Electronic Supplementary Data

Synthesis, characterisation and redox properties of anti-bimetallic permethylpentalene complexes

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1. General details

General methods and materials

Air- and moisture-sensitive reactions were performed on a dual-manifold vacuum/N_2 line using standard Schlenk techniques, or in a N_2 filled MBraun Unilab glovebox. All glassware was heated in an oven at 170 °C for at least 1 hour prior to use. Hexane, pentane, dichloromethane, benzene, and toluene were dried using a MBraun SPS-800 solvent purification system. Diethyl ether was distilled from potassium, and tetrahydrofuran was dried over Na/benzophenone until purple, and distilled under N_2. Dry solvents were stored under N_2 in oven dried ampoules with a Rotaflo cap containing K mirrors (pentane, hexane, benzene, toluene, ether) or 3 Å molecular sieves dried for 12 hours at 140 °C (THF, dichloromethane). Deuterated NMR spectroscopic solvents were purchased from Goss Scientific or Cambridge Isotopes Laboratories and stored in the glovebox after drying. Benzene-d_6 and toluene-d_8 were either stirred over NaK for at least 3 days then distilled, or dried over a potassium mirror and freeze–thaw–degassed three times. THF-d_8, pyridine-d_5, chloroform-d_1, and dichloromethane-d_2 were stirred over powdered calcium hydride for at least three days then distilled. All solvents were degassed prior to use.

Reagents were purchased from Sigma Aldrich or Alfa Aesar and used without further purification unless otherwise stated. Metal(II) acetylacetonates were dried at 10^{-2} mbar overnight and stored in the glovebox and freshly sublimed prior to use. $Li_2Pn^*TMEDA_x$,[1] Cp*FeCl·TMEDA,[2] Cp*Fe(acac),[3,4] Cp*Co(acac),[4] and Cp*Ni(acac),[4] were prepared according to literature methods.

NMR spectroscopy

^1H and $^{13}C\{^1H\}$ NMR spectra were obtained either on a Agilent Mercury VX-Works 300 MHz spectrometer running Varian software, or on a Bruker AVIII 400 MHz running ICON automation of TOPSPIN software. Air sensitive NMR samples were prepared in a glovebox under a nitrogen atmosphere and sealed in 5 mm tubes with Young type concentric stopcocks. ^1H and $^{13}C\{^1H\}$ shifts (in parts per million, ppm) are referenced internally to residual protio-solvent relative to TMS ($\delta = 0$. *J* values are given in Hz.

^1H and 2D spectra of paramagnetic molecules, variable temperature, and Evans NMR studies were conducted on a Bruker AVIII 500 MHz running TOPSPIN software.

For Evans' NMR measurements, a concentrated toluene-d_8 solution of a paramagnetic complex and a sealed glass capilliary containing pure toluene-d_8 were placed in an NMR tube sealed with a Young's concentric stopcock. The samples were heated as required to ensure full solvation of the complex.

Mass spectroscopy and elemental analysis

Electrospray ionisation spectra of air- and moisture-stable samples diluted in methanol or acetonitrile were collected in positive and negative modes on an Agilent Technologies 6120 Quadrupole LCMS spectrometer. Electrospray ionisation mass spectra of air and moisture sensitive samples were recorded by Colin Sparrow of the Chemistry Research Laboratory, University of Oxford, using a Bruker μTOF spectrometer. Elemental analyses were carried out by Stephen Boyer of London Metropolitan University.

Single crystal X-ray crystallography

A typical crystal was mounted on a MiTeGen Micromounts using perfluoropolyether oil and cooled rapidly to 150 K in a stream of nitrogen gas using an Oxford Cryosystems Cryostream unit.[5] Data were collected with an Enraf-Nonius KappaCCD diffractometer (using graphite-monochromated Mo K_α radiation, λ = 0.71073 Å) or on an Agilent SuperNova A diffractomenter (Cu K_α radiation, λ = 1.54180 Å). Raw frame data were reduced using the DENZO-SMN package or using CrysAlisPro.[6,7] Intensity data were corrected using multi-scan method with SCALEPACK (within DENZO-SMN). The structure was solved using direct methods with SIR92[8] or Superflip[9] and refined using full-matrix least squares refinement on all F^2 data using the CRYSTALS program suite.[10-12] In general distances and angles were calculated using the full variance–covariance matrix. Dihedral angles were calculated using PLATON.[13]

DFT Calculations

All DFT calculations were performed with the ADF program package.[14,15] Geometry optimisation calculations were carried out at BP,[16,17] and B3LYP,[18] and MO6L[19] levels of DFT. For geometry optimisations the triple-zeta[20] Slater type basis sets were used.

Electrochemical measurements

Cyclic voltammetry measurements were carried out in a three-electrode configuration, with a silver quasi-reference electrode, a glassy-carbon working electrode and a platinum auxiliary electrode, all sourced from Bioanalytical Systems®, within a Saffron Omega Scientific glovebox under anhydrous Nitrogen on a PARAMETEK® VersaSTAT 3 potentiostat. The supporting electrolyte (0.1 M $[NBu_4][PF_6]$ in THF) was prepared from recrystallised salt with freshly distilled THF, thoroughly degassed, and tested prior to use. The electrodes were immersed in 10 mL of a 1 mM solution of the analyte, prepared in the glovebox. Voltammograms were collected, typically scanning a potential range between −2.5 and 1.5 V *vs* Ag at scan rates ranging from 0.1 to 10 V s^{-1}. All potentials were referenced to the internal ferrocene/ferrocenium ($Fc^{0/+}$) couple by addition of ferrocene to each sample and recording its potential under identical conditions.

2. X-ray crystallography

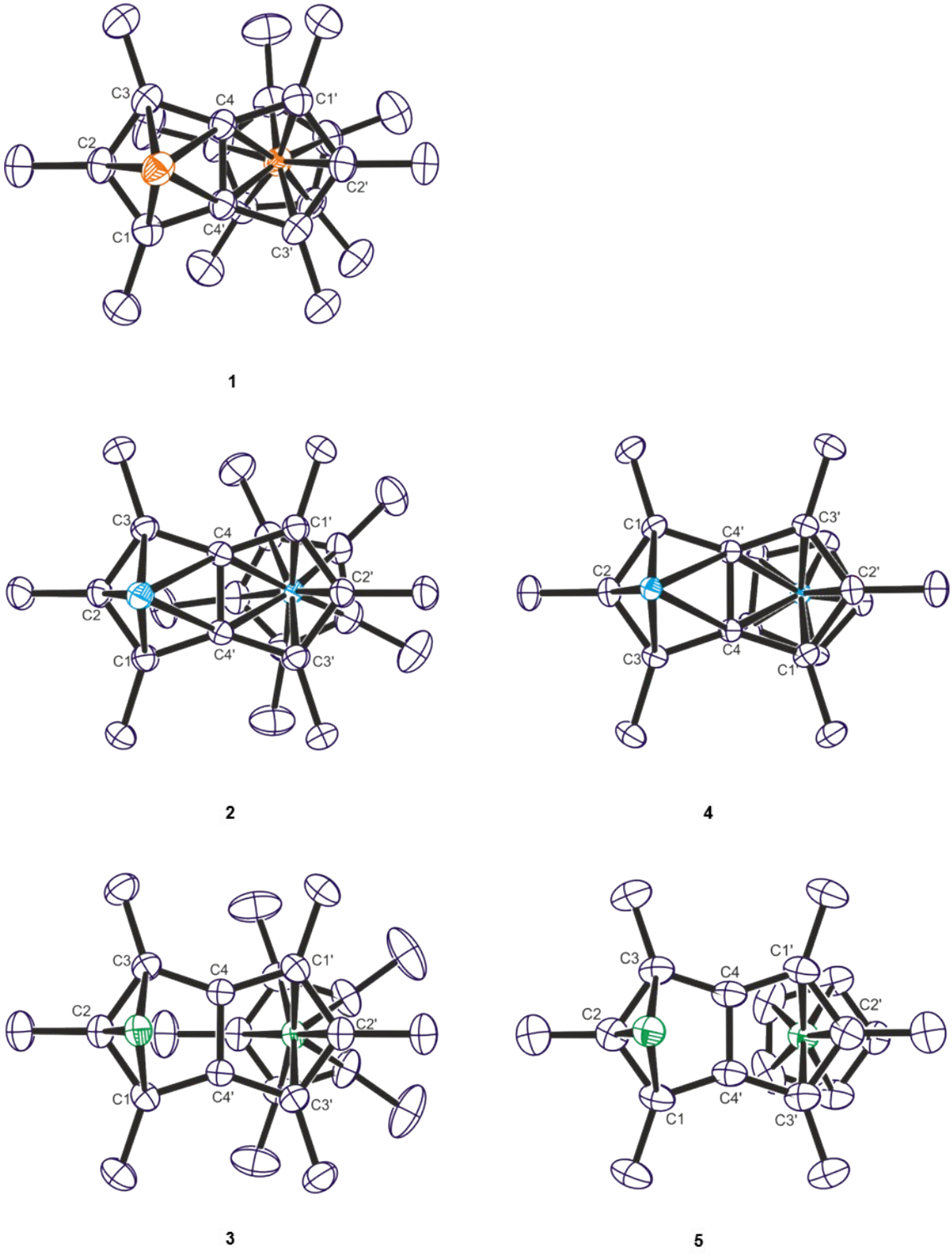

Fig. S1. Plan views of the *anti*-bimetallic complexes *anti*-$(MCp^*)_2Pn^*$ (M = Fe (**1**), Co (**2**) and Ni (**3**)) and *anti*-$(MCp)_2Pn^*$ (M = Co (**4**) and Ni (**5**)), showing the staggered (**1**-**3**) and eclipsing (**4**-**5**) capping groups. One capping group has been removed to show the perpendicular projection of the metal atom onto the Pn* plane.

Table S1. Selected bond lengths, angles and distances for $(FeCp^*)_2Pn^*$ (**1**).

Fe1–C1	2.050(3)
Fe1–C2	2.018(3)
Fe1–C3	2.050(3)
Fe1–C4	2.185(2)
Fe1–C4’	2.185(3)
Fe1–C8	2.065(3)
Fe1–C9	2.073(3)
Fe1–C10	2.056(3)
Fe1–C11	2.060(3)
Fe1–C12	2.071(3)
C4–C4’	1.453(3)
Fe1–P_{cent}	1.703
Fe1–C_{cent}	1.673
Fe1–Fe1’	4.1208(7)
C_{cent}–Fe1–P_{cent}	176.52
Tilt angle	2.39
Hinge angle	6.20
$(C4C4')_{cent}$–C2–C6	175.64

Tilt angle = angle between mean planes of C1,2,3,4,4’ and C8,9,10,11,12; Hinge angle = angle between mean planes of C1,3,4,4’ and C1,2,3; $\delta(\%) = \frac{[(M-C)-(M-C2)]}{(M-C2)} \times 100$

Table S2. Selected bond lengths, angles and distances for $(CoCp^*)_2Pn^*$ (**2**) and $(CoCp)_2Pn^*$ (**4**).

	2	**4**
Co1–C1	2.059(3)	2.055(2)
Co1–C2	1.991(3)	2.008(3)
Co1–C3	2.055(2)	2.052(3)
Co1–C4	2.265(2)	2.249(2)
Co1–C4’	2.267(2)	2.251(2)
Co1–C8	2.056(3)	2.081(1)
Co1–C9	2.103(3)	2.144(2)
Co1–C10	2.092(3)	2.097(3)
Co1–C11	2.065(3)	2.070(3)
Co1–C12	2.082(3)	2.076(2)
C4–C4’	1.422(4)	1.425(3)
Co1–Pn^*_{cent}	1.745	1.739
Co1–Cp_{cent}	1.691	1.710
Co1–Co1’	4.3032(5)	4.2697(4)
Cp^*_{cent}–Co1–Pn^*_{cent}	172.48	171.42
Tilt angle	1.06	2.15
Hinge angle	6.84	7.33
$(C4C4')_{cent}$–C2–C6	173.38	174.41

Table S3. Selected bond lengths, angles and distances for $(NiCp^*)_2Pn^*$ (**3**) and $(NiCp)_2Pn^*$ (**5**).

	3	**5**
Ni1–C1	2.131(3)	2.142(4)
Ni1–C2	1.996(3)	1.998(3)
Ni1–C3	2.147(3)	2.145(3)
Ni1–C4	2.353(3)	2.390(3)
Ni1–C4’	2.360(2)	2.392(3)
Ni1–C8	2.141(3)	2.182(4)
Ni1–C9	2.145(3)	2.185(3)
Ni1–C10	2.151(3)	2.181(4)
Ni1–C11	2.146(3)	2.133(6)
Ni1–C12	2.118(3)	2.128(4)
C4–C4’	1.463(3)	1.470(4)
Ni1–Pn^*_{cent}	1.830	1.850
Ni1–C_{cent}	1.769	1.800
Ni1–Ni1’	4.4806(6)	4.5495(6)
C_{cent}–Ni1–Pn^*_{cent}	171.27	175.95
Tilt angle	2.34	6.48
Hinge angle	2.06	3.21
$(C_{cent}$–C4–C4’–$C_{cent})$	C2–C6 173.64	173.99

Table S4. Distortions towards η^3 coordination

Complex	(%)	Ref
1	8.2	[a]
2	13.8	[a]
3	18.1	[a]
4	12.1	[a]
5	19.7	[a]

[a] This work

Complex	(%)	Ref
$(FeCp^*)_2Pn$	5.08	21
$(CoCp^*)_2Pn$	16.2	22
$(FePnH)Pn(CoCp^*)$	Fe 4.9 Co 13.05	23
$[Ni(allyl)]_2Pn$	11.8	24

Table S5. Selected experimental crystallographic data for $(FeCp^*)_2Pn^*$ (**1**), $(CoCp^*)_2Pn^*$ (**2**), $(NiCp^*)_2Pn^*$ (**3**), $(CoCp)_2Pn^*$ (**4**) and $(NiCp)_2Pn^*$ (**5**).

Complex	**1**	**2**	**3**	**4**	**5**
			Crystal data		
Chemical formula	$C_{34}H_{48}Fe_2$	$C_{34}H_{48}Co_2$	$C_{34}H_{48}Ni_2$	$C_{24}H_{28}Co_2$	$C_{24}H_{28}Ni_2$
M_r	568.45	574.62	574.17	434.35	433.91
Crystal system, space group	Monoclinic, $P2_1/n$	Monoclinic, $C2/c$	Monoclinic, $P2_1/n$ c	Triclinic, $P\bar{1}$	Triclinic, $P\bar{1}$
Temperature (K)	150	150	150	150	150
a, b, c (Å)	9.1531 (3), 15.1021 (4), 11.1714 (3)	16.7219 (4), 8.6986 (2), 20.5957 (5)	8.8663 (3), 15.1452 (7), 11.5069 (4)	7.9066 (2), 8.1643 (2), 9.3165 (4)	7.6274 (4), 8.2173 (4), 9.6561 (7)
α, β, γ (°)	90, 109.768 (3), 90	90, 104.8732 (10), 90	90, 104.974 (3), 90	67.9417 (14), 83.4571 (14), 61.8652 (17)	68.600 (3), 87.710 (3), 62.426 (4)
V (Å^3)	1453.23 (7)	2895.42 (12)	1492.70 (10)	490.05 (3)	493.33 (5)
Z	2	4	2	1	1
Radiation type	Cu $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	8.13	1.17	1.28	1.70	1.91
Crystal size (mm)	0.30 × 0.08 × 0.08	0.16 × 0.16 × 0.05	0.20 × 0.08 × 0.08	0.42 × 0.40 × 0.40	0.16 × 0.16 × 0.10
			Data Collection		
Diffractometer	SuperNova, Dual, Cu at zero, Atlas diffractometer	Nonius KappaCCD	Nonius KappaCCD	Nonius KappaCCD	Nonius KappaCCD
Absorption correction	Multi-scan.	Multi-scan *DENZO*/*SCALEPACK* (Otwinowski & Minor, 1997).	Multi-scan *DENZO*/*SCALEPACK* (Otwinowski & Minor, 1997).	Multi-scan *DENZO*/*SCALEPACK* (Otwinowski & Minor, 1997).	Multi-scan *DENZO*/*SCALEPACK* (Otwinowski & Minor, 1997).

T_{min}, T_{max}		0.87, 0.94	0.84, 0.90	0.43, 0.51	0.74, 0.83
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7782, 3013, 2281	17044, 3296, 2456	13864, 5069, 2466	6663, 2232, 2013	6788, 2245, 2099
R_{int}	0.044	0.029	0.027	0.019	0.029
			Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.117, 0.98	0.036, 0.098, 0.94	0.040, 0.107, 0.95	0.029, 0.066, 0.89	0.040, 0.102, 0.88
No. of reflections	3001	3296	3387	2232	2245
No. of parameters	163	163	163	118	119
No. of restraints	0	0	0	0	0
$(\Delta/\sigma)_{max}$	0.001	0.0004	0.001	0.0004	0.001
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.75, -0.45	0.86, -0.58	0.66, -0.65	0.50, -0.39	0.87, -0.64

Computer programs: *CrysAlis PRO*, Agilent Technologies, Version 1.171.35.21 (release 20-01-2012 CrysAlis171 .NET) (compiled Jan 23 2012, 18:06:46), *CrysAlis PRO* 1.171.38.41 (Rigaku OD, 2015), Collect (Nonius BV, 1997-2000), *HKL SCALEPACK* (Otwinowski & Minor 1997), *HKL DENZO* and *SCALEPACK* (Otwinowski & Minor 1997), SUPERFLIP. Palatinus, L.; Chapuis, G. J. Appl. Cryst. 2007, 40, 786-790, Sir-92. Altomare, A.; Cascarano, G.; Giacovazzo, C.; Guagliardi, A. J. Appl. Cryst. 1994, 27, 435., *SHELXL2014* (Sheldrick, 2014), *ORTEP-3 for Windows*. Farrugia, L. J. J. Appl. Cryst. 1997, 30, 565.

3. Magnetic studies

The size of the magnetisation, *m(*T*)*, is proportional to the difference in population between the ground and excited states. For molecules with a diamagnetic ground state therefore, $(T) \propto \frac{p(T)}{T}$, where *p(*T*)* is the Boltzmann population of the excited state, and the factor T^{-1} accounts for the temperature-dependent Curie behaviour of the excited state. Assuming relaxation of electron spin is fast, the nuclei in the molecules will experience a magnetic field proportional to this magnetisation, which augments the field applied inside a spectrometer, causing the chemical shifts to have a temperature-dependent contribution (the isotropic shift). The Boltzmann population, $p(T)$, of a state that differs in energy from the ground state by $\Delta\varepsilon = 2J$, is found by normalising the population of that state $(g_i e^{\Delta\varepsilon/kT}$, where g_i is the multiplicity of state *i*) by the partition function for the system $(Z = \sum_i g_i e^{-\varepsilon_i/kT})$. For a two level system containing a singlet ground and a triply degenerate triplet excited state, this results in the expression $p(T) = 3e^{2J/kT}/(1 + 3e^{2J/kT})$, which is valid when the Zeeman splitting of the triplet state is small compared to *k*T.

The temperature-dependence of the chemical shifts of a given nucleus can therefore be modelled using the expression

$$\delta(T) = \delta_0 + \delta_P \cdot m(T) = \delta_0 + \delta_P \cdot \frac{3e^{2J/kT}}{T\left(1 + 3e^{2J/kT}\right)}$$

where *δ(*T*)* is the position of the chemical shift at temperature T, and δ_p is a constant that relates the temperature-dependence of the high-spin state and hyperfine coupling constant of the described nucleus to the isotropic chemical shift.

In the solid state, both on **3** and **5** appear to be paramagnetic. There is no evidence of a singlet ground state.

Inverse molar magnetic susceptibility data (as χ_{mol}^{-1}) and the derived effective magnetic moment for **3** are plotted in Fig S2a. Compound **3** obeys the Curie-Weiss law below 40 K with a magnetic moment, μ_B = 2.04 μ_{BM} and Weiss constant of 1 K indicating negligible spin-spin interactions at low temperature. Above 40 K, there is a small deviation from the Cure-Weiss law which may be tentatively attributed to TIP. The observed magnetic moment is slightly low for a species with a triplet ground state ($\mu_{s.o.}$=2.83 μ_{BM}).

Inverse molar magnetic susceptibility data and the derived effective magnetic moment for **5** is shown in Fig S2b. Compound **5**, obeys the Curie-Weiss law below 210 K. The effective magnetic moment, μ_{eff} = 3.49 μ_{BM} with a Weiss constant of −14.6 K suggesting weak antiferromagnetic spin-spin interactions between neighbouring spins. The magnetic moment is higher than the spin-only value of 2.83 μ_B of an $S = 1$ species and is consistent with two

unpaired electrons occupying orbitals where the spatial component of angular momentum is not fully quenched. Using $(\mu_{eff})^2 = g^2S(S+1)$; g is estimated to be 2.467.

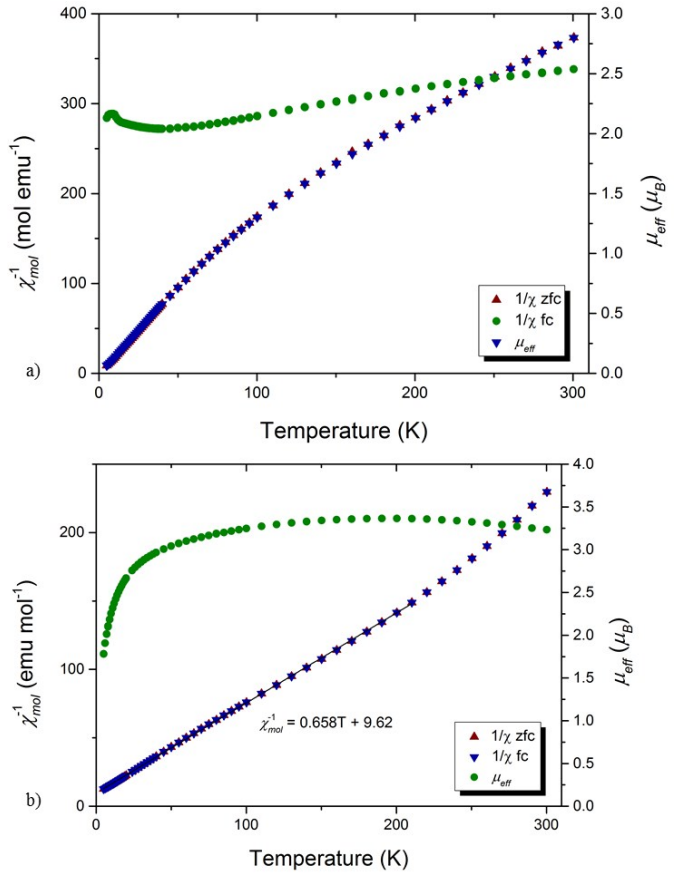

Fig. S2. Plot of effective magnetic moment and inverse magnetic susceptibility for a) $(NiCp^*)_2Pn^*$ (**3**) and $(NiCp)_2Pn$ (**5**) between 5 and 300 K.

4. DFT studies and electronic studies

Table S6. Comparison of calculated and observed structural data for **1** – **5**

	1		**2**		**4**	
	calcd	**obsd**	**calcd**	**obsd**	**calcd**	**obsd**
M—C1/3	2.055	2.050(3)	2.079	2.057	2.064	2.054
M—C2	2.041	2.018(3)	1.968	1.991(3)	1.968	2.008(3)
M—C4/4’	2.175	2.185(3)	2.382	2.266	2.352	2.25
delta (%)	6.6	8.3	21.0	13.8	19.5	12.1
C4—C4’	1.477	1.453(3)	1.435	1.422(4)	1.435	1.425(3)
Tilt angle	5.14	2.39	6.64	1.06	5.04	2.15
Hinge angle	6.81	6.2	8.21	6.84	8.37	7.33

	3			**5**		
	calcd (S = 0)	**calcd** (S = 1)	**obsd**	**calcd** (S = 0)	**calcd** (S = 1)	**obsd**
M—C1/3	2.179	2.192	2.139	2.175	2.157	2.144
M—C2	1.967	2.014	1.996(3)	1.968	1.997	1.998(3)
M—C4/4’	2.551	2.448	2.357	2.531	2.537	2.391
delta (%)	29.7	21.5	18.1	28.6	27.0	19.7
C4—C4’	1.479	1.472	1.463(3)	1.479	1.437	1.470(4)
Tilt angle	10.47	6.25	2.34	10.93	6.75	6.48
Hinge angle	5.47	1.98	2.06	5.24	8.64	3.21

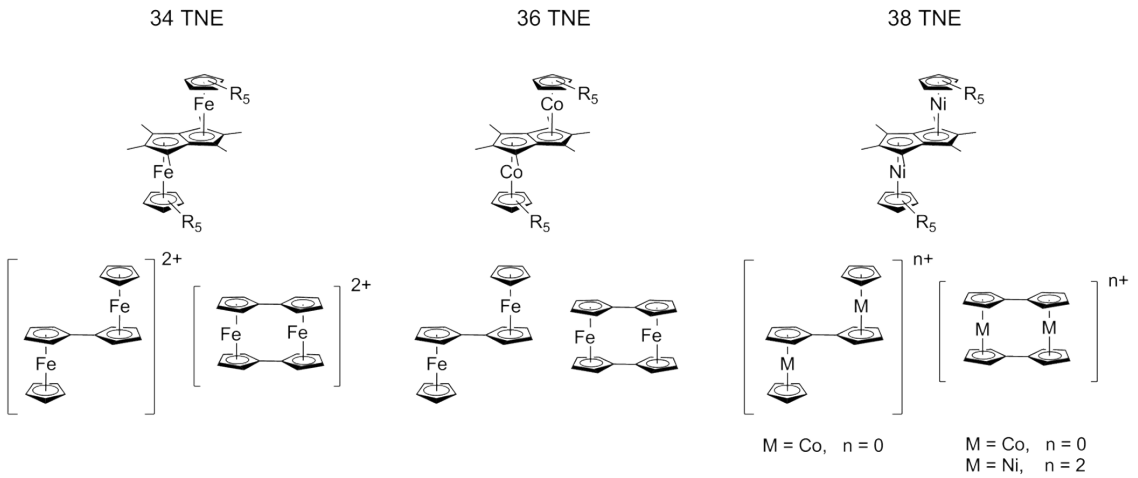

Fig. S3. Classification of linked and fused bimetallics according to the total number of electrons (TNE) for comparison of magnetic properties.

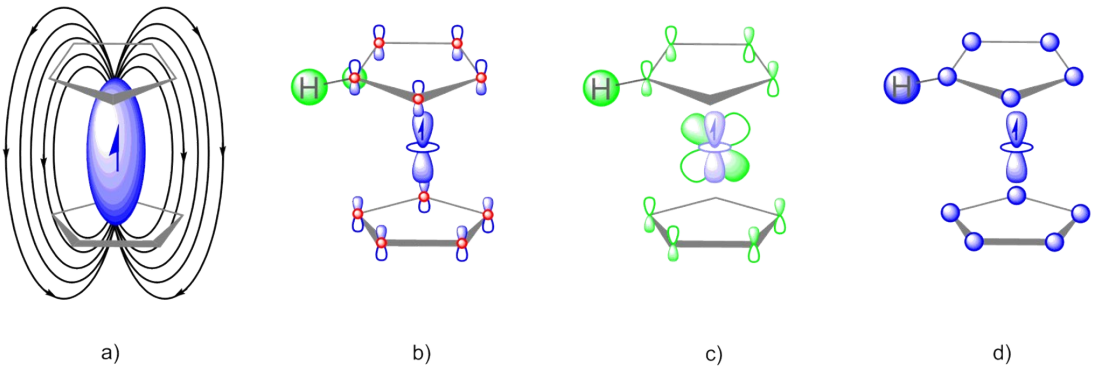

Fig. S4. Illustrations depicting visualisations of a) the pseudocontact shift mechanism, nuclei interact with a magnetic field generated by the molecules anisotropic spin density; b), c) and d) Fermi contact shift mechanisms: b) electron spin density in mixed Md-Lπ molecular orbitals (depicted blue) results in polarisation of the ring carbon nuclei (depicted red). The spin polarisation mechanism[25] (depicted green) transmits this polarisation to ring substituents through bonds that have electron density at both nuclei; c) electrons in bonding orbitals (green) that overlap with the metal atom are polarised through exchange interactions with the metal-based spin density (blue); d) mixing between the metal based orbital(s) housing the unpaired electron(s) and ligand σ-networks directly causes spin density to reside on the ring protons.

Table S7. Calculated spin densities of **3** and **5** with S=1. $\mathbf{3^1}$ corresponds to the first excited state with a $b_g^1b_u^1$ configuration and $\mathbf{3^2}$ to the second excited state with a $b_g^1a_u^1$ configuration.

	$\mathbf{3^1}$	$\mathbf{3^2}$	**5**
Ni	0.5724	0.5024	0.6183
Pn* ring C WT	0.0696	-0.0434	0.0777
Pn* Me C WT	-0.0068	0.0032	-0.0065
Pn* Me H WT	0.0013	-0.0013	0.002
Pn* ring C NWT	-0.0398	0.1510	-0.0460
Pn* Me C NWT	0.0025	-0.0140	0.0034
Pn* Me H Pn* NWT	-0.0011	0.0056	-0.0014
Cp* ring C	0.0603	0.0432	
Cp* Me C	-0.0057	-0.0038	
Cp* Me H	0.0021	0.0022	
Cp ring C			0.0486
Cp H			-0.0039

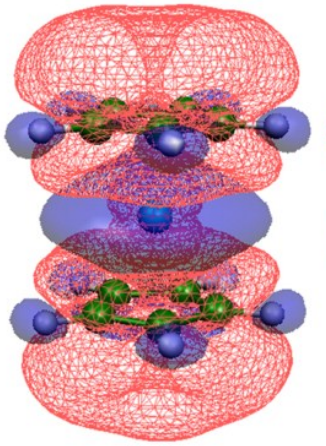

Fig. S5. Spin-density distribution in nickelocene calculated by Hrobárik *et al.* with DFT methods, +/−0.0001 a.u. isosurfaces; red "chickenwire" indicates positive spin density, blue "transparent" indicates negative spin density.[26]

5. Cyclic voltammetry

Table S8. Peak potentials of reversible ET events obtained from cyclic voltammograms of **1**.

	$E_{½}$	$E_{½}$	$E_{½}$	$(E_{½})$
vs Ag	−2.60 [a]	0.12	0.58	1.05
vs $Fc^{0/+}$	−4.20 [a]	−1.48	−1.02	−0.55

Using $E_{½} = (E_{pa}+E_{pc})/2$ [a] E_{pc}

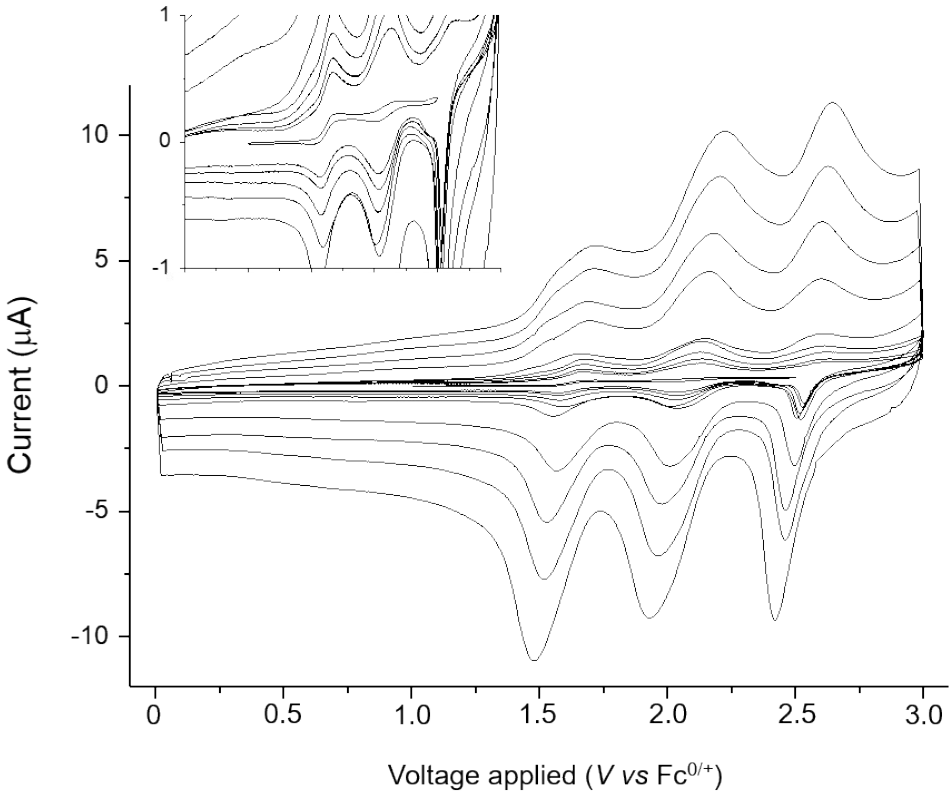

Fig. S6. Overlaid cyclic voltammograms (1 cycle) obtained by scanning a 0.1 mM solution of **1** in THF containing 0.1 M $[NBu_4][PF_6]$ over the region 0 to 3.0 V at scan rates ranging from 0.1 to 10 V s^{-1}.

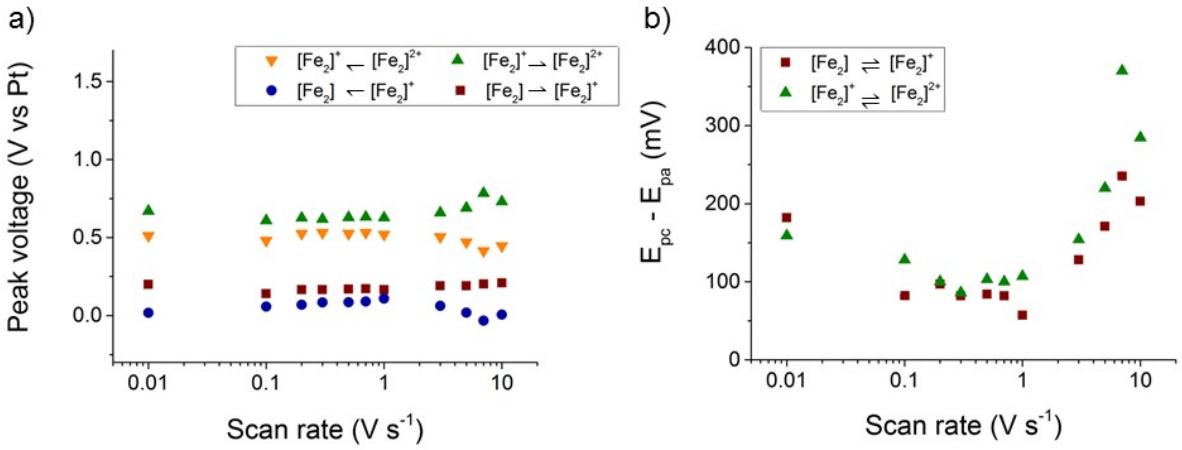

Fig. S7. Plots of a) peak potentials of ET events versus scan rate for **1**, and b) difference in peak potentials, $\Delta E=(E_{pa}-E_{pc})/2$, for the ET events shown in a).

Table S9. Peak potentials of reversible ET events obtained from cyclic voltammograms of **5**.

	$E_{½}$(I)	$E_{½}$(II)	$E_{½}$(III)	$E_{½}$(IV)	$E_{½}$(V)
vs Ag	−1.86	−1.48 [a]	0.08	0.39	0.87
vs $Fc^{0/+}$	−3.48	−3.10 [a]	−1.54	−1.15	−0.75

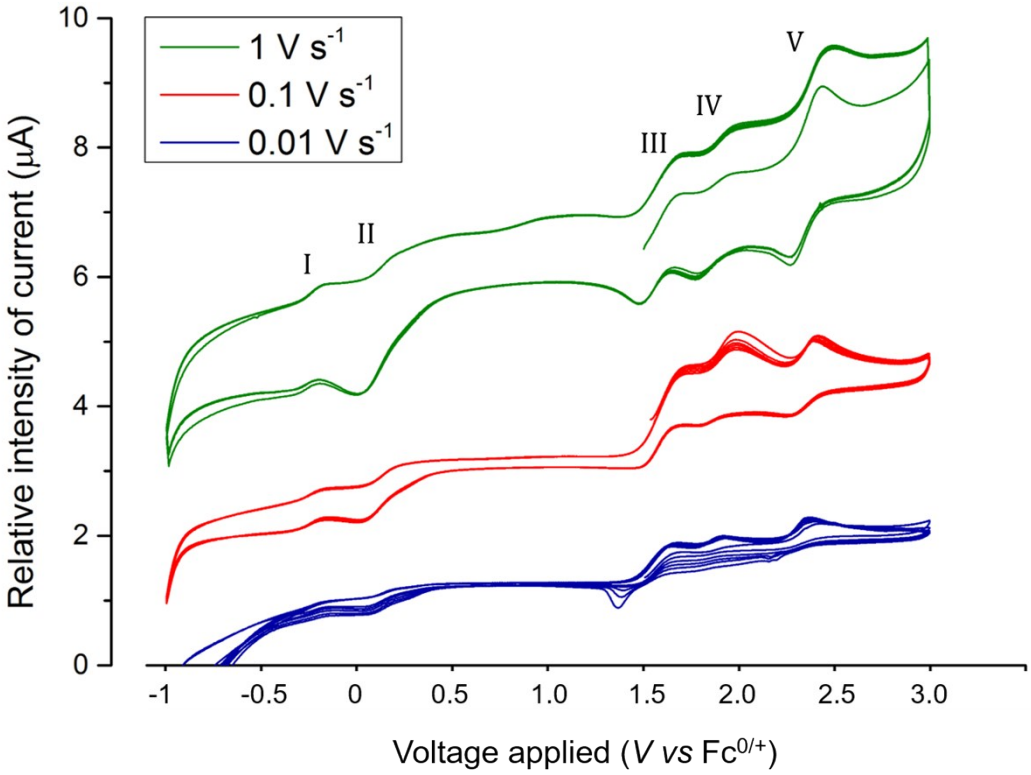

Fig. S8. Offset plot of overlaid cyclic voltammograms (5 cycles) obtained by scanning a 0.1 mM solution of **5** in THF containing 0.1 M $[NBu_4][PF_6]$ over the region −1.0 to 3.0 V at scan rates of 0.01, 0.1, and 1 V s^{-1}.

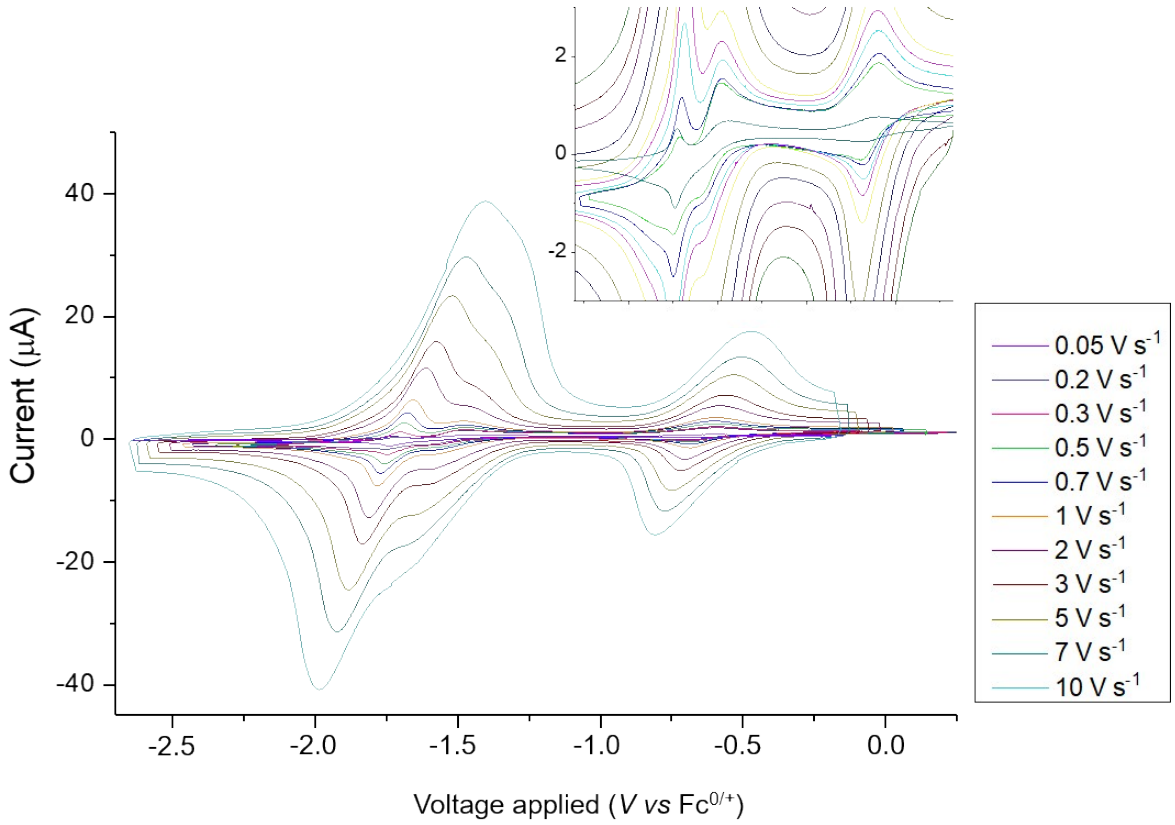

Fig. S9. Overlaid cyclic voltammograms (1 cycle) obtained by scanning a 0.1 mM solution of **2** in THF containing 0.1 M $[NBu_4][PF_6]$ over the region −2.75 to −0.5 V at scan rates ranging from 0.05 to 10 V s^{-1}.

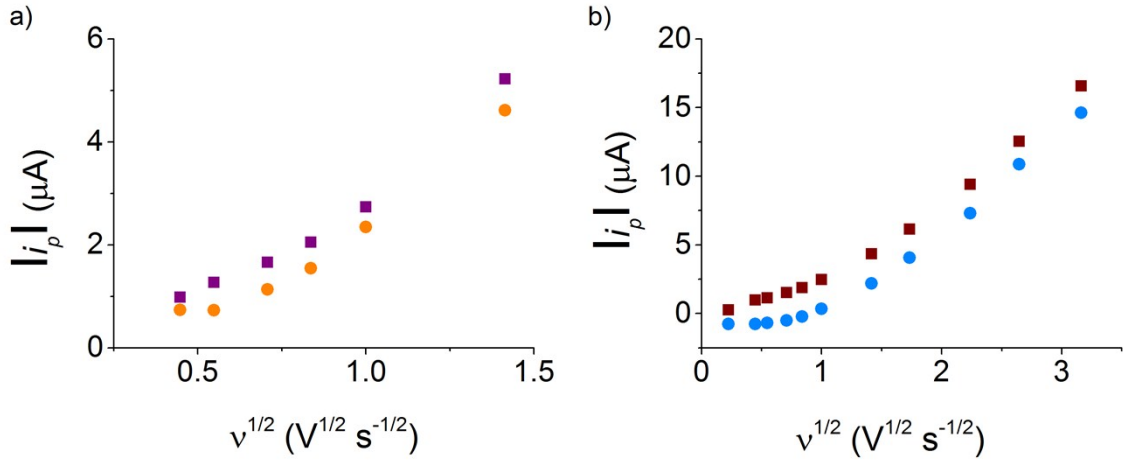

Fig. S10. Plots of the modulus peak currents *vs* the square root of the scan rate for the two events, a) $E_{½}$=−0.03 V, b) $E_{½}$=0.86 V, ■ indicates an anodic peak current (i_{pa}), ● indicates the modulus of a cathodic peak current (i_{pc}).

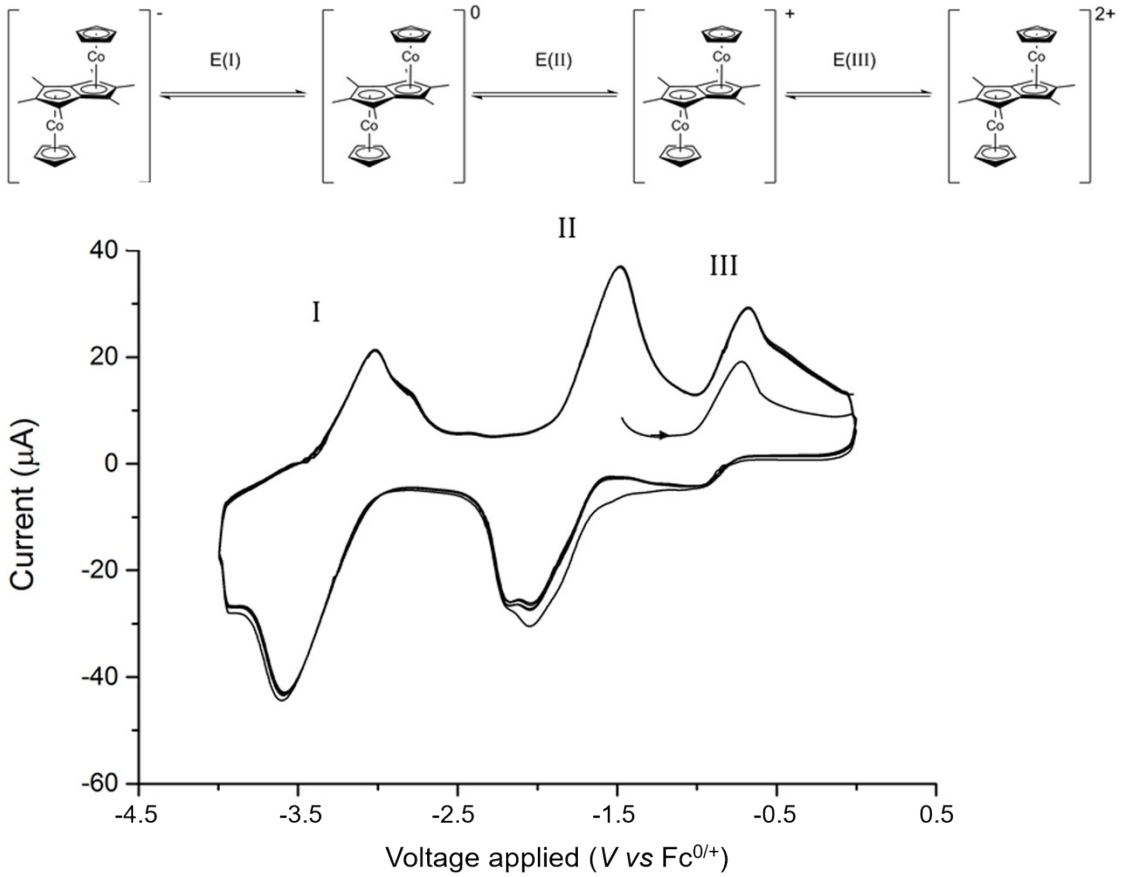

Fig. S11. Overlaid cyclic voltammograms (5 cycles) obtained by scanning a 0.1 mM solution of **4** in THF containing 0.1 M $[NBu_4][PF_6]$ over the region −4.0 to 0 V at a scan rate of 5 V s^{-1}, and an inset scheme showing the three ET events corresponding to the peaks observed.

6. Cartesian coordinates for optimised structures

$Fe_2Pn^*Cp^*_2$ 1

84

Fe	-2.04269908	0.10488581	-0.00000000
C	-1.10434374	1.91761897	-0.00000000
C	-0.74193864	1.16437701	-1.18767805
C	0.00000000	-0.00000000	-0.73873347
C	-0.74193864	1.16437701	1.18767805
C	-0.89595117	1.62891371	-2.60851049
C	-1.71108392	3.29347222	-0.00000000
C	-3.37340862	-1.00586169	-1.16901856
C	-3.00675850	-1.76051470	-0.00000000
C	-3.37340862	-1.00586169	1.16901856
C	-3.96137327	0.23329693	0.72354005
C	-3.96137327	0.23329693	-0.72354005
C	-4.59732808	1.27115999	-1.60392216
C	-4.59732808	1.27115999	1.60392216
C	-3.27638604	-1.47602595	2.59310542
C	-2.39847988	-3.13376788	-0.00000000
C	-3.27638604	-1.47602595	-2.59310542
C	-0.89595117	1.62891371	2.60851049
H	-1.01694944	0.78021650	-3.29640588
H	-1.77052876	2.28372877	-2.72875582
H	-0.01251927	2.19930278	-2.94624872
H	-2.33804504	3.46106489	0.88682790
H	-2.33804504	3.46106489	-0.88682790
H	-0.93036902	4.07419770	-0.00000000
H	-4.56685046	2.27000868	-1.14627031
H	-5.65903068	1.03220471	-1.79272226
H	-4.10091586	1.33599221	-2.58257998
H	-4.56685046	2.27000868	1.14627031
H	-5.65903068	1.03220471	1.79272226
H	-4.10091586	1.33599221	2.58257998
H	-3.13641159	-0.63872290	3.29145169
H	-4.19544974	-2.00631939	2.89990962
H	-2.43711465	-2.17088620	2.73503833
H	-1.77004290	-3.29872584	0.88610133
H	-3.18293981	-3.91068574	-0.00000000
H	-1.77004290	-3.29872584	-0.88610133
H	-3.13641159	-0.63872290	-3.29145169
H	-4.19544974	-2.00631939	-2.89990962
H	-2.43711465	-2.17088620	-2.73503833
H	-1.01694944	0.78021650	3.29640588
H	-1.77052876	2.28372877	2.72875582
H	-0.01251927	2.19930278	2.94624872
C	1.10434374	-1.91761897	-0.00000000
C	0.74193864	-1.16437701	1.18767805
C	0.00000000	-0.00000000	0.73873347
C	0.74193864	-1.16437701	-1.18767805
C	0.89595117	-1.62891371	2.60851049
C	1.71108392	-3.29347222	-0.00000000
C	0.89595117	-1.62891371	-2.60851049
H	1.01694944	-0.78021650	3.29640588
H	1.77052876	-2.28372877	2.72875582
H	0.01251927	-2.19930278	2.94624872

H	2.33804504	-3.46106489	-0.88682790
H	2.33804504	-3.46106489	0.88682790
H	0.93036902	-4.07419770	-0.00000000
H	1.01694944	-0.78021650	-3.29640588
H	1.77052876	-2.28372877	-2.72875582
H	0.01251927	-2.19930278	-2.94624872
Fe	2.04269908	-0.10488581	-0.00000000
C	3.37340862	1.00586169	1.16901856
C	3.00675850	1.76051470	-0.00000000
C	3.37340862	1.00586169	-1.16901856
C	3.96137327	-0.23329693	-0.72354005
C	3.96137327	-0.23329693	0.72354005
C	4.59732808	-1.27115999	1.60392216
C	4.59732808	-1.27115999	-1.60392216
C	3.27638604	1.47602595	-2.59310542
C	2.39847988	3.13376788	-0.00000000
C	3.27638604	1.47602595	2.59310542
H	4.56685046	-2.27000868	1.14627031
H	5.65903068	-1.03220471	1.79272226
H	4.10091586	-1.33599221	2.58257998
H	4.56685046	-2.27000868	-1.14627031
H	5.65903068	-1.03220471	-1.79272226
H	4.10091586	-1.33599221	-2.58257998
H	3.13641159	0.63872290	-3.29145169
H	4.19544974	2.00631939	-2.89990962
H	2.43711465	2.17088620	-2.73503833
H	1.77004290	3.29872584	-0.88610133
H	3.18293981	3.91068574	-0.00000000
H	1.77004290	3.29872584	0.88610133
H	3.13641159	0.63872290	3.29145169
H	4.19544974	2.00631939	2.89990962
H	2.43711465	2.17088620	2.73503833

$Co_2Pn^*Cp^*_2$ 2

84

Co	2.25850491	6.19768328	12.08162494
C	0.32896210	6.00305825	11.74735431
C	1.01262004	5.05825024	10.87237505
C	1.63186363	5.82627444	9.81368776
C	0.69972534	7.34915735	11.32697780
C	0.84092673	3.56400083	10.89952882
C	-0.71992761	5.65305066	12.76628648
C	3.97590492	5.13874218	12.61556708
C	4.36266162	6.47615502	12.25917125
C	3.63599037	7.37012224	13.12122329
C	2.86318220	6.58356139	14.06346733
C	3.06951936	5.20297665	13.74835156
C	2.53163064	4.02486813	14.50906555
C	2.07686044	7.12667088	15.22237893
C	3.77687554	8.86602271	13.14711461
C	5.38097360	6.86842771	11.22734471
C	4.53621562	3.87615234	12.02331308
C	0.14727588	8.62548393	11.89999926
H	1.74249279	3.04694413	10.54145715
H	0.62901485	3.20089697	11.91485754
H	0.00365986	3.24116844	10.25552605

H	-0.76329924	6.39840028	13.57270047
H	-0.52075545	4.67684582	13.22988015
H	-1.72471462	5.60212075	12.31050230
H	1.57040133	4.25525077	14.99044249
H	3.22698358	3.70868722	15.30697245
H	2.37652354	3.15482689	13.85524974
H	1.24902457	6.45943175	15.50225255
H	2.71264412	7.24847660	16.11737125
H	1.64746013	8.11310723	14.99656169
H	2.85461733	9.35868726	13.48550942
H	4.58239206	9.17320164	13.83687028
H	4.02592346	9.26624329	12.15479303
H	5.14890160	7.84451251	10.77871761
H	6.39278308	6.94028413	11.66552378
H	5.43070790	6.13667670	10.40879800
H	3.80963523	3.05206060	12.05301141
H	5.42912343	3.54296051	12.58062096
H	4.83786797	4.01887505	10.97663602
H	0.86858565	9.45099044	11.81842897
H	-0.11003847	8.51184105	12.96240622
H	-0.77024178	8.94158207	11.37271024
C	2.74546806	7.04484175	8.15831221
C	2.06181012	7.98964976	9.03329148
C	1.44256653	7.22162556	10.09197876
C	2.37470482	5.69874265	8.57868872
C	2.23350343	9.48389917	9.00613770
C	3.79435777	7.39484934	7.13938005
C	2.92715428	4.42241607	8.00566726
H	1.33193737	10.00095587	9.36420937
H	2.44541531	9.84700303	7.99080898
H	3.07077030	9.80673156	9.65014047
H	3.83772940	6.64949972	6.33296605
H	3.59518561	8.37105418	6.67578637
H	4.79914478	7.44577925	7.59516422
H	2.20584451	3.59690956	8.08723755
H	3.18446863	4.53605895	6.94326030
H	3.84467194	4.10631793	8.53295629
Co	0.81592525	6.85021672	7.82404159
C	-0.90147476	7.90915782	7.29009945
C	-1.28823146	6.57174498	7.64649528
C	-0.56156021	5.67777776	6.78444323
C	0.21124796	6.46433861	5.84219920
C	0.00491080	7.84492335	6.15731497
C	0.54279953	9.02303187	5.39660097
C	0.99756972	5.92122912	4.68328759
C	-0.70244538	4.18187729	6.75855191
C	-2.30654344	6.17947229	8.67832181
C	-1.46178546	9.17174766	7.88235344
H	1.50402883	8.79264923	4.91522403
H	-0.15255342	9.33921278	4.59869407
H	0.69790662	9.89307311	6.05041679
H	1.82540559	6.58846825	4.40341397
H	0.36178604	5.79942340	3.78829527
H	1.42697003	4.93479277	4.90910483
H	0.21981283	3.68921274	6.42015711
H	-1.50796190	3.87469836	6.06879625
H	-0.95149330	3.78165671	7.75087349
H	-2.07447144	5.20338749	9.12694891

H	-3.31835292	6.10761587	8.24014274
H	-2.35627774	6.91122330	9.49686852
H	-0.73520507	9.99583940	7.85265511
H	-2.35469326	9.50493949	7.32504557
H	-1.76343780	9.02902495	8.92903050

$Ni_2Pn^*Cp^*_2$ 3 S=0

84

C	-0.83023000	1.06696000	1.18645000
C	-1.28878000	1.78895000	0.00000000
C	-0.83023000	1.06696000	-1.18645000
C	0.00000000	0.00000000	-0.73947000
C	-1.01025000	1.54094000	2.60350000
C	-1.84674000	3.18691000	0.00000000
C	-1.01025000	1.54094000	-2.60350000
C	-3.90138000	-0.94157000	1.16762000
C	-4.48505000	0.29122000	0.72447000
C	-4.48505000	0.29122000	-0.72447000
C	-3.90138000	-0.94157000	-1.16762000
C	-3.51412000	-1.69215000	0.00000000
C	-3.78766000	-1.41458000	2.58990000
C	-5.12700000	1.33449000	1.59649000
C	-5.12700000	1.33449000	-1.59649000
C	-3.78766000	-1.41458000	-2.58990000
C	-2.94000000	-3.08157000	0.00000000
Ni	-2.43362000	0.18939000	0.00000000
H	-1.03671000	0.70003000	3.30970000
H	-0.18398000	2.20401000	2.91379000
H	-1.94449000	2.10628000	2.72560000
H	-2.46801000	3.37510000	0.88646000
H	-1.03742000	3.93830000	0.00000000
H	-2.46801000	3.37510000	-0.88646000
H	-1.03671000	0.70003000	-3.30970000
H	-0.18398000	2.20401000	-2.91379000
H	-1.94449000	2.10628000	-2.72560000
H	-5.05274000	2.33971000	1.15681000
H	-6.20176000	1.12776000	1.74574000
H	-4.66733000	1.37421000	2.59437000
H	-5.05274000	2.33971000	-1.15681000
H	-6.20176000	1.12776000	-1.74574000
H	-4.66733000	1.37421000	-2.59437000
H	-3.70660000	-0.57603000	-3.29624000
H	-4.67048000	-2.00658000	-2.89043000
H	-2.90600000	-2.05483000	-2.73512000
H	-2.31542000	-3.26394000	-0.88558000
H	-3.73765000	-3.84584000	0.00000000
H	-2.31542000	-3.26394000	0.88558000
H	-3.70660000	-0.57603000	3.29624000
H	-4.67048000	-2.00658000	2.89043000
H	-2.90600000	-2.05483000	2.73512000
C	0.83023000	-1.06696000	-1.18645000
C	1.28878000	-1.78895000	0.00000000
C	0.83023000	-1.06696000	1.18645000
C	0.00000000	0.00000000	0.73947000
C	1.01025000	-1.54094000	-2.60350000
C	1.84674000	-3.18691000	0.00000000

C	1.01025000	-1.54094000	2.60350000
H	1.03671000	-0.70003000	-3.30970000
H	0.18398000	-2.20401000	-2.91379000
H	1.94449000	-2.10628000	-2.72560000
H	2.46801000	-3.37510000	-0.88646000
H	1.03742000	-3.93830000	0.00000000
H	2.46801000	-3.37510000	0.88646000
H	1.03671000	-0.70003000	3.30970000
H	0.18398000	-2.20401000	2.91379000
H	1.94449000	-2.10628000	2.72560000
C	3.90138000	0.94157000	-1.16762000
C	4.48505000	-0.29122000	-0.72447000
C	4.48505000	-0.29122000	0.72447000
C	3.90138000	0.94157000	1.16762000
C	3.51412000	1.69215000	0.00000000
C	3.78766000	1.41458000	-2.58990000
C	5.12700000	-1.33449000	-1.59649000
C	5.12700000	-1.33449000	1.59649000
C	3.78766000	1.41458000	2.58990000
C	2.94000000	3.08157000	0.00000000
Ni	2.43362000	-0.18939000	0.00000000
H	5.05274000	-2.33971000	-1.15681000
H	6.20176000	-1.12776000	-1.74574000
H	4.66733000	-1.37421000	-2.59437000
H	5.05274000	-2.33971000	1.15681000
H	6.20176000	-1.12776000	1.74574000
H	4.66733000	-1.37421000	2.59437000
H	3.70660000	0.57603000	3.29624000
H	4.67048000	2.00658000	2.89043000
H	2.90600000	2.05483000	2.73512000
H	2.31542000	3.26394000	0.88558000
H	3.73765000	3.84584000	0.00000000
H	2.31542000	3.26394000	-0.88558000
H	3.70660000	0.57603000	-3.29624000
H	4.67048000	2.00658000	-2.89043000
H	2.90600000	2.05483000	-2.73512000

Ni_2Pn*Cp*$_2$ 3 S=1

84

C	-0.77543027	1.11717878	1.19191285
C	-1.22930179	1.82195532	0.00000000
C	-0.77543027	1.11717878	-1.19191285
C	0.00000000	0.00000000	-0.73594146
C	-0.93447024	1.59309694	2.60973824
C	-1.84443125	3.19527937	0.00000000
C	-0.93447024	1.59309694	-2.60973824
C	-3.78374333	-1.02422209	1.16628342
C	-4.41459898	0.18490685	0.72225111
C	-4.41459898	0.18490685	-0.72225111
C	-3.78374333	-1.02422209	-1.16628342
C	-3.37231335	-1.76484694	0.00000000
C	-3.64988488	-1.48385627	2.59137114
C	-5.07368641	1.21594106	1.59539511
C	-5.07368641	1.21594106	-1.59539511
C	-3.64988488	-1.48385627	-2.59137114
C	-2.75749081	-3.13618728	0.00000000

Ni	-2.33116184	0.13573049	0.00000000
H	-1.00450745	0.75144351	3.31328024
H	-0.08125301	2.21627921	2.93544208
H	-1.84186502	2.20134076	2.73393762
H	-2.47155363	3.35981085	0.88691123
H	-1.06425807	3.97598483	0.00000000
H	-2.47155363	3.35981085	-0.88691123
H	-1.00450745	0.75144351	-3.31328024
H	-0.08125301	2.21627921	-2.93544208
H	-1.84186502	2.20134076	-2.73393762
H	-5.03008670	2.21939833	1.14779327
H	-6.14084796	0.98260546	1.75818355
H	-4.60282699	1.27348178	2.58700272
H	-5.03008670	2.21939833	-1.14779327
H	-6.14084796	0.98260546	-1.75818355
H	-4.60282699	1.27348178	-2.58700272
H	-3.59191656	-0.63763933	-3.29043653
H	-4.51411391	-2.09895555	-2.89856314
H	-2.74910816	-2.09655806	-2.73774646
H	-2.12730553	-3.29856500	-0.88557675
H	-3.53191509	-3.92381093	0.00000000
H	-2.12730553	-3.29856500	0.88557675
H	-3.59191656	-0.63763933	3.29043653
H	-4.51411391	-2.09895555	2.89856314
H	-2.74910816	-2.09655806	2.73774646
C	0.77543027	-1.11717878	-1.19191285
C	1.22930179	-1.82195532	0.00000000
C	0.77543027	-1.11717878	1.19191285
C	0.00000000	0.00000000	0.73594146
C	0.93447024	-1.59309694	-2.60973824
C	1.84443125	-3.19527937	0.00000000
C	0.93447024	-1.59309694	2.60973824
H	1.00450745	-0.75144351	-3.31328024
H	0.08125301	-2.21627921	-2.93544208
H	1.84186502	-2.20134076	-2.73393762
H	2.47155363	-3.35981085	-0.88691123
H	1.06425807	-3.97598483	0.00000000
H	2.47155363	-3.35981085	0.88691123
H	1.00450745	-0.75144351	3.31328024
H	0.08125301	-2.21627921	2.93544208
H	1.84186502	-2.20134076	2.73393762
C	3.78374333	1.02422209	-1.16628342
C	4.41459898	-0.18490685	-0.72225111
C	4.41459898	-0.18490685	0.72225111
C	3.78374333	1.02422209	1.16628342
C	3.37231335	1.76484694	0.00000000
C	3.64988488	1.48385627	-2.59137114
C	5.07368641	-1.21594106	-1.59539511
C	5.07368641	-1.21594106	1.59539511
C	3.64988488	1.48385627	2.59137114
C	2.75749081	3.13618728	0.00000000
Ni	2.33116184	-0.13573049	0.00000000
H	5.03008670	-2.21939833	-1.14779327
H	6.14084796	-0.98260546	-1.75818355
H	4.60282699	-1.27348178	-2.58700272
H	5.03008670	-2.21939833	1.14779327
H	6.14084796	-0.98260546	1.75818355
H	4.60282699	-1.27348178	2.58700272

H	3.59191656	0.63763933	3.29043653
H	4.51411391	2.09895555	2.89856314
H	2.74910816	2.09655806	2.73774646
H	2.12730553	3.29856500	0.88557675
H	3.53191509	3.92381093	0.00000000
H	2.12730553	3.29856500	-0.88557675
H	3.59191656	0.63763933	-3.29043653
H	4.51411391	2.09895555	-2.89856314
H	2.74910816	2.09655806	-2.73774646

$Fe_2Pn^*Cp_2$ 54

Fe	-2.00838723	-0.00965556	0.00000000
Fe	2.00838723	0.00965556	0.00000000
C	-0.80068574	1.12527033	-1.18929217
C	-1.20266730	1.85659950	0.00000000
C	-0.80068574	1.12527033	1.18929217
C	0.80068574	-1.12527033	1.18929217
C	1.20266730	-1.85659950	0.00000000
C	0.80068574	-1.12527033	-1.18929217
C	0.00000000	0.00000000	0.74221325
C	0.00000000	0.00000000	-0.74221325
C	-0.99248086	1.56744667	-2.61223395
C	-1.91414428	3.18139502	0.00000000
C	-0.99248086	1.56744667	2.61223395
C	0.99248086	-1.56744667	2.61223395
C	1.91414428	-3.18139502	0.00000000
C	0.99248086	-1.56744667	-2.61223395
C	-3.64826150	-0.52249726	-1.16217336
C	-4.05898078	0.21545478	0.00000000
C	-3.64826150	-0.52249726	1.16217336
C	-2.97539892	-1.70491777	0.71988437
C	-2.97539892	-1.70491777	-0.71988437
C	3.64826150	0.52249726	1.16217336
C	4.05898078	-0.21545478	0.00000000
C	3.64826150	0.52249726	-1.16217336
C	2.97539892	1.70491777	-0.71988437
C	2.97539892	1.70491777	0.71988437
H	-1.07643184	0.70586175	-3.28901748
H	-1.90205831	2.17280093	-2.73040349
H	-0.14140235	2.17928654	-2.95982879
H	-2.55296945	3.29824099	0.88630700
H	-2.55296945	3.29824099	-0.88630700
H	-1.19541199	4.01921780	0.00000000
H	-1.07643184	0.70586175	3.28901748
H	-1.90205831	2.17280093	2.73040349
H	-0.14140235	2.17928654	2.95982879
H	1.07643184	-0.70586175	3.28901748
H	0.14140235	-2.17928654	2.95982879
H	1.90205831	-2.17280093	2.73040349
H	2.55296945	-3.29824099	-0.88630700
H	1.19541199	-4.01921780	0.00000000
H	2.55296945	-3.29824099	0.88630700
H	1.07643184	-0.70586175	-3.28901748
H	0.14140235	-2.17928654	-2.95982879
H	1.90205831	-2.17280093	-2.73040349
H	-3.80699943	-0.22526826	-2.19631004
H	-4.58809818	1.16593352	0.00000000

H	-3.80699943	-0.22526826	2.19631004
H	-2.53047279	-2.46520840	1.35757971
H	-2.53047279	-2.46520840	-1.35757971
H	3.80699943	0.22526826	2.19631004
H	4.58809818	-1.16593352	0.00000000
H	3.80699943	0.22526826	-2.19631004
H	2.53047279	2.46520840	-1.35757971
H	2.53047279	2.46520840	1.35757971

$Co_2Pn^*Cp_2$ 4

54

Co	-2.23950352	0.04380602	0.00000000
Co	2.23950352	-0.04380602	0.00000000
C	-0.87835004	1.05448387	-1.17775890
C	-1.32562674	1.78651565	0.00000000
C	-0.87835004	1.05448387	1.17775890
C	0.87835004	-1.05448387	1.17775890
C	1.32562674	-1.78651565	0.00000000
C	0.87835004	-1.05448387	-1.17775890
C	-0.00000000	0.00000000	0.71725772
C	-0.00000000	0.00000000	-0.71725772
C	-1.05347846	1.49715529	-2.60391300
C	-1.98703150	3.13681688	0.00000000
C	-1.05347846	1.49715529	2.60391300
C	1.05347846	-1.49715529	2.60391300
C	1.98703150	-3.13681688	0.00000000
C	1.05347846	-1.49715529	-2.60391300
C	-3.89886680	-0.51940773	-1.15181076
C	-4.37931759	0.17567507	0.00000000
C	-3.89886680	-0.51940773	1.15181076
C	-3.17870602	-1.69136347	0.71188494
C	-3.17870602	-1.69136347	-0.71188494
C	3.89886680	0.51940773	1.15181076
C	4.37931759	-0.17567507	0.00000000
C	3.89886680	0.51940773	-1.15181076
C	3.17870602	1.69136347	-0.71188494
C	3.17870602	1.69136347	0.71188494
H	-1.10671594	0.63914639	-3.28823643
H	-1.97310501	2.08391845	-2.73401447
H	-0.20884001	2.12861730	-2.93173199
H	-2.62200708	3.27362436	0.88592230
H	-2.62200708	3.27362436	-0.88592230
H	-1.23904008	3.94925050	0.00000000
H	-1.10671594	0.63914639	3.28823643
H	-1.97310501	2.08391845	2.73401447
H	-0.20884001	2.12861730	2.93173199
H	1.10671594	-0.63914639	3.28823643
H	0.20884001	-2.12861730	2.93173199
H	1.97310501	-2.08391845	2.73401447
H	2.62200708	-3.27362436	-0.88592230
H	1.23904008	-3.94925050	0.00000000
H	2.62200708	-3.27362436	0.88592230
H	1.10671594	-0.63914639	-3.28823643
H	0.20884001	-2.12861730	-2.93173199
H	1.97310501	-2.08391845	-2.73401447
H	-4.06897255	-0.23230403	-2.18701338

H	-4.96274109	1.09288751	0.00000000
H	-4.06897255	-0.23230403	2.18701338
H	-2.71756780	-2.43616099	1.35548420
H	-2.71756780	-2.43616099	-1.35548420
H	4.06897255	0.23230403	2.18701338
H	4.96274109	-1.09288751	0.00000000
H	4.06897255	0.23230403	-2.18701338
H	2.71756780	2.43616099	-1.35548420
H	2.71756780	2.43616099	1.35548420

$Ni_2Pn^*Cp_2$ 5 S=0

54

Ni	2.42098389	-0.00068369	-0.00000000
Ni	-2.42098389	0.00068369	-0.00000000
C	0.90125225	-1.00537163	-1.18731735
C	1.41011304	-1.68978996	-0.00000000
C	0.90125225	-1.00537163	1.18731735
C	-0.90125225	1.00537163	1.18731735
C	-1.41011304	1.68978996	-0.00000000
C	-0.90125225	1.00537163	-1.18731735
C	-0.00000000	0.00000000	0.73958646
C	-0.00000000	0.00000000	-0.73958646
C	1.10883728	-1.46521289	-2.60429062
C	2.07760205	-3.03835463	-0.00000000
C	1.10883728	-1.46521289	2.60429062
C	-1.10883728	1.46521289	2.60429062
C	-2.07760205	3.03835463	-0.00000000
C	-1.10883728	1.46521289	-2.60429062
C	4.21087264	0.56020718	-1.16104596
C	4.60411436	-0.18071804	-0.00000000
C	4.21087264	0.56020718	1.16104596
C	3.53188024	1.73408397	0.71806901
C	3.53188024	1.73408397	-0.71806901
C	-4.21087264	-0.56020718	1.16104596
C	-4.60411436	0.18071804	-0.00000000
C	-4.21087264	-0.56020718	-1.16104596
C	-3.53188024	-1.73408397	-0.71806901
C	-3.53188024	-1.73408397	0.71806901
H	1.07819060	-0.62380538	-3.30902327
H	2.07698537	-1.96859532	-2.72951540
H	0.32300587	-2.17909560	-2.90734036
H	2.71096672	-3.17662951	0.88639952
H	2.71096672	-3.17662951	-0.88639952
H	1.32564530	-3.84700283	-0.00000000
H	1.07819060	-0.62380538	3.30902327
H	2.07698537	-1.96859532	2.72951540
H	0.32300587	-2.17909560	2.90734036
H	-1.07819060	0.62380538	3.30902327
H	-0.32300587	2.17909560	2.90734036
H	-2.07698537	1.96859532	2.72951540
H	-2.71096672	3.17662951	-0.88639952
H	-1.32564530	3.84700283	-0.00000000
H	-2.71096672	3.17662951	0.88639952
H	-1.07819060	0.62380538	-3.30902327
H	-0.32300587	2.17909560	-2.90734036

H	-2.07698537	1.96859532	-2.72951540
H	4.38906519	0.27287517	-2.19418651
H	5.14867399	-1.12216698	-0.00000000
H	4.38906519	0.27287517	2.19418651
H	3.10730295	2.50743711	1.35327899
H	3.10730295	2.50743711	-1.35327899
H	-4.38906519	-0.27287517	2.19418651
H	-5.14867399	1.12216698	-0.00000000
H	-4.38906519	-0.27287517	-2.19418651
H	-3.10730295	-2.50743711	-1.35327899
H	-3.10730295	-2.50743711	1.35327899

$Ni_2Pn^*Cp_2$ 5 S=1

54

Ni	2.43301879	-0.02344785	-0.00000000
Ni	-2.43301879	0.02344785	-0.00000000
C	0.91889025	-1.01262585	-1.17496647
C	1.39463510	-1.72918616	-0.00000000
C	0.91889025	-1.01262585	1.17496647
C	-0.91889025	1.01262585	1.17496647
C	-1.39463510	1.72918616	-0.00000000
C	-0.91889025	1.01262585	-1.17496647
C	0.00000000	-0.00000000	0.71843988
C	0.00000000	-0.00000000	-0.71843988
C	1.11547222	-1.45686932	-2.59827802
C	2.08057983	-3.06874352	-0.00000000
C	1.11547222	-1.45686932	2.59827802
C	-1.11547222	1.45686932	2.59827802
C	-2.08057983	3.06874352	-0.00000000
C	-1.11547222	1.45686932	-2.59827802
C	4.22311230	0.56094372	-1.15021156
C	4.70346382	-0.12936521	-0.00000000
C	4.22311230	0.56094372	1.15021156
C	3.48875977	1.71932434	0.71148579
C	3.48875977	1.71932434	-0.71148579
C	-4.22311230	-0.56094372	1.15021156
C	-4.70346382	0.12936521	-0.00000000
C	-4.22311230	-0.56094372	-1.15021156
C	-3.48875977	-1.71932434	-0.71148579
C	-3.48875977	-1.71932434	0.71148579
H	1.14403471	-0.60280151	-3.28811349
H	2.05003992	-2.01994889	-2.72282928
H	0.28829037	-2.11288199	-2.92159416
H	2.71946347	-3.19670916	0.88454862
H	2.71946347	-3.19670916	-0.88454862
H	1.34721218	-3.89459957	-0.00000000
H	1.14403471	-0.60280151	3.28811349
H	2.05003992	-2.01994889	2.72282928
H	0.28829037	-2.11288199	2.92159416
H	-1.14403471	0.60280151	3.28811349
H	-0.28829037	2.11288199	2.92159416
H	-2.05003992	2.01994889	2.72282928
H	-2.71946347	3.19670916	-0.88454862
H	-1.34721218	3.89459957	-0.00000000
H	-2.71946347	3.19670916	0.88454862
H	-1.14403471	0.60280151	-3.28811349

H	-0.28829037	2.11288199	-2.92159416
H	-2.05003992	2.01994889	-2.72282928
H	4.40471697	0.28118465	-2.18533797
H	5.29172987	-1.04344815	-0.00000000
H	4.40471697	0.28118465	2.18533797
H	3.03260095	2.46781547	1.35420569
H	3.03260095	2.46781547	-1.35420569
H	-4.40471697	-0.28118465	2.18533797
H	-5.29172987	1.04344815	-0.00000000
H	-4.40471697	-0.28118465	-2.18533797
H	-3.03260095	-2.46781547	-1.35420569
H	-3.03260095	-2.46781547	1.35420569

7. References

1. S. H. Bertz, J. M. Cook, A. Gawish, U. Weiss, T. K. Jones, S. E. Denmark, S. V Govindan, and R. M. Coates, *Org. Synth.*, 1986, **64**, 27.
2. K. Jonas, P. Klusmann, and R. Goddard, *Z. Naturforsch., B: Chem. Sci.*, 1995, **50**, 394.
3. J. M. Manriquez, E. E. Bunel, B. Oelckers, C. Vasquez, and J. S. Miller, in *Inorganic Syntheses*, ed. A. H. Cowley, John Wiley & Sons, Inc., 1997, vol. 31, p. 215.
4. E. E. Bunel, L. Valle, and J. M. Manriquez, *Organometallics*, 1985, **4**, 1680.
5. J. Cosier and A. M. Glazer, *J. Appl. Cryst.*, 1986, **19**, 105.
6. Z. Otwinowski and W. Minor, in *Methods in Enzymol.*, eds. C. W. Carter and R. M. Sweet, Academic Press, 1997, p. 276.
7. *CrysAlis PRO*, Oxford Diffraction /Agilent Technologies UK Ltd, Yarnton, England.
8. A. Altomare, G. Cascarano, C. Giacovazzo, A. Guagliardi, M. C. Burla, G. Polidori, and M. Camalli, *J. Appl. Cryst.*, 1994, **27**, 435.
9. L. Palatinus and G. Chapuis, *J. Appl. Cryst.*, 2007, **40**, 786.
10. P. W. Betteridge, J. R. Carruthers, R. I. Cooper, K. Prout, and D. J. Watkin, *J. Appl. Cryst.*, 2003, **36**, 1487.
11. R. I. Cooper, A. L. Thompson, and D. J. Watkin, *J. Appl. Cryst.*, 2010, **43**, 1100.
12. J. R. Carruthers and D. J. Watkin, *Acta Crystallogr. Sect. A*, 1979, **35**, 698.
13. A. L. Spek, *J. Appl. Cryst.*, 2003, **36**, 7.
14. A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098.
15. J. P. Perdew and W. Yue, *Phys. Rev. B*, 1986, **33**, 8800.
16. S. H. Vosko, L. Wilk, and M. Nusair, *Can. J. Phys.*, 1980, **58**, 1200.
17. C. Lee, W. Yang, and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785.
18. B. Miehlich, A. Savin, H. Stoll, and H. Preuss, *Chem. Phys. Lett.*, 1989, **157**, 200.
19. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2007, **120**, 215.
20. R. A. Kendall, T. H. Dunning, and R. J. Harrison, *J. Chem. Phys.*, 1992, **96**, 6796.
21 E. E. Bunel, L. Valle, N. L. Jones, P. J. Carroll, C. Barra, M. Gonzalez, N. Munoz, G. Visconti, A. Aizman and J. M. Manriquez, *J. Am. Chem. Soc.*, 1988, **110**, 6596.
22 J. M. Manriquez, M. D. Ward, W. M. Reiff, J. C. Calabrese, N. L. Jones, P. J. Carroll, E. E. Bunel and J. S. Miller, *J. Am. Chem. Soc.*, 1995, **117**, 6182.
23 C. Miravitlles, E. Molins, W. Maniukiewicz, M. Mas, J. M. Manríquez, I. Chávez, B. Oelckers, A. Alvarez-Larena and J. L. Briansó, *Acta Crystallogr. Sect. C Cryst. Struct. Commun.*, 1996, **52**, 3047.
24 Y. Kitano, M. Kashiwagi and Y. Kinoshita, *Bull. Chem. Soc. Jpn.*, 1973, **46**, 723.
25 H. M. McConnell and D. B. Chesnut, *J. Chem. Phys.*, 1958, **28**, 107.
26 P. Hrobárik, R. Reviakine, A. V. Arbuznikov, O. L. Malkina, V. G. Malkin, F. H. Köhler and M. Kaupp, *J. Chem. Phys.*, 2007, **126**, 024107.