Supporting information for

C-O and C-C Bond Cleavage of α,β-Unsaturated Esters by the Assist of Gallane(pyridyl)iron Complex

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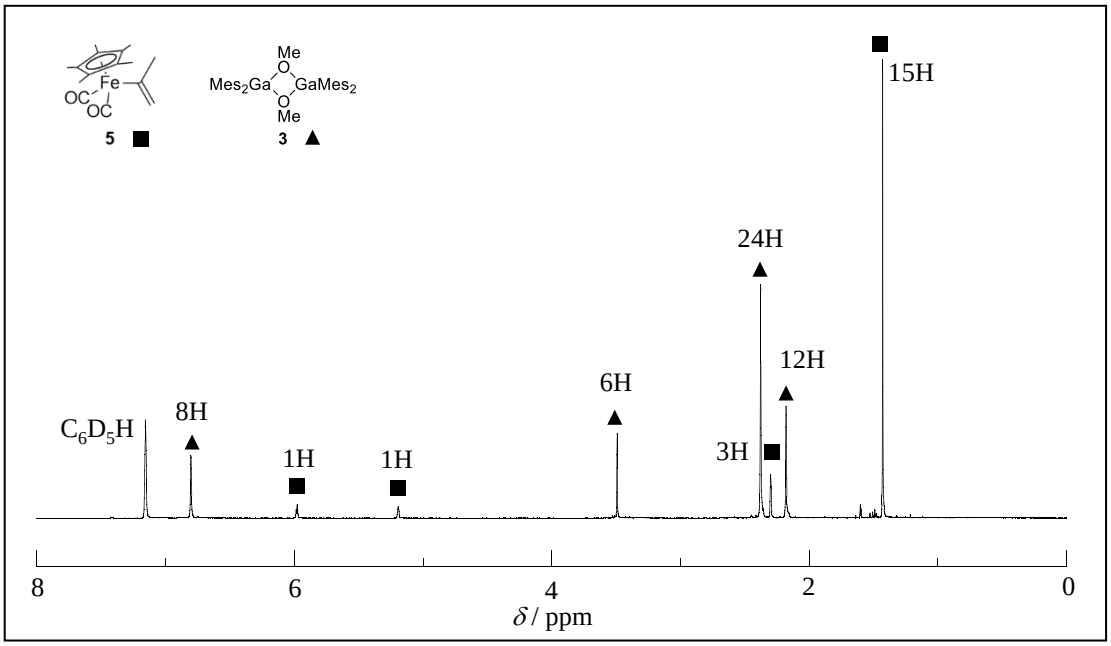

Figure S1. ^{1}H NMR spectrum of the reaction mixture obtained by the reaction of **1** with methyl methacrylate after removal of the volatiles in vacuo (300 MHz, C_6D_6).

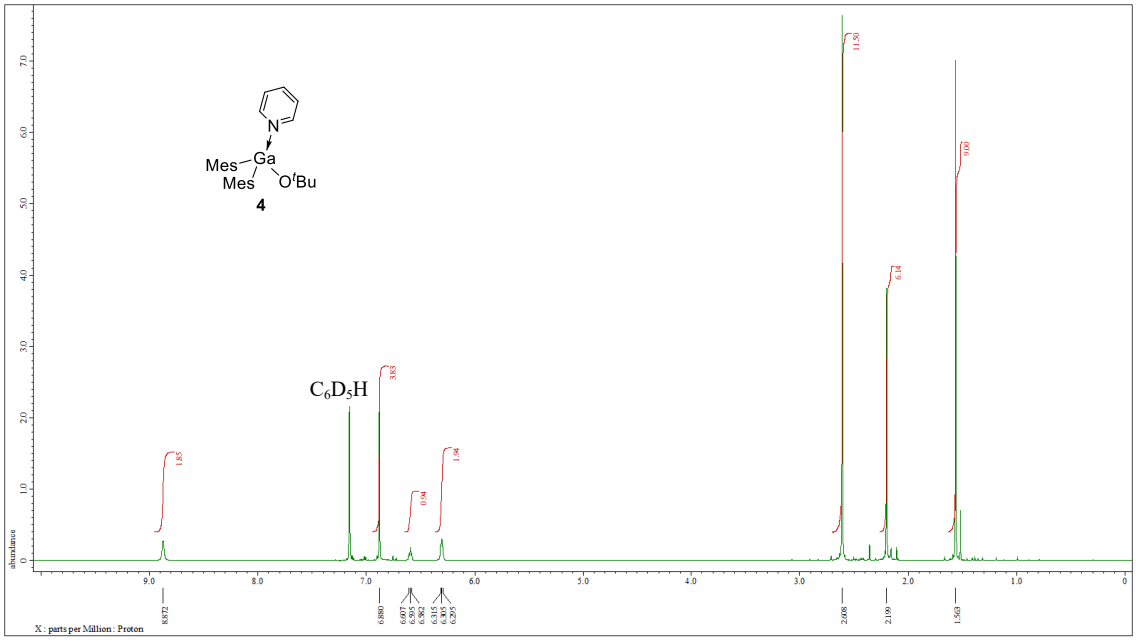

Figure S2. ^{1}H NMR spectrum of **4** (600 MHz, C_6D_6).

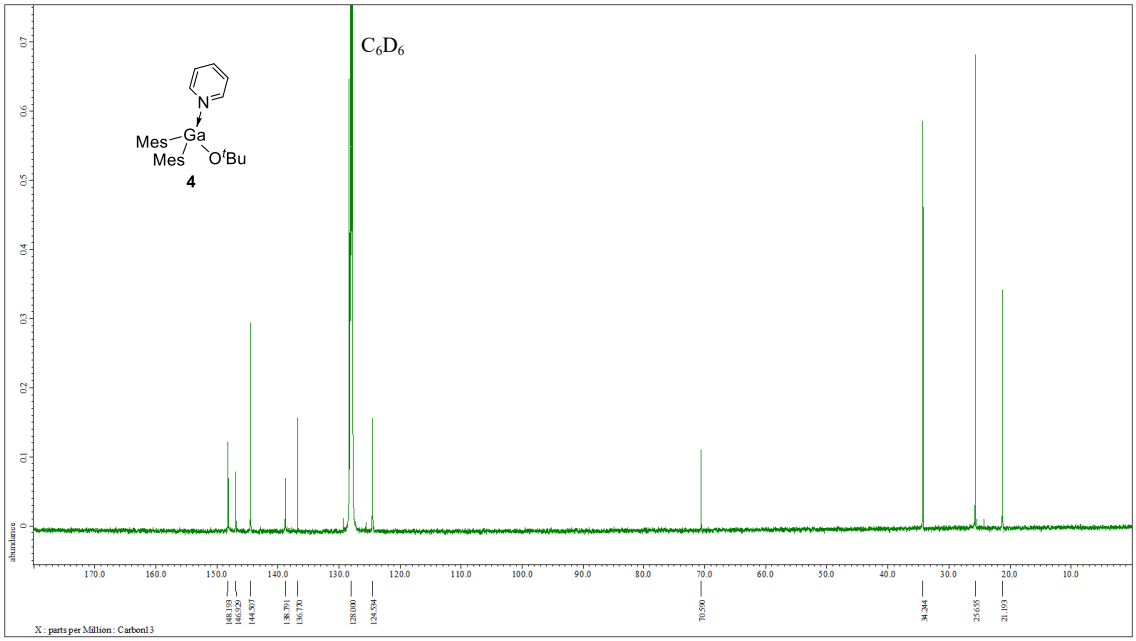

Figure S3. ^{13}C NMR spectrum of **4** (150.6 MHz, C_6D_6).

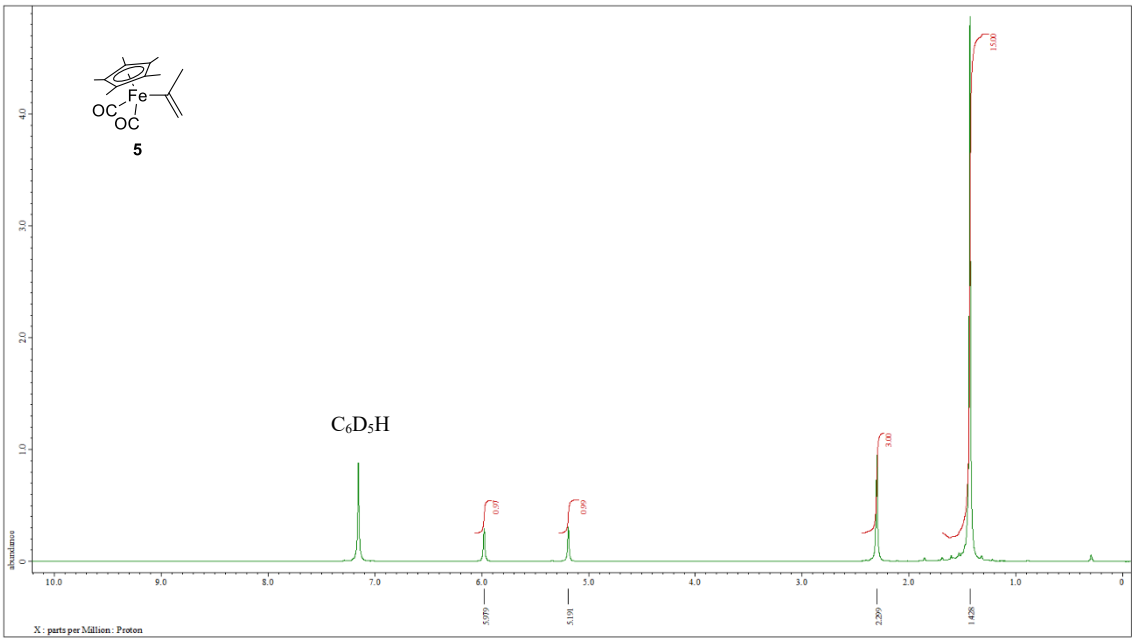

Figure S4. ^{1}H NMR spectrum of **5** (400 MHz, C_6D_6).

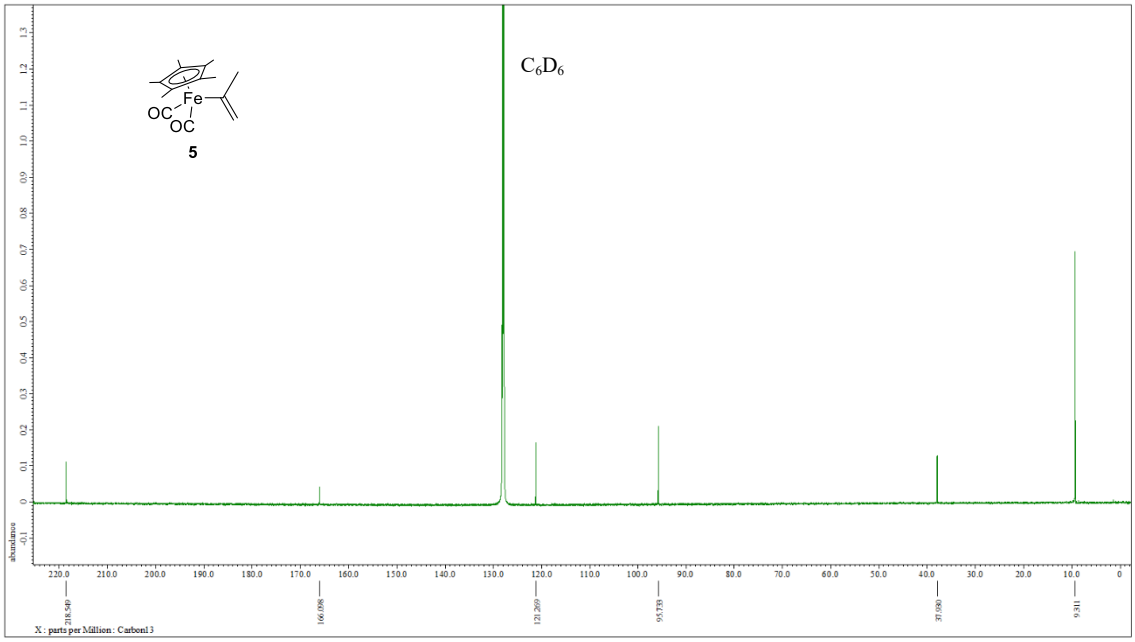

Figure S5. ^{13}C NMR spectrum of **5** (150.6 MHz, C_6D_6).

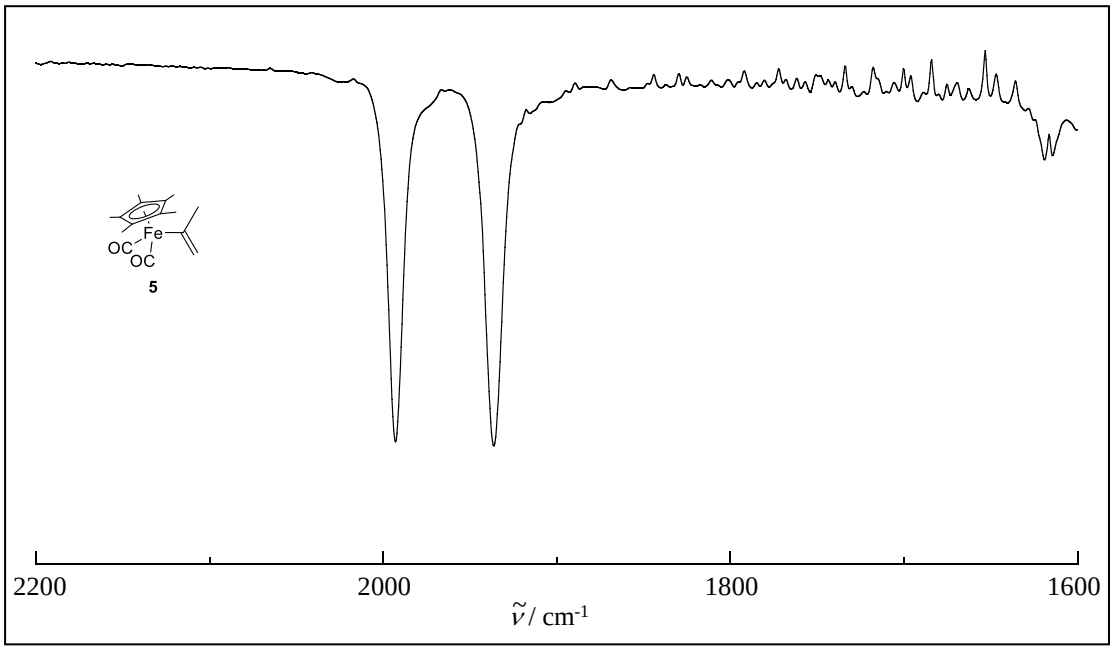

Figure S6. IR spectrum of **5** (C_6D_6).

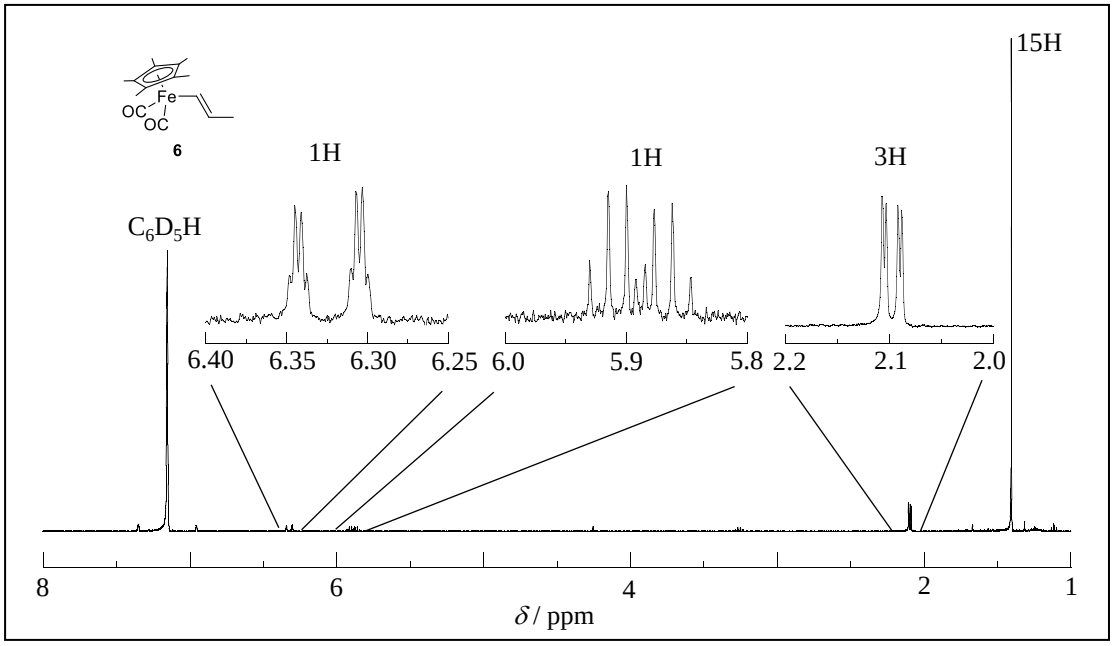

Figure S7. ^{1}H NMR spectrum of crude **6** (400 MHz, C_6D_6).

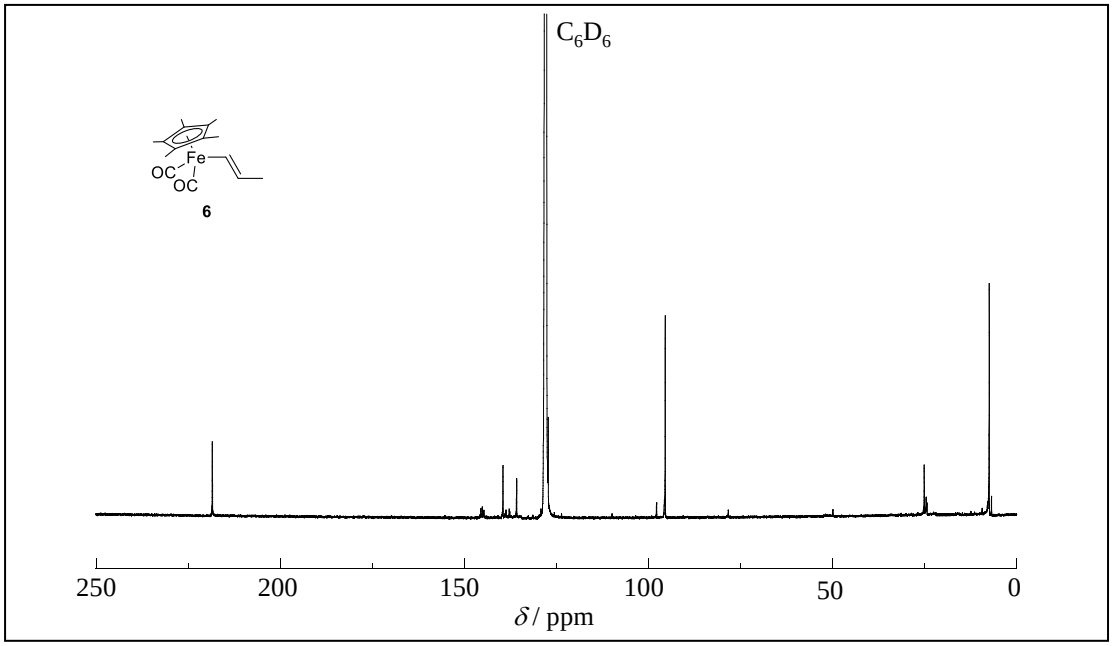

Figure S8. ^{13}C NMR spectrum of crude **6** (100.4 MHz, C_6D_6).

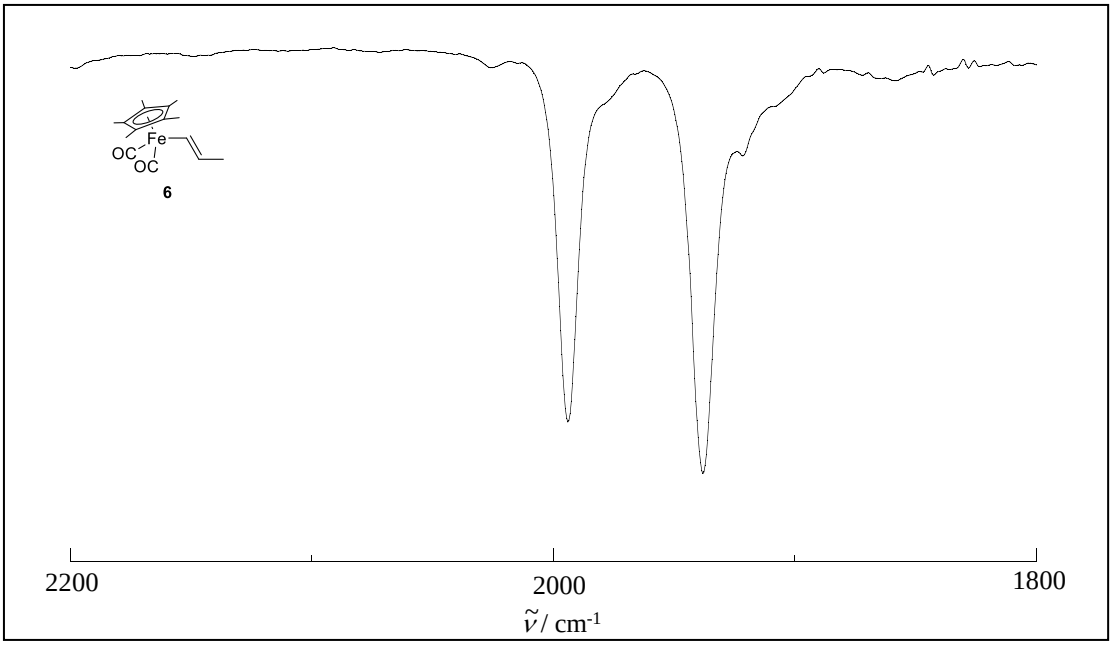

Figure S9. IR spectrum of crude **6** (C_6H_6).

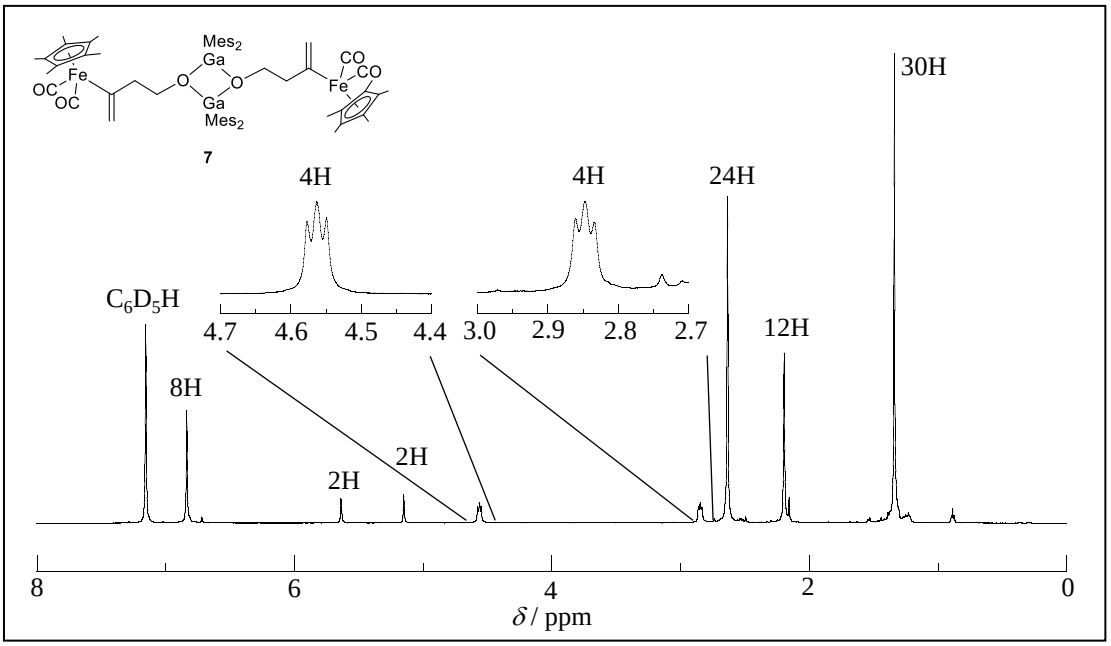

Figure S10. ^{1}H NMR spectrum of **7** (600 MHz, C_6D_6).

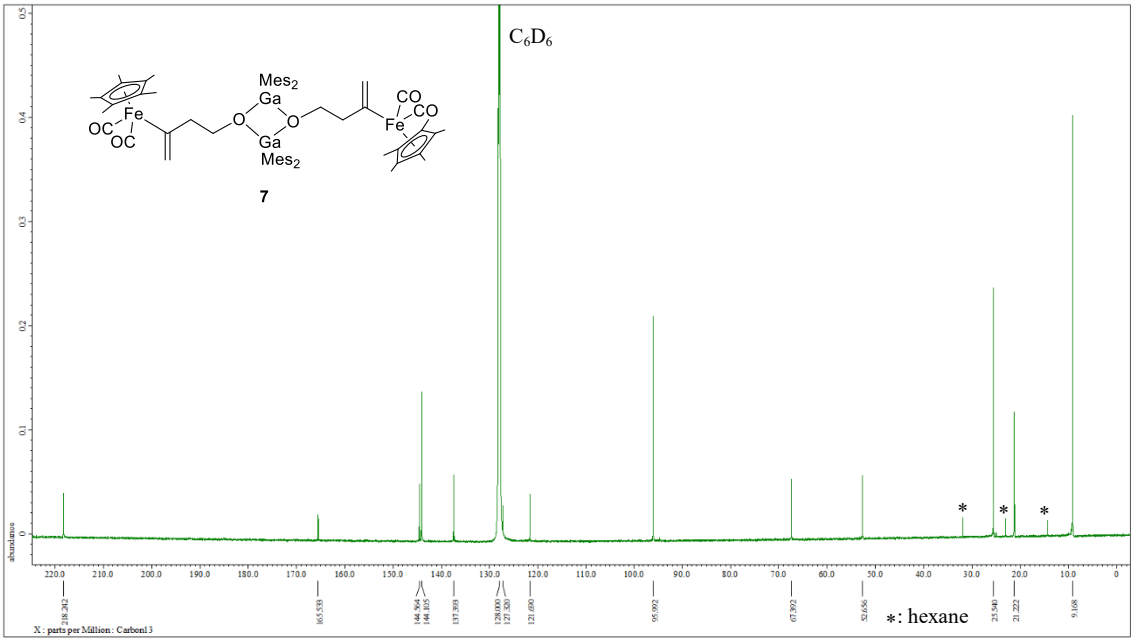

Figure S11. ^{13}C NMR spectrum of **7** (150.6 MHz, C_6D_6).

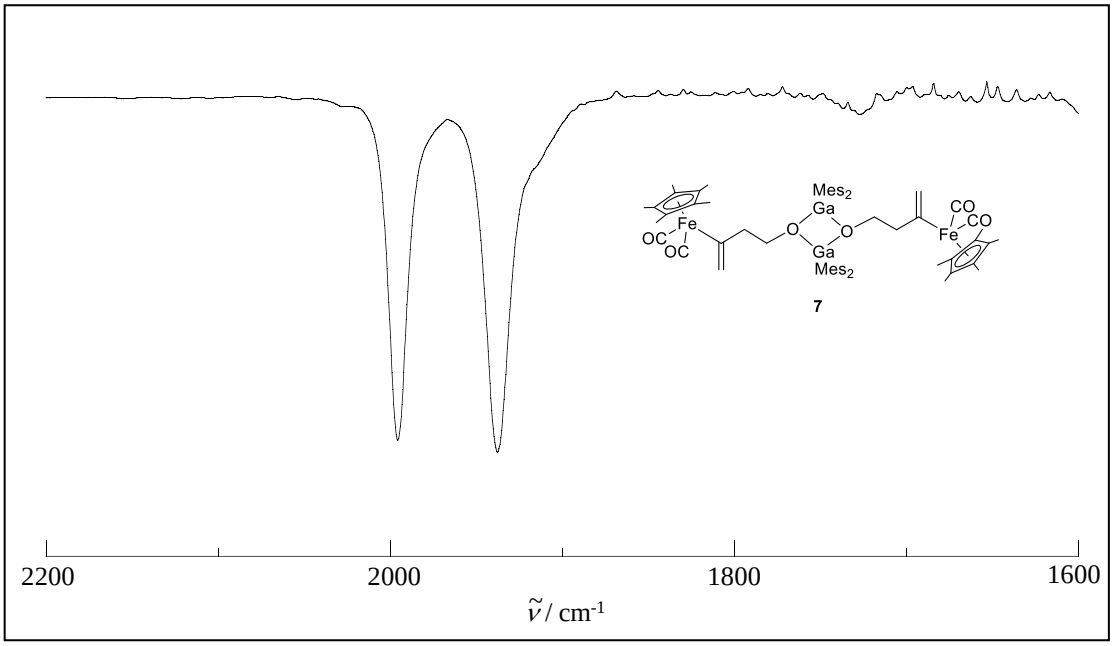

Figure S12. IR spectrum of **7** (CH_2Cl_2).

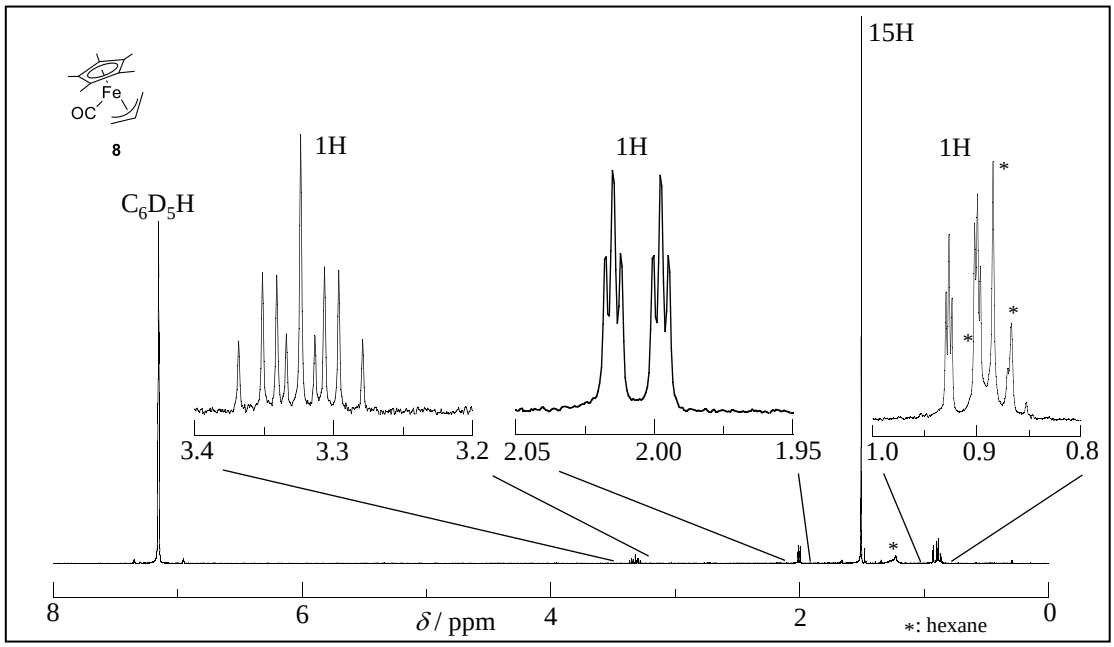

Figure S13. ^{1}H NMR spectrum of **8** (400 MHz, C_6D_6).

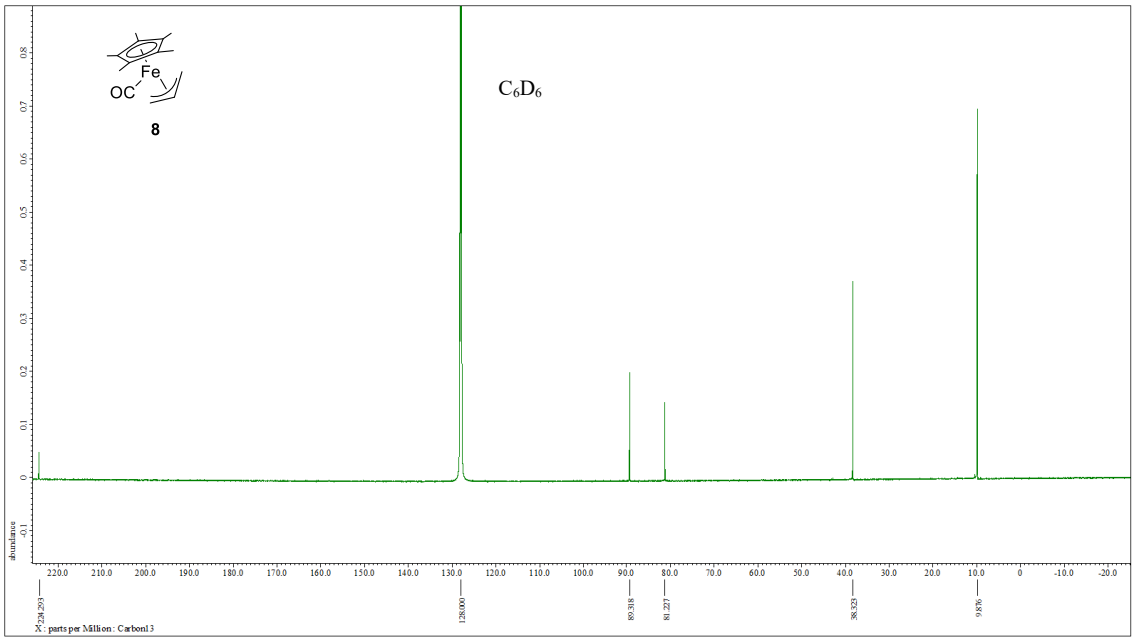

Figure S14. ^{13}C NMR spectrum of **8** (150.6 MHz, C_6D_6).

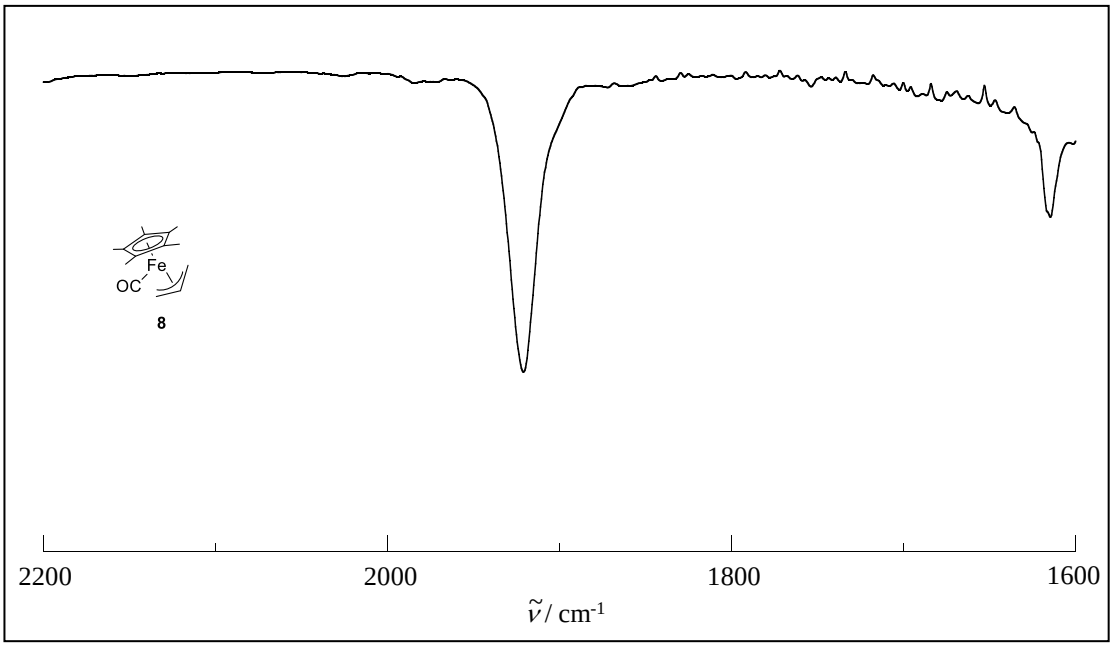

Figure S15. IR spectrum of **8** (C_6D_6).

Table S1. Crystal data and structure refinement for complex **7·toluene**.

Complex	$[Cp^*(OC)_2FeC(=CH_2)CH_2CH_2OGaMes_2]_2 \cdot C_7H_8$ (**7·toluene**)
Empirical formula	$C_{75}H_{94}Fe_2Ga_2O_6$
Formula weight	1342.64
Temperature (K)	93(2)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 13.572(3) Å b = 28.859(5) Å β = 99.767(5)° c = 17.651(3) Å
Volume (Å^3)	6813(2)
Z	4
D_{calc} (Mg / m^3)	1.309
Absorption coefficient (mm^{-1})	1.250
F(000)	2824
Crystal Size (mm^3)	0.30 × 0.15 × 0.05
θ Range for data collection (°)	2.734 – 27.584
Index ranges	$-17 \le h \le 17$, $-37 \le k \le 37$, $-22 \le l \le 22$
Reflections collected	117960
Independent reflections [R(int)]	15691 [0.1118]
Absorption correction	Semi-empirical from equivalents
Maximum and minimum transmission	1.000 and 0.722
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	15691 / 0 / 789
Goodness-of-fit on F^2	1.034
Final R indices[a] [$I > 2\sigma(I)$]	$R1$ = 0.0368, w$R2$ = 0.0975
R indices[a] (all data)	$R1$ = 0.0510, w$R2$ = 0.1024
Largest difference in peak and hole (eÅ^{-3})	1.097 and -0.384

[a]$R1 = \Sigma||Fo| - |Fc|| / \Sigma|Fo|$.
$wR2 = [\Sigma[w\,(Fo^2 - Fc^2)^2] / \Sigma[w\,(Fo^2)^2]]^{0.5}$,
calc $w = 1 / [\sigma^2(Fo^2) + (0.0559\,P)^2]$ where $P = (Fo^2 + 2Fc^2) / 3$.

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **7·toluene**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	*U*(eq)
Fe(1)	2468(1)	6370(1)	1549(1)	25(1)
Ga(1)	3428(1)	4281(1)	2550(1)	19(1)
O(1)	617(1)	5856(1)	1466(1)	45(1)
O(2)	2101(2)	6992(1)	2759(1)	50(1)
O(3)	2519(1)	4752(1)	2850(1)	21(1)
C(1)	1365(2)	6048(1)	1525(1)	31(1)
C(2)	2243(2)	6741(1)	2285(2)	33(1)
C(3)	2123(2)	6493(1)	360(1)	30(1)
C(4)	2509(2)	6901(1)	738(1)	31(1)
C(5)	3506(2)	6803(1)	1130(2)	33(1)
C(6)	3729(2)	6336(1)	971(1)	33(1)
C(7)	2877(2)	6139(1)	510(1)	32(1)
C(8)	1129(2)	6433(1)	-150(2)	43(1)
C(9)	2008(2)	7364(1)	698(2)	43(1)
C(10)	4214(2)	7152(1)	1554(2)	50(1)
C(11)	4730(2)	6106(1)	1201(2)	46(1)
C(12)	2813(2)	5663(1)	172(2)	46(1)
C(13)	3259(2)	5965(1)	2355(1)	26(1)
C(14)	3149(2)	5441(1)	2277(1)	24(1)
C(15)	2575(2)	5249(1)	2871(1)	24(1)
C(16)	3909(2)	6131(1)	2942(2)	38(1)
C(17)	3231(2)	4309(1)	1405(1)	21(1)
C(18)	4016(2)	4478(1)	1048(1)	23(1)
C(19)	3873(2)	4547(1)	257(1)	25(1)
C(20)	2953(2)	4470(1)	-212(1)	26(1)
C(21)	2190(2)	4299(1)	135(1)	24(1)
C(22)	2311(2)	4206(1)	923(1)	22(1)
C(23)	5042(2)	4586(1)	1501(1)	28(1)
C(24)	2795(2)	4569(1)	-1063(1)	33(1)
C(25)	1446(2)	3975(1)	1211(1)	27(1)
C(26)	4726(2)	4150(1)	3231(1)	21(1)

C(27)	5159(2)	4441(1)	3841(1)	23(1)
C(28)	6013(2)	4303(1)	4345(1)	24(1)
C(29)	6462(2)	3878(1)	4266(1)	26(1)
C(30)	6056(2)	3597(1)	3659(1)	26(1)
C(31)	5200(2)	3727(1)	3137(1)	23(1)
C(32)	4718(2)	4908(1)	3963(1)	28(1)
C(33)	7390(2)	3736(1)	4823(1)	32(1)
C(34)	4831(2)	3399(1)	2481(1)	27(1)
Fe(2)	1559(1)	2152(1)	2127(1)	25(1)
Ga(2)	1745(1)	4395(1)	3476(1)	20(1)
O(4)	3304(2)	1578(1)	2069(2)	66(1)
O(5)	1575(2)	2625(1)	679(1)	60(1)
O(6)	2500(1)	3916(1)	3043(1)	21(1)
C(35)	2616(2)	1807(1)	2087(2)	42(1)
C(36)	1613(2)	2446(1)	1264(2)	38(1)
C(37)	524(2)	2271(1)	2892(1)	25(1)
C(38)	51(2)	2327(1)	2120(1)	27(1)
C(39)	110(2)	1894(1)	1731(1)	28(1)
C(40)	643(2)	1579(1)	2260(1)	28(1)
C(41)	918(2)	1814(1)	2980(1)	27(1)
C(42)	547(2)	2622(1)	3519(1)	33(1)
C(43)	-517(2)	2743(1)	1778(2)	37(1)
C(44)	-387(2)	1786(1)	924(1)	41(1)
C(45)	850(2)	1079(1)	2110(2)	40(1)
C(46)	1417(2)	1610(1)	3729(1)	40(1)
C(47)	2461(2)	2601(1)	2783(1)	25(1)
C(48)	2278(2)	3111(1)	2603(1)	23(1)
C(49)	2664(2)	3437(1)	3261(1)	23(1)
C(50)	3152(2)	2466(1)	3368(1)	32(1)
C(51)	335(2)	4250(1)	3027(1)	23(1)
C(52)	-193(2)	4425(1)	2327(1)	24(1)
C(53)	-1120(2)	4242(1)	2007(1)	27(1)
C(54)	-1575(2)	3896(1)	2368(1)	28(1)
C(55)	-1088(2)	3744(1)	3080(1)	28(1)
C(56)	-151(2)	3914(1)	3411(1)	24(1)
C(57)	201(2)	4832(1)	1929(1)	30(1)

C(58)	-2583(2)	3704(1)	2017(2)	37(1)
C(59)	306(2)	3743(1)	4201(1)	28(1)
C(60)	2098(2)	4586(1)	4572(1)	22(1)
C(61)	1564(2)	4964(1)	4809(1)	24(1)
C(62)	1703(2)	5095(1)	5581(1)	27(1)
C(63)	2381(2)	4868(1)	6137(1)	29(1)
C(64)	2908(2)	4499(1)	5903(1)	28(1)
C(65)	2783(2)	4356(1)	5138(1)	23(1)
C(66)	835(2)	5244(1)	4243(1)	29(1)
C(67)	2558(2)	5027(1)	6961(1)	41(1)
C(68)	3395(2)	3950(1)	4954(1)	33(1)
C(71)	4561(2)	2112(1)	5453(1)	35(1)
C(72)	4395(2)	2586(1)	5419(2)	49(1)
C(73)	5187(3)	2898(1)	5537(2)	64(1)
C(74)	6156(2)	2738(1)	5711(2)	51(1)
C(75)	6329(2)	2270(1)	5754(2)	43(1)
C(76)	5540(2)	1963(1)	5616(1)	36(1)
C(77)	3718(2)	1777(1)	5317(2)	50(1)

Table S3. Bond lengths [Å] and angles [°] for **7·toluene**.

Fe(1)-C(2)	1.749(3)	C(20)-C(21)	1.381(3)
Fe(1)-C(1)	1.756(2)	C(20)-C(24)	1.508(3)
Fe(1)-C(13)	2.006(2)	C(21)-C(22)	1.398(3)
Fe(1)-C(3)	2.100(2)	C(22)-C(25)	1.513(3)
Fe(1)-C(4)	2.104(2)	C(26)-C(31)	1.404(3)
Fe(1)-C(5)	2.108(2)	C(26)-C(27)	1.412(3)
Fe(1)-C(7)	2.112(2)	C(27)-C(28)	1.394(3)
Fe(1)-C(6)	2.138(2)	C(27)-C(32)	1.504(3)
Ga(1)-O(6)	1.9556(14)	C(28)-C(29)	1.389(3)
Ga(1)-O(3)	1.9688(14)	C(29)-C(30)	1.380(3)
Ga(1)-C(26)	1.993(2)	C(29)-C(33)	1.517(3)
Ga(1)-C(17)	1.995(2)	C(30)-C(31)	1.405(3)
O(1)-C(1)	1.146(3)	C(31)-C(34)	1.513(3)
O(2)-C(2)	1.149(3)	Fe(2)-C(36)	1.755(3)
O(3)-C(15)	1.435(2)	Fe(2)-C(35)	1.758(3)
O(3)-Ga(2)	1.9448(14)	Fe(2)-C(47)	2.010(2)
C(3)-C(4)	1.408(3)	Fe(2)-C(41)	2.102(2)
C(3)-C(7)	1.439(3)	Fe(2)-C(40)	2.106(2)
C(3)-C(8)	1.500(3)	Fe(2)-C(38)	2.106(2)
C(4)-C(5)	1.439(3)	Fe(2)-C(39)	2.108(2)
C(4)-C(9)	1.497(3)	Fe(2)-C(37)	2.135(2)
C(5)-C(6)	1.420(3)	Ga(2)-O(6)	1.9539(14)
C(5)-C(10)	1.501(4)	Ga(2)-C(51)	1.988(2)
C(6)-C(7)	1.415(4)	Ga(2)-C(60)	1.990(2)
C(6)-C(11)	1.505(3)	O(4)-C(35)	1.148(3)
C(7)-C(12)	1.494(3)	O(5)-C(36)	1.148(3)
C(13)-C(16)	1.332(3)	O(6)-C(49)	1.440(2)
C(13)-C(14)	1.522(3)	C(37)-C(38)	1.414(3)
C(14)-C(15)	1.514(3)	C(37)-C(41)	1.423(3)
C(17)-C(18)	1.413(3)	C(37)-C(42)	1.496(3)
C(17)-C(22)	1.417(3)	C(38)-C(39)	1.434(3)
C(18)-C(19)	1.390(3)	C(38)-C(43)	1.499(3)
C(18)-C(23)	1.516(3)	C(39)-C(40)	1.413(3)
C(19)-C(20)	1.394(3)	C(39)-C(44)	1.502(3)

C(40)-C(41)	1.433(3)	C(60)-C(61)	1.412(3)
C(40)-C(45)	1.501(3)	C(61)-C(62)	1.395(3)
C(41)-C(46)	1.499(3)	C(61)-C(66)	1.514(3)
C(47)-C(50)	1.330(3)	C(62)-C(63)	1.390(3)
C(47)-C(48)	1.517(3)	C(63)-C(64)	1.383(3)
C(48)-C(49)	1.519(3)	C(63)-C(67)	1.506(3)
C(51)-C(56)	1.409(3)	C(64)-C(65)	1.395(3)
C(51)-C(52)	1.412(3)	C(65)-C(68)	1.505(3)
C(52)-C(53)	1.394(3)	C(71)-C(76)	1.380(3)
C(52)-C(57)	1.511(3)	C(71)-C(72)	1.385(4)
C(53)-C(54)	1.384(3)	C(71)-C(77)	1.486(4)
C(54)-C(55)	1.388(3)	C(72)-C(73)	1.391(4)
C(54)-C(58)	1.509(3)	C(73)-C(74)	1.378(5)
C(55)-C(56)	1.396(3)	C(74)-C(75)	1.373(4)
C(56)-C(59)	1.510(3)	C(75)-C(76)	1.379(4)
C(60)-C(65)	1.411(3)		

C(2)-Fe(1)-C(1)	94.89(11)	C(4)-Fe(1)-C(7)	66.26(9)
C(2)-Fe(1)-C(13)	88.22(10)	C(5)-Fe(1)-C(7)	65.98(10)
C(1)-Fe(1)-C(13)	93.43(10)	C(2)-Fe(1)-C(6)	129.56(11)
C(2)-Fe(1)-C(3)	126.92(10)	C(1)-Fe(1)-C(6)	135.47(11)
C(1)-Fe(1)-C(3)	91.23(10)	C(13)-Fe(1)-C(6)	86.36(9)
C(13)-Fe(1)-C(3)	143.99(9)	C(3)-Fe(1)-C(6)	65.95(9)
C(2)-Fe(1)-C(4)	95.07(11)	C(4)-Fe(1)-C(6)	65.99(9)
C(1)-Fe(1)-C(4)	119.33(10)	C(5)-Fe(1)-C(6)	39.06(9)
C(13)-Fe(1)-C(4)	146.54(9)	C(7)-Fe(1)-C(6)	38.90(10)
C(3)-Fe(1)-C(4)	39.12(9)	O(6)-Ga(1)-O(3)	76.86(6)
C(2)-Fe(1)-C(5)	96.25(11)	O(6)-Ga(1)-C(26)	101.50(7)
C(1)-Fe(1)-C(5)	157.34(10)	O(3)-Ga(1)-C(26)	119.89(7)
C(13)-Fe(1)-C(5)	106.57(9)	O(6)-Ga(1)-C(17)	119.14(7)
C(3)-Fe(1)-C(5)	66.34(9)	O(3)-Ga(1)-C(17)	105.19(7)
C(4)-Fe(1)-C(5)	39.97(9)	C(26)-Ga(1)-C(17)	124.88(8)
C(2)-Fe(1)-C(7)	160.47(10)	C(15)-O(3)-Ga(2)	123.13(12)
C(1)-Fe(1)-C(7)	99.30(11)	C(15)-O(3)-Ga(1)	131.58(12)
C(13)-Fe(1)-C(7)	104.16(9)	Ga(2)-O(3)-Ga(1)	102.13(6)
C(3)-Fe(1)-C(7)	39.94(9)	O(1)-C(1)-Fe(1)	175.3(2)

O(2)-C(2)-Fe(1)	178.5(2)	C(18)-C(17)-C(22)	117.27(19)
C(4)-C(3)-C(7)	108.1(2)	C(18)-C(17)-Ga(1)	118.97(15)
C(4)-C(3)-C(8)	127.3(2)	C(22)-C(17)-Ga(1)	123.53(15)
C(7)-C(3)-C(8)	124.5(2)	C(19)-C(18)-C(17)	120.66(19)
C(4)-C(3)-Fe(1)	70.57(13)	C(19)-C(18)-C(23)	117.35(19)
C(7)-C(3)-Fe(1)	70.47(13)	C(17)-C(18)-C(23)	121.98(19)
C(8)-C(3)-Fe(1)	127.29(17)	C(18)-C(19)-C(20)	122.1(2)
C(3)-C(4)-C(5)	107.9(2)	C(21)-C(20)-C(19)	117.2(2)
C(3)-C(4)-C(9)	126.5(2)	C(21)-C(20)-C(24)	121.3(2)
C(5)-C(4)-C(9)	125.4(2)	C(19)-C(20)-C(24)	121.5(2)
C(3)-C(4)-Fe(1)	70.31(13)	C(20)-C(21)-C(22)	122.6(2)
C(5)-C(4)-Fe(1)	70.16(13)	C(21)-C(22)-C(17)	120.02(19)
C(9)-C(4)-Fe(1)	128.18(17)	C(21)-C(22)-C(25)	116.82(18)
C(6)-C(5)-C(4)	107.8(2)	C(17)-C(22)-C(25)	123.08(19)
C(6)-C(5)-C(10)	126.5(2)	C(31)-C(26)-C(27)	117.85(19)
C(4)-C(5)-C(10)	125.3(2)	C(31)-C(26)-Ga(1)	118.00(15)
C(6)-C(5)-Fe(1)	71.63(14)	C(27)-C(26)-Ga(1)	123.97(15)
C(4)-C(5)-Fe(1)	69.86(13)	C(28)-C(27)-C(26)	120.72(19)
C(10)-C(5)-Fe(1)	129.27(19)	C(28)-C(27)-C(32)	118.17(19)
C(7)-C(6)-C(5)	108.3(2)	C(26)-C(27)-C(32)	121.11(18)
C(7)-C(6)-C(11)	126.2(2)	C(29)-C(28)-C(27)	121.3(2)
C(5)-C(6)-C(11)	125.3(2)	C(30)-C(29)-C(28)	118.21(19)
C(7)-C(6)-Fe(1)	69.55(14)	C(30)-C(29)-C(33)	121.5(2)
C(5)-C(6)-Fe(1)	69.31(13)	C(28)-C(29)-C(33)	120.24(19)
C(11)-C(6)-Fe(1)	130.62(18)	C(29)-C(30)-C(31)	122.0(2)
C(6)-C(7)-C(3)	107.9(2)	C(26)-C(31)-C(30)	119.92(19)
C(6)-C(7)-C(12)	125.8(2)	C(26)-C(31)-C(34)	122.38(19)
C(3)-C(7)-C(12)	126.1(2)	C(30)-C(31)-C(34)	117.70(19)
C(6)-C(7)-Fe(1)	71.55(14)	C(36)-Fe(2)-C(35)	94.87(13)
C(3)-C(7)-Fe(1)	69.59(13)	C(36)-Fe(2)-C(47)	94.47(10)
C(12)-C(7)-Fe(1)	129.05(18)	C(35)-Fe(2)-C(47)	88.10(10)
C(16)-C(13)-C(14)	118.0(2)	C(36)-Fe(2)-C(41)	158.25(11)
C(16)-C(13)-Fe(1)	123.14(17)	C(35)-Fe(2)-C(41)	101.83(12)
C(14)-C(13)-Fe(1)	118.82(15)	C(47)-Fe(2)-C(41)	99.87(9)
C(15)-C(14)-C(13)	110.84(18)	C(36)-Fe(2)-C(40)	126.07(10)
O(3)-C(15)-C(14)	112.36(17)	C(35)-Fe(2)-C(40)	93.47(11)

C(47)-Fe(2)-C(40)	139.02(9)	C(42)-C(37)-Fe(2)	130.10(15)
C(41)-Fe(2)-C(40)	39.81(9)	C(37)-C(38)-C(39)	108.08(19)
C(36)-Fe(2)-C(38)	93.61(11)	C(37)-C(38)-C(43)	126.7(2)
C(35)-Fe(2)-C(38)	159.14(10)	C(39)-C(38)-C(43)	124.9(2)
C(47)-Fe(2)-C(38)	110.20(9)	C(37)-C(38)-Fe(2)	71.64(13)
C(41)-Fe(2)-C(38)	66.14(9)	C(39)-C(38)-Fe(2)	70.15(12)
C(40)-Fe(2)-C(38)	66.25(9)	C(43)-C(38)-Fe(2)	128.84(17)
C(36)-Fe(2)-C(39)	93.24(10)	C(40)-C(39)-C(38)	107.92(19)
C(35)-Fe(2)-C(39)	120.58(10)	C(40)-C(39)-C(44)	126.2(2)
C(47)-Fe(2)-C(39)	149.49(9)	C(38)-C(39)-C(44)	125.7(2)
C(41)-Fe(2)-C(39)	66.30(8)	C(40)-C(39)-Fe(2)	70.35(13)
C(40)-Fe(2)-C(39)	39.19(9)	C(38)-C(39)-Fe(2)	70.07(12)
C(38)-Fe(2)-C(39)	39.78(9)	C(44)-C(39)-Fe(2)	129.24(17)
C(36)-Fe(2)-C(37)	126.85(11)	C(39)-C(40)-C(41)	107.98(19)
C(35)-Fe(2)-C(37)	138.19(12)	C(39)-C(40)-C(45)	126.3(2)
C(47)-Fe(2)-C(37)	86.15(8)	C(41)-C(40)-C(45)	125.7(2)
C(41)-Fe(2)-C(37)	39.22(8)	C(39)-C(40)-Fe(2)	70.46(13)
C(40)-Fe(2)-C(37)	65.91(9)	C(41)-C(40)-Fe(2)	69.95(12)
C(38)-Fe(2)-C(37)	38.93(8)	C(45)-C(40)-Fe(2)	127.08(17)
C(39)-Fe(2)-C(37)	65.80(8)	C(37)-C(41)-C(40)	107.82(19)
O(3)-Ga(2)-O(6)	77.46(6)	C(37)-C(41)-C(46)	124.4(2)
O(3)-Ga(2)-C(51)	117.50(8)	C(40)-C(41)-C(46)	127.3(2)
O(6)-Ga(2)-C(51)	103.21(7)	C(37)-C(41)-Fe(2)	71.65(12)
O(3)-Ga(2)-C(60)	109.95(7)	C(40)-C(41)-Fe(2)	70.25(13)
O(6)-Ga(2)-C(60)	121.38(7)	C(46)-C(41)-Fe(2)	129.37(17)
C(51)-Ga(2)-C(60)	120.18(9)	C(50)-C(47)-C(48)	121.05(19)
C(49)-O(6)-Ga(2)	129.86(12)	C(50)-C(47)-Fe(2)	122.63(17)
C(49)-O(6)-Ga(1)	123.64(12)	C(48)-C(47)-Fe(2)	116.24(15)
Ga(2)-O(6)-Ga(1)	102.29(6)	C(47)-C(48)-C(49)	114.71(17)
O(4)-C(35)-Fe(2)	179.1(3)	O(6)-C(49)-C(48)	111.81(16)
O(5)-C(36)-Fe(2)	174.7(2)	C(56)-C(51)-C(52)	117.27(19)
C(38)-C(37)-C(41)	108.13(19)	C(56)-C(51)-Ga(2)	116.78(15)
C(38)-C(37)-C(42)	125.9(2)	C(52)-C(51)-Ga(2)	125.74(16)
C(41)-C(37)-C(42)	125.9(2)	C(53)-C(52)-C(51)	120.5(2)
C(38)-C(37)-Fe(2)	69.43(13)	C(53)-C(52)-C(57)	118.2(2)
C(41)-C(37)-Fe(2)	69.12(12)	C(51)-C(52)-C(57)	121.24(19)

C(54)-C(53)-C(52)	122.0(2)	C(64)-C(63)-C(62)	117.8(2)
C(53)-C(54)-C(55)	117.7(2)	C(64)-C(63)-C(67)	121.1(2)
C(53)-C(54)-C(58)	121.3(2)	C(62)-C(63)-C(67)	121.1(2)
C(55)-C(54)-C(58)	121.0(2)	C(63)-C(64)-C(65)	122.1(2)
C(54)-C(55)-C(56)	121.8(2)	C(64)-C(65)-C(60)	120.31(19)
C(55)-C(56)-C(51)	120.5(2)	C(64)-C(65)-C(68)	117.37(19)
C(55)-C(56)-C(59)	118.3(2)	C(60)-C(65)-C(68)	122.31(19)
C(51)-C(56)-C(59)	121.13(19)	C(76)-C(71)-C(72)	117.5(2)
C(65)-C(60)-C(61)	117.53(19)	C(76)-C(71)-C(77)	121.2(2)
C(65)-C(60)-Ga(2)	125.49(15)	C(72)-C(71)-C(77)	121.3(3)
C(61)-C(60)-Ga(2)	116.83(15)	C(71)-C(72)-C(73)	121.1(3)
C(62)-C(61)-C(60)	120.6(2)	C(74)-C(73)-C(72)	120.1(3)
C(62)-C(61)-C(66)	117.71(19)	C(75)-C(74)-C(73)	119.3(3)
C(60)-C(61)-C(66)	121.73(19)	C(74)-C(75)-C(76)	120.2(3)
C(63)-C(62)-C(61)	121.7(2)	C(71)-C(76)-C(75)	121.9(2)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **7·toluene**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe(1)	23(1)	23(1)	28(1)	2(1)	5(1)	0(1)
Ga(1)	18(1)	23(1)	17(1)	-1(1)	2(1)	-1(1)
O(1)	28(1)	43(1)	62(1)	20(1)	0(1)	-6(1)
O(2)	48(1)	56(1)	47(1)	-17(1)	7(1)	11(1)
O(3)	21(1)	20(1)	22(1)	0(1)	5(1)	0(1)
C(1)	31(1)	30(1)	31(1)	9(1)	3(1)	2(1)
C(2)	28(1)	34(1)	39(1)	1(1)	5(1)	3(1)
C(3)	33(1)	30(1)	29(1)	7(1)	8(1)	2(1)
C(4)	32(1)	26(1)	38(1)	9(1)	14(1)	1(1)
C(5)	27(1)	32(1)	42(1)	4(1)	10(1)	-4(1)
C(6)	31(1)	36(1)	36(1)	7(1)	13(1)	7(1)
C(7)	40(1)	30(1)	26(1)	6(1)	9(1)	5(1)
C(8)	44(2)	45(2)	36(1)	10(1)	-2(1)	1(1)
C(9)	49(2)	29(1)	53(2)	11(1)	19(1)	8(1)
C(10)	39(2)	46(2)	65(2)	-1(1)	11(1)	-14(1)
C(11)	36(1)	56(2)	50(2)	11(1)	16(1)	15(1)
C(12)	74(2)	33(1)	32(1)	0(1)	9(1)	10(1)
C(13)	25(1)	25(1)	28(1)	3(1)	5(1)	-1(1)
C(14)	25(1)	24(1)	23(1)	2(1)	3(1)	1(1)
C(15)	24(1)	21(1)	26(1)	0(1)	1(1)	2(1)
C(16)	40(1)	26(1)	44(2)	3(1)	-5(1)	-2(1)
C(17)	21(1)	23(1)	19(1)	-1(1)	2(1)	1(1)
C(18)	23(1)	24(1)	21(1)	0(1)	4(1)	2(1)
C(19)	26(1)	26(1)	24(1)	1(1)	9(1)	0(1)
C(20)	33(1)	22(1)	21(1)	-1(1)	3(1)	-1(1)
C(21)	26(1)	27(1)	20(1)	-3(1)	-1(1)	0(1)
C(22)	23(1)	24(1)	20(1)	-2(1)	3(1)	1(1)
C(23)	23(1)	35(1)	27(1)	1(1)	6(1)	-3(1)
C(24)	42(1)	37(1)	20(1)	1(1)	3(1)	-4(1)
C(25)	23(1)	36(1)	22(1)	0(1)	0(1)	-4(1)
C(26)	19(1)	26(1)	19(1)	0(1)	4(1)	-1(1)
C(27)	22(1)	26(1)	21(1)	1(1)	3(1)	0(1)
C(28)	23(1)	28(1)	21(1)	-1(1)	-1(1)	-2(1)

C(29)	22(1)	29(1)	24(1)	4(1)	-1(1)	-2(1)
C(30)	24(1)	24(1)	28(1)	2(1)	4(1)	2(1)
C(31)	20(1)	27(1)	23(1)	0(1)	4(1)	-3(1)
C(32)	28(1)	27(1)	26(1)	-5(1)	-3(1)	2(1)
C(33)	29(1)	32(1)	31(1)	4(1)	-5(1)	2(1)
C(34)	25(1)	28(1)	27(1)	-4(1)	3(1)	1(1)
Fe(2)	26(1)	24(1)	26(1)	-4(1)	5(1)	-2(1)
Ga(2)	19(1)	22(1)	18(1)	-1(1)	3(1)	0(1)
O(4)	39(1)	54(1)	104(2)	-35(1)	10(1)	10(1)
O(5)	83(2)	68(1)	29(1)	2(1)	14(1)	-30(1)
O(6)	21(1)	20(1)	22(1)	-1(1)	6(1)	0(1)
C(35)	36(1)	35(1)	54(2)	-18(1)	8(1)	-5(1)
C(36)	44(2)	40(1)	31(1)	-9(1)	11(1)	-16(1)
C(37)	23(1)	26(1)	27(1)	-2(1)	5(1)	-6(1)
C(38)	22(1)	30(1)	29(1)	1(1)	5(1)	-2(1)
C(39)	27(1)	31(1)	24(1)	0(1)	1(1)	-4(1)
C(40)	29(1)	24(1)	31(1)	0(1)	2(1)	-4(1)
C(41)	28(1)	26(1)	25(1)	2(1)	1(1)	-4(1)
C(42)	34(1)	37(1)	31(1)	-6(1)	13(1)	-6(1)
C(43)	34(1)	33(1)	43(2)	8(1)	1(1)	4(1)
C(44)	48(2)	46(2)	26(1)	-3(1)	-4(1)	-10(1)
C(45)	47(2)	24(1)	47(2)	-6(1)	3(1)	-4(1)
C(46)	46(2)	36(1)	33(1)	7(1)	-8(1)	-6(1)
C(47)	24(1)	24(1)	26(1)	-4(1)	6(1)	-3(1)
C(48)	21(1)	25(1)	22(1)	0(1)	3(1)	-2(1)
C(49)	25(1)	21(1)	22(1)	0(1)	5(1)	0(1)
C(50)	29(1)	24(1)	39(1)	-1(1)	0(1)	-2(1)
C(51)	22(1)	24(1)	23(1)	-3(1)	6(1)	2(1)
C(52)	22(1)	25(1)	27(1)	-3(1)	6(1)	2(1)
C(53)	23(1)	31(1)	25(1)	-3(1)	1(1)	4(1)
C(54)	20(1)	33(1)	31(1)	-7(1)	5(1)	-1(1)
C(55)	25(1)	29(1)	32(1)	-4(1)	14(1)	-3(1)
C(56)	24(1)	25(1)	24(1)	-4(1)	8(1)	2(1)
C(57)	27(1)	32(1)	29(1)	5(1)	-1(1)	-1(1)
C(58)	25(1)	43(1)	41(1)	-5(1)	3(1)	-6(1)
C(59)	30(1)	31(1)	25(1)	0(1)	9(1)	-4(1)

C(60)	22(1)	25(1)	19(1)	-2(1)	5(1)	-1(1)
C(61)	22(1)	25(1)	25(1)	-2(1)	7(1)	-2(1)
C(62)	30(1)	25(1)	29(1)	-5(1)	12(1)	-1(1)
C(63)	37(1)	29(1)	21(1)	-4(1)	10(1)	-5(1)
C(64)	32(1)	30(1)	20(1)	1(1)	2(1)	-1(1)
C(65)	25(1)	25(1)	21(1)	-1(1)	7(1)	0(1)
C(66)	26(1)	30(1)	31(1)	-4(1)	5(1)	4(1)
C(67)	57(2)	42(1)	23(1)	-6(1)	9(1)	1(1)
C(68)	39(1)	34(1)	23(1)	-3(1)	-2(1)	11(1)
C(71)	37(1)	40(1)	27(1)	3(1)	4(1)	-1(1)
C(72)	47(2)	41(2)	56(2)	-4(1)	-3(1)	11(1)
C(73)	73(2)	37(2)	72(2)	-4(2)	-11(2)	6(2)
C(74)	52(2)	48(2)	51(2)	1(1)	-1(1)	-14(1)
C(75)	35(1)	55(2)	38(1)	5(1)	6(1)	0(1)
C(76)	39(1)	37(1)	32(1)	3(1)	6(1)	7(1)
C(77)	45(2)	57(2)	45(2)	11(1)	0(1)	-8(1)

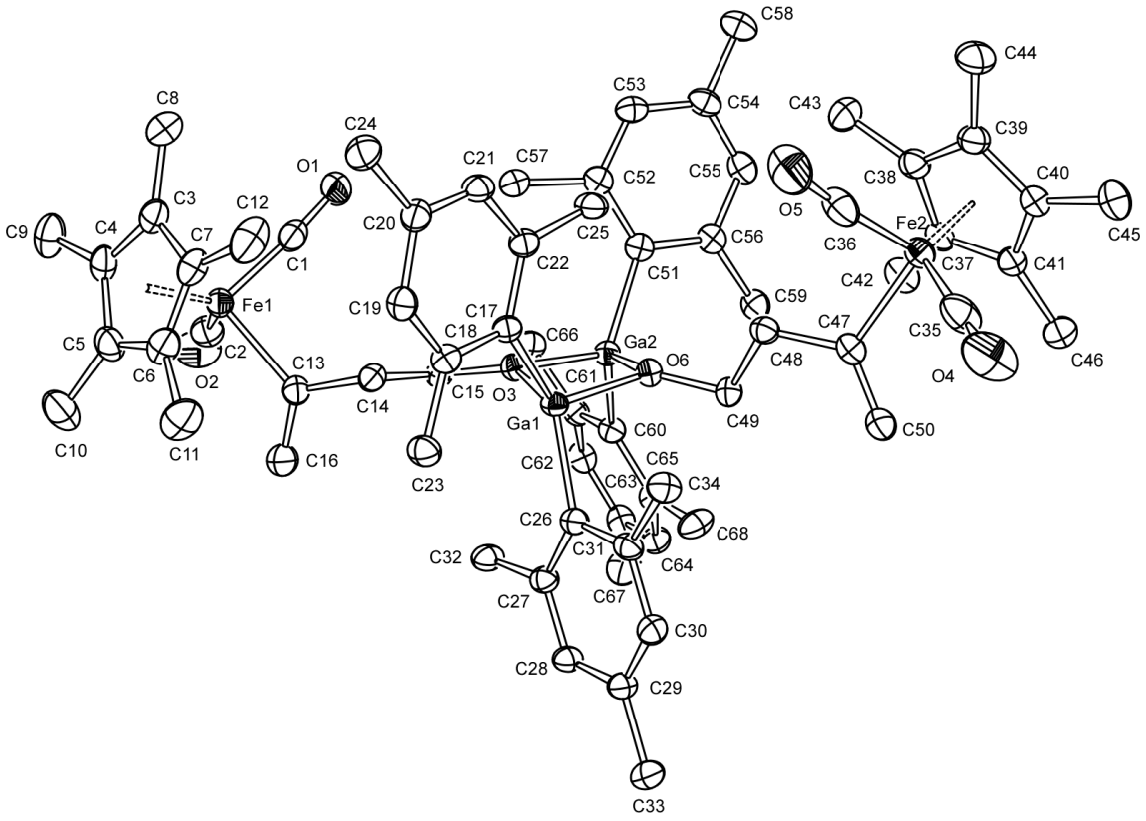

Figure S16. ORTEP drawing of **7** (thermal ellipsoids at the 50% probability level). Hydrogen atoms are omitted for clarity.