

Table 1. Crystal data and structure refinement for FcC 1.

Identification code	JVB-9-Fe	
Empirical formula	C ₁₉ H ₁₅ Cl Fe O	
Formula weight	350.61	
Temperature	293(2) K	
Wavelength	0.56083 Å	
Crystal system	Orthorhombic	
Space group	P2 ₁ 2 ₁ 2 ₁	
Unit cell dimensions	a = 5.8022(3) Å	α = 90°.
	b = 10.5286(5) Å	β = 90°.
	c = 25.5874(12) Å	γ = 90°.
Volume	1563.11(13) Å ³	
Z	4	
Density (calculated)	1.490 Mg/m ³	
Absorption coefficient	0.591 mm ⁻¹	
F(000)	720	
Theta range for data collection	1.977 to 20.517°.	
Index ranges	-7 ≤ h ≤ 7, -13 ≤ k ≤ 13, -31 ≤ l ≤ 31	
Reflections collected	42477	
Independent reflections	3196 [R(int) = 0.0951]	
Completeness to theta = 19.664°	99.9 %	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3196 / 0 / 199	
Goodness-of-fit on F ²	1.019	
Final R indices [I > 2σ(I)]	R1 = 0.0500, wR2 = 0.1175	
R indices (all data)	R1 = 0.0595, wR2 = 0.1257	
Absolute structure parameter	0.08(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.971 and -0.246 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for FeC

1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Fe(1)	5177(1)	4980(1)	4128(1)	48(1)
Cl(1)	5508(4)	7735(2)	7786(1)	95(1)
O(1)	1012(6)	4912(4)	5261(2)	73(1)
C(1)	3764(8)	3957(5)	4719(2)	51(1)
C(2)	2993(9)	4573(5)	5202(2)	57(1)
C(3)	4730(9)	4752(5)	5618(2)	59(1)
C(4)	4236(9)	5362(5)	6055(2)	56(1)
C(5)	5765(9)	5580(5)	6500(2)	52(1)
C(6)	5043(10)	6402(4)	6889(2)	56(1)
C(7)	6440(10)	6630(5)	7317(2)	63(1)
C(8)	8529(10)	6048(6)	7377(2)	70(2)
C(9)	9232(10)	5209(5)	6992(2)	69(1)
C(10)	7900(8)	4991(6)	6555(2)	59(1)
C(11)	2381(9)	3849(5)	4261(2)	56(1)
C(12)	3752(12)	3309(5)	3862(2)	63(2)
C(13)	5995(11)	3089(5)	4063(2)	63(1)
C(14)	6001(10)	3486(4)	4590(2)	55(1)
C(15)	5574(12)	6805(5)	4382(3)	76(2)
C(16)	4117(13)	6772(6)	3941(3)	79(2)
C(17)	5370(14)	6242(6)	3527(3)	84(2)
C(18)	7589(12)	5955(6)	3713(3)	78(2)
C(19)	7705(10)	6307(5)	4239(3)	70(2)

Table 3. Bond lengths [Å] and angles [°] for FcC 1.

Fe(1)-C(14)	2.025(5)
Fe(1)-C(1)	2.028(5)
Fe(1)-C(18)	2.035(6)
Fe(1)-C(17)	2.036(5)
Fe(1)-C(15)	2.041(5)
Fe(1)-C(11)	2.041(5)
Fe(1)-C(16)	2.041(6)
Fe(1)-C(19)	2.045(5)
Fe(1)-C(13)	2.053(5)
Fe(1)-C(12)	2.061(6)
Cl(1)-C(7)	1.758(6)
O(1)-C(2)	1.213(7)
C(1)-C(11)	1.424(7)
C(1)-C(14)	1.427(7)
C(1)-C(2)	1.466(8)
C(2)-C(3)	1.479(7)
C(3)-C(4)	1.320(8)
C(3)-H(3)	0.9300
C(4)-C(5)	1.463(7)
C(4)-H(4)	0.9300
C(5)-C(6)	1.383(7)
C(5)-C(10)	1.393(7)
C(6)-C(7)	1.383(8)
C(6)-H(6)	0.9300
C(7)-C(8)	1.367(8)
C(8)-C(9)	1.384(8)
C(8)-H(8)	0.9300
C(9)-C(10)	1.378(8)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
C(11)-C(12)	1.414(8)
C(11)-H(11)	0.9300
C(12)-C(13)	1.419(9)
C(12)-H(12)	0.9300
C(13)-C(14)	1.412(8)
C(13)-H(13)	0.9300

C(14)-H(14)	0.9300
C(15)-C(19)	1.392(9)
C(15)-C(16)	1.411(10)
C(15)-H(15)	0.9300
C(16)-C(17)	1.400(10)
C(16)-H(16)	0.9300
C(17)-C(18)	1.406(10)
C(17)-H(17)	0.9300
C(18)-C(19)	1.396(10)
C(18)-H(18)	0.9300
C(19)-H(19)	0.9300

C(14)-Fe(1)-C(1)	41.2(2)
C(14)-Fe(1)-C(18)	122.3(2)
C(1)-Fe(1)-C(18)	159.2(2)
C(14)-Fe(1)-C(17)	159.3(3)
C(1)-Fe(1)-C(17)	158.7(3)
C(18)-Fe(1)-C(17)	40.4(3)
C(14)-Fe(1)-C(15)	121.3(3)
C(1)-Fe(1)-C(15)	108.0(2)
C(18)-Fe(1)-C(15)	67.3(3)
C(17)-Fe(1)-C(15)	67.7(3)
C(14)-Fe(1)-C(11)	68.7(2)
C(1)-Fe(1)-C(11)	41.0(2)
C(18)-Fe(1)-C(11)	158.1(3)
C(17)-Fe(1)-C(11)	123.4(3)
C(15)-Fe(1)-C(11)	125.9(3)
C(14)-Fe(1)-C(16)	157.9(3)
C(1)-Fe(1)-C(16)	123.0(3)
C(18)-Fe(1)-C(16)	67.6(3)
C(17)-Fe(1)-C(16)	40.2(3)
C(15)-Fe(1)-C(16)	40.5(3)
C(11)-Fe(1)-C(16)	109.8(3)
C(14)-Fe(1)-C(19)	106.3(2)
C(1)-Fe(1)-C(19)	123.4(2)
C(18)-Fe(1)-C(19)	40.0(3)
C(17)-Fe(1)-C(19)	67.6(3)
C(15)-Fe(1)-C(19)	39.8(3)

C(11)-Fe(1)-C(19)	161.0(3)
C(16)-Fe(1)-C(19)	67.5(3)
C(14)-Fe(1)-C(13)	40.5(2)
C(1)-Fe(1)-C(13)	68.8(2)
C(18)-Fe(1)-C(13)	106.7(3)
C(17)-Fe(1)-C(13)	124.0(3)
C(15)-Fe(1)-C(13)	155.8(3)
C(11)-Fe(1)-C(13)	68.4(2)
C(16)-Fe(1)-C(13)	161.2(3)
C(19)-Fe(1)-C(13)	120.5(2)
C(14)-Fe(1)-C(12)	67.9(2)
C(1)-Fe(1)-C(12)	68.3(2)
C(18)-Fe(1)-C(12)	122.3(3)
C(17)-Fe(1)-C(12)	109.2(3)
C(15)-Fe(1)-C(12)	162.7(3)
C(11)-Fe(1)-C(12)	40.3(2)
C(16)-Fe(1)-C(12)	126.2(3)
C(19)-Fe(1)-C(12)	156.5(3)
C(13)-Fe(1)-C(12)	40.4(2)
C(11)-C(1)-C(14)	107.2(4)
C(11)-C(1)-C(2)	123.8(5)
C(14)-C(1)-C(2)	128.7(5)
C(11)-C(1)-Fe(1)	70.0(3)
C(14)-C(1)-Fe(1)	69.3(3)
C(2)-C(1)-Fe(1)	121.1(3)
O(1)-C(2)-C(1)	121.6(5)
O(1)-C(2)-C(3)	121.3(5)
C(1)-C(2)-C(3)	117.1(4)
C(4)-C(3)-C(2)	121.6(5)
C(4)-C(3)-H(3)	119.2
C(2)-C(3)-H(3)	119.2
C(3)-C(4)-C(5)	127.2(5)
C(3)-C(4)-H(4)	116.4
C(5)-C(4)-H(4)	116.4
C(6)-C(5)-C(10)	118.4(5)
C(6)-C(5)-C(4)	118.3(5)
C(10)-C(5)-C(4)	123.2(5)
C(5)-C(6)-C(7)	120.0(5)

C(5)-C(6)-H(6)	120.0
C(7)-C(6)-H(6)	120.0
C(8)-C(7)-C(6)	122.1(5)
C(8)-C(7)-Cl(1)	119.5(5)
C(6)-C(7)-Cl(1)	118.4(5)
C(7)-C(8)-C(9)	117.8(5)
C(7)-C(8)-H(8)	121.1
C(9)-C(8)-H(8)	121.1
C(10)-C(9)-C(8)	121.2(5)
C(10)-C(9)-H(9)	119.4
C(8)-C(9)-H(9)	119.4
C(9)-C(10)-C(5)	120.4(5)
C(9)-C(10)-H(10)	119.8
C(5)-C(10)-H(10)	119.8
C(12)-C(11)-C(1)	108.0(5)
C(12)-C(11)-Fe(1)	70.6(3)
C(1)-C(11)-Fe(1)	69.0(3)
C(12)-C(11)-H(11)	126.0
C(1)-C(11)-H(11)	126.0
Fe(1)-C(11)-H(11)	126.0
C(11)-C(12)-C(13)	108.6(5)
C(11)-C(12)-Fe(1)	69.1(3)
C(13)-C(12)-Fe(1)	69.6(3)
C(11)-C(12)-H(12)	125.7
C(13)-C(12)-H(12)	125.7
Fe(1)-C(12)-H(12)	127.2
C(14)-C(13)-C(12)	107.5(5)
C(14)-C(13)-Fe(1)	68.7(3)
C(12)-C(13)-Fe(1)	70.1(3)
C(14)-C(13)-H(13)	126.2
C(12)-C(13)-H(13)	126.2
Fe(1)-C(13)-H(13)	126.5
C(13)-C(14)-C(1)	108.7(5)
C(13)-C(14)-Fe(1)	70.8(3)
C(1)-C(14)-Fe(1)	69.5(3)
C(13)-C(14)-H(14)	125.7
C(1)-C(14)-H(14)	125.7
Fe(1)-C(14)-H(14)	125.6

C(19)-C(15)-C(16)	108.2(6)
C(19)-C(15)-Fe(1)	70.3(3)
C(16)-C(15)-Fe(1)	69.8(3)
C(19)-C(15)-H(15)	125.9
C(16)-C(15)-H(15)	125.9
Fe(1)-C(15)-H(15)	125.6
C(17)-C(16)-C(15)	107.7(6)
C(17)-C(16)-Fe(1)	69.7(3)
C(15)-C(16)-Fe(1)	69.8(3)
C(17)-C(16)-H(16)	126.2
C(15)-C(16)-H(16)	126.2
Fe(1)-C(16)-H(16)	125.9
C(16)-C(17)-C(18)	107.7(6)
C(16)-C(17)-Fe(1)	70.1(3)
C(18)-C(17)-Fe(1)	69.7(3)
C(16)-C(17)-H(17)	126.1
C(18)-C(17)-H(17)	126.1
Fe(1)-C(17)-H(17)	125.6
C(19)-C(18)-C(17)	108.3(6)
C(19)-C(18)-Fe(1)	70.4(3)
C(17)-C(18)-Fe(1)	69.9(3)
C(19)-C(18)-H(18)	125.9
C(17)-C(18)-H(18)	125.9
Fe(1)-C(18)-H(18)	125.4
C(15)-C(19)-C(18)	108.1(6)
C(15)-C(19)-Fe(1)	69.9(3)
C(18)-C(19)-Fe(1)	69.6(3)
C(15)-C(19)-H(19)	125.9
C(18)-C(19)-H(19)	125.9
Fe(1)-C(19)-H(19)	126.2

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for FeC **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	45(1)	44(1)	55(1)	6(1)	-3(1)	-2(1)
Cl(1)	100(1)	107(1)	77(1)	-31(1)	8(1)	-1(1)
O(1)	51(2)	96(3)	72(2)	-7(2)	-1(2)	6(2)
C(1)	51(3)	47(2)	56(2)	8(2)	2(2)	-6(2)
C(2)	53(3)	59(3)	58(3)	6(2)	0(2)	-2(2)
C(3)	53(3)	68(3)	56(2)	1(2)	-3(2)	8(2)
C(4)	47(3)	58(3)	63(3)	8(2)	2(2)	2(2)
C(5)	52(3)	49(2)	55(2)	9(2)	4(2)	-4(2)
C(6)	52(3)	56(3)	61(2)	3(2)	5(2)	2(2)
C(7)	64(3)	68(3)	57(3)	-4(3)	11(2)	-9(3)
C(8)	67(4)	80(4)	64(3)	4(3)	-9(3)	-9(3)
C(9)	57(3)	74(4)	77(3)	10(3)	-6(2)	6(3)
C(10)	54(3)	58(3)	65(3)	1(3)	3(2)	1(3)
C(11)	48(3)	55(3)	64(3)	7(2)	-2(2)	-14(2)
C(12)	72(4)	55(3)	61(3)	-5(2)	-5(3)	-11(3)
C(13)	70(3)	47(3)	73(3)	-2(2)	8(3)	3(2)
C(14)	61(3)	44(2)	60(3)	10(2)	-6(2)	1(2)
C(15)	80(5)	41(2)	105(5)	-6(3)	7(4)	-7(3)
C(16)	62(4)	53(3)	123(6)	30(3)	-6(4)	4(3)
C(17)	99(5)	72(3)	80(4)	37(3)	-12(4)	-20(4)
C(18)	68(4)	69(4)	96(4)	20(3)	17(3)	-9(3)
C(19)	54(3)	58(3)	98(4)	4(3)	-14(3)	-17(3)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for FcC **1**.

	x	y	z	U(eq)
H(3)	6206	4428	5571	71
H(4)	2752	5689	6082	67
H(6)	3618	6801	6862	67
H(8)	9448	6210	7667	85
H(9)	10629	4786	7029	83
H(10)	8431	4447	6295	71
H(11)	845	4090	4230	67
H(12)	3264	3128	3524	75
H(13)	7236	2747	3881	76
H(14)	7253	3446	4817	66
H(15)	5179	7106	4712	91
H(16)	2597	7051	3927	95
H(17)	4831	6105	3189	100
H(18)	8776	5592	3520	93
H(19)	8984	6224	4455	84

Table 6. Torsion angles [°] for FcC 1.

C(11)-C(1)-C(2)-O(1)	8.2(8)
C(14)-C(1)-C(2)-O(1)	-178.8(5)
Fe(1)-C(1)-C(2)-O(1)	93.8(6)
C(11)-C(1)-C(2)-C(3)	-172.4(4)
C(14)-C(1)-C(2)-C(3)	0.5(7)
Fe(1)-C(1)-C(2)-C(3)	-86.8(5)
O(1)-C(2)-C(3)-C(4)	-4.6(8)
C(1)-C(2)-C(3)-C(4)	176.0(5)
C(2)-C(3)-C(4)-C(5)	178.5(4)
C(3)-C(4)-C(5)-C(6)	170.5(5)
C(3)-C(4)-C(5)-C(10)	-10.2(8)
C(10)-C(5)-C(6)-C(7)	0.6(7)
C(4)-C(5)-C(6)-C(7)	179.9(5)
C(5)-C(6)-C(7)-C(8)	-1.2(8)
C(5)-C(6)-C(7)-Cl(1)	177.2(4)
C(6)-C(7)-C(8)-C(9)	0.1(9)
Cl(1)-C(7)-C(8)-C(9)	-178.3(4)
C(7)-C(8)-C(9)-C(10)	1.6(9)
C(8)-C(9)-C(10)-C(5)	-2.3(8)
C(6)-C(5)-C(10)-C(9)	1.1(7)
C(4)-C(5)-C(10)-C(9)	-178.1(5)
C(14)-C(1)-C(11)-C(12)	0.5(5)
C(2)-C(1)-C(11)-C(12)	174.7(5)
Fe(1)-C(1)-C(11)-C(12)	60.0(4)
C(14)-C(1)-C(11)-Fe(1)	-59.6(3)
C(2)-C(1)-C(11)-Fe(1)	114.7(5)
C(1)-C(11)-C(12)-C(13)	-0.6(6)
Fe(1)-C(11)-C(12)-C(13)	58.5(4)
C(1)-C(11)-C(12)-Fe(1)	-59.1(3)
C(11)-C(12)-C(13)-C(14)	0.5(6)
Fe(1)-C(12)-C(13)-C(14)	58.7(4)
C(11)-C(12)-C(13)-Fe(1)	-58.2(4)
C(12)-C(13)-C(14)-C(1)	-0.2(6)
Fe(1)-C(13)-C(14)-C(1)	59.4(3)
C(12)-C(13)-C(14)-Fe(1)	-59.6(4)
C(11)-C(1)-C(14)-C(13)	-0.2(5)

C(2)-C(1)-C(14)-C(13)	-174.1(5)
Fe(1)-C(1)-C(14)-C(13)	-60.2(3)
C(11)-C(1)-C(14)-Fe(1)	60.0(3)
C(2)-C(1)-C(14)-Fe(1)	-113.9(5)
C(19)-C(15)-C(16)-C(17)	0.4(7)
Fe(1)-C(15)-C(16)-C(17)	-59.6(4)
C(19)-C(15)-C(16)-Fe(1)	60.0(4)
C(15)-C(16)-C(17)-C(18)	-0.2(7)
Fe(1)-C(16)-C(17)-C(18)	-59.8(4)
C(15)-C(16)-C(17)-Fe(1)	59.7(4)
C(16)-C(17)-C(18)-C(19)	-0.1(7)
Fe(1)-C(17)-C(18)-C(19)	-60.2(4)
C(16)-C(17)-C(18)-Fe(1)	60.1(4)
C(16)-C(15)-C(19)-C(18)	-0.5(7)
Fe(1)-C(15)-C(19)-C(18)	59.3(4)
C(16)-C(15)-C(19)-Fe(1)	-59.7(4)
C(17)-C(18)-C(19)-C(15)	0.4(7)
Fe(1)-C(18)-C(19)-C(15)	-59.5(4)
C(17)-C(18)-C(19)-Fe(1)	59.8(4)

Symmetry transformations used to generate equivalent atoms:

Table 7. Crystal data and structure refinement for FcC 2.

Identification code	JVB-10-Fe	
Empirical formula	C ₂₀ H ₁₈ Fe O	
Formula weight	330.19	
Temperature	295(1) K	
Wavelength	0.56083 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 28.5538(16) Å	α = 90°.
	b = 5.9183(2) Å	β = 110.119(4)°.
	c = 19.7317(11) Å	γ = 90°.
Volume	3131.0(3) Å ³	
Z	8	
Density (calculated)	1.401 Mg/m ³	
Absorption coefficient	0.505 mm ⁻¹	
F(000)	1376	
Theta range for data collection	2.398 to 20.518°.	
Index ranges	-35 ≤ h ≤ 35, -7 ≤ k ≤ 7, -24 ≤ l ≤ 24	
Reflections collected	54422	
Independent reflections	6415 [R(int) = 0.0889]	
Completeness to theta = 19.664°	99.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	6415 / 0 / 400	
Goodness-of-fit on F ²	0.969	
Final R indices [I > 2σ(I)]	R1 = 0.0470, wR2 = 0.1043	
R indices (all data)	R1 = 0.0627, wR2 = 0.1087	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.509 and -0.269 e.Å ⁻³	

Table 8. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for FeC 2. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Fe(1)	6879(1)	11368(1)	10934(1)	42(1)
O(1)	6507(1)	15500(5)	9362(2)	60(1)
C(1)	7012(2)	12664(7)	10065(2)	40(1)
C(2)	6608(2)	13465(7)	9429(3)	47(1)
C(3)	6344(2)	11803(7)	8878(2)	47(1)
C(4)	5979(2)	12411(7)	8269(2)	44(1)
C(5)	5720(2)	11021(6)	7647(2)	43(1)
C(6)	5328(2)	11955(8)	7099(3)	49(1)
C(7)	5091(2)	10819(8)	6458(3)	56(1)
C(8)	5259(2)	8646(8)	6383(3)	63(1)
C(9)	5642(2)	7695(8)	6935(3)	56(1)
C(10)	5880(2)	8847(7)	7548(3)	51(1)
C(11)	7257(2)	14013(7)	10701(3)	51(1)
C(12)	7588(2)	12647(9)	11192(3)	55(1)
C(13)	7566(2)	10415(8)	10930(3)	54(1)
C(14)	7213(2)	10426(8)	10228(2)	48(1)
C(15)	6128(2)	11110(9)	10698(3)	62(1)
C(16)	6335(2)	12477(9)	11307(4)	69(2)
C(17)	6684(2)	11169(10)	11839(3)	70(2)
C(18)	6690(2)	9035(8)	11549(3)	60(1)
C(19)	6349(2)	8970(7)	10844(3)	60(1)
C(20)	4679(2)	11927(11)	5852(3)	82(2)
Fe(2)	8150(1)	8245(1)	9033(1)	40(1)
O(51)	8466(1)	4115(5)	7764(2)	58(1)
C(51)	7966(2)	6881(7)	8033(2)	44(1)
C(52)	8360(2)	6112(6)	7758(2)	42(1)
C(53)	8615(2)	7848(7)	7470(2)	43(1)
C(54)	8994(2)	7349(6)	7254(2)	43(1)
C(55)	9262(2)	8790(6)	6911(2)	42(1)
C(56)	9675(2)	7918(7)	6769(2)	45(1)
C(57)	9912(2)	9131(8)	6381(3)	52(1)
C(58)	9744(2)	11281(8)	6152(3)	56(1)
C(59)	9341(2)	12226(8)	6290(3)	53(1)

C(60)	9095(2)	10981(7)	6670(2)	46(1)
C(61)	7769(2)	5514(7)	8468(3)	47(1)
C(62)	7442(2)	6899(7)	8703(3)	57(1)
C(63)	7437(2)	9084(7)	8409(3)	51(1)
C(64)	7765(2)	9082(7)	8003(2)	45(1)
C(65)	8912(2)	8615(7)	9442(3)	59(1)
C(66)	8749(2)	7129(8)	9880(3)	59(1)
C(67)	8415(2)	8264(9)	10132(3)	66(1)
C(68)	8365(2)	10538(8)	9857(3)	58(1)
C(69)	8674(2)	10702(7)	9428(3)	61(1)
C(70)	10331(2)	8099(10)	6190(4)	79(2)

Table 9. Bond lengths [Å] and angles [°] for FcC 2.

Fe(1)-C(14)	2.018(4)
Fe(1)-C(18)	2.029(5)
Fe(1)-C(1)	2.030(4)
Fe(1)-C(15)	2.036(5)
Fe(1)-C(19)	2.037(5)
Fe(1)-C(11)	2.042(4)
Fe(1)-C(16)	2.042(5)
Fe(1)-C(13)	2.045(5)
Fe(1)-C(17)	2.048(5)
Fe(1)-C(12)	2.054(4)
O(1)-C(2)	1.235(5)
C(1)-C(14)	1.435(6)
C(1)-C(11)	1.447(6)
C(1)-C(2)	1.461(7)
C(2)-C(3)	1.467(6)
C(3)-C(4)	1.342(6)
C(3)-H(3)	0.9300
C(4)-C(5)	1.451(6)
C(4)-H(4)	0.9300
C(5)-C(6)	1.377(6)
C(5)-C(10)	1.402(5)
C(6)-C(7)	1.387(7)
C(6)-H(6)	0.9300
C(7)-C(8)	1.398(7)
C(7)-C(20)	1.509(7)
C(8)-C(9)	1.372(8)
C(8)-H(8)	0.9300
C(9)-C(10)	1.351(7)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
C(11)-C(12)	1.363(7)
C(11)-H(11)	0.9300
C(12)-C(13)	1.412(7)
C(12)-H(12)	0.9300
C(13)-C(14)	1.404(6)
C(13)-H(13)	0.9300

C(14)-H(14)	0.9300
C(15)-C(19)	1.400(6)
C(15)-C(16)	1.400(8)
C(15)-H(15)	0.9300
C(16)-C(17)	1.405(8)
C(16)-H(16)	0.9300
C(17)-C(18)	1.389(7)
C(17)-H(17)	0.9300
C(18)-C(19)	1.397(7)
C(18)-H(18)	0.9300
C(19)-H(19)	0.9300
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
Fe(2)-C(64)	2.012(4)
Fe(2)-C(51)	2.026(4)
Fe(2)-C(67)	2.037(5)
Fe(2)-C(69)	2.039(4)
Fe(2)-C(68)	2.043(5)
Fe(2)-C(63)	2.046(5)
Fe(2)-C(66)	2.046(5)
Fe(2)-C(61)	2.051(4)
Fe(2)-C(65)	2.055(5)
Fe(2)-C(62)	2.061(4)
O(51)-C(52)	1.219(5)
C(51)-C(64)	1.416(6)
C(51)-C(61)	1.428(6)
C(51)-C(52)	1.479(6)
C(52)-C(53)	1.480(6)
C(53)-C(54)	1.327(6)
C(53)-H(53)	0.9300
C(54)-C(55)	1.458(6)
C(54)-H(54)	0.9300
C(55)-C(56)	1.401(6)
C(55)-C(60)	1.407(5)
C(56)-C(57)	1.383(7)
C(56)-H(56)	0.9300
C(57)-C(58)	1.380(7)

C(57)-C(70)	1.504(7)
C(58)-C(59)	1.388(7)
C(58)-H(58)	0.9300
C(59)-C(60)	1.400(7)
C(59)-H(59)	0.9300
C(60)-H(60)	0.9300
C(61)-C(62)	1.435(7)
C(61)-H(61)	0.9300
C(62)-C(63)	1.416(6)
C(62)-H(62)	0.9300
C(63)-C(64)	1.428(6)
C(63)-H(63)	0.9300
C(64)-H(64)	0.9300
C(65)-C(69)	1.405(6)
C(65)-C(66)	1.418(7)
C(65)-H(65)	0.9300
C(66)-C(67)	1.392(7)
C(66)-H(66)	0.9300
C(67)-C(68)	1.440(7)
C(67)-H(67)	0.9300
C(68)-C(69)	1.422(7)
C(68)-H(68)	0.9300
C(69)-H(69)	0.9300
C(70)-H(70A)	0.9600
C(70)-H(70B)	0.9600
C(70)-H(70C)	0.9600
C(14)-Fe(1)-C(18)	120.7(2)
C(14)-Fe(1)-C(1)	41.53(17)
C(18)-Fe(1)-C(1)	158.03(19)
C(14)-Fe(1)-C(15)	122.1(2)
C(18)-Fe(1)-C(15)	67.1(2)
C(1)-Fe(1)-C(15)	108.9(2)
C(14)-Fe(1)-C(19)	105.1(2)
C(18)-Fe(1)-C(19)	40.2(2)
C(1)-Fe(1)-C(19)	122.61(19)
C(15)-Fe(1)-C(19)	40.21(19)
C(14)-Fe(1)-C(11)	69.17(18)
C(18)-Fe(1)-C(11)	157.9(2)

C(1)-Fe(1)-C(11)	41.64(18)
C(15)-Fe(1)-C(11)	127.0(2)
C(19)-Fe(1)-C(11)	161.6(2)
C(14)-Fe(1)-C(16)	159.4(2)
C(18)-Fe(1)-C(16)	67.2(2)
C(1)-Fe(1)-C(16)	124.7(2)
C(15)-Fe(1)-C(16)	40.2(2)
C(19)-Fe(1)-C(16)	67.8(2)
C(11)-Fe(1)-C(16)	111.15(19)
C(14)-Fe(1)-C(13)	40.43(18)
C(18)-Fe(1)-C(13)	105.5(2)
C(1)-Fe(1)-C(13)	69.01(18)
C(15)-Fe(1)-C(13)	156.1(2)
C(19)-Fe(1)-C(13)	119.49(19)
C(11)-Fe(1)-C(13)	68.19(18)
C(16)-Fe(1)-C(13)	160.1(3)
C(14)-Fe(1)-C(17)	156.9(2)
C(18)-Fe(1)-C(17)	39.8(2)
C(1)-Fe(1)-C(17)	160.7(2)
C(15)-Fe(1)-C(17)	67.4(2)
C(19)-Fe(1)-C(17)	67.7(2)
C(11)-Fe(1)-C(17)	124.3(2)
C(16)-Fe(1)-C(17)	40.2(2)
C(13)-Fe(1)-C(17)	122.5(2)
C(14)-Fe(1)-C(12)	67.2(2)
C(18)-Fe(1)-C(12)	123.0(2)
C(1)-Fe(1)-C(12)	67.4(2)
C(15)-Fe(1)-C(12)	162.6(2)
C(19)-Fe(1)-C(12)	156.5(2)
C(11)-Fe(1)-C(12)	38.9(2)
C(16)-Fe(1)-C(12)	126.8(2)
C(13)-Fe(1)-C(12)	40.3(2)
C(17)-Fe(1)-C(12)	110.2(2)
C(14)-C(1)-C(11)	106.2(4)
C(14)-C(1)-C(2)	129.0(4)
C(11)-C(1)-C(2)	124.6(4)
C(14)-C(1)-Fe(1)	68.8(2)
C(11)-C(1)-Fe(1)	69.6(3)

C(2)-C(1)-Fe(1)	121.8(3)
O(1)-C(2)-C(1)	119.7(4)
O(1)-C(2)-C(3)	122.2(4)
C(1)-C(2)-C(3)	118.1(4)
C(4)-C(3)-C(2)	121.8(4)
C(4)-C(3)-H(3)	119.1
C(2)-C(3)-H(3)	119.1
C(3)-C(4)-C(5)	128.3(4)
C(3)-C(4)-H(4)	115.9
C(5)-C(4)-H(4)	115.9
C(6)-C(5)-C(10)	118.4(4)
C(6)-C(5)-C(4)	118.5(4)
C(10)-C(5)-C(4)	122.8(4)
C(5)-C(6)-C(7)	122.1(4)
C(5)-C(6)-H(6)	118.9
C(7)-C(6)-H(6)	118.9
C(6)-C(7)-C(8)	117.8(5)
C(6)-C(7)-C(20)	121.0(5)
C(8)-C(7)-C(20)	121.2(5)
C(9)-C(8)-C(7)	120.1(5)
C(9)-C(8)-H(8)	119.9
C(7)-C(8)-H(8)	119.9
C(10)-C(9)-C(8)	121.5(5)
C(10)-C(9)-H(9)	119.2
C(8)-C(9)-H(9)	119.2
C(9)-C(10)-C(5)	120.0(5)
C(9)-C(10)-H(10)	120.0
C(5)-C(10)-H(10)	120.0
C(12)-C(11)-C(1)	107.4(4)
C(12)-C(11)-Fe(1)	71.1(3)
C(1)-C(11)-Fe(1)	68.7(2)
C(12)-C(11)-H(11)	126.3
C(1)-C(11)-H(11)	126.3
Fe(1)-C(11)-H(11)	125.4
C(11)-C(12)-C(13)	111.2(4)
C(11)-C(12)-Fe(1)	70.1(3)
C(13)-C(12)-Fe(1)	69.5(3)
C(11)-C(12)-H(12)	124.4

C(13)-C(12)-H(12)	124.4
Fe(1)-C(12)-H(12)	127.8
C(14)-C(13)-C(12)	106.4(4)
C(14)-C(13)-Fe(1)	68.8(3)
C(12)-C(13)-Fe(1)	70.2(3)
C(14)-C(13)-H(13)	126.8
C(12)-C(13)-H(13)	126.8
Fe(1)-C(13)-H(13)	125.8
C(13)-C(14)-C(1)	108.8(4)
C(13)-C(14)-Fe(1)	70.8(3)
C(1)-C(14)-Fe(1)	69.7(2)
C(13)-C(14)-H(14)	125.6
C(1)-C(14)-H(14)	125.6
Fe(1)-C(14)-H(14)	125.5
C(19)-C(15)-C(16)	108.6(5)
C(19)-C(15)-Fe(1)	69.9(3)
C(16)-C(15)-Fe(1)	70.1(3)
C(19)-C(15)-H(15)	125.7
C(16)-C(15)-H(15)	125.7
Fe(1)-C(15)-H(15)	125.8
C(15)-C(16)-C(17)	107.7(5)
C(15)-C(16)-Fe(1)	69.7(3)
C(17)-C(16)-Fe(1)	70.1(3)
C(15)-C(16)-H(16)	126.2
C(17)-C(16)-H(16)	126.2
Fe(1)-C(16)-H(16)	125.6
C(18)-C(17)-C(16)	107.4(5)
C(18)-C(17)-Fe(1)	69.4(3)
C(16)-C(17)-Fe(1)	69.7(3)
C(18)-C(17)-H(17)	126.3
C(16)-C(17)-H(17)	126.3
Fe(1)-C(17)-H(17)	126.2
C(17)-C(18)-C(19)	109.4(5)
C(17)-C(18)-Fe(1)	70.8(3)
C(19)-C(18)-Fe(1)	70.2(3)
C(17)-C(18)-H(18)	125.3
C(19)-C(18)-H(18)	125.3
Fe(1)-C(18)-H(18)	125.3

C(18)-C(19)-C(15)	106.9(4)
C(18)-C(19)-Fe(1)	69.6(3)
C(15)-C(19)-Fe(1)	69.9(3)
C(18)-C(19)-H(19)	126.6
C(15)-C(19)-H(19)	126.6
Fe(1)-C(19)-H(19)	125.5
C(7)-C(20)-H(20A)	109.5
C(7)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(7)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(64)-Fe(2)-C(51)	41.05(17)
C(64)-Fe(2)-C(67)	161.5(2)
C(51)-Fe(2)-C(67)	156.3(2)
C(64)-Fe(2)-C(69)	106.5(2)
C(51)-Fe(2)-C(69)	124.5(2)
C(67)-Fe(2)-C(69)	68.6(2)
C(64)-Fe(2)-C(68)	123.40(19)
C(51)-Fe(2)-C(68)	161.0(2)
C(67)-Fe(2)-C(68)	41.3(2)
C(69)-Fe(2)-C(68)	40.8(2)
C(64)-Fe(2)-C(63)	41.18(18)
C(51)-Fe(2)-C(63)	68.86(18)
C(67)-Fe(2)-C(63)	124.6(2)
C(69)-Fe(2)-C(63)	120.31(19)
C(68)-Fe(2)-C(63)	106.35(19)
C(64)-Fe(2)-C(66)	156.5(2)
C(51)-Fe(2)-C(66)	122.1(2)
C(67)-Fe(2)-C(66)	39.9(2)
C(69)-Fe(2)-C(66)	67.7(2)
C(68)-Fe(2)-C(66)	68.1(2)
C(63)-Fe(2)-C(66)	161.6(2)
C(64)-Fe(2)-C(61)	68.99(18)
C(51)-Fe(2)-C(61)	41.00(18)
C(67)-Fe(2)-C(61)	121.1(2)
C(69)-Fe(2)-C(61)	162.3(2)
C(68)-Fe(2)-C(61)	156.01(19)

C(63)-Fe(2)-C(61)	68.37(18)
C(66)-Fe(2)-C(61)	109.14(19)
C(64)-Fe(2)-C(65)	120.50(19)
C(51)-Fe(2)-C(65)	108.09(19)
C(67)-Fe(2)-C(65)	68.0(2)
C(69)-Fe(2)-C(65)	40.15(17)
C(68)-Fe(2)-C(65)	68.26(19)
C(63)-Fe(2)-C(65)	155.62(19)
C(66)-Fe(2)-C(65)	40.46(19)
C(61)-Fe(2)-C(65)	126.16(18)
C(64)-Fe(2)-C(62)	68.9(2)
C(51)-Fe(2)-C(62)	69.0(2)
C(67)-Fe(2)-C(62)	107.6(2)
C(69)-Fe(2)-C(62)	155.2(2)
C(68)-Fe(2)-C(62)	120.0(2)
C(63)-Fe(2)-C(62)	40.34(18)
C(66)-Fe(2)-C(62)	125.9(2)
C(61)-Fe(2)-C(62)	40.85(19)
C(65)-Fe(2)-C(62)	163.11(19)
C(64)-C(51)-C(61)	108.0(4)
C(64)-C(51)-C(52)	128.0(4)
C(61)-C(51)-C(52)	123.6(4)
C(64)-C(51)-Fe(2)	69.0(2)
C(61)-C(51)-Fe(2)	70.4(3)
C(52)-C(51)-Fe(2)	120.3(3)
O(51)-C(52)-C(51)	120.8(4)
O(51)-C(52)-C(53)	121.6(4)
C(51)-C(52)-C(53)	117.6(4)
C(54)-C(53)-C(52)	122.1(4)
C(54)-C(53)-H(53)	118.9
C(52)-C(53)-H(53)	118.9
C(53)-C(54)-C(55)	129.5(4)
C(53)-C(54)-H(54)	115.3
C(55)-C(54)-H(54)	115.3
C(56)-C(55)-C(60)	118.9(4)
C(56)-C(55)-C(54)	119.3(4)
C(60)-C(55)-C(54)	121.7(4)
C(57)-C(56)-C(55)	121.7(4)

C(57)-C(56)-H(56)	119.2
C(55)-C(56)-H(56)	119.2
C(58)-C(57)-C(56)	118.6(4)
C(58)-C(57)-C(70)	120.6(5)
C(56)-C(57)-C(70)	120.8(4)
C(57)-C(58)-C(59)	121.7(4)
C(57)-C(58)-H(58)	119.2
C(59)-C(58)-H(58)	119.2
C(58)-C(59)-C(60)	119.7(4)
C(58)-C(59)-H(59)	120.1
C(60)-C(59)-H(59)	120.1
C(59)-C(60)-C(55)	119.5(4)
C(59)-C(60)-H(60)	120.3
C(55)-C(60)-H(60)	120.3
C(51)-C(61)-C(62)	107.8(4)
C(51)-C(61)-Fe(2)	68.6(2)
C(62)-C(61)-Fe(2)	69.9(2)
C(51)-C(61)-H(61)	126.1
C(62)-C(61)-H(61)	126.1
Fe(2)-C(61)-H(61)	127.0
C(63)-C(62)-C(61)	107.7(4)
C(63)-C(62)-Fe(2)	69.3(3)
C(61)-C(62)-Fe(2)	69.2(2)
C(63)-C(62)-H(62)	126.2
C(61)-C(62)-H(62)	126.2
Fe(2)-C(62)-H(62)	126.9
C(62)-C(63)-C(64)	108.4(4)
C(62)-C(63)-Fe(2)	70.4(3)
C(64)-C(63)-Fe(2)	68.2(3)
C(62)-C(63)-H(63)	125.8
C(64)-C(63)-H(63)	125.8
Fe(2)-C(63)-H(63)	127.2
C(51)-C(64)-C(63)	108.1(4)
C(51)-C(64)-Fe(2)	70.0(2)
C(63)-C(64)-Fe(2)	70.7(3)
C(51)-C(64)-H(64)	126.0
C(63)-C(64)-H(64)	126.0
Fe(2)-C(64)-H(64)	125.0

C(69)-C(65)-C(66)	107.4(5)
C(69)-C(65)-Fe(2)	69.3(3)
C(66)-C(65)-Fe(2)	69.4(3)
C(69)-C(65)-H(65)	126.3
C(66)-C(65)-H(65)	126.3
Fe(2)-C(65)-H(65)	126.5
C(67)-C(66)-C(65)	109.1(4)
C(67)-C(66)-Fe(2)	69.7(3)
C(65)-C(66)-Fe(2)	70.1(3)
C(67)-C(66)-H(66)	125.4
C(65)-C(66)-H(66)	125.4
Fe(2)-C(66)-H(66)	126.3
C(66)-C(67)-C(68)	107.9(5)
C(66)-C(67)-Fe(2)	70.4(3)
C(68)-C(67)-Fe(2)	69.6(3)
C(66)-C(67)-H(67)	126.1
C(68)-C(67)-H(67)	126.1
Fe(2)-C(67)-H(67)	125.6
C(69)-C(68)-C(67)	106.7(4)
C(69)-C(68)-Fe(2)	69.5(3)
C(67)-C(68)-Fe(2)	69.1(3)
C(69)-C(68)-H(68)	126.7
C(67)-C(68)-H(68)	126.7
Fe(2)-C(68)-H(68)	126.3
C(65)-C(69)-C(68)	108.8(4)
C(65)-C(69)-Fe(2)	70.5(3)
C(68)-C(69)-Fe(2)	69.8(3)
C(65)-C(69)-H(69)	125.6
C(68)-C(69)-H(69)	125.6
Fe(2)-C(69)-H(69)	125.7
C(57)-C(70)-H(70A)	109.5
C(57)-C(70)-H(70B)	109.5
H(70A)-C(70)-H(70B)	109.5
C(57)-C(70)-H(70C)	109.5
H(70A)-C(70)-H(70C)	109.5
H(70B)-C(70)-H(70C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 10. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for FeC **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Fe(1)	42(1)	45(1)	42(1)	-6(1)	16(1)	-3(1)
O(1)	71(2)	41(2)	62(2)	0(1)	17(2)	1(2)
C(1)	36(3)	42(2)	41(3)	0(2)	14(2)	-4(2)
C(2)	48(3)	50(3)	51(3)	-8(2)	28(2)	-8(2)
C(3)	50(3)	43(2)	49(3)	2(2)	20(2)	1(2)
C(4)	46(3)	42(2)	44(3)	2(2)	15(2)	2(2)
C(5)	41(2)	42(2)	47(3)	3(2)	17(2)	1(2)
C(6)	45(3)	52(2)	51(3)	5(2)	16(2)	1(2)
C(7)	46(3)	70(3)	52(3)	10(2)	15(2)	-8(2)
C(8)	67(4)	68(3)	55(3)	-13(2)	24(3)	-22(3)
C(9)	63(4)	46(2)	65(4)	-14(2)	31(3)	-11(2)
C(10)	51(3)	48(2)	57(3)	7(2)	22(2)	0(2)
C(11)	48(3)	45(2)	59(3)	-8(2)	18(2)	-9(2)
C(12)	42(3)	78(3)	41(3)	-12(2)	9(2)	-16(3)
C(13)	50(3)	65(3)	48(3)	-4(2)	16(2)	9(2)
C(14)	42(3)	61(3)	44(3)	-7(2)	19(2)	5(2)
C(15)	37(3)	82(3)	67(4)	10(3)	18(3)	0(2)
C(16)	73(4)	55(3)	106(5)	-4(3)	64(4)	0(3)
C(17)	76(4)	90(4)	54(3)	-16(3)	36(3)	-19(3)
C(18)	61(3)	57(3)	65(3)	12(2)	25(3)	-3(2)
C(19)	60(3)	54(2)	68(3)	-7(2)	25(3)	-11(2)
C(20)	62(4)	110(5)	56(4)	14(3)	-3(3)	-4(4)
Fe(2)	40(1)	42(1)	39(1)	1(1)	16(1)	-3(1)
O(51)	65(2)	47(2)	70(2)	-4(2)	33(2)	2(2)
C(51)	37(2)	56(2)	35(2)	-3(2)	9(2)	0(2)
C(52)	46(3)	41(2)	39(2)	-5(2)	13(2)	0(2)
C(53)	45(3)	43(2)	44(3)	1(2)	17(2)	4(2)
C(54)	46(3)	35(2)	45(3)	-1(2)	13(2)	-2(2)
C(55)	43(2)	44(2)	37(2)	-3(2)	10(2)	1(2)
C(56)	42(3)	44(2)	48(3)	-5(2)	14(2)	2(2)
C(57)	47(3)	59(3)	50(3)	-10(2)	16(2)	-7(2)
C(58)	57(3)	64(3)	50(3)	-4(2)	21(3)	-19(3)
C(59)	59(3)	43(2)	50(3)	-1(2)	9(3)	-4(2)

C(60)	45(3)	43(2)	50(3)	-4(2)	15(2)	-2(2)
C(61)	50(3)	39(2)	55(3)	-5(2)	21(2)	-12(2)
C(62)	47(3)	71(3)	56(3)	11(3)	21(3)	-17(2)
C(63)	41(3)	56(2)	53(3)	-5(2)	14(2)	7(2)
C(64)	43(3)	47(2)	44(3)	4(2)	14(2)	1(2)
C(65)	43(3)	74(3)	56(3)	-11(3)	13(2)	1(2)
C(66)	57(3)	56(3)	53(3)	9(2)	5(3)	5(2)
C(67)	63(4)	94(4)	37(3)	-4(2)	15(3)	-5(3)
C(68)	59(3)	51(2)	62(3)	-15(2)	17(3)	-1(2)
C(69)	57(3)	47(2)	81(4)	-7(2)	26(3)	-13(2)
C(70)	65(4)	92(4)	94(5)	-14(3)	46(4)	-10(3)

Table 11. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for FcC 2.

	x	y	z	U(eq)
H(3)	6433	10287	8954	56
H(4)	5880	13915	8241	53
H(6)	5218	13394	7161	59
H(8)	5110	7843	5957	75
H(9)	5740	6223	6887	67
H(10)	6151	8198	7905	61
H(11)	7198	15533	10762	61
H(12)	7801	13123	11641	66
H(13)	7749	9181	11173	65
H(14)	7124	9188	9920	57
H(15)	5885	11550	10268	74
H(16)	6256	13981	11352	83
H(17)	6876	11644	12300	84
H(18)	6890	7836	11787	72
H(19)	6282	7740	10532	72
H(20A)	4377	11922	5964	123
H(20B)	4626	11108	5412	123
H(20C)	4771	13457	5794	123
H(53)	8505	9337	7440	52
H(54)	9105	5862	7331	51
H(56)	9793	6488	6939	54
H(58)	9904	12118	5898	67
H(59)	9235	13680	6132	64
H(60)	8823	11597	6762	56
H(61)	7840	3997	8579	57
H(62)	7265	6444	8997	69
H(63)	7252	10310	8470	61
H(64)	7835	10313	7760	54
H(65)	9136	8271	9208	70
H(66)	8849	5634	9981	71
H(67)	8253	7661	10427	79
H(68)	8168	11677	9943	69
H(69)	8713	11982	9179	73

H(70A)	10494	6965	6540	119
H(70B)	10567	9253	6188	119
H(70C)	10201	7421	5720	119

Table 12. Torsion angles [°] for FcC 2.

C(14)-C(1)-C(2)-O(1)	-175.4(4)
C(11)-C(1)-C(2)-O(1)	11.3(7)
Fe(1)-C(1)-C(2)-O(1)	97.3(4)
C(14)-C(1)-C(2)-C(3)	3.0(7)
C(11)-C(1)-C(2)-C(3)	-170.3(4)
Fe(1)-C(1)-C(2)-C(3)	-84.4(4)
O(1)-C(2)-C(3)-C(4)	0.3(7)
C(1)-C(2)-C(3)-C(4)	-178.0(4)
C(2)-C(3)-C(4)-C(5)	173.3(4)
C(3)-C(4)-C(5)-C(6)	175.0(5)
C(3)-C(4)-C(5)-C(10)	-11.4(7)
C(10)-C(5)-C(6)-C(7)	-0.2(7)
C(4)-C(5)-C(6)-C(7)	173.7(4)
C(5)-C(6)-C(7)-C(8)	0.9(7)
C(5)-C(6)-C(7)-C(20)	-177.0(5)
C(6)-C(7)-C(8)-C(9)	0.6(7)
C(20)-C(7)-C(8)-C(9)	178.4(5)
C(7)-C(8)-C(9)-C(10)	-2.8(8)
C(8)-C(9)-C(10)-C(5)	3.5(7)
C(6)-C(5)-C(10)-C(9)	-1.9(6)
C(4)-C(5)-C(10)-C(9)	-175.6(4)
C(14)-C(1)-C(11)-C(12)	1.5(5)
C(2)-C(1)-C(11)-C(12)	176.1(4)
Fe(1)-C(1)-C(11)-C(12)	60.9(3)
C(14)-C(1)-C(11)-Fe(1)	-59.4(3)
C(2)-C(1)-C(11)-Fe(1)	115.2(4)
C(1)-C(11)-C(12)-C(13)	-2.2(6)
Fe(1)-C(11)-C(12)-C(13)	57.2(4)
C(1)-C(11)-C(12)-Fe(1)	-59.4(3)
C(11)-C(12)-C(13)-C(14)	2.0(6)
Fe(1)-C(12)-C(13)-C(14)	59.5(3)
C(11)-C(12)-C(13)-Fe(1)	-57.6(4)
C(12)-C(13)-C(14)-C(1)	-0.9(5)
Fe(1)-C(13)-C(14)-C(1)	59.5(3)
C(12)-C(13)-C(14)-Fe(1)	-60.5(3)
C(11)-C(1)-C(14)-C(13)	-0.3(5)

C(2)-C(1)-C(14)-C(13)	-174.6(4)
Fe(1)-C(1)-C(14)-C(13)	-60.2(3)
C(11)-C(1)-C(14)-Fe(1)	59.9(3)
C(2)-C(1)-C(14)-Fe(1)	-114.4(5)
C(19)-C(15)-C(16)-C(17)	-0.6(6)
Fe(1)-C(15)-C(16)-C(17)	-60.1(4)
C(19)-C(15)-C(16)-Fe(1)	59.5(4)
C(15)-C(16)-C(17)-C(18)	0.5(6)
Fe(1)-C(16)-C(17)-C(18)	-59.3(4)
C(15)-C(16)-C(17)-Fe(1)	59.8(4)
C(16)-C(17)-C(18)-C(19)	-0.3(6)
Fe(1)-C(17)-C(18)-C(19)	-59.8(4)
C(16)-C(17)-C(18)-Fe(1)	59.5(4)
C(17)-C(18)-C(19)-C(15)	-0.1(6)
Fe(1)-C(18)-C(19)-C(15)	-60.2(3)
C(17)-C(18)-C(19)-Fe(1)	60.2(4)
C(16)-C(15)-C(19)-C(18)	0.4(6)
Fe(1)-C(15)-C(19)-C(18)	60.1(3)
C(16)-C(15)-C(19)-Fe(1)	-59.7(4)
C(64)-C(51)-C(52)-O(51)	-173.4(4)
C(61)-C(51)-C(52)-O(51)	15.2(7)
Fe(2)-C(51)-C(52)-O(51)	100.7(5)
C(64)-C(51)-C(52)-C(53)	5.9(7)
C(61)-C(51)-C(52)-C(53)	-165.5(4)
Fe(2)-C(51)-C(52)-C(53)	-80.0(5)
O(51)-C(52)-C(53)-C(54)	-5.0(7)
C(51)-C(52)-C(53)-C(54)	175.7(4)
C(52)-C(53)-C(54)-C(55)	175.1(4)
C(53)-C(54)-C(55)-C(56)	176.0(5)
C(53)-C(54)-C(55)-C(60)	-8.9(7)
C(60)-C(55)-C(56)-C(57)	-1.8(6)
C(54)-C(55)-C(56)-C(57)	173.4(4)
C(55)-C(56)-C(57)-C(58)	2.1(7)
C(55)-C(56)-C(57)-C(70)	-175.7(5)
C(56)-C(57)-C(58)-C(59)	-1.1(7)
C(70)-C(57)-C(58)-C(59)	176.7(5)
C(57)-C(58)-C(59)-C(60)	-0.2(7)
C(58)-C(59)-C(60)-C(55)	0.5(7)

C(56)-C(55)-C(60)-C(59)	0.5(6)
C(54)-C(55)-C(60)-C(59)	-174.6(4)
C(64)-C(51)-C(61)-C(62)	0.2(5)
C(52)-C(51)-C(61)-C(62)	173.1(4)
Fe(2)-C(51)-C(61)-C(62)	59.1(3)
C(64)-C(51)-C(61)-Fe(2)	-58.9(3)
C(52)-C(51)-C(61)-Fe(2)	114.0(4)
C(51)-C(61)-C(62)-C(63)	0.5(6)
Fe(2)-C(61)-C(62)-C(63)	58.8(3)
C(51)-C(61)-C(62)-Fe(2)	-58.3(3)
C(61)-C(62)-C(63)-C(64)	-1.0(6)
Fe(2)-C(62)-C(63)-C(64)	57.7(3)
C(61)-C(62)-C(63)-Fe(2)	-58.7(3)
C(61)-C(51)-C(64)-C(63)	-0.8(5)
C(52)-C(51)-C(64)-C(63)	-173.3(4)
Fe(2)-C(51)-C(64)-C(63)	-60.7(3)
C(61)-C(51)-C(64)-Fe(2)	59.8(3)
C(52)-C(51)-C(64)-Fe(2)	-112.6(5)
C(62)-C(63)-C(64)-C(51)	1.2(5)
Fe(2)-C(63)-C(64)-C(51)	60.2(3)
C(62)-C(63)-C(64)-Fe(2)	-59.1(4)
C(69)-C(65)-C(66)-C(67)	0.1(6)
Fe(2)-C(65)-C(66)-C(67)	-59.0(4)
C(69)-C(65)-C(66)-Fe(2)	59.1(4)
C(65)-C(66)-C(67)-C(68)	-0.5(6)
Fe(2)-C(66)-C(67)-C(68)	-59.7(4)
C(65)-C(66)-C(67)-Fe(2)	59.2(4)
C(66)-C(67)-C(68)-C(69)	0.6(6)
Fe(2)-C(67)-C(68)-C(69)	-59.6(3)
C(66)-C(67)-C(68)-Fe(2)	60.2(4)
C(66)-C(65)-C(69)-C(68)	0.3(6)
Fe(2)-C(65)-C(69)-C(68)	59.5(3)
C(66)-C(65)-C(69)-Fe(2)	-59.2(4)
C(67)-C(68)-C(69)-C(65)	-0.6(6)
Fe(2)-C(68)-C(69)-C(65)	-59.9(3)
C(67)-C(68)-C(69)-Fe(2)	59.4(3)

Symmetry transformations used to generate equivalent atoms: