Supporting information of the manuscript entitled:

Triple-decker sandwich complexes with a bent *cyclo*-P_5 middle-deck

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Contents

General Procedures: All manipulations were performed with rigorous exclusion of oxygen and moisture in Schlenk-type glassware on a dual manifold Schlenk line in argon atmosphere or in Ar filled glove box with a high-capacity recirculator (< 0.1ppm O_2). THF, toluene, *n*-hexane, and DME were distilled from sodium benzophenoneketyl. Deuterated solvents were degassed, dried and distilled prior to use. The complex [Cp*Fe(η^5-P_5)] (**I**), [Li][**1a**] and [Li][**1b**] were prepared according to their published procedures.[1] NMR spectra were recorded on a Bruker Avance 300 MHz and Bruker Avance 400 MHz spectrometer. Chemical shifts were measured at ambient temperature and are given in ppm; they are referenced to TMS for ^{1}H and ^{13}C, and 85 % H_3PO_4 for ^{31}P as external standard. Elemental analyses (CHN) were determined using in-house facility. The X-Band EPR measurements were carried out with a MiniScope MS400 device with a frequency of 9.44 GHz and a rectangular resonator TE102 of the company Magnettech GmbH.

All cyclic voltammetry measurements were performed at 295 K in a three electrode setup, with a platinum disc electrode (working electrode, 3 mm diameter), an Ag-wire (pseudo-reference electrode) and a Pt-wire (auxiliary electrode), in combination with a *Methrom Autolab PGSTAT101* potentiostat. Bu_4NPF_6 (0.1 mol/L) was used as supporting electrolyte and all cyclic voltammograms are referenced against the Cp_2Fe/Cp_2Fe^+ redox couple.

The molar magnetic susceptibility χ_P and the effective magnetic moment μ_{eff} for **2a** and **2b** were determined on a Bruker Avance 400 MHz spectrometer (^{1}H: 400.130 MHz) by Evans method (equations (1) and (2)).[2] The diamagnetic contribution was calculated using Pascal's constants.[3] Pure solvent was used as an internal reference.

Equation:

$$\chi_P = \frac{3000\,\Delta f}{4\,\pi\,f\,c} - \chi_D \qquad (1)$$

$$\mu_{eff} = \sqrt{8\,\chi_P\,T} \qquad (2)$$

X_p: molar susceptibility of the sample in $m^3 \cdot mol^{-1}$.

Δf: chemical shift difference between solvent in presence of paramagnetic solute and pure solvent in Hz.

f: operating frequency of NMR spectrometer in Hz.

c: concentration of the paramagnetic sample in $mol \cdot L^{-1}$ (0.01 mol/L)

T: absolute temperature in K.

μ_{eff}: effective magnetic moment in μ_B.

1. Experimental details: complex syntheses and characterization

All the transition metal compounds [Cp'''MX]$_2$ (M = Cr, Fe, Co, Ni; X = Cl, Br) were prepared in situ in THF by mixing the MX_2 salt with NaCp''' in the right stoichiometrie and adding the solvent at room temperature.[4] The suspension was stirred overnight, the solvent removed, the product solved in *n*-hexane, filtered through a well dried frit and used for subsequent reactions. As a side note: For the synthesis of [Cp'''CrCl]$_2$ it is important to use very fresh $CrCl_2$, otherwise the reaction is likely to fail.

Synthesis of [2a]: To 234 mg (0.4 mmol) of **1a**·2 Et_2O in 20 mL THF, 130 mg (0.2 mmol) of [Cp'''CoCl]$_2$ in 20 mL THF were added and the solution was stirred overnight. The solvent was removed and **2a** extracted with *n*-hexane, filtered and the solvent removed. **2a** was obtained in 35 % (103 mg) crystalline yield from a CH_2Cl_2 (5 mL) : MeCN (30 mL) mixture at 0° C, and in 80 % yield (234 mg) as a powder. Single crystals suitable for X-ray measurements were obtained from a saturated solution of **2a** in MeCN. $C_{31}H_{55}CoFeP_5Si$ (725.50): calcd. C 51.31, H 7.64; found C 51.39, H 7.19. X-band EPR (toluene, 77 K): g_{iso} = 2.069. Evans (C_6D_6, 300 K): μ_{eff} = 2.14 μ_B.

Synthesis of [2b]: To 170 mg (0.3 mmol) of **1b**·2 THF in 20 mL THF, 103 mg (0.15 mmol) of [Cp'''CoCl]$_2$ in 20 mL THF was added and the solution was stirred overnight. The solvent was removed, **2b** extracted with *n*-hexane, filtered and the solvent was concentrated to 5 mL. By removing the solvent slowly over the course of two weeks **2b** was obtained in 15 % (31 mg) crystalline yield. Higher yields were obtained by isolating **2b** as a powder (64 %, 126 mg). $C_{29}H_{50}CoFeP_5N$ (682.36): calcd. C 51.04, H 7.39, N 2.05; found C 51.12, H 7.32, N 2.16. X-band EPR (toluene, 77 K): g_{iso} = 2.076. Evans (C_6D_6, 300 K): μ_{eff} = 1.83 μ_B.

Synthesis of [3]: To 213 mg (0.3 mmol) of **1b**·3 THF in 20 mL THF, 129 mg (0.15 mmol) of [Cp'''NiBr]$_2$ in 20 mL THF was added and stirred overnight. The solvent was removed and **3** was extracted with *n*-hexane and filtered through a frit. The solution was concentrated to the first precipitation (5 mL) and stored over night at -30° C. **3** was isolated in 51 % crystalline yield (118 mg). FD-MS: 681.1 (M^+, 100 %). $C_{29}H_{50}FeNiP_5N$ (682.12): calcd. C 51.06, H 7.39, N 2.05; found C 50.99, H 7.42, N 1.93.^{1}H NMR (400.13 MHz, C_6D_6): δ [ppm] = 1.45 (s, 9 H, Cp'''), 1.61 (s, 18 H, Cp'''), 1.68 (s, 15 H, Cp*), 2.107 (d, 6 H, NMe_2), 5.04 (s, 2 H, Cp'''). ^{13}C{^{1}H} NMR (100.62 MHz, C_6D_6): δ = 11.5 (s, $C_5(CH_3)_5$), 31.68 (s, $C(CH_3)_3$), 32.26 (s, $C(CH_3)_3$), 33.55 (s, $C(CH_3)_3$), 33.67 (s, $C(CH_3)_3$), 36.32 (t, NMe_2), 90.82 (s, CH), 91.69 (*s*, $C_5(CH_3)_5$), 116.69 (s, *C*-$C(CH_3)_3$), 118.06 (s, *C*-$C(CH_3)_3$). ^{31}P NMR (161.97 MHz, C_6D_6): δ = -53.87 (m, 2 P), -30.28 (m, 2 P), 40.63 (t, 1 P).

Synthesis of [4]: To 180 mg (0.33 mmol) of **1b**·2 THF in 20 mL THF, 245 mg (0.16 mmol) of [Cp'''FeBr]$_2$ in 20 mL THF was added and stirred overnight. The solvent was removed, **4** extracted with *n*-hexane, filtered and the solvent was concentrated to 5 mL and stored over night at -30° C. **4** was isolated in 58 % crystalline yield (131 mg). $C_{29}H_{50}Fe_2P_5N$ (679.27): calcd. C 51.28, H 7.42, N 2.06; found C 51.34, H 7.47, N 2.36. ^{1}H NMR (400.13 MHz, THF-d_8): δ [ppm] = 1.19 (s, 9 H, Cp'''), 1.42 (s 18 H, Cp'''), 1.62 (s, 15 H, Cp*), 2.51 (d, 6 H, NMe_2), 3.78 (s, 2 H, Cp'''). ^{13}C{^{1}H} NMR (100.62 MHz, THF-d_8): δ = 10.74 (s, $C_5(CH_3)_5$), 31.61(s, $C(CH_3)_3$), 32.19 (s, $C(CH_3)_3$), 34.105 (s, $C(CH_3)_3$), 34.34(s, $C(CH_3)_3$), 40.73 (s, NMe_2), 74.76 (s, CH), 85.85 (*s*, $C_5(CH_3)_5$), 103.93(s, *C*-$C(CH_3)_3$), 106.07 (s, *C*-$C(CH_3)_3$). ^{31}P NMR (161.97 MHz, THF-d_8): δ = -151.5 (broad, 2 P), -131.2 (broad, 2 P), 73.75 (s, 1 P).

Synthesis of [5]: To 173 mg (0.3 mmol) of **1a**·2 Et_2O in 20 mL THF, 95 mg (0.15 mmol) of [Cp'''CrCl]$_2$ in 20 mL was added and stirred overnight. The solvent was removed, **5** extracted with *n*-hexane, filtered and the solvent was concentrated to 5 mL and stored over night at -30° C. **5** was isolated in 47 % crystalline yield (100 mg). $C_{31}H_{55}CrFeP_5Si$ (718.56): calcd. C 51.82, H 7.71; found C 51.43, H 7.86. ^{1}H NMR (400.13 MHz, C_6D_6): δ [ppm] = 0.34 (s, 9 H, $SiMe_3$), 1.32 (s, 9 H, Cp'''), 1.49 (s, 18 H, Cp'''), 1.52

(s broad, 15 H, Cp*), 1.58 (s, 2 H, CH_2SiMe_3), 3.41 (s, 1 H, CH), 4.62 (s, 1 H, CH). ^{31}P NMR (161.97 MHz, C_6D_6): δ = -66.73 (tt, 1 P), 9.46 (d broad, 2 P), 281.16 (dd broad, 2 P).

Synthesis of [6][PF$_6$]: To 300 mg (0.41 mmol) of **2a** in THF 130 mg (0.4 mmol) of [Cp_2Fe][PF_6] was added at -50° C. The mixture was stirred and warmed up to room temperature overnight. The solvent was removed and the residue washed five times with *n*-hexane. **6** is poorly soluble in Et_2O and after the repeatedly extraction with Et_2O, removing of solvent and washing with *n*-hexane, very few crystals of **6**, suitable for single crystal measurement, were obtained (3 mg, 1 %).

2. Experimental and simulated NMR spectra

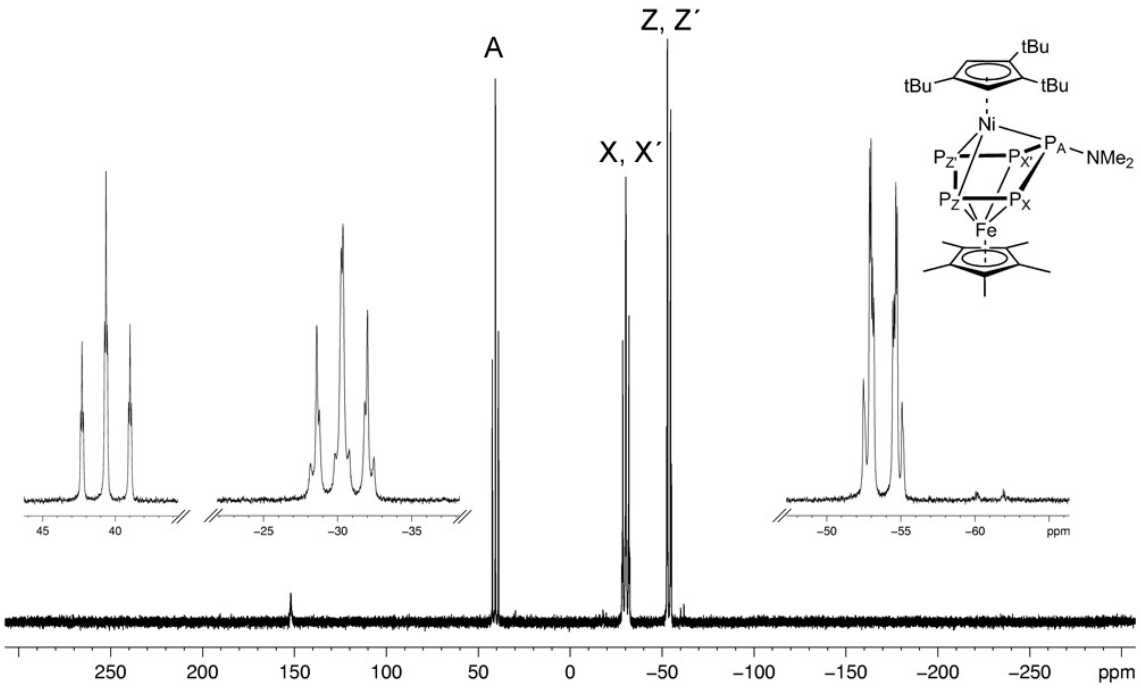


Figure S1. ^{31}P NMR (161.97 MHz, C_6D_6) spectrum of **3**.

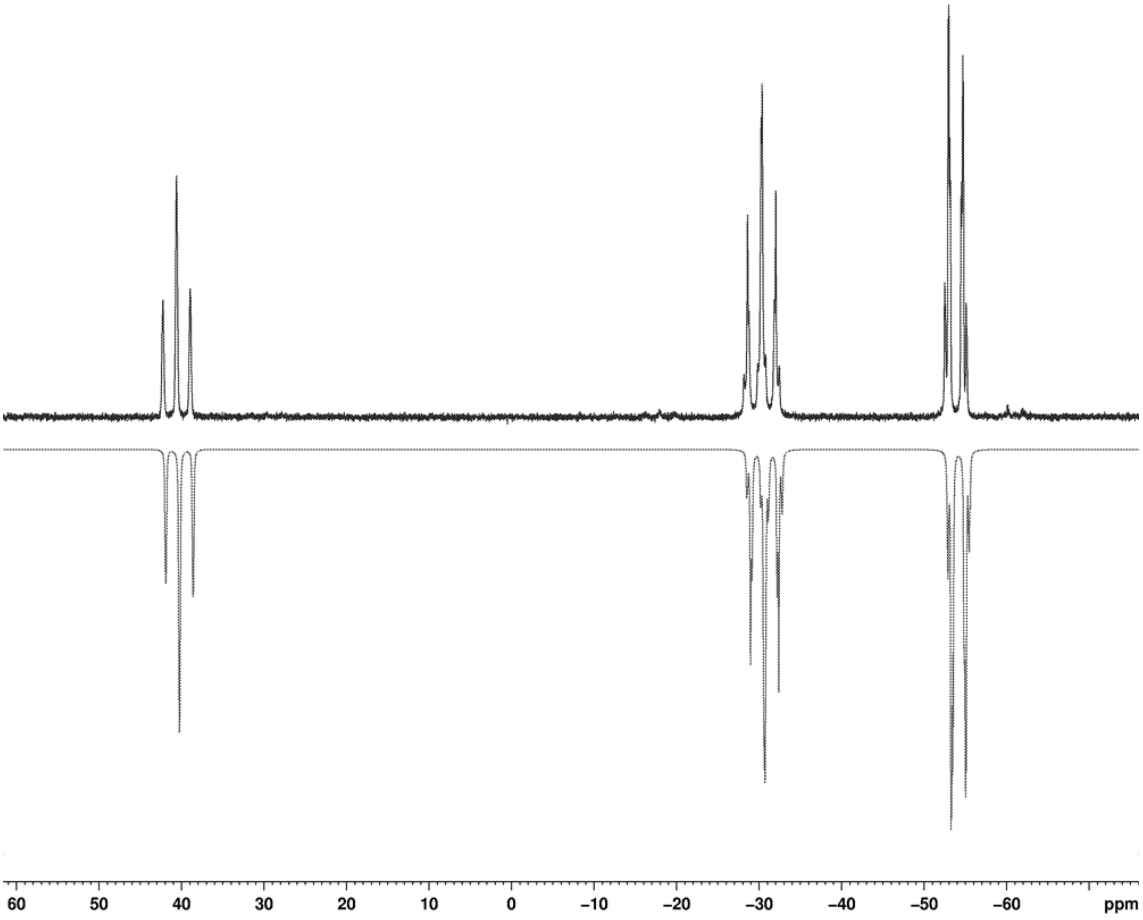


Figure S2. Experimental (top) and simulated (bottom) ^{31}P NMR (161.97 MHz, C_6D_6) spectrum of **3**.

Table S1. ^{31}P NMR chemical shifts and coupling constants for **3** obtained from the simulation.

	J (Hz)			δ (ppm)	
$^{1}J_{PA\text{-}PX}$	269.83	$^{1}J_{PX\text{-}PZ}$	290.36	A, A'	40.61
$^{1}J_{PA\text{-}PX'}$	267.89	$^{2}J_{PX\text{-}PZ'}$	-17.13	X, X'	30.37
$^{2}J_{PA\text{-}PZ}$	-14.13	$^{2}J_{PX'\text{-}PZ}$	-2.62	Z, Z'	-53.79
$^{2}J_{PA\text{-}PZ'}$	-17.22	$^{1}J_{PX'\text{-}PZ'}$	302.00		
$^{1}J_{PX\text{-}PX'}$	98.94	$^{1}J_{PZ'\text{-}PZ'}$	11.08		

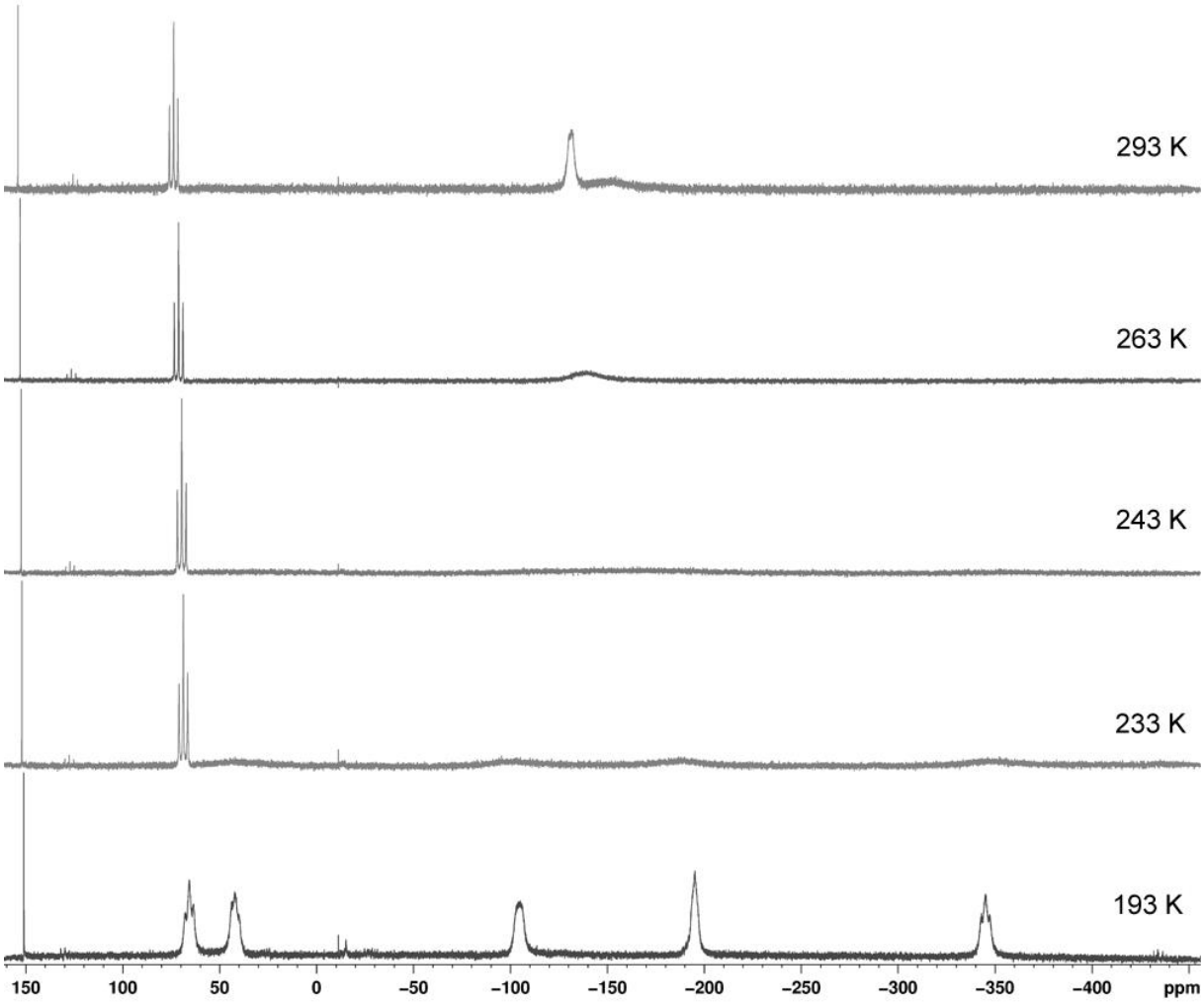


Figure S3. ^{31}P NMR (161.97 MHz, C_6D_6) spectrum of **4** at different temperatures.

Due to the big linewidth of the signals of **4** in the ^{31}P NMR spectrum at 193 K, the coupling constant was neglected for the calculation of the rate constant k_C. 243 K was determined as the coalescence temperature. $\Delta\nu$ is 62715.1 Hz. Therefore the value of the free activation enthalpy results in a value of 35.2 KJ mol^{-1}, according to the literature.[5]

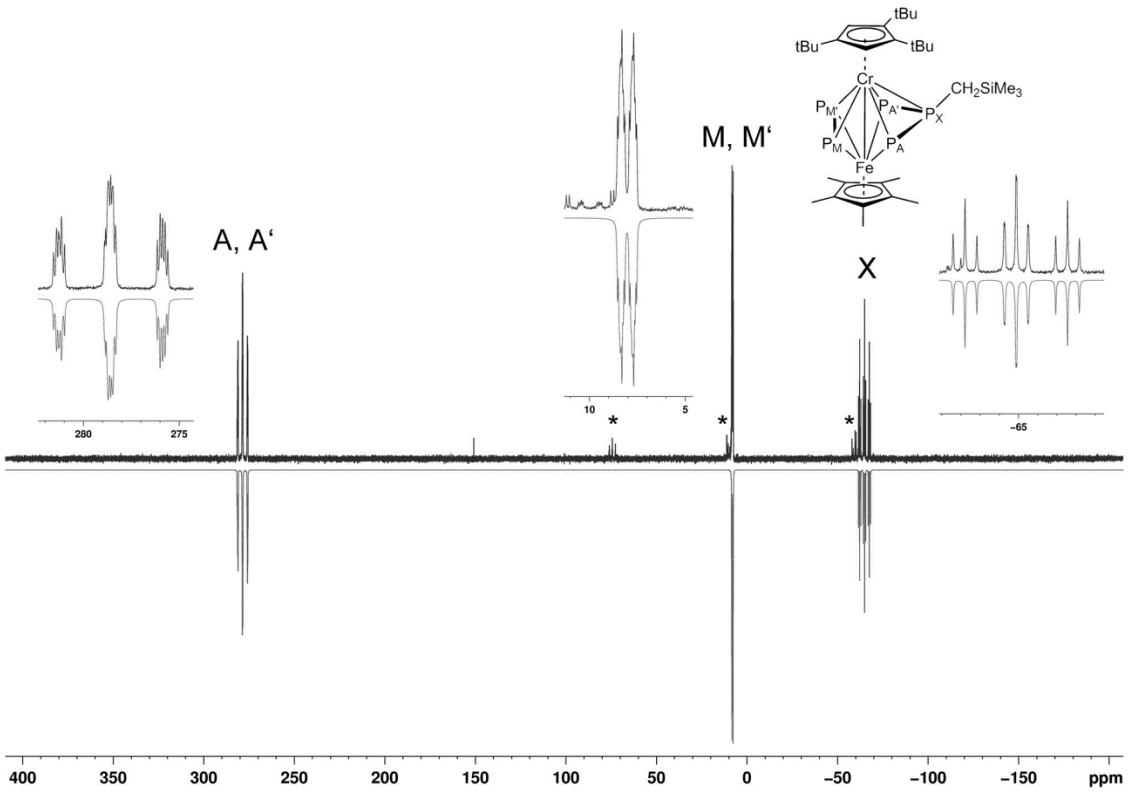


Figure S4. ^{31}P NMR (161.97 MHz, C_6D_6) spectrum of **5** at 253 K. Impurities are marked with *.

Table S2. ^{31}P NMR chemical shifts and coupling constants for **5** at 253 K obtained from the simulation

	J (Hz)			δ (ppm)	
$^1J_{PA\text{-}PX}$	429.62	$^2J_{PA'\text{-}PM}$	-25.62	A	279.93
$^1J_{PA'\text{-}PX}$	437.11	$^2J_{PX\text{-}PM}$	99.70	A’	277.22
$^1J_{PA\text{-}PM}$	22.66	$^2J_{PX\text{-}PM'}$	100.13	M	7.9928
$^1J_{PA'\text{-}PM'}$	21.16	$^1J_{PM\text{-}PM'}$	3.36	M’	8.0736
$^2J_{PA\text{-}PM'}$	-27.48	$^2J_{PA\text{-}PA'}$	42.20	X	-64.87

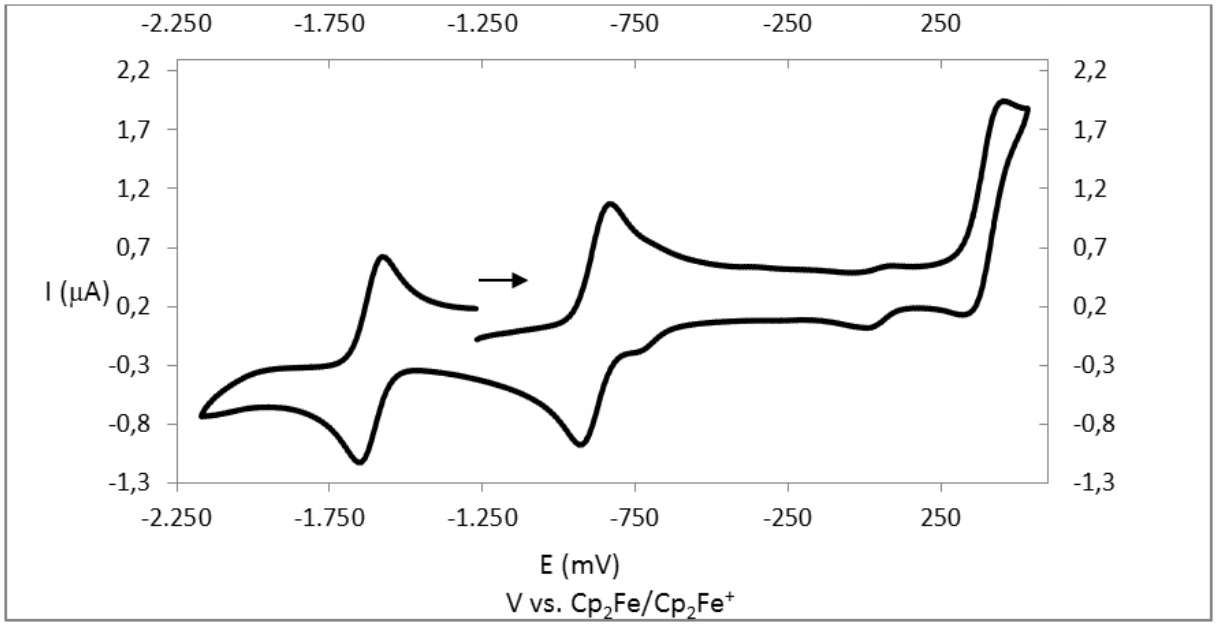


Figure S5. Cyclic voltammogram of **2b** recorded at a platinum disc electrode in 1,3-difluorobenzene at 100 mV/s and referenced against fc/fc+; supporting electrolyte $[Bu_4N][PF_6]$ (0.1 mol/L).

3. EPR spectra

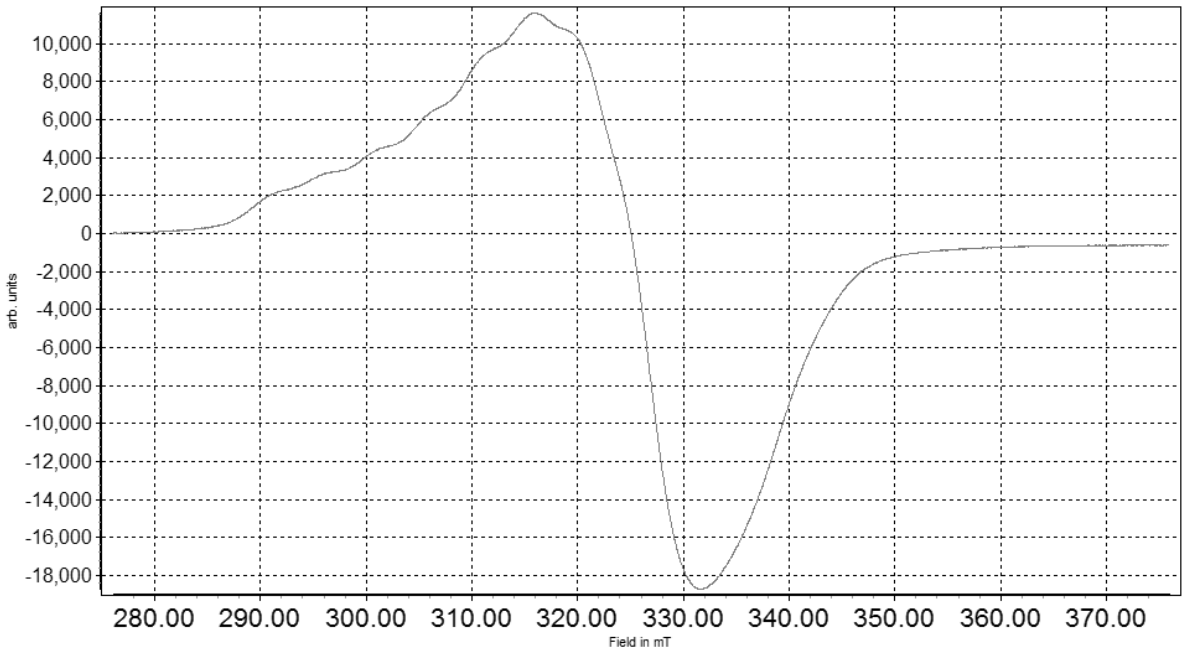


Figure S6. X-band EPR spectrum of **2a**, in toluene at 77 K.

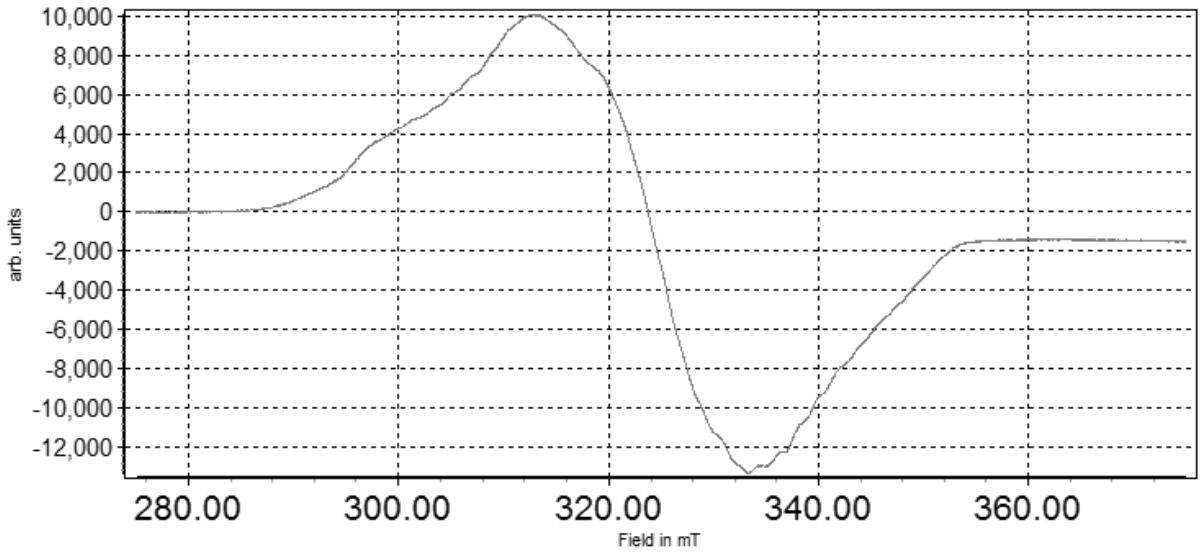


Figure S7. X-band EPR spectrum of **2b**, in toluene at 77 K.

4. Details on X-ray structure determinations and ortep plots

The diffraction data were collected on a Gemini R-Ultra diffractometer (**2a**, **2b**, **3**) equipped with Ruby detector or SuperNova diffractometers (Agilent Technologies) equipped with Atlas (**5**-**6**) detectors, respectively, and micro-focus SuperNova sourse (CuK_α radiation, λ = 1.54178 Å) using ω scans of 1° (**5**, **6**), 0.5° (**2a**, **2b**, **3**) or 0.25° (**4**) frames. The diffraction experiment for **4** was performed on a SuperNova equipped with CCD detector Eos with Mo *K*α radiation (λ = 0.71073Å) using ω scans of 0.25° frames. All measurements were performed at 123 K. All structures were solved by direct methods with ShelXT[6] or Olex2[7] programs and refined by full-matrix least-squares method against $|F|^2$ in anisotropic approximation using SHELXTL or its multiprocessor version SHELX2013[6]. Absorption corrections were applied analytically using *CrysAlis PRO* Software (Table S1).[8] All non-hydrogen atoms were refined in anisotropic approximation. Hydrogen atoms were refined in calculated positions using riding on pivot atom model.

The supplementary crystallographic data for this publication (Tables S1-S2) can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; Fax: + 44-1223-336-033; e-mail: deposit@ccdc.cam.ac.uk). The data are deposited at the under the deposition codes CCDC 1499116-1499121. All drawings for **2a**, **2b**-**6** were made in Olex2.[7]

Table S3. Crystal data, data collection parameters, and convergence results for **2a**, **2b** - **4**.

	2a	**2b**	**3**	**4**
CCDC Code	CCDC-1499116	CCDC-1499117	CCDC-1499118	CCDC-1499119
Crystal data				
Chemical formula	$C_{31}H_{55}CoFeP_5Si$	$C_{29}H_{50}CoFeNP_5$	$C_{29}H_{50}FeNNiP_5$	$C_{29}H_{50}Fe_2NP_5$
M_r	725.47	682.33	682.11	679.25
Crystal system, space group	Triclinic, $P\bar{1}$	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/c$
Temperature (K)	123	123	123	123
a, b, c (Å)	10.1595 (3), 12.5137 (4), 15.7867 (5)	12.7300 (1), 15.5790 (1), 17.3044 (1)	12.7483 (1), 15.4746 (1), 17.3699 (2)	17.2557 (3), 12.4359 (2), 16.6796 (3)
α, β, γ (°)	100.375 (2), 100.066 (2), 108.045 (3)	90, 108.258 (1), 90	90, 107.710 (1), 90	90, 114.972 (2), 90
V (Å^3)	1819.16 (10)	3259.05 (4)	3264.25 (5)	3244.67 (11)
Z	2	4	4	4
F(000)	766	1436	1440	1432
D_x (Mg m^{-3})	1.324	1.391	1.388	1.390
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	9.30	10.02	6.74	1.16
Crystal shape and colour	Black block	Black block	Brown plate	Dark green trapezoid
Crystal size (mm)	0.31 × 0.13 × 0.11	0.12 × 0.10 × 0.09	0.19 × 0.17 × 0.06	0.10 × 0.07 × 0.05
Data collection				
Diffractometer	Xcalibur, Ruby, Gemini ultra diffractometer	Xcalibur, Ruby, Gemini ultra diffractometer	Xcalibur, Ruby, Gemini ultra diffractometer	SuperNova, Single source at offset, Eos diffractometer
Absorption correction	Analytical	Analytical	Analytical	Analytical
T_{min}, T_{max}	0.179, 0.518	0.463, 0.555	0.434, 0.734	0.914, 0.958
No. of measured, independent and observed [> 2σ(I)] reflections	13401, 7013, 6204	17145, 5732, 4810	15331, 5591, 4600	20562, 10520, 6944
R_{int}	0.021	0.032	0.027	0.028
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.624	0.595	0.594	0.754
Range of h, k, l	h = -12→8, k = -15→15, l = -18→19	h = -15→13, k = -17→18, l = -16→20	h = -15→15, k = -15→17, l = -20→18	h = -25→24, k = -17→14, l = -25→20
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.026, 0.080, 1.09	0.029, 0.068, 0.93	0.024, 0.056, 0.91	0.030, 0.061, 0.84
No. of reflections	7013	5732	5591	10520
No. of parameters	369	350	350	350
No. of restraints	0	0	0	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.32, -0.43	0.61, -0.40	0.32, -0.25	0.47, -0.29

Table S4. Crystal data, data collection parameters, and convergence results for **5** and **6**.

	5	**6**
CCDC Code	CCDC-1499120	CCDC-1499121
Crystal data		
Chemical formula	$C_{31}H_{55}CrFeP_5Si$	$C_{31}H_{55}CoFeP_5Si \cdot F_6P$
M_r	718.54	870.44
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/n$
Temperature (K)	123	123
a, b, c (Å)	19.9256 (2), 11.6275 (1), 16.4157 (2)	14.9545 (1), 16.8539 (1), 15.7381 (1)
α, β, γ (°)	90, 106.491 (1), 90	90, 98.016 (1), 90
V (Å^3)	3646.82 (7)	3927.90 (4)
Z	4	4
$F(000)$	1520	1808
D_x (Mg m^{-3})	1.309	1.472
Radiation type	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	8.17	9.31
Crystal shape and colour	Dark green plate	Dark brown needle
Crystal size (mm)	0.16 × 0.12 × 0.06	0.30 × 0.25 × 0.12
Data collection		
Diffractometer	SuperNova, Single source at offset, Atlas diffractometer	SuperNova, Single source at offset, Atlas diffractometer
Absorption correction	Analytical	Analytical
T_{min}, T_{max}	0.422, 0.700	0.174, 0.517
No. of measured, independent and observed [$> 2\sigma(I)$] reflections	63463, 7334, 6576	129446, 7934, 7215
R_{int}	0.046	0.045
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.625	0.623
Range of h, k, l	h = -24→24, k = -14→14, l = -20→19	h = -18→18, k = -20→20, l = -19→19
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.028, 0.078, 1.09	0.024, 0.066, 1.08
No. of reflections	7334	7934
No. of parameters	369	432
No. of restraints	0	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.69, -0.41	0.41, -0.34

Computer programs: *CrysAlis PRO*, Agilent Technologies, Version 1.171.37.34 (release 22-05-2014 CrysAlis171.NET) (compiled May 22 2014,16:03:01), *SHELXL97* (Sheldrick, 1997), *SHELXL2013* (Sheldrick, 2013).

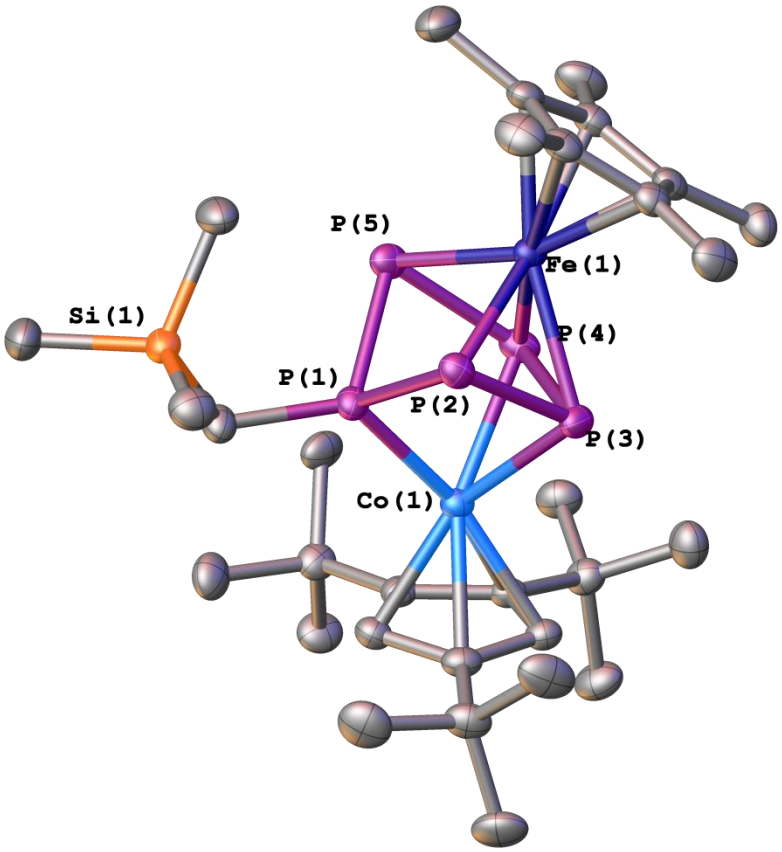


Figure S8. Molecular structure (ellipsoids at 50 % probability) and enumeration scheme for **2a**

Table S5. Selected geometric parameters (Å, º) for **2a**

Fe1—P4	2.3475 (5)	P4—P3	2.3530 (7)
Fe1—P2	2.2822 (6)	P2—P1	2.1928 (7)
Fe1—P5	2.2726 (6)	P2—P3	2.1911 (7)
Fe1—P3	2.3158 (6)	P5—P1	2.1771 (7)
Co1—P4	2.3555 (6)	Si1—C28	1.899 (2)
Co1—P1	2.1691 (6)	Si1—C31	1.861 (3)
Co1—P3	2.3136 (6)	Si1—C30	1.866 (2)
P4—P5	2.1790 (7)	Si1—C29	1.868 (2)

P5—P4—P3	101.38 (3)	P5—P1—P2	91.86 (3)
P3—P2—P1	86.00 (3)	P2—P3—P4	99.27 (3)
P1—P5—P4	83.17 (3)		

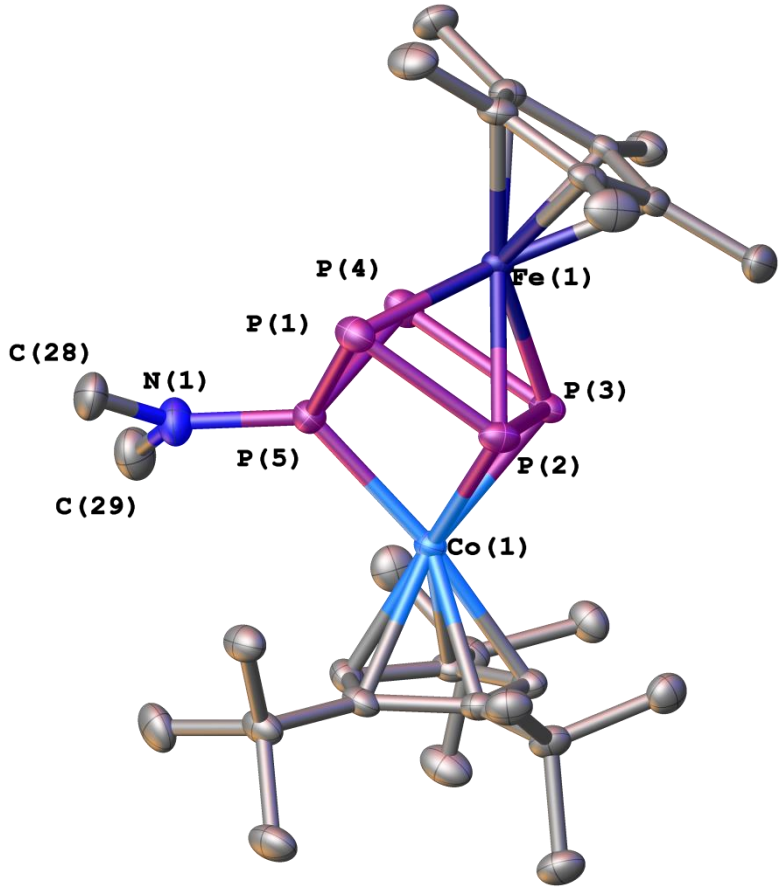


Figure S9. Molecular structure (ellipsoids at 50 % probability) and enumeration scheme for **2b**

Table S6. Selected geometric parameters (Å, º) for **2b**

P1—Fe1	2.3139 (6)	P4—P5	2.2004 (8)
P2—Fe1	2.3278 (6)	P3—Co1	2.2774 (6)
P3—Fe1	2.3048 (6)	P2—Co1	2.3596 (6)
P4—Fe1	2.2752 (6)	P5—Co1	2.1743 (6)
P1—P2	2.1854 (8)	N1—P5	1.6649 (19)
P1—P5	2.1569 (8)	C28—N1	1.452 (3)
P2—P3	2.4132 (8)	C29—N1	1.454 (3)
P3—P4	2.1855 (8)		

C28—N1—C29	115.41 (19)	P4—P3—P2	97.02 (3)
C28—N1—P5	124.47 (16)	P3—P4—P5	86.75 (3)
C29—N1—P5	120.11 (16)	N1—P5—P1	115.09 (8)
P5—P1—P2	79.71 (3)	N1—P5—P4	115.63 (8)
P1—P2—P3	103.96 (3)	P1—P5—P4	95.21 (3)

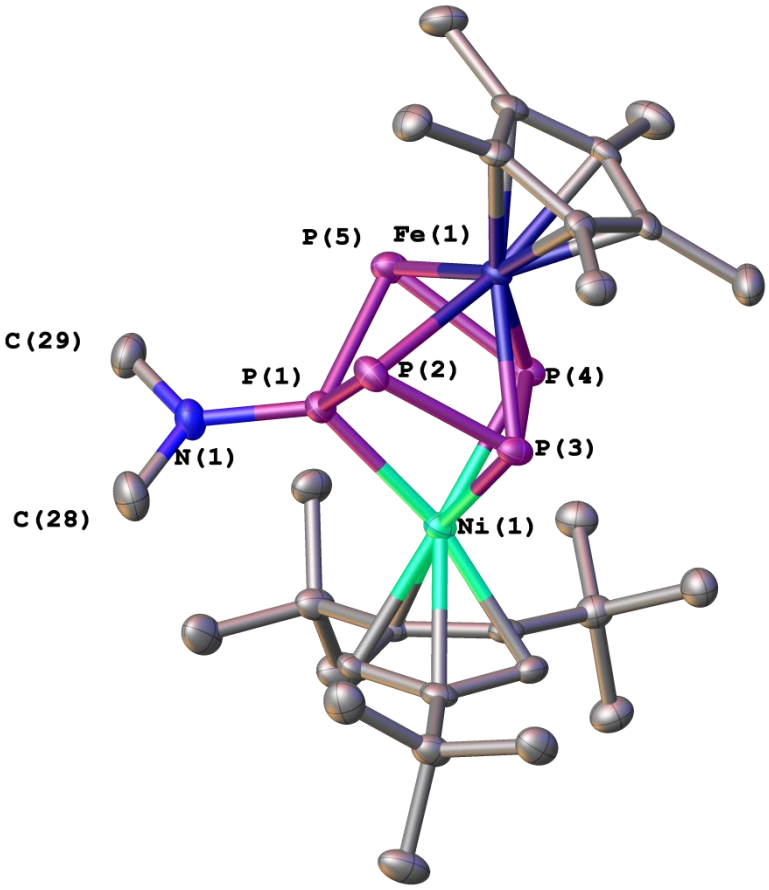


Figure S10. Molecular structure (ellipsoids at 50 % probability) and enumeration scheme for **3**

Table S7. Selected geometric parameters (Å, º) for **3**

P2—Fe1	2.2923 (5)	P5—P1	2.1620 (7)
P3—Fe1	2.2912 (5)	P1—Ni1	2.1998 (6)
P4—Fe1	2.2968 (5)	P3—Ni1	2.2846 (5)
P5—Fe1	2.3106 (6)	P4—Ni1	2.2972 (5)
P2—P1	2.1791 (7)	N1—P1	1.6706 (17)
P2—P3	2.1738 (7)	C28—N1	1.455 (3)
P3—P4	2.4739 (7)	C29—N1	1.451 (3)
P4—P5	2.1753 (7)		

P3—P2—P1	82.05 (2)	N1—P1—P2	116.15 (6)
P2—P3—P4	99.18 (2)	N1—P1—P5	114.89 (7)
P5—P4—P3	100.75 (2)	P5—P1—P2	96.03 (3)
P1—P5—P4	80.56 (2)		

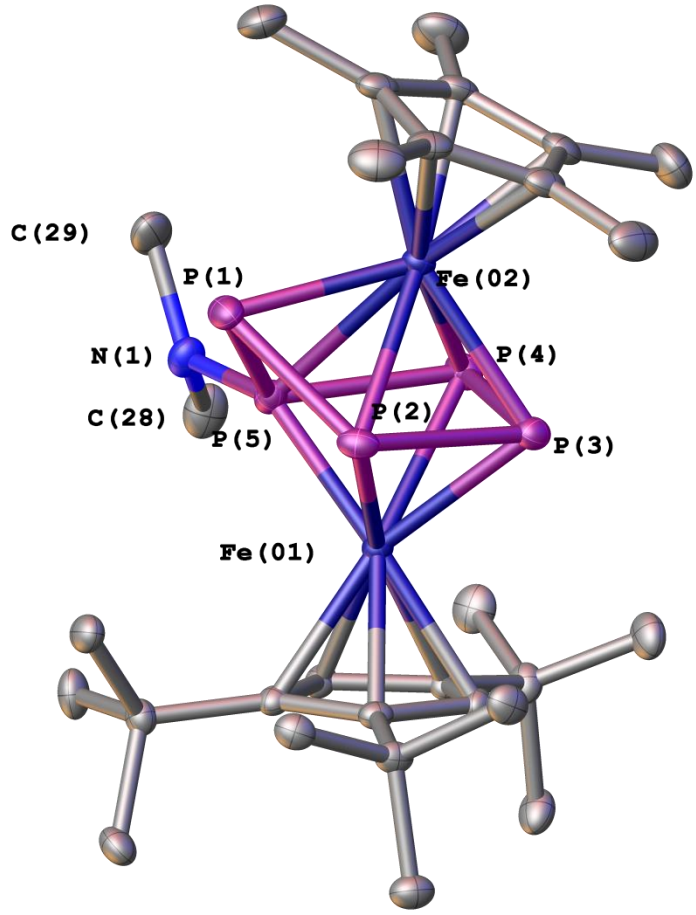


Figure S11. Molecular structure (ellipsoids at 50 % probability) and enumeration scheme for **4**

Table S8. Selected geometric parameters (Å, º) for **4**

Fe01—P5	2.1362 (5)	P5—P4	2.3187 (6)
Fe01—P3	2.3252 (5)	P5—P1	2.0952 (6)
Fe01—P4	2.4690 (5)	P3—P4	2.1054 (6)
Fe01—P2	2.3685 (5)	P3—P2	2.3587 (6)
Fe02—P5	2.6313 (5)	P2—P1	2.2063 (6)
Fe02—P3	2.3472 (5)	P5—N1	1.6804 (14)
Fe02—P4	2.4120 (5)	N1—C29	1.469 (2)
Fe02—P2	2.4323 (5)	N1—C28	1.460 (2)
Fe02—P1	2.3169 (5)	P5...P2	2.6552 (6)

P4—P5—P2	86.423 (19)	N1—P5—P1	113.58 (5)
P1—P5—P4	115.21 (2)	C29—N1—P5	117.52 (12)
P1—P5—P2	53.793 (18)	C28—N1—P5	119.79 (12)
N1—P5—P4	106.21 (5)	C28—N1—C29	112.81 (14)
N1—P5—P2	165.87 (5)		

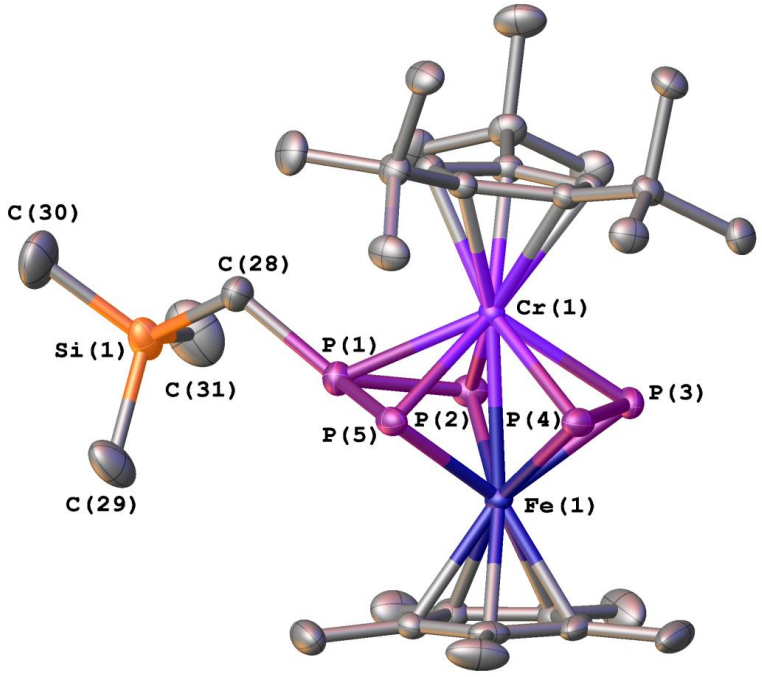


Figure S12. Molecular structure (ellipsoids at 50 % probability) and enumeration scheme for **5**

Table S9. Selected geometric parameters (Å, º) for **5**

Fe1—Cr1	2.6252 (4)	P5—P4	2.6258 (7)
Fe1—P5	2.2936 (5)	P5—P1	2.1549 (6)
Fe1—P2	2.2885 (5)	P2—P1	2.1558 (7)
Fe1—P4	2.2822 (5)	P2—P3	2.6328 (7)
Fe1—P3	2.2820 (5)	P4—P3	2.1040 (7)
Cr1—P5	2.3053 (5)	P1—C28	1.8574 (19)
Cr1—P2	2.2969 (5)	Si1—C28	1.878 (2)
Cr1—P4	2.3744 (5)	Si1—C29	1.856 (2)
Cr1—P1	2.5066 (5)	Si1—C30	1.865 (3)
Cr1—P3	2.3776 (5)	Si1—C31	1.851 (3)

P1—P2—P3	117.41 (2)	P3—P4—P5	102.78 (2)
P5—P1—P2	97.72 (2)	C28—P1—P5	125.15 (7)
P4—P3—P2	102.31 (2)	C28—P1—P2	128.44 (7)

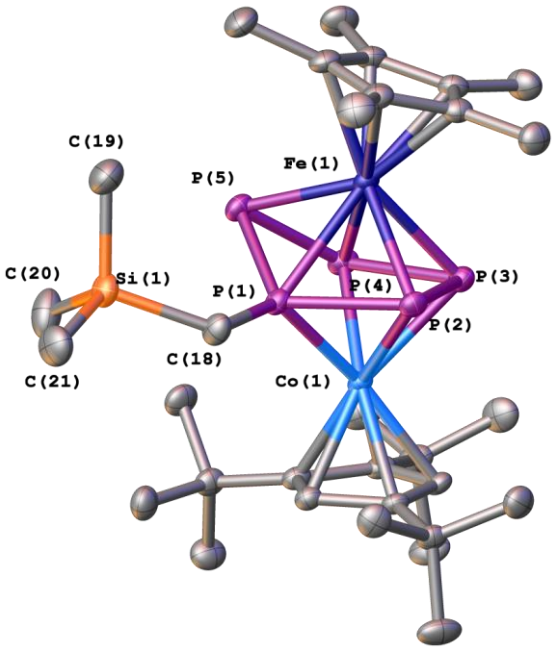


Figure S13. Cationic complex (ellipsoids at 50 % probability) and enumeration scheme for **6**

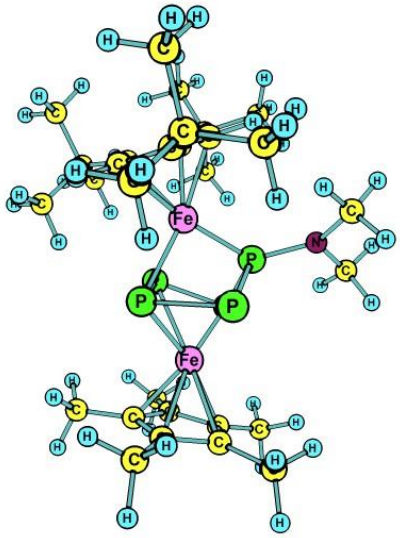
Table S10. Selected geometric parameters (Å, º) for **6**

C18—Si1	1.9046 (15)	P1—Fe1	2.4339 (4)
C18—P1	1.8233 (15)	P1—Co1	2.1924 (4)
C19—Si1	1.852 (2)	P2—P3	2.1045 (5)
C20—Si1	1.862 (2)	P2—Fe1	2.3647 (4)
C21—Si1	1.8564 (19)	P2—Co1	2.3842 (4)
F1—P6	1.5991 (13)	P3—P4	2.2715 (5)
F2—P6	1.6056 (13)	P3—Fe1	2.3547 (4)
F3—P6	1.5866 (15)	P3—Co1	2.3193 (4)
F4—P6	1.5894 (14)	P4—P5	2.1986 (5)
F5—P6	1.5969 (13)	P4—Fe1	2.4871 (4)
F6—P6	1.5964 (14)	P4—Co1	2.3447 (4)
P1—P2	2.2811 (5)	P5—Fe1	2.2918 (4)
P1—P5	2.1089 (5)		

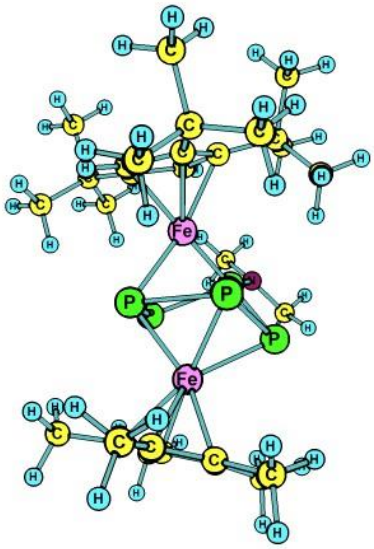
P1—C18—Si1	118.83 (9)	C18—P1—P5	122.07 (5)
C19—Si1—C18	109.24 (8)	C18—P1—Fe1	129.16 (6)
C19—Si1—C20	110.87 (10)	C18—P1—Co1	127.73 (5)
C19—Si1—C21	109.83 (10)	P5—P1—P2	118.59 (2)
C20—Si1—C18	110.11 (8)	P3—P2—P1	94.402 (19)
C21—Si1—C18	107.37 (8)	P2—P3—P4	102.07 (2)
C21—Si1—C20	109.35 (10)	P5—P4—P3	113.80 (2)
C18—P1—P2	105.45 (5)	P1—P5—P4	79.579 (18)

5. Details on DFT calculations

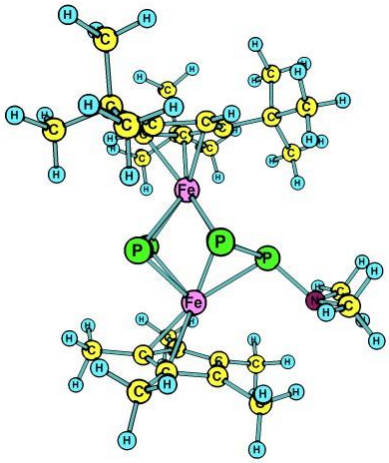
The geometries of the compounds have been fully optimized with gradient-corrected density functional theory (DFT) in form of Becke's three-parameter hybrid method B3LYP[9] with def2-SVP all electron basis set.[10] Gaussian 03 program package[11] was used throughout. All structures correspond to minima on their respective potential energy surfaces.



3fefe 0 kJ mol^{-1}

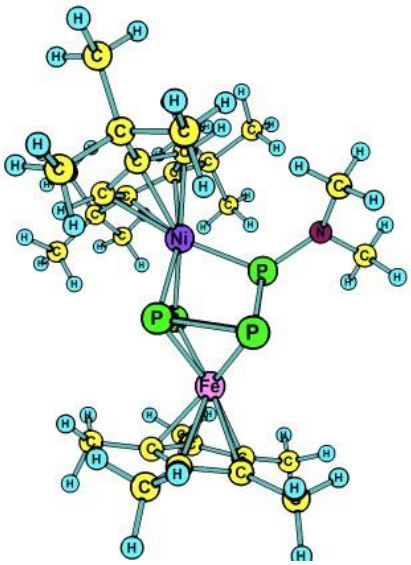


4 0 kJ mol^{-1}

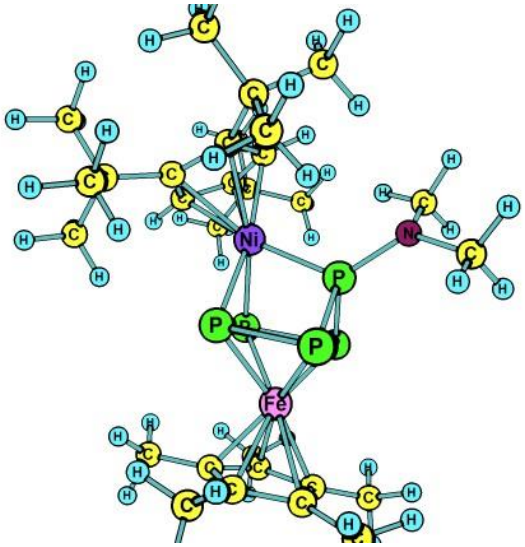


5fefe +55.9 kJ mol^{-1}

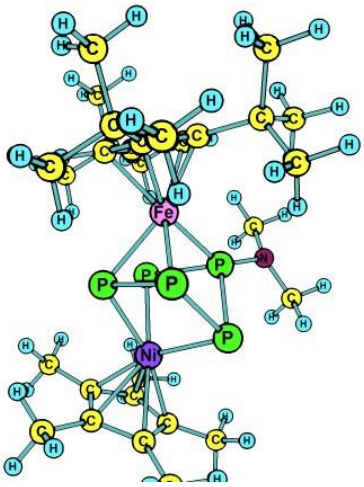
Figure S14. Optimized structures and relative energies of the compound **4** and its isomers **3**fefe and **5**fefe.



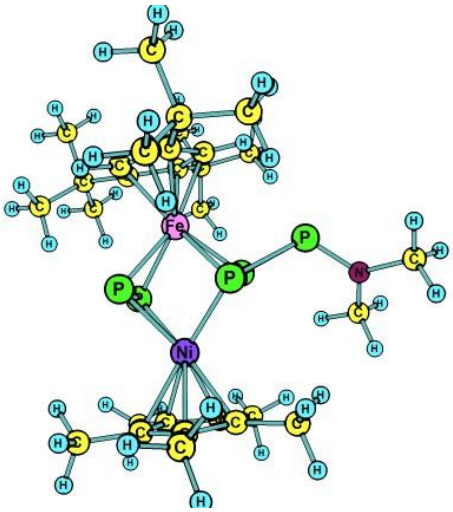
3 0 kJ mol^{-1}



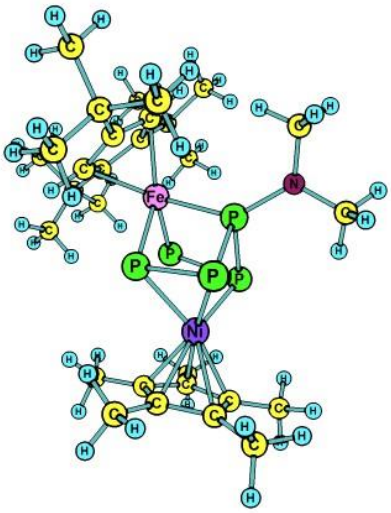
4nife 0 kJ mol^{-1}



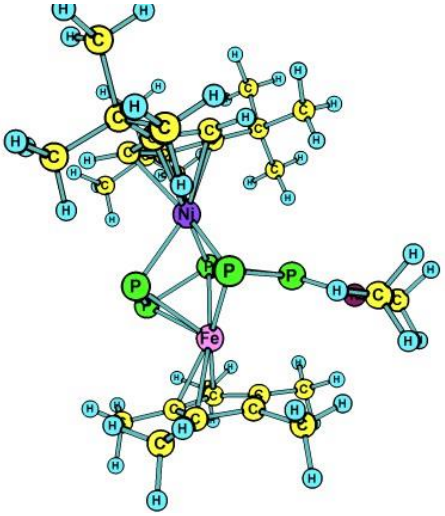
4feni 44.4 kJ mol^{-1}



5nife 90.2 kJ mol^{-1}

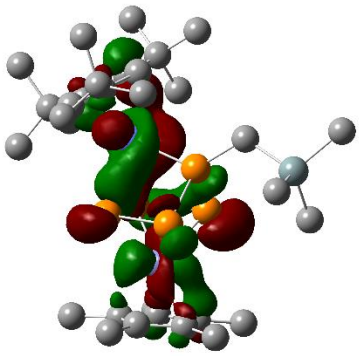


3feni 106.9 kJ mol^{-1}

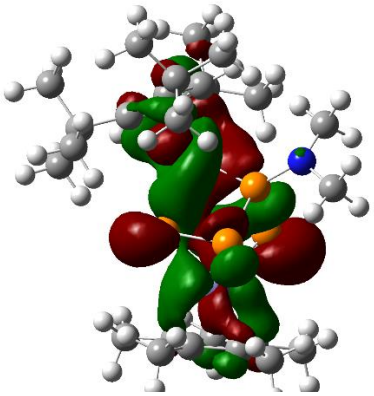


5feni 106.8 kJ mol^{-1}

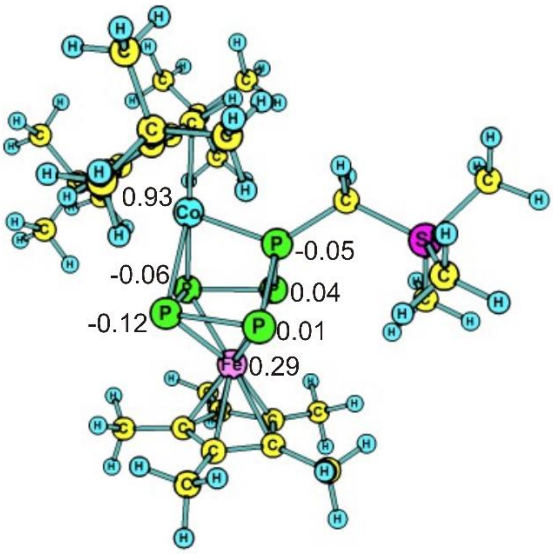
Figure S15. Optimized structures and relative energies of the isomers.



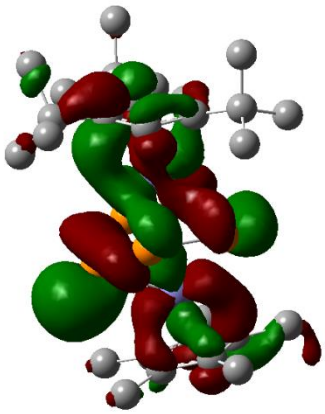
SOMO_**2a**



SOMO_**2b**



Atomic spin density for **2a**



SOMO_**8**

Figure S16. Isosurface of the single-occupied molecular orbitals (SOMO) in **2a**, **2b** and **8**.

Table S11. Wiberg bond indexes (WBI): (numbering of atoms corresponds to the Figures 1, 2 and 5 in the manuscript).

		M-P1	M-P2	M-P3	M-P4	M-P5
2a	Co	0.75	0.06	0.48	0.53	0.07
	Fe	0.05	0.80	0.66	0.65	0.80
2b	Co	0.76	0.05	0.46	0.53	0.08
	Fe	0.06	0.79	0.67	0.66	0.80
3	Ni	0.72	0.08	0.61	0.59	0.07
	Fe	0.08	0.77	0.70	0.70	0.77
5	Cr	0.64	0.94	0.77	0.78	0.96
	Fe	0.11	0.73	0.76	0.76	0.72

Table S12. Wiberg bond indexes (WBI): (numbering of atoms corresponds to the Figures 1, 2 and 5 in the manuscript).

	M-M	P1-P2	P2-P3	P3-P4	P4-P5	P5-P1	P2-P5
2a	0.12	0.93	1.00	0.70	0.98	0.92	0.07
2b	0.12	0.94	1.01	0.67	1.00	0.85	0.07
3	0.13	0.88	1.03	0.51	1.01	0.95	0.07
5	0.47	0.91	0.22	1.14	0.22	0.90	0.07

Table S13. Mulliken atomic charges and atomic spin densities (numbering of atoms corresponds to the Figures 1, 2 and 5 in the manuscript).

	Mulliken atomic charge				Atomic Spin density	
	2a	**2b**	**3**	**5**	**2a**	**2b**
Co/Fe1/Cr/Ni	-0.021	-0.029	-0.052	-0.790	0.930	0.926
Fe	-0.407	-0.414	-0.432	-0.431	0.295	0.278
P1	0.027	0.183	0.231	0.075	-0.055	-0.050
P2	-0.015	-0.015	-0.022	0.098	0.005	0.0006
P3	-0.012	-0.048	0.015	0.083	-0.128	-0.122
P4	-0.051	-0.029	-0.011	0.068	-0.060	-0.057
P5	0.001	-0.005	-0.021	0.108	0.041	0.048
N		-0.480	-0.479			-0.003
C	-0.303			-0.334	-0.003	

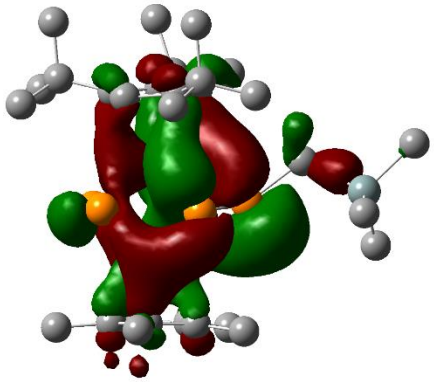


Figure S17. Isosurface of the HOMO-3 of **5**

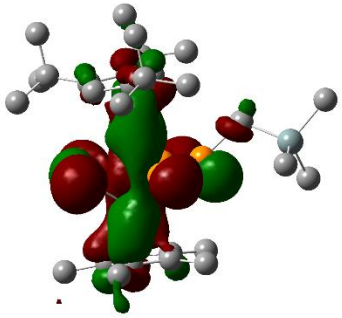


Figure S18. Isosurface of the HOMO of **5**

Table S14. Comparison of sum of valence angles around N and N-P bond distance.

Compound	Sum of angles on N atom	N-P, Å	WBI (N-P)
2b	351.29	1.712	0.813
3	351.68	1.715	0.795
3fefe (converged to **4**)	355.45	1.706	
3feni	353.67	1.714	
4	355.44	1.706	0.818
4feni	351.44	1.713	
4nife (converged to **3**)	351.70	1.715	
5fefe	336.12	1.801	0.672
5feni	358.25	1.734	
5nife	359.93	1.708	

With the exception of **5fefe** all compounds feature almost a planar NMe_2 group (sum of angles greater than 351 degree) with short P-N distances (1.706-1.734 Å). In **5fefe** the NMe_2 group is pyramidal (sum of angles 336 degrees) and the P-N distance is prolonged with 1.801 Å. These structural changes are also reflected in the Wiberg bond indexes (WBI): 0.813 and 0.818 for **2b** and **4** and only 0.67 for **5fefe** (table S3). Thus, in all compounds except for **5fefe** the lone pair of the nitrogen atom is involved in the conjugation with the P atom of the complex, which leads to a shorter N-P bond and a larger WBI.

Table S15. Total energies E^{o}_{0}, sum of electronic and thermal enthalpies H^{o}_{298} (Hartree) and standard entropies S^{o}_{298} (cal $mol^{-1}K^{-1}$) for studied compounds. B3LYP/def2-SVP level of theory.

Compound	$E°_{0}$, Hartree	$H°_{298}$, Hartree	$S°_{298}$, cal mol^{-1} K^{-1}
2a	-5855.69586	-5854.851566	292.52
2b	-5541.765076	-5540.9811	268.41
3fefe (converged to **4**)	-5422.700466	-5421.916178	264.475
3feni	-5667.263255	-5666.479909	269.063
3	-5667.303973	-5666.519976	264.939
4feni	-5667.287074	-5666.503693	269.237
4nife (converged to **3**)	-5667.303973	-5666.519978	264.972
4	-5422.700467	-5421.916183	264.52
5fefe	-5422.679187	-5421.895554	263.898
5feni	-5667.263289	-5666.480117	269.542
5nife	-5667.269627	-5666.486312	273.926
5	-5517.379123	-5516.534161	284.233
6_cation_singlet_state	-5855.492431	-5854.646552	288.401
6_cation_triplet_state	-5855.498774	-5854.653552	293.229

The triplet state of the cation of $[\mathbf{6}]^{+}$ in the gas phase is by 16.7 kJ mol^{-1} lower in energy than the singlet state.

Table S16. Optimized geometries of theoretically studied compounds. xyz coordinates in angstroms. B3LYP/def2-SVP level of theory.

2a

Fe	8.2129833715	0.8363907219	12.5639483764
Co	6.5217957562	-2.3243029867	11.2463316017
P	8.6534315523	-1.3380458634	11.8187622388
P	5.8795563147	0.7834236717	12.3714987031
P	8.2781190749	0.2326521403	10.3034098735
P	6.1334642626	-0.2952064245	10.45668308
P	6.8766377107	-0.9545036785	13.2993729785
Si	4.743853449	2.0326983711	8.6414848757
C	6.5494494452	-4.1415945445	10.0521201497
C	8.1480941455	-5.2542927103	12.0192950883
C	3.3776395104	-3.2648480158	12.0364612066
C	10.2130145016	1.3898685101	12.9891979201
C	8.3961402907	1.9439363786	14.3305388295
C	6.9671515881	-4.4614252593	11.4081789032
C	7.1934880552	-4.3581599156	8.6607370705
C	7.4813953539	-5.8597400668	8.4300443937
H	8.2418461179	-6.2548106471	9.1140201947
H	7.8472408941	-6.0213733751	7.4027932583
H	6.5667152894	-6.45979516	8.5611209987
C	8.4753256862	-3.5219420057	8.4471530899
H	8.2545929564	-2.4456787755	8.5077411173
H	8.8963393529	-3.7269986651	7.4486204677
H	9.2522736773	-3.7338995654	9.1880108666
C	4.7853661559	-3.5723929961	11.5335847176
C	9.5335277133	2.4997822135	12.3824408898
C	9.5092855018	1.0438701549	14.1933458115

C	7.7694967708	-6.7571934285	11.9880604019
H	8.5550717197	-7.3606666039	12.4732699775
H	7.6432460823	-7.1291565837	10.9618389411
H	6.8250104961	-6.9353145669	12.5258371845
C	9.5123232285	-5.0575933481	11.3320880304
H	9.8079938882	-3.9985033646	11.3339963199
H	9.5292818461	-5.4241933797	10.2993725531
H	10.281337528	-5.6220812641	11.8834876429
C	9.9954282734	3.2468087073	11.1658966591
H	9.1578311121	3.7087515995	10.6242879862
H	10.5212830898	2.5901874891	10.4581935509
H	10.693092856	4.05513907	11.4510399686
C	5.0887986806	0.183800378	9.0114511652
H	4.1214096124	-0.3344838451	9.1291879975
H	5.5832689421	-0.2712041718	8.1341567003
C	8.412762263	2.8423277363	13.2066683315
C	11.4868810875	0.7723809711	12.4907156963
H	11.6414137643	-0.2322016944	12.9083334032
H	12.3593786414	1.3893199479	12.7707199471
H	11.4930882432	0.6754577086	11.394088007
C	3.5065657319	2.7084688684	9.8977161931
H	3.8959714297	2.6440568092	10.9264231406
H	2.556846287	2.1490070976	9.8631885828
H	3.2782376492	3.766737341	9.6861298253
C	6.2110878861	-3.9338911308	7.5436117879
H	5.2740589552	-4.5109881348	7.572643017
H	6.6781009189	-4.1091351459	6.5619811601
H	5.9612192376	-2.8635391543	7.5989951732
C	6.3485186529	3.0243421639	8.6939135093
H	6.1581705888	4.0809131743	8.4408523968

H 7.0916039 2.6339448233 7.979777358

H 6.8018169763 2.9912854055 9.69775107

C 3.369491937 -3.0421095325 13.5602120205

H 3.696999603 -3.9418788822 14.1040450323

H 2.3495011114 -2.8054742833 13.9034680751

H 4.0289131273 -2.2090140878 13.8475328505

C 9.9259323947 -0.0005520325 15.1860797083

H 10.4298672409 -0.8470117191 14.6972250253

H 9.0632905215 -0.4062662518 15.7338949878

H 10.6268650367 0.4204001205 15.9288288566

C 2.787705271 -2.0176090777 11.3496985909

H 3.357436738 -1.1126370777 11.6101944642

H 1.7452450778 -1.8626662329 11.6723714057

H 2.7767610991 -2.1217349038 10.2527725892

C 7.5012067267 4.0174938258 13.0075073137

H 7.9108344552 4.9149156041 13.5059126609

H 6.5006540228 3.8344111319 13.4241253694

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H	-5.411219806	0.6447369935	3.202361591
H	-5.7052959918	0.4286322585	1.4592559939
C	-2.6229159232	0.663309624	3.1118763022
H	-1.7086362703	0.0532701848	3.1394900547
H	-3.0777472507	0.6348204324	4.1161038499
H	-2.3161433031	1.6926961195	2.9100528178
C	-3.8609109862	-1.3686098355	2.4536153122
H	-4.6349959555	-1.8409354712	1.8294498274
H	-4.2062111842	-1.4197630294	3.4980664643
H	-2.9382678863	-1.9626485186	2.3841603872
C	4.0632083567	1.5020361455	0.7096163817
C	4.4049917047	0.10761409	0.8185126537
C	4.2912380193	-0.4792824612	-0.4796117349
C	3.9115823859	0.5523490221	-1.4089362104
C	3.7667391824	1.775273887	-0.671513324
C	4.1193486703	2.5144887472	1.8165481073
H	3.8839723528	2.0653233997	2.7929724256

H	3.4040441589	3.3332505735	1.6516001832
H	5.1264470354	2.9624373813	1.8943640844
C	4.8994152097	-0.5867618143	2.0533477758
H	6.0017715133	-0.531313062	2.110528293
H	4.6238432861	-1.6515018687	2.0623781803
H	4.4954565594	-0.1337754617	2.9693994521
C	4.6108552098	-1.9019353058	-0.8348926938
H	5.6764683379	-2.007505813	-1.1083478044
H	4.0139265103	-2.2528607709	-1.6890190418
H	4.4174607679	-2.5853033716	0.0048311768
C	3.7779953428	0.3784409503	-2.8923599047
H	3.1788322375	1.181140548	-3.3446990022
H	3.2904939839	-0.5749429271	-3.149073791
H	4.7686663776	0.3842897677	-3.3808488464
C	3.448100044	3.1229978839	-1.248026844
H	4.3729716309	3.6560522294	-1.5323381545
H	2.9088126263	3.7543896237	-0.5271634808
H	2.8208998346	3.0425416744	-2.1474486883
C	-0.9004250218	-3.7804411898	1.1812996962
H	-0.1931070514	-4.5055171944	0.7330970337
H	-1.5064448078	-3.3595689431	0.3703437642
H	-1.5684408833	-4.3327091672	1.8658054701
C	0.673924584	-3.1916896996	2.9550337612
H	0.0993461606	-3.8078608311	3.6683695826
H	1.1015464932	-2.3421925769	3.5062081421
H	1.5081206278	-3.8099939494	2.5665842304
N	-0.2044652113	-2.7219841844	1.8955954941
P	0.9297424532	-1.3901763467	-0.9457363626
P	0.6753187785	0.7322398083	-1.3445841009
P	0.43296976	1.5647546015	0.855993106

P	1.41828628	0.0823127257	2.1820929986
P	0.04790472	-1.2098941041	1.1477223311
Fe	2.4360096354	0.3675206865	0.0770550431
Fe	-1.1755125015	-0.0305695428	-0.1891339178

4

Fe	1.2277907908	7.0735407333	8.0742235351
Fe	0.6424922231	4.4755440015	5.5875175864
P	-0.6987652491	6.1401024725	7.7711070637
P	2.3039102449	5.4478592252	6.8320127327
P	0.8313872337	4.4862033752	8.1108461808
P	0.9209915774	6.9205973077	5.6028568628
P	-1.1159871836	6.0404923829	5.66551782
N	-2.070439029	5.9931098259	8.7743419434
C	3.0392268333	7.9679816385	8.7502553652
H	4.0394200507	7.6581444076	8.4669703871
C	2.2586710419	8.9476628477	8.0413980112
C	0.9865440384	9.0590414733	8.7491022909
C	1.0692335908	8.1313762722	9.8547614215
H	0.2923035443	7.990424275	10.5976310748
C	2.3324658816	7.4770146096	9.8763401015
C	2.973301201	9.7898691341	6.9526585805
C	-0.4248372584	3.0975682925	4.3811734899
C	4.0151620965	8.936212261	6.1885614096
H	4.8134254785	8.5516462806	6.8387448785
H	4.5011365869	9.5583894523	5.420717123
H	3.5439448675	8.0826818159	5.6802570311
C	2.0815601099	10.4393448276	5.8785555105
H	1.5142973616	9.6833555072	5.317740414
H	2.7220837504	10.9758000941	5.1603368508

H	1.3799044848	11.1739915306	6.2895841448
C	0.3856750948	2.3935980084	5.324608207
C	1.7593205728	2.7614841515	5.1018052122
C	-0.9629622713	9.9056794118	7.2684541821
H	-0.3084895928	10.024820351	6.4012787538
H	-1.7508265983	10.6749420592	7.2079706756
H	-1.4456318349	8.9221535555	7.1762900387
C	1.7892852616	3.7168707985	4.0309866676
C	-0.2164252497	10.0257774285	8.6142902473
C	3.7452577067	10.9072145645	7.7033655327
H	3.0677771354	11.5715054156	8.2582023061
H	4.3140562734	11.5226789911	6.9868970945
H	4.458471545	10.4800041425	8.42524149
C	2.8966074092	6.5918725885	10.9851671026
C	0.4378245333	3.9338246048	3.587679085
C	0.2564939048	11.4813943161	8.8445855985
H	0.7888347294	11.5745389165	9.8048400065
H	-0.6114410807	12.1602293243	8.8732878892
H	0.9270439599	11.8404984653	8.0543198449
C	3.9816650517	5.6388284886	10.4487196245
H	3.5794561214	4.9676087379	9.6757060015
H	4.3789807696	5.0197322039	11.2692094367
H	4.8309301779	6.1885512853	10.0142714216
C	3.534465512	7.5404159459	12.0312776409
H	4.3335010222	8.1494979727	11.5802321114
H	3.9730855672	6.9609119525	12.8606063409
H	2.7856872262	8.2287539408	12.4544276917
C	-1.2666098955	9.7341761122	9.7124217551
H	-1.6601930183	8.7102745686	9.6368396616
H	-2.1175581443	10.4225716063	9.5911114019

H	-0.8646559843	9.8860670611	10.7259423288
C	-3.3419217066	5.5274648662	8.2441474835
H	-3.4337131209	5.7861959513	7.1797508659
H	-4.171284289	6.0133974785	8.7869844082
H	-3.4643568154	4.4304685603	8.3475276328
C	1.7972243384	5.7620092162	11.6733204097
H	1.0169475635	6.4021797908	12.1147549247
H	2.2313022735	5.1680191153	12.4936385479
H	1.32262831	5.0682820632	10.9633185289
C	-1.9076699742	5.7898243109	10.2050996664
H	-2.0148364798	4.7226478291	10.4818208687
H	-2.6654961936	6.3661084199	10.7649018476
H	-0.9132346762	6.120508323	10.527258166
C	2.9415339536	2.1767949871	5.8153504545
H	3.8298001574	2.8177970617	5.7257643529
H	3.2008419713	1.1857357785	5.4022571799
H	2.7441921495	2.0434318102	6.8904264322
C	0.0164454104	4.7896536097	2.4285907688
H	-1.000307373	5.1878735506	2.5634362813
H	0.0217836849	4.2125875396	1.4862963578
H	0.689748769	5.648778504	2.2951189054
C	-1.9007558862	2.9123858019	4.1840965041
H	-2.412686068	2.6718060955	5.1273710544
H	-2.0938862312	2.0801126978	3.4829714481
H	-2.3764234032	3.812725562	3.7709816212
C	-0.0964795417	1.3700250492	6.3105771442
H	0.5365612767	1.339546108	7.2090941826
H	-0.0867195875	0.3596916111	5.8626988974
H	-1.1258155663	1.5739867426	6.639801476
C	3.0186917214	4.3205710399	3.4191125539

H	2.8200035572	5.3252125865	3.0186920936
H	3.3887459042	3.6962756831	2.5862293994
H	3.833245699	4.414370243	4.1516023814

4nife

Ni	-1.0905069324	0.1730300081	-0.2266925339
Fe	2.6017342941	-0.0258328294	-0.146700175
P	0.1952437253	1.6771968332	0.7457859081
P	0.809725553	0.0652117575	-1.6188241236
P	1.6328516792	1.9791808393	-0.9229480946
P	0.7039890958	-1.159352919	0.5457882209
P	1.5102207397	0.360211358	1.9106652941
N	-0.4001690434	3.0326306336	1.6116646567
C	-2.5427693151	-0.9012157015	-1.4169091773
H	-2.2655208531	-1.5644683486	-2.2295245
C	-2.7777187079	-1.3414948972	-0.0548630746
C	-3.0940278332	-0.1612133206	0.7005815338
C	-3.0537742913	0.9466629588	-0.2515421315
H	-3.2955735097	1.9728225503	0.0036127005
C	-2.802992577	0.4833968621	-1.5691721467
C	-2.8093081967	-2.8613947771	0.2327962532
C	4.5501505137	-0.1609868592	0.6952967199
C	-1.9017134889	-3.6213539108	-0.7672046482
H	-2.2691331702	-3.5602189132	-1.8017788143
H	-1.8781898259	-4.6892728219	-0.4998087885
H	-0.8691561037	-3.2432989864	-0.7414177393
C	-2.3449037935	-3.2819465016	1.6398122347
H	-1.3161890744	-2.9457872867	1.8361564852
H	-2.3592029175	-4.381230852	1.7135247596
H	-2.9948497784	-2.9003699907	2.4350792183

C	4.6110037245	0.5489919289	-0.5434287468
C	4.1062466415	-0.3143774916	-1.5786237498
C	-2.4107706103	-0.223003034	3.1874159256
H	-2.0476819826	-1.2537399978	3.132989424
H	-2.777497158	-0.0470942911	4.2126290691
H	-1.547362068	0.4366975308	3.0202898047
C	3.7376933665	-1.564845938	-0.9722345345
C	-3.5315306081	0.0785652305	2.1671613002
C	-4.2611609043	-3.3546085014	0.0006629545
H	-4.9709366055	-2.8962529358	0.7028309951
H	-4.3174152762	-4.449030483	0.1266732733
H	-4.5995091078	-3.1142592137	-1.0196266698
C	-2.9262315401	1.2690711062	-2.8720658241
C	4.0088366022	-1.469386999	0.436351254
C	-4.7977442852	-0.7450858884	2.4990909215
H	-5.6043748352	-0.5369030422	1.7780833001
H	-5.1660062066	-0.4782855465	3.503205995
H	-4.6146409455	-1.8263297712	2.4965406047
C	-2.2221842904	0.5351467439	-4.0289201781
H	-1.1521851564	0.3857069639	-3.8192263403
H	-2.3118977503	1.1194392703	-4.9588176495
H	-2.6747648453	-0.4509999355	-4.2179973156
C	-4.4334751713	1.3926572451	-3.2054546427
H	-4.8972383408	0.3995118901	-3.3141251984
H	-4.5791677074	1.9429092003	-4.1503159164
H	-4.9757583825	1.9305333028	-2.4115658717
C	-3.9150929503	1.5626074806	2.3784779544
H	-3.0592766914	2.2309016668	2.2053943829
H	-4.2400237923	1.7075693563	3.4206412398
H	-4.7469473157	1.8741891091	1.7277712732

C	0.3474219018	3.5603069281	2.7457059086
H	0.8395785467	2.7451540538	3.2945700334
H	-0.3458966836	4.067475473	3.4387773096
H	1.1206977102	4.2947508107	2.4416028156
C	-2.3279733994	2.6830649576	-2.7371904657
H	-2.8393548634	3.265589801	-1.954198242
H	-2.4456686774	3.2390940206	-3.6814455259
H	-1.2549005031	2.6437632744	-2.4954676928
C	-1.131458425	4.0469260667	0.8655713574
H	-0.4629203797	4.8316509726	0.4586755092
H	-1.875131057	4.5364759962	1.5182159389
H	-1.6629062041	3.5908552775	0.0204241804
C	4.0906769148	-0.0012133878	-3.0464882827
H	3.3337830817	-0.5927954028	-3.5810729608
H	5.0710391117	-0.2213701527	-3.5057908732
H	3.8722451636	1.0606776494	-3.2358296173
C	3.8679718512	-2.5692450734	1.4483448607
H	3.5477361078	-2.1854806317	2.4291019103
H	4.8298132025	-3.0911710137	1.5996613791
H	3.1290853481	-3.3198714979	1.1339161332
C	5.0725583175	0.3249242398	2.0152412304
H	4.9945647139	1.4176264418	2.1091753815
H	6.1383882084	0.0570075864	2.1321219282
H	4.5254001871	-0.1169753465	2.8600760917
C	5.2109449927	1.9086457993	-0.7487167598
H	4.7485916731	2.4370423014	-1.594430997
H	6.2931766825	1.826872167	-0.9574823096
H	5.0932895467	2.5452252977	0.139938847
C	3.2455726636	-2.7820389342	-1.698016047
H	2.6328131197	-3.4213009363	-1.0460034828

H	4.090120442	-3.3917072781	-2.0657791715
H	2.6262527094	-2.5114073012	-2.5657124582

4feni

Fe	-1.2272570972	-0.1017033011	-0.018177709
Ni	2.5577277164	-0.2061643758	0.0037572725
P	0.1024329268	1.1532933715	1.1720125703
P	0.653474492	-1.2311989985	-0.940519537
P	0.7927371388	1.0538257254	-0.9373417647
P	0.1043618937	-1.7032184559	1.1397988666
P	1.5464798204	-0.1996830117	2.0799932445
N	0.0087866286	2.7097335877	1.8813069968
C	-2.5973644157	-0.8767978225	-1.4360977898
H	-2.35258429	-1.5070388916	-2.2850347633
C	-2.9321538916	-1.3696389073	-0.1262264098
C	-3.1838740274	-0.1931505652	0.7067983301
C	-3.013855535	0.94801418	-0.165072532
H	-3.1634899017	1.9785149908	0.1378131965
C	-2.6763950019	0.5414754072	-1.4831893047
C	-3.2143393716	-2.8864535264	0.026716197
C	4.5830173696	0.3874668782	0.4863061797
C	-2.2744047764	-3.7174188898	-0.8802412359
H	-2.4049773595	-3.4958283351	-1.9487168392
H	-2.4939743384	-4.7883738667	-0.7473462744
H	-1.2164932635	-3.5597941761	-0.6240033143
C	-3.0851791701	-3.4818347036	1.4404135611
H	-2.0688782707	-3.3531410621	1.8379686124
H	-3.2919382435	-4.5628421148	1.3917572618
H	-3.7994644878	-3.0523570417	2.1518035172
C	4.3430609836	0.8122202522	-0.840140075

C	3.9688230712	-0.3565241617	-1.6034881277
C	-2.7998745384	-0.6192536516	3.2384776096
H	-2.6031081678	-1.6841353192	3.0899224281
H	-3.2697915759	-0.4971618644	4.2287679186
H	-1.8281524755	-0.1047975083	3.2612370672
C	4.1253152393	-1.5266325517	-0.7742769178
C	-3.7113807932	-0.0078230196	2.1520978799
C	-4.6667323069	-3.109875128	-0.4721697614
H	-5.3970825546	-2.5597241255	0.1384017933
H	-4.9240981179	-4.1810786532	-0.4267234134
H	-4.7851077068	-2.7763789077	-1.5148286772
C	-2.6549894471	1.407698644	-2.7406392926
C	4.4418970673	-1.0744339254	0.5304126004
C	-5.1443771561	-0.5833196014	2.2609775118
H	-5.8027764366	-0.1432412862	1.4948928149
H	-5.5728661197	-0.3476597491	3.2489481734
H	-5.1757942016	-1.673780194	2.1424910266
C	-1.7206929014	0.8222679984	-3.8159792988
H	-0.6829337934	0.7703184428	-3.4553506181
H	-1.7413433575	1.4532606067	-4.7193416919
H	-2.029281868	-0.1906102908	-4.1177202787
C	-4.1033882285	1.4255329601	-3.2918303194
H	-4.4504991056	0.4080614841	-3.5308970419
H	-4.1599082964	2.0303570715	-4.2122498105
H	-4.8034220752	1.8547733749	-2.5574777286
C	-3.8219645765	1.4968433826	2.4951466228
H	-2.8460368335	2.0002909721	2.4338890721
H	-4.1823052562	1.605690009	3.5299451383
H	-4.5359214017	2.0244364674	1.8443610778
C	1.1125245961	3.1943747848	2.6966644902

H	1.5352882583	2.3750652432	3.295786617
H	0.7416713485	3.9681927033	3.3902548848
H	1.9285824232	3.6405333453	2.091440137
C	-2.2279156123	2.8544545056	-2.4327252258
H	-2.9006971339	3.3324523665	-1.703033472
H	-2.2599073409	3.462769285	-3.3509840988
H	-1.2018089862	2.8916165383	-2.0380024258
C	-0.6839155815	3.7533863665	1.1418445785
H	-0.014178246	4.2767246192	0.4292967344
H	-1.096252882	4.5014411155	1.8403508679
H	-1.5147759401	3.3248559957	0.5676122735
C	3.6366413942	-0.3693009366	-3.0648219055
H	2.9049809302	-1.155552543	-3.3063105064
H	4.5379977671	-0.5580915695	-3.6754846977
H	3.2120268597	0.5909667319	-3.3932454822
C	4.7560894202	-1.9253870706	1.7249921133
H	4.4471094743	-1.4411434614	2.6631551216
H	5.8418364239	-2.1191796051	1.7976881424
H	4.2498229979	-2.9006406106	1.6758505959
C	5.049449023	1.2275527554	1.6381148106
H	4.8123519042	2.2916200939	1.4909912177
H	6.1441281336	1.1490476825	1.7687827502
H	4.5859971177	0.9126637873	2.5854786145
C	4.4354867865	2.2080300828	-1.381867966
H	3.5636771569	2.465149262	-2.0042267962
H	5.3349922865	2.3379801514	-2.0100321799
H	4.4917171697	2.9534547092	-0.5752221423
C	3.9688178516	-2.9479130185	-1.2271646973
H	3.7674490885	-3.6229993495	-0.3825934472
H	4.882845118	-3.3127096818	-1.7298931846

H	3.1369405795	-3.0606701016	-1.9393487363

5

Fe	1.6620024119	8.948900108	8.0021691634
Cr	2.0415561498	6.3699978951	8.047365611
P	0.9279672186	7.4844091685	9.6722607703
P	3.735655262	7.8792695514	8.0571897482
P	0.1401022402	7.4646110861	7.1084829192
P	3.0809947788	7.4946207436	10.1162967883
P	1.9590589313	7.7106073454	6.0711996635
Si	5.1840520289	7.2861204446	12.507459929
C	1.2834410455	4.2677009887	8.5890591749
C	2.3945569845	4.6892155286	6.6050395542
H	2.593353571	4.8242638172	5.5477287199
C	1.0979814741	4.4133754432	7.1509783956
C	1.3330257649	10.6226535289	9.341570306
C	3.4000103388	4.6476765173	7.6023881427
C	2.6939983271	4.4278753989	8.8206114143
H	3.1605186305	4.3359865925	9.7940563882
C	0.3517780975	3.7474755907	9.7182288056
C	2.5757632017	10.7985730442	8.6623339754
C	0.2909246221	10.5306164075	8.352937837
C	-0.0187293904	3.9843961906	6.1554495192
C	0.2503020822	2.488111547	5.8334827926
H	1.245695999	2.3548777699	5.382287742
H	-0.4989279942	2.1174908525	5.114324355
H	0.2032248902	1.854238598	6.7284196671
C	3.9399210002	6.3869784388	11.3672142568
H	4.4614648757	5.5571260063	10.8677879779
H	3.1462724234	5.9477371746	11.9953624387

C	4.8945216948	4.4563577389	7.3260456051
C	-1.4733710464	4.133060335	6.6359968229
H	-1.7140278408	3.4717649759	7.4764109857
H	-2.1527749752	3.861882937	5.8124406522
H	-1.6982765283	5.16910827	6.9265822321
C	0.8983111091	10.6757973629	7.0605381765
C	0.074080085	4.7459608223	4.8101793461
H	-0.0992974249	5.8231161153	4.9305923282
H	-0.6962129791	4.3546593656	4.1270471543
H	1.0412390715	4.6104712359	4.3062076763
C	-0.9504229843	4.5503268448	9.9282763314
H	-0.7354662883	5.5365356575	10.3611823606
H	-1.6049645035	4.0078715443	10.6307398293
H	-1.5129469938	4.7148867622	9.0066543553
C	2.314463234	10.8177655966	7.246363217
C	0.0083382918	2.2621216434	9.4400569494
H	-0.6580341817	2.1384447502	8.5774581175
H	-0.5040792164	1.8270205765	10.3136277255
H	0.9190325679	1.6708120621	9.253552867
C	1.0843784248	3.7715440032	11.0788288059
H	1.9561649882	3.1001285281	11.102780156
H	0.3932340901	3.4369772396	11.8678411515
H	1.4143352003	4.7870776531	11.3380073165
C	5.3484403837	5.2247800594	6.0704459022
H	4.7983264067	4.9044893397	5.1722083969
H	6.4178762708	5.0374285137	5.8813625259
H	5.2048555201	6.3079866495	6.1895441544
C	1.1338463802	10.690007619	10.8256522269
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H	1.9520874557	10.1972718561	11.369638195
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H	6.8358391847	4.6688296524	8.2860698534
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C	5.0975166751	2.9392444501	7.0760526857
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H	4.5002786302	2.5939625988	6.2177491006
C	3.8927959352	11.0843115929	9.3183422013
H	4.0022455056	10.5347511344	10.2639327194
H	3.9791734587	12.1618998813	9.547131186
H	4.7404165849	10.8111447832	8.6744947426
C	-1.1787197662	10.4584943783	8.643435481
H	-1.7415502882	10.0556291299	7.7901479669
H	-1.5819508717	11.4617790073	8.8705337879
H	-1.3884410017	9.8114897151	9.5080820374
C	0.1657668273	10.7752713035	5.7550571325
H	0.7962442402	10.4687811912	4.9089160925
H	-0.1537634324	11.8170376157	5.5748404779
H	-0.7332595418	10.1428849505	5.7405332079
C	3.3301656471	11.1042000514	6.180750299
H	4.2965572978	10.629117275	6.4048902549
H	3.5052701121	12.1913942732	6.0908274021
H	3.0046963387	10.7348721784	5.198470992
C	4.3059738244	8.6418622242	13.4905889654
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H	5.0058382429	9.1322274157	14.1878593796
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H	5.0969359754	5.540528355	14.3162967962
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Fe	1.10567802	-0.3889213502	-0.1080166847
P	-0.2455801416	0.9025995485	1.3285733555
P	-0.3338668403	0.3388697248	-1.8612204432
P	-0.6150775702	-1.3251337741	1.2251077622
P	-0.7002667344	2.016108074	-0.5424981744
P	-0.6999006814	-1.6920598422	-0.8890220037
C	3.0387688084	0.5532581053	-0.0204971709
C	2.6690839202	-1.7081886416	0.3616233761
H	2.5312315253	-2.6594049303	0.8670072798
C	2.9116928834	-0.4598722532	1.0328853353
C	-3.9043052864	1.0337140219	0.5532592359
C	2.6689082458	-1.5411338417	-1.0478680285
C	2.8564658794	-0.1469162848	-1.2610551532
H	2.8860645929	0.3179114514	-2.2407161876
C	3.5274645372	2.0265131109	-0.028664814
C	-4.0026453379	0.7041252917	-0.8414415238
C	-3.7249326185	-0.1842352411	1.2829081973
C	3.2585327518	-0.499890877	2.5440308029
C	4.7501907145	-0.9116285294	2.6539086027
H	4.9237133613	-1.893610367	2.1870568113

H	5.0501967673	-0.9808143872	3.712973848
H	5.4134722426	-0.1871518687	2.1609412642
N	-1.8096766178	3.367182258	-0.9733923674
C	2.7443594974	-2.6408720652	-2.1067730412
C	3.0475968716	0.8078857275	3.3270949715
H	3.7150384145	1.6122980535	2.9968375719
H	3.2655970498	0.6293828151	4.3923291711
H	2.00798775	1.1597569352	3.2543099446
C	-3.7280565397	-1.269376173	0.341254734
C	2.4281229608	-1.5778698149	3.280833122
H	1.3512931395	-1.363425596	3.234137871
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C	2.6723079964	3.0103215508	0.7965092655
H	1.6719292126	3.1168042726	0.356153384
H	3.1509698323	4.0040045241	0.794522411
H	2.5431542134	2.7049514412	1.837572931
C	-3.8787278052	-0.7151933603	-0.9726171995
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H	5.4128073963	3.0795554718	0.3122990653
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C	3.5291510014	2.5806350906	-1.4739919284
H	4.2301156772	2.0408874868	-2.1285968894
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C	2.1407545093	-3.9634319001	-1.5982955317
H	2.6702542831	-4.3356576792	-0.707297215
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C	-4.1282274223	2.3825425143	1.1655897325
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H	0.9669800738	-2.097518619	-3.2823547131
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H	2.4574298397	-1.2938852063	-3.8250108828
C	4.2502112832	-2.8685816571	-2.3966122144
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C	-4.3835936825	1.6331719369	-1.9527401542
H	-4.1598479859	2.6753027365	-1.6993769912
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H	-3.8627501448	1.3892388428	-2.890120261
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H	-3.128015242	-1.2085151062	3.0944932129
H	-4.6868018389	-0.3579998185	3.2006423624
H	-3.1612457367	0.5570880697	3.2331856837
C	-4.0102870287	-1.4859844211	-2.2524846956
H	-3.6009113581	-0.926613921	-3.106187362
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H	-3.4808338851	-2.4481622916	-2.20738627
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H	-1.8696774325	2.8103284952	-3.0136920425
H	-2.5862593748	4.395468285	-2.6418422803
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H	-2.4160335585	5.2484092585	-0.2399668865

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H	-0.6404761132	5.0679664494	-0.35072839
C	-3.6998403137	-2.7302210677	0.6767134454
H	-4.7292937522	-3.1104812131	0.8005855327
H	-3.217920539	-3.3237148487	-0.113795203
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5feni

Fe	-2.1662666115	-0.0627241517	0.3300619876
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P	-0.5506012017	0.1574872609	-1.4689089987
P	-1.1237796259	-1.4218879228	1.9849389403
P	-0.7946533219	2.0845000552	-0.5721046862
P	-0.6141724298	-1.8829803165	-0.0629490651
C	3.1216578247	0.6122722899	0.1684797246
C	2.8440701161	-1.6966978441	0.1220878031
H	2.770336914	-2.7353360001	0.4285133352
C	3.0575802682	-0.6003861363	1.0149666963
C	-3.8845871957	1.1869843828	0.593110379
C	2.7633818364	-1.2467233499	-1.2236275525
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C	3.5091398737	2.0847011247	0.4575564646
C	-3.9263359036	0.5714533892	-0.7116304316
C	-3.8845418734	0.1418628153	1.5635022949
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H	5.5557244052	-0.3305654411	2.2152223931
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C	2.7834594308	-2.1174268444	-2.4789692386
C	3.1081341556	0.1898366224	3.5097350314
H	3.6901190409	1.1056602923	3.3534805264
H	3.3496855319	-0.1734924387	4.5214765748
H	2.0390430801	0.4490839465	3.4922813921
C	-3.9336660715	-1.1194872628	0.8610787956
C	2.7118724231	-2.1888973497	2.9707711686
H	1.6195828647	-2.0897321835	2.8925571861
H	2.9607053712	-2.370462036	4.0281284106
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C	2.54299707	2.8247903396	1.4073636045
H	1.5507627726	2.9287178702	0.9467063409
H	2.9308778055	3.8367324694	1.6126499332
H	2.4043360999	2.3188143882	2.3669698488
C	-3.9463583472	-0.8469825846	-0.5430032449
C	4.9515689745	2.145437572	1.0148788789
H	5.0351368862	1.7025376548	2.0150236907
H	5.2809104975	3.1947120433	1.0927770777
H	5.6552292826	1.6183047238	0.3509687449
C	3.5159749851	2.9002331916	-0.857416298
H	4.2598394893	2.5258761978	-1.5771979668
H	3.771139045	3.9477531372	-0.6331894137
H	2.5283184589	2.8971512745	-1.3429460846
C	2.0809392263	-3.4681573806	-2.2428835714
H	2.571271756	-4.0496966719	-1.4463879604
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H	1.0260392692	-3.3339690205	-1.9610986418

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H	-5.0532962343	2.9022819495	1.1628452303
H	-3.7239387276	3.2752990676	0.0476974112
C	2.1225304032	-1.4059932238	-3.675139951
H	1.0653569004	-1.1761889536	-3.4757547312
H	2.1738082672	-2.0462518076	-4.5708707364
H	2.6331922951	-0.4613558502	-3.9202645404
C	4.2707553126	-2.3857693848	-2.8222690817
H	4.8106283907	-1.4452729554	-3.0152220642
H	4.3517067943	-3.0175086086	-3.7230420322
H	4.7816767605	-2.9032623645	-1.995057433
C	-4.1566623572	1.2685074846	-2.0169953525
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H	-5.2291181441	1.2204000021	-2.2776730339
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C	-3.9605400741	0.3348404579	3.0495137415
H	-3.5274323492	-0.5150315265	3.5957341562
H	-5.0110507838	0.4421035742	3.3744030865
H	-3.4225490326	1.2397552824	3.3678830255
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H	-3.5792818016	-2.8104447152	-1.3705213824
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H	-1.2638166773	1.7784750887	-3.4538390964
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C	-1.7285135177	4.4780455257	-1.4685993426
H	-2.7709990843	4.7652103964	-1.7091281185

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H	-3.5711192447	-3.2565055698	0.9528735442
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Ni	-2.1660049976	-0.2271753151	0.3660093745
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P	-0.3452685341	-0.2005353081	1.8965118248
P	0.1141895013	2.0889599389	-2.3695364764
P	-0.4747442724	-1.7939796	0.5864392891
C	3.0640241956	0.6539926613	0.3284922833
C	2.6242204442	-1.6032780001	0.0617599797
H	2.4748113177	-2.6567138029	0.2797224718
C	2.9401918252	-0.6068630784	1.0495460259
C	-3.9091347573	0.9779904008	0.8005902022
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H	2.8812047946	1.0633745411	-1.8758193364
C	3.5520507304	2.0650531149	0.752894114
C	-4.05119557	0.2798209017	-0.451540843
C	-3.7431215735	-0.0108745572	1.809705916
C	3.3145527736	-1.0794022752	2.4786003757
C	4.8211325816	-1.4486888787	2.4557015114
H	5.0206241705	-2.2318262361	1.7076576558
H	5.1338028544	-1.8336844728	3.4408627841

H	5.4566646756	-0.5872668093	2.2114873208
N	-0.9259531894	3.3344967767	-2.9021858987
C	2.5629613876	-1.8344154979	-2.5539198309
C	3.057426797	-0.0716923558	3.6143510988
H	3.6816535694	0.8258188087	3.5381894404
H	3.2956851277	-0.5455509504	4.5800384576
H	2.00197034	0.2372953194	3.6458428736
C	-3.8782838252	-1.3268227495	1.1925536582
C	2.544243779	-2.3666162333	2.8647917868
H	1.4562468983	-2.2115281081	2.8645044985
H	2.8400191021	-2.6718750655	3.8808670249
H	2.7708480374	-3.2139722225	2.2022391862
C	2.6463762591	2.7709757358	1.7863852752
H	1.6580403104	2.9872208878	1.3560160963
H	3.1024410095	3.7297525298	2.085381339
H	2.4843323918	2.1807834155	2.6927155136
C	-4.09164101	-1.1455631835	-0.192268365
C	4.9980980549	1.977440934	1.2997249814
H	5.0555079543	1.4611751127	2.2657650583
H	5.4052880233	2.9911540212	1.4470629855
H	5.6581239697	1.4494340945	0.5931521746
C	3.6187822877	3.0017477823	-0.4762411438
H	4.3399754432	2.6472053079	-1.2283297839
H	3.9449332596	4.0025199574	-0.1522867576
H	2.6388464408	3.1130798084	-0.9615835193
C	1.5156875465	-2.9638793333	-2.5165329158
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