Supporting Information for:

Formation of a paramagnetic Al complex and extrusion of Fe during the reaction of (diiminepyridine)Fe with AlR_3 (R = Me, Et).

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Complex 1

Synthesis

Method A: A solution of Me_3Al (2.0 M, 4.2 mL, 8.2 mmol) was added to a suspension of {2,6-[2,6-(i-$Pr)_2PhN=C(CH_3)]_2(C_5H_3N)$}$FeCl_2$ (0.50 g, 0.82 mmol) in toluene (20mL) at -35ºC. The color instantly became purple and eventually dark green after about 30 minutes at room temperature. The mixture was evaporated to dryness under reduced pressure and the dark green mass was washed with hexanes. The resulting product was then dissolved in toluene and centrifuged to remove any insoluble material. Orange crystals of **1** (0.23 g, 0.32 mmol, 38%) were isolated after crystallization at -35ºC for 2 days.

Method B: A solution of Me_3Al (2 M, 0.35 mL, 0.7 mmol) was added to a suspension of {2,6-[2,6-(i-$Pr)_2PhN=C(CH_3)]_2$-(C_5H_3N)}$Fe(CH_2SiMe_3)_2$ (0.10 g, 0.14 mmol) in toluene at -35ºC. The colour became dark yellow-brown and grew orange-brown after stirring for a period of time. The mixture was stirred overnight, evaporated to dryness, washed with hexane and placed in the freezer to crystallize (0.040 g, 0.05 mmol, 39%).

Method C: The ligand {2,6-[2,6-(i-$Pr)_2PhN=C(CH_3)]_2(C_5H_3N)$} (0.40g, 0.83 mmol) was reacted with 1 equivalent of Na (0.019 g, 0.83 mmol) in THF. The resulting dark purple solution was evaporated to dryness and dissolved in toluene. A solution of Me_2AlCl (1 M, 0.84 mL, 0.83 mmol) was added at -35ºC and the solution became dark orange. Centrifugation and freezing allowed the isolation of orange crystals of **1** (0.45 g, 0.62 mmol, 76%). Anal. Calcd. (found) for $C_{49}H_{65}AlN_3$: C, 81.40(81.06); H, 9.06(9.12); N, 5.81(5.56). [μ_{eff} = 1.73 μ_{BM}]. [m.p. (dec) = 165-67C].

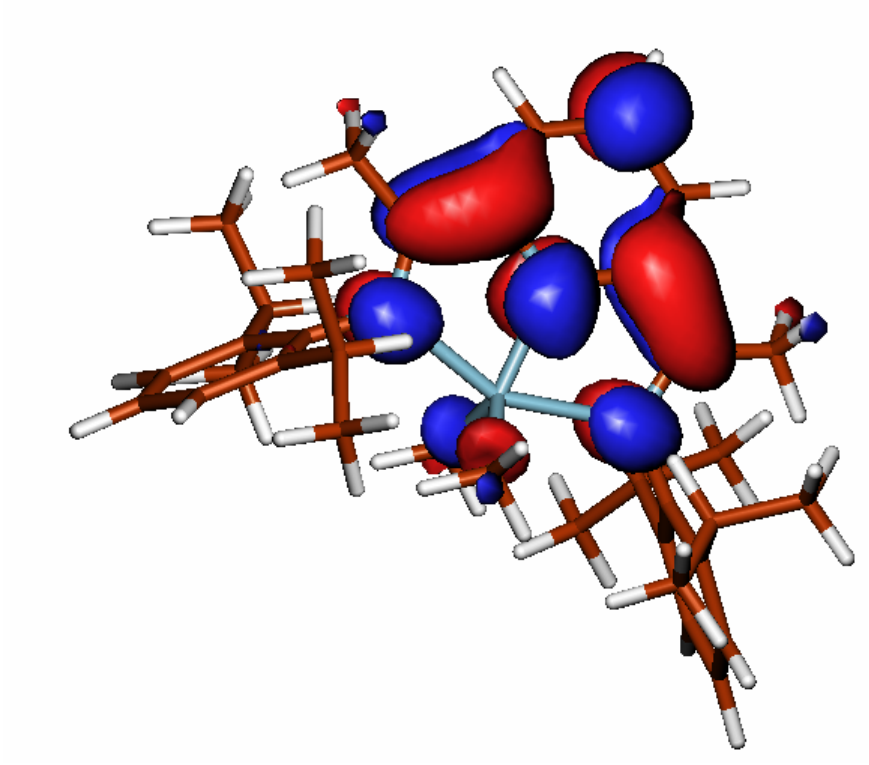

Figure S1. SOMO of **1** (Turbomole/Molden, b3-lyp, TZVP basis set)

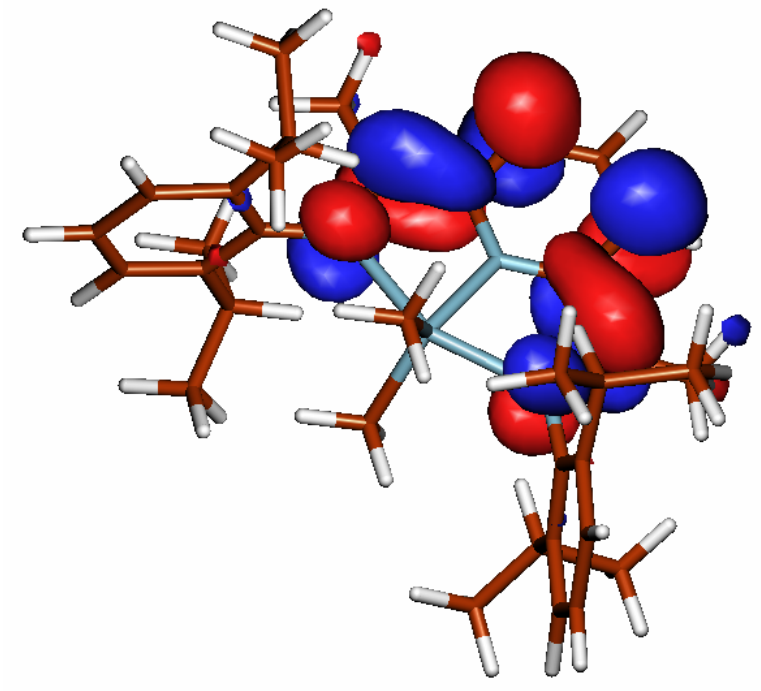

Figure S2. LUMO of **1** (Turbomole/Molden, b3-lyp, TZVP basis set)

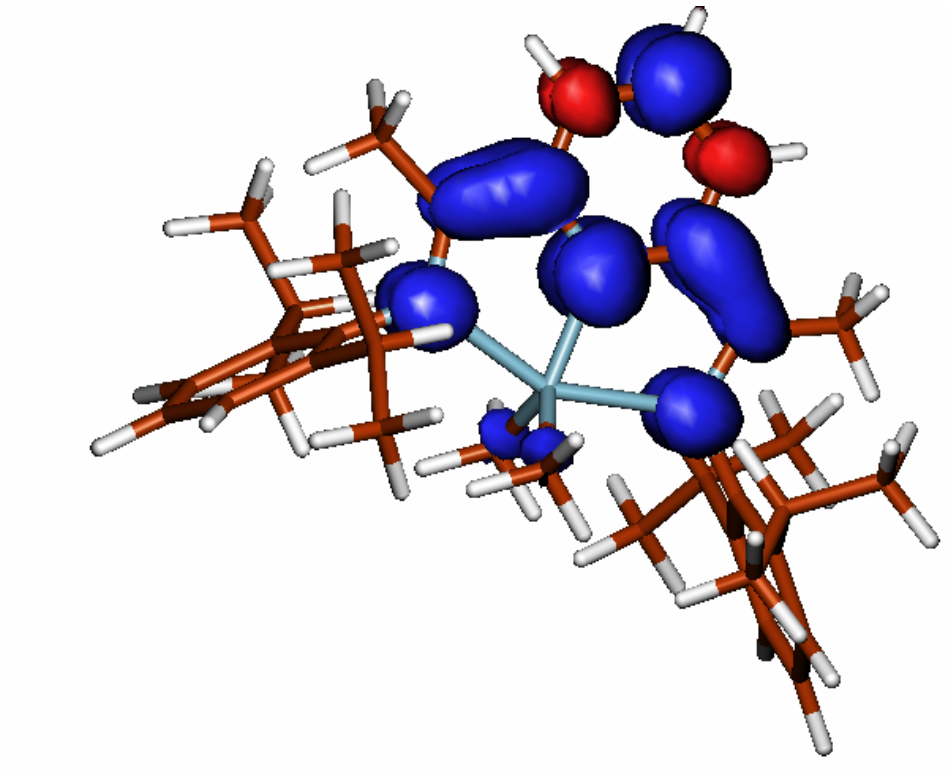

Figure S3. Spin density plot of **1** (Turbomole/Molden, b3-lyp, TZVP basis set)

DFT geometry optimizations and EPR parameter calculations

The geometry optimization of **1** was carried out with the Turbomole program[1a] coupled to the PQS Baker optimizer.[2] Geometries were fully optimized as minima at the bp86[3] level using the Turbomole SV(P)

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[1] (a) R. Ahlrichs, M. Bär, H.-P. Baron, R. Bauernschmitt, S. Böcker, M. Ehrig, K. Eichkorn, S. Elliott, F. Furche, F. Haase, M. Häser, C. Hättig, H. Horn, C. Huber, U. Huniar, M. Kattannek, A. Köhn, C. Kölmel, M. Kollwitz, K. May, C. Ochsenfeld, H. Öhm, A. Schäfer, U. Schneider, O. Treutler, K. Tsereteli, B. Unterreiner, M. von Arnim, F. Weigend, P. Weis, H. Weiss Turbomole Version 5, january **2002**. Theoretical Chemistry Group, University of Karlsruhe; (b) O. Treutler, R. Ahlrichs *J. Chem. Phys.* **1995**, *102*, 346-354; (c) Turbomole basisset library, Turbomole Version 5, see (a); (d) A. Schäfer, H. Horn, R. Ahlrichs *J. Chem. Phys.* **1992**, *97*, 2571-2577; (e) D. Andrae, U. Haeussermann, M. Dolg, H. Stoll, H. Preuss *Theor. Chim. Acta* **1990**, *77*, 123-141; (f) A. Schäfer, C. Huber, R. Ahlrichs *J. Chem. Phys.* **1994**, *100*, 5829-5835. g) Ahlrichs, R.; May, K. *Chem. Phys.*, **2000**, *2*, 943.

basisset[1c,d] on all atoms. Improved energies were obtained from single-point calculations at the b3-lyp level[4] using the polarized triple-ξ TZVP basis set[1c,f,g] (Ahlrichs polarization functions on all atoms).[5] Orbitals and spin densities were visualized with the Molden program.[6]

The EPR parameters[7] of **1** were calculated from a single point SCF calculation with the program ORCA[8], using the b3-lyp[4] functional and TZVP[1c,f,g] basis set (identical to those in Turbomole) supplied with the program. The coordinates from the structure optimized in Turbomole were used as input for the ORCA calculations, performed according to the spin unrestricted coupled-perturbed Kohn-Sham

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[2] (a) PQS version 2.4, **2001**, Parallel Quantum Solutions, Fayetteville, Arkansas, USA (the Baker optimizer is available separately from PQS upon request); (b) J. Baker *J. Comput. Chem.* **1986**, *7*, 385-395.

[3] (a) A.D. Becke *Phys. Rev. A* **1988**, *38*, 3098-3100; (b) J.P. Perdew *Phys. Rev. B* **1986**, *33*, 8822-8824.

[4] (a) C. Lee, W. Yang, R.G. Parr, *Phys. Rev. B* **1988**, *37*, 785-789; (b) A.D. Becke *J. Chem. Phys.* **1993**, *98*, 1372-1377; (c) A.D. Becke *J. Chem. Phys.* **1993**, *98*, 5648-5652; (d) All calculations were performed using the Turbomole functional "b3-lyp", which is not identical to the Gaussian "B3LYP" functional.

[5] Ahlrichs and coworkers, unpublished.

[6] G.Schaftenaar and J.H. Noordik, "Molden: a pre- and post-processing program for molecular and electronic structures", *J. Comput.-Aided Mol. Design*, **2000**, *14*, 123-134.

[7] Some references and reviews on DFT approaches to EPR parameters: (a) van Lenthe, E.; van der Avoird, A.; Wormer, P.E.S.; *J. Chem. Phys.* **1997**, *107*, 2488. (b) van Lenthe, E.; van der Avoird, A.; Wormer, P.E.S.; *J. Chem. Phys.* **1998**, *108*, 4783. (c) Neese, F., Curr. Opin. Chem. Biol. 2003, 7, 125. (d) Neese, F.; Solomon, E. In Magnetoscience- From Molecules to amterials; Miller, J.S. Drillon, M., Eds.; Wiley: New York, 2003; pp 345-466. (e) Peng, G.; Nichols, J.; McCullough, E.A.; Spence, J. *Inorg. Chem.*, **1994**, 33, 2857-2864.

[8] Neese, F. *ORCA- an ab initio, Density Functionla and Semiempirical Program Package*, version 2.4, Revision 35; Max-Planck Institute für Bioanorganische Chemie: Mülheim an der Ruhr, Germany, May 2005.

formalism, which expresses the g-tensor as a second-order response property with respect to homogeneous external magnetic field and spin-orbit coupling (SOC) perturbations.[9] Calculation of the hyperfine interactions takes the appropriate SOC effects into account.[10]

[11]EPR properties were also calculated with the ADF[12] program system using the BP86[3] functional with the ZORA/V basis sets supplied with the program (triple-ξ plus two polarisation functions on all atoms), again using the optimized geometry from Turbomole as input.

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[9] Neese, F. *J. Chem. Phys.* **2001**, *115*, 11080.

[10] Neese, F. *J. Chem. Phys.* **2003**, *118*, 3939.

[11]

[12] ADF2000.02. (a) Baerends, E. J.; Ellis, D. E. ; Ros, P.; *Chem. Phys.* **1973**, *2*, 41. (b) Versluis, L.; Ziegler, T.; *J. Chem. Phys.*, **1988**, *88*, 322. (c) te Velde, G.; Baerends, E. J.; *J. Comput. Phys.*, **1992**, *99(1)*, 84. (d) Fonseca Guerra, C.; Snijders, J. G.; te Velde, G; Baerends, E. J.; *Theor. Chem. Acc.*, **1998**, *99*, 391.

Table 1. Crystal data and structure refinement for sg2378.

Identification code	sg2378
Empirical formula	C49 H65 Al N3
Formula weight	723.02
Temperature	213(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, Pc
Unit cell dimensions	a = 10.727(6) A alpha = 90 deg. b = 12.871(7) A beta = 98.068(10) deg. c = 16.300(9) A gamma = 90 deg.
Volume	2228(2) A^3
Z, Calculated density	2, 1.078 Mg/m^3
Absorption coefficient	0.080 mm^-1
F(000)	786
Crystal size	0.10 x 0.05 x 0.02 mm
Theta range for data collection	2.49 to 18.86 deg.
Limiting indices	-9<=h<=9, -11<=k<=11, -14<=l<=14
Reflections collected / unique	8193 / 3453 [R(int) = 0.1378]
Completeness to theta = 18.86	99.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9984 and 0.9920
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3453 / 357 / 297
Goodness-of-fit on F^2	1.040

Final R indices [I>2sigma(I)]	R1 = 0.0758, wR2 = 0.1360
R indices (all data)	R1 = 0.1492, wR2 = 0.1612
Absolute structure parameter	1.1(5)
Largest diff. peak and hole	0.200 and -0.204 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for sg2378.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Al(1)	8722(3)	4290(2)	7245(2)	42(1)
N(1)	8803(8)	5788(6)	7916(5)	32(2)
N(2)	8685(8)	3900(6)	8360(5)	35(2)
N(3)	8717(7)	2611(6)	7188(5)	33(2)
C(1)	8753(9)	6587(8)	9292(6)	63(4)
C(2)	8741(10)	5691(9)	8701(7)	37(3)
C(3)	8690(10)	4639(8)	8967(7)	38(3)
C(4)	8617(10)	4384(8)	9770(6)	47(3)
C(5)	8556(11)	3347(9)	9989(7)	56(4)
C(6)	8581(9)	2573(8)	9398(6)	42(3)
C(7)	8612(9)	2870(8)	8585(6)	32(3)
C(8)	8675(10)	2170(8)	7922(7)	39(3)
C(9)	8670(10)	986(7)	8053(6)	50(3)
C(10)	10109(5)	7204(5)	7495(4)	44(3)
C(11)	10231(6)	8154(6)	7110(4)	54(3)
C(12)	9164(8)	8707(4)	6780(4)	62(4)
C(13)	7975(6)	8308(5)	6835(4)	56(3)
C(14)	7852(5)	7358(6)	7221(5)	39(3)
C(15)	8919(7)	6805(4)	7551(4)	35(3)
C(16)	11283(2)	6682(1)	7901(2)	58(3)
C(17)	11826(2)	7200(1)	8727(2)	97(5)
C(18)	12363(2)	6675(1)	7311(2)	79(4)
C(19)	6517(2)	6997(1)	7337(2)	46(3)
C(20)	5959(2)	7651(1)	8005(2)	88(4)
C(21)	5560(2)	7099(1)	6513(2)	74(4)
C(22)	9949(2)	1726(1)	6251(2)	36(3)
C(23)	10028(2)	1149(1)	5539(2)	48(3)
C(24)	8937(2)	814(1)	5049(2)	47(3)
C(25)	7766(2)	1058(1)	5270(2)	47(3)
C(26)	7687(2)	1635(1)	5981(2)	40(3)
C(27)	8778(2)	1970(1)	6472(2)	36(3)
C(28)	11202(2)	2022(1)	6803(2)	50(3)
C(29)	12199(2)	2448(1)	6264(2)	73(4)
C(30)	11759(2)	1036(1)	7297(2)	80(4)
C(31)	6375(2)	1895(1)	6233(2)	49(3)
C(32)	5468(2)	2364(1)	5489(2)	70(4)
C(33)	5780(2)	806(1)	6526(2)	97(5)
C(34)	7110(2)	4528(1)	6514(2)	29(2)
C(35)	10269(2)	4547(1)	6711(2)	28(2)
C(36)	4141(2)	1724(1)	9620(2)	97(5)
C(37)	5062(2)	1406(1)	9153(2)	111(5)
C(38)	5017(2)	414(1)	8814(2)	105(5)
C(39)	4050(2)	-261(1)	8941(2)	78(4)
C(40)	3129(2)	57(1)	9407(2)	89(4)
C(41)	3174(2)	1049(1)	9746(2)	98(5)
C(42)	2140(2)	1380(1)	10224(2)	138(6)

C(43)	4464(2)	5174(1)	4677(2)	85(4)
C(44)	3543(2)	5108(1)	5196(2)	122(5)
C(45)	2331(2)	5464(1)	4926(2)	126(5)
C(46)	2040(2)	5886(1)	4137(2)	105(5)
C(47)	2961(2)	5952(1)	3618(2)	82(4)
C(48)	4172(2)	5597(1)	3888(2)	98(5)
C(49)	5112(2)	5750(1)	3321(2)	154(7)

Table 3. Bond lengths [A] and angles [deg] for sg2378.

Al(1)-N(2)	1.892(8)
Al(1)-C(34)	1.982(4)
Al(1)-C(35)	2.007(4)
Al(1)-N(3)	2.163(8)
Al(1)-N(1)	2.212(8)
N(1)-C(2)	1.297(10)
N(1)-C(15)	1.451(8)
N(2)-C(7)	1.381(10)
N(2)-C(3)	1.371(11)
N(3)-C(8)	1.331(11)
N(3)-C(27)	1.439(8)
C(1)-C(2)	1.501(13)
C(2)-C(3)	1.425(13)
C(3)-C(4)	1.362(12)
C(4)-C(5)	1.386(12)
C(5)-C(6)	1.389(12)
C(6)-C(7)	1.383(12)
C(7)-C(8)	1.416(12)
C(8)-C(9)	1.539(12)
C(10)-C(11)	1.3900
C(10)-C(15)	1.3900
C(10)-C(16)	1.497(6)
C(11)-C(12)	1.3900
C(12)-C(13)	1.3900
C(13)-C(14)	1.3900
C(14)-C(15)	1.3900
C(14)-C(19)	1.542(6)
C(16)-C(17)	1.5419
C(16)-C(18)	1.6058
C(19)-C(20)	1.5612
C(19)-C(21)	1.5774
C(22)-C(27)	1.3900
C(22)-C(23)	1.3901
C(22)-C(28)	1.5573
C(23)-C(24)	1.3899
C(24)-C(25)	1.3900
C(25)-C(26)	1.3899
C(26)-C(27)	1.3901
C(26)-C(31)	1.5568
C(28)-C(30)	1.5747
C(28)-C(29)	1.5749
C(31)-C(32)	1.5654
C(31)-C(33)	1.6379
C(36)-C(37)	1.3899
C(36)-C(41)	1.3901
C(37)-C(38)	1.3900
C(38)-C(39)	1.3901
C(39)-C(40)	1.3899
C(40)-C(41)	1.3900
C(41)-C(42)	1.5037
C(43)-C(48)	1.3900
C(43)-C(44)	1.3901
C(44)-C(45)	1.3900

C(45)-C(46)	1.3899
C(46)-C(47)	1.3900
C(47)-C(48)	1.3900
C(48)-C(49)	1.4729

N(2)-Al(1)-C(34)	119.0(3)
N(2)-Al(1)-C(35)	126.2(3)
C(34)-Al(1)-C(35)	114.72(18)
N(2)-Al(1)-N(3)	77.1(3)
C(34)-Al(1)-N(3)	97.6(3)
C(35)-Al(1)-N(3)	98.2(3)
N(2)-Al(1)-N(1)	76.2(4)
C(34)-Al(1)-N(1)	97.6(3)
C(35)-Al(1)-N(1)	95.4(3)
N(3)-Al(1)-N(1)	153.1(3)
C(2)-N(1)-C(15)	120.8(9)
C(2)-N(1)-Al(1)	113.6(7)
C(15)-N(1)-Al(1)	125.7(6)
C(7)-N(2)-C(3)	118.0(8)
C(7)-N(2)-Al(1)	121.3(7)
C(3)-N(2)-Al(1)	120.7(7)
C(8)-N(3)-C(27)	119.7(7)
C(8)-N(3)-Al(1)	112.8(7)
C(27)-N(3)-Al(1)	127.5(5)
N(1)-C(2)-C(3)	113.7(10)
N(1)-C(2)-C(1)	124.2(10)
C(3)-C(2)-C(1)	122.2(10)
C(4)-C(3)-N(2)	122.1(9)
C(4)-C(3)-C(2)	122.1(11)
N(2)-C(3)-C(2)	115.8(9)
C(3)-C(4)-C(5)	119.4(9)
C(6)-C(5)-C(4)	120.4(10)
C(5)-C(6)-C(7)	118.2(10)
N(2)-C(7)-C(6)	122.0(10)
N(2)-C(7)-C(8)	113.4(9)
C(6)-C(7)-C(8)	124.4(10)
N(3)-C(8)-C(7)	115.2(9)
N(3)-C(8)-C(9)	123.3(9)
C(7)-C(8)-C(9)	121.5(10)
C(11)-C(10)-C(15)	120.0
C(11)-C(10)-C(16)	117.9(5)
C(15)-C(10)-C(16)	121.9(5)
C(12)-C(11)-C(10)	120.0
C(11)-C(12)-C(13)	120.0
C(14)-C(13)-C(12)	120.0
C(13)-C(14)-C(15)	120.0
C(13)-C(14)-C(19)	118.0(5)
C(15)-C(14)-C(19)	121.8(5)
C(14)-C(15)-C(10)	120.0
C(14)-C(15)-N(1)	120.4(6)
C(10)-C(15)-N(1)	119.5(6)
C(10)-C(16)-C(17)	112.5(3)
C(10)-C(16)-C(18)	111.8(3)
C(17)-C(16)-C(18)	108.0
C(14)-C(19)-C(20)	112.2(3)
C(14)-C(19)-C(21)	112.0(3)
C(20)-C(19)-C(21)	106.4

C(27)-C(22)-C(23)	120.0
C(27)-C(22)-C(28)	122.2
C(23)-C(22)-C(28)	117.7
C(24)-C(23)-C(22)	120.0
C(23)-C(24)-C(25)	120.0
C(26)-C(25)-C(24)	120.0
C(25)-C(26)-C(27)	120.0
C(25)-C(26)-C(31)	119.9
C(27)-C(26)-C(31)	120.1
C(22)-C(27)-C(26)	120.0
C(22)-C(27)-N(3)	119.0(3)
C(26)-C(27)-N(3)	120.9(3)
C(22)-C(28)-C(30)	109.4
C(22)-C(28)-C(29)	111.2
C(30)-C(28)-C(29)	109.1
C(26)-C(31)-C(32)	111.4
C(26)-C(31)-C(33)	107.3
C(32)-C(31)-C(33)	109.3
C(37)-C(36)-C(41)	120.0
C(36)-C(37)-C(38)	120.0
C(37)-C(38)-C(39)	120.0
C(40)-C(39)-C(38)	120.0
C(39)-C(40)-C(41)	120.0
C(40)-C(41)-C(36)	120.0
C(40)-C(41)-C(42)	118.6
C(36)-C(41)-C(42)	121.3
C(48)-C(43)-C(44)	120.0
C(45)-C(44)-C(43)	120.0
C(46)-C(45)-C(44)	120.0
C(45)-C(46)-C(47)	120.0
C(48)-C(47)-C(46)	120.0
C(47)-C(48)-C(43)	120.0
C(47)-C(48)-C(49)	116.7
C(43)-C(48)-C(49)	123.2

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for sg2378. 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
Al(1)	48(2)	44(2)	36(2)	1(2)	11(2)	-7(2)
N(1)	36(5)	29(4)	31(5)	1(4)	1(4)	-6(4)
N(2)	54(6)	21(4)	30(4)	4(4)	2(5)	-5(5)
N(3)	34(6)	37(4)	29(4)	1(4)	8(4)	4(5)
C(1)	54(10)	64(7)	75(9)	-37(7)	25(8)	-13(7)
C(2)	46(8)	29(5)	40(6)	-2(4)	22(7)	3(6)
C(3)	45(8)	40(5)	27(5)	7(4)	2(6)	-12(7)
C(4)	80(9)	32(6)	31(6)	-3(5)	9(7)	2(8)
C(5)	92(10)	51(7)	25(6)	10(5)	8(7)	-2(8)
C(6)	60(9)	35(6)	33(6)	4(5)	9(7)	-21(7)
C(7)	31(7)	39(5)	26(5)	5(4)	7(6)	3(6)
C(8)	47(8)	39(5)	31(5)	-5(5)	3(7)	-2(7)
C(9)	67(8)	49(6)	32(8)	17(6)	7(7)	-8(7)
C(10)	55(5)	26(6)	48(8)	-5(5)	-1(6)	-18(5)
C(11)	84(8)	26(7)	55(8)	-6(5)	23(7)	-10(6)
C(12)	99(9)	31(7)	61(8)	12(6)	33(9)	1(6)
C(13)	84(8)	32(7)	57(8)	-6(6)	27(7)	11(6)
C(14)	59(5)	19(6)	39(8)	-18(5)	9(6)	4(5)
C(15)	46(5)	24(5)	36(7)	-6(5)	6(6)	-8(5)
C(16)	45(6)	60(8)	66(8)	8(6)	-5(6)	-20(6)
C(17)	89(11)	119(13)	74(8)	-11(8)	-26(7)	-25(9)
C(18)	61(8)	59(9)	117(10)	-12(8)	14(7)	-18(7)
C(19)	54(6)	34(7)	50(7)	1(6)	8(6)	16(6)
C(20)	78(10)	118(11)	76(8)	-30(8)	38(7)	3(9)
C(21)	72(8)	73(9)	73(8)	-20(8)	-8(6)	8(8)
C(22)	49(5)	26(7)	38(7)	9(5)	22(5)	2(6)
C(23)	56(7)	35(8)	60(8)	-2(5)	31(6)	1(6)
C(24)	75(8)	37(7)	32(7)	-4(6)	21(6)	-2(7)
C(25)	61(7)	52(8)	27(7)	1(5)	7(6)	-6(6)
C(26)	54(5)	28(7)	34(7)	1(5)	-6(5)	9(5)
C(27)	32(5)	53(7)	25(6)	2(5)	6(5)	8(6)
C(28)	40(6)	54(8)	56(8)	-4(6)	8(5)	17(6)
C(29)	62(8)	84(9)	79(9)	-24(7)	32(7)	-13(7)
C(30)	46(9)	87(9)	108(11)	27(7)	9(7)	30(7)
C(31)	36(6)	52(8)	56(7)	-14(6)	-6(5)	0(6)
C(32)	59(8)	59(8)	84(9)	1(6)	-19(7)	-4(7)
C(33)	74(10)	89(10)	131(12)	37(8)	24(9)	4(8)
C(34)	48(6)	17(6)	23(6)	-9(5)	6(5)	6(5)
C(35)	37(6)	17(6)	30(6)	-13(5)	3(5)	3(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for sg2378.

	x	y	z	U(eq)
H(1A)	8783	7234	8991	95
H(1B)	9487	6536	9711	95
H(1C)	7997	6569	9555	95
H(4A)	8609	4907	10172	57
H(5A)	8496	3165	10541	67
H(6A)	8578	1867	9545	51
H(9A)	8713	638	7530	74
H(9B)	7902	785	8262	74
H(9C)	9391	789	8450	74
H(11A)	11036	8424	7072	64
H(12A)	9247	9350	6519	74
H(13A)	7253	8682	6612	67
H(16A)	11074	5952	8017	70
H(17A)	11189	7213	9094	146
H(17B)	12081	7905	8622	146
H(17C)	12550	6808	8983	146
H(18A)	12042	6352	6786	118
H(18B)	13083	6286	7576	118
H(18C)	12615	7383	7215	118
H(19A)	6556	6260	7512	55
H(20A)	6518	7612	8527	132
H(20B)	5139	7377	8079	132
H(20C)	5873	8369	7826	132
H(21A)	5868	6703	6076	111
H(21B)	5478	7824	6352	111
H(21C)	4745	6832	6604	111
H(23A)	10820	984	5390	58
H(24A)	8990	424	4568	56
H(25A)	7028	831	4938	56
H(28A)	11029	2565	7202	60
H(29A)	11861	3056	5959	109
H(29B)	12385	1915	5878	109
H(29C)	12965	2635	6623	109
H(30A)	11149	770	7630	121
H(30B)	12526	1225	7654	121
H(30C)	11946	505	6909	121
H(31A)	6476	2393	6701	59
H(32A)	5819	3008	5315	105
H(32B)	4653	2498	5660	105
H(32C)	5372	1875	5031	105
H(33A)	6340	514	6987	146
H(33B)	5684	318	6068	146
H(33C)	4965	941	6696	146
H(34A)	6907	3923	6166	43
H(34B)	7189	5131	6168	43
H(34C)	6446	4647	6850	43
H(35A)	10421	3953	6372	43

H(35B)	10987	4649	7136	43
H(35C)	10146	5163	6366	43
H(36A)	4172	2395	9849	116
H(37A)	5716	1862	9068	133
H(38A)	5640	199	8499	126
H(39A)	4020	-932	8711	94
H(40A)	2476	-400	9493	106
H(42A)	1556	809	10248	207
H(42B)	1697	1970	9951	207
H(42C)	2500	1575	10782	207
H(43A)	5283	4934	4859	102
H(44A)	3740	4823	5729	147
H(45A)	1709	5419	5277	151
H(46A)	1221	6127	3955	126
H(47A)	2764	6238	3085	99
H(49A)	4707	6053	2807	231
H(49B)	5479	5086	3207	231
H(49C)	5769	6212	3576	231

Table 6. Torsion angles [deg] for sg2378.

N(2)-Al(1)-N(1)-C(2)	-2.4(7)
C(34)-Al(1)-N(1)-C(2)	115.7(7)
C(35)-Al(1)-N(1)-C(2)	-128.4(7)
N(3)-Al(1)-N(1)-C(2)	-8.2(12)
N(2)-Al(1)-N(1)-C(15)	177.4(8)
C(34)-Al(1)-N(1)-C(15)	-64.6(7)
C(35)-Al(1)-N(1)-C(15)	51.3(7)
N(3)-Al(1)-N(1)-C(15)	171.6(7)
C(34)-Al(1)-N(2)-C(7)	88.4(8)
C(35)-Al(1)-N(2)-C(7)	-93.9(8)
N(3)-Al(1)-N(2)-C(7)	-3.1(8)
N(1)-Al(1)-N(2)-C(7)	179.5(8)
C(34)-Al(1)-N(2)-C(3)	-89.5(8)
C(35)-Al(1)-N(2)-C(3)	88.1(8)
N(3)-Al(1)-N(2)-C(3)	178.9(8)
N(1)-Al(1)-N(2)-C(3)	1.6(7)
N(2)-Al(1)-N(3)-C(8)	0.8(8)
C(34)-Al(1)-N(3)-C(8)	-117.3(7)
C(35)-Al(1)-N(3)-C(8)	126.2(7)
N(1)-Al(1)-N(3)-C(8)	6.6(12)
N(2)-Al(1)-N(3)-C(27)	-177.8(7)
C(34)-Al(1)-N(3)-C(27)	64.1(6)
C(35)-Al(1)-N(3)-C(27)	-52.4(6)
N(1)-Al(1)-N(3)-C(27)	-172.0(6)
C(15)-N(1)-C(2)-C(3)	-177.1(8)
Al(1)-N(1)-C(2)-C(3)	2.6(11)
C(15)-N(1)-C(2)-C(1)	1.4(15)
Al(1)-N(1)-C(2)-C(1)	-178.9(8)
C(7)-N(2)-C(3)-C(4)	-0.5(15)
Al(1)-N(2)-C(3)-C(4)	177.5(9)
C(7)-N(2)-C(3)-C(2)	-178.8(9)
Al(1)-N(2)-C(3)-C(2)	-0.8(12)
N(1)-C(2)-C(3)-C(4)	-179.8(10)
C(1)-C(2)-C(3)-C(4)	1.7(16)
N(1)-C(2)-C(3)-N(2)	-1.4(14)
C(1)-C(2)-C(3)-N(2)	-180.0(9)
N(2)-C(3)-C(4)-C(5)	1.0(17)
C(2)-C(3)-C(4)-C(5)	179.2(10)
C(3)-C(4)-C(5)-C(6)	0.7(17)
C(4)-C(5)-C(6)-C(7)	-2.9(17)
C(3)-N(2)-C(7)-C(6)	-1.8(14)
Al(1)-N(2)-C(7)-C(6)	-179.8(8)
C(3)-N(2)-C(7)-C(8)	-177.1(9)
Al(1)-N(2)-C(7)-C(8)	4.9(12)
C(5)-C(6)-C(7)-N(2)	3.5(15)
C(5)-C(6)-C(7)-C(8)	178.2(10)
C(27)-N(3)-C(8)-C(7)	-179.8(7)
Al(1)-N(3)-C(8)-C(7)	1.5(12)
C(27)-N(3)-C(8)-C(9)	-0.9(15)
Al(1)-N(3)-C(8)-C(9)	-179.7(8)
N(2)-C(7)-C(8)-N(3)	-3.9(14)
C(6)-C(7)-C(8)-N(3)	-179.0(10)
N(2)-C(7)-C(8)-C(9)	177.2(9)

C(6)-C(7)-C(8)-C(9)	2.1(17)
C(15)-C(10)-C(11)-C(12)	0.0
C(16)-C(10)-C(11)-C(12)	-175.1(5)
C(10)-C(11)-C(12)-C(13)	0.0
C(11)-C(12)-C(13)-C(14)	0.0
C(12)-C(13)-C(14)-C(15)	0.0
C(12)-C(13)-C(14)-C(19)	174.5(5)
C(13)-C(14)-C(15)-C(10)	0.0
C(19)-C(14)-C(15)-C(10)	-174.3(5)
C(13)-C(14)-C(15)-N(1)	-176.8(7)
C(19)-C(14)-C(15)-N(1)	8.9(7)
C(11)-C(10)-C(15)-C(14)	0.0
C(16)-C(10)-C(15)-C(14)	174.9(5)
C(11)-C(10)-C(15)-N(1)	176.8(7)
C(16)-C(10)-C(15)-N(1)	-8.3(6)
C(2)-N(1)-C(15)-C(14)	-91.4(9)
Al(1)-N(1)-C(15)-C(14)	88.9(7)
C(2)-N(1)-C(15)-C(10)	91.8(9)
Al(1)-N(1)-C(15)-C(10)	-87.9(7)
C(11)-C(10)-C(16)-C(17)	74.8(4)
C(15)-C(10)-C(16)-C(17)	-100.2(4)
C(11)-C(10)-C(16)-C(18)	-46.9(4)
C(15)-C(10)-C(16)-C(18)	138.1(3)
C(13)-C(14)-C(19)-C(20)	-71.0(4)
C(15)-C(14)-C(19)-C(20)	103.4(4)
C(13)-C(14)-C(19)-C(21)	48.6(4)
C(15)-C(14)-C(19)-C(21)	-137.0(3)
C(27)-C(22)-C(23)-C(24)	0.0
C(28)-C(22)-C(23)-C(24)	176.4
C(22)-C(23)-C(24)-C(25)	0.0
C(23)-C(24)-C(25)-C(26)	0.0
C(24)-C(25)-C(26)-C(27)	0.0
C(24)-C(25)-C(26)-C(31)	-179.2
C(23)-C(22)-C(27)-C(26)	0.0
C(28)-C(22)-C(27)-C(26)	-176.2
C(23)-C(22)-C(27)-N(3)	-177.0(4)
C(28)-C(22)-C(27)-N(3)	6.8(4)
C(25)-C(26)-C(27)-C(22)	0.0
C(31)-C(26)-C(27)-C(22)	179.2
C(25)-C(26)-C(27)-N(3)	176.9(4)
C(31)-C(26)-C(27)-N(3)	-3.9(4)
C(8)-N(3)-C(27)-C(22)	-93.2(8)
Al(1)-N(3)-C(27)-C(22)	85.4(6)
C(8)-N(3)-C(27)-C(26)	89.9(9)
Al(1)-N(3)-C(27)-C(26)	-91.6(6)
C(27)-C(22)-C(28)-C(30)	101.8
C(23)-C(22)-C(28)-C(30)	-74.5
C(27)-C(22)-C(28)-C(29)	-137.6
C(23)-C(22)-C(28)-C(29)	46.1
C(25)-C(26)-C(31)-C(32)	-50.1
C(27)-C(26)-C(31)-C(32)	130.7
C(25)-C(26)-C(31)-C(33)	69.5
C(27)-C(26)-C(31)-C(33)	-109.8
C(41)-C(36)-C(37)-C(38)	0.0
C(36)-C(37)-C(38)-C(39)	0.0
C(37)-C(38)-C(39)-C(40)	0.0
C(38)-C(39)-C(40)-C(41)	0.0

C(39)-C(40)-C(41)-C(36)	0.0
C(39)-C(40)-C(41)-C(42)	178.0
C(37)-C(36)-C(41)-C(40)	0.0
C(37)-C(36)-C(41)-C(42)	-178.0
C(48)-C(43)-C(44)-C(45)	0.0
C(43)-C(44)-C(45)-C(46)	0.0
C(44)-C(45)-C(46)-C(47)	0.0
C(45)-C(46)-C(47)-C(48)	0.0
C(46)-C(47)-C(48)-C(43)	0.0
C(46)-C(47)-C(48)-C(49)	-176.5
C(44)-C(43)-C(48)-C(47)	0.0
C(44)-C(43)-C(48)-C(49)	176.3

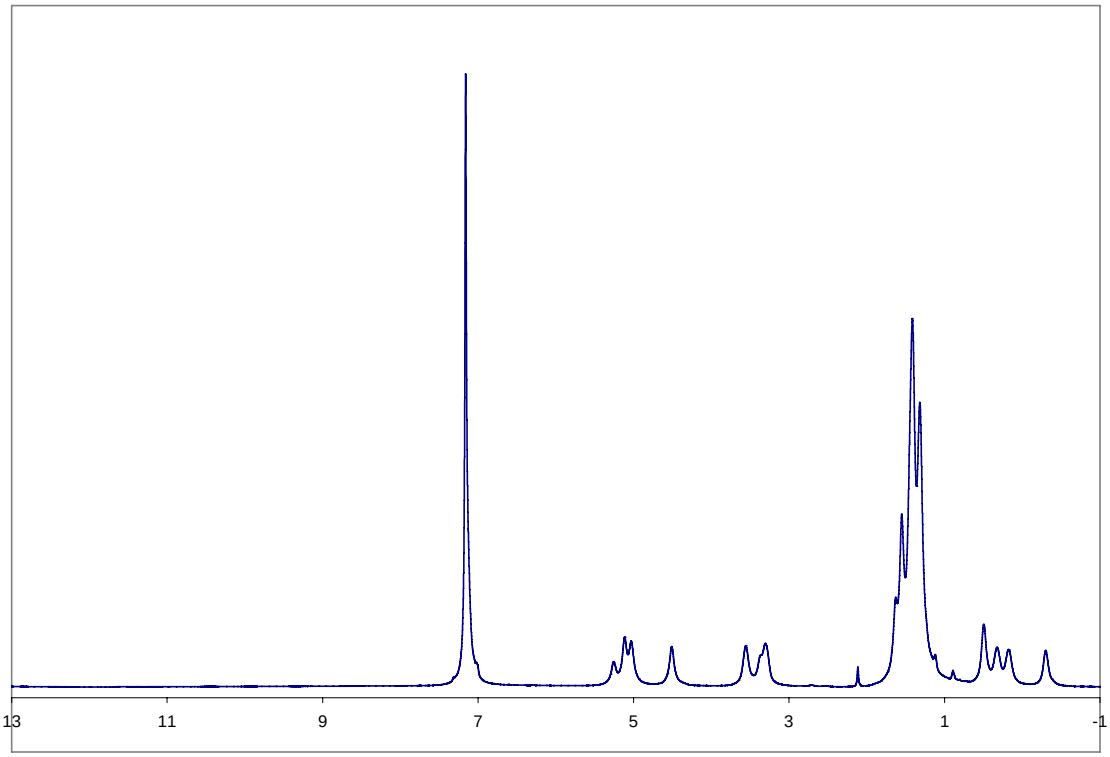
Symmetry transformations used to generate equivalent atoms:

Complex 2

Synthesis

{2,6-[2,6-(i-Pr)$_2$PhN=C(CH$_3$)]$_2$(C$_5$H$_3$N)}FeCl$_2$ was prepared in-situ by stirring FeCl$_2$(THF)$_{1.5}$ (0.200 g, 0.85 mmol) with {2,6-[2,6-(i-Pr)$_2$PhN=C(CH$_3$)]$_2$(C$_5$H$_3$N)} (0.410 g, 0.85 mmol) in toluene overnight. The resulting dark-blue suspension was cooled to -35ºC and treated with 5 equivalents of AlEt$_3$ (4.25mL of a 1M solution, 4.25mmol). The initially blue color became dark-green and then dark-orange during eight hour stirring at room temperature. The solvent was evaporated and the residue washed with hexane to remove a dark greenish-brown solution. The residual precipitate was dissolved in ether, centrifuged to remove traces of insoluble material, concentrated, and allowed to stand at room temperature for 2 days. Crystals of **3** separated which were washed with several portions of hexane to obtain a 41% yield of crystalline **3** (0.280 g, 0.34 mmol). Anal. Calcd. (found) for C$_{46}$H$_{66}$N$_3$Al$_2$ClFe: C, 68.52(67.98); H, 8.25(8.01); N, 5.21(5.02). IR (Nujol mull, cm^{-1}): ν 2918 (s), 2854 (s), 1597 (s), 1584 (s), 1509 (s), 1305 (s), 1272 (m), 1236 (w), 1219 (w), 1192 (m), 1171 (m), 1108 (m), 1073 (w), 1054 (w), 1033 (w), 992 (m), 971 (m), 947 (m), 902 (w), 847 (m), 820 (s), 803 (m), 793 (m), 777 (s), 724 (m), 690 (m). [μ_{eff} = 1.41 μ_B]. [m.p.(dec) = 157-9C].

^{1}H NMR of **2**.



Details of calculations

Density functional calculations on model complexes were performed with the TURBOMOLE program[1] in combination with the OPTIMIZE routine of Baker and co-workers.[2] All relevant structures were fully optimized at the restricted or unrestricted b3-lyp[3] level, employing the standard SV(P) basis sets.[4] Improved electronic energies were calculated at the SV(P) optimized geometries using the TZVPP basis set on all atoms.[5] Orbital plots were prepared using Molden.[6]

(1) a) Ahlrichs, R.; Bär, M.; Häser, M.; Horn, H.; Kölmel, C. *Chem. Phys. Lett.* **1989**, *162*, 165; b) Treutler, O.; Ahlrichs, R. *J. Chem. Phys.*, 1995, *102*, 346; c) Ahlrichs, R.; Bär, M.; Baron, H.-P.; Bauernschmitt, R.; Böcker, S.; Ehrig, M.; Eichkorn, K.; Elliott, S.; Furche, F.; Haase, F.; Häser, M.; Hättig, C.; Horn, H.; Huber, C.; Huniar, U.; Kattannek, M.; Köhn, A.; Kölmel, C.; Kollwitz, M.; May, K.; Ochsenfeld, C.; Öhm, H.; Schäfer, A.; Schneider, U.; Treutler, O.; Tsereteli, K.; Unterreiner, B.; Von Arnim, M.; Weigend, F.; Weis, P.; Weiss H. Turbomole Version 5, January **2002**. Theoretical Chemistry Group, University of Karlsruhe

(2) Baker, J. *J. Comput. Chem.* **1986**, *7*, 385; PQS version 2.4, **2001**, Parallel Quantum Solutions, Fayetteville, Arkansas, USA; the Baker optimizer is available separately from PQS upon request

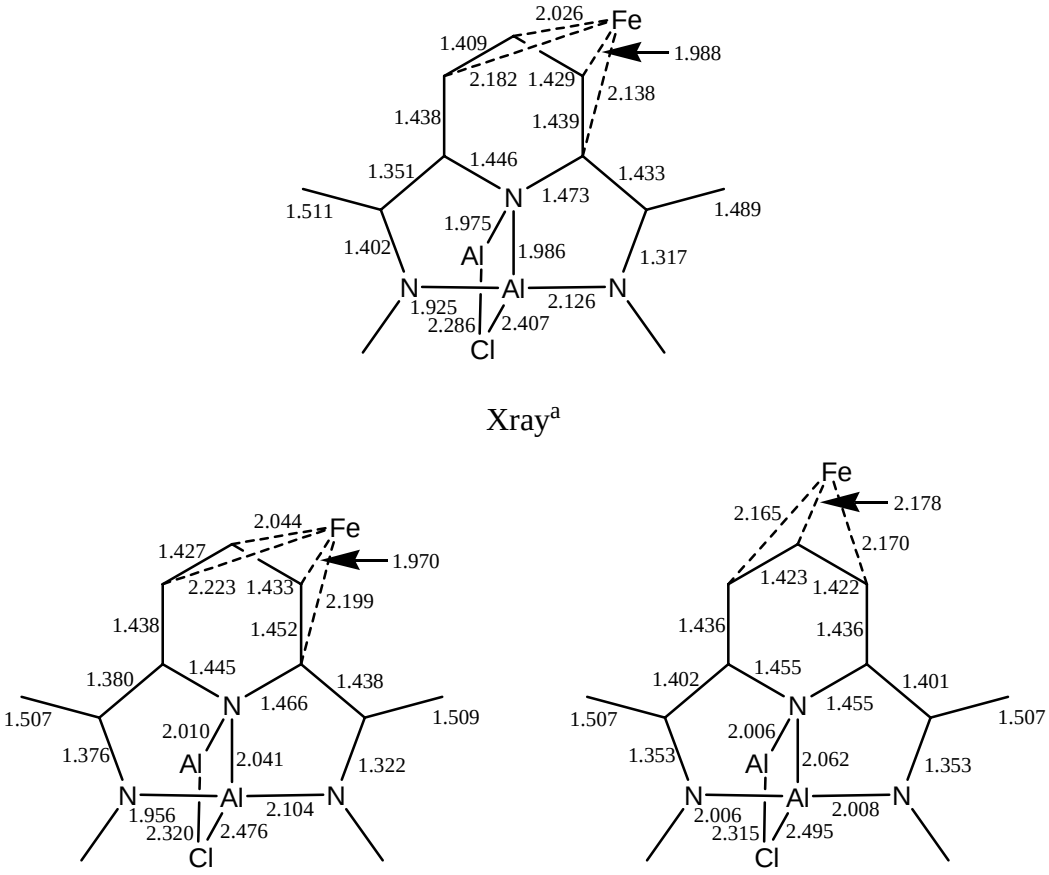
(3) a) Lee, C.; Yang, W.; Parr, R.G. *Phys. Rev. B* **1988**, *37*, 785; b) Becke, A.D. *J. Chem. Phys.* **1993**, *98*, 1372; c) Becke, A.D. *J. Chem. Phys.* **1993**, *98*, 5648; note that the Turbomole functional "b3-lyp" is not identical to the Gaussian "B3LYP" functional

(4) Schäfer, A.; Horn, H.; Ahlrichs, R. *J. Chem. Phys.* **1992**, *97*, 2571

(5) Schäfer, A.; Huber, C. Ahlrichs, R. *J. Chem. Phys.* **1994**, *100*, 5829

(6) Schaftenaar, G.; Noordik, J.H. *J. Comput.-Aided Mol. Design*, **2000**, *14*, 123

Figure S1. Comparison of observed and calculated bond lengths (Å).



[a] Ordered molecule of the X-ray structure. The other molecule has disorder between "Fe-left" and "Fe-right" structures and therefore shows averaged bond lengths for the ligand skeleton.

Table S1. Total (a.u.) and relative (kcal/mol) energies for states of $(C_6H_6)FeLAl_2Me_3Cl$, calculated at different levels of theory.

	ri-bp86/SV(P)		b3-lyp/SV(P)		b3-lyp/TZVPP//SV(P)	
State	Etot	Erel	Etot	Erel	Etot	Erel
RDFT	-3692.98499	(0)	-3691.37144	(0)	-3693.57088	(0)
UDFT (S = 1)	-3692.97114	8.69	-3691.37921	-4.87	-3693.58010	-5.78
UDFT (S = 2)	-3692.92716	36.29	-3691.35594	9.73	-3693.55163	12.08

Table S2. Total energies (a.u.) and relative $(C_6H_6)Fe$ binding energies of butadiene-like ligands

	b3-lyp/SV(P)			b3-lyp/TZVPP//SV(P)		
Ligand	Lig	$(C_6H_6)Fe(Lig)$	$E_b(rel)$	Lig	$(C_6H_6)Fe(Lig)$	$E_b(rel)$
Butadiene	-155.75135	-1651.16446	0.00	-155.94321	-1651.78869	0.00
1,2-dihydro-pyridine	-249.09733	-1744.49826	7.64	-249.39380	-1745.22571	8.51
2-Methylene-1,2-dihydro-pyridine	-287.15952	-1782.54950	14.51	-287.49712	-1783.31868	15.01
LAl_2Me_3Cl	-2195.98244	-3691.37144	15.12	-2197.75289	-3693.57088	17.24

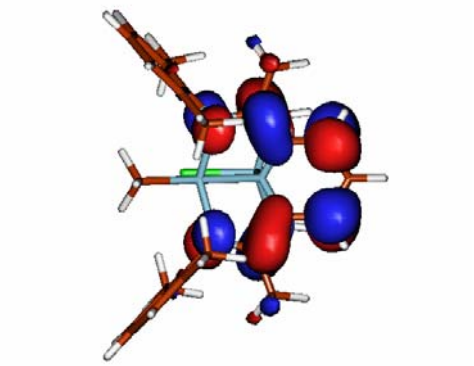
Orbital plots

For the Fe complexes, two views of each relevant orbital are give. The left picture shows a "standard orientation", while the picture on the right is rotated to make the contribution of the Fe better recognizable. Descriptions are indicative only. The coordinate system chosen to assign approximate labels has the *z* axis perpendicular to the pyridine ring, the *x* axis along the pyridine N-C4 line and the *y* axis along the imine-imine vector.

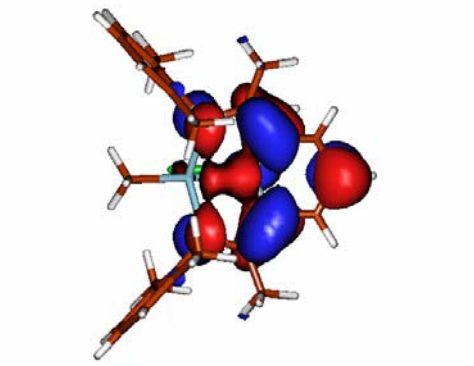
LAl$_2$Me$_3$Cl fragment, without Fe attached

Highest π-orbitals

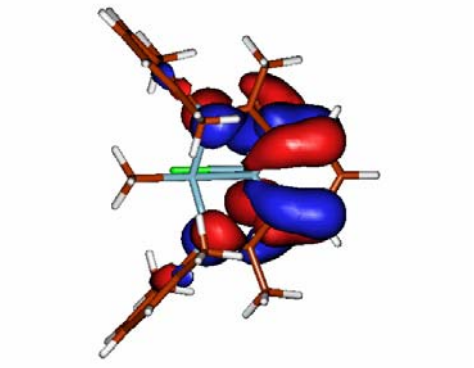
135 (LUMO): π^*_a, (imine π*)-(imine π*)



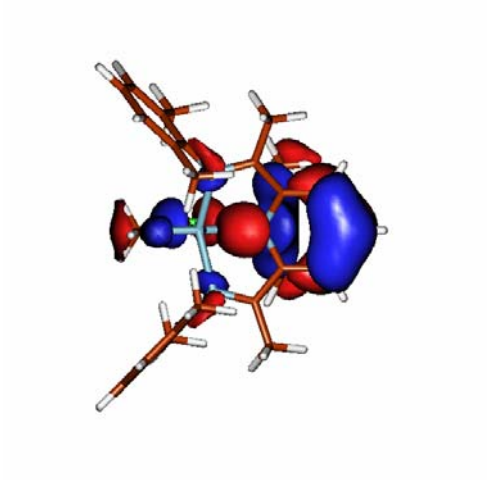
134 (HOMO): π^*_s, (imine π*)+(imine π*)



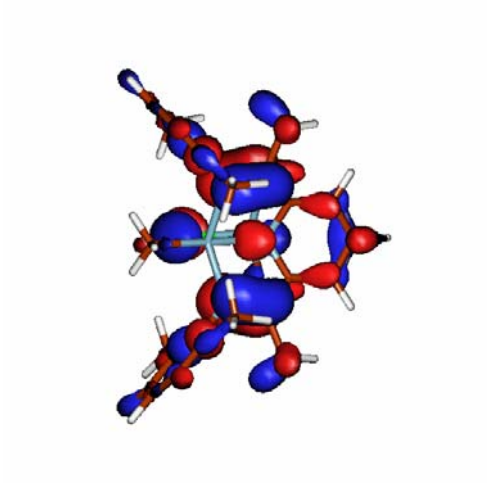
127: Py π_a



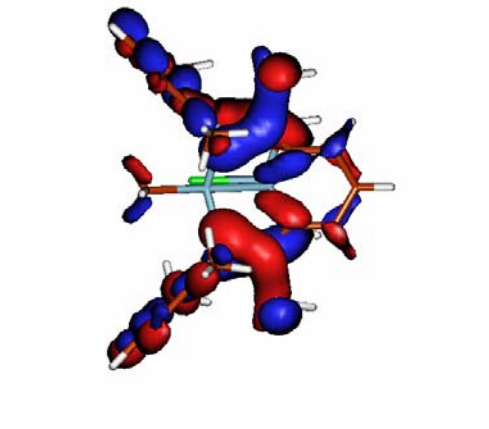
124: Py π_s



123: (imine)+(imine π)



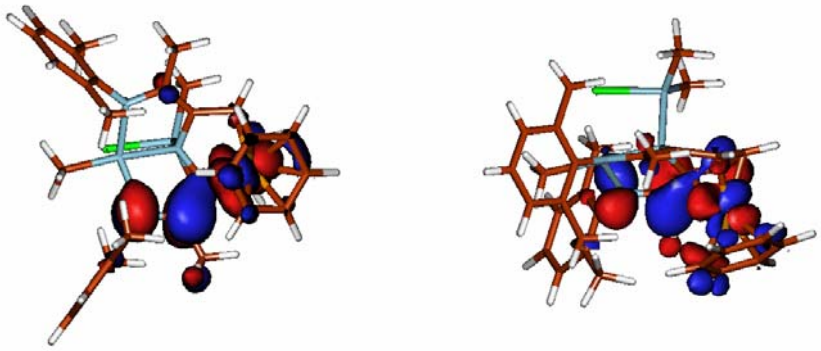
121: (imine)-(imine π)



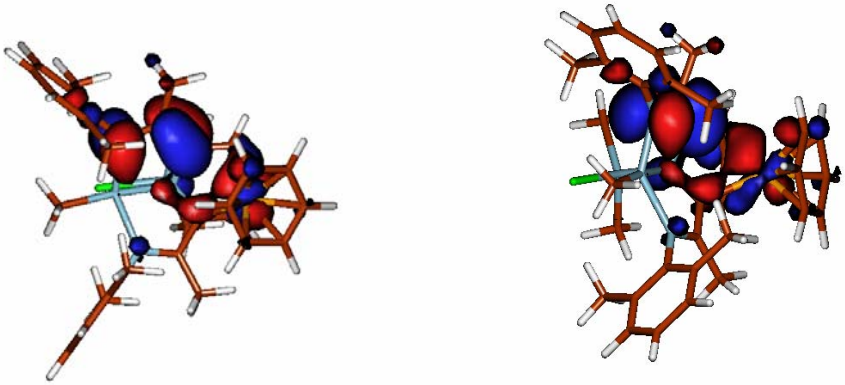
Singlet (C_6H_6)FeLAl$_2$Me$_3$Cl

Highest Fe-containing orbitals

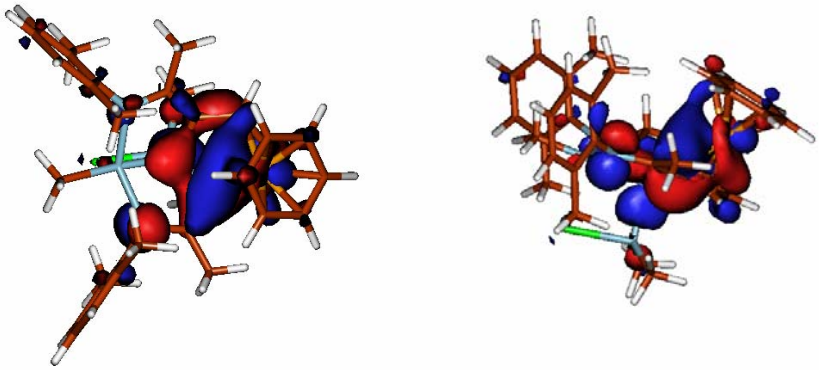
169 (LUMO): imine2 π*



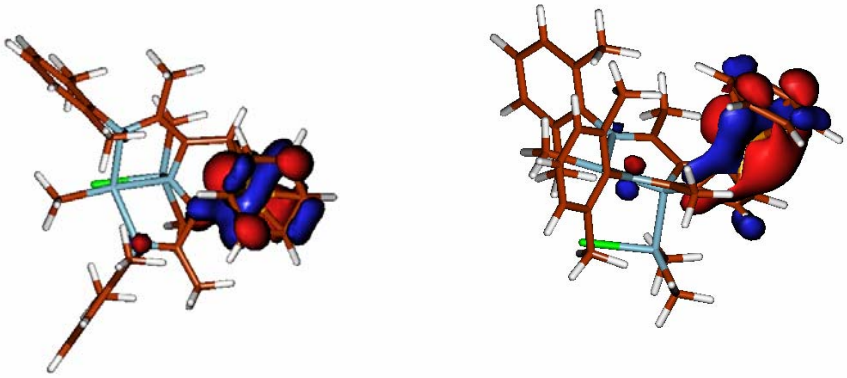
168 (HOMO): imine1 π* donating into Fe d_{yz}



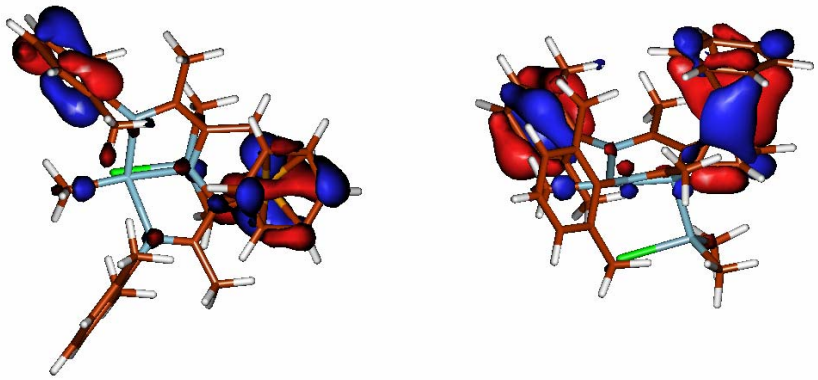
167: Py π donating into "d_{z^2}"



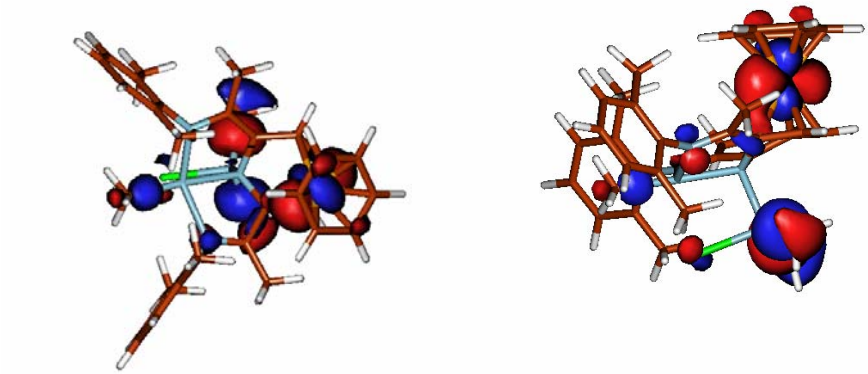
165: Fe $d_{x^2-y^2}$



163: Fe d_{xy}



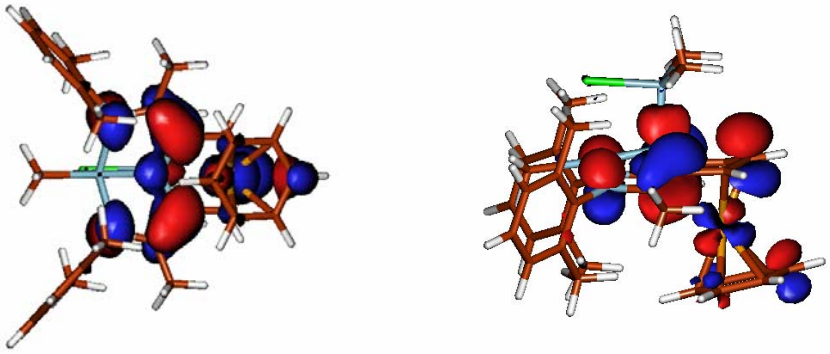
160: Fe d_{xz}



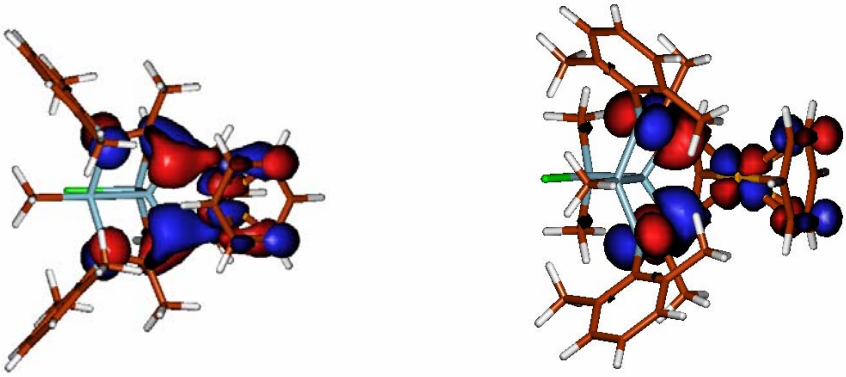
Triplet (C_6H_6)FeLAl$_2$Me$_3$Cl

Highest Fe-containing α orbitals

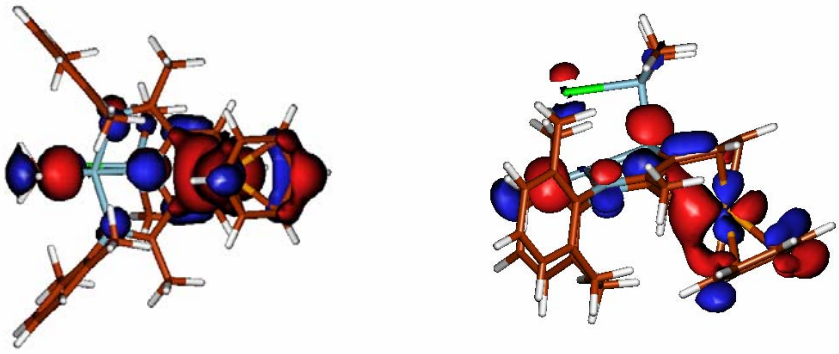
α169 (SOMO): π*$_s$ - Fe d_{xz}



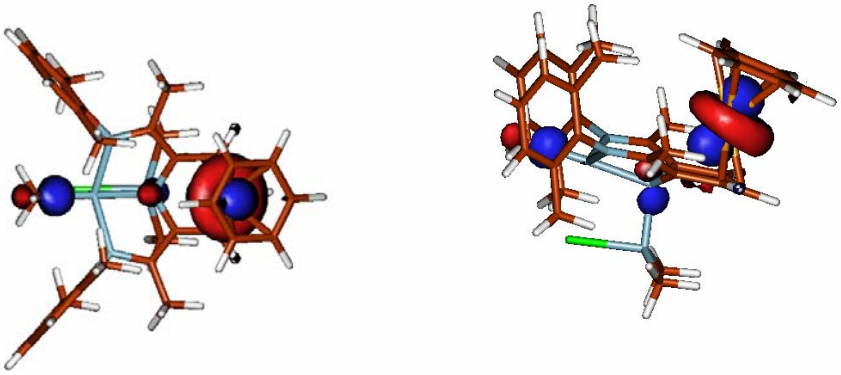
α168: π*$_a$ - Fe d_{yz} (partially paired with β167)



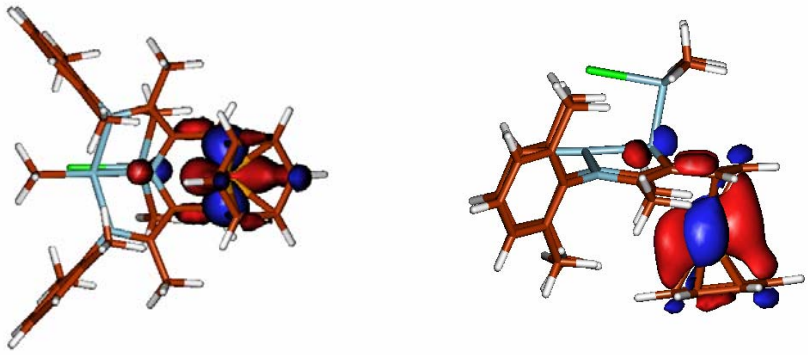
α165: Fe d_{xz} + ...



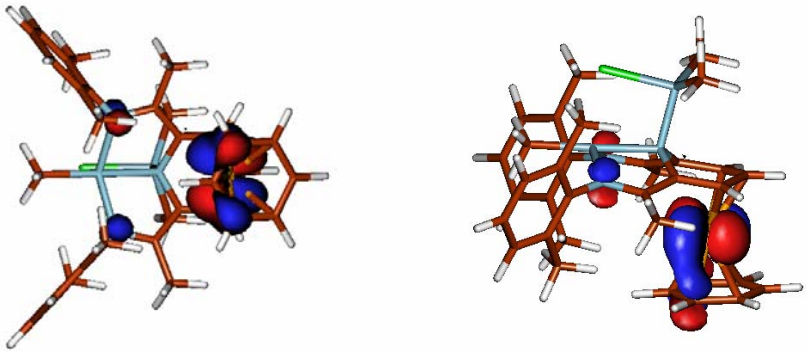
α163: Fe d_{z^2} (paired with β165)



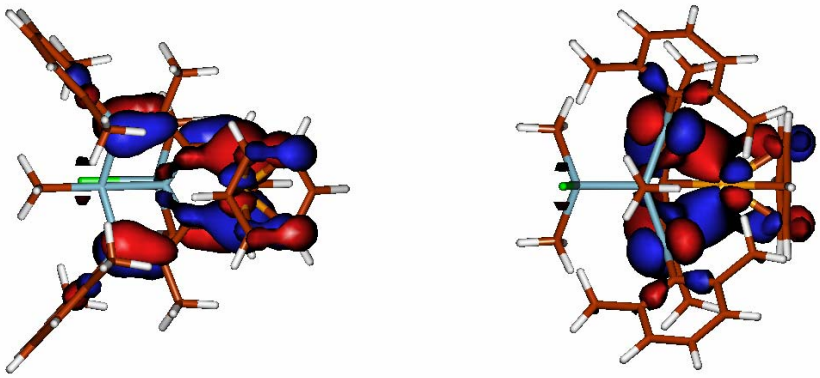
α159: Fe $d_{x^2-y^2}$ (paired with Fe parts of β164/166)



α158: Fe d_{xy} (partially paired with β167)

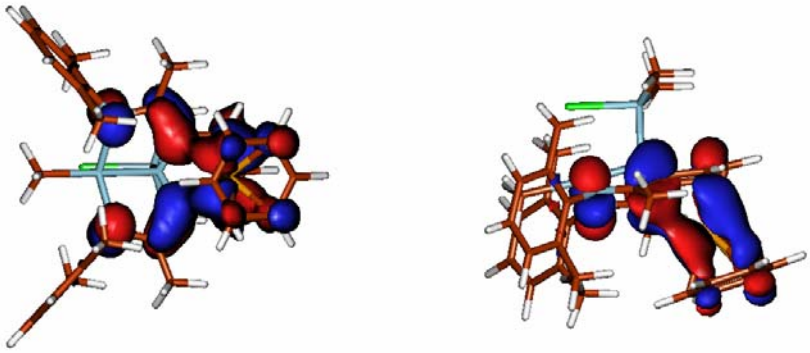


α156: L π_a + Fe d_{yz}

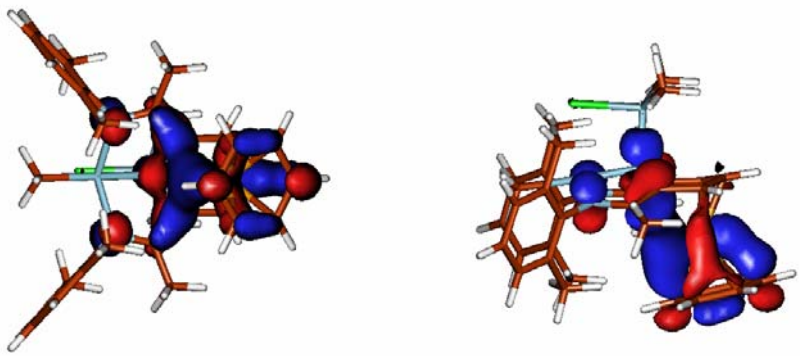


Highest Fe-containing β orbitals

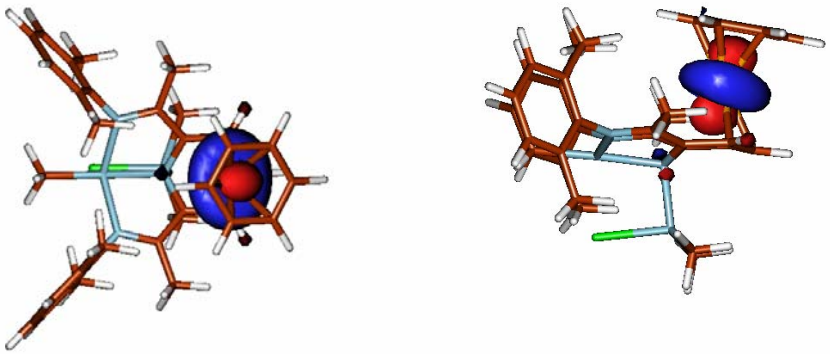
β167 (singly occ): Fe d_{xy} + π^*_a



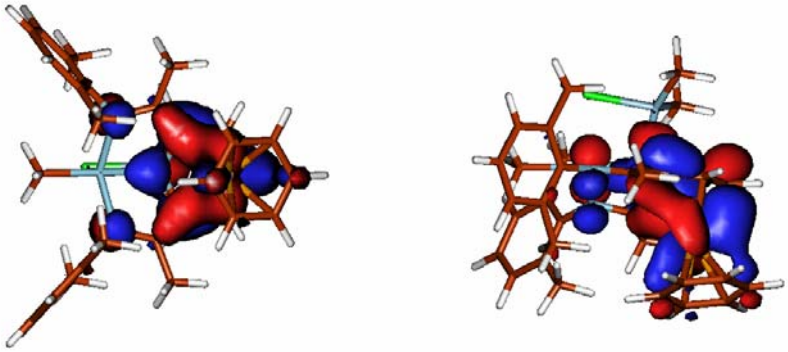
β166: Fe $d_{x^2-y^2}$, C_6H_6 π*



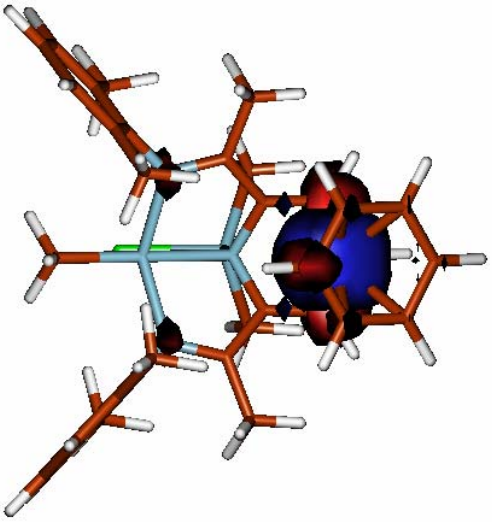
β165: Fe d_{z^2}



β164: Py π, Fe $d_{x^2-y^2}$



Total spin density (α - β density)



X-ray Crystallography

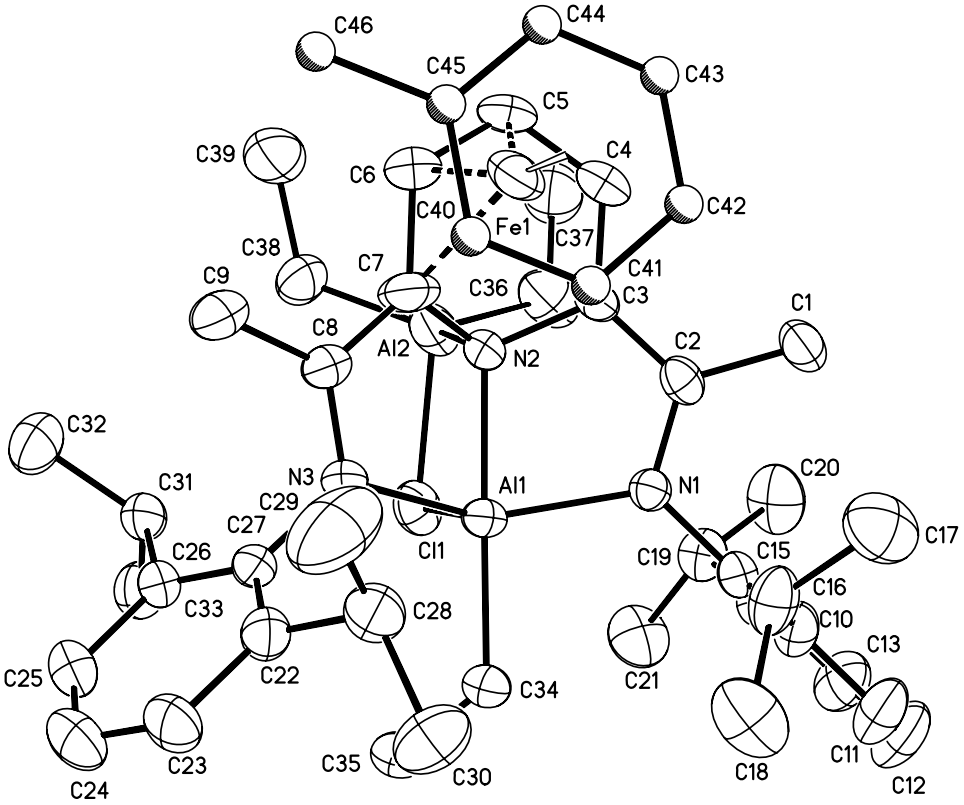


Table 1. Crystal data and structure refinement for sg2714.

Identification code	sg2714
Empirical formula	C92 H132 Al4 Cl2 Fe2 N6
Formula weight	1612.56
Temperature	207(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 10.676(4) A alpha = 82.262(6) deg. b = 19.708(7) A beta = 89.088(6) deg. c = 21.150(7) A gamma = 87.984(6) deg.
Volume	4407(3) A^3
Z, Calculated density	2, 1.215 Mg/m^3
Absorption coefficient	0.477 mm^-1
F(000)	1728
Crystal size	0.35 x 0.30 x 0.20 mm
Theta range for data collection	2.09 to 21.97 deg.
Limiting indices	-11<=h<=11, -20<=k<=20, -22<=l<=22
Reflections collected / unique	31293 / 10504 [R(int) = 0.0499]
Completeness to theta = 21.97	97.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9106 and 0.8508
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10504 / 39 / 928
Goodness-of-fit on F^2	1.013
Final R indices [I>2sigma(I)]	R1 = 0.0673, wR2 = 0.1660
R indices (all data)	R1 = 0.1016, wR2 = 0.1880
Largest diff. peak and hole	0.753 and -0.316 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for sg2714.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	-161(3)	7305(1)	5763(1)	74(1)
Fe(1')	301(2)	6875(1)	5761(1)	69(1)
Al(1)	2301(1)	7664(1)	3992(1)	45(1)
Al(2)	4119(2)	7539(1)	5138(1)	84(1)
Cl(1)	4522(1)	7859(1)	4086(1)	71(1)
N(1)	2151(4)	6650(2)	4071(2)	44(1)
N(2)	2346(4)	7433(2)	4938(2)	54(1)
N(3)	1399(4)	8508(2)	4261(2)	51(1)
C(1)	1936(6)	5559(3)	4812(3)	66(2)
C(2)	2032(5)	6323(3)	4671(3)	50(1)
C(3)	2024(5)	6731(3)	5157(3)	55(1)
C(4)	1849(10)	6555(4)	5808(3)	108(3)
C(5)	1740(9)	7050(4)	6227(3)	100(3)
C(6)	1427(7)	7710(4)	5936(3)	79(2)
C(7)	1538(8)	7883(4)	5263(3)	88(2)
C(8)	1164(6)	8484(3)	4879(3)	66(2)
C(9)	506(7)	9063(3)	5174(3)	83(2)
C(10)	1078(6)	6119(3)	3243(3)	61(2)
C(11)	1140(7)	5722(4)	2750(4)	85(2)
C(12)	2249(9)	5447(4)	2561(4)	103(3)
C(13)	3342(8)	5556(4)	2854(4)	89(2)
C(14)	3352(5)	5960(3)	3360(3)	61(2)
C(15)	2188(5)	6231(2)	3551(3)	48(1)
C(16)	-190(6)	6404(3)	3433(3)	72(2)
C(17)	-1001(7)	5848(4)	3770(4)	104(3)
C(18)	-884(7)	6783(4)	2866(4)	104(3)
C(19)	4565(5)	6087(3)	3654(3)	67(2)
C(20)	5254(7)	5417(4)	3953(4)	105(3)
C(21)	5410(7)	6520(4)	3176(4)	100(2)
C(22)	-8(6)	9222(3)	3495(3)	60(2)
C(23)	-224(7)	9829(3)	3090(3)	75(2)
C(24)	597(8)	10343(4)	3028(4)	92(2)
C(25)	1702(7)	10264(3)	3370(3)	77(2)
C(26)	1980(6)	9665(3)	3783(3)	58(2)
C(27)	1112(6)	9144(3)	3841(2)	52(1)
C(28)	-990(6)	8680(3)	3569(3)	72(2)
C(29)	-2060(10)	8867(6)	3997(5)	153(4)
C(30)	-1565(7)	8570(4)	2937(4)	95(2)
C(31)	3173(6)	9628(3)	4163(3)	63(2)
C(32)	3144(7)	10168(4)	4627(4)	90(2)
C(33)	4341(7)	9708(4)	3741(3)	83(2)
C(34)	2212(5)	7882(3)	3055(2)	56(1)
C(35)	3026(7)	8427(4)	2688(3)	87(2)
C(36')	4860(40)	6835(19)	5681(18)	116(11)
C(37')	5490(60)	6340(30)	5300(20)	122(15)
C(38)	4770(19)	8252(10)	5519(10)	80(5)

C(36)	5099(15)	6648(8)	5307(7)	95(5)
C(37)	5454(14)	6422(6)	5978(6)	129(4)
C(38')	4096(19)	8437(11)	5616(11)	74(6)
C(39)	4596(10)	8261(5)	6270(4)	126(3)
Fe(2)	5316(1)	7104(1)	10718(1)	68(1)
Al(3)	2831(1)	7634(1)	9038(1)	38(1)
Al(4)	1214(2)	7604(1)	10272(1)	59(1)
Cl(2)	664(1)	7925(1)	9232(1)	56(1)
N(4)	3806(3)	8468(2)	9313(2)	40(1)
N(5)	2933(3)	7395(2)	9979(2)	40(1)
N(6)	2881(4)	6653(2)	9063(2)	43(1)
C(47)	4769(5)	8947(3)	10204(3)	65(2)
C(48)	4151(4)	8400(3)	9913(2)	44(1)
C(49)	3845(4)	7772(3)	10300(2)	44(1)
C(50)	3858(5)	7657(4)	10986(3)	62(2)
C(51)	3703(5)	6952(4)	11228(3)	67(2)
C(52)	3660(5)	6479(3)	10786(3)	58(2)
C(53)	3161(5)	6667(3)	10156(2)	45(1)
C(54)	3077(4)	6289(3)	9672(2)	43(1)
C(55)	3169(6)	5515(3)	9768(3)	62(2)
C(56)	5221(5)	9148(3)	8558(3)	56(2)
C(57)	5429(6)	9757(3)	8155(3)	77(2)
C(58)	4568(7)	10286(3)	8084(4)	84(2)
C(59)	3450(6)	10228(3)	8423(3)	67(2)
C(60)	3176(5)	9642(3)	8837(3)	51(1)
C(61)	4076(5)	9098(2)	8899(2)	45(1)
C(62)	6229(5)	8586(3)	8610(3)	67(2)
C(63)	7448(7)	8827(5)	8885(4)	107(3)
C(64)	6551(6)	8332(4)	7987(4)	87(2)
C(65)	1950(5)	9622(3)	9210(3)	49(1)
C(66)	1910(6)	10164(3)	9674(3)	67(2)
C(67)	815(6)	9729(3)	8771(3)	68(2)
C(68)	3758(5)	6142(3)	8148(3)	57(2)
C(69)	3565(7)	5783(3)	7636(3)	75(2)
C(70)	2401(8)	5543(4)	7523(4)	87(2)
C(71)	1394(7)	5674(3)	7910(3)	75(2)
C(72)	1525(5)	6033(3)	8426(3)	56(2)
C(73)	2723(5)	6268(2)	8544(2)	46(1)
C(74)	5064(5)	6366(3)	8268(3)	65(2)
C(75)	5796(6)	6608(4)	7663(3)	83(2)
C(76)	5825(6)	5799(4)	8664(4)	95(2)
C(77)	385(5)	6159(3)	8828(3)	62(2)
C(78)	-209(7)	5502(4)	9127(4)	94(2)
C(79)	-592(6)	6626(4)	8451(4)	89(2)
C(80)	2904(6)	7958(3)	8107(2)	60(2)
C'81	2094(18)	8449(9)	7735(7)	77(5)
C(81)	1742(11)	7917(7)	7716(5)	71(3)
C(82)	203(7)	6792(5)	10567(5)	128(4)
C(83)	268(9)	6404(5)	11150(6)	153(4)
C(84)	1036(6)	8438(4)	10686(3)	78(2)
C(85)	654(8)	8328(5)	11393(3)	116(3)
C(86)	6918(7)	7518(3)	10493(3)	82(3)
C(87)	6740(8)	7034(3)	10084(2)	74(5)
C(88)	6515(7)	6359(3)	10332(3)	72(3)
C(89)	6469(6)	6168(2)	10989(3)	78(3)
C(90)	6647(6)	6651(3)	11398(2)	72(3)

C(91)	6871(5)	7326(3)	11150(3)	85(3)
C(92)	6980(9)	7810(4)	11606(4)	124(4)
C(86')	6907(8)	7122(3)	11321(3)	8(3)
C(87')	6984(9)	7734(3)	10911(4)	28(3)
C(88')	6938(11)	7732(4)	10255(4)	38(4)
C(89')	6815(14)	7119(5)	10009(3)	49(8)
C(90')	6738(12)	6507(4)	10418(3)	43(5)
C(91')	6784(6)	6509(3)	11074(3)	18(3)
C(92')	6530(10)	5778(4)	11524(4)	31(3)
C(40)	-1797(13)	7808(6)	5379(7)	130(6)
C(41)	-1608(13)	7212(7)	5102(5)	104(5)
C(42)	-1408(14)	6588(6)	5484(7)	158(8)
C(43)	-1397(12)	6560(6)	6145(6)	113(6)
C(44)	-1586(14)	7157(8)	6422(5)	139(8)
C(45)	-1786(14)	7781(6)	6039(7)	147(8)
C(46)	-1700(30)	8390(8)	6348(11)	2000(600)
C(40')	-913(8)	6517(3)	6499(3)	71(3)
C(41')	-800(9)	6033(3)	6079(4)	79(4)
C(42')	-988(9)	6228(4)	5430(4)	83(4)
C(43')	-1288(9)	6908(4)	5202(3)	75(4)
C(44')	-1401(8)	7392(3)	5621(3)	60(3)
C(45')	-1214(6)	7197(3)	6270(3)	81(4)
C(46')	-1409(11)	7715(4)	6702(4)	88(4)

Table 3. Bond lengths [A] and angles [deg] for sg2714.

Fe(1)-C(6)	1.959(8)
Fe(1)-C(5)	2.278(9)
Fe(1)-C(7)	2.338(9)
Fe(1')-C(4)	1.748(10)
Fe(1')-C(5)	1.905(9)
Fe(1')-C(6)	2.146(7)
Fe(1')-C(3)	2.254(6)
Al(1)-C(34)	1.974(5)
Al(1)-N(2)	1.993(4)
Al(1)-N(1)	1.996(4)
Al(1)-N(3)	2.035(5)
Al(1)-Cl(1)	2.430(2)
Al(2)-C(38)	1.87(2)
Al(2)-C(36')	1.84(3)
Al(2)-N(2)	1.970(5)
Al(2)-C(36)	2.005(16)
Al(2)-C(38')	2.15(2)
Al(2)-Cl(1)	2.268(3)
N(1)-C(2)	1.351(7)
N(1)-C(15)	1.460(7)
N(2)-C(7)	1.447(8)
N(2)-C(3)	1.449(7)
N(3)-C(8)	1.322(7)
N(3)-C(27)	1.461(7)
C(1)-C(2)	1.503(7)
C(2)-C(3)	1.386(8)
C(3)-C(4)	1.385(9)
C(4)-C(5)	1.406(10)
C(5)-C(6)	1.393(9)
C(6)-C(7)	1.422(8)
C(7)-C(8)	1.393(9)
C(8)-C(9)	1.518(8)
C(10)-C(11)	1.386(9)
C(10)-C(15)	1.399(8)
C(10)-C(16)	1.516(8)
C(11)-C(12)	1.362(10)
C(12)-C(13)	1.366(10)
C(13)-C(14)	1.417(9)
C(14)-C(15)	1.410(8)
C(14)-C(19)	1.489(8)
C(16)-C(17)	1.516(9)
C(16)-C(18)	1.513(9)
C(19)-C(21)	1.536(9)
C(19)-C(20)	1.550(9)
C(22)-C(23)	1.390(8)
C(22)-C(27)	1.405(8)
C(22)-C(28)	1.514(9)
C(23)-C(24)	1.353(10)
C(24)-C(25)	1.388(10)
C(25)-C(26)	1.396(8)
C(26)-C(27)	1.399(8)
C(26)-C(31)	1.511(8)
C(28)-C(29)	1.514(11)

C(28)-C(30)	1.524(9)
C(31)-C(33)	1.522(9)
C(31)-C(32)	1.541(8)
C(34)-C(35)	1.527(8)
C(36')-C(37')	1.48(2)
C(38)-C(39)	1.60(2)
C(36)-C(37)	1.481(15)
C(38')-C(39)	1.48(2)
Fe(2)-C(50)	1.988(6)
Fe(2)-C(51)	2.026(6)
Fe(2)-C(49)	2.138(5)
Fe(2)-C(52)	2.182(6)
Al(3)-N(6)	1.925(4)
Al(3)-N(5)	1.986(4)
Al(3)-C(80)	1.989(5)
Al(3)-N(4)	2.126(4)
Al(3)-Cl(2)	2.407(2)
Al(4)-C(84)	1.965(7)
Al(4)-N(5)	1.975(4)
Al(4)-C(82)	1.986(9)
Al(4)-Cl(2)	2.286(2)
N(4)-C(48)	1.317(6)
N(4)-C(61)	1.453(6)
N(5)-C(53)	1.446(6)
N(5)-C(49)	1.473(6)
N(6)-C(54)	1.402(6)
N(6)-C(73)	1.432(6)
C(47)-C(48)	1.489(7)
C(48)-C(49)	1.433(7)
C(49)-C(50)	1.439(7)
C(50)-C(51)	1.429(9)
C(51)-C(52)	1.409(8)
C(52)-C(53)	1.438(7)
C(53)-C(54)	1.351(7)
C(54)-C(55)	1.511(7)
C(56)-C(57)	1.397(8)
C(56)-C(61)	1.409(7)
C(56)-C(62)	1.511(8)
C(57)-C(58)	1.361(9)
C(58)-C(59)	1.382(9)
C(59)-C(60)	1.389(8)
C(60)-C(61)	1.409(7)
C(60)-C(65)	1.516(7)
C(62)-C(64)	1.501(9)
C(62)-C(63)	1.550(9)
C(65)-C(67)	1.529(8)
C(65)-C(66)	1.543(7)
C(68)-C(69)	1.392(8)
C(68)-C(73)	1.410(8)
C(68)-C(74)	1.513(8)
C(69)-C(70)	1.381(9)
C(70)-C(71)	1.379(9)
C(71)-C(72)	1.390(8)
C(72)-C(73)	1.413(7)
C(72)-C(77)	1.507(8)
C(74)-C(76)	1.523(9)
C(74)-C(75)	1.519(9)

C(77)-C(78)	1.518(9)
C(77)-C(79)	1.527(8)
C(80)-C'81	1.435(15)
C(80)-C(81)	1.511(12)
C(82)-C(83)	1.363(12)
C(84)-C(85)	1.532(9)
C(86)-C(87)	1.3900
C(86)-C(91)	1.3900
C(87)-C(88)	1.3900
C(88)-C(89)	1.3900
C(89)-C(90)	1.3900
C(90)-C(91)	1.3900
C(91)-C(92)	1.4536
C(86')-C(87')	1.3900
C(86')-C(91')	1.3900
C(87')-C(88')	1.3900
C(88')-C(89')	1.3900
C(89')-C(90')	1.3900
C(90')-C(91')	1.3900
C(91')-C(92')	1.6439
C(40)-C(41)	1.3900
C(40)-C(45)	1.3900
C(41)-C(42)	1.3900
C(42)-C(43)	1.3900
C(43)-C(44)	1.3900
C(44)-C(45)	1.3900
C(45)-C(46)	1.4484
C(40')-C(41')	1.3900
C(40')-C(45')	1.3900
C(41')-C(42')	1.3900
C(42')-C(43')	1.3900
C(43')-C(44')	1.3900
C(44')-C(45')	1.3900
C(45')-C(46')	1.4661

C(6)-Fe(1)-C(5)	37.4(3)
C(6)-Fe(1)-C(7)	37.4(2)
C(5)-Fe(1)-C(7)	64.0(3)
C(4)-Fe(1')-C(5)	45.0(3)
C(4)-Fe(1')-C(6)	73.6(3)
C(5)-Fe(1')-C(6)	39.7(3)
C(4)-Fe(1')-C(3)	37.9(3)
C(5)-Fe(1')-C(3)	71.3(3)
C(6)-Fe(1')-C(3)	77.4(2)
C(34)-Al(1)-N(2)	178.4(2)
C(34)-Al(1)-N(1)	99.1(2)
N(2)-Al(1)-N(1)	80.11(17)
C(34)-Al(1)-N(3)	100.4(2)
N(2)-Al(1)-N(3)	79.55(18)
N(1)-Al(1)-N(3)	140.54(19)
C(34)-Al(1)-Cl(1)	97.03(18)
N(2)-Al(1)-Cl(1)	84.49(15)
N(1)-Al(1)-Cl(1)	105.80(14)
N(3)-Al(1)-Cl(1)	105.45(14)
C(38)-Al(2)-C(36')	96.4(15)
C(38)-Al(2)-N(2)	126.3(6)
C(36')-Al(2)-N(2)	116.0(14)

C(38)-Al(2)-C(36)	114.4(8)
C(36')-Al(2)-C(36)	28.1(12)
N(2)-Al(2)-C(36)	113.7(5)
C(38)-Al(2)-C(38')	22.4(6)
C(36')-Al(2)-C(38')	107.2(14)
N(2)-Al(2)-C(38')	104.0(6)
C(36)-Al(2)-C(38')	131.2(7)
C(38)-Al(2)-Cl(1)	102.8(7)
C(36')-Al(2)-Cl(1)	128.6(13)
N(2)-Al(2)-Cl(1)	89.49(15)
C(36)-Al(2)-Cl(1)	101.8(5)
C(38')-Al(2)-Cl(1)	108.6(6)
Al(2)-Cl(1)-Al(1)	82.73(8)
C(2)-N(1)-C(15)	117.5(4)
C(2)-N(1)-Al(1)	115.7(3)
C(15)-N(1)-Al(1)	126.7(3)
C(7)-N(2)-C(3)	108.4(5)
C(7)-N(2)-Al(2)	111.0(4)
C(3)-N(2)-Al(2)	108.2(3)
C(7)-N(2)-Al(1)	112.8(3)
C(3)-N(2)-Al(1)	113.1(3)
Al(2)-N(2)-Al(1)	103.3(2)
C(8)-N(3)-C(27)	118.8(5)
C(8)-N(3)-Al(1)	115.6(4)
C(27)-N(3)-Al(1)	125.4(3)
N(1)-C(2)-C(3)	116.3(5)
N(1)-C(2)-C(1)	122.2(5)
C(3)-C(2)-C(1)	121.5(5)
C(4)-C(3)-C(2)	129.8(5)
C(4)-C(3)-N(2)	116.9(5)
C(2)-C(3)-N(2)	113.2(4)
C(4)-C(3)-Fe(1')	50.8(5)
C(2)-C(3)-Fe(1')	121.9(4)
N(2)-C(3)-Fe(1')	101.9(4)
C(3)-C(4)-C(5)	122.1(6)
C(3)-C(4)-Fe(1')	91.3(5)
C(5)-C(4)-Fe(1')	73.4(6)
C(4)-C(5)-C(6)	114.6(6)
C(4)-C(5)-Fe(1')	61.6(5)
C(6)-C(5)-Fe(1')	79.5(5)
C(4)-C(5)-Fe(1)	84.4(6)
C(6)-C(5)-Fe(1)	58.8(4)
Fe(1')-C(5)-Fe(1)	24.67(13)
C(5)-C(6)-C(7)	120.7(6)
C(5)-C(6)-Fe(1)	83.8(5)
C(7)-C(6)-Fe(1)	85.9(5)
C(5)-C(6)-Fe(1')	60.8(4)
C(7)-C(6)-Fe(1')	87.6(5)
Fe(1)-C(6)-Fe(1')	26.71(12)
C(8)-C(7)-C(6)	129.3(6)
C(8)-C(7)-N(2)	113.6(5)
C(6)-C(7)-N(2)	116.0(6)
C(8)-C(7)-Fe(1)	112.3(5)
C(6)-C(7)-Fe(1)	56.7(4)
N(2)-C(7)-Fe(1)	111.6(5)
N(3)-C(8)-C(7)	116.4(5)
N(3)-C(8)-C(9)	123.5(5)

C(7)-C(8)-C(9)	120.1(5)
C(11)-C(10)-C(15)	118.5(6)
C(11)-C(10)-C(16)	118.6(6)
C(15)-C(10)-C(16)	122.9(5)
C(12)-C(11)-C(10)	121.4(6)
C(11)-C(12)-C(13)	120.7(7)
C(12)-C(13)-C(14)	121.0(7)
C(15)-C(14)-C(13)	117.0(6)
C(15)-C(14)-C(19)	123.4(5)
C(13)-C(14)-C(19)	119.6(6)
C(10)-C(15)-C(14)	121.3(5)
C(10)-C(15)-N(1)	119.6(5)
C(14)-C(15)-N(1)	119.1(5)
C(17)-C(16)-C(10)	111.7(6)
C(17)-C(16)-C(18)	109.6(6)
C(10)-C(16)-C(18)	112.1(6)
C(14)-C(19)-C(21)	111.1(6)
C(14)-C(19)-C(20)	112.8(5)
C(21)-C(19)-C(20)	111.4(6)
C(23)-C(22)-C(27)	118.0(6)
C(23)-C(22)-C(28)	119.8(6)
C(27)-C(22)-C(28)	122.2(5)
C(24)-C(23)-C(22)	122.2(6)
C(23)-C(24)-C(25)	119.6(6)
C(24)-C(25)-C(26)	121.1(6)
C(27)-C(26)-C(25)	118.1(6)
C(27)-C(26)-C(31)	123.6(5)
C(25)-C(26)-C(31)	118.2(6)
C(26)-C(27)-C(22)	120.9(5)
C(26)-C(27)-N(3)	118.9(5)
C(22)-C(27)-N(3)	120.2(5)
C(22)-C(28)-C(29)	111.3(6)
C(22)-C(28)-C(30)	113.1(6)
C(29)-C(28)-C(30)	106.8(6)
C(33)-C(31)-C(26)	112.7(5)
C(33)-C(31)-C(32)	109.6(5)
C(26)-C(31)-C(32)	111.3(5)
C(35)-C(34)-Al(1)	121.4(4)
C(37')-C(36')-Al(2)	109(3)
C(39)-C(38)-Al(2)	119.8(13)
C(37)-C(36)-Al(2)	116.3(12)
C(39)-C(38')-Al(2)	110.1(12)
C(38')-C(39)-C(38)	30.9(8)
C(50)-Fe(2)-C(51)	41.7(2)
C(50)-Fe(2)-C(49)	40.6(2)
C(51)-Fe(2)-C(49)	69.5(2)
C(50)-Fe(2)-C(52)	71.2(3)
C(51)-Fe(2)-C(52)	38.9(2)
C(49)-Fe(2)-C(52)	75.0(2)
N(6)-Al(3)-N(5)	82.57(17)
N(6)-Al(3)-C(80)	102.4(2)
N(5)-Al(3)-C(80)	172.6(2)
N(6)-Al(3)-N(4)	143.70(17)
N(5)-Al(3)-N(4)	77.44(16)
C(80)-Al(3)-N(4)	95.5(2)
N(6)-Al(3)-Cl(2)	104.45(13)
N(5)-Al(3)-Cl(2)	85.33(12)

C(80)-Al(3)-Cl(2)	98.55(19)
N(4)-Al(3)-Cl(2)	103.77(12)
C(84)-Al(4)-N(5)	114.7(3)
C(84)-Al(4)-C(82)	120.8(4)
N(5)-Al(4)-C(82)	115.1(3)
C(84)-Al(4)-Cl(2)	105.9(2)
N(5)-Al(4)-Cl(2)	88.92(13)
C(82)-Al(4)-Cl(2)	105.1(3)
Al(4)-Cl(2)-Al(3)	82.68(7)
C(48)-N(4)-C(61)	119.0(4)
C(48)-N(4)-Al(3)	115.6(3)
C(61)-N(4)-Al(3)	125.3(3)
C(53)-N(5)-C(49)	109.3(4)
C(53)-N(5)-Al(4)	106.7(3)
C(49)-N(5)-Al(4)	110.2(3)
C(53)-N(5)-Al(3)	111.2(3)
C(49)-N(5)-Al(3)	115.9(3)
Al(4)-N(5)-Al(3)	103.06(18)
C(54)-N(6)-C(73)	117.9(4)
C(54)-N(6)-Al(3)	114.3(3)
C(73)-N(6)-Al(3)	127.8(3)
N(4)-C(48)-C(49)	116.5(4)
N(4)-C(48)-C(47)	123.4(5)
C(49)-C(48)-C(47)	120.0(5)
C(50)-C(49)-C(48)	125.3(5)
C(50)-C(49)-N(5)	117.2(5)
C(48)-C(49)-N(5)	111.0(4)
C(50)-C(49)-Fe(2)	64.1(3)
C(48)-C(49)-Fe(2)	119.6(3)
N(5)-C(49)-Fe(2)	111.3(3)
C(51)-C(50)-C(49)	111.9(5)
C(51)-C(50)-Fe(2)	70.6(3)
C(49)-C(50)-Fe(2)	75.3(3)
C(52)-C(51)-C(50)	118.0(5)
C(52)-C(51)-Fe(2)	76.5(3)
C(50)-C(51)-Fe(2)	67.7(3)
C(51)-C(52)-C(53)	121.9(5)
C(51)-C(52)-Fe(2)	64.6(4)
C(53)-C(52)-Fe(2)	100.3(4)
C(54)-C(53)-C(52)	129.7(5)
C(54)-C(53)-N(5)	114.7(4)
C(52)-C(53)-N(5)	114.5(5)
C(53)-C(54)-N(6)	116.4(4)
C(53)-C(54)-C(55)	122.9(5)
N(6)-C(54)-C(55)	120.7(5)
C(57)-C(56)-C(61)	117.5(5)
C(57)-C(56)-C(62)	118.7(5)
C(61)-C(56)-C(62)	123.7(5)
C(58)-C(57)-C(56)	122.2(6)
C(59)-C(58)-C(57)	119.4(6)
C(58)-C(59)-C(60)	121.9(6)
C(59)-C(60)-C(61)	117.7(5)
C(59)-C(60)-C(65)	119.0(5)
C(61)-C(60)-C(65)	123.2(5)
C(60)-C(61)-C(56)	121.2(5)
C(60)-C(61)-N(4)	119.3(4)
C(56)-C(61)-N(4)	119.5(5)

C(64)-C(62)-C(56)	113.8(6)
C(64)-C(62)-C(63)	108.1(5)
C(56)-C(62)-C(63)	111.0(5)
C(60)-C(65)-C(67)	112.0(5)
C(60)-C(65)-C(66)	110.7(4)
C(67)-C(65)-C(66)	110.0(5)
C(69)-C(68)-C(73)	118.3(5)
C(69)-C(68)-C(74)	119.1(5)
C(73)-C(68)-C(74)	122.6(5)
C(70)-C(69)-C(68)	121.3(6)
C(69)-C(70)-C(71)	120.0(6)
C(70)-C(71)-C(72)	121.4(6)
C(71)-C(72)-C(73)	118.2(6)
C(71)-C(72)-C(77)	118.6(5)
C(73)-C(72)-C(77)	123.2(5)
C(72)-C(73)-C(68)	120.9(5)
C(72)-C(73)-N(6)	119.4(5)
C(68)-C(73)-N(6)	119.7(5)
C(68)-C(74)-C(76)	111.4(5)
C(68)-C(74)-C(75)	113.8(5)
C(76)-C(74)-C(75)	108.9(5)
C(72)-C(77)-C(78)	112.9(5)
C(72)-C(77)-C(79)	111.7(5)
C(78)-C(77)-C(79)	110.0(5)
C'81-C(80)-C(81)	45.1(8)
C'81-C(80)-Al(3)	128.8(7)
C(81)-C(80)-Al(3)	118.6(6)
C(83)-C(82)-Al(4)	126.1(9)
C(85)-C(84)-Al(4)	115.7(5)
C(87)-C(86)-C(91)	120.0
C(88)-C(87)-C(86)	120.0
C(89)-C(88)-C(87)	120.0
C(88)-C(89)-C(90)	120.0
C(89)-C(90)-C(91)	120.0
C(90)-C(91)-C(86)	120.0
C(90)-C(91)-C(92)	116.9
C(86)-C(91)-C(92)	123.1
C(87')-C(86')-C(91')	120.0
C(88')-C(87')-C(86')	120.0
C(87')-C(88')-C(89')	120.0
C(90')-C(89')-C(88')	120.0
C(91')-C(90')-C(89')	120.0
C(90')-C(91')-C(86')	120.0
C(90')-C(91')-C(92')	116.6
C(86')-C(91')-C(92')	123.0
C(41)-C(40)-C(45)	120.0
C(40)-C(41)-C(42)	120.0
C(43)-C(42)-C(41)	120.0
C(42)-C(43)-C(44)	120.0
C(45)-C(44)-C(43)	120.0
C(44)-C(45)-C(40)	120.0
C(44)-C(45)-C(46)	116.4
C(40)-C(45)-C(46)	122.1
C(41')-C(40')-C(45')	120.0
C(40')-C(41')-C(42')	120.0
C(43')-C(42')-C(41')	120.0
C(42')-C(43')-C(44')	120.0

C(43')-C(44')-C(45')	120.0
C(44')-C(45')-C(40')	120.0
C(44')-C(45')-C(46')	118.4
C(40')-C(45')-C(46')	121.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for sg2714.
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
Fe(1)	100(2)	53(2)	62(2)	11(1)	33(1)	7(1)
Fe(1')	100(2)	65(1)	41(1)	-2(1)	18(1)	-23(1)
Al(1)	45(1)	51(1)	37(1)	-2(1)	-1(1)	-4(1)
Al(2)	105(2)	69(1)	74(1)	14(1)	-45(1)	-31(1)
Cl(1)	60(1)	65(1)	85(1)	-1(1)	-9(1)	-16(1)
N(1)	45(3)	45(2)	43(3)	-4(2)	-3(2)	-6(2)
N(2)	79(3)	41(3)	41(3)	0(2)	-6(2)	-6(2)
N(3)	65(3)	49(3)	38(3)	-3(2)	-7(2)	-5(2)
C(1)	76(4)	50(4)	69(4)	8(3)	-1(3)	-10(3)
C(2)	42(3)	47(3)	60(4)	2(3)	-2(3)	-9(2)
C(3)	71(4)	48(3)	42(3)	6(3)	-4(3)	-12(3)
C(4)	200(10)	66(5)	52(5)	15(4)	10(5)	-29(5)
C(5)	183(9)	79(5)	33(4)	10(4)	-2(4)	-11(5)
C(6)	117(6)	77(5)	41(4)	-5(3)	-1(3)	-9(4)
C(7)	146(7)	79(5)	35(4)	-5(3)	-2(4)	24(5)
C(8)	102(5)	56(4)	42(4)	-10(3)	0(3)	5(3)
C(9)	123(6)	76(5)	52(4)	-16(3)	10(4)	10(4)
C(10)	62(4)	51(4)	71(4)	-15(3)	-12(3)	-4(3)
C(11)	88(5)	77(5)	98(6)	-42(4)	-33(4)	12(4)
C(12)	122(7)	91(6)	106(6)	-56(5)	-34(6)	22(5)
C(13)	98(6)	80(5)	92(5)	-34(4)	-2(5)	21(4)
C(14)	58(4)	58(4)	67(4)	-9(3)	1(3)	2(3)
C(15)	52(4)	38(3)	53(3)	-4(3)	-1(3)	0(2)
C(16)	55(4)	67(4)	100(5)	-28(4)	-18(4)	-8(3)
C(17)	86(5)	119(7)	104(6)	4(5)	4(5)	-19(5)
C(18)	64(5)	102(6)	136(7)	22(5)	-17(5)	2(4)
C(19)	55(4)	67(4)	79(4)	-15(3)	1(3)	6(3)
C(20)	81(5)	83(5)	148(8)	-14(5)	-20(5)	29(4)
C(21)	75(5)	109(6)	114(6)	-10(5)	37(5)	-9(4)
C(22)	71(4)	50(4)	59(4)	-9(3)	-11(3)	1(3)
C(23)	86(5)	61(4)	73(4)	5(4)	-24(4)	9(4)
C(24)	120(7)	64(5)	86(5)	14(4)	-21(5)	11(5)
C(25)	105(6)	49(4)	75(5)	0(3)	-7(4)	-5(4)
C(26)	83(4)	41(3)	51(3)	-5(3)	-2(3)	3(3)
C(27)	73(4)	42(3)	41(3)	-4(3)	-9(3)	6(3)
C(28)	76(5)	68(4)	69(4)	-3(3)	-18(4)	11(3)
C(29)	145(9)	204(11)	127(8)	-79(8)	57(7)	-75(8)
C(30)	81(5)	123(6)	86(5)	-34(5)	-23(4)	-4(4)
C(31)	80(4)	53(4)	56(4)	-5(3)	-8(3)	-15(3)
C(32)	105(6)	81(5)	90(5)	-29(4)	-10(4)	-10(4)
C(33)	86(5)	76(5)	88(5)	-15(4)	3(4)	-18(4)
C(34)	66(4)	57(4)	45(3)	-2(3)	2(3)	-7(3)
C(35)	122(6)	85(5)	52(4)	-1(3)	15(4)	-27(4)
C(36')	120(20)	140(20)	70(20)	40(18)	-44(19)	8(18)
C(37')	150(40)	120(30)	90(30)	30(20)	-60(20)	0(20)
C(38)	99(15)	78(11)	66(11)	-18(8)	-17(12)	0(11)

C(36)	75(9)	106(12)	97(10)	20(9)	-36(8)	-24(8)
C(37)	181(13)	103(9)	101(9)	2(7)	-51(9)	-4(8)
C(38')	81(14)	74(14)	66(11)	0(10)	-8(12)	-33(11)
C(39)	188(10)	116(7)	77(6)	-4(5)	-35(6)	-51(6)
Fe(2)	49(1)	115(1)	40(1)	-15(1)	-12(1)	27(1)
Al(3)	36(1)	42(1)	35(1)	0(1)	-5(1)	-1(1)
Al(4)	41(1)	73(1)	55(1)	12(1)	10(1)	14(1)
Cl(2)	41(1)	56(1)	69(1)	-6(1)	-16(1)	7(1)
N(4)	35(2)	47(3)	39(3)	-8(2)	0(2)	0(2)
N(5)	34(2)	50(3)	34(2)	-1(2)	0(2)	2(2)
N(6)	41(2)	46(2)	41(3)	-1(2)	-5(2)	-4(2)
C(47)	58(4)	82(4)	62(4)	-31(3)	-6(3)	-3(3)
C(48)	31(3)	60(4)	45(3)	-19(3)	-2(2)	4(2)
C(49)	38(3)	60(3)	36(3)	-12(3)	-4(2)	9(2)
C(50)	54(4)	95(5)	37(3)	-17(3)	-8(3)	14(3)
C(51)	60(4)	104(5)	32(3)	4(4)	-4(3)	30(4)
C(52)	58(4)	76(4)	37(3)	1(3)	-3(3)	23(3)
C(53)	42(3)	51(3)	38(3)	6(3)	3(2)	7(2)
C(54)	40(3)	44(3)	42(3)	7(3)	2(2)	5(2)
C(55)	69(4)	43(3)	68(4)	9(3)	-3(3)	4(3)
C(56)	53(4)	56(4)	60(4)	-13(3)	15(3)	-11(3)
C(57)	72(5)	71(5)	89(5)	-10(4)	40(4)	-18(4)
C(58)	97(5)	51(4)	99(5)	9(4)	41(4)	-8(4)
C(59)	70(4)	50(4)	78(4)	-3(3)	13(4)	-6(3)
C(60)	58(4)	44(3)	53(3)	-10(3)	7(3)	-7(3)
C(61)	47(3)	40(3)	49(3)	-13(2)	7(3)	-10(3)
C(62)	47(4)	80(4)	73(4)	-11(3)	17(3)	-3(3)
C(63)	62(5)	146(7)	124(7)	-58(6)	0(4)	5(5)
C(64)	70(5)	92(5)	104(6)	-35(4)	15(4)	6(4)
C(65)	48(3)	43(3)	57(3)	-11(3)	5(3)	-2(2)
C(66)	64(4)	63(4)	80(4)	-29(3)	10(3)	0(3)
C(67)	66(4)	60(4)	78(4)	-5(3)	-6(3)	-1(3)
C(68)	63(4)	48(3)	60(4)	-7(3)	-1(3)	-5(3)
C(69)	82(5)	81(5)	69(4)	-30(4)	11(4)	-16(4)
C(70)	104(6)	87(5)	81(5)	-43(4)	-6(5)	-17(4)
C(71)	72(5)	75(4)	82(5)	-24(4)	-12(4)	-18(3)
C(72)	58(4)	43(3)	69(4)	-7(3)	-13(3)	-9(3)
C(73)	54(4)	36(3)	47(3)	-3(2)	-8(3)	-3(2)
C(74)	58(4)	68(4)	74(4)	-26(3)	8(3)	-3(3)
C(75)	72(5)	88(5)	86(5)	2(4)	11(4)	-6(4)
C(76)	67(5)	124(6)	86(5)	21(5)	-2(4)	-9(4)
C(77)	48(4)	63(4)	77(4)	-14(3)	0(3)	-15(3)
C(78)	88(5)	83(5)	113(6)	-7(4)	10(4)	-28(4)
C(79)	61(4)	89(5)	120(6)	-25(4)	-26(4)	1(4)
C(80)	75(4)	63(4)	39(3)	7(3)	-12(3)	-14(3)
C'81	123(15)	74(11)	32(8)	-7(8)	-13(8)	18(11)
C(81)	87(8)	72(8)	55(7)	-8(6)	-15(6)	-1(7)
C(82)	56(5)	158(8)	143(8)	64(7)	38(5)	21(5)
C(83)	123(8)	119(8)	193(11)	64(8)	37(7)	1(6)
C(84)	74(4)	102(5)	55(4)	-7(4)	7(3)	32(4)
C(85)	128(7)	155(8)	58(5)	-10(5)	17(4)	48(6)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for sg2714.

	x	y	z	U(eq)
H(1A)	1956	5363	4414	99
H(1B)	1156	5449	5037	99
H(1C)	2635	5370	5074	99
H(4A)	1803	6090	5974	129
H(5A)	1867	6945	6669	120
H(6A)	1140	8044	6187	94
H(9A)	295	9436	4841	125
H(9B)	1056	9224	5478	125
H(9C)	-255	8898	5391	125
H(11A)	400	5640	2542	102
H(12A)	2264	5179	2225	123
H(13A)	4098	5360	2719	106
H(16A)	-47	6735	3735	87
H(17A)	-562	5612	4138	156
H(17B)	-1178	5523	3480	156
H(17C)	-1781	6052	3908	156
H(18A)	-361	7136	2649	156
H(18B)	-1653	6991	3012	156
H(18C)	-1082	6463	2574	156
H(19A)	4369	6360	4006	80
H(20A)	4704	5161	4259	157
H(20B)	6001	5530	4167	157
H(20C)	5489	5143	3619	157
H(21A)	4965	6942	3011	150
H(21B)	5635	6265	2827	150
H(21C)	6164	6625	3388	150
H(23A)	-965	9886	2852	90
H(24A)	419	10750	2754	111
H(25A)	2273	10620	3324	92
H(28A)	-593	8241	3764	86
H(29A)	-1734	8934	4409	229
H(29B)	-2652	8501	4053	229
H(29C)	-2479	9287	3804	229
H(30A)	-908	8443	2649	142
H(30B)	-1991	8990	2749	142
H(30C)	-2161	8206	3011	142
H(31A)	3233	9170	4421	75
H(32A)	2403	10113	4898	135
H(32B)	3123	10623	4386	135
H(32C)	3887	10107	4889	135
H(33A)	4374	9357	3460	124
H(33B)	5080	9661	4007	124
H(33C)	4314	10157	3488	124
H(34A)	2395	7454	2878	67
H(34B)	1338	8015	2952	67
H(35A)	2845	8465	2236	130
H(35B)	3903	8297	2755	130
H(35C)	2847	8864	2838	130

H(36A)	5469	7017	5948	139
H(36B)	4216	6604	5961	139
H(37A)	5769	5936	5585	183
H(37B)	6200	6550	5075	183
H(37C)	4902	6207	4998	183
H(38A)	5671	8259	5425	96
H(38B)	4400	8683	5304	96
H(36C)	4605	6290	5161	114
H(36D)	5867	6685	5046	114
H(37D)	5910	5985	6007	194
H(37E)	4704	6375	6243	194
H(37F)	5981	6760	6124	194
H(38C)	4608	8788	5374	88
H(38D)	3236	8624	5637	88
H(39A)	5014	8651	6394	190
H(39B)	4957	7842	6498	190
H(39C)	3710	8296	6375	190
H(39D)	4625	8673	6473	190
H(39E)	5434	8059	6248	190
H(39F)	4055	7937	6517	190
H(47A)	4918	9333	9878	97
H(47B)	5561	8770	10387	97
H(47C)	4230	9096	10536	97
H(50A)	3957	8003	11244	74
H(51A)	3632	6808	11668	81
H(52A)	3966	6027	10905	70
H(55A)	3302	5352	10216	93
H(55B)	3867	5362	9518	93
H(55C)	2398	5336	9632	93
H(57A)	6189	9802	7926	93
H(58A)	4732	10688	7807	101
H(59A)	2859	10595	8371	80
H(62A)	5924	8195	8909	80
H(63A)	8079	8458	8915	161
H(63B)	7277	8954	9306	161
H(63C)	7753	9220	8606	161
H(64A)	5810	8153	7819	131
H(64B)	7197	7972	8055	131
H(64C)	6854	8707	7686	131
H(65A)	1898	9165	9466	59
H(66A)	2629	10091	9952	101
H(66B)	1146	10122	9928	101
H(66C)	1931	10618	9432	101
H(67A)	841	9383	8485	103
H(67B)	834	10180	8524	103
H(67C)	52	9691	9026	103
H(69A)	4240	5703	7363	90
H(70A)	2296	5291	7182	105
H(71A)	602	5516	7824	89
H(74A)	4977	6756	8517	78
H(75A)	6616	6750	7774	125
H(75B)	5348	6993	7422	125
H(75C)	5893	6237	7406	125
H(76A)	5377	5651	9059	143
H(76B)	6631	5970	8762	143
H(76C)	5952	5415	8426	143
H(77A)	661	6399	9181	74

H(78A)	419	5208	9364	142
H(78B)	-542	5268	8795	142
H(78C)	-882	5610	9414	142
H(79A)	-209	7048	8269	133
H(79B)	-1276	6730	8734	133
H(79C)	-912	6397	8112	133
H(39A)	3750	8130	8027	90
H(39B)	2877	7542	7901	90
H(39C)	3146	8438	8052	90
H(39D)	3579	7696	7922	90
H(81D)	2365	8497	7291	115
H(81E)	2131	8888	7891	115
H(81F)	1241	8294	7770	115
H(81A)	1919	8086	7273	107
H(81B)	1069	8195	7874	107
H(81C)	1494	7445	7751	107
H(82A)	-675	6950	10517	153
H(82B)	358	6474	10254	153
H(83A)	-311	6034	11169	229
H(83B)	49	6687	11479	229
H(83C)	1114	6215	11218	229
H(84A)	1837	8669	10646	93
H(84B)	410	8746	10454	93
H(85A)	603	8766	11554	173
H(85B)	1273	8031	11632	173
H(85C)	-157	8119	11440	173
H(86A)	7070	7974	10326	98
H(87A)	6771	7164	9640	88
H(88A)	6395	6032	10055	86
H(89A)	6317	5711	11156	93
H(90A)	6615	6522	11842	86
H(92A)	6923	7569	12036	187
H(92B)	6308	8156	11540	187
H(92C)	7781	8028	11546	187
H(86')	6938	7124	11765	9
H(87')	7067	8148	11078	34
H(88')	6989	8145	9978	46
H(89')	6784	7117	9565	58
H(90')	6655	6093	10252	51
H(92D)	5884	5540	11334	47
H(92E)	6260	5866	11946	47
H(92F)	7297	5498	11556	47
H(40A)	-1933	8230	5120	155
H(41A)	-1616	7230	4655	124
H(42A)	-1280	6184	5297	190
H(43A)	-1262	6138	6403	135
H(44A)	-1579	7138	6868	167
H(46A)	-1703	8263	6807	3000
H(46B)	-2402	8700	6226	3000
H(46C)	-921	8614	6217	3000
H(40B)	-787	6385	6938	86
H(41B)	-597	5573	6234	95
H(42B)	-911	5900	5147	99
H(43B)	-1415	7040	4763	90
H(44B)	-1604	7852	5467	73
H(46D)	-1609	8156	6456	132
H(46E)	-651	7746	6942	132

H(46F)	-2096	7586	6995	132

Table 6. Torsion angles [deg] for sg2714.

C(38)-Al(2)-Cl(1)-Al(1)	-128.1(6)
C(36')-Al(2)-Cl(1)-Al(1)	122.7(18)
N(2)-Al(2)-Cl(1)-Al(1)	-0.89(14)
C(36)-Al(2)-Cl(1)-Al(1)	113.2(5)
C(38')-Al(2)-Cl(1)-Al(1)	-105.5(6)
C(34)-Al(1)-Cl(1)-Al(2)	-178.72(19)
N(2)-Al(1)-Cl(1)-Al(2)	0.89(14)
N(1)-Al(1)-Cl(1)-Al(2)	-77.18(15)
N(3)-Al(1)-Cl(1)-Al(2)	78.43(15)
C(34)-Al(1)-N(1)-C(2)	-172.7(4)
N(2)-Al(1)-N(1)-C(2)	6.0(4)
N(3)-Al(1)-N(1)-C(2)	-53.9(5)
Cl(1)-Al(1)-N(1)-C(2)	87.3(3)
C(34)-Al(1)-N(1)-C(15)	9.0(4)
N(2)-Al(1)-N(1)-C(15)	-172.4(4)
N(3)-Al(1)-N(1)-C(15)	127.7(4)
Cl(1)-Al(1)-N(1)-C(15)	-91.1(4)
C(38)-Al(2)-N(2)-C(7)	-14.3(9)
C(36')-Al(2)-N(2)-C(7)	106.5(14)
C(36)-Al(2)-N(2)-C(7)	137.3(6)
C(38')-Al(2)-N(2)-C(7)	-10.9(7)
Cl(1)-Al(2)-N(2)-C(7)	-120.0(4)
C(38)-Al(2)-N(2)-C(3)	-133.2(9)
C(36')-Al(2)-N(2)-C(3)	-12.4(15)
C(36)-Al(2)-N(2)-C(3)	18.5(6)
C(38')-Al(2)-N(2)-C(3)	-129.8(7)
Cl(1)-Al(2)-N(2)-C(3)	121.2(3)
C(38)-Al(2)-N(2)-Al(1)	106.7(8)
C(36')-Al(2)-N(2)-Al(1)	-132.5(14)
C(36)-Al(2)-N(2)-Al(1)	-101.6(5)
C(38')-Al(2)-N(2)-Al(1)	110.1(6)
Cl(1)-Al(2)-N(2)-Al(1)	1.11(18)
C(34)-Al(1)-N(2)-C(7)	-76(9)
N(1)-Al(1)-N(2)-C(7)	-134.1(5)
N(3)-Al(1)-N(2)-C(7)	11.9(5)
Cl(1)-Al(1)-N(2)-C(7)	118.8(5)
C(34)-Al(1)-N(2)-C(3)	48(9)
N(1)-Al(1)-N(2)-C(3)	-10.6(4)
N(3)-Al(1)-N(2)-C(3)	135.4(4)
Cl(1)-Al(1)-N(2)-C(3)	-117.7(4)
C(34)-Al(1)-N(2)-Al(2)	164(9)
N(1)-Al(1)-N(2)-Al(2)	106.1(2)
N(3)-Al(1)-N(2)-Al(2)	-107.9(2)
Cl(1)-Al(1)-N(2)-Al(2)	-1.04(17)
C(34)-Al(1)-N(3)-C(8)	172.2(4)
N(2)-Al(1)-N(3)-C(8)	-6.2(4)
N(1)-Al(1)-N(3)-C(8)	53.9(5)
Cl(1)-Al(1)-N(3)-C(8)	-87.4(4)
C(34)-Al(1)-N(3)-C(27)	-14.1(5)
N(2)-Al(1)-N(3)-C(27)	167.5(4)
N(1)-Al(1)-N(3)-C(27)	-132.4(4)
Cl(1)-Al(1)-N(3)-C(27)	86.3(4)
C(15)-N(1)-C(2)-C(3)	178.8(5)

Al(1)-N(1)-C(2)-C(3)	0.2(6)
C(15)-N(1)-C(2)-C(1)	-0.2(7)
Al(1)-N(1)-C(2)-C(1)	-178.7(4)
N(1)-C(2)-C(3)-C(4)	176.1(7)
C(1)-C(2)-C(3)-C(4)	-5.0(10)
N(1)-C(2)-C(3)-N(2)	-9.2(7)
C(1)-C(2)-C(3)-N(2)	169.7(5)
N(1)-C(2)-C(3)-Fe(1')	112.8(5)
C(1)-C(2)-C(3)-Fe(1')	-68.2(6)
C(7)-N(2)-C(3)-C(4)	-44.9(8)
Al(2)-N(2)-C(3)-C(4)	75.6(7)
Al(1)-N(2)-C(3)-C(4)	-170.7(6)
C(7)-N(2)-C(3)-C(2)	139.7(5)
Al(2)-N(2)-C(3)-C(2)	-99.9(5)
Al(1)-N(2)-C(3)-C(2)	13.9(6)
C(7)-N(2)-C(3)-Fe(1')	7.1(5)
Al(2)-N(2)-C(3)-Fe(1')	127.5(3)
Al(1)-N(2)-C(3)-Fe(1')	-118.8(3)
C(5)-Fe(1')-C(3)-C(4)	38.7(5)
C(6)-Fe(1')-C(3)-C(4)	79.4(5)
C(4)-Fe(1')-C(3)-C(2)	117.7(7)
C(5)-Fe(1')-C(3)-C(2)	156.4(5)
C(6)-Fe(1')-C(3)-C(2)	-162.9(5)
C(4)-Fe(1')-C(3)-N(2)	-115.1(6)
C(5)-Fe(1')-C(3)-N(2)	-76.4(4)
C(6)-Fe(1')-C(3)-N(2)	-35.6(3)
C(2)-C(3)-C(4)-C(5)	-173.2(8)
N(2)-C(3)-C(4)-C(5)	12.3(12)
Fe(1')-C(3)-C(4)-C(5)	-71.2(9)
C(2)-C(3)-C(4)-Fe(1')	-102.0(7)
N(2)-C(3)-C(4)-Fe(1')	83.5(6)
C(5)-Fe(1')-C(4)-C(3)	-123.2(6)
C(6)-Fe(1')-C(4)-C(3)	-90.4(4)
C(6)-Fe(1')-C(4)-C(5)	32.8(4)
C(3)-Fe(1')-C(4)-C(5)	123.2(6)
C(3)-C(4)-C(5)-C(6)	19.2(13)
Fe(1')-C(4)-C(5)-C(6)	-61.6(7)
C(3)-C(4)-C(5)-Fe(1')	80.8(8)
C(3)-C(4)-C(5)-Fe(1)	71.0(9)
Fe(1')-C(4)-C(5)-Fe(1)	-9.80(16)
C(6)-Fe(1')-C(5)-C(4)	-125.5(6)
C(3)-Fe(1')-C(5)-C(4)	-32.9(4)
C(4)-Fe(1')-C(5)-C(6)	125.5(6)
C(3)-Fe(1')-C(5)-C(6)	92.7(4)
C(4)-Fe(1')-C(5)-Fe(1)	156.1(4)
C(6)-Fe(1')-C(5)-Fe(1)	30.5(5)
C(3)-Fe(1')-C(5)-Fe(1)	123.2(2)
C(6)-Fe(1)-C(5)-C(4)	-123.3(6)
C(7)-Fe(1)-C(5)-C(4)	-88.1(4)
C(7)-Fe(1)-C(5)-C(6)	35.2(4)
C(6)-Fe(1)-C(5)-Fe(1')	-144.3(5)
C(7)-Fe(1)-C(5)-Fe(1')	-109.1(3)
C(4)-C(5)-C(6)-C(7)	-15.3(12)
Fe(1')-C(5)-C(6)-C(7)	-67.2(7)
Fe(1)-C(5)-C(6)-C(7)	-81.6(7)

C(4)-C(5)-C(6)-Fe(1)	66.2(8)
Fe(1')-C(5)-C(6)-Fe(1)	14.4(2)
C(4)-C(5)-C(6)-Fe(1')	51.9(7)
Fe(1)-C(5)-C(6)-Fe(1')	-14.4(2)
C(7)-Fe(1)-C(6)-C(5)	-121.5(6)
C(5)-Fe(1)-C(6)-C(7)	121.5(6)
C(5)-Fe(1)-C(6)-Fe(1')	28.8(4)
C(7)-Fe(1)-C(6)-Fe(1')	-92.7(4)
C(4)-Fe(1')-C(6)-C(5)	-36.9(5)
C(3)-Fe(1')-C(6)-C(5)	-75.9(4)
C(4)-Fe(1')-C(6)-C(7)	90.6(5)
C(5)-Fe(1')-C(6)-C(7)	127.5(7)
C(3)-Fe(1')-C(6)-C(7)	51.6(4)
C(4)-Fe(1')-C(6)-Fe(1)	176.4(3)
C(5)-Fe(1')-C(6)-Fe(1)	-146.7(5)
C(3)-Fe(1')-C(6)-Fe(1)	137.4(3)
C(5)-C(6)-C(7)-C(8)	173.1(8)
Fe(1)-C(6)-C(7)-C(8)	92.7(9)
Fe(1')-C(6)-C(7)-C(8)	119.5(9)
C(5)-C(6)-C(7)-N(2)	-19.4(11)
Fe(1)-C(6)-C(7)-N(2)	-99.8(6)
Fe(1')-C(6)-C(7)-N(2)	-73.1(6)
C(5)-C(6)-C(7)-Fe(1)	80.4(7)
Fe(1')-C(6)-C(7)-Fe(1)	26.70(11)
C(3)-N(2)-C(7)-C(8)	-142.4(6)
Al(2)-N(2)-C(7)-C(8)	98.9(6)
Al(1)-N(2)-C(7)-C(8)	-16.4(8)
C(3)-N(2)-C(7)-C(6)	48.2(8)
Al(2)-N(2)-C(7)-C(6)	-70.5(7)
Al(1)-N(2)-C(7)-C(6)	174.2(5)
C(3)-N(2)-C(7)-Fe(1)	-14.2(5)
Al(2)-N(2)-C(7)-Fe(1)	-132.9(3)
Al(1)-N(2)-C(7)-Fe(1)	111.8(3)
C(6)-Fe(1)-C(7)-C(8)	-123.4(7)
C(5)-Fe(1)-C(7)-C(8)	-158.6(6)
C(5)-Fe(1)-C(7)-C(6)	-35.2(4)
C(6)-Fe(1)-C(7)-N(2)	107.7(6)
C(5)-Fe(1)-C(7)-N(2)	72.5(4)
C(27)-N(3)-C(8)-C(7)	-175.5(6)
Al(1)-N(3)-C(8)-C(7)	-1.4(8)
C(27)-N(3)-C(8)-C(9)	5.6(9)
Al(1)-N(3)-C(8)-C(9)	179.7(5)
C(6)-C(7)-C(8)-N(3)	179.3(7)
N(2)-C(7)-C(8)-N(3)	11.6(10)
Fe(1)-C(7)-C(8)-N(3)	-116.2(5)
C(6)-C(7)-C(8)-C(9)	-1.7(13)
N(2)-C(7)-C(8)-C(9)	-169.4(6)
Fe(1)-C(7)-C(8)-C(9)	62.7(8)
C(15)-C(10)-C(11)-C(12)	-0.5(11)
C(16)-C(10)-C(11)-C(12)	-179.5(7)
C(10)-C(11)-C(12)-C(13)	0.0(13)
C(11)-C(12)-C(13)-C(14)	-0.3(13)
C(12)-C(13)-C(14)-C(15)	1.1(10)
C(12)-C(13)-C(14)-C(19)	-178.1(7)
C(11)-C(10)-C(15)-C(14)	1.4(9)
C(16)-C(10)-C(15)-C(14)	-179.7(5)

C(11)-C(10)-C(15)-N(1)	179.8(5)
C(16)-C(10)-C(15)-N(1)	-1.2(8)
C(13)-C(14)-C(15)-C(10)	-1.6(8)
C(19)-C(14)-C(15)-C(10)	177.5(5)
C(13)-C(14)-C(15)-N(1)	179.9(5)
C(19)-C(14)-C(15)-N(1)	-1.0(8)
C(2)-N(1)-C(15)-C(10)	93.1(6)
Al(1)-N(1)-C(15)-C(10)	-88.5(6)
C(2)-N(1)-C(15)-C(14)	-88.4(6)
Al(1)-N(1)-C(15)-C(14)	90.0(5)
C(11)-C(10)-C(16)-C(17)	71.4(8)
C(15)-C(10)-C(16)-C(17)	-107.5(7)
C(11)-C(10)-C(16)-C(18)	-52.1(8)
C(15)-C(10)-C(16)-C(18)	129.0(6)
C(15)-C(14)-C(19)-C(21)	-113.3(7)
C(13)-C(14)-C(19)-C(21)	65.8(8)
C(15)-C(14)-C(19)-C(20)	120.7(7)
C(13)-C(14)-C(19)-C(20)	-60.1(8)
C(27)-C(22)-C(23)-C(24)	-0.8(10)
C(28)-C(22)-C(23)-C(24)	177.1(7)
C(22)-C(23)-C(24)-C(25)	0.8(12)
C(23)-C(24)-C(25)-C(26)	-0.5(11)
C(24)-C(25)-C(26)-C(27)	0.1(10)
C(24)-C(25)-C(26)-C(31)	-177.3(6)
C(25)-C(26)-C(27)-C(22)	-0.1(8)
C(31)-C(26)-C(27)-C(22)	177.1(5)
C(25)-C(26)-C(27)-N(3)	178.8(5)
C(31)-C(26)-C(27)-N(3)	-4.0(8)
C(23)-C(22)-C(27)-C(26)	0.4(9)
C(28)-C(22)-C(27)-C(26)	-177.3(5)
C(23)-C(22)-C(27)-N(3)	-178.4(5)
C(28)-C(22)-C(27)-N(3)	3.8(8)
C(8)-N(3)-C(27)-C(26)	82.7(7)
Al(1)-N(3)-C(27)-C(26)	-90.8(5)
C(8)-N(3)-C(27)-C(22)	-98.4(7)
Al(1)-N(3)-C(27)-C(22)	88.1(6)
C(23)-C(22)-C(28)-C(29)	-77.3(9)
C(27)-C(22)-C(28)-C(29)	100.4(8)
C(23)-C(22)-C(28)-C(30)	43.0(8)
C(27)-C(22)-C(28)-C(30)	-139.3(6)
C(27)-C(26)-C(31)-C(33)	122.6(6)
C(25)-C(26)-C(31)-C(33)	-60.1(7)
C(27)-C(26)-C(31)-C(32)	-113.9(6)
C(25)-C(26)-C(31)-C(32)	63.4(7)
N(2)-Al(1)-C(34)-C(35)	161(8)
N(1)-Al(1)-C(34)-C(35)	-141.0(5)
N(3)-Al(1)-C(34)-C(35)	73.5(5)
Cl(1)-Al(1)-C(34)-C(35)	-33.7(5)
C(38)-Al(2)-C(36')-C(37')	-131(4)
N(2)-Al(2)-C(36')-C(37')	93(4)
C(36)-Al(2)-C(36')-C(37')	2(4)
C(38')-Al(2)-C(36')-C(37')	-151(4)
Cl(1)-Al(2)-C(36')-C(37')	-19(5)
C(36')-Al(2)-C(38)-C(39)	-52.4(18)

N(2)-Al(2)-C(38)-C(39)	76.6(14)
C(36)-Al(2)-C(38)-C(39)	-74.9(14)
C(38')-Al(2)-C(38)-C(39)	68(3)
Cl(1)-Al(2)-C(38)-C(39)	175.6(11)
C(38)-Al(2)-C(36)-C(37)	47.2(15)
C(36')-Al(2)-C(36)-C(37)	-7(3)
N(2)-Al(2)-C(36)-C(37)	-108.0(11)
C(38')-Al(2)-C(36)-C(37)	29.3(16)
Cl(1)-Al(2)-C(36)-C(37)	157.3(11)
C(38)-Al(2)-C(38')-C(39)	-67(3)
C(36')-Al(2)-C(38')-C(39)	-3.6(19)
N(2)-Al(2)-C(38')-C(39)	119.8(11)
C(36)-Al(2)-C(38')-C(39)	-20.4(17)
Cl(1)-Al(2)-C(38')-C(39)	-145.9(10)
Al(2)-C(38')-C(39)-C(38)	53(2)
Al(2)-C(38)-C(39)-C(38')	-86(3)
C(84)-Al(4)-Cl(2)-Al(3)	114.8(2)
N(5)-Al(4)-Cl(2)-Al(3)	-0.57(13)
C(82)-Al(4)-Cl(2)-Al(3)	-116.3(3)
N(6)-Al(3)-Cl(2)-Al(4)	81.65(14)
N(5)-Al(3)-Cl(2)-Al(4)	0.56(13)
C(80)-Al(3)-Cl(2)-Al(4)	-173.08(18)
N(4)-Al(3)-Cl(2)-Al(4)	-75.28(13)
N(6)-Al(3)-N(4)-C(48)	-49.8(5)
N(5)-Al(3)-N(4)-C(48)	8.4(3)
C(80)-Al(3)-N(4)-C(48)	-169.4(4)
Cl(2)-Al(3)-N(4)-C(48)	90.4(3)
N(6)-Al(3)-N(4)-C(61)	132.1(4)
N(5)-Al(3)-N(4)-C(61)	-169.7(4)
C(80)-Al(3)-N(4)-C(61)	12.5(4)
Cl(2)-Al(3)-N(4)-C(61)	-87.8(4)
C(84)-Al(4)-N(5)-C(53)	136.5(3)
C(82)-Al(4)-N(5)-C(53)	-10.3(5)
Cl(2)-Al(4)-N(5)-C(53)	-116.5(3)
C(84)-Al(4)-N(5)-C(49)	18.0(4)
C(82)-Al(4)-N(5)-C(49)	-128.8(4)
Cl(2)-Al(4)-N(5)-C(49)	125.0(3)
C(84)-Al(4)-N(5)-Al(3)	-106.3(3)
C(82)-Al(4)-N(5)-Al(3)	106.9(4)
Cl(2)-Al(4)-N(5)-Al(3)	0.70(16)
N(6)-Al(3)-N(5)-C(53)	8.0(3)
C(80)-Al(3)-N(5)-C(53)	-124.8(17)
N(4)-Al(3)-N(5)-C(53)	-141.5(3)
Cl(2)-Al(3)-N(5)-C(53)	113.3(3)
N(6)-Al(3)-N(5)-C(49)	133.7(3)
C(80)-Al(3)-N(5)-C(49)	0.9(19)
N(4)-Al(3)-N(5)-C(49)	-15.8(3)
Cl(2)-Al(3)-N(5)-C(49)	-121.1(3)
N(6)-Al(3)-N(5)-Al(4)	-105.9(2)
C(80)-Al(3)-N(5)-Al(4)	121.3(17)
N(4)-Al(3)-N(5)-Al(4)	104.6(2)
Cl(2)-Al(3)-N(5)-Al(4)	-0.67(15)
N(5)-Al(3)-N(6)-C(54)	-5.8(3)
C(80)-Al(3)-N(6)-C(54)	168.7(3)
N(4)-Al(3)-N(6)-C(54)	51.0(5)
Cl(2)-Al(3)-N(6)-C(54)	-89.0(3)
N(5)-Al(3)-N(6)-C(73)	173.2(4)

C(80)-Al(3)-N(6)-C(73)	-12.4(5)
N(4)-Al(3)-N(6)-C(73)	-130.1(4)
Cl(2)-Al(3)-N(6)-C(73)	90.0(4)
C(61)-N(4)-C(48)-C(49)	179.2(4)
Al(3)-N(4)-C(48)-C(49)	1.0(5)
C(61)-N(4)-C(48)-C(47)	2.3(7)
Al(3)-N(4)-C(48)-C(47)	-176.0(4)
N(4)-C(48)-C(49)-C(50)	-164.3(5)
C(47)-C(48)-C(49)-C(50)	12.7(7)
N(4)-C(48)-C(49)-N(5)	-13.6(6)
C(47)-C(48)-C(49)-N(5)	163.4(4)
N(4)-C(48)-C(49)-Fe(2)	118.1(4)
C(47)-C(48)-C(49)-Fe(2)	-64.9(6)
C(53)-N(5)-C(49)-C(50)	-59.0(5)
Al(4)-N(5)-C(49)-C(50)	57.9(5)
Al(3)-N(5)-C(49)-C(50)	174.4(4)
C(53)-N(5)-C(49)-C(48)	147.7(4)
Al(4)-N(5)-C(49)-C(48)	-95.4(4)
Al(3)-N(5)-C(49)-C(48)	21.1(5)
C(53)-N(5)-C(49)-Fe(2)	11.9(4)
Al(4)-N(5)-C(49)-Fe(2)	128.8(2)
Al(3)-N(5)-C(49)-Fe(2)	-114.7(3)
C(51)-Fe(2)-C(49)-C(50)	37.9(4)
C(52)-Fe(2)-C(49)-C(50)	78.5(4)
C(50)-Fe(2)-C(49)-C(48)	117.6(6)
C(51)-Fe(2)-C(49)-C(48)	155.5(5)
C(52)-Fe(2)-C(49)-C(48)	-164.0(4)
C(50)-Fe(2)-C(49)-N(5)	-110.8(5)
C(51)-Fe(2)-C(49)-N(5)	-72.9(4)
C(52)-Fe(2)-C(49)-N(5)	-32.4(3)
C(48)-C(49)-C(50)-C(51)	-170.8(5)
N(5)-C(49)-C(50)-C(51)	40.1(6)
Fe(2)-C(49)-C(50)-C(51)	-61.6(4)
C(48)-C(49)-C(50)-Fe(2)	-109.1(5)
N(5)-C(49)-C(50)-Fe(2)	101.8(4)
C(49)-Fe(2)-C(50)-C(51)	120.0(5)
C(52)-Fe(2)-C(50)-C(51)	31.3(3)
C(51)-Fe(2)-C(50)-C(49)	-120.0(5)
C(52)-Fe(2)-C(50)-C(49)	-88.7(3)
C(49)-C(50)-C(51)-C(52)	4.7(7)
Fe(2)-C(50)-C(51)-C(52)	-59.8(5)
C(49)-C(50)-C(51)-Fe(2)	64.5(4)
C(50)-Fe(2)-C(51)-C(52)	128.3(5)
C(49)-Fe(2)-C(51)-C(52)	91.4(3)
C(49)-Fe(2)-C(51)-C(50)	-37.0(3)
C(52)-Fe(2)-C(51)-C(50)	-128.3(5)
C(50)-C(51)-C(52)-C(53)	-31.1(8)
Fe(2)-C(51)-C(52)-C(53)	-86.4(5)
C(50)-C(51)-C(52)-Fe(2)	55.3(5)
C(50)-Fe(2)-C(52)-C(51)	-33.4(3)
C(49)-Fe(2)-C(52)-C(51)	-75.8(3)
C(50)-Fe(2)-C(52)-C(53)	87.1(4)
C(51)-Fe(2)-C(52)-C(53)	120.5(5)
C(49)-Fe(2)-C(52)-C(53)	44.7(3)
C(51)-C(52)-C(53)-C(54)	178.1(6)
Fe(2)-C(52)-C(53)-C(54)	111.8(6)
C(51)-C(52)-C(53)-N(5)	10.9(7)

Fe(2)-C(52)-C(53)-N(5)	-55.5(4)
C(49)-N(5)-C(53)-C(54)	-138.4(4)
Al(4)-N(5)-C(53)-C(54)	102.5(4)
Al(3)-N(5)-C(53)-C(54)	-9.2(5)
C(49)-N(5)-C(53)-C(52)	30.8(5)
Al(4)-N(5)-C(53)-C(52)	-88.3(4)
Al(3)-N(5)-C(53)-C(52)	160.0(4)
C(52)-C(53)-C(54)-N(6)	-162.4(5)
N(5)-C(53)-C(54)-N(6)	4.8(6)
C(52)-C(53)-C(54)-C(55)	18.4(9)
N(5)-C(53)-C(54)-C(55)	-174.4(4)
C(73)-N(6)-C(54)-C(53)	-176.9(4)
Al(3)-N(6)-C(54)-C(53)	2.2(5)
C(73)-N(6)-C(54)-C(55)	2.4(7)
Al(3)-N(6)-C(54)-C(55)	-178.6(4)
C(61)-C(56)-C(57)-C(58)	-0.4(10)
C(62)-C(56)-C(57)-C(58)	-179.9(6)
C(56)-C(57)-C(58)-C(59)	0.5(11)
C(57)-C(58)-C(59)-C(60)	0.1(11)
C(58)-C(59)-C(60)-C(61)	-0.6(9)
C(58)-C(59)-C(60)-C(65)	178.0(6)
C(59)-C(60)-C(61)-C(56)	0.6(8)
C(65)-C(60)-C(61)-C(56)	-177.9(5)
C(59)-C(60)-C(61)-N(4)	-178.1(5)
C(65)-C(60)-C(61)-N(4)	3.4(8)
C(57)-C(56)-C(61)-C(60)	-0.1(8)
C(62)-C(56)-C(61)-C(60)	179.3(5)
C(57)-C(56)-C(61)-N(4)	178.5(5)
C(62)-C(56)-C(61)-N(4)	-2.0(8)
C(48)-N(4)-C(61)-C(60)	-91.7(6)
Al(3)-N(4)-C(61)-C(60)	86.4(5)
C(48)-N(4)-C(61)-C(56)	89.6(6)
Al(3)-N(4)-C(61)-C(56)	-92.3(5)
C(57)-C(56)-C(62)-C(64)	-59.6(8)
C(61)-C(56)-C(62)-C(64)	120.9(6)
C(57)-C(56)-C(62)-C(63)	62.6(8)
C(61)-C(56)-C(62)-C(63)	-116.9(7)
C(59)-C(60)-C(65)-C(67)	59.1(7)
C(61)-C(60)-C(65)-C(67)	-122.4(6)
C(59)-C(60)-C(65)-C(66)	-64.0(7)
C(61)-C(60)-C(65)-C(66)	114.5(6)
C(73)-C(68)-C(69)-C(70)	-1.4(9)
C(74)-C(68)-C(69)-C(70)	177.3(6)
C(68)-C(69)-C(70)-C(71)	1.8(11)
C(69)-C(70)-C(71)-C(72)	-1.3(11)
C(70)-C(71)-C(72)-C(73)	0.4(9)
C(70)-C(71)-C(72)-C(77)	179.9(6)
C(71)-C(72)-C(73)-C(68)	0.0(8)
C(77)-C(72)-C(73)-C(68)	-179.4(5)
C(71)-C(72)-C(73)-N(6)	178.7(5)
C(77)-C(72)-C(73)-N(6)	-0.8(8)
C(69)-C(68)-C(73)-C(72)	0.5(8)
C(74)-C(68)-C(73)-C(72)	-178.2(5)
C(69)-C(68)-C(73)-N(6)	-178.2(5)
C(74)-C(68)-C(73)-N(6)	3.2(8)
C(54)-N(6)-C(73)-C(72)	84.5(6)
Al(3)-N(6)-C(73)-C(72)	-94.4(5)

C(54)-N(6)-C(73)-C(68)	-96.8(5)
Al(3)-N(6)-C(73)-C(68)	84.3(5)
C(69)-C(68)-C(74)-C(76)	-85.2(7)
C(73)-C(68)-C(74)-C(76)	93.5(7)
C(69)-C(68)-C(74)-C(75)	38.4(8)
C(73)-C(68)-C(74)-C(75)	-142.9(6)
C(71)-C(72)-C(77)-C(78)	59.3(8)
C(73)-C(72)-C(77)-C(78)	-121.3(6)
C(71)-C(72)-C(77)-C(79)	-65.4(7)
C(73)-C(72)-C(77)-C(79)	114.0(6)
N(6)-Al(3)-C(80)-C'81	128.7(12)
N(5)-Al(3)-C(80)-C'81	-100(2)
N(4)-Al(3)-C(80)-C'81	-83.1(12)
Cl(2)-Al(3)-C(80)-C'81	21.7(12)
N(6)-Al(3)-C(80)-C(81)	75.0(7)
N(5)-Al(3)-C(80)-C(81)	-153.1(16)
N(4)-Al(3)-C(80)-C(81)	-136.7(7)
Cl(2)-Al(3)-C(80)-C(81)	-31.9(7)
C(84)-Al(4)-C(82)-C(83)	-64.3(9)
N(5)-Al(4)-C(82)-C(83)	80.3(9)
Cl(2)-Al(4)-C(82)-C(83)	176.3(8)
N(5)-Al(4)-C(84)-C(85)	-115.5(5)
C(82)-Al(4)-C(84)-C(85)	29.3(7)
Cl(2)-Al(4)-C(84)-C(85)	148.3(5)
C(91)-C(86)-C(87)-C(88)	0.0
C(86)-C(87)-C(88)-C(89)	0.0
C(87)-C(88)-C(89)-C(90)	0.0
C(88)-C(89)-C(90)-C(91)	0.0
C(89)-C(90)-C(91)-C(86)	0.0
C(89)-C(90)-C(91)-C(92)	176.7
C(87)-C(86)-C(91)-C(90)	0.0
C(87)-C(86)-C(91)-C(92)	-176.5
C(91')-C(86')-C(87')-C(88')	0.0
C(86')-C(87')-C(88')-C(89')	0.0
C(87')-C(88')-C(89')-C(90')	0.0
C(88')-C(89')-C(90')-C(91')	0.0
C(89')-C(90')-C(91')-C(86')	0.0
C(89')-C(90')-C(91')-C(92')	173.4
C(87')-C(86')-C(91')-C(90')	0.0
C(87')-C(86')-C(91')-C(92')	-173.0
C(45)-C(40)-C(41)-C(42)	0.0
C(40)-C(41)-C(42)-C(43)	0.0
C(41)-C(42)-C(43)-C(44)	0.0
C(42)-C(43)-C(44)-C(45)	0.0
C(43)-C(44)-C(45)-C(40)	0.0
C(43)-C(44)-C(45)-C(46)	-166.6
C(41)-C(40)-C(45)-C(44)	0.0
C(41)-C(40)-C(45)-C(46)	165.9
C(45')-C(40')-C(41')-C(42')	0.0
C(40')-C(41')-C(42')-C(43')	0.0
C(41')-C(42')-C(43')-C(44')	0.0
C(42')-C(43')-C(44')-C(45')	0.0
C(43')-C(44')-C(45')-C(40')	0.0
C(43')-C(44')-C(45')-C(46')	-176.7
C(41')-C(40')-C(45')-C(44')	0.0
C(41')-C(40')-C(45')-C(46')	176.6

Symmetry transformations used to generate equivalent atoms: