Supporting information of the manuscript entitled:

Cyclo-E₅-bridged Trinuclear Triple-decker Complexes (E = P, As) Containing a Triply-bonded Mo₂ Unit and Their Isomerisation

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Contents

1. List of figures

2. List of tables

3. Syntheses and characterisation of compounds

Unless stated otherwise, all operations were performed at room temperature, using standard Schlenk techniques or in a glovebox under an inert atmosphere of nitrogen. Et_2O and THF were distilled from purple sodium benzophenone ketyl. n-Hexane, toluene and dichloromethane were passed through columns of solvent purification systems to remove oxygen and moisture. All deuterated solvents were purchased in ampoules from Sigma-Aldrich and stored over 3 Å molecular sieves in Schlenk tubes. 3 Å molecular sieves and celite were dried in a vacuum for 3 days at a temperature just above 170 °C. $Mo_2[\mu,\kappa^2\text{-PhB(N-2,6-}^i Pr_2 C_6 H_3)_2]_2$ (**1**)[1] and $Cp^*Fe(\eta^5\text{-}E_5)$ (E = P (**2**),[2] As (**3**)[3]) was synthesized based on literature methods. All other commercially available chemicals were used without further purification. Elemental analyses were performed with the Elementar vario EL cube. NMR spectra were recorded with Bruker Avance 400 NMR spectrometer or Bruker Avance 500 NMR spectrometer and graphed by the Bruker TopSpin 3.6.2 program. The spectra are referenced relative to residual protio-solvent resonances.[4] Because commonly-utilized solvents were frequently used in the glove box for experimental operations, the deuterated solvents stored in the glovebox were inevitably contaminated with trace solvent vapors. The NMR resonances of common solvents were ignored for clarity when labeling the NMR spectral signals in each deuterated solvent matrix.[4]

3-1. Cp*Fe($\mu_3,\eta^{5:2:2}$-P$_5$)Mo$_2$[μ,κ^2-PhB(N-2,6-^{i}Pr$_2$C$_6$H$_3$)$_2$]$_2$ (4)

To a 20 mL of vial was charged with **1** (105.9 mg, 0.099 mmol) and **2** (34.3 mg, 0.099 mmol). 4 mL of Et$_2$O of −30 °C was then added to the vial and the resultant solution was allowed to react at ambient temperature for 30 min by stirring. The color of the solution changed from burgundy to deep brown along with the emersion of a deep brown precipitate. After the reaction went to completion, all volatile materials were removed under vacuum. The residual solid was washed with Et$_2$O of −30 °C and was collected in a vial. A saturated dichloromethane solution of the collected brown solid was layered with n-hexane for liquid/liquid diffusion, by which deep brown crystals of **4** were isolated (89.7 mg, 0.063 mmol). The isolated yield was 64.0%. Anal. Calcd for C$_{70}$H$_{93}$B$_2$FeMo$_2$N$_4$P$_5$: C, 59.43; H, 6.63; N, 3.96%. Found: C, 59.92; H, 7.27; N, 4.31%. ^{1}H NMR (400.2 MHz, 300.0 K, toluene-d_8): δ 7.52 (m, 2 H, PhB(N-2,6-^{i}Pr$_2$C$_6$$H_3$)$_2$)), 7.20-7.12 (m, 6 H, PhB(N-2,6-^{i}Pr$_2$C$_6$$H_3$)$_2$)), 6.91-6.70 (m, 14 H, PhB(N-2,6-^{i}Pr$_2$C$_6$$H_3$)$_2$)), 4.44 (sept, 2 H, C$HMe_2$), 4.07 (sept, 2 H, C$HMe_2$), 3.52 (sept, 2 H, C$HMe_2$), 1.85 (sept, 2 H, C$HMe_2$), 1.66 (d, 6 H, CH$Me_2$), 1.62 (d, 6 H, CH$Me_2$), 1.53 (m, 12 H, two CH$Me_2$ overlapped), 1.17(s, 15 H, Cp*), 0.94 (d, 6 H, CHMe_2), 0.44 (m, 12 H, two CHMe_2 overlapped), 0.21 (d, 6 H, CHMe_2) ppm. ^{31}P NMR (162.0 MHz, 298.0 K, THF-d_8): δ 25.2 ppm.

Fig. S1. The ^{1}H NMR spectrum of **4**.

Fig. S2. Thermolysis of **4** monitored by the ^{1}H NMR (400.2 MHz, 300.0 K, toluene-d_8) spectroscopy. The experimental conditions were: (a) 15 °C; (b) 27 °C for 2 hours; (c) 27 °C for 1 day; (d) 37 °C for 2 hours; (e) 37 °C for 3 days; (f) 47 °C for 1 day. Signals marked with @ are assigned to **4**, and signals marked with * are assigned to unknown intermediates, and signals marked with # are assigned to **6**.

—25.2

450 400 350 300 250 200 150 100 50 0 −50 ppm
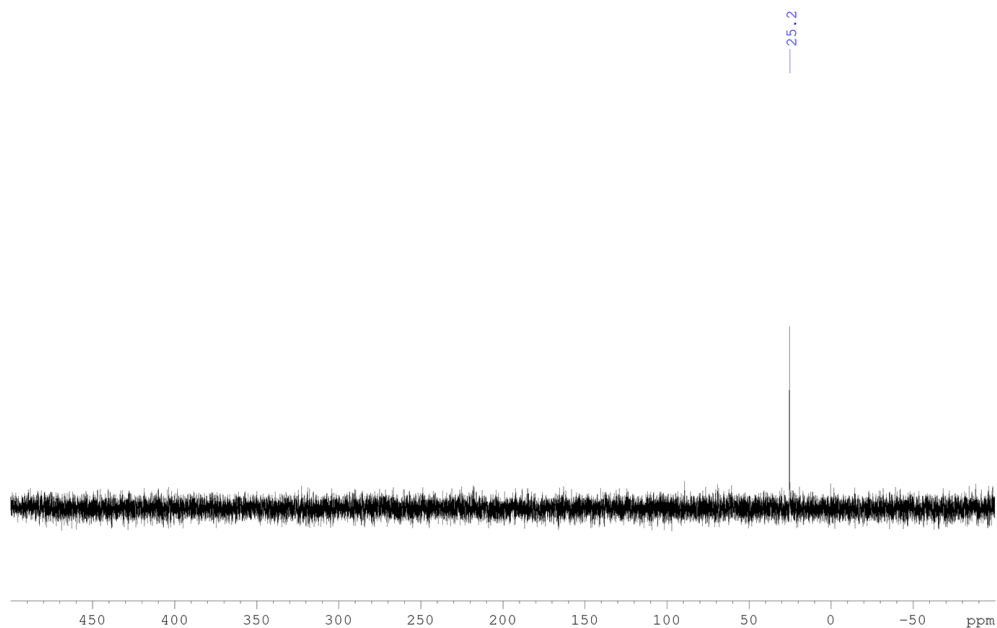
Fig. S3. The ^{31}P NMR spectrum of **4**.

273 K

253 K

233 K

213 K

193 K

150 100 50 0 -50 -100 ppm
Scale: 13.11 ppm/cm, 2124 Hz/cm
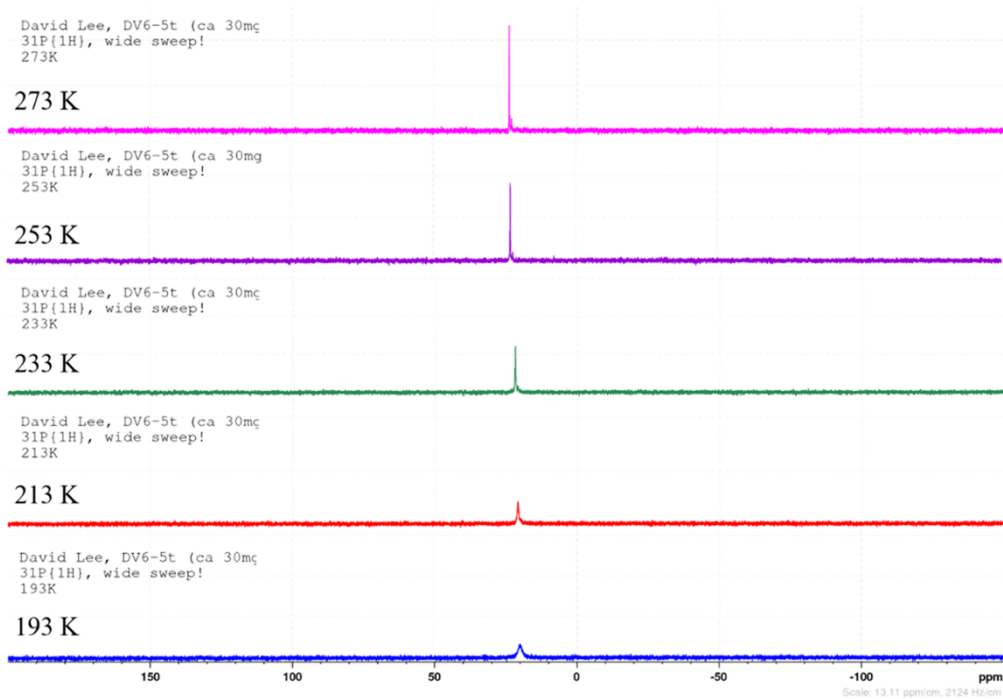
Fig. S4. The ^{31}P{^{1}H} VT-NMR (162.0 MHz, 273-193 K, toluene-d_8) spectra of **4**.

6
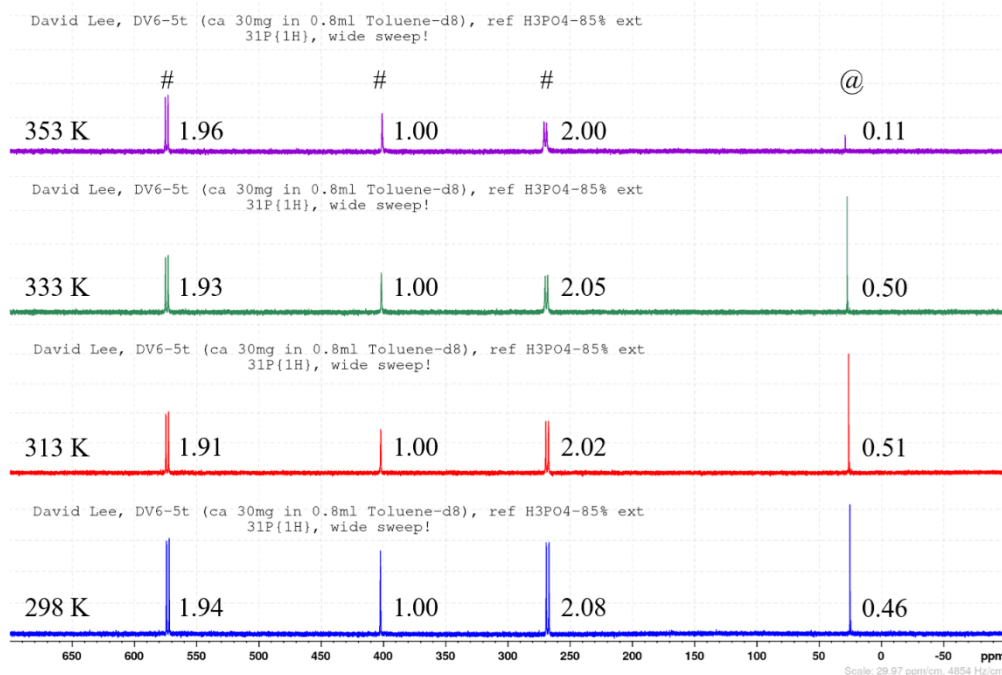
Fig. S5. The $^{31}P\{^1H\}$ VT-NMR (162.0 MHz, 298-353 K, toluene-d_8) spectra of mixture **4** and **6**. Signals marked with @ are assigned to **4**, and signals marked with # are assigned to **6**. The integral ratio is marked next to each signal.

3-2. Cp*Fe($\mu_3,\eta^{5:2:2}$-As$_5$)Mo$_2[\mu,\kappa^2$-PhB(N-2,6-^{i}Pr$_2$C$_6$H$_3$)$_2]_2$ (5)

To a 100 mL of Schlenk tube was charged with **1** (276.2 mg, 0.258 mmol), **3** (146.2 mg, 0.258 mmol), and 10 mL Et$_2$O. The resultant mixture was allowed to react at ambient temperature for 4 hours by stirring. The color of the solution changed from burgundy to deep brown along with the emersion of a deep brown precipitate. After the reaction went to completion, all volatile materials were removed under vacuum. The residual solid was washed with *n*-hexane, and was then dissolved in THF. A saturated THF solution was layered with *n*-hexane for liquid/liquid diffusion, by which deep

7

brown crystals of **5** were collected (253.3 mg, 0.155 mmol). The isolated yield was 60.0%. Anal. Calcd for $C_{70}H_{93}As_5B_2FeMo_2N_4$: C, 51.44; H, 5.74; N, 3.43%. Found: C, 51.61; H, 5.70; N, 3.27%. ^{1}H NMR (400.3 MHz, 298.0 K, toluene-d_8): δ 7.55 (br, 2 H, *Ph*B(N-2,6-^{i}Pr$_2$C$_6$*H*$_3$)$_2$), 7.29-7.11 (m, 7 H, *Ph*B(N-2,6-^{i}Pr$_2$C$_6$*H*$_3$)$_2$), 6.97-6.75 (m, 13 H, *Ph*B(N-2,6-^{i}Pr$_2$C$_6$*H*$_3$)$_2$), 4.64 (sept, 2 H, C*H*Me$_2$), 3.92 (sept, 2 H, C*H*Me$_2$), 3.57 (sept, 2 H, C*H*Me$_2$), 1.90 (sept, 2 H, C*H*Me$_2$), 1.70 (d, 6 H, CH*Me*$_2$), 1.67 (d, 6 H, CH*Me*$_2$), 1.56 (d, 6 H, CH*Me*$_2$), 1.46 (d, 6 H, CH*Me*$_2$), 1.14 (s, 15 H, *Cp**), 0.95 (d, 6 H, CH*Me*$_2$), 0.57 (d, 6 H, CH*Me*$_2$), 0.39 (d, 6 H, CH*Me*$_2$), 0.17 (d, 6 H, CH*Me*$_2$) ppm.
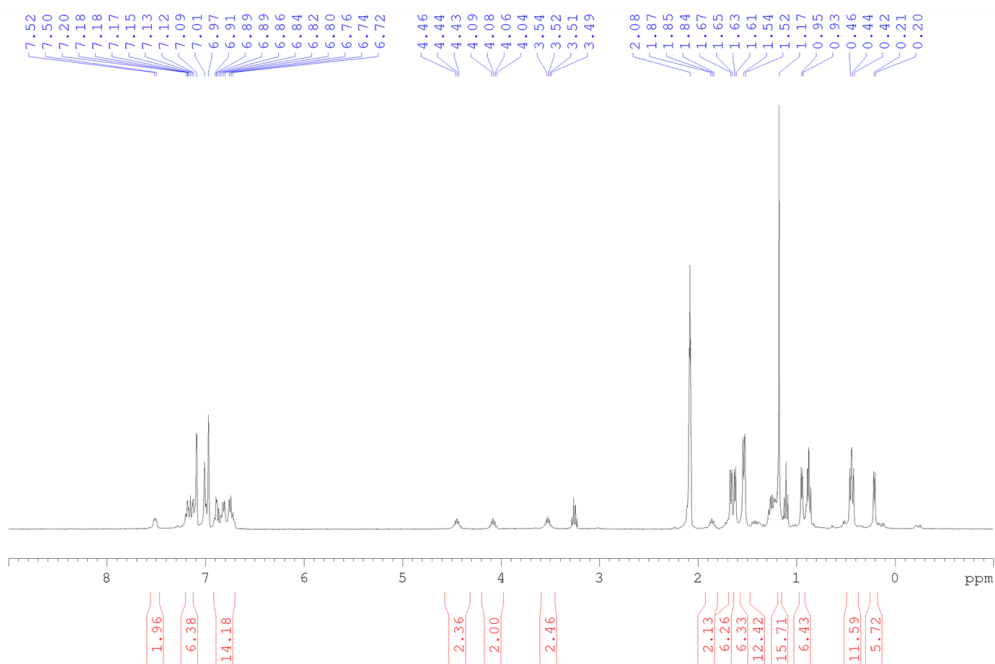

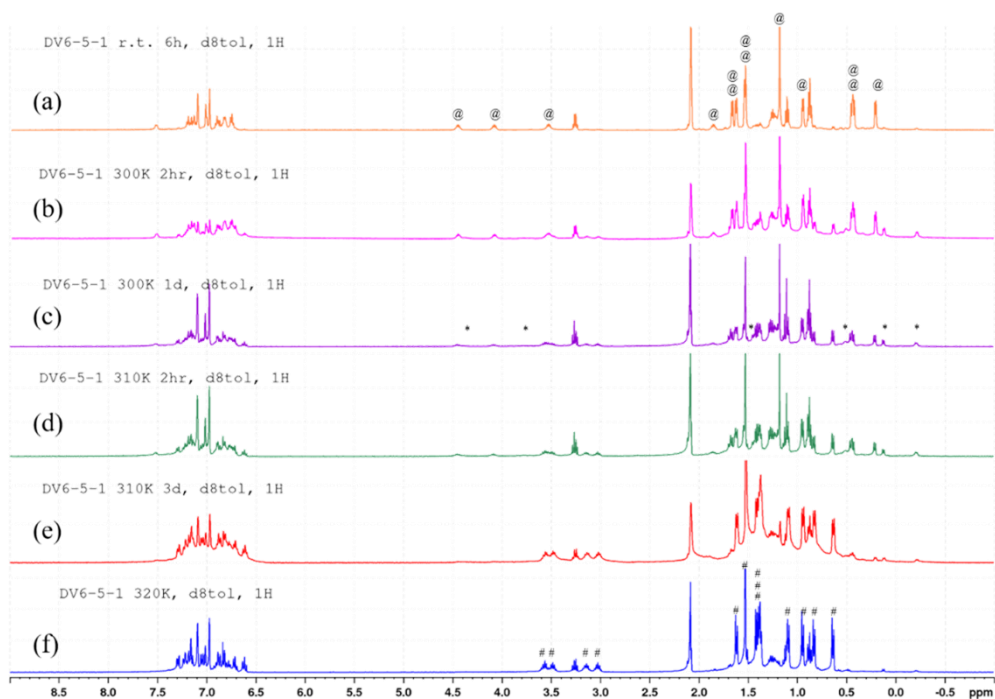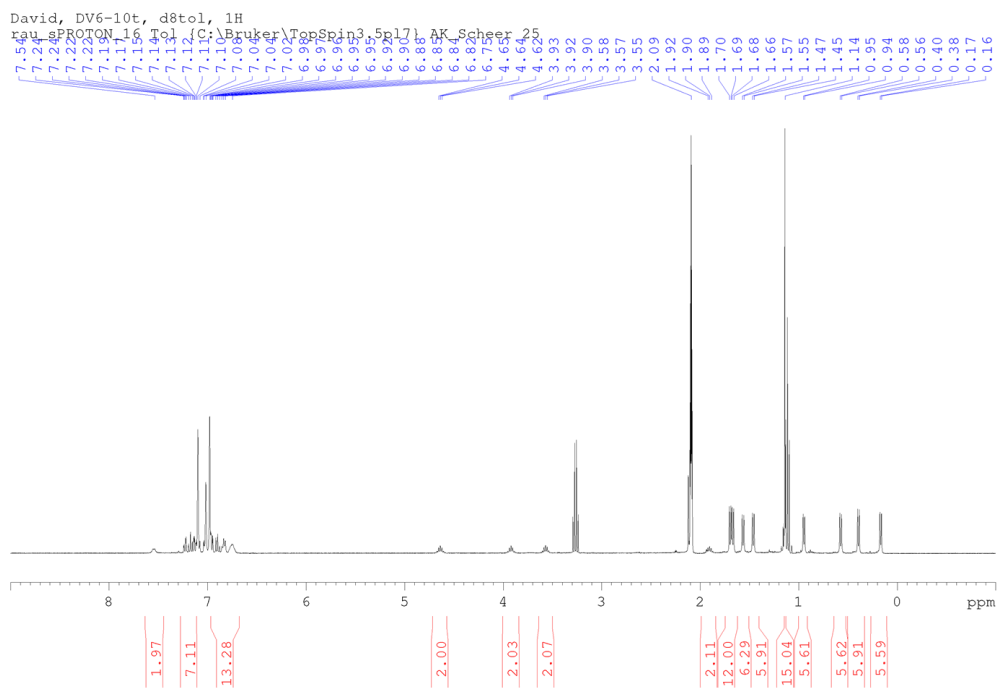**Fig. S6.**　The ^{1}H NMR spectrum of **5**.
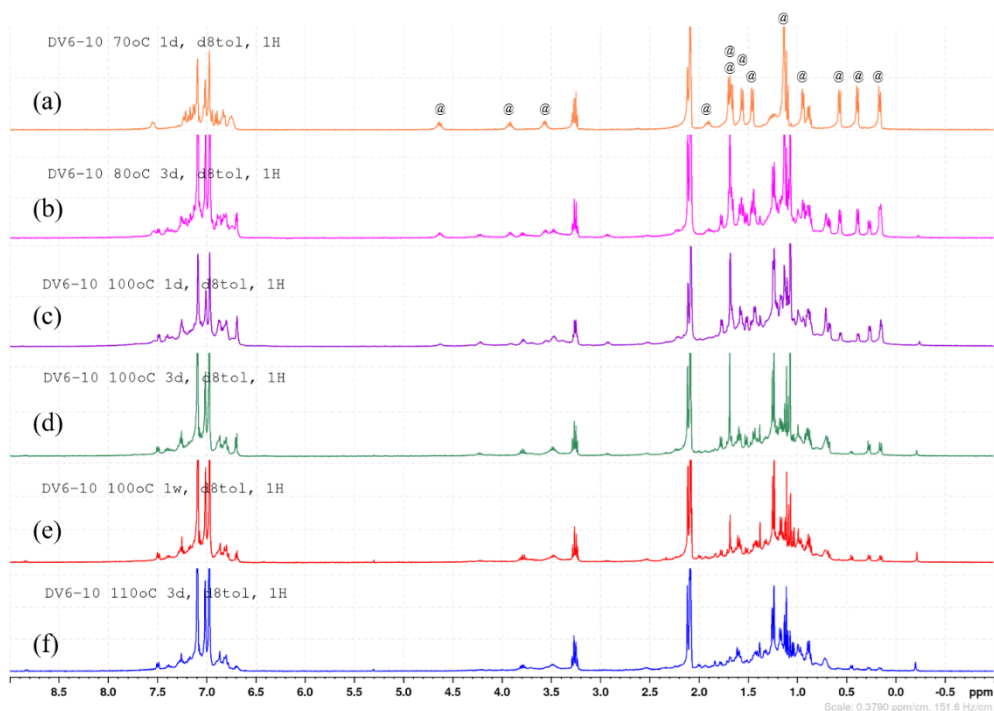
Fig. S7. Thermolysis of **5** monitored by the ^{1}H NMR (400.3 MHz, 298.0 K, toluene-d_8) spectroscopy. The experimental conditions were: (a) 70 °C for 1 day; (b) 80 °C for 3 days; (c) 100 °C for 1 day; (d) 100 °C for 3 days; (e) 100 °C for 7 days; (f) 110 °C for 1 day. Signals marked with @ are assigned to **5**.

3-3. Cp*FeMo$_2$[κ^2-PhB(N-2,6-^{i}Pr$_2$C$_6$H$_3$)$_2$]($\mu_3,\kappa:\kappa:\eta^2$-P$_2$)[$\mu_3,\kappa:\kappa:\eta^3\kappa$-P$_3$PhB(N-2,6-^{i}Pr$_2C_6H_3$)$_2$] (6)

To a 100 mL of Schlenk tube was charged with **4** (79.2 mg, 0.056 mmol) and 10 mL toluene. The resultant solution was allowed to react at 57 °C for 1 day by stirring. After the reaction went to completion, all volatile materials were removed under vacuum. The solid residual was washed with *n*-hexane and extracted with Et$_2$O. The filtrate was vaporized for recrystallization, by which deep brown crystals of **6** were isolated (69.8 mg, 0.049 mmol). The isolated yield was 87.5%. Anal. Calcd for

$C_{70}H_{93}B_2FeMo_2N_4P_5$: C, 59.43; H, 6.63; N, 3.96%. Found: C, 59.81; H, 6.91; N, 3.81%.

^{1}H NMR (400.2 MHz, 300.0 K, toluene-d_8): δ 7.27-6.97 (m, 12 H, *Ph*B(N-2,6-^{i}Pr$_2$C$_6$H$_3$)$_2$), 6.85-6.76 (m, 6 H, *Ph*B(N-2,6-^{i}Pr$_2$C$_6$*H*$_3$)$_2$), 6.68 (t, 2 H, *Ph*B(N-2,6-^{i}Pr$_2$C$_6$*H*$_3$)$_2$), 6.61 (the , 2 H, *Ph*B(N-2,6-^{i}Pr$_2$C$_6$*H*$_3$)$_2$), 3.54 (sept, 2 H, C*H*Me$_2$), 3.46 (sept, 2 H, C*H*Me$_2$), 3.12 (sept, 2 H, C*H*Me$_2$), 3.00 (sept, 2 H, C*H*Me$_2$), 1.59 (d, 6 H, CH*Me$_2$*), 1.52 (s, 15 H, *Cp**), 1.39 (d, 6 H, CH*Me$_2$*), 1.37 (d, 6 H, CH*Me$_2$*), 1.35 (d, 6 H, CH*Me$_2$*), 1.06 (d, 6 H, CH*Me$_2$*), 0.92 (d, 6 H, CH*Me$_2$*), 0.80 (d, 6 H, CH*Me$_2$*), 0.62 (d, 6 H, CH*Me$_2$*) ppm. ^{13}C{^{1}H} NMR (100.6 MHz, 300.0 K, toluene-d_8): δ 162.0,150.7, 145.8, 141.2, 140.9, 136.7, 130.4, 130.2, 129.4, 127.9, 127.2, 126.4, 126.1, 126.0, 124.6, 123.8, 122.7 (*Ph*B(N-2,6-^{i}Pr$_2$C$_6$H$_3$)$_2$), 98.2 (*Cp**), 29.7, 29.6, 29.1, 29.1, 27.7, 26.8, 25.6, 25.0, 24.5, 24.2, 24.1, 23.4 (CH*Me$_2$*), 12.4 (*Cp**) ppm. ^{31}P NMR (202.5 MHz, 300.0 K, toluene-d_8): δ 572.5 (dddd), 401.6 (dddd), 267.3 (dddd) ppm. The coupling constants were listed in Table S1.

DV6-5e, d8tol, 1H
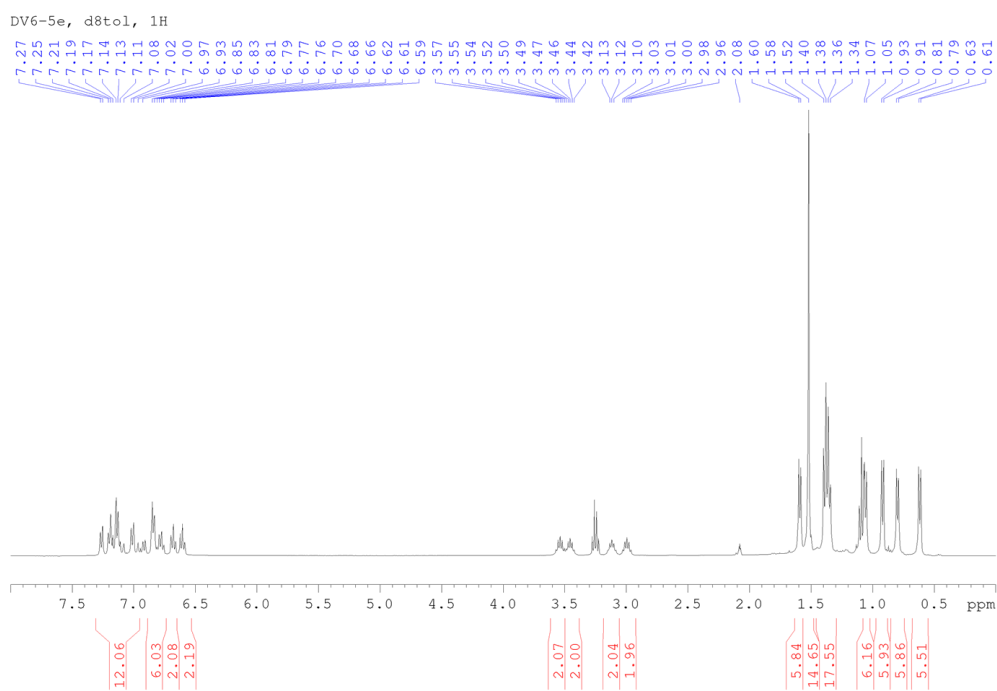
Fig. S8. The ^{1}H NMR spectrum of **6**.

DV6-5e, d8tol, 13C
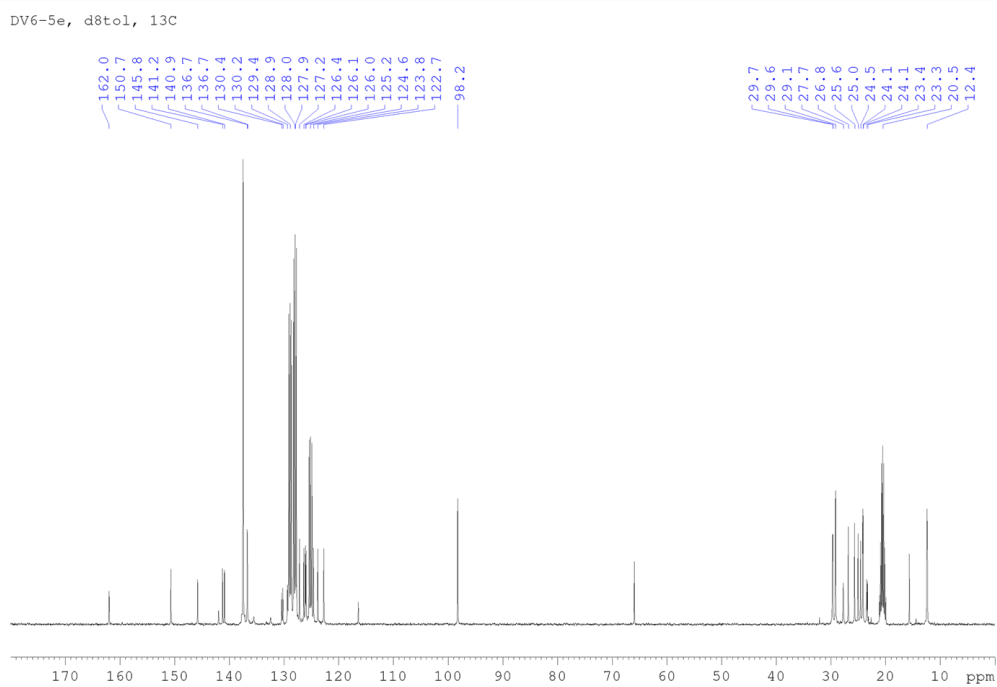
Fig. S9. The ^{13}C{^{1}H} NMR spectrum of **6**.

DV 6-5
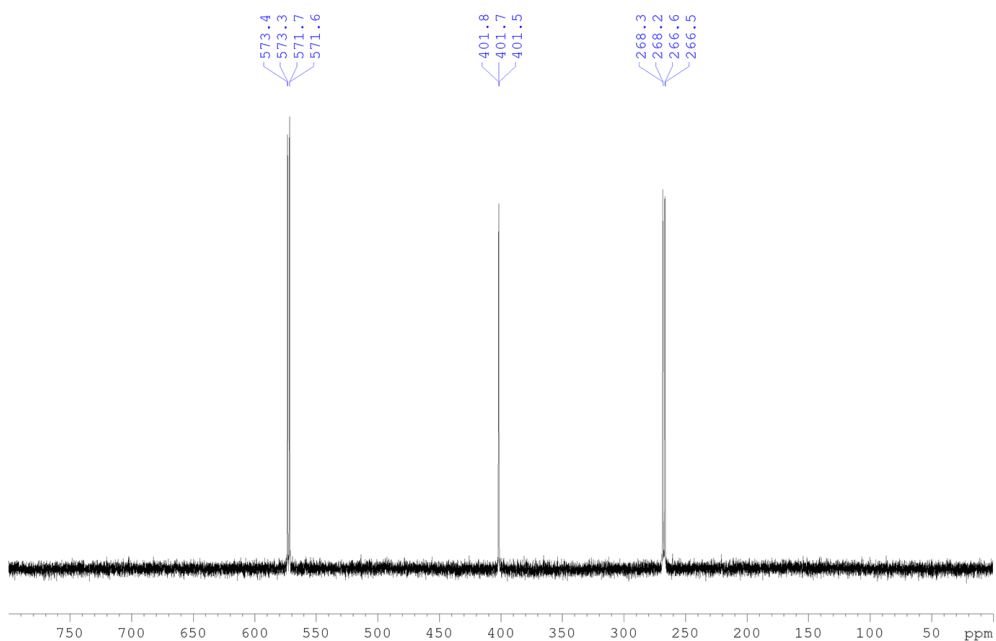
Fig. S10. The ^{31}P NMR spectrum of **6**.
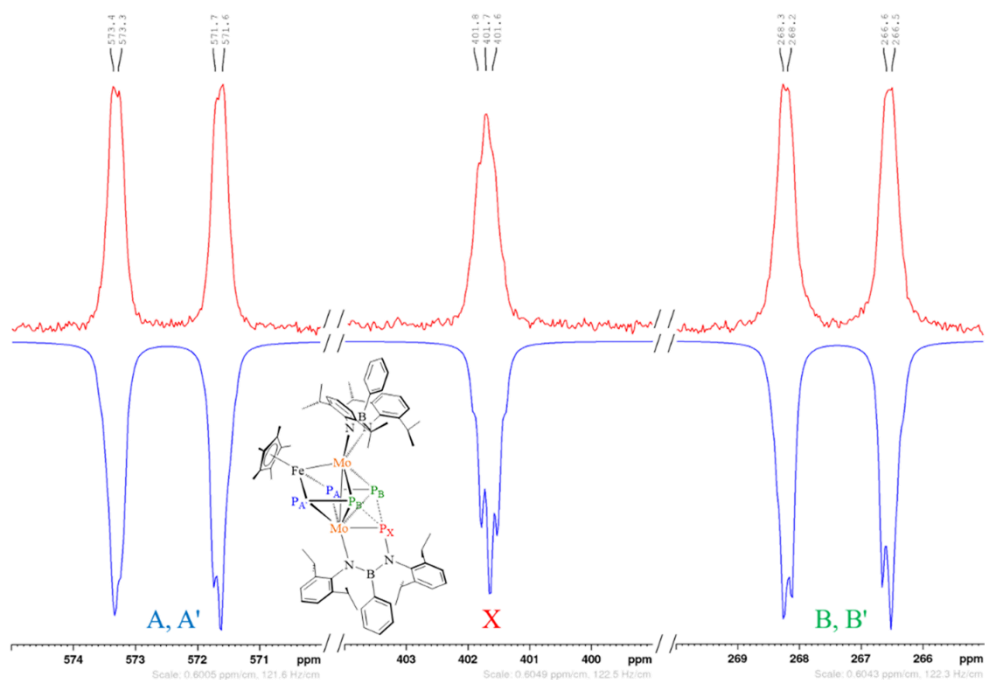
Fig. S11. The experimental (top) and simulated (bottom) ^{31}P NMR spectra of **6**.

12

Table S1. Chemical shifts, coupling constants, and linewidth data obtained from simulation of the ^{31}P NMR spectrum of **6**.

δ (ppm)		J (Hz)			
P_A	572.4	$^1J_{AB}$	340.9	$^2J_{BA'}$	−20.8
P_B	267.3	$^1J_{A'B'}$	341.8	$^2J_{XA'}$	24.2
P_X	401.6	$^2J_{AX}$	25.0	$^2J_{AB'}$	−19.3
$P_{A'}$	572.5	$^2J_{BX}$	−31.5	$^2J_{BB'}$	14.6
$P_{B'}$	267.3	$^2J_{AA'}$	28.5	$^2J_{XB'}$	−26.8
* Simulations were performed using the Bruker TopSpin 3.6.2 program.				Linewidth	20.0
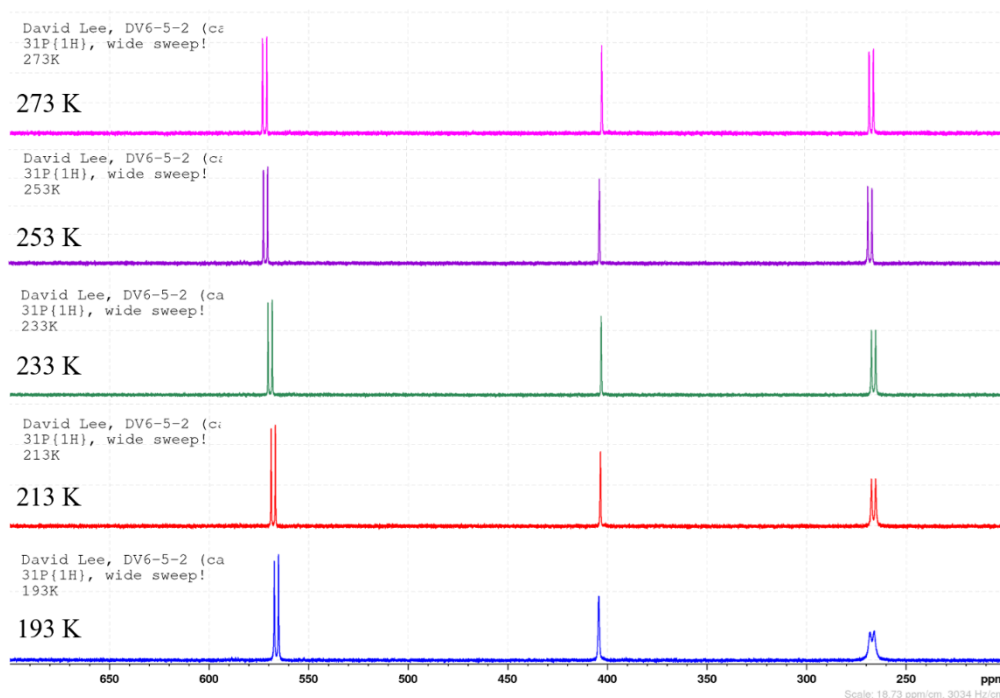
Fig. S12. The ^{31}P{^{1}H} VT-NMR (162.0 MHz, 273-193 K, toluene-d_8) spectra of **6**.

13
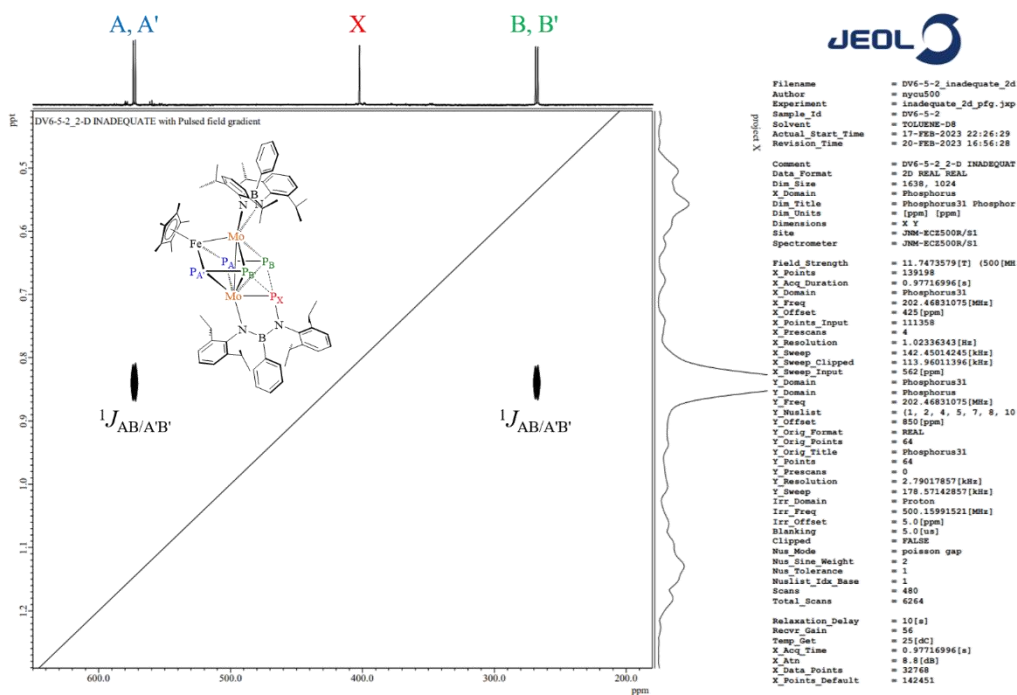
Fig. S13. The ^{31}P-^{31}P INADEQUATE (202.5 MHz, 298.2 K, toluene-d_8) spectrum of **6**.
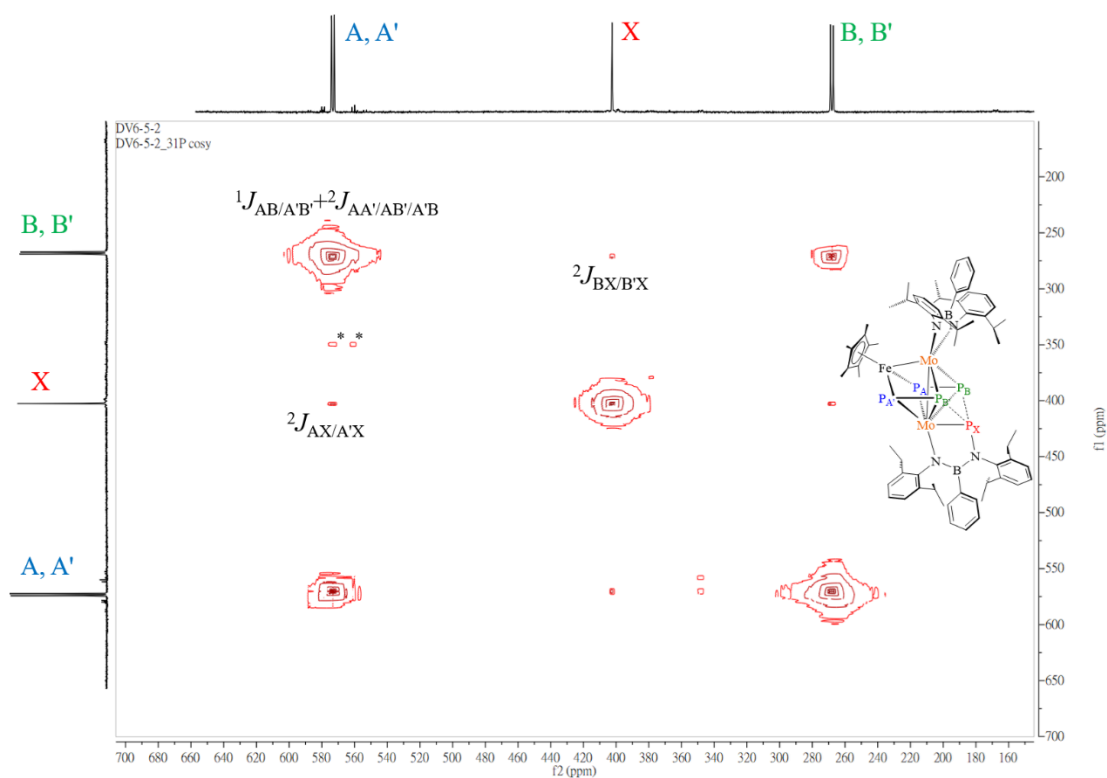
Fig. S14. The ^{31}P-^{31}P COSY (202.5 MHz, 298.2 K, toluene-d_8) spectrum of **6**. *Signals from impurities.

4. Details of crystallographic structure data and DFT calculations

Single crystals data of **4** and **5** were collected on a GV1000, TitanS2 diffractometer, and those of **6** were collected on an XtaLAB Synergy R, DW system, HyPix-Arc 150 diffractometer. Using Olex2 [5], the structure was solved with the SHELXT [6] structure solution program using Intrinsic Phasing and refined with the SHELXL [7] refinement package using Least Squares minimization. Images of crystallographic structures were illustrated by the Diamond 3.2 program.

All calculations were performed with the ORCA 5.0 program.[8] The geometry was optimised starting from the X-ray coordinates at the BP86 [9–11]/def2-SVP [12,13] level, followed by single point calculation using the def2-TZVP [12,13] basis set for Mo, P, N, B, carbon atoms bonded to Mo and the C atom of the N_2CH unit. Dispersion correction was included via the Grimme's D4 model.[14,15] The NBO analysis was performed with NBO 7.0.[16] The Intrinsic Bonding Orbitals [17] were calculated as implemented in ORCA and visualized using ChemCraft.

Table S2. Crystallographic data for compound **4-6**.

Compound	$4 \cdot 2\ CH_2Cl_2$	$5 \cdot 1.3\ C_4H_8O$	$6 \cdot Et_2O$
Identification code	abs_gaus_error	res462_cub2_twin1_hklf4	230119lt_auto
Empirical formula	$C_{72}H_{97}B_2Cl_4FeMo_2N_4P_5$	$C_{70}H_{93}B_2FeMo_2N_4As_5 \cdot 1.3\ C_4H_8O$	$C_{74}H_{103}B_2FeMo_2N_4OP_5$
Formula weight	1584.53	1728.16	1488.80
Temperature (K)	89.9(4)	123.00(10)	100.00(10)
Crystal system	triclinic	monoclinic	monoclinic
Space group	P-1	C2/c	P2$_1$/c
a (Å)	12.7702(3)	23.4267(2)	11.1538(1)
b (Å)	13.1154(3)	12.7561(1)	17.6318(2)
c (Å)	24.2746(4)	48.9677(5)	37.3554(4)
α (°)	90.203(2)	90	90
β (°)	90.567(2)	93.741(1)	90.889(1)
γ (°)	117.810(2)	90	90
Volume (Å^3)	3595.75(14)	14602.0(2)	7345.49(13)
Z	2	8	4
ρ_{calc} (g/cm^3)	1.463	1.572	1.346
μ (mm^{-1})	7.168	5.376	5.685
F(000)	1640.0	7024	3112.0
Crystal size (mm^3)	0.317 × 0.059 × 0.033	0.16 × 0.09 × 0.04 × 0.05	0.17 × 0.16 × 0.12
Radiation λ (Å)	1.54184 (Cu Kα)	1.39222 (Cu Kβ)	1.54184 (Cu Kα)
2Θ range for data collection (°)	7.284 to 148.638	7.376 to 135.440	4.732 to 134.158
Index ranges	$-15 \le h \le 13$ $-10 \le k \le 16$ $-29 \le l \le 29$	$-30 \le h \le 29$ $-10 \le k \le 16$ $-64 \le l \le 64$	$-13 \le h \le 9$ $-21 \le k \le 21$ $-42 \le l \le 44$
Reflections collected	25909	34483	65913
Independent reflections, R(int)	13807, 0.0306	32515, 0.0518	13043, 0.0295
Data/restraints/parameters	13807/0/832	32515/0/824	13043/381/921
Goodness-of-fit on F^2	1.021	0.961	1.019
Final R$_1$, wR$_2$ [I≥2σ (I)]	0.0349, 0.0912	0.0385, 0.1002	0.0268, 0.0701
Final R$_1$, wR$_2$ [all data]	0.0423, 0.0932	0.0467, 0.1026	0.0285, 0.0710
Largest diff. peak/hole (e · Å^{-3})	1.00/−1.03	0.685/−0.629	0.56/−0.70
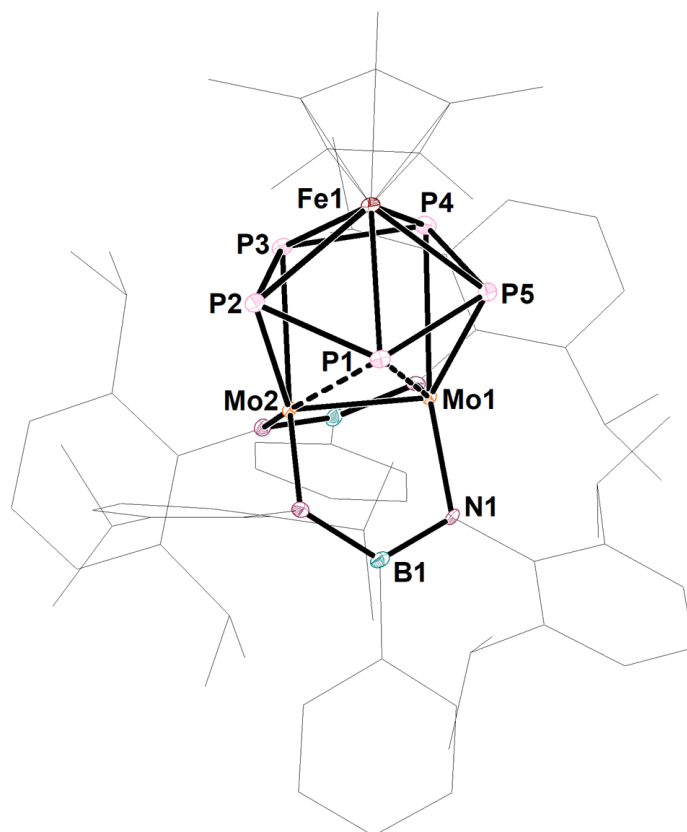
Fig. S15. The solid-state molecular structure of **4**. Thermal ellipsoids are drawn at the 30% probability level. The boraamidinato and Cp* ligands are displayed in the wireframe model; hydrogen atoms are omitted for clarity.
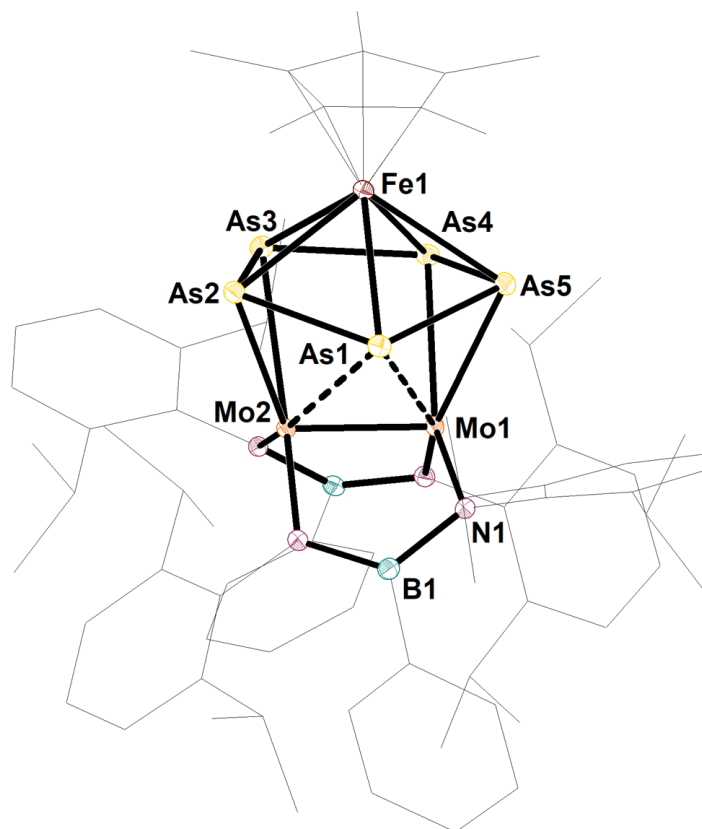
Fig. S16. The solid-state molecular structure of **5**. Thermal ellipsoids are drawn at the 30% probability level. The boraamidinato and Cp* ligands are displayed in the wireframe model; hydrogen atoms are omitted for clarity.

Table S1. Selected bond lengths (Å) and angles (°) of **4** and **5**.

E = P (**4**), As (**5**)	**4**	**5**
Mo1−Mo2	2.1989(3)	2.2026(3)
Mo1−E1	2.8305(7)	2.9256(4)
Mo2−E1	2.7973(8)	2.9249(4)
Mo1−E4	2.6433(7)	2.6115(4)
Mo1−E5	2.5156(7)	2.7037(4)
Mo2−E2	2.5782(7)	2.6625(4)
Mo2−E3	2.5031(7)	2.7577(4)
Fe1−E1	2.4152(8)	2.5178(6)
Fe1−E2	2.3402(8)	2.4404(6)
Fe1−E3	2.4664(8)	2.5655(6)
Fe1−E4	2.3875(8)	2.6042(6)
Fe1−E5	2.3010(8)	2.4951(6)
E1−E2	2.1534(10)	2.3740(5)
E1−E5	2.1697(10)	2.3697(5)
E2−E3	2.2270(10)	2.3796(5)
E3−E4	2.2464(9)	2.4627(5)
E4−E5	2.1994(11)	2.4162(5)
E1−E2−E3	98.14(4)	102.49(2)
E2−E3−E4	110.50(4)	106.18(2)
E3−E4−E5	105.55(4)	111.06(2)
E1−E5−E4	103.28(4)	97.52(2)
E2−E1−E5	114.61(4)	115.25(2)
E2−E3−E4−E5	10.94(6)	−7.86(5)
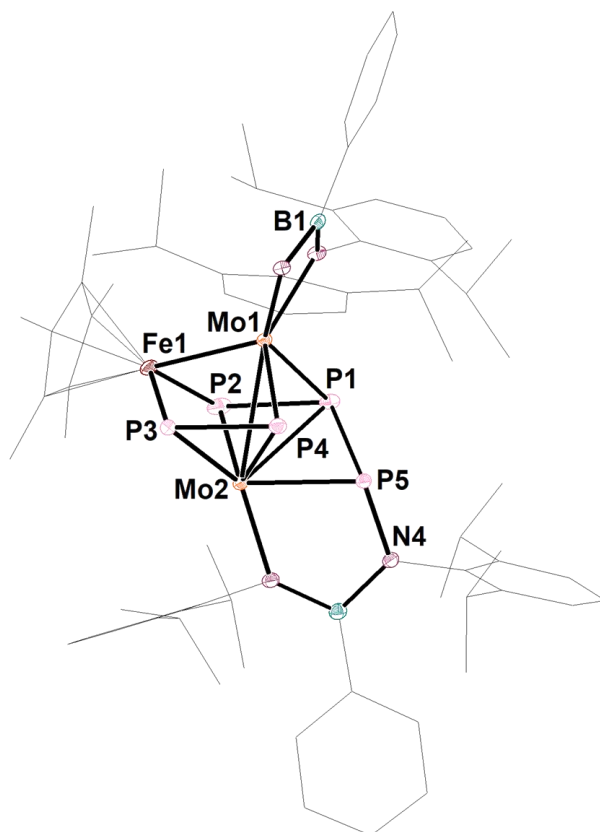
Fig. S17. The solid-state molecular structure of **6**. Thermal ellipsoids are drawn at the 30% probability level. The boraamidinato and Cp* ligands are displayed in the wireframe model; hydrogen atoms are omitted for clarity. Selected bond lengths (Å) were labeled in the figure.

Table S2. Selected bond lengths (Å) and angles (°) of the experimental, optimised structures of **6**, and the transition state structure of **6-TS**.

	Exp. **6**	Calc. **6**	**6-TS**
Mo1−Mo2	2.8484(2)	2.879	2.863
Mo1−Fe1	2.4022(9)	2.378	2.384
Mo1−P1	2.4179(5)	2.429	2.420
Mo1−P4	2.3602(5)	2.364	2.407
Mo2−P1	2.5902(5)	2.638	2.615
Mo2−P2	2.3466(5)	2.350	2.366
Mo2−P3	2.4136(5)	2.464	2.379
Mo2−P4	2.5618(5)	2.575	2.591
Mo2−P5	2.4070(5)	2.442	2.416
Fe1−P2	2.2044(7)	2.207	2.216
Fe1−P3	2.2215(6)	2.230	2.216
N4−P5	1.7183(16)	1.763	2.473
P1−P2	2.2278(7)	2.256	2.263
P1−P5	2.2730(6)	2.240	2.389
P3−P4	2.1798(7)	2.201	2.257
Fe−C	2.051(7)-2.242(7)	2.110-2.165	2.108-2.157
Mo2···Fe1	2.8445(10)	2.866	2.834
Mo1···P2	2.7975(5)	2.921	2.825
Mo1···P3	2.7388(5)	2.769	2.777
P2···P3	3.5954(8)	3.623	3.602
P1···P4	3.5194(7)	3.612	3.532
P4···P5	2.6550(6)	2.913	2.473
P1−P2−P3−P4	−2.05(3)	−6.22	−1.71

Table S3. The calculated Mayer bond orders (MBOs) of **4-6**.

E = P (**4**), As (**5**)	**4**	**5**	**6**	
Mo1−Mo2	2.41	2.51	Mo1−Mo2	0.44
Mo1−E1	0.28	0.26	Mo1−Fe1	0.97
Mo2−E1	0.29	0.32	Mo1−P1	0.85
Mo1−E4	0.47	0.55	Mo1−P4	1.07
Mo1−E5	0.57	0.48	Mo2−P1	0.52
Mo2−E2	0.60	0.59	Mo2−P2	0.98
Mo2−E3	0.77	0.69	Mo2−P3	0.78
Fe1−E1	0.56	0.58	Mo2−P4	0.70
Fe1−E2	0.59	0.59	Mo2−P5	0.94
Fe1−E3	0.47	0.50	Fe1−P2	0.91
Fe1−E4	0.57	0.55	Fe1−P3	0.85
Fe1−E5	0.60	0.63	N4−P5	1.02
E1−E2	0.94	0.85	P1−P2	0.84
E1−E5	0.92	0.87	P1−P5	0.90
E2−E3	0.74	0.70	P3−P4	0.95
E3−E4	0.87	0.73	Mo2···Fe1	0.35
E4−E5	0.82	0.75	Mo1···P2	0.26
			Mo1···P3	0.39
			P4···P5	0.12
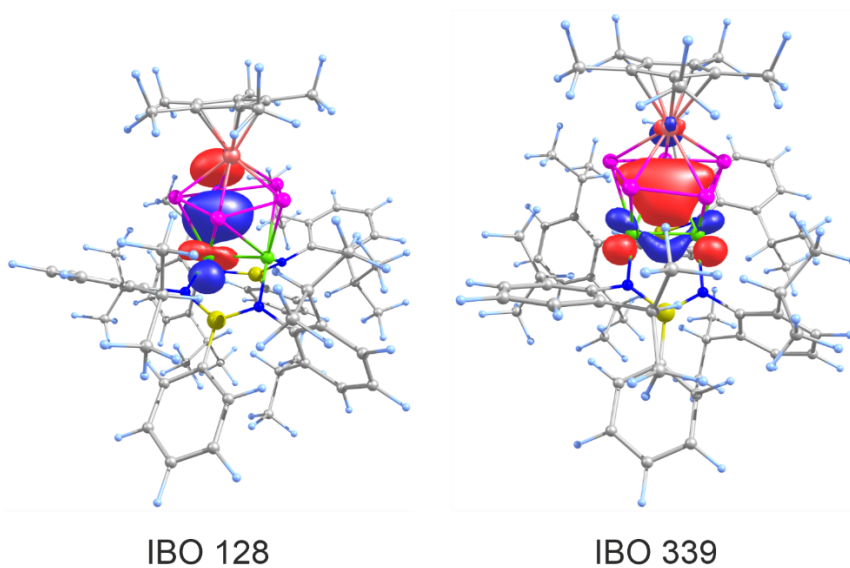
IBO 128   IBO 339

Fig. S18. Selected Intrinsic Bonding Orbitals representing the 2c-2e Mo−P bond (IBO 128) and the 3c-2e Mo_2−P bond (IBO 339) of **4**. Only one IBO from each type is depicted.

IBO 382   IBO 378   IBO 173
(3c-2e bond)

IBO 170   IBO 172
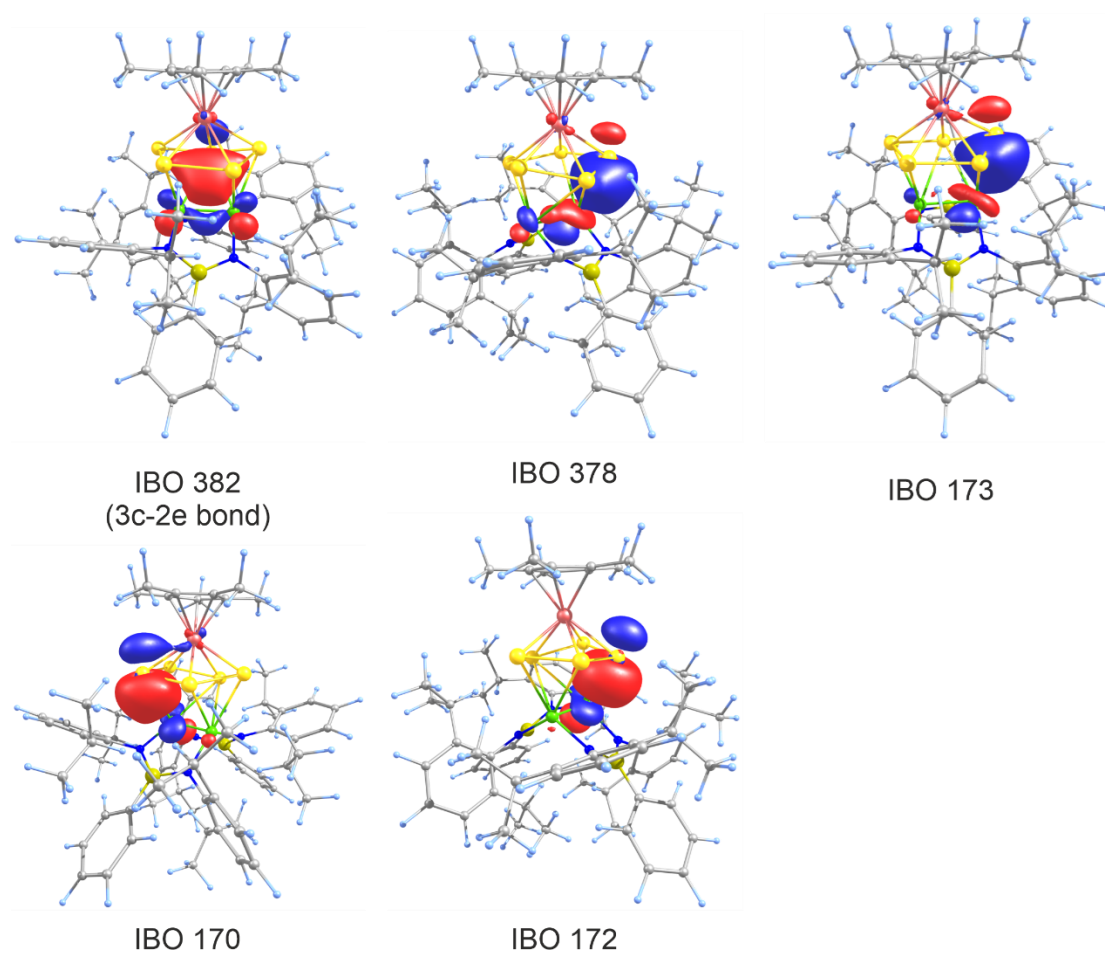
Fig. S19. Selected Intrinsic Bonding Orbitals representing the Mo−As bonding of **5**.
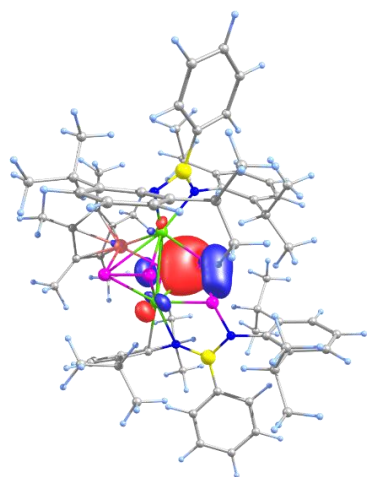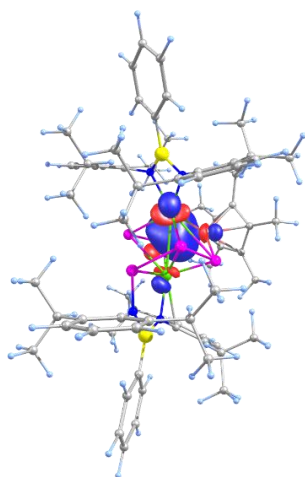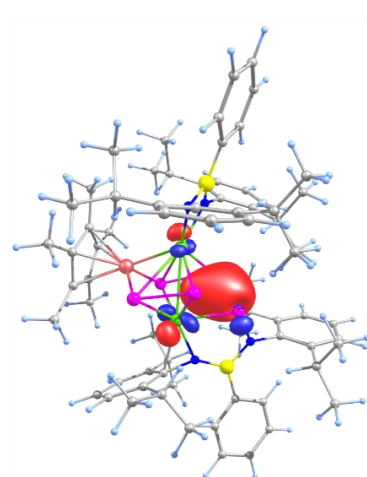
IBO 339   IBO 337   IBO 335
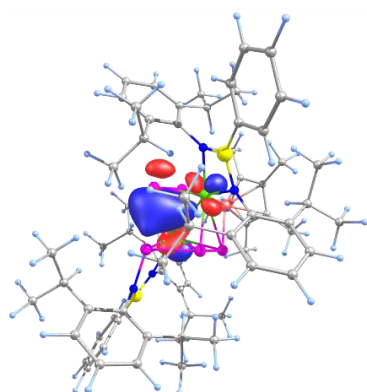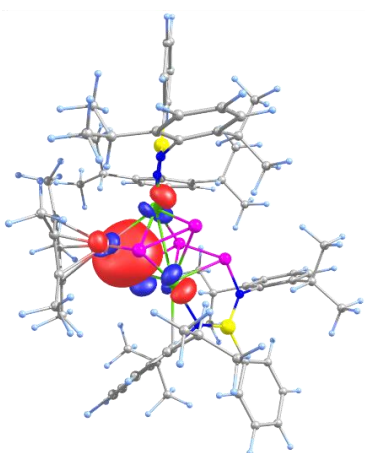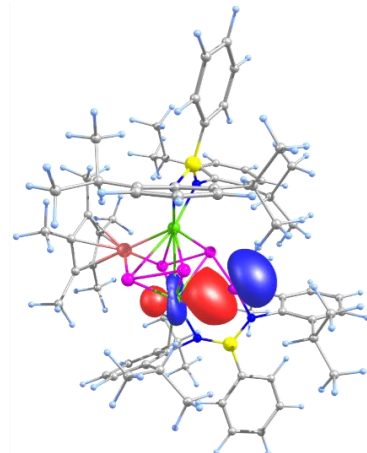
IBO 330   IBO 313   IBO 127

Fig. S20. Selected Intrinsic Bonding Orbitals of **6**.
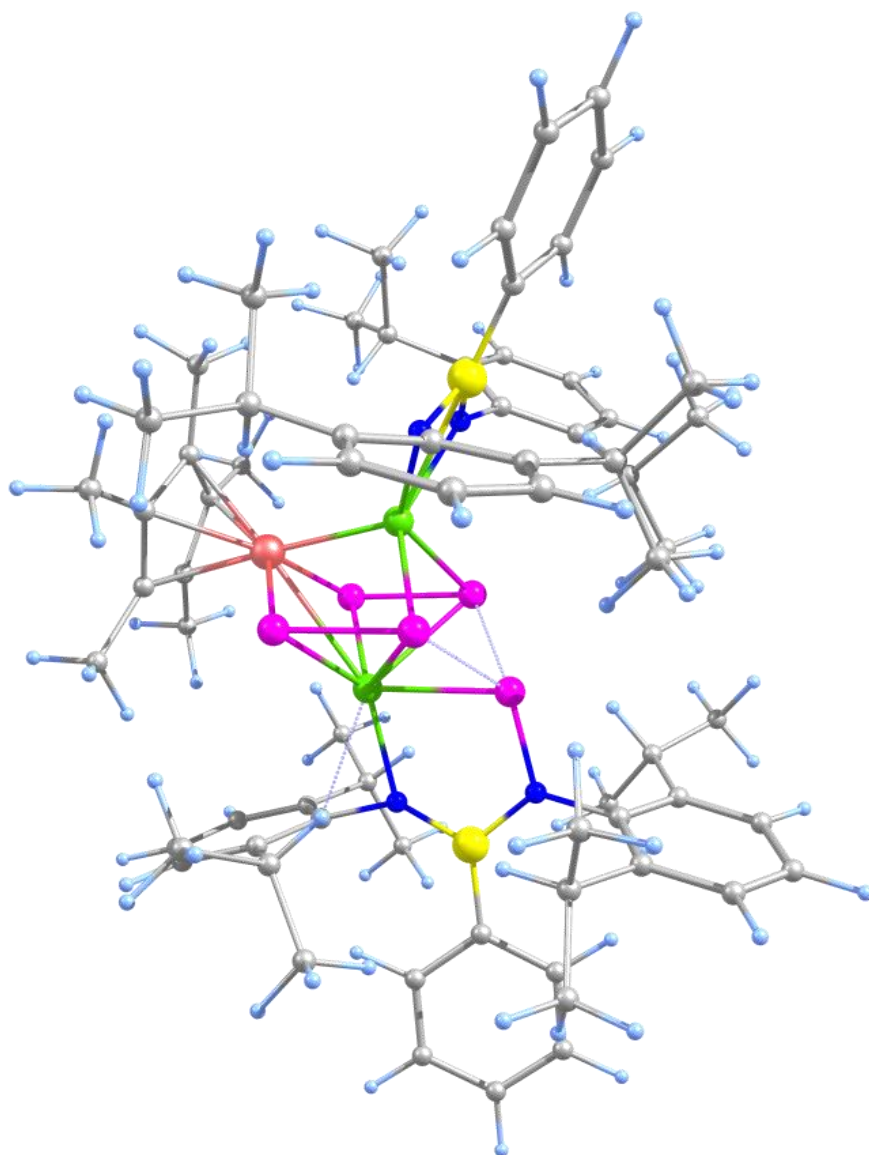
Fig. S21. The DFT-optimised transition state structure of **6-TS** calculated at the BP86-D4/def2-SVP CPCM(THF) level of theory.

4-1. Cartesian coordinates of the optimised 4

FINAL SINGLE POINT ENERGY   -6098.977810973585 a.u.

Mo	0.844087000	6.821638000	18.345267000
Mo	-0.134488000	8.795454000	18.408497000
Fe	-1.793388000	6.741037000	21.112848000
P	-1.395613000	8.963411000	20.544043000
P	0.375591000	7.728470000	21.037598000
P	0.210823000	5.611143000	20.531443000
P	-1.365902000	5.813928000	18.878209000
P	-2.558226000	7.728509000	19.091484000
N	1.652293000	9.720036000	18.828602000
N	2.605742000	7.438809000	19.296689000
N	-0.881383000	8.653145000	16.535967000
N	0.615168000	6.658431000	16.324063000
B	2.821348000	8.874152000	19.102865000
B	-0.185965000	7.687842000	15.667001000
C	-2.543587000	5.052814000	22.084048000
C	-1.774744000	5.860689000	23.008546000
C	-2.376276000	7.169568000	23.060728000
C	-3.525841000	7.167463000	22.179143000
C	-3.624325000	5.858919000	21.571690000
C	-2.307354000	3.609915000	21.764313000
H	-1.249070000	3.324153000	21.919207000
H	-2.930509000	2.966089000	22.422003000
H	-2.574080000	3.376246000	20.715062000
C	-0.603031000	5.399200000	23.814994000
H	-0.945514000	4.958871000	24.776202000
H	-0.017382000	4.625734000	23.280555000
H	0.082412000	6.235635000	24.053962000
C	-1.923969000	8.304897000	23.924944000
H	-0.823469000	8.301448000	24.053372000
H	-2.211686000	9.284654000	23.497144000
H	-2.380929000	8.230012000	24.935211000
C	-4.488017000	8.298203000	21.987207000
H	-4.005770000	9.278332000	22.168584000
H	-4.902550000	8.307648000	20.960613000

H	-5.336873000	8.202610000	22.697873000
C	-4.692091000	5.389884000	20.633240000
H	-4.293482000	4.664138000	19.897229000
H	-5.504530000	4.882095000	21.197186000
H	-5.142357000	6.231807000	20.074035000
C	4.308366000	9.433725000	19.126142000
C	3.245995000	4.909051000	14.313441000
H	4.205951000	5.139401000	13.825182000
C	2.241360000	13.105125000	17.339507000
H	2.586988000	13.544086000	16.390389000
C	3.107295000	7.355741000	14.916646000
H	2.335685000	8.035087000	15.328682000
C	-0.290206000	7.852662000	14.093010000
C	2.210204000	11.705166000	17.473865000
C	1.308260000	5.637397000	15.609566000
C	1.742656000	11.136500000	18.699552000
C	2.544054000	5.941270000	14.960917000
C	2.737123000	10.849223000	16.327461000
H	2.766217000	9.799775000	16.680831000
C	0.757653000	4.324719000	15.502701000
C	-1.366012000	11.563099000	16.981781000
H	-0.411311000	11.004453000	17.105425000
C	5.381494000	8.550475000	18.847256000
H	5.165080000	7.498721000	18.619315000
C	3.492325000	8.387109000	22.114580000
H	2.920434000	9.006022000	21.391420000
C	3.701230000	6.999247000	21.510296000
C	-2.162663000	9.202116000	16.254312000
C	-2.430283000	10.584952000	16.510152000
C	1.863611000	13.950984000	18.390008000
H	1.893607000	15.044326000	18.264031000
C	1.410155000	11.992948000	19.793376000
C	4.336861000	6.067755000	22.356090000
H	4.593330000	6.376418000	23.381158000
C	-0.655012000	9.108952000	13.546773000
H	-0.852767000	9.952627000	14.221110000
C	-3.112914000	6.892570000	15.449724000
H	-2.071104000	6.571060000	15.660494000

C	-0.655117000	3.986543000	15.967447000
H	-1.097447000	4.915473000	16.379413000
C	1.471280000	13.387975000	19.610141000
H	1.213197000	14.049228000	20.452218000
C	4.658593000	10.771503000	19.437178000
H	3.876989000	11.501327000	19.678076000
C	3.702595000	5.280238000	19.746596000
C	-0.074049000	6.799541000	13.168724000
H	0.190113000	5.798944000	13.530240000
C	3.466983000	4.766299000	18.334506000
H	2.943595000	5.561982000	17.755158000
C	4.852354000	9.070423000	22.372075000
H	5.408913000	8.536565000	23.170535000
H	5.486713000	9.086171000	21.467475000
H	4.708542000	10.116472000	22.710833000
C	2.242547000	11.815434000	22.157314000
H	2.349768000	12.915373000	22.261955000
H	2.042006000	11.401167000	23.166529000
H	3.212792000	11.414358000	21.808711000
C	1.502344000	3.325856000	14.845221000
H	1.084768000	2.309120000	14.773958000
C	4.654368000	4.771956000	21.943084000
H	5.144600000	4.066176000	22.631190000
C	2.746403000	3.600854000	14.265948000
H	3.314890000	2.804893000	13.760564000
C	3.346415000	6.604853000	20.169636000
C	-3.724584000	11.099156000	16.310710000
H	-3.908294000	12.166449000	16.509112000
C	-3.240929000	8.373462000	15.789006000
C	2.689260000	8.344850000	23.429781000
H	1.705930000	7.854566000	23.288892000
H	3.238235000	7.796721000	24.222409000
H	2.506882000	9.372014000	23.804858000
C	7.034027000	10.305978000	19.166659000
H	8.082702000	10.642834000	19.180964000
C	4.342782000	4.397165000	20.633300000
H	4.605750000	3.387246000	20.282174000
C	-0.206247000	6.989500000	11.784045000

H	-0.036889000	6.143818000	11.099051000
C	5.994530000	11.202771000	19.464693000
H	6.223397000	12.249211000	19.720942000
C	3.407892000	7.813397000	13.478640000
H	4.197032000	7.191502000	13.006948000
H	2.503454000	7.764058000	12.840468000
H	3.773571000	8.860885000	13.478315000
C	-4.041634000	6.009236000	16.305962000
H	-3.883312000	6.177480000	17.388735000
H	-5.109398000	6.215142000	16.084218000
H	-3.856689000	4.935979000	16.098163000
C	1.096323000	11.463782000	21.188430000
H	1.037866000	10.358602000	21.122264000
C	-1.112892000	12.662416000	15.933694000
H	-0.889752000	12.231574000	14.938066000
H	-2.003578000	13.316410000	15.828102000
H	-0.254570000	13.295600000	16.234436000
C	-0.555281000	8.251180000	11.273412000
H	-0.655526000	8.404419000	10.187192000
C	6.719776000	8.971380000	18.855922000
H	7.522085000	8.252750000	18.625517000
C	-1.515721000	3.534932000	14.770764000
H	-1.161032000	2.565270000	14.363146000
H	-2.573037000	3.398645000	15.078099000
H	-1.490302000	4.274373000	13.946931000
C	4.347474000	7.479838000	15.812465000
H	4.093995000	7.227054000	16.856712000
H	5.157116000	6.798251000	15.479777000
H	4.746779000	8.512491000	15.803507000
C	-4.516585000	8.941628000	15.609703000
H	-5.336839000	8.297146000	15.257320000
C	-3.399623000	6.656991000	13.953012000
H	-4.460848000	6.883648000	13.719797000
H	-2.765330000	7.294828000	13.310108000
H	-3.217743000	5.599558000	13.677401000
C	4.169972000	11.252519000	15.933003000
H	4.207639000	12.292006000	15.545736000
H	4.863116000	11.180701000	16.793549000

H	4.548680000	10.591637000	15.126526000
C	-0.780033000	9.314872000	12.164714000
H	-1.060523000	10.308617000	11.781386000
C	-4.775485000	10.290801000	15.867770000
H	-5.784410000	10.706982000	15.723813000
C	1.803019000	10.895788000	15.109644000
H	0.798292000	10.523790000	15.373470000
H	1.697022000	11.928801000	14.719166000
H	2.189824000	10.261094000	14.288163000
C	2.582791000	3.510989000	18.330404000
H	3.068712000	2.679504000	18.880863000
H	1.608911000	3.710600000	18.819336000
H	2.386039000	3.170177000	17.297098000
C	-0.699474000	2.927072000	17.080661000
H	-1.751016000	2.695090000	17.347956000
H	-0.211519000	1.981291000	16.763528000
H	-0.193130000	3.279849000	17.998809000
C	-1.733302000	12.178870000	18.341094000
H	-2.664192000	12.777857000	18.267214000
H	-1.902994000	11.392669000	19.105107000
H	-0.924678000	12.840153000	18.703842000
C	4.800110000	4.493883000	17.612703000
H	5.471385000	5.374663000	17.643008000
H	5.335748000	3.644663000	18.086078000
H	4.617263000	4.236966000	16.550641000
C	-0.236808000	11.985167000	21.752781000
H	-0.205667000	13.083308000	21.914064000
H	-1.086076000	11.762677000	21.080474000
H	-0.449622000	11.510737000	22.733187000

4-2. Cartesian coordinates of the optimised 5

FINAL SINGLE POINT ENERGY   -15572.794197007026 a.u.

Mo	11.864082000	7.235004000	30.543364000
Mo	13.748897000	6.086810000	30.517151000
Fe	13.968587000	8.804051000	27.723936000
As	12.758466000	6.597783000	27.767658000
As	11.571689000	8.619978000	28.305449000
As	13.006158000	9.687143000	29.926924000
As	15.069256000	8.282558000	29.998653000
As	15.110649000	6.595117000	28.209443000
N	13.989306000	6.256480000	32.539103000
N	12.118706000	7.918741000	32.434412000
N	10.764591000	5.524163000	30.127415000
N	12.943200000	4.388346000	29.572087000
B	13.046308000	7.122474000	33.250249000
B	11.502325000	4.290399000	29.832044000
C	15.026174000	10.548496000	27.284979000
C	15.681642000	9.411650000	26.686955000
C	14.743397000	8.772492000	25.785506000
C	13.511967000	9.519913000	25.824029000
C	13.687327000	10.623784000	26.745984000
C	15.660695000	11.517756000	28.234130000
H	16.261500000	12.271573000	27.680136000
H	16.340698000	11.000457000	28.939662000
H	14.901000000	12.059218000	28.829594000
C	17.117505000	9.039717000	26.897321000
H	17.424063000	9.189862000	27.951366000
H	17.772069000	9.676510000	26.263410000
H	17.316469000	7.984144000	26.630534000
C	15.018103000	7.603732000	24.891141000
H	15.813405000	6.948824000	25.296640000
H	15.346139000	7.952831000	23.888034000
H	14.111647000	6.981972000	24.749608000
C	12.304966000	9.250457000	24.979934000
H	12.150991000	8.164015000	24.825501000
H	12.419831000	9.718691000	23.978238000

H	11.383660000	9.659558000	25.437861000
C	12.700069000	11.720272000	27.002474000
H	12.796404000	12.125465000	28.028439000
H	11.655357000	11.376154000	26.871185000
H	12.867604000	12.556538000	26.289442000
C	9.351267000	5.527293000	30.323790000
C	10.825032000	2.850346000	29.837678000
C	8.803920000	5.071794000	31.565233000
C	11.666715000	9.221914000	32.785885000
C	12.945432000	7.199783000	34.832827000
C	14.968378000	5.472122000	33.223422000
C	9.229511000	8.612248000	32.127312000
H	9.712785000	7.625317000	31.951673000
C	7.412053000	5.128094000	31.761736000
H	6.994567000	4.792612000	32.724071000
C	11.736637000	7.632186000	35.433827000
H	10.882702000	7.896402000	34.796617000
C	9.454392000	2.606044000	29.570599000
H	8.781050000	3.442372000	29.351936000
C	15.001308000	3.134471000	29.054001000
C	16.326486000	5.906484000	33.301322000
C	10.298040000	9.592777000	32.585063000
C	11.818205000	3.497042000	26.807086000
H	11.266460000	4.124916000	27.537305000
C	13.684905000	3.571579000	28.680936000
C	13.885758000	7.017065000	37.106509000
H	14.744469000	6.782513000	37.755106000
C	11.589634000	7.742411000	36.824688000
H	10.630146000	8.076919000	37.249697000
C	17.835843000	7.248837000	31.731787000
H	18.743969000	6.698759000	32.057285000
H	18.144166000	8.277665000	31.453834000
H	17.451587000	6.756348000	30.818423000
C	8.158816000	8.406249000	33.215777000
H	8.612151000	8.137096000	34.189813000
H	7.464718000	7.593745000	32.922558000
H	7.564084000	9.331952000	33.363456000
C	16.911179000	3.855220000	34.509959000

H	17.668650000	3.216344000	34.989714000
C	14.015635000	6.902074000	35.713505000
H	14.984130000	6.586448000	35.309420000
C	12.668290000	7.432691000	37.671337000
H	12.561491000	7.519745000	38.764226000
C	14.061536000	9.987181000	33.549086000
H	14.307621000	8.938134000	33.280924000
C	14.578252000	4.266849000	33.883658000
C	11.627698000	1.709787000	30.089366000
H	12.701795000	1.838573000	30.275011000
C	8.464963000	5.932565000	29.277963000
C	8.575744000	9.051221000	30.807044000
H	8.063963000	10.029351000	30.917099000
H	7.828095000	8.305084000	30.478394000
H	9.328414000	9.153672000	29.999359000
C	15.563578000	3.473452000	34.498339000
H	15.262873000	2.535913000	34.991541000
C	7.078366000	5.956569000	29.522250000
H	6.399381000	6.272149000	28.714668000
C	12.582922000	10.226044000	33.256759000
C	6.544573000	5.577509000	30.759076000
H	5.458375000	5.614670000	30.934957000
C	16.776885000	7.289430000	32.845700000
H	15.883622000	7.810257000	32.445992000
C	12.110355000	11.531244000	33.494582000
H	12.821037000	12.292593000	33.851679000
C	11.837873000	4.245767000	25.459141000
H	12.410944000	5.192352000	25.515616000
H	10.804088000	4.491536000	25.143608000
H	12.286966000	3.624703000	24.657446000
C	17.274909000	5.075081000	33.929396000
H	18.324567000	5.405431000	33.977708000
C	15.571340000	3.306941000	30.454529000
H	14.860110000	3.924181000	31.050826000
C	8.944307000	6.234997000	27.863561000
H	10.051152000	6.274235000	27.892029000
C	13.217123000	3.225906000	27.359669000
C	9.883286000	10.912840000	32.839375000

H	8.825920000	11.177847000	32.682739000
C	15.811494000	2.442675000	28.136514000
H	16.816006000	2.119382000	28.450143000
C	9.663275000	4.465894000	32.669475000
H	10.691294000	4.360303000	32.271063000
C	14.348074000	10.190942000	35.051358000
H	14.217634000	11.257767000	35.328843000
H	15.391037000	9.909063000	35.296874000
H	13.670030000	9.589752000	35.683872000
C	11.101443000	0.409136000	30.102004000
H	11.761863000	-0.447122000	30.311686000
C	8.917104000	1.308806000	29.562889000
H	7.847898000	1.163916000	29.341591000
C	13.123128000	3.828924000	33.979922000
H	12.500328000	4.666278000	33.609800000
C	11.047205000	2.172040000	26.621933000
H	9.998503000	2.369096000	26.319290000
H	11.032652000	1.564479000	27.544142000
H	11.517308000	1.565294000	25.820105000
C	9.167237000	3.065006000	33.072797000
H	8.147864000	3.103769000	33.510241000
H	9.833814000	2.629551000	33.844849000
H	9.142296000	2.375576000	32.206858000
C	12.700213000	3.540653000	35.430902000
H	11.620499000	3.289081000	35.474144000
H	12.876969000	4.416945000	36.085284000
H	13.253650000	2.677369000	35.855556000
C	10.775840000	11.890865000	33.287736000
H	10.435331000	12.920881000	33.474783000
C	15.370060000	2.149178000	26.843937000
H	16.019995000	1.618802000	26.131099000
C	16.931104000	4.018695000	30.447590000
H	17.286632000	4.192665000	31.480048000
H	16.867730000	4.998795000	29.934500000
H	17.697229000	3.414405000	29.920344000
C	8.424507000	7.576978000	27.318893000
H	7.324988000	7.553515000	27.166513000
H	8.890081000	7.799573000	26.336480000

H	8.653478000	8.418347000	28.000205000
C	14.990440000	10.898873000	32.721966000
H	14.800786000	10.814601000	31.634098000
H	16.051995000	10.633441000	32.901567000
H	14.861900000	11.964903000	33.002791000
C	9.736386000	0.201440000	29.838519000
H	9.316788000	-0.817029000	29.839882000
C	15.684966000	1.942994000	31.162766000
H	16.441424000	1.306487000	30.658080000
H	14.723115000	1.394913000	31.152939000
H	15.993607000	2.078326000	32.218300000
C	17.300546000	8.106424000	34.042892000
H	16.559880000	8.147114000	34.864874000
H	17.526348000	9.147909000	33.733897000
H	18.235677000	7.671070000	34.453184000
C	8.541031000	5.095345000	26.907446000
H	8.950670000	4.120624000	27.233152000
H	8.909871000	5.297624000	25.880973000
H	7.436466000	4.996522000	26.854773000
C	14.077273000	2.533509000	26.482982000
H	13.711424000	2.286534000	25.474720000
C	9.733208000	5.385734000	33.895635000
H	10.179586000	6.357995000	33.627353000
H	10.356168000	4.940084000	34.695501000
H	8.724499000	5.573416000	34.317252000
C	12.858524000	2.622419000	33.071085000
H	13.485315000	1.754491000	33.361772000
H	13.089344000	2.875238000	32.022191000
H	11.799082000	2.305855000	33.114759000

4-3. Cartesian coordinates of the optimised 6

FINAL SINGLE POINT ENERGY   -6098.988431987543 a.u.)

Mo	1.51820564344526	-0.32895464625666	-1.02681165315302
Mo	-1.09222923245626	0.87303999866319	-0.85482454303447
Fe	0.53403952649512	2.18333985434314	-1.99204074301270
P	0.37350202205817	0.26900655429566	-3.12472185989605
P	-0.73182793705407	-1.20568730373308	-1.92122265287260
P	0.46993504318652	-1.72535036676683	0.68047565154119
P	0.23152631663863	0.45397432472644	1.13861843625207
P	1.55899236610854	1.81774566344270	-0.07198695109589
N	-3.03224074397127	0.69439811562510	-1.51640875892630
B	-3.55340476870749	1.27481626402753	-0.28129001541167
N	-2.42591203707789	1.64004253198940	0.54183392565852
N	3.06987230597031	-1.34003988551787	-0.21516058406954
B	3.14695206360472	-2.19231849730747	0.93859066372633
N	1.86022937257846	-2.30176388111877	1.59768824543942
C	3.96092783328850	-0.77547232758058	-1.12485794719451
C	3.76571390315496	-1.10419355909030	-2.51716164411976
C	4.95562614064194	0.18225279102555	-0.71848015358141
C	-3.13712136503993	1.31307766245015	-5.86229281441963
C	-0.43074308121815	3.06309833145461	-5.07617147724441
C	2.58635364199851	2.31833496279072	-4.61367757349205
C	2.45154410415611	-2.25992705766409	-4.39220579658234
C	-4.16372448107535	-1.05129980873002	-4.61256949991641
C	-3.28735231365657	1.32055949601763	-4.33546772851600
C	-4.28814927134475	2.41733932038664	-3.91569621510384
C	0.30818107464389	3.30202847537973	-3.80212090482236
C	-4.60782130450439	-2.27939217963028	-4.10495580524062
C	1.70474221452342	2.98832674442245	-3.60833779806847
C	-3.68888728771158	-0.03287774382918	-3.76560168011003
C	4.57010444637591	-0.44977377675719	-3.47438424192319
C	5.55077131830481	0.46361234430402	-3.07933299071434
C	-1.51051391950653	4.68473867748300	-2.53435021516965
C	-0.15618515959108	4.06014414812697	-2.66662823735425
C	2.83518863813247	-2.25691833490491	-2.91093547490227
C	3.41473437915198	-3.61617450838444	-2.47899934276243

C	2.12360859717907	3.60010982860700	-2.38276931896211
C	-4.61236914032262	-2.47981240092470	-2.72197345955107
C	-3.63596722029844	-0.26239293979599	-2.35283960270470
C	0.97952010103099	4.26724361462863	-1.80081275531944
C	3.53479138880590	3.66957695549366	-1.88776106254834
C	5.74308141507171	0.76532889535341	-1.71686572729864
C	-4.15485405869767	-1.49197706891169	-1.82914661069253
C	1.03541497680989	5.14391151874878	-0.59152448076789
C	-6.08080507136806	1.27632979508649	-0.94062254768013
C	-7.44251497634381	1.49893631227481	-0.67787864965034
C	-4.25603290993798	-1.79582392782726	-0.34010568162425
C	-5.08372080308125	1.51550376121396	0.03730942925686
C	-7.84802409521447	1.96479796200557	0.58467061149628
C	-5.71136167718946	-2.10476827068572	0.05911937858452
C	-3.56304815463378	4.71763041482298	0.57643330200143
C	5.48291267799108	-3.18033056852046	0.39787314155532
C	6.61242434408713	-3.96405549551636	0.67942216405900
C	-3.31056269597651	-2.93126095176767	0.08890367620781
C	1.66434519339662	-6.32232353727904	2.06129428688071
C	5.18346485503676	0.51283102789888	0.75019334907031
C	-6.87932457346766	2.21619340795834	1.57283213812139
C	-5.52070275929954	1.99871067421828	1.29680854175873
C	-2.16271367589963	4.46222167115039	1.16970391310905
C	5.03833882836123	2.01558541682113	1.04666116158005
C	-0.66130828733537	-5.32582490867295	1.72125163788018
C	4.42621643976012	-3.02221425160976	1.33162597317261
C	0.83705697887256	-5.03112104203404	1.91983299757976
C	-1.56425402644401	5.79529800033620	1.64302302341582
C	6.55611668044019	0.00358987357086	1.23208776878266
C	6.72742997468507	-4.60904095887582	1.92280563495851
C	-2.34265229160082	2.00912546016874	1.89594011785728
C	4.56877176216263	-3.68891999445401	2.57608653867027
C	-2.18017698729336	3.38762137852414	2.24883412545779
C	5.70086151681598	-4.46456986850961	2.87196590956431
C	1.06369680858578	-4.09165535978157	3.09661792237873
C	1.58426450453370	-2.78515955600161	2.91238893359422
C	-2.66862522444086	-0.45299676032138	2.67134642841620
C	-2.38201433123717	1.02157803612476	2.93598240557793

C	-4.15164775603696	-0.75548305266373	2.96541812534340
C	-2.06339393824032	3.74342855652930	3.60541649854971
C	0.77424741739832	-4.51252223373340	4.40933167432411
C	-1.78584870111405	-1.40939924123523	3.48910275220333
C	1.80557862730358	-1.90715310506280	4.01068469915107
C	2.37589733107788	-0.50627405207018	3.80833822102145
C	-2.25018106382627	1.43300079117030	4.27740127036849
C	3.86683944373387	-0.45139882410086	4.19310669847964
C	-2.09218584467124	2.77840458646415	4.62127761478949
C	1.00004691145290	-3.66860143738750	5.50546809123867
C	1.51514915533762	-2.37918151142118	5.30386909424374
C	1.56965399018345	0.57594568626419	4.54544913820007
H	-4.09969498900477	1.07698265810828	-6.36204357169850
H	-2.82817124991217	2.31054500474063	-6.22951101844307
H	-2.38471669323035	0.57361744253267	-6.20438390574601
H	0.01703065979036	3.68748744978570	-5.87972795060316
H	-4.19499004040314	-0.88406310071817	-5.69759467429337
H	2.91384745571217	3.05142176033562	-5.38326450033676
H	-0.37215770259016	2.00851419909287	-5.40908152170160
H	-1.49271040372550	3.34651743970395	-4.98865078521742
H	3.32356685025720	-2.50067483641077	-5.03478198578535
H	2.05964356763035	1.49902030385719	-5.14267483437332
H	2.03987893054418	-1.28024711096527	-4.70759790573742
H	1.67753491199132	-3.03083241250863	-4.57771739529072
H	-4.96420633300217	-3.06764286021899	-4.78625338993560
H	-3.99939859927216	3.39759343817571	-4.34954120946027
H	-5.30969840835837	2.17825958109827	-4.27957658533408
H	4.44310973753045	-0.68062432810527	-4.54069451526241
H	3.49301140605326	1.89361162965377	-4.14554161921861
H	-1.55985795722948	5.63624974757345	-3.10787410446606
H	-2.30676571678595	1.57592627780549	-3.87492321344179
H	6.18030521905493	0.95151419669433	-3.83900459036338
H	-2.30522938773750	4.01921440510471	-2.91702876075464
H	4.41265574654719	-3.77809861239604	-2.93671551592039
H	-4.32946466754762	2.52905157842925	-2.81623658262484
H	2.74286014876735	-4.43474357113155	-2.80718397324699
H	4.10082700526933	4.42885692901256	-2.47007922550420
H	1.86700042808484	-2.16950951823676	-2.34081017821102

H	4.05841149237664	2.70197297973171	-2.00200566647081
H	-4.98713090079344	-3.43241293106829	-2.31527903675780
H	-1.74831296014966	4.91679550292423	-1.48210521099469
H	-5.78926731917842	0.90117721567152	-1.93157557146229
H	3.52426424800125	-3.68692761170402	-1.38109523914850
H	-8.19171505204477	1.30364649121447	-1.46133268981688
H	6.52496466375728	1.48644964235905	-1.43189966718032
H	1.51477256775919	6.11278218278847	-0.85024279961124
H	3.58813461496183	3.96202935192002	-0.82299484836264
H	0.02801761380018	5.36311039082385	-0.20483912326057
H	-3.52915592466577	5.55232754559298	-0.15442312821430
H	5.42625067014607	-2.68339035802714	-0.58091340595838
H	-6.08667542669100	-3.01410312678336	-0.45422093674963
H	-6.38404925322938	-1.26344843099957	-0.19891975539849
H	7.40892280368088	-4.06753584368870	-0.07387540064023
H	-3.96018412081377	3.82750619956226	0.05782223732262
H	1.53931041312116	-6.96387637403261	1.16443067292948
H	1.62542370071313	4.69090108857043	0.23013158872455
H	-8.91527025777142	2.13576577021177	0.79742048165862
H	-3.53427979611782	-3.87268548391597	-0.45534063382974
H	-0.82013085641790	-5.97249911134818	0.83337082027562
H	-1.52705194457885	4.05250194838422	0.35142776137137
H	-1.47426388571818	6.49750874521020	0.78933195828207
H	-3.94721483443735	-0.88732854782660	0.21342420349232
H	-2.25203086267008	-2.66736023428453	-0.10303854995772
H	5.80472629703983	2.61437606901871	0.51158319336477
H	1.19690062299178	-4.51107314027815	1.00893903519463
H	4.03636396400998	2.38590865511026	0.75401950030372
H	-4.28325284050091	4.99618717718839	1.37376527249847
H	7.38045754018980	0.52889879911067	0.70553875749197
H	2.74379035073449	-6.09363306243092	2.17274159474331
H	-5.78877323074939	-2.28319087332158	1.14992363744857
H	6.67439789140425	-1.08292342434168	1.06057387423636
H	1.34895874226700	-6.91674160936154	2.94455373045846
H	7.61370108388897	-5.22159358835986	2.15139079286344
H	4.40097832008457	-0.01541666182566	1.33177318868924
H	-1.23234557447052	-4.38819180594436	1.56734148378582
H	-3.41336350434568	-3.13705766685444	1.17395013930828

H	-7.18534920929339	2.58742542337409	2.56371572390306
H	-4.78068549709494	2.21883166487037	2.07924513353744
H	-0.55996186147645	5.67134648961183	2.09550100054797
H	-1.09226439763614	-5.84780007838438	2.60155768096546
H	-2.21744266284600	6.28940403808107	2.39210979369195
H	-2.47488057991130	-0.64845325682704	1.59706765568699
H	5.16604710889828	2.20144157991009	2.13298340879783
H	6.67397881707199	0.19341243555320	2.31862135381277
H	-4.83246006425241	-0.17052705454887	2.32024167116041
H	3.78147012983726	-3.60338603266620	3.33644230133282
H	5.77978849041184	-4.96273935170305	3.85094568481498
H	-4.37066836159697	-1.83155180966546	2.81149811469993
H	2.30381565578086	-0.27874666384053	2.72438933295212
H	-1.93653130066326	-2.45285809741890	3.14608153422343
H	-1.94647923366002	4.80100008852297	3.88065950992714
H	4.46426937762212	-1.17933988235071	3.61026758478551
H	0.36963766908762	-5.52325468086297	4.57667954183276
H	-0.70934907303515	-1.17999500443530	3.38812298820970
H	-4.39203437514990	-0.51136920360686	4.02149854103494
H	4.27912026613112	0.56073408878793	4.00209832781613
H	-2.03702264994164	-1.38080675492006	4.56969719511172
H	-2.28753614172744	0.67358400618521	5.07324719688601
H	4.00921794835175	-0.68080447144525	5.27033322633717
H	1.96264067884359	1.58224660755707	4.29242603173523
H	0.50012480561382	0.55246325178708	4.25670027645687
H	-1.99436232983225	3.07795728598773	5.67631785641080
H	0.77080138994895	-4.01651419233021	6.52481519429714
H	1.68669031191974	-1.72210444311625	6.17058482207778
H	1.63192700689515	0.46249576793108	5.64805245728675

4-4. Cartesian coordinates of the calculated 6-TS

The DFT-optimised transition state geometry was calculated at the BP86-D4/def2-SVP

CPCM(THF) level of theory.

FINAL SINGLE POINT ENERGY   -6097.888273406011 a.u.

Mo	1.664950000	0.044518000	-0.569832000
Mo	-0.993355000	1.104211000	-0.497644000
Fe	0.520800000	2.244048000	-1.943115000
P	0.491225000	0.139379000	-2.637352000
P	-0.551704000	-1.175704000	-1.128835000
P	0.564106000	-1.345344000	1.072041000
P	0.375122000	0.998390000	1.495547000
P	1.496824000	2.323573000	0.044344000
N	-2.917624000	0.638095000	-1.082660000
B	-3.473199000	1.472166000	-0.031715000
N	-2.367930000	2.123896000	0.647193000
N	3.116763000	-1.222159000	-0.036609000
B	3.146094000	-2.286237000	0.928776000
N	1.857746000	-2.403425000	1.602985000
C	4.025725000	-0.634787000	-0.931186000
C	4.060422000	-1.090696000	-2.299202000
C	4.855756000	0.454741000	-0.482160000
C	-2.949245000	0.199950000	-5.454321000
C	-0.420432000	2.375321000	-5.146235000
C	2.641667000	1.938351000	-4.496536000
C	2.786774000	-2.124985000	-4.255293000
C	-3.799695000	-1.881311000	-3.681702000
C	-3.126344000	0.555402000	-3.972256000
C	-4.207667000	1.645421000	-3.820292000
C	0.282998000	2.934285000	-3.953974000
C	-4.169149000	-2.983962000	-2.900177000
C	1.690554000	2.755462000	-3.681247000
C	-3.442839000	-0.651249000	-3.098322000
C	4.976850000	-0.475327000	-3.168198000
C	5.815032000	0.559386000	-2.727619000

C	-1.638592000	4.451755000	-3.049567000
C	-0.252582000	3.886788000	-3.013439000
C	3.180827000	-2.245199000	-2.776230000
C	3.833541000	-3.616122000	-2.505405000
C	2.041186000	3.625050000	-2.600799000
C	-4.218559000	-2.845239000	-1.510166000
C	-3.431017000	-0.530613000	-1.670345000
C	0.845767000	4.332496000	-2.189222000
C	3.429944000	3.877555000	-2.101419000
C	5.742790000	1.027952000	-1.407350000
C	-3.872878000	-1.637951000	-0.873570000
C	0.831675000	5.447422000	-1.194390000
C	-5.977984000	1.161822000	-0.662377000
C	-7.355820000	1.346486000	-0.464019000
C	-4.001655000	-1.585591000	0.643357000
C	-5.017213000	1.673840000	0.245051000
C	-7.814791000	2.047044000	0.664851000
C	-5.455287000	-1.854094000	1.080026000
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