Supplementary materials

for crystal structures (I) - (II)

Figures 1 and 2.

ORTEP II plot for (**I**)-(**II**).

Tables 1-1; 2-1.

Crystal data and structure refinement for (**I**)-(**II**).

Tables 1-2; 2-2.

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for (**I**)-(**II**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Tables 1-3; 2-3.

Selected bond lengths [Å] and angles [deg] for (**I**)-(**II**).

Tables 1-4; 2-4.

Bond lengths [Å] and angles [deg] for (**I**)-(**II**).

Tables 1-5; 2-5.

Anisotropic displacement parameters (Å^2 x 10^3) for (**I**)-(**II**).The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

Table 1-6.

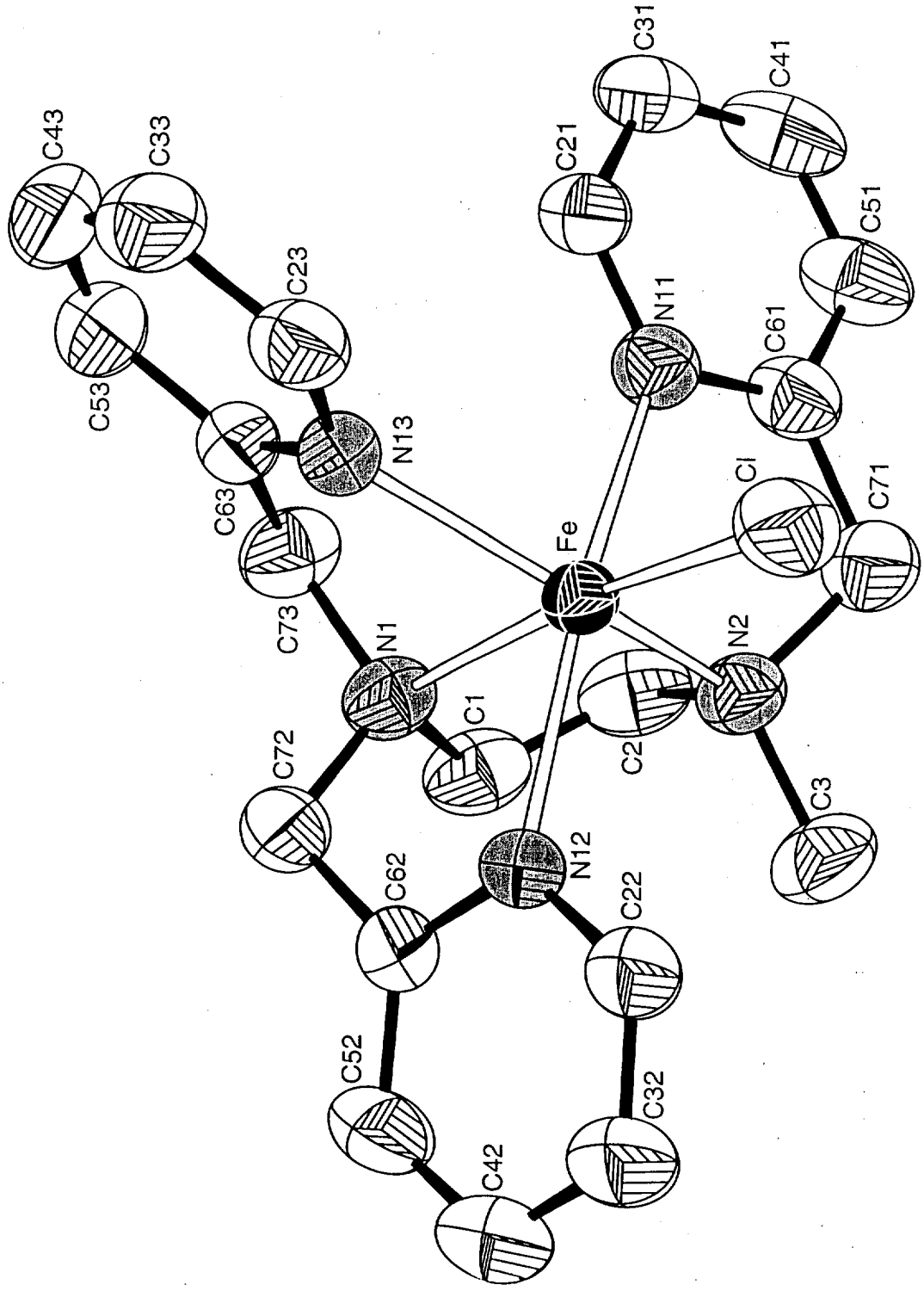
Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for (**I**).

Table 2-6.

Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for (**II**).

Tables 1-7; 2-7.

Observed and calculated structure factors for (**I**)-(**II**).


C31
C41
C43
C33
C21
C51
C23
N11
C53
C61
N13
Cl
C71
C63
Fe
C73
N1
N2
C1
C2
C72
C3
N12
C62
C22
C52
C32
C42

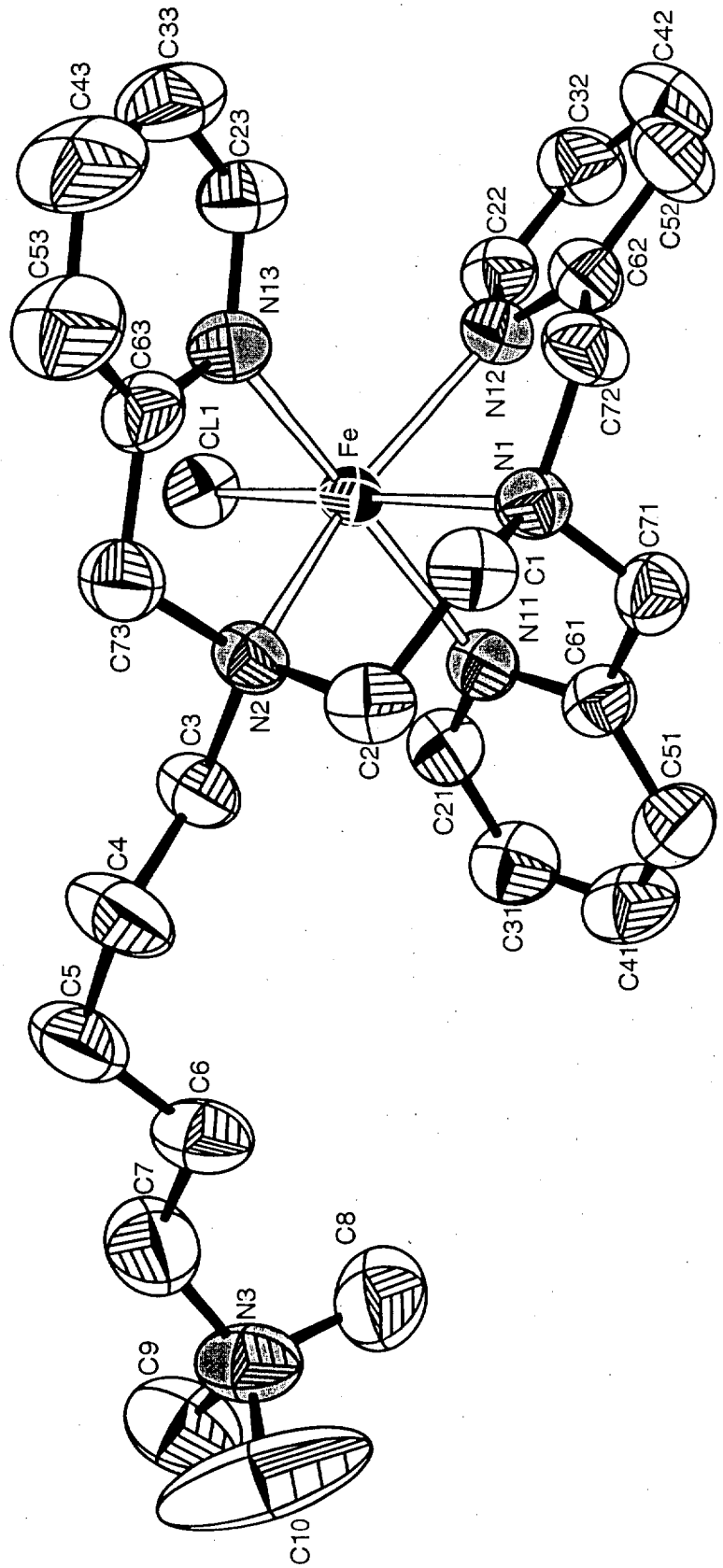

C33
C43
C23
C42
C32
C22
C52
C62
C53
N13
C63
N12
C72
CL1
Fe
N1
C71
C73
N11
C1
C61
N2
C2
C3
C21
C51
C4
C31
C41
C5
C6
C7
C8
N3
C9
C10

Table 1-1. Crystal data and structure refinement for (I).

Identification code	(I)	
Empirical formula	C45 H45 B Cl Fe N5	
Formula weight	757.97	
Temperature	294(2) K	
Wavelength	0.71073 A	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 17.645(7) Å	α = 90 deg.
	b = 16.077(6) Å	β = 90 deg.
	c = 13.934(5) Å	γ = 90 deg.
Volume	3953(3) $Å^3$	
Z	4	
Density (calculated)	1.274 Mg/m^3	
Absorption coefficient	0.488 mm^{-1}	
F(000)	1592	
Crystal size	0.50 x 0.50 x 0.50 mm	
Theta range for data collection	2.25 to 28.00 deg.	
Index ranges	-23<=h<=23, 0<=k<=21, 0<=l<=18	
Reflections collected	10241	
Independent reflections	9559 [R(int) = 0.0301]	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9353 / 0 / 614	
Goodness-of-fit on F^2	1.057	
Final R indices [I>2sigma(I)]	R1 = 0.0500, wR2 = 0.0756	
R indices (all data)	R1 = 0.0974, wR2 = 0.1072	
Absolute structure parameter	-0.04(2)	
Extinction coefficient	0.0027(4)	
Largest difference peak and hole	0.195 and -0.192 $e.Å^{-3}$	

Table 1-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (I). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Fe	4568(1)	7070(1)	9812(1)	40(1)
Cl	5668(1)	7860(1)	9642(1)	62(1)
N(1)	3392(2)	6494(2)	9876(2)	51(1)
C(1)	3118(2)	6476(3)	10886(3)	64(1)
C(2)	3770(3)	6405(3)	11576(3)	67(1)
N(2)	4344(2)	7061(2)	11400(2)	52(1)
C(3)	4105(3)	7858(3)	11835(3)	70(1)
N(11)	5227(2)	5969(2)	10400(2)	50(1)
C(21)	5492(2)	5291(2)	9951(3)	54(1)
C(31)	5904(2)	4682(2)	10400(4)	61(1)
C(41)	6054(2)	4771(3)	11364(4)	73(1)
C(51)	5804(2)	5462(3)	11834(3)	71(1)
C(61)	5385(2)	6055(2)	11345(2)	54(1)
C(71)	5084(3)	6818(3)	11825(3)	66(1)
N(12)	3795(1)	8120(2)	9554(2)	44(1)
C(22)	3983(2)	8919(2)	9693(3)	54(1)
C(32)	3454(2)	9532(2)	9805(4)	68(1)
C(42)	2704(2)	9329(3)	9783(4)	79(1)
C(52)	2496(2)	8519(3)	9609(3)	68(1)
C(62)	3055(2)	7927(2)	9492(2)	49(1)
C(72)	2893(2)	7030(3)	9284(3)	59(1)
N(13)	4451(2)	6340(2)	8510(2)	45(1)
C(23)	4909(2)	6396(2)	7742(3)	53(1)
C(33)	4900(3)	5800(3)	7018(3)	68(1)
C(43)	4434(3)	5139(3)	7089(3)	74(1)
C(53)	3956(3)	5083(3)	7866(3)	68(1)
C(63)	3970(2)	5692(2)	8564(3)	50(1)
C(73)	3478(2)	5657(2)	9452(3)	62(1)
B	7796(2)	7874(2)	4768(3)	41(1)
C(11')	7132(2)	8362(2)	4160(2)	44(1)
C(21')	6364(2)	8271(2)	4328(3)	60(1)
C(31')	5815(2)	8623(3)	3737(4)	74(1)
C(41')	6025(3)	9106(3)	2957(4)	75(1)
C(51')	6779(3)	9215(3)	2772(3)	71(1)
C(61')	7315(2)	8854(3)	3361(3)	59(1)
C(12')	8501(2)	8491(2)	5075(2)	41(1)
C(22')	9201(2)	8174(2)	5371(3)	51(1)
C(32')	9794(2)	8672(3)	5662(3)	63(1)
C(42')	9707(3)	9518(3)	5709(3)	67(1)
C(52')	9028(3)	9862(3)	5452(3)	67(1)
C(62')	8438(2)	9353(2)	5121(3)	53(1)
C(13')	8073(2)	7125(2)	4041(2)	45(1)
C(23')	8769(2)	7088(3)	3575(3)	60(1)
C(33')	8975(3)	6437(3)	2965(3)	71(1)
C(43')	8491(3)	5805(3)	2793(3)	73(1)
C(53')	7784(3)	5820(3)	3203(3)	72(1)
C(63')	7584(2)	6468(3)	3812(4)	66(1)
C(14')	7457(2)	7523(2)	5790(3)	41(1)
C(24')	7149(3)	8067(3)	6453(3)	64(1)
C(34')	6852(2)	7819(3)	7338(3)	66(1)

Table 1-3. Selected bond lengths [Å] and angles [deg] for (I).

Fe-N(13)	2.171(3)
Fe-N(12)	2.200(3)
Fe-N(2)	2.248(3)
Fe-N(11)	2.270(3)
Fe-N(1)	2.274(3)
Fe-Cl	2.3302(11)
N(13)-Fe-N(12)	102.63(10)
N(13)-Fe-N(2)	143.35(11)
N(12)-Fe-N(2)	93.26(10)
N(13)-Fe-N(11)	85.92(10)
N(12)-Fe-N(11)	167.04(10)
N(2)-Fe-N(11)	74.32(10)
N(13)-Fe-N(1)	74.05(11)
N(12)-Fe-N(1)	75.67(10)
N(2)-Fe-N(1)	78.36(11)
N(11)-Fe-N(1)	97.77(10)
N(13)-Fe-Cl	106.79(8)
N(12)-Fe-Cl	94.70(8)
N(2)-Fe-Cl	104.51(8)
N(11)-Fe-Cl	92.05(8)
N(1)-Fe-Cl	170.18(8)

Table 1-4. Bond lengths [Å] and angles [deg] for (I).

Fe-N(13)	2.171(3)
Fe-N(12)	2.200(3)
Fe-N(2)	2.248(3)
Fe-N(11)	2.270(3)
Fe-N(1)	2.274(3)
Fe-Cl	2.3302(11)
N(1)-C(73)	1.478(5)
N(1)-C(72)	1.483(5)
N(1)-C(1)	1.488(5)
C(1)-C(2)	1.504(6)
C(2)-N(2)	1.482(5)
N(2)-C(3)	1.479(5)
N(2)-C(71)	1.485(5)
N(11)-C(21)	1.342(4)
N(11)-C(61)	1.353(4)
C(21)-C(31)	1.370(5)
C(31)-C(41)	1.376(6)
C(41)-C(51)	1.364(6)
C(51)-C(61)	1.386(5)
C(61)-C(71)	1.494(5)
N(12)-C(22)	1.341(4)
N(12)-C(62)	1.344(4)
C(22)-C(32)	1.368(5)
C(32)-C(42)	1.364(5)
C(42)-C(52)	1.375(5)
C(52)-C(62)	1.381(5)
C(62)-C(72)	1.499(5)
N(13)-C(23)	1.344(4)
N(13)-C(63)	1.346(4)
C(23)-C(33)	1.391(5)
C(33)-C(43)	1.348(6)
C(43)-C(53)	1.375(6)
C(53)-C(63)	1.381(5)
C(63)-C(73)	1.513(5)
B-C(11')	1.645(5)
B-C(14')	1.646(5)
B-C(12')	1.647(5)
B-C(13')	1.647(5)
C(11')-C(21')	1.383(5)
C(11')-C(61')	1.403(5)
C(21')-C(31')	1.391(6)
C(31')-C(41')	1.385(6)
C(41')-C(51')	1.366(6)
C(51')-C(61')	1.381(6)
C(12')-C(62')	1.392(4)
C(12')-C(22')	1.398(4)
C(22')-C(32')	1.380(5)
C(32')-C(42')	1.370(6)
C(42')-C(52')	1.367(6)
C(52')-C(62')	1.402(5)
C(13')-C(23')	1.392(5)
C(13')-C(63')	1.401(5)
C(23')-C(33')	1.397(5)
C(33')-C(43')	1.348(6)
C(43')-C(53')	1.373(6)
C(53')-C(63')	1.389(6)

C(14')-C(64')	1.379(4)
C(14')-C(24')	1.383(5)
C(24')-C(34')	1.397(5)
C(34')-C(44')	1.359(6)
C(44')-C(54')	1.359(6)
C(54')-C(64')	1.406(6)
N(13)-Fe-N(12)	102.63(10)
N(13)-Fe-N(2)	143.35(11)
N(12)-Fe-N(2)	93.26(10)
N(13)-Fe-N(11)	85.92(10)
N(12)-Fe-N(11)	167.04(10)
N(2)-Fe-N(11)	74.32(10)
N(13)-Fe-N(1)	74.05(11)
N(12)-Fe-N(1)	75.67(10)
N(2)-Fe-N(1)	78.36(11)
N(11)-Fe-N(1)	97.77(10)
N(13)-Fe-Cl	106.79(8)
N(12)-Fe-Cl	94.70(8)
N(2)-Fe-Cl	104.51(8)
N(11)-Fe-Cl	92.05(8)
N(1)-Fe-Cl	170.18(8)
C(73)-N(1)-C(72)	111.5(3)
C(73)-N(1)-C(1)	113.2(3)
C(72)-N(1)-C(1)	110.1(3)
C(73)-N(1)-Fe	105.2(2)
C(72)-N(1)-Fe	106.5(2)
C(1)-N(1)-Fe	110.0(2)
N(1)-C(1)-C(2)	110.9(3)
N(2)-C(2)-C(1)	111.3(3)
C(3)-N(2)-C(2)	110.7(3)
C(3)-N(2)-C(71)	108.4(3)
C(2)-N(2)-C(71)	110.3(3)
C(3)-N(2)-Fe	116.6(2)
C(2)-N(2)-Fe	106.7(2)
C(71)-N(2)-Fe	103.9(2)
C(21)-N(11)-C(61)	117.7(3)
C(21)-N(11)-Fe	130.1(2)
C(61)-N(11)-Fe	112.1(2)
N(11)-C(21)-C(31)	123.5(4)
C(21)-C(31)-C(41)	118.3(4)
C(51)-C(41)-C(31)	119.4(4)
C(41)-C(51)-C(61)	119.8(4)
N(11)-C(61)-C(51)	121.2(4)
N(11)-C(61)-C(71)	116.5(3)
C(51)-C(61)-C(71)	122.3(4)
N(2)-C(71)-C(61)	110.4(3)
C(22)-N(12)-C(62)	118.1(3)
C(22)-N(12)-Fe	123.9(2)
C(62)-N(12)-Fe	115.9(2)
N(12)-C(22)-C(32)	122.5(3)
C(42)-C(32)-C(22)	119.2(4)
C(32)-C(42)-C(52)	119.3(4)
C(42)-C(52)-C(62)	118.9(4)
N(12)-C(62)-C(52)	121.9(3)
N(12)-C(62)-C(72)	114.8(3)
C(52)-C(62)-C(72)	123.3(3)
N(1)-C(72)-C(62)	109.7(3)
C(23)-N(13)-C(63)	118.4(3)
C(23)-N(13)-Fe	124.9(2)

C(63)-N(13)-Fe	115.6(2)
N(13)-C(23)-C(33)	121.6(4)
C(43)-C(33)-C(23)	119.8(4)
C(33)-C(43)-C(53)	119.0(4)
C(43)-C(53)-C(63)	119.8(4)
N(13)-C(63)-C(53)	121.5(4)
N(13)-C(63)-C(73)	115.9(3)
C(53)-C(63)-C(73)	122.6(4)
N(1)-C(73)-C(63)	110.6(3)
C(11')-B-C(14')	110.5(2)
C(11')-B-C(12')	112.6(3)
C(14')-B-C(12')	104.9(3)
C(11')-B-C(13')	104.1(3)
C(14')-B-C(13')	112.9(3)
C(12')-B-C(13')	112.1(2)
C(21')-C(11')-C(61')	114.8(3)
C(21')-C(11')-B	124.1(3)
C(61')-C(11')-B	120.9(3)
C(11')-C(21')-C(31')	122.6(4)
C(41')-C(31')-C(21')	120.4(4)
C(51')-C(41')-C(31')	118.7(4)
C(41')-C(51')-C(61')	120.0(4)
C(51')-C(61')-C(11')	123.4(4)
C(62')-C(12')-C(22')	114.9(3)
C(62')-C(12')-B	123.4(3)
C(22')-C(12')-B	121.6(3)
C(32')-C(22')-C(12')	123.1(4)
C(42')-C(32')-C(22')	120.3(4)
C(52')-C(42')-C(32')	119.2(4)
C(42')-C(52')-C(62')	120.1(4)
C(12')-C(62')-C(52')	122.4(4)
C(23')-C(13')-C(63')	113.9(3)
C(23')-C(13')-B	125.4(3)
C(63')-C(13')-B	120.6(3)
C(13')-C(23')-C(33')	123.1(4)
C(43')-C(33')-C(23')	120.6(4)
C(33')-C(43')-C(53')	119.3(4)
C(43')-C(53')-C(63')	119.9(4)
C(53')-C(63')-C(13')	123.3(4)
C(64')-C(14')-C(24')	114.1(3)
C(64')-C(14')-B	125.6(3)
C(24')-C(14')-B	120.3(3)
C(14')-C(24')-C(34')	123.8(4)
C(44')-C(34')-C(24')	120.0(4)
C(34')-C(44')-C(54')	118.6(4)
C(44')-C(54')-C(64')	120.7(4)
C(14')-C(64')-C(54')	122.8(4)

Table 1-5. Anisotropic displacement parameters ($Å^2 \times 10^3$) for (I).
The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U11 + \ldots + 2 h k a^* b^* U12]$$

Atom	U11	U22	U33	U23	U13	U12
Fe	38(1)	40(1)	41(1)	-3(1)	3(1)	0(1)
Cl	43(1)	59(1)	85(1)	-7(1)	7(1)	-6(1)
N(1)	50(2)	46(2)	58(2)	-3(2)	12(2)	-2(1)
C(1)	61(3)	59(3)	72(3)	-4(2)	26(2)	-1(2)
C(2)	78(3)	64(3)	57(3)	7(2)	27(2)	9(2)
N(2)	59(2)	53(2)	43(2)	-5(2)	4(1)	9(2)
C(3)	91(3)	68(3)	52(2)	-16(3)	7(2)	16(3)
N(11)	53(2)	50(2)	48(2)	1(1)	-1(1)	7(1)
C(21)	47(2)	54(2)	60(2)	-4(2)	3(2)	6(2)
C(31)	48(2)	53(2)	83(3)	-1(2)	11(2)	11(2)
C(41)	56(3)	78(3)	84(4)	34(3)	16(2)	23(2)
C(51)	62(3)	96(3)	55(3)	20(3)	7(2)	22(2)
C(61)	50(2)	62(2)	50(2)	7(2)	0(2)	10(2)
C(71)	78(3)	79(3)	40(2)	-5(2)	-4(2)	21(2)
N(12)	41(1)	42(2)	49(2)	-3(1)	-2(1)	5(1)
C(22)	51(2)	47(2)	63(2)	-1(2)	-6(2)	5(2)
C(32)	67(3)	49(2)	88(3)	-1(3)	-12(3)	13(2)
C(42)	69(3)	65(3)	104(4)	-8(3)	-15(3)	27(2)
C(52)	43(2)	72(3)	89(4)	-3(3)	-6(2)	13(2)
C(62)	44(2)	53(2)	49(2)	-7(2)	-5(2)	4(2)
C(72)	37(2)	66(2)	75(3)	-16(3)	0(2)	0(2)
N(13)	43(2)	49(2)	44(2)	-4(1)	-1(1)	3(1)
C(23)	51(2)	59(2)	49(2)	5(2)	1(2)	12(2)
C(33)	78(3)	83(3)	43(2)	0(2)	2(2)	27(3)
C(43)	92(4)	72(3)	57(3)	-21(2)	-19(3)	21(3)
C(53)	67(3)	57(3)	78(3)	-20(2)	-13(3)	4(2)
C(63)	45(2)	46(2)	58(2)	-9(2)	-6(2)	3(2)
C(73)	57(2)	47(2)	81(3)	-11(2)	13(2)	-11(2)
B	50(2)	35(2)	38(2)	2(2)	2(2)	7(2)
C(11')	50(2)	36(2)	47(2)	-5(2)	2(2)	3(2)
C(21')	52(2)	53(2)	74(3)	11(2)	1(2)	3(2)
C(31')	51(2)	75(3)	97(4)	6(3)	-6(3)	6(2)
C(41')	67(3)	74(3)	84(3)	7(3)	-22(3)	20(2)
C(51')	88(3)	71(3)	55(3)	15(2)	-5(2)	5(3)
C(61')	57(2)	64(3)	55(2)	11(2)	2(2)	8(2)
C(12')	49(2)	41(2)	34(2)	0(1)	8(2)	0(1)
C(22')	58(2)	53(2)	43(2)	4(2)	2(2)	3(2)
C(32')	57(2)	84(3)	48(2)	7(2)	0(2)	-5(2)
C(42')	70(3)	89(3)	42(2)	-2(2)	3(2)	-31(3)
C(52')	98(3)	48(2)	54(3)	-10(2)	11(2)	-20(2)
C(62')	63(2)	44(2)	52(2)	-5(2)	7(2)	-1(2)
C(13')	59(2)	34(2)	43(2)	1(2)	-1(2)	0(2)
C(23')	75(3)	47(2)	57(2)	-7(2)	19(2)	-7(2)
C(33')	81(3)	69(3)	62(3)	-13(2)	30(2)	3(3)
C(43')	97(4)	61(3)	60(3)	-25(2)	2(3)	9(3)
C(53')	81(3)	57(3)	79(3)	-29(2)	-15(3)	-1(2)
C(63')	58(3)	61(3)	79(3)	-22(2)	-3(2)	1(2)
C(14')	41(2)	37(2)	46(2)	3(2)	0(2)	-2(2)
C(24')	99(3)	44(2)	49(2)	3(2)	16(2)	3(2)
C(34')	83(3)	66(3)	48(2)	1(2)	14(2)	-1(2)
C(44')	49(2)	81(3)	49(2)	20(3)	2(2)	-6(2)
C(54')	70(3)	53(2)	83(3)	29(3)	16(2)	1(2)
C(64')	58(2)	45(2)	66(3)	9(2)	15(2)	8(2)

Table 1-6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (I).

Atom	x	y	z	U(eq)
H(1A)	2765(21)	5909(25)	10957(26)	77
H(1B)	2857(21)	7025(27)	10975(25)	77
H(2A)	3613(23)	6466(24)	12195(31)	80
H(2B)	4045(24)	5866(27)	11544(28)	80
H(3A)	3998(21)	7804(26)	12477(32)	84
H(3B)	3582(24)	7995(28)	11549(28)	84
H(3C)	4530(25)	8287(24)	11709(27)	84
H(21)	5335(20)	5266(20)	9247(26)	64
H(31)	6058(20)	4238(22)	10059(29)	74
H(41)	6287(25)	4390(28)	11713(31)	87
H(51)	5867(22)	5529(25)	12504(31)	85
H(71A)	5059(21)	6733(23)	12519(31)	79
H(71B)	5460(22)	7275(25)	11725(27)	79
H(22)	4545(20)	9021(19)	9711(24)	64
H(32)	3616(21)	10085(23)	9894(30)	82
H(42)	2328(23)	9778(25)	9892(32)	95
H(52)	1978(22)	8337(22)	9592(29)	82
H(72A)	2371(22)	6907(21)	9399(25)	71
H(72B)	3008(20)	6908(24)	8613(28)	71
H(23)	5208(19)	6917(23)	7711(23)	64
H(33)	5250(22)	5879(24)	6457(28)	82
H(43)	4416(23)	4702(26)	6569(30)	88
H(53)	3580(24)	4633(26)	7953(30)	81
H(73A)	2989(23)	5383(23)	9224(28)	74
H(73B)	3727(21)	5297(22)	9871(30)	74
H(21')	6214(18)	7901(21)	4856(26)	71
H(31')	5304(26)	8559(26)	3899(30)	89
H(41')	5659(24)	9372(26)	2582(30)	90
H(51')	6928(25)	9567(26)	2246(32)	86
H(61')	7847(22)	8909(23)	3206(26)	70
H(22')	9254(17)	7561(21)	5364(26)	61
H(32')	10239(22)	8424(23)	5826(27)	75
H(42')	10133(23)	9842(24)	5873(28)	80
H(52')	8968(21)	10401(24)	5440(31)	80
H(62')	7987(19)	9583(20)	4911(27)	64
H(23')	9151(20)	7486(23)	3722(28)	71
H(33')	9443(24)	6493(25)	2691(29)	85
H(43')	8584(24)	5369(27)	2384(32)	87
H(53')	7411(24)	5355(25)	3099(31)	87
H(63')	7183(24)	6468(28)	4026(31)	79
H(24')	7155(22)	8662(26)	6253(28)	77
H(34')	6644(21)	8246(24)	7803(29)	79
H(44')	6728(20)	6873(23)	8253(28)	72
H(54')	7222(23)	5875(27)	7084(31)	82
H(64')	7672(21)	6330(22)	5647(28)	68

Table 2-1. Crystal data and structure refinement for (II).

Identification code	(II)
Empirical formula	C28 H41 Cl3 Fe N6 O8
Formula weight	751.87
Temperature	294(2) K
Wavelength	0.71073 A
Crystal system	Monoclinic
Space group	P21/a
Unit cell dimensions	a = 14.691(2) Å α = 90 deg. b = 13.545(2) Å β = 93.43(1) deg. c = 17.430(2) Å γ = 90 deg.
Volume	3462(1) $Å^3$
Z	4
Density (calculated)	1.44 Mg/m^2
Absorption coefficient	0.722 mm^{-1}
F(000)	1568
Crystal size	0.75 x 0.25 x 0.20 mm
Theta range for data collection	2.05 to 24.96 deg.
Index ranges	-17<=h<=17, -16<=k<=16, 0<=l<=20
Reflections collected	12574
Independent reflections	6078 [R(int) = 0.0373]
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6077 / 109 / 396
Goodness-of-fit on F^2	1.031
Final R indices [I>2sigma(I)]	R1 = 0.0520, wR2 = 0.1377
R indices (all data)	R1 = 0.0958, wR2 = 0.1628
Largest difference peak and hole	0.558 and -0.329 $e.Å^{-3}$

Table 2-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (11). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Fe	3896(1)	1727(1)	1889(1)	41(1)
Cl(1)	2545(1)	801(1)	1829(1)	55(1)
N(11)	4716(3)	672(3)	1284(2)	48(1)
C(21)	4492(4)	-281(4)	1162(3)	57(1)
C(31)	5102(5)	-966(5)	922(4)	71(2)
C(41)	5975(5)	-661(5)	798(4)	77(2)
C(51)	6213(4)	297(5)	929(4)	69(2)
C(61)	5564(4)	962(4)	1156(3)	50(1)
C(71)	5762(4)	2050(4)	1234(3)	56(1)
N(12)	3662(3)	2694(3)	891(3)	48(1)
C(22)	2989(4)	2611(5)	339(3)	56(1)
C(32)	2829(5)	3300(6)	-239(4)	73(2)
C(42)	3367(5)	4128(6)	-230(4)	87(2)
C(52)	4065(5)	4224(5)	327(4)	78(2)
C(62)	4211(4)	3490(4)	872(3)	56(1)
C(72)	4970(4)	3558(4)	1496(4)	59(2)
N(13)	3483(3)	2878(3)	2684(3)	51(1)
C(23)	3072(4)	3737(4)	2495(4)	61(2)
C(33)	2936(5)	4471(5)	3012(5)	83(2)
C(43)	3262(7)	4349(6)	3748(6)	107(3)
C(53)	3701(6)	3481(6)	3961(4)	94(2)
C(63)	3784(4)	2756(4)	3418(3)	58(2)
C(73)	4193(5)	1764(5)	3636(3)	65(2)
N(1)	5211(3)	2566(3)	1785(3)	48(1)
C(1)	5674(4)	2603(4)	2564(3)	56(1)
C(2)	5617(4)	1619(4)	2965(3)	55(1)
N(2)	4658(3)	1278(3)	3015(2)	48(1)
C(3)	4649(4)	189(4)	3136(3)	59(2)
C(4)	5114(6)	-188(5)	3884(4)	89(2)
C(5)	5096(7)	-1300(6)	3939(4)	97(3)
C(6)	5747(5)	-1832(5)	3446(4)	75(2)
C(7)	5658(8)	-2920(6)	3523(6)	117(3)
N(3)	6348(4)	-3562(4)	3189(3)	81(2)
C(8)	6430(8)	-3328(8)	2350(6)	101(3)
C(9)	5953(8)	-4614(7)	3174(7)	108(4)
C(10)	7160(2)	-3569(4)	3633(2)	208(11)
C(11)	7220(1)	-3093(9)	2802(1)	121(16)
C(12)	6804(4)	-4415(3)	3617(6)	156(23)
C(13)	5813(4)	-3884(8)	2614(5)	141(20)
Cl(2)	1252(1)	1554(1)	8541(1)	108(1)
O(12)	1156(1)	2441(1)	8114(1)	152(3)
O(22)	670(1)	826(1)	8231(1)	189(4)
O(32)	1105(1)	1739(1)	9330(1)	178(4)
O(42)	2142(1)	1235(1)	8493(1)	236(6)
Cl(3)	1667(1)	1754(1)	4847(1)	96(1)
O(13)	1750(1)	1538(2)	4056(1)	210(6)
O(23)	921(1)	1252(1)	4967(1)	266(9)

Table 2-3. Selected bond lengths [Å] and angles [deg] for (II).

Fe-N(11)	2.181(4)
Fe-N(12)	2.188(4)
Fe-N(13)	2.196(4)
Fe-N(1)	2.258(4)
Fe-N(2)	2.283(4)
Fe-Cl(1)	2.3449(14)
N(11)-Fe-N(12)	94.2(2)
N(11)-Fe-N(13)	162.2(2)
N(12)-Fe-N(13)	92.3(2)
N(11)-Fe-N(1)	78.0(2)
N(12)-Fe-N(1)	74.3(2)
N(13)-Fe-N(1)	87.9(2)
N(11)-Fe-N(2)	89.1(2)
N(12)-Fe-N(2)	152.6(2)
N(13)-Fe-N(2)	77.6(2)
N(1)-Fe-N(2)	79.9(2)
N(11)-Fe-Cl(1)	96.82(12)
N(12)-Fe-Cl(1)	101.12(12)
N(13)-Fe-Cl(1)	98.19(12)
N(1)-Fe-Cl(1)	172.63(12)
N(2)-Fe-Cl(1)	105.42(12)

Table 2-4. Bond lengths [Å] and angles [deg] for (II).

Fe-N(11)	2.181(4)
Fe-N(12)	2.188(4)
Fe-N(13)	2.196(4)
Fe-N(1)	2.258(4)
Fe-N(2)	2.283(4)
Fe-Cl(1)	2.3449(14)
N(11)-C(61)	1.338(7)
N(11)-C(21)	1.345(7)
C(21)-C(31)	1.373(9)
C(31)-C(41)	1.377(10)
C(41)-C(51)	1.360(9)
C(51)-C(61)	1.386(8)
C(61)-C(71)	1.506(8)
C(71)-N(1)	1.470(7)
N(12)-C(22)	1.343(7)
N(12)-C(62)	1.348(7)
C(22)-C(32)	1.383(9)
C(32)-C(42)	1.371(11)
C(42)-C(52)	1.376(10)
C(52)-C(62)	1.384(8)
C(62)-C(72)	1.513(8)
C(72)-N(1)	1.471(7)
N(13)-C(63)	1.338(7)
N(13)-C(23)	1.344(7)
C(23)-C(33)	1.364(9)
C(33)-C(43)	1.351(11)
C(43)-C(53)	1.381(11)
C(53)-C(63)	1.374(9)
C(63)-C(73)	1.511(8)
C(73)-N(2)	1.470(7)
N(1)-C(1)	1.482(7)
C(1)-C(2)	1.510(8)
C(2)-N(2)	1.490(7)
N(2)-C(3)	1.491(7)
C(3)-C(4)	1.524(8)
C(4)-C(5)	1.509(10)
C(5)-C(6)	1.506(10)
C(6)-C(7)	1.486(11)
C(7)-N(3)	1.480(9)
N(3)-C(13)	1.311(6)
N(3)-C(10)	1.383(6)
N(3)-C(8)	1.508(11)
N(3)-C(12)	1.511(8)
N(3)-C(9)	1.539(11)
N(3)-C(11)	1.613(9)
Cl(2)-O(42)	1.39
Cl(2)-O(22)	1.39
Cl(2)-O(12)	1.42
Cl(2)-O(32)	1.43
Cl(3)-O(33)	1.25
Cl(3)-O(23')	1.30
Cl(3)-O(43')	1.32
Cl(3)-O(23)	1.32
Cl(3)-O(33')	1.34

Cl(3)-O(13')	1.36
Cl(3)-O(13)	1.42
Cl(3)-O(43)	1.47
N(11)-Fe-N(12)	94.2(2)
N(11)-Fe-N(13)	162.2(2)
N(12)-Fe-N(13)	92.3(2)
N(11)-Fe-N(1)	78.0(2)
N(12)-Fe-N(1)	74.3(2)
N(13)-Fe-N(1)	87.9(2)
N(11)-Fe-N(2)	89.1(2)
N(12)-Fe-N(2)	152.6(2)
N(13)-Fe-N(2)	77.6(2)
N(1)-Fe-N(2)	79.9(2)
N(11)-Fe-Cl(1)	96.82(12)
N(12)-Fe-Cl(1)	101.12(12)
N(13)-Fe-Cl(1)	98.19(12)
N(1)-Fe-Cl(1)	172.63(12)
N(2)-Fe-Cl(1)	105.42(12)
C(61)-N(11)-C(21)	118.5(5)
C(61)-N(11)-Fe	115.8(3)
C(21)-N(11)-Fe	124.6(4)
N(11)-C(21)-C(31)	122.6(6)
C(21)-C(31)-C(41)	118.5(6)
C(51)-C(41)-C(31)	119.5(6)
C(41)-C(51)-C(61)	119.5(6)
N(11)-C(61)-C(51)	121.3(6)
N(11)-C(61)-C(71)	116.7(5)
C(51)-C(61)-C(71)	121.9(5)
N(1)-C(71)-C(61)	114.5(4)
C(22)-N(12)-C(62)	117.7(5)
C(22)-N(12)-Fe	126.4(4)
C(62)-N(12)-Fe	115.7(4)
N(12)-C(22)-C(32)	123.4(6)
C(42)-C(32)-C(22)	118.2(6)
C(32)-C(42)-C(52)	119.3(6)
C(42)-C(52)-C(62)	119.7(7)
N(12)-C(62)-C(52)	121.6(6)
N(12)-C(62)-C(72)	116.6(5)
C(52)-C(62)-C(72)	121.8(6)
N(1)-C(72)-C(62)	110.0(4)
C(63)-N(13)-C(23)	117.3(5)
C(63)-N(13)-Fe	115.3(4)
C(23)-N(13)-Fe	126.7(4)
N(13)-C(23)-C(33)	123.4(6)
C(43)-C(33)-C(23)	118.7(7)
C(33)-C(43)-C(53)	119.5(7)
C(63)-C(53)-C(43)	118.9(7)
N(13)-C(63)-C(53)	122.2(6)
N(13)-C(63)-C(73)	117.0(5)
C(53)-C(63)-C(73)	120.8(6)
N(2)-C(73)-C(63)	114.1(5)
C(71)-N(1)-C(72)	109.9(5)
C(71)-N(1)-C(1)	111.9(4)
C(72)-N(1)-C(1)	111.8(4)
C(71)-N(1)-Fe	108.6(3)
C(72)-N(1)-Fe	107.4(3)
C(1)-N(1)-Fe	107.0(3)

N(1)-C(1)-C(2)	111.1(4)
N(2)-C(2)-C(1)	112.3(4)
C(73)-N(2)-C(2)	112.7(5)
C(73)-N(2)-C(3)	109.3(4)
C(2)-N(2)-C(3)	109.4(4)
C(73)-N(2)-Fe	106.8(3)
C(2)-N(2)-Fe	106.5(3)
C(3)-N(2)-Fe	112.2(3)
N(2)-C(3)-C(4)	116.5(5)
C(5)-C(4)-C(3)	112.3(6)
C(6)-C(5)-C(4)	115.3(7)
C(7)-C(6)-C(5)	111.2(7)
N(3)-C(7)-C(6)	118.8(8)
C(13)-N(3)-C(7)	95.9(6)
C(10)-N(3)-C(7)	111.9(6)
C(10)-N(3)-C(8)	115.4(7)
C(7)-N(3)-C(8)	110.7(6)
C(13)-N(3)-C(12)	110.5(6)
C(7)-N(3)-C(12)	123.3(7)
C(10)-N(3)-C(9)	108.3(6)
C(7)-N(3)-C(9)	106.5(7)
C(8)-N(3)-C(9)	103.3(7)
C(13)-N(3)-C(11)	105.4(6)
C(7)-N(3)-C(11)	120.9(7)
C(12)-N(3)-C(11)	99.6(3)
O(42)-Cl(2)-O(22)	108.4
O(42)-Cl(2)-O(12)	107.3
O(22)-Cl(2)-O(12)	111.0
O(42)-Cl(2)-O(32)	108.1
O(22)-Cl(2)-O(32)	112.0
O(12)-Cl(2)-O(32)	109.9
O(23')-Cl(3)-O(43')	90.8
O(33)-Cl(3)-O(23)	110.7
O(23')-Cl(3)-O(33')	123.8
O(43')-Cl(3)-O(33')	126.1
O(23')-Cl(3)-O(13')	101.7
O(43')-Cl(3)-O(13')	120.5
O(33')-Cl(3)-O(13')	93.8
O(33)-Cl(3)-O(13)	118.0
O(23)-Cl(3)-O(13)	99.7
O(33)-Cl(3)-O(43)	107.8
O(23)-Cl(3)-O(43)	119.0
O(13)-Cl(3)-O(43)	101.8

Table 2-5. Anisotropic displacement parameters ($Å^2 \times 10^3$) for (II). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

Atom	U11	U22	U33	U23	U13	U12
Fe	43(1)	34(1)	45(1)	-2(1)	0(1)	-3(1)
Cl	45(1)	47(1)	72(1)	-6(1)	2(1)	-11(1)
N(11)	56(3)	46(3)	43(2)	-5(2)	2(2)	1(2)
C(21)	70(4)	47(3)	53(3)	-11(3)	3(3)	-4(3)
C(31)	91(5)	58(4)	64(4)	-19(3)	1(3)	6(4)
C(41)	91(5)	70(5)	71(4)	-22(4)	5(4)	24(4)
C(51)	60(4)	79(5)	68(4)	-5(4)	8(3)	9(3)
C(61)	50(3)	58(4)	42(3)	-4(3)	1(2)	7(3)
C(71)	47(3)	62(4)	60(3)	2(3)	7(3)	-5(3)
N(12)	51(2)	41(3)	52(3)	2(2)	1(2)	1(2)
C(22)	61(3)	55(4)	51(3)	-5(3)	0(3)	6(3)
C(32)	83(4)	81(5)	53(4)	8(4)	-9(3)	15(4)
C(42)	100(6)	84(6)	76(5)	32(4)	1(4)	12(4)
C(52)	82(5)	67(4)	85(5)	31(4)	5(4)	-8(3)
C(62)	53(3)	51(4)	65(4)	12(3)	6(3)	1(3)
C(72)	56(3)	39(3)	80(4)	11(3)	-2(3)	-7(3)
N(13)	54(3)	41(3)	57(3)	-8(2)	-3(2)	1(2)
C(23)	58(3)	49(3)	75(4)	-2(3)	0(3)	5(3)
C(33)	82(5)	50(4)	118(7)	-15(4)	13(4)	15(3)
C(43)	146(8)	66(5)	108(7)	-39(5)	8(6)	24(5)
C(53)	128(7)	86(6)	67(5)	-29(4)	4(4)	20(5)
C(63)	66(4)	50(3)	60(4)	-13(3)	12(3)	3(3)
C(73)	85(4)	63(4)	48(3)	-1(3)	5(3)	13(3)
N(1)	45(2)	40(2)	58(3)	0(2)	1(2)	-3(2)
C(1)	52(3)	51(3)	64(4)	-5(3)	-7(3)	-8(3)
C(2)	56(3)	56(4)	52(3)	-7(3)	-12(3)	2(3)
N(2)	61(3)	40(2)	41(2)	-1(2)	0(2)	2(2)
C(3)	81(4)	46(3)	49(3)	5(3)	0(3)	6(3)
C(4)	161(7)	58(4)	47(4)	6(3)	-4(4)	32(5)
C(5)	157(8)	68(5)	69(5)	19(4)	21(5)	45(5)
C(6)	94(5)	53(4)	76(4)	-1(3)	-8(4)	15(3)
C(7)	176(9)	71(5)	111(7)	19(5)	58(6)	47(6)
N(3)	100(4)	64(4)	76(4)	-14(3)	-15(3)	28(3)
C(8)	119(8)	76(7)	110(8)	-9(6)	36(7)	9(6)
C(9)	154(10)	54(6)	114(9)	-4(6)	-10(7)	5(6)
C(10)	134(11)	200(17)	272(20)	-149(15)	-136(13)	102(11)
Cl(2)	90(1)	72(1)	155(2)	-28(1)	-43(1)	9(1)
O(12)	190(7)	88(5)	177(7)	11(5)	11(6)	8(5)
O(22)	193(8)	104(6)	256(11)	-22(6)	-110(7)	-30(5)
O(32)	285(12)	117(6)	129(7)	-24(5)	0(7)	-30(6)
O(42)	133(7)	216(11)	346(15)	-96(10)	-89(8)	72(7)
Cl(3)	104(2)	95(2)	86(1)	15(1)	-24(1)	-13(1)
O(13)	361(20)	152(11)	111(8)	-49(7)	20(10)	13(11)
O(23)	153(11)	258(19)	386(26)	91(19)	3(13)	-51(12)
O(33)	329(19)	100(8)	399(23)	63(11)	-295(19)	-45(9)
O(43)	196(10)	78(6)	113(6)	14(5)	-23(6)	8(6)

Table 2-6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (11).

Atom	x	y	z	U(eq)
H(21)	3900(4)	-483(4)	1243(3)	68
H(31)	4929(5)	-1620(5)	845(4)	85
H(41)	6399(5)	-1107(5)	627(4)	93
H(51)	6808(4)	505(5)	866(4)	83
H(71A)	6401(4)	2135(4)	1392(3)	68
H(71B)	5658(4)	2357(4)	734(3)	68
H(22)	2610(4)	2061(5)	345(3)	67
H(32)	2370(5)	3205(6)	-622(4)	88
H(42)	3260(5)	4620(6)	-598(4)	104
H(52)	4437(5)	4781(5)	337(4)	93
H(72A)	5501(4)	3866(4)	1292(4)	70
H(72B)	4775(4)	3965(4)	1914(4)	70
H(23)	2869(4)	3837(4)	1986(4)	73
H(33)	2625(5)	5044(5)	2862(5)	100
H(43)	3192(7)	4846(6)	4107(6)	128
H(53)	3936(6)	3388(6)	4463(4)	112
H(73A)	4627(5)	1852(5)	4073(3)	78
H(73B)	3713(5)	1334(5)	3797(3)	78
H(1A)	5392(4)	3108(4)	2865(3)	67
H(1B)	6309(4)	2780(4)	2523(3)	67
H(2A)	5953(4)	1131(4)	2690(3)	66
H(2B)	5902(4)	1675(4)	3480(3)	66
H(3A)	4939(4)	-121(4)	2712(3)	71
H(3B)	4019(4)	-29(4)	3113(3)	71
H(4A)	5743(6)	35(5)	3920(4)	107
H(4B)	4812(6)	90(5)	4314(4)	107
H(5A)	5234(7)	-1487(6)	4470(4)	117
H(5B)	4482(7)	-1525(6)	3796(4)	117
H(6A)	5623(5)	-1645(5)	2913(4)	90
H(6B)	6367(5)	-1637(5)	3598(4)	90
H(7A)	5656(8)	-3072(6)	4066(6)	141
H(7B)	5066(8)	-3107(6)	3292(6)	141
H(8A)	6795(37)	-3823(26)	2122(10)	121
H(8B)	6712(39)	-2693(22)	2301(6)	121
H(8C)	5833(9)	-3318(46)	2092(9)	121
H(9A)	5892(43)	-4838(20)	3691(7)	130
H(9B)	6354(23)	-5048(12)	2920(34)	130
H(9C)	5365(21)	-4612(11)	2902(33)	130
H(10A)	7039(2)	-3463(2)	4162(2)	250
H(10B)	7550(1)	-3054(8)	3464(1)	250
H(10C)	7455(4)	-4196(6)	3581(6)	250