Supplementary Material (ESI) for Chemical Communications

Monomeric, two-coordinate Mn, Fe and Co(II) complexes featuring 2,6-(2,4,6-trimethylphenyl)phenyl ligands

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Supporting information (16 pages)

Synthetic, Spectroscopic and Crystallographic Data for 1, 2 and 3

Supporting information

Preparative, spectroscopic and crystallographic data for 1

*Synthesis of (2,6-$Mes_2C_6H_3)_2Mn$ (**1**)*
A solution of [2,6-$Mes_2C_6H_3Li]_2$ (0.250 g, 0.37 mmol) in toluene (10 cm^3) was added dropwise to a suspension of $MnCl_2$ (0.046 g, 0.37 mmol) in a mixture of toluene (10 cm^3) and THF (2 cm^3) at –78 °C and the resulting mixture warmed slowly to room temperature and stirred overnight. The solution was filtered and volatiles were removed *in vacuo*. The resultant solid was extracted into hexanes (15 cm^3) and cooled to –35 °C for several days, whereupon colourless crystals of **1** suitable for X-ray diffraction were formed (0.157 g, 62%). Mp: 240–250 °C (from hexane, melts and turns black). ^{1}H NMR (300 MHz, C_6D_6, Me_4Si) δ 10.5 (s, br, obscured by benzene peak), 16.9 (s, br, $\Delta\nu_{½}$ = 904 Hz), 27.4 (s, v br, $\Delta\nu_{½}$ = 2000 Hz). μ_{eff} = 5.894(4) μ_B. UV/vis (hexane): strong absorption between 200 and 400 nm ($\varepsilon > 1 \times 10^5$ dm^3 mol^{-1} cm^{-1}). EI-MS: M^+ = 681 (10%), fragment ion peaks at *m/z* 368 [(2,6-$Mes_2C_6H_3Mn)^+$, 25], 313 [(2,6-$Mes_2C_6H_3)^+$, 20], 298 [(2,6-$Mes_2C_6H_3$ – Me)$^+$, 20], 283 [(2,6-$Mes_2C_6H_3$ – 2Me)$^+$, 20], 268 [(2,6-$Mes_2C_6H_3$ – 3Me)$^+$, 15], 253 [(2,6-$Mes_2C_6H_3$ – 4Me)$^+$, 10]; exact mass: calcd for 681.3288 measd 681.3283.

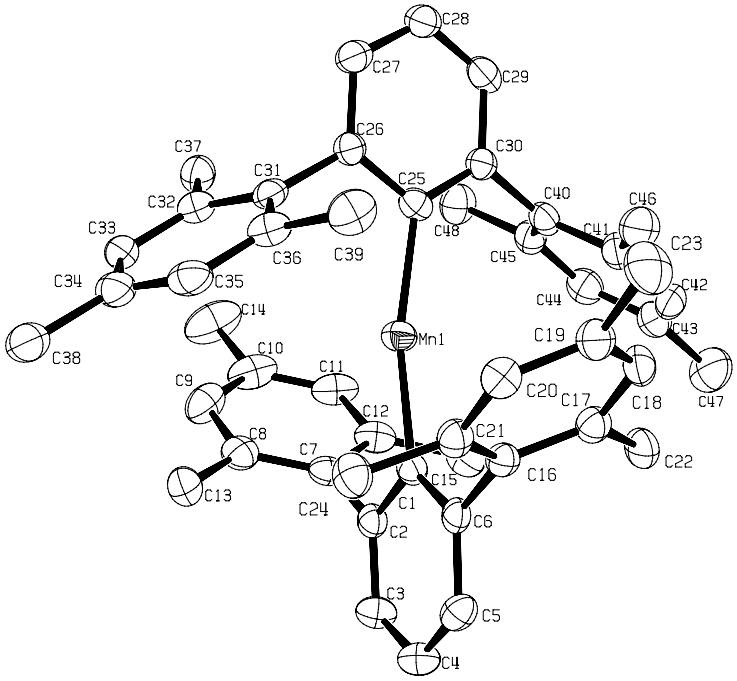

Figure S1. Thermal ellipsoid plot at 40% probability of one of the two crystallographically-distinct molecules of **1**. Hydrogen atoms have been omitted.

Crystals of **1** were grown by controlled cooling of a saturated hexane solution to –35 °C. A single crystal having dimensions approximately 0.03 x 0.28 x 0.30 mm was mounted on a glass fibre using perfluoropolyether oil and cooled rapidly to 150K in a stream of cold N_2 using an Oxford Cryosystems CRYOSTREAM unit. Diffraction data were measured using an Enraf-Nonius KappaCCD diffractometer (graphite-monochromated MoK_α radiation, λ = 0.71073 Å). Intensity data were processed using the DENZO-SMN package[1].

Examination of the systematic absences of the intensity data showed the space group to be *P* $2_1/c$. The structure was solved using the direct-methods program SIR92[2], which located all non-hydrogen atoms. Subsequent full-matrix least-squares

refinement was carried out using the CRYSTALS program suite[3]. Coordinates and anisotropic thermal parameters of all non-hydrogen atoms were refined. Hydrogen atoms were positioned geometrically after each cycle of refinement. A 3-term Chebychev polynomial weighting scheme was applied. Refinement converged satisfactorily to give R = 0.0575, wR = 0.0641.

A summary of crystallographic data is given below, as are full lists of atomic coordinates, anisotropic thermal parameters and those bond lengths and angles not concerning H atoms.

The asymmetric unit contains two crystallographically-distinct molecules, neither of which have any crystallographic symmetry. The geometries of these are similar but differ slightly in the orientation of the mesityl groups. Both are significantly distorted from the idealised $\bar{4}2m$ (D_{2d}) point symmetry, as shown by the C-Mn-C and Mn-C-C angles listed in Table S6 below.

Table S1.: Crystal data and refinement details for **1**

Crystal identification	**1**
Chemical formula	$C_{48}H_{50}Mn$
Formula weight	681.85
Temperature (K)	150
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	$P\,2_1/c$
a (Å)	10.5378(2)
b (Å)	38.4153(7)
c (Å)	19.0976(4)
α (°)	90
β (°)	91.6501(8)
γ (°)	90
Cell volume (Å^3)	7727.7(3)
Z	8
Calculated density (Mg/m^3)	1.172
Absorption coefficient (mm^{-1})	0.373
F_{000}	2904
Crystal size (mm)	0.03 x 0.28 x 0.30
Description of crystal	Colourless plate
Absorption correction	Semi-empirical from equivalent reflections
Transmission coefficients (min,max)	0.89, 0.99
θ range for data collection (°)	$5.0 \le \theta \le 27.5$
Index ranges	$-13 \le h \le 13$, $0 \le k \le 49$, $0 \le l \le 24$
Reflections measured	53601
Unique reflections	15914
R_{int}	0.066
Observed reflections (I > 2σ(I))	8184
Refinement method	Full-matrix least-squares on F
Parameters refined	883
Weighting scheme	Chebychev 3-term polynomial

Goodness of fit	1.1057
R	0.0575
wR	0.0641
Residual electron density (min,max) ($eÅ^{-3}$)	-0.28, 0.39

Table S2. Bond lengths (Å) for **1**.

Mn(1) - C(1)	2.098(3)	Mn(2) - C(49)	2.092(3)
Mn(1) - C(25)	2.093(3)	Mn(2) - C(73)	2.096(3)
C(1) - C(2)	1.410(5)	C(49) - C(50)	1.406(5)
C(1) - C(6)	1.410(5)	C(49) - C(54)	1.414(5)
C(2) - C(3)	1.394(5)	C(50) - C(51)	1.404(5)
C(2) - C(7)	1.499(5)	C(50) - C(55)	1.493(5)
C(3) - C(4)	1.384(5)	C(51) - C(52)	1.380(6)
C(4) - C(5)	1.381(5)	C(52) - C(53)	1.379(6)
C(5) - C(6)	1.403(5)	C(53) - C(54)	1.388(5)
C(6) - C(16)	1.502(5)	C(54) - C(64)	1.499(5)
C(7) - C(8)	1.397(6)	C(55) - C(56)	1.407(5)
C(7) - C(12)	1.419(5)	C(55) - C(60)	1.408(5)
C(8) - C(9)	1.393(6)	C(56) - C(57)	1.392(5)
C(8) - C(13)	1.496(6)	C(56) - C(61)	1.519(5)
C(9) - C(10)	1.388(7)	C(57) - C(58)	1.387(6)
C(10) - C(11)	1.386(6)	C(58) - C(59)	1.382(6)
C(10) - C(14)	1.518(6)	C(58) - C(62)	1.513(6)
C(11) - C(12)	1.394(5)	C(59) - C(60)	1.391(6)
C(12) - C(15)	1.505(6)	C(60) - C(63)	1.506(6)
C(16) - C(17)	1.402(5)	C(64) - C(65)	1.404(5)
C(16) - C(21)	1.398(5)	C(64) - C(69)	1.403(5)
C(17) - C(18)	1.399(5)	C(65) - C(66)	1.388(5)
C(17) - C(22)	1.509(5)	C(65) - C(70)	1.506(5)
C(18) - C(19)	1.389(5)	C(66) - C(67)	1.384(5)
C(19) - C(20)	1.391(5)	C(67) - C(68)	1.388(5)
C(19) - C(23)	1.508(5)	C(67) - C(71)	1.508(5)
C(20) - C(21)	1.394(5)	C(68) - C(69)	1.393(5)
C(21) - C(24)	1.511(5)	C(69) - C(72)	1.516(5)
C(25) - C(26)	1.418(5)	C(73) - C(74)	1.402(5)
C(25) - C(30)	1.408(5)	C(73) - C(78)	1.407(5)
C(26) - C(27)	1.402(5)	C(74) - C(75)	1.399(5)
C(26) - C(31)	1.495(5)	C(74) - C(79)	1.496(5)
C(27) - C(28)	1.382(6)	C(75) - C(76)	1.389(5)
C(28) - C(29)	1.381(6)	C(76) - C(77)	1.380(5)
C(29) - C(30)	1.401(5)	C(77) - C(78)	1.392(5)
C(30) - C(40)	1.501(5)	C(78) - C(88)	1.500(5)
C(31) - C(32)	1.408(5)	C(79) - C(80)	1.415(5)
C(31) - C(36)	1.412(5)	C(79) - C(84)	1.396(5)
C(32) - C(33)	1.388(5)	C(80) - C(81)	1.396(5)
C(32) - C(37)	1.507(5)	C(80) - C(85)	1.504(5)
C(33) - C(34)	1.389(6)	C(81) - C(82)	1.382(5)

C(34) - C(35)	1.376(6)	C(82) - C(83)	1.385(5)
C(34) - C(38)	1.526(6)	C(82) - C(86)	1.513(5)
C(35) - C(36)	1.402(6)	C(83) - C(84)	1.390(5)
C(36) - C(39)	1.512(6)	C(84) - C(87)	1.518(5)
C(40) - C(41)	1.402(5)	C(88) - C(89)	1.411(5)
C(40) - C(45)	1.401(5)	C(88) - C(93)	1.389(5)
C(41) - C(42)	1.387(6)	C(89) - C(90)	1.400(5)
C(41) - C(46)	1.518(6)	C(89) - C(94)	1.505(6)
C(42) - C(43)	1.378(6)	C(90) - C(91)	1.385(6)
C(43) - C(44)	1.392(6)	C(91) - C(92)	1.385(5)
C(43) - C(47)	1.516(6)	C(91) - C(95)	1.512(6)
C(44) - C(45)	1.395(6)	C(92) - C(93)	1.391(5)
C(45) - C(48)	1.514(5)	C(93) - C(96)	1.523(5)

Note – H atoms have been excluded

Table S3. Bond angles (°) for **1**.

C(1) - Mn(1) - C(25)	166.41(13)	C(49) - Mn(2) - C(73)	173.00(13)
Mn(1) - C(1) - C(2)	108.1(2)	Mn(2) - C(49) - C(50)	109.3(2)
Mn(1) - C(1) - C(6)	134.9(3)	Mn(2) - C(49) - C(54)	133.5(3)
C(2) - C(1) - C(6)	116.8(3)	C(50) - C(49) - C(54)	117.1(3)
C(1) - C(2) - C(3)	122.2(3)	C(49) - C(50) - C(51)	121.5(3)
C(1) - C(2) - C(7)	115.0(3)	C(49) - C(50) - C(55)	116.4(3)
C(3) - C(2) - C(7)	122.7(3)	C(51) - C(50) - C(55)	122.1(3)
C(2) - C(3) - C(4)	119.4(3)	C(50) - C(51) - C(52)	119.7(3)
C(3) - C(4) - C(5)	120.1(3)	C(51) - C(52) - C(53)	119.8(3)
C(4) - C(5) - C(6)	120.7(3)	C(52) - C(53) - C(54)	121.2(4)
C(1) - C(6) - C(5)	120.7(3)	C(49) - C(54) - C(53)	120.7(3)
C(1) - C(6) - C(16)	118.8(3)	C(49) - C(54) - C(64)	119.9(3)
C(5) - C(6) - C(16)	120.6(3)	C(53) - C(54) - C(64)	119.4(3)
C(2) - C(7) - C(8)	119.8(3)	C(50) - C(55) - C(56)	120.5(3)
C(2) - C(7) - C(12)	119.3(3)	C(50) - C(55) - C(60)	120.3(3)
C(8) - C(7) - C(12)	120.6(3)	C(56) - C(55) - C(60)	119.2(3)
C(7) - C(8) - C(9)	118.5(4)	C(55) - C(56) - C(57)	119.4(3)
C(7) - C(8) - C(13)	120.6(3)	C(55) - C(56) - C(61)	119.7(3)
C(9) - C(8) - C(13)	120.9(4)	C(57) - C(56) - C(61)	120.9(3)
C(8) - C(9) - C(10)	122.2(4)	C(56) - C(57) - C(58)	121.9(4)
C(9) - C(10) - C(11)	118.4(4)	C(57) - C(58) - C(59)	117.9(4)
C(9) - C(10) - C(14)	120.0(5)	C(57) - C(58) - C(62)	120.7(4)
C(11) - C(10) - C(14)	121.6(5)	C(59) - C(58) - C(62)	121.4(4)
C(10) - C(11) - C(12)	122.0(4)	C(58) - C(59) - C(60)	122.4(4)
C(7) - C(12) - C(11)	118.2(4)	C(55) - C(60) - C(59)	119.0(4)
C(7) - C(12) - C(15)	120.8(3)	C(55) - C(60) - C(63)	120.7(3)
C(11) - C(12) - C(15)	120.9(4)	C(59) - C(60) - C(63)	120.3(3)
C(6) - C(16) - C(17)	119.4(3)	C(54) - C(64) - C(65)	120.2(3)
C(6) - C(16) - C(21)	121.0(3)	C(54) - C(64) - C(69)	120.0(3)
C(17) - C(16) - C(21)	119.6(3)	C(65) - C(64) - C(69)	119.7(3)
C(16) - C(17) - C(18)	119.5(3)	C(64) - C(65) - C(66)	118.9(3)
C(16) - C(17) - C(22)	121.1(3)	C(64) - C(65) - C(70)	120.4(3)
C(18) - C(17) - C(22)	119.4(3)	C(66) - C(65) - C(70)	120.7(3)
C(17) - C(18) - C(19)	121.4(3)	C(65) - C(66) - C(67)	122.5(3)
C(18) - C(19) - C(20)	118.4(3)	C(66) - C(67) - C(68)	117.8(3)
C(18) - C(19) - C(23)	121.1(4)	C(66) - C(67) - C(71)	121.4(3)

C(20) - C(19) - C(23)	120.5(4)	C(68) - C(67) - C(71)	120.7(3)
C(19) - C(20) - C(21)	121.4(3)	C(67) - C(68) - C(69)	121.9(3)
C(16) - C(21) - C(20)	119.7(3)	C(64) - C(69) - C(68)	119.2(3)
C(16) - C(21) - C(24)	120.6(3)	C(64) - C(69) - C(72)	120.5(3)
C(20) - C(21) - C(24)	119.7(3)	C(68) - C(69) - C(72)	120.3(3)
Mn(1) - C(25) - C(26)	112.2(2)	Mn(2) - C(73) - C(74)	113.7(2)
Mn(1) - C(25) - C(30)	130.8(3)	Mn(2) - C(73) - C(78)	128.6(3)
C(26) - C(25) - C(30)	116.9(3)	C(74) - C(73) - C(78)	117.6(3)
C(25) - C(26) - C(27)	121.6(3)	C(73) - C(74) - C(75)	121.6(3)
C(25) - C(26) - C(31)	116.5(3)	C(73) - C(74) - C(79)	118.0(3)
C(27) - C(26) - C(31)	121.8(3)	C(75) - C(74) - C(79)	120.3(3)
C(26) - C(27) - C(28)	119.7(3)	C(74) - C(75) - C(76)	119.6(3)
C(27) - C(28) - C(29)	120.1(3)	C(75) - C(76) - C(77)	119.6(3)
C(28) - C(29) - C(30)	120.7(3)	C(76) - C(77) - C(78)	121.2(3)
C(25) - C(30) - C(29)	120.9(3)	C(73) - C(78) - C(77)	120.4(3)
C(25) - C(30) - C(40)	118.6(3)	C(73) - C(78) - C(88)	119.7(3)
C(29) - C(30) - C(40)	120.5(3)	C(77) - C(78) - C(88)	119.9(3)
C(26) - C(31) - C(32)	119.0(3)	C(74) - C(79) - C(80)	119.7(3)
C(26) - C(31) - C(36)	121.7(3)	C(74) - C(79) - C(84)	120.1(3)
C(32) - C(31) - C(36)	119.2(3)	C(80) - C(79) - C(84)	120.1(3)
C(31) - C(32) - C(33)	119.8(3)	C(79) - C(80) - C(81)	118.3(3)
C(31) - C(32) - C(37)	120.5(3)	C(79) - C(80) - C(85)	121.3(3)
C(33) - C(32) - C(37)	119.7(4)	C(81) - C(80) - C(85)	120.4(3)
C(32) - C(33) - C(34)	121.4(4)	C(80) - C(81) - C(82)	122.3(3)
C(33) - C(34) - C(35)	118.8(4)	C(81) - C(82) - C(83)	118.2(3)
C(33) - C(34) - C(38)	119.7(4)	C(81) - C(82) - C(86)	121.5(3)
C(35) - C(34) - C(38)	121.5(4)	C(83) - C(82) - C(86)	120.4(4)
C(34) - C(35) - C(36)	121.8(4)	C(82) - C(83) - C(84)	122.1(3)
C(31) - C(36) - C(35)	119.0(4)	C(79) - C(84) - C(83)	119.0(3)
C(31) - C(36) - C(39)	120.4(4)	C(79) - C(84) - C(87)	121.1(3)
C(35) - C(36) - C(39)	120.5(4)	C(83) - C(84) - C(87)	119.9(3)
C(30) - C(40) - C(41)	120.8(3)	C(78) - C(88) - C(89)	119.1(3)
C(30) - C(40) - C(45)	119.4(3)	C(78) - C(88) - C(93)	121.3(3)
C(41) - C(40) - C(45)	119.8(4)	C(89) - C(88) - C(93)	119.6(3)
C(40) - C(41) - C(42)	118.9(4)	C(88) - C(89) - C(90)	118.9(3)
C(40) - C(41) - C(46)	120.2(4)	C(88) - C(89) - C(94)	121.2(3)
C(42) - C(41) - C(46)	120.9(3)	C(90) - C(89) - C(94)	119.9(3)
C(41) - C(42) - C(43)	122.7(4)	C(89) - C(90) - C(91)	121.8(3)
C(42) - C(43) - C(44)	117.6(4)	C(90) - C(91) - C(92)	118.2(3)
C(42) - C(43) - C(47)	122.0(4)	C(90) - C(91) - C(95)	120.8(4)
C(44) - C(43) - C(47)	120.4(4)	C(92) - C(91) - C(95)	121.0(4)
C(43) - C(44) - C(45)	121.9(4)	C(91) - C(92) - C(93)	121.8(3)
C(40) - C(45) - C(44)	119.0(3)	C(88) - C(93) - C(92)	119.8(3)
C(40) - C(45) - C(48)	121.1(3)	C(88) - C(93) - C(96)	120.8(3)
C(44) - C(45) - C(48)	119.9(4)	C(92) - C(93) - C(96)	119.4(3)

Note – H atoms have been excluded

Preparative, spectroscopic and crystallographic data for 2

*Synthesis of (2,6-$Mes_2C_6H_3)_2Fe$ (**2**)*

A solution of [2,6-$Mes_2C_6H_3Li]_2$ (0.300 g, 0.49 mmol) in toluene (10 cm^3) was added dropwise to a suspension of $FeCl_2(THF)_{1.5}$ (0.108 g, 0.49 mmol) in a mixture of toluene (10 cm^3) and THF (2 cm^3) at –78 °C and the resulting mixture warmed slowly to room temperature and stirred overnight. The solution was filtered and volatiles removed *in vacuo*. The resultant solid was extracted into hexanes (15 cm^3) and cooled

to –35 °C for several days, whereupon yellow-green crystals of **2** suitable for X-ray diffraction were formed (0.184 g, 56%). Mp: 200–210°C (from hexane, melts and turns black, darkens at 140 °C). ^{1}H NMR (300 MHz, C_6D_6, Me_4Si) δ –56.2 (s, br, $\Delta\nu_{½}$ = 205 Hz, 8H, *m*-H of Mes), –36.2 (s, br, $\Delta\nu_{½}$ = 1242 Hz, 24H, *o*-CH_3 of Mes), –11.6 (s, $\Delta\nu_{½}$ = 38 Hz, 12H, *p*-CH_3 of Mes), 33.7 (s, br, $\Delta\nu_{½}$ = 269 Hz, 2H, *p*-H of C_6H_3), 139.0 (s, br, $\Delta\nu_{½}$ = 950 Hz, 4H, *m*-H of C_6H_3). μ_{eff} = 4.900(4) μ_B. UV/vis (hexane): strong absorption between 200 and 400 nm; λ_{max}/nm (ε dm^3 mol^{-1} cm^{-1}) 353 (1313) sh, 366 (1107) sh, 382 (738) sh, 411 (517). EI-MS: M^+ = 682 (95%), fragment ion peaks at *m/z* 369 [(2,6-$Mes_2C_6H_3Fe)^+$, 10], 313 [(2,6-$Mes_2C_6H_3)^+$, 60], 298 [(2,6-$Mes_2C_6H_3$ – $Me)^+$, 30], 283 [(2,6-$Mes_2C_6H_3$ – $2Me)^+$, 40], 268 [(2,6-$Mes_2C_6H_3$ – $3Me)^+$, 40], 253 [(2,6-$Mes_2C_6H_3$ – $4Me)^+$, 35]; exact mass: calcd for 682.3256 measd 682.3251.

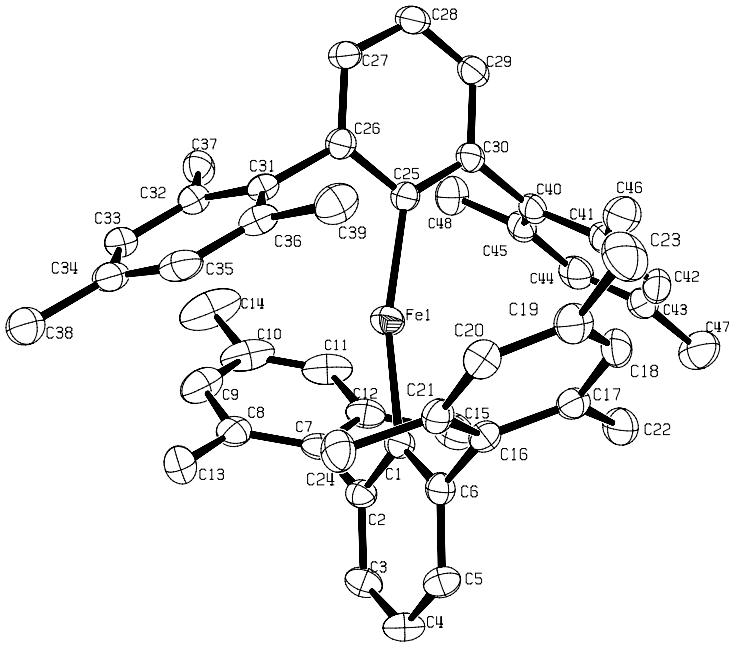

Figure S2. Thermal ellipsoid plot at 40% probability of one of the two crystallographically-distinct molecules of **2**. Hydrogen atoms have been omitted.

Crystals of **2** were grown by the controlled cooling of a saturated hexane solution to –35 °C. A single crystal having dimensions approximately 0.03 x 0.30 x 0.30 mm was mounted on a glass fibre using perfluoropolyether oil and cooled rapidly to 150K in a stream of cold N_2 using an Oxford Cryosystems CRYOSTREAM unit. Diffraction data were measured using an Enraf-Nonius KappaCCD diffractometer (graphite-monochromated MoK_α radiation, λ = 0.71073 Å). Intensity data were processed using the DENZO-SMN package[1].

Examination of the systematic absences of the intensity data showed the space group to be *P* $2_1/c$. The structure was solved using the direct-methods program SIR92[2], which located all non-hydrogen atoms. Subsequent full-matrix least-squares refinement was carried out using the CRYSTALS program suite[3]. Coordinates and anisotropic thermal parameters of all non-hydrogen atoms were refined. Hydrogen atoms were positioned geometrically after each cycle of refinement. A 3-term Chebychev polynomial weighting scheme was applied. Refinement converged satisfactorily to give R = 0.0463, wR = 0.0512.

A summary of crystallographic data is given below, as are full lists of atomic coordinates, anisotropic thermal parameters and those bond lengths and angles not concerning H atoms.

The asymmetric unit contains two crystallographically-distinct molecules, neither of which have any crystallographic symmetry. The geometries of these are similar but differ slightly in the orientation of the mesityl groups. Both are significantly distorted from the idealised $\bar{4}2m$ (D_{2d}) point symmetry as shown by the C-Fe-C and Fe-C-C angles listed in Table S12 below.

Table S4. Crystal data and refinement details for **2**

Crystal identification	**2**
Chemical formula	$C_{48}H_{50}Fe$
Formula weight	682.77
Temperature (K)	150
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	$P\,2_1/c$
a (Å)	10.4641(2)
b (Å)	38.4046(3)
c (Å)	19.1887(2)
α (°)	90
β (°)	92.1247(3)
γ (°)	90
Cell volume (Å^3)	7706.05(18)
Z	8
Calculated density (Mg/m^3)	1.177
Absorption coefficient (mm^{-1})	0.423
F_{000}	2912
Crystal size (mm)	0.03 x 0.30 x 0.30
Description of crystal	Green-yellow plate
Absorption correction	Semi-empirical from equivalent reflections
Transmission coefficients (min,max)	0.88, 0.99
θ range for data collection (°)	$5.0 \le \theta \le 27.5$
Index ranges	$-13 \le h \le 13$, $0 \le k \le 49$, $0 \le l \le 24$
Reflections measured	84689
Unique reflections	17822
R_{int}	0.068
Observed reflections (I > 3σ(I))	8216
Refinement method	Full-matrix least-squares on F
Parameters refined	883
Weighting scheme	Chebychev 3-term polynomial
Goodness of fit	1.1098
R	0.0463
wR	0.0512
Residual electron density (min,max) (eÅ^{-3})	-0.45, 0.38

Table S5. Bond lengths (Å) for **2**

Fe(1) - C(1)	2.042(3)	Fe(2) - C(49)	2.037(3)
Fe(1) - C(25)	2.040(3)	Fe(2) - C(73)	2.040(3)
C(1) - C(2)	1.408(4)	C(49) - C(50)	1.409(4)
C(1) - C(6)	1.404(4)	C(49) - C(54)	1.408(4)
C(2) - C(3)	1.398(4)	C(50) - C(51)	1.392(4)
C(2) - C(7)	1.497(4)	C(50) - C(55)	1.499(4)
C(3) - C(4)	1.385(5)	C(51) - C(52)	1.388(5)
C(4) - C(5)	1.380(5)	C(52) - C(53)	1.383(5)
C(5) - C(6)	1.403(4)	C(53) - C(54)	1.394(4)
C(6) - C(16)	1.495(4)	C(54) - C(64)	1.499(4)
C(7) - C(8)	1.410(5)	C(55) - C(56)	1.403(4)
C(7) - C(12)	1.413(5)	C(55) - C(60)	1.412(4)
C(8) - C(9)	1.397(5)	C(56) - C(57)	1.387(5)
C(8) - C(13)	1.500(5)	C(56) - C(61)	1.519(5)
C(9) - C(10)	1.376(6)	C(57) - C(58)	1.394(5)
C(10) - C(11)	1.385(6)	C(58) - C(59)	1.380(5)
C(10) - C(14)	1.515(6)	C(58) - C(62)	1.513(5)
C(11) - C(12)	1.395(5)	C(59) - C(60)	1.391(5)
C(12) - C(15)	1.503(6)	C(60) - C(63)	1.508(5)
C(16) - C(17)	1.404(4)	C(64) - C(65)	1.397(5)
C(16) - C(21)	1.403(4)	C(64) - C(69)	1.407(4)
C(17) - C(18)	1.394(5)	C(65) - C(66)	1.389(4)
C(17) - C(22)	1.509(5)	C(65) - C(70)	1.516(5)
C(18) - C(19)	1.389(5)	C(66) - C(67)	1.390(5)
C(19) - C(20)	1.380(5)	C(67) - C(68)	1.394(5)
C(19) - C(23)	1.507(5)	C(67) - C(71)	1.506(5)
C(20) - C(21)	1.400(4)	C(68) - C(69)	1.391(5)
C(21) - C(24)	1.505(4)	C(69) - C(72)	1.513(5)
C(25) - C(26)	1.412(4)	C(73) - C(74)	1.406(4)
C(25) - C(30)	1.409(4)	C(73) - C(78)	1.404(4)
C(26) - C(27)	1.398(4)	C(74) - C(75)	1.395(4)
C(26) - C(31)	1.501(4)	C(74) - C(79)	1.499(4)
C(27) - C(28)	1.380(5)	C(75) - C(76)	1.388(5)
C(28) - C(29)	1.384(5)	C(76) - C(77)	1.383(5)
C(29) - C(30)	1.400(4)	C(77) - C(78)	1.399(4)
C(30) - C(40)	1.500(4)	C(78) - C(88)	1.497(4)
C(31) - C(32)	1.413(4)	C(79) - C(80)	1.415(4)
C(31) - C(36)	1.406(5)	C(79) - C(84)	1.401(4)
C(32) - C(33)	1.388(5)	C(80) - C(81)	1.389(4)
C(32) - C(37)	1.505(5)	C(80) - C(85)	1.499(5)
C(33) - C(34)	1.393(5)	C(81) - C(82)	1.387(5)
C(34) - C(35)	1.381(5)	C(82) - C(83)	1.381(5)
C(34) - C(38)	1.512(5)	C(82) - C(86)	1.512(5)
C(35) - C(36)	1.399(5)	C(83) - C(84)	1.396(5)
C(36) - C(39)	1.509(5)	C(84) - C(87)	1.511(5)
C(40) - C(41)	1.410(4)	C(88) - C(89)	1.406(4)
C(40) - C(45)	1.398(5)	C(88) - C(93)	1.405(4)
C(41) - C(42)	1.387(5)	C(89) - C(90)	1.392(5)
C(41) - C(46)	1.507(5)	C(89) - C(94)	1.516(5)
C(42) - C(43)	1.388(6)	C(90) - C(91)	1.391(5)
C(43) - C(44)	1.387(5)	C(91) - C(92)	1.386(5)
C(43) - C(47)	1.506(5)	C(91) - C(95)	1.507(5)
C(44) - C(45)	1.392(5)	C(92) - C(93)	1.395(5)
C(45) - C(48)	1.514(5)	C(93) - C(96)	1.509(5)

Note – H atoms have been excluded

Table S6. Bond angles (°) for **2**

C(1) - Fe(1) - C(25)	164.44(12)	C(49) - Fe(2) - C(73)	171.06(12)
Fe(1) - C(1) - C(2)	106.7(2)	Fe(2) - C(49) - C(50)	107.2(2)
Fe(1) - C(1) - C(6)	136.1(2)	Fe(2) - C(49) - C(54)	135.5(2)
C(2) - C(1) - C(6)	117.1(3)	C(50) - C(49) - C(54)	117.2(3)
C(1) - C(2) - C(3)	122.4(3)	C(49) - C(50) - C(51)	121.9(3)
C(1) - C(2) - C(7)	115.8(3)	C(49) - C(50) - C(55)	116.5(3)
C(3) - C(2) - C(7)	121.8(3)	C(51) - C(50) - C(55)	121.5(3)
C(2) - C(3) - C(4)	118.9(3)	C(50) - C(51) - C(52)	119.6(3)
C(3) - C(4) - C(5)	120.3(3)	C(51) - C(52) - C(53)	119.6(3)
C(4) - C(5) - C(6)	120.9(3)	C(52) - C(53) - C(54)	121.1(3)
C(1) - C(6) - C(5)	120.3(3)	C(49) - C(54) - C(53)	120.5(3)
C(1) - C(6) - C(16)	119.7(3)	C(49) - C(54) - C(64)	120.6(3)
C(5) - C(6) - C(16)	119.9(3)	C(53) - C(54) - C(64)	118.9(3)
C(2) - C(7) - C(8)	119.4(3)	C(50) - C(55) - C(56)	120.5(3)
C(2) - C(7) - C(12)	119.9(3)	C(50) - C(55) - C(60)	119.9(3)
C(8) - C(7) - C(12)	120.5(3)	C(56) - C(55) - C(60)	119.6(3)
C(7) - C(8) - C(9)	117.9(3)	C(55) - C(56) - C(57)	119.3(3)
C(7) - C(8) - C(13)	120.3(3)	C(55) - C(56) - C(61)	120.2(3)
C(9) - C(8) - C(13)	121.8(3)	C(57) - C(56) - C(61)	120.5(3)
C(8) - C(9) - C(10)	122.7(4)	C(56) - C(57) - C(58)	121.9(3)
C(9) - C(10) - C(11)	118.6(3)	C(57) - C(58) - C(59)	118.1(3)
C(9) - C(10) - C(14)	120.2(5)	C(57) - C(58) - C(62)	120.4(4)
C(11) - C(10) - C(14)	121.1(5)	C(59) - C(58) - C(62)	121.5(3)
C(10) - C(11) - C(12)	121.9(4)	C(58) - C(59) - C(60)	122.2(3)
C(7) - C(12) - C(11)	118.5(4)	C(55) - C(60) - C(59)	118.9(3)
C(7) - C(12) - C(15)	120.4(3)	C(55) - C(60) - C(63)	121.1(3)
C(11) - C(12) - C(15)	121.1(3)	C(59) - C(60) - C(63)	120.0(3)
C(6) - C(16) - C(17)	120.1(3)	C(54) - C(64) - C(65)	120.3(3)
C(6) - C(16) - C(21)	120.6(3)	C(54) - C(64) - C(69)	119.7(3)
C(17) - C(16) - C(21)	119.4(3)	C(65) - C(64) - C(69)	120.0(3)
C(16) - C(17) - C(18)	119.2(3)	C(64) - C(65) - C(66)	119.2(3)
C(16) - C(17) - C(22)	120.4(3)	C(64) - C(65) - C(70)	120.8(3)
C(18) - C(17) - C(22)	120.4(3)	C(66) - C(65) - C(70)	120.0(3)
C(17) - C(18) - C(19)	122.1(3)	C(65) - C(66) - C(67)	122.2(3)
C(18) - C(19) - C(20)	118.1(3)	C(66) - C(67) - C(68)	117.7(3)
C(18) - C(19) - C(23)	120.9(3)	C(66) - C(67) - C(71)	121.6(3)
C(20) - C(19) - C(23)	121.0(3)	C(68) - C(67) - C(71)	120.7(3)
C(19) - C(20) - C(21)	121.8(3)	C(67) - C(68) - C(69)	122.0(3)
C(16) - C(21) - C(20)	119.4(3)	C(64) - C(69) - C(68)	119.0(3)
C(16) - C(21) - C(24)	120.5(3)	C(64) - C(69) - C(72)	120.7(3)
C(20) - C(21) - C(24)	120.1(3)	C(68) - C(69) - C(72)	120.3(3)
Fe(1) - C(25) - C(26)	111.8(2)	Fe(2) - C(73) - C(74)	114.5(2)
Fe(1) - C(25) - C(30)	130.8(2)	Fe(2) - C(73) - C(78)	128.0(2)
C(26) - C(25) - C(30)	117.3(3)	C(74) - C(73) - C(78)	117.4(3)
C(25) - C(26) - C(27)	121.5(3)	C(73) - C(74) - C(75)	121.8(3)
C(25) - C(26) - C(31)	116.7(3)	C(73) - C(74) - C(79)	118.0(3)
C(27) - C(26) - C(31)	121.6(3)	C(75) - C(74) - C(79)	120.2(3)
C(26) - C(27) - C(28)	119.9(3)	C(74) - C(75) - C(76)	119.7(3)
C(27) - C(28) - C(29)	119.8(3)	C(75) - C(76) - C(77)	119.6(3)
C(28) - C(29) - C(30)	121.0(3)	C(76) - C(77) - C(78)	120.9(3)
C(25) - C(30) - C(29)	120.4(3)	C(73) - C(78) - C(77)	120.6(3)
C(25) - C(30) - C(40)	119.7(3)	C(73) - C(78) - C(88)	120.0(3)
C(29) - C(30) - C(40)	119.8(3)	C(77) - C(78) - C(88)	119.4(3)
C(26) - C(31) - C(32)	118.4(3)	C(74) - C(79) - C(80)	120.3(3)

C(26) - C(31) - C(36)	121.8(3)	C(74) - C(79) - C(84)	119.6(3)
C(32) - C(31) - C(36)	119.8(3)	C(80) - C(79) - C(84)	120.0(3)
C(31) - C(32) - C(33)	119.0(3)	C(79) - C(80) - C(81)	118.6(3)
C(31) - C(32) - C(37)	120.8(3)	C(79) - C(80) - C(85)	120.4(3)
C(33) - C(32) - C(37)	120.2(3)	C(81) - C(80) - C(85)	121.0(3)
C(32) - C(33) - C(34)	122.2(3)	C(80) - C(81) - C(82)	122.4(3)
C(33) - C(34) - C(35)	117.8(3)	C(81) - C(82) - C(83)	118.0(3)
C(33) - C(34) - C(38)	120.2(3)	C(81) - C(82) - C(86)	121.3(3)
C(35) - C(34) - C(38)	121.9(3)	C(83) - C(82) - C(86)	120.7(3)
C(34) - C(35) - C(36)	122.5(3)	C(82) - C(83) - C(84)	122.4(3)
C(31) - C(36) - C(35)	118.7(3)	C(79) - C(84) - C(83)	118.6(3)
C(31) - C(36) - C(39)	120.3(3)	C(79) - C(84) - C(87)	121.1(3)
C(35) - C(36) - C(39)	121.0(3)	C(83) - C(84) - C(87)	120.2(3)
C(30) - C(40) - C(41)	120.1(3)	C(78) - C(88) - C(89)	120.0(3)
C(30) - C(40) - C(45)	120.2(3)	C(78) - C(88) - C(93)	120.4(3)
C(41) - C(40) - C(45)	119.7(3)	C(89) - C(88) - C(93)	119.6(3)
C(40) - C(41) - C(42)	118.8(3)	C(88) - C(89) - C(90)	119.6(3)
C(40) - C(41) - C(46)	120.2(3)	C(88) - C(89) - C(94)	120.9(3)
C(42) - C(41) - C(46)	121.0(3)	C(90) - C(89) - C(94)	119.5(3)
C(41) - C(42) - C(43)	122.6(3)	C(89) - C(90) - C(91)	121.6(3)
C(42) - C(43) - C(44)	117.5(3)	C(90) - C(91) - C(92)	118.1(3)
C(42) - C(43) - C(47)	121.6(4)	C(90) - C(91) - C(95)	120.7(3)
C(44) - C(43) - C(47)	120.9(4)	C(92) - C(91) - C(95)	121.2(3)
C(43) - C(44) - C(45)	122.3(3)	C(91) - C(92) - C(93)	122.3(3)
C(40) - C(45) - C(44)	119.1(3)	C(88) - C(93) - C(92)	118.9(3)
C(40) - C(45) - C(48)	120.3(3)	C(88) - C(93) - C(96)	121.3(3)
C(44) - C(45) - C(48)	120.6(3)	C(92) - C(93) - C(96)	119.9(3)

Note – H atoms have been excluded

Preparative, spectroscopic and crystallographic data for 3

*Synthesis of (2,6-$Mes_2C_6H_3)_2Co$ (**3**)*

A solution of [2,6-$Mes_2C_6H_3Li]_2$ (0.225 g, 0.33 mmol) in toluene (10 cm^3) was added dropwise to a suspension of $CoBr_2$(DME) (0.108 g, 0.33 mmol) in a mixture of toluene (10 cm^3) and THF (2 cm^3) at –78 °C and the resulting mixture warmed slowly to room temperature and stirred overnight. The solution was filtered and volatiles were removed *in vacuo*. The resultant solid was extracted into hexanes (15 cm^3) and cooled to –35 °C for several days, whereupon dark purple crystals of **3** suitable for X-ray diffraction were formed (0.110 g, 48%). Mp: 148–155 °C (from hexane, melts and turns black). ^{1}H NMR (300 MHz, C_6D_6, Me_4Si) δ –100.2 (s, br, $\Delta\nu_{½}$ = 320 Hz, 8H, *m*-H of Mes), –74.3 (s, br, $\Delta\nu_{½}$ = 1535 Hz, 24H, *o*-CH_3 of Mes), –29.6 (s, br, $\Delta\nu_{½}$ = 109 Hz, 12H, *p*-CH_3 of Mes), 142.6 (s, br, $\Delta\nu_{½}$ = 889 Hz, 2H, *m*-H of C_6H_3), *p*-H of C_6H_3 not observed. μ_{eff} = 3.814(9) μ_B. UV/vis (hexane): strong absorption between 200 and 400 nm; λ_{max}/nm (ε dm^3 mol^{-1} cm^{-1}) 385 (2017) sh, 521 (497). EI-MS: M^+ = 685 (25%), fragment ion peaks at m/z 373 [(2,6-$Mes_2C_6H_3Co)^+$, 20], 313 [(2,6-$Mes_2C_6H_3)^+$, 55], 298 [(2,6-$Mes_2C_6H_3$ – Me)$^+$, 80], 283 [(2,6-$Mes_2C_6H_3$ – 2Me)$^+$, 25], 268 [(2,6-$Mes_2C_6H_3$ – 3Me)$^+$, 20], 253 [(2,6-$Mes_2C_6H_3$ – 4Me)$^+$, 5]; exact mass: calcd for 685.3239 measd 685.3239.

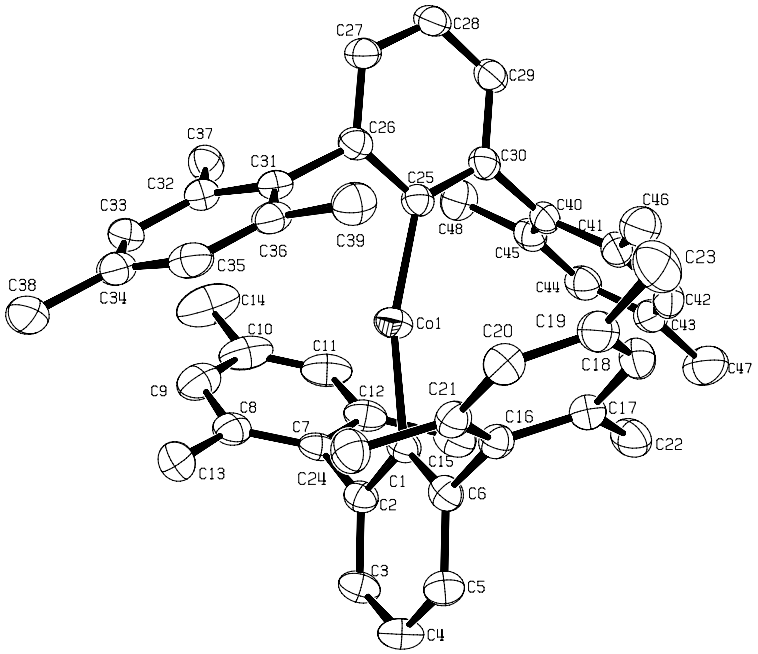

Figure S3. Thermal ellipsoid plot at 40% probability of one of the two crystallographically-distinct molecules of **3**. Hydrogen atoms have been omitted.

Crystals of **3** were grown by the controlled cooling of a saturated hexane solution to –35 °C. A single crystal having dimensions approximately 0.03 x 0.26 x 0.26 mm was mounted on a glass fibre using perfluoropolyether oil and cooled rapidly to 150K in a stream of cold N_2 using an Oxford Cryosystems CRYOSTREAM unit. Diffraction data were measured using an Enraf-Nonius KappaCCD diffractometer (graphite-monochromated MoK_α radiation, λ = 0.71073 Å). Intensity data were processed using the DENZO-SMN package[1].

Examination of the systematic absences of the intensity data showed the space group to be $P\ 2_1/c$. The structure was solved using the direct-methods program SIR92[2], which located all non-hydrogen atoms. Subsequent full-matrix least-squares refinement was carried out using the CRYSTALS program suite[3]. Coordinates and anisotropic thermal parameters of all non-hydrogen atoms were refined. Hydrogen atoms were positioned geometrically after each cycle of refinement. A 3-term Chebychev polynomial weighting scheme was applied. Refinement converged satisfactorily to give R = 0.0452, wR = 0.0510.

A summary of crystallographic data is given below, as are full lists of atomic coordinates, anisotropic thermal parameters and those bond lengths and angles not concerning H atoms.

Comment:

The complex is isomorphous with the Fe analogue and shows similar deviations from the idealised 42*m* (D_{2d}) point symmetry.

Table S7. Crystal data and refinement details for **3**

Crystal identification	**3**
Chemical formula	$C_{48}H_{50}Co$
Formula weight	685.86
Temperature (K)	150

Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	$P\,2_1/c$
a (Å)	10.4123(2)
b (Å)	38.5032(6)
c (Å)	19.1871(3)
α (°)	90
β (°)	92.4695
γ (°)	90
Cell volume (Å^3)	7685.1(2)
Z	8
Calculated density (Mg/m^3)	1.185
Absorption coefficient (mm^{-1})	0.478
F_{000}	2920
Crystal size (mm)	0.03 x 0.26 x 0.26
Description of crystal	Dark-purple plate
Absorption correction	Semi-empirical from equivalent reflections
Transmission coefficients (min,max)	0.88, 0.99
θ range for data collection (°)	$5.0 \le \theta \le 27.5$
Index ranges	$-13 \le h \le 13$, $0 \le k \le 49$, $0 \le l \le 24$
Reflections measured	55484
Unique reflections	17289
R_{int}	0.047
Observed reflections (I > 3σ(I))	9572
Refinement method	Full-matrix least-squares on F
Parameters refined	883
Weighting scheme	Chebychev 3-term polynomial
Goodness of fit	1.1009
R	0.0452
wR	0.0510
Residual electron density (min,max) (eÅ^{-3})	-0.32, 0.31

Table S8. Bond lengths (Å) for **3**

Co(1) - C(1)	2.003(3)	Co(2) - C(49)	2.000(2)
Co(1) - C(25)	2.000(3)	Co(2) - C(73)	1.999(2)
C(1) - C(2)	1.406(3)	C(49) - C(50)	1.402(4)
C(1) - C(6)	1.408(4)	C(49) - C(54)	1.406(4)
C(2) - C(3)	1.396(4)	C(50) - C(51)	1.390(4)
C(2) - C(7)	1.499(4)	C(50) - C(55)	1.508(4)
C(3) - C(4)	1.388(4)	C(51) - C(52)	1.389(4)
C(4) - C(5)	1.386(4)	C(52) - C(53)	1.387(4)
C(5) - C(6)	1.397(4)	C(53) - C(54)	1.398(4)
C(6) - C(16)	1.502(3)	C(54) - C(64)	1.499(4)
C(7) - C(8)	1.404(4)	C(55) - C(56)	1.410(4)
C(7) - C(12)	1.414(4)	C(55) - C(60)	1.402(4)
C(8) - C(9)	1.396(4)	C(56) - C(57)	1.387(4)
C(8) - C(13)	1.500(5)	C(56) - C(61)	1.514(4)
C(9) - C(10)	1.387(5)	C(57) - C(58)	1.386(4)

C(10) - C(11)	1.375(5)	C(58) - C(59)	1.390(4)
C(10) - C(14)	1.517(5)	C(58) - C(62)	1.510(4)
C(11) - C(12)	1.388(4)	C(59) - C(60)	1.395(4)
C(12) - C(15)	1.511(5)	C(60) - C(63)	1.508(4)
C(16) - C(17)	1.407(4)	C(64) - C(65)	1.398(4)
C(16) - C(21)	1.391(4)	C(64) - C(69)	1.408(4)
C(17) - C(18)	1.396(4)	C(65) - C(66)	1.395(4)
C(17) - C(22)	1.506(4)	C(65) - C(70)	1.516(4)
C(18) - C(19)	1.390(4)	C(66) - C(67)	1.384(4)
C(19) - C(20)	1.383(4)	C(67) - C(68)	1.389(4)
C(19) - C(23)	1.511(4)	C(67) - C(71)	1.505(4)
C(20) - C(21)	1.396(4)	C(68) - C(69)	1.389(4)
C(21) - C(24)	1.511(4)	C(69) - C(72)	1.510(4)
C(25) - C(26)	1.411(4)	C(73) - C(74)	1.409(4)
C(25) - C(30)	1.411(4)	C(73) - C(78)	1.405(4)
C(26) - C(27)	1.398(4)	C(74) - C(75)	1.400(3)
C(26) - C(31)	1.499(4)	C(74) - C(79)	1.492(4)
C(27) - C(28)	1.384(4)	C(75) - C(76)	1.389(4)
C(28) - C(29)	1.382(4)	C(76) - C(77)	1.382(4)
C(29) - C(30)	1.399(4)	C(77) - C(78)	1.399(4)
C(30) - C(40)	1.499(4)	C(78) - C(88)	1.498(4)
C(31) - C(32)	1.416(4)	C(79) - C(80)	1.411(4)
C(31) - C(36)	1.406(4)	C(79) - C(84)	1.405(4)
C(32) - C(33)	1.391(4)	C(80) - C(81)	1.390(4)
C(32) - C(37)	1.499(4)	C(80) - C(85)	1.510(4)
C(33) - C(34)	1.389(4)	C(81) - C(82)	1.393(4)
C(34) - C(35)	1.390(4)	C(82) - C(83)	1.383(4)
C(34) - C(38)	1.512(4)	C(82) - C(86)	1.511(4)
C(35) - C(36)	1.401(4)	C(83) - C(84)	1.391(4)
C(36) - C(39)	1.514(4)	C(84) - C(87)	1.519(4)
C(40) - C(41)	1.401(4)	C(88) - C(89)	1.407(4)
C(40) - C(45)	1.400(4)	C(88) - C(93)	1.405(4)
C(41) - C(42)	1.396(4)	C(89) - C(90)	1.391(4)
C(41) - C(46)	1.510(5)	C(89) - C(94)	1.509(4)
C(42) - C(43)	1.380(5)	C(90) - C(91)	1.386(4)
C(43) - C(44)	1.384(5)	C(91) - C(92)	1.395(4)
C(43) - C(47)	1.514(5)	C(91) - C(95)	1.511(4)
C(44) - C(45)	1.395(4)	C(92) - C(93)	1.391(4)
C(45) - C(48)	1.518(4)	C(93) - C(96)	1.511(4)

Note – H atoms have been excluded

Table S9. Bond angles (°) for **3**

C(1) - Co(1) - C(25)	162.84(10)	C(49) - Co(2) - C(73)	172.17(11)
Co(1) - C(1) - C(2)	106.62(18)	Co(2) - C(49) - C(50)	108.08(18)
Co(1) - C(1) - C(6)	136.37(19)	Co(2) - C(49) - C(54)	134.6(2)
C(2) - C(1) - C(6)	117.0(2)	C(50) - C(49) - C(54)	117.3(2)
C(1) - C(2) - C(3)	122.7(2)	C(49) - C(50) - C(51)	122.7(2)
C(1) - C(2) - C(7)	115.1(2)	C(49) - C(50) - C(55)	116.0(2)
C(3) - C(2) - C(7)	122.1(2)	C(51) - C(50) - C(55)	121.4(2)
C(2) - C(3) - C(4)	118.8(2)	C(50) - C(51) - C(52)	119.2(3)
C(3) - C(4) - C(5)	120.0(2)	C(51) - C(52) - C(53)	119.4(2)
C(4) - C(5) - C(6)	121.0(3)	C(52) - C(53) - C(54)	121.3(3)
C(1) - C(6) - C(5)	120.4(2)	C(49) - C(54) - C(53)	120.1(3)
C(1) - C(6) - C(16)	120.2(2)	C(49) - C(54) - C(64)	121.7(2)

C(5) - C(6) - C(16)	119.4(2)	C(53) - C(54) - C(64)	118.2(2)
C(2) - C(7) - C(8)	119.4(3)	C(50) - C(55) - C(56)	120.1(2)
C(2) - C(7) - C(12)	119.9(3)	C(50) - C(55) - C(60)	119.9(2)
C(8) - C(7) - C(12)	120.5(3)	C(56) - C(55) - C(60)	120.0(2)
C(7) - C(8) - C(9)	118.0(3)	C(55) - C(56) - C(57)	118.9(3)
C(7) - C(8) - C(13)	120.7(3)	C(55) - C(56) - C(61)	120.5(2)
C(9) - C(8) - C(13)	121.4(3)	C(57) - C(56) - C(61)	120.6(3)
C(8) - C(9) - C(10)	122.4(3)	C(56) - C(57) - C(58)	122.2(3)
C(9) - C(10) - C(11)	118.3(3)	C(57) - C(58) - C(59)	118.2(3)
C(9) - C(10) - C(14)	119.9(4)	C(57) - C(58) - C(62)	121.2(3)
C(11) - C(10) - C(14)	121.8(4)	C(59) - C(58) - C(62)	120.6(3)
C(10) - C(11) - C(12)	122.4(3)	C(58) - C(59) - C(60)	121.8(3)
C(7) - C(12) - C(11)	118.4(3)	C(55) - C(60) - C(59)	119.0(3)
C(7) - C(12) - C(15)	120.0(3)	C(55) - C(60) - C(63)	121.3(3)
C(11) - C(12) - C(15)	121.4(3)	C(59) - C(60) - C(63)	119.7(3)
C(6) - C(16) - C(17)	119.3(2)	C(54) - C(64) - C(65)	120.1(2)
C(6) - C(16) - C(21)	120.9(2)	C(54) - C(64) - C(69)	119.8(2)
C(17) - C(16) - C(21)	119.9(2)	C(65) - C(64) - C(69)	120.0(3)
C(16) - C(17) - C(18)	118.7(3)	C(64) - C(65) - C(66)	118.9(2)
C(16) - C(17) - C(22)	120.9(2)	C(64) - C(65) - C(70)	120.7(3)
C(18) - C(17) - C(22)	120.4(2)	C(66) - C(65) - C(70)	120.3(3)
C(17) - C(18) - C(19)	122.0(3)	C(65) - C(66) - C(67)	122.0(3)
C(18) - C(19) - C(20)	118.1(2)	C(66) - C(67) - C(68)	118.1(3)
C(18) - C(19) - C(23)	121.0(3)	C(66) - C(67) - C(71)	121.3(3)
C(20) - C(19) - C(23)	120.9(3)	C(68) - C(67) - C(71)	120.5(3)
C(19) - C(20) - C(21)	121.7(3)	C(67) - C(68) - C(69)	122.0(3)
C(16) - C(21) - C(20)	119.6(2)	C(64) - C(69) - C(68)	118.9(3)
C(16) - C(21) - C(24)	120.9(2)	C(64) - C(69) - C(72)	120.5(3)
C(20) - C(21) - C(24)	119.5(2)	C(68) - C(69) - C(72)	120.6(3)
Co(1) - C(25) - C(26)	110.68(18)	Co(2) - C(73) - C(74)	113.75(18)
Co(1) - C(25) - C(30)	132.1(2)	Co(2) - C(73) - C(78)	128.85(19)
C(26) - C(25) - C(30)	117.0(2)	C(74) - C(73) - C(78)	117.3(2)
C(25) - C(26) - C(27)	122.0(2)	C(73) - C(74) - C(75)	121.7(2)
C(25) - C(26) - C(31)	116.6(2)	C(73) - C(74) - C(79)	118.2(2)
C(27) - C(26) - C(31)	121.3(2)	C(75) - C(74) - C(79)	120.1(2)
C(26) - C(27) - C(28)	119.6(3)	C(74) - C(75) - C(76)	119.7(2)
C(27) - C(28) - C(29)	119.8(2)	C(75) - C(76) - C(77)	119.6(2)
C(28) - C(29) - C(30)	121.1(3)	C(76) - C(77) - C(78)	121.1(2)
C(25) - C(30) - C(29)	120.4(3)	C(73) - C(78) - C(77)	120.6(2)
C(25) - C(30) - C(40)	120.1(2)	C(73) - C(78) - C(88)	120.1(2)
C(29) - C(30) - C(40)	119.5(2)	C(77) - C(78) - C(88)	119.3(2)
C(26) - C(31) - C(32)	118.8(2)	C(74) - C(79) - C(80)	120.8(2)
C(26) - C(31) - C(36)	121.8(2)	C(74) - C(79) - C(84)	119.6(2)
C(32) - C(31) - C(36)	119.4(2)	C(80) - C(79) - C(84)	119.6(2)
C(31) - C(32) - C(33)	119.0(3)	C(79) - C(80) - C(81)	119.1(2)
C(31) - C(32) - C(37)	120.6(2)	C(79) - C(80) - C(85)	120.6(2)
C(33) - C(32) - C(37)	120.4(3)	C(81) - C(80) - C(85)	120.2(2)
C(32) - C(33) - C(34)	122.3(3)	C(80) - C(81) - C(82)	121.9(3)
C(33) - C(34) - C(35)	118.1(3)	C(81) - C(82) - C(83)	118.1(3)
C(33) - C(34) - C(38)	120.2(3)	C(81) - C(82) - C(86)	121.2(3)
C(35) - C(34) - C(38)	121.7(3)	C(83) - C(82) - C(86)	120.7(3)
C(34) - C(35) - C(36)	121.7(3)	C(82) - C(83) - C(84)	122.3(3)
C(31) - C(36) - C(35)	119.3(3)	C(79) - C(84) - C(83)	119.0(3)
C(31) - C(36) - C(39)	120.3(3)	C(79) - C(84) - C(87)	120.7(2)
C(35) - C(36) - C(39)	120.2(3)	C(83) - C(84) - C(87)	120.2(2)
C(30) - C(40) - C(41)	120.1(2)	C(78) - C(88) - C(89)	119.9(2)
C(30) - C(40) - C(45)	119.8(2)	C(78) - C(88) - C(93)	120.4(2)

C(41) - C(40) - C(45)	120.1(3)	C(89) - C(88) - C(93)	119.7(2)
C(40) - C(41) - C(42)	118.7(3)	C(88) - C(89) - C(90)	119.4(3)
C(40) - C(41) - C(46)	120.6(3)	C(88) - C(89) - C(94)	121.1(2)
C(42) - C(41) - C(46)	120.7(3)	C(90) - C(89) - C(94)	119.4(3)
C(41) - C(42) - C(43)	122.0(3)	C(89) - C(90) - C(91)	121.8(3)
C(42) - C(43) - C(44)	118.5(3)	C(90) - C(91) - C(92)	118.2(3)
C(42) - C(43) - C(47)	121.0(3)	C(90) - C(91) - C(95)	120.7(3)
C(44) - C(43) - C(47)	120.5(3)	C(92) - C(91) - C(95)	121.0(3)
C(43) - C(44) - C(45)	121.7(3)	C(91) - C(92) - C(93)	121.8(3)
C(40) - C(45) - C(44)	119.1(3)	C(88) - C(93) - C(92)	119.1(3)
C(40) - C(45) - C(48)	120.5(3)	C(88) - C(93) - C(96)	121.0(2)
C(44) - C(45) - C(48)	120.4(3)	C(92) - C(93) - C(96)	119.9(3)

Note – H atoms have been excluded

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