
H	-1.426759	-2.121781	4.393263
H	-0.911184	-0.785334	3.351765
C	-0.842155	-3.543735	-0.454874
H	-0.323172	-3.322298	-1.391648
H	-0.511732	-4.532556	-0.116055
C	-2.354535	-3.528297	-0.682605
H	-2.905438	-3.813341	0.217892
H	-2.622479	-4.237635	-1.470123
H	-2.692610	-2.541965	-1.000866
C	-3.591883	-0.043759	0.841716
H	-3.579259	-1.111558	0.603727
H	-3.179634	0.046734	1.852975
C	-5.020320	0.500944	0.778186
H	-5.065299	1.566843	1.017933
H	-5.654303	-0.021351	1.500301
H	-5.463226	0.359607	-0.210808
C	-3.185570	0.862689	-1.925749
H	-4.067932	1.499383	-1.798010
H	-2.499616	1.401713	-2.587148
C	-3.568003	-0.480126	-2.552026
H	-2.685111	-1.098672	-2.724551
H	-4.056508	-0.316259	-3.516137
H	-4.267286	-1.036692	-1.920747
C	1.421616	2.477267	2.292572
H	2.459077	2.351094	1.966688
H	1.297958	3.529589	2.568126
C	1.125128	1.575189	3.491672
H	0.092276	1.683944	3.835306
H	1.779292	1.835612	4.327947
H	1.284794	0.523364	3.244945
C	1.008801	3.369948	-0.456298
H	1.963655	2.958829	-0.801209
H	0.329746	3.311572	-1.313976
C	1.175030	4.823482	-0.003312
H	0.232512	5.253443	0.346431
H	1.520396	5.433946	-0.842138
H	1.911216	4.919696	0.798352
P	2.373398	-0.849817	-0.429035
P	-0.238607	-2.307866	0.786019
P	-2.340374	0.741659	-0.279255
P	0.363400	2.170777	0.809736
Mo	0.033594	-0.049076	-0.127336
H	0.950538	-0.205684	1.263545
H	-0.743842	0.136733	1.349470
H	0.344010	1.036158	-1.676227
C	0.010409	0.286652	-2.577685
O	0.008037	0.834532	-3.653520
O	-0.236617	-0.880527	-2.140460

Sum of electronic and zero-point Energies= -2414.572249
Sum of electronic and thermal Free Energies= -2414.643506

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INT4-I

C	-0.057332	-0.025538	-3.061904
H	-0.102308	-0.131378	-4.153137
C	2.670178	-2.359132	0.420973
H	2.510582	-3.112118	-0.357900
H	3.707996	-2.456437	0.748969
C	1.690688	-2.572003	1.575393
H	1.948145	-1.930699	2.425031
H	1.697414	-3.608183	1.929408
C	-1.306389	2.508828	1.397040
H	-1.514753	1.905186	2.286703
H	-1.230593	3.547472	1.733031
C	-2.416719	2.340386	0.356894
H	-2.219183	2.973228	-0.514714
H	-3.386031	2.643404	0.763146
C	3.204703	-0.916105	-2.025718
H	4.169994	-1.411056	-1.877965
H	2.568529	-1.600138	-2.592760
C	3.380836	0.405908	-2.780834
H	2.437230	0.951759	-2.867287
H	3.759789	0.225076	-3.790540
H	4.095434	1.064197	-2.277816
C	3.594694	0.394904	0.516842
H	3.445348	1.408094	0.131303
H	3.278622	0.409030	1.563031
C	5.075041	0.014746	0.419163
H	5.267225	-0.993429	0.795341
H	5.677638	0.704189	1.017765
H	5.442973	0.064276	-0.608081
C	-1.065941	-2.334791	2.505362
H	-2.097682	-2.413624	2.151646
H	-0.804681	-3.304823	2.943810
C	-0.950403	-1.222058	3.545722
H	0.056852	-1.163314	3.964944
H	-1.644352	-1.391181	4.373812
H	-1.180273	-0.247094	3.105424
C	-0.480127	-3.586281	-0.015168
H	0.251246	-3.652730	-0.826228
H	-0.351359	-4.472797	0.616979
C	-1.893022	-3.536728	-0.602120
H	-2.656889	-3.472909	0.178582
H	-2.096227	-4.440453	-1.183488
H	-2.012480	-2.679962	-1.268513
C	-3.669149	-0.260471	0.871463
H	-3.645839	-1.318939	0.593305
H	-3.228966	-0.202438	1.873186
C	-5.107594	0.262322	0.877914
H	-5.157656	1.324497	1.133684
H	-5.703210	-0.279682	1.617857
H	-5.589332	0.127611	-0.093794
C	-3.377456	0.746097	-1.869713
H	-4.305018	1.298092	-1.685802
H	-2.742522	1.368445	-2.505676
C	-3.664933	-0.597318	-2.545246
H	-2.741187	-1.135183	-2.775741
H	-4.202843	-0.441479	-3.484175
H	-4.281901	-1.246059	-1.916377
C	1.452580	2.422774	2.156484
H	2.472300	2.505066	1.774934
H	1.158680	3.426065	2.481647
C	1.390683	1.449483	3.332716
H	0.403941	1.448787	3.802246
H	2.119302	1.727545	4.099120
H	1.603599	0.425796	3.013940
C	0.781941	3.270092	-0.532913

H	1.795256	3.022464	-0.868476
H	0.139295	3.088068	-1.396057
C	0.701428	4.727866	-0.073337
H	-0.311113	5.002998	0.235575
H	0.978130	5.389360	-0.899181
H	1.378882	4.940437	0.757418
O	0.173060	-1.072769	-2.346373
O	-0.219783	1.074225	-2.489119
P	2.379967	-0.693976	-0.379248
P	-0.011461	-2.091787	0.997634
P	-2.470298	0.588859	-0.263026
P	0.355911	1.971312	0.723750
Mo	-0.055196	-0.174064	-0.440117

Sum of electronic and zero-point Energies= -2413.391949
Sum of electronic and thermal Free Energies= -2413.463052

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INT4

C	0.429114	-0.897459	-2.289858
C	2.610181	-2.375531	-0.224403
H	2.303712	-2.739499	-1.208880
H	3.650257	-2.670901	-0.067873
C	1.699658	-2.908931	0.880612
H	2.044241	-2.573240	1.864039
H	1.676170	-4.002843	0.899915
C	-1.125093	2.721895	1.419688
H	-0.966748	2.197791	2.366439
H	-1.091918	3.796077	1.626986
C	-2.455320	2.315366	0.792346
H	-2.691416	2.973969	-0.049169
H	-3.273156	2.417294	1.509907
C	3.566654	-0.055778	-1.657496
H	4.574657	-0.405752	-1.412579
H	3.214830	-0.627361	-2.519488
C	3.569479	1.438909	-1.977432
H	2.571505	1.771898	-2.276141
H	4.247635	1.649219	-2.808543
H	3.898231	2.045587	-1.127196
C	3.357524	-0.017492	1.263068
H	3.513582	1.060217	1.190434
H	2.668982	-0.169655	2.098687
C	4.694780	-0.713865	1.531465
H	4.565894	-1.777221	1.748104
H	5.182367	-0.261380	2.399699
H	5.383014	-0.623092	0.686864
C	-0.845231	-2.648665	2.237072
H	-1.925265	-2.611218	2.080865
H	-0.596372	-3.692122	2.464725
C	-0.440548	-1.736549	3.395977
H	0.638668	-1.761026	3.574180
H	-0.934179	-2.056637	4.317601
H	-0.716811	-0.697942	3.198958
C	-0.708224	-3.589340	-0.506878
H	-0.110350	-3.551589	-1.422727
H	-0.498158	-4.549850	-0.021548
C	-2.193562	-3.462692	-0.838033
H	-2.818283	-3.544488	0.056671
H	-2.495544	-4.261614	-1.520426
H	-2.402265	-2.512070	-1.326906
C	-3.438861	-0.403396	1.297768
H	-3.431840	-1.431155	0.924080
H	-2.883204	-0.411692	2.241311
C	-4.879002	0.068657	1.515970
H	-4.925893	1.092826	1.895619
H	-5.374644	-0.572353	2.250482
H	-5.462799	0.025292	0.593560
C	-3.516397	0.800581	-1.372749
H	-4.350619	1.428841	-1.041377
H	-2.937262	1.390013	-2.091264
C	-4.036980	-0.471173	-2.044835
H	-3.226079	-1.017149	-2.525936
H	-4.767321	-0.206375	-2.814571
H	-4.537914	-1.136195	-1.335368
C	1.720002	3.073192	1.135416
H	2.620262	2.771633	0.596458
H	1.603390	4.149046	0.968486
C	1.833774	2.789265	2.637871
H	1.040530	3.293085	3.194936
H	2.788571	3.159450	3.020152
H	1.774681	1.721479	2.859076
C	0.038810	3.224809	-1.248064
H	0.989725	3.172774	-1.786401
H	-0.688893	2.682551	-1.862124
C	-0.395015	4.684218	-1.068393
H	-1.374849	4.765405	-0.591109
H	-0.462538	5.171062	-2.044970
H	0.320186	5.252881	-0.468407
O	-0.827230	-0.556962	-2.255022
O	1.125763	-1.458540	-3.107711
P	2.441914	-0.531140	-0.271812
P	-0.031684	-2.276102	0.618657
P	-2.409906	0.575445	0.103630
P	0.286207	2.242911	0.316719
Mo	-0.003511	-0.075342	-0.416591
H	0.220001	-0.018406	1.310875

Sum of electronic and zero-point Energies= -2413.389960
Sum of electronic and thermal Free Energies= -2413.459720

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INT4'

C	-0.244140	1.462737	-2.077325
H	-0.008133	-1.229503	-1.960341
C	2.224135	-2.825421	-0.211070
H	1.931098	-3.269453	-1.168388
H	3.188179	-3.260501	0.063610
C	1.168545	-3.092119	0.860384
H	1.467735	-2.636417	1.809308
H	1.034356	-4.163477	1.042886
C	-1.045321	2.658265	1.470045
H	-1.293492	2.093383	2.374781
H	-0.898002	3.699414	1.772252
C	-2.160734	2.534117	0.434504
H	-1.931453	3.124717	-0.456902
H	-3.112019	2.896693	0.832329
C	3.317357	-0.849839	-2.052112
H	4.038443	-1.674178	-2.082161
H	2.597419	-1.011932	-2.859091
C	4.027255	0.495176	-2.245210
H	3.315646	1.321340	-2.220743
H	4.525124	0.511582	-3.218442
H	4.793920	0.664381	-1.484221
C	3.585034	-0.475211	0.822940
H	3.749937	0.593647	0.656567
H	3.084025	-0.561194	1.790936
C	4.924071	-1.218735	0.843445
H	4.801808	-2.272486	1.106639
H	5.587661	-0.773785	1.590343
H	5.434680	-1.170014	-0.121417
C	-1.490871	-2.777691	1.869521
H	-2.533339	-2.556658	1.638685
H	-1.420596	-3.865701	1.985561
C	-1.070960	-2.079444	3.162893
H	-0.063655	-2.368660	3.473721
H	-1.753520	-2.350407	3.972830
H	-1.084511	-0.993134	3.056381
C	-1.074425	-3.651643	-0.833523
H	-0.448613	-3.571660	-1.727863
H	-0.870092	-4.631024	-0.385903
C	-2.552766	-3.533688	-1.206920
H	-3.201199	-3.675088	-0.337733

H	-2.818999	-4.298624	-1.941025
H	-2.777782	-2.560597	-1.643791
C	-3.393827	-0.038523	1.115045
H	-3.606223	-1.037102	0.720766
H	-2.767263	-0.179962	1.999164
C	-4.704411	0.656195	1.494744
H	-4.533305	1.644401	1.929102
H	-5.238674	0.061186	2.241125
H	-5.368578	0.774862	0.635453
C	-3.510916	1.032168	-1.577422
H	-4.370039	1.581686	-1.179141
H	-2.993857	1.693212	-2.273882
C	-3.967397	-0.240572	-2.286211
H	-3.122254	-0.753613	-2.754558
H	-4.675980	0.007121	-3.081138
H	-4.466259	-0.941018	-1.609180
C	1.589956	1.927061	2.355513
H	2.631914	1.821110	2.043822
H	1.503101	2.915892	2.816788
C	1.218646	0.846885	3.370460
H	0.198248	0.975791	3.742273
H	1.888841	0.893148	4.233405
H	1.285168	-0.153584	2.938609
C	1.303894	3.368965	-0.147178
H	2.171700	2.950117	-0.666244
H	0.584275	3.621016	-0.930927
C	1.692892	4.620246	0.645518
H	0.848619	5.033902	1.204994
H	2.036282	5.397368	-0.042711
H	2.504071	4.425566	1.351284
O	-0.922530	2.307057	-2.620137
O	0.951485	1.058376	-2.145053
P	2.360334	-0.995735	-0.471794
P	-0.476143	-2.370137	0.372099
P	-2.335087	0.785632	-0.168835
P	0.554099	1.972634	0.818721
Mo	0.006435	-0.056862	-0.548487
H	-0.108421	-0.190630	1.146582
H	-0.802006	-0.885894	-1.967571

Sum of electronic and zero-point Energies= -2414.567755
Sum of electronic and thermal Free Energies= -2414.636727

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INT5-I

C	0.121724	-0.089972	2.801932
H	0.167393	-0.099440	3.897976
C	-2.577378	-2.565744	0.496020
H	-2.215482	-2.966031	1.449579
H	-3.621827	-2.873646	0.395230
C	-1.731998	-3.091175	-0.669463
H	-2.098870	-2.685774	-1.616292
H	-1.782828	-4.182749	-0.736937
C	1.384961	2.961646	-0.959879
H	1.602593	2.529249	-1.937985
H	1.410701	4.049442	-1.063793
C	2.416165	2.487589	0.066023
H	2.238029	2.966990	1.035251
H	3.426529	2.768771	-0.244079
C	-3.218860	-0.366349	2.257614
H	-4.153458	-0.934117	2.318321
H	-2.550672	-0.791471	3.014306
C	-3.462853	1.120957	2.525233
H	-2.525526	1.679700	2.498448
H	-3.914206	1.259858	3.511314
H	-4.146684	1.554066	1.789276
C	-3.659850	-0.069704	-0.627886
H	-3.636127	1.019781	-0.522012
H	-3.230677	-0.286424	-1.610050
C	-5.095407	-0.589066	-0.519573
H	-5.151990	-1.669321	-0.676886
H	-5.721062	-0.117255	-1.282383
H	-5.539402	-0.365322	0.454357
C	0.854216	-3.117306	-2.069904
H	1.804768	-2.580611	-2.136164
H	1.092053	-4.177519	-1.927636
C	0.055147	-2.937437	-3.365570
H	-0.860906	-3.533804	-3.357734
H	0.660150	-3.279061	-4.209627
H	-0.209403	-1.895790	-3.546597
C	0.719289	-3.746149	0.746247
H	0.290518	-3.492650	1.717190
H	0.357560	-4.741984	0.464895
C	2.248035	-3.728293	0.819097
H	2.703222	-4.058897	-0.118306
H	2.598757	-4.396434	1.610194
H	2.616659	-2.726759	1.042226
C	3.613747	-0.129485	-0.718551
H	3.575790	-1.201369	-0.495539
H	3.218746	-0.011527	-1.729958
C	5.046658	0.397149	-0.609821
H	5.109283	1.462103	-0.850336
H	5.687995	-0.130877	-1.321016
H	5.470628	0.250872	0.387141
C	3.173126	0.638111	2.065903
H	4.043177	1.298711	1.983603
H	2.481419	1.132688	2.754226
C	3.597672	-0.728347	2.606552
H	2.740424	-1.388309	2.747700
H	4.097091	-0.609479	3.572339
H	4.303088	-1.225812	1.935372
C	-1.424992	2.766753	-1.919849
H	-2.108309	1.919195	-1.999825
H	-2.017330	3.643132	-1.638012
C	-0.736529	3.001768	-3.268991
H	-0.079000	3.874569	-3.241372
H	-1.494878	3.184414	-4.035366
H	-0.148265	2.136188	-3.580296
C	-0.867413	3.552362	0.843671
H	-1.932132	3.339267	0.988209
H	-0.371256	3.259128	1.770327
C	-0.646358	5.037643	0.542272
H	0.416597	5.291530	0.526213
H	-1.115840	5.648108	1.318755
H	-1.078447	5.336757	-0.417239
O	0.294749	-1.150051	2.134328
O	-0.101569	0.984347	2.170061
P	-2.449355	-0.713368	0.612660
P	0.039602	-2.555623	-0.493988
P	2.359902	0.647656	0.394461
P	-0.313127	2.381754	-0.479501
Mo	-0.054549	-0.075731	0.176656
C	0.490493	0.023074	-1.841800
O	-0.780607	-0.204216	-1.806521
O	1.278619	0.197946	-2.748707

Sum of electronic and zero-point Energies= -2601.995038
Sum of electronic and thermal Free Energies= -2602.067630

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INT5

C	0.429898	1.201062	-2.075318
C	2.095307	-2.878275	0.084440
H	1.758120	-3.405454	-0.814247
H	3.063016	-3.305248	0.362401
C	1.070768	-3.030252	1.211579
H	1.403906	-2.491645	2.105123
H	0.953226	-4.082324	1.492068
C	-0.985500	2.714076	1.459367
H	-1.192733	2.047140	2.301060
H	-0.878691	3.725141	1.863472
C	-2.117269	2.646565	0.432468

H	-1.912579	3.314619	-0.411001
H	-3.066054	2.969961	0.869966
C	3.154507	-1.231596	-2.046129
H	3.907276	-2.024592	-1.975853
H	2.386312	-1.567901	-2.749316
C	3.791319	0.076071	-2.524281
H	3.057964	0.882820	-2.588221
H	4.217593	-0.058413	-3.521726
H	4.599920	0.400073	-1.862805
C	3.582747	-0.426065	0.735490
H	3.737779	0.614123	0.433055
H	3.134716	-0.396324	1.731838
C	4.918453	-1.175175	0.765070
H	4.802271	-2.201542	1.121922
H	5.613038	-0.671446	1.443057
H	5.388090	-1.211826	-0.220942
C	-1.556484	-2.511888	2.271173
H	-2.609141	-2.371287	2.011751
H	-1.453604	-3.551745	2.603153
C	-1.159703	-1.550590	3.394448
H	-0.123707	-1.701435	3.710644
H	-1.795811	-1.705089	4.270535
H	-1.254119	-0.508739	3.078889
C	-1.251928	-3.667029	-0.376654
H	-0.618418	-3.683501	-1.267462
H	-1.139092	-4.626110	0.141652
C	-2.704561	-3.432375	-0.798635
H	-3.385185	-3.423629	0.058596
H	-3.039126	-4.227950	-1.469970
H	-2.796601	-2.485987	-1.333830
C	-3.542482	0.103911	0.806437
H	-3.591217	-0.931283	0.457942
H	-3.108078	0.070152	1.810890
C	-4.941238	0.725868	0.830669
H	-4.924066	1.769760	1.156297
H	-5.582338	0.178309	1.527135
H	-5.416011	0.686953	-0.152809
C	-3.147288	1.232034	-1.876311
H	-4.035448	1.841896	-1.678161
H	-2.461979	1.841640	-2.473945
C	-3.510704	-0.049514	-2.629054
H	-2.618901	-0.649651	-2.826774
H	-3.977275	0.199068	-3.585890
H	-4.223284	-0.658277	-2.064228
C	1.767277	2.205996	2.177196
H	2.781926	2.059986	1.796600
H	1.728471	3.225324	2.573160
C	1.457122	1.208070	3.293778
H	0.487688	1.411116	3.756302
H	2.215830	1.279336	4.078357
H	1.430564	0.181223	2.925569
C	1.175580	3.645515	-0.271930
H	2.085314	3.340506	-0.801680
H	0.419356	3.790700	-1.050061
C	1.413602	4.955346	0.485244
H	0.532722	5.269851	1.052325
H	1.645884	5.755326	-0.223291
H	2.254117	4.880748	1.179065
O	-0.404713	-1.171752	-1.934339
O	0.628292	1.881246	-2.984490
P	2.298288	-1.101188	-0.412201
P	-0.577534	-2.326091	0.704854
P	-2.285429	0.936530	-0.266848
P	0.625056	2.162350	0.713799
Mo	-0.019697	-0.120695	-0.568459
H	0.094732	-0.045672	1.196966

Sum of electronic and zero-point Energies= -2413.391515
Sum of electronic and thermal Free Energies= -2413.463310

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INT6-I

C	-0.339334	1.384737	-1.991945
C	3.385353	-1.242619	-0.779734
H	3.162679	-1.621092	-1.782786
H	4.470867	-1.122403	-0.713006
C	2.871740	-2.206172	0.297540
H	3.094356	-1.810779	1.292261
H	3.377932	-3.173347	0.215004
C	-2.217285	1.766313	1.705472
H	-1.759477	1.235903	2.535918
H	-2.749385	2.629173	2.116896
C	-3.196983	0.833613	0.981858
H	-3.853141	1.409561	0.321501
H	-3.837271	0.338108	1.716118
C	3.187154	1.347406	-2.108865
H	4.259805	1.153865	-2.216362
H	2.691895	0.916491	-2.985197
C	2.917054	2.853078	-2.016849
H	1.858809	3.063145	-1.839092
H	3.197511	3.345583	-2.951119
H	3.494655	3.315558	-1.211844
C	3.313739	1.216008	0.826434
H	2.857506	2.207577	0.899110
H	2.948247	0.657008	1.690351
C	4.841013	1.318504	0.817208
H	5.314709	0.333334	0.813063
H	5.184583	1.841298	1.714101
H	5.210573	1.873740	-0.049237
C	0.583797	-3.487959	1.661567
H	-0.417577	-3.181204	1.966558
H	0.520253	-4.525597	1.318161
C	1.538698	-3.401225	2.856342
H	2.528887	-3.795850	2.614970
H	1.141172	-3.989516	3.687609
H	1.663189	-2.376561	3.215213
C	0.927770	-3.666242	-1.219957
H	1.325361	-3.168650	-2.108045
H	1.593892	-4.501605	-0.974625
C	-0.489847	-4.166574	-1.504043
H	-0.937561	-4.644960	-0.627106
H	-0.477802	-4.906748	-2.308780
H	-1.132781	-3.343396	-1.820079
C	-2.968074	-2.108954	0.609423
H	-2.459517	-2.880853	0.025604
H	-2.554353	-2.141081	1.617728
C	-4.481389	-2.341939	0.611198
H	-5.016874	-1.557571	1.154235
H	-4.706895	-3.290099	1.107222
H	-4.892679	-2.393892	-0.400061
C	-3.375476	-0.309415	-1.653459
H	-4.438502	-0.324037	-1.388953
H	-3.157307	0.692186	-2.038389
C	-3.067319	-1.366612	-2.714869
H	-2.010614	-1.355047	-2.992166
H	-3.657992	-1.177731	-3.615356
H	-3.318959	-2.371069	-2.362138
C	0.185493	3.496494	1.588832
H	1.021556	3.782277	0.940288
H	-0.398379	4.406439	1.759380
C	0.697576	2.953014	2.924696
H	-0.128328	2.683782	3.588772
H	1.287662	3.721454	3.431775
H	1.321647	2.072016	2.784724
C	-1.779465	3.560903	-0.526357
H	-1.013389	4.081671	-1.110897
H	-2.353926	2.971631	-1.246852
C	-2.704915	4.569168	0.161835
H	-3.554730	4.078122	0.642836
H	-3.107795	5.263007	-0.581150
H	-2.188945	5.166931	0.917677

O	0.173358	-0.935051	-2.054714
O	-0.483090	2.075234	-2.901978
P	2.557773	0.409025	-0.649691
P	1.025831	-2.449819	0.172262
P	-2.405868	-0.489043	-0.080285
P	-0.876265	2.356578	0.575271
Mo	0.070517	-0.062675	-0.579182
C	0.017784	-0.388619	2.640216
O	-1.073817	-0.937643	2.750228
O	0.556028	0.071094	1.552385
H	0.650308	-0.222053	3.531805

Sum of electronic and zero-point Energies= -2601.988271
Sum of electronic and thermal Free Energies= -2602.063346

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INT6

C	2.509512	-2.584164	-0.285257
H	2.240594	-2.976659	-1.271852
H	3.522636	-2.931090	-0.065313
C	1.513567	-3.060215	0.775446
H	1.799242	-2.692371	1.765675
H	1.475512	-4.153052	0.826927
C	-1.060546	2.593542	1.554619
H	-0.847714	1.991930	2.442273
H	-1.033585	3.646403	1.851489
C	-2.423251	2.213398	0.972605
H	-2.760966	2.973150	0.261005
H	-3.178105	2.159522	1.761380
C	3.337608	-0.357410	-1.979679
H	4.294651	-0.888765	-1.991651
H	2.710800	-0.771409	-2.774957
C	3.533653	1.145705	-2.195237
H	2.567995	1.658205	-2.218451
H	4.034456	1.334268	-3.148327
H	4.146457	1.594409	-1.406575
C	3.595276	-0.200302	0.947050
H	3.553202	0.887967	0.995961
H	3.144939	-0.559964	1.877343
C	5.049721	-0.662066	0.819804
H	5.138394	-1.750787	0.779608
H	5.625059	-0.321137	1.685166
H	5.527143	-0.252459	-0.074160
C	-1.159395	-2.880292	1.890025
H	-2.215987	-2.815048	1.620548
H	-0.946769	-3.941087	2.069553
C	-0.876853	-2.053760	3.145539
H	0.171921	-2.122263	3.446946
H	-1.487520	-2.415021	3.977830
H	-1.093919	-0.995938	2.981891
C	-0.752427	-3.619787	-0.885402
H	-0.107170	-3.471884	-1.757113
H	-0.552667	-4.624649	-0.494871
C	-2.218557	-3.480017	-1.294584
H	-2.894337	-3.672146	-0.455735
H	-2.463355	-4.199597	-2.080491
H	-2.421527	-2.481598	-1.683258
C	-3.613602	-0.482590	0.894175
H	-3.576189	-1.452475	0.390071
H	-3.241248	-0.644167	1.911386
C	-5.048676	0.051405	0.915617
H	-5.113642	1.041454	1.375714
H	-5.689621	-0.620171	1.493476
H	-5.467510	0.119477	-0.091410
C	-3.150981	1.050410	-1.564275
H	-4.100205	1.540946	-1.323457
H	-2.499760	1.810845	-2.005145
C	-3.358049	-0.095602	-2.552095
H	-2.401500	-0.544112	-2.830044
H	-3.831948	0.279790	-3.463247
H	-4.009515	-0.871942	-2.140233
C	1.794934	2.896128	1.243497
H	2.661528	2.657383	0.620090
H	1.707148	3.987573	1.246192
C	1.967749	2.377672	2.675008
H	1.222498	2.816571	3.343055
H	2.953803	2.648571	3.061943
H	1.863479	1.291599	2.723121
C	0.095675	3.409315	-1.049517
H	1.047072	3.393346	-1.592978
H	-0.638885	2.967975	-1.728491
C	-0.296801	4.842842	-0.681713
H	-1.282110	4.884079	-0.208895
H	-0.338573	5.461812	-1.582168
H	0.421585	5.306392	-0.000280
O	0.101206	-0.230814	-2.153045
P	2.450290	-0.730098	-0.406240
P	-0.183659	-2.399934	0.393564
P	-2.354606	0.583604	0.049037
P	0.314440	2.219527	0.364112
Mo	0.024550	-0.094841	-0.436903
H	0.495156	-0.175795	1.373863

Sum of electronic and zero-point Energies= -2300.077126
Sum of electronic and thermal Free Energies= -2300.146722

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TS1

C	2.619179	2.003493	-1.136065
H	2.768801	1.420105	-2.049602
H	3.004646	3.010135	-1.323155
C	3.332052	1.339820	0.041849
H	3.260839	1.964078	0.938736
H	4.395727	1.191925	-0.165119
C	3.142208	-0.609274	2.162751
H	4.226365	-0.453353	2.161340
H	2.700476	0.167640	2.794268
C	2.802998	-1.998806	2.707894
H	1.722759	-2.142314	2.791372
H	3.233279	-2.128519	3.704537
H	3.201638	-2.794166	2.071062
C	3.419910	-1.516334	-0.605702
H	2.874331	-2.458594	-0.495585
H	3.243599	-1.193772	-1.637384
C	4.912715	-1.706765	-0.329795
H	5.470907	-0.770103	-0.418197
H	5.340561	-2.408492	-1.051288
H	5.094183	-2.111975	0.668925
C	0.606138	3.511948	0.313701
H	-0.424965	3.499765	0.678782
H	1.223190	3.267682	1.184836
C	0.962581	4.889745	-0.248727
H	0.278101	5.192741	-1.045058
H	1.979726	4.919380	-0.650022
H	0.902823	5.644583	0.540433
C	0.101802	2.643253	-2.437792
H	-0.950716	2.886504	-2.259184
H	0.607733	3.578109	-2.699100
C	0.226322	1.631947	-3.579487
H	-0.238611	2.029421	-4.485820
H	-0.261011	0.688297	-3.324068
H	1.272032	1.414604	-3.815156
C	-3.152336	-1.511022	-0.417473
H	-3.414019	-0.923184	-1.304327
H	-3.796706	-2.394919	-0.410017
C	-3.345106	-0.678311	0.854027
H	-3.155874	-1.291646	1.741149
H	-4.370824	-0.306573	0.930753
C	-2.940097	2.016925	-0.143227
H	-2.229850	2.844289	-0.231118
H	-5.037740	1.739213	0.423459
H	-4.234906	3.067522	1.270318

C	-1.286479	-3.586882	0.364792
H	-1.474289	-3.321017	1.410432
H	-2.114886	-4.226453	0.043149
C	0.046415	-4.327666	0.231591
H	0.237272	-4.626055	-0.803361
H	0.041297	-5.233905	0.843090
H	0.881877	-3.703612	0.560382
C	-1.226984	-2.539643	-2.367229
H	-1.367541	-1.628057	-2.956914
H	-0.183365	-2.833741	-2.514121
C	-2.185536	-3.645063	-2.816200
H	-2.042640	-3.856348	-3.879568
H	-3.231949	-3.359317	-2.676350
H	-2.014516	-4.577917	-2.272160
Mo	0.081129	-0.144855	0.135730
H	-0.822821	0.159340	-1.278051
H	0.512245	0.826900	1.507803
H	0.552278	-1.565656	0.996971
H	0.857881	-0.819373	-1.233895
H	-0.210789	-1.074568	1.575411
P	0.787555	2.053556	-0.822562
P	2.524806	-0.285242	0.449215
P	-1.367983	-2.009333	-0.604496
P	-2.121089	0.723984	0.911739
C	-2.293938	1.385068	2.630577
H	-1.797928	2.362140	2.633135
H	-3.357515	1.562601	2.820382
C	-1.697681	0.488327	3.717399
H	-2.171683	-0.498005	3.733750
H	-1.848470	0.940282	4.701662
H	-0.626355	0.346336	3.561306
H	-3.006206	1.573706	-1.142997
C	-4.303249	2.541912	0.314682
H	-4.700611	3.247747	-0.420305

Sum of electronic and zero-point Energies= -2227.167198
Sum of electronic and thermal Free Energies= -2227.236354

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TS2B

C	2.319131	-2.710076	-0.073972
H	1.975582	-3.271257	-0.950872
H	3.342181	-3.039532	0.128421
C	1.404339	-2.989155	1.123323
H	1.785411	-2.485540	2.017692
H	1.360589	-4.060696	1.344810
C	-0.876655	3.162792	0.768368
H	-1.226881	2.895272	1.770912
H	-0.626226	4.227807	0.786187
C	-1.955186	2.863399	-0.269710
H	-1.628868	3.191305	-1.262946
H	-2.882467	3.396822	-0.043038
C	3.052711	-0.975771	-2.253524
H	3.990179	-1.536902	-2.184502
H	2.372878	-1.561384	-2.878216
C	3.281806	0.403408	-2.874335
H	2.341614	0.955530	-2.952828
H	3.705441	0.306268	-3.877568
H	3.980977	1.001947	-2.281365
C	3.618939	-0.144804	0.478206
H	3.604962	0.925781	0.251679
H	3.274776	-0.238979	1.513730
C	5.038260	-0.694303	0.321260
H	5.089969	-1.766439	0.529421
H	5.714542	-0.194714	1.020850
H	5.427960	-0.528163	-0.686222
C	-1.160659	-2.538698	2.440469
H	-2.222033	-2.343806	2.258414
H	-1.070265	-3.595038	2.721388
C	-0.653177	-1.633402	3.562021
H	0.408715	-1.795007	3.769772
H	-1.201919	-1.834721	4.486187
H	-0.789954	-0.581559	3.304646
C	-1.073624	-3.704694	-0.180861
H	-0.571421	-3.730626	-1.152331
H	-0.826649	-4.643680	0.327945
C	-2.589256	-3.579283	-0.360855
H	-3.115014	-3.706962	0.588822
H	-2.956311	-4.348675	-1.045411
H	-2.865322	-2.605474	-0.770418
C	-3.522932	0.672208	0.903753
H	-3.784448	-0.384668	0.778941
H	-2.976416	0.732982	1.850309
C	-4.778690	1.546142	0.945120
H	-4.538729	2.586755	1.179236
H	-5.461905	1.188516	1.720820
H	-5.323148	1.534263	-0.002520
C	-3.283968	1.019365	-1.988795
H	-3.868107	1.946428	-2.001013
H	-2.569258	1.086475	-2.815298
C	-4.214802	-0.182195	-2.173996
H	-3.670809	-1.127027	-2.167684
H	-4.732127	-0.106970	-3.134557
H	-4.978815	-0.226616	-1.393981
C	1.604407	2.450462	2.025498
H	2.653285	2.214970	1.822667
H	1.556884	3.527516	2.216293
C	1.116551	1.675676	3.247996
H	0.055134	1.852687	3.446368
H	1.674585	1.983100	4.136825
H	1.251256	0.601049	3.114757
C	1.606912	3.166159	-0.776118
H	2.449429	2.545340	-1.093532
H	0.952256	3.240413	-1.650366
C	2.089845	4.547979	-0.329444
H	1.268887	5.177251	0.026454
H	2.555439	5.068572	-1.171126
H	2.834332	4.483275	0.467842
P	2.287133	-0.907488	-0.568552
P	-0.311059	-2.326980	0.809403
P	-2.275184	1.034654	-0.422824
P	0.658337	2.153742	0.456971
Mo	-0.045844	-0.067311	-0.235820
H	0.847341	-0.161274	1.176069
H	-0.873836	0.174767	1.197780
H	0.119465	1.032530	-1.571517
C	-0.175289	-1.203997	-2.411984
O	-1.298507	-1.423882	-2.477873

Sum of electronic and zero-point Energies= -2339.284475
Sum of electronic and thermal Free Energies= -2339.354456

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TS2

C	-0.322875	0.975229	-3.099679
H	0.450345	-1.429498	-1.553190
C	2.064386	-2.934107	0.376509
H	1.960548	-3.512555	-0.547265
H	2.964640	-3.296078	0.879016
C	0.827046	-3.104932	1.259420
H	0.964405	-2.576674	2.207767
H	0.643283	-4.159793	1.488999
C	-0.698616	3.244003	0.617788
H	-1.066628	3.226391	1.648069
H	-0.345219	4.260648	0.424969
C	-1.813450	2.837860	-0.344140
H	-1.512558	3.000558	-1.385291
H	-2.715707	3.433124	-0.177331
C	3.401634	-1.320217	-1.591040
H	4.197044	-2.027379	-1.332351
H	2.801103	-1.784170	-2.379774
C	3.995547	0.001354	-2.084521

H	3.211813	0.696427	-2.393190
H	4.645612	-0.172012	-2.946528
H	4.602456	0.486125	-1.313191
C	3.394443	-0.465899	1.184971
H	3.568324	0.580870	0.917828
H	2.808887	-0.454583	2.110191
C	4.736778	-1.169744	1.401798
H	4.611265	-2.213142	1.701637
H	5.299023	-0.669940	2.195995
H	5.354937	-1.151297	0.500680
C	-2.006534	-2.596941	1.662522
H	-2.904802	-2.138535	1.238538
H	-2.205215	-3.672944	1.726467
C	-1.708035	-2.033372	3.054083
H	-0.929749	-2.612531	3.557561
H	-2.602498	-2.072675	3.682109
H	-1.375672	-0.994368	3.004804
C	-1.035783	-3.707704	-0.809517
H	-0.168884	-3.765953	-1.474266
H	-1.080986	-4.647505	-0.246258
C	-2.307452	-3.522128	-1.634501
H	-3.200213	-3.514522	-1.002475
H	-2.419441	-4.344346	-2.346794
H	-2.274975	-2.587912	-2.200621
C	-2.918521	0.972801	1.554800
H	-3.256399	-0.055032	1.704828
H	-2.100428	1.116456	2.265216
C	-4.059810	1.954785	1.828053
H	-3.726277	2.994857	1.776395
H	-4.464301	1.792547	2.831433
H	-4.883265	1.832536	1.119380
C	-3.614082	0.774874	-1.257124
H	-4.248977	1.663659	-1.179091
H	-3.226787	0.743977	-2.278141
C	-4.424962	-0.486685	-0.954683
H	-3.793818	-1.375807	-0.976496
H	-5.211344	-0.619741	-1.702477
H	-4.908687	-0.432379	0.024609
C	1.473600	2.240401	2.222398
H	2.519274	1.930258	2.173594
H	1.473871	3.310524	2.454010
C	0.739240	1.461171	3.313480
H	-0.300580	1.786785	3.413364
H	1.224309	1.619875	4.280559
H	0.730358	0.390029	3.099543
C	1.965294	2.969440	-0.556384
H	2.771388	2.264188	-0.775479
H	1.455416	3.143029	-1.508632
C	2.531238	4.279300	-0.000317
H	1.745135	4.995238	0.256070
H	3.170659	4.753485	-0.750071
H	3.138810	4.112789	0.892389
O	-1.275278	1.100749	-3.757749
O	0.722803	0.951732	-2.544382
P	2.271402	-1.151540	-0.130875
P	-0.655296	-2.360890	0.415016
P	-2.154666	1.015047	-0.140980
P	0.751249	2.064470	0.521638
Mo	-0.004106	-0.212274	-0.456289
H	-0.137701	-0.359656	1.228406
H	-1.164404	-0.720905	-1.589816

Sum of electronic and zero-point Energies= -2414.555902
Sum of electronic and thermal Free Energies= -2414.625505

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TS2-outer-sphere

C	-3.395933	0.440045	-1.369843
H	-3.153661	0.607892	-2.425208
H	-4.415041	0.045837	-1.334752
C	-3.266687	1.738143	-0.578885
H	-3.662900	1.620259	0.435061
H	-3.814251	2.561584	-1.048738
C	2.360876	-1.009041	1.926054
H	2.433186	0.033606	2.249198
H	2.691886	-1.646650	2.751068
C	3.207864	-1.248987	0.671561
H	3.375355	-2.318495	0.510381
H	4.190873	-0.780724	0.767052
C	-2.348324	-2.116964	-2.057590
H	-3.417935	-2.283465	-2.221494
H	-1.948760	-1.668082	-2.973531
C	-1.636812	-3.436473	-1.762843
H	-0.564525	-3.279722	-1.623358
H	-1.771490	-4.134822	-2.593100
H	-2.030109	-3.916140	-0.861532
C	-3.053957	-1.535108	0.725786
H	-2.366584	-2.254281	1.178719
H	-3.134524	-0.710716	1.443074
C	-4.415936	-2.188235	0.481495
H	-5.136957	-1.489072	0.049707
H	-4.836457	-2.544225	1.426405
H	-4.339332	-3.048898	-0.187909
C	-1.518350	3.691158	0.660034
H	-0.583494	4.226586	0.491590
H	-2.341692	4.312111	0.286722
C	-1.693502	3.374088	2.147320
H	-2.539873	2.704473	2.332849
H	-1.878706	4.296387	2.703814
H	-0.794568	2.910609	2.556588
C	-0.965415	2.760723	-2.116214
H	-1.756913	2.496706	-2.823912
H	-0.835120	3.845697	-2.152848
C	0.341153	2.028565	-2.454014
H	1.161328	2.395280	-1.838540
H	0.618467	2.134260	-3.507317
H	0.199027	0.921849	-2.341426
C	3.622277	0.552203	-1.644090
H	4.459533	-0.103810	-1.912511
H	3.190221	0.905940	-2.585538
C	4.117257	1.730391	-0.806609
H	3.343524	2.481916	-0.660106
H	4.955260	2.210201	-1.319746
H	4.476619	1.413977	0.176935
C	2.465941	-2.014737	-2.040525
H	3.513295	-2.333068	-2.100300
H	1.902426	-2.835138	-1.587041
C	1.911113	-1.707684	-3.433132
H	0.862170	-1.401061	-3.375308
H	1.966474	-2.596278	-4.067487
H	2.474923	-0.914366	-3.931117
C	-0.229638	-1.211968	3.217902
H	-1.196428	-1.720810	3.139711
H	0.391506	-1.817347	3.885146
C	-0.406612	0.197935	3.784581
H	0.499082	0.799972	3.684288
H	-0.668248	0.141675	4.844864
H	-1.210557	0.726206	3.268908
C	0.500132	-3.124903	1.187504
H	-0.550868	-3.365081	1.004888
H	1.000784	-3.266503	0.226321
C	1.090163	-4.064913	2.242544
H	2.142782	-3.846189	2.441833
H	1.031874	-5.100436	1.895105
H	0.548996	-4.006636	3.189727
P	-2.167800	-0.821307	-0.747394
P	-1.478249	2.200066	-0.422990
P	2.374600	-0.583849	-0.863866
P	0.567271	-1.301479	1.551390
Mo	0.004133	0.210198	-0.279827
H	-0.841621	0.380164	1.162995
H	1.135240	1.367582	0.574160

H	-0.019193	-1.118429	-1.324725
C	1.611278	2.540361	1.177994
O	1.949129	2.224767	2.292249
O	1.532460	3.445522	0.377988

Sum of electronic and zero-point Energies= -2414.521606
Sum of electronic and thermal Free Energies= -2414.591660

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TS3B

C	-0.320424	-1.939176	-1.492960
H	-0.581742	-0.141634	-2.019807
C	-3.199024	0.612189	1.361849
H	-3.784902	1.478593	1.043970
H	-3.880929	-0.034476	1.920741
C	-2.033408	1.057906	2.263809
H	-1.681753	0.215325	2.863545
H	-2.365020	1.844222	2.947798
C	3.179102	-0.962022	0.817165
H	3.265487	-0.052556	1.421312
H	3.920444	-1.673327	1.192384
C	3.394519	-0.648273	-0.665251
H	3.373990	-1.567296	-1.259904
H	4.365321	-0.176456	-0.837966
C	-3.618122	0.529811	-1.526428
H	-4.666050	0.583559	-1.212210
H	-3.245361	1.557106	-1.591205
C	-3.493178	-0.164177	-2.885041
H	-2.452791	-0.195617	-3.219950
H	-4.073502	0.372246	-3.640429
H	-3.863877	-1.192449	-2.850812
C	-3.436228	-1.968071	-0.036880
H	-3.051161	-2.569335	-0.866274
H	-3.016258	-2.405976	0.874923
C	-4.966015	-1.994582	-0.009499
H	-5.375106	-1.371503	0.791651
H	-5.319577	-3.015731	0.157849
H	-5.394973	-1.650649	-0.954012
C	0.643728	2.412778	2.362728
H	1.407372	1.666498	2.583550
H	1.136545	3.181871	1.758078
C	0.096498	3.024058	3.655030
H	-0.684586	3.764049	3.458476
H	0.896287	3.530772	4.202419
H	-0.323089	2.259821	4.314889
C	-1.385065	3.156561	0.480032
H	-2.314492	2.829449	0.008102
H	-1.668419	3.810756	1.312465
C	-0.547674	3.924169	-0.540137
H	0.383816	4.300555	-0.107708
H	-1.105133	4.788914	-0.910898
H	-0.302540	3.291734	-1.397953
C	2.637856	2.140403	-0.832982
H	1.837058	2.834145	-1.093978
H	2.700231	2.149197	0.260616
C	3.960324	2.593619	-1.457120
H	4.787803	1.923466	-1.208986
H	4.227474	3.588547	-1.089386
H	3.892624	2.654697	-2.546116
C	2.235710	0.369647	-3.124630
H	3.296509	0.505799	-3.360355
H	1.965328	-0.650624	-3.415762
C	1.378370	1.386312	-3.883959
H	0.314994	1.240697	-3.677177
H	1.529708	1.279190	-4.961167
H	1.637560	2.414744	-3.614760
C	1.276288	-1.937185	2.845043
H	0.366364	-2.539749	2.942807
H	2.113658	-2.575182	3.142824
C	1.206425	-0.719980	3.762656
H	2.105681	-0.101891	3.687361
H	1.121183	-1.042224	4.804112
H	0.341001	-0.096193	3.538178
C	1.596930	-3.367261	0.390608
H	0.585627	-3.783779	0.434720
H	1.835274	-3.283405	-0.672837
C	2.593760	-4.297111	1.087559
H	3.607585	-3.886509	1.096080
H	2.635603	-5.250947	0.554286
H	2.306253	-4.514249	2.118669
O	-0.479284	-2.863912	-2.182800
P	-2.645176	-0.300243	-0.185415
P	-0.602015	1.633698	1.215753
P	2.025117	0.447738	-1.288769
P	1.460139	-1.625616	1.028077
Mo	-0.196458	-0.306424	-0.381972
H	-0.922529	-1.191004	0.911292
H	-0.570714	1.086591	-1.302458

Sum of electronic and zero-point Energies= -2339.344278
Sum of electronic and thermal Free Energies= -2339.413876

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TS3

C	-2.281708	-2.754118	-0.085673
H	-1.971286	-3.319295	0.800735
H	-3.294827	-3.085329	-0.330541
C	-1.316700	-3.023534	-1.246296
H	-1.676949	-2.540130	-2.160098
H	-1.239195	-4.096702	-1.450109
C	1.010905	3.073825	-1.087530
H	1.328694	2.724631	-2.075506
H	0.828166	4.149654	-1.166809
C	2.086806	2.773038	-0.043566
H	1.810032	3.218063	0.918939
H	3.048131	3.208469	-0.330872
C	-3.002617	-1.039726	2.125037
H	-3.885620	-1.686890	2.097066
H	-2.267113	-1.551129	2.755852
C	-3.353799	0.333224	2.706434
H	-2.486716	0.998484	2.712717
H	-3.710212	0.234213	3.735053
H	-4.146088	0.819113	2.129383
C	-3.638744	-0.193552	-0.588219
H	-3.630934	0.873885	-0.344804
H	-3.311845	-0.268571	-1.630691
C	-5.044200	-0.771584	-0.411484
H	-5.082356	-1.837328	-0.652691
H	-5.746694	-0.262459	-1.077454
H	-5.411105	-0.645237	0.610290
C	1.305831	-2.587384	-2.444431
H	2.355524	-2.376679	-2.218644
H	1.236662	-3.653734	-2.690688
C	0.844224	-1.725906	-3.620771
H	-0.201646	-1.915483	-3.879526
H	1.446004	-1.942884	-4.507513
H	0.944555	-0.663391	-3.389144
C	1.074358	-3.603624	0.256094
H	0.527524	-3.537574	1.201448
H	0.849825	-4.584413	-0.178649
C	2.576985	-3.454645	0.505439
H	3.155710	-3.627263	-0.406023
H	2.914652	-4.180378	1.250347
H	2.817685	-2.457299	0.877056
C	3.566094	0.376457	-0.914465
H	3.663274	-0.703106	-0.757415
H	3.116257	0.493607	-1.906568
C	4.934126	1.058209	-0.847874
H	4.862910	2.136264	-1.016844
H	5.596384	0.652132	-1.617863
H	5.420972	0.901974	0.118291
C	3.164497	1.013596	1.911248

H	3.960527	1.759473	1.811613
H	2.455184	1.418365	2.641162
C	3.744691	-0.314783	2.402087
H	2.966783	-1.064856	2.560383
H	4.268477	-0.171699	3.351173
H	4.464683	-0.727619	1.689783
C	-1.556934	2.424320	-2.242070
H	-2.600342	2.208998	-1.990127
H	-1.503995	3.491414	-2.481419
C	-1.120639	1.591140	-3.446812
H	-0.071907	1.766973	-3.704514
H	-1.722770	1.850997	-4.321869
H	-1.238024	0.523199	-3.253853
C	-1.432674	3.272829	0.525402
H	-2.306977	2.710719	0.869371
H	-0.762127	3.331286	1.388880
C	-1.835472	4.669232	0.046051
H	-0.980829	5.235783	-0.335022
H	-2.258653	5.240356	0.877273
H	-2.591448	4.628782	-0.741953
P	-2.278158	-0.952433	0.419105
P	0.367806	-2.312122	-0.874112
P	2.266314	0.942132	0.283933
P	-0.570346	2.170094	-0.693833
Mo	0.003426	-0.051375	0.093948
H	-0.904670	-0.240165	-1.301238
H	0.749685	0.272079	-1.375141
H	-0.304707	1.021223	1.449928
C	0.205278	-0.230790	2.904046
O	0.067758	0.436949	3.849853
O	0.433586	-1.137597	2.157492

Sum of electronic and zero-point Energies= -2414.561989
Sum of electronic and thermal Free Energies= -2414.632992

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TS4-I

C	-0.138691	0.135087	-2.958630
H	-0.212191	0.201743	-4.050559
C	2.693160	-2.314665	-0.872633
H	2.330598	-2.559722	-1.876943
H	3.751115	-2.588747	-0.834415
C	1.891397	-3.070067	0.192338
H	2.292752	-2.849551	1.185981
H	1.950518	-4.154262	0.052015
C	-1.360215	2.622253	1.546630
H	-1.252542	2.064327	2.480287
H	-1.444459	3.675654	1.830709
C	-2.592646	2.152755	0.768804
H	-2.835539	2.887314	-0.005324
H	-3.463889	2.092061	1.425610
C	3.356072	0.225443	-2.095083
H	4.328737	-0.268472	-2.188315
H	2.775494	-0.044438	-2.983191
C	3.514406	1.745548	-2.012265
H	2.536174	2.224707	-1.934208
H	4.009934	2.132291	-2.906983
H	4.118543	2.041271	-1.148795
C	3.583093	-0.106109	0.792002
H	3.498206	0.970513	0.966348
H	3.135957	-0.584293	1.670262
C	5.053277	-0.507496	0.651584
H	5.172008	-1.586261	0.519538
H	5.611386	-0.226347	1.549630
H	5.528663	-0.011488	-0.198712
C	-0.652367	-3.283571	1.680424
H	-1.505735	-2.660444	1.962732
H	-1.074502	-4.245722	1.373340
C	0.282497	-3.509002	2.875212
H	1.035999	-4.267272	2.650755
H	-0.292244	-3.861444	3.735887
H	0.816868	-2.604893	3.179784
C	-0.565787	-3.610204	-1.191412
H	-0.092198	-3.299523	-2.124213
H	-0.226528	-4.626611	-0.959340
C	-2.085895	-3.560590	-1.333982
H	-2.594365	-3.875299	-0.417273
H	-2.411242	-4.231178	-2.134166
H	-2.413659	-2.553384	-1.586410
C	-3.496106	-0.639031	0.801818
H	-3.380872	-1.619449	0.329893
H	-3.093625	-0.740554	1.814998
C	-4.975040	-0.247595	0.864840
H	-5.122946	0.725200	1.342018
H	-5.535963	-0.983235	1.448918
H	-5.427053	-0.202776	-0.128721
C	-3.299721	0.876537	-1.669571
H	-4.197841	1.431517	-1.377655
H	-2.674468	1.570842	-2.242362
C	-3.679834	-0.327377	-2.533816
H	-2.796685	-0.869087	-2.874330
H	-4.238209	0.002611	-3.415004
H	-4.318148	-1.029330	-1.989768
C	1.530267	3.119686	1.489940
H	2.426281	3.048093	0.864098
H	1.299788	4.185275	1.588594
C	1.790887	2.523620	2.876080
H	0.899799	2.573201	3.509971
H	2.576782	3.089837	3.383204
H	2.116120	1.484104	2.817570
C	-0.065696	3.591060	-0.867468
H	0.886366	3.615982	-1.404807
H	-0.779914	3.156955	-1.568240
C	-0.497033	4.999173	-0.450611
H	-1.492168	5.005538	0.002337
H	-0.538682	5.642446	-1.334147
H	0.197615	5.463058	0.254434
O	-0.426774	-0.932003	-2.343039
O	0.238680	1.122260	-2.264261
P	2.450572	-0.478283	-0.640420
P	0.107171	-2.521096	0.147154
P	-2.333377	0.498781	-0.115818
P	0.155177	2.355350	0.502094
Mo	0.068223	-0.017048	-0.351587
O	0.552188	-0.270849	2.109075
C	-0.414472	-0.282376	2.784763
O	-1.322578	-0.299970	3.508563

Sum of electronic and zero-point Energies= -2601.956285
Sum of electronic and thermal Free Energies= -2602.029393

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TS4

C	-0.222092	1.428404	-2.119643
H	0.186351	-1.284516	-1.765463
C	2.152496	-2.883624	-0.281576
H	1.847922	-3.267129	-1.260762
H	3.100603	-3.362339	-0.024349
C	1.085127	-3.166145	0.773778
H	1.394810	-2.759430	1.741362
H	0.926443	-4.240849	0.910619
C	-0.953625	2.723989	1.456795
H	-1.190719	2.171595	2.371683
H	-0.788804	3.766575	1.745021
C	-2.089072	2.601611	0.444751
H	-1.867049	3.173057	-0.461084
H	-3.026804	2.987653	0.853020
C	3.328684	-0.858412	-2.016442
H	4.043007	-1.687413	-2.067945
H	2.614882	-0.983205	-2.834838
C	4.050926	0.486943	-2.146594
H	3.344269	1.316833	-2.099418

H	4.560478	0.539446	-3.112343
H	4.808918	0.621001	-1.369878
C	3.561537	-0.615159	0.879895
H	3.763410	0.452954	0.757696
H	3.040676	-0.721484	1.835363
C	4.877569	-1.399290	0.892950
H	4.719155	-2.459394	1.106227
H	5.538317	-1.007298	1.671286
H	5.408463	-1.322793	-0.059180
C	-1.522950	-2.766990	1.862536
H	-2.566481	-2.517721	1.667051
H	-1.480552	-3.856717	1.976886
C	-1.042743	-2.081214	3.141640
H	-0.036303	-2.401985	3.423408
H	-1.708598	-2.329469	3.972566
H	-1.024454	-0.994875	3.033589
C	-1.225647	-3.639440	-0.859946
H	-0.641876	-3.546012	-1.780417
H	-1.016739	-4.629194	-0.437827
C	-2.717744	-3.493889	-1.160435
H	-3.327980	-3.644926	-0.265417
H	-3.027902	-4.240191	-1.896518
H	-2.945374	-2.509915	-1.569236
C	-3.352702	0.057520	1.188943
H	-3.573684	-0.947288	0.816795
H	-2.713299	-0.070370	2.066212
C	-4.654886	0.767202	1.569662
H	-4.474579	1.767550	1.971533
H	-5.177808	0.195990	2.342102
H	-5.332458	0.861650	0.717893
C	-3.504807	1.105213	-1.514829
H	-4.329667	1.698251	-1.106139
H	-2.979279	1.729921	-2.237612
C	-4.031094	-0.160589	-2.185375
H	-3.218846	-0.714820	-2.663086
H	-4.749500	0.103691	-2.966045
H	-4.541513	-0.825803	-1.481972
C	1.685500	1.969351	2.303222
H	2.717714	1.817439	1.978355
H	1.643568	2.969758	2.745546
C	1.287573	0.922814	3.344489
H	0.285116	1.108244	3.740543
H	1.981533	0.948455	4.189212
H	1.292016	-0.085414	2.926396
C	1.366876	3.384874	-0.222407
H	2.223347	2.949498	-0.746815
H	0.635325	3.623062	-0.999864
C	1.777189	4.650493	0.535868
H	0.944164	5.083536	1.097493
H	2.117931	5.409197	-0.173819
H	2.596219	4.463725	1.234720
O	-0.911658	2.264980	-2.654185
O	0.958357	1.006173	-2.182593
P	2.352511	-1.052833	-0.457269
P	-0.548063	-2.387897	0.329805
P	-2.310914	0.849245	-0.125537
P	0.624809	2.015215	0.783486
Mo	-0.003944	-0.097330	-0.558994
H	-0.094219	-0.245747	1.136043
H	-1.019917	-0.742048	-1.757595

Sum of electronic and zero-point Energies= -2414.566195
Sum of electronic and thermal Free Energies= -2414.635363

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TS5-I

C	-0.185120	-0.069312	-2.689532
H	-0.265586	-0.022818	-3.784521
C	3.156227	-1.651146	-0.891499
H	2.793972	-2.032509	-1.852329
H	4.249026	-1.642275	-0.939913
C	2.663956	-2.531882	0.258825
H	3.017937	-2.135323	1.214263
H	3.045960	-3.553878	0.165868
C	-2.163426	2.507029	1.018196
H	-2.291981	1.986871	1.971300
H	-2.489755	3.540111	1.165816
C	-2.994194	1.830933	-0.078620
H	-2.862802	2.353471	-1.032224
H	-4.061037	1.870066	0.160325
C	3.049364	0.788770	-2.375920
H	4.106104	0.531024	-2.507892
H	2.501291	0.243629	-3.151705
C	2.833991	2.295231	-2.524789
H	1.773644	2.541998	-2.460586
H	3.205708	2.636185	-3.494935
H	3.370895	2.857470	-1.754800
C	3.564414	0.919249	0.513028
H	3.291498	1.979458	0.463942
H	3.201797	0.561011	1.480483
C	5.077914	0.745366	0.371845
H	5.378908	-0.298322	0.495882
H	5.595042	1.325641	1.141142
H	5.443201	1.089402	-0.600192
C	0.450786	-3.392289	1.964026
H	-0.623812	-3.279616	2.137023
H	0.637482	-4.463292	1.822126
C	1.234657	-2.876276	3.176576
H	2.298221	-3.115790	3.094296
H	0.861645	-3.358362	4.084193
H	1.134682	-1.797378	3.296281
C	0.320080	-3.863657	-0.876376
H	0.548890	-3.480987	-1.872401
H	0.946362	-4.744996	-0.695715
C	-1.164796	-4.225486	-0.771218
H	-1.398740	-4.698310	0.186514
H	-1.446437	-4.924888	-1.562867
H	-1.791760	-3.337144	-0.874166
C	-3.599799	-0.953942	0.721714
H	-3.262093	-1.990277	0.614032
H	-3.354247	-0.664620	1.745288
C	-5.107792	-0.843166	0.478827
H	-5.463545	0.186886	0.571387
H	-5.641740	-1.437242	1.225445
H	-5.398972	-1.213896	-0.506458
C	-3.255559	-0.199672	-2.074121
H	-4.268675	0.214068	-2.022370
H	-2.699665	0.440035	-2.764178
C	-3.290261	-1.647833	-2.568014
H	-2.284292	-2.057006	-2.667076
H	-3.777806	-1.695393	-3.545715
H	-3.855983	-2.293049	-1.890492
C	0.543200	3.118518	2.043293
H	1.600987	2.909722	1.853487
H	0.419301	4.206227	2.014032
C	0.141747	2.573478	3.416827
H	-0.906085	2.784297	3.646784
H	0.746795	3.055278	4.189978
H	0.303211	1.497912	3.481939
C	-0.130208	3.729007	-0.708978
H	0.952383	3.887302	-0.763742
H	-0.421555	3.286326	-1.662831
C	-0.856932	5.056131	-0.471793
H	-1.941837	4.940009	-0.542460
H	-0.557965	5.784713	-1.230663
H	-0.628013	5.489861	0.505857
O	-0.051491	-1.172805	-2.101552
O	-0.235202	0.996313	-2.006789
P	2.509105	0.084956	-0.750634
P	0.809311	-2.562491	0.340252
P	-2.516071	0.055079	-0.392275
P	-0.360727	2.421921	0.585493

Mo	0.041353	-0.083500	0.056711
C	-0.804397	-0.382193	1.832423
O	0.932064	-0.046269	1.676358
O	-1.269718	-0.528205	2.899463

Sum of electronic and zero-point Energies= -2601.961127
Sum of electronic and thermal Free Energies= -2602.035144

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TS5

C	0.796850	-0.412170	-2.312391
C	1.888520	-3.020667	0.021348
H	1.829384	-3.217266	-1.054358
H	2.748455	-3.575372	0.405779
C	0.596169	-3.427637	0.725483
H	0.689516	-3.285009	1.805598
H	0.351417	-4.480700	0.554875
C	-0.553028	3.307030	0.457581
H	-0.707390	3.264015	1.539206
H	-0.274028	4.336350	0.212925
C	-1.824214	2.879491	-0.273646
H	-1.689209	2.927710	-1.359366
H	-2.664788	3.530973	-0.019178
C	3.666399	-0.947756	-0.817262
H	4.335303	-1.786534	-0.596826
H	3.349973	-1.053219	-1.858329
C	4.402338	0.376691	-0.612499
H	3.774632	1.230957	-0.872400
H	5.286511	0.415361	-1.254054
H	4.741708	0.500656	0.420279
C	2.721060	-1.032420	1.966880
H	2.954843	0.022438	2.122497
H	1.844063	-1.234367	2.590041
C	3.909026	-1.904424	2.381182
H	3.678266	-2.970784	2.315939
H	4.181913	-1.694080	3.419104
H	4.791336	-1.712380	1.764814
C	-2.147684	-2.672347	1.340354
H	-3.020146	-2.112655	0.994823
H	-2.410347	-3.735553	1.290383
C	-1.785445	-2.267660	2.773111
H	-1.029459	-2.932219	3.199617
H	-2.667068	-2.324578	3.417130
H	-1.398205	-1.246410	2.809613
C	-1.309003	-3.280299	-1.418483
H	-0.411156	-3.324279	-2.043476
H	-1.540322	-4.306280	-1.107682
C	-2.468380	-2.675716	-2.209909
H	-3.401965	-2.713803	-1.643833
H	-2.620984	-3.244983	-3.130636
H	-2.261445	-1.638794	-2.484730
C	-2.871095	1.156610	1.842564
H	-3.255345	0.153620	2.052612
H	-1.996120	1.279759	2.488797
C	-3.933408	2.216329	2.146864
H	-3.530944	3.228785	2.056173
H	-4.301277	2.101979	3.170454
H	-4.793389	2.137939	1.476139
C	-3.704331	0.849324	-0.977889
H	-4.218685	1.811659	-1.072218
H	-3.291525	0.608419	-1.962394
C	-4.688397	-0.225020	-0.512171
H	-4.206265	-1.198613	-0.409880
H	-5.493113	-0.338657	-1.243540
H	-5.148071	0.027428	0.447040
C	2.079442	2.543108	1.378354
H	2.984183	1.971287	1.162009
H	2.349773	3.600262	1.294413
C	1.556328	2.240563	2.788038
H	0.800722	2.967026	3.096489
H	2.372948	2.296884	3.512926
H	1.109874	1.245252	2.848443
C	1.541170	2.921402	-1.519925
H	2.234303	2.193531	-1.949120
H	0.688242	2.949753	-2.207149
C	2.201428	4.296423	-1.394809
H	1.540883	5.034026	-0.929776
H	2.461085	4.672685	-2.388014
H	3.123651	4.251227	-0.809502
O	-0.790121	0.286806	-2.177415
O	1.285626	-0.601219	-3.363095
P	2.145506	-1.191624	0.211496
P	-0.799605	-2.364716	0.114604
P	-2.225474	1.106769	0.107525
P	0.862043	2.172732	0.037809
Mo	-0.045030	-0.083104	-0.493466
H	-0.144025	-0.000313	1.269854

Sum of electronic and zero-point Energies= -2413.374377
Sum of electronic and thermal Free Energies= -2413.444812

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TS6-II

C	-1.352828	-0.598399	-2.126206
C	0.777712	3.365111	-0.862005
H	1.140078	3.159646	-1.874777
H	0.533302	4.430482	-0.814644
C	1.837458	2.997651	0.183989
H	1.464286	3.183162	1.194875
H	2.730762	3.612714	0.041419
C	-1.612721	-2.345229	1.702024
H	-1.055112	-1.870379	2.507728
H	-2.447871	-2.895967	2.144260
C	-0.696332	-3.285909	0.915753
H	-1.269741	-3.860940	0.181339
H	-0.225682	-4.009683	1.586544
C	-1.799401	2.834431	-2.116420
H	-1.744772	3.919998	-2.250659
H	-1.321571	2.375806	-2.987795
C	-3.256647	2.379435	-1.990232
H	-3.327203	1.308705	-1.777480
H	-3.794833	2.565062	-2.922940
H	-3.777545	2.917958	-1.193809
C	-1.632221	3.104370	0.797257
H	-2.568653	2.553592	0.912772
H	-1.021239	2.867402	1.669481
C	-1.905627	4.608660	0.702006
H	-0.980461	5.188224	0.653052
H	-2.447609	4.938861	1.592334
H	-2.514211	4.866017	-0.169029
C	3.372626	0.952363	1.586227
H	2.755163	1.160574	2.461400
H	3.626985	-0.110638	1.629233
C	4.641215	1.811661	1.637490
H	5.325869	1.586031	0.816587
H	5.175566	1.624905	2.573312
H	4.408973	2.879467	1.602170
C	3.496328	1.175942	-1.315233
H	2.919466	1.374883	-2.220675
H	4.195939	2.005175	-1.172024
C	4.243336	-0.151184	-1.460890
H	4.832911	-0.390864	-0.570631
H	4.932208	-0.109509	-2.309030
H	3.545219	-0.969077	-1.644941
C	2.194549	-2.619964	0.924187
H	2.959409	-2.056350	0.382050
H	2.029800	-2.100992	1.872133
C	2.647577	-4.065886	1.143919
H	1.895343	-4.657614	1.673059
H	3.555909	-4.080118	1.752423
H	2.874272	-4.570753	0.201235
C	0.807784	-3.476191	-1.531366

H	0.935594	-4.505412	-1.177975
H	-0.157892	-3.430212	-2.045846
C	1.936867	-3.079446	-2.482371
H	1.813557	-2.052135	-2.834198
H	1.940391	-3.740017	-3.353404
H	2.914668	-3.167281	-2.000201
C	-3.429414	-0.032892	1.654747
H	-3.789031	0.795688	1.035418
H	-4.294235	-0.677831	1.836281
C	-2.880849	0.472836	2.990200
H	-2.535108	-0.350671	3.619887
H	-3.673297	0.990875	3.537432
H	-2.056304	1.172177	2.863109
C	-3.448663	-1.939022	-0.507588
H	-3.984472	-1.183450	-1.092493
H	-2.849700	-2.504226	-1.226119
C	-4.438612	-2.883805	0.180757
H	-3.929633	-3.707074	0.688592
H	-5.101742	-3.324021	-0.569048
H	-5.070642	-2.374755	0.912315
O	0.901175	0.164919	-2.153817
O	-1.984389	-0.832139	-3.058943
P	-0.769224	2.366545	-0.655598
P	2.293458	1.193363	0.090620
P	0.634069	-2.394700	-0.037722
P	-2.260192	-1.011848	0.594567
Mo	0.001647	-0.032923	-0.680696
H	0.002151	0.214470	1.194331
C	0.409529	0.424520	2.660660
O	0.633501	-0.670187	3.093855
O	0.377201	1.611923	2.826751

Sum of electronic and zero-point Energies= -2601.956164
Sum of electronic and thermal Free Energies= -2602.030577

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TS6-I

C	-0.287942	1.597041	2.384205
C	-2.728055	-2.307596	0.803346
H	-2.419532	-2.518467	1.832714
H	-3.778299	-2.599225	0.712889
C	-1.855213	-3.070546	-0.199907
H	-2.173769	-2.848193	-1.221389
H	-1.951441	-4.151451	-0.057769
C	1.380543	2.414404	-1.776825
H	1.122332	1.798745	-2.634480
H	1.534085	3.434333	-2.140577
C	2.663582	1.871633	-1.133246
H	3.143543	2.646061	-0.526674
H	3.370831	1.586324	-1.915365
C	-3.489905	0.267029	1.943923
H	-4.434574	-0.275909	2.054431
H	-2.906190	0.083347	2.851610
C	-3.748990	1.765451	1.757004
H	-2.822535	2.312757	1.558052
H	-4.197625	2.190603	2.658210
H	-4.433710	1.952758	0.925280
C	-3.512295	-0.110373	-0.968814
H	-3.457335	0.972010	-1.111487
H	-2.950493	-0.547328	-1.797118
C	-4.969201	-0.579407	-0.955732
H	-5.047343	-1.667550	-0.887159
H	-5.465899	-0.275491	-1.881353
H	-5.532652	-0.148007	-0.123694
C	0.802021	-3.371550	-1.482760
H	1.552916	-2.661353	-1.828122
H	1.332724	-4.243242	-1.087145
C	-0.087801	-3.798677	-2.654476
H	-0.800654	-4.574963	-2.365152
H	0.535221	-4.202859	-3.456658
H	-0.652339	-2.960633	-3.070663
C	0.461748	-3.624519	1.399806
H	-0.119562	-3.292482	2.263701
H	0.168472	-4.655874	1.171193
C	1.955302	-3.542704	1.717927
H	2.571153	-3.862469	0.871533
H	2.198353	-4.193669	2.562063
H	2.236315	-2.524814	1.989504
C	3.600907	-0.897996	-0.613822
H	3.435237	-1.782857	0.007441
H	3.263989	-1.138934	-1.622681
C	5.079392	-0.498805	-0.601328
H	5.261590	0.411992	-1.179194
H	5.680195	-1.293959	-1.051560
H	5.454941	-0.337174	0.412258
C	3.204486	1.007390	1.555544
H	4.189710	1.404670	1.288032
H	2.601123	1.858211	1.888195
C	3.327835	-0.025962	2.674948
H	2.348876	-0.411924	2.968511
H	3.791984	0.427223	3.555331
H	3.954765	-0.869674	2.372206
C	-1.474111	3.072199	-1.564843
H	-2.353910	2.965814	-0.920798
H	-1.300434	4.147203	-1.675848
C	-1.726293	2.446295	-2.939398
H	-0.881082	2.613749	-3.612256
H	-2.605937	2.904726	-3.399933
H	-1.893009	1.372473	-2.866363
C	0.335634	3.781572	0.562531
H	-0.579171	3.961492	1.138904
H	1.078661	3.414586	1.276149
C	0.830878	5.086440	-0.068542
H	1.810344	4.961487	-0.537124
H	0.933326	5.854207	0.703299
H	0.142773	5.474250	-0.824306
O	0.152814	-0.747104	2.058097
O	-0.536235	1.820511	3.474592
P	-2.533606	-0.480986	0.551741
P	-0.063607	-2.581209	-0.033531
P	2.415957	0.389556	-0.013502
P	-0.046318	2.376482	-0.598852
Mo	-0.034767	-0.099176	0.490108
C	0.215345	-0.459769	-2.731041
O	1.441232	-0.491759	-2.798929
O	-0.502117	-0.289456	-1.664149
H	-0.394905	-0.569630	-3.646892

Sum of electronic and zero-point Energies= -2601.980620
Sum of electronic and thermal Free Energies= -2602.054717

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TS6

C	0.239504	1.589675	-2.697628
C	2.522054	-2.579991	-0.040176
H	2.259613	-3.067155	-0.985203
H	3.536477	-2.896997	0.214376
C	1.521376	-2.957443	1.054308
H	1.791708	-2.485664	2.004443
H	1.497955	-4.039778	1.216898
C	-1.255079	2.340487	1.797953
H	-1.218168	1.583033	2.585197
H	-1.258543	3.320491	2.284205
C	-2.493137	2.144607	0.923817
H	-2.577087	2.953605	0.191019
H	-3.407383	2.162503	1.523089
C	3.283077	-0.571852	-2.003086
H	4.150221	-1.239812	-2.041959
H	2.552088	-0.934564	-2.732015
C	3.695389	0.869380	-2.316463
H	2.858670	1.561823	-2.184259
H	4.034324	0.952717	-3.352160

H	4.513668	1.204548	-1.672875
C	3.671195	-0.038888	0.844436
H	3.713779	1.031931	0.629439
H	3.229958	-0.136847	1.839475
C	5.082322	-0.633512	0.811279
H	5.090216	-1.687503	1.099303
H	5.727347	-0.099799	1.514889
H	5.536830	-0.551141	-0.179488
C	-1.169114	-2.757632	2.099340
H	-2.221297	-2.761032	1.805351
H	-0.918037	-3.790890	2.367430
C	-0.952076	-1.827429	3.293401
H	0.094285	-1.812470	3.610871
H	-1.554192	-2.159031	4.144140
H	-1.229008	-0.799374	3.050040
C	-0.703691	-3.682437	-0.605598
H	-0.022006	-3.605189	-1.457020
H	-0.535531	-4.653754	-0.125914
C	-2.145659	-3.557523	-1.098250
H	-2.867253	-3.668526	-0.282869
H	-2.363978	-4.338417	-1.831824
H	-2.302596	-2.592772	-1.582208
C	-3.633630	-0.550230	0.803575
H	-3.533780	-1.534152	0.338673
H	-3.293747	-0.658507	1.838980
C	-5.091377	-0.084357	0.753538
H	-5.220747	0.918352	1.170943
H	-5.721473	-0.763105	1.335072
H	-5.475419	-0.075199	-0.269403
C	-3.174069	0.989621	-1.645437
H	-4.141301	1.455773	-1.429075
H	-2.534517	1.764373	-2.079999
C	-3.330535	-0.179401	-2.618280
H	-2.361797	-0.631153	-2.846046
H	-3.773871	0.169593	-3.554748
H	-3.988536	-0.953310	-2.211796
C	1.608512	2.518499	2.024319
H	2.568078	2.440288	1.508298
H	1.492742	3.568778	2.307769
C	1.585492	1.639461	3.278361
H	0.723647	1.873047	3.908971
H	2.484758	1.810847	3.876284
H	1.529324	0.578336	3.025145
C	0.292637	3.640562	-0.307158
H	1.247887	3.622594	-0.843822
H	-0.473417	3.471011	-1.068474
C	0.074498	4.997299	0.367971
H	-0.899348	5.054443	0.862113
H	0.105938	5.792898	-0.381835
H	0.843430	5.222019	1.111077
O	-0.089845	-0.904949	-1.961188
O	0.214840	1.552556	-3.834480
P	2.458350	-0.750224	-0.357861
P	-0.179412	-2.363955	0.586067
P	-2.386905	0.544177	-0.025971
P	0.286442	2.131760	0.781753
Mo	0.012689	-0.161664	-0.389586
H	0.333951	-0.247575	1.396311

Sum of electronic and zero-point Energies= -2413.383185
Sum of electronic and thermal Free Energies= -2413.456044

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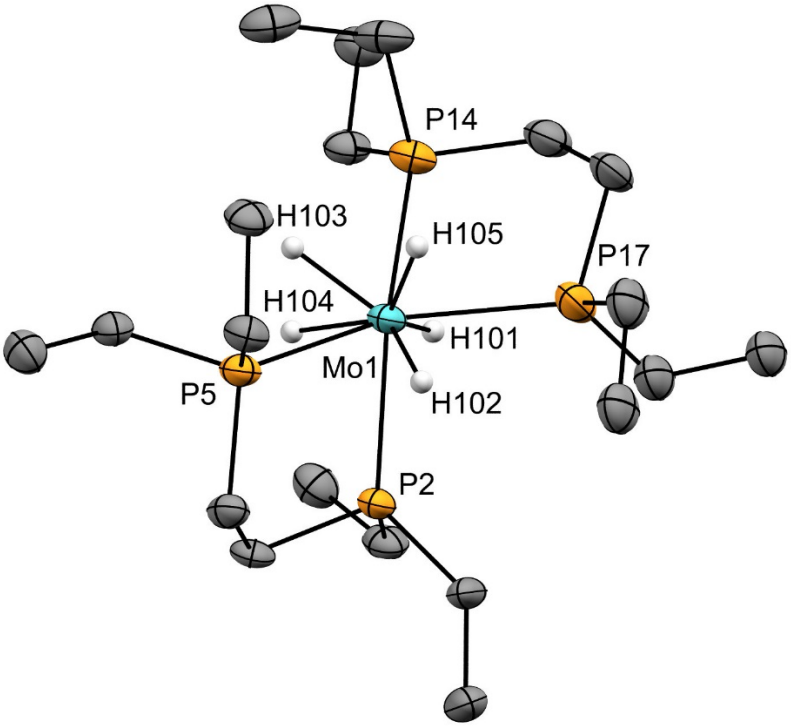
TS7

C	-2.229495	-2.675864	0.419132
H	-2.098290	-2.626698	1.504768
H	-3.185188	-3.171822	0.229347
C	-1.070390	-3.419737	-0.241654
H	-1.216199	-3.482612	-1.325338
H	-0.983783	-4.442782	0.139114
C	0.986906	3.330307	0.144179
H	1.288645	3.622861	-0.865719
H	0.761772	4.248708	0.694151
C	2.098181	2.532341	0.825957
H	1.845920	2.313309	1.867869
H	3.043990	3.081319	0.819995
C	-3.590327	-0.223237	0.951655
H	-4.302599	-1.033433	1.142304
H	-3.090793	-0.027689	1.904553
C	-4.339435	1.006588	0.434005
H	-3.668165	1.835491	0.205335
H	-5.046663	1.358494	1.189935
H	-4.909295	0.781698	-0.470723
C	-3.113124	-1.018826	-1.841429
H	-3.263236	0.019141	-2.157279
H	-2.359322	-1.421631	-2.523632
C	-4.418921	-1.812949	-1.916206
H	-4.258744	-2.875082	-1.712502
H	-4.845917	-1.735975	-2.920072
H	-5.169178	-1.445955	-1.210305
C	1.718911	-3.445693	-1.001882
H	2.718023	-3.291194	-0.585414
H	1.489326	-4.510556	-0.875791
C	1.683095	-3.047353	-2.478665
H	0.693111	-3.204133	-2.915955
H	2.398137	-3.646750	-3.048386
H	1.928617	-1.991473	-2.612416
C	0.905799	-3.098311	1.774734
H	0.037195	-2.844013	2.387007
H	0.950286	-4.191994	1.710570
C	2.175370	-2.546132	2.419052
H	3.064787	-2.752819	1.818661
H	2.325180	-3.009409	3.397947
H	2.099648	-1.469407	2.572786
C	2.941762	1.318403	-1.712903
H	3.178351	0.364736	-2.194608
H	2.092116	1.722970	-2.269081
C	4.137341	2.272344	-1.759856
H	3.890974	3.253929	-1.345575
H	4.451090	2.424264	-2.796376
H	4.997811	1.882304	-1.209855
C	3.802173	0.221447	0.860894
H	4.482301	1.063851	1.025746
H	3.468023	-0.107596	1.846738
C	4.520643	-0.901288	0.111675
H	3.832420	-1.699489	-0.171656
H	5.301529	-1.338955	0.738882
H	4.996114	-0.535179	-0.801777
C	-1.515147	3.103797	-1.341734
H	-2.518649	2.669749	-1.327180
H	-1.616865	4.162613	-1.082012
C	-0.893565	2.942755	-2.732604
H	0.096156	3.406159	-2.788752
H	-1.523211	3.435655	-3.478129
H	-0.791882	1.890465	-3.006499
C	-1.402329	2.680263	1.606642
H	-2.135911	1.897360	1.796633
H	-0.629391	2.561455	2.371285
C	-2.048279	4.065251	1.691372
H	-1.338307	4.867244	1.468543
H	-2.424635	4.235486	2.703653
H	-2.892724	4.162524	1.004142
P	-2.299640	-0.921233	-0.178371
P	0.524608	-2.511304	0.061400
P	2.316038	0.891251	-0.013577
P	-0.548103	2.285321	0.009569
Mo	0.049558	-0.101768	-0.483366
H	-0.232965	-0.199631	1.394990
C	-0.209470	-0.091330	3.101417
O	0.717287	0.624779	3.308371
O	-1.137443	-0.782071	3.372022
O	-0.047692	-0.248762	-2.181211

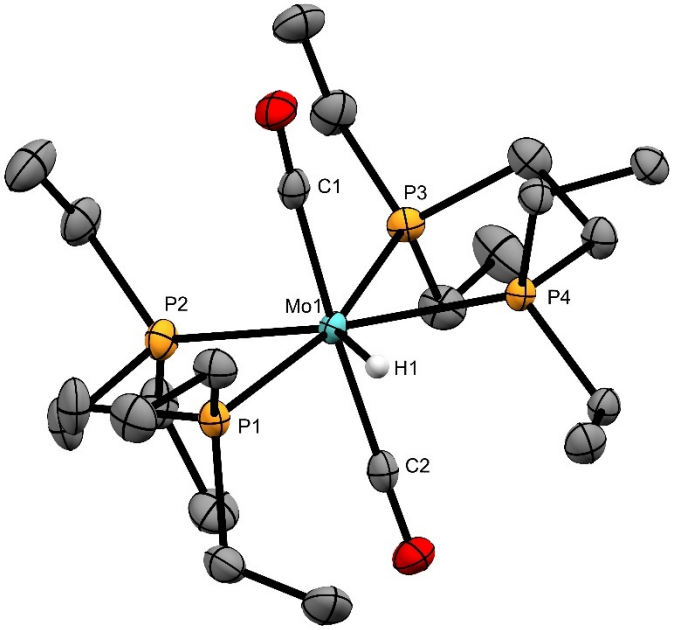
Sum of electronic and zero-point Energies= -2488.654229
Sum of electronic and thermal Free Energies= -2488.727678

IV. Crystallographic data

IV.1. $[Mo(depe)_2H_5][B(C_6H_5)_4]$ (1.BPh_4) – Molecular structure



IV.2. $[Mo(depe)_2(CO)_2H][B(C_6H_5)_4]$ (4.BPh_4) – Molecular structure



IV.3. $[Mo(depe)_2H_5][B(C_6H_5)_4]$ (1.BPh_4) – Tables

Crystal Data	
Chemical Formula	$C_{20}H_{53}MoP_4 \cdot C_{24}H_{20}B$
M_r	828.79
Crystal system, space group	monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	13.9330 (3), 16.7804 (4), 19.2576 (5)
α, β, γ (°)	90, 95.774 (2), 90
V (Å^3)	4479.61 (19)
Z	4
Radiation type	Cu *K*α radiation, λ = 1.54184 Å
μ (mm^{-1})	3.96
Crystal size (mm)	0.10 × 0.07 × 0.02
Data Collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix
Absorption Correction	multi-scan CrysAlisPro 1.171.41.120a (Rigaku Oxford Diffraction, 2021) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.774, 1.000
No. of measured, independent and observed [I > 2σ(I)] reflections	30591, 7622, 5143
R_{int}	0.150
θ_{max} (°)	65.1
Refinement	
R[F^2 > 2σ(F^2)], wR(F^2), S	**0.078**, 0.280, 1.16
No. of reflections	7622
No. of parameters	479
H-atom treatement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.32, −1.94

IV.4. $[Mo(depe)_2(HCOO)H_2][B(C_6H_5)_4]$ (3.BPh_4) – Tables

Crystal Data	
Chemical Formula	$2(C_{21}H_{49}MoO_2P_4)\cdot 2(C_{24}H20B)\cdot C_4H_8O$
M_r	1817.37
Crystal system, space group	triclinic, P -1
Temperature (K)	100
a, b, c (Å)	15.332 (3), 15.378 (3), 23.433 (5)
α, β, γ (°)	101.532 (6), 99.455 (5), 108.140 (5)
V ($Å^3$)	4989.8 (16)
Z	2
Radiation type	Mo *K*α radiation, λ = 0.71073 Å
μ (mm^{-1})	0.43
Crystal size (mm)	0.10 × 0.08 × 0.02
Data Collection	
Diffractometer	Bruker Kappa Apex2 diffractometer
Absorption Correction	multi-scan *SADABS* (Siemens, 1996)
T_{min}, T_{max}	0.676, 0.740
No. of measured, independent and observed [I > 2σ(I)] reflections	105966, 16987, 11913
R_{int}	0.124
θ_{max} (°)	24.7
Refinement	
R[F^2 > 2σ(F^2)], wR(F^2), S	**0.099**, 0.225, 1.19
No. of reflections	16987
No. of parameters	1016
H-atom treatement	H atoms parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å−3)	1.21, -1.73

IV.5. $[Mo(depe)_2(CO)_2H][B(C_6H_5)_4]$ (4.BPh_4) – Tables

Crystal Data	
Chemical Formula	$C_{22}H_{49}MoO_2P_4 \cdot C_{24}H_{20}B$
M_r	884.64
Crystal system, space group	monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	21.5133 (2), 18.8557 (2), 22.6970 (2)
α, β, γ (°)	90, 99.354 (1), 90
V (Å^3)	9084.57 (15)
Z	8
Radiation type	Cu $K\alpha$ radiation, λ = 1.54184 Å
μ (mm^{-1})	3.96
Crystal size (mm)	0.20 × 0.15 × 0.04
Data Collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix
Absorption Correction	multi-scan CrysAlisPro 1.171.41.120a (Rigaku Oxford Diffraction, 2021) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.432, 1.000
No. of measured, independent and observed [I > 2σ(I)] reflections	162235, 17141, 15649
R_{int}	0.051
θ_{max} (°)	70.1
Refinement	
R[F^2 > 2σ(F^2)], wR(F^2), S	**0.030**, 0.075, 1.02
No. of reflections	17141
No. of parameters	1000
H-atom treatement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.93, −0.79

IV.6. [Mo(depe)$_2$(^{i}PrNCHN^{i}Pr)H$_2$] (7.BPh$_4$) – Tables

Crystal Data	
Chemical Formula	$C_{27}H_{63}MoN_2P_4 \cdot C_{24}H_{20}B$
M_r	954.82
Crystal system, space group	monoclinic, $P2_1$
Temperature (K)	100
a, b, c (Å)	11.2886 (1), 25.1547 (2), 20.9232 (2)
α, β, γ (°)	90, 90.436 (1), 90
V (Å^3)	5941.21 (9)
Z	4
Radiation type	Cu *K*α radiation, λ = 1.54184 Å
μ (mm^{-1})	3.04
Crystal size (mm)	0.15 × 0.09 × 0.02
Data Collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix
Absorption Correction	multi-scan *CrysAlis PRO* 1.171.41.93a (Rigaku Oxford Diffraction, 2020) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.801, 1.000
No. of measured, independent and observed [I > 2σ(I)] reflections	112023, 19997, 19255
R_{int}	0.055
θ_{max} (°)	65.1
Refinement	
R[F^2 > 2σ(F^2)], wR(F^2), S	**0.055**, 0.136, 1.05
No. of reflections	19997
No. of parameters	1035
H-atom treatement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å−3)	1.06, -0.82

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