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Supporting Information

The Trinuclear Gallium-Bridged Ferrocenophane $[\{Fe(\eta^5\text{-}C_5H_4)_2\}_3Ga_2]$: Synthesis, Bonding, Structure and Coordination Chemistry

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Table 1. Atomic coordinates for **3**.

Figure 1. Molecular structure and crystallographic numbering scheme of [**3c**·DMSO].

Table 2. Crystal data and structure refinement for [**3c**·DMSO].

Table 3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for [**3c**·DMSO].

U(eq) is defined as one third of the trace of the Orthogonalized Uij tensor.

Table 4. Bond lengths [A] and angles [deg] for [**3c**·DMSO].

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for [**3c**·DMSO].

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for [**3c**·DMSO].

Figure 3. Molecular structure and crystallographic numbering scheme of [**3d**·0.75 toluene].

Table 7. Crystal data and structure refinement for [**3d**·0.75 toluene].

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for [**3d**·0.75 toluene].

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Table 9. Bond lengths [A] and angles [deg] for [**3d**·0.75 toluene].

Table 10. Anisotropic displacement parameters (A^2 x 10^3) for [**3d**·0.75 toluene].The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

Table 11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for [**3d**·0.75 toluene].

Table 1. Atomic coordinates for **3**.

	x	y	z
Ga1	0.000000	0.000000	1.689792
Ga2	0.000000	0.000000	-1.689792
Fe1	0.000000	3.156772	0.000000
Fe2	-2.733845	-1.578386	0.000000
Fe3	2.733845	-1.578386	0.000000
C1	0.000000	1.948447	1.689936
C2	1.145873	2.819654	1.669803
C3	0.713212	4.175727	1.639986
C4	-0.713212	4.175727	1.639986
C5	-1.145873	2.819654	1.669803
C6	0.000000	1.948447	-1.689936
C7	-1.145873	2.819654	-1.669803
C8	-0.713212	4.175727	-1.639986
C9	0.713212	4.175727	-1.639986
C10	1.145873	2.819654	-1.669803
C11	-1.687404	-.974223	1.689936
C12	-3.014829	-.417472	1.669803
C13	-3.972892	-1.470204	1.639986
C14	-3.259679	-2.705523	1.639986
C15	-1.868956	-2.402183	1.669803
C16	-1.687404	-0.974223	-1.689936
C17	-3.014829	-0.417472	-1.669803
C18	-3.972892	-1.470204	-1.639986
C19	-3.259679	-2.705523	-1.639986
C20	-1.868956	-2.402183	-1.669803
C21	1.687404	-0.974223	1.689936
C22	1.868956	-2.402183	1.669803
C23	3.259679	-2.705523	1.639986
C24	3.972892	-1.470204	1.639986
C25	3.014829	-0.417472	1.669803
C26	1.687404	-0.974223	-1.689936
C27	1.868956	-2.402183	-1.669803
C28	3.259679	-2.705523	-1.639986
C29	3.972892	-1.470204	-1.639986
C30	3.014829	-0.417472	-1.669803
H1	2.178595	2.498954	1.664448
H2	1.351559	5.049682	1.609114
H3	-1.351559	5.049682	1.609114
H4	-2.178595	2.498954	1.664448
H5	-2.178595	2.498954	-1.664448
H6	-1.351559	5.049682	-1.609114
H7	1.351559	5.049682	-1.609114
H8	2.178595	2.498954	-1.664448
H9	-3.253456	.637242	1.664448

H10	-5.048933	-1.354356	1.609114
H11	-3.697373	-3.695326	1.609114
H12	-1.074860	-3.136196	1.664448
H13	-3.253456	0.637242	-1.664448
H14	-5.048933	-1.354356	-1.609114
H15	-3.697373	-3.695326	-1.609114
H16	-1.074860	-3.136196	-1.664448
H17	1.074860	-3.136196	1.664448
H18	3.697373	-3.695326	1.609114
H19	5.048933	-1.354356	1.609114
H20	3.253456	0.637242	1.664448
H21	1.074860	-3.136196	-1.664448
H22	3.697373	-3.695326	-1.609114
H23	5.048933	-1.354356	-1.609114
H24	3.253456	0.637242	-1.664448

Figure 1. Molecular structure and crystallographic numbering scheme of [**3c**·DMSO].

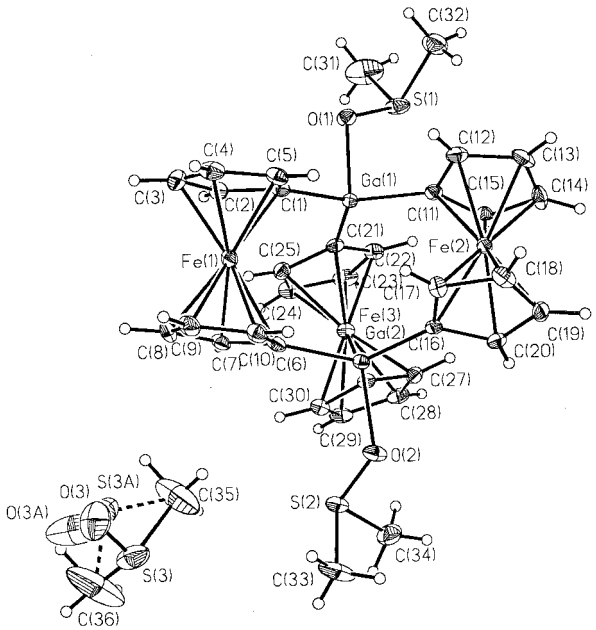

Table 2. Crystal data and structure refinement for [**3c**·DMSO].

Measurement device	Nonius KappaCCD
Empirical formula	C34 H36 Fe3 Ga2 O2 S2 x C2H6SO
Formula weight	925.87
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic P b c a
Unit cell dimensions	a = 10.12100(10) A alpha = 90 deg. b = 21.7770(2) A beta = 90 deg. c = 32.8060(3) A gamma = 90 deg.
Volume	7230.61(12) A^3
Z, Calculated density	8, 1.701 Mg/m^3
Absorption coefficient	2.855 mm^-1
F(000)	3760
Crystal size, colour and habit	0.23 x 0.16 x 0.09 mm^3, orange plates
Theta range for data collection	3.02 to 27.49 deg.
Index ranges	-13<=h<=13, -28<=k<=28, -42<=l<=42
Reflections collected / unique	54475 / 8263 [R(int) = 0.051]
Completeness to theta = 27.49	99.6%
Absorption correction	Mulit-Scan
Max. and min. transmission	0.7832 and 0.5597
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8263 / 0 / 611
Goodness-of-fit on F^2	0.963
Final R indices [I>2sigma(I)]	R1 = 0.0267, wR2 = 0.0538 [6423]
R indices (all data)	R1 = 0.0445, wR2 = 0.0585
Largest diff. peak and hole	0.509 and -0.410 e.A^-3
remarks	all hydrogen atoms were refined isotropically. Disordered solvent. S(3),O(3):S(3A),O(3A) 57:43

Table 3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for [**3c**·DMSO].
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ga(1)	3309(1)	329(1)	1107(1)	12(1)
Ga(2)	3827(1)	2052(1)	1175(1)	12(1)
Fe(1)	2008(1)	1193(1)	1963(1)	15(1)
Fe(2)	2130(1)	1330(1)	298(1)	13(1)
Fe(3)	6657(1)	1014(1)	1190(1)	14(1)
S(1)	3795(1)	-896(1)	668(1)	25(1)
S(2)	5140(1)	3286(1)	1433(1)	19(1)
O(1)	3154(2)	-628(1)	1051(1)	19(1)
O(2)	4044(1)	3008(1)	1166(1)	20(1)
C(1)	2138(2)	435(1)	1575(1)	15(1)
C(2)	2500(2)	277(1)	1986(1)	18(1)
C(3)	1428(3)	405(1)	2252(1)	26(1)
C(4)	379(2)	648(1)	2015(1)	24(1)
C(5)	806(2)	664(1)	1601(1)	19(1)
C(6)	3049(2)	1935(1)	1717(1)	16(1)
C(7)	3657(2)	1702(1)	2078(1)	17(1)
C(8)	2760(2)	1739(1)	2413(1)	21(1)
C(9)	1564(2)	1992(1)	2262(1)	22(1)
C(10)	1734(2)	2108(1)	1838(1)	18(1)
C(11)	2702(2)	504(1)	552(1)	14(1)
C(12)	1364(2)	482(1)	410(1)	20(1)
C(13)	1321(2)	612(1)	-15(1)	23(1)
C(14)	2638(3)	717(1)	-146(1)	22(1)
C(15)	3476(2)	647(1)	200(1)	18(1)
C(16)	2665(2)	2032(1)	698(1)	13(1)
C(17)	1263(2)	1945(1)	680(1)	16(1)
C(18)	809(2)	2031(1)	275(1)	21(1)
C(19)	1919(3)	2170(1)	29(1)	23(1)
C(20)	3054(2)	2166(1)	288(1)	19(1)
C(21)	5213(2)	336(1)	1212(1)	14(1)
C(22)	6227(2)	192(1)	920(1)	18(1)
C(23)	7477(2)	161(1)	1126(1)	23(1)
C(24)	7257(2)	289(1)	1543(1)	22(1)
C(25)	5880(2)	398(1)	1594(1)	17(1)
C(26)	5709(2)	1851(1)	1119(1)	14(1)
C(27)	6434(2)	1682(1)	760(1)	16(1)
C(28)	7801(2)	1604(1)	860(1)	20(1)
C(29)	7943(2)	1728(1)	1283(1)	20(1)
C(30)	6672(2)	1878(1)	1442(1)	17(1)
C(31)	4499(4)	-1597(1)	842(1)	51(1)

C(32)	2449(3)	-1202(1)	383(1)	37(1)
C(33)	4638(3)	4067(1)	1498(1)	38(1)
C(34)	6480(3)	3420(1)	1092(1)	30(1)
C(35)	3861(4)	3261(2)	2458(2)	76(1)
C(36)	4850(7)	3908(2)	3045(2)	110(2)
S(3)	3526(1)	3889(1)	2764(1)	40(1)
O(3)	2169(8)	3748(5)	2948(3)	48(2)
S(3A)	3571(2)	3391(1)	2918(1)	47(1)
O(3A)	2585(14)	3732(6)	3082(5)	123(6)

Table 4. Bond lengths [A] and angles [deg] for [**3c**·DMSO].

Ga(1)-C(1)	1.952(2)
Ga(1)-C(21)	1.957(2)
Ga(1)-C(11)	1.958(2)
Ga(1)-O(1)	2.0984(13)
Ga(2)-C(16)	1.959(2)
Ga(2)-C(6)	1.962(2)
Ga(2)-C(26)	1.963(2)
Ga(2)-O(2)	2.0929(14)
Fe(1)-C(7)	2.038(2)
Fe(1)-C(4)	2.039(2)
Fe(1)-C(8)	2.041(2)
Fe(1)-C(3)	2.046(2)
Fe(1)-C(9)	2.047(2)
Fe(1)-C(5)	2.054(2)
Fe(1)-C(10)	2.054(2)
Fe(1)-C(2)	2.056(2)
Fe(1)-C(1)	2.089(2)
Fe(1)-C(6)	2.091(2)
Fe(2)-C(18)	2.030(2)
Fe(2)-C(17)	2.033(2)
Fe(2)-C(12)	2.036(2)
Fe(2)-C(19)	2.042(2)
Fe(2)-C(14)	2.043(2)
Fe(2)-C(13)	2.043(2)
Fe(2)-C(15)	2.044(2)
Fe(2)-C(20)	2.047(2)
Fe(2)-C(11)	2.0665(19)
Fe(2)-C(16)	2.0844(19)
Fe(3)-C(27)	2.039(2)
Fe(3)-C(28)	2.041(2)
Fe(3)-C(25)	2.043(2)
Fe(3)-C(22)	2.043(2)
Fe(3)-C(23)	2.044(2)

Fe(3)-C(24)	2.049(2)
Fe(3)-C(29)	2.052(2)
Fe(3)-C(30)	2.054(2)
Fe(3)-C(26)	2.074(2)
Fe(3)-C(21)	2.079(2)
S(1)-O(1)	1.5289(15)
S(1)-C(31)	1.779(3)
S(1)-C(32)	1.783(3)
S(2)-O(2)	1.5384(15)
S(2)-C(34)	1.782(3)
S(2)-C(33)	1.789(3)
C(1)-C(5)	1.440(3)
C(1)-C(2)	1.441(3)
C(2)-C(3)	1.419(3)
C(2)-H(2)	0.99(2)
C(3)-C(4)	1.418(3)
C(3)-H(3)	0.91(2)
C(4)-C(5)	1.423(3)
C(4)-H(4)	0.94(2)
C(5)-H(5)	0.96(2)
C(6)-C(7)	1.428(3)
C(6)-C(10)	1.439(3)
C(7)-C(8)	1.426(3)
C(7)-H(7)	0.94(2)
C(8)-C(9)	1.419(3)
C(8)-H(8)	0.96(2)
C(9)-C(10)	1.426(3)
C(9)-H(9)	0.95(2)
C(10)-H(10)	0.97(2)
C(11)-C(15)	1.431(3)
C(11)-C(12)	1.434(3)
C(12)-C(13)	1.421(3)
C(12)-H(12)	0.90(2)
C(13)-C(14)	1.420(3)
C(13)-H(13)	0.95(2)
C(14)-C(15)	1.424(3)
C(14)-H(14)	0.94(2)
C(15)-H(15)	0.94(2)
C(16)-C(20)	1.429(3)
C(16)-C(17)	1.432(3)
C(17)-C(18)	1.420(3)
C(17)-H(17)	0.84(2)
C(18)-C(19)	1.416(3)
C(18)-H(18)	0.89(2)
C(19)-C(20)	1.430(3)
C(19)-H(19)	0.92(2)
C(20)-H(20)	0.93(2)
C(21)-C(25)	1.432(3)
C(21)-C(22)	1.437(3)
C(22)-C(23)	1.435(3)
C(22)-H(22)	0.95(2)
C(23)-C(24)	1.415(3)

C(23)-H(23)	0.93(2)
C(24)-C(25)	1.423(3)
C(24)-H(24)	0.99(2)
C(25)-H(25)	0.92(2)
C(26)-C(27)	1.434(3)
C(26)-C(30)	1.441(3)
C(27)-C(28)	1.432(3)
C(27)-H(27)	0.93(2)
C(28)-C(29)	1.421(3)
C(28)-H(28)	0.98(2)
C(29)-C(30)	1.425(3)
C(29)-H(29)	0.93(2)
C(30)-H(30)	0.983(19)
C(31)-H(31A)	0.91(4)
C(31)-H(31B)	0.97(3)
C(31)-H(31C)	0.94(3)
C(32)-H(32A)	0.98(3)
C(32)-H(32B)	0.95(2)
C(32)-H(32C)	0.92(3)
C(33)-H(33A)	0.97(2)
C(33)-H(33B)	0.94(3)
C(33)-H(33C)	0.88(3)
C(34)-H(34A)	0.94(3)
C(34)-H(34B)	0.94(2)
C(34)-H(34C)	0.93(2)
C(35)-S(3A)	1.564(5)
C(35)-S(3)	1.731(4)
C(35)-H(35A)	0.86(3)
C(35)-H(35B)	1.09(7)
C(35)-H(35C)	0.99(3)
C(36)-S(3)	1.626(6)
C(36)-S(3A)	1.765(6)
C(36)-H(36A)	0.81(5)
C(36)-H(36B)	0.99(3)
C(36)-H(36C)	1.09(8)
S(3)-O(3)	1.530(9)
S(3A)-O(3A)	1.356(13)
S(3A)-H(35B)	1.51(7)
S(3A)-H(36C)	1.57(8)

C(1)-Ga(1)-C(21)	117.34(9)
C(1)-Ga(1)-C(11)	121.10(9)
C(21)-Ga(1)-C(11)	118.07(9)
C(1)-Ga(1)-O(1)	98.10(7)
C(21)-Ga(1)-O(1)	95.53(7)
C(11)-Ga(1)-O(1)	95.05(7)
C(16)-Ga(2)-C(6)	118.75(9)
C(16)-Ga(2)-C(26)	120.18(8)
C(6)-Ga(2)-C(26)	116.46(9)
C(16)-Ga(2)-O(2)	94.24(7)
C(6)-Ga(2)-O(2)	100.58(7)
C(26)-Ga(2)-O(2)	96.79(7)

C(7)-Fe(1)-C(4)	164.43(9)
C(7)-Fe(1)-C(8)	40.92(9)
C(4)-Fe(1)-C(8)	125.51(9)
C(7)-Fe(1)-C(3)	127.27(10)
C(4)-Fe(1)-C(3)	40.62(10)
C(8)-Fe(1)-C(3)	105.16(10)
C(7)-Fe(1)-C(9)	68.24(9)
C(4)-Fe(1)-C(9)	106.09(9)
C(8)-Fe(1)-C(9)	40.60(9)
C(3)-Fe(1)-C(9)	115.31(10)
C(7)-Fe(1)-C(5)	153.80(9)
C(4)-Fe(1)-C(5)	40.69(9)
C(8)-Fe(1)-C(5)	164.84(9)
C(3)-Fe(1)-C(5)	68.06(10)
C(9)-Fe(1)-C(5)	128.58(9)
C(7)-Fe(1)-C(10)	67.68(9)
C(4)-Fe(1)-C(10)	118.18(9)
C(8)-Fe(1)-C(10)	68.27(9)
C(3)-Fe(1)-C(10)	150.18(9)
C(9)-Fe(1)-C(10)	40.69(9)
C(5)-Fe(1)-C(10)	110.42(9)
C(7)-Fe(1)-C(2)	108.80(9)
C(4)-Fe(1)-C(2)	68.17(9)
C(8)-Fe(1)-C(2)	116.61(9)
C(3)-Fe(1)-C(2)	40.48(9)
C(9)-Fe(1)-C(2)	149.23(9)
C(5)-Fe(1)-C(2)	67.70(9)
C(10)-Fe(1)-C(2)	168.80(9)
C(7)-Fe(1)-C(1)	119.42(8)
C(4)-Fe(1)-C(1)	68.98(8)
C(8)-Fe(1)-C(1)	151.32(9)
C(3)-Fe(1)-C(1)	68.76(9)
C(9)-Fe(1)-C(1)	167.79(9)
C(5)-Fe(1)-C(1)	40.65(8)
C(10)-Fe(1)-C(1)	130.77(9)
C(2)-Fe(1)-C(1)	40.66(8)
C(7)-Fe(1)-C(6)	40.42(8)
C(4)-Fe(1)-C(6)	152.81(9)
C(8)-Fe(1)-C(6)	68.93(9)
C(3)-Fe(1)-C(6)	166.27(10)
C(9)-Fe(1)-C(6)	68.85(9)
C(5)-Fe(1)-C(6)	120.63(9)
C(10)-Fe(1)-C(6)	40.63(8)
C(2)-Fe(1)-C(6)	129.91(9)
C(1)-Fe(1)-C(6)	110.10(8)
C(18)-Fe(2)-C(17)	40.92(9)
C(18)-Fe(2)-C(12)	115.99(10)
C(17)-Fe(2)-C(12)	108.82(9)
C(18)-Fe(2)-C(19)	40.68(10)
C(17)-Fe(2)-C(19)	68.43(9)
C(12)-Fe(2)-C(19)	148.22(10)
C(18)-Fe(2)-C(14)	129.08(9)

C(17)-Fe(2)-C(14)	168.30(9)
C(12)-Fe(2)-C(14)	68.33(10)
C(19)-Fe(2)-C(14)	107.62(9)
C(18)-Fe(2)-C(13)	107.04(9)
C(17)-Fe(2)-C(13)	129.91(10)
C(12)-Fe(2)-C(13)	40.78(9)
C(19)-Fe(2)-C(13)	115.22(9)
C(14)-Fe(2)-C(13)	40.67(10)
C(18)-Fe(2)-C(15)	168.65(9)
C(17)-Fe(2)-C(15)	149.86(9)
C(12)-Fe(2)-C(15)	67.76(9)
C(19)-Fe(2)-C(15)	130.79(10)
C(14)-Fe(2)-C(15)	40.79(9)
C(13)-Fe(2)-C(15)	68.27(9)
C(18)-Fe(2)-C(20)	68.38(10)
C(17)-Fe(2)-C(20)	67.75(9)
C(12)-Fe(2)-C(20)	169.61(9)
C(19)-Fe(2)-C(20)	40.93(9)
C(14)-Fe(2)-C(20)	117.06(10)
C(13)-Fe(2)-C(20)	148.89(10)
C(15)-Fe(2)-C(20)	109.91(9)
C(18)-Fe(2)-C(11)	148.73(9)
C(17)-Fe(2)-C(11)	116.48(9)
C(12)-Fe(2)-C(11)	40.90(8)
C(19)-Fe(2)-C(11)	169.67(9)
C(14)-Fe(2)-C(11)	69.36(9)
C(13)-Fe(2)-C(11)	69.39(9)
C(15)-Fe(2)-C(11)	40.75(8)
C(20)-Fe(2)-C(11)	130.77(9)
C(18)-Fe(2)-C(16)	69.12(8)
C(17)-Fe(2)-C(16)	40.69(8)
C(12)-Fe(2)-C(16)	130.65(9)
C(19)-Fe(2)-C(16)	69.07(8)
C(14)-Fe(2)-C(16)	149.57(9)
C(13)-Fe(2)-C(16)	169.01(9)
C(15)-Fe(2)-C(16)	117.40(9)
C(20)-Fe(2)-C(16)	40.47(8)
C(11)-Fe(2)-C(16)	108.20(8)
C(27)-Fe(3)-C(28)	41.09(8)
C(27)-Fe(3)-C(25)	151.04(9)
C(28)-Fe(3)-C(25)	167.40(9)
C(27)-Fe(3)-C(22)	107.52(9)
C(28)-Fe(3)-C(22)	116.23(9)
C(25)-Fe(3)-C(22)	67.96(9)
C(27)-Fe(3)-C(23)	128.38(9)
C(28)-Fe(3)-C(23)	106.64(9)
C(25)-Fe(3)-C(23)	68.12(9)
C(22)-Fe(3)-C(23)	41.10(9)
C(27)-Fe(3)-C(24)	166.66(9)
C(28)-Fe(3)-C(24)	128.05(9)
C(25)-Fe(3)-C(24)	40.70(9)
C(22)-Fe(3)-C(24)	68.53(9)

C(23)-Fe(3)-C(24)	40.45(9)
C(27)-Fe(3)-C(29)	68.39(9)
C(28)-Fe(3)-C(29)	40.63(9)
C(25)-Fe(3)-C(29)	130.22(9)
C(22)-Fe(3)-C(29)	149.70(9)
C(23)-Fe(3)-C(29)	116.50(9)
C(24)-Fe(3)-C(29)	108.17(9)
C(27)-Fe(3)-C(30)	67.98(9)
C(28)-Fe(3)-C(30)	68.39(9)
C(25)-Fe(3)-C(30)	110.12(9)
C(22)-Fe(3)-C(30)	167.85(8)
C(23)-Fe(3)-C(30)	150.48(9)
C(24)-Fe(3)-C(30)	118.45(9)
C(29)-Fe(3)-C(30)	40.62(8)
C(27)-Fe(3)-C(26)	40.80(8)
C(28)-Fe(3)-C(26)	69.41(8)
C(25)-Fe(3)-C(26)	118.25(9)
C(22)-Fe(3)-C(26)	128.49(9)
C(23)-Fe(3)-C(26)	167.01(9)
C(24)-Fe(3)-C(26)	151.45(9)
C(29)-Fe(3)-C(26)	69.11(8)
C(30)-Fe(3)-C(26)	40.85(8)
C(27)-Fe(3)-C(21)	116.90(8)
C(28)-Fe(3)-C(21)	149.78(9)
C(25)-Fe(3)-C(21)	40.66(8)
C(22)-Fe(3)-C(21)	40.80(8)
C(23)-Fe(3)-C(21)	69.15(9)
C(24)-Fe(3)-C(21)	69.05(8)
C(29)-Fe(3)-C(21)	168.50(9)
C(30)-Fe(3)-C(21)	129.98(8)
C(26)-Fe(3)-C(21)	107.67(8)
O(1)-S(1)-C(31)	103.48(15)
O(1)-S(1)-C(32)	104.47(12)
C(31)-S(1)-C(32)	98.80(18)
O(2)-S(2)-C(34)	104.77(12)
O(2)-S(2)-C(33)	103.72(11)
C(34)-S(2)-C(33)	97.75(16)
S(1)-O(1)-Ga(1)	114.75(8)
S(2)-O(2)-Ga(2)	117.36(8)
C(5)-C(1)-C(2)	105.29(19)
C(5)-C(1)-Ga(1)	131.11(16)
C(2)-C(1)-Ga(1)	123.60(16)
C(5)-C(1)-Fe(1)	68.34(11)
C(2)-C(1)-Fe(1)	68.44(12)
Ga(1)-C(1)-Fe(1)	127.64(10)
C(3)-C(2)-C(1)	109.5(2)
C(3)-C(2)-Fe(1)	69.35(13)
C(1)-C(2)-Fe(1)	70.90(12)
C(3)-C(2)-H(2)	120.8(14)
C(1)-C(2)-H(2)	129.7(14)
Fe(1)-C(2)-H(2)	127.9(13)
C(4)-C(3)-C(2)	108.0(2)

C(4)-C(3)-Fe(1)	69.45(13)
C(2)-C(3)-Fe(1)	70.17(13)
C(4)-C(3)-H(3)	128.4(16)
C(2)-C(3)-H(3)	123.6(16)
Fe(1)-C(3)-H(3)	124.6(16)
C(3)-C(4)-C(5)	107.7(2)
C(3)-C(4)-Fe(1)	69.93(13)
C(5)-C(4)-Fe(1)	70.19(12)
C(3)-C(4)-H(4)	125.6(13)
C(5)-C(4)-H(4)	126.4(13)
Fe(1)-C(4)-H(4)	120.7(13)
C(4)-C(5)-C(1)	109.5(2)
C(4)-C(5)-Fe(1)	69.12(13)
C(1)-C(5)-Fe(1)	71.01(12)
C(4)-C(5)-H(5)	124.6(13)
C(1)-C(5)-H(5)	125.6(14)
Fe(1)-C(5)-H(5)	121.5(13)
C(7)-C(6)-C(10)	105.28(19)
C(7)-C(6)-Ga(2)	128.72(16)
C(10)-C(6)-Ga(2)	125.91(16)
C(7)-C(6)-Fe(1)	67.80(12)
C(10)-C(6)-Fe(1)	68.30(12)
Ga(2)-C(6)-Fe(1)	130.71(10)
C(8)-C(7)-C(6)	110.1(2)
C(8)-C(7)-Fe(1)	69.65(12)
C(6)-C(7)-Fe(1)	71.77(12)
C(8)-C(7)-H(7)	125.1(13)
C(6)-C(7)-H(7)	124.8(13)
Fe(1)-C(7)-H(7)	125.3(12)
C(9)-C(8)-C(7)	107.3(2)
C(9)-C(8)-Fe(1)	69.93(13)
C(7)-C(8)-Fe(1)	69.43(12)
C(9)-C(8)-H(8)	126.1(12)
C(7)-C(8)-H(8)	126.5(12)
Fe(1)-C(8)-H(8)	125.4(12)
C(8)-C(9)-C(10)	107.8(2)
C(8)-C(9)-Fe(1)	69.47(13)
C(10)-C(9)-Fe(1)	69.90(12)
C(8)-C(9)-H(9)	127.3(14)
C(10)-C(9)-H(9)	124.9(14)
Fe(1)-C(9)-H(9)	124.7(14)
C(9)-C(10)-C(6)	109.5(2)
C(9)-C(10)-Fe(1)	69.41(13)
C(6)-C(10)-Fe(1)	71.08(12)
C(9)-C(10)-H(10)	126.9(13)
C(6)-C(10)-H(10)	123.6(13)
Fe(1)-C(10)-H(10)	127.1(12)
C(15)-C(11)-C(12)	105.06(19)
C(15)-C(11)-Ga(1)	128.44(16)
C(12)-C(11)-Ga(1)	126.43(16)
C(15)-C(11)-Fe(2)	68.76(11)
C(12)-C(11)-Fe(2)	68.39(12)

Ga(1)-C(11)-Fe(2)	129.21(10)
C(13)-C(12)-C(11)	110.0(2)
C(13)-C(12)-Fe(2)	69.90(12)
C(11)-C(12)-Fe(2)	70.71(12)
C(13)-C(12)-H(12)	124.6(14)
C(11)-C(12)-H(12)	125.1(14)
Fe(2)-C(12)-H(12)	122.2(13)
C(14)-C(13)-C(12)	107.4(2)
C(14)-C(13)-Fe(2)	69.64(13)
C(12)-C(13)-Fe(2)	69.31(12)
C(14)-C(13)-H(13)	127.9(15)
C(12)-C(13)-H(13)	124.5(15)
Fe(2)-C(13)-H(13)	123.4(13)
C(13)-C(14)-C(15)	107.5(2)
C(13)-C(14)-Fe(2)	69.70(13)
C(15)-C(14)-Fe(2)	69.64(12)
C(13)-C(14)-H(14)	124.2(13)
C(15)-C(14)-H(14)	128.2(13)
Fe(2)-C(14)-H(14)	123.1(13)
C(14)-C(15)-C(11)	110.0(2)
C(14)-C(15)-Fe(2)	69.57(13)
C(11)-C(15)-Fe(2)	70.48(12)
C(14)-C(15)-H(15)	126.0(13)
C(11)-C(15)-H(15)	124.0(13)
Fe(2)-C(15)-H(15)	124.7(12)
C(20)-C(16)-C(17)	105.24(18)
C(20)-C(16)-Ga(2)	125.51(16)
C(17)-C(16)-Ga(2)	129.00(16)
C(20)-C(16)-Fe(2)	68.35(12)
C(17)-C(16)-Fe(2)	67.71(11)
Ga(2)-C(16)-Fe(2)	132.41(10)
C(18)-C(17)-C(16)	109.9(2)
C(18)-C(17)-Fe(2)	69.46(12)
C(16)-C(17)-Fe(2)	71.60(12)
C(18)-C(17)-H(17)	125.9(15)
C(16)-C(17)-H(17)	124.2(15)
Fe(2)-C(17)-H(17)	124.7(14)
C(19)-C(18)-C(17)	107.8(2)
C(19)-C(18)-Fe(2)	70.10(13)
C(17)-C(18)-Fe(2)	69.62(12)
C(19)-C(18)-H(18)	125.6(15)
C(17)-C(18)-H(18)	126.6(15)
Fe(2)-C(18)-H(18)	125.0(14)
C(18)-C(19)-C(20)	107.3(2)
C(18)-C(19)-Fe(2)	69.22(12)
C(20)-C(19)-Fe(2)	69.72(12)
C(18)-C(19)-H(19)	127.2(14)
C(20)-C(19)-H(19)	125.6(14)
Fe(2)-C(19)-H(19)	125.4(13)
C(16)-C(20)-C(19)	109.8(2)
C(16)-C(20)-Fe(2)	71.18(11)
C(19)-C(20)-Fe(2)	69.35(12)

C(16)-C(20)-H(20)	126.7(13)
C(19)-C(20)-H(20)	123.5(13)
Fe(2)-C(20)-H(20)	124.5(13)
C(25)-C(21)-C(22)	105.46(19)
C(25)-C(21)-Ga(1)	128.25(16)
C(22)-C(21)-Ga(1)	125.79(16)
C(25)-C(21)-Fe(3)	68.32(12)
C(22)-C(21)-Fe(3)	68.26(12)
Ga(1)-C(21)-Fe(3)	133.73(10)
C(23)-C(22)-C(21)	109.1(2)
C(23)-C(22)-Fe(3)	69.50(13)
C(21)-C(22)-Fe(3)	70.93(12)
C(23)-C(22)-H(22)	120.2(14)
C(21)-C(22)-H(22)	130.7(14)
Fe(3)-C(22)-H(22)	124.0(13)
C(24)-C(23)-C(22)	107.9(2)
C(24)-C(23)-Fe(3)	69.94(12)
C(22)-C(23)-Fe(3)	69.39(12)
C(24)-C(23)-H(23)	126.6(14)
C(22)-C(23)-H(23)	125.5(14)
Fe(3)-C(23)-H(23)	126.4(14)
C(23)-C(24)-C(25)	107.5(2)
C(23)-C(24)-Fe(3)	69.61(13)
C(25)-C(24)-Fe(3)	69.42(12)
C(23)-C(24)-H(24)	128.9(14)
C(25)-C(24)-H(24)	123.5(14)
Fe(3)-C(24)-H(24)	124.5(13)
C(24)-C(25)-C(21)	110.0(2)
C(24)-C(25)-Fe(3)	69.88(13)
C(21)-C(25)-Fe(3)	71.02(12)
C(24)-C(25)-H(25)	123.9(14)
C(21)-C(25)-H(25)	126.0(14)
Fe(3)-C(25)-H(25)	122.7(13)
C(27)-C(26)-C(30)	105.48(19)
C(27)-C(26)-Ga(2)	129.12(16)
C(30)-C(26)-Ga(2)	125.34(15)
C(27)-C(26)-Fe(3)	68.27(12)
C(30)-C(26)-Fe(3)	68.83(11)
Ga(2)-C(26)-Fe(3)	129.33(10)
C(28)-C(27)-C(26)	109.7(2)
C(28)-C(27)-Fe(3)	69.54(12)
C(26)-C(27)-Fe(3)	70.93(12)
C(28)-C(27)-H(27)	124.5(12)
C(26)-C(27)-H(27)	125.7(12)
Fe(3)-C(27)-H(27)	123.5(12)
C(29)-C(28)-C(27)	107.4(2)
C(29)-C(28)-Fe(3)	70.09(13)
C(27)-C(28)-Fe(3)	69.37(12)
C(29)-C(28)-H(28)	128.3(13)
C(27)-C(28)-H(28)	124.2(13)
Fe(3)-C(28)-H(28)	122.9(13)
C(28)-C(29)-C(30)	107.9(2)

C(28)-C(29)-Fe(3)	69.28(12)
C(30)-C(29)-Fe(3)	69.78(12)
C(28)-C(29)-H(29)	128.9(14)
C(30)-C(29)-H(29)	123.1(14)
Fe(3)-C(29)-H(29)	123.1(14)
C(29)-C(30)-C(26)	109.5(2)
C(29)-C(30)-Fe(3)	69.60(12)
C(26)-C(30)-Fe(3)	70.32(12)
C(29)-C(30)-H(30)	123.2(11)
C(26)-C(30)-H(30)	127.3(11)
Fe(3)-C(30)-H(30)	125.7(11)
S(1)-C(31)-H(31A)	106(2)
S(1)-C(31)-H(31B)	108.3(18)
H(31A)-C(31)-H(31B)	109(3)
S(1)-C(31)-H(31C)	108(2)
H(31A)-C(31)-H(31C)	112(3)
H(31B)-C(31)-H(31C)	113(3)
S(1)-C(32)-H(32A)	103.2(17)
S(1)-C(32)-H(32B)	111.0(14)
H(32A)-C(32)-H(32B)	115(2)
S(1)-C(32)-H(32C)	107.5(18)
H(32A)-C(32)-H(32C)	108(2)
H(32B)-C(32)-H(32C)	112(2)
S(2)-C(33)-H(33A)	103.2(14)
S(2)-C(33)-H(33B)	107.2(16)
H(33A)-C(33)-H(33B)	108(2)
S(2)-C(33)-H(33C)	108.4(16)
H(33A)-C(33)-H(33C)	114(2)
H(33B)-C(33)-H(33C)	116(2)
S(2)-C(34)-H(34A)	111.0(16)
S(2)-C(34)-H(34B)	106.8(16)
H(34A)-C(34)-H(34B)	113(2)
S(2)-C(34)-H(34C)	107.8(15)
H(34A)-C(34)-H(34C)	105(2)
H(34B)-C(34)-H(34C)	112(2)
S(3A)-C(35)-S(3)	42.20(12)
S(3A)-C(35)-H(35A)	122(2)
S(3)-C(35)-H(35A)	114(2)
S(3A)-C(35)-H(35B)	67(4)
S(3)-C(35)-H(35B)	109(4)
H(35A)-C(35)-H(35B)	100(4)
S(3A)-C(35)-H(35C)	121.8(17)
S(3)-C(35)-H(35C)	114.0(16)
H(35A)-C(35)-H(35C)	116(3)
H(35B)-C(35)-H(35C)	102(4)
S(3)-C(36)-S(3A)	41.05(15)
S(3)-C(36)-H(36A)	114(4)
S(3A)-C(36)-H(36A)	122(4)
S(3)-C(36)-H(36B)	121.3(18)
S(3A)-C(36)-H(36B)	115.6(16)
H(36A)-C(36)-H(36B)	120(4)
S(3)-C(36)-H(36C)	100(5)

S(3A)-C(36)-H(36C)	61(5)
H(36A)-C(36)-H(36C)	90(5)
H(36B)-C(36)-H(36C)	103(5)
O(3)-S(3)-C(36)	121.5(4)
O(3)-S(3)-C(35)	104.2(4)
C(36)-S(3)-C(35)	100.8(3)
O(3A)-S(3A)-C(35)	128.4(7)
O(3A)-S(3A)-C(36)	95.5(6)
C(35)-S(3A)-C(36)	101.9(3)
O(3A)-S(3A)-H(35B)	143(3)
C(35)-S(3A)-H(35B)	41(2)
C(36)-S(3A)-H(35B)	121(3)
O(3A)-S(3A)-H(36C)	99(3)
C(35)-S(3A)-H(36C)	124(3)
C(36)-S(3A)-H(36C)	38(3)
H(35B)-S(3A)-H(36C)	115(4)

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for [**3c**·DMSO].
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ga(1)	12(1)	11(1)	12(1)	-1(1)	0(1)	0(1)
Ga(2)	11(1)	12(1)	14(1)	-1(1)	0(1)	-1(1)
Fe(1)	13(1)	18(1)	14(1)	-3(1)	3(1)	-2(1)
Fe(2)	15(1)	11(1)	12(1)	0(1)	-2(1)	0(1)
Fe(3)	10(1)	14(1)	18(1)	-1(1)	0(1)	1(1)
S(1)	26(1)	15(1)	34(1)	-8(1)	12(1)	-4(1)
S(2)	18(1)	13(1)	25(1)	-3(1)	-5(1)	-1(1)
O(1)	24(1)	12(1)	20(1)	-2(1)	6(1)	-1(1)
O(2)	18(1)	13(1)	28(1)	-2(1)	-8(1)	-1(1)
C(1)	14(1)	13(1)	17(1)	-3(1)	2(1)	-2(1)
C(2)	20(1)	16(1)	19(1)	0(1)	-1(1)	-2(1)
C(3)	32(1)	26(1)	19(1)	-1(1)	8(1)	-8(1)
C(4)	15(1)	25(1)	31(1)	-9(1)	8(1)	-6(1)
C(5)	14(1)	20(1)	23(1)	-5(1)	-2(1)	-2(1)
C(6)	16(1)	16(1)	16(1)	-7(1)	2(1)	-3(1)
C(7)	14(1)	18(1)	18(1)	-6(1)	-1(1)	-5(1)
C(8)	26(1)	24(1)	13(1)	-6(1)	0(1)	-3(1)

C(9)	23(1)	21(1)	21(1)	-9(1)	7(1)	-1(1)
C(10)	16(1)	19(1)	19(1)	-5(1)	2(1)	0(1)
C(11)	17(1)	9(1)	17(1)	0(1)	-2(1)	1(1)
C(12)	20(1)	13(1)	26(1)	1(1)	-2(1)	-3(1)
C(13)	30(1)	13(1)	27(1)	-4(1)	-16(1)	0(1)
C(14)	38(2)	18(1)	12(1)	-3(1)	-4(1)	9(1)
C(15)	23(1)	17(1)	15(1)	-2(1)	0(1)	5(1)
C(16)	17(1)	8(1)	15(1)	0(1)	-1(1)	0(1)
C(17)	15(1)	17(1)	16(1)	-1(1)	0(1)	4(1)
C(18)	23(1)	15(1)	25(1)	-4(1)	-10(1)	6(1)
C(19)	44(2)	11(1)	14(1)	2(1)	-5(1)	0(1)
C(20)	26(1)	13(1)	19(1)	1(1)	3(1)	-5(1)
C(21)	15(1)	10(1)	18(1)	2(1)	-1(1)	-1(1)
C(22)	16(1)	14(1)	24(1)	-2(1)	3(1)	2(1)
C(23)	14(1)	14(1)	40(2)	0(1)	2(1)	4(1)
C(24)	16(1)	19(1)	32(2)	4(1)	-8(1)	2(1)
C(25)	17(1)	17(1)	17(1)	2(1)	-1(1)	-1(1)
C(26)	14(1)	11(1)	17(1)	0(1)	2(1)	0(1)
C(27)	18(1)	16(1)	16(1)	1(1)	2(1)	-1(1)
C(28)	14(1)	16(1)	30(1)	1(1)	7(1)	-2(1)
C(29)	11(1)	17(1)	32(1)	0(1)	-3(1)	-4(1)
C(30)	16(1)	15(1)	20(1)	-3(1)	-1(1)	0(1)
C(31)	47(2)	20(2)	88(3)	-5(2)	7(2)	11(1)
C(32)	41(2)	37(2)	32(2)	-14(1)	9(1)	-14(1)
C(33)	35(2)	17(1)	61(2)	-15(1)	-20(2)	3(1)
C(34)	29(2)	29(2)	34(2)	5(1)	0(1)	-11(1)
C(35)	53(2)	90(3)	84(3)	-58(3)	15(2)	-22(2)
C(36)	122(5)	68(3)	140(5)	-65(4)	-52(4)	20(3)
S(3)	45(1)	21(1)	52(1)	3(1)	19(1)	1(1)
O(3)	34(2)	65(4)	44(3)	0(2)	17(2)	3(2)
S(3A)	78(2)	28(1)	36(1)	4(1)	20(1)	-2(1)
O(3A)	140(13)	45(6)	184(15)	-41(8)	137(10	-28(7)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for [**3c**·DMSO].

	x	y	z	U(eq)
H(2)	3320(2)	92(10)	2091(7)	28(7)
H(3)	1460(2)	345(11)	2526(8)	35(7)
H(4)	-420(2)	806(10)	2118(6)	22(6)
H(5)	310(2)	839(10)	1381(7)	22(6)
H(7)	4520(2)	1548(9)	2092(6)	15(6)
H(8)	2930(19)	1612(9)	2689(6)	10(5)
H(9)	780(2)	2062(10)	2410(7)	27(7)
H(10)	1090(2)	2286(9)	1652(7)	21(6)
H(12)	650(2)	427(9)	568(6)	16(6)
H(13)	530(2)	644(10)	-171(7)	28(7)
H(14)	2870(2)	835(10)	-411(7)	18(6)
H(15)	4390(2)	700(9)	204(6)	15(6)
H(17)	790(2)	1850(9)	883(6)	13(6)
H(18)	-20(2)	1999(9)	187(7)	19(6)
H(19)	1930(2)	2242(10)	-248(7)	19(6)
H(20)	3910(2)	2231(9)	194(6)	17(6)
H(22)	6180(2)	132(10)	633(7)	25(7)
H(23)	8280(2)	71(10)	1004(7)	20(6)
H(24)	7910(2)	320(10)	1767(8)	31(7)
H(25)	5500(2)	514(9)	1837(7)	18(6)
H(27)	6072(19)	1611(9)	503(6)	10(5)
H(28)	8480(2)	1464(10)	667(7)	22(6)
H(29)	8700(2)	1696(10)	1446(7)	23(6)
H(30)	6513(18)	1976(8)	1730(6)	4(5)
H(31A)	5210(4)	-1488(16)	995(11)	80(13)
H(31B)	4790(3)	-1830(14)	606(9)	67(10)
H(31C)	3860(3)	-1806(15)	995(10)	66(11)
H(32A)	2020(3)	-835(14)	270(9)	61(10)
H(32B)	1890(2)	-1448(10)	551(7)	23(6)
H(32C)	2800(3)	-1426(12)	170(9)	52(9)
H(33A)	3810(2)	4032(10)	1648(7)	26(7)
H(33B)	4430(3)	4223(12)	1237(8)	40(8)
H(33C)	5270(3)	4265(11)	1632(7)	35(8)
H(34A)	6880(3)	3046(13)	1014(8)	44(8)
H(34B)	7060(3)	3691(11)	1224(7)	31(7)
H(34C)	6130(2)	3586(10)	853(8)	26(7)
H(35A)	3240(3)	3179(15)	2284(10)	63(11)
H(35B)	3830(6)	2850(3)	2643(19)	240(3)
H(35C)	4770(3)	3253(12)	2349(9)	56(9)
H(36A)	4790(5)	4140(2)	3239(15)	130(2)
H(36B)	5730(3)	3811(12)	2931(8)	39(9)
H(36C)	4670(8)	3520(4)	3250(2)	300(5)

Figure 3. Molecular structure and crystallographic numbering scheme of [**3d**·0.75 toluene].

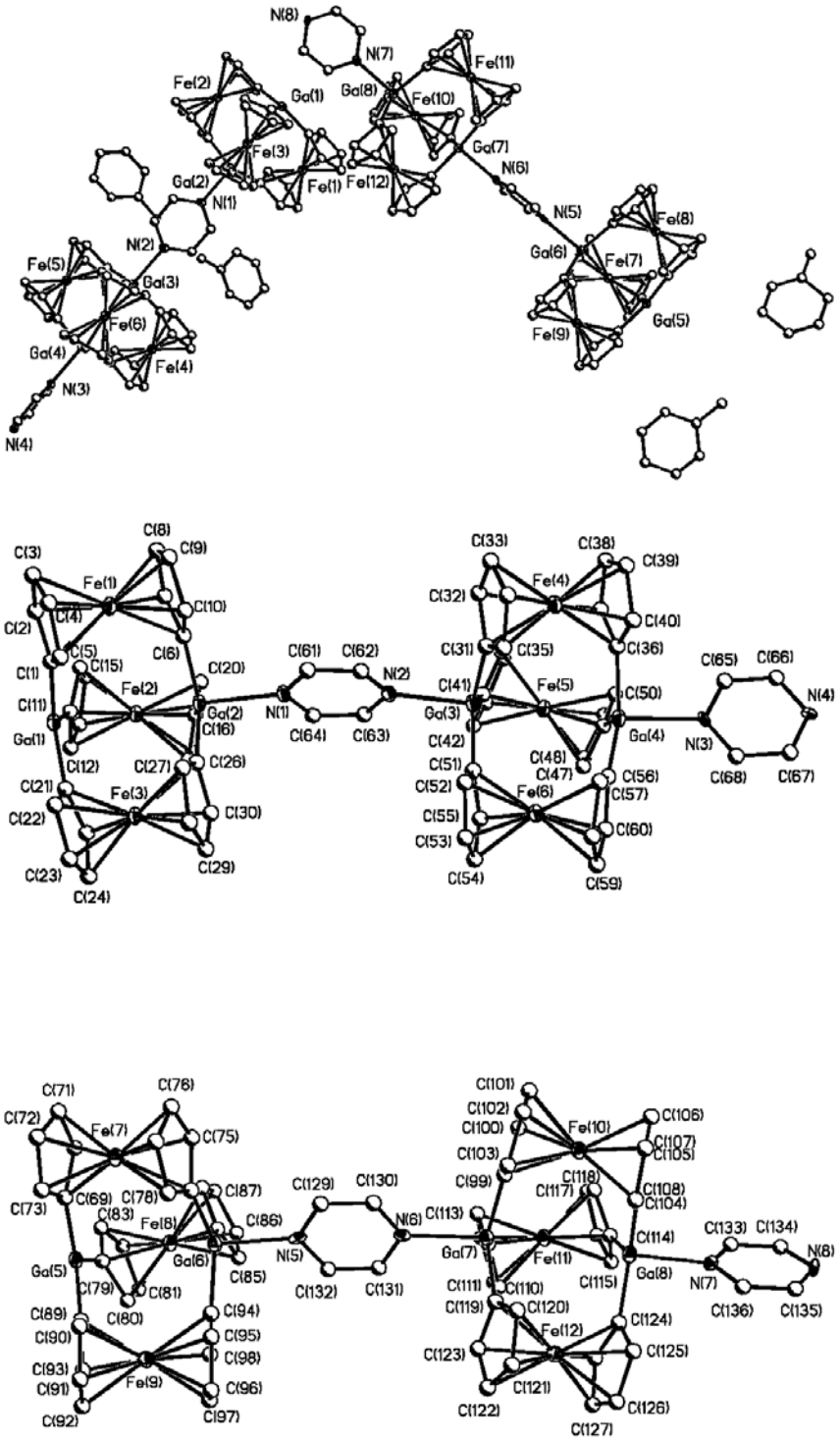

Table 7. Crystal data and structure refinement for [**3d**·0.75 toluene].

Measurement device	Nonius KappaCCD
Empirical formula	C34 H28 Fe3 Ga2 N2 + 3/4 C7H8
Formula weight	840.67
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic P -1
Unit cell dimensions	a = 15.5930(2) A alpha = 86.8150(6) deg. b = 15.5960(2) A beta = 80.4920(6) deg. c = 27.0290(5) A gamma = 89.9790(6) deg.
Volume	6472.57(17) A^3
Z, Calculated density	8, 1.725 Mg/m^3
Absorption coefficient	2.989 mm^-1
F(000)	3388
Crystal size, colour and habit	0.13 x 0.12 x 0.02 mm^3, brownplate
Theta range for data collection	2.96 to 25.00 deg.
Index ranges	-18<=h<=18,-18<=k<=18,-32<=l<=32
Reflections collected / unique	150458 / 22760 [R(int) = 0.190]
Completeness to theta = 25.00	99.7%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9426 and 0.6973
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	22760 / 0 / 882
Goodness-of-fit on F^2	1.010
Final R indices [I>2sigma(I)]	R1 = 0.0666, wR2 = 0.1068[11786]
R indices (all data)	R1 = 0.1642, wR2 = 0.1310
Largest diff. peak and hole	1.142 and -0.754 e.A^-3
remarks	Disorder of 2 toluene at 2 inversion centers.

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for [**3d**·0.75 toluene]. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ga(1)	-838(1)	-3328(1)	1700(1)	17(1)
Ga(2)	931(1)	-5028(1)	1503(1)	17(1)
Ga(3)	4167(1)	-8324(1)	1555(1)	17(1)
Ga(4)	5870(1)	-10044(1)	1775(1)	18(1)
Ga(5)	5311(1)	6503(1)	3505(1)	17(1)
Ga(6)	3666(1)	4803(1)	3301(1)	17(1)
Ga(7)	404(1)	1533(1)	3227(1)	17(1)
Ga(8)	-1383(1)	-238(1)	3439(1)	17(1)
Fe(1)	1366(1)	-2843(1)	999(1)	18(1)
Fe(2)	-1116(1)	-5227(1)	1010(1)	18(1)
Fe(3)	-123(1)	-4503(1)	2758(1)	16(1)
Fe(4)	6470(1)	-8009(1)	1061(1)	18(1)
Fe(5)	4098(1)	-10405(1)	1047(1)	19(1)
Fe(6)	4493(1)	-9108(1)	2818(1)	17(1)
Fe(7)	5041(1)	5930(1)	2244(1)	17(1)
Fe(8)	3027(1)	6733(1)	4003(1)	17(1)
Fe(9)	5425(1)	4267(1)	3998(1)	17(1)
Fe(10)	-342(1)	570(1)	2182(1)	16(1)
Fe(11)	-1773(1)	1880(1)	3932(1)	17(1)
Fe(12)	597(1)	-525(1)	3955(1)	18(1)
N(1)	1943(4)	-6042(4)	1402(2)	17(2)
N(2)	3217(4)	-7297(4)	1429(2)	16(2)
N(3)	6868(4)	-11064(4)	1804(2)	14(2)
N(4)	8147(4)	-12315(4)	1761(2)	13(2)
N(5)	2675(4)	3818(4)	3235(2)	15(2)
N(6)	1433(4)	2544(4)	3195(2)	14(2)
N(7)	-2437(4)	-1234(4)	3559(2)	14(2)
N(8)	-3695(4)	-2516(4)	3606(2)	15(2)
C(1)	146(5)	-2581(5)	1408(3)	15(2)
C(2)	278(5)	-2143(5)	920(3)	17(2)
C(3)	1018(5)	-1589(5)	870(3)	21(2)
C(4)	1373(5)	-1694(5)	1321(3)	19(2)
C(5)	843(5)	-2293(5)	1652(3)	17(2)
C(6)	1612(5)	-4167(5)	1066(3)	18(2)
C(7)	1458(5)	-3892(5)	565(3)	17(2)
C(8)	2076(5)	-3256(5)	350(3)	19(2)
C(9)	2626(5)	-3088(5)	700(3)	19(2)
C(10)	2339(5)	-3629(5)	1135(3)	20(2)
C(11)	-1370(5)	-3991(5)	1237(3)	16(2)
C(12)	-2133(5)	-4542(4)	1363(3)	15(2)

C(13)	-2340(5)	-4850(5)	913(3)	19(2)
C(14)	-1730(5)	-4524(5)	500(3)	20(2)
C(15)	-1137(5)	-4001(5)	695(3)	19(2)
C(16)	35(5)	-5654(5)	1239(3)	16(2)
C(17)	-718(5)	-6090(5)	1520(3)	20(2)
C(18)	-1146(5)	-6519(5)	1192(3)	16(2)
C(19)	-719(5)	-6353(5)	704(3)	21(2)
C(20)	5(5)	-5820(5)	729(3)	18(2)
C(21)	-958(5)	-3702(5)	2410(3)	16(2)
C(22)	-597(5)	-3283(5)	2790(3)	18(2)
C(23)	-817(5)	-3747(5)	3260(3)	22(2)
C(24)	-1336(5)	-4477(5)	3194(3)	22(2)
C(25)	-1399(5)	-4453(5)	2667(3)	22(2)
C(26)	834(5)	-5029(5)	2230(3)	17(2)
C(27)	1200(5)	-4449(5)	2535(3)	18(2)
C(28)	983(5)	-4736(5)	3051(3)	20(2)
C(29)	480(5)	-5478(5)	3077(3)	21(2)
C(30)	394(5)	-5667(5)	2586(3)	20(2)
C(31)	5214(5)	-7623(5)	1319(3)	17(2)
C(32)	5522(5)	-7269(5)	821(3)	22(2)
C(33)	6271(5)	-6760(5)	815(3)	22(2)
C(34)	6450(5)	-6798(5)	1313(3)	20(2)
C(35)	5799(5)	-7313(4)	1616(3)	15(2)
C(36)	6649(5)	-9273(5)	1289(3)	18(2)
C(37)	6545(5)	-9198(5)	778(3)	20(2)
C(38)	7204(5)	-8661(5)	505(3)	23(2)
C(39)	7729(5)	-8398(5)	847(3)	21(2)
C(40)	7374(5)	-8776(5)	1328(3)	22(2)
C(41)	3785(5)	-9120(5)	1108(3)	16(2)
C(42)	3015(5)	-9666(5)	1171(3)	22(2)
C(43)	3024(5)	-10127(5)	730(3)	24(2)
C(44)	3784(5)	-9892(5)	391(3)	25(2)
C(45)	4239(5)	-9276(5)	610(3)	18(2)
C(46)	5063(5)	-10733(5)	1470(3)	20(2)
C(47)	4230(5)	-11074(5)	1699(3)	20(2)
C(48)	3900(5)	-11618(5)	1362(3)	21(2)
C(49)	4530(5)	-11633(4)	930(3)	14(2)
C(50)	5223(5)	-11089(5)	986(3)	22(2)
C(51)	3843(5)	-8468(5)	2285(3)	16(2)
C(52)	4098(5)	-7902(5)	2632(3)	19(2)
C(53)	3719(5)	-8169(5)	3130(3)	16(2)
C(54)	3217(5)	-8918(5)	3102(3)	19(2)
C(55)	3304(5)	-9107(5)	2592(3)	19(2)
C(56)	5548(5)	-9828(5)	2478(3)	18(2)
C(57)	5825(5)	-9154(5)	2771(3)	20(2)
C(58)	5404(5)	-9254(5)	3276(3)	20(2)
C(59)	4865(5)	-9986(5)	3317(3)	26(2)
C(60)	4935(5)	-10334(5)	2847(3)	22(2)
C(61)	2784(6)	-5840(5)	1400(3)	27(2)
C(62)	3409(5)	-6468(5)	1421(3)	21(2)
C(63)	2381(5)	-7508(5)	1411(3)	23(2)
C(64)	1745(5)	-6884(5)	1406(3)	16(2)

C(65)	7317(5)	-11294(5)	1372(3)	24(2)
C(66)	7957(5)	-11913(5)	1348(3)	19(2)
C(67)	7702(5)	-12094(5)	2193(3)	17(2)
C(68)	7050(5)	-11471(5)	2216(3)	18(2)
C(69)	5480(5)	6674(5)	2775(3)	13(2)
C(70)	4962(5)	7174(5)	2465(3)	16(2)
C(71)	5353(5)	7146(5)	1955(3)	18(2)
C(72)	6116(5)	6639(5)	1932(3)	19(2)
C(73)	6182(5)	6361(5)	2423(3)	17(2)
C(74)	4173(5)	4970(5)	2593(3)	19(2)
C(75)	3818(5)	5484(5)	2218(3)	21(2)
C(76)	4354(5)	5442(5)	1744(3)	26(2)
C(77)	5070(5)	4900(5)	1813(3)	19(2)
C(78)	4963(5)	4623(5)	2322(3)	18(2)
C(79)	4338(5)	7011(5)	3942(3)	15(2)
C(80)	3987(5)	6654(5)	4440(3)	14(2)
C(81)	3297(5)	7191(5)	4661(3)	22(2)
C(82)	3219(5)	7862(5)	4303(3)	18(2)
C(83)	3835(5)	7764(5)	3871(3)	16(2)
C(84)	2849(5)	5677(4)	3591(3)	12(2)
C(85)	2314(5)	5611(5)	4078(3)	17(2)
C(86)	1757(5)	6338(5)	4119(3)	22(2)
C(87)	1941(5)	6868(5)	3674(3)	19(2)
C(88)	2612(5)	6462(5)	3351(3)	18(2)
C(89)	5881(5)	5511(5)	3778(3)	19(2)
C(90)	6388(5)	4870(5)	3492(3)	18(2)
C(91)	6745(5)	4303(5)	3823(3)	17(2)
C(92)	6487(5)	4543(5)	4308(3)	22(2)
C(93)	5951(5)	5289(5)	4288(3)	21(2)
C(94)	4235(5)	4089(5)	3762(3)	17(2)
C(95)	4818(5)	3384(5)	3647(3)	16(2)
C(96)	5039(5)	3008(5)	4089(3)	19(2)
C(97)	4631(5)	3462(5)	4498(3)	21(2)
C(98)	4132(5)	4122(5)	4305(3)	17(2)
C(99)	317(5)	1491(5)	2517(3)	17(2)
C(100)	-322(5)	1874(5)	2243(3)	22(2)
C(101)	-142(5)	1679(5)	1744(3)	19(2)
C(102)	620(5)	1149(5)	1673(3)	25(2)
C(103)	904(5)	1019(4)	2146(3)	13(2)
C(104)	-1091(5)	-292(5)	2709(3)	17(2)
C(105)	-1586(5)	99(5)	2352(3)	20(2)
C(106)	-1197(5)	-97(4)	1860(3)	15(2)
C(107)	-453(5)	-598(5)	1896(3)	19(2)
C(108)	-390(5)	-701(5)	2414(3)	16(2)
C(109)	-450(5)	2118(5)	3705(3)	15(2)
C(110)	-653(5)	1834(5)	4220(3)	20(2)
C(111)	-1223(5)	2400(5)	4490(3)	26(2)
C(112)	-1419(5)	3049(5)	4149(3)	23(2)
C(113)	-942(5)	2873(5)	3671(3)	21(2)
C(114)	-2126(5)	721(5)	3680(3)	17(2)
C(115)	-2570(5)	841(5)	4171(3)	18(2)
C(116)	-3057(5)	1607(5)	4173(3)	20(2)

C(117)	-2924(5)	1963(5)	3676(3)	20(2)
C(118)	-2359(5)	1437(5)	3373(3)	21(2)
C(119)	1038(5)	604(5)	3537(3)	14(2)
C(120)	1410(5)	-144(5)	3307(3)	18(2)
C(121)	1878(5)	-605(5)	3647(3)	21(2)
C(122)	1785(5)	-156(5)	4091(3)	25(2)
C(123)	1269(5)	583(5)	4025(3)	17(2)
C(124)	-684(5)	-801(5)	3888(3)	14(2)
C(125)	-116(5)	-1549(5)	3821(3)	24(2)
C(126)	256(6)	-1712(5)	4257(3)	28(2)
C(127)	-47(5)	-1089(5)	4602(3)	23(2)
C(128)	-624(5)	-548(5)	4383(3)	21(2)
C(129)	2526(5)	3529(5)	2803(3)	21(2)
C(130)	1913(5)	2885(5)	2785(3)	18(2)
C(131)	1566(5)	2833(5)	3630(3)	19(2)
C(132)	2179(5)	3458(5)	3651(3)	16(2)
C(133)	-3282(5)	-1052(5)	3621(3)	19(2)
C(134)	-3895(6)	-1690(5)	3646(3)	24(2)
C(135)	-2853(5)	-2700(5)	3567(3)	18(2)
C(136)	-2235(6)	-2059(5)	3547(3)	23(2)
C(137)	2048(9)	-8043(8)	67(5)	76(4)
C(138)	2014(8)	-8908(8)	-46(4)	74(4)
C(139)	1345(8)	-9385(7)	28(4)	65(3)
C(140)	499(9)	-9081(8)	246(5)	83(4)
C(141)	488(8)	-8259(7)	364(4)	69(4)
C(142)	1194(8)	-7747(7)	274(4)	66(3)
C(143)	2826(9)	-7535(8)	-30(5)	114(5)
C(144)	4746(10)	-5655(9)	-267(5)	89(4)
C(145)	5574(9)	-5461(8)	-261(5)	81(4)
C(146)	5879(9)	-4891(9)	-46(5)	93(5)
C(147)	4421(17)	-6259(16)	-468(9)	91(9)
C(148)	8067(9)	7040(8)	4915(5)	74(4)
C(149)	8903(7)	7001(7)	5043(4)	60(3)
C(150)	9400(8)	6346(7)	4956(4)	76(4)
C(151)	9160(9)	5609(8)	4710(4)	81(4)
C(152)	8347(8)	5634(8)	4598(4)	71(4)
C(153)	7821(7)	6299(6)	4679(4)	55(3)
C(154)	7520(9)	7751(8)	5011(5)	111(5)
C(155)	4367(9)	10370(9)	4769(5)	88(4)
C(156)	4536(7)	9521(7)	4764(4)	63(3)
C(157)	5125(7)	9100(7)	4966(4)	74(4)
C(158)	3812(7)	10775(7)	4587(4)	88(9)

Table 9. Bond lengths [A] and angles [deg] for [**3d**·0.75 toluene].

Ga(1)-C(11)	1.952(7)
Ga(1)-C(21)	1.953(8)
Ga(1)-C(1)	1.958(7)
Ga(1)-N(4)#1	2.229(6)
Ga(2)-C(6)	1.933(7)
Ga(2)-C(26)	1.945(8)
Ga(2)-C(16)	1.955(7)
Ga(2)-N(1)	2.229(6)
Ga(3)-C(41)	1.940(7)
Ga(3)-C(51)	1.956(8)
Ga(3)-C(31)	1.961(7)
Ga(3)-N(2)	2.231(6)
Ga(4)-C(56)	1.930(8)
Ga(4)-C(46)	1.966(8)
Ga(4)-C(36)	1.987(7)
Ga(4)-N(3)	2.232(6)
Ga(5)-C(69)	1.948(7)
Ga(5)-C(89)	1.953(8)
Ga(5)-C(79)	1.958(8)
Ga(5)-N(8)#2	2.238(6)
Ga(6)-C(94)	1.945(8)
Ga(6)-C(74)	1.951(8)
Ga(6)-C(84)	1.970(7)
Ga(6)-N(5)	2.214(6)
Ga(7)-C(99)	1.951(8)
Ga(7)-C(109)	1.959(8)
Ga(7)-C(119)	1.978(8)
Ga(7)-N(6)	2.239(6)
Ga(8)-C(124)	1.938(8)
Ga(8)-C(104)	1.956(8)
Ga(8)-C(114)	1.965(8)
Ga(8)-N(7)	2.234(6)
Fe(1)-C(10)	2.019(8)
Fe(1)-C(4)	2.036(7)
Fe(1)-C(9)	2.043(8)
Fe(1)-C(5)	2.051(8)
Fe(1)-C(2)	2.051(8)
Fe(1)-C(8)	2.051(8)
Fe(1)-C(3)	2.056(8)
Fe(1)-C(7)	2.057(7)
Fe(1)-C(1)	2.088(8)
Fe(1)-C(6)	2.104(8)
Fe(2)-C(20)	2.031(8)
Fe(2)-C(19)	2.036(8)
Fe(2)-C(12)	2.043(8)
Fe(2)-C(17)	2.044(8)
Fe(2)-C(18)	2.047(7)
Fe(2)-C(13)	2.050(8)

Fe(2)-C(15)	2.051(8)
Fe(2)-C(14)	2.070(8)
Fe(2)-C(11)	2.074(7)
Fe(2)-C(16)	2.091(8)
Fe(3)-C(29)	2.015(8)
Fe(3)-C(23)	2.024(8)
Fe(3)-C(30)	2.032(8)
Fe(3)-C(28)	2.038(8)
Fe(3)-C(22)	2.042(8)
Fe(3)-C(25)	2.046(8)
Fe(3)-C(27)	2.052(8)
Fe(3)-C(24)	2.058(8)
Fe(3)-C(26)	2.089(8)
Fe(3)-C(21)	2.101(8)
Fe(4)-C(32)	2.041(8)
Fe(4)-C(37)	2.041(8)
Fe(4)-C(34)	2.042(7)
Fe(4)-C(40)	2.044(8)
Fe(4)-C(35)	2.046(8)
Fe(4)-C(38)	2.049(8)
Fe(4)-C(39)	2.054(8)
Fe(4)-C(33)	2.062(8)
Fe(4)-C(36)	2.065(8)
Fe(4)-C(31)	2.069(8)
Fe(5)-C(48)	2.033(8)
Fe(5)-C(42)	2.036(8)
Fe(5)-C(44)	2.037(8)
Fe(5)-C(47)	2.037(8)
Fe(5)-C(43)	2.038(8)
Fe(5)-C(50)	2.041(8)
Fe(5)-C(49)	2.054(7)
Fe(5)-C(45)	2.056(8)
Fe(5)-C(41)	2.071(8)
Fe(5)-C(46)	2.082(8)
Fe(6)-C(59)	2.019(8)
Fe(6)-C(53)	2.028(8)
Fe(6)-C(60)	2.033(8)
Fe(6)-C(58)	2.037(8)
Fe(6)-C(54)	2.039(8)
Fe(6)-C(52)	2.042(8)
Fe(6)-C(55)	2.046(8)
Fe(6)-C(57)	2.061(8)
Fe(6)-C(51)	2.103(8)
Fe(6)-C(56)	2.103(8)
Fe(7)-C(77)	2.034(8)
Fe(7)-C(76)	2.038(8)
Fe(7)-C(71)	2.038(7)
Fe(7)-C(78)	2.039(7)
Fe(7)-C(73)	2.042(8)
Fe(7)-C(72)	2.043(8)
Fe(7)-C(75)	2.045(8)
Fe(7)-C(70)	2.058(7)

Fe(7)-C(69)	2.094(7)
Fe(7)-C(74)	2.094(7)
Fe(8)-C(82)	2.023(7)
Fe(8)-C(83)	2.023(7)
Fe(8)-C(88)	2.042(8)
Fe(8)-C(86)	2.043(8)
Fe(8)-C(87)	2.045(8)
Fe(8)-C(80)	2.054(8)
Fe(8)-C(85)	2.055(7)
Fe(8)-C(81)	2.059(8)
Fe(8)-C(79)	2.068(8)
Fe(8)-C(84)	2.083(7)
Fe(9)-C(92)	2.033(8)
Fe(9)-C(95)	2.034(7)
Fe(9)-C(91)	2.035(8)
Fe(9)-C(96)	2.043(7)
Fe(9)-C(93)	2.044(8)
Fe(9)-C(90)	2.047(8)
Fe(9)-C(97)	2.048(8)
Fe(9)-C(98)	2.057(8)
Fe(9)-C(94)	2.084(8)
Fe(9)-C(89)	2.087(7)
Fe(10)-C(106)	2.025(7)
Fe(10)-C(102)	2.035(8)
Fe(10)-C(101)	2.035(8)
Fe(10)-C(107)	2.036(7)
Fe(10)-C(108)	2.043(7)
Fe(10)-C(105)	2.045(8)
Fe(10)-C(100)	2.051(8)
Fe(10)-C(103)	2.052(7)
Fe(10)-C(99)	2.096(7)
Fe(10)-C(104)	2.107(7)
Fe(11)-C(110)	2.027(8)
Fe(11)-C(117)	2.028(8)
Fe(11)-C(113)	2.037(8)
Fe(11)-C(116)	2.038(8)
Fe(11)-C(118)	2.041(8)
Fe(11)-C(112)	2.050(8)
Fe(11)-C(115)	2.052(7)
Fe(11)-C(111)	2.058(8)
Fe(11)-C(114)	2.073(7)
Fe(11)-C(109)	2.080(8)
Fe(12)-C(126)	2.017(8)
Fe(12)-C(127)	2.022(8)
Fe(12)-C(125)	2.029(8)
Fe(12)-C(122)	2.036(8)
Fe(12)-C(121)	2.039(8)
Fe(12)-C(120)	2.045(8)
Fe(12)-C(123)	2.055(7)
Fe(12)-C(128)	2.058(8)
Fe(12)-C(124)	2.083(8)
Fe(12)-C(119)	2.091(7)

N(1)-C(61)	1.348(10)
N(1)-C(64)	1.348(8)
N(2)-C(62)	1.326(9)
N(2)-C(63)	1.354(9)
N(3)-C(68)	1.323(9)
N(3)-C(65)	1.326(9)
N(4)-C(67)	1.318(9)
N(4)-C(66)	1.327(9)
N(4)-Ga(1)#3	2.229(6)
N(5)-C(129)	1.332(9)
N(5)-C(132)	1.347(9)
N(6)-C(130)	1.316(9)
N(6)-C(131)	1.329(9)
N(7)-C(136)	1.326(9)
N(7)-C(133)	1.333(9)
N(8)-C(134)	1.332(9)
N(8)-C(135)	1.332(9)
N(8)-Ga(5)#4	2.238(6)
C(1)-C(2)	1.435(10)
C(1)-C(5)	1.443(10)
C(2)-C(3)	1.427(10)
C(3)-C(4)	1.422(10)
C(4)-C(5)	1.421(10)
C(6)-C(10)	1.453(10)
C(6)-C(7)	1.456(10)
C(7)-C(8)	1.416(10)
C(8)-C(9)	1.413(10)
C(9)-C(10)	1.420(10)
C(11)-C(15)	1.450(10)
C(11)-C(12)	1.451(10)
C(12)-C(13)	1.417(10)
C(13)-C(14)	1.413(10)
C(14)-C(15)	1.417(10)
C(16)-C(20)	1.426(10)
C(16)-C(17)	1.438(10)
C(17)-C(18)	1.395(10)
C(18)-C(19)	1.386(10)
C(19)-C(20)	1.416(10)
C(21)-C(22)	1.437(10)
C(21)-C(25)	1.443(10)
C(22)-C(23)	1.417(10)
C(23)-C(24)	1.433(10)
C(24)-C(25)	1.442(10)
C(26)-C(30)	1.436(10)
C(26)-C(27)	1.438(10)
C(27)-C(28)	1.426(10)
C(28)-C(29)	1.390(10)
C(29)-C(30)	1.403(10)
C(31)-C(35)	1.412(10)
C(31)-C(32)	1.431(10)
C(32)-C(33)	1.409(10)
C(33)-C(34)	1.418(10)

C(34)-C(35)	1.414(10)
C(36)-C(40)	1.393(10)
C(36)-C(37)	1.414(10)
C(37)-C(38)	1.409(10)
C(38)-C(39)	1.409(10)
C(39)-C(40)	1.421(10)
C(41)-C(45)	1.446(10)
C(41)-C(42)	1.453(10)
C(42)-C(43)	1.424(10)
C(43)-C(44)	1.408(10)
C(44)-C(45)	1.407(10)
C(46)-C(47)	1.432(10)
C(46)-C(50)	1.432(10)
C(47)-C(48)	1.434(10)
C(48)-C(49)	1.397(10)
C(49)-C(50)	1.407(10)
C(51)-C(52)	1.424(10)
C(51)-C(55)	1.437(10)
C(52)-C(53)	1.418(10)
C(53)-C(54)	1.419(10)
C(54)-C(55)	1.409(10)
C(56)-C(60)	1.458(10)
C(56)-C(57)	1.459(10)
C(57)-C(58)	1.413(10)
C(58)-C(59)	1.407(10)
C(59)-C(60)	1.397(10)
C(61)-C(62)	1.386(11)
C(63)-C(64)	1.390(10)
C(65)-C(66)	1.385(11)
C(67)-C(68)	1.402(10)
C(69)-C(73)	1.431(10)
C(69)-C(70)	1.455(10)
C(70)-C(71)	1.416(10)
C(71)-C(72)	1.423(10)
C(72)-C(73)	1.394(10)
C(74)-C(75)	1.439(11)
C(74)-C(78)	1.447(10)
C(75)-C(76)	1.416(10)
C(76)-C(77)	1.430(11)
C(77)-C(78)	1.402(10)
C(79)-C(83)	1.434(10)
C(79)-C(80)	1.449(10)
C(80)-C(81)	1.435(10)
C(81)-C(82)	1.405(10)
C(82)-C(83)	1.400(10)
C(84)-C(88)	1.430(10)
C(84)-C(85)	1.435(10)
C(85)-C(86)	1.427(10)
C(86)-C(87)	1.410(10)
C(87)-C(88)	1.420(10)
C(89)-C(93)	1.425(10)
C(89)-C(90)	1.451(10)

C(90)-C(91)	1.403(10)
C(91)-C(92)	1.379(10)
C(92)-C(93)	1.435(11)
C(94)-C(95)	1.441(10)
C(94)-C(98)	1.456(10)
C(95)-C(96)	1.396(10)
C(96)-C(97)	1.407(10)
C(97)-C(98)	1.416(10)
C(99)-C(100)	1.445(11)
C(99)-C(103)	1.471(10)
C(100)-C(101)	1.383(10)
C(101)-C(102)	1.440(11)
C(102)-C(103)	1.427(10)
C(104)-C(108)	1.417(10)
C(104)-C(105)	1.442(10)
C(105)-C(106)	1.418(10)
C(106)-C(107)	1.411(10)
C(107)-C(108)	1.419(10)
C(109)-C(113)	1.411(10)
C(109)-C(110)	1.422(10)
C(110)-C(111)	1.400(10)
C(111)-C(112)	1.398(11)
C(112)-C(113)	1.421(10)
C(114)-C(115)	1.415(10)
C(114)-C(118)	1.436(10)
C(115)-C(116)	1.415(10)
C(116)-C(117)	1.406(10)
C(117)-C(118)	1.398(10)
C(119)-C(123)	1.421(10)
C(119)-C(120)	1.430(10)
C(120)-C(121)	1.430(10)
C(121)-C(122)	1.410(10)
C(122)-C(123)	1.426(11)
C(124)-C(128)	1.433(10)
C(124)-C(125)	1.465(11)
C(125)-C(126)	1.408(11)
C(126)-C(127)	1.412(11)
C(127)-C(128)	1.410(11)
C(129)-C(130)	1.394(10)
C(131)-C(132)	1.376(10)
C(133)-C(134)	1.372(10)
C(135)-C(136)	1.381(10)
C(137)-C(138)	1.403(14)
C(137)-C(143)	1.428(15)
C(137)-C(142)	1.444(15)
C(138)-C(139)	1.264(13)
C(139)-C(140)	1.445(15)
C(140)-C(141)	1.337(14)
C(141)-C(142)	1.341(13)
C(144)-C(147)	1.26(2)
C(144)-C(145)	1.329(15)
C(144)-C(146)#5	1.483(16)

C(145)-C(146)	1.225(14)
C(146)-C(144)#5	1.483(16)
C(148)-C(149)	1.404(15)
C(148)-C(154)	1.408(16)
C(148)-C(153)	1.433(13)
C(149)-C(150)	1.290(14)
C(150)-C(151)	1.439(14)
C(151)-C(152)	1.350(15)
C(152)-C(153)	1.327(14)
C(155)-C(158)	1.224(17)
C(155)-C(156)	1.349(14)
C(155)-C(157)#6	1.443(14)
C(156)-C(157)	1.304(14)
C(157)-C(155)#6	1.443(14)

C(11)-Ga(1)-C(21)	120.6(3)
C(11)-Ga(1)-C(1)	117.0(3)
C(21)-Ga(1)-C(1)	118.4(3)
C(11)-Ga(1)-N(4)#1	94.5(3)
C(21)-Ga(1)-N(4)#1	98.6(3)
C(1)-Ga(1)-N(4)#1	97.0(3)
C(6)-Ga(2)-C(26)	121.5(3)
C(6)-Ga(2)-C(16)	118.4(3)
C(26)-Ga(2)-C(16)	117.0(3)
C(6)-Ga(2)-N(1)	95.3(3)
C(26)-Ga(2)-N(1)	95.6(3)
C(16)-Ga(2)-N(1)	96.7(3)
C(41)-Ga(3)-C(51)	122.2(3)
C(41)-Ga(3)-C(31)	119.1(3)
C(51)-Ga(3)-C(31)	115.0(3)
C(41)-Ga(3)-N(2)	96.0(3)
C(51)-Ga(3)-N(2)	97.3(3)
C(31)-Ga(3)-N(2)	96.1(3)
C(56)-Ga(4)-C(46)	117.5(3)
C(56)-Ga(4)-C(36)	123.4(3)
C(46)-Ga(4)-C(36)	114.3(3)
C(56)-Ga(4)-N(3)	101.4(3)
C(46)-Ga(4)-N(3)	96.2(3)
C(36)-Ga(4)-N(3)	94.2(3)
C(69)-Ga(5)-C(89)	116.7(3)
C(69)-Ga(5)-C(79)	122.4(3)
C(89)-Ga(5)-C(79)	117.7(3)
C(69)-Ga(5)-N(8)#2	95.0(3)
C(89)-Ga(5)-N(8)#2	96.8(3)
C(79)-Ga(5)-N(8)#2	96.1(3)
C(94)-Ga(6)-C(74)	120.9(3)
C(94)-Ga(6)-C(84)	117.6(3)
C(74)-Ga(6)-C(84)	117.6(3)
C(94)-Ga(6)-N(5)	94.3(3)
C(74)-Ga(6)-N(5)	98.8(3)
C(84)-Ga(6)-N(5)	96.7(3)
C(99)-Ga(7)-C(109)	122.7(3)

C(99)-Ga(7)-C(119)	118.3(3)
C(109)-Ga(7)-C(119)	114.2(3)
C(99)-Ga(7)-N(6)	100.9(3)
C(109)-Ga(7)-N(6)	94.4(3)
C(119)-Ga(7)-N(6)	96.3(3)
C(124)-Ga(8)-C(104)	121.9(3)
C(124)-Ga(8)-C(114)	118.7(3)
C(104)-Ga(8)-C(114)	115.9(3)
C(124)-Ga(8)-N(7)	95.6(3)
C(104)-Ga(8)-N(7)	97.0(3)
C(114)-Ga(8)-N(7)	96.2(3)
C(10)-Fe(1)-C(4)	113.9(3)
C(10)-Fe(1)-C(9)	40.9(3)
C(4)-Fe(1)-C(9)	106.5(3)
C(10)-Fe(1)-C(5)	109.0(3)
C(4)-Fe(1)-C(5)	40.7(3)
C(9)-Fe(1)-C(5)	131.1(3)
C(10)-Fe(1)-C(2)	173.0(3)
C(4)-Fe(1)-C(2)	68.4(3)
C(9)-Fe(1)-C(2)	145.8(3)
C(5)-Fe(1)-C(2)	68.1(3)
C(10)-Fe(1)-C(8)	67.9(3)
C(4)-Fe(1)-C(8)	130.6(3)
C(9)-Fe(1)-C(8)	40.4(3)
C(5)-Fe(1)-C(8)	169.8(3)
C(2)-Fe(1)-C(8)	116.1(3)
C(10)-Fe(1)-C(3)	145.1(3)
C(4)-Fe(1)-C(3)	40.7(3)
C(9)-Fe(1)-C(3)	113.1(3)
C(5)-Fe(1)-C(3)	68.2(3)
C(2)-Fe(1)-C(3)	40.7(3)
C(8)-Fe(1)-C(3)	108.4(3)
C(10)-Fe(1)-C(7)	68.0(3)
C(4)-Fe(1)-C(7)	170.3(3)
C(9)-Fe(1)-C(7)	68.3(3)
C(5)-Fe(1)-C(7)	148.7(3)
C(2)-Fe(1)-C(7)	110.9(3)
C(8)-Fe(1)-C(7)	40.3(3)
C(3)-Fe(1)-C(7)	132.7(3)
C(10)-Fe(1)-C(1)	133.2(3)
C(4)-Fe(1)-C(1)	68.9(3)
C(9)-Fe(1)-C(1)	171.3(3)
C(5)-Fe(1)-C(1)	40.8(3)
C(2)-Fe(1)-C(1)	40.6(3)
C(8)-Fe(1)-C(1)	148.1(3)
C(3)-Fe(1)-C(1)	68.6(3)
C(7)-Fe(1)-C(1)	117.3(3)
C(10)-Fe(1)-C(6)	41.2(3)
C(4)-Fe(1)-C(6)	146.3(3)
C(9)-Fe(1)-C(6)	69.7(3)
C(5)-Fe(1)-C(6)	115.7(3)
C(2)-Fe(1)-C(6)	133.5(3)

C(8)-Fe(1)-C(6)	68.9(3)
C(3)-Fe(1)-C(6)	172.5(3)
C(7)-Fe(1)-C(6)	40.9(3)
C(1)-Fe(1)-C(6)	109.7(3)
C(20)-Fe(2)-C(19)	40.7(3)
C(20)-Fe(2)-C(12)	171.2(3)
C(19)-Fe(2)-C(12)	146.6(3)
C(20)-Fe(2)-C(17)	67.5(3)
C(19)-Fe(2)-C(17)	67.5(3)
C(12)-Fe(2)-C(17)	108.9(3)
C(20)-Fe(2)-C(18)	67.1(3)
C(19)-Fe(2)-C(18)	39.7(3)
C(12)-Fe(2)-C(18)	115.8(3)
C(17)-Fe(2)-C(18)	39.9(3)
C(20)-Fe(2)-C(13)	147.9(3)
C(19)-Fe(2)-C(13)	115.0(3)
C(12)-Fe(2)-C(13)	40.5(3)
C(17)-Fe(2)-C(13)	130.7(3)
C(18)-Fe(2)-C(13)	108.5(3)
C(20)-Fe(2)-C(15)	110.5(3)
C(19)-Fe(2)-C(15)	131.4(3)
C(12)-Fe(2)-C(15)	68.3(3)
C(17)-Fe(2)-C(15)	150.6(3)
C(18)-Fe(2)-C(15)	168.8(3)
C(13)-Fe(2)-C(15)	67.3(3)
C(20)-Fe(2)-C(14)	116.7(3)
C(19)-Fe(2)-C(14)	108.0(3)
C(12)-Fe(2)-C(14)	68.4(3)
C(17)-Fe(2)-C(14)	168.3(3)
C(18)-Fe(2)-C(14)	130.0(3)
C(13)-Fe(2)-C(14)	40.1(3)
C(15)-Fe(2)-C(14)	40.2(3)
C(20)-Fe(2)-C(11)	132.1(3)
C(19)-Fe(2)-C(11)	171.0(3)
C(12)-Fe(2)-C(11)	41.3(3)
C(17)-Fe(2)-C(11)	116.9(3)
C(18)-Fe(2)-C(11)	148.5(3)
C(13)-Fe(2)-C(11)	68.8(3)
C(15)-Fe(2)-C(11)	41.2(3)
C(14)-Fe(2)-C(11)	69.2(3)
C(20)-Fe(2)-C(16)	40.4(3)
C(19)-Fe(2)-C(16)	68.5(3)
C(12)-Fe(2)-C(16)	131.7(3)
C(17)-Fe(2)-C(16)	40.7(3)
C(18)-Fe(2)-C(16)	67.8(3)
C(13)-Fe(2)-C(16)	170.0(3)
C(15)-Fe(2)-C(16)	118.1(3)
C(14)-Fe(2)-C(16)	149.3(3)
C(11)-Fe(2)-C(16)	109.2(3)
C(29)-Fe(3)-C(23)	113.8(3)
C(29)-Fe(3)-C(30)	40.6(3)
C(23)-Fe(3)-C(30)	149.6(3)

C(29)-Fe(3)-C(28)	40.1(3)
C(23)-Fe(3)-C(28)	103.3(3)
C(30)-Fe(3)-C(28)	67.5(3)
C(29)-Fe(3)-C(22)	148.8(3)
C(23)-Fe(3)-C(22)	40.8(3)
C(30)-Fe(3)-C(22)	169.3(3)
C(28)-Fe(3)-C(22)	116.9(3)
C(29)-Fe(3)-C(25)	127.3(3)
C(23)-Fe(3)-C(25)	68.8(3)
C(30)-Fe(3)-C(25)	111.0(3)
C(28)-Fe(3)-C(25)	162.5(3)
C(22)-Fe(3)-C(25)	67.9(3)
C(29)-Fe(3)-C(27)	68.0(3)
C(23)-Fe(3)-C(27)	125.5(3)
C(30)-Fe(3)-C(27)	67.3(3)
C(28)-Fe(3)-C(27)	40.8(3)
C(22)-Fe(3)-C(27)	109.1(3)
C(25)-Fe(3)-C(27)	156.2(3)
C(29)-Fe(3)-C(24)	104.1(3)
C(23)-Fe(3)-C(24)	41.1(3)
C(30)-Fe(3)-C(24)	118.0(3)
C(28)-Fe(3)-C(24)	122.9(3)
C(22)-Fe(3)-C(24)	68.6(3)
C(25)-Fe(3)-C(24)	41.1(3)
C(27)-Fe(3)-C(24)	161.9(3)
C(29)-Fe(3)-C(26)	69.3(3)
C(23)-Fe(3)-C(26)	165.1(3)
C(30)-Fe(3)-C(26)	40.8(3)
C(28)-Fe(3)-C(26)	69.1(3)
C(22)-Fe(3)-C(26)	130.0(3)
C(25)-Fe(3)-C(26)	122.0(3)
C(27)-Fe(3)-C(26)	40.6(3)
C(24)-Fe(3)-C(26)	153.8(3)
C(29)-Fe(3)-C(21)	167.1(3)
C(23)-Fe(3)-C(21)	69.1(3)
C(30)-Fe(3)-C(21)	131.7(3)
C(28)-Fe(3)-C(21)	152.8(3)
C(22)-Fe(3)-C(21)	40.6(3)
C(25)-Fe(3)-C(21)	40.7(3)
C(27)-Fe(3)-C(21)	121.4(3)
C(24)-Fe(3)-C(21)	69.4(3)
C(26)-Fe(3)-C(21)	111.4(3)
C(32)-Fe(4)-C(37)	113.0(3)
C(32)-Fe(4)-C(34)	67.5(3)
C(37)-Fe(4)-C(34)	176.9(3)
C(32)-Fe(4)-C(40)	177.2(3)
C(37)-Fe(4)-C(40)	66.8(3)
C(34)-Fe(4)-C(40)	112.9(3)
C(32)-Fe(4)-C(35)	67.0(3)
C(37)-Fe(4)-C(35)	142.7(3)
C(34)-Fe(4)-C(35)	40.5(3)
C(40)-Fe(4)-C(35)	111.3(3)

C(32)-Fe(4)-C(38)	114.1(3)
C(37)-Fe(4)-C(38)	40.3(3)
C(34)-Fe(4)-C(38)	136.6(3)
C(40)-Fe(4)-C(38)	67.7(3)
C(35)-Fe(4)-C(38)	176.6(3)
C(32)-Fe(4)-C(39)	142.2(3)
C(37)-Fe(4)-C(39)	67.3(3)
C(34)-Fe(4)-C(39)	110.3(3)
C(40)-Fe(4)-C(39)	40.6(3)
C(35)-Fe(4)-C(39)	137.0(3)
C(38)-Fe(4)-C(39)	40.2(3)
C(32)-Fe(4)-C(33)	40.2(3)
C(37)-Fe(4)-C(33)	138.0(3)
C(34)-Fe(4)-C(33)	40.4(3)
C(40)-Fe(4)-C(33)	141.8(3)
C(35)-Fe(4)-C(33)	67.7(3)
C(38)-Fe(4)-C(33)	111.0(3)
C(39)-Fe(4)-C(33)	112.7(3)
C(32)-Fe(4)-C(36)	138.4(3)
C(37)-Fe(4)-C(36)	40.3(3)
C(34)-Fe(4)-C(36)	141.3(3)
C(40)-Fe(4)-C(36)	39.6(3)
C(35)-Fe(4)-C(36)	113.2(3)
C(38)-Fe(4)-C(36)	68.2(3)
C(39)-Fe(4)-C(36)	67.8(3)
C(33)-Fe(4)-C(36)	178.2(3)
C(32)-Fe(4)-C(31)	40.7(3)
C(37)-Fe(4)-C(31)	114.0(3)
C(34)-Fe(4)-C(31)	68.5(3)
C(40)-Fe(4)-C(31)	136.5(3)
C(35)-Fe(4)-C(31)	40.1(3)
C(38)-Fe(4)-C(31)	142.7(3)
C(39)-Fe(4)-C(31)	176.6(3)
C(33)-Fe(4)-C(31)	68.7(3)
C(36)-Fe(4)-C(31)	110.9(3)
C(48)-Fe(5)-C(42)	112.8(3)
C(48)-Fe(5)-C(44)	129.4(3)
C(42)-Fe(5)-C(44)	68.5(3)
C(48)-Fe(5)-C(47)	41.2(3)
C(42)-Fe(5)-C(47)	108.9(3)
C(44)-Fe(5)-C(47)	169.4(3)
C(48)-Fe(5)-C(43)	105.6(3)
C(42)-Fe(5)-C(43)	40.9(3)
C(44)-Fe(5)-C(43)	40.4(3)
C(47)-Fe(5)-C(43)	131.1(3)
C(48)-Fe(5)-C(50)	68.0(3)
C(42)-Fe(5)-C(50)	173.9(3)
C(44)-Fe(5)-C(50)	116.0(3)
C(47)-Fe(5)-C(50)	67.5(3)
C(43)-Fe(5)-C(50)	145.1(3)
C(48)-Fe(5)-C(49)	40.0(3)
C(42)-Fe(5)-C(49)	143.9(3)

C(44)-Fe(5)-C(49)	108.1(3)
C(47)-Fe(5)-C(49)	67.6(3)
C(43)-Fe(5)-C(49)	112.6(3)
C(50)-Fe(5)-C(49)	40.2(3)
C(48)-Fe(5)-C(45)	169.2(3)
C(42)-Fe(5)-C(45)	68.2(3)
C(44)-Fe(5)-C(45)	40.2(3)
C(47)-Fe(5)-C(45)	149.5(3)
C(43)-Fe(5)-C(45)	67.7(3)
C(50)-Fe(5)-C(45)	112.3(3)
C(49)-Fe(5)-C(45)	133.4(3)
C(48)-Fe(5)-C(41)	146.2(3)
C(42)-Fe(5)-C(41)	41.4(3)
C(44)-Fe(5)-C(41)	69.3(3)
C(47)-Fe(5)-C(41)	116.0(3)
C(43)-Fe(5)-C(41)	69.5(3)
C(50)-Fe(5)-C(41)	135.0(3)
C(49)-Fe(5)-C(41)	173.5(3)
C(45)-Fe(5)-C(41)	41.0(3)
C(48)-Fe(5)-C(46)	69.5(3)
C(42)-Fe(5)-C(46)	133.5(3)
C(44)-Fe(5)-C(46)	148.1(3)
C(47)-Fe(5)-C(46)	40.7(3)
C(43)-Fe(5)-C(46)	171.4(3)
C(50)-Fe(5)-C(46)	40.6(3)
C(49)-Fe(5)-C(46)	68.5(3)
C(45)-Fe(5)-C(46)	118.2(3)
C(41)-Fe(5)-C(46)	110.4(3)
C(59)-Fe(6)-C(53)	114.7(3)
C(59)-Fe(6)-C(60)	40.3(3)
C(53)-Fe(6)-C(60)	149.9(3)
C(59)-Fe(6)-C(58)	40.6(3)
C(53)-Fe(6)-C(58)	103.4(3)
C(60)-Fe(6)-C(58)	68.3(3)
C(59)-Fe(6)-C(54)	103.1(3)
C(53)-Fe(6)-C(54)	40.9(3)
C(60)-Fe(6)-C(54)	117.2(3)
C(58)-Fe(6)-C(54)	121.4(3)
C(59)-Fe(6)-C(52)	151.3(3)
C(53)-Fe(6)-C(52)	40.8(3)
C(60)-Fe(6)-C(52)	168.0(3)
C(58)-Fe(6)-C(52)	119.3(3)
C(54)-Fe(6)-C(52)	68.1(3)
C(59)-Fe(6)-C(55)	124.3(3)
C(53)-Fe(6)-C(55)	68.2(3)
C(60)-Fe(6)-C(55)	109.0(3)
C(58)-Fe(6)-C(55)	159.6(3)
C(54)-Fe(6)-C(55)	40.4(3)
C(52)-Fe(6)-C(55)	67.4(3)
C(59)-Fe(6)-C(57)	67.6(3)
C(53)-Fe(6)-C(57)	125.3(3)
C(60)-Fe(6)-C(57)	67.8(3)

C(58)-Fe(6)-C(57)	40.3(3)
C(54)-Fe(6)-C(57)	160.1(3)
C(52)-Fe(6)-C(57)	111.2(3)
C(55)-Fe(6)-C(57)	159.2(3)
C(59)-Fe(6)-C(51)	163.6(3)
C(53)-Fe(6)-C(51)	68.7(3)
C(60)-Fe(6)-C(51)	129.8(3)
C(58)-Fe(6)-C(51)	155.8(3)
C(54)-Fe(6)-C(51)	68.5(3)
C(52)-Fe(6)-C(51)	40.2(3)
C(55)-Fe(6)-C(51)	40.5(3)
C(57)-Fe(6)-C(51)	124.7(3)
C(59)-Fe(6)-C(56)	69.1(3)
C(53)-Fe(6)-C(56)	164.9(3)
C(60)-Fe(6)-C(56)	41.2(3)
C(58)-Fe(6)-C(56)	69.4(3)
C(54)-Fe(6)-C(56)	154.2(3)
C(52)-Fe(6)-C(56)	130.1(3)
C(55)-Fe(6)-C(56)	122.9(3)
C(57)-Fe(6)-C(56)	41.0(3)
C(51)-Fe(6)-C(56)	112.0(3)
C(77)-Fe(7)-C(76)	41.1(3)
C(77)-Fe(7)-C(71)	123.1(3)
C(76)-Fe(7)-C(71)	103.7(3)
C(77)-Fe(7)-C(78)	40.3(3)
C(76)-Fe(7)-C(78)	68.3(3)
C(71)-Fe(7)-C(78)	161.7(3)
C(77)-Fe(7)-C(73)	118.7(3)
C(76)-Fe(7)-C(73)	150.6(3)
C(71)-Fe(7)-C(73)	67.5(3)
C(78)-Fe(7)-C(73)	110.8(3)
C(77)-Fe(7)-C(72)	104.5(3)
C(76)-Fe(7)-C(72)	115.1(3)
C(71)-Fe(7)-C(72)	40.8(3)
C(78)-Fe(7)-C(72)	126.0(3)
C(73)-Fe(7)-C(72)	39.9(3)
C(77)-Fe(7)-C(75)	68.3(3)
C(76)-Fe(7)-C(75)	40.6(3)
C(71)-Fe(7)-C(75)	117.6(3)
C(78)-Fe(7)-C(75)	67.8(3)
C(73)-Fe(7)-C(75)	168.5(3)
C(72)-Fe(7)-C(75)	150.4(3)
C(77)-Fe(7)-C(70)	161.4(3)
C(76)-Fe(7)-C(70)	124.9(3)
C(71)-Fe(7)-C(70)	40.5(3)
C(78)-Fe(7)-C(70)	157.4(3)
C(73)-Fe(7)-C(70)	67.5(3)
C(72)-Fe(7)-C(70)	68.2(3)
C(75)-Fe(7)-C(70)	109.1(3)
C(77)-Fe(7)-C(69)	154.2(3)
C(76)-Fe(7)-C(69)	164.6(3)
C(71)-Fe(7)-C(69)	68.9(3)

C(78)-Fe(7)-C(69)	122.6(3)
C(73)-Fe(7)-C(69)	40.5(3)
C(72)-Fe(7)-C(69)	68.7(3)
C(75)-Fe(7)-C(69)	129.7(3)
C(70)-Fe(7)-C(69)	41.0(3)
C(77)-Fe(7)-C(74)	69.0(3)
C(76)-Fe(7)-C(74)	69.1(3)
C(71)-Fe(7)-C(74)	153.5(3)
C(78)-Fe(7)-C(74)	40.9(3)
C(73)-Fe(7)-C(74)	130.8(3)
C(72)-Fe(7)-C(74)	165.5(3)
C(75)-Fe(7)-C(74)	40.7(3)
C(70)-Fe(7)-C(74)	121.9(3)
C(69)-Fe(7)-C(74)	111.2(3)
C(82)-Fe(8)-C(83)	40.5(3)
C(82)-Fe(8)-C(88)	131.4(3)
C(83)-Fe(8)-C(88)	109.0(3)
C(82)-Fe(8)-C(86)	113.9(3)
C(83)-Fe(8)-C(86)	144.8(3)
C(88)-Fe(8)-C(86)	67.6(3)
C(82)-Fe(8)-C(87)	107.0(3)
C(83)-Fe(8)-C(87)	113.4(3)
C(88)-Fe(8)-C(87)	40.7(3)
C(86)-Fe(8)-C(87)	40.3(3)
C(82)-Fe(8)-C(80)	68.0(3)
C(83)-Fe(8)-C(80)	68.4(3)
C(88)-Fe(8)-C(80)	148.6(3)
C(86)-Fe(8)-C(80)	133.2(3)
C(87)-Fe(8)-C(80)	170.5(3)
C(82)-Fe(8)-C(85)	146.1(3)
C(83)-Fe(8)-C(85)	173.1(3)
C(88)-Fe(8)-C(85)	68.0(3)
C(86)-Fe(8)-C(85)	40.8(3)
C(87)-Fe(8)-C(85)	68.6(3)
C(80)-Fe(8)-C(85)	110.8(3)
C(82)-Fe(8)-C(81)	40.3(3)
C(83)-Fe(8)-C(81)	68.4(3)
C(88)-Fe(8)-C(81)	169.7(3)
C(86)-Fe(8)-C(81)	108.4(3)
C(87)-Fe(8)-C(81)	130.2(3)
C(80)-Fe(8)-C(81)	40.8(3)
C(85)-Fe(8)-C(81)	115.8(3)
C(82)-Fe(8)-C(79)	68.8(3)
C(83)-Fe(8)-C(79)	41.0(3)
C(88)-Fe(8)-C(79)	115.7(3)
C(86)-Fe(8)-C(79)	173.3(3)
C(87)-Fe(8)-C(79)	145.8(3)
C(80)-Fe(8)-C(79)	41.1(3)
C(85)-Fe(8)-C(79)	133.9(3)
C(81)-Fe(8)-C(79)	69.3(3)
C(82)-Fe(8)-C(84)	171.3(3)
C(83)-Fe(8)-C(84)	133.2(3)

C(88)-Fe(8)-C(84)	40.6(3)
C(86)-Fe(8)-C(84)	68.2(3)
C(87)-Fe(8)-C(84)	68.8(3)
C(80)-Fe(8)-C(84)	117.3(3)
C(85)-Fe(8)-C(84)	40.6(3)
C(81)-Fe(8)-C(84)	148.2(3)
C(79)-Fe(8)-C(84)	110.1(3)
C(92)-Fe(9)-C(95)	146.2(3)
C(92)-Fe(9)-C(91)	39.6(3)
C(95)-Fe(9)-C(91)	115.7(3)
C(92)-Fe(9)-C(96)	114.7(3)
C(95)-Fe(9)-C(96)	40.1(3)
C(91)-Fe(9)-C(96)	108.0(3)
C(92)-Fe(9)-C(93)	41.2(3)
C(95)-Fe(9)-C(93)	171.5(3)
C(91)-Fe(9)-C(93)	67.8(3)
C(96)-Fe(9)-C(93)	147.9(3)
C(92)-Fe(9)-C(90)	67.5(3)
C(95)-Fe(9)-C(90)	109.5(3)
C(91)-Fe(9)-C(90)	40.2(3)
C(96)-Fe(9)-C(90)	130.7(3)
C(93)-Fe(9)-C(90)	67.7(3)
C(92)-Fe(9)-C(97)	108.1(3)
C(95)-Fe(9)-C(97)	67.9(3)
C(91)-Fe(9)-C(97)	129.8(3)
C(96)-Fe(9)-C(97)	40.2(3)
C(93)-Fe(9)-C(97)	116.6(3)
C(90)-Fe(9)-C(97)	168.5(3)
C(92)-Fe(9)-C(98)	131.7(3)
C(95)-Fe(9)-C(98)	68.0(3)
C(91)-Fe(9)-C(98)	168.9(3)
C(96)-Fe(9)-C(98)	67.5(3)
C(93)-Fe(9)-C(98)	110.2(3)
C(90)-Fe(9)-C(98)	150.3(3)
C(97)-Fe(9)-C(98)	40.4(3)
C(92)-Fe(9)-C(94)	171.6(3)
C(95)-Fe(9)-C(94)	41.0(3)
C(91)-Fe(9)-C(94)	148.1(3)
C(96)-Fe(9)-C(94)	68.5(3)
C(93)-Fe(9)-C(94)	132.2(3)
C(90)-Fe(9)-C(94)	116.9(3)
C(97)-Fe(9)-C(94)	69.1(3)
C(98)-Fe(9)-C(94)	41.2(3)
C(92)-Fe(9)-C(89)	68.9(3)
C(95)-Fe(9)-C(89)	132.3(3)
C(91)-Fe(9)-C(89)	68.7(3)
C(96)-Fe(9)-C(89)	170.4(3)
C(93)-Fe(9)-C(89)	40.3(3)
C(90)-Fe(9)-C(89)	41.1(3)
C(97)-Fe(9)-C(89)	148.7(3)
C(98)-Fe(9)-C(89)	117.4(3)
C(94)-Fe(9)-C(89)	109.2(3)

C(106)-Fe(10)-C(102)	113.1(3)
C(106)-Fe(10)-C(101)	103.8(3)
C(102)-Fe(10)-C(101)	41.4(3)
C(106)-Fe(10)-C(107)	40.7(3)
C(102)-Fe(10)-C(107)	102.5(3)
C(101)-Fe(10)-C(107)	122.9(3)
C(106)-Fe(10)-C(108)	68.0(3)
C(102)-Fe(10)-C(108)	125.5(3)
C(101)-Fe(10)-C(108)	162.1(3)
C(107)-Fe(10)-C(108)	40.7(3)
C(106)-Fe(10)-C(105)	40.8(3)
C(102)-Fe(10)-C(105)	149.1(3)
C(101)-Fe(10)-C(105)	117.6(3)
C(107)-Fe(10)-C(105)	68.3(3)
C(108)-Fe(10)-C(105)	67.4(3)
C(106)-Fe(10)-C(100)	126.2(3)
C(102)-Fe(10)-C(100)	68.3(3)
C(101)-Fe(10)-C(100)	39.6(3)
C(107)-Fe(10)-C(100)	161.2(3)
C(108)-Fe(10)-C(100)	157.7(3)
C(105)-Fe(10)-C(100)	110.8(3)
C(106)-Fe(10)-C(103)	148.0(3)
C(102)-Fe(10)-C(103)	40.9(3)
C(101)-Fe(10)-C(103)	69.0(3)
C(107)-Fe(10)-C(103)	115.6(3)
C(108)-Fe(10)-C(103)	108.9(3)
C(105)-Fe(10)-C(103)	169.8(3)
C(100)-Fe(10)-C(103)	68.8(3)
C(106)-Fe(10)-C(99)	166.2(3)
C(102)-Fe(10)-C(99)	69.1(3)
C(101)-Fe(10)-C(99)	68.4(3)
C(107)-Fe(10)-C(99)	153.1(3)
C(108)-Fe(10)-C(99)	122.7(3)
C(105)-Fe(10)-C(99)	131.6(3)
C(100)-Fe(10)-C(99)	40.8(3)
C(103)-Fe(10)-C(99)	41.5(3)
C(106)-Fe(10)-C(104)	68.7(3)
C(102)-Fe(10)-C(104)	164.7(3)
C(101)-Fe(10)-C(104)	153.9(3)
C(107)-Fe(10)-C(104)	68.5(3)
C(108)-Fe(10)-C(104)	39.9(3)
C(105)-Fe(10)-C(104)	40.6(3)
C(100)-Fe(10)-C(104)	123.9(3)
C(103)-Fe(10)-C(104)	130.6(3)
C(99)-Fe(10)-C(104)	113.0(3)
C(110)-Fe(11)-C(117)	176.9(3)
C(110)-Fe(11)-C(113)	66.6(3)
C(117)-Fe(11)-C(113)	113.4(3)
C(110)-Fe(11)-C(116)	137.6(3)
C(117)-Fe(11)-C(116)	40.5(3)
C(113)-Fe(11)-C(116)	141.9(3)
C(110)-Fe(11)-C(118)	142.9(3)

C(117)-Fe(11)-C(118)	40.2(3)
C(113)-Fe(11)-C(118)	111.3(3)
C(116)-Fe(11)-C(118)	68.1(3)
C(110)-Fe(11)-C(112)	67.2(3)
C(117)-Fe(11)-C(112)	110.7(3)
C(113)-Fe(11)-C(112)	40.7(3)
C(116)-Fe(11)-C(112)	112.3(3)
C(118)-Fe(11)-C(112)	137.0(3)
C(110)-Fe(11)-C(115)	112.6(3)
C(117)-Fe(11)-C(115)	67.5(3)
C(113)-Fe(11)-C(115)	177.1(3)
C(116)-Fe(11)-C(115)	40.5(3)
C(118)-Fe(11)-C(115)	67.5(3)
C(112)-Fe(11)-C(115)	141.9(3)
C(110)-Fe(11)-C(111)	40.1(3)
C(117)-Fe(11)-C(111)	136.9(3)
C(113)-Fe(11)-C(111)	67.1(3)
C(116)-Fe(11)-C(111)	110.9(3)
C(118)-Fe(11)-C(111)	176.4(3)
C(112)-Fe(11)-C(111)	39.8(3)
C(115)-Fe(11)-C(111)	114.2(3)
C(110)-Fe(11)-C(114)	113.9(3)
C(117)-Fe(11)-C(114)	68.3(3)
C(113)-Fe(11)-C(114)	137.3(3)
C(116)-Fe(11)-C(114)	68.5(3)
C(118)-Fe(11)-C(114)	40.9(3)
C(112)-Fe(11)-C(114)	177.5(3)
C(115)-Fe(11)-C(114)	40.1(3)
C(111)-Fe(11)-C(114)	142.5(3)
C(110)-Fe(11)-C(109)	40.5(3)
C(117)-Fe(11)-C(109)	141.5(3)
C(113)-Fe(11)-C(109)	40.1(3)
C(116)-Fe(11)-C(109)	177.7(3)
C(118)-Fe(11)-C(109)	112.8(3)
C(112)-Fe(11)-C(109)	68.7(3)
C(115)-Fe(11)-C(109)	137.5(3)
C(111)-Fe(11)-C(109)	68.4(3)
C(114)-Fe(11)-C(109)	110.6(3)
C(126)-Fe(12)-C(127)	40.9(3)
C(126)-Fe(12)-C(125)	40.7(3)
C(127)-Fe(12)-C(125)	68.7(3)
C(126)-Fe(12)-C(122)	112.1(3)
C(127)-Fe(12)-C(122)	107.1(3)
C(125)-Fe(12)-C(122)	143.9(3)
C(126)-Fe(12)-C(121)	105.3(3)
C(127)-Fe(12)-C(121)	129.2(3)
C(125)-Fe(12)-C(121)	112.9(3)
C(122)-Fe(12)-C(121)	40.5(3)
C(126)-Fe(12)-C(120)	130.4(3)
C(127)-Fe(12)-C(120)	169.1(3)
C(125)-Fe(12)-C(120)	108.8(3)
C(122)-Fe(12)-C(120)	68.2(3)

C(121)-Fe(12)-C(120)	41.0(3)
C(126)-Fe(12)-C(123)	145.6(3)
C(127)-Fe(12)-C(123)	115.9(3)
C(125)-Fe(12)-C(123)	173.6(3)
C(122)-Fe(12)-C(123)	40.8(3)
C(121)-Fe(12)-C(123)	68.2(3)
C(120)-Fe(12)-C(123)	67.6(3)
C(126)-Fe(12)-C(128)	68.1(3)
C(127)-Fe(12)-C(128)	40.4(3)
C(125)-Fe(12)-C(128)	68.1(3)
C(122)-Fe(12)-C(128)	132.8(3)
C(121)-Fe(12)-C(128)	169.4(3)
C(120)-Fe(12)-C(128)	149.6(3)
C(123)-Fe(12)-C(128)	112.0(3)
C(126)-Fe(12)-C(124)	69.6(3)
C(127)-Fe(12)-C(124)	69.2(3)
C(125)-Fe(12)-C(124)	41.7(3)
C(122)-Fe(12)-C(124)	172.7(3)
C(121)-Fe(12)-C(124)	146.7(3)
C(120)-Fe(12)-C(124)	116.5(3)
C(123)-Fe(12)-C(124)	134.3(3)
C(128)-Fe(12)-C(124)	40.5(3)
C(126)-Fe(12)-C(119)	170.7(3)
C(127)-Fe(12)-C(119)	148.4(3)
C(125)-Fe(12)-C(119)	133.8(3)
C(122)-Fe(12)-C(119)	68.4(3)
C(121)-Fe(12)-C(119)	68.7(3)
C(120)-Fe(12)-C(119)	40.5(3)
C(123)-Fe(12)-C(119)	40.1(3)
C(128)-Fe(12)-C(119)	118.9(3)
C(124)-Fe(12)-C(119)	111.1(3)
C(61)-N(1)-C(64)	116.6(7)
C(61)-N(1)-Ga(2)	120.1(5)
C(64)-N(1)-Ga(2)	122.7(5)
C(62)-N(2)-C(63)	117.0(7)
C(62)-N(2)-Ga(3)	122.7(5)
C(63)-N(2)-Ga(3)	120.0(5)
C(68)-N(3)-C(65)	116.5(7)
C(68)-N(3)-Ga(4)	125.7(5)
C(65)-N(3)-Ga(4)	117.8(5)
C(67)-N(4)-C(66)	117.0(7)
C(67)-N(4)-Ga(1)#3	123.4(5)
C(66)-N(4)-Ga(1)#3	119.7(5)
C(129)-N(5)-C(132)	115.3(6)
C(129)-N(5)-Ga(6)	124.5(5)
C(132)-N(5)-Ga(6)	120.2(5)
C(130)-N(6)-C(131)	116.9(7)
C(130)-N(6)-Ga(7)	126.0(5)
C(131)-N(6)-Ga(7)	117.1(5)
C(136)-N(7)-C(133)	116.3(7)
C(136)-N(7)-Ga(8)	119.9(5)
C(133)-N(7)-Ga(8)	123.8(5)

C(134)-N(8)-C(135)	115.7(7)
C(134)-N(8)-Ga(5)#4	121.5(5)
C(135)-N(8)-Ga(5)#4	122.2(5)
C(2)-C(1)-C(5)	105.8(6)
C(2)-C(1)-Ga(1)	126.5(6)
C(5)-C(1)-Ga(1)	127.5(6)
C(2)-C(1)-Fe(1)	68.3(4)
C(5)-C(1)-Fe(1)	68.2(4)
Ga(1)-C(1)-Fe(1)	131.9(4)
C(3)-C(2)-C(1)	109.5(7)
C(3)-C(2)-Fe(1)	69.9(5)
C(1)-C(2)-Fe(1)	71.1(5)
C(4)-C(3)-C(2)	107.5(7)
C(4)-C(3)-Fe(1)	68.9(4)
C(2)-C(3)-Fe(1)	69.5(4)
C(5)-C(4)-C(3)	108.2(7)
C(5)-C(4)-Fe(1)	70.2(4)
C(3)-C(4)-Fe(1)	70.4(4)
C(4)-C(5)-C(1)	109.0(7)
C(4)-C(5)-Fe(1)	69.1(4)
C(1)-C(5)-Fe(1)	71.0(4)
C(10)-C(6)-C(7)	103.3(6)
C(10)-C(6)-Ga(2)	132.1(6)
C(7)-C(6)-Ga(2)	124.6(6)
C(10)-C(6)-Fe(1)	66.3(4)
C(7)-C(6)-Fe(1)	67.8(4)
Ga(2)-C(6)-Fe(1)	127.5(4)
C(8)-C(7)-C(6)	109.9(7)
C(8)-C(7)-Fe(1)	69.6(4)
C(6)-C(7)-Fe(1)	71.2(4)
C(9)-C(8)-C(7)	108.9(7)
C(9)-C(8)-Fe(1)	69.5(4)
C(7)-C(8)-Fe(1)	70.1(4)
C(8)-C(9)-C(10)	106.8(7)
C(8)-C(9)-Fe(1)	70.1(5)
C(10)-C(9)-Fe(1)	68.6(4)
C(9)-C(10)-C(6)	111.1(7)
C(9)-C(10)-Fe(1)	70.5(5)
C(6)-C(10)-Fe(1)	72.5(5)
C(15)-C(11)-C(12)	104.8(6)
C(15)-C(11)-Ga(1)	128.4(5)
C(12)-C(11)-Ga(1)	126.7(6)
C(15)-C(11)-Fe(2)	68.6(4)
C(12)-C(11)-Fe(2)	68.2(4)
Ga(1)-C(11)-Fe(2)	130.1(4)
C(13)-C(12)-C(11)	108.6(7)
C(13)-C(12)-Fe(2)	70.0(4)
C(11)-C(12)-Fe(2)	70.5(4)
C(14)-C(13)-C(12)	109.5(7)
C(14)-C(13)-Fe(2)	70.7(5)
C(12)-C(13)-Fe(2)	69.5(4)
C(13)-C(14)-C(15)	106.9(7)

C(13)-C(14)-Fe(2)	69.2(5)
C(15)-C(14)-Fe(2)	69.2(5)
C(14)-C(15)-C(11)	110.2(7)
C(14)-C(15)-Fe(2)	70.6(4)
C(11)-C(15)-Fe(2)	70.2(4)
C(20)-C(16)-C(17)	104.6(6)
C(20)-C(16)-Ga(2)	127.8(6)
C(17)-C(16)-Ga(2)	127.5(6)
C(20)-C(16)-Fe(2)	67.5(4)
C(17)-C(16)-Fe(2)	67.9(4)
Ga(2)-C(16)-Fe(2)	130.6(4)
C(18)-C(17)-C(16)	109.1(7)
C(18)-C(17)-Fe(2)	70.2(5)
C(16)-C(17)-Fe(2)	71.4(5)
C(19)-C(18)-C(17)	109.3(7)
C(19)-C(18)-Fe(2)	69.7(4)
C(17)-C(18)-Fe(2)	70.0(4)
C(18)-C(19)-C(20)	107.2(7)
C(18)-C(19)-Fe(2)	70.6(5)
C(20)-C(19)-Fe(2)	69.4(4)
C(19)-C(20)-C(16)	109.8(7)
C(19)-C(20)-Fe(2)	69.8(5)
C(16)-C(20)-Fe(2)	72.0(5)
C(22)-C(21)-C(25)	104.9(7)
C(22)-C(21)-Ga(1)	126.5(6)
C(25)-C(21)-Ga(1)	128.6(6)
C(22)-C(21)-Fe(3)	67.5(4)
C(25)-C(21)-Fe(3)	67.6(4)
Ga(1)-C(21)-Fe(3)	127.8(4)
C(23)-C(22)-C(21)	110.2(7)
C(23)-C(22)-Fe(3)	68.9(4)
C(21)-C(22)-Fe(3)	71.9(4)
C(22)-C(23)-C(24)	108.4(7)
C(22)-C(23)-Fe(3)	70.3(5)
C(24)-C(23)-Fe(3)	70.7(5)
C(23)-C(24)-C(25)	106.2(7)
C(23)-C(24)-Fe(3)	68.2(5)
C(25)-C(24)-Fe(3)	69.0(4)
C(24)-C(25)-C(21)	110.2(7)
C(24)-C(25)-Fe(3)	69.9(5)
C(21)-C(25)-Fe(3)	71.7(5)
C(30)-C(26)-C(27)	103.9(7)
C(30)-C(26)-Ga(2)	126.0(6)
C(27)-C(26)-Ga(2)	130.0(6)
C(30)-C(26)-Fe(3)	67.5(4)
C(27)-C(26)-Fe(3)	68.3(4)
Ga(2)-C(26)-Fe(3)	129.8(4)
C(28)-C(27)-C(26)	109.6(7)
C(28)-C(27)-Fe(3)	69.0(4)
C(26)-C(27)-Fe(3)	71.1(4)
C(29)-C(28)-C(27)	107.8(7)
C(29)-C(28)-Fe(3)	69.1(5)

C(27)-C(28)-Fe(3)	70.1(5)
C(28)-C(29)-C(30)	108.2(7)
C(28)-C(29)-Fe(3)	70.8(5)
C(30)-C(29)-Fe(3)	70.4(5)
C(29)-C(30)-C(26)	110.5(7)
C(29)-C(30)-Fe(3)	69.1(4)
C(26)-C(30)-Fe(3)	71.8(4)
C(35)-C(31)-C(32)	105.1(7)
C(35)-C(31)-Ga(3)	126.7(6)
C(32)-C(31)-Ga(3)	128.1(6)
C(35)-C(31)-Fe(4)	69.1(4)
C(32)-C(31)-Fe(4)	68.6(4)
Ga(3)-C(31)-Fe(4)	129.3(4)
C(33)-C(32)-C(31)	110.3(7)
C(33)-C(32)-Fe(4)	70.7(5)
C(31)-C(32)-Fe(4)	70.7(5)
C(32)-C(33)-C(34)	106.7(7)
C(32)-C(33)-Fe(4)	69.1(5)
C(34)-C(33)-Fe(4)	69.0(4)
C(35)-C(34)-C(33)	107.8(7)
C(35)-C(34)-Fe(4)	69.9(4)
C(33)-C(34)-Fe(4)	70.6(4)
C(31)-C(35)-C(34)	110.0(7)
C(31)-C(35)-Fe(4)	70.8(4)
C(34)-C(35)-Fe(4)	69.6(4)
C(40)-C(36)-C(37)	106.4(7)
C(40)-C(36)-Ga(4)	133.2(6)
C(37)-C(36)-Ga(4)	120.3(6)
C(40)-C(36)-Fe(4)	69.4(4)
C(37)-C(36)-Fe(4)	68.9(4)
Ga(4)-C(36)-Fe(4)	129.3(4)
C(38)-C(37)-C(36)	109.5(7)
C(38)-C(37)-Fe(4)	70.2(4)
C(36)-C(37)-Fe(4)	70.8(4)
C(37)-C(38)-C(39)	107.2(7)
C(37)-C(38)-Fe(4)	69.6(5)
C(39)-C(38)-Fe(4)	70.1(5)
C(38)-C(39)-C(40)	107.3(7)
C(38)-C(39)-Fe(4)	69.7(5)
C(40)-C(39)-Fe(4)	69.3(5)
C(36)-C(40)-C(39)	109.5(7)
C(36)-C(40)-Fe(4)	71.0(5)
C(39)-C(40)-Fe(4)	70.1(5)
C(45)-C(41)-C(42)	104.5(6)
C(45)-C(41)-Ga(3)	124.9(5)
C(42)-C(41)-Ga(3)	130.6(6)
C(45)-C(41)-Fe(5)	68.9(4)
C(42)-C(41)-Fe(5)	68.0(4)
Ga(3)-C(41)-Fe(5)	127.8(4)
C(43)-C(42)-C(41)	109.1(7)
C(43)-C(42)-Fe(5)	69.6(5)
C(41)-C(42)-Fe(5)	70.6(5)

C(44)-C(43)-C(42)	108.1(7)
C(44)-C(43)-Fe(5)	69.8(5)
C(42)-C(43)-Fe(5)	69.4(5)
C(45)-C(44)-C(43)	108.3(7)
C(45)-C(44)-Fe(5)	70.6(5)
C(43)-C(44)-Fe(5)	69.8(5)
C(44)-C(45)-C(41)	110.0(7)
C(44)-C(45)-Fe(5)	69.2(4)
C(41)-C(45)-Fe(5)	70.0(4)
C(47)-C(46)-C(50)	104.5(7)
C(47)-C(46)-Ga(4)	127.9(6)
C(50)-C(46)-Ga(4)	127.2(6)
C(47)-C(46)-Fe(5)	68.0(5)
C(50)-C(46)-Fe(5)	68.1(5)
Ga(4)-C(46)-Fe(5)	132.7(4)
C(46)-C(47)-C(48)	109.8(7)
C(46)-C(47)-Fe(5)	71.3(5)
C(48)-C(47)-Fe(5)	69.2(5)
C(49)-C(48)-C(47)	107.0(7)
C(49)-C(48)-Fe(5)	70.8(4)
C(47)-C(48)-Fe(5)	69.5(4)
C(48)-C(49)-C(50)	108.5(7)
C(48)-C(49)-Fe(5)	69.2(4)
C(50)-C(49)-Fe(5)	69.4(4)
C(49)-C(50)-C(46)	110.1(7)
C(49)-C(50)-Fe(5)	70.4(5)
C(46)-C(50)-Fe(5)	71.2(5)
C(52)-C(51)-C(55)	104.8(7)
C(52)-C(51)-Ga(3)	124.7(6)
C(55)-C(51)-Ga(3)	130.5(6)
C(52)-C(51)-Fe(6)	67.6(4)
C(55)-C(51)-Fe(6)	67.6(4)
Ga(3)-C(51)-Fe(6)	129.9(4)
C(53)-C(52)-C(51)	110.3(7)
C(53)-C(52)-Fe(6)	69.1(4)
C(51)-C(52)-Fe(6)	72.2(4)
C(52)-C(53)-C(54)	107.1(7)
C(52)-C(53)-Fe(6)	70.1(4)
C(54)-C(53)-Fe(6)	70.0(4)
C(55)-C(54)-C(53)	107.7(7)
C(55)-C(54)-Fe(6)	70.1(5)
C(53)-C(54)-Fe(6)	69.2(4)
C(54)-C(55)-C(51)	110.0(7)
C(54)-C(55)-Fe(6)	69.5(5)
C(51)-C(55)-Fe(6)	71.9(5)
C(60)-C(56)-C(57)	103.1(7)
C(60)-C(56)-Ga(4)	126.2(5)
C(57)-C(56)-Ga(4)	130.7(6)
C(60)-C(56)-Fe(6)	66.8(4)
C(57)-C(56)-Fe(6)	67.9(4)
Ga(4)-C(56)-Fe(6)	127.9(4)
C(58)-C(57)-C(56)	110.4(7)

C(58)-C(57)-Fe(6)	68.9(5)
C(56)-C(57)-Fe(6)	71.0(4)
C(59)-C(58)-C(57)	107.3(7)
C(59)-C(58)-Fe(6)	69.0(5)
C(57)-C(58)-Fe(6)	70.7(5)
C(60)-C(59)-C(58)	109.2(7)
C(60)-C(59)-Fe(6)	70.4(5)
C(58)-C(59)-Fe(6)	70.4(5)
C(59)-C(60)-C(56)	110.1(7)
C(59)-C(60)-Fe(6)	69.3(5)
C(56)-C(60)-Fe(6)	72.0(4)
N(1)-C(61)-C(62)	121.7(8)
N(2)-C(62)-C(61)	121.9(8)
N(2)-C(63)-C(64)	121.4(7)
N(1)-C(64)-C(63)	121.3(7)
N(3)-C(65)-C(66)	122.5(8)
N(4)-C(66)-C(65)	121.1(8)
N(4)-C(67)-C(68)	121.8(8)
N(3)-C(68)-C(67)	121.1(8)
C(73)-C(69)-C(70)	104.1(7)
C(73)-C(69)-Ga(5)	127.0(6)
C(70)-C(69)-Ga(5)	128.8(6)
C(73)-C(69)-Fe(7)	67.8(4)
C(70)-C(69)-Fe(7)	68.2(4)
Ga(5)-C(69)-Fe(7)	129.7(4)
C(71)-C(70)-C(69)	109.0(7)
C(71)-C(70)-Fe(7)	69.0(4)
C(69)-C(70)-Fe(7)	70.8(4)
C(70)-C(71)-C(72)	108.2(7)
C(70)-C(71)-Fe(7)	70.5(4)
C(72)-C(71)-Fe(7)	69.8(4)
C(73)-C(72)-C(71)	107.2(7)
C(73)-C(72)-Fe(7)	70.0(4)
C(71)-C(72)-Fe(7)	69.4(4)
C(72)-C(73)-C(69)	111.5(7)
C(72)-C(73)-Fe(7)	70.1(5)
C(69)-C(73)-Fe(7)	71.7(4)
C(75)-C(74)-C(78)	104.3(7)
C(75)-C(74)-Ga(6)	126.1(6)
C(78)-C(74)-Ga(6)	129.6(6)
C(75)-C(74)-Fe(7)	67.8(4)
C(78)-C(74)-Fe(7)	67.5(4)
Ga(6)-C(74)-Fe(7)	128.5(4)
C(76)-C(75)-C(74)	110.3(8)
C(76)-C(75)-Fe(7)	69.4(5)
C(74)-C(75)-Fe(7)	71.5(5)
C(75)-C(76)-C(77)	107.2(8)
C(75)-C(76)-Fe(7)	70.0(5)
C(77)-C(76)-Fe(7)	69.3(5)
C(78)-C(77)-C(76)	107.9(7)
C(78)-C(77)-Fe(7)	70.1(4)
C(76)-C(77)-Fe(7)	69.6(4)

C(77)-C(78)-C(74)	110.3(7)
C(77)-C(78)-Fe(7)	69.6(4)
C(74)-C(78)-Fe(7)	71.6(4)
C(83)-C(79)-C(80)	105.3(7)
C(83)-C(79)-Ga(5)	131.4(6)
C(80)-C(79)-Ga(5)	123.4(6)
C(83)-C(79)-Fe(8)	67.8(4)
C(80)-C(79)-Fe(8)	68.9(4)
Ga(5)-C(79)-Fe(8)	127.9(4)
C(81)-C(80)-C(79)	109.0(7)
C(81)-C(80)-Fe(8)	69.8(5)
C(79)-C(80)-Fe(8)	70.0(4)
C(82)-C(81)-C(80)	106.7(7)
C(82)-C(81)-Fe(8)	68.5(4)
C(80)-C(81)-Fe(8)	69.4(4)
C(83)-C(82)-C(81)	109.7(7)
C(83)-C(82)-Fe(8)	69.8(4)
C(81)-C(82)-Fe(8)	71.3(4)
C(82)-C(83)-C(79)	109.3(7)
C(82)-C(83)-Fe(8)	69.7(4)
C(79)-C(83)-Fe(8)	71.2(4)
C(88)-C(84)-C(85)	106.1(7)
C(88)-C(84)-Ga(6)	127.7(6)
C(85)-C(84)-Ga(6)	126.0(6)
C(88)-C(84)-Fe(8)	68.2(4)
C(85)-C(84)-Fe(8)	68.7(4)
Ga(6)-C(84)-Fe(8)	131.5(4)
C(86)-C(85)-C(84)	108.0(7)
C(86)-C(85)-Fe(8)	69.2(4)
C(84)-C(85)-Fe(8)	70.8(4)
C(87)-C(86)-C(85)	109.2(7)
C(87)-C(86)-Fe(8)	69.9(4)
C(85)-C(86)-Fe(8)	70.1(5)
C(86)-C(87)-C(88)	106.8(7)
C(86)-C(87)-Fe(8)	69.7(5)
C(88)-C(87)-Fe(8)	69.5(5)
C(87)-C(88)-C(84)	109.9(7)
C(87)-C(88)-Fe(8)	69.8(5)
C(84)-C(88)-Fe(8)	71.3(4)
C(93)-C(89)-C(90)	104.7(7)
C(93)-C(89)-Ga(5)	128.6(6)
C(90)-C(89)-Ga(5)	126.5(6)
C(93)-C(89)-Fe(9)	68.2(4)
C(90)-C(89)-Fe(9)	68.0(4)
Ga(5)-C(89)-Fe(9)	131.1(4)
C(91)-C(90)-C(89)	109.2(7)
C(91)-C(90)-Fe(9)	69.4(4)
C(89)-C(90)-Fe(9)	71.0(4)
C(92)-C(91)-C(90)	109.1(7)
C(92)-C(91)-Fe(9)	70.1(5)
C(90)-C(91)-Fe(9)	70.4(5)
C(91)-C(92)-C(93)	107.9(7)

C(91)-C(92)-Fe(9)	70.3(5)
C(93)-C(92)-Fe(9)	69.8(5)
C(89)-C(93)-C(92)	109.2(7)
C(89)-C(93)-Fe(9)	71.5(4)
C(92)-C(93)-Fe(9)	69.0(4)
C(95)-C(94)-C(98)	104.3(7)
C(95)-C(94)-Ga(6)	128.1(6)
C(98)-C(94)-Ga(6)	127.5(6)
C(95)-C(94)-Fe(9)	67.7(4)
C(98)-C(94)-Fe(9)	68.4(4)
Ga(6)-C(94)-Fe(9)	129.7(4)
C(96)-C(95)-C(94)	109.9(7)
C(96)-C(95)-Fe(9)	70.3(4)
C(94)-C(95)-Fe(9)	71.4(4)
C(95)-C(96)-C(97)	108.8(8)
C(95)-C(96)-Fe(9)	69.6(4)
C(97)-C(96)-Fe(9)	70.1(4)
C(96)-C(97)-C(98)	107.7(7)
C(96)-C(97)-Fe(9)	69.7(4)
C(98)-C(97)-Fe(9)	70.2(4)
C(97)-C(98)-C(94)	109.2(7)
C(97)-C(98)-Fe(9)	69.5(5)
C(94)-C(98)-Fe(9)	70.4(4)
C(100)-C(99)-C(103)	105.3(7)
C(100)-C(99)-Ga(7)	129.3(6)
C(103)-C(99)-Ga(7)	125.4(6)
C(100)-C(99)-Fe(10)	67.9(4)
C(103)-C(99)-Fe(10)	67.6(4)
Ga(7)-C(99)-Fe(10)	127.2(4)
C(101)-C(100)-C(99)	110.3(7)
C(101)-C(100)-Fe(10)	69.6(4)
C(99)-C(100)-Fe(10)	71.3(4)
C(100)-C(101)-C(102)	108.6(8)
C(100)-C(101)-Fe(10)	70.8(5)
C(102)-C(101)-Fe(10)	69.3(4)
C(103)-C(102)-C(101)	107.8(7)
C(103)-C(102)-Fe(10)	70.2(4)
C(101)-C(102)-Fe(10)	69.3(4)
C(102)-C(103)-C(99)	108.0(7)
C(102)-C(103)-Fe(10)	68.9(4)
C(99)-C(103)-Fe(10)	70.8(4)
C(108)-C(104)-C(105)	105.0(7)
C(108)-C(104)-Ga(8)	130.0(6)
C(105)-C(104)-Ga(8)	125.0(6)
C(108)-C(104)-Fe(10)	67.6(4)
C(105)-C(104)-Fe(10)	67.4(4)
Ga(8)-C(104)-Fe(10)	129.1(4)
C(106)-C(105)-C(104)	109.2(7)
C(106)-C(105)-Fe(10)	68.9(4)
C(104)-C(105)-Fe(10)	72.0(4)
C(107)-C(106)-C(105)	108.1(7)
C(107)-C(106)-Fe(10)	70.1(4)

C(105)-C(106)-Fe(10)	70.4(4)
C(106)-C(107)-C(108)	107.0(7)
C(106)-C(107)-Fe(10)	69.3(4)
C(108)-C(107)-Fe(10)	69.9(4)
C(104)-C(108)-C(107)	110.6(7)
C(104)-C(108)-Fe(10)	72.5(4)
C(107)-C(108)-Fe(10)	69.4(4)
C(113)-C(109)-C(110)	104.0(7)
C(113)-C(109)-Ga(7)	133.8(6)
C(110)-C(109)-Ga(7)	122.0(6)
C(113)-C(109)-Fe(11)	68.3(4)
C(110)-C(109)-Fe(11)	67.7(4)
Ga(7)-C(109)-Fe(11)	130.2(4)
C(111)-C(110)-C(109)	110.9(7)
C(111)-C(110)-Fe(11)	71.2(5)
C(109)-C(110)-Fe(11)	71.8(5)
C(112)-C(111)-C(110)	107.5(8)
C(112)-C(111)-Fe(11)	69.8(5)
C(110)-C(111)-Fe(11)	68.8(5)
C(111)-C(112)-C(113)	106.9(8)
C(111)-C(112)-Fe(11)	70.4(5)
C(113)-C(112)-Fe(11)	69.2(4)
C(109)-C(113)-C(112)	110.6(7)
C(109)-C(113)-Fe(11)	71.6(4)
C(112)-C(113)-Fe(11)	70.1(4)
C(115)-C(114)-C(118)	105.7(7)
C(115)-C(114)-Ga(8)	128.7(6)
C(118)-C(114)-Ga(8)	125.5(6)
C(115)-C(114)-Fe(11)	69.1(4)
C(118)-C(114)-Fe(11)	68.4(4)
Ga(8)-C(114)-Fe(11)	128.9(4)
C(114)-C(115)-C(116)	109.7(7)
C(114)-C(115)-Fe(11)	70.7(4)
C(116)-C(115)-Fe(11)	69.2(4)
C(117)-C(116)-C(115)	106.9(7)
C(117)-C(116)-Fe(11)	69.4(4)
C(115)-C(116)-Fe(11)	70.3(5)
C(118)-C(117)-C(116)	109.0(8)
C(118)-C(117)-Fe(11)	70.4(5)
C(116)-C(117)-Fe(11)	70.1(5)
C(117)-C(118)-C(114)	108.7(7)
C(117)-C(118)-Fe(11)	69.4(5)
C(114)-C(118)-Fe(11)	70.8(4)
C(123)-C(119)-C(120)	106.2(7)
C(123)-C(119)-Ga(7)	126.3(6)
C(120)-C(119)-Ga(7)	127.3(6)
C(123)-C(119)-Fe(12)	68.6(4)
C(120)-C(119)-Fe(12)	68.0(4)
Ga(7)-C(119)-Fe(12)	131.4(4)
C(121)-C(120)-C(119)	109.1(7)
C(121)-C(120)-Fe(12)	69.3(4)
C(119)-C(120)-Fe(12)	71.5(4)

C(122)-C(121)-C(120)	107.4(7)
C(122)-C(121)-Fe(12)	69.7(5)
C(120)-C(121)-Fe(12)	69.7(5)
C(121)-C(122)-C(123)	108.1(8)
C(121)-C(122)-Fe(12)	69.9(5)
C(123)-C(122)-Fe(12)	70.3(5)
C(119)-C(123)-C(122)	109.2(7)
C(119)-C(123)-Fe(12)	71.3(4)
C(122)-C(123)-Fe(12)	68.9(4)
C(128)-C(124)-C(125)	104.4(7)
C(128)-C(124)-Ga(8)	125.2(6)
C(125)-C(124)-Ga(8)	130.4(6)
C(128)-C(124)-Fe(12)	68.8(4)
C(125)-C(124)-Fe(12)	67.2(4)
Ga(8)-C(124)-Fe(12)	127.7(4)
C(126)-C(125)-C(124)	109.1(7)
C(126)-C(125)-Fe(12)	69.1(5)
C(124)-C(125)-Fe(12)	71.1(4)
C(125)-C(126)-C(127)	108.3(8)
C(125)-C(126)-Fe(12)	70.1(5)
C(127)-C(126)-Fe(12)	69.7(5)
C(128)-C(127)-C(126)	108.0(8)
C(128)-C(127)-Fe(12)	71.2(5)
C(126)-C(127)-Fe(12)	69.3(5)
C(127)-C(128)-C(124)	110.2(7)
C(127)-C(128)-Fe(12)	68.4(5)
C(124)-C(128)-Fe(12)	70.7(4)
N(5)-C(129)-C(130)	122.0(7)
N(6)-C(130)-C(129)	121.8(7)
N(6)-C(131)-C(132)	121.6(7)
N(5)-C(132)-C(131)	122.4(7)
N(7)-C(133)-C(134)	120.9(8)
N(8)-C(134)-C(133)	123.1(8)
N(8)-C(135)-C(136)	121.2(8)
N(7)-C(136)-C(135)	122.6(8)
C(138)-C(137)-C(143)	123.6(13)
C(138)-C(137)-C(142)	110.5(11)
C(143)-C(137)-C(142)	125.9(12)
C(139)-C(138)-C(137)	126.2(13)
C(138)-C(139)-C(140)	122.4(13)
C(141)-C(140)-C(139)	114.4(12)
C(140)-C(141)-C(142)	123.2(13)
C(141)-C(142)-C(137)	123.2(12)
C(147)-C(144)-C(145)	130(2)
C(147)-C(144)-C(146)#5	116.0(19)
C(145)-C(144)-C(146)#5	113.7(13)
C(146)-C(145)-C(144)	129.3(15)
C(145)-C(146)-C(144)#5	117.0(14)
C(149)-C(148)-C(154)	122.5(12)
C(149)-C(148)-C(153)	114.4(12)
C(154)-C(148)-C(153)	123.2(13)
C(150)-C(149)-C(148)	122.2(12)

C(149)-C(150)-C(151)	123.4(13)
C(152)-C(151)-C(150)	114.5(13)
C(153)-C(152)-C(151)	123.6(13)
C(152)-C(153)-C(148)	121.8(12)
C(158)-C(155)-C(156)	129.0(15)
C(158)-C(155)-C(157)#6	112.7(13)
C(156)-C(155)-C(157)#6	118.3(13)
C(157)-C(156)-C(155)	128.1(12)
C(156)-C(157)-C(155)#6	113.6(11)

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y+1,z #2 x+1,y+1,z #3 x+1,y-1,z

#4 x-1,y-1,z #5 -x+1,-y-1,-z #6 -x+1,-y+2,-z+1

Table 10. Anisotropic displacement parameters (A^2 x 10^3) for [**3d**·0.75 toluene].
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ga(1)	14(1)	14(1)	23(1)	-2(1)	-3(1)	2(1)
Ga(2)	13(1)	14(1)	24(1)	-2(1)	-4(1)	3(1)
Ga(3)	12(1)	15(1)	25(1)	-2(1)	-4(1)	3(1)
Ga(4)	15(1)	14(1)	24(1)	-2(1)	-4(1)	3(1)
Ga(5)	14(1)	13(1)	24(1)	-2(1)	-4(1)	0(1)
Ga(6)	13(1)	15(1)	23(1)	-2(1)	-4(1)	0(1)
Ga(7)	14(1)	15(1)	22(1)	-2(1)	-4(1)	-1(1)
Ga(8)	15(1)	13(1)	23(1)	-3(1)	-2(1)	0(1)
Fe(1)	16(1)	14(1)	23(1)	-2(1)	-3(1)	2(1)
Fe(2)	14(1)	15(1)	24(1)	-2(1)	-5(1)	2(1)
Fe(3)	14(1)	14(1)	21(1)	-1(1)	-3(1)	3(1)
Fe(4)	14(1)	14(1)	25(1)	-2(1)	-2(1)	2(1)
Fe(5)	18(1)	15(1)	24(1)	-2(1)	-6(1)	2(1)
Fe(6)	14(1)	16(1)	22(1)	-2(1)	-3(1)	1(1)
Fe(7)	17(1)	14(1)	22(1)	-2(1)	-3(1)	0(1)
Fe(8)	14(1)	16(1)	22(1)	-3(1)	-2(1)	1(1)
Fe(9)	14(1)	14(1)	24(1)	-1(1)	-5(1)	1(1)
Fe(10)	14(1)	14(1)	21(1)	-2(1)	-3(1)	0(1)
Fe(11)	15(1)	14(1)	24(1)	-5(1)	-5(1)	1(1)
Fe(12)	15(1)	17(1)	22(1)	0(1)	-4(1)	2(1)
N(1)	13(4)	16(4)	22(4)	-2(3)	-3(3)	4(3)
N(2)	15(4)	18(4)	16(4)	-2(3)	-2(3)	3(3)
N(3)	10(4)	12(4)	18(4)	-3(3)	2(3)	3(3)
N(4)	12(4)	14(4)	11(4)	-1(3)	2(3)	-2(3)
N(5)	16(4)	10(4)	19(4)	4(3)	-3(3)	8(3)
N(6)	18(4)	11(4)	14(4)	-2(3)	-6(3)	6(3)
N(7)	16(4)	12(4)	14(4)	-2(3)	-1(3)	1(3)
N(8)	19(4)	6(4)	20(4)	-6(3)	-1(3)	-2(3)

Table 11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for [**3d**·0.75 toluene].

	x	y	z	U(eq)
H(2)	-74	-2213	669	21
H(3)	1235	-1217	586	25
H(4)	1877	-1412	1390	22
H(5)	933	-2475	1981	21
H(7)	1009	-4108	406	21
H(8)	2114	-2986	23	23
H(9)	3097	-2689	652	23
H(10)	2589	-3638	1433	24
H(12)	-2441	-4675	1691	18
H(13)	-2816	-5219	892	23
H(14)	-1719	-4634	157	24
H(15)	-657	-3700	499	23
H(17)	-896	-6087	1874	24
H(18)	-1651	-6870	1287	19
H(19)	-882	-6559	408	25
H(20)	410	-5604	448	21
H(22)	-259	-2769	2735	22
H(23)	-650	-3599	3567	27
H(24)	-1588	-4892	3446	26
H(25)	-1690	-4872	2512	26
H(27)	1536	-3951	2412	21
H(28)	1151	-4468	3328	25
H(29)	237	-5802	3375	25
H(30)	87	-6150	2501	24
H(32)	5260	-7365	536	26
H(33)	6593	-6452	532	26
H(34)	6924	-6526	1424	24
H(35)	5760	-7433	1967	18
H(37)	6100	-9469	640	25
H(38)	7281	-8505	156	28
H(39)	8228	-8035	771	26
H(40)	7597	-8701	1629	26
H(42)	2577	-9709	1461	26
H(43)	2593	-10523	674	29
H(44)	3960	-10112	69	30
H(45)	4767	-9002	454	22
H(47)	3940	-10957	2025	24
H(48)	3356	-11912	1421	25
H(49)	4495	-11957	646	17
H(50)	5724	-10974	739	26
H(52)	4469	-7416	2542	23

H(53)	3789	-7897	3427	19
H(54)	2882	-9236	3377	23
H(55)	3045	-9585	2469	23
H(57)	6231	-8711	2642	24
H(58)	5473	-8893	3539	25
H(59)	4510	-10209	3616	31
H(60)	4629	-10828	2777	26
H(61)	2953	-5253	1383	32
H(62)	3991	-6299	1429	26
H(63)	2225	-8095	1402	28
H(64)	1161	-7054	1405	19
H(65)	7195	-11024	1068	28
H(66)	8266	-12053	1029	23
H(67)	7826	-12365	2496	21
H(68)	6734	-11339	2534	22
H(70)	4444	7471	2585	19
H(71)	5143	7419	1676	21
H(72)	6507	6513	1637	23
H(73)	6635	6009	2513	20
H(75)	3297	5805	2280	25
H(76)	4257	5722	1437	31
H(77)	5535	4754	1558	23
H(78)	5354	4260	2468	22
H(80)	4182	6146	4596	16
H(81)	2959	7109	4987	26
H(82)	2810	8315	4348	22
H(83)	3908	8137	3577	19
H(85)	2329	5163	4328	21
H(86)	1329	6448	4401	26
H(87)	1669	7396	3603	23
H(88)	2866	6679	3024	21
H(90)	6466	4840	3138	22
H(91)	7107	3829	3728	21
H(92)	6638	4265	4603	27
H(93)	5685	5586	4570	25
H(95)	5022	3202	3319	19
H(96)	5405	2526	4111	23
H(97)	4680	3347	4841	26
H(98)	3785	4522	4501	20
H(100)	-797	2211	2386	27
H(101)	-467	1864	1490	23
H(102)	885	925	1365	30
H(103)	1389	687	2211	16
H(105)	-2093	435	2433	24
H(106)	-1400	78	1558	19
H(107)	-68	-824	1626	23
H(108)	60	-1003	2545	19
H(110)	-431	1326	4362	24
H(111)	-1437	2353	4840	31
H(112)	-1799	3518	4224	28
H(113)	-953	3216	3371	25
H(115)	-2546	464	4457	22

H(116)	-3407	1838	4455	24
H(117)	-3177	2477	3564	24
H(118)	-2163	1536	3023	26
H(120)	1355	-307	2980	21
H(121)	2193	-1121	3585	25
H(122)	2025	-317	4383	30
H(123)	1106	996	4268	20
H(125)	-15	-1872	3529	29
H(126)	645	-2165	4310	33
H(127)	110	-1042	4924	28
H(128)	-929	-82	4541	25
H(129)	2846	3769	2497	25
H(130)	1841	2687	2469	21
H(131)	1231	2602	3934	23
H(132)	2256	3644	3970	19
H(133)	-3462	-472	3648	23
H(134)	-4491	-1536	3694	29
H(135)	-2674	-3282	3553	21
H(136)	-1641	-2216	3523	28
H(138)	2545	-9160	-192	89
H(139)	1400	-9964	-64	78
H(140)	-7	-9435	302	100
H(141)	-46	-8026	520	83
H(142)	1128	-7160	349	79
H(14A)	2695	-6951	74	171
H(14B)	3059	-7516	-390	171
H(14C)	3256	-7790	159	171
H(144)	4572	-6103	-454	134
H(145)	5988	-5813	-450	98
H(146)	6489	-4804	-78	112
H(14D)	3786	-6226	-397	136
H(14E)	4608	-6810	-332	136
H(14F)	4618	-6209	-833	136
H(149)	9110	7472	5200	71
H(150)	9954	6351	5059	91
H(151)	9542	5143	4633	97
H(152)	8141	5149	4454	85
H(153)	7267	6283	4577	66
H(15A)	6970	7651	4892	166
H(15B)	7804	8268	4835	166
H(15C)	7405	7830	5373	166
H(155)	3926	10611	4602	132
H(156)	4181	9190	4591	75
H(157)	5211	8500	4940	88
H(15D)	3847	11381	4660	132
H(15E)	3234	10546	4732	132
H(15F)	3908	10723	4222	132