Supplementary Material (ESI) for Dalton Transactions

Iron indenyl carbonyl compounds: CO-releasing molecules

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Table S1. X-ray crystal data for $[(\eta\text{-}C_9H_7)Fe(CO)_2L][BF_4]$, L = $P(OPh)_3$, PPh_3, $MeC_3N_2H_3$, NCMe, CO and NC_5H_5.

Compound	$[(\eta\text{-}C_9H_7)Fe(CO)_2 P(OPh)_3][BF_4]$	$[(\eta\text{-}C_9H_7)Fe(CO)_2 PPh_3][BF_4]\bullet CHCl_3$	$[(\eta\text{-}C_9H_7)Fe(CO)_2 MeC_3N_2H_3][BF_4]$
Empirical formula	C29 H22 B F4 Fe O5 P	C30 H23 B Cl3 F4 Fe O2 P	C15 H13 B F4 Fe N2 O2
Formula weight	624.10	695.46	395.93
Temperature	150(2) K	150(2) K	100(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Orthorhombic	Triclinic
Space group	C c	$P2_12_12_1$	P-1
Unit cell dimensions	a = 13.092(12) Å	a = 9.4217(5) Å	a = 7.0213(5) Å
	b = 20.322(12) Å	b = 11.0573(5) Å	b = 10.6698(8) Å
	c = 21.77(2) Å	c = 28.4413(13) Å	c = 11.1259(8) Å
	α= 90°.	α= 90°	α= 78.540(3)°.
	β= 107.458(17)°.	β= 90°	β= 83.572(3)°.
	γ = 90°	γ = 90°	γ = 81.108(3)°.
Volume	5525(8) $Å^3$	2963.0(2) $Å^3$	804.23(10) $Å^3$
Z	8	4	2
Density (calculated)	1.501 Mg/m^3	1.559 Mg/m^3	1.635 Mg/m^3
Absorption coefficient	0.669 mm^{-1}	0.887 mm^{-1}	0.992 mm^{-1}
F(000)	2544	1408	400
Crystal size	0.32 x 0.12 x 0.12 mm^3	0.22 x 0.17 x 0.17 mm^3	0.30 x 0.10 x 0.04 mm^3
Theta range for data collection	1.91 to 27.67°.	1.98 to 27.48°	1.87 to 36.17°
Index ranges	-17<=h<=16,	-12<=h<=12,	-11<=h<=11,
	-26<=k<=26,	-13<=k<=14,	-17<=k<=17,
	-27<=l<=28	-36<=l<=36	-18<=l<=18
Reflections collected	31374	58444	21878
Independent reflections	12567 [R(int) = 0.0967]	6787 [R(int) = 0.0387]	7270 [R(int) = 0.0269]
Completeness to	theta = 27.67°, 98.8%	theta = 27.48°, 99.9%	theta = 25.00°, 99.9%
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	0.9240 and 0.8143	0.8638 and 0.8288	0.9614 and 0.7552
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	12567 / 2 / 740	6787 / 0 / 379	7270 / 0 / 227
Goodness-of-fit on F^2	1.029	1.029	1.048
Final R indices [I>2sigma(I)]	R1 = 0.0683, wR2 = 0.1600	R1 = 0.0253, wR2 = 0.0611	R1 = 0.0446, wR2 = 0.1102
R indices (all data)	R1 = 0.1050, wR2 = 0.1794	R1 = 0.0274, wR2 = 0.0621	R1 = 0.0561, wR2 = 0.1172
Absolute structure parameter	0.512(19)	0.004(9)	
Largest diff. peak and hole	1.681 and -0.455 e.$Å^{-3}$	0.633 and -0.409 e.$Å^{-3}$	1.266 and -0.974 e.$Å^{-3}$
Weighting scheme	$1/[\sigma^2(Fo^2)$ $+(0.1040*P)^2+0.000*P]$	$1/[\sigma^2(Fo^2)+(0.7977*P)^2+0.0351*P]$	$1/[\sigma^2(Fo^2)+(0.0562*P)^2+$ $0.5342*P]$
CCDC Reference Number	766624	766623	766625

[a] $P=(Fo^2+2*Fc^2)/3$

Table S1 Continued.

Compound	$[(\eta\text{-}C_9H_7)Fe(CO)_2(NCMe)][BF_4]$	$[(\eta\text{-}C_9H_7)Fe(CO)_3][BF_4]$	$[(\eta\text{-}C_9H_7)Fe(CO)_2(NC_5H_5)][BF_4]$
Empirical formula	C13 H10 B F4 Fe N O2	C12 H7 B F4 Fe O3	C16 H12 B F4 Fe N O2
Formula weight	354.88	341.84	392.93
Temperature	100(2) K	150(2) K	150(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Orthorhombic	Triclinic
Space group	$P2_1/c$	$P2_12_12_1$	P-1
Unit cell dimensions	a = 9.6851(8) Å	a = 8.4741(3) Å	a = 7.9950(16) Å
	b = 18.7238(16)	b = 10.5865(4) Å	b = 9.5420(19) Å
	c = 7.7446(7) Å	c = 14.1233(6) Å	c = 10.832(2) Å
	α= 90°	α = 90°	α = 89.32(3)°
	β= 95.239(4) °	β = 90°	β = 78.41(3)°
	γ = 90°	γ = 90°	γ = 82.82(3)°
Volume	1398.6(2) $Å^3$	1267.02(8) $Å^3$	803.1(3) $Å^3$
Z	4	4	2
Density (calculated)	1.685 Mg/m^3	1.792 Mg/m^3	1.625 Mg/m^3
Absorption coefficient	1.128 mm^{-1}	1.245 mm^{-1}	0.991 mm^{-1}
F(000)	712	680	396
Crystal size	0.43 x 0.20 x 0.20 mm^3	0.38 x 0.21 x 0.21 mm^3	0.25 x 0.12 x 0.12 mm^3
Theta range for data collection	2.11 to 36.42°	2.40 to 27.50°	1.92 to 27.53°
Index ranges	-16<=h<=15,	-10<=h<=11,	-10<=h<=10,
	-26<=k<=30,	-12<=k<=13,	-12<=k<=12,
	-12<=l<=12	-18<=l<=18	-14<=l<=14
Reflections collected	47413	9153	18344
Independent reflections	6726 [R(int) = 0.0270]	2867 [R(int) = 0.0310]	3675 [R(int) = 0.0320]
Completeness to	theta = 36.42 °, 98.7 %	theta = 25.00°, 99.7%	theta = 27.53°, 99.1%
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	0.8059 and 0.6427	0.7801 and 0.6491	0.8903 and 0.7898
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	6726 / 7 / 210	2867 / 3 / 190	3675 / 0 / 226
Goodness-of-fit on F^2	1.166	1.427	1.095
Final R indices [I>2sigma(I)]	R1 = 0.0372, wR2 = 0.0871	R1 = 0.0228, wR2 = 0.0557	R1 = 0.0310, wR2 = 0.0788
R indices (all data)	R1 = 0.0436, wR2 = 0.0894	R1 = 0.0238, wR2 = 0.0561	R1 = 0.0377, wR2 = 0.0824
Absolute structure parameter		0.012(13)	
Largest diff. peak and hole	0.795 and -0.496 e.Å-3	0.274 and -0.340 $e.Å^{-3}$	0.882 and -0.539 $e.Å^{-3}$
Weighting Scheme[a]	$1/[\sigma^2(Fo^2) +(0.0268*P)^2+ 0.9580*P]$	$1/[\sigma^2(Fo^2) +(0.0000*P)^2+ 0.0000*P]$	$1/[\sigma^2(Fo^2) + (0.0435*P)^2 + 0.2310*P]$
CCDC Reference Number	766622	766621	766626

[a] $P=(Fo^2+ 2 * Fc^2)/3$.