Electronic Supplementary Information for Dalton Transactions

Long-range Solid-State Ordering and High Geometric Distortions Induced in Phthalocyanines by Small Fluoroalkyl Groups

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Supporting Information

Structural details and tables for complexes **2** and **3**.

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Structure of $H_8(CF_3)_8PcH_2$

The crystal was a dark purple prism mounted on a glass fiber with epoxy cement. X-ray data collection was carried out using a Bruker single-crystal diffractometer equipped with an APEX CCD area detector and controlled by SMART version 5 (1) software. Data reduction was performed by SAINT version 6 (1) and absorption corrections were applied by SADABS version 2 (2).

The compound crystallizes in a body-centered tetragonal cell that contains sixteen equivalents of the independent unit. The structure was determined by direct methods and refined on F squared by use of programs in the SHELXTL version 5 (1) package, which were also used for all figures. All three independent hydrogen atoms appeared in a difference map, and were sufficiently well-defined that they could be refined without restraints, except that the site occupancy factor of one hydrogen atom was fixed at one-half.

The molecule consists of four equivalents of the independent unit, and is centered on a 4-bar (S4) symmetry element. The molecule is saddle-shaped, rather than planar, as expected. In the center there are expected to be two hydrogen atoms, on chemical grounds, but four symmetry-equivalent atoms are apparent there. When refined as full atoms, the displacement factor was large (0.13), so the occupancy was set at one-half; then the displacement factor was small (0.03), even a little smaller than expected (0.06). Naturally, hydrogen atoms are not well determined, but the model with half-hydrogens fits the data better than the model with full hydrogens. There are four whole molecules in the unit cell.

ORTEP representation at 40% probability

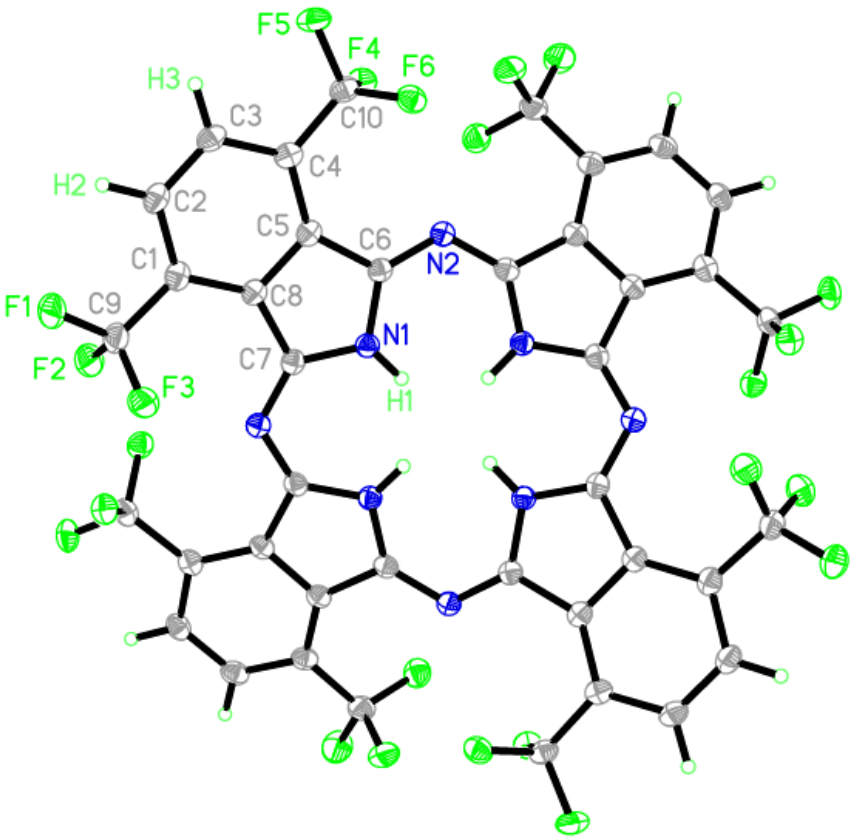


Table 1. Crystal data and structure refinement for $(CF_3)_8PcH_2$.

Empirical formula	C40 H10 F24 N8	
Formula weight	1058.56	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	I4(1)/a	
Unit cell dimensions	a = 15.2835(6) Å	α= 90°.
	b = 15.2835(6) Å	β= 90°.
	c = 16.8165(12) Å	γ = 90°.
Volume	3928.1(4) $Å^3$	
Z	4	
Density (calculated)	1.790 g/cm^3	
Absorption coefficient	0.189 mm^{-1}	
F(000)	2088	
Crystal size	0.18 x 0.14 x 0.07 mm^3	
Theta range for data collection	2.67 to 25.04°.	
Index ranges	-18<=h<=18, -18<=k<=17, -20<=l<=20	
Reflections collected	16471	
Independent reflections	1736 [R(int) = 0.0429]	
Completeness to theta = 25.04°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9869 and 0.9667	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1736 / 0 / 175	
Goodness-of-fit on F^2	1.010	
Final R indices [I>2sigma(I)]	R1 = 0.0357, wR2 = 0.0784	
R indices (all data)	R1 = 0.0567, wR2 = 0.0880	
Largest diff. peak and hole	0.171 and -0.137 $eÅ^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for $(CF_3)_8PcH_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	4154(1)	8452(1)	1184(1)	41(1)
C(1)	4371(1)	9312(1)	1141(1)	39(1)
C(2)	3608(1)	9794(1)	840(1)	41(1)
C(3)	3456(1)	10681(1)	670(1)	46(1)
C(4)	4126(2)	11379(1)	801(1)	52(1)
F(1)	4883(1)	11208(1)	440(1)	64(1)
F(2)	4291(1)	11496(1)	1572(1)	64(1)
F(3)	3860(1)	12153(1)	518(1)	76(1)
C(5)	2643(2)	10919(2)	393(1)	56(1)
C(6)	2002(2)	10302(2)	246(2)	57(1)
C(7)	2137(1)	9425(1)	389(1)	50(1)
C(8)	1430(2)	8796(2)	168(2)	69(1)
F(4)	1724(1)	8086(1)	-193(1)	83(1)
F(5)	987(1)	8536(1)	803(1)	98(1)
F(6)	849(1)	9161(1)	-322(1)	116(1)
C(9)	2944(1)	9174(1)	718(1)	42(1)
C(10)	3299(1)	8331(1)	993(1)	41(1)
N(2)	2828(1)	7617(1)	1126(1)	42(1)

Table 3. Bond lengths [Å] and angles [°] for $(CF_3)_8PcH_2$.

N(1)-C(1)	1.357(3)	F(1)-C(4)-F(3)	106.00(18)
N(1)-C(10)	1.358(3)	F(2)-C(4)-C(3)	111.62(18)
C(1)-N(2)#1	1.325(2)	F(1)-C(4)-C(3)	112.76(17)
C(1)-C(2)	1.470(3)	F(3)-C(4)-C(3)	111.67(19)
C(2)-C(9)	1.404(3)	C(3)-C(5)-C(6)	121.4(2)
C(2)-C(3)	1.404(3)	C(7)-C(6)-C(5)	121.8(2)
C(3)-C(5)	1.375(3)	C(6)-C(7)-C(9)	117.7(2)
C(3)-C(4)	1.496(3)	C(6)-C(7)-C(8)	118.3(2)
C(4)-F(2)	1.332(2)	C(9)-C(7)-C(8)	124.0(2)
C(4)-F(1)	1.333(2)	F(4)-C(8)-F(5)	107.3(2)
C(4)-F(3)	1.338(2)	F(4)-C(8)-F(6)	106.6(2)
C(5)-C(6)	1.382(3)	F(5)-C(8)-F(6)	106.5(2)
C(6)-C(7)	1.378(3)	F(4)-C(8)-C(7)	113.3(2)
C(7)-C(9)	1.405(3)	F(5)-C(8)-C(7)	111.2(2)
C(7)-C(8)	1.493(3)	F(6)-C(8)-C(7)	111.5(2)
C(8)-F(4)	1.321(3)	C(2)-C(9)-C(7)	120.57(19)
C(8)-F(5)	1.325(3)	C(2)-C(9)-C(10)	106.22(17)
C(8)-F(6)	1.334(3)	C(7)-C(9)-C(10)	133.20(19)
C(9)-C(10)	1.472(3)	N(2)-C(10)-N(1)	126.48(18)
C(10)-N(2)	1.327(2)	N(2)-C(10)-C(9)	125.00(18)
N(2)-C(1)#2	1.325(2)	N(1)-C(10)-C(9)	107.97(17)
C(1)-N(1)-C(10)	110.81(17)	C(1)#2-N(2)-C(10)	122.15(17)
N(2)#1-C(1)-N(1)	126.68(18)		
N(2)#1-C(1)-C(2)	125.18(17)		
N(1)-C(1)-C(2)	108.02(17)		
C(9)-C(2)-C(3)	120.12(18)		
C(9)-C(2)-C(1)	106.58(16)		
C(3)-C(2)-C(1)	133.30(19)		
C(5)-C(3)-C(2)	118.3(2)		
C(5)-C(3)-C(4)	118.67(19)		
C(2)-C(3)-C(4)	123.01(19)		
F(2)-C(4)-F(1)	107.81(19)		
F(2)-C(4)-F(3)	106.61(17)		

Symmetry transformations used to generate equivalent atoms:

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

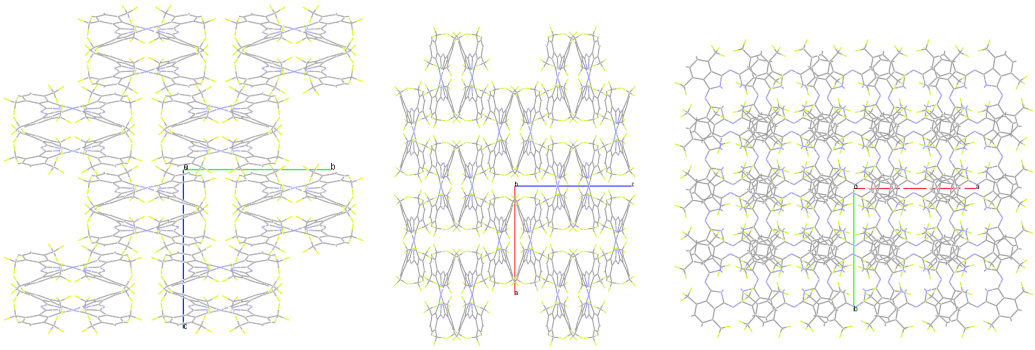
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $(CF_3)_8PcH_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	36(1)	37(1)	52(1)	2(1)	0(1)	1(1)
C(1)	39(1)	37(1)	42(1)	-1(1)	3(1)	1(1)
C(2)	42(1)	40(1)	41(1)	2(1)	2(1)	4(1)
C(3)	53(1)	40(1)	45(1)	3(1)	5(1)	6(1)
C(4)	67(2)	41(1)	49(1)	4(1)	1(1)	5(1)
F(1)	68(1)	58(1)	64(1)	3(1)	13(1)	-12(1)
F(2)	78(1)	59(1)	54(1)	-6(1)	-4(1)	1(1)
F(3)	100(1)	38(1)	89(1)	11(1)	-18(1)	2(1)
C(5)	60(2)	46(1)	60(2)	11(1)	3(1)	13(1)
C(6)	46(1)	62(2)	64(2)	14(1)	-2(1)	10(1)
C(7)	41(1)	52(1)	56(1)	8(1)	1(1)	4(1)
C(8)	44(1)	70(2)	92(2)	17(2)	-12(1)	4(1)
F(4)	79(1)	74(1)	95(1)	-8(1)	-26(1)	-5(1)
F(5)	58(1)	96(1)	140(2)	20(1)	24(1)	-10(1)
F(6)	82(1)	92(1)	175(2)	32(1)	-72(1)	-5(1)
C(9)	39(1)	44(1)	44(1)	2(1)	3(1)	4(1)
C(10)	36(1)	41(1)	45(1)	-2(1)	2(1)	3(1)
N(2)	37(1)	40(1)	49(1)	0(1)	0(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $(CF_3)_8PcH_2$.

	x	y	z	U(eq)
H(1)	4470(20)	8040(20)	1280(20)	28(10)
H(5A)	2533(15)	11519(16)	292(13)	66(7)
H(6A)	1461(15)	10463(14)	31(14)	61(7)

Packing diagrams, along a, b and c axes.



Structure of **$[H_8(CF_3)_8PcFe]_2O$**

Data collection

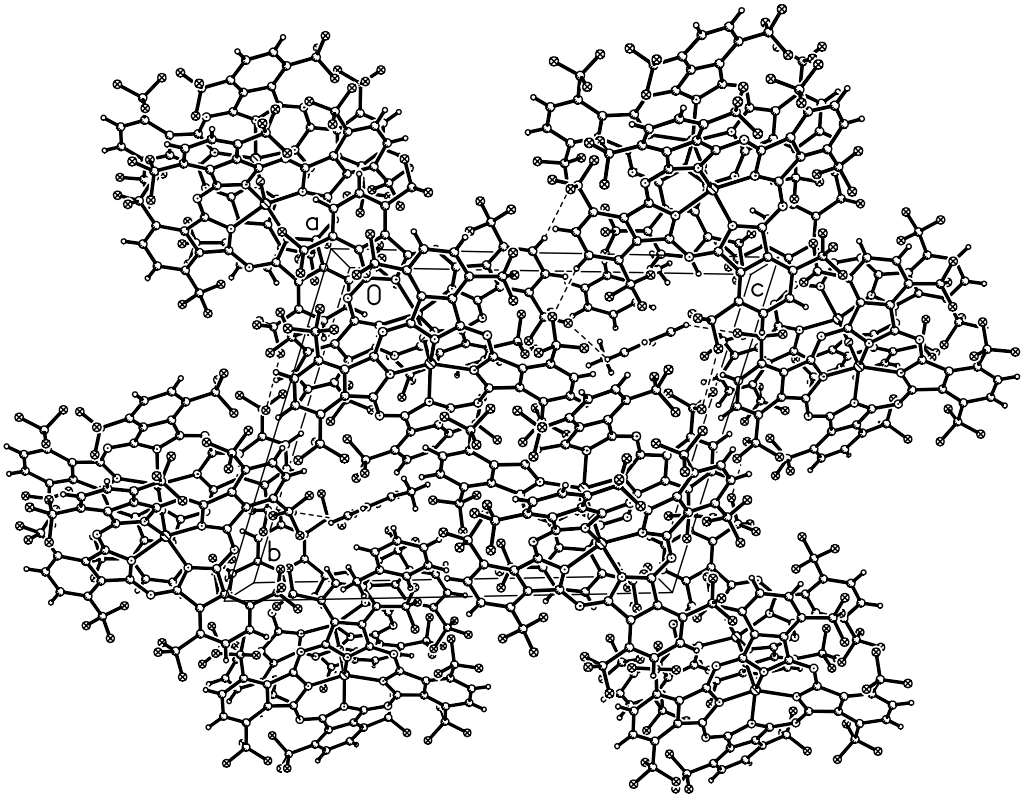
A crystal (approximate dimensions 0.36 x 0.28 x 0.18 mm^3) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a Bruker SMART Platform CCD diffractometer for a data collection at 173(2) K. A preliminary set of cell constants was calculated from reflections harvested from three sets of 20 frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced initial orientation matrices determined from 161 reflections. The data collection was carried out using MoKα radiation (graphite monochromator) with a frame time of 25 seconds and a detector distance of 4.94 cm. A randomly oriented region of reciprocal space was surveyed to the extent of 1.5 hemispheres and to a resolution of 0.84 Å. Three major sections of frames were collected with 0.30º steps in ω at three different ϕ settings and a detector position of -28º in 2θ. The intensity data were corrected for absorption and decay (SADABS).[1] Final cell constants were calculated from the xyz centroids of 1922 strong reflections from the actual data collection after integration (SAINT).[2] Please refer to Table 1 for additional crystal and refinement information.

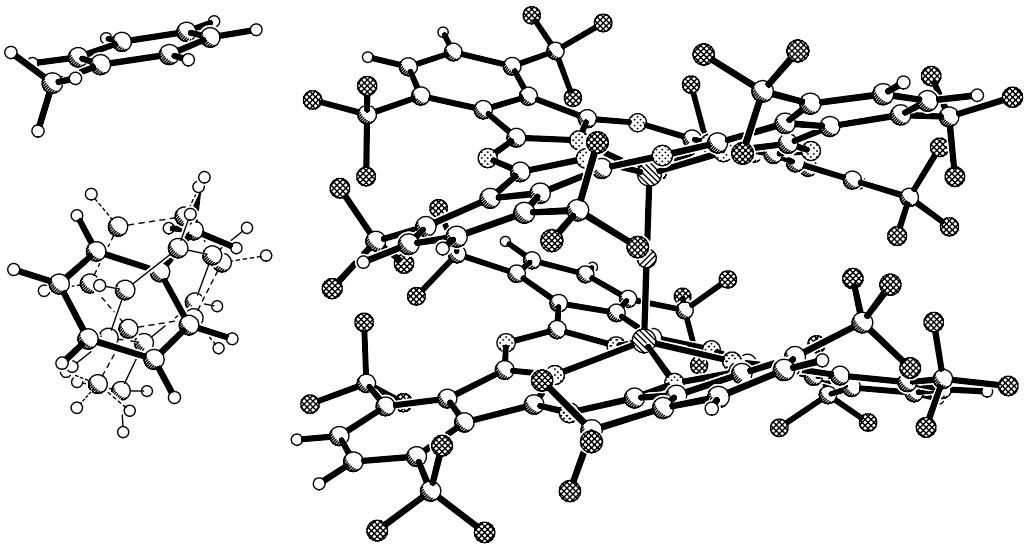
Structure solution and refinement

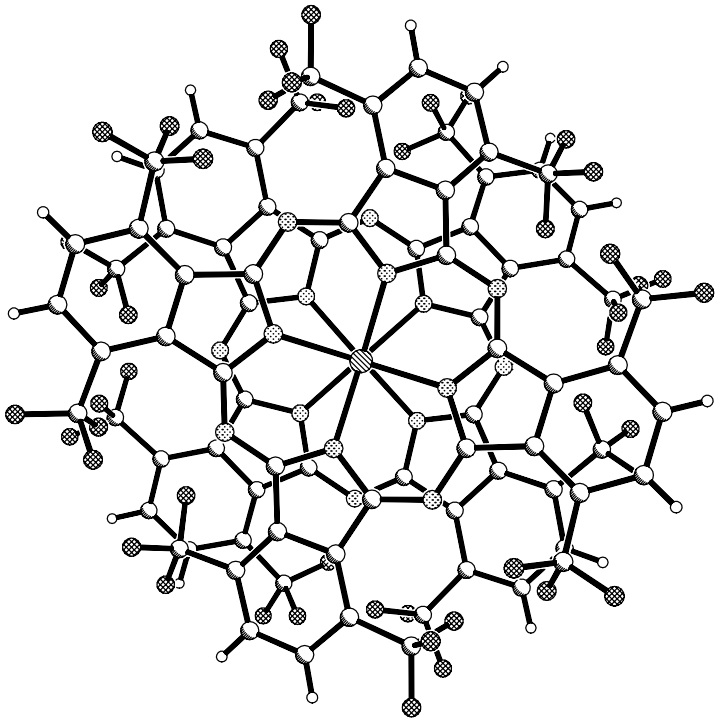
The structure was solved using SIR97[3] and refined using SHELXL-97.[4] The space group *P*-1 was determined based on the lack of systematic absences and intensity statistics. A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The final full matrix least squares refinement converged to $R1 = 0.0419$ and $wR2 = 0.1150$ (F^2, all data).

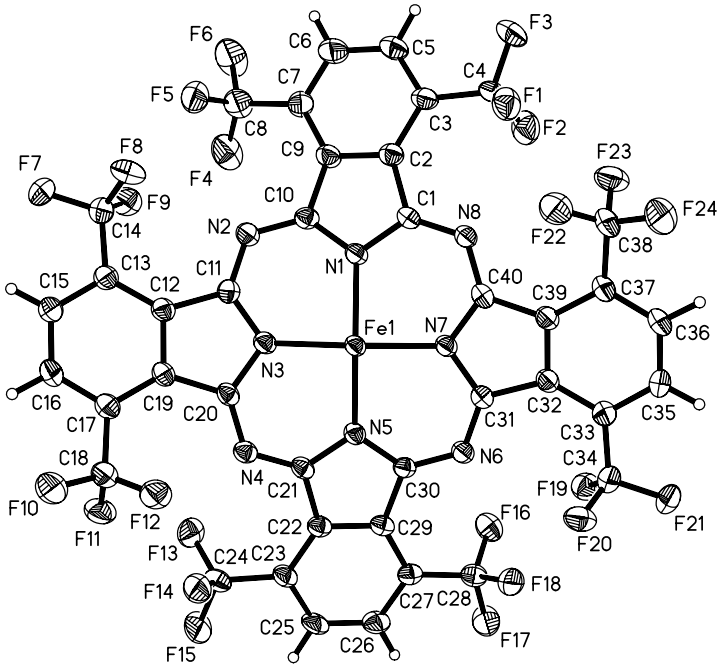
Structure description

The structure is the one suggested. One of the toluene solvent molecules is disordered over three positions (41:17:42). The phthalocyanine ligands, which are in twisted saddle conformations, are rotated about the Fe-O-Fe vector approximately 30 degrees with respect to each other. All atoms lie on general positions.









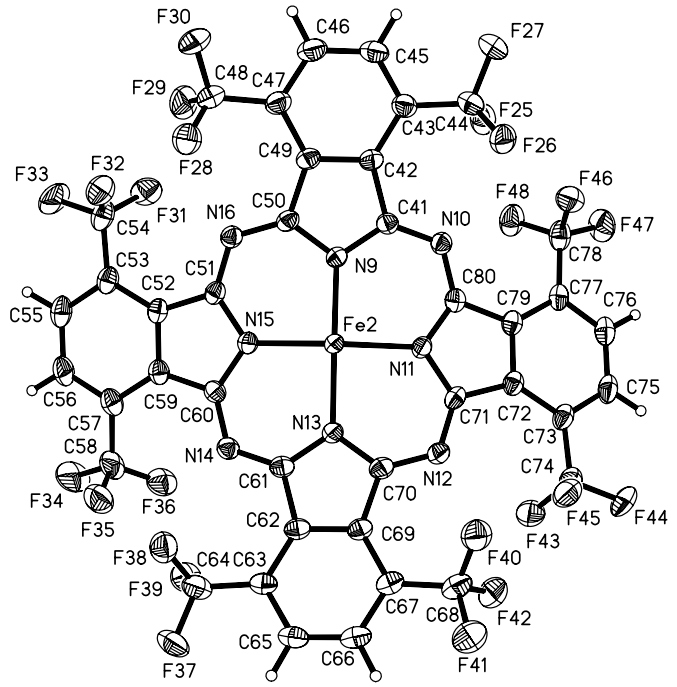


Table 1. Crystal data and structure refinement for 03029.

Identification code	03029	
Empirical formula	C94 H32 F48 Fe2 N16 O	
Formula weight	2425.06	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	*a*= 13.703(3) Å	α= 105.260(3)°
	b= 16.673(3) Å	β= 106.060(3)°
	c= 21.513(4) Å	γ = 94.236(3)°
Volume	4499(2) Å^3	
Z	2	
Density (calculated)	1.790 Mg/m^3	
Absorption coefficient	0.484 mm^{-1}	
F(000)	2400	
Crystal color, morphology	dark red, parallelopiped	
Crystal size	0.36 x 0.28 x 0.18 mm^3	
Theta range for data collection	1.28 to 25.04°.	
Index ranges	$-16 \le h \le 16$, $-19 \le k \le 19$, $-25 \le l \le 22$	
Reflections collected	33075	
Independent reflections	15789 [*R*(int) = 0.0410]	
Observed reflections	11656	
Completeness to theta = 25.04°	99.2%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000000 and 0.878530	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15789 / 81 / 1484	
Goodness-of-fit on F^2	0.992	
Final *R* indices [*I*>2sigma(*I*)]	*R*1 = 0.0419, *wR*2 = 0.1007	
R indices (all data)	*R*1 = 0.0653, *wR*2 = 0.1150	
Largest diff. peak and hole	0.449 and -0.510 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 03029. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Fe1	1345(1)	6819(1)	7147(1)	22(1)
Fe2	3592(1)	8342(1)	7853(1)	21(1)
O1	2456(1)	7590(1)	7497(1)	27(1)
N1	1132(2)	6498(1)	7960(1)	24(1)
N2	2044(2)	5302(1)	7939(1)	27(1)
N3	1891(2)	5711(1)	6928(1)	26(1)
N4	1979(2)	5680(2)	5819(1)	26(1)
N5	823(2)	6625(1)	6123(1)	24(1)
N6	-396(2)	7603(2)	6053(1)	26(1)
N7	178(2)	7493(1)	7189(1)	24(1)
N8	353(2)	7696(2)	8372(1)	25(1)
C1	728(2)	6995(2)	8416(1)	25(1)
C2	781(2)	6620(2)	8968(2)	28(1)
C3	510(2)	6867(2)	9575(2)	32(1)
C4	123(2)	7671(2)	9807(2)	35(1)
F1	784(1)	8340(1)	9893(1)	44(1)
F2	-771(1)	7710(1)	9378(1)	50(1)
F3	-59(2)	7750(2)	10400(1)	68(1)
C5	655(3)	6353(2)	9986(2)	41(1)
C6	1005(3)	5590(2)	9807(2)	47(1)
C7	1258(3)	5334(2)	9217(2)	39(1)
C8	1579(3)	4482(2)	9046(2)	51(1)
F4	1154(2)	4051(1)	8392(1)	58(1)
F5	2591(2)	4520(1)	9199(1)	60(1)
F6	1268(2)	4006(1)	9397(1)	82(1)
C9	1189(2)	5869(2)	8803(2)	30(1)
C10	1466(2)	5837(2)	8185(1)	26(1)
C11	2300(2)	5296(2)	7385(1)	25(1)
C12	3075(2)	4826(2)	7162(1)	27(1)
C13	3701(2)	4274(2)	7407(2)	31(1)
C14	3633(3)	3982(2)	8000(2)	38(1)

F7	4271(2)	3423(2)	8110(1)	62(1)
F8	3904(2)	4612(1)	8575(1)	47(1)
F9	2694(2)	3599(1)	7900(1)	45(1)
C15	4408(2)	3980(2)	7087(2)	36(1)
C16	4536(2)	4252(2)	6552(2)	36(1)
C17	3922(2)	4775(2)	6291(2)	30(1)
C18	4149(2)	5067(2)	5737(2)	36(1)
F10	5133(2)	5039(2)	5756(1)	59(1)
F11	3575(2)	4577(1)	5123(1)	46(1)
F12	4005(1)	5857(1)	5775(1)	42(1)
C19	3151(2)	5035(2)	6582(1)	27(1)
C20	2325(2)	5529(2)	6410(1)	25(1)
C21	1212(2)	6111(2)	5670(1)	25(1)
C22	671(2)	6128(2)	4984(1)	26(1)
C23	758(2)	5713(2)	4345(2)	29(1)
C24	1518(3)	5130(2)	4237(2)	39(1)
F13	1475(1)	4510(1)	4523(1)	41(1)
F14	2476(2)	5535(1)	4470(1)	51(1)
F15	1337(2)	4741(2)	3575(1)	72(1)
C25	130(2)	5879(2)	3784(2)	34(1)
C26	-602(2)	6404(2)	3840(2)	34(1)
C27	-720(2)	6792(2)	4460(1)	27(1)
C28	-1572(2)	7300(2)	4466(2)	33(1)
F16	-2178(1)	7073(1)	4801(1)	42(1)
F17	-2184(2)	7214(1)	3837(1)	55(1)
F18	-1214(2)	8122(1)	4744(1)	43(1)
C29	-57(2)	6668(2)	5047(1)	25(1)
C30	77(2)	7005(2)	5779(1)	24(1)
C31	-288(2)	7868(2)	6713(1)	24(1)
C32	-658(2)	8623(2)	7053(2)	27(1)
C33	-1197(2)	9231(2)	6828(2)	32(1)
C34	-1556(3)	9228(2)	6104(2)	37(1)
F19	-2197(1)	8527(1)	5702(1)	41(1)
F20	-768(1)	9313(1)	5861(1)	42(1)
F21	-2071(2)	9868(1)	6025(1)	60(1)
C35	-1381(3)	9893(2)	7304(2)	44(1)

C36	-990(3)	9986(2)	7992(2)	46(1)
C37	-446(2)	9412(2)	8227(2)	35(1)
C38	28(3)	9612(2)	8981(2)	43(1)
F22	950(2)	9380(1)	9150(1)	46(1)
F23	-561(2)	9254(2)	9261(1)	57(1)
F24	180(2)	10443(1)	9277(1)	77(1)
C39	-325(2)	8692(2)	7749(2)	27(1)
C40	130(2)	7937(2)	7815(1)	26(1)
N9	4447(2)	8013(1)	8657(1)	24(1)
N10	5501(2)	7141(2)	8136(1)	25(1)
N11	4602(2)	7857(1)	7365(1)	24(1)
N12	3946(2)	8253(2)	6344(1)	27(1)
N13	3362(2)	9084(1)	7230(1)	25(1)
N14	2646(2)	10185(1)	7843(1)	26(1)
N15	3336(2)	9328(1)	8558(1)	24(1)
N16	3763(2)	8778(2)	9516(1)	26(1)
C41	5006(2)	7364(2)	8592(1)	24(1)
C42	5032(2)	6985(2)	9143(1)	27(1)
C43	5467(2)	6308(2)	9324(2)	31(1)
C44	6108(3)	5801(2)	8954(2)	39(1)
F25	7010(1)	6256(1)	9042(1)	45(1)
F26	5632(1)	5488(1)	8289(1)	41(1)
F27	6338(2)	5137(1)	9180(1)	60(1)
C45	5316(3)	6107(2)	9874(2)	40(1)
C46	4726(3)	6537(2)	10237(2)	40(1)
C47	4291(2)	7204(2)	10076(2)	33(1)
C48	3653(3)	7625(2)	10490(2)	43(1)
F28	2777(1)	7774(1)	10110(1)	47(1)
F29	4161(2)	8354(1)	10939(1)	59(1)
F30	3381(2)	7143(2)	10842(1)	81(1)
C49	4467(2)	7450(2)	9529(1)	27(1)
C50	4160(2)	8126(2)	9232(1)	25(1)
C51	3477(2)	9370(2)	9224(1)	25(1)
C52	3223(2)	10179(2)	9569(1)	26(1)
C53	3185(2)	10545(2)	10231(2)	31(1)
C54	3462(2)	10139(2)	10785(2)	38(1)

F31	4412(1)	9935(1)	10892(1)	46(1)
F32	2808(1)	9448(1)	10668(1)	44(1)
F33	3459(2)	10661(1)	11381(1)	62(1)
C55	2869(2)	11323(2)	10379(2)	38(1)
C56	2649(2)	11761(2)	9904(2)	38(1)
C57	2712(2)	11429(2)	9258(2)	33(1)
C58	2520(3)	11963(2)	8791(2)	43(1)
F34	2613(2)	12778(1)	9142(1)	68(1)
F35	1571(2)	11757(1)	8356(1)	55(1)
F36	3193(2)	11936(1)	8444(1)	47(1)
C59	2958(2)	10608(2)	9080(2)	27(1)
C60	2994(2)	10039(2)	8440(1)	25(1)
C61	2746(2)	9693(2)	7273(2)	26(1)
C62	2245(2)	9746(2)	6590(2)	28(1)
C63	1550(2)	10250(2)	6330(2)	31(1)
C64	1152(3)	10917(2)	6765(2)	40(1)
F37	417(2)	11243(1)	6392(1)	63(1)
F38	714(1)	10620(1)	7163(1)	44(1)
F39	1880(2)	11564(1)	7160(1)	48(1)
C65	1215(2)	10115(2)	5640(2)	38(1)
C66	1497(2)	9476(2)	5201(2)	38(1)
C67	2154(2)	8958(2)	5436(2)	33(1)
C68	2350(3)	8245(2)	4922(2)	43(1)
F40	2383(2)	7537(1)	5106(1)	45(1)
F41	1599(2)	8045(2)	4330(1)	71(1)
F42	3227(2)	8419(1)	4792(1)	56(1)
C69	2571(2)	9125(2)	6143(2)	27(1)
C70	3329(2)	8754(2)	6567(2)	27(1)
C71	4604(2)	7910(2)	6743(1)	25(1)
C72	5459(2)	7520(2)	6568(2)	27(1)
C73	5820(2)	7402(2)	6001(2)	31(1)
C74	5272(3)	7602(2)	5370(2)	38(1)
F43	5236(2)	8425(1)	5474(1)	47(1)
F44	5731(2)	7376(1)	4888(1)	55(1)
F45	4308(2)	7192(1)	5100(1)	44(1)
C75	6707(2)	7051(2)	6023(2)	36(1)

C76	7226(2)	6814(2)	6578(2)	35(1)
C77	6870(2)	6895(2)	7127(2)	29(1)
C78	7454(2)	6602(2)	7699(2)	36(1)
F46	6965(1)	5887(1)	7712(1)	43(1)
F47	8384(1)	6437(1)	7645(1)	50(1)
F48	7633(1)	7173(1)	8298(1)	48(1)
C79	5960(2)	7245(2)	7119(1)	26(1)
C80	5365(2)	7426(2)	7601(1)	25(1)
C81	4817(3)	9426(3)	3055(2)	63(1)
C82	5410(3)	8843(3)	2831(2)	66(1)
C83	6016(4)	8485(3)	3275(3)	83(2)
C84	6071(4)	8695(4)	3941(3)	89(2)
C85	5504(5)	9269(4)	4162(3)	96(2)
C86	4872(4)	9629(3)	3732(2)	71(1)
C87	4161(4)	9806(4)	2591(3)	111(2)
C88	2417(5)	7226(4)	2742(3)	84(4)
C89	2603(4)	7541(5)	2242(4)	97(2)
C90	1822(6)	7826(5)	1829(3)	63(3)
C91	854(5)	7795(5)	1917(4)	83(4)
C92	667(4)	7480(5)	2417(4)	80(3)
C93	1448(5)	7195(5)	2830(3)	101(5)
C94	3326(6)	7051(7)	3199(5)	114(3)
C88'	1918(13)	5834(11)	2232(9)	74(2)
C89'	1633(15)	6492(12)	1973(9)	83(3)
C90'	2023(19)	7320(11)	2364(12)	97(2)
C91'	2699(18)	7491(13)	3014(12)	114(3)
C92'	2984(18)	6833(16)	3274(9)	82(3)
C93'	2593(17)	6005(14)	2883(10)	70(2)
C94'	1470(20)	5023(11)	1768(12)	90(4)
C88"	2101(5)	5984(4)	2144(3)	74(2)
C89"	2562(6)	6647(5)	1991(3)	83(3)
C90"	3222(7)	7311(5)	2509(5)	97(2)
C91"	3422(6)	7313(5)	3179(4)	114(3)
C92"	2961(7)	6650(6)	3331(3)	82(3)
C93"	2301(6)	5985(5)	2814(4)	70(2)
C94"	1432(8)	5323(6)	1598(5)	90(4)

Table 3. Bond lengths [Å] and angles [°] for 03029.

Fe(1)-O(1)	1.7626(19)	C(5)-C(6)	1.390(5)
Fe(1)-N(7)	2.031(2)	C(5)-H(5A)	0.9500
Fe(1)-N(3)	2.033(2)	C(6)-C(7)	1.378(5)
Fe(1)-N(1)	2.046(2)	C(6)-H(6A)	0.9500
Fe(1)-N(5)	2.046(2)	C(7)-C(9)	1.408(4)
Fe(2)-O(1)	1.7691(19)	C(7)-C(8)	1.501(5)
Fe(2)-N(13)	2.030(2)	C(8)-F(5)	1.326(4)
Fe(2)-N(9)	2.034(2)	C(8)-F(4)	1.336(4)
Fe(2)-N(11)	2.047(2)	C(8)-F(6)	1.351(4)
Fe(2)-N(15)	2.047(2)	C(9)-C(10)	1.468(4)
N(1)-C(10)	1.376(4)	C(11)-C(12)	1.477(4)
N(1)-C(1)	1.376(3)	C(12)-C(19)	1.408(4)
N(2)-C(11)	1.330(4)	C(12)-C(13)	1.409(4)
N(2)-C(10)	1.338(4)	C(13)-C(15)	1.383(4)
N(3)-C(11)	1.367(4)	C(13)-C(14)	1.502(4)
N(3)-C(20)	1.381(4)	C(14)-F(9)	1.328(4)
N(4)-C(20)	1.324(4)	C(14)-F(8)	1.333(4)
N(4)-C(21)	1.331(4)	C(14)-F(7)	1.345(4)
N(5)-C(21)	1.373(3)	C(15)-C(16)	1.392(4)
N(5)-C(30)	1.384(3)	C(15)-H(15A)	0.9500
N(6)-C(30)	1.327(3)	C(16)-C(17)	1.374(4)
N(6)-C(31)	1.334(4)	C(16)-H(16A)	0.9500
N(7)-C(31)	1.372(4)	C(17)-C(19)	1.409(4)
N(7)-C(40)	1.377(4)	C(17)-C(18)	1.498(4)
N(8)-C(1)	1.326(4)	C(18)-F(12)	1.331(4)
N(8)-C(40)	1.327(4)	C(18)-F(11)	1.338(4)
C(1)-C(2)	1.468(4)	C(18)-F(10)	1.342(3)
C(2)-C(9)	1.409(4)	C(19)-C(20)	1.471(4)
C(2)-C(3)	1.422(4)	C(21)-C(22)	1.466(4)
C(3)-C(5)	1.372(4)	C(22)-C(29)	1.402(4)
C(3)-C(4)	1.493(4)	C(22)-C(23)	1.411(4)
C(4)-F(1)	1.321(4)	C(23)-C(25)	1.382(4)
C(4)-F(2)	1.332(4)	C(23)-C(24)	1.500(4)
C(4)-F(3)	1.342(4)	C(24)-F(14)	1.325(4)

C(24)-F(13)	1.341(4)	N(12)-C(70)	1.327(4)
C(24)-F(15)	1.343(4)	N(12)-C(71)	1.335(4)
C(25)-C(26)	1.388(4)	N(13)-C(61)	1.368(4)
C(25)-H(25A)	0.9500	N(13)-C(70)	1.375(4)
C(26)-C(27)	1.381(4)	N(14)-C(61)	1.331(4)
C(26)-H(26A)	0.9500	N(14)-C(60)	1.333(4)
C(27)-C(29)	1.411(4)	N(15)-C(60)	1.365(3)
C(27)-C(28)	1.494(4)	N(15)-C(51)	1.374(4)
C(28)-F(18)	1.335(4)	N(16)-C(51)	1.330(4)
C(28)-F(16)	1.335(4)	N(16)-C(50)	1.330(4)
C(28)-F(17)	1.344(3)	C(41)-C(42)	1.476(4)
C(29)-C(30)	1.479(4)	C(42)-C(43)	1.408(4)
C(31)-C(32)	1.480(4)	C(42)-C(49)	1.412(4)
C(32)-C(33)	1.407(4)	C(43)-C(45)	1.376(4)
C(32)-C(39)	1.408(4)	C(43)-C(44)	1.504(4)
C(33)-C(35)	1.385(4)	C(44)-F(26)	1.336(4)
C(33)-C(34)	1.497(4)	C(44)-F(25)	1.340(4)
C(34)-F(19)	1.334(4)	C(44)-F(27)	1.346(4)
C(34)-F(20)	1.339(4)	C(45)-C(46)	1.383(5)
C(34)-F(21)	1.344(3)	C(45)-H(45A)	0.9500
C(35)-C(36)	1.388(5)	C(46)-C(47)	1.378(4)
C(35)-H(35A)	0.9500	C(46)-H(46A)	0.9500
C(36)-C(37)	1.372(4)	C(47)-C(49)	1.418(4)
C(36)-H(36A)	0.9500	C(47)-C(48)	1.497(4)
C(37)-C(39)	1.414(4)	C(48)-F(28)	1.333(4)
C(37)-C(38)	1.503(5)	C(48)-F(29)	1.335(4)
C(38)-F(23)	1.325(4)	C(48)-F(30)	1.338(4)
C(38)-F(22)	1.331(4)	C(49)-C(50)	1.468(4)
C(38)-F(24)	1.337(4)	C(51)-C(52)	1.475(4)
C(39)-C(40)	1.468(4)	C(52)-C(59)	1.405(4)
N(9)-C(50)	1.371(4)	C(52)-C(53)	1.412(4)
N(9)-C(41)	1.372(3)	C(53)-C(55)	1.384(4)
N(10)-C(80)	1.330(4)	C(53)-C(54)	1.495(5)
N(10)-C(41)	1.332(4)	C(54)-F(32)	1.329(4)
N(11)-C(71)	1.365(4)	C(54)-F(31)	1.343(4)
N(11)-C(80)	1.370(3)	C(54)-F(33)	1.348(4)

C(55)-C(56)	1.388(5)	C(75)-C(76)	1.381(5)
C(55)-H(55A)	0.9500	C(75)-H(75A)	0.9500
C(56)-C(57)	1.382(4)	C(76)-C(77)	1.377(4)
C(56)-H(56A)	0.9500	C(76)-H(76A)	0.9500
C(57)-C(59)	1.413(4)	C(77)-C(79)	1.413(4)
C(57)-C(58)	1.495(5)	C(77)-C(78)	1.491(4)
C(58)-F(35)	1.332(4)	C(78)-F(48)	1.332(4)
C(58)-F(36)	1.333(4)	C(78)-F(46)	1.335(4)
C(58)-F(34)	1.346(4)	C(78)-F(47)	1.352(3)
C(59)-C(60)	1.468(4)	C(79)-C(80)	1.473(4)
C(61)-C(62)	1.470(4)	C(81)-C(86)	1.384(6)
C(62)-C(69)	1.405(4)	C(81)-C(82)	1.388(6)
C(62)-C(63)	1.414(4)	C(81)-C(87)	1.458(6)
C(63)-C(65)	1.378(4)	C(82)-C(83)	1.375(7)
C(63)-C(64)	1.493(5)	C(82)-H(82A)	0.9500
C(64)-F(39)	1.330(4)	C(83)-C(84)	1.362(7)
C(64)-F(38)	1.342(4)	C(83)-H(83A)	0.9500
C(64)-F(37)	1.348(4)	C(84)-C(85)	1.349(7)
C(65)-C(66)	1.382(5)	C(84)-H(84A)	0.9500
C(65)-H(65A)	0.9500	C(85)-C(86)	1.376(7)
C(66)-C(67)	1.380(4)	C(85)-H(85A)	0.9500
C(66)-H(66A)	0.9500	C(86)-H(86A)	0.9500
C(67)-C(69)	1.412(4)	C(87)-H(87A)	0.9800
C(67)-C(68)	1.492(5)	C(87)-H(87B)	0.9800
C(68)-F(42)	1.336(4)	C(87)-H(87C)	0.9800
C(68)-F(41)	1.340(4)	C(88)-C(89)	1.3900
C(68)-F(40)	1.340(4)	C(88)-C(93)	1.3900
C(69)-C(70)	1.469(4)	C(88)-C(94)	1.4597
C(71)-C(72)	1.472(4)	C(89)-C(90)	1.3900
C(72)-C(79)	1.403(4)	C(89)-H(89)	0.9500
C(72)-C(73)	1.411(4)	C(90)-C(91)	1.3900
C(73)-C(75)	1.383(4)	C(90)-H(90)	0.9500
C(73)-C(74)	1.492(4)	C(91)-C(92)	1.3900
C(74)-F(45)	1.335(4)	C(91)-H(91)	0.9500
C(74)-F(43)	1.339(4)	C(92)-C(93)	1.3900
C(74)-F(44)	1.341(4)	C(92)-H(92)	0.9500

C(93)-H(93)	0.9500	N(7)-Fe(1)-N(3)	151.88(10)
C(94)-H(94A)	0.9800	O(1)-Fe(1)-N(1)	104.31(9)
C(94)-H(94B)	0.9800	N(7)-Fe(1)-N(1)	86.40(9)
C(94)-H(94C)	0.9800	N(3)-Fe(1)-N(1)	85.60(9)
C(88')-C(89')	1.3900	O(1)-Fe(1)-N(5)	108.94(9)
C(88')-C(93')	1.3900	N(7)-Fe(1)-N(5)	85.77(9)
C(88')-C(94')	1.4257	N(3)-Fe(1)-N(5)	86.28(9)
C(89')-C(90')	1.3900	N(1)-Fe(1)-N(5)	146.75(9)
C(89')-H(89')	0.9500	O(1)-Fe(2)-N(13)	102.19(9)
C(90')-C(91')	1.3900	O(1)-Fe(2)-N(9)	105.48(9)
C(90')-H(90')	0.9500	N(13)-Fe(2)-N(9)	152.32(10)
C(91')-C(92')	1.3900	O(1)-Fe(2)-N(11)	105.51(9)
C(91')-H(91')	0.9500	N(13)-Fe(2)-N(11)	85.83(9)
C(92')-C(93')	1.3900	N(9)-Fe(2)-N(11)	86.28(9)
C(92')-H(92')	0.9500	O(1)-Fe(2)-N(15)	107.86(9)
C(93')-H(93')	0.9500	N(13)-Fe(2)-N(15)	86.24(9)
C(94')-H(94D)	0.9800	N(9)-Fe(2)-N(15)	85.88(9)
C(94')-H(94E)	0.9800	N(11)-Fe(2)-N(15)	146.61(9)
C(94')-H(94F)	0.9800	Fe(1)-O(1)-Fe(2)	178.40(13)
C(88")-C(89")	1.3900	C(10)-N(1)-C(1)	109.7(2)
C(88")-C(93")	1.3900	C(10)-N(1)-Fe(1)	126.93(18)
C(88")-C(94")	1.417(8)	C(1)-N(1)-Fe(1)	122.97(19)
C(89")-C(90")	1.3900	C(11)-N(2)-C(10)	123.1(2)
C(89")-H(89")	0.9500	C(11)-N(3)-C(20)	109.3(2)
C(90")-C(91")	1.3900	C(11)-N(3)-Fe(1)	125.38(19)
C(90")-H(90")	0.9500	C(20)-N(3)-Fe(1)	118.93(18)
C(91")-C(92")	1.3900	C(20)-N(4)-C(21)	123.8(2)
C(91")-H(91")	0.9500	C(21)-N(5)-C(30)	109.3(2)
C(92")-C(93")	1.3900	C(21)-N(5)-Fe(1)	123.76(18)
C(92")-H(92")	0.9500	C(30)-N(5)-Fe(1)	126.93(18)
C(93")-H(93")	0.9500	C(30)-N(6)-C(31)	123.6(2)
C(94")-H(94G)	0.9800	C(31)-N(7)-C(40)	109.8(2)
C(94")-H(94H)	0.9800	C(31)-N(7)-Fe(1)	125.28(18)
C(94")-H(94I)	0.9800	C(40)-N(7)-Fe(1)	118.46(18)
O(1)-Fe(1)-N(7)	103.80(9)	C(1)-N(8)-C(40)	123.9(2)
O(1)-Fe(1)-N(3)	104.29(9)	N(8)-C(1)-N(1)	126.5(3)

N(8)-C(1)-C(2)	125.1(3)	N(2)-C(11)-C(12)	124.9(3)
N(1)-C(1)-C(2)	108.4(2)	N(3)-C(11)-C(12)	108.8(2)
C(9)-C(2)-C(3)	120.2(3)	C(19)-C(12)-C(13)	119.4(3)
C(9)-C(2)-C(1)	106.6(2)	C(19)-C(12)-C(11)	106.3(2)
C(3)-C(2)-C(1)	133.2(3)	C(13)-C(12)-C(11)	134.3(3)
C(5)-C(3)-C(2)	118.1(3)	C(15)-C(13)-C(12)	118.8(3)
C(5)-C(3)-C(4)	118.1(3)	C(15)-C(13)-C(14)	118.2(3)
C(2)-C(3)-C(4)	123.8(3)	C(12)-C(13)-C(14)	123.0(3)
F(1)-C(4)-F(2)	108.2(3)	F(9)-C(14)-F(8)	108.7(3)
F(1)-C(4)-F(3)	107.0(3)	F(9)-C(14)-F(7)	106.5(3)
F(2)-C(4)-F(3)	105.3(3)	F(8)-C(14)-F(7)	105.8(3)
F(1)-C(4)-C(3)	112.4(3)	F(9)-C(14)-C(13)	111.9(3)
F(2)-C(4)-C(3)	112.2(3)	F(8)-C(14)-C(13)	112.3(3)
F(3)-C(4)-C(3)	111.3(3)	F(7)-C(14)-C(13)	111.5(3)
C(3)-C(5)-C(6)	121.9(3)	C(13)-C(15)-C(16)	120.9(3)
C(3)-C(5)-H(5A)	119.1	C(13)-C(15)-H(15A)	119.5
C(6)-C(5)-H(5A)	119.1	C(16)-C(15)-H(15A)	119.5
C(7)-C(6)-C(5)	120.9(3)	C(17)-C(16)-C(15)	121.6(3)
C(7)-C(6)-H(6A)	119.6	C(17)-C(16)-H(16A)	119.2
C(5)-C(6)-H(6A)	119.6	C(15)-C(16)-H(16A)	119.2
C(6)-C(7)-C(9)	119.1(3)	C(16)-C(17)-C(19)	118.1(3)
C(6)-C(7)-C(8)	117.3(3)	C(16)-C(17)-C(18)	117.8(3)
C(9)-C(7)-C(8)	123.6(3)	C(19)-C(17)-C(18)	124.1(3)
F(5)-C(8)-F(4)	108.5(3)	F(12)-C(18)-F(11)	107.8(2)
F(5)-C(8)-F(6)	106.3(3)	F(12)-C(18)-F(10)	106.2(3)
F(4)-C(8)-F(6)	105.9(3)	F(11)-C(18)-F(10)	106.2(3)
F(5)-C(8)-C(7)	112.8(3)	F(12)-C(18)-C(17)	113.4(3)
F(4)-C(8)-C(7)	112.3(3)	F(11)-C(18)-C(17)	111.8(3)
F(6)-C(8)-C(7)	110.6(3)	F(10)-C(18)-C(17)	111.0(3)
C(7)-C(9)-C(2)	119.6(3)	C(12)-C(19)-C(17)	120.7(3)
C(7)-C(9)-C(10)	133.8(3)	C(12)-C(19)-C(20)	106.2(2)
C(2)-C(9)-C(10)	106.6(3)	C(17)-C(19)-C(20)	133.0(3)
N(2)-C(10)-N(1)	126.9(3)	N(4)-C(20)-N(3)	125.9(3)
N(2)-C(10)-C(9)	124.4(3)	N(4)-C(20)-C(19)	125.1(3)
N(1)-C(10)-C(9)	108.4(2)	N(3)-C(20)-C(19)	108.6(2)
N(2)-C(11)-N(3)	126.3(3)	N(4)-C(21)-N(5)	126.4(3)

N(4)-C(21)-C(22)	124.4(2)	N(6)-C(31)-C(32)	125.2(3)
N(5)-C(21)-C(22)	109.2(2)	N(7)-C(31)-C(32)	108.6(2)
C(29)-C(22)-C(23)	121.1(3)	C(33)-C(32)-C(39)	120.0(3)
C(29)-C(22)-C(21)	106.6(2)	C(33)-C(32)-C(31)	134.1(3)
C(23)-C(22)-C(21)	132.3(3)	C(39)-C(32)-C(31)	105.9(2)
C(25)-C(23)-C(22)	117.9(3)	C(35)-C(33)-C(32)	118.5(3)
C(25)-C(23)-C(24)	117.9(3)	C(35)-C(33)-C(34)	117.4(3)
C(22)-C(23)-C(24)	124.2(3)	C(32)-C(33)-C(34)	124.1(3)
F(14)-C(24)-F(13)	108.1(3)	F(19)-C(34)-F(20)	108.2(3)
F(14)-C(24)-F(15)	106.7(3)	F(19)-C(34)-F(21)	105.9(3)
F(13)-C(24)-F(15)	105.4(3)	F(20)-C(34)-F(21)	106.1(3)
F(14)-C(24)-C(23)	112.0(3)	F(19)-C(34)-C(33)	112.5(3)
F(13)-C(24)-C(23)	113.1(3)	F(20)-C(34)-C(33)	111.7(3)
F(15)-C(24)-C(23)	111.1(3)	F(21)-C(34)-C(33)	112.0(3)
C(23)-C(25)-C(26)	121.4(3)	C(33)-C(35)-C(36)	121.0(3)
C(23)-C(25)-H(25A)	119.3	C(33)-C(35)-H(35A)	119.5
C(26)-C(25)-H(25A)	119.3	C(36)-C(35)-H(35A)	119.5
C(27)-C(26)-C(25)	121.3(3)	C(37)-C(36)-C(35)	121.7(3)
C(27)-C(26)-H(26A)	119.4	C(37)-C(36)-H(36A)	119.1
C(25)-C(26)-H(26A)	119.4	C(35)-C(36)-H(36A)	119.1
C(26)-C(27)-C(29)	118.8(3)	C(36)-C(37)-C(39)	118.2(3)
C(26)-C(27)-C(28)	117.5(3)	C(36)-C(37)-C(38)	117.5(3)
C(29)-C(27)-C(28)	123.7(3)	C(39)-C(37)-C(38)	124.2(3)
F(18)-C(28)-F(16)	108.2(2)	F(23)-C(38)-F(22)	108.0(3)
F(18)-C(28)-F(17)	106.0(3)	F(23)-C(38)-F(24)	107.5(3)
F(16)-C(28)-F(17)	106.4(2)	F(22)-C(38)-F(24)	105.5(3)
F(18)-C(28)-C(27)	111.7(3)	F(23)-C(38)-C(37)	112.3(3)
F(16)-C(28)-C(27)	112.2(3)	F(22)-C(38)-C(37)	112.6(3)
F(17)-C(28)-C(27)	111.9(2)	F(24)-C(38)-C(37)	110.5(3)
C(22)-C(29)-C(27)	119.5(3)	C(32)-C(39)-C(37)	120.1(3)
C(22)-C(29)-C(30)	106.8(2)	C(32)-C(39)-C(40)	107.0(2)
C(27)-C(29)-C(30)	133.7(3)	C(37)-C(39)-C(40)	132.9(3)
N(6)-C(30)-N(5)	126.6(3)	N(8)-C(40)-N(7)	126.8(3)
N(6)-C(30)-C(29)	125.3(2)	N(8)-C(40)-C(39)	124.6(3)
N(5)-C(30)-C(29)	108.1(2)	N(7)-C(40)-C(39)	108.2(2)
N(6)-C(31)-N(7)	126.2(3)	C(50)-N(9)-C(41)	109.9(2)

C(50)-N(9)-Fe(2)	120.72(18)	C(46)-C(47)-C(49)	118.4(3)
C(41)-N(9)-Fe(2)	123.19(18)	C(46)-C(47)-C(48)	117.9(3)
C(80)-N(10)-C(41)	123.3(2)	C(49)-C(47)-C(48)	123.7(3)
C(71)-N(11)-C(80)	109.5(2)	F(28)-C(48)-F(29)	108.0(3)
C(71)-N(11)-Fe(2)	124.48(18)	F(28)-C(48)-F(30)	105.9(3)
C(80)-N(11)-Fe(2)	126.06(19)	F(29)-C(48)-F(30)	106.7(3)
C(70)-N(12)-C(71)	122.7(2)	F(28)-C(48)-C(47)	112.6(3)
C(61)-N(13)-C(70)	109.2(2)	F(29)-C(48)-C(47)	112.0(3)
C(61)-N(13)-Fe(2)	123.23(19)	F(30)-C(48)-C(47)	111.2(3)
C(70)-N(13)-Fe(2)	119.33(18)	C(42)-C(49)-C(47)	119.7(3)
C(61)-N(14)-C(60)	123.0(2)	C(42)-C(49)-C(50)	106.9(2)
C(60)-N(15)-C(51)	109.6(2)	C(47)-C(49)-C(50)	133.4(3)
C(60)-N(15)-Fe(2)	125.57(19)	N(16)-C(50)-N(9)	126.4(3)
C(51)-N(15)-Fe(2)	124.83(18)	N(16)-C(50)-C(49)	125.0(3)
C(51)-N(16)-C(50)	123.1(2)	N(9)-C(50)-C(49)	108.3(2)
N(10)-C(41)-N(9)	126.1(3)	N(16)-C(51)-N(15)	126.7(3)
N(10)-C(41)-C(42)	125.2(2)	N(16)-C(51)-C(52)	124.7(3)
N(9)-C(41)-C(42)	108.6(2)	N(15)-C(51)-C(52)	108.6(2)
C(43)-C(42)-C(49)	120.1(3)	C(59)-C(52)-C(53)	120.1(3)
C(43)-C(42)-C(41)	134.0(3)	C(59)-C(52)-C(51)	106.1(2)
C(49)-C(42)-C(41)	105.9(2)	C(53)-C(52)-C(51)	133.8(3)
C(45)-C(43)-C(42)	118.6(3)	C(55)-C(53)-C(52)	118.4(3)
C(45)-C(43)-C(44)	118.0(3)	C(55)-C(53)-C(54)	117.7(3)
C(42)-C(43)-C(44)	123.4(3)	C(52)-C(53)-C(54)	123.9(3)
F(26)-C(44)-F(25)	108.0(3)	F(32)-C(54)-F(31)	108.0(3)
F(26)-C(44)-F(27)	106.2(3)	F(32)-C(54)-F(33)	106.2(3)
F(25)-C(44)-F(27)	106.1(3)	F(31)-C(54)-F(33)	105.7(3)
F(26)-C(44)-C(43)	112.7(3)	F(32)-C(54)-C(53)	112.7(3)
F(25)-C(44)-C(43)	111.8(3)	F(31)-C(54)-C(53)	112.4(3)
F(27)-C(44)-C(43)	111.6(3)	F(33)-C(54)-C(53)	111.4(3)
C(43)-C(45)-C(46)	121.6(3)	C(53)-C(55)-C(56)	121.3(3)
C(43)-C(45)-H(45A)	119.2	C(53)-C(55)-H(55A)	119.4
C(46)-C(45)-H(45A)	119.2	C(56)-C(55)-H(55A)	119.4
C(47)-C(46)-C(45)	121.5(3)	C(57)-C(56)-C(55)	121.4(3)
C(47)-C(46)-H(46A)	119.3	C(57)-C(56)-H(56A)	119.3
C(45)-C(46)-H(46A)	119.3	C(55)-C(56)-H(56A)	119.3

C(56)-C(57)-C(59)	118.2(3)	C(66)-C(67)-C(69)	117.9(3)
C(56)-C(57)-C(58)	117.9(3)	C(66)-C(67)-C(68)	117.5(3)
C(59)-C(57)-C(58)	123.9(3)	C(69)-C(67)-C(68)	124.6(3)
F(35)-C(58)-F(36)	108.9(3)	F(42)-C(68)-F(41)	106.5(3)
F(35)-C(58)-F(34)	106.2(3)	F(42)-C(68)-F(40)	107.5(3)
F(36)-C(58)-F(34)	105.9(3)	F(41)-C(68)-F(40)	105.4(3)
F(35)-C(58)-C(57)	112.2(3)	F(42)-C(68)-C(67)	112.8(3)
F(36)-C(58)-C(57)	112.8(3)	F(41)-C(68)-C(67)	111.4(3)
F(34)-C(58)-C(57)	110.6(3)	F(40)-C(68)-C(67)	112.7(3)
C(52)-C(59)-C(57)	120.3(3)	C(62)-C(69)-C(67)	120.7(3)
C(52)-C(59)-C(60)	106.7(2)	C(62)-C(69)-C(70)	106.4(2)
C(57)-C(59)-C(60)	133.0(3)	C(67)-C(69)-C(70)	132.9(3)
N(14)-C(60)-N(15)	127.3(3)	N(12)-C(70)-N(13)	126.3(3)
N(14)-C(60)-C(59)	123.6(3)	N(12)-C(70)-C(69)	124.7(3)
N(15)-C(60)-C(59)	108.8(2)	N(13)-C(70)-C(69)	108.7(2)
N(14)-C(61)-N(13)	125.8(3)	N(12)-C(71)-N(11)	126.7(3)
N(14)-C(61)-C(62)	125.2(3)	N(12)-C(71)-C(72)	124.2(3)
N(13)-C(61)-C(62)	109.0(2)	N(11)-C(71)-C(72)	109.1(2)
C(69)-C(62)-C(63)	119.7(3)	C(79)-C(72)-C(73)	120.6(3)
C(69)-C(62)-C(61)	106.4(2)	C(79)-C(72)-C(71)	106.1(2)
C(63)-C(62)-C(61)	133.9(3)	C(73)-C(72)-C(71)	133.4(3)
C(65)-C(63)-C(62)	118.2(3)	C(75)-C(73)-C(72)	117.9(3)
C(65)-C(63)-C(64)	118.3(3)	C(75)-C(73)-C(74)	118.4(3)
C(62)-C(63)-C(64)	123.5(3)	C(72)-C(73)-C(74)	123.6(3)
F(39)-C(64)-F(38)	107.9(3)	F(45)-C(74)-F(43)	107.8(3)
F(39)-C(64)-F(37)	106.0(3)	F(45)-C(74)-F(44)	106.2(3)
F(38)-C(64)-F(37)	105.6(3)	F(43)-C(74)-F(44)	106.2(3)
F(39)-C(64)-C(63)	112.7(3)	F(45)-C(74)-C(73)	111.7(3)
F(38)-C(64)-C(63)	112.4(3)	F(43)-C(74)-C(73)	112.5(3)
F(37)-C(64)-C(63)	111.8(3)	F(44)-C(74)-C(73)	112.0(3)
C(63)-C(65)-C(66)	121.8(3)	C(76)-C(75)-C(73)	121.6(3)
C(63)-C(65)-H(65A)	119.1	C(76)-C(75)-H(75A)	119.2
C(66)-C(65)-H(65A)	119.1	C(73)-C(75)-H(75A)	119.2
C(67)-C(66)-C(65)	121.4(3)	C(77)-C(76)-C(75)	121.6(3)
C(67)-C(66)-H(66A)	119.3	C(77)-C(76)-H(76A)	119.2
C(65)-C(66)-H(66A)	119.3	C(75)-C(76)-H(76A)	119.2

C(76)-C(77)-C(79)	118.4(3)	C(81)-C(87)-H(87C)	109.5
C(76)-C(77)-C(78)	118.6(3)	H(87A)-C(87)-H(87C)	109.5
C(79)-C(77)-C(78)	123.0(3)	H(87B)-C(87)-H(87C)	109.5
F(48)-C(78)-F(46)	108.4(3)	C(89)-C(88)-C(93)	120.0
F(48)-C(78)-F(47)	106.3(2)	C(89)-C(88)-C(94)	114.9
F(46)-C(78)-F(47)	106.0(3)	C(93)-C(88)-C(94)	124.6
F(48)-C(78)-C(77)	112.4(3)	C(88)-C(89)-C(90)	120.0
F(46)-C(78)-C(77)	111.8(2)	C(88)-C(89)-H(89)	120.0
F(47)-C(78)-C(77)	111.6(3)	C(90)-C(89)-H(89)	120.0
C(72)-C(79)-C(77)	119.8(3)	C(91)-C(90)-C(89)	120.0
C(72)-C(79)-C(80)	106.6(2)	C(91)-C(90)-H(90)	120.0
C(77)-C(79)-C(80)	133.5(3)	C(89)-C(90)-H(90)	120.0
N(10)-C(80)-N(11)	126.7(2)	C(90)-C(91)-C(92)	120.0
N(10)-C(80)-C(79)	124.5(3)	C(90)-C(91)-H(91)	120.0
N(11)-C(80)-C(79)	108.5(2)	C(92)-C(91)-H(91)	120.0
C(86)-C(81)-C(82)	117.4(4)	C(93)-C(92)-C(91)	120.0
C(86)-C(81)-C(87)	121.7(5)	C(93)-C(92)-H(92)	120.0
C(82)-C(81)-C(87)	120.9(5)	C(91)-C(92)-H(92)	120.0
C(83)-C(82)-C(81)	120.1(5)	C(92)-C(93)-C(88)	120.0
C(83)-C(82)-H(82A)	120.0	C(92)-C(93)-H(93)	120.0
C(81)-C(82)-H(82A)	120.0	C(88)-C(93)-H(93)	120.0
C(84)-C(83)-C(82)	122.0(5)	C(88)-C(94)-H(94A)	109.5
C(84)-C(83)-H(83A)	119.0	C(88)-C(94)-H(94B)	109.5
C(82)-C(83)-H(83A)	119.0	H(94A)-C(94)-H(94B)	109.5
C(85)-C(84)-C(83)	118.1(5)	C(88)-C(94)-H(94C)	109.5
C(85)-C(84)-H(84A)	121.0	H(94A)-C(94)-H(94C)	109.5
C(83)-C(84)-H(84A)	121.0	H(94B)-C(94)-H(94C)	109.5
C(84)-C(85)-C(86)	121.8(5)	C(89')-C(88')-C(93')	120.0
C(84)-C(85)-H(85A)	119.1	C(89')-C(88')-C(94')	113.4
C(86)-C(85)-H(85A)	119.1	C(93')-C(88')-C(94')	126.6
C(85)-C(86)-C(81)	120.6(5)	C(88')-C(89')-C(90')	120.0
C(85)-C(86)-H(86A)	119.7	C(88')-C(89')-H(89')	120.0
C(81)-C(86)-H(86A)	119.7	C(90')-C(89')-H(89')	120.0
C(81)-C(87)-H(87A)	109.5	C(91')-C(90')-C(89')	120.0
C(81)-C(87)-H(87B)	109.5	C(91')-C(90')-H(90')	120.0
H(87A)-C(87)-H(87B)	109.5	C(89')-C(90')-H(90')	120.0

C(90')-C(91')-C(92')	120.0	C(90")-C(89")-H(89")	120.0
C(90')-C(91')-H(91')	120.0	C(91")-C(90")-C(89")	120.0
C(92')-C(91')-H(91')	120.0	C(91")-C(90")-H(90")	120.0
C(93')-C(92')-C(91')	120.0	C(89")-C(90")-H(90")	120.0
C(93')-C(92')-H(92')	120.0	C(92")-C(91")-C(90")	120.0
C(91')-C(92')-H(92')	120.0	C(92")-C(91")-H(91")	120.0
C(92')-C(93')-C(88')	120.0	C(90")-C(91")-H(91")	120.0
C(92')-C(93')-H(93')	120.0	C(91")-C(92")-C(93")	120.0
C(88')-C(93')-H(93')	120.0	C(91")-C(92")-H(92")	120.0
C(88')-C(94')-H(94D)	109.5	C(93")-C(92")-H(92")	120.0
C(88')-C(94')-H(94E)	109.5	C(92")-C(93")-C(88")	120.0
H(94D)-C(94')-H(94E)	109.5	C(92")-C(93")-H(93")	120.0
C(88')-C(94')-H(94F)	109.5	C(88")-C(93")-H(93")	120.0
H(94D)-C(94')-H(94F)	109.5	C(88")-C(94")-H(94G)	109.5
H(94E)-C(94')-H(94F)	109.5	C(88")-C(94")-H(94H)	109.5
C(89")-C(88")-C(93")	120.0	H(94G)-C(94")-H(94H)	109.5
C(89")-C(88")-C(94")	117.7(6)	C(88")-C(94")-H(94I)	109.5
C(93")-C(88")-C(94")	122.3(6)	H(94G)-C(94")-H(94I)	109.5
C(88")-C(89")-C(90")	120.0	H(94H)-C(94")-H(94I)	109.5
C(88")-C(89")-H(89")	120.0		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 03029. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe1	25(1)	20(1)	20(1)	4(1)	9(1)	4(1)
Fe2	24(1)	22(1)	18(1)	6(1)	7(1)	4(1)
O1	31(1)	27(1)	24(1)	6(1)	10(1)	5(1)
N1	29(1)	23(1)	22(1)	5(1)	11(1)	3(1)
N2	35(1)	22(1)	29(1)	7(1)	15(1)	4(1)
N3	31(1)	23(1)	23(1)	5(1)	11(1)	4(1)
N4	32(1)	23(1)	24(1)	5(1)	11(1)	3(1)
N5	28(1)	22(1)	22(1)	4(1)	9(1)	4(1)
N6	29(1)	25(1)	25(1)	6(1)	11(1)	5(1)
N7	25(1)	26(1)	20(1)	5(1)	8(1)	5(1)
N8	27(1)	26(1)	23(1)	5(1)	10(1)	5(1)
C1	26(1)	26(2)	21(2)	4(1)	9(1)	3(1)
C2	28(2)	33(2)	26(2)	10(1)	10(1)	4(1)
C3	31(2)	41(2)	24(2)	11(1)	11(1)	6(1)
C4	42(2)	45(2)	22(2)	9(2)	14(1)	14(2)
F1	41(1)	39(1)	42(1)	2(1)	6(1)	8(1)
F2	35(1)	59(1)	55(1)	13(1)	13(1)	16(1)
F3	116(2)	72(2)	44(1)	25(1)	53(1)	47(2)
C5	52(2)	48(2)	34(2)	16(2)	26(2)	13(2)
C6	67(2)	51(2)	44(2)	28(2)	33(2)	18(2)
C7	47(2)	40(2)	44(2)	24(2)	26(2)	15(2)
C8	76(3)	42(2)	62(3)	32(2)	46(2)	21(2)
F4	80(2)	32(1)	75(2)	14(1)	44(1)	8(1)
F5	72(2)	70(2)	67(2)	41(1)	40(1)	39(1)
F6	141(2)	56(2)	115(2)	60(2)	101(2)	46(2)
C9	35(2)	32(2)	30(2)	11(1)	17(1)	6(1)
C10	32(2)	23(2)	25(2)	8(1)	11(1)	1(1)
C11	31(2)	15(1)	26(2)	3(1)	9(1)	2(1)
C12	34(2)	23(2)	23(2)	3(1)	9(1)	4(1)
C13	38(2)	27(2)	26(2)	5(1)	9(1)	8(1)
C14	47(2)	37(2)	37(2)	15(2)	18(2)	16(2)

F7	83(2)	77(2)	59(1)	47(1)	39(1)	54(1)
F8	59(1)	56(1)	27(1)	8(1)	18(1)	7(1)
F9	60(1)	34(1)	48(1)	17(1)	23(1)	7(1)
C15	47(2)	35(2)	29(2)	8(2)	14(2)	17(2)
C16	39(2)	39(2)	33(2)	7(2)	17(2)	16(2)
C17	32(2)	29(2)	26(2)	4(1)	10(1)	4(1)
C18	35(2)	42(2)	32(2)	12(2)	15(1)	10(2)
F10	44(1)	90(2)	70(2)	45(1)	35(1)	25(1)
F11	68(1)	42(1)	29(1)	7(1)	21(1)	13(1)
F12	51(1)	34(1)	47(1)	16(1)	22(1)	4(1)
C19	31(2)	22(2)	23(2)	1(1)	9(1)	4(1)
C20	30(2)	20(2)	25(2)	3(1)	12(1)	3(1)
C21	29(2)	21(2)	22(2)	1(1)	10(1)	1(1)
C22	31(2)	24(2)	23(2)	6(1)	9(1)	1(1)
C23	35(2)	28(2)	23(2)	3(1)	12(1)	4(1)
C24	53(2)	43(2)	23(2)	6(2)	17(2)	15(2)
F13	53(1)	27(1)	40(1)	5(1)	11(1)	8(1)
F14	49(1)	59(1)	66(1)	34(1)	35(1)	22(1)
F15	112(2)	82(2)	27(1)	7(1)	25(1)	62(2)
C25	45(2)	34(2)	19(2)	1(1)	14(1)	4(2)
C26	39(2)	38(2)	20(2)	6(1)	4(1)	3(1)
C27	31(2)	27(2)	23(2)	8(1)	7(1)	1(1)
C28	38(2)	37(2)	21(2)	5(1)	6(1)	5(1)
F16	37(1)	47(1)	44(1)	9(1)	18(1)	7(1)
F17	57(1)	73(2)	26(1)	8(1)	1(1)	32(1)
F18	61(1)	32(1)	41(1)	12(1)	20(1)	13(1)
C29	28(2)	25(2)	21(2)	5(1)	9(1)	1(1)
C30	28(1)	23(2)	21(2)	6(1)	8(1)	2(1)
C31	23(1)	24(2)	25(2)	5(1)	8(1)	2(1)
C32	30(2)	26(2)	27(2)	7(1)	13(1)	5(1)
C33	37(2)	31(2)	34(2)	12(1)	16(1)	10(1)
C34	45(2)	32(2)	37(2)	13(2)	13(2)	15(2)
F19	40(1)	44(1)	36(1)	11(1)	9(1)	6(1)
F20	53(1)	41(1)	34(1)	11(1)	19(1)	0(1)
F21	96(2)	52(1)	45(1)	24(1)	24(1)	45(1)
C35	64(2)	38(2)	43(2)	18(2)	25(2)	30(2)

C36	74(3)	39(2)	35(2)	8(2)	29(2)	27(2)
C37	47(2)	30(2)	31(2)	6(1)	19(2)	13(2)
C38	64(2)	33(2)	34(2)	3(2)	22(2)	17(2)
F22	51(1)	41(1)	36(1)	2(1)	6(1)	2(1)
F23	64(1)	86(2)	38(1)	27(1)	28(1)	30(1)
F24	136(2)	40(1)	37(1)	-9(1)	13(1)	31(1)
C39	30(2)	26(2)	27(2)	6(1)	13(1)	5(1)
C40	24(1)	25(2)	26(2)	2(1)	10(1)	3(1)
N9	25(1)	25(1)	19(1)	6(1)	6(1)	5(1)
N10	25(1)	27(1)	23(1)	6(1)	7(1)	5(1)
N11	27(1)	25(1)	21(1)	6(1)	10(1)	5(1)
N12	31(1)	28(1)	24(1)	10(1)	11(1)	5(1)
N13	30(1)	24(1)	22(1)	7(1)	9(1)	6(1)
N14	29(1)	23(1)	26(1)	7(1)	7(1)	4(1)
N15	26(1)	23(1)	22(1)	4(1)	8(1)	4(1)
N16	24(1)	29(1)	22(1)	7(1)	6(1)	5(1)
C41	23(1)	26(2)	21(2)	6(1)	3(1)	5(1)
C42	28(2)	29(2)	23(2)	9(1)	5(1)	4(1)
C43	34(2)	30(2)	29(2)	10(1)	7(1)	7(1)
C44	49(2)	34(2)	39(2)	16(2)	13(2)	16(2)
F25	38(1)	52(1)	41(1)	7(1)	11(1)	14(1)
F26	51(1)	35(1)	35(1)	4(1)	14(1)	5(1)
F27	92(2)	50(1)	61(1)	32(1)	35(1)	42(1)
C45	51(2)	38(2)	36(2)	20(2)	11(2)	15(2)
C46	50(2)	44(2)	31(2)	19(2)	12(2)	9(2)
C47	35(2)	39(2)	26(2)	13(1)	9(1)	7(1)
C48	55(2)	52(2)	37(2)	25(2)	23(2)	18(2)
F28	38(1)	56(1)	56(1)	23(1)	22(1)	12(1)
F29	71(1)	70(2)	29(1)	4(1)	11(1)	29(1)
F30	115(2)	100(2)	94(2)	75(2)	82(2)	59(2)
C49	28(2)	31(2)	21(2)	9(1)	4(1)	4(1)
C50	25(1)	30(2)	19(2)	7(1)	5(1)	3(1)
C51	22(1)	29(2)	23(2)	5(1)	8(1)	3(1)
C52	23(1)	29(2)	25(2)	3(1)	9(1)	2(1)
C53	28(2)	34(2)	27(2)	1(1)	10(1)	1(1)
C54	37(2)	43(2)	28(2)	-1(2)	12(1)	1(2)

F31	37(1)	59(1)	36(1)	15(1)	2(1)	3(1)
F32	43(1)	48(1)	46(1)	15(1)	19(1)	2(1)
F33	102(2)	58(1)	25(1)	3(1)	25(1)	16(1)
C55	36(2)	38(2)	32(2)	-5(2)	13(2)	3(2)
C56	38(2)	30(2)	38(2)	-3(2)	12(2)	10(1)
C57	29(2)	28(2)	37(2)	2(1)	8(1)	6(1)
C58	56(2)	26(2)	40(2)	0(2)	11(2)	16(2)
F34	113(2)	29(1)	55(1)	5(1)	17(1)	27(1)
F35	52(1)	63(1)	46(1)	14(1)	7(1)	26(1)
F36	56(1)	32(1)	52(1)	15(1)	15(1)	5(1)
C59	22(1)	28(2)	29(2)	3(1)	7(1)	3(1)
C60	24(1)	22(2)	28(2)	7(1)	7(1)	4(1)
C61	29(2)	24(2)	28(2)	11(1)	9(1)	1(1)
C62	30(2)	27(2)	27(2)	13(1)	8(1)	1(1)
C63	34(2)	31(2)	32(2)	16(1)	8(1)	5(1)
C64	41(2)	38(2)	39(2)	15(2)	5(2)	11(2)
F37	72(2)	69(2)	48(1)	19(1)	5(1)	46(1)
F38	40(1)	48(1)	44(1)	10(1)	14(1)	10(1)
F39	60(1)	32(1)	48(1)	9(1)	14(1)	6(1)
C65	39(2)	42(2)	36(2)	22(2)	6(2)	11(2)
C66	40(2)	46(2)	28(2)	18(2)	5(1)	6(2)
C67	35(2)	37(2)	27(2)	13(1)	9(1)	3(1)
C68	49(2)	51(2)	25(2)	12(2)	7(2)	8(2)
F40	55(1)	36(1)	39(1)	7(1)	11(1)	4(1)
F41	82(2)	81(2)	27(1)	-2(1)	-7(1)	29(1)
F42	74(2)	65(1)	51(1)	29(1)	40(1)	25(1)
C69	30(2)	27(2)	26(2)	11(1)	9(1)	2(1)
C70	30(2)	26(2)	27(2)	11(1)	10(1)	1(1)
C71	30(2)	24(2)	20(2)	3(1)	10(1)	0(1)
C72	32(2)	21(2)	27(2)	3(1)	13(1)	0(1)
C73	41(2)	25(2)	30(2)	5(1)	19(1)	1(1)
C74	48(2)	35(2)	36(2)	10(2)	24(2)	8(2)
F43	68(1)	38(1)	48(1)	22(1)	27(1)	12(1)
F44	72(1)	75(2)	36(1)	21(1)	37(1)	24(1)
F45	53(1)	47(1)	31(1)	10(1)	14(1)	6(1)
C75	45(2)	30(2)	39(2)	5(2)	27(2)	6(2)

C76	36(2)	30(2)	40(2)	4(2)	20(2)	6(1)
C77	30(2)	25(2)	30(2)	1(1)	13(1)	3(1)
C78	26(2)	40(2)	37(2)	0(2)	10(1)	6(1)
F46	45(1)	44(1)	45(1)	19(1)	14(1)	13(1)
F47	30(1)	66(1)	54(1)	13(1)	14(1)	18(1)
F48	40(1)	59(1)	32(1)	-1(1)	5(1)	12(1)
C79	25(1)	24(2)	26(2)	2(1)	9(1)	0(1)
C80	23(1)	26(2)	25(2)	4(1)	8(1)	3(1)
C81	56(2)	57(3)	70(3)	28(2)	6(2)	-10(2)
C82	64(3)	66(3)	60(3)	4(2)	29(2)	-11(2)
C83	69(3)	63(3)	129(5)	29(3)	45(3)	13(2)
C84	87(4)	93(4)	104(5)	58(4)	28(3)	20(3)
C85	131(5)	93(4)	75(4)	36(3)	36(4)	17(4)
C86	91(3)	61(3)	62(3)	11(2)	33(3)	17(3)
C87	80(4)	113(5)	127(5)	77(4)	-19(3)	-21(3)
C88	92(9)	91(10)	80(9)	28(7)	30(8)	56(8)
C89	86(5)	114(5)	92(5)	43(4)	21(4)	-1(4)
C90	74(7)	60(7)	62(7)	26(5)	26(6)	12(5)
C91	100(10)	80(9)	75(9)	26(7)	29(7)	29(7)
C92	76(8)	85(9)	70(8)	6(7)	23(6)	19(7)
C93	57(7)	156(14)	100(11)	50(10)	29(7)	23(8)
C94	94(5)	126(6)	105(4)	15(4)	23(4)	16(4)
C88'	79(5)	86(5)	60(4)	35(4)	16(4)	8(4)
C89'	86(5)	105(5)	68(5)	50(4)	20(4)	-6(5)
C90'	86(5)	114(5)	92(5)	43(4)	21(4)	-1(4)
C91'	94(5)	126(6)	105(4)	15(4)	23(4)	16(4)
C92'	85(5)	92(6)	73(4)	30(4)	24(4)	24(4)
C93'	79(5)	77(4)	64(4)	30(4)	32(4)	16(4)
C94'	97(8)	89(10)	93(9)	61(7)	10(7)	23(7)
C88"	79(5)	86(5)	60(4)	35(4)	16(4)	8(4)
C89"	86(5)	105(5)	68(5)	50(4)	20(4)	-6(5)
C90"	86(5)	114(5)	92(5)	43(4)	21(4)	-1(4)
C91"	94(5)	126(6)	105(4)	15(4)	23(4)	16(4)
C92"	85(5)	92(6)	73(4)	30(4)	24(4)	24(4)
C93"	79(5)	77(4)	64(4)	30(4)	32(4)	16(4)
C94"	97(8)	89(10)	93(9)	61(7)	10(7)	23(7)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 03029.

	x	y	z	U(eq)
H5A	511	6523	10405	49
H6A	1071	5240	10096	57
H15A	4811	3586	7235	43
H16A	5061	4073	6363	43
H25A	201	5629	3351	40
H26A	-1030	6498	3444	41
H35A	-1781	10289	7158	53
H36A	-1102	10460	8307	55
H45A	5623	5662	10009	48
H46A	4619	6368	10605	48
H55A	2801	11562	10814	46
H56A	2451	12300	10024	45
H65A	779	10471	5461	45
H66A	1233	9391	4727	45
H75A	6966	6971	5648	43
H76A	7844	6590	6581	42
H82A	5398	8691	2371	79
H83A	6408	8080	3112	100
H84A	6497	8444	4242	107
H85A	5543	9429	4627	116
H86A	4469	10020	3901	85
H87A	4560	10021	2339	167
H87B	3900	10270	2849	167
H87C	3582	9381	2273	167
H89	3265	7562	2182	117
H90	1949	8042	1487	75
H91	319	7990	1635	100
H92	5	7459	2477	96
H93	1321	6979	3172	121
H94A	3126	6832	3534	171

H94B	3821	7572	3432	171
H94C	3641	6633	2939	171
H89'	1171	6375	1528	100
H90'	1829	7770	2186	117
H91'	2966	8057	3282	137
H92'	3445	6950	3719	98
H93'	2788	5555	3061	83
H94D	1696	4588	1980	134
H94E	1678	4953	1360	134
H94F	716	4970	1645	134
H89"	2425	6646	1533	100
H90"	3537	7765	2404	117
H91"	3874	7768	3532	137
H92"	3098	6651	3789	98
H93"	1985	5532	2918	83
H94G	1153	4903	1774	134
H94H	1815	5057	1297	134
H94I	867	5551	1344	134

Table 6. Torsion angles [°] for 03029.

N7-Fe1-O1-Fe2	158(5)	N1-Fe1-N7-C31	-171.3(2)
N3-Fe1-O1-Fe2	-21(5)	N5-Fe1-N7-C31	-23.7(2)
N1-Fe1-O1-Fe2	68(5)	O1-Fe1-N7-C40	-64.0(2)
N5-Fe1-O1-Fe2	-112(5)	N3-Fe1-N7-C40	113.5(2)
N13-Fe2-O1-Fe1	142(5)	N1-Fe1-N7-C40	39.8(2)
N9-Fe2-O1-Fe1	-37(5)	N5-Fe1-N7-C40	-172.5(2)
N11-Fe2-O1-Fe1	53(5)	C40-N8-C1-N1	13.6(4)
N15-Fe2-O1-Fe1	-128(5)	C40-N8-C1-C2	-166.5(3)
O1-Fe1-N1-C10	-94.9(2)	C10-N1-C1-N8	178.5(3)
N7-Fe1-N1-C10	161.8(2)	Fe1-N1-C1-N8	5.6(4)
N3-Fe1-N1-C10	8.7(2)	C10-N1-C1-C2	-1.4(3)
N5-Fe1-N1-C10	85.1(3)	Fe1-N1-C1-C2	-174.32(18)
O1-Fe1-N1-C1	76.7(2)	N8-C1-C2-C9	177.7(3)
N7-Fe1-N1-C1	-26.6(2)	N1-C1-C2-C9	-2.4(3)
N3-Fe1-N1-C1	-179.6(2)	N8-C1-C2-C3	-2.1(5)
N5-Fe1-N1-C1	-103.3(2)	N1-C1-C2-C3	177.8(3)
O1-Fe1-N3-C11	79.5(2)	C9-C2-C3-C5	-0.3(4)
N7-Fe1-N3-C11	-98.0(3)	C1-C2-C3-C5	179.4(3)
N1-Fe1-N3-C11	-24.1(2)	C9-C2-C3-C4	176.9(3)
N5-Fe1-N3-C11	-171.9(2)	C1-C2-C3-C4	-3.4(5)
O1-Fe1-N3-C20	-69.3(2)	C5-C3-C4-F1	118.0(3)
N7-Fe1-N3-C20	113.1(2)	C2-C3-C4-F1	-59.1(4)
N1-Fe1-N3-C20	-173.0(2)	C5-C3-C4-F2	-119.7(3)
N5-Fe1-N3-C20	39.3(2)	C2-C3-C4-F2	63.1(4)
O1-Fe1-N5-C21	82.2(2)	C5-C3-C4-F3	-2.0(4)
N7-Fe1-N5-C21	-174.6(2)	C2-C3-C4-F3	-179.1(3)
N3-Fe1-N5-C21	-21.6(2)	C2-C3-C5-C6	-3.2(5)
N1-Fe1-N5-C21	-97.8(3)	C4-C3-C5-C6	179.5(3)
O1-Fe1-N5-C30	-94.6(2)	C3-C5-C6-C7	2.4(6)
N7-Fe1-N5-C30	8.6(2)	C5-C6-C7-C9	2.0(6)
N3-Fe1-N5-C30	161.6(2)	C5-C6-C7-C8	-177.0(3)
N1-Fe1-N5-C30	85.4(3)	C6-C7-C8-F5	-100.2(4)
O1-Fe1-N7-C31	84.8(2)	C9-C7-C8-F5	80.8(4)
N3-Fe1-N7-C31	-97.6(3)	C6-C7-C8-F4	136.8(3)

C9-C7-C8-F4	-42.1(5)	C12-C13-C14-F9	57.5(4)
C6-C7-C8-F6	18.7(5)	C15-C13-C14-F8	115.6(3)
C9-C7-C8-F6	-160.2(3)	C12-C13-C14-F8	-64.9(4)
C6-C7-C9-C2	-5.4(5)	C15-C13-C14-F7	-2.9(4)
C8-C7-C9-C2	173.5(3)	C12-C13-C14-F7	176.6(3)
C6-C7-C9-C10	174.3(3)	C12-C13-C15-C16	3.0(5)
C8-C7-C9-C10	-6.8(6)	C14-C13-C15-C16	-177.5(3)
C3-C2-C9-C7	4.6(5)	C13-C15-C16-C17	-4.6(5)
C1-C2-C9-C7	-175.2(3)	C15-C16-C17-C19	0.2(5)
C3-C2-C9-C10	-175.2(3)	C15-C16-C17-C18	177.2(3)
C1-C2-C9-C10	5.0(3)	C16-C17-C18-F12	-143.2(3)
C11-N2-C10-N1	-6.6(5)	C19-C17-C18-F12	33.7(4)
C11-N2-C10-C9	-178.7(3)	C16-C17-C18-F11	94.7(3)
C1-N1-C10-N2	-168.5(3)	C19-C17-C18-F11	-88.5(4)
Fe1-N1-C10-N2	4.0(4)	C16-C17-C18-F10	-23.8(4)
C1-N1-C10-C9	4.6(3)	C19-C17-C18-F10	153.1(3)
Fe1-N1-C10-C9	177.15(19)	C13-C12-C19-C17	-7.2(4)
C7-C9-C10-N2	-12.4(5)	C11-C12-C19-C17	171.8(3)
C2-C9-C10-N2	167.3(3)	C13-C12-C19-C20	173.3(3)
C7-C9-C10-N1	174.2(3)	C11-C12-C19-C20	-7.7(3)
C2-C9-C10-N1	-6.0(3)	C16-C17-C19-C12	5.6(4)
C10-N2-C11-N3	-11.7(4)	C18-C17-C19-C12	-171.2(3)
C10-N2-C11-C12	168.9(3)	C16-C17-C19-C20	-175.0(3)
C20-N3-C11-N2	-178.0(3)	C18-C17-C19-C20	8.2(5)
Fe1-N3-C11-N2	30.7(4)	C21-N4-C20-N3	7.1(5)
C20-N3-C11-C12	1.5(3)	C21-N4-C20-C19	178.1(3)
Fe1-N3-C11-C12	-149.82(19)	C11-N3-C20-N4	165.9(3)
N2-C11-C12-C19	-176.4(3)	Fe1-N3-C20-N4	-40.7(4)
N3-C11-C12-C19	4.1(3)	C11-N3-C20-C19	-6.4(3)
N2-C11-C12-C13	2.4(5)	Fe1-N3-C20-C19	147.06(19)
N3-C11-C12-C13	-177.1(3)	C12-C19-C20-N4	-163.5(3)
C19-C12-C13-C15	2.8(4)	C17-C19-C20-N4	17.1(5)
C11-C12-C13-C15	-175.9(3)	C12-C19-C20-N3	8.9(3)
C19-C12-C13-C14	-176.7(3)	C17-C19-C20-N3	-170.5(3)
C11-C12-C13-C14	4.6(5)	C20-N4-C21-N5	16.4(5)
C15-C13-C14-F9	-122.0(3)	C20-N4-C21-C22	-166.0(3)

C30-N5-C21-N4	176.0(3)	C28-C27-C29-C30	-5.5(5)
Fe1-N5-C21-N4	-1.3(4)	C31-N6-C30-N5	-7.1(5)
C30-N5-C21-C22	-1.9(3)	C31-N6-C30-C29	177.2(3)
Fe1-N5-C21-C22	-179.24(18)	C21-N5-C30-N6	-172.9(3)
N4-C21-C22-C29	-178.3(3)	Fe1-N5-C30-N6	4.3(4)
N5-C21-C22-C29	-0.3(3)	C21-N5-C30-C29	3.4(3)
N4-C21-C22-C23	2.9(5)	Fe1-N5-C30-C29	-179.44(18)
N5-C21-C22-C23	-179.1(3)	C22-C29-C30-N6	172.8(3)
C29-C22-C23-C25	2.3(4)	C27-C29-C30-N6	-6.6(5)
C21-C22-C23-C25	-179.1(3)	C22-C29-C30-N5	-3.5(3)
C29-C22-C23-C24	179.8(3)	C27-C29-C30-N5	177.1(3)
C21-C22-C23-C24	-1.6(5)	C30-N6-C31-N7	-10.9(4)
C25-C23-C24-F14	108.5(3)	C30-N6-C31-C32	169.3(3)
C22-C23-C24-F14	-69.0(4)	C40-N7-C31-N6	-179.0(3)
C25-C23-C24-F13	-129.1(3)	Fe1-N7-C31-N6	29.8(4)
C22-C23-C24-F13	53.5(4)	C40-N7-C31-C32	0.8(3)
C25-C23-C24-F15	-10.8(4)	Fe1-N7-C31-C32	-150.32(19)
C22-C23-C24-F15	171.7(3)	N6-C31-C32-C33	1.3(5)
C22-C23-C25-C26	-3.2(5)	N7-C31-C32-C33	-178.6(3)
C24-C23-C25-C26	179.2(3)	N6-C31-C32-C39	-176.4(3)
C23-C25-C26-C27	1.0(5)	N7-C31-C32-C39	3.7(3)
C25-C26-C27-C29	2.0(5)	C39-C32-C33-C35	0.4(5)
C25-C26-C27-C28	-176.1(3)	C31-C32-C33-C35	-177.0(3)
C26-C27-C28-F18	-111.0(3)	C39-C32-C33-C34	178.1(3)
C29-C27-C28-F18	70.9(4)	C31-C32-C33-C34	0.7(5)
C26-C27-C28-F16	127.2(3)	C35-C33-C34-F19	-122.9(3)
C29-C27-C28-F16	-50.9(4)	C32-C33-C34-F19	59.4(4)
C26-C27-C28-F17	7.7(4)	C35-C33-C34-F20	115.2(3)
C29-C27-C28-F17	-170.4(3)	C32-C33-C34-F20	-62.5(4)
C23-C22-C29-C27	0.7(4)	C35-C33-C34-F21	-3.7(4)
C21-C22-C29-C27	-178.2(3)	C32-C33-C34-F21	178.6(3)
C23-C22-C29-C30	-178.8(3)	C32-C33-C35-C36	3.9(5)
C21-C22-C29-C30	2.3(3)	C34-C33-C35-C36	-173.9(3)
C26-C27-C29-C22	-2.8(4)	C33-C35-C36-C37	-2.8(6)
C28-C27-C29-C22	175.2(3)	C35-C36-C37-C39	-2.7(5)
C26-C27-C29-C30	176.4(3)	C35-C36-C37-C38	174.5(3)

C36-C37-C38-F23	95.8(4)	O1-Fe2-N11-C80	-97.8(2)
C39-C37-C38-F23	-87.2(4)	N13-Fe2-N11-C80	160.7(2)
C36-C37-C38-F22	-141.9(3)	N9-Fe2-N11-C80	7.3(2)
C39-C37-C38-F22	35.1(5)	N15-Fe2-N11-C80	84.0(3)
C36-C37-C38-F24	-24.2(5)	O1-Fe2-N13-C61	78.8(2)
C39-C37-C38-F24	152.8(3)	N9-Fe2-N13-C61	-102.4(3)
C33-C32-C39-C37	-5.9(4)	N11-Fe2-N13-C61	-176.2(2)
C31-C32-C39-C37	172.2(3)	N15-Fe2-N13-C61	-28.7(2)
C33-C32-C39-C40	175.4(3)	O1-Fe2-N13-C70	-66.3(2)
C31-C32-C39-C40	-6.5(3)	N9-Fe2-N13-C70	112.5(2)
C36-C37-C39-C32	7.0(5)	N11-Fe2-N13-C70	38.7(2)
C38-C37-C39-C32	-169.9(3)	N15-Fe2-N13-C70	-173.8(2)
C36-C37-C39-C40	-174.8(3)	O1-Fe2-N15-C60	-92.8(2)
C38-C37-C39-C40	8.3(6)	N13-Fe2-N15-C60	8.8(2)
C1-N8-C40-N7	4.6(4)	N9-Fe2-N15-C60	162.2(2)
C1-N8-C40-C39	177.3(3)	N11-Fe2-N15-C60	85.4(3)
C31-N7-C40-N8	168.8(3)	O1-Fe2-N15-C51	86.6(2)
Fe1-N7-C40-N8	-37.8(4)	N13-Fe2-N15-C51	-171.8(2)
C31-N7-C40-C39	-4.9(3)	N9-Fe2-N15-C51	-18.3(2)
Fe1-N7-C40-C39	148.47(19)	N11-Fe2-N15-C51	-95.2(3)
C32-C39-C40-N8	-166.7(3)	C80-N10-C41-N9	-12.6(4)
C37-C39-C40-N8	14.9(5)	C80-N10-C41-C42	171.8(3)
C32-C39-C40-N7	7.2(3)	C50-N9-C41-N10	-172.2(3)
C37-C39-C40-N7	-171.2(3)	Fe2-N9-C41-N10	35.5(4)
O1-Fe2-N9-C50	-71.5(2)	C50-N9-C41-C42	4.0(3)
N13-Fe2-N9-C50	109.7(3)	Fe2-N9-C41-C42	-148.30(19)
N11-Fe2-N9-C50	-176.6(2)	N10-C41-C42-C43	-4.9(5)
N15-Fe2-N9-C50	35.9(2)	N9-C41-C42-C43	178.9(3)
O1-Fe2-N9-C41	77.9(2)	N10-C41-C42-C49	175.9(3)
N13-Fe2-N9-C41	-100.9(3)	N9-C41-C42-C49	-0.3(3)
N11-Fe2-N9-C41	-27.2(2)	C49-C42-C43-C45	0.9(4)
N15-Fe2-N9-C41	-174.7(2)	C41-C42-C43-C45	-178.2(3)
O1-Fe2-N11-C71	81.4(2)	C49-C42-C43-C44	-177.9(3)
N13-Fe2-N11-C71	-20.1(2)	C41-C42-C43-C44	3.0(5)
N9-Fe2-N11-C71	-173.6(2)	C45-C43-C44-F26	127.2(3)
N15-Fe2-N11-C71	-96.8(3)	C42-C43-C44-F26	-54.0(4)

C45-C43-C44-F25	-110.8(3)	Fe2-N15-C51-N16	-2.5(4)
C42-C43-C44-F25	68.0(4)	C60-N15-C51-C52	-1.0(3)
C45-C43-C44-F27	7.9(4)	Fe2-N15-C51-C52	179.42(17)
C42-C43-C44-F27	-173.3(3)	N16-C51-C52-C59	-179.6(3)
C42-C43-C45-C46	1.9(5)	N15-C51-C52-C59	-1.5(3)
C44-C43-C45-C46	-179.3(3)	N16-C51-C52-C53	-1.1(5)
C43-C45-C46-C47	-2.1(5)	N15-C51-C52-C53	177.0(3)
C45-C46-C47-C49	-0.5(5)	C59-C52-C53-C55	0.9(4)
C45-C46-C47-C48	179.2(3)	C51-C52-C53-C55	-177.4(3)
C46-C47-C48-F28	-135.4(3)	C59-C52-C53-C54	-179.5(3)
C49-C47-C48-F28	44.4(5)	C51-C52-C53-C54	2.2(5)
C46-C47-C48-F29	102.6(4)	C55-C53-C54-F32	112.5(3)
C49-C47-C48-F29	-77.6(4)	C52-C53-C54-F32	-67.1(4)
C46-C47-C48-F30	-16.6(5)	C55-C53-C54-F31	-125.1(3)
C49-C47-C48-F30	163.1(3)	C52-C53-C54-F31	55.2(4)
C43-C42-C49-C47	-3.5(4)	C55-C53-C54-F33	-6.7(4)
C41-C42-C49-C47	175.9(3)	C52-C53-C54-F33	173.7(3)
C43-C42-C49-C50	177.5(3)	C52-C53-C55-C56	-3.7(5)
C41-C42-C49-C50	-3.1(3)	C54-C53-C55-C56	176.7(3)
C46-C47-C49-C42	3.3(4)	C53-C55-C56-C57	1.7(5)
C48-C47-C49-C42	-176.5(3)	C55-C56-C57-C59	3.1(5)
C46-C47-C49-C50	-178.0(3)	C55-C56-C57-C58	-176.6(3)
C48-C47-C49-C50	2.2(5)	C56-C57-C58-F35	-100.0(3)
C51-N16-C50-N9	8.2(4)	C59-C57-C58-F35	80.4(4)
C51-N16-C50-C49	-178.7(3)	C56-C57-C58-F36	136.6(3)
C41-N9-C50-N16	168.1(3)	C59-C57-C58-F36	-43.0(4)
Fe2-N9-C50-N16	-38.8(4)	C56-C57-C58-F34	18.3(4)
C41-N9-C50-C49	-6.0(3)	C59-C57-C58-F34	-161.3(3)
Fe2-N9-C50-C49	147.12(19)	C53-C52-C59-C57	3.9(4)
C42-C49-C50-N16	-168.5(3)	C51-C52-C59-C57	-177.4(3)
C47-C49-C50-N16	12.6(5)	C53-C52-C59-C60	-175.5(3)
C42-C49-C50-N9	5.6(3)	C51-C52-C59-C60	3.2(3)
C47-C49-C50-N9	-173.2(3)	C56-C57-C59-C52	-5.8(4)
C50-N16-C51-N15	14.6(4)	C58-C57-C59-C52	173.9(3)
C50-N16-C51-C52	-167.7(3)	C56-C57-C59-C60	173.4(3)
C60-N15-C51-N16	177.0(3)	C58-C57-C59-C60	-7.0(5)

C61-N14-C60-N15	-11.8(4)	C69-C67-C68-F42	-83.6(4)
C61-N14-C60-C59	175.3(3)	C66-C67-C68-F41	-21.4(4)
C51-N15-C60-N14	-170.7(3)	C69-C67-C68-F41	156.7(3)
Fe2-N15-C60-N14	8.9(4)	C66-C67-C68-F40	-139.7(3)
C51-N15-C60-C59	3.1(3)	C69-C67-C68-F40	38.4(4)
Fe2-N15-C60-C59	-177.36(18)	C63-C62-C69-C67	-4.6(4)
C52-C59-C60-N14	170.0(3)	C61-C62-C69-C67	174.3(3)
C57-C59-C60-N14	-9.2(5)	C63-C62-C69-C70	176.5(3)
C52-C59-C60-N15	-4.0(3)	C61-C62-C69-C70	-4.6(3)
C57-C59-C60-N15	176.7(3)	C66-C67-C69-C62	6.1(4)
C60-N14-C61-N13	-12.8(4)	C68-C67-C69-C62	-172.0(3)
C60-N14-C61-C62	170.2(3)	C66-C67-C69-C70	-175.3(3)
C70-N13-C61-N14	-175.3(3)	C68-C67-C69-C70	6.6(5)
Fe2-N13-C61-N14	36.6(4)	C71-N12-C70-N13	9.5(5)
C70-N13-C61-C62	2.2(3)	C71-N12-C70-C69	-178.0(3)
Fe2-N13-C61-C62	-145.93(19)	C61-N13-C70-N12	168.4(3)
N14-C61-C62-C69	179.2(3)	Fe2-N13-C70-N12	-42.1(4)
N13-C61-C62-C69	1.7(3)	C61-N13-C70-C69	-5.1(3)
N14-C61-C62-C63	-2.1(5)	Fe2-N13-C70-C69	144.43(19)
N13-C61-C62-C63	-179.6(3)	C62-C69-C70-N12	-167.5(3)
C69-C62-C63-C65	-0.2(4)	C67-C69-C70-N12	13.7(5)
C61-C62-C63-C65	-178.8(3)	C62-C69-C70-N13	6.1(3)
C69-C62-C63-C64	179.2(3)	C67-C69-C70-N13	-172.7(3)
C61-C62-C63-C64	0.6(5)	C70-N12-C71-N11	15.1(5)
C65-C63-C64-F39	-113.1(3)	C70-N12-C71-C72	-165.1(3)
C62-C63-C64-F39	67.4(4)	C80-N11-C71-N12	177.0(3)
C65-C63-C64-F38	124.7(3)	Fe2-N11-C71-N12	-2.3(4)
C62-C63-C64-F38	-54.7(4)	C80-N11-C71-C72	-2.8(3)
C65-C63-C64-F37	6.2(4)	Fe2-N11-C71-C72	177.90(18)
C62-C63-C64-F37	-173.2(3)	N12-C71-C72-C79	179.7(3)
C62-C63-C65-C66	3.6(5)	N11-C71-C72-C79	-0.5(3)
C64-C63-C65-C66	-175.9(3)	N12-C71-C72-C73	0.4(5)
C63-C65-C66-C67	-2.0(5)	N11-C71-C72-C73	-179.8(3)
C65-C66-C67-C69	-2.8(5)	C79-C72-C73-C75	-3.4(4)
C65-C66-C67-C68	175.4(3)	C71-C72-C73-C75	175.7(3)
C66-C67-C68-F42	98.3(3)	C79-C72-C73-C74	173.9(3)

C71-C72-C73-C74	-6.9(5)	C86-C81-C82-C83	0.5(6)
C75-C73-C74-F45	120.9(3)	C87-C81-C82-C83	-179.3(4)
C72-C73-C74-F45	-56.4(4)	C81-C82-C83-C84	-1.1(7)
C75-C73-C74-F43	-117.7(3)	C82-C83-C84-C85	0.3(8)
C72-C73-C74-F43	65.0(4)	C83-C84-C85-C86	1.0(9)
C75-C73-C74-F44	1.9(4)	C84-C85-C86-C81	-1.6(9)
C72-C73-C74-F44	-175.4(3)	C82-C81-C86-C85	0.8(7)
C72-C73-C75-C76	0.6(5)	C87-C81-C86-C85	-179.3(5)
C74-C73-C75-C76	-176.9(3)	C93-C88-C89-C90	0.0
C73-C75-C76-C77	1.8(5)	C94-C88-C89-C90	-172.2
C75-C76-C77-C79	-1.2(5)	C88-C89-C90-C91	0.0
C75-C76-C77-C78	178.2(3)	C89-C90-C91-C92	0.0
C76-C77-C78-F48	131.2(3)	C90-C91-C92-C93	0.0
C79-C77-C78-F48	-49.5(4)	C91-C92-C93-C88	0.0
C76-C77-C78-F46	-106.7(3)	C89-C88-C93-C92	0.0
C79-C77-C78-F46	72.7(4)	C94-C88-C93-C92	171.4
C76-C77-C78-F47	11.8(4)	C93'-C88'-C89'-C90'	0.0
C79-C77-C78-F47	-168.8(3)	C94'-C88'-C89'-C90'	-179.1
C73-C72-C79-C77	4.0(4)	C88'-C89'-C90'-C91'	0.0
C71-C72-C79-C77	-175.3(3)	C89'-C90'-C91'-C92'	0.0
C73-C72-C79-C80	-177.3(3)	C90'-C91'-C92'-C93'	0.0
C71-C72-C79-C80	3.3(3)	C91'-C92'-C93'-C88'	0.0
C76-C77-C79-C72	-1.7(4)	C89'-C88'-C93'-C92'	0.0
C78-C77-C79-C72	179.0(3)	C94'-C88'-C93'-C92'	179.0
C76-C77-C79-C80	-179.9(3)	C93"-C88"-C89"-C90"	0.0
C78-C77-C79-C80	0.7(5)	C94"-C88"-C89"-C90"	179.90(13)
C41-N10-C80-N11	-12.0(5)	C88"-C89"-C90"-C91"	0.0
C41-N10-C80-C79	174.8(3)	C89"-C90"-C91"-C92"	0.0
C71-N11-C80-N10	-169.2(3)	C90"-C91"-C92"-C93"	0.0
Fe2-N11-C80-N10	10.1(4)	C91"-C92"-C93"-C88"	0.0
C71-N11-C80-C79	4.9(3)	C89"-C88"-C93"-C92"	0.0
Fe2-N11-C80-C79	-175.81(18)	C94"-C88"-C93"-C92"	-179.89(14)
C72-C79-C80-N10	169.1(3)		
C77-C79-C80-N10	-12.5(5)		
C72-C79-C80-N11	-5.2(3)		
C77-C79-C80-N11	173.3(3)		

Symmetry transformations used to generate equivalent atoms: