Table of Contents

Appendix 1

Crystallographic data of Complex 3

Table 1. Crystal data and structure refinement for Complex **3**.

Identification code	kgc2l_ac2c	
Empirical formula	C_{26} H_{18} Cr_2 Fe O_{12}	
Formula weight	682.25	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 12.3910(15) Å	a= 90°.
	b = 14.6211(17) Å	b= 90.047(2)°.
	c = 14.9681(18) Å	g = 90°.
Volume	2711.8(6) $Å^3$	
Z	4	
Density (calculated)	1.671 Mg/m^3	
Absorption coefficient	1.379 mm^{-1}	
F(000)	1376	
Crystal size	0.34 x 0.08 x 0.06 mm^3	
Theta range for data collection	2.55 to 26.43°.	
Index ranges	-14<=h<=12, -17<=k<=14, -11<=l<=18	
Reflections collected	7163	
Independent reflections	2537 [R(int) = 0.0273]	
Completeness to θ = 25.00°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.921 and 0.769	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2537 / 0 / 201	
Goodness-of-fit on F^2	1.076	
Final R indices [I>2σ(I)]	R1 = 0.0374, wR2 = 0.1075	
R indices (all data)	R1 = 0.0408, wR2 = 0.1122	
Extinction coefficient	0	
Largest diff. peak and hole	0.512 and -0.317 $e.Å^{-3}$	

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

	x	y	z	U(eq)
Cr(1)	2869(1)	10030(1)	6259(1)	32(1)
Fe(1)	0	8513(1)	7500	29(1)
C(1)	4375(3)	10037(2)	6248(5)	45(1)
O(1)	5301(2)	10028(2)	6201(5)	76(1)
C(2)	3006(4)	9106(2)	7146(2)	42(1)
O(2)	3201(3)	8573(2)	7666(3)	69(1)
C(3)	2881(4)	10912(2)	7192(2)	45(1)
O(3)	2930(4)	11427(2)	7746(2)	79(1)
C(4)	2961(4)	10952(2)	5361(2)	42(1)
O(4)	3126(3)	11492(2)	4839(2)	66(1)
C(5)	2864(4)	9119(3)	5343(2)	48(1)
O(5)	2898(5)	8585(2)	4795(3)	83(1)
C(6)	1189(2)	9996(2)	6282(4)	33(1)
O(6)	497(2)	10682(2)	6262(3)	48(1)
C(7)	539(3)	9178(2)	6330(3)	36(1)
C(8)	922(3)	8240(3)	6363(3)	47(1)
C(9)	-3(4)	7651(2)	6398(2)	54(1)
C(10)	-909(3)	8176(3)	6399(3)	35(1)
C(11)	-619(4)	9100(3)	6353(4)	34(1)
C(18)	805(3)	11634(2)	6176(4)	56(1)
C(19)	-183(4)	12184(3)	6159(3)	71(1)
Fe(1A)	0	11463(4)	7500	29(1)
Fe(1B)	-40(12)	11477(3)	5013(2)	24(1)
C(10A)	-937(18)	11798(16)	6316(19)	69(5)
C(11A)	-630(20)	10862(17)	6230(30)	84(6)

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

Cr(1)-C(1)	1.866(4)	Fe(1B)-C(10A)	2.29(3)
Cr(1)-C(3)	1.901(3)	C(10A)-C(11A)	1.42(3)
Cr(1)-C(2)	1.902(3)		
Cr(1)-C(4)	1.908(3)	C(1)-Cr(1)-C(3)	89.7(2)
Cr(1)-C(5)	1.910(4)	C(1)-Cr(1)-C(2)	85.5(2)
Cr(1)-C(6)	2.083(3)	C(3)-Cr(1)-C(2)	88.17(18)
Fe(1)-C(10)	2.056(4)	C(1)-Cr(1)-C(4)	86.0(2)
Fe(1)-C(11)	2.067(5)	C(3)-Cr(1)-C(4)	92.17(14)
Fe(1)-C(9)	2.076(3)	C(2)-Cr(1)-C(4)	171.42(13)
Fe(1)-C(8)	2.089(5)	C(1)-Cr(1)-C(5)	90.0(2)
Fe(1)-C(7)	2.112(4)	C(3)-Cr(1)-C(5)	178.52(16)
C(1)-O(1)	1.151(5)	C(2)-Cr(1)-C(5)	90.35(15)
C(2)-O(2)	1.128(5)	C(4)-Cr(1)-C(5)	89.27(17)
C(3)-O(3)	1.121(4)	C(1)-Cr(1)-C(6)	178.87(16)
C(4)-O(4)	1.130(4)	C(3)-Cr(1)-C(6)	90.7(2)
C(5)-O(5)	1.134(5)	C(2)-Cr(1)-C(6)	93.48(19)
C(6)-O(6)	1.320(3)	C(4)-Cr(1)-C(6)	95.09(19)
C(6)-C(7)	1.443(4)	C(5)-Cr(1)-C(6)	89.6(2)
O(6)-C(18)	1.449(4)	C(10)-Fe(1)-C(10)#1	152.2(3)
C(7)-C(11)	1.439(4)	C(10)-Fe(1)-C(11)#1	165.60(18)
C(7)-C(8)	1.452(5)	C(10)-Fe(1)-C(11)	39.72(17)
C(8)-C(9)	1.434(6)	C(11)#1-Fe(1)-C(11)	130.9(2)
C(8)-H(8)	0.9300	C(10)-Fe(1)-C(9)	38.4(2)
C(9)-C(10)	1.360(7)	C(11)-Fe(1)-C(9)	65.88(17)
C(9)-H(9)	0.9300	C(10)-Fe(1)-C(9)#1	119.45(19)
C(10)-C(11)	1.401(6)	C(11)-Fe(1)-C(9)#1	155.9(2)
C(10)-H(10)	0.9300	C(9)-Fe(1)-C(9)#1	105.23(18)
C(11)-H(11)	0.9300	C(10)-Fe(1)-C(8)	66.48(12)
C(18)-C(19)	1.465(5)	C(11)-Fe(1)-C(8)	66.76(18)
C(18)-H(18A)	0.9700	C(9)-Fe(1)-C(8)	40.29(16)
C(18)-H(18B)	0.9700	C(10)-Fe(1)-C(8)#1	107.89(12)
C(19)-H(19A)	0.9600	C(11)-Fe(1)-C(8)#1	123.61(18)
C(19)-H(19B)	0.9600	C(9)-Fe(1)-C(8)#1	122.04(17)
C(19)-H(19C)	0.9600	C(8)-Fe(1)-C(8)#1	157.9(2)
Fe(1A)-C(10A)	2.17(3)	C(10)-Fe(1)-C(7)	67.61(16)
Fe(1A)-C(11A)	2.23(4)	C(11)-Fe(1)-C(7)	40.27(12)
Fe(1B)-C(11A)	2.17(3)	C(9)-Fe(1)-C(7)	67.71(13)

C(8)-Fe(1)-C(7)	40.45(14)	C(9)-C(10)-C(11)	109.4(3)
C(10)-Fe(1)-C(7)#1	127.01(17)	C(9)-C(10)-Fe(1)	71.6(2)
C(11)-Fe(1)-C(7)#1	112.39(11)	C(11)-C(10)-Fe(1)	70.6(3)
C(9)-Fe(1)-C(7)#1	159.74(18)	C(9)-C(10)-H(10)	125.3
C(8)-Fe(1)-C(7)#1	159.57(15)	C(11)-C(10)-H(10)	125.3
C(7)-Fe(1)-C(7)#1	125.21(19)	Fe(1)-C(10)-H(10)	124.1
O(1)-C(1)-Cr(1)	176.8(9)	C(10)-C(11)-C(7)	109.5(3)
O(2)-C(2)-Cr(1)	172.8(4)	C(10)-C(11)-Fe(1)	69.7(3)
O(3)-C(3)-Cr(1)	177.3(5)	C(7)-C(11)-Fe(1)	71.6(3)
O(4)-C(4)-Cr(1)	173.0(4)	C(10)-C(11)-H(11)	125.2
O(5)-C(5)-Cr(1)	177.6(5)	C(7)-C(11)-H(11)	125.2
O(6)-C(6)-C(7)	105.6(3)	Fe(1)-C(11)-H(11)	125.1
O(6)-C(6)-Cr(1)	129.10(19)	O(6)-C(18)-C(19)	107.9(3)
C(7)-C(6)-Cr(1)	125.3(2)	O(6)-C(18)-H(18A)	110.1
C(6)-O(6)-C(18)	124.1(3)	C(19)-C(18)-H(18A)	110.1
C(6)-C(7)-C(11)	128.5(3)	O(6)-C(18)-H(18B)	110.1
C(6)-C(7)-C(8)	127.0(3)	C(19)-C(18)-H(18B)	110.1
C(11)-C(7)-C(8)	104.5(3)	H(18A)-C(18)-H(18B)	108.4
C(6)-C(7)-Fe(1)	126.8(4)	C(18)-C(19)-H(19A)	109.5
C(11)-C(7)-Fe(1)	68.2(3)	C(18)-C(19)-H(19B)	109.5
C(8)-C(7)-Fe(1)	68.9(3)	H(19A)-C(19)-H(19B)	109.5
C(9)-C(8)-C(7)	107.9(3)	C(18)-C(19)-H(19C)	109.5
C(9)-C(8)-Fe(1)	69.4(2)	H(19A)-C(19)-H(19C)	109.5
C(7)-C(8)-Fe(1)	70.6(2)	H(19B)-C(19)-H(19C)	109.5
C(9)-C(8)-H(8)	126.1	C(10A)-Fe(1A)-C(10A)#1	154.0(13)
C(7)-C(8)-H(8)	126.1	C(10A)-Fe(1A)-C(11A)	37.7(9)
Fe(1)-C(8)-H(8)	125.5	C(10A)-Fe(1A)-C(11A)#1	165.6(10)
C(10)-C(9)-C(8)	108.8(2)	C(11A)-Fe(1A)-C(11A)#1	133.6(14)
C(10)-C(9)-Fe(1)	70.0(2)	C(11A)-Fe(1B)-C(10A)	37.1(8)
C(8)-C(9)-Fe(1)	70.3(2)	C(11A)-C(10A)-Fe(1A)	73.3(18)
C(10)-C(9)-H(9)	125.6	C(11A)-C(10A)-Fe(1B)	66.6(17)
C(8)-C(9)-H(9)	125.6	C(10A)-C(11A)-Fe(1B)	76.3(18)
Fe(1)-C(9)-H(9)	125.7	C(10A)-C(11A)-Fe(1A)	69.0(17)

Symmetry transformations used to generate equivalent atoms:

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

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	31(1)	32(1)	33(1)	1(1)	0(1)	-1(1)
Fe(1)	31(1)	23(1)	31(1)	0	0(1)	0
C(1)	43(2)	44(2)	49(2)	2(1)	12(3)	3(1)
O(1)	36(2)	86(2)	106(3)	3(2)	-6(3)	0(1)
C(2)	40(2)	41(2)	46(2)	2(1)	-5(2)	1(2)
O(2)	79(2)	60(2)	67(3)	24(2)	-12(2)	1(1)
C(3)	48(2)	43(2)	44(2)	-1(1)	-7(2)	-6(2)
O(3)	110(3)	65(2)	61(2)	-23(2)	-21(2)	0(2)
C(4)	40(2)	42(2)	44(2)	3(1)	0(2)	3(2)
O(4)	77(3)	61(2)	59(2)	22(2)	15(2)	6(2)
C(5)	50(2)	50(2)	42(2)	4(2)	3(2)	-9(2)
O(5)	117(3)	71(2)	59(2)	-27(2)	12(2)	-19(2)
C(6)	37(1)	25(1)	37(2)	2(1)	1(2)	2(1)
O(6)	40(1)	39(1)	65(1)	4(1)	0(1)	3(1)
C(7)	34(2)	36(2)	38(2)	-4(2)	-3(2)	-4(1)
C(8)	44(2)	33(2)	63(3)	-8(2)	3(2)	-6(1)
C(9)	58(2)	39(1)	66(2)	-9(1)	-3(3)	-17(2)
C(10)	34(2)	37(2)	34(3)	2(2)	-7(2)	-13(2)
C(11)	28(2)	33(2)	41(3)	2(2)	-8(2)	2(2)
C(18)	46(2)	32(2)	91(3)	7(2)	1(2)	6(1)
C(19)	66(3)	55(2)	93(3)	13(2)	7(3)	24(2)

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

	x	y	z	U(eq)
H(8)	1640	8054	6363	56
H(9)	15	7015	6416	65
H(10)	-1612	7955	6426	42
H(11)	-1099	9588	6339	41
H(18A)	1212	11726	5630	67
H(18B)	1255	11814	6677	67
H(19A)	2	12821	6121	107
H(19B)	-588	12077	6695	107
H(19C)	-610	12016	5650	107

Table 6. Torsion angles [°] for Complex **3**.

C(3)-Cr(1)-C(6)-O(6)	49.8(6)
C(2)-Cr(1)-C(6)-O(6)	138.0(5)
C(4)-Cr(1)-C(6)-O(6)	-42.5(6)
C(5)-Cr(1)-C(6)-O(6)	-131.7(6)
C(3)-Cr(1)-C(6)-C(7)	-129.9(5)
C(2)-Cr(1)-C(6)-C(7)	-41.6(5)
C(4)-Cr(1)-C(6)-C(7)	137.9(5)
C(5)-Cr(1)-C(6)-C(7)	48.7(5)
C(7)-C(6)-O(6)-C(18)	-177.4(4)
Cr(1)-C(6)-O(6)-C(18)	2.9(8)
O(6)-C(6)-C(7)-C(11)	0.0(10)
Cr(1)-C(6)-C(7)-C(11)	179.7(6)
O(6)-C(6)-C(7)-C(8)	179.8(4)
Cr(1)-C(6)-C(7)-C(8)	-0.5(8)
O(6)-C(6)-C(7)-Fe(1)	-90.1(5)
Cr(1)-C(6)-C(7)-Fe(1)	89.5(5)
C(6)-C(7)-C(8)-C(9)	-179.4(5)
C(11)-C(7)-C(8)-C(9)	0.4(6)
C(7)-C(8)-C(9)-C(10)	-0.8(4)
C(8)-C(9)-C(10)-C(11)	0.9(5)
C(9)-C(10)-C(11)-C(7)	-0.6(7)
C(6)-O(6)-C(18)-C(19)	178.7(5)

Appendix 2

Crystallographic data of Complex 5

Table 1. Crystal data and structure refinement for Complex **5**.

Identification code	db52bc2_abs	
Empirical formula	C_{27} H_{21} Cl_3 Cr Fe O_6 Ti	
Formula weight	703.54	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2_1/n	
Unit cell dimensions	a = 10.2230(7) Å	a= 90°.
	b = 26.2984(19) Å	b= 90.7190(10)°.
	c = 10.5587(8) Å	g = 90°.
Volume	2838.5(4) $Å^3$	
Z	4	
Density (calculated)	1.646 Mg/m^3	
Absorption coefficient	1.477 mm^{-1}	
F(000)	1416	
Crystal size	0.44 x 0.40 x 0.08 mm^3	
Theta range for data collection	2.47 to 26.38°.	
Index ranges	-5<=h<=12, -32<=k<=32, -10<=l<=12	
Reflections collected	14859	
Independent reflections	5143 [R(int) = 0.0414]	
Completeness to theta = 25.00°	97.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.889 and 0.544	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5143 / 0 / 352	
Goodness-of-fit on F^2	1.035	
Final R indices [I>2sigma(I)]	R1 = 0.0488, wR2 = 0.1224	
R indices (all data)	R1 = 0.0798, wR2 = 0.1423	
Extinction coefficient	0	
Largest diff. peak and hole	0.590 and -0.623 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Complex **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cr(1)	-802(1)	1296(1)	8269(1)	42(1)
C(1)	-2270(5)	1083(2)	7349(5)	62(1)
O(1)	-3194(4)	951(2)	6809(5)	99(2)
C(2)	-199(5)	623(2)	8399(5)	55(1)
O(2)	101(4)	205(1)	8440(4)	84(1)
C(3)	167(5)	1345(2)	6749(5)	50(1)
O(3)	729(4)	1346(2)	5826(4)	73(1)
C(4)	-1464(4)	1977(2)	8170(4)	49(1)
O(4)	-1918(4)	2368(1)	8159(4)	67(1)
C(5)	-1759(4)	1204(2)	9754(5)	49(1)
O(5)	-2371(3)	1132(2)	10633(4)	72(1)
C(6)	826(4)	1587(2)	9244(4)	37(1)
O(6)	1451(3)	1967(1)	8784(3)	43(1)
Fe(1)	2733(1)	894(1)	10901(1)	53(1)
C(7)	1330(4)	1429(2)	10496(4)	40(1)
C(8)	817(4)	1025(2)	11267(4)	47(1)
C(9)	1541(5)	1012(2)	12406(5)	63(1)
C(10)	2514(6)	1392(2)	12370(5)	67(2)
C(11)	2416(4)	1647(2)	11202(5)	49(1)
C(12)	3430(8)	561(3)	9289(8)	97(2)
C(13)	2889(6)	194(2)	10063(7)	83(2)
C(14)	3547(6)	200(2)	11200(8)	86(2)
C(15)	4536(6)	573(3)	11148(9)	103(3)
C(16)	4443(7)	796(3)	9952(10)	109(3)
Ti(1)	2339(1)	2535(1)	8077(1)	36(1)
Cl(1)	819(1)	2667(1)	6374(1)	58(1)
C(17)	1723(4)	2869(2)	10081(4)	47(1)
C(18)	3011(5)	3018(2)	9839(4)	51(1)
C(19)	2961(5)	3355(2)	8797(5)	57(1)
C(20)	1680(5)	3397(2)	8390(5)	56(1)
C(21)	906(4)	3089(2)	9180(4)	49(1)
C(22)	3620(6)	1831(2)	7346(7)	72(2)

C(23)	4333(5)	2082(3)	8250(5)	70(2)
C(24)	4634(5)	2554(3)	7799(7)	77(2)
C(25)	4030(5)	2602(2)	6605(6)	75(2)
C(26)	3420(5)	2143(3)	6351(5)	71(2)
Cl(2)	3635(5)	509(2)	5445(5)	264(2)
Cl(3)	1491(11)	-148(3)	5542(11)	472(7)
C(27)	2930(20)	-153(6)	5890(30)	380(20)

Table 3. Bond lengths [Å] and angles [°] for Complex **5**.

Cr(1)-C(1)	1.863(5)	C(12)-C(16)	1.388(10)
Cr(1)-C(5)	1.875(5)	C(12)-H(12)	0.9300
Cr(1)-C(2)	1.880(6)	C(13)-C(14)	1.369(9)
Cr(1)-C(3)	1.900(5)	C(13)-H(13)	0.9300
Cr(1)-C(4)	1.917(5)	C(14)-C(15)	1.411(9)
Cr(1)-C(6)	2.090(4)	C(14)-H(14)	0.9300
C(1)-O(1)	1.151(6)	C(15)-C(16)	1.394(11)
C(2)-O(2)	1.141(6)	C(15)-H(15)	0.9300
C(3)-O(3)	1.137(6)	C(16)-H(16)	0.9300
C(4)-O(4)	1.128(5)	Ti(1)-C(25)	2.345(5)
C(5)-O(5)	1.141(6)	Ti(1)-C(18)	2.348(4)
C(6)-O(6)	1.286(5)	Ti(1)-C(23)	2.367(5)
C(6)-C(7)	1.472(6)	Ti(1)-C(24)	2.368(5)
O(6)-Ti(1)	1.905(3)	Ti(1)-C(19)	2.372(5)
Fe(1)-C(14)	2.029(5)	Ti(1)-C(26)	2.378(5)
Fe(1)-C(8)	2.031(4)	Ti(1)-C(21)	2.381(4)
Fe(1)-C(11)	2.032(4)	Ti(1)-C(17)	2.384(4)
Fe(1)-C(9)	2.038(5)	Ti(1)-Cl(1)	2.3870(13)
Fe(1)-C(15)	2.040(6)	Ti(1)-C(20)	2.390(5)
Fe(1)-C(16)	2.042(7)	Ti(1)-C(22)	2.400(5)
Fe(1)-C(10)	2.044(6)	C(17)-C(21)	1.384(6)
Fe(1)-C(13)	2.049(6)	C(17)-C(18)	1.400(6)
Fe(1)-C(12)	2.049(7)	C(17)-H(17)	0.9300
Fe(1)-C(7)	2.050(4)	C(18)-C(19)	1.413(7)
C(7)-C(8)	1.440(6)	C(18)-H(18)	0.9300
C(7)-C(11)	1.449(6)	C(19)-C(20)	1.377(7)
C(8)-C(9)	1.405(7)	C(19)-H(19)	0.9300
C(8)-H(8)	0.9300	C(20)-C(21)	1.413(7)
C(9)-C(10)	1.411(7)	C(20)-H(20)	0.9300
C(9)-H(9)	0.9300	C(21)-H(21)	0.9300
C(10)-C(11)	1.405(7)	C(22)-C(26)	1.346(8)
C(10)-H(10)	0.9300	C(22)-C(23)	1.364(8)
C(11)-H(11)	0.9300	C(22)-H(22)	0.9300
C(12)-C(13)	1.384(9)	C(23)-C(24)	1.365(8)

C(23)-H(23)	0.9300	C(14)-Fe(1)-C(11)	156.7(3)
C(24)-C(25)	1.402(9)	C(8)-Fe(1)-C(11)	69.40(19)
C(24)-H(24)	0.9300	C(14)-Fe(1)-C(9)	105.3(3)
C(25)-C(26)	1.384(8)	C(8)-Fe(1)-C(9)	40.39(19)
C(25)-H(25)	0.9300	C(11)-Fe(1)-C(9)	68.4(2)
C(26)-H(26)	0.9300	C(14)-Fe(1)-C(15)	40.6(2)
Cl(2)-C(27)	1.94(2)	C(8)-Fe(1)-C(15)	156.6(3)
Cl(3)-C(27)	1.516(17)	C(11)-Fe(1)-C(15)	121.9(2)
C(27)-H(27A)	0.9700	C(9)-Fe(1)-C(15)	120.7(3)
C(27)-H(27B)	0.9700	C(14)-Fe(1)-C(16)	67.1(3)
		C(8)-Fe(1)-C(16)	161.5(3)
C(1)-Cr(1)-C(5)	88.4(2)	C(11)-Fe(1)-C(16)	109.8(2)
C(1)-Cr(1)-C(2)	90.9(2)	C(9)-Fe(1)-C(16)	157.8(3)
C(5)-Cr(1)-C(2)	89.5(2)	C(15)-Fe(1)-C(16)	39.9(3)
C(1)-Cr(1)-C(3)	90.3(2)	C(14)-Fe(1)-C(10)	120.5(3)
C(5)-Cr(1)-C(3)	176.4(2)	C(8)-Fe(1)-C(10)	68.4(2)
C(2)-Cr(1)-C(3)	87.2(2)	C(11)-Fe(1)-C(10)	40.3(2)
C(1)-Cr(1)-C(4)	88.3(2)	C(9)-Fe(1)-C(10)	40.5(2)
C(5)-Cr(1)-C(4)	88.74(19)	C(15)-Fe(1)-C(10)	106.0(3)
C(2)-Cr(1)-C(4)	178.1(2)	C(16)-Fe(1)-C(10)	123.8(3)
C(3)-Cr(1)-C(4)	94.5(2)	C(14)-Fe(1)-C(13)	39.2(3)
C(1)-Cr(1)-C(6)	175.9(2)	C(8)-Fe(1)-C(13)	108.4(2)
C(5)-Cr(1)-C(6)	93.18(18)	C(11)-Fe(1)-C(13)	163.0(3)
C(2)-Cr(1)-C(6)	92.88(19)	C(9)-Fe(1)-C(13)	121.6(2)
C(3)-Cr(1)-C(6)	88.36(18)	C(15)-Fe(1)-C(13)	67.0(3)
C(4)-Cr(1)-C(6)	87.92(17)	C(16)-Fe(1)-C(13)	66.6(3)
O(1)-C(1)-Cr(1)	178.3(5)	C(10)-Fe(1)-C(13)	155.9(3)
O(2)-C(2)-Cr(1)	176.0(5)	C(14)-Fe(1)-C(12)	66.4(3)
O(3)-C(3)-Cr(1)	176.1(4)	C(8)-Fe(1)-C(12)	125.2(3)
O(4)-C(4)-Cr(1)	175.6(4)	C(11)-Fe(1)-C(12)	127.2(3)
O(5)-C(5)-Cr(1)	177.1(4)	C(9)-Fe(1)-C(12)	158.4(3)
O(6)-C(6)-C(7)	112.9(3)	C(15)-Fe(1)-C(12)	66.8(3)
O(6)-C(6)-Cr(1)	119.7(3)	C(16)-Fe(1)-C(12)	39.6(3)
C(7)-C(6)-Cr(1)	127.3(3)	C(10)-Fe(1)-C(12)	161.1(3)
C(6)-O(6)-Ti(1)	178.5(3)	C(13)-Fe(1)-C(12)	39.5(3)
C(14)-Fe(1)-C(8)	121.2(2)	C(14)-Fe(1)-C(7)	159.0(2)

C(8)-Fe(1)-C(7)	41.31(16)	C(7)-C(11)-H(11)	126.0
C(11)-Fe(1)-C(7)	41.57(17)	Fe(1)-C(11)-H(11)	125.4
C(9)-Fe(1)-C(7)	68.59(19)	C(13)-C(12)-C(16)	108.3(7)
C(15)-Fe(1)-C(7)	159.8(2)	C(13)-C(12)-Fe(1)	70.3(4)
C(16)-Fe(1)-C(7)	125.8(3)	C(16)-C(12)-Fe(1)	69.9(4)
C(10)-Fe(1)-C(7)	68.65(19)	C(13)-C(12)-H(12)	125.9
C(13)-Fe(1)-C(7)	125.7(2)	C(16)-C(12)-H(12)	125.9
C(12)-Fe(1)-C(7)	111.7(2)	Fe(1)-C(12)-H(12)	125.6
C(8)-C(7)-C(11)	106.4(4)	C(14)-C(13)-C(12)	108.4(7)
C(8)-C(7)-C(6)	126.2(4)	C(14)-C(13)-Fe(1)	69.6(4)
C(11)-C(7)-C(6)	127.4(4)	C(12)-C(13)-Fe(1)	70.3(4)
C(8)-C(7)-Fe(1)	68.6(2)	C(14)-C(13)-H(13)	125.8
C(11)-C(7)-Fe(1)	68.5(2)	C(12)-C(13)-H(13)	125.8
C(6)-C(7)-Fe(1)	128.1(3)	Fe(1)-C(13)-H(13)	125.9
C(9)-C(8)-C(7)	108.2(4)	C(13)-C(14)-C(15)	108.5(7)
C(9)-C(8)-Fe(1)	70.1(3)	C(13)-C(14)-Fe(1)	71.2(3)
C(7)-C(8)-Fe(1)	70.1(2)	C(15)-C(14)-Fe(1)	70.2(3)
C(9)-C(8)-H(8)	125.9	C(13)-C(14)-H(14)	125.7
C(7)-C(8)-H(8)	125.9	C(15)-C(14)-H(14)	125.7
Fe(1)-C(8)-H(8)	125.5	Fe(1)-C(14)-H(14)	124.5
C(8)-C(9)-C(10)	108.8(4)	C(16)-C(15)-C(14)	106.7(7)
C(8)-C(9)-Fe(1)	69.5(3)	C(16)-C(15)-Fe(1)	70.1(3)
C(10)-C(9)-Fe(1)	70.0(3)	C(14)-C(15)-Fe(1)	69.3(3)
C(8)-C(9)-H(9)	125.6	C(16)-C(15)-H(15)	126.7
C(10)-C(9)-H(9)	125.6	C(14)-C(15)-H(15)	126.7
Fe(1)-C(9)-H(9)	126.5	Fe(1)-C(15)-H(15)	125.5
C(11)-C(10)-C(9)	108.6(5)	C(12)-C(16)-C(15)	108.2(7)
C(11)-C(10)-Fe(1)	69.4(3)	C(12)-C(16)-Fe(1)	70.5(4)
C(9)-C(10)-Fe(1)	69.5(3)	C(15)-C(16)-Fe(1)	70.0(4)
C(11)-C(10)-H(10)	125.7	C(12)-C(16)-H(16)	125.9
C(9)-C(10)-H(10)	125.7	C(15)-C(16)-H(16)	125.9
Fe(1)-C(10)-H(10)	127.0	Fe(1)-C(16)-H(16)	125.3
C(10)-C(11)-C(7)	108.0(4)	O(6)-Ti(1)-C(25)	132.63(18)
C(10)-C(11)-Fe(1)	70.3(3)	O(6)-Ti(1)-C(18)	104.46(15)
C(7)-C(11)-Fe(1)	69.9(2)	C(25)-Ti(1)-C(18)	105.9(2)
C(10)-C(11)-H(11)	126.0	O(6)-Ti(1)-C(23)	89.38(19)

C(25)-Ti(1)-C(23)	56.5(2)	C(24)-Ti(1)-Cl(1)	122.70(19)
C(18)-Ti(1)-C(23)	88.2(2)	C(19)-Ti(1)-Cl(1)	106.20(14)
O(6)-Ti(1)-C(24)	122.8(2)	C(26)-Ti(1)-Cl(1)	77.89(14)
C(25)-Ti(1)-C(24)	34.6(2)	C(21)-Ti(1)-Cl(1)	83.18(12)
C(18)-Ti(1)-C(24)	78.86(19)	C(17)-Ti(1)-Cl(1)	116.02(12)
C(23)-Ti(1)-C(24)	33.5(2)	O(6)-Ti(1)-C(20)	123.59(15)
O(6)-Ti(1)-C(19)	135.61(15)	C(25)-Ti(1)-C(20)	103.40(19)
C(25)-Ti(1)-C(19)	87.0(2)	C(18)-Ti(1)-C(20)	57.11(17)
C(18)-Ti(1)-C(19)	34.84(17)	C(23)-Ti(1)-C(20)	135.3(2)
C(23)-Ti(1)-C(19)	101.9(2)	C(24)-Ti(1)-C(20)	106.2(2)
C(24)-Ti(1)-C(19)	76.07(19)	C(19)-Ti(1)-C(20)	33.61(17)
O(6)-Ti(1)-C(26)	100.9(2)	C(26)-Ti(1)-C(20)	130.7(2)
C(25)-Ti(1)-C(26)	34.1(2)	C(21)-Ti(1)-C(20)	34.45(16)
C(18)-Ti(1)-C(26)	135.03(18)	C(17)-Ti(1)-C(20)	56.56(16)
C(23)-Ti(1)-C(26)	55.4(2)	Cl(1)-Ti(1)-C(20)	77.58(13)
C(24)-Ti(1)-C(26)	56.2(2)	O(6)-Ti(1)-C(22)	77.63(16)
C(19)-Ti(1)-C(26)	121.0(2)	C(25)-Ti(1)-C(22)	55.6(2)
O(6)-Ti(1)-C(21)	89.37(15)	C(18)-Ti(1)-C(22)	121.1(2)
C(25)-Ti(1)-C(21)	137.84(19)	C(23)-Ti(1)-C(22)	33.3(2)
C(18)-Ti(1)-C(21)	57.10(16)	C(24)-Ti(1)-C(22)	55.3(2)
C(23)-Ti(1)-C(21)	143.61(19)	C(19)-Ti(1)-C(22)	131.28(19)
C(24)-Ti(1)-C(21)	131.65(19)	C(26)-Ti(1)-C(22)	32.7(2)
C(19)-Ti(1)-C(21)	56.66(16)	C(21)-Ti(1)-C(22)	166.08(19)
C(26)-Ti(1)-C(21)	159.23(19)	C(17)-Ti(1)-C(22)	136.1(2)
O(6)-Ti(1)-C(17)	78.97(14)	Cl(1)-Ti(1)-C(22)	102.83(18)
C(25)-Ti(1)-C(17)	140.0(2)	C(20)-Ti(1)-C(22)	158.77(19)
C(18)-Ti(1)-C(17)	34.41(15)	C(21)-C(17)-C(18)	108.5(4)
C(23)-Ti(1)-C(17)	110.73(18)	C(21)-C(17)-Ti(1)	73.0(3)
C(24)-Ti(1)-C(17)	112.06(19)	C(18)-C(17)-Ti(1)	71.4(3)
C(19)-Ti(1)-C(17)	56.80(16)	C(21)-C(17)-H(17)	125.7
C(26)-Ti(1)-C(17)	166.09(18)	C(18)-C(17)-H(17)	125.7
C(21)-Ti(1)-C(17)	33.78(15)	Ti(1)-C(17)-H(17)	121.6
O(6)-Ti(1)-Cl(1)	95.74(10)	C(17)-C(18)-C(19)	107.0(4)
C(25)-Ti(1)-Cl(1)	88.18(17)	C(17)-C(18)-Ti(1)	74.2(3)
C(18)-Ti(1)-Cl(1)	134.39(13)	C(19)-C(18)-Ti(1)	73.5(3)
C(23)-Ti(1)-Cl(1)	133.10(15)	C(17)-C(18)-H(18)	126.5

C(19)-C(18)-H(18)	126.5	C(25)-C(24)-H(24)	126.3
Ti(1)-C(18)-H(18)	117.9	Ti(1)-C(24)-H(24)	120.5
C(20)-C(19)-C(18)	108.6(4)	C(26)-C(25)-C(24)	106.7(5)
C(20)-C(19)-Ti(1)	73.9(3)	C(26)-C(25)-Ti(1)	74.3(3)
C(18)-C(19)-Ti(1)	71.7(3)	C(24)-C(25)-Ti(1)	73.6(3)
C(20)-C(19)-H(19)	125.7	C(26)-C(25)-H(25)	126.7
C(18)-C(19)-H(19)	125.7	C(24)-C(25)-H(25)	126.7
Ti(1)-C(19)-H(19)	120.4	Ti(1)-C(25)-H(25)	117.6
C(19)-C(20)-C(21)	107.9(4)	C(22)-C(26)-C(25)	108.5(5)
C(19)-C(20)-Ti(1)	72.4(3)	C(22)-C(26)-Ti(1)	74.6(3)
C(21)-C(20)-Ti(1)	72.4(3)	C(25)-C(26)-Ti(1)	71.7(3)
C(19)-C(20)-H(20)	126.1	C(22)-C(26)-H(26)	125.8
C(21)-C(20)-H(20)	126.1	C(25)-C(26)-H(26)	125.8
Ti(1)-C(20)-H(20)	120.8	Ti(1)-C(26)-H(26)	119.8
C(17)-C(21)-C(20)	107.9(4)	Cl(3)-C(27)-Cl(2)	107.1(11)
C(17)-C(21)-Ti(1)	73.2(3)	Cl(3)-C(27)-H(27A)	110.3
C(20)-C(21)-Ti(1)	73.1(3)	Cl(2)-C(27)-H(27A)	110.3
C(17)-C(21)-H(21)	126.0	Cl(3)-C(27)-H(27B)	110.3
C(20)-C(21)-H(21)	126.0	Cl(2)-C(27)-H(27B)	110.3
Ti(1)-C(21)-H(21)	119.5	H(27A)-C(27)-H(27B)	108.5
C(26)-C(22)-C(23)	109.0(5)		
C(26)-C(22)-Ti(1)	72.7(3)		
C(23)-C(22)-Ti(1)	72.0(3)		
C(26)-C(22)-H(22)	125.5		
C(23)-C(22)-H(22)	125.5		
Ti(1)-C(22)-H(22)	121.4		
C(22)-C(23)-C(24)	108.4(5)		
C(22)-C(23)-Ti(1)	74.7(3)		
C(24)-C(23)-Ti(1)	73.3(3)		
C(22)-C(23)-H(23)	125.8		
C(24)-C(23)-H(23)	125.8		
Ti(1)-C(23)-H(23)	118.1		
C(23)-C(24)-C(25)	107.3(5)		
C(23)-C(24)-Ti(1)	73.2(3)		
C(25)-C(24)-Ti(1)	71.8(3)		
C(23)-C(24)-H(24)	126.3		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for Complex **5**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	40(1)	39(1)	47(1)	-3(1)	0(1)	-6(1)
C(1)	63(3)	57(3)	65(3)	7(3)	-12(3)	-11(3)
O(1)	86(3)	108(4)	103(3)	5(3)	-36(3)	-36(3)
C(2)	60(3)	50(3)	54(3)	-1(2)	5(2)	-10(2)
O(2)	105(3)	40(2)	108(3)	-1(2)	2(3)	2(2)
C(3)	55(3)	44(3)	50(3)	-5(2)	-3(2)	-1(2)
O(3)	78(3)	82(3)	58(2)	-3(2)	15(2)	1(2)
C(4)	38(2)	57(3)	51(3)	-1(2)	1(2)	-9(2)
O(4)	68(2)	51(2)	82(3)	4(2)	2(2)	11(2)
C(5)	37(2)	46(3)	64(3)	-4(2)	0(2)	-2(2)
O(5)	59(2)	80(3)	77(3)	-3(2)	26(2)	-6(2)
C(6)	36(2)	33(2)	44(2)	-4(2)	9(2)	1(2)
O(6)	42(2)	40(2)	47(2)	5(1)	3(1)	-8(1)
Fe(1)	41(1)	37(1)	80(1)	8(1)	-4(1)	4(1)
C(7)	38(2)	33(2)	49(3)	2(2)	3(2)	4(2)
C(8)	42(2)	44(3)	56(3)	10(2)	5(2)	1(2)
C(9)	73(3)	60(3)	56(3)	16(3)	1(3)	2(3)
C(10)	81(4)	53(3)	65(3)	5(3)	-28(3)	2(3)
C(11)	51(3)	35(2)	61(3)	0(2)	-12(2)	-1(2)
C(12)	92(5)	85(5)	116(6)	-1(4)	36(5)	42(4)
C(13)	71(4)	48(3)	129(6)	-9(4)	17(4)	12(3)
C(14)	78(4)	54(4)	125(6)	25(4)	-1(4)	22(3)
C(15)	56(4)	62(4)	189(8)	11(5)	-26(4)	19(3)
C(16)	58(4)	61(4)	210(10)	30(5)	41(5)	20(3)
Ti(1)	32(1)	39(1)	38(1)	4(1)	3(1)	-4(1)
Cl(1)	51(1)	71(1)	53(1)	7(1)	-12(1)	-2(1)
C(17)	56(3)	46(3)	39(2)	-3(2)	6(2)	-1(2)
C(18)	51(3)	51(3)	51(3)	-12(2)	-11(2)	-2(2)
C(19)	55(3)	44(3)	72(3)	-7(3)	13(2)	-14(2)
C(20)	73(3)	42(3)	52(3)	8(2)	6(2)	8(2)
C(21)	43(2)	51(3)	54(3)	-3(2)	5(2)	5(2)
C(22)	68(3)	49(3)	100(5)	-8(3)	35(3)	3(3)

C(23)	54(3)	97(5)	59(3)	10(3)	7(3)	35(3)
C(24)	35(3)	89(5)	107(5)	-37(4)	12(3)	-9(3)
C(25)	60(3)	79(4)	86(4)	33(3)	44(3)	21(3)
C(26)	55(3)	109(5)	48(3)	-18(3)	7(2)	10(3)
Cl(2)	272(5)	262(5)	256(5)	-81(4)	-28(4)	83(4)
Cl(3)	547(14)	264(7)	614(16)	-73(9)	362(13)	-11(9)
C(27)	370(30)	143(13)	620(40)	-190(20)	-330(30)	112(17)

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

	x	y	z	U(eq)
H(8)	127	811	11049	57
H(9)	1402	789	13074	76
H(10)	3120	1462	13011	80
H(11)	2954	1909	10932	59
H(12)	3160	637	8466	117
H(13)	2198	-20	9847	99
H(14)	3371	-7	11891	103
H(15)	5133	655	11787	123
H(16)	4970	1056	9650	131
H(17)	1461	2658	10737	56
H(18)	3758	2915	10279	61
H(19)	3673	3521	8446	68
H(20)	1379	3594	7715	67
H(21)	7	3042	9108	59
H(22)	3319	1498	7407	86
H(23)	4575	1953	9039	84
H(24)	5144	2798	8208	92
H(25)	4038	2888	6085	89
H(26)	2952	2063	5617	85
H(27A)	3381	-419	5433	460
H(27B)	3048	-214	6793	460

Table 6. Torsion angles [°] for Complex **5**

C(5)-Cr(1)-C(6)-O(6)	-139.1(3)
C(2)-Cr(1)-C(6)-O(6)	131.2(3)
C(3)-Cr(1)-C(6)-O(6)	44.1(3)
C(4)-Cr(1)-C(6)-O(6)	-50.5(3)
C(5)-Cr(1)-C(6)-C(7)	36.2(4)
C(2)-Cr(1)-C(6)-C(7)	-53.5(4)
C(3)-Cr(1)-C(6)-C(7)	-140.6(4)
C(4)-Cr(1)-C(6)-C(7)	124.8(4)
O(6)-C(6)-C(7)-C(8)	178.3(4)
Cr(1)-C(6)-C(7)-C(8)	2.7(6)
O(6)-C(6)-C(7)-C(11)	-1.0(6)
Cr(1)-C(6)-C(7)-C(11)	-176.5(3)
C(11)-C(7)-C(8)-C(9)	1.6(5)
C(6)-C(7)-C(8)-C(9)	-177.7(4)
C(7)-C(8)-C(9)-C(10)	-0.8(6)
C(8)-C(9)-C(10)-C(11)	-0.3(6)
C(9)-C(10)-C(11)-C(7)	1.4(6)
C(8)-C(7)-C(11)-C(10)	-1.8(5)
C(6)-C(7)-C(11)-C(10)	177.5(4)
C(12)-C(13)-C(14)-C(15)	-0.7(7)
C(13)-C(14)-C(15)-C(16)	0.7(7)
C(13)-C(12)-C(16)-C(15)	0.0(7)
C(21)-C(17)-C(18)-C(19)	2.7(5)
C(17)-C(18)-C(19)-C(20)	-1.9(5)
C(18)-C(19)-C(20)-C(21)	0.4(6)
C(18)-C(17)-C(21)-C(20)	-2.4(5)
C(19)-C(20)-C(21)-C(17)	1.2(5)
C(26)-C(22)-C(23)-C(24)	-2.4(6)
C(22)-C(23)-C(24)-C(25)	2.9(6)
C(23)-C(24)-C(25)-C(26)	-2.4(6)
C(23)-C(22)-C(26)-C(25)	0.8(6)
C(24)-C(25)-C(26)-C(22)	1.0(6)

Symmetry transformations used to generate equivalent atoms:

Table 7. Selected least-squares planes and deviations from the planes (Åx10^3) for Complex **5**

Plane 1	-6.199(7)x + 17.075(36)y + 4.927(18)z = 6.777(11)						
Atoms *	Cr(1)	C(6)	O(6)	C(7)		rms	[Ti(1)]
Deviations	7(1)	-26(3)	10(1)	9(1)		15	[81(6)]
Plane 2	-6.507(20)x + 17.165(50)y + 4.423(24) z = 6.219(28)						
Atoms *	C(7)	C(8)	C(9)	C(10)	C(11)	rms	[Fe(1)]
Deviations	10(3)	-7(3)	2(3)	5(3)	-9(3)	7	[-1642(2)]
Plane 3	-6.603(24)x + 17.832(59)y + 3.789(31)z = 2.254(36)						
Atoms *	C(12)	C(13)	C(14)	C(15)	C(16)	rms	[Fe(1)]
Deviations	1(4)	-3(4)	4(4)	-3(4)	1(4)	3	[1665(3)]
Plane 4	-1.356(23)x + 20.460(39)y + 6.501(20)z = 12.176(11)						
Atoms *	C(17)	C(18)	C(19)	C(20)	C(21)	rms	[Ti(1)]
Deviations	15(3)	-13(3)	7(3)	2(3)	-10(3)	10	[-2056(2)]
Plane 5	-8.588(14)x + 9.142(64)y + 4.507(24)z = 1.885(27)						
Atoms *	C(22)	C(23)	C(24)	C(25)	C(26)	rms	[Ti(1)]
Deviations	-9(3)	15(3)	-15(3)	10(3)	-1(3)	11	[2064(2)]

Dihedral angles between planes (º):

Planes 1 and 2: 3.26(33) Planes 4 and 5: 50.39(23)

Planes 2 and 3: 17.14(17)

* rms = root mean square deviation from the plane;
atoms not involved in calculating the plane are shown in brackets [ ].

Appendix 3

Crystallographic data of Complex 6

Table 1. Crystal data and structure refinement for Complex **6**.

Identification code	bvdw01_pna21	
Empirical formula	C_{26} H_{19} Cl Fe O_6 Ti W	
Formula weight	750.46	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$Pna2_1$	
Unit cell dimensions	a = 23.220(3) Å	a= 90°.
	b = 10.0663(14) Å	b= 90°.
	c = 10.8634(15) Å	g = 90°.
Volume	2539.2(6) $Å^3$	
Z	4	
Density (calculated)	1.963 Mg/m^3	
Absorption coefficient	5.535 mm^{-1}	
F(000)	1448	
Crystal size	0.22 x 0.18 x 0.01 mm^3	
Theta range for data collection	2.57 to 26.43°.	
Index ranges	-28<=h<=13, -11<=k<=12, -12<=l<=11	
Reflections collected	12791	
Independent reflections	4518 [R(int) = 0.0616]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.946 and 0.328	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4518 / 1 / 325	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2σ(I)]	R1 = 0.0413, wR2 = 0.0885	
R indices (all data)	R1 = 0.0667, wR2 = 0.0996	
Absolute structure parameter	0.027(14)	
Extinction coefficient	0	
Largest diff. peak and hole	0.977 and -2.287 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Complex **6**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
W(1)	1151(1)	9655(1)	10737(1)	36(1)
C(1)	939(5)	11270(13)	11722(12)	52(3)
O(1)	837(5)	12207(10)	12297(10)	89(3)
C(2)	1981(4)	10294(9)	10785(19)	46(2)
O(2)	2438(3)	10740(7)	10844(12)	61(2)
C(3)	1043(5)	10684(12)	9171(12)	47(3)
O(3)	946(5)	11256(10)	8323(11)	83(3)
C(4)	311(4)	9255(11)	10687(18)	59(3)
O(4)	-186(4)	9095(11)	10684(18)	123(5)
C(5)	1190(5)	8544(13)	12321(12)	51(3)
O(5)	1153(4)	7884(12)	13190(9)	83(4)
C(6)	1469(4)	7829(9)	9749(9)	32(2)
O(6)	1886(3)	7180(7)	10218(6)	36(2)
Fe(1)	587(1)	5952(2)	8470(1)	38(1)
C(7)	1249(4)	7279(11)	8592(10)	35(3)
C(8)	1437(5)	6093(11)	7984(9)	43(3)
C(9)	1093(5)	5896(14)	6933(11)	55(3)
C(10)	689(5)	6970(13)	6866(9)	54(3)
C(11)	778(5)	7785(11)	7858(9)	46(3)
C(12)	-237(5)	5211(13)	8419(13)	55(3)
C(13)	-179(5)	6052(13)	9438(11)	54(3)
C(14)	264(5)	5586(13)	10190(12)	58(3)
C(15)	471(5)	4373(13)	9645(14)	64(4)
C(16)	170(5)	4152(12)	8528(14)	56(3)
Ti(1)	2547(1)	6325(2)	10877(2)	31(1)
Cl(1)	2705(1)	7881(3)	12518(2)	44(1)
C(17)	2087(7)	4239(11)	10772(18)	70(4)
C(18)	2623(6)	3996(11)	11284(18)	83(6)
C(19)	2626(8)	4698(14)	12421(17)	87(6)
C(20)	2076(8)	5227(13)	12543(14)	69(4)
C(21)	1775(6)	4931(14)	11557(17)	70(5)
C(22)	3071(5)	5677(12)	9146(11)	52(3)

C(23)	3464(4)	5724(11)	10106(12)	51(3)
C(24)	3518(4)	7043(11)	10487(11)	47(3)
C(25)	3138(4)	7778(11)	9736(10)	44(3)
C(26)	2870(5)	6958(12)	8883(10)	49(3)

Table 3. Bond lengths [Å] and angles [°] for Complex **6**.

W(1)-C(4)	1.993(10)	C(12)-C(16)	1.430(17)
W(1)-C(3)	2.008(13)	C(12)-H(12)	0.9300
W(1)-C(1)	2.008(13)	C(13)-C(14)	1.395(16)
W(1)-C(2)	2.033(10)	C(13)-H(13)	0.9300
W(1)-C(5)	2.053(14)	C(14)-C(15)	1.440(18)
W(1)-C(6)	2.253(9)	C(14)-H(14)	0.9300
C(1)-O(1)	1.155(14)	C(15)-C(16)	1.419(18)
C(2)-O(2)	1.154(11)	C(15)-H(15)	0.9300
C(3)-O(3)	1.109(14)	C(16)-H(16)	0.9300
C(4)-O(4)	1.163(12)	Ti(1)-C(22)	2.332(11)
C(5)-O(5)	1.158(15)	Ti(1)-C(19)	2.351(13)
C(6)-O(6)	1.273(11)	Ti(1)-C(25)	2.358(10)
C(6)-C(7)	1.465(15)	Ti(1)-C(17)	2.359(10)
O(6)-Ti(1)	1.901(6)	Ti(1)-C(23)	2.366(10)
Fe(1)-C(11)	2.011(11)	Ti(1)-C(26)	2.380(11)
Fe(1)-C(10)	2.036(11)	Ti(1)-C(20)	2.386(13)
Fe(1)-C(7)	2.042(11)	Ti(1)-C(18)	2.392(11)
Fe(1)-C(9)	2.042(12)	Ti(1)-C(21)	2.393(13)
Fe(1)-C(8)	2.047(11)	Ti(1)-Cl(1)	2.402(3)
Fe(1)-C(14)	2.047(12)	Ti(1)-C(24)	2.404(10)
Fe(1)-C(12)	2.054(12)	C(17)-C(21)	1.32(2)
Fe(1)-C(16)	2.055(12)	C(17)-C(18)	1.387(19)
Fe(1)-C(15)	2.056(13)	C(17)-H(17)	0.9300
Fe(1)-C(13)	2.069(11)	C(18)-C(19)	1.42(2)
C(7)-C(8)	1.432(14)	C(18)-H(18)	0.9300
C(7)-C(11)	1.447(14)	C(19)-C(20)	1.39(2)
C(8)-C(9)	1.407(15)	C(19)-H(19)	0.9300
C(8)-H(8)	0.9300	C(20)-C(21)	1.31(2)
C(9)-C(10)	1.433(17)	C(20)-H(20)	0.9300
C(9)-H(9)	0.9300	C(21)-H(21)	0.9300
C(10)-C(11)	1.370(15)	C(22)-C(23)	1.386(16)
C(10)-H(10)	0.9300	C(22)-C(26)	1.401(16)
C(11)-H(11)	0.9300	C(22)-H(22)	0.9300
C(12)-C(13)	1.400(17)	C(23)-C(24)	1.396(14)

C(23)-H(23)	0.9300	C(7)-Fe(1)-C(9)	68.8(5)
C(24)-C(25)	1.411(14)	C(11)-Fe(1)-C(8)	68.8(5)
C(24)-H(24)	0.9300	C(10)-Fe(1)-C(8)	68.4(5)
C(25)-C(26)	1.389(15)	C(7)-Fe(1)-C(8)	41.0(4)
C(25)-H(25)	0.9300	C(9)-Fe(1)-C(8)	40.3(4)
C(26)-H(26)	0.9300	C(11)-Fe(1)-C(14)	123.2(5)
		C(10)-Fe(1)-C(14)	156.1(5)
C(4)-W(1)-C(3)	87.6(7)	C(7)-Fe(1)-C(14)	109.6(5)
C(4)-W(1)-C(1)	86.5(5)	C(9)-Fe(1)-C(14)	162.3(5)
C(3)-W(1)-C(1)	90.2(6)	C(8)-Fe(1)-C(14)	127.0(5)
C(4)-W(1)-C(2)	173.2(4)	C(11)-Fe(1)-C(12)	121.9(5)
C(3)-W(1)-C(2)	88.7(6)	C(10)-Fe(1)-C(12)	105.5(5)
C(1)-W(1)-C(2)	87.8(5)	C(7)-Fe(1)-C(12)	160.2(5)
C(4)-W(1)-C(5)	87.5(6)	C(9)-Fe(1)-C(12)	120.2(5)
C(3)-W(1)-C(5)	175.1(5)	C(8)-Fe(1)-C(12)	156.3(5)
C(1)-W(1)-C(5)	90.3(5)	C(14)-Fe(1)-C(12)	67.5(5)
C(2)-W(1)-C(5)	96.2(6)	C(11)-Fe(1)-C(16)	157.3(5)
C(4)-W(1)-C(6)	98.3(4)	C(10)-Fe(1)-C(16)	121.6(5)
C(3)-W(1)-C(6)	93.3(4)	C(7)-Fe(1)-C(16)	158.4(4)
C(1)-W(1)-C(6)	174.2(4)	C(9)-Fe(1)-C(16)	105.8(6)
C(2)-W(1)-C(6)	87.7(4)	C(8)-Fe(1)-C(16)	121.6(5)
C(5)-W(1)-C(6)	86.6(4)	C(14)-Fe(1)-C(16)	69.0(6)
O(1)-C(1)-W(1)	177.7(11)	C(12)-Fe(1)-C(16)	40.7(5)
O(2)-C(2)-W(1)	175.2(10)	C(11)-Fe(1)-C(15)	160.6(5)
O(3)-C(3)-W(1)	175.5(12)	C(10)-Fe(1)-C(15)	159.4(5)
O(4)-C(4)-W(1)	176.1(10)	C(7)-Fe(1)-C(15)	124.4(5)
O(5)-C(5)-W(1)	172.8(10)	C(9)-Fe(1)-C(15)	124.2(6)
O(6)-C(6)-C(7)	114.5(8)	C(8)-Fe(1)-C(15)	109.9(5)
O(6)-C(6)-W(1)	118.5(7)	C(14)-Fe(1)-C(15)	41.1(5)
C(7)-C(6)-W(1)	127.0(7)	C(12)-Fe(1)-C(15)	67.3(5)
C(6)-O(6)-Ti(1)	175.4(7)	C(16)-Fe(1)-C(15)	40.4(5)
C(11)-Fe(1)-C(10)	39.6(4)	C(11)-Fe(1)-C(13)	108.2(5)
C(11)-Fe(1)-C(7)	41.8(4)	C(10)-Fe(1)-C(13)	120.6(5)
C(10)-Fe(1)-C(7)	68.8(5)	C(7)-Fe(1)-C(13)	125.6(5)
C(11)-Fe(1)-C(9)	68.2(5)	C(9)-Fe(1)-C(13)	155.7(5)
C(10)-Fe(1)-C(9)	41.2(5)	C(8)-Fe(1)-C(13)	163.0(4)

C(14)-Fe(1)-C(13)	39.6(5)	C(16)-C(12)-Fe(1)	69.7(7)
C(12)-Fe(1)-C(13)	39.7(5)	C(13)-C(12)-H(12)	125.6
C(16)-Fe(1)-C(13)	67.8(5)	C(16)-C(12)-H(12)	125.6
C(15)-Fe(1)-C(13)	67.0(5)	Fe(1)-C(12)-H(12)	125.6
C(8)-C(7)-C(11)	105.6(9)	C(14)-C(13)-C(12)	109.3(12)
C(8)-C(7)-C(6)	127.2(9)	C(14)-C(13)-Fe(1)	69.3(7)
C(11)-C(7)-C(6)	127.1(9)	C(12)-C(13)-Fe(1)	69.6(7)
C(8)-C(7)-Fe(1)	69.7(6)	C(14)-C(13)-H(13)	125.3
C(11)-C(7)-Fe(1)	68.0(6)	C(12)-C(13)-H(13)	125.3
C(6)-C(7)-Fe(1)	124.4(7)	Fe(1)-C(13)-H(13)	127.3
C(9)-C(8)-C(7)	108.6(10)	C(13)-C(14)-C(15)	106.9(11)
C(9)-C(8)-Fe(1)	69.7(7)	C(13)-C(14)-Fe(1)	71.0(7)
C(7)-C(8)-Fe(1)	69.3(6)	C(15)-C(14)-Fe(1)	69.8(7)
C(9)-C(8)-H(8)	125.7	C(13)-C(14)-H(14)	126.5
C(7)-C(8)-H(8)	125.7	C(15)-C(14)-H(14)	126.5
Fe(1)-C(8)-H(8)	126.9	Fe(1)-C(14)-H(14)	124.3
C(8)-C(9)-C(10)	107.9(10)	C(16)-C(15)-C(14)	108.7(11)
C(8)-C(9)-Fe(1)	70.0(7)	C(16)-C(15)-Fe(1)	69.8(7)
C(10)-C(9)-Fe(1)	69.2(6)	C(14)-C(15)-Fe(1)	69.1(7)
C(8)-C(9)-H(9)	126.1	C(16)-C(15)-H(15)	125.7
C(10)-C(9)-H(9)	126.1	C(14)-C(15)-H(15)	125.7
Fe(1)-C(9)-H(9)	126.2	Fe(1)-C(15)-H(15)	127.0
C(11)-C(10)-C(9)	108.2(10)	C(15)-C(16)-C(12)	106.2(12)
C(11)-C(10)-Fe(1)	69.2(6)	C(15)-C(16)-Fe(1)	69.8(7)
C(9)-C(10)-Fe(1)	69.6(7)	C(12)-C(16)-Fe(1)	69.6(8)
C(11)-C(10)-H(10)	125.9	C(15)-C(16)-H(16)	126.9
C(9)-C(10)-H(10)	125.9	C(12)-C(16)-H(16)	126.9
Fe(1)-C(10)-H(10)	126.8	Fe(1)-C(16)-H(16)	125.3
C(10)-C(11)-C(7)	109.7(10)	O(6)-Ti(1)-C(22)	104.2(4)
C(10)-C(11)-Fe(1)	71.2(7)	O(6)-Ti(1)-C(19)	130.3(5)
C(7)-C(11)-Fe(1)	70.2(6)	C(22)-Ti(1)-C(19)	109.9(6)
C(10)-C(11)-H(11)	125.1	O(6)-Ti(1)-C(25)	89.5(4)
C(7)-C(11)-H(11)	125.1	C(22)-Ti(1)-C(25)	56.4(4)
Fe(1)-C(11)-H(11)	125.0	C(19)-Ti(1)-C(25)	139.7(5)
C(13)-C(12)-C(16)	108.8(11)	O(6)-Ti(1)-C(17)	91.1(5)
C(13)-C(12)-Fe(1)	70.7(7)	C(22)-Ti(1)-C(17)	87.1(6)

C(19)-Ti(1)-C(17)	56.6(5)	C(18)-Ti(1)-C(21)	54.8(4)
C(25)-Ti(1)-C(17)	142.3(6)	O(6)-Ti(1)-Cl(1)	96.1(2)
O(6)-Ti(1)-C(23)	135.2(4)	C(22)-Ti(1)-Cl(1)	134.5(3)
C(22)-Ti(1)-C(23)	34.3(4)	C(19)-Ti(1)-Cl(1)	85.0(5)
C(19)-Ti(1)-C(23)	90.3(6)	C(25)-Ti(1)-Cl(1)	84.1(3)
C(25)-Ti(1)-C(23)	56.6(4)	C(17)-Ti(1)-Cl(1)	133.3(5)
C(17)-Ti(1)-C(23)	99.4(5)	C(23)-Ti(1)-Cl(1)	107.0(3)
O(6)-Ti(1)-C(26)	77.9(4)	C(26)-Ti(1)-Cl(1)	116.9(3)
C(22)-Ti(1)-C(26)	34.6(4)	C(20)-Ti(1)-Cl(1)	79.0(4)
C(19)-Ti(1)-C(26)	144.3(6)	C(18)-Ti(1)-Cl(1)	119.4(5)
C(25)-Ti(1)-C(26)	34.1(4)	C(21)-Ti(1)-Cl(1)	105.5(5)
C(17)-Ti(1)-C(26)	109.7(6)	O(6)-Ti(1)-C(24)	123.7(3)
C(23)-Ti(1)-C(26)	57.5(4)	C(22)-Ti(1)-C(24)	56.8(4)
O(6)-Ti(1)-C(20)	97.2(5)	C(19)-Ti(1)-C(24)	105.2(5)
C(22)-Ti(1)-C(20)	136.2(5)	C(25)-Ti(1)-C(24)	34.4(3)
C(19)-Ti(1)-C(20)	34.1(6)	C(17)-Ti(1)-C(24)	133.2(5)
C(25)-Ti(1)-C(20)	162.3(5)	C(23)-Ti(1)-C(24)	34.0(3)
C(17)-Ti(1)-C(20)	54.3(6)	C(26)-Ti(1)-C(24)	57.6(4)
C(23)-Ti(1)-C(20)	124.3(5)	C(20)-Ti(1)-C(24)	134.7(5)
C(26)-Ti(1)-C(20)	163.6(5)	C(18)-Ti(1)-C(24)	105.0(4)
O(6)-Ti(1)-C(18)	125.0(5)	C(21)-Ti(1)-C(24)	158.9(4)
C(22)-Ti(1)-C(18)	80.6(5)	Cl(1)-Ti(1)-C(24)	78.0(3)
C(19)-Ti(1)-C(18)	34.9(6)	C(21)-C(17)-C(18)	109.1(16)
C(25)-Ti(1)-C(18)	131.5(4)	C(21)-C(17)-Ti(1)	75.4(8)
C(17)-Ti(1)-C(18)	33.9(5)	C(18)-C(17)-Ti(1)	74.3(6)
C(23)-Ti(1)-C(18)	75.4(4)	C(21)-C(17)-H(17)	125.5
C(26)-Ti(1)-C(18)	114.1(5)	C(18)-C(17)-H(17)	125.5
C(20)-Ti(1)-C(18)	55.9(5)	Ti(1)-C(17)-H(17)	116.8
O(6)-Ti(1)-C(21)	77.1(4)	C(17)-C(18)-C(19)	105.3(13)
C(22)-Ti(1)-C(21)	118.4(6)	C(17)-C(18)-Ti(1)	71.7(6)
C(19)-Ti(1)-C(21)	55.2(5)	C(19)-C(18)-Ti(1)	71.0(7)
C(25)-Ti(1)-C(21)	164.1(5)	C(17)-C(18)-H(18)	127.3
C(17)-Ti(1)-C(21)	32.2(5)	C(19)-C(18)-H(18)	127.3
C(23)-Ti(1)-C(21)	129.3(5)	Ti(1)-C(18)-H(18)	121.8
C(26)-Ti(1)-C(21)	132.4(6)	C(20)-C(19)-C(18)	105.6(13)
C(20)-Ti(1)-C(21)	31.9(5)	C(20)-C(19)-Ti(1)	74.3(8)

C(18)-C(19)-Ti(1)	74.1(8)	C(22)-C(23)-Ti(1)	71.5(6)
C(20)-C(19)-H(19)	127.2	C(24)-C(23)-Ti(1)	74.5(6)
C(18)-C(19)-H(19)	127.2	C(22)-C(23)-H(23)	125.8
Ti(1)-C(19)-H(19)	116.7	C(24)-C(23)-H(23)	125.8
C(21)-C(20)-C(19)	108.9(14)	Ti(1)-C(23)-H(23)	119.9
C(21)-C(20)-Ti(1)	74.3(8)	C(23)-C(24)-C(25)	105.8(10)
C(19)-C(20)-Ti(1)	71.6(8)	C(23)-C(24)-Ti(1)	71.5(6)
C(21)-C(20)-H(20)	125.6	C(25)-C(24)-Ti(1)	71.0(6)
C(19)-C(20)-H(20)	125.6	C(23)-C(24)-H(24)	127.1
Ti(1)-C(20)-H(20)	120.2	C(25)-C(24)-H(24)	127.1
C(20)-C(21)-C(17)	110.9(14)	Ti(1)-C(24)-H(24)	122.2
C(20)-C(21)-Ti(1)	73.8(9)	C(26)-C(25)-C(24)	110.7(10)
C(17)-C(21)-Ti(1)	72.5(7)	C(26)-C(25)-Ti(1)	73.8(6)
C(20)-C(21)-H(21)	124.5	C(24)-C(25)-Ti(1)	74.6(6)
C(17)-C(21)-H(21)	124.5	C(26)-C(25)-H(25)	124.6
Ti(1)-C(21)-H(21)	120.8	C(24)-C(25)-H(25)	124.6
C(23)-C(22)-C(26)	110.0(11)	Ti(1)-C(25)-H(25)	118.6
C(23)-C(22)-Ti(1)	74.2(7)	C(25)-C(26)-C(22)	105.2(11)
C(26)-C(22)-Ti(1)	74.6(6)	C(25)-C(26)-Ti(1)	72.1(6)
C(23)-C(22)-H(22)	125.0	C(22)-C(26)-Ti(1)	70.9(6)
C(26)-C(22)-H(22)	125.0	C(25)-C(26)-H(26)	127.4
Ti(1)-C(22)-H(22)	118.0	C(22)-C(26)-H(26)	127.4
C(22)-C(23)-C(24)	108.3(10)	Ti(1)-C(26)-H(26)	121.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for Complex **6**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
W(1)	37(1)	31(1)	42(1)	-6(1)	-1(1)	4(1)
C(1)	50(7)	50(8)	56(8)	-6(7)	-10(6)	7(6)
O(1)	105(8)	65(7)	98(8)	-46(6)	-5(6)	42(6)
C(2)	45(5)	32(5)	61(7)	1(8)	-8(10)	13(4)
O(2)	45(4)	49(4)	90(6)	-4(6)	-8(6)	-9(3)
C(3)	58(8)	37(7)	46(7)	11(6)	1(6)	5(5)
O(3)	100(8)	66(7)	84(8)	13(6)	-1(6)	9(6)
C(4)	38(5)	66(7)	71(7)	-32(12)	3(9)	2(5)
O(4)	47(5)	134(10)	188(12)	-80(14)	5(10)	-9(5)
C(5)	44(7)	49(8)	61(8)	-11(7)	2(6)	-6(5)
O(5)	121(10)	83(9)	44(6)	26(6)	2(5)	-12(6)
C(6)	39(6)	25(5)	33(5)	6(4)	9(4)	-3(5)
O(6)	33(4)	31(4)	42(4)	-3(3)	-7(3)	7(3)
Fe(1)	42(1)	32(1)	41(1)	-1(1)	-7(1)	0(1)
C(7)	37(6)	34(6)	34(6)	2(5)	-1(4)	1(4)
C(8)	42(6)	47(7)	39(6)	-5(5)	-1(5)	2(5)
C(9)	66(8)	53(7)	45(7)	-18(6)	-1(6)	1(6)
C(10)	75(9)	66(9)	21(6)	0(5)	-9(5)	4(7)
C(11)	55(7)	40(7)	41(7)	0(5)	-14(5)	1(5)
C(12)	47(7)	53(8)	66(9)	-1(7)	-12(6)	-15(6)
C(13)	43(7)	48(8)	71(8)	-3(7)	1(6)	-1(6)
C(14)	68(8)	56(8)	51(7)	2(6)	4(6)	-14(6)
C(15)	56(8)	57(9)	80(10)	26(7)	-24(7)	-13(6)
C(16)	52(7)	26(6)	90(10)	-2(7)	-15(7)	2(5)
Ti(1)	35(1)	24(1)	35(1)	1(1)	-3(1)	2(1)
Cl(1)	57(2)	35(2)	40(1)	-11(1)	-6(1)	-3(1)
C(17)	113(11)	47(7)	50(7)	7(11)	-5(13)	-44(7)
C(18)	72(9)	12(5)	165(19)	26(8)	44(10)	7(6)
C(19)	113(14)	38(8)	110(14)	42(9)	-53(11)	-43(9)
C(20)	106(12)	47(8)	53(8)	18(7)	13(9)	-2(8)
C(21)	48(8)	59(9)	102(12)	56(9)	15(8)	10(6)
C(22)	49(7)	46(7)	60(8)	-12(6)	11(6)	-3(5)

C(23)	28(5)	45(7)	79(8)	9(6)	9(5)	5(5)
C(24)	41(5)	44(6)	56(9)	8(6)	-5(5)	-9(4)
C(25)	50(6)	24(6)	57(7)	0(5)	4(5)	-10(5)
C(26)	61(7)	47(7)	40(6)	10(6)	9(5)	-5(6)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Complex **6**.

	x	y	z	U(eq)
H(8)	1736	5544	8241	51
H(9)	1122	5194	6381	66
H(10)	414	7093	6254	65
H(11)	567	8547	8033	55
H(12)	-497	5323	7776	66
H(13)	-401	6804	9589	65
H(14)	399	5983	10907	70
H(15)	755	3826	9972	77
H(16)	226	3458	7976	67
H(17)	1966	3959	9998	84
H(18)	2919	3483	10955	99
H(19)	2931	4784	12968	105
H(20)	1943	5712	13214	83
H(21)	1394	5176	11430	84
H(22)	2958	4909	8738	62
H(23)	3658	5001	10439	61
H(24)	3755	7369	11107	56
H(25)	3076	8688	9804	52
H(26)	2613	7206	8268	59

Table 6. Torsion angles [°] for Complex **6**.

C(4)-W(1)-C(6)-O(6)	-132.0(9)
C(3)-W(1)-C(6)-O(6)	139.9(8)
C(2)-W(1)-C(6)-O(6)	51.4(9)
C(5)-W(1)-C(6)-O(6)	-45.0(7)
C(4)-W(1)-C(6)-C(7)	48.1(10)
C(3)-W(1)-C(6)-C(7)	-39.9(9)
C(2)-W(1)-C(6)-C(7)	-128.5(10)
C(5)-W(1)-C(6)-C(7)	135.1(9)
O(6)-C(6)-C(7)-C(8)	2.6(15)
W(1)-C(6)-C(7)-C(8)	-177.5(8)
O(6)-C(6)-C(7)-C(11)	179.1(9)
W(1)-C(6)-C(7)-C(11)	-1.0(15)
C(11)-C(7)-C(8)-C(9)	0.0(12)
C(6)-C(7)-C(8)-C(9)	177.1(10)
C(7)-C(8)-C(9)-C(10)	0.6(13)
C(8)-C(9)-C(10)-C(11)	-1.0(14)
C(9)-C(10)-C(11)-C(7)	1.0(14)
C(8)-C(7)-C(11)-C(10)	-0.6(12)
C(6)-C(7)-C(11)-C(10)	-177.7(10)
C(16)-C(12)-C(13)-C(14)	1.4(15)
C(12)-C(13)-C(14)-C(15)	-2.7(14)
C(13)-C(14)-C(15)-C(16)	3.0(15)
C(14)-C(15)-C(16)-C(12)	-2.1(16)
C(21)-C(17)-C(18)-C(19)	-4.5(14)
C(17)-C(18)-C(19)-C(20)	4.2(13)
C(18)-C(19)-C(20)-C(21)	-2.5(15)
C(19)-C(20)-C(21)-C(17)	-0.3(16)
C(18)-C(17)-C(21)-C(20)	3.1(16)
C(26)-C(22)-C(23)-C(24)	0.6(13)
C(22)-C(23)-C(24)-C(25)	0.9(12)
C(23)-C(24)-C(25)-C(26)	-2.1(12)
C(24)-C(25)-C(26)-C(22)	2.5(12)
C(23)-C(22)-C(26)-C(25)	-1.9(13)

Appendix 4

Crystallographic data of Complex 8

Table 1. Crystal data and structure refinement for Complex **8**.

Identification code	db52a3n_abs	
Empirical formula	C_{32} H_{18} Cr_2 Fe O_{12} Ti	
Formula weight	802.21	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2_1/c	
Unit cell dimensions	a = 9.9813(4) Å	a= 90°.
	b = 15.8650(7) Å	b= 101.723(1)°.
	c = 20.1457(9) Å	g = 90°.
Volume	3123.6(2) $Å^3$	
Z	4	
Density (calculated)	1.706 Mg/m^3	
Absorption coefficient	1.444 mm^{-1}	
F(000)	1608	
Crystal size	0.42 x 0.12 x 0.12 mm^3	
Theta range for data collection	2.43 to 26.53°.	
Index ranges	-4<=h<=12, -17<=k<=19, -24<=l<=25	
Reflections collected	16699	
Independent reflections	5958 [R(int) = 0.0290]	
Completeness to theta = 25.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.841 and 0.725	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5958 / 0 / 433	
Goodness-of-fit on F^2	1.076	
Final R indices [I>2σ(I)]	R1 = 0.0314, wR2 = 0.0824	
R indices (all data)	R1 = 0.0409, wR2 = 0.0911	
Extinction coefficient	0	
Largest diff. peak and hole	0.407 and -0.286 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Complex **8**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cr(1)	-244(1)	5514(1)	3626(1)	39(1)
C(1)	-1290(3)	6024(2)	4194(1)	58(1)
O(1)	-1921(2)	6339(2)	4539(1)	91(1)
C(2)	-1865(2)	5526(1)	2939(1)	42(1)
O(2)	-2876(2)	5529(1)	2559(1)	56(1)
C(3)	411(3)	6552(2)	3369(1)	55(1)
O(3)	877(3)	7165(2)	3229(1)	96(1)
C(4)	1247(3)	5528(2)	4366(1)	55(1)
O(4)	2093(2)	5566(2)	4841(1)	91(1)
C(5)	-607(2)	4393(2)	3862(1)	47(1)
O(5)	-759(2)	3706(1)	3994(1)	68(1)
C(6)	826(2)	4957(1)	2967(1)	35(1)
O(6)	1881(1)	4499(1)	3166(1)	39(1)
Cr(2)	5224(1)	3626(1)	1256(1)	37(1)
C(7)	6273(3)	3115(2)	695(1)	57(1)
O(7)	6929(3)	2805(2)	362(1)	93(1)
C(8)	6753(2)	3639(2)	1986(1)	45(1)
O(8)	7667(2)	3607(1)	2427(1)	69(1)
C(9)	4813(3)	2546(2)	1543(1)	49(1)
O(9)	4616(3)	1868(1)	1683(1)	79(1)
C(10)	3575(3)	3535(2)	607(1)	50(1)
O(10)	2553(2)	3441(2)	239(1)	79(1)
C(11)	5754(2)	4678(2)	924(1)	47(1)
O(11)	6116(2)	5281(1)	714(1)	72(1)
C(12)	4119(2)	4276(1)	1862(1)	35(1)
O(12)	3952(1)	4006(1)	2435(1)	39(1)
Fe(1)	1515(1)	5426(1)	1565(1)	38(1)
C(13)	378(2)	4998(2)	2221(1)	39(1)
C(14)	-312(2)	5688(2)	1828(1)	49(1)
C(15)	-548(3)	5475(2)	1139(1)	58(1)
C(16)	-29(3)	4657(2)	1078(1)	56(1)
C(17)	544(2)	4362(2)	1739(1)	44(1)

C(18)	3529(2)	5124(1)	1687(1)	39(1)
C(19)	3308(2)	5768(1)	2158(1)	43(1)
C(20)	2711(3)	6479(2)	1785(2)	56(1)
C(21)	2538(3)	6290(2)	1088(2)	59(1)
C(22)	3036(2)	5472(2)	1020(1)	51(1)
Ti(1)	3454(1)	3743(1)	3300(1)	31(1)
C(23)	4393(3)	4893(2)	4005(2)	68(1)
C(24)	4335(4)	4198(3)	4403(1)	97(2)
C(25)	5289(5)	3611(3)	4236(3)	120(2)
C(26)	5816(3)	3980(3)	3726(2)	83(1)
C(27)	5269(3)	4751(2)	3613(2)	64(1)
C(28)	2063(3)	2720(2)	3711(1)	58(1)
C(29)	3337(3)	2353(2)	3749(2)	65(1)
C(30)	3610(3)	2287(2)	3100(2)	59(1)
C(31)	2435(3)	2576(2)	2644(1)	49(1)
C(32)	1492(2)	2834(2)	3022(1)	50(1)

Table 3. Bond lengths [Å] and angles [°] for Complex **8**.

Cr(1)-C(4)	1.881(3)	Fe(1)-C(20)	2.049(3)
Cr(1)-C(1)	1.882(3)	Fe(1)-C(16)	2.052(3)
Cr(1)-C(3)	1.883(3)	Fe(1)-C(21)	2.059(2)
Cr(1)-C(5)	1.895(3)	Fe(1)-C(15)	2.065(2)
Cr(1)-C(2)	1.904(2)	C(13)-C(17)	1.432(3)
Cr(1)-C(6)	2.063(2)	C(13)-C(14)	1.443(3)
C(1)-O(1)	1.144(3)	C(14)-C(15)	1.400(4)
C(2)-O(2)	1.136(3)	C(14)-H(14)	0.9300
C(3)-O(3)	1.137(3)	C(15)-C(16)	1.411(4)
C(4)-O(4)	1.141(3)	C(15)-H(15)	0.9300
C(5)-O(5)	1.139(3)	C(16)-C(17)	1.417(3)
C(6)-O(6)	1.276(2)	C(16)-H(16)	0.9300
C(6)-C(13)	1.480(3)	C(17)-H(17)	0.9300
O(6)-Ti(1)	1.9507(14)	C(18)-C(19)	1.442(3)
Cr(2)-C(7)	1.873(3)	C(18)-C(22)	1.444(3)
Cr(2)-C(9)	1.880(3)	C(19)-C(20)	1.419(3)
Cr(2)-C(10)	1.888(3)	C(19)-H(19)	0.9300
Cr(2)-C(8)	1.893(2)	C(20)-C(21)	1.411(4)
Cr(2)-C(11)	1.912(3)	C(20)-H(20)	0.9300
Cr(2)-C(12)	2.077(2)	C(21)-C(22)	1.406(4)
C(7)-O(7)	1.141(3)	C(21)-H(21)	0.9300
C(8)-O(8)	1.137(3)	C(22)-H(22)	0.9300
C(9)-O(9)	1.139(3)	Ti(1)-C(24)	2.330(3)
C(10)-O(10)	1.143(3)	Ti(1)-C(25)	2.355(3)
C(11)-O(11)	1.135(3)	Ti(1)-C(30)	2.356(2)
C(12)-O(12)	1.274(2)	Ti(1)-C(26)	2.369(3)
C(12)-C(18)	1.483(3)	Ti(1)-C(31)	2.380(2)
O(12)-Ti(1)	1.9514(15)	Ti(1)-C(23)	2.383(3)
Fe(1)-C(17)	2.014(2)	Ti(1)-C(28)	2.390(2)
Fe(1)-C(19)	2.014(2)	Ti(1)-C(29)	2.396(3)
Fe(1)-C(13)	2.027(2)	Ti(1)-C(27)	2.403(3)
Fe(1)-C(18)	2.032(2)	Ti(1)-C(32)	2.405(2)
Fe(1)-C(14)	2.043(2)	C(23)-C(27)	1.311(4)
Fe(1)-C(22)	2.047(2)	C(23)-C(24)	1.372(5)

C(23)-H(23)	0.9300	O(3)-C(3)-Cr(1)	176.3(3)
C(24)-C(25)	1.421(6)	O(4)-C(4)-Cr(1)	175.2(2)
C(24)-H(24)	0.9300	O(5)-C(5)-Cr(1)	176.2(2)
C(25)-C(26)	1.376(6)	O(6)-C(6)-C(13)	113.81(18)
C(25)-H(25)	0.9300	O(6)-C(6)-Cr(1)	122.91(15)
C(26)-C(27)	1.341(5)	C(13)-C(6)-Cr(1)	123.12(14)
C(26)-H(26)	0.9300	C(6)-O(6)-Ti(1)	169.76(15)
C(27)-H(27)	0.9300	C(7)-Cr(2)-C(9)	88.55(12)
C(28)-C(29)	1.387(4)	C(7)-Cr(2)-C(10)	93.72(12)
C(28)-C(32)	1.400(4)	C(9)-Cr(2)-C(10)	85.97(11)
C(28)-H(28)	0.9300	C(7)-Cr(2)-C(8)	90.70(11)
C(29)-C(30)	1.393(4)	C(9)-Cr(2)-C(8)	87.89(10)
C(29)-H(29)	0.9300	C(10)-Cr(2)-C(8)	172.34(11)
C(30)-C(31)	1.411(4)	C(7)-Cr(2)-C(11)	86.44(12)
C(30)-H(30)	0.9300	C(9)-Cr(2)-C(11)	174.94(11)
C(31)-C(32)	1.388(4)	C(10)-Cr(2)-C(11)	95.05(10)
C(31)-H(31)	0.9300	C(8)-Cr(2)-C(11)	91.47(10)
C(32)-H(32)	0.9300	C(7)-Cr(2)-C(12)	175.84(11)
		C(9)-Cr(2)-C(12)	95.55(10)
C(4)-Cr(1)-C(1)	87.70(12)	C(10)-Cr(2)-C(12)	87.28(10)
C(4)-Cr(1)-C(3)	86.81(12)	C(8)-Cr(2)-C(12)	88.75(9)
C(1)-Cr(1)-C(3)	93.27(13)	C(11)-Cr(2)-C(12)	89.45(9)
C(4)-Cr(1)-C(5)	88.48(12)	O(7)-C(7)-Cr(2)	178.9(3)
C(1)-Cr(1)-C(5)	95.34(12)	O(8)-C(8)-Cr(2)	176.7(2)
C(3)-Cr(1)-C(5)	170.01(11)	O(9)-C(9)-Cr(2)	175.0(2)
C(4)-Cr(1)-C(2)	174.26(10)	O(10)-C(10)-Cr(2)	175.7(2)
C(1)-Cr(1)-C(2)	86.69(11)	O(11)-C(11)-Cr(2)	176.6(2)
C(3)-Cr(1)-C(2)	94.75(10)	O(12)-C(12)-C(18)	113.66(18)
C(5)-Cr(1)-C(2)	90.80(10)	O(12)-C(12)-Cr(2)	123.29(15)
C(4)-Cr(1)-C(6)	94.97(10)	C(18)-C(12)-Cr(2)	122.93(15)
C(1)-Cr(1)-C(6)	177.32(10)	C(12)-O(12)-Ti(1)	170.09(14)
C(3)-Cr(1)-C(6)	86.78(11)	C(17)-Fe(1)-C(19)	121.56(9)
C(5)-Cr(1)-C(6)	84.86(9)	C(17)-Fe(1)-C(13)	41.52(9)
C(2)-Cr(1)-C(6)	90.63(9)	C(19)-Fe(1)-C(13)	104.52(9)
O(1)-C(1)-Cr(1)	179.5(3)	C(17)-Fe(1)-C(18)	106.29(9)
O(2)-C(2)-Cr(1)	175.9(2)	C(19)-Fe(1)-C(18)	41.76(9)

C(13)-Fe(1)-C(18)	120.86(9)	C(22)-Fe(1)-C(15)	124.20(11)
C(17)-Fe(1)-C(14)	68.81(10)	C(20)-Fe(1)-C(15)	123.18(11)
C(19)-Fe(1)-C(14)	121.55(10)	C(16)-Fe(1)-C(15)	40.08(11)
C(13)-Fe(1)-C(14)	41.52(9)	C(21)-Fe(1)-C(15)	109.20(11)
C(18)-Fe(1)-C(14)	158.40(9)	C(17)-C(13)-C(14)	105.8(2)
C(17)-Fe(1)-C(22)	124.01(10)	C(17)-C(13)-C(6)	127.2(2)
C(19)-Fe(1)-C(22)	69.07(10)	C(14)-C(13)-C(6)	127.0(2)
C(13)-Fe(1)-C(22)	159.41(9)	C(17)-C(13)-Fe(1)	68.76(13)
C(18)-Fe(1)-C(22)	41.46(9)	C(14)-C(13)-Fe(1)	69.86(13)
C(14)-Fe(1)-C(22)	158.46(9)	C(6)-C(13)-Fe(1)	125.68(15)
C(17)-Fe(1)-C(20)	157.84(11)	C(15)-C(14)-C(13)	109.0(2)
C(19)-Fe(1)-C(20)	40.86(10)	C(15)-C(14)-Fe(1)	70.94(14)
C(13)-Fe(1)-C(20)	120.74(11)	C(13)-C(14)-Fe(1)	68.62(12)
C(18)-Fe(1)-C(20)	69.38(10)	C(15)-C(14)-H(14)	125.5
C(14)-Fe(1)-C(20)	106.80(11)	C(13)-C(14)-H(14)	125.5
C(22)-Fe(1)-C(20)	67.93(11)	Fe(1)-C(14)-H(14)	126.5
C(17)-Fe(1)-C(16)	40.79(10)	C(14)-C(15)-C(16)	108.5(2)
C(19)-Fe(1)-C(16)	159.10(10)	C(14)-C(15)-Fe(1)	69.22(14)
C(13)-Fe(1)-C(16)	69.24(10)	C(16)-C(15)-Fe(1)	69.44(14)
C(18)-Fe(1)-C(16)	123.13(11)	C(14)-C(15)-H(15)	125.7
C(14)-Fe(1)-C(16)	67.72(11)	C(16)-C(15)-H(15)	125.7
C(22)-Fe(1)-C(16)	109.43(11)	Fe(1)-C(15)-H(15)	127.2
C(20)-Fe(1)-C(16)	159.44(11)	C(15)-C(16)-C(17)	107.9(2)
C(17)-Fe(1)-C(21)	160.31(11)	C(15)-C(16)-Fe(1)	70.48(15)
C(19)-Fe(1)-C(21)	68.47(11)	C(17)-C(16)-Fe(1)	68.16(13)
C(13)-Fe(1)-C(21)	157.48(11)	C(15)-C(16)-H(16)	126.0
C(18)-Fe(1)-C(21)	69.01(10)	C(17)-C(16)-H(16)	126.0
C(14)-Fe(1)-C(21)	122.59(10)	Fe(1)-C(16)-H(16)	126.9
C(22)-Fe(1)-C(21)	40.05(10)	C(16)-C(17)-C(13)	108.8(2)
C(20)-Fe(1)-C(21)	40.19(11)	C(16)-C(17)-Fe(1)	71.05(15)
C(16)-Fe(1)-C(21)	124.66(12)	C(13)-C(17)-Fe(1)	69.72(13)
C(17)-Fe(1)-C(15)	68.20(11)	C(16)-C(17)-H(17)	125.6
C(19)-Fe(1)-C(15)	157.97(11)	C(13)-C(17)-H(17)	125.6
C(13)-Fe(1)-C(15)	68.86(10)	Fe(1)-C(17)-H(17)	125.2
C(18)-Fe(1)-C(15)	159.68(11)	C(19)-C(18)-C(22)	105.9(2)
C(14)-Fe(1)-C(15)	39.84(10)	C(19)-C(18)-C(12)	126.4(2)

C(22)-C(18)-C(12)	127.7(2)	C(24)-Ti(1)-C(30)	116.19(16)
C(19)-C(18)-Fe(1)	68.47(12)	C(25)-Ti(1)-C(30)	88.96(13)
C(22)-C(18)-Fe(1)	69.85(13)	O(6)-Ti(1)-C(26)	131.79(11)
C(12)-C(18)-Fe(1)	125.33(15)	O(12)-Ti(1)-C(26)	82.78(12)
C(20)-C(19)-C(18)	108.6(2)	C(24)-Ti(1)-C(26)	56.70(13)
C(20)-C(19)-Fe(1)	70.89(15)	C(25)-Ti(1)-C(26)	33.86(15)
C(18)-C(19)-Fe(1)	69.78(13)	C(30)-Ti(1)-C(26)	97.02(12)
C(20)-C(19)-H(19)	125.7	O(6)-Ti(1)-C(31)	99.22(8)
C(18)-C(19)-H(19)	125.7	O(12)-Ti(1)-C(31)	80.08(8)
Fe(1)-C(19)-H(19)	125.2	C(24)-Ti(1)-C(31)	143.70(13)
C(21)-C(20)-C(19)	108.1(2)	C(25)-Ti(1)-C(31)	123.37(12)
C(21)-C(20)-Fe(1)	70.27(16)	C(30)-Ti(1)-C(31)	34.67(9)
C(19)-C(20)-Fe(1)	68.25(14)	C(26)-Ti(1)-C(31)	127.31(11)
C(21)-C(20)-H(20)	125.9	O(6)-Ti(1)-C(23)	79.63(9)
C(19)-C(20)-H(20)	125.9	O(12)-Ti(1)-C(23)	103.15(10)
Fe(1)-C(20)-H(20)	127.1	C(24)-Ti(1)-C(23)	33.82(13)
C(22)-C(21)-C(20)	108.6(2)	C(25)-Ti(1)-C(23)	56.23(14)
C(22)-C(21)-Fe(1)	69.54(14)	C(30)-Ti(1)-C(23)	145.19(11)
C(20)-C(21)-Fe(1)	69.54(14)	C(26)-Ti(1)-C(23)	54.62(12)
C(22)-C(21)-H(21)	125.7	C(31)-Ti(1)-C(23)	176.63(10)
C(20)-C(21)-H(21)	125.7	O(6)-Ti(1)-C(28)	87.58(8)
Fe(1)-C(21)-H(21)	126.8	O(12)-Ti(1)-C(28)	136.47(9)
C(21)-C(22)-C(18)	108.8(2)	C(24)-Ti(1)-C(28)	90.78(11)
C(21)-C(22)-Fe(1)	70.40(14)	C(25)-Ti(1)-C(28)	94.29(14)
C(18)-C(22)-Fe(1)	68.69(13)	C(30)-Ti(1)-C(28)	57.07(10)
C(21)-C(22)-H(22)	125.6	C(26)-Ti(1)-C(28)	126.01(13)
C(18)-C(22)-H(22)	125.6	C(31)-Ti(1)-C(28)	56.71(10)
Fe(1)-C(22)-H(22)	126.9	C(23)-Ti(1)-C(28)	119.98(11)
O(6)-Ti(1)-O(12)	95.07(6)	O(6)-Ti(1)-C(29)	121.27(9)
O(6)-Ti(1)-C(24)	94.54(14)	O(12)-Ti(1)-C(29)	125.06(9)
O(12)-Ti(1)-C(24)	132.04(10)	C(24)-Ti(1)-C(29)	87.88(15)
O(6)-Ti(1)-C(25)	129.73(17)	C(25)-Ti(1)-C(29)	72.87(12)
O(12)-Ti(1)-C(25)	115.83(18)	C(30)-Ti(1)-C(29)	34.07(11)
C(24)-Ti(1)-C(25)	35.29(16)	C(26)-Ti(1)-C(29)	97.51(14)
O(6)-Ti(1)-C(30)	131.19(8)	C(31)-Ti(1)-C(29)	56.31(10)
O(12)-Ti(1)-C(30)	91.09(9)	C(23)-Ti(1)-C(29)	121.57(12)

C(28)-Ti(1)-C(29)	33.69(10)	C(24)-C(25)-Ti(1)	71.39(17)
O(6)-Ti(1)-C(27)	99.76(9)	C(26)-C(25)-H(25)	127.1
O(12)-Ti(1)-C(27)	77.10(9)	C(24)-C(25)-H(25)	127.1
C(24)-Ti(1)-C(27)	54.97(11)	Ti(1)-C(25)-H(25)	119.9
C(25)-Ti(1)-C(27)	55.07(13)	C(27)-C(26)-C(25)	108.2(4)
C(30)-Ti(1)-C(27)	128.71(11)	C(27)-C(26)-Ti(1)	75.07(15)
C(26)-Ti(1)-C(27)	32.63(12)	C(25)-C(26)-Ti(1)	72.51(19)
C(31)-Ti(1)-C(27)	151.39(10)	C(27)-C(26)-H(26)	125.9
C(23)-Ti(1)-C(27)	31.79(10)	C(25)-C(26)-H(26)	125.9
C(28)-Ti(1)-C(27)	145.24(10)	Ti(1)-C(26)-H(26)	118.4
C(29)-Ti(1)-C(27)	127.31(11)	C(23)-C(27)-C(26)	110.6(3)
O(6)-Ti(1)-C(32)	75.04(8)	C(23)-C(27)-Ti(1)	73.29(16)
O(12)-Ti(1)-C(32)	105.25(8)	C(26)-C(27)-Ti(1)	72.30(17)
C(24)-Ti(1)-C(32)	122.62(10)	C(23)-C(27)-H(27)	124.7
C(25)-Ti(1)-C(32)	126.66(13)	C(26)-C(27)-H(27)	124.7
C(30)-Ti(1)-C(32)	56.70(9)	Ti(1)-C(27)-H(27)	121.3
C(26)-Ti(1)-C(32)	152.00(13)	C(29)-C(28)-C(32)	107.1(3)
C(31)-Ti(1)-C(32)	33.72(9)	C(29)-C(28)-Ti(1)	73.37(15)
C(23)-Ti(1)-C(32)	143.20(10)	C(32)-C(28)-Ti(1)	73.60(14)
C(28)-Ti(1)-C(32)	33.95(9)	C(29)-C(28)-H(28)	126.5
C(29)-Ti(1)-C(32)	55.67(9)	C(32)-C(28)-H(28)	126.5
C(27)-Ti(1)-C(32)	174.37(10)	Ti(1)-C(28)-H(28)	118.6
C(27)-C(23)-C(24)	109.1(3)	C(28)-C(29)-C(30)	109.3(3)
C(27)-C(23)-Ti(1)	74.92(17)	C(28)-C(29)-Ti(1)	72.94(15)
C(24)-C(23)-Ti(1)	70.96(17)	C(30)-C(29)-Ti(1)	71.41(14)
C(27)-C(23)-H(23)	125.5	C(28)-C(29)-H(29)	125.3
C(24)-C(23)-H(23)	125.5	C(30)-C(29)-H(29)	125.3
Ti(1)-C(23)-H(23)	120.3	Ti(1)-C(29)-H(29)	122.0
C(23)-C(24)-C(25)	106.2(3)	C(29)-C(30)-C(31)	107.0(3)
C(23)-C(24)-Ti(1)	75.22(17)	C(29)-C(30)-Ti(1)	74.52(15)
C(25)-C(24)-Ti(1)	73.31(19)	C(31)-C(30)-Ti(1)	73.58(14)
C(23)-C(24)-H(24)	126.9	C(29)-C(30)-H(30)	126.5
C(25)-C(24)-H(24)	126.9	C(31)-C(30)-H(30)	126.5
Ti(1)-C(24)-H(24)	116.8	Ti(1)-C(30)-H(30)	117.5
C(26)-C(25)-C(24)	105.9(3)	C(32)-C(31)-C(30)	107.8(2)
C(26)-C(25)-Ti(1)	73.63(17)	C(32)-C(31)-Ti(1)	74.13(14)

C(30)-C(31)-Ti(1)	71.75(14)	C(31)-C(32)-Ti(1)	72.14(13)
C(32)-C(31)-H(31)	126.1	C(28)-C(32)-Ti(1)	72.45(14)
C(30)-C(31)-H(31)	126.1	C(31)-C(32)-H(32)	125.7
Ti(1)-C(31)-H(31)	119.8	C(28)-C(32)-H(32)	125.7
C(31)-C(32)-C(28)	108.7(2)	Ti(1)-C(32)-H(32)	121.4

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for Complex **8**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	36(1)	44(1)	39(1)	-1(1)	11(1)	2(1)
C(1)	56(2)	67(2)	53(2)	-3(1)	16(1)	9(1)
O(1)	90(2)	109(2)	83(2)	-17(1)	43(1)	30(1)
C(2)	40(1)	39(1)	49(1)	2(1)	16(1)	2(1)
O(2)	42(1)	57(1)	65(1)	8(1)	3(1)	2(1)
C(3)	52(1)	50(2)	58(2)	1(1)	1(1)	-5(1)
O(3)	102(2)	71(2)	101(2)	21(1)	-15(2)	-35(1)
C(4)	48(1)	74(2)	45(2)	-7(1)	15(1)	3(1)
O(4)	62(1)	153(2)	51(1)	-16(1)	-3(1)	1(1)
C(5)	40(1)	59(2)	44(1)	4(1)	14(1)	4(1)
O(5)	70(1)	59(1)	77(1)	17(1)	23(1)	1(1)
C(6)	30(1)	34(1)	40(1)	3(1)	9(1)	-2(1)
O(6)	34(1)	42(1)	41(1)	6(1)	7(1)	4(1)
Cr(2)	40(1)	41(1)	31(1)	-1(1)	8(1)	1(1)
C(7)	67(2)	62(2)	45(1)	-8(1)	17(1)	4(1)
O(7)	108(2)	110(2)	73(2)	-24(1)	47(1)	18(2)
C(8)	47(1)	42(1)	45(1)	-6(1)	11(1)	5(1)
O(8)	62(1)	69(1)	63(1)	-9(1)	-16(1)	11(1)
C(9)	54(1)	47(2)	43(1)	-2(1)	7(1)	3(1)
O(9)	104(2)	45(1)	86(2)	9(1)	16(1)	-2(1)
C(10)	62(2)	48(1)	38(1)	5(1)	4(1)	-2(1)
O(10)	73(1)	84(2)	64(1)	6(1)	-21(1)	-15(1)
C(11)	42(1)	54(2)	45(1)	4(1)	11(1)	1(1)
O(11)	66(1)	70(1)	81(2)	23(1)	21(1)	-12(1)
C(12)	30(1)	41(1)	31(1)	2(1)	4(1)	-5(1)
O(12)	39(1)	45(1)	33(1)	7(1)	10(1)	3(1)
Fe(1)	37(1)	42(1)	34(1)	8(1)	8(1)	6(1)
C(13)	31(1)	47(1)	38(1)	6(1)	8(1)	3(1)
C(14)	40(1)	61(2)	48(1)	13(1)	12(1)	16(1)
C(15)	42(1)	81(2)	46(2)	16(1)	0(1)	14(1)
C(16)	48(1)	76(2)	39(1)	-3(1)	-2(1)	-7(1)
C(17)	42(1)	47(1)	40(1)	0(1)	5(1)	-5(1)

C(18)	36(1)	43(1)	41(1)	7(1)	14(1)	1(1)
C(19)	40(1)	39(1)	49(1)	2(1)	8(1)	-4(1)
C(20)	60(2)	35(1)	77(2)	7(1)	22(1)	0(1)
C(21)	64(2)	53(2)	65(2)	30(1)	25(1)	9(1)
C(22)	52(1)	61(2)	44(1)	17(1)	19(1)	10(1)
Ti(1)	31(1)	34(1)	28(1)	3(1)	5(1)	1(1)
C(23)	54(2)	75(2)	73(2)	-31(2)	7(1)	-16(1)
C(24)	89(2)	173(4)	26(1)	-14(2)	6(2)	-70(3)
C(25)	129(4)	77(3)	106(3)	36(2)	-87(3)	-26(2)
C(26)	35(1)	117(3)	86(2)	-32(2)	-14(2)	9(2)
C(27)	42(1)	83(2)	61(2)	-2(2)	-3(1)	-23(1)
C(28)	65(2)	53(2)	59(2)	13(1)	22(1)	-12(1)
C(29)	77(2)	46(2)	66(2)	25(1)	0(2)	-4(1)
C(30)	59(2)	33(1)	83(2)	0(1)	14(1)	6(1)
C(31)	56(1)	35(1)	53(2)	-5(1)	7(1)	-8(1)
C(32)	44(1)	41(1)	65(2)	2(1)	8(1)	-12(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Complex **8**.

	x	y	z	U(eq)
H(14)	-560	6194	2003	59
H(15)	-976	5814	782	69
H(16)	-58	4364	676	67
H(17)	959	3840	1843	52
H(19)	3521	5724	2628	52
H(20)	2475	6983	1967	67
H(21)	2157	6646	733	71
H(22)	3047	5200	612	61
H(23)	3892	5386	4012	82
H(24)	3782	4125	4718	116
H(25)	5512	3084	4431	144
H(26)	6443	3737	3500	100
H(27)	5482	5133	3300	77
H(28)	1663	2864	4074	69
H(29)	3919	2178	4146	78
H(30)	4413	2089	2988	70
H(31)	2315	2591	2174	59
H(32)	624	3048	2847	60

Table 6. Torsion angles [°] for Complex **8**.

C(4)-Cr(1)-C(6)-O(6)	24.79(19)	C(19)-C(20)-C(21)-C(22)	-0.8(3)
C(3)-Cr(1)-C(6)-O(6)	111.30(18)	C(20)-C(21)-C(22)-C(18)	0.6(3)
C(5)-Cr(1)-C(6)-O(6)	-63.23(18)	C(19)-C(18)-C(22)-C(21)	-0.2(3)
C(2)-Cr(1)-C(6)-O(6)	-153.98(18)	C(12)-C(18)-C(22)-C(21)	178.8(2)
C(4)-Cr(1)-C(6)-C(13)	-160.13(18)	C(27)-C(23)-C(24)-C(25)	1.5(3)
C(3)-Cr(1)-C(6)-C(13)	-73.62(18)	C(23)-C(24)-C(25)-C(26)	-2.5(3)
C(5)-Cr(1)-C(6)-C(13)	111.85(18)	C(24)-C(25)-C(26)-C(27)	2.6(4)
C(2)-Cr(1)-C(6)-C(13)	21.10(18)	C(24)-C(23)-C(27)-C(26)	0.1(3)
C(9)-Cr(2)-C(12)-O(12)	30.81(18)	C(25)-C(26)-C(27)-C(23)	-1.8(3)
C(10)-Cr(2)-C(12)-O(12)	116.49(18)	C(32)-C(28)-C(29)-C(30)	3.9(3)
C(8)-Cr(2)-C(12)-O(12)	-56.94(18)	C(28)-C(29)-C(30)-C(31)	-3.5(3)
C(11)-Cr(2)-C(12)-O(12)	-148.42(17)	C(29)-C(30)-C(31)-C(32)	1.7(3)
C(9)-Cr(2)-C(12)-C(18)	-153.40(17)	C(30)-C(31)-C(32)-C(28)	0.7(3)
C(10)-Cr(2)-C(12)-C(18)	-67.72(18)	C(29)-C(28)-C(32)-C(31)	-2.8(3)
C(8)-Cr(2)-C(12)-C(18)	118.84(18)		
C(11)-Cr(2)-C(12)-C(18)	27.36(18)		
O(6)-C(6)-C(13)-C(17)	29.5(3)		
Cr(1)-C(6)-C(13)-C(17)	-145.97(19)		
O(6)-C(6)-C(13)-C(14)	-150.2(2)		
Cr(1)-C(6)-C(13)-C(14)	34.3(3)		
C(17)-C(13)-C(14)-C(15)	-0.1(3)		
C(6)-C(13)-C(14)-C(15)	179.7(2)		
C(13)-C(14)-C(15)-C(16)	0.2(3)		
C(14)-C(15)-C(16)-C(17)	-0.3(3)		
C(15)-C(16)-C(17)-C(13)	0.3(3)		
C(14)-C(13)-C(17)-C(16)	-0.1(3)		
C(6)-C(13)-C(17)-C(16)	-179.9(2)		
O(12)-C(12)-C(18)-C(19)	25.9(3)		
Cr(2)-C(12)-C(18)-C(19)	-150.22(18)		
O(12)-C(12)-C(18)-C(22)	-152.8(2)		
Cr(2)-C(12)-C(18)-C(22)	31.0(3)		
C(22)-C(18)-C(19)-C(20)	-0.3(3)		
C(12)-C(18)-C(19)-C(20)	-179.3(2)		
C(18)-C(19)-C(20)-C(21)	0.7(3)		

Table 7. Selected least-squares planes and deviations from the planes (Åx10^4) for Complex **8**.

Plane 1	5.711(6) x + 13.012(7) y - 2.240(19) z = 6.230(5)						
Atoms forming the Plane*	Cr(1)	C(6)	O(6)	C(13)	rms	[Ti(1)]	
Deviations	-72(4)	270(16)	-106(6)	-92(6)	156	[-1265(29)]	
Plane 2	7.670 (3) x + 6.946(15) y + 6.060(14) z = 7.280 (3)						
Atoms forming the Plane*	Cr(2)	C(12)	O(12)	C(18)	rms	[Ti(1)]	
Deviations	61(4)	-231(16)	92(6)	78(5)	134	[-309(29)]	
Plane 3	9.151 (5) x + 6.243 (20) y - 5.085(34) z = 2.336 (14)						
Atoms forming the Plane*	C(13)	C(14)	C(15)	C(16)	C(17)	rms	[C(6)]
Deviations	4(17)	-2(9)	-2(9)	2(11)	-2(11)	3	[55(46)]
Plane 4	9.267(5) x + 5.893 (18) y - 3.786(25) z = 5.651(10)						
Atoms forming the Plane*	C(18)	C(19)	C(20)	C(21)	C(22)	rms	[C(12)]
Deviations	6(14)	-31(15)	45(16)	-41(16)	21(16)	32	[-189(37)]
Plane 5	6.034 (11) x + 6.159 (22) y + 11.245 (25) z = 10.164(6)						
Atoms forming the Plane*	C(23)	C(24)	C(25)	C(26)	C(27)	rms	
Deviations	46(17)	-118(18)	148(19)	-127(19)	52(17)	106	
Plane 6	3.899(12) x + 14.573(8) y - 0.340(26) z = 4.601(8)						
Atoms forming the Plane*	C(28)	C(29)	C(30)	C(31)	C(32)	rms	
Deviations	189(16)	-210(17)	147(16)	-30(15)	-97(15)	150	

Dihedral angles between planes (º):

Planes 1 and 2:	36.76(9)	Planes 3 and 4:	4.21(12)
Planes 1 and 3:	32.12(11)	Planes 5 and 6:	50.58(13)
Planes 2 and 4:	28.78(9)		

* rms = root mean square deviation from the plane;
atoms not involved in calculating the plane are shown in brackets [ ].

Appendix 5

Crystallographic data of Complex 12

Table 1. Crystal data and structure refinement for Complex **12**.

Identification code	db100f2_abs	
Empirical formula	C_{20} H_{13} Cl Cr O_6 S Ti	
Formula weight	516.71	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2_1/c	
Unit cell dimensions	a = 10.7477(5) Å	a= 90°.
	b = 13.5857(7) Å	b= 104.0110(10)°.
	c = 14.9790(7) Å	g = 90°.
Volume	2122.09(18) $Å^3$	
Z	4	
Density (calculated)	1.617 Mg/m^3	
Absorption coefficient	1.147 mm^{-1}	
F(000)	1040	
Crystal size	0.32 x 0.22 x 0.20 mm^3	
Theta range for data collection	2.46 to 26.46°.	
Index ranges	-11<=h<=13, -15<=k<=16, -18<=l<=6	
Reflections collected	11215	
Independent reflections	4000 [R(int) = 0.0286]	
Completeness to θ = 25.00°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.795 and 0.685	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4000 / 0 / 293	
Goodness-of-fit on F^2	1.057	
Final R indices [I>2σ(I)]	R1 = 0.0351, wR2 = 0.0930	
R indices (all data)	R1 = 0.0399, wR2 = 0.0990	
Extinction coefficient	0	
Largest diff. peak and hole	0.365 and -0.276 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Complex **12**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cr(1)	5107(1)	2680(1)	10332(1)	36(1)
C(1)	6353(2)	3333(2)	11220(2)	54(1)
O(1)	7140(2)	3736(2)	11750(2)	84(1)
C(2)	5950(2)	3047(2)	9424(2)	49(1)
O(2)	6472(2)	3262(2)	8872(2)	83(1)
C(3)	6141(2)	1545(2)	10596(2)	51(1)
O(3)	6845(2)	912(2)	10802(2)	83(1)
C(4)	4185(2)	2234(2)	11197(2)	47(1)
O(4)	3650(2)	1933(2)	11701(1)	74(1)
C(5)	4158(2)	3875(2)	10125(2)	41(1)
O(5)	3634(2)	4609(1)	10000(1)	59(1)
C(6)	3671(2)	2052(2)	9304(1)	34(1)
O(6)	2496(1)	2293(1)	9229(1)	39(1)
C(7)	3908(4)	1373(7)	8624(4)	38(1)
C(8)	5072(3)	980(7)	8520(6)	84(6)
C(9)	4862(5)	400(10)	7723(8)	64(2)
C(10)	3605(5)	355(9)	7208(7)	57(3)
S(1)	2615(3)	1032(3)	7714(2)	60(1)
C(7A)	3777(4)	1382(6)	8554(5)	38(1)
C(8A)	2832(3)	1059(7)	7790(5)	67(5)
C(9A)	3365(5)	405(9)	7261(6)	49(2)
C(10A)	4655(5)	198(8)	7598(5)	48(2)
S(1A)	5272(3)	835(3)	8596(2)	62(1)
Ti(1)	698(1)	2530(1)	9090(1)	34(1)
Cl(1)	932(1)	3485(1)	10449(1)	53(1)
C(11)	860(3)	796(2)	9347(3)	69(1)
C(12)	-211(3)	978(2)	8614(2)	63(1)
C(13)	-1105(3)	1475(2)	8958(2)	66(1)
C(14)	-611(3)	1631(2)	9874(2)	67(1)
C(15)	605(3)	1225(2)	10131(2)	63(1)
C(16)	1068(3)	3326(3)	7764(2)	87(1)
C(17)	-73(4)	2837(3)	7503(2)	70(1)

C(18)	-916(3)	3264(3)	7916(2)	66(1)
C(19)	-340(3)	4009(2)	8463(2)	71(1)
C(20)	925(4)	4067(2)	8392(3)	87(1)

Table 3. Bond lengths [Å] and angles [°] for Complex **12**.

Cr(1)-C(1)	1.866(3)	Ti(1)-C(20)	2.374(3)
Cr(1)-C(2)	1.876(2)	Ti(1)-Cl(1)	2.3753(7)
Cr(1)-C(3)	1.885(2)	Ti(1)-C(15)	2.378(2)
Cr(1)-C(5)	1.902(2)	Ti(1)-C(14)	2.378(2)
Cr(1)-C(4)	1.911(2)	Ti(1)-C(16)	2.378(3)
Cr(1)-C(6)	2.081(2)	Ti(1)-C(19)	2.379(3)
C(1)-O(1)	1.150(3)	Ti(1)-C(13)	2.380(3)
C(2)-O(2)	1.143(3)	Ti(1)-C(11)	2.386(2)
C(3)-O(3)	1.139(3)	C(11)-C(15)	1.396(4)
C(4)-O(4)	1.130(3)	C(11)-C(12)	1.406(4)
C(5)-O(5)	1.138(3)	C(11)-H(11)	0.9300
C(6)-O(6)	1.283(2)	C(12)-C(13)	1.373(4)
C(6)-C(7)	1.442(5)	C(12)-H(12)	0.9300
C(6)-C(7A)	1.472(5)	C(13)-C(14)	1.362(4)
O(6)-Ti(1)	1.9192(15)	C(13)-H(13)	0.9300
C(7)-C(8)	1.4034	C(14)-C(15)	1.384(4)
C(7)-S(1)	1.7571	C(14)-H(14)	0.9300
C(8)-C(9)	1.4021	C(15)-H(15)	0.9300
C(8)-H(8)	0.9300	C(16)-C(17)	1.366(5)
C(9)-C(10)	1.3852	C(16)-C(20)	1.411(5)
C(9)-H(9)	0.9300	C(16)-H(16)	0.9300
C(10)-S(1)	1.7155	C(17)-C(18)	1.346(4)
C(10)-H(10)	0.9300	C(17)-H(17)	0.9300
C(7A)-C(8A)	1.4034	C(18)-C(19)	1.354(5)
C(7A)-S(1A)	1.7571	C(18)-H(18)	0.9300
C(8A)-C(9A)	1.4021	C(19)-C(20)	1.392(5)
C(8A)-H(8A)	0.9300	C(19)-H(19)	0.9300
C(9A)-C(10A)	1.3852	C(20)-H(20)	0.9300
C(9A)-H(9A)	0.9300		
C(10A)-S(1A)	1.7155	C(1)-Cr(1)-C(2)	90.10(12)
C(10A)-H(10A)	0.9300	C(1)-Cr(1)-C(3)	87.39(12)
Ti(1)-C(17)	2.359(3)	C(2)-Cr(1)-C(3)	90.33(10)
Ti(1)-C(12)	2.361(3)	C(1)-Cr(1)-C(5)	88.57(10)
Ti(1)-C(18)	2.371(3)	C(2)-Cr(1)-C(5)	89.38(10)

C(3)-Cr(1)-C(5)	175.95(11)	C(6)-C(7A)-S(1A)	118.2(3)
C(1)-Cr(1)-C(4)	93.90(11)	C(9A)-C(8A)-C(7A)	110.2
C(2)-Cr(1)-C(4)	175.79(11)	C(9A)-C(8A)-H(8A)	124.9
C(3)-Cr(1)-C(4)	88.51(10)	C(7A)-C(8A)-H(8A)	124.9
C(5)-Cr(1)-C(4)	92.06(10)	C(10A)-C(9A)-C(8A)	115.6
C(1)-Cr(1)-C(6)	175.86(10)	C(10A)-C(9A)-H(9A)	122.2
C(2)-Cr(1)-C(6)	88.52(10)	C(8A)-C(9A)-H(9A)	122.2
C(3)-Cr(1)-C(6)	96.52(10)	C(9A)-C(10A)-S(1A)	110.9
C(5)-Cr(1)-C(6)	87.51(9)	C(9A)-C(10A)-H(10A)	124.6
C(4)-Cr(1)-C(6)	87.59(9)	S(1A)-C(10A)-H(10A)	124.6
O(1)-C(1)-Cr(1)	178.2(3)	C(10A)-S(1A)-C(7A)	91.4
O(2)-C(2)-Cr(1)	179.3(2)	O(6)-Ti(1)-C(17)	103.76(10)
O(3)-C(3)-Cr(1)	174.0(3)	O(6)-Ti(1)-C(12)	102.40(9)
O(4)-C(4)-Cr(1)	177.3(2)	C(17)-Ti(1)-C(12)	80.50(12)
O(5)-C(5)-Cr(1)	177.28(19)	O(6)-Ti(1)-C(18)	133.42(9)
O(6)-C(6)-C(7)	116.1(2)	C(17)-Ti(1)-C(18)	33.06(11)
O(6)-C(6)-C(7A)	110.3(2)	C(12)-Ti(1)-C(18)	88.68(11)
O(6)-C(6)-Cr(1)	119.92(15)	O(6)-Ti(1)-C(20)	89.28(11)
C(7)-C(6)-Cr(1)	123.95(19)	C(17)-Ti(1)-C(20)	56.53(12)
C(7A)-C(6)-Cr(1)	129.6(2)	C(12)-Ti(1)-C(20)	137.02(11)
C(6)-O(6)-Ti(1)	174.81(14)	C(18)-Ti(1)-C(20)	55.78(11)
C(8)-C(7)-C(6)	129.6(3)	O(6)-Ti(1)-Cl(1)	95.98(5)
C(8)-C(7)-S(1)	111.8	C(17)-Ti(1)-Cl(1)	134.89(9)
C(6)-C(7)-S(1)	118.4(3)	C(12)-Ti(1)-Cl(1)	134.18(7)
C(9)-C(8)-C(7)	110.2	C(18)-Ti(1)-Cl(1)	108.21(9)
C(9)-C(8)-H(8)	124.9	C(20)-Ti(1)-Cl(1)	84.06(11)
C(7)-C(8)-H(8)	124.9	O(6)-Ti(1)-C(15)	90.29(9)
C(10)-C(9)-C(8)	115.6	C(17)-Ti(1)-C(15)	137.08(12)
C(10)-C(9)-H(9)	122.2	C(12)-Ti(1)-C(15)	56.77(10)
C(8)-C(9)-H(9)	122.2	C(18)-Ti(1)-C(15)	131.32(11)
C(9)-C(10)-S(1)	110.9	C(20)-Ti(1)-C(15)	165.77(12)
C(9)-C(10)-H(10)	124.6	Cl(1)-Ti(1)-C(15)	81.84(8)
S(1)-C(10)-H(10)	124.6	O(6)-Ti(1)-C(14)	124.12(10)
C(10)-S(1)-C(7)	91.4	C(17)-Ti(1)-C(14)	118.90(13)
C(8A)-C(7A)-C(6)	129.9(3)	C(12)-Ti(1)-C(14)	55.88(10)
C(8A)-C(7A)-S(1A)	111.8	C(18)-Ti(1)-C(14)	99.69(12)

C(20)-Ti(1)-C(14)	143.67(14)	C(15)-Ti(1)-C(11)	34.07(11)
Cl(1)-Ti(1)-C(14)	79.03(8)	C(14)-Ti(1)-C(11)	56.07(10)
C(15)-Ti(1)-C(14)	33.84(11)	C(16)-Ti(1)-C(11)	124.28(14)
O(6)-Ti(1)-C(16)	78.44(9)	C(19)-Ti(1)-C(11)	155.02(12)
C(17)-Ti(1)-C(16)	33.51(13)	C(13)-Ti(1)-C(11)	56.27(10)
C(12)-Ti(1)-C(16)	107.12(14)	C(15)-C(11)-C(12)	107.0(3)
C(18)-Ti(1)-C(16)	55.17(11)	C(15)-C(11)-Ti(1)	72.64(15)
C(20)-Ti(1)-C(16)	34.54(13)	C(12)-C(11)-Ti(1)	71.77(15)
Cl(1)-Ti(1)-C(16)	117.59(13)	C(15)-C(11)-H(11)	126.5
C(15)-Ti(1)-C(16)	158.18(13)	C(12)-C(11)-H(11)	126.5
C(14)-Ti(1)-C(16)	152.22(14)	Ti(1)-C(11)-H(11)	120.9
O(6)-Ti(1)-C(19)	123.25(10)	C(13)-C(12)-C(11)	107.9(3)
C(17)-Ti(1)-C(19)	55.63(11)	C(13)-C(12)-Ti(1)	73.93(16)
C(12)-Ti(1)-C(19)	121.01(12)	C(11)-C(12)-Ti(1)	73.77(15)
C(18)-Ti(1)-C(19)	33.13(11)	C(13)-C(12)-H(12)	126.0
C(20)-Ti(1)-C(19)	34.05(13)	C(11)-C(12)-H(12)	126.0
Cl(1)-Ti(1)-C(19)	79.57(8)	Ti(1)-C(12)-H(12)	118.2
C(15)-Ti(1)-C(19)	142.94(12)	C(14)-C(13)-C(12)	108.5(3)
C(14)-Ti(1)-C(19)	110.59(12)	C(14)-C(13)-Ti(1)	73.27(15)
C(16)-Ti(1)-C(19)	56.17(11)	C(12)-C(13)-Ti(1)	72.40(15)
O(6)-Ti(1)-C(13)	133.30(9)	C(14)-C(13)-H(13)	125.7
C(17)-Ti(1)-C(13)	86.70(12)	C(12)-C(13)-H(13)	125.7
C(12)-Ti(1)-C(13)	33.67(10)	Ti(1)-C(13)-H(13)	120.3
C(18)-Ti(1)-C(13)	75.94(11)	C(13)-C(14)-C(15)	109.2(3)
C(20)-Ti(1)-C(13)	131.41(11)	C(13)-C(14)-Ti(1)	73.44(15)
Cl(1)-Ti(1)-C(13)	108.37(8)	C(15)-C(14)-Ti(1)	73.10(14)
C(15)-Ti(1)-C(13)	56.13(10)	C(13)-C(14)-H(14)	125.4
C(14)-Ti(1)-C(13)	33.28(10)	C(15)-C(14)-H(14)	125.4
C(16)-Ti(1)-C(13)	120.11(14)	Ti(1)-C(14)-H(14)	119.8
C(19)-Ti(1)-C(13)	100.44(12)	C(14)-C(15)-C(11)	107.3(3)
O(6)-Ti(1)-C(11)	77.57(8)	C(14)-C(15)-Ti(1)	73.06(15)
C(17)-Ti(1)-C(11)	109.36(13)	C(11)-C(15)-Ti(1)	73.29(14)
C(12)-Ti(1)-C(11)	34.46(11)	C(14)-C(15)-H(15)	126.3
C(18)-Ti(1)-C(11)	123.13(12)	C(11)-C(15)-H(15)	126.3
C(20)-Ti(1)-C(11)	158.11(15)	Ti(1)-C(15)-H(15)	119.2
Cl(1)-Ti(1)-C(11)	114.36(9)	C(17)-C(16)-C(20)	107.6(3)

C(17)-C(16)-Ti(1)	72.45(16)	C(19)-C(18)-H(18)	125.0
C(20)-C(16)-Ti(1)	72.55(16)	Ti(1)-C(18)-H(18)	119.9
C(17)-C(16)-H(16)	126.2	C(18)-C(19)-C(20)	107.9(3)
C(20)-C(16)-H(16)	126.2	C(18)-C(19)-Ti(1)	73.11(17)
Ti(1)-C(16)-H(16)	120.6	C(20)-C(19)-Ti(1)	72.77(16)
C(18)-C(17)-C(16)	108.4(3)	C(18)-C(19)-H(19)	126.1
C(18)-C(17)-Ti(1)	73.98(16)	C(20)-C(19)-H(19)	126.1
C(16)-C(17)-Ti(1)	74.04(17)	Ti(1)-C(19)-H(19)	119.9
C(18)-C(17)-H(17)	125.8	C(19)-C(20)-C(16)	106.1(3)
C(16)-C(17)-H(17)	125.8	C(19)-C(20)-Ti(1)	73.18(17)
Ti(1)-C(17)-H(17)	118.1	C(16)-C(20)-Ti(1)	72.91(16)
C(17)-C(18)-C(19)	110.0(3)	C(19)-C(20)-H(20)	126.9
C(17)-C(18)-Ti(1)	72.97(16)	C(16)-C(20)-H(20)	126.9
C(19)-C(18)-Ti(1)	73.76(15)	Ti(1)-C(20)-H(20)	119.0
C(17)-C(18)-H(18)	125.0		

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	30(1)	35(1)	43(1)	5(1)	8(1)	1(1)
C(1)	45(1)	57(2)	55(1)	6(1)	1(1)	4(1)
O(1)	62(1)	90(2)	82(1)	-10(1)	-20(1)	-11(1)
C(2)	45(1)	37(1)	67(2)	7(1)	20(1)	3(1)
O(2)	99(2)	63(1)	110(2)	19(1)	71(2)	3(1)
C(3)	46(1)	51(1)	59(1)	14(1)	21(1)	5(1)
O(3)	78(1)	70(1)	108(2)	40(1)	38(1)	40(1)
C(4)	47(1)	46(1)	48(1)	6(1)	14(1)	7(1)
O(4)	77(1)	82(1)	76(1)	22(1)	43(1)	12(1)
C(5)	36(1)	39(1)	49(1)	0(1)	10(1)	-5(1)
O(5)	50(1)	38(1)	88(1)	5(1)	14(1)	5(1)
C(6)	33(1)	29(1)	43(1)	7(1)	13(1)	2(1)
O(6)	31(1)	39(1)	46(1)	-1(1)	10(1)	2(1)
C(7)	36(1)	35(1)	44(1)	2(1)	14(1)	2(1)
C(8)	115(12)	60(7)	80(8)	-24(5)	29(7)	0(6)
C(9)	70(5)	43(6)	89(6)	-20(4)	39(4)	-8(4)
C(10)	80(6)	45(4)	60(5)	-15(4)	42(5)	4(5)
S(1)	75(1)	61(2)	45(1)	-15(1)	19(1)	0(1)
C(7A)	36(1)	35(1)	44(1)	2(1)	14(1)	2(1)
C(8A)	104(9)	52(7)	50(7)	11(5)	27(5)	5(6)
C(9A)	51(3)	59(5)	43(4)	-5(3)	18(3)	-7(3)
C(10A)	54(4)	36(5)	58(4)	-21(3)	24(3)	-9(3)
S(1A)	48(1)	64(1)	79(2)	-23(1)	24(1)	5(1)
Ti(1)	29(1)	37(1)	35(1)	1(1)	8(1)	0(1)
Cl(1)	61(1)	53(1)	47(1)	-11(1)	16(1)	-2(1)
C(11)	62(2)	31(1)	126(3)	14(1)	44(2)	0(1)
C(12)	79(2)	51(2)	59(2)	-12(1)	17(1)	-24(1)
C(13)	41(1)	70(2)	85(2)	-1(2)	11(1)	-19(1)
C(14)	67(2)	69(2)	78(2)	-7(2)	43(2)	-24(2)
C(15)	73(2)	56(2)	55(1)	15(1)	9(1)	-23(1)
C(16)	72(2)	117(3)	87(2)	70(2)	49(2)	43(2)
C(17)	95(2)	75(2)	39(1)	9(1)	12(1)	16(2)

C(18)	46(1)	86(2)	59(2)	17(2)	-1(1)	9(1)
C(19)	85(2)	67(2)	56(2)	10(1)	5(1)	40(2)
C(20)	84(2)	61(2)	90(2)	45(2)	-30(2)	-26(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Complex **12**.

	x	y	z	U(eq)
H(8)	5867	1088	8921	101
H(9)	5524	68	7551	77
H(10)	3335	6	6662	69
H(8A)	1976	1252	7654	81
H(9A)	2883	128	6720	59
H(10A)	5125	-229	7321	57
H(11)	1598	455	9316	83
H(12)	-298	793	8004	75
H(13)	-1911	1672	8623	79
H(14)	-1026	1958	10265	80
H(15)	1151	1237	10716	75
H(16)	1805	3194	7564	104
H(17)	-240	2301	7106	84
H(18)	-1767	3076	7837	79
H(19)	-722	4411	8823	85
H(20)	1550	4504	8696	104

Table 6. Torsion angles [°] for Complex **12**.

C(2)-Cr(1)-C(6)-O(6)	-126.85(17)	C(8A)-C(7A)-S(1A)-C(10A)	0.9
C(3)-Cr(1)-C(6)-O(6)	142.99(16)	C(6)-C(7A)-S(1A)-C(10A)	178.5(9)
C(5)-Cr(1)-C(6)-O(6)	-37.40(16)	C(15)-C(11)-C(12)-C(13)	-2.0(3)
C(4)-Cr(1)-C(6)-O(6)	54.76(16)	C(11)-C(12)-C(13)-C(14)	1.6(3)
C(2)-Cr(1)-C(6)-C(7)	50.5(5)	C(12)-C(13)-C(14)-C(15)	-0.6(3)
C(3)-Cr(1)-C(6)-C(7)	-39.7(5)	C(13)-C(14)-C(15)-C(11)	-0.7(3)
C(5)-Cr(1)-C(6)-C(7)	139.9(5)	C(12)-C(11)-C(15)-C(14)	1.7(3)
C(4)-Cr(1)-C(6)-C(7)	-127.9(5)	C(20)-C(16)-C(17)-C(18)	2.0(3)
C(2)-Cr(1)-C(6)-C(7A)	48.1(5)	C(16)-C(17)-C(18)-C(19)	-1.6(3)
C(3)-Cr(1)-C(6)-C(7A)	-42.0(5)	C(17)-C(18)-C(19)-C(20)	0.5(3)
C(5)-Cr(1)-C(6)-C(7A)	137.6(5)	C(18)-C(19)-C(20)-C(16)	0.8(3)
C(4)-Cr(1)-C(6)-C(7A)	-130.3(5)	C(17)-C(16)-C(20)-C(19)	-1.7(3)
O(6)-C(6)-C(7)-C(8)	179.6(6)		
Cr(1)-C(6)-C(7)-C(8)	2.2(10)		
O(6)-C(6)-C(7)-S(1)	5.5(8)		
Cr(1)-C(6)-C(7)-S(1)	-171.9(3)		
C(6)-C(7)-C(8)-C(9)	-175.9(12)		
S(1)-C(7)-C(8)-C(9)	-1.5		
C(7)-C(8)-C(9)-C(10)	1.5		
C(8)-C(9)-C(10)-S(1)	-0.9		
C(9)-C(10)-S(1)-C(7)	0.0		
C(8)-C(7)-S(1)-C(10)	0.9		
C(6)-C(7)-S(1)-C(10)	176.0(10)		
O(6)-C(6)-C(7A)-C(8A)	4.8(8)		
C(7)-C(6)-C(7A)-C(8A)	171(8)		
Cr(1)-C(6)-C(7A)-C(8A)	-170.5(5)		
O(6)-C(6)-C(7A)-S(1A)	-172.3(4)		
C(7)-C(6)-C(7A)-S(1A)	-7(7)		
Cr(1)-C(6)-C(7A)-S(1A)	12.4(9)		
C(6)-C(7A)-C(8A)-C(9A)	-178.8(11)		
S(1A)-C(7A)-C(8A)-C(9A)	-1.5		
C(7A)-C(8A)-C(9A)-C(10A)	1.5		
C(8A)-C(9A)-C(10A)-S(1A)	-0.9		
C(9A)-C(10A)-S(1A)-C(7A)	0.0		

Appendix 6

Crystallographic data of Complex 13

Table 1. Crystal data and structure refinement for Complex **13**.

Identification code	db76a_abs	
Empirical formula	C_{25} H_{15} Cl Cr_2 O_9 Ti	
Formula weight	646.72	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 14.9820(8) Å	a= 90°.
	b = 15.3296(8) Å	b= 90°.
	c = 21.8203(12) Å	g = 90°.
Volume	5011.4(5) $Å^3$	
Z	8	
Density (calculated)	1.714 Mg/m^3	
Absorption coefficient	1.323 mm^{-1}	
F(000)	2592	
Crystal size	0.28 x 0.20 x 0.10 mm^3	
Theta range for data collection	2.66 to 26.53°.	
Index ranges	-18<=h<=18, -5<=k<=18, -27<=l<=26	
Reflections collected	21839	
Independent reflections	4680 [R(int) = 0.0404]	
Completeness to θ = 25.00°	98.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.876 and 0.688	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4680 / 0 / 343	
Goodness-of-fit on F^2	1.136	
Final R indices [I>2σ(I)]	R1 = 0.0388, wR2 = 0.0946	
R indices (all data)	R1 = 0.0616, wR2 = 0.1180	
Extinction coefficient	0	
Largest diff. peak and hole	0.570 and -0.475 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Complex **13**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cr(1)	5488(1)	837(1)	6040(1)	36(1)
C(1)	4322(3)	722(2)	5732(2)	48(1)
O(1)	3612(2)	674(2)	5541(2)	70(1)
C(2)	5205(3)	2032(2)	6170(2)	44(1)
O(2)	4990(2)	2740(2)	6237(1)	64(1)
C(3)	5134(3)	511(2)	6837(2)	47(1)
O(3)	4935(2)	261(2)	7309(1)	73(1)
C(4)	5643(2)	-382(2)	5926(2)	44(1)
O(4)	5680(2)	-1123(2)	5882(2)	66(1)
C(5)	5931(3)	1114(2)	5239(2)	44(1)
O(5)	6188(2)	1277(2)	4766(1)	58(1)
C(6)	6745(2)	1066(2)	6396(1)	32(1)
O(6)	6841(2)	1587(1)	6854(1)	35(1)
Cr(2)	8568(1)	1089(1)	5460(1)	33(1)
C(7)	8349(3)	920(2)	4639(2)	46(1)
O(7)	8226(3)	802(2)	4128(1)	74(1)
C(8)	7985(3)	2155(2)	5393(2)	47(1)
O(8)	7618(2)	2801(2)	5338(2)	74(1)
C(9)	9631(3)	1637(2)	5264(2)	47(1)
O(9)	10300(2)	1952(2)	5151(2)	69(1)
C(10)	7629(2)	684(2)	6195(1)	33(1)
C(11)	8448(2)	968(2)	6464(2)	38(1)
C(12)	9257(3)	610(2)	6284(2)	45(1)
C(13)	9287(3)	-52(2)	5837(2)	46(1)
C(14)	8500(3)	-339(2)	5569(2)	42(1)
C(15)	7676(2)	25(2)	5742(2)	37(1)
Ti(1)	6907(1)	2276(1)	7594(1)	31(1)
Cl(1)	5340(1)	2333(1)	7780(1)	52(1)
C(16)	8135(3)	1665(3)	8098(2)	51(1)
C(17)	7626(3)	961(2)	7903(2)	46(1)
C(18)	6804(3)	985(2)	8203(2)	51(1)
C(19)	6822(3)	1690(3)	8610(2)	60(1)
C(20)	7637(3)	2110(3)	8544(2)	59(1)
C(21)	7903(3)	3215(2)	7062(2)	65(1)
C(22)	7061(4)	3358(2)	6809(2)	60(1)
C(23)	6530(3)	3709(2)	7263(2)	63(1)

C(24)	7034(4)	3772(2)	7796(2)	70(1)
C(25)	7888(4)	3488(3)	7658(3)	72(1)

Table 3. Bond lengths [Å] and angles [°] for Complex **13**.

Cr(1)-C(1)	1.879(4)	Ti(1)-C(24)	2.342(4)
Cr(1)-C(3)	1.886(4)	Ti(1)-C(20)	2.357(4)
Cr(1)-C(4)	1.900(4)	Ti(1)-C(25)	2.373(4)
Cr(1)-C(2)	1.901(4)	Ti(1)-C(21)	2.376(4)
Cr(1)-C(5)	1.916(4)	Ti(1)-C(23)	2.381(4)
Cr(1)-C(6)	2.067(3)	Ti(1)-C(17)	2.383(3)
C(1)-O(1)	1.146(5)	Ti(1)-Cl(1)	2.3833(11)
C(2)-O(2)	1.141(4)	Ti(1)-C(18)	2.389(3)
C(3)-O(3)	1.139(5)	Ti(1)-C(19)	2.394(4)
C(4)-O(4)	1.141(4)	Ti(1)-C(22)	2.396(4)
C(5)-O(5)	1.130(4)	C(16)-C(17)	1.389(5)
C(6)-O(6)	1.287(4)	C(16)-C(20)	1.405(6)
C(6)-C(10)	1.513(5)	C(16)-H(16)	0.9300
O(6)-Ti(1)	1.933(2)	C(17)-C(18)	1.395(6)
Cr(2)-C(7)	1.840(4)	C(17)-H(17)	0.9300
Cr(2)-C(9)	1.852(4)	C(18)-C(19)	1.399(6)
Cr(2)-C(8)	1.859(4)	C(18)-H(18)	0.9300
Cr(2)-C(15)	2.197(3)	C(19)-C(20)	1.388(6)
Cr(2)-C(12)	2.198(3)	C(19)-H(19)	0.9300
Cr(2)-C(14)	2.204(3)	C(20)-H(20)	0.9300
Cr(2)-C(11)	2.206(3)	C(21)-C(25)	1.365(7)
Cr(2)-C(13)	2.213(3)	C(21)-C(22)	1.394(7)
Cr(2)-C(10)	2.221(3)	C(21)-H(21)	0.9300
C(7)-O(7)	1.144(4)	C(22)-C(23)	1.380(6)
C(8)-O(8)	1.139(4)	C(22)-H(22)	0.9300
C(9)-O(9)	1.140(5)	C(23)-C(24)	1.390(7)
C(10)-C(15)	1.416(4)	C(23)-H(23)	0.9300
C(10)-C(11)	1.428(5)	C(24)-C(25)	1.384(7)
C(11)-C(12)	1.387(5)	C(24)-H(24)	0.9300
C(11)-H(11)	0.9300	C(25)-H(25)	0.9300
C(12)-C(13)	1.409(5)		
C(12)-H(12)	0.9300	C(1)-Cr(1)-C(3)	92.49(17)
C(13)-C(14)	1.388(5)	C(1)-Cr(1)-C(4)	88.52(16)
C(13)-H(13)	0.9300	C(3)-Cr(1)-C(4)	83.90(16)
C(14)-C(15)	1.408(5)	C(1)-Cr(1)-C(2)	86.44(16)
C(14)-H(14)	0.9300	C(3)-Cr(1)-C(2)	93.16(16)
C(15)-H(15)	0.9300	C(4)-Cr(1)-C(2)	174.05(16)
Ti(1)-C(16)	2.339(4)	C(1)-Cr(1)-C(5)	91.00(17)

C(3)-Cr(1)-C(5)	175.39(17)	C(9)-Cr(2)-C(13)	91.44(15)
C(4)-Cr(1)-C(5)	93.19(15)	C(8)-Cr(2)-C(13)	162.39(16)
C(2)-Cr(1)-C(5)	90.06(15)	C(15)-Cr(2)-C(13)	66.77(14)
C(1)-Cr(1)-C(6)	175.44(14)	C(12)-Cr(2)-C(13)	37.25(14)
C(3)-Cr(1)-C(6)	87.37(15)	C(14)-Cr(2)-C(13)	36.62(14)
C(4)-Cr(1)-C(6)	96.00(14)	C(11)-Cr(2)-C(13)	66.71(13)
C(2)-Cr(1)-C(6)	89.01(14)	C(7)-Cr(2)-C(10)	123.43(16)
C(5)-Cr(1)-C(6)	89.39(14)	C(9)-Cr(2)-C(10)	146.98(15)
O(1)-C(1)-Cr(1)	178.2(4)	C(8)-Cr(2)-C(10)	90.29(14)
O(2)-C(2)-Cr(1)	176.3(4)	C(15)-Cr(2)-C(10)	37.37(12)
O(3)-C(3)-Cr(1)	175.7(3)	C(12)-Cr(2)-C(10)	67.31(13)
O(4)-C(4)-Cr(1)	174.9(4)	C(14)-Cr(2)-C(10)	67.45(12)
O(5)-C(5)-Cr(1)	179.7(4)	C(11)-Cr(2)-C(10)	37.65(12)
O(6)-C(6)-C(10)	111.5(3)	C(13)-Cr(2)-C(10)	79.64(13)
O(6)-C(6)-Cr(1)	119.9(2)	O(7)-C(7)-Cr(2)	178.5(4)
C(10)-C(6)-Cr(1)	128.5(2)	O(8)-C(8)-Cr(2)	178.2(4)
C(6)-O(6)-Ti(1)	173.6(2)	O(9)-C(9)-Cr(2)	177.8(4)
C(7)-Cr(2)-C(9)	89.55(18)	C(15)-C(10)-C(11)	117.5(3)
C(7)-Cr(2)-C(8)	87.87(16)	C(15)-C(10)-C(6)	121.5(3)
C(9)-Cr(2)-C(8)	89.22(17)	C(11)-C(10)-C(6)	121.0(3)
C(7)-Cr(2)-C(15)	93.45(15)	C(15)-C(10)-Cr(2)	70.38(18)
C(9)-Cr(2)-C(15)	157.72(15)	C(11)-C(10)-Cr(2)	70.60(19)
C(8)-Cr(2)-C(15)	112.93(15)	C(6)-C(10)-Cr(2)	131.0(2)
C(7)-Cr(2)-C(12)	146.41(16)	C(12)-C(11)-C(10)	120.9(3)
C(9)-Cr(2)-C(12)	86.34(16)	C(12)-C(11)-Cr(2)	71.3(2)
C(8)-Cr(2)-C(12)	125.33(16)	C(10)-C(11)-Cr(2)	71.76(18)
C(15)-Cr(2)-C(12)	78.99(14)	C(12)-C(11)-H(11)	119.6
C(7)-Cr(2)-C(14)	87.54(15)	C(10)-C(11)-H(11)	119.6
C(9)-Cr(2)-C(14)	120.99(15)	Cr(2)-C(11)-H(11)	129.9
C(8)-Cr(2)-C(14)	149.38(16)	C(11)-C(12)-C(13)	120.7(4)
C(15)-Cr(2)-C(14)	37.32(13)	C(11)-C(12)-Cr(2)	71.9(2)
C(12)-Cr(2)-C(14)	66.57(14)	C(13)-C(12)-Cr(2)	71.9(2)
C(7)-Cr(2)-C(11)	160.22(16)	C(11)-C(12)-H(12)	119.7
C(9)-Cr(2)-C(11)	109.73(15)	C(13)-C(12)-H(12)	119.7
C(8)-Cr(2)-C(11)	96.54(15)	Cr(2)-C(12)-H(12)	128.8
C(15)-Cr(2)-C(11)	67.05(13)	C(14)-C(13)-C(12)	119.5(3)
C(12)-Cr(2)-C(11)	36.72(13)	C(14)-C(13)-Cr(2)	71.4(2)
C(14)-Cr(2)-C(11)	78.84(13)	C(12)-C(13)-Cr(2)	70.8(2)
C(7)-Cr(2)-C(13)	109.73(15)	C(14)-C(13)-H(13)	120.2

C(12)-C(13)-H(13)	120.2	C(25)-Ti(1)-C(17)	111.47(17)
Cr(2)-C(13)-H(13)	130.1	C(21)-Ti(1)-C(17)	111.53(15)
C(13)-C(14)-C(15)	120.4(3)	C(23)-Ti(1)-C(17)	166.87(16)
C(13)-C(14)-Cr(2)	72.0(2)	O(6)-Ti(1)-Cl(1)	96.41(7)
C(15)-C(14)-Cr(2)	71.05(18)	C(16)-Ti(1)-Cl(1)	135.20(11)
C(13)-C(14)-H(14)	119.8	C(24)-Ti(1)-Cl(1)	90.72(15)
C(15)-C(14)-H(14)	119.8	C(20)-Ti(1)-Cl(1)	108.13(13)
Cr(2)-C(14)-H(14)	129.6	C(25)-Ti(1)-Cl(1)	124.84(15)
C(14)-C(15)-C(10)	121.0(3)	C(21)-Ti(1)-Cl(1)	132.79(12)
C(14)-C(15)-Cr(2)	71.63(19)	C(23)-Ti(1)-Cl(1)	77.53(12)
C(10)-C(15)-Cr(2)	72.25(18)	C(17)-Ti(1)-Cl(1)	115.33(10)
C(14)-C(15)-H(15)	119.5	O(6)-Ti(1)-C(18)	90.49(12)
C(10)-C(15)-H(15)	119.5	C(16)-Ti(1)-C(18)	57.16(14)
Cr(2)-C(15)-H(15)	129.0	C(24)-Ti(1)-C(18)	135.39(16)
O(6)-Ti(1)-C(16)	102.34(12)	C(20)-Ti(1)-C(18)	56.72(15)
O(6)-Ti(1)-C(24)	134.12(14)	C(25)-Ti(1)-C(18)	131.00(16)
C(16)-Ti(1)-C(24)	103.88(18)	C(21)-Ti(1)-C(18)	144.51(16)
O(6)-Ti(1)-C(20)	134.39(13)	C(23)-Ti(1)-C(18)	156.64(16)
C(16)-Ti(1)-C(20)	34.81(15)	C(17)-Ti(1)-C(18)	34.00(14)
C(24)-Ti(1)-C(20)	84.43(17)	Cl(1)-Ti(1)-C(18)	82.66(11)
O(6)-Ti(1)-C(25)	120.58(16)	O(6)-Ti(1)-C(19)	124.44(13)
C(16)-Ti(1)-C(25)	78.40(16)	C(16)-Ti(1)-C(19)	57.12(15)
C(24)-Ti(1)-C(25)	34.12(18)	C(24)-Ti(1)-C(19)	101.41(16)
C(20)-Ti(1)-C(25)	75.28(16)	C(20)-Ti(1)-C(19)	33.95(16)
O(6)-Ti(1)-C(21)	87.43(14)	C(25)-Ti(1)-C(19)	105.82(18)
C(16)-Ti(1)-C(21)	88.74(16)	C(21)-Ti(1)-C(19)	135.46(19)
C(24)-Ti(1)-C(21)	56.46(17)	C(23)-Ti(1)-C(19)	127.90(16)
C(20)-Ti(1)-C(21)	101.76(18)	C(17)-Ti(1)-C(19)	56.30(14)
C(25)-Ti(1)-C(21)	33.42(16)	Cl(1)-Ti(1)-C(19)	78.69(12)
O(6)-Ti(1)-C(23)	103.82(14)	C(18)-Ti(1)-C(19)	34.01(14)
C(16)-Ti(1)-C(23)	134.34(16)	O(6)-Ti(1)-C(22)	77.64(12)
C(24)-Ti(1)-C(23)	34.21(17)	C(16)-Ti(1)-C(22)	122.50(16)
C(20)-Ti(1)-C(23)	118.46(16)	C(24)-Ti(1)-C(22)	56.54(15)
C(25)-Ti(1)-C(23)	56.10(17)	C(20)-Ti(1)-C(22)	131.21(16)
C(21)-Ti(1)-C(23)	56.07(16)	C(25)-Ti(1)-C(22)	55.95(16)
O(6)-Ti(1)-C(17)	78.27(11)	C(21)-Ti(1)-C(22)	33.97(16)
C(16)-Ti(1)-C(17)	34.19(13)	C(23)-Ti(1)-C(22)	33.59(16)
C(24)-Ti(1)-C(17)	137.59(17)	C(17)-Ti(1)-C(22)	138.11(15)
C(20)-Ti(1)-C(17)	56.67(14)	Cl(1)-Ti(1)-C(22)	101.02(13)

C(18)-Ti(1)-C(22)	167.85(14)	Ti(1)-C(20)-H(20)	119.6
C(19)-Ti(1)-C(22)	157.91(15)	C(25)-C(21)-C(22)	108.3(4)
C(17)-C(16)-C(20)	107.3(4)	C(25)-C(21)-Ti(1)	73.2(3)
C(17)-C(16)-Ti(1)	74.6(2)	C(22)-C(21)-Ti(1)	73.8(2)
C(20)-C(16)-Ti(1)	73.3(2)	C(25)-C(21)-H(21)	125.8
C(17)-C(16)-H(16)	126.3	C(22)-C(21)-H(21)	125.8
C(20)-C(16)-H(16)	126.3	Ti(1)-C(21)-H(21)	119.1
Ti(1)-C(16)-H(16)	117.8	C(23)-C(22)-C(21)	107.4(4)
C(16)-C(17)-C(18)	108.7(3)	C(23)-C(22)-Ti(1)	72.6(2)
C(16)-C(17)-Ti(1)	71.16(19)	C(21)-C(22)-Ti(1)	72.2(2)
C(18)-C(17)-Ti(1)	73.2(2)	C(23)-C(22)-H(22)	126.3
C(16)-C(17)-H(17)	125.6	C(21)-C(22)-H(22)	126.3
C(18)-C(17)-H(17)	125.6	Ti(1)-C(22)-H(22)	120.7
Ti(1)-C(17)-H(17)	121.6	C(22)-C(23)-C(24)	108.2(4)
C(17)-C(18)-C(19)	107.6(4)	C(22)-C(23)-Ti(1)	73.8(2)
C(17)-C(18)-Ti(1)	72.78(19)	C(24)-C(23)-Ti(1)	71.4(2)
C(19)-C(18)-Ti(1)	73.2(2)	C(22)-C(23)-H(23)	125.9
C(17)-C(18)-H(18)	126.2	C(24)-C(23)-H(23)	125.9
C(19)-C(18)-H(18)	126.2	Ti(1)-C(23)-H(23)	120.7
Ti(1)-C(18)-H(18)	119.7	C(25)-C(24)-C(23)	107.4(4)
C(20)-C(19)-C(18)	108.1(4)	C(25)-C(24)-Ti(1)	74.2(2)
C(20)-C(19)-Ti(1)	71.6(2)	C(23)-C(24)-Ti(1)	74.4(2)
C(18)-C(19)-Ti(1)	72.8(2)	C(25)-C(24)-H(24)	126.3
C(20)-C(19)-H(19)	126.0	C(23)-C(24)-H(24)	126.3
C(18)-C(19)-H(19)	126.0	Ti(1)-C(24)-H(24)	117.2
Ti(1)-C(19)-H(19)	121.4	C(21)-C(25)-C(24)	108.6(5)
C(19)-C(20)-C(16)	108.3(4)	C(21)-C(25)-Ti(1)	73.4(2)
C(19)-C(20)-Ti(1)	74.5(2)	C(24)-C(25)-Ti(1)	71.7(2)
C(16)-C(20)-Ti(1)	71.9(2)	C(21)-C(25)-H(25)	125.7
C(19)-C(20)-H(20)	125.8	C(24)-C(25)-H(25)	125.7
C(16)-C(20)-H(20)	125.8	Ti(1)-C(25)-H(25)	120.9

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for Complex **13**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	34(1)	35(1)	39(1)	-6(1)	-2(1)	1(1)
C(1)	44(2)	48(2)	51(2)	-17(2)	-2(2)	4(2)
O(1)	44(2)	86(2)	79(2)	-29(2)	-17(2)	9(2)
C(2)	43(2)	46(2)	41(2)	-2(2)	-4(2)	3(2)
O(2)	83(2)	45(2)	65(2)	-4(1)	-4(2)	18(2)
C(3)	44(2)	44(2)	52(2)	-6(2)	4(2)	-9(2)
O(3)	92(3)	73(2)	55(2)	1(2)	19(2)	-27(2)
C(4)	37(2)	47(2)	49(2)	-5(2)	-1(2)	0(2)
O(4)	69(2)	37(2)	92(2)	-9(1)	-6(2)	1(1)
C(5)	43(2)	42(2)	48(2)	-8(2)	-8(2)	6(2)
O(5)	62(2)	68(2)	43(2)	3(1)	3(1)	5(2)
C(6)	38(2)	26(1)	32(2)	3(1)	0(1)	-2(1)
O(6)	38(1)	33(1)	35(1)	-6(1)	-1(1)	1(1)
Cr(2)	36(1)	28(1)	34(1)	0(1)	2(1)	1(1)
C(7)	56(2)	41(2)	41(2)	0(2)	-3(2)	4(2)
O(7)	108(3)	72(2)	40(2)	-2(1)	-14(2)	7(2)
C(8)	53(2)	39(2)	48(2)	3(2)	7(2)	1(2)
O(8)	91(3)	41(2)	91(2)	7(1)	6(2)	23(2)
C(9)	51(2)	39(2)	49(2)	4(2)	0(2)	-5(2)
O(9)	53(2)	73(2)	82(2)	14(2)	7(2)	-20(2)
C(10)	38(2)	29(1)	31(2)	3(1)	2(1)	0(1)
C(11)	39(2)	45(2)	31(2)	-1(1)	2(2)	0(2)
C(12)	37(2)	57(2)	39(2)	11(2)	-4(2)	2(2)
C(13)	41(2)	44(2)	52(2)	11(2)	9(2)	15(2)
C(14)	48(2)	28(2)	49(2)	0(1)	11(2)	5(2)
C(15)	43(2)	28(1)	40(2)	-1(1)	6(2)	-1(1)
Ti(1)	37(1)	24(1)	33(1)	-2(1)	-1(1)	1(1)
Cl(1)	42(1)	54(1)	59(1)	-2(1)	7(1)	6(1)
C(16)	45(2)	56(2)	53(2)	18(2)	-10(2)	5(2)
C(17)	59(3)	34(2)	46(2)	7(2)	-3(2)	14(2)
C(18)	59(3)	41(2)	51(2)	19(2)	2(2)	-4(2)
C(19)	75(3)	67(3)	37(2)	11(2)	10(2)	21(2)
C(20)	80(3)	52(2)	46(2)	0(2)	-18(2)	1(2)
C(21)	65(3)	34(2)	94(4)	16(2)	25(3)	-3(2)
C(22)	99(4)	34(2)	48(2)	14(2)	-4(2)	-7(2)
C(23)	67(3)	28(2)	95(4)	16(2)	-1(3)	7(2)

C(24)	119(5)	26(2)	64(3)	-10(2)	10(3)	-9(2)
C(25)	85(4)	42(2)	89(4)	13(2)	-28(3)	-26(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Complex **13**.

	x	y	z	U(eq)
H(11)	8439	1398	6765	46
H(12)	9784	809	6460	53
H(13)	9831	-295	5722	55
H(14)	8518	-775	5272	50
H(15)	7154	-171	5557	44
H(16)	8702	1814	7958	61
H(17)	7803	542	7619	55
H(18)	6330	602	8144	61
H(19)	6367	1850	8877	71
H(20)	7821	2602	8759	71
H(21)	8391	2975	6860	77
H(22)	6889	3239	6408	72
H(23)	5936	3876	7220	76
H(24)	6835	3968	8175	83
H(25)	8370	3484	7926	86

Table 6. Torsion angles [°] for Complex **13**.

C(3)-Cr(1)-C(6)-O(6)	-55.0(3)	Cr(2)-C(10)-C(11)-C(12)	-53.9(3)
C(4)-Cr(1)-C(6)-O(6)	-138.5(2)	C(15)-C(10)-C(11)-Cr(2)	54.2(3)
C(2)-Cr(1)-C(6)-O(6)	38.2(3)	C(6)-C(10)-C(11)-Cr(2)	-126.8(3)
C(5)-Cr(1)-C(6)-O(6)	128.3(2)	C(7)-Cr(2)-C(11)-C(12)	112.9(5)
C(3)-Cr(1)-C(6)-C(10)	124.2(3)	C(9)-Cr(2)-C(11)-C(12)	-53.6(3)
C(4)-Cr(1)-C(6)-C(10)	40.6(3)	C(8)-Cr(2)-C(11)-C(12)	-145.1(2)
C(2)-Cr(1)-C(6)-C(10)	-142.6(3)	C(15)-Cr(2)-C(11)-C(12)	102.8(2)
C(5)-Cr(1)-C(6)-C(10)	-52.5(3)	C(14)-Cr(2)-C(11)-C(12)	65.6(2)
O(6)-C(6)-C(10)-C(15)	173.2(3)	C(13)-Cr(2)-C(11)-C(12)	29.3(2)
Cr(1)-C(6)-C(10)-C(15)	-6.0(4)	C(10)-Cr(2)-C(11)-C(12)	133.0(3)
O(6)-C(6)-C(10)-C(11)	-5.7(4)	C(7)-Cr(2)-C(11)-C(10)	-20.1(5)
Cr(1)-C(6)-C(10)-C(11)	175.1(2)	C(9)-Cr(2)-C(11)-C(10)	173.5(2)
O(6)-C(6)-C(10)-Cr(2)	-96.2(3)	C(8)-Cr(2)-C(11)-C(10)	81.9(2)
Cr(1)-C(6)-C(10)-Cr(2)	84.6(3)	C(15)-Cr(2)-C(11)-C(10)	-30.24(18)
C(7)-Cr(2)-C(10)-C(15)	41.8(3)	C(12)-Cr(2)-C(11)-C(10)	-133.0(3)
C(9)-Cr(2)-C(10)-C(15)	-141.5(3)	C(14)-Cr(2)-C(11)-C(10)	-67.4(2)
C(8)-Cr(2)-C(10)-C(15)	129.4(2)	C(13)-Cr(2)-C(11)-C(10)	-103.7(2)
C(12)-Cr(2)-C(10)-C(15)	-101.9(2)	C(10)-C(11)-C(12)-C(13)	-1.0(5)
C(14)-Cr(2)-C(10)-C(15)	-28.9(2)	Cr(2)-C(11)-C(12)-C(13)	-55.1(3)
C(11)-Cr(2)-C(10)-C(15)	-130.2(3)	C(10)-C(11)-C(12)-Cr(2)	54.1(3)
C(13)-Cr(2)-C(10)-C(15)	-65.1(2)	C(7)-Cr(2)-C(12)-C(11)	-145.7(3)
C(7)-Cr(2)-C(10)-C(11)	172.0(2)	C(9)-Cr(2)-C(12)-C(11)	130.6(2)
C(9)-Cr(2)-C(10)-C(11)	-11.4(3)	C(8)-Cr(2)-C(12)-C(11)	44.2(3)
C(8)-Cr(2)-C(10)-C(11)	-100.4(2)	C(15)-Cr(2)-C(12)-C(11)	-66.2(2)
C(15)-Cr(2)-C(10)-C(11)	130.2(3)	C(14)-Cr(2)-C(12)-C(11)	-103.2(2)
C(12)-Cr(2)-C(10)-C(11)	28.3(2)	C(13)-Cr(2)-C(12)-C(11)	-132.1(3)
C(14)-Cr(2)-C(10)-C(11)	101.2(2)	C(10)-Cr(2)-C(12)-C(11)	-29.0(2)
C(13)-Cr(2)-C(10)-C(11)	65.1(2)	C(7)-Cr(2)-C(12)-C(13)	-13.6(4)
C(7)-Cr(2)-C(10)-C(6)	-73.3(3)	C(9)-Cr(2)-C(12)-C(13)	-97.2(2)
C(9)-Cr(2)-C(10)-C(6)	103.3(4)	C(8)-Cr(2)-C(12)-C(13)	176.3(2)
C(8)-Cr(2)-C(10)-C(6)	14.3(3)	C(15)-Cr(2)-C(12)-C(13)	65.9(2)
C(15)-Cr(2)-C(10)-C(6)	-115.1(4)	C(14)-Cr(2)-C(12)-C(13)	28.9(2)
C(12)-Cr(2)-C(10)-C(6)	143.0(3)	C(11)-Cr(2)-C(12)-C(13)	132.1(3)
C(14)-Cr(2)-C(10)-C(6)	-144.1(3)	C(10)-Cr(2)-C(12)-C(13)	103.2(2)
C(11)-Cr(2)-C(10)-C(6)	114.7(4)	C(11)-C(12)-C(13)-C(14)	0.9(5)
C(13)-Cr(2)-C(10)-C(6)	179.8(3)	Cr(2)-C(12)-C(13)-C(14)	-54.1(3)
C(15)-C(10)-C(11)-C(12)	0.4(5)	C(11)-C(12)-C(13)-Cr(2)	55.1(3)
C(6)-C(10)-C(11)-C(12)	179.3(3)	C(7)-Cr(2)-C(13)-C(14)	-56.0(3)

C(9)-Cr(2)-C(13)-C(14)	-146.1(2)	C(9)-Cr(2)-C(15)-C(14)	-15.9(5)
C(8)-Cr(2)-C(13)-C(14)	122.0(5)	C(8)-Cr(2)-C(15)-C(14)	170.5(2)
C(15)-Cr(2)-C(13)-C(14)	29.1(2)	C(12)-Cr(2)-C(15)-C(14)	-65.6(2)
C(12)-Cr(2)-C(13)-C(14)	131.9(3)	C(11)-Cr(2)-C(15)-C(14)	-102.0(2)
C(11)-Cr(2)-C(13)-C(14)	103.0(2)	C(13)-Cr(2)-C(15)-C(14)	-28.6(2)
C(10)-Cr(2)-C(13)-C(14)	65.9(2)	C(10)-Cr(2)-C(15)-C(14)	-132.5(3)
C(7)-Cr(2)-C(13)-C(12)	172.1(2)	C(7)-Cr(2)-C(15)-C(10)	-146.1(2)
C(9)-Cr(2)-C(13)-C(12)	82.0(2)	C(9)-Cr(2)-C(15)-C(10)	116.6(4)
C(8)-Cr(2)-C(13)-C(12)	-9.9(6)	C(8)-Cr(2)-C(15)-C(10)	-57.0(2)
C(15)-Cr(2)-C(13)-C(12)	-102.8(2)	C(12)-Cr(2)-C(15)-C(10)	66.9(2)
C(14)-Cr(2)-C(13)-C(12)	-131.9(3)	C(14)-Cr(2)-C(15)-C(10)	132.5(3)
C(11)-Cr(2)-C(13)-C(12)	-28.9(2)	C(11)-Cr(2)-C(15)-C(10)	30.44(19)
C(10)-Cr(2)-C(13)-C(12)	-66.0(2)	C(13)-Cr(2)-C(15)-C(10)	103.9(2)
C(12)-C(13)-C(14)-C(15)	-0.2(5)	O(6)-Ti(1)-C(16)-C(17)	-46.2(2)
Cr(2)-C(13)-C(14)-C(15)	-54.1(3)	C(24)-Ti(1)-C(16)-C(17)	171.8(2)
C(12)-C(13)-C(14)-Cr(2)	53.9(3)	C(20)-Ti(1)-C(16)-C(17)	113.9(4)
C(7)-Cr(2)-C(14)-C(13)	128.6(2)	C(25)-Ti(1)-C(16)-C(17)	-165.3(3)
C(9)-Cr(2)-C(14)-C(13)	40.6(3)	C(21)-Ti(1)-C(16)-C(17)	-133.3(3)
C(8)-Cr(2)-C(14)-C(13)	-149.7(3)	C(23)-Ti(1)-C(16)-C(17)	-169.9(3)
C(15)-Cr(2)-C(14)-C(13)	-132.4(3)	Cl(1)-Ti(1)-C(16)-C(17)	66.3(3)
C(12)-Cr(2)-C(14)-C(13)	-29.4(2)	C(18)-Ti(1)-C(16)-C(17)	36.3(2)
C(11)-Cr(2)-C(14)-C(13)	-65.8(2)	C(19)-Ti(1)-C(16)-C(17)	77.0(3)
C(10)-Cr(2)-C(14)-C(13)	-103.4(2)	C(22)-Ti(1)-C(16)-C(17)	-129.3(2)
C(7)-Cr(2)-C(14)-C(15)	-99.0(2)	O(6)-Ti(1)-C(16)-C(20)	-160.0(2)
C(9)-Cr(2)-C(14)-C(15)	173.0(2)	C(24)-Ti(1)-C(16)-C(20)	58.0(3)
C(8)-Cr(2)-C(14)-C(15)	-17.3(4)	C(25)-Ti(1)-C(16)-C(20)	80.8(3)
C(12)-Cr(2)-C(14)-C(15)	103.0(2)	C(21)-Ti(1)-C(16)-C(20)	112.9(3)
C(11)-Cr(2)-C(14)-C(15)	66.6(2)	C(23)-Ti(1)-C(16)-C(20)	76.2(3)
C(13)-Cr(2)-C(14)-C(15)	132.4(3)	C(17)-Ti(1)-C(16)-C(20)	-113.9(4)
C(10)-Cr(2)-C(14)-C(15)	29.0(2)	Cl(1)-Ti(1)-C(16)-C(20)	-47.5(3)
C(13)-C(14)-C(15)-C(10)	-0.4(5)	C(18)-Ti(1)-C(16)-C(20)	-77.5(3)
Cr(2)-C(14)-C(15)-C(10)	-55.0(3)	C(19)-Ti(1)-C(16)-C(20)	-36.8(2)
C(13)-C(14)-C(15)-Cr(2)	54.5(3)	C(22)-Ti(1)-C(16)-C(20)	116.9(3)
C(11)-C(10)-C(15)-C(14)	0.4(5)	C(20)-C(16)-C(17)-C(18)	2.5(4)
C(6)-C(10)-C(15)-C(14)	-178.6(3)	Ti(1)-C(16)-C(17)-C(18)	-64.1(3)
Cr(2)-C(10)-C(15)-C(14)	54.7(3)	C(20)-C(16)-C(17)-Ti(1)	66.6(3)
C(11)-C(10)-C(15)-Cr(2)	-54.3(3)	O(6)-Ti(1)-C(17)-C(16)	134.0(2)
C(6)-C(10)-C(15)-Cr(2)	126.7(3)	C(24)-Ti(1)-C(17)-C(16)	-11.8(4)
C(7)-Cr(2)-C(15)-C(14)	81.4(2)	C(20)-Ti(1)-C(17)-C(16)	-38.7(2)

C(25)-Ti(1)-C(17)-C(16)	15.5(3)	C(22)-Ti(1)-C(18)-C(19)	170.9(7)
C(21)-Ti(1)-C(17)-C(16)	51.5(3)	C(17)-C(18)-C(19)-C(20)	1.8(4)
C(23)-Ti(1)-C(17)-C(16)	33.4(8)	Ti(1)-C(18)-C(19)-C(20)	-63.3(3)
Cl(1)-Ti(1)-C(17)-C(16)	-134.5(2)	C(17)-C(18)-C(19)-Ti(1)	65.2(2)
C(18)-Ti(1)-C(17)-C(16)	-117.2(3)	O(6)-Ti(1)-C(19)-C(20)	120.0(3)
C(19)-Ti(1)-C(17)-C(16)	-79.7(3)	C(16)-Ti(1)-C(19)-C(20)	37.8(2)
C(22)-Ti(1)-C(17)-C(16)	77.9(3)	C(24)-Ti(1)-C(19)-C(20)	-61.5(3)
O(6)-Ti(1)-C(17)-C(18)	-108.9(2)	C(25)-Ti(1)-C(19)-C(20)	-26.6(3)
C(16)-Ti(1)-C(17)-C(18)	117.2(3)	C(21)-Ti(1)-C(19)-C(20)	-8.3(4)
C(24)-Ti(1)-C(17)-C(18)	105.3(3)	C(23)-Ti(1)-C(19)-C(20)	-85.7(3)
C(20)-Ti(1)-C(17)-C(18)	78.5(3)	C(17)-Ti(1)-C(19)-C(20)	78.9(3)
C(25)-Ti(1)-C(17)-C(18)	132.7(3)	Cl(1)-Ti(1)-C(19)-C(20)	-149.9(3)
C(21)-Ti(1)-C(17)-C(18)	168.7(3)	C(18)-Ti(1)-C(19)-C(20)	116.4(4)
C(23)-Ti(1)-C(17)-C(18)	150.5(7)	C(22)-Ti(1)-C(19)-C(20)	-58.5(5)
Cl(1)-Ti(1)-C(17)-C(18)	-17.3(3)	O(6)-Ti(1)-C(19)-C(18)	3.6(3)
C(19)-Ti(1)-C(17)-C(18)	37.5(2)	C(16)-Ti(1)-C(19)-C(18)	-78.7(3)
C(22)-Ti(1)-C(17)-C(18)	-164.9(3)	C(24)-Ti(1)-C(19)-C(18)	-177.9(3)
C(16)-C(17)-C(18)-C(19)	-2.7(4)	C(20)-Ti(1)-C(19)-C(18)	-116.4(4)
Ti(1)-C(17)-C(18)-C(19)	-65.4(3)	C(25)-Ti(1)-C(19)-C(18)	-143.1(3)
C(16)-C(17)-C(18)-Ti(1)	62.7(2)	C(21)-Ti(1)-C(19)-C(18)	-124.7(3)
O(6)-Ti(1)-C(18)-C(17)	67.9(2)	C(23)-Ti(1)-C(19)-C(18)	157.9(3)
C(16)-Ti(1)-C(18)-C(17)	-36.5(2)	C(17)-Ti(1)-C(19)-C(18)	-37.5(2)
C(24)-Ti(1)-C(18)-C(17)	-112.2(3)	Cl(1)-Ti(1)-C(19)-C(18)	93.6(3)
C(20)-Ti(1)-C(18)-C(17)	-78.3(3)	C(22)-Ti(1)-C(19)-C(18)	-174.9(4)
C(25)-Ti(1)-C(18)-C(17)	-65.1(3)	C(18)-C(19)-C(20)-C(16)	-0.3(4)
C(21)-Ti(1)-C(18)-C(17)	-18.4(4)	Ti(1)-C(19)-C(20)-C(16)	-64.4(3)
C(23)-Ti(1)-C(18)-C(17)	-163.6(4)	C(18)-C(19)-C(20)-Ti(1)	64.1(3)
Cl(1)-Ti(1)-C(18)-C(17)	164.3(2)	C(17)-C(16)-C(20)-C(19)	-1.4(4)
C(19)-Ti(1)-C(18)-C(17)	-115.1(4)	Ti(1)-C(16)-C(20)-C(19)	66.1(3)
C(22)-Ti(1)-C(18)-C(17)	55.8(9)	C(17)-C(16)-C(20)-Ti(1)	-67.5(2)
O(6)-Ti(1)-C(18)-C(19)	-177.0(3)	O(6)-Ti(1)-C(20)-C(19)	-87.9(3)
C(16)-Ti(1)-C(18)-C(19)	78.5(3)	C(16)-Ti(1)-C(20)-C(19)	-115.7(4)
C(24)-Ti(1)-C(18)-C(19)	2.9(4)	C(24)-Ti(1)-C(20)-C(19)	120.1(3)
C(20)-Ti(1)-C(18)-C(19)	36.7(3)	C(25)-Ti(1)-C(20)-C(19)	153.5(3)
C(25)-Ti(1)-C(18)-C(19)	50.0(4)	C(21)-Ti(1)-C(20)-C(19)	174.1(3)
C(21)-Ti(1)-C(18)-C(19)	96.7(4)	C(23)-Ti(1)-C(20)-C(19)	116.5(3)
C(23)-Ti(1)-C(18)-C(19)	-48.6(5)	C(17)-Ti(1)-C(20)-C(19)	-77.8(3)
C(17)-Ti(1)-C(18)-C(19)	115.1(4)	Cl(1)-Ti(1)-C(20)-C(19)	31.1(3)
Cl(1)-Ti(1)-C(18)-C(19)	-80.6(3)	C(18)-Ti(1)-C(20)-C(19)	-36.8(2)

C(22)-Ti(1)-C(20)-C(19)	154.8(3)	C(21)-Ti(1)-C(22)-C(23)	-115.4(4)
O(6)-Ti(1)-C(20)-C(16)	27.8(3)	C(17)-Ti(1)-C(22)-C(23)	-163.3(3)
C(24)-Ti(1)-C(20)-C(16)	-124.2(3)	Cl(1)-Ti(1)-C(22)-C(23)	46.3(3)
C(25)-Ti(1)-C(20)-C(16)	-90.8(3)	C(18)-Ti(1)-C(22)-C(23)	152.9(7)
C(21)-Ti(1)-C(20)-C(16)	-70.2(3)	C(19)-Ti(1)-C(22)-C(23)	-40.8(6)
C(23)-Ti(1)-C(20)-C(16)	-127.8(3)	O(6)-Ti(1)-C(22)-C(21)	-104.1(3)
C(17)-Ti(1)-C(20)-C(16)	38.0(2)	C(16)-Ti(1)-C(22)-C(21)	-7.2(3)
Cl(1)-Ti(1)-C(20)-C(16)	146.8(2)	C(24)-Ti(1)-C(22)-C(21)	78.2(3)
C(18)-Ti(1)-C(20)-C(16)	78.9(3)	C(20)-Ti(1)-C(22)-C(21)	35.4(4)
C(19)-Ti(1)-C(20)-C(16)	115.7(4)	C(25)-Ti(1)-C(22)-C(21)	36.9(3)
C(22)-Ti(1)-C(20)-C(16)	-89.5(3)	C(23)-Ti(1)-C(22)-C(21)	115.4(4)
O(6)-Ti(1)-C(21)-C(25)	-173.0(3)	C(17)-Ti(1)-C(22)-C(21)	-47.9(3)
C(16)-Ti(1)-C(21)-C(25)	-70.6(3)	Cl(1)-Ti(1)-C(22)-C(21)	161.7(2)
C(24)-Ti(1)-C(21)-C(25)	37.0(3)	C(18)-Ti(1)-C(22)-C(21)	-91.7(8)
C(20)-Ti(1)-C(21)-C(25)	-38.1(3)	C(19)-Ti(1)-C(22)-C(21)	74.6(5)
C(23)-Ti(1)-C(21)-C(25)	78.4(3)	C(21)-C(22)-C(23)-C(24)	-0.8(4)
C(17)-Ti(1)-C(21)-C(25)	-96.7(3)	Ti(1)-C(22)-C(23)-C(24)	63.5(3)
Cl(1)-Ti(1)-C(21)-C(25)	90.6(3)	C(21)-C(22)-C(23)-Ti(1)	-64.3(3)
C(18)-Ti(1)-C(21)-C(25)	-85.8(4)	O(6)-Ti(1)-C(23)-C(22)	-39.8(3)
C(19)-Ti(1)-C(21)-C(25)	-33.4(4)	C(16)-Ti(1)-C(23)-C(22)	83.5(4)
C(22)-Ti(1)-C(21)-C(25)	115.5(4)	C(24)-Ti(1)-C(23)-C(22)	116.2(4)
O(6)-Ti(1)-C(21)-C(22)	71.5(3)	C(20)-Ti(1)-C(23)-C(22)	122.6(3)
C(16)-Ti(1)-C(21)-C(22)	173.9(3)	C(25)-Ti(1)-C(23)-C(22)	78.0(3)
C(24)-Ti(1)-C(21)-C(22)	-78.5(3)	C(21)-Ti(1)-C(23)-C(22)	37.5(3)
C(20)-Ti(1)-C(21)-C(22)	-153.6(3)	C(17)-Ti(1)-C(23)-C(22)	57.9(8)
C(25)-Ti(1)-C(21)-C(22)	-115.5(4)	Cl(1)-Ti(1)-C(23)-C(22)	-133.4(3)
C(23)-Ti(1)-C(21)-C(22)	-37.0(3)	C(18)-Ti(1)-C(23)-C(22)	-166.0(4)
C(17)-Ti(1)-C(21)-C(22)	147.8(2)	C(19)-Ti(1)-C(23)-C(22)	161.9(3)
Cl(1)-Ti(1)-C(21)-C(22)	-24.8(3)	O(6)-Ti(1)-C(23)-C(24)	-156.0(3)
C(18)-Ti(1)-C(21)-C(22)	158.8(3)	C(16)-Ti(1)-C(23)-C(24)	-32.8(4)
C(19)-Ti(1)-C(21)-C(22)	-148.9(3)	C(20)-Ti(1)-C(23)-C(24)	6.3(4)
C(25)-C(21)-C(22)-C(23)	-1.0(4)	C(25)-Ti(1)-C(23)-C(24)	-38.2(3)
Ti(1)-C(21)-C(22)-C(23)	64.6(3)	C(21)-Ti(1)-C(23)-C(24)	-78.8(3)
C(25)-C(21)-C(22)-Ti(1)	-65.6(3)	C(17)-Ti(1)-C(23)-C(24)	-58.4(8)
O(6)-Ti(1)-C(22)-C(23)	140.5(3)	Cl(1)-Ti(1)-C(23)-C(24)	110.4(3)
C(16)-Ti(1)-C(22)-C(23)	-122.6(3)	C(18)-Ti(1)-C(23)-C(24)	77.7(5)
C(24)-Ti(1)-C(22)-C(23)	-37.2(3)	C(19)-Ti(1)-C(23)-C(24)	45.6(4)
C(20)-Ti(1)-C(22)-C(23)	-80.0(4)	C(22)-Ti(1)-C(23)-C(24)	-116.2(4)
C(25)-Ti(1)-C(22)-C(23)	-78.5(3)	C(22)-C(23)-C(24)-C(25)	2.3(4)

Ti(1)-C(23)-C(24)-C(25)	67.4(3)	C(16)-Ti(1)-C(25)-C(24)	-137.7(3)
C(22)-C(23)-C(24)-Ti(1)	-65.1(3)	C(20)-Ti(1)-C(25)-C(24)	-102.1(3)
O(6)-Ti(1)-C(24)-C(25)	-80.3(4)	C(21)-Ti(1)-C(25)-C(24)	116.6(4)
C(16)-Ti(1)-C(24)-C(25)	42.8(3)	C(23)-Ti(1)-C(25)-C(24)	38.3(3)
C(20)-Ti(1)-C(24)-C(25)	71.9(3)	C(17)-Ti(1)-C(25)-C(24)	-146.5(3)
C(21)-Ti(1)-C(24)-C(25)	-36.2(3)	Cl(1)-Ti(1)-C(25)-C(24)	0.0(4)
C(23)-Ti(1)-C(24)-C(25)	-113.7(4)	C(18)-Ti(1)-C(25)-C(24)	-113.5(3)
C(17)-Ti(1)-C(24)-C(25)	49.6(4)	C(19)-Ti(1)-C(25)-C(24)	-87.0(3)
Cl(1)-Ti(1)-C(24)-C(25)	-180.0(3)	C(22)-Ti(1)-C(25)-C(24)	79.1(3)
C(18)-Ti(1)-C(24)-C(25)	99.8(3)		
C(19)-Ti(1)-C(24)-C(25)	101.4(3)		
C(22)-Ti(1)-C(24)-C(25)	-77.2(3)		
O(6)-Ti(1)-C(24)-C(23)	33.4(4)		
C(16)-Ti(1)-C(24)-C(23)	156.5(3)		
C(20)-Ti(1)-C(24)-C(23)	-174.4(3)		
C(25)-Ti(1)-C(24)-C(23)	113.7(4)		
C(21)-Ti(1)-C(24)-C(23)	77.5(3)		
C(17)-Ti(1)-C(24)-C(23)	163.3(3)		
Cl(1)-Ti(1)-C(24)-C(23)	-66.3(3)		
C(18)-Ti(1)-C(24)-C(23)	-146.5(3)		
C(19)-Ti(1)-C(24)-C(23)	-144.9(3)		
C(22)-Ti(1)-C(24)-C(23)	36.5(3)		
C(22)-C(21)-C(25)-C(24)	2.4(5)		
Ti(1)-C(21)-C(25)-C(24)	-63.6(3)		
C(22)-C(21)-C(25)-Ti(1)	66.0(3)		
C(23)-C(24)-C(25)-C(21)	-2.9(5)		
Ti(1)-C(24)-C(25)-C(21)	64.7(3)		
C(23)-C(24)-C(25)-Ti(1)	-67.6(3)		
O(6)-Ti(1)-C(25)-C(21)	8.1(4)		
C(16)-Ti(1)-C(25)-C(21)	105.7(3)		
C(24)-Ti(1)-C(25)-C(21)	-116.6(4)		
C(20)-Ti(1)-C(25)-C(21)	141.3(3)		
C(23)-Ti(1)-C(25)-C(21)	-78.3(3)		
C(17)-Ti(1)-C(25)-C(21)	96.9(3)		
Cl(1)-Ti(1)-C(25)-C(21)	-116.6(3)		
C(18)-Ti(1)-C(25)-C(21)	129.9(3)		
C(19)-Ti(1)-C(25)-C(21)	156.3(3)		
C(22)-Ti(1)-C(25)-C(21)	-37.5(3)		
O(6)-Ti(1)-C(25)-C(24)	124.7(3)		

Appendix 7

Crystallographic data of Complex 23

Table 1. Crystal data and structure refinement for Complex **23**.

Identification code	db78a1_pn	
Empirical formula	C_{30} H_{28} Fe Mn_2 O_6	
Formula weight	650.25	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P n	
Unit cell dimensions	a = 11.9498(11) Å	a= 90°.
	b = 9.7620(9) Å	b= 115.7030(10)°.
	c = 12.9245(12) Å	g = 90°.
Volume	1358.5(2) $Å^3$	
Z	2	
Density (calculated)	1.590 Mg/m^3	
Absorption coefficient	1.485 mm^{-1}	
F(000)	664	
Crystal size	0.36 x 0.30 x 0.015 mm^3	
Theta range for data collection	2.72 to 26.44°.	
Index ranges	-14<=h<=12, -11<=k<=12, -15<=l<=12	
Reflections collected	6873	
Independent reflections	3294 [R(int) = 0.0264]	
Completeness to theta = 25.00°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.978 and 0.590	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3294 / 2 / 371	
Goodness-of-fit on F^2	1.066	
Final R indices [I>2σ(I)]	R1 = 0.0317, wR2 = 0.0779	
R indices (all data)	R1 = 0.0384, wR2 = 0.0829	
Absolute structure parameter	0.53(3)	
Extinction coefficient	0	
Largest diff. peak and hole	0.295 and -0.303 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Complex **23**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mn(1)	5227(1)	8821(1)	5965(1)	53(1)
C(1)	6903(4)	8781(4)	6121(4)	45(1)
O(1)	7873(3)	8115(3)	6922(3)	61(1)
C(2)	4513(5)	8856(6)	4465(5)	66(1)
O(2)	3938(4)	8823(5)	3462(4)	96(2)
C(3)	5063(5)	7017(6)	5903(5)	68(1)
O(3)	4902(5)	5838(4)	5804(5)	96(1)
C(4)	5826(5)	10283(6)	7336(5)	75(2)
C(5)	5260(7)	9185(6)	7634(6)	76(2)
C(6)	4051(6)	9127(6)	6791(6)	75(2)
C(7)	3837(5)	10146(6)	5995(5)	73(2)
C(8)	4954(7)	10898(6)	6326(6)	79(2)
Mn(2)	10481(1)	5899(1)	4946(1)	53(1)
C(9)	8777(4)	6120(4)	4655(4)	44(1)
O(9)	8129(3)	5430(3)	5109(3)	59(1)
C(10)	11087(5)	5953(4)	6457(5)	60(1)
O(10)	11548(5)	6037(4)	7441(4)	90(1)
C(11)	10750(4)	7673(5)	4961(5)	59(1)
O(11)	11027(4)	8823(4)	5005(4)	83(1)
C(12)	9906(6)	4317(10)	3685(8)	106(3)
C(13)	10814(8)	3777(7)	4697(8)	94(2)
C(14)	11893(6)	4527(8)	4960(7)	96(2)
C(15)	11654(7)	5499(9)	4120(8)	100(2)
C(16)	10435(8)	5373(9)	3333(6)	96(2)
Fe(1)	7442(1)	8953(1)	3976(1)	39(1)
C(17)	7391(4)	9586(4)	5469(4)	46(1)
C(18)	6708(5)	10490(4)	4527(5)	61(1)
C(19)	7521(7)	11047(5)	4124(6)	69(2)
C(20)	8694(5)	10494(5)	4754(5)	59(1)
C(21)	8636(5)	9600(5)	5580(4)	47(1)
C(22)	7860(4)	6956(4)	3767(4)	41(1)
C(23)	6575(4)	7113(4)	3497(4)	41(1)

C(24)	6014(4)	8063(5)	2588(4)	48(1)
C(25)	6939(5)	8517(6)	2281(4)	55(1)
C(26)	8066(4)	7870(4)	2984(3)	48(1)
C(27)	7767(5)	7230(6)	7766(5)	74(2)
C(28)	9007(6)	6717(7)	8505(5)	87(2)
C(29)	8679(6)	4346(6)	5944(6)	75(2)
C(30)	7646(7)	3737(6)	6144(7)	83(2)
Fe(2)	8285(6)	5994(5)	6802(5)	25(1)
C(31)	9720(40)	6870(40)	8200(30)	25(1)
C(32)	9190(40)	7810(40)	7260(30)	25(1)
C(33)	6940(40)	4480(40)	6010(30)	25(1)
C(34)	7030(40)	5340(40)	5140(30)	25(1)

Table 3. Bond lengths [Å] and angles [°] for Complex **23**.

Mn(1)-C(2)	1.747(5)	C(9)-C(22)	1.446(6)
Mn(1)-C(3)	1.770(6)	O(9)-C(34)	1.33(4)
Mn(1)-C(1)	1.924(5)	O(9)-C(29)	1.450(6)
Mn(1)-C(7)	2.118(5)	O(9)-Fe(2)	2.184(7)
Mn(1)-C(6)	2.122(5)	C(10)-O(10)	1.149(7)
Mn(1)-C(8)	2.137(5)	C(11)-O(11)	1.164(6)
Mn(1)-C(4)	2.142(5)	C(12)-C(16)	1.386(11)
Mn(1)-C(5)	2.170(6)	C(12)-C(13)	1.391(12)
C(1)-O(1)	1.340(5)	C(12)-H(12)	0.9300
C(1)-C(17)	1.447(6)	C(13)-C(14)	1.390(10)
O(1)-C(27)	1.439(5)	C(13)-H(13)	0.9300
O(1)-C(32)	1.46(4)	C(14)-C(15)	1.375(10)
O(1)-Fe(2)	2.149(6)	C(14)-H(14)	0.9300
C(2)-O(2)	1.175(7)	C(15)-C(16)	1.374(10)
C(3)-O(3)	1.165(6)	C(15)-H(15)	0.9300
C(4)-C(8)	1.403(9)	C(16)-H(16)	0.9300
C(4)-C(5)	1.407(8)	Fe(1)-C(18)	2.018(4)
C(4)-H(4)	0.9300	Fe(1)-C(23)	2.031(4)
C(5)-C(6)	1.383(9)	Fe(1)-C(26)	2.037(4)
C(5)-H(5)	0.9300	Fe(1)-C(21)	2.041(5)
C(6)-C(7)	1.373(8)	Fe(1)-C(25)	2.049(5)
C(6)-H(6)	0.9300	Fe(1)-C(20)	2.052(5)
C(7)-C(8)	1.417(8)	Fe(1)-C(19)	2.052(5)
C(7)-H(7)	0.9300	Fe(1)-C(17)	2.052(4)
C(8)-H(8)	0.9300	Fe(1)-C(24)	2.057(5)
Mn(2)-C(11)	1.761(5)	Fe(1)-C(22)	2.059(4)
Mn(2)-C(10)	1.764(6)	C(17)-C(21)	1.432(6)
Mn(2)-C(9)	1.916(5)	C(17)-C(18)	1.437(7)
Mn(2)-C(16)	2.125(6)	C(18)-C(19)	1.396(8)
Mn(2)-C(12)	2.131(6)	C(18)-H(18)	0.9300
Mn(2)-C(15)	2.134(6)	C(19)-C(20)	1.389(9)
Mn(2)-C(14)	2.149(6)	C(19)-H(19)	0.9300
Mn(2)-C(13)	2.159(6)	C(20)-C(21)	1.403(7)
C(9)-O(9)	1.338(5)	C(20)-H(20)	0.9300

C(21)-H(21)	0.9300
C(22)-C(23)	1.427(6)
C(22)-C(26)	1.449(6)
C(23)-C(24)	1.416(6)
C(23)-H(23)	0.9300
C(24)-C(25)	1.399(7)
C(24)-H(24)	0.9300
C(25)-C(26)	1.406(6)
C(25)-H(25)	0.9300
C(26)-H(26)	0.9300
C(27)-C(28)	1.460(8)
C(27)-H(27A)	0.9700
C(27)-H(27B)	0.9700
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600
C(29)-C(30)	1.489(8)
C(29)-H(29A)	0.9700
C(29)-H(29B)	0.9700
C(30)-H(30A)	0.9600
C(30)-H(30B)	0.9600
C(30)-H(30C)	0.9600
Fe(2)-C(32)	2.03(4)
Fe(2)-C(31)	2.06(4)
Fe(2)-C(33)	2.09(4)
Fe(2)-C(34)	2.11(4)
C(31)-C(32)	1.43(5)
C(33)-C(34)	1.44(5)

C(2)-Mn(1)-C(3)	88.8(3)
C(2)-Mn(1)-C(1)	95.8(2)
C(3)-Mn(1)-C(1)	94.2(2)
C(2)-Mn(1)-C(7)	90.0(2)
C(3)-Mn(1)-C(7)	122.4(3)
C(1)-Mn(1)-C(7)	143.0(2)
C(2)-Mn(1)-C(6)	116.4(3)
C(3)-Mn(1)-C(6)	94.5(3)
C(1)-Mn(1)-C(6)	146.7(2)
C(7)-Mn(1)-C(6)	37.8(2)
C(2)-Mn(1)-C(8)	100.2(3)
C(3)-Mn(1)-C(8)	158.3(3)
C(1)-Mn(1)-C(8)	104.3(2)
C(7)-Mn(1)-C(8)	38.9(2)
C(6)-Mn(1)-C(8)	63.9(2)
C(2)-Mn(1)-C(4)	137.1(3)
C(3)-Mn(1)-C(4)	133.7(3)
C(1)-Mn(1)-C(4)	88.15(19)
C(7)-Mn(1)-C(4)	64.0(2)
C(6)-Mn(1)-C(4)	63.1(2)
C(8)-Mn(1)-C(4)	38.3(2)
C(2)-Mn(1)-C(5)	152.9(3)
C(3)-Mn(1)-C(5)	99.3(3)
C(1)-Mn(1)-C(5)	109.2(2)
C(7)-Mn(1)-C(5)	63.8(2)
C(6)-Mn(1)-C(5)	37.6(2)
C(8)-Mn(1)-C(5)	64.3(2)
C(4)-Mn(1)-C(5)	38.1(2)
O(1)-C(1)-C(17)	106.3(4)
O(1)-C(1)-Mn(1)	127.1(3)
C(17)-C(1)-Mn(1)	126.3(3)
C(1)-O(1)-C(27)	123.1(4)
C(1)-O(1)-C(32)	141.8(14)
C(27)-O(1)-C(32)	94.8(14)
C(1)-O(1)-Fe(2)	124.0(3)
C(27)-O(1)-Fe(2)	64.8(3)
C(32)-O(1)-Fe(2)	65.1(14)
O(2)-C(2)-Mn(1)	173.6(5)
O(3)-C(3)-Mn(1)	176.3(6)
C(8)-C(4)-C(5)	109.3(6)
C(8)-C(4)-Mn(1)	70.7(3)
C(5)-C(4)-Mn(1)	72.0(3)
C(8)-C(4)-H(4)	125.4

C(5)-C(4)-H(4)	125.4	C(11)-Mn(2)-C(15)	91.6(3)
Mn(1)-C(4)-H(4)	123.5	C(10)-Mn(2)-C(15)	121.0(3)
C(6)-C(5)-C(4)	106.1(6)	C(9)-Mn(2)-C(15)	142.7(3)
C(6)-C(5)-Mn(1)	69.3(3)	C(16)-Mn(2)-C(15)	37.6(3)
C(4)-C(5)-Mn(1)	69.9(3)	C(12)-Mn(2)-C(15)	63.2(3)
C(6)-C(5)-H(5)	127.0	C(11)-Mn(2)-C(14)	118.3(3)
C(4)-C(5)-H(5)	127.0	C(10)-Mn(2)-C(14)	93.7(3)
Mn(1)-C(5)-H(5)	125.4	C(9)-Mn(2)-C(14)	146.7(3)
C(7)-C(6)-C(5)	110.6(6)	C(16)-Mn(2)-C(14)	62.8(3)
C(7)-C(6)-Mn(1)	71.0(3)	C(12)-Mn(2)-C(14)	63.0(3)
C(5)-C(6)-Mn(1)	73.1(3)	C(15)-Mn(2)-C(14)	37.5(3)
C(7)-C(6)-H(6)	124.7	C(11)-Mn(2)-C(13)	154.2(3)
C(5)-C(6)-H(6)	124.7	C(10)-Mn(2)-C(13)	100.3(3)
Mn(1)-C(6)-H(6)	122.8	C(9)-Mn(2)-C(13)	109.2(3)
C(6)-C(7)-C(8)	107.7(6)	C(16)-Mn(2)-C(13)	63.3(3)
C(6)-C(7)-Mn(1)	71.3(3)	C(12)-Mn(2)-C(13)	37.8(3)
C(8)-C(7)-Mn(1)	71.3(3)	C(15)-Mn(2)-C(13)	63.0(3)
C(6)-C(7)-H(7)	126.2	C(14)-Mn(2)-C(13)	37.6(3)
C(8)-C(7)-H(7)	126.2	O(9)-C(9)-C(22)	104.4(4)
Mn(1)-C(7)-H(7)	123.0	O(9)-C(9)-Mn(2)	128.7(3)
C(4)-C(8)-C(7)	106.4(6)	C(22)-C(9)-Mn(2)	126.4(3)
C(4)-C(8)-Mn(1)	71.1(3)	C(34)-O(9)-C(9)	144.1(16)
C(7)-C(8)-Mn(1)	69.9(3)	C(34)-O(9)-C(29)	93.7(16)
C(4)-C(8)-H(8)	126.8	C(9)-O(9)-C(29)	122.1(4)
C(7)-C(8)-H(8)	126.8	C(34)-O(9)-Fe(2)	69.0(16)
Mn(1)-C(8)-H(8)	123.9	C(9)-O(9)-Fe(2)	119.9(3)
C(11)-Mn(2)-C(10)	88.5(2)	C(29)-O(9)-Fe(2)	67.9(3)
C(11)-Mn(2)-C(9)	93.73(19)	O(10)-C(10)-Mn(2)	175.4(6)
C(10)-Mn(2)-C(9)	96.0(2)	O(11)-C(11)-Mn(2)	174.7(4)
C(11)-Mn(2)-C(16)	100.1(3)	C(16)-C(12)-C(13)	108.0(7)
C(10)-Mn(2)-C(16)	156.4(3)	C(16)-C(12)-Mn(2)	70.8(4)
C(9)-Mn(2)-C(16)	105.2(3)	C(13)-C(12)-Mn(2)	72.2(4)
C(11)-Mn(2)-C(12)	135.9(4)	C(16)-C(12)-H(12)	126.0
C(10)-Mn(2)-C(12)	135.2(4)	C(13)-C(12)-H(12)	126.0
C(9)-Mn(2)-C(12)	88.2(2)	Mn(2)-C(12)-H(12)	122.7
C(16)-Mn(2)-C(12)	38.0(3)	C(14)-C(13)-C(12)	107.0(8)

C(14)-C(13)-Mn(2)	70.8(4)	C(21)-Fe(1)-C(20)	40.1(2)
C(12)-C(13)-Mn(2)	70.0(4)	C(25)-Fe(1)-C(20)	119.3(2)
C(14)-C(13)-H(13)	126.5	C(18)-Fe(1)-C(19)	40.1(2)
C(12)-C(13)-H(13)	126.5	C(23)-Fe(1)-C(19)	155.0(2)
Mn(2)-C(13)-H(13)	124.4	C(26)-Fe(1)-C(19)	124.1(2)
C(15)-C(14)-C(13)	108.5(7)	C(21)-Fe(1)-C(19)	67.2(2)
C(15)-C(14)-Mn(2)	70.7(4)	C(25)-Fe(1)-C(19)	106.7(2)
C(13)-C(14)-Mn(2)	71.6(4)	C(20)-Fe(1)-C(19)	39.6(3)
C(15)-C(14)-H(14)	125.7	C(18)-Fe(1)-C(17)	41.34(19)
C(13)-C(14)-H(14)	125.7	C(23)-Fe(1)-C(17)	109.52(17)
Mn(2)-C(14)-H(14)	123.6	C(26)-Fe(1)-C(17)	156.46(18)
C(16)-C(15)-C(14)	108.3(7)	C(21)-Fe(1)-C(17)	40.95(17)
C(16)-C(15)-Mn(2)	70.8(3)	C(25)-Fe(1)-C(17)	162.4(2)
C(14)-C(15)-Mn(2)	71.8(4)	C(20)-Fe(1)-C(17)	68.3(2)
C(16)-C(15)-H(15)	125.9	C(19)-Fe(1)-C(17)	68.3(2)
C(14)-C(15)-H(15)	125.9	C(18)-Fe(1)-C(24)	107.4(2)
Mn(2)-C(15)-H(15)	123.1	C(23)-Fe(1)-C(24)	40.53(18)
C(15)-C(16)-C(12)	108.1(7)	C(26)-Fe(1)-C(24)	67.87(18)
C(15)-C(16)-Mn(2)	71.6(4)	C(21)-Fe(1)-C(24)	165.19(19)
C(12)-C(16)-Mn(2)	71.2(4)	C(25)-Fe(1)-C(24)	39.8(2)
C(15)-C(16)-H(16)	125.9	C(20)-Fe(1)-C(24)	152.9(2)
C(12)-C(16)-H(16)	125.9	C(19)-Fe(1)-C(24)	119.3(3)
Mn(2)-C(16)-H(16)	123.0	C(17)-Fe(1)-C(24)	126.57(19)
C(18)-Fe(1)-C(23)	121.5(2)	C(18)-Fe(1)-C(22)	156.61(18)
C(18)-Fe(1)-C(26)	160.45(18)	C(23)-Fe(1)-C(22)	40.85(16)
C(23)-Fe(1)-C(26)	68.08(17)	C(26)-Fe(1)-C(22)	41.42(16)
C(18)-Fe(1)-C(21)	68.3(2)	C(21)-Fe(1)-C(22)	108.89(18)
C(23)-Fe(1)-C(21)	128.54(19)	C(25)-Fe(1)-C(22)	68.81(19)
C(26)-Fe(1)-C(21)	120.96(18)	C(20)-Fe(1)-C(22)	126.3(2)
C(18)-Fe(1)-C(25)	124.1(2)	C(19)-Fe(1)-C(22)	162.1(2)
C(23)-Fe(1)-C(25)	67.4(2)	C(17)-Fe(1)-C(22)	121.09(18)
C(26)-Fe(1)-C(25)	40.25(18)	C(24)-Fe(1)-C(22)	69.04(18)
C(21)-Fe(1)-C(25)	154.36(19)	C(21)-C(17)-C(18)	105.2(4)
C(18)-Fe(1)-C(20)	67.5(2)	C(21)-C(17)-C(1)	127.7(4)
C(23)-Fe(1)-C(20)	164.8(2)	C(18)-C(17)-C(1)	127.1(4)
C(26)-Fe(1)-C(20)	107.5(2)	C(21)-C(17)-Fe(1)	69.1(2)

C(18)-C(17)-Fe(1)	68.0(2)	C(22)-C(23)-H(23)	124.9
C(1)-C(17)-Fe(1)	124.6(3)	Fe(1)-C(23)-H(23)	125.4
C(19)-C(18)-C(17)	108.9(5)	C(25)-C(24)-C(23)	107.1(4)
C(19)-C(18)-Fe(1)	71.3(3)	C(25)-C(24)-Fe(1)	69.8(3)
C(17)-C(18)-Fe(1)	70.6(2)	C(23)-C(24)-Fe(1)	68.8(3)
C(19)-C(18)-H(18)	125.5	C(25)-C(24)-H(24)	126.4
C(17)-C(18)-H(18)	125.5	C(23)-C(24)-H(24)	126.4
Fe(1)-C(18)-H(18)	124.2	Fe(1)-C(24)-H(24)	126.5
C(20)-C(19)-C(18)	108.6(5)	C(24)-C(25)-C(26)	109.1(4)
C(20)-C(19)-Fe(1)	70.2(3)	C(24)-C(25)-Fe(1)	70.4(3)
C(18)-C(19)-Fe(1)	68.6(3)	C(26)-C(25)-Fe(1)	69.4(2)
C(20)-C(19)-H(19)	125.7	C(24)-C(25)-H(25)	125.4
C(18)-C(19)-H(19)	125.7	C(26)-C(25)-H(25)	125.4
Fe(1)-C(19)-H(19)	127.0	Fe(1)-C(25)-H(25)	126.4
C(19)-C(20)-C(21)	108.5(5)	C(25)-C(26)-C(22)	108.8(4)
C(19)-C(20)-Fe(1)	70.2(3)	C(25)-C(26)-Fe(1)	70.3(2)
C(21)-C(20)-Fe(1)	69.5(3)	C(22)-C(26)-Fe(1)	70.1(2)
C(19)-C(20)-H(20)	125.8	C(25)-C(26)-H(26)	125.6
C(21)-C(20)-H(20)	125.8	C(22)-C(26)-H(26)	125.6
Fe(1)-C(20)-H(20)	126.1	Fe(1)-C(26)-H(26)	125.5
C(20)-C(21)-C(17)	108.8(5)	O(1)-C(27)-C(28)	107.7(5)
C(20)-C(21)-Fe(1)	70.4(3)	O(1)-C(27)-H(27A)	110.2
C(17)-C(21)-Fe(1)	69.9(3)	C(28)-C(27)-H(27A)	110.2
C(20)-C(21)-H(21)	125.6	O(1)-C(27)-H(27B)	110.2
C(17)-C(21)-H(21)	125.6	C(28)-C(27)-H(27B)	110.2
Fe(1)-C(21)-H(21)	125.7	H(27A)-C(27)-H(27B)	108.5
C(23)-C(22)-C(9)	128.2(4)	C(27)-C(28)-H(28A)	109.5
C(23)-C(22)-C(26)	104.7(4)	C(27)-C(28)-H(28B)	109.5
C(9)-C(22)-C(26)	127.0(4)	H(28A)-C(28)-H(28B)	109.5
C(23)-C(22)-Fe(1)	68.5(2)	C(27)-C(28)-H(28C)	109.5
C(9)-C(22)-Fe(1)	125.0(3)	H(28A)-C(28)-H(28C)	109.5
C(26)-C(22)-Fe(1)	68.5(2)	H(28B)-C(28)-H(28C)	109.5
C(24)-C(23)-C(22)	110.2(4)	O(9)-C(29)-C(30)	106.1(5)
C(24)-C(23)-Fe(1)	70.7(3)	O(9)-C(29)-H(29A)	110.5
C(22)-C(23)-Fe(1)	70.6(2)	C(30)-C(29)-H(29A)	110.5
C(24)-C(23)-H(23)	124.9	C(34)-C(29)-H(29A)	119.5

O(9)-C(29)-H(29B)	110.5	H(30A)-C(30)-H(30B)	109.5
C(30)-C(29)-H(29B)	110.5	C(29)-C(30)-H(30C)	109.5
H(29A)-C(29)-H(29B)	108.7	H(30A)-C(30)-H(30C)	109.5
C(29)-C(30)-H(30A)	109.5	H(30B)-C(30)-H(30C)	109.5
C(29)-C(30)-H(30B)	109.5		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for Complex **23**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn(1)	40(1)	71(1)	50(1)	-11(1)	22(1)	0(1)
C(1)	47(3)	50(2)	40(2)	-4(2)	22(2)	3(2)
O(1)	48(2)	80(2)	58(2)	11(2)	27(2)	4(2)
C(2)	43(3)	95(4)	55(3)	-8(3)	18(3)	14(2)
O(2)	56(3)	160(5)	59(3)	-5(2)	12(2)	18(2)
C(3)	53(3)	92(4)	61(3)	-12(3)	26(2)	-6(3)
O(3)	97(4)	79(3)	99(3)	-21(2)	31(3)	-25(2)
C(4)	58(3)	99(4)	78(4)	-41(3)	38(3)	-7(3)
C(5)	82(5)	95(4)	69(4)	-12(3)	49(4)	-1(3)
C(6)	59(4)	100(4)	81(4)	-8(3)	44(3)	0(3)
C(7)	55(3)	100(4)	70(4)	-13(3)	34(3)	15(3)
C(8)	89(5)	74(4)	95(5)	-10(3)	59(4)	7(3)
Mn(2)	38(1)	60(1)	57(1)	-8(1)	17(1)	5(1)
C(9)	48(3)	40(2)	47(2)	-8(2)	23(2)	-2(2)
O(9)	55(2)	54(2)	72(2)	13(2)	32(2)	5(2)
C(10)	50(3)	50(3)	64(4)	-6(2)	12(3)	4(2)
O(10)	91(3)	85(3)	61(3)	-1(2)	4(2)	-7(2)
C(11)	35(3)	70(3)	64(3)	-5(3)	14(2)	-5(2)
O(11)	60(3)	73(2)	104(3)	3(2)	23(3)	-17(2)
C(12)	62(4)	122(6)	123(6)	-81(5)	30(4)	-3(4)
C(13)	106(6)	75(4)	111(6)	-12(4)	58(5)	22(4)
C(14)	55(4)	117(5)	102(5)	-24(5)	22(3)	32(4)
C(15)	81(5)	123(6)	123(6)	-24(5)	69(5)	6(4)
C(16)	106(6)	124(6)	64(4)	-12(4)	41(4)	37(5)
Fe(1)	39(1)	38(1)	41(1)	2(1)	19(1)	-1(1)
C(17)	47(3)	42(2)	54(3)	-10(2)	27(2)	-4(2)
C(18)	76(3)	43(2)	84(4)	5(2)	53(3)	10(2)
C(19)	99(5)	42(2)	79(4)	8(2)	52(4)	5(3)
C(20)	62(3)	49(3)	69(3)	-8(2)	33(3)	-21(3)
C(21)	49(3)	47(2)	46(2)	-9(2)	21(2)	-5(2)
C(22)	33(2)	39(2)	46(2)	-7(2)	13(2)	-1(2)
C(23)	39(2)	39(2)	46(2)	-3(2)	18(2)	-7(2)

C(24)	36(2)	54(3)	48(3)	-1(2)	12(2)	0(2)
C(25)	52(3)	74(3)	34(2)	7(2)	15(2)	5(2)
C(26)	48(3)	57(2)	41(2)	-2(2)	22(2)	-2(2)
C(27)	61(3)	86(4)	73(3)	27(3)	28(3)	10(3)
C(28)	64(4)	106(5)	71(4)	23(3)	12(3)	-3(3)
C(29)	74(4)	63(3)	91(4)	30(3)	38(3)	13(3)
C(30)	88(5)	65(3)	105(5)	22(3)	51(4)	0(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Complex **23**.

	x	y	z	U(eq)
H(4)	6647	10558	7743	90
H(5)	5626	8614	8270	91
H(6)	3464	8486	6766	90
H(7)	3093	10313	5353	87
H(8)	5084	11649	5950	95
H(12)	9087	4021	3311	127
H(13)	10718	3052	5119	112
H(14)	12649	4393	5596	115
H(15)	12221	6133	4091	120
H(16)	10034	5905	2677	115
H(18)	5863	10674	4234	74
H(19)	7312	11682	3533	83
H(20)	9399	10684	4647	70
H(21)	9298	9099	6111	56
H(23)	6165	6657	3864	50
H(24)	5186	8334	2258	58
H(25)	6827	9146	1704	66
H(26)	8820	8006	2951	57
H(27A)	7213	6473	7391	88
H(27B)	7434	7733	8217	88
H(28A)	8953	6057	9032	130
H(28B)	9526	7465	8926	130
H(28C)	9357	6292	8042	130
H(29A)	9313	4712	6654	91
H(29B)	9054	3660	5650	91
H(30A)	7927	2907	6579	125
H(30B)	6960	3537	5419	125
H(30C)	7386	4375	6562	125

Table 6. Torsion angles [°] for Complex **23**.

C(2)-Mn(1)-C(1)-O(1)	-144.7(4)	C(2)-Mn(1)-C(4)-C(8)	19.5(5)
C(3)-Mn(1)-C(1)-O(1)	-55.5(4)	C(3)-Mn(1)-C(4)-C(8)	-149.8(4)
C(7)-Mn(1)-C(1)-O(1)	117.6(4)	C(1)-Mn(1)-C(4)-C(8)	116.1(4)
C(6)-Mn(1)-C(1)-O(1)	49.3(6)	C(7)-Mn(1)-C(4)-C(8)	-38.8(4)
C(8)-Mn(1)-C(1)-O(1)	113.2(4)	C(6)-Mn(1)-C(4)-C(8)	-81.2(4)
C(4)-Mn(1)-C(1)-O(1)	78.2(4)	C(5)-Mn(1)-C(4)-C(8)	-118.8(5)
C(5)-Mn(1)-C(1)-O(1)	45.9(4)	C(2)-Mn(1)-C(4)-C(5)	138.3(4)
C(2)-Mn(1)-C(1)-C(17)	42.6(4)	C(3)-Mn(1)-C(4)-C(5)	-31.0(5)
C(3)-Mn(1)-C(1)-C(17)	131.8(4)	C(1)-Mn(1)-C(4)-C(5)	-125.1(4)
C(7)-Mn(1)-C(1)-C(17)	-55.2(5)	C(7)-Mn(1)-C(4)-C(5)	80.0(4)
C(6)-Mn(1)-C(1)-C(17)	-123.4(4)	C(6)-Mn(1)-C(4)-C(5)	37.6(4)
C(8)-Mn(1)-C(1)-C(17)	-59.5(4)	C(8)-Mn(1)-C(4)-C(5)	118.8(5)
C(4)-Mn(1)-C(1)-C(17)	-94.6(4)	C(8)-C(4)-C(5)-C(6)	0.9(6)
C(5)-Mn(1)-C(1)-C(17)	-126.9(4)	Mn(1)-C(4)-C(5)-C(6)	-60.2(4)
C(17)-C(1)-O(1)-C(27)	178.3(4)	C(8)-C(4)-C(5)-Mn(1)	61.2(4)
Mn(1)-C(1)-O(1)-C(27)	4.4(6)	C(2)-Mn(1)-C(5)-C(6)	20.5(7)
C(17)-C(1)-O(1)-C(32)	-10(2)	C(3)-Mn(1)-C(5)-C(6)	-85.3(4)
Mn(1)-C(1)-O(1)-C(32)	176(2)	C(1)-Mn(1)-C(5)-C(6)	176.9(4)
C(17)-C(1)-O(1)-Fe(2)	-101.7(4)	C(7)-Mn(1)-C(5)-C(6)	36.4(4)
Mn(1)-C(1)-O(1)-Fe(2)	84.4(4)	C(8)-Mn(1)-C(5)-C(6)	79.9(4)
C(3)-Mn(1)-C(2)-O(2)	60(4)	C(4)-Mn(1)-C(5)-C(6)	116.9(6)
C(1)-Mn(1)-C(2)-O(2)	154(4)	C(2)-Mn(1)-C(5)-C(4)	-96.5(6)
C(7)-Mn(1)-C(2)-O(2)	-63(4)	C(3)-Mn(1)-C(5)-C(4)	157.8(4)
C(6)-Mn(1)-C(2)-O(2)	-35(4)	C(1)-Mn(1)-C(5)-C(4)	60.0(4)
C(8)-Mn(1)-C(2)-O(2)	-100(4)	C(7)-Mn(1)-C(5)-C(4)	-80.5(4)
C(4)-Mn(1)-C(2)-O(2)	-112(4)	C(6)-Mn(1)-C(5)-C(4)	-116.9(6)
C(5)-Mn(1)-C(2)-O(2)	-48(5)	C(8)-Mn(1)-C(5)-C(4)	-37.1(4)
C(2)-Mn(1)-C(3)-O(3)	-25(9)	C(4)-C(5)-C(6)-C(7)	-0.8(6)
C(1)-Mn(1)-C(3)-O(3)	-120(9)	Mn(1)-C(5)-C(6)-C(7)	-61.4(4)
C(7)-Mn(1)-C(3)-O(3)	65(9)	C(4)-C(5)-C(6)-Mn(1)	60.6(4)
C(6)-Mn(1)-C(3)-O(3)	92(9)	C(2)-Mn(1)-C(6)-C(7)	-50.1(4)
C(8)-Mn(1)-C(3)-O(3)	91(9)	C(3)-Mn(1)-C(6)-C(7)	-141.0(4)
C(4)-Mn(1)-C(3)-O(3)	148(8)	C(1)-Mn(1)-C(6)-C(7)	114.3(5)
C(5)-Mn(1)-C(3)-O(3)	129(9)	C(8)-Mn(1)-C(6)-C(7)	38.5(4)

C(4)-Mn(1)-C(6)-C(7)	81.5(4)	C(3)-Mn(1)-C(8)-C(7)	-36.1(10)
C(5)-Mn(1)-C(6)-C(7)	119.6(6)	C(1)-Mn(1)-C(8)-C(7)	175.8(4)
C(2)-Mn(1)-C(6)-C(5)	-169.7(4)	C(6)-Mn(1)-C(8)-C(7)	-37.5(4)
C(3)-Mn(1)-C(6)-C(5)	99.4(4)	C(4)-Mn(1)-C(8)-C(7)	-116.3(5)
C(1)-Mn(1)-C(6)-C(5)	-5.3(6)	C(5)-Mn(1)-C(8)-C(7)	-79.4(4)
C(7)-Mn(1)-C(6)-C(5)	-119.6(6)	C(11)-Mn(2)-C(9)-O(9)	-139.0(4)
C(8)-Mn(1)-C(6)-C(5)	-81.1(4)	C(10)-Mn(2)-C(9)-O(9)	-50.1(4)
C(4)-Mn(1)-C(6)-C(5)	-38.1(4)	C(16)-Mn(2)-C(9)-O(9)	119.5(5)
C(5)-C(6)-C(7)-C(8)	0.4(6)	C(12)-Mn(2)-C(9)-O(9)	85.2(5)
Mn(1)-C(6)-C(7)-C(8)	-62.3(4)	C(15)-Mn(2)-C(9)-O(9)	123.4(5)
C(5)-C(6)-C(7)-Mn(1)	62.7(4)	C(14)-Mn(2)-C(9)-O(9)	56.2(7)
C(2)-Mn(1)-C(7)-C(6)	136.6(4)	C(13)-Mn(2)-C(9)-O(9)	53.1(5)
C(3)-Mn(1)-C(7)-C(6)	48.1(5)	C(11)-Mn(2)-C(9)-C(22)	50.3(4)
C(1)-Mn(1)-C(7)-C(6)	-123.8(4)	C(10)-Mn(2)-C(9)-C(22)	139.1(4)
C(8)-Mn(1)-C(7)-C(6)	-117.0(5)	C(16)-Mn(2)-C(9)-C(22)	-51.2(4)
C(4)-Mn(1)-C(7)-C(6)	-78.8(4)	C(12)-Mn(2)-C(9)-C(22)	-85.6(5)
C(5)-Mn(1)-C(7)-C(6)	-36.2(4)	C(15)-Mn(2)-C(9)-C(22)	-47.3(6)
C(2)-Mn(1)-C(7)-C(8)	-106.4(4)	C(14)-Mn(2)-C(9)-C(22)	-114.6(6)
C(3)-Mn(1)-C(7)-C(8)	165.1(4)	C(13)-Mn(2)-C(9)-C(22)	-117.7(4)
C(1)-Mn(1)-C(7)-C(8)	-6.7(6)	C(22)-C(9)-O(9)-C(34)	-11(3)
C(6)-Mn(1)-C(7)-C(8)	117.0(5)	Mn(2)-C(9)-O(9)-C(34)	177(3)
C(4)-Mn(1)-C(7)-C(8)	38.2(4)	C(22)-C(9)-O(9)-C(29)	172.4(4)
C(5)-Mn(1)-C(7)-C(8)	80.8(4)	Mn(2)-C(9)-O(9)-C(29)	0.1(6)
C(5)-C(4)-C(8)-C(7)	-0.7(6)	C(22)-C(9)-O(9)-Fe(2)	-106.2(4)
Mn(1)-C(4)-C(8)-C(7)	61.3(3)	Mn(2)-C(9)-O(9)-Fe(2)	81.4(4)
C(5)-C(4)-C(8)-Mn(1)	-62.0(4)	C(11)-Mn(2)-C(10)-O(10)	-48(6)
C(6)-C(7)-C(8)-C(4)	0.2(6)	C(9)-Mn(2)-C(10)-O(10)	-142(6)
Mn(1)-C(7)-C(8)-C(4)	-62.1(3)	C(16)-Mn(2)-C(10)-O(10)	64(6)
C(6)-C(7)-C(8)-Mn(1)	62.3(4)	C(12)-Mn(2)-C(10)-O(10)	124(6)
C(2)-Mn(1)-C(8)-C(4)	-166.6(4)	C(15)-Mn(2)-C(10)-O(10)	42(6)
C(3)-Mn(1)-C(8)-C(4)	80.2(9)	C(14)-Mn(2)-C(10)-O(10)	70(6)
C(1)-Mn(1)-C(8)-C(4)	-67.9(4)	C(13)-Mn(2)-C(10)-O(10)	107(6)
C(7)-Mn(1)-C(8)-C(4)	116.3(5)	C(10)-Mn(2)-C(11)-O(11)	72(5)
C(6)-Mn(1)-C(8)-C(4)	78.9(4)	C(9)-Mn(2)-C(11)-O(11)	168(5)
C(5)-Mn(1)-C(8)-C(4)	36.9(3)	C(16)-Mn(2)-C(11)-O(11)	-86(5)
C(2)-Mn(1)-C(8)-C(7)	77.0(4)	C(12)-Mn(2)-C(11)-O(11)	-101(5)

C(15)-Mn(2)-C(11)-O(11)	-49(5)	C(16)-Mn(2)-C(14)-C(15)	37.5(5)
C(14)-Mn(2)-C(11)-O(11)	-21(6)	C(12)-Mn(2)-C(14)-C(15)	80.4(6)
C(13)-Mn(2)-C(11)-O(11)	-39(6)	C(13)-Mn(2)-C(14)-C(15)	118.1(7)
C(11)-Mn(2)-C(12)-C(16)	24.2(6)	C(11)-Mn(2)-C(14)-C(13)	-167.6(5)
C(10)-Mn(2)-C(12)-C(16)	-145.5(5)	C(10)-Mn(2)-C(14)-C(13)	102.1(5)
C(9)-Mn(2)-C(12)-C(16)	117.7(5)	C(9)-Mn(2)-C(14)-C(13)	-4.9(8)
C(15)-Mn(2)-C(12)-C(16)	-37.4(5)	C(16)-Mn(2)-C(14)-C(13)	-80.7(6)
C(14)-Mn(2)-C(12)-C(16)	-79.6(5)	C(12)-Mn(2)-C(14)-C(13)	-37.8(5)
C(13)-Mn(2)-C(12)-C(16)	-117.2(7)	C(15)-Mn(2)-C(14)-C(13)	-118.1(7)
C(11)-Mn(2)-C(12)-C(13)	141.3(5)	C(13)-C(14)-C(15)-C(16)	0.1(7)
C(10)-Mn(2)-C(12)-C(13)	-28.3(7)	Mn(2)-C(14)-C(15)-C(16)	-61.8(4)
C(9)-Mn(2)-C(12)-C(13)	-125.1(5)	C(13)-C(14)-C(15)-Mn(2)	61.9(5)
C(16)-Mn(2)-C(12)-C(13)	117.2(7)	C(11)-Mn(2)-C(15)-C(16)	-104.4(6)
C(15)-Mn(2)-C(12)-C(13)	79.8(5)	C(10)-Mn(2)-C(15)-C(16)	166.4(5)
C(14)-Mn(2)-C(12)-C(13)	37.6(5)	C(9)-Mn(2)-C(15)-C(16)	-6.1(8)
C(16)-C(12)-C(13)-C(14)	0.6(7)	C(12)-Mn(2)-C(15)-C(16)	37.8(5)
Mn(2)-C(12)-C(13)-C(14)	-61.4(5)	C(14)-Mn(2)-C(15)-C(16)	117.6(7)
C(16)-C(12)-C(13)-Mn(2)	62.1(4)	C(13)-Mn(2)-C(15)-C(16)	80.4(6)
C(11)-Mn(2)-C(13)-C(14)	25.7(10)	C(11)-Mn(2)-C(15)-C(14)	137.9(5)
C(10)-Mn(2)-C(13)-C(14)	-82.7(5)	C(10)-Mn(2)-C(15)-C(14)	48.8(5)
C(9)-Mn(2)-C(13)-C(14)	177.2(5)	C(9)-Mn(2)-C(15)-C(14)	-123.7(5)
C(16)-Mn(2)-C(13)-C(14)	79.4(5)	C(16)-Mn(2)-C(15)-C(14)	-117.6(7)
C(12)-Mn(2)-C(13)-C(14)	117.2(7)	C(12)-Mn(2)-C(15)-C(14)	-79.8(5)
C(15)-Mn(2)-C(13)-C(14)	37.0(5)	C(13)-Mn(2)-C(15)-C(14)	-37.2(5)
C(11)-Mn(2)-C(13)-C(12)	-91.5(9)	C(14)-C(15)-C(16)-C(12)	0.3(7)
C(10)-Mn(2)-C(13)-C(12)	160.1(5)	Mn(2)-C(15)-C(16)-C(12)	-62.2(4)
C(9)-Mn(2)-C(13)-C(12)	60.0(6)	C(14)-C(15)-C(16)-Mn(2)	62.5(5)
C(16)-Mn(2)-C(13)-C(12)	-37.8(5)	C(13)-C(12)-C(16)-C(15)	-0.6(7)
C(15)-Mn(2)-C(13)-C(12)	-80.2(6)	Mn(2)-C(12)-C(16)-C(15)	62.4(5)
C(14)-Mn(2)-C(13)-C(12)	-117.2(7)	C(13)-C(12)-C(16)-Mn(2)	-63.0(5)
C(12)-C(13)-C(14)-C(15)	-0.5(7)	C(11)-Mn(2)-C(16)-C(15)	79.5(6)
Mn(2)-C(13)-C(14)-C(15)	-61.4(4)	C(10)-Mn(2)-C(16)-C(15)	-30.3(12)
C(12)-C(13)-C(14)-Mn(2)	60.9(4)	C(9)-Mn(2)-C(16)-C(15)	176.2(5)
C(11)-Mn(2)-C(14)-C(15)	-49.5(6)	C(12)-Mn(2)-C(16)-C(15)	-117.4(7)
C(10)-Mn(2)-C(14)-C(15)	-139.8(5)	C(14)-Mn(2)-C(16)-C(15)	-37.3(5)
C(9)-Mn(2)-C(14)-C(15)	113.2(6)	C(13)-Mn(2)-C(16)-C(15)	-79.7(6)

C(11)-Mn(2)-C(16)-C(12)	-163.2(5)	C(22)-Fe(1)-C(17)-C(1)	-38.8(4)
C(10)-Mn(2)-C(16)-C(12)	87.0(10)	C(21)-C(17)-C(18)-C(19)	-1.8(5)
C(9)-Mn(2)-C(16)-C(12)	-66.5(5)	C(1)-C(17)-C(18)-C(19)	-178.8(4)
C(15)-Mn(2)-C(16)-C(12)	117.4(7)	Fe(1)-C(17)-C(18)-C(19)	-61.3(3)
C(14)-Mn(2)-C(16)-C(12)	80.1(5)	C(21)-C(17)-C(18)-Fe(1)	59.5(3)
C(13)-Mn(2)-C(16)-C(12)	37.7(4)	C(1)-C(17)-C(18)-Fe(1)	-117.5(4)
O(1)-C(1)-C(17)-C(21)	4.7(6)	C(23)-Fe(1)-C(18)-C(19)	-157.2(4)
Mn(1)-C(1)-C(17)-C(21)	178.7(3)	C(26)-Fe(1)-C(18)-C(19)	-42.4(8)
O(1)-C(1)-C(17)-C(18)	-179.0(4)	C(21)-Fe(1)-C(18)-C(19)	80.0(4)
Mn(1)-C(1)-C(17)-C(18)	-5.0(6)	C(25)-Fe(1)-C(18)-C(19)	-74.5(5)
O(1)-C(1)-C(17)-Fe(1)	93.8(4)	C(20)-Fe(1)-C(18)-C(19)	36.5(4)
Mn(1)-C(1)-C(17)-Fe(1)	-92.2(4)	C(17)-Fe(1)-C(18)-C(19)	118.8(5)
C(18)-Fe(1)-C(17)-C(21)	-117.2(4)	C(24)-Fe(1)-C(18)-C(19)	-115.1(4)
C(23)-Fe(1)-C(17)-C(21)	126.9(3)	C(22)-Fe(1)-C(18)-C(19)	167.6(5)
C(26)-Fe(1)-C(17)-C(21)	47.1(5)	C(23)-Fe(1)-C(18)-C(17)	84.0(3)
C(25)-Fe(1)-C(17)-C(21)	-156.4(6)	C(26)-Fe(1)-C(18)-C(17)	-161.2(5)
C(20)-Fe(1)-C(17)-C(21)	-37.0(3)	C(21)-Fe(1)-C(18)-C(17)	-38.9(3)
C(19)-Fe(1)-C(17)-C(21)	-79.8(4)	C(25)-Fe(1)-C(18)-C(17)	166.6(3)
C(24)-Fe(1)-C(17)-C(21)	169.1(3)	C(20)-Fe(1)-C(18)-C(17)	-82.3(3)
C(22)-Fe(1)-C(17)-C(21)	83.2(3)	C(19)-Fe(1)-C(18)-C(17)	-118.8(5)
C(23)-Fe(1)-C(17)-C(18)	-115.9(3)	C(24)-Fe(1)-C(18)-C(17)	126.1(3)
C(26)-Fe(1)-C(17)-C(18)	164.3(4)	C(22)-Fe(1)-C(18)-C(17)	48.8(7)
C(21)-Fe(1)-C(17)-C(18)	117.2(4)	C(17)-C(18)-C(19)-C(20)	1.9(6)
C(25)-Fe(1)-C(17)-C(18)	-39.2(7)	Fe(1)-C(18)-C(19)-C(20)	-59.0(4)
C(20)-Fe(1)-C(17)-C(18)	80.1(3)	C(17)-C(18)-C(19)-Fe(1)	60.9(3)
C(19)-Fe(1)-C(17)-C(18)	37.4(3)	C(18)-Fe(1)-C(19)-C(20)	120.3(5)
C(24)-Fe(1)-C(17)-C(18)	-73.8(3)	C(23)-Fe(1)-C(19)-C(20)	171.7(4)
C(22)-Fe(1)-C(17)-C(18)	-159.6(3)	C(26)-Fe(1)-C(19)-C(20)	-75.5(4)
C(18)-Fe(1)-C(17)-C(1)	120.7(5)	C(21)-Fe(1)-C(19)-C(20)	37.4(3)
C(23)-Fe(1)-C(17)-C(1)	4.8(4)	C(25)-Fe(1)-C(19)-C(20)	-116.1(3)
C(26)-Fe(1)-C(17)-C(1)	-74.9(6)	C(17)-Fe(1)-C(19)-C(20)	81.8(3)
C(21)-Fe(1)-C(17)-C(1)	-122.1(5)	C(24)-Fe(1)-C(19)-C(20)	-157.4(3)
C(25)-Fe(1)-C(17)-C(1)	81.5(8)	C(22)-Fe(1)-C(19)-C(20)	-43.6(9)
C(20)-Fe(1)-C(17)-C(1)	-159.1(4)	C(23)-Fe(1)-C(19)-C(18)	51.4(7)
C(19)-Fe(1)-C(17)-C(1)	158.1(5)	C(26)-Fe(1)-C(19)-C(18)	164.2(3)
C(24)-Fe(1)-C(17)-C(1)	47.0(5)	C(21)-Fe(1)-C(19)-C(18)	-82.9(4)

C(25)-Fe(1)-C(19)-C(18)	123.6(4)	C(19)-Fe(1)-C(21)-C(20)	-36.9(3)
C(20)-Fe(1)-C(19)-C(18)	-120.3(5)	C(17)-Fe(1)-C(21)-C(20)	-119.6(4)
C(17)-Fe(1)-C(19)-C(18)	-38.5(3)	C(24)-Fe(1)-C(21)-C(20)	-156.3(7)
C(24)-Fe(1)-C(19)-C(18)	82.3(4)	C(22)-Fe(1)-C(21)-C(20)	124.4(3)
C(22)-Fe(1)-C(19)-C(18)	-163.9(6)	C(18)-Fe(1)-C(21)-C(17)	39.2(3)
C(18)-C(19)-C(20)-C(21)	-1.2(6)	C(23)-Fe(1)-C(21)-C(17)	-74.6(3)
Fe(1)-C(19)-C(20)-C(21)	-59.2(3)	C(26)-Fe(1)-C(21)-C(17)	-160.0(3)
C(18)-C(19)-C(20)-Fe(1)	58.0(4)	C(25)-Fe(1)-C(21)-C(17)	163.8(4)
C(18)-Fe(1)-C(20)-C(19)	-37.0(3)	C(20)-Fe(1)-C(21)-C(17)	119.6(4)
C(23)-Fe(1)-C(20)-C(19)	-166.6(7)	C(19)-Fe(1)-C(21)-C(17)	82.7(3)
C(26)-Fe(1)-C(20)-C(19)	122.8(3)	C(24)-Fe(1)-C(21)-C(17)	-36.6(9)
C(21)-Fe(1)-C(20)-C(19)	-119.6(5)	C(22)-Fe(1)-C(21)-C(17)	-116.0(3)
C(25)-Fe(1)-C(20)-C(19)	80.6(4)	O(9)-C(9)-C(22)-C(23)	5.1(6)
C(17)-Fe(1)-C(20)-C(19)	-81.8(4)	Mn(2)-C(9)-C(22)-C(23)	177.7(3)
C(24)-Fe(1)-C(20)-C(19)	47.4(6)	O(9)-C(9)-C(22)-C(26)	-177.8(4)
C(22)-Fe(1)-C(20)-C(19)	164.8(3)	Mn(2)-C(9)-C(22)-C(26)	-5.2(6)
C(18)-Fe(1)-C(20)-C(21)	82.6(3)	O(9)-C(9)-C(22)-Fe(1)	94.1(4)
C(23)-Fe(1)-C(20)-C(21)	-47.0(9)	Mn(2)-C(9)-C(22)-Fe(1)	-93.3(4)
C(26)-Fe(1)-C(20)-C(21)	-117.6(3)	C(18)-Fe(1)-C(22)-C(23)	48.7(6)
C(25)-Fe(1)-C(20)-C(21)	-159.8(3)	C(26)-Fe(1)-C(22)-C(23)	-116.6(4)
C(19)-Fe(1)-C(20)-C(21)	119.6(5)	C(21)-Fe(1)-C(22)-C(23)	127.7(3)
C(17)-Fe(1)-C(20)-C(21)	37.8(3)	C(25)-Fe(1)-C(22)-C(23)	-79.5(3)
C(24)-Fe(1)-C(20)-C(21)	166.9(4)	C(20)-Fe(1)-C(22)-C(23)	168.9(3)
C(22)-Fe(1)-C(20)-C(21)	-75.6(3)	C(19)-Fe(1)-C(22)-C(23)	-158.0(7)
C(19)-C(20)-C(21)-C(17)	0.0(5)	C(17)-Fe(1)-C(22)-C(23)	84.2(3)
Fe(1)-C(20)-C(21)-C(17)	-59.6(3)	C(24)-Fe(1)-C(22)-C(23)	-36.7(3)
C(19)-C(20)-C(21)-Fe(1)	59.6(4)	C(18)-Fe(1)-C(22)-C(9)	-73.7(7)
C(18)-C(17)-C(21)-C(20)	1.1(5)	C(23)-Fe(1)-C(22)-C(9)	-122.5(5)
C(1)-C(17)-C(21)-C(20)	178.0(4)	C(26)-Fe(1)-C(22)-C(9)	120.9(5)
Fe(1)-C(17)-C(21)-C(20)	59.9(3)	C(21)-Fe(1)-C(22)-C(9)	5.2(4)
C(18)-C(17)-C(21)-Fe(1)	-58.8(3)	C(25)-Fe(1)-C(22)-C(9)	158.0(4)
C(1)-C(17)-C(21)-Fe(1)	118.2(4)	C(20)-Fe(1)-C(22)-C(9)	46.5(5)
C(18)-Fe(1)-C(21)-C(20)	-80.4(3)	C(19)-Fe(1)-C(22)-C(9)	79.5(9)
C(23)-Fe(1)-C(21)-C(20)	165.8(3)	C(17)-Fe(1)-C(22)-C(9)	-38.3(4)
C(26)-Fe(1)-C(21)-C(20)	80.3(3)	C(24)-Fe(1)-C(22)-C(9)	-159.2(4)
C(25)-Fe(1)-C(21)-C(20)	44.1(6)	C(18)-Fe(1)-C(22)-C(26)	165.4(5)

C(23)-Fe(1)-C(22)-C(26)	116.6(4)	C(19)-Fe(1)-C(24)-C(25)	80.8(4)
C(21)-Fe(1)-C(22)-C(26)	-115.7(3)	C(17)-Fe(1)-C(24)-C(25)	164.5(3)
C(25)-Fe(1)-C(22)-C(26)	37.1(3)	C(22)-Fe(1)-C(24)-C(25)	-81.7(3)
C(20)-Fe(1)-C(22)-C(26)	-74.4(3)	C(18)-Fe(1)-C(24)-C(23)	-118.5(3)
C(19)-Fe(1)-C(22)-C(26)	-41.4(8)	C(26)-Fe(1)-C(24)-C(23)	81.7(3)
C(17)-Fe(1)-C(22)-C(26)	-159.2(2)	C(21)-Fe(1)-C(24)-C(23)	-47.7(9)
C(24)-Fe(1)-C(22)-C(26)	79.9(3)	C(25)-Fe(1)-C(24)-C(23)	118.7(4)
C(9)-C(22)-C(23)-C(24)	178.1(4)	C(20)-Fe(1)-C(24)-C(23)	167.0(4)
C(26)-C(22)-C(23)-C(24)	0.5(5)	C(19)-Fe(1)-C(24)-C(23)	-160.5(3)
Fe(1)-C(22)-C(23)-C(24)	59.8(3)	C(17)-Fe(1)-C(24)-C(23)	-76.9(3)
C(9)-C(22)-C(23)-Fe(1)	118.3(4)	C(22)-Fe(1)-C(24)-C(23)	37.0(3)
C(26)-C(22)-C(23)-Fe(1)	-59.3(3)	C(23)-C(24)-C(25)-C(26)	-0.1(5)
C(18)-Fe(1)-C(23)-C(24)	79.7(3)	Fe(1)-C(24)-C(25)-C(26)	58.7(3)
C(26)-Fe(1)-C(23)-C(24)	-81.1(3)	C(23)-C(24)-C(25)-Fe(1)	-58.9(3)
C(21)-Fe(1)-C(23)-C(24)	166.0(3)	C(18)-Fe(1)-C(25)-C(24)	-75.6(4)
C(25)-Fe(1)-C(23)-C(24)	-37.5(3)	C(23)-Fe(1)-C(25)-C(24)	38.1(3)
C(20)-Fe(1)-C(23)-C(24)	-156.9(7)	C(26)-Fe(1)-C(25)-C(24)	120.4(4)
C(19)-Fe(1)-C(23)-C(24)	43.5(6)	C(21)-Fe(1)-C(25)-C(24)	172.0(4)
C(17)-Fe(1)-C(23)-C(24)	123.9(3)	C(20)-Fe(1)-C(25)-C(24)	-157.0(3)
C(22)-Fe(1)-C(23)-C(24)	-120.8(4)	C(19)-Fe(1)-C(25)-C(24)	-116.0(3)
C(18)-Fe(1)-C(23)-C(22)	-159.5(3)	C(17)-Fe(1)-C(25)-C(24)	-45.3(8)
C(26)-Fe(1)-C(23)-C(22)	39.6(2)	C(22)-Fe(1)-C(25)-C(24)	82.3(3)
C(21)-Fe(1)-C(23)-C(22)	-73.2(3)	C(18)-Fe(1)-C(25)-C(26)	164.0(3)
C(25)-Fe(1)-C(23)-C(22)	83.3(3)	C(23)-Fe(1)-C(25)-C(26)	-82.3(3)
C(20)-Fe(1)-C(23)-C(22)	-36.2(8)	C(21)-Fe(1)-C(25)-C(26)	51.6(6)
C(19)-Fe(1)-C(23)-C(22)	164.3(5)	C(20)-Fe(1)-C(25)-C(26)	82.6(3)
C(17)-Fe(1)-C(23)-C(22)	-115.3(3)	C(19)-Fe(1)-C(25)-C(26)	123.6(3)
C(24)-Fe(1)-C(23)-C(22)	120.8(4)	C(17)-Fe(1)-C(25)-C(26)	-165.7(6)
C(22)-C(23)-C(24)-C(25)	-0.2(5)	C(24)-Fe(1)-C(25)-C(26)	-120.4(4)
Fe(1)-C(23)-C(24)-C(25)	59.5(3)	C(22)-Fe(1)-C(25)-C(26)	-38.1(3)
C(22)-C(23)-C(24)-Fe(1)	-59.7(3)	C(24)-C(25)-C(26)-C(22)	0.5(5)
C(18)-Fe(1)-C(24)-C(25)	122.8(3)	Fe(1)-C(25)-C(26)-C(22)	59.8(3)
C(23)-Fe(1)-C(24)-C(25)	-118.7(4)	C(24)-C(25)-C(26)-Fe(1)	-59.3(3)
C(26)-Fe(1)-C(24)-C(25)	-37.0(3)	C(23)-C(22)-C(26)-C(25)	-0.6(4)
C(21)-Fe(1)-C(24)-C(25)	-166.4(7)	C(9)-C(22)-C(26)-C(25)	-178.3(4)
C(20)-Fe(1)-C(24)-C(25)	48.3(6)	Fe(1)-C(22)-C(26)-C(25)	-59.9(3)

C(23)-C(22)-C(26)-Fe(1)	59.3(3)
C(9)-C(22)-C(26)-Fe(1)	-118.3(4)
C(18)-Fe(1)-C(26)-C(25)	-43.0(7)
C(23)-Fe(1)-C(26)-C(25)	80.5(3)
C(21)-Fe(1)-C(26)-C(25)	-156.7(3)
C(20)-Fe(1)-C(26)-C(25)	-115.0(3)
C(19)-Fe(1)-C(26)-C(25)	-74.7(4)
C(17)-Fe(1)-C(26)-C(25)	169.2(4)
C(24)-Fe(1)-C(26)-C(25)	36.6(3)
C(22)-Fe(1)-C(26)-C(25)	119.6(4)
C(18)-Fe(1)-C(26)-C(22)	-162.6(6)
C(23)-Fe(1)-C(26)-C(22)	-39.1(2)
C(21)-Fe(1)-C(26)-C(22)	83.7(3)
C(25)-Fe(1)-C(26)-C(22)	-119.6(4)
C(20)-Fe(1)-C(26)-C(22)	125.5(3)
C(19)-Fe(1)-C(26)-C(22)	165.8(3)
C(17)-Fe(1)-C(26)-C(22)	49.7(5)
C(24)-Fe(1)-C(26)-C(22)	-82.9(3)
C(1)-O(1)-C(27)-C(28)	-178.6(5)
C(9)-O(9)-C(29)-C(30)	-174.1(5)

Appendix 8

Crystallographic data of Complex 27

Table 1. Crystal data and structure refinement for Complex **27**.

Identification code	db61a5_abs	
Empirical formula	C_{34} H_{18} Fe O_{20} Re_4	
Formula weight	1547.13	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P$\bar{1}$	
Unit cell dimensions	a = 15.5600(14) Å	a= 98.175(1)°.
	b = 16.0269(14) Å	b= 91.337(1)°.
	c = 16.5632(14) Å	g = 90.100(1)°.
Volume	4087.4(6) Å^3	
Z	4	
Density (calculated)	2.514 Mg/m^3	
Absorption coefficient	12.227 mm^{-1}	
F(000)	2832	
Crystal size	0.34 x 0.08 x 0.01 mm^3	
Theta range for data collection	2.34 to 26.52°.	
Index ranges	-19<=h<=19, -19<=k<=20, -20<=l<=6	
Reflections collected	22399	
Independent reflections	14796 [R(int) = 0.0532]	
Completeness to θ = 25.00°	97.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.885 and 0.348	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14796 / 0 / 1064	
Goodness-of-fit on F^2	0.997	
Final R indices [I>2σ(I)]	R1 = 0.0545, wR2 = 0.1265	
R indices (all data)	R1 = 0.0995, wR2 = 0.1568	
Extinction coefficient	0.00078(6)	
Largest diff. peak and hole	2.547 and -2.452 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Complex **27**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	5620(1)	2995(1)	4048(1)	46(1)
Re(2)	7212(1)	1853(1)	3705(1)	47(1)
C(1)	4676(13)	3721(12)	4400(11)	70(5)
O(1)	4098(10)	4123(9)	4637(8)	93(4)
C(2)	6485(12)	3893(11)	4397(10)	57(4)
O(2)	7027(10)	4406(8)	4534(9)	90(4)
C(3)	5642(16)	3297(14)	2910(11)	94(7)
O(3)	5631(10)	3485(10)	2283(8)	102(5)
C(4)	4828(11)	2065(11)	3606(10)	59(4)
O(4)	4381(8)	1533(9)	3333(8)	87(4)
C(5)	5673(16)	2640(13)	5136(12)	88(7)
O(5)	5631(10)	2408(9)	5763(8)	93(5)
C(6)	8134(13)	1115(11)	3340(10)	68(5)
O(6)	8688(9)	672(9)	3128(9)	90(4)
C(7)	6954(14)	1287(12)	4667(10)	79(6)
O(7)	6927(10)	1038(8)	5287(7)	85(4)
C(8)	7945(13)	2572(11)	4483(13)	76(5)
O(8)	8412(12)	2990(10)	4920(10)	124(6)
C(9)	7493(12)	2719(11)	3014(10)	61(4)
O(9)	7680(9)	3266(8)	2670(8)	83(4)
C(10)	6384(10)	1129(9)	2848(9)	48(4)
O(10)	5883(7)	460(7)	2944(6)	60(3)
Re(3)	9018(1)	-1125(1)	-2004(1)	55(1)
Re(4)	7478(1)	64(1)	-1765(1)	45(1)
C(11)	10006(13)	-1855(12)	-2158(10)	72(5)
O(11)	10600(10)	-2306(10)	-2269(9)	105(5)
C(12)	9317(11)	-605(11)	-2976(10)	63(5)
O(12)	9426(9)	-333(9)	-3566(7)	88(4)
C(13)	8251(15)	-1937(13)	-2691(13)	86(7)
O(13)	7820(12)	-2418(11)	-3090(11)	140(8)
C(14)	8610(13)	-1560(13)	-1013(12)	88(7)
O(14)	8426(13)	-1853(10)	-469(9)	136(8)

C(15)	9668(12)	-210(13)	-1308(12)	72(5)
O(15)	10046(9)	287(11)	-892(10)	106(5)
C(16)	6491(12)	767(11)	-1624(10)	64(5)
O(16)	5889(9)	1191(9)	-1508(8)	91(4)
C(17)	8204(12)	910(11)	-2154(9)	61(4)
O(17)	8638(9)	1371(8)	-2474(8)	86(4)
C(18)	7274(11)	-262(11)	-2952(10)	61(5)
O(18)	7132(10)	-420(9)	-3640(7)	98(5)
C(19)	6877(11)	-988(11)	-1627(9)	56(4)
O(19)	6547(9)	-1627(8)	-1628(7)	74(3)
C(20)	7791(9)	359(9)	-511(8)	44(3)
O(20)	8292(7)	973(7)	-138(6)	58(3)
Fe(1)	6662(2)	462(1)	1006(1)	48(1)
C(21)	6257(11)	1241(10)	1994(8)	53(4)
C(22)	6775(11)	1684(10)	1490(8)	54(4)
C(23)	6383(15)	1617(12)	691(10)	76(6)
C(24)	5614(14)	1120(14)	691(10)	84(7)
C(25)	5523(11)	875(12)	1468(10)	69(5)
C(26)	7478(10)	-91(9)	156(9)	50(4)
C(27)	6732(14)	-586(11)	168(9)	70(5)
C(28)	6631(17)	-856(12)	959(11)	88(7)
C(29)	7331(15)	-486(12)	1423(11)	83(7)
C(30)	7862(12)	-25(11)	974(10)	65(5)
C(31)	5863(11)	117(10)	3707(9)	60(4)
C(32)	5219(15)	-594(13)	3558(13)	100(7)
C(33)	8596(12)	1687(11)	-494(10)	68(5)
C(34)	8933(16)	2306(12)	186(13)	104(8)
Re(41)	6038(1)	3816(1)	-2014(1)	53(1)
Re(42)	7546(1)	5077(1)	-1841(1)	45(1)
C(41)	5093(13)	3049(12)	-2156(11)	73(5)
O(41)	4499(9)	2589(9)	-2228(9)	99(5)
C(42)	6488(10)	3424(11)	-992(11)	62(5)
O(42)	6747(10)	3187(9)	-424(9)	102(5)
C(43)	6804(13)	3001(11)	-2672(12)	72(5)
O(43)	7253(12)	2551(11)	-3038(11)	133(7)
C(44)	5723(11)	4308(12)	-3019(10)	65(5)

O(44)	5588(9)	4571(9)	-3609(8)	97(5)
C(45)	5346(14)	4660(14)	-1366(11)	81(6)
O(45)	4910(10)	5129(10)	-959(10)	106(5)
C(46)	8514(11)	5808(11)	-1702(11)	64(5)
O(46)	9124(9)	6240(9)	-1572(9)	93(4)
C(47)	6808(10)	5928(10)	-2281(10)	53(4)
O(47)	6417(9)	6358(8)	-2633(8)	88(4)
C(48)	7731(10)	4670(10)	-3020(8)	54(4)
O(48)	7840(9)	4459(9)	-3676(7)	88(4)
C(49)	8173(11)	4062(10)	-1601(8)	53(4)
O(49)	8510(7)	3437(7)	-1527(7)	65(3)
C(50)	7258(9)	5414(9)	-606(8)	42(3)
O(50)	6689(7)	5943(7)	-247(6)	63(3)
Re(43)	9363(1)	8021(1)	4155(1)	46(1)
Re(44)	7759(1)	6867(1)	3817(1)	45(1)
C(51)	10304(13)	8773(12)	4545(10)	65(5)
O(51)	10873(10)	9189(9)	4772(9)	106(6)
C(52)	10148(11)	7121(11)	3684(11)	62(5)
O(52)	10635(9)	6647(9)	3385(8)	92(5)
C(53)	9268(12)	8370(11)	3053(9)	66(5)
O(53)	9267(10)	8608(9)	2434(8)	95(5)
C(54)	8472(13)	8877(12)	4517(11)	67(5)
O(54)	7940(10)	9363(8)	4692(9)	91(4)
C(55)	9411(14)	7594(11)	5216(11)	74(5)
O(55)	9400(10)	7383(9)	5840(7)	89(4)
C(56)	6830(12)	6122(11)	3416(11)	66(5)
O(56)	6288(9)	5671(9)	3151(10)	104(5)
C(57)	8078(11)	6188(12)	4718(10)	63(5)
O(57)	8188(11)	5933(8)	5301(8)	98(5)
C(58)	7045(13)	7527(12)	4661(11)	71(5)
O(58)	6590(12)	7930(10)	5096(10)	122(6)
C(59)	7450(10)	7758(10)	3165(9)	52(4)
O(59)	7202(8)	8333(7)	2886(7)	73(3)
C(60)	8551(10)	6255(9)	2920(8)	49(4)
O(60)	9067(7)	5600(7)	2936(6)	59(3)
Fe(41)	8347(2)	5713(2)	1015(1)	55(1)

C(61)	7657(11)	5051(11)	52(10)	62(5)
C(62)	7297(12)	4944(10)	821(10)	62(5)
C(63)	7921(15)	4593(11)	1310(12)	81(6)
C(64)	8694(18)	4472(13)	878(13)	108(10)
C(65)	8541(13)	4746(13)	105(10)	85(6)
C(66)	8604(12)	6494(10)	2078(8)	55(4)
C(67)	7945(13)	6801(10)	1615(9)	64(5)
C(68)	8275(18)	6964(13)	861(11)	94(8)
C(69)	9123(16)	6700(17)	867(12)	107(9)
C(70)	9317(13)	6402(13)	1588(12)	81(6)
C(71)	6241(11)	6569(10)	-671(11)	62(5)
C(72)	5694(15)	7074(13)	-51(13)	100(7)
C(73)	9168(13)	5156(11)	3628(11)	77(6)
C(74)	9766(19)	4455(14)	3412(15)	140(11)

Table 3. Bond lengths [Å] and angles [°] for Complex **27**.

Re(1)-C(1)	1.924(19)	C(11)-O(11)	1.18(2)
Re(1)-C(5)	1.96(2)	C(12)-O(12)	1.142(18)
Re(1)-C(4)	1.979(19)	C(13)-O(13)	1.15(2)
Re(1)-C(2)	1.99(2)	C(14)-O(14)	1.117(19)
Re(1)-C(3)	2.013(18)	C(15)-O(15)	1.13(2)
Re(1)-Re(2)	3.0974(9)	C(16)-O(16)	1.161(19)
Re(2)-C(6)	1.915(19)	C(17)-O(17)	1.187(19)
Re(2)-C(8)	1.95(2)	C(18)-O(18)	1.147(18)
Re(2)-C(9)	1.975(18)	C(19)-O(19)	1.146(18)
Re(2)-C(7)	1.991(17)	C(20)-O(20)	1.327(16)
Re(2)-C(10)	2.111(15)	C(20)-C(26)	1.493(19)
C(1)-O(1)	1.15(2)	O(20)-C(33)	1.444(18)
C(2)-O(2)	1.17(2)	Fe(1)-C(22)	2.014(15)
C(3)-O(3)	1.121(19)	Fe(1)-C(25)	2.021(16)
C(4)-O(4)	1.135(19)	Fe(1)-C(30)	2.024(18)
C(5)-O(5)	1.16(2)	Fe(1)-C(27)	2.026(17)
C(6)-O(6)	1.15(2)	Fe(1)-C(21)	2.027(15)
C(7)-O(7)	1.156(18)	Fe(1)-C(26)	2.028(14)
C(8)-O(8)	1.16(2)	Fe(1)-C(29)	2.035(18)
C(9)-O(9)	1.152(18)	Fe(1)-C(23)	2.038(17)
C(10)-O(10)	1.355(17)	Fe(1)-C(24)	2.041(17)
C(10)-C(21)	1.460(19)	Fe(1)-C(28)	2.104(19)
O(10)-C(31)	1.449(16)	C(21)-C(22)	1.43(2)
Re(3)-C(11)	1.93(2)	C(21)-C(25)	1.49(2)
Re(3)-C(12)	1.979(16)	C(22)-C(23)	1.43(2)
Re(3)-C(13)	1.98(2)	C(22)-H(22)	0.9300
Re(3)-C(14)	1.989(17)	C(23)-C(24)	1.44(3)
Re(3)-C(15)	1.99(2)	C(23)-H(23)	0.9300
Re(3)-Re(4)	3.0632(9)	C(24)-C(25)	1.41(2)
Re(4)-C(16)	1.905(18)	C(24)-H(24)	0.9300
Re(4)-C(17)	1.952(18)	C(25)-H(25)	0.9300
Re(4)-C(19)	1.970(18)	C(26)-C(27)	1.41(2)
Re(4)-C(18)	1.980(16)	C(26)-C(30)	1.46(2)
Re(4)-C(20)	2.108(14)	C(27)-C(28)	1.45(2)

C(27)-H(27)	0.9300	C(48)-O(48)	1.109(16)
C(28)-C(29)	1.40(3)	C(49)-O(49)	1.151(17)
C(28)-H(28)	0.9300	C(50)-O(50)	1.319(17)
C(29)-C(30)	1.40(2)	C(50)-C(61)	1.44(2)
C(29)-H(29)	0.9300	O(50)-C(71)	1.471(18)
C(30)-H(30)	0.9300	Re(43)-C(51)	1.93(2)
C(31)-C(32)	1.51(2)	Re(43)-C(55)	1.975(19)
C(31)-H(31A)	0.9700	Re(43)-C(52)	1.98(2)
C(31)-H(31B)	0.9700	Re(43)-C(53)	1.986(16)
C(32)-H(32A)	0.9600	Re(43)-C(54)	1.99(2)
C(32)-H(32B)	0.9600	Re(43)-Re(44)	3.0962(9)
C(32)-H(32C)	0.9600	Re(44)-C(56)	1.919(19)
C(33)-C(34)	1.48(2)	Re(44)-C(59)	1.963(17)
C(33)-H(33A)	0.9700	Re(44)-C(58)	1.991(19)
C(33)-H(33B)	0.9700	Re(44)-C(57)	2.021(17)
C(34)-H(34A)	0.9600	Re(44)-C(60)	2.090(15)
C(34)-H(34B)	0.9600	C(51)-O(51)	1.13(2)
C(34)-H(34C)	0.9600	C(52)-O(52)	1.14(2)
Re(41)-C(41)	1.904(19)	C(53)-O(53)	1.143(18)
Re(41)-C(45)	1.95(2)	C(54)-O(54)	1.15(2)
Re(41)-C(44)	1.993(17)	C(55)-O(55)	1.133(19)
Re(41)-C(43)	1.99(2)	C(56)-O(56)	1.148(19)
Re(41)-C(42)	2.000(17)	C(57)-O(57)	1.111(18)
Re(41)-Re(42)	3.0771(9)	C(58)-O(58)	1.15(2)
Re(42)-C(46)	1.895(16)	C(59)-O(59)	1.151(17)
Re(42)-C(49)	1.983(17)	C(60)-O(60)	1.324(17)
Re(42)-C(47)	1.989(16)	C(60)-C(66)	1.502(19)
Re(42)-C(48)	1.997(14)	O(60)-C(73)	1.440(19)
Re(42)-C(50)	2.100(14)	Fe(41)-C(67)	1.990(17)
C(41)-O(41)	1.17(2)	Fe(41)-C(70)	2.007(18)
C(42)-O(42)	1.130(18)	Fe(41)-C(65)	2.031(18)
C(43)-O(43)	1.13(2)	Fe(41)-C(69)	2.03(2)
C(44)-O(44)	1.132(19)	Fe(41)-C(62)	2.036(16)
C(45)-O(45)	1.17(2)	Fe(41)-C(63)	2.039(19)
C(46)-O(46)	1.172(18)	Fe(41)-C(66)	2.041(14)
C(47)-O(47)	1.133(18)	Fe(41)-C(64)	2.045(19)

Fe(41)-C(68)	2.06(2)	C(1)-Re(1)-C(2)	92.7(8)
Fe(41)-C(61)	2.062(16)	C(5)-Re(1)-C(2)	90.6(7)
C(61)-C(62)	1.44(2)	C(4)-Re(1)-C(2)	174.3(6)
C(61)-C(65)	1.47(2)	C(1)-Re(1)-C(3)	95.6(8)
C(62)-C(63)	1.42(2)	C(5)-Re(1)-C(3)	175.6(10)
C(62)-H(62)	0.9300	C(4)-Re(1)-C(3)	86.9(8)
C(63)-C(64)	1.41(3)	C(2)-Re(1)-C(3)	89.2(8)
C(63)-H(63)	0.9300	C(1)-Re(1)-Re(2)	172.9(5)
C(64)-C(65)	1.43(3)	C(5)-Re(1)-Re(2)	84.9(7)
C(64)-H(64)	0.9300	C(4)-Re(1)-Re(2)	91.8(5)
C(65)-H(65)	0.9300	C(2)-Re(1)-Re(2)	84.2(4)
C(66)-C(70)	1.39(2)	C(3)-Re(1)-Re(2)	90.7(7)
C(66)-C(67)	1.40(2)	C(6)-Re(2)-C(8)	93.3(8)
C(67)-C(68)	1.42(2)	C(6)-Re(2)-C(9)	95.4(7)
C(67)-H(67)	0.9300	C(8)-Re(2)-C(9)	81.5(7)
C(68)-C(69)	1.39(3)	C(6)-Re(2)-C(7)	95.0(8)
C(68)-H(68)	0.9300	C(8)-Re(2)-C(7)	83.6(8)
C(69)-C(70)	1.38(3)	C(9)-Re(2)-C(7)	162.3(7)
C(69)-H(69)	0.9300	C(6)-Re(2)-C(10)	89.0(7)
C(70)-H(70)	0.9300	C(8)-Re(2)-C(10)	177.1(6)
C(71)-C(72)	1.50(2)	C(9)-Re(2)-C(10)	96.5(6)
C(71)-H(71A)	0.9700	C(7)-Re(2)-C(10)	98.0(7)
C(71)-H(71B)	0.9700	C(6)-Re(2)-Re(1)	172.0(5)
C(72)-H(72A)	0.9600	C(8)-Re(2)-Re(1)	93.3(5)
C(72)-H(72B)	0.9600	C(9)-Re(2)-Re(1)	81.3(5)
C(72)-H(72C)	0.9600	C(7)-Re(2)-Re(1)	90.1(6)
C(73)-C(74)	1.47(3)	C(10)-Re(2)-Re(1)	84.2(4)
C(73)-H(73A)	0.9700	O(1)-C(1)-Re(1)	176.3(17)
C(73)-H(73B)	0.9700	O(2)-C(2)-Re(1)	173.9(15)
C(74)-H(74A)	0.9600	O(3)-C(3)-Re(1)	178(2)
C(74)-H(74B)	0.9600	O(4)-C(4)-Re(1)	178.3(16)
C(74)-H(74C)	0.9600	O(5)-C(5)-Re(1)	174(2)
		O(6)-C(6)-Re(2)	179.4(17)
C(1)-Re(1)-C(5)	88.9(8)	O(7)-C(7)-Re(2)	168.0(19)
C(1)-Re(1)-C(4)	91.8(8)	O(8)-C(8)-Re(2)	177(2)
C(5)-Re(1)-C(4)	93.0(8)	O(9)-C(9)-Re(2)	174.3(15)

O(10)-C(10)-C(21)	104.8(13)	O(13)-C(13)-Re(3)	179(2)
O(10)-C(10)-Re(2)	129.2(10)	O(14)-C(14)-Re(3)	174.5(17)
C(21)-C(10)-Re(2)	125.9(12)	O(15)-C(15)-Re(3)	177.2(18)
C(10)-O(10)-C(31)	122.0(12)	O(16)-C(16)-Re(4)	177.5(16)
C(11)-Re(3)-C(12)	90.5(7)	O(17)-C(17)-Re(4)	172.6(15)
C(11)-Re(3)-C(13)	93.4(8)	O(18)-C(18)-Re(4)	176.9(17)
C(12)-Re(3)-C(13)	90.0(8)	O(19)-C(19)-Re(4)	173.0(13)
C(11)-Re(3)-C(14)	95.9(7)	O(20)-C(20)-C(26)	104.9(12)
C(12)-Re(3)-C(14)	173.7(7)	O(20)-C(20)-Re(4)	128.7(10)
C(13)-Re(3)-C(14)	89.8(9)	C(26)-C(20)-Re(4)	126.4(11)
C(11)-Re(3)-C(15)	93.7(8)	C(20)-O(20)-C(33)	125.5(12)
C(12)-Re(3)-C(15)	89.2(7)	C(22)-Fe(1)-C(25)	70.7(7)
C(13)-Re(3)-C(15)	172.9(8)	C(22)-Fe(1)-C(30)	106.8(7)
C(14)-Re(3)-C(15)	90.3(9)	C(25)-Fe(1)-C(30)	158.8(6)
C(11)-Re(3)-Re(4)	178.8(6)	C(22)-Fe(1)-C(27)	158.7(6)
C(12)-Re(3)-Re(4)	88.7(5)	C(25)-Fe(1)-C(27)	121.2(8)
C(13)-Re(3)-Re(4)	87.5(6)	C(30)-Fe(1)-C(27)	68.7(8)
C(14)-Re(3)-Re(4)	84.9(5)	C(22)-Fe(1)-C(21)	41.5(6)
C(15)-Re(3)-Re(4)	85.4(5)	C(25)-Fe(1)-C(21)	43.1(6)
C(16)-Re(4)-C(17)	95.1(7)	C(30)-Fe(1)-C(21)	121.2(7)
C(16)-Re(4)-C(19)	95.8(7)	C(27)-Fe(1)-C(21)	158.8(7)
C(17)-Re(4)-C(19)	164.4(6)	C(22)-Fe(1)-C(26)	122.1(6)
C(16)-Re(4)-C(18)	94.5(7)	C(25)-Fe(1)-C(26)	156.9(7)
C(17)-Re(4)-C(18)	81.4(6)	C(30)-Fe(1)-C(26)	42.2(6)
C(19)-Re(4)-C(18)	86.6(6)	C(27)-Fe(1)-C(26)	40.6(7)
C(16)-Re(4)-C(20)	90.1(6)	C(21)-Fe(1)-C(26)	158.7(7)
C(17)-Re(4)-C(20)	97.7(6)	C(22)-Fe(1)-C(29)	123.8(8)
C(19)-Re(4)-C(20)	93.4(6)	C(25)-Fe(1)-C(29)	122.6(7)
C(18)-Re(4)-C(20)	175.3(7)	C(30)-Fe(1)-C(29)	40.4(7)
C(16)-Re(4)-Re(3)	177.8(5)	C(27)-Fe(1)-C(29)	67.1(8)
C(17)-Re(4)-Re(3)	86.9(5)	C(21)-Fe(1)-C(29)	107.3(7)
C(19)-Re(4)-Re(3)	82.1(5)	C(26)-Fe(1)-C(29)	68.7(6)
C(18)-Re(4)-Re(3)	84.7(5)	C(22)-Fe(1)-C(23)	41.5(6)
C(20)-Re(4)-Re(3)	90.7(4)	C(25)-Fe(1)-C(23)	69.6(8)
O(11)-C(11)-Re(3)	178.5(18)	C(30)-Fe(1)-C(23)	123.2(8)
O(12)-C(12)-Re(3)	174.3(17)	C(27)-Fe(1)-C(23)	122.3(7)

C(21)-Fe(1)-C(23)	70.1(6)	C(24)-C(23)-H(23)	126.1
C(26)-Fe(1)-C(23)	106.3(7)	Fe(1)-C(23)-H(23)	127.5
C(29)-Fe(1)-C(23)	160.3(10)	C(25)-C(24)-C(23)	109.1(17)
C(22)-Fe(1)-C(24)	69.7(8)	C(25)-C(24)-Fe(1)	69.0(9)
C(25)-Fe(1)-C(24)	40.6(7)	C(23)-C(24)-Fe(1)	69.3(10)
C(30)-Fe(1)-C(24)	159.7(7)	C(25)-C(24)-H(24)	125.5
C(27)-Fe(1)-C(24)	106.9(8)	C(23)-C(24)-H(24)	125.5
C(21)-Fe(1)-C(24)	70.3(7)	Fe(1)-C(24)-H(24)	127.9
C(26)-Fe(1)-C(24)	121.6(6)	C(24)-C(25)-C(21)	107.8(17)
C(29)-Fe(1)-C(24)	157.8(10)	C(24)-C(25)-Fe(1)	70.5(10)
C(23)-Fe(1)-C(24)	41.2(8)	C(21)-C(25)-Fe(1)	68.6(9)
C(22)-Fe(1)-C(28)	158.6(7)	C(24)-C(25)-H(25)	126.1
C(25)-Fe(1)-C(28)	105.6(9)	C(21)-C(25)-H(25)	126.1
C(30)-Fe(1)-C(28)	68.7(9)	Fe(1)-C(25)-H(25)	126.4
C(27)-Fe(1)-C(28)	41.0(6)	C(27)-C(26)-C(30)	105.9(14)
C(21)-Fe(1)-C(28)	121.6(6)	C(27)-C(26)-C(20)	128.7(14)
C(26)-Fe(1)-C(28)	69.5(7)	C(30)-C(26)-C(20)	125.2(15)
C(29)-Fe(1)-C(28)	39.5(8)	C(27)-C(26)-Fe(1)	69.6(9)
C(23)-Fe(1)-C(28)	158.5(9)	C(30)-C(26)-Fe(1)	68.8(9)
C(24)-Fe(1)-C(28)	121.8(10)	C(20)-C(26)-Fe(1)	121.6(10)
C(22)-C(21)-C(10)	129.7(15)	C(26)-C(27)-C(28)	111.1(18)
C(22)-C(21)-C(25)	106.2(13)	C(26)-C(27)-Fe(1)	69.8(9)
C(10)-C(21)-C(25)	124.1(15)	C(28)-C(27)-Fe(1)	72.4(10)
C(22)-C(21)-Fe(1)	68.8(8)	C(26)-C(27)-H(27)	124.4
C(10)-C(21)-Fe(1)	126.8(11)	C(28)-C(27)-H(27)	124.4
C(25)-C(21)-Fe(1)	68.3(8)	Fe(1)-C(27)-H(27)	125.0
C(21)-C(22)-C(23)	109.1(16)	C(29)-C(28)-C(27)	103.8(18)
C(21)-C(22)-Fe(1)	69.7(9)	C(29)-C(28)-Fe(1)	67.6(11)
C(23)-C(22)-Fe(1)	70.2(10)	C(27)-C(28)-Fe(1)	66.6(10)
C(21)-C(22)-H(22)	125.4	C(29)-C(28)-H(28)	128.1
C(23)-C(22)-H(22)	125.4	C(27)-C(28)-H(28)	128.1
Fe(1)-C(22)-H(22)	126.2	Fe(1)-C(28)-H(28)	129.1
C(22)-C(23)-C(24)	107.7(16)	C(28)-C(29)-C(30)	112.5(17)
C(22)-C(23)-Fe(1)	68.4(9)	C(28)-C(29)-Fe(1)	72.9(12)
C(24)-C(23)-Fe(1)	69.5(10)	C(30)-C(29)-Fe(1)	69.4(10)
C(22)-C(23)-H(23)	126.1	C(28)-C(29)-H(29)	123.8

C(30)-C(29)-H(29)	123.8	C(45)-Re(41)-C(43)	176.6(7)
Fe(1)-C(29)-H(29)	125.5	C(44)-Re(41)-C(43)	89.4(7)
C(29)-C(30)-C(26)	106.6(18)	C(41)-Re(41)-C(42)	94.8(7)
C(29)-C(30)-Fe(1)	70.2(11)	C(45)-Re(41)-C(42)	89.9(8)
C(26)-C(30)-Fe(1)	69.1(9)	C(44)-Re(41)-C(42)	172.4(7)
C(29)-C(30)-H(30)	126.7	C(43)-Re(41)-C(42)	90.0(7)
C(26)-C(30)-H(30)	126.7	C(41)-Re(41)-Re(42)	178.0(5)
Fe(1)-C(30)-H(30)	125.6	C(45)-Re(41)-Re(42)	89.1(5)
O(10)-C(31)-C(32)	104.9(14)	C(44)-Re(41)-Re(42)	85.2(5)
O(10)-C(31)-H(31A)	110.8	C(43)-Re(41)-Re(42)	87.5(5)
C(32)-C(31)-H(31A)	110.8	C(42)-Re(41)-Re(42)	87.2(5)
O(10)-C(31)-H(31B)	110.8	C(46)-Re(42)-C(49)	95.7(7)
C(32)-C(31)-H(31B)	110.8	C(46)-Re(42)-C(47)	93.0(7)
H(31A)-C(31)-H(31B)	108.8	C(49)-Re(42)-C(47)	167.7(6)
C(31)-C(32)-H(32A)	109.5	C(46)-Re(42)-C(48)	95.6(7)
C(31)-C(32)-H(32B)	109.5	C(49)-Re(42)-C(48)	87.2(6)
H(32A)-C(32)-H(32B)	109.5	C(47)-Re(42)-C(48)	83.3(6)
C(31)-C(32)-H(32C)	109.5	C(46)-Re(42)-C(50)	90.0(7)
H(32A)-C(32)-H(32C)	109.5	C(49)-Re(42)-C(50)	91.4(6)
H(32B)-C(32)-H(32C)	109.5	C(47)-Re(42)-C(50)	97.3(6)
O(20)-C(33)-C(34)	106.7(14)	C(48)-Re(42)-C(50)	174.3(6)
O(20)-C(33)-H(33A)	110.4	C(46)-Re(42)-Re(41)	176.5(5)
C(34)-C(33)-H(33A)	110.4	C(49)-Re(42)-Re(41)	80.9(5)
O(20)-C(33)-H(33B)	110.4	C(47)-Re(42)-Re(41)	90.5(5)
C(34)-C(33)-H(33B)	110.4	C(48)-Re(42)-Re(41)	85.2(5)
H(33A)-C(33)-H(33B)	108.6	C(50)-Re(42)-Re(41)	89.1(4)
C(33)-C(34)-H(34A)	109.5	O(41)-C(41)-Re(41)	178(2)
C(33)-C(34)-H(34B)	109.5	O(42)-C(42)-Re(41)	178.5(17)
H(34A)-C(34)-H(34B)	109.5	O(43)-C(43)-Re(41)	178.5(18)
C(33)-C(34)-H(34C)	109.5	O(44)-C(44)-Re(41)	176.0(17)
H(34A)-C(34)-H(34C)	109.5	O(45)-C(45)-Re(41)	176.1(18)
H(34B)-C(34)-H(34C)	109.5	O(46)-C(46)-Re(42)	175.9(16)
C(41)-Re(41)-C(45)	91.0(8)	O(47)-C(47)-Re(42)	170.6(14)
C(41)-Re(41)-C(44)	92.8(7)	O(48)-C(48)-Re(42)	178.6(17)
C(45)-Re(41)-C(44)	90.3(8)	O(49)-C(49)-Re(42)	173.9(12)
C(41)-Re(41)-C(43)	92.4(8)	O(50)-C(50)-C(61)	104.2(12)

O(50)-C(50)-Re(42)	131.3(10)	O(54)-C(54)-Re(43)	177.0(15)
C(61)-C(50)-Re(42)	124.4(11)	O(55)-C(55)-Re(43)	175.8(19)
C(50)-O(50)-C(71)	122.7(12)	O(56)-C(56)-Re(44)	177.7(18)
C(51)-Re(43)-C(55)	88.2(7)	O(57)-C(57)-Re(44)	167.3(18)
C(51)-Re(43)-C(52)	92.7(7)	O(58)-C(58)-Re(44)	174(2)
C(55)-Re(43)-C(52)	90.8(8)	O(59)-C(59)-Re(44)	169.6(14)
C(51)-Re(43)-C(53)	95.9(7)	O(60)-C(60)-C(66)	106.3(13)
C(55)-Re(43)-C(53)	175.6(7)	O(60)-C(60)-Re(44)	130.4(10)
C(52)-Re(43)-C(53)	87.5(7)	C(66)-C(60)-Re(44)	123.3(11)
C(51)-Re(43)-C(54)	93.3(7)	C(60)-O(60)-C(73)	123.6(12)
C(55)-Re(43)-C(54)	93.2(7)	C(67)-Fe(41)-C(70)	67.8(8)
C(52)-Re(43)-C(54)	172.9(6)	C(67)-Fe(41)-C(65)	161.4(7)
C(53)-Re(43)-C(54)	88.1(7)	C(70)-Fe(41)-C(65)	122.5(9)
C(51)-Re(43)-Re(44)	170.8(5)	C(67)-Fe(41)-C(69)	67.3(9)
C(55)-Re(43)-Re(44)	84.3(6)	C(70)-Fe(41)-C(69)	39.8(7)
C(52)-Re(43)-Re(44)	92.8(5)	C(65)-Fe(41)-C(69)	109.6(9)
C(53)-Re(43)-Re(44)	91.7(5)	C(67)-Fe(41)-C(62)	106.6(7)
C(54)-Re(43)-Re(44)	81.8(5)	C(70)-Fe(41)-C(62)	160.9(7)
C(56)-Re(44)-C(59)	95.8(7)	C(65)-Fe(41)-C(62)	68.6(8)
C(56)-Re(44)-C(58)	93.2(8)	C(69)-Fe(41)-C(62)	156.8(8)
C(59)-Re(44)-C(58)	84.0(7)	C(67)-Fe(41)-C(63)	120.8(9)
C(56)-Re(44)-C(57)	93.0(7)	C(70)-Fe(41)-C(63)	125.0(7)
C(59)-Re(44)-C(57)	165.8(7)	C(65)-Fe(41)-C(63)	68.2(9)
C(58)-Re(44)-C(57)	84.4(8)	C(69)-Fe(41)-C(63)	161.9(10)
C(56)-Re(44)-C(60)	90.0(7)	C(62)-Fe(41)-C(63)	40.7(7)
C(59)-Re(44)-C(60)	93.2(6)	C(67)-Fe(41)-C(66)	40.5(6)
C(58)-Re(44)-C(60)	176.0(7)	C(70)-Fe(41)-C(66)	40.0(7)
C(57)-Re(44)-C(60)	97.9(6)	C(65)-Fe(41)-C(66)	157.0(7)
C(56)-Re(44)-Re(43)	170.0(5)	C(69)-Fe(41)-C(66)	66.9(7)
C(59)-Re(44)-Re(43)	79.9(4)	C(62)-Fe(41)-C(66)	124.0(7)
C(58)-Re(44)-Re(43)	95.2(5)	C(63)-Fe(41)-C(66)	107.7(7)
C(57)-Re(44)-Re(43)	93.1(5)	C(67)-Fe(41)-C(64)	155.9(8)
C(60)-Re(44)-Re(43)	81.4(4)	C(70)-Fe(41)-C(64)	108.3(9)
O(51)-C(51)-Re(43)	177.6(17)	C(65)-Fe(41)-C(64)	41.0(8)
O(52)-C(52)-Re(43)	174.7(17)	C(69)-Fe(41)-C(64)	126.0(12)
O(53)-C(53)-Re(43)	174.8(16)	C(62)-Fe(41)-C(64)	68.8(9)

C(63)-Fe(41)-C(64)	40.5(9)	Fe(41)-C(63)-H(63)	126.7
C(66)-Fe(41)-C(64)	121.1(7)	C(63)-C(64)-C(65)	106.9(17)
C(67)-Fe(41)-C(68)	41.0(7)	C(63)-C(64)-Fe(41)	69.5(11)
C(70)-Fe(41)-C(68)	67.5(9)	C(65)-C(64)-Fe(41)	69.0(11)
C(65)-Fe(41)-C(68)	124.8(8)	C(63)-C(64)-H(64)	126.6
C(69)-Fe(41)-C(68)	39.6(9)	C(65)-C(64)-H(64)	126.6
C(62)-Fe(41)-C(68)	121.1(9)	Fe(41)-C(64)-H(64)	126.5
C(63)-Fe(41)-C(68)	156.6(11)	C(64)-C(65)-C(61)	109.8(19)
C(66)-Fe(41)-C(68)	68.2(7)	C(64)-C(65)-Fe(41)	70.1(10)
C(64)-Fe(41)-C(68)	161.6(11)	C(61)-C(65)-Fe(41)	70.2(10)
C(67)-Fe(41)-C(61)	122.7(7)	C(64)-C(65)-H(65)	125.1
C(70)-Fe(41)-C(61)	157.5(8)	C(61)-C(65)-H(65)	125.1
C(65)-Fe(41)-C(61)	41.9(6)	Fe(41)-C(65)-H(65)	126.3
C(69)-Fe(41)-C(61)	121.9(7)	C(70)-C(66)-C(67)	106.4(14)
C(62)-Fe(41)-C(61)	41.0(6)	C(70)-C(66)-C(60)	125.8(16)
C(63)-Fe(41)-C(61)	69.3(7)	C(67)-C(66)-C(60)	127.7(17)
C(66)-Fe(41)-C(61)	159.9(7)	C(70)-C(66)-Fe(41)	68.7(10)
C(64)-Fe(41)-C(61)	70.3(7)	C(67)-C(66)-Fe(41)	67.8(9)
C(68)-Fe(41)-C(61)	106.3(7)	C(60)-C(66)-Fe(41)	125.5(11)
C(62)-C(61)-C(50)	127.9(15)	C(66)-C(67)-C(68)	109.3(19)
C(62)-C(61)-C(65)	104.4(15)	C(66)-C(67)-Fe(41)	71.7(10)
C(50)-C(61)-C(65)	127.6(16)	C(68)-C(67)-Fe(41)	72.1(12)
C(62)-C(61)-Fe(41)	68.5(9)	C(66)-C(67)-H(67)	125.4
C(50)-C(61)-Fe(41)	125.2(12)	C(68)-C(67)-H(67)	125.4
C(65)-C(61)-Fe(41)	67.9(9)	Fe(41)-C(67)-H(67)	122.4
C(63)-C(62)-C(61)	109.8(18)	C(69)-C(68)-C(67)	105.3(19)
C(63)-C(62)-Fe(41)	69.8(11)	C(69)-C(68)-Fe(41)	69.2(15)
C(61)-C(62)-Fe(41)	70.5(10)	C(67)-C(68)-Fe(41)	66.8(10)
C(63)-C(62)-H(62)	125.1	C(69)-C(68)-H(68)	127.4
C(61)-C(62)-H(62)	125.1	C(67)-C(68)-H(68)	127.4
Fe(41)-C(62)-H(62)	126.2	Fe(41)-C(68)-H(68)	128.0
C(64)-C(63)-C(62)	109.1(18)	C(70)-C(69)-C(68)	109.9(19)
C(64)-C(63)-Fe(41)	70.0(13)	C(70)-C(69)-Fe(41)	69.0(12)
C(62)-C(63)-Fe(41)	69.5(10)	C(68)-C(69)-Fe(41)	71.2(13)
C(64)-C(63)-H(63)	125.4	C(70)-C(69)-H(69)	125.1
C(62)-C(63)-H(63)	125.4	C(68)-C(69)-H(69)	125.1

Fe(41)-C(69)-H(69)	126.3	C(71)-C(72)-H(72C)	109.5
C(69)-C(70)-C(66)	108.9(19)	H(72A)-C(72)-H(72C)	109.5
C(69)-C(70)-Fe(41)	71.2(12)	H(72B)-C(72)-H(72C)	109.5
C(66)-C(70)-Fe(41)	71.3(10)	O(60)-C(73)-C(74)	108.1(16)
C(69)-C(70)-H(70)	125.5	O(60)-C(73)-H(73A)	110.1
C(66)-C(70)-H(70)	125.5	C(74)-C(73)-H(73A)	110.1
Fe(41)-C(70)-H(70)	123.6	O(60)-C(73)-H(73B)	110.1
O(50)-C(71)-C(72)	106.5(15)	C(74)-C(73)-H(73B)	110.1
O(50)-C(71)-H(71A)	110.4	H(73A)-C(73)-H(73B)	108.4
C(72)-C(71)-H(71A)	110.4	C(73)-C(74)-H(74A)	109.5
O(50)-C(71)-H(71B)	110.4	C(73)-C(74)-H(74B)	109.5
C(72)-C(71)-H(71B)	110.4	H(74A)-C(74)-H(74B)	109.5
H(71A)-C(71)-H(71B)	108.6	C(73)-C(74)-H(74C)	109.5
C(71)-C(72)-H(72A)	109.5	H(74A)-C(74)-H(74C)	109.5
C(71)-C(72)-H(72B)	109.5	H(74B)-C(74)-H(74C)	109.5
H(72A)-C(72)-H(72B)	109.5		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for Complex **27**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Re(1)	45(1)	48(1)	45(1)	8(1)	5(1)	9(1)
Re(2)	47(1)	48(1)	48(1)	10(1)	5(1)	11(1)
C(1)	80(14)	65(12)	67(11)	11(9)	7(10)	29(11)
O(1)	107(12)	82(9)	96(9)	28(8)	47(9)	45(9)
C(2)	61(11)	54(10)	59(9)	12(8)	17(9)	21(9)
O(2)	87(10)	68(9)	112(11)	4(8)	-14(9)	-21(8)
C(3)	120(20)	110(18)	58(11)	30(11)	19(12)	5(15)
O(3)	116(13)	133(13)	69(8)	50(9)	15(8)	22(10)
C(4)	53(11)	62(11)	57(9)	-5(8)	6(8)	11(9)
O(4)	55(8)	104(11)	92(9)	-15(8)	16(7)	-7(8)
C(5)	130(20)	74(14)	61(12)	-7(10)	1(12)	-10(13)
O(5)	128(13)	92(10)	63(8)	24(7)	6(8)	0(9)
C(6)	80(14)	59(11)	67(11)	12(9)	7(10)	15(10)
O(6)	66(9)	88(10)	116(11)	9(8)	22(8)	33(8)
C(7)	108(17)	82(14)	49(10)	16(9)	20(10)	-2(12)
O(7)	113(12)	87(9)	60(7)	28(7)	5(7)	18(8)
C(8)	72(14)	53(11)	105(15)	15(10)	-2(12)	18(10)
O(8)	132(15)	110(13)	118(12)	-14(10)	-55(11)	-11(11)
C(9)	66(12)	54(11)	63(10)	4(8)	-4(9)	10(9)
O(9)	98(11)	65(9)	92(9)	27(7)	16(8)	-8(8)
C(10)	39(9)	49(9)	59(9)	12(7)	6(7)	13(7)
O(10)	62(8)	58(7)	62(6)	15(5)	4(6)	-2(6)
Re(3)	55(1)	57(1)	56(1)	20(1)	18(1)	16(1)
Re(4)	43(1)	47(1)	45(1)	11(1)	6(1)	4(1)
C(11)	84(14)	86(13)	52(9)	27(9)	38(9)	16(12)
O(11)	91(11)	120(12)	112(11)	31(9)	41(9)	56(10)
C(12)	52(11)	75(12)	67(10)	22(9)	24(9)	-4(9)
O(12)	95(11)	116(11)	61(7)	33(7)	19(7)	17(9)
C(13)	95(17)	67(13)	95(15)	0(11)	60(13)	9(12)
O(13)	121(15)	122(14)	153(16)	-63(12)	48(12)	-52(12)
C(14)	77(14)	113(16)	90(13)	58(12)	59(11)	60(13)
O(14)	200(20)	116(12)	112(12)	79(10)	88(12)	76(13)

C(15)	46(11)	92(15)	85(13)	36(11)	14(10)	18(11)
O(15)	60(10)	135(14)	113(12)	-19(10)	-9(9)	18(9)
C(16)	68(12)	54(10)	67(10)	0(8)	4(9)	18(9)
O(16)	81(10)	90(10)	100(10)	9(8)	6(8)	39(8)
C(17)	73(12)	62(11)	50(9)	18(8)	1(9)	6(9)
O(17)	91(11)	82(9)	92(9)	38(8)	24(8)	-8(8)
C(18)	63(12)	72(12)	52(9)	15(8)	8(8)	-15(9)
O(18)	115(13)	123(12)	56(8)	16(8)	8(8)	-16(10)
C(19)	53(10)	64(11)	46(8)	-7(8)	8(8)	-7(9)
O(19)	83(10)	60(8)	76(8)	0(6)	17(7)	-19(7)
C(20)	37(8)	43(8)	53(8)	10(7)	-6(7)	3(7)
O(20)	47(7)	60(7)	69(7)	15(6)	5(6)	-5(6)
Fe(1)	49(1)	57(1)	41(1)	10(1)	8(1)	8(1)
C(21)	55(10)	63(10)	44(8)	15(7)	8(7)	5(8)
C(22)	61(11)	56(10)	43(8)	3(7)	17(8)	7(8)
C(23)	102(17)	71(13)	59(10)	18(9)	8(11)	33(12)
C(24)	81(15)	121(18)	51(10)	21(11)	-1(10)	57(14)
C(25)	43(10)	105(15)	57(10)	6(9)	17(8)	15(10)
C(26)	51(10)	37(8)	67(9)	20(7)	26(8)	23(7)
C(27)	100(16)	66(12)	48(9)	14(8)	30(10)	-1(11)
C(28)	140(20)	62(13)	61(11)	2(9)	39(13)	-6(13)
C(29)	120(19)	78(14)	59(11)	33(10)	43(12)	41(13)
C(30)	73(13)	66(11)	60(10)	21(9)	22(9)	22(10)
C(31)	67(12)	65(11)	55(9)	24(8)	35(8)	0(9)
C(32)	100(18)	96(17)	114(17)	41(13)	24(14)	-20(14)
C(33)	71(13)	64(12)	71(11)	18(9)	-6(10)	-4(10)
C(34)	130(20)	60(13)	121(18)	15(12)	-11(16)	-40(14)
Re(41)	50(1)	48(1)	62(1)	11(1)	-9(1)	-2(1)
Re(42)	40(1)	50(1)	45(1)	8(1)	1(1)	4(1)
C(41)	77(14)	61(12)	86(12)	29(10)	-23(11)	-11(11)
O(41)	73(10)	88(10)	135(12)	20(9)	-15(9)	-44(9)
C(42)	43(10)	66(11)	77(11)	10(9)	-13(9)	6(9)
O(42)	115(13)	96(11)	103(10)	47(9)	-41(10)	-23(9)
C(43)	70(13)	50(11)	92(13)	4(10)	-30(11)	-9(10)
O(43)	129(15)	111(13)	140(15)	-43(11)	-29(12)	67(12)
C(44)	39(10)	91(14)	67(11)	14(10)	-15(8)	6(9)

O(44)	88(11)	118(12)	95(10)	52(9)	-29(8)	-14(9)
C(45)	80(15)	92(16)	71(12)	6(11)	7(11)	-48(13)
O(45)	83(11)	105(12)	128(13)	-4(10)	55(10)	8(9)
C(46)	37(9)	67(12)	91(12)	20(10)	3(9)	-14(9)
O(46)	58(9)	105(11)	115(11)	17(9)	0(8)	-29(8)
C(47)	48(10)	46(9)	63(9)	0(8)	13(8)	14(8)
O(47)	98(11)	71(9)	100(10)	33(7)	-18(8)	16(8)
C(48)	55(10)	73(11)	33(7)	5(7)	4(7)	21(9)
O(48)	94(11)	114(11)	59(8)	25(7)	15(7)	27(9)
C(49)	65(11)	56(10)	34(7)	-3(7)	0(7)	-3(9)
O(49)	61(8)	64(8)	66(7)	2(6)	-9(6)	19(6)
C(50)	39(8)	44(8)	42(7)	-1(6)	-6(7)	-9(7)
O(50)	66(8)	65(7)	57(6)	10(5)	9(6)	26(6)
Re(43)	45(1)	43(1)	50(1)	8(1)	-2(1)	-4(1)
Re(44)	49(1)	43(1)	45(1)	8(1)	3(1)	-6(1)
C(51)	70(13)	69(12)	58(10)	17(9)	-9(9)	9(10)
O(51)	105(12)	83(10)	136(13)	41(9)	-60(11)	-41(9)
C(52)	47(10)	69(12)	71(11)	9(9)	-8(9)	-8(9)
O(52)	71(9)	120(12)	74(8)	-21(8)	4(7)	41(9)
C(53)	77(13)	74(12)	47(9)	10(8)	0(9)	-25(10)
O(53)	101(11)	115(11)	75(8)	41(8)	-14(8)	-28(9)
C(54)	74(13)	61(12)	68(11)	21(9)	-21(10)	-16(10)
O(54)	90(11)	55(8)	122(11)	-6(8)	8(9)	30(8)
C(55)	103(17)	58(12)	57(10)	-3(9)	1(11)	-8(11)
O(55)	120(13)	95(10)	54(7)	19(7)	-2(8)	-10(9)
C(56)	62(12)	59(11)	76(11)	11(9)	2(10)	-4(10)
O(56)	79(10)	92(11)	139(13)	19(9)	-41(10)	-30(9)
C(57)	50(10)	87(13)	54(9)	16(9)	-2(8)	-11(10)
O(57)	160(15)	68(9)	68(8)	28(7)	-28(9)	-30(9)
C(58)	69(13)	67(12)	76(12)	1(10)	30(10)	-12(10)
O(58)	124(14)	111(13)	123(13)	-21(10)	71(11)	-4(11)
C(59)	34(9)	61(11)	60(9)	7(8)	6(7)	2(8)
O(59)	77(9)	53(7)	90(8)	15(6)	-8(7)	7(7)
C(60)	53(10)	52(9)	42(7)	10(7)	-5(7)	8(8)
O(60)	71(8)	57(7)	46(6)	4(5)	-12(5)	14(6)
Fe(41)	58(2)	70(2)	37(1)	7(1)	2(1)	-5(1)

C(61)	50(11)	73(12)	61(10)	-7(8)	10(8)	9(9)
C(62)	66(12)	43(9)	76(11)	0(8)	-4(10)	-17(9)
C(63)	107(18)	59(12)	76(13)	17(10)	-44(13)	-8(12)
C(64)	140(20)	78(15)	90(15)	-20(11)	-76(16)	51(15)
C(65)	67(13)	134(18)	44(9)	-15(10)	-14(9)	16(12)
C(66)	72(12)	56(10)	36(7)	8(7)	-6(8)	-16(9)
C(67)	86(14)	50(10)	57(9)	13(8)	-6(9)	-12(9)
C(68)	150(20)	85(15)	51(10)	26(10)	-8(13)	-57(16)
C(69)	92(18)	180(30)	54(11)	36(14)	9(12)	-56(19)
C(70)	59(13)	105(16)	80(13)	18(12)	-11(11)	-16(12)
C(71)	54(11)	49(10)	85(12)	11(9)	9(9)	17(8)
C(72)	109(19)	79(15)	112(17)	8(13)	9(15)	33(14)
C(73)	80(14)	70(12)	78(12)	10(10)	-18(10)	34(11)
C(74)	210(30)	82(17)	130(20)	34(15)	20(20)	60(19)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Complex **27**.

	x	y	z	U(eq)
H(22)	7284	1969	1654	64
H(23)	6590	1853	251	92
H(24)	5236	983	248	100
H(25)	5083	543	1624	82
H(27)	6354	-722	-275	84
H(28)	6201	-1197	1120	106
H(29)	7433	-539	1968	100
H(30)	8361	266	1161	78
H(31A)	5684	542	4147	72
H(31B)	6425	-90	3846	72
H(32A)	5176	-856	4042	151
H(32B)	5403	-1002	3116	151
H(32C)	4668	-376	3422	151
H(33A)	8129	1930	-781	82
H(33B)	9046	1516	-878	82
H(34A)	9148	2792	-25	157
H(34B)	9389	2056	468	157
H(34C)	8480	2473	558	157
H(62)	6739	5083	975	75
H(63)	7835	4464	1832	97
H(64)	9204	4255	1062	129
H(65)	8942	4733	-304	102
H(67)	7380	6886	1776	76
H(68)	7985	7198	451	113
H(69)	9503	6721	445	129
H(70)	9841	6175	1725	98
H(71A)	5887	6290	-1119	75
H(71B)	6652	6931	-885	75
H(72A)	5391	7495	-301	151
H(72B)	6052	7341	391	151
H(72C)	5288	6708	153	151
H(73A)	8616	4941	3769	92

H(73B)	9393	5534	4095	92
H(74A)	9838	4147	3865	209
H(74B)	10312	4674	3281	209
H(74C)	9539	4087	2948	209

Table 6. Torsion angles [°] for Complex **27**.

C(5)-Re(1)-Re(2)-C(8)	-66.7(8)	C(13)-Re(3)-Re(4)-C(18)	-44.2(7)
C(4)-Re(1)-Re(2)-C(8)	-159.5(8)	C(14)-Re(3)-Re(4)-C(18)	-134.2(9)
C(2)-Re(1)-Re(2)-C(8)	24.4(7)	C(15)-Re(3)-Re(4)-C(18)	135.2(7)
C(3)-Re(1)-Re(2)-C(8)	113.5(9)	C(12)-Re(3)-Re(4)-C(20)	-133.4(7)
C(5)-Re(1)-Re(2)-C(9)	-147.6(8)	C(13)-Re(3)-Re(4)-C(20)	136.5(7)
C(4)-Re(1)-Re(2)-C(9)	119.6(7)	C(14)-Re(3)-Re(4)-C(20)	46.5(8)
C(2)-Re(1)-Re(2)-C(9)	-56.4(6)	C(15)-Re(3)-Re(4)-C(20)	-44.2(7)
C(3)-Re(1)-Re(2)-C(9)	32.7(8)	C(16)-Re(4)-C(20)-O(20)	-91.6(14)
C(5)-Re(1)-Re(2)-C(7)	16.9(8)	C(17)-Re(4)-C(20)-O(20)	3.5(14)
C(4)-Re(1)-Re(2)-C(7)	-75.9(7)	C(19)-Re(4)-C(20)-O(20)	172.6(13)
C(2)-Re(1)-Re(2)-C(7)	108.0(7)	Re(3)-Re(4)-C(20)-O(20)	90.5(13)
C(3)-Re(1)-Re(2)-C(7)	-162.9(9)	C(16)-Re(4)-C(20)-C(26)	87.9(13)
C(5)-Re(1)-Re(2)-C(10)	114.9(7)	C(17)-Re(4)-C(20)-C(26)	-177.0(12)
C(4)-Re(1)-Re(2)-C(10)	22.1(6)	C(19)-Re(4)-C(20)-C(26)	-8.0(13)
C(2)-Re(1)-Re(2)-C(10)	-154.0(6)	Re(3)-Re(4)-C(20)-C(26)	-90.1(12)
C(3)-Re(1)-Re(2)-C(10)	-64.9(8)	C(26)-C(20)-O(20)-C(33)	-165.8(14)
C(6)-Re(2)-C(10)-O(10)	91.6(14)	Re(4)-C(20)-O(20)-C(33)	14(2)
C(9)-Re(2)-C(10)-O(10)	-173.1(13)	O(10)-C(10)-C(21)-C(22)	-161.1(16)
C(7)-Re(2)-C(10)-O(10)	-3.3(14)	Re(2)-C(10)-C(21)-C(22)	17(2)
C(6)-Re(2)-C(10)-C(21)	-86.2(14)	O(10)-C(10)-C(21)-C(25)	18(2)
C(9)-Re(2)-C(10)-C(21)	9.1(14)	Re(2)-C(10)-C(21)-C(25)	-164.0(12)
C(7)-Re(2)-C(10)-C(21)	178.9(14)	O(10)-C(10)-C(21)-Fe(1)	-69.2(16)
Re(1)-Re(2)-C(10)-C(21)	89.6(13)	Re(2)-C(10)-C(21)-Fe(1)	109.1(14)
C(21)-C(10)-O(10)-C(31)	176.8(13)	C(25)-Fe(1)-C(21)-C(22)	-118.5(14)
Re(2)-C(10)-O(10)-C(31)	-1(2)	C(30)-Fe(1)-C(21)-C(22)	80.0(11)
C(12)-Re(3)-Re(4)-C(17)	-35.7(7)	C(27)-Fe(1)-C(21)-C(22)	-167.2(19)
C(13)-Re(3)-Re(4)-C(17)	-125.8(7)	C(26)-Fe(1)-C(21)-C(22)	46.4(19)
C(14)-Re(3)-Re(4)-C(17)	144.2(9)	C(29)-Fe(1)-C(21)-C(22)	121.9(11)
C(15)-Re(3)-Re(4)-C(17)	53.6(7)	C(23)-Fe(1)-C(21)-C(22)	-37.4(11)
C(12)-Re(3)-Re(4)-C(19)	133.2(7)	C(24)-Fe(1)-C(21)-C(22)	-81.4(11)
C(13)-Re(3)-Re(4)-C(19)	43.1(7)	C(28)-Fe(1)-C(21)-C(22)	162.7(11)
C(14)-Re(3)-Re(4)-C(19)	-46.9(8)	C(22)-Fe(1)-C(21)-C(10)	-124.4(19)
C(15)-Re(3)-Re(4)-C(19)	-137.5(7)	C(25)-Fe(1)-C(21)-C(10)	117.1(19)
C(12)-Re(3)-Re(4)-C(18)	45.9(7)	C(30)-Fe(1)-C(21)-C(10)	-44.4(17)

C(27)-Fe(1)-C(21)-C(10)	68(3)	Fe(1)-C(22)-C(23)-C(24)	58.5(13)
C(26)-Fe(1)-C(21)-C(10)	-78(2)	C(21)-C(22)-C(23)-Fe(1)	-59.0(11)
C(29)-Fe(1)-C(21)-C(10)	-2.5(17)	C(25)-Fe(1)-C(23)-C(22)	83.5(11)
C(23)-Fe(1)-C(21)-C(10)	-161.9(17)	C(30)-Fe(1)-C(23)-C(22)	-77.4(12)
C(24)-Fe(1)-C(21)-C(10)	154.2(17)	C(27)-Fe(1)-C(23)-C(22)	-161.7(11)
C(28)-Fe(1)-C(21)-C(10)	38.2(18)	C(21)-Fe(1)-C(23)-C(22)	37.5(10)
C(22)-Fe(1)-C(21)-C(25)	118.5(14)	C(26)-Fe(1)-C(23)-C(22)	-120.4(11)
C(30)-Fe(1)-C(21)-C(25)	-161.5(10)	C(29)-Fe(1)-C(23)-C(22)	-48(3)
C(27)-Fe(1)-C(21)-C(25)	-49(2)	C(24)-Fe(1)-C(23)-C(22)	119.9(16)
C(26)-Fe(1)-C(21)-C(25)	164.9(15)	C(28)-Fe(1)-C(23)-C(22)	164.4(19)
C(29)-Fe(1)-C(21)-C(25)	-119.6(12)	C(22)-Fe(1)-C(23)-C(24)	-119.9(16)
C(23)-Fe(1)-C(21)-C(25)	81.1(11)	C(25)-Fe(1)-C(23)-C(24)	-36.3(10)
C(24)-Fe(1)-C(21)-C(25)	37.1(11)	C(30)-Fe(1)-C(23)-C(24)	162.7(10)
C(28)-Fe(1)-C(21)-C(25)	-78.8(13)	C(27)-Fe(1)-C(23)-C(24)	78.4(13)
C(10)-C(21)-C(22)-C(23)	-179.9(16)	C(21)-Fe(1)-C(23)-C(24)	-82.4(11)
C(25)-C(21)-C(22)-C(23)	1.1(18)	C(26)-Fe(1)-C(23)-C(24)	119.7(11)
Fe(1)-C(21)-C(22)-C(23)	59.3(11)	C(29)-Fe(1)-C(23)-C(24)	-168.2(18)
C(10)-C(21)-C(22)-Fe(1)	120.8(17)	C(28)-Fe(1)-C(23)-C(24)	45(3)
C(25)-C(21)-C(22)-Fe(1)	-58.2(11)	C(22)-C(23)-C(24)-C(25)	0(2)
C(25)-Fe(1)-C(22)-C(21)	39.5(9)	Fe(1)-C(23)-C(24)-C(25)	57.5(13)
C(30)-Fe(1)-C(22)-C(21)	-118.3(9)	C(22)-C(23)-C(24)-Fe(1)	-57.8(12)
C(27)-Fe(1)-C(22)-C(21)	167(2)	C(22)-Fe(1)-C(24)-C(25)	-83.6(12)
C(26)-Fe(1)-C(22)-C(21)	-161.9(9)	C(30)-Fe(1)-C(24)-C(25)	-167(2)
C(29)-Fe(1)-C(22)-C(21)	-77.4(12)	C(27)-Fe(1)-C(24)-C(25)	118.5(12)
C(23)-Fe(1)-C(22)-C(21)	120.3(15)	C(21)-Fe(1)-C(24)-C(25)	-39.3(11)
C(24)-Fe(1)-C(22)-C(21)	82.8(10)	C(26)-Fe(1)-C(24)-C(25)	160.4(11)
C(28)-Fe(1)-C(22)-C(21)	-44(3)	C(29)-Fe(1)-C(24)-C(25)	48(3)
C(25)-Fe(1)-C(22)-C(23)	-80.8(12)	C(23)-Fe(1)-C(24)-C(25)	-121.4(17)
C(30)-Fe(1)-C(22)-C(23)	121.4(12)	C(28)-Fe(1)-C(24)-C(25)	76.2(14)
C(27)-Fe(1)-C(22)-C(23)	47(3)	C(22)-Fe(1)-C(24)-C(23)	37.7(10)
C(21)-Fe(1)-C(22)-C(23)	-120.3(15)	C(25)-Fe(1)-C(24)-C(23)	121.4(17)
C(26)-Fe(1)-C(22)-C(23)	77.8(13)	C(30)-Fe(1)-C(24)-C(23)	-46(3)
C(29)-Fe(1)-C(22)-C(23)	162.3(12)	C(27)-Fe(1)-C(24)-C(23)	-120.1(11)
C(24)-Fe(1)-C(22)-C(23)	-37.5(11)	C(21)-Fe(1)-C(24)-C(23)	82.0(11)
C(28)-Fe(1)-C(22)-C(23)	-164(2)	C(26)-Fe(1)-C(24)-C(23)	-78.3(13)
C(21)-C(22)-C(23)-C(24)	0(2)	C(29)-Fe(1)-C(24)-C(23)	169.5(18)

C(28)-Fe(1)-C(24)-C(23)	-162.4(10)	C(23)-Fe(1)-C(26)-C(27)	-121.0(11)
C(23)-C(24)-C(25)-C(21)	1(2)	C(24)-Fe(1)-C(26)-C(27)	-78.8(13)
Fe(1)-C(24)-C(25)-C(21)	58.6(12)	C(28)-Fe(1)-C(26)-C(27)	36.8(11)
C(23)-C(24)-C(25)-Fe(1)	-57.7(13)	C(22)-Fe(1)-C(26)-C(30)	79.4(11)
C(22)-C(21)-C(25)-C(24)	-1.2(19)	C(25)-Fe(1)-C(26)-C(30)	-162.1(17)
C(10)-C(21)-C(25)-C(24)	179.7(15)	C(27)-Fe(1)-C(26)-C(30)	-117.2(13)
Fe(1)-C(21)-C(25)-C(24)	-59.8(12)	C(21)-Fe(1)-C(26)-C(30)	44.8(19)
C(22)-C(21)-C(25)-Fe(1)	58.6(11)	C(29)-Fe(1)-C(26)-C(30)	-38.1(11)
C(10)-C(21)-C(25)-Fe(1)	-120.5(15)	C(23)-Fe(1)-C(26)-C(30)	121.8(11)
C(22)-Fe(1)-C(25)-C(24)	81.1(13)	C(24)-Fe(1)-C(26)-C(30)	164.0(12)
C(30)-Fe(1)-C(25)-C(24)	168(2)	C(28)-Fe(1)-C(26)-C(30)	-80.5(11)
C(27)-Fe(1)-C(25)-C(24)	-79.3(14)	C(22)-Fe(1)-C(26)-C(20)	-39.7(15)
C(21)-Fe(1)-C(25)-C(24)	119.2(17)	C(25)-Fe(1)-C(26)-C(20)	79(2)
C(26)-Fe(1)-C(25)-C(24)	-47(2)	C(30)-Fe(1)-C(26)-C(20)	-119.1(17)
C(29)-Fe(1)-C(25)-C(24)	-160.5(14)	C(27)-Fe(1)-C(26)-C(20)	123.7(17)
C(23)-Fe(1)-C(25)-C(24)	36.9(12)	C(21)-Fe(1)-C(26)-C(20)	-74(2)
C(28)-Fe(1)-C(25)-C(24)	-121.0(14)	C(29)-Fe(1)-C(26)-C(20)	-157.1(16)
C(22)-Fe(1)-C(25)-C(21)	-38.1(9)	C(23)-Fe(1)-C(26)-C(20)	2.7(15)
C(30)-Fe(1)-C(25)-C(21)	49(3)	C(24)-Fe(1)-C(26)-C(20)	44.9(17)
C(27)-Fe(1)-C(25)-C(21)	161.5(9)	C(28)-Fe(1)-C(26)-C(20)	160.4(16)
C(26)-Fe(1)-C(25)-C(21)	-166.0(14)	C(30)-C(26)-C(27)-C(28)	-1.3(19)
C(29)-Fe(1)-C(25)-C(21)	80.3(13)	C(20)-C(26)-C(27)-C(28)	-175.5(15)
C(23)-Fe(1)-C(25)-C(21)	-82.3(10)	Fe(1)-C(26)-C(27)-C(28)	-60.8(13)
C(24)-Fe(1)-C(25)-C(21)	-119.2(17)	C(30)-C(26)-C(27)-Fe(1)	59.5(10)
C(28)-Fe(1)-C(25)-C(21)	119.8(10)	C(20)-C(26)-C(27)-Fe(1)	-114.8(15)
O(20)-C(20)-C(26)-C(27)	156.1(15)	C(22)-Fe(1)-C(27)-C(26)	42(3)
Re(4)-C(20)-C(26)-C(27)	-23(2)	C(25)-Fe(1)-C(27)-C(26)	161.1(9)
O(20)-C(20)-C(26)-C(30)	-17.1(19)	C(30)-Fe(1)-C(27)-C(26)	-39.8(9)
Re(4)-C(20)-C(26)-C(30)	163.3(11)	C(21)-Fe(1)-C(27)-C(26)	-162.0(16)
O(20)-C(20)-C(26)-Fe(1)	67.9(15)	C(29)-Fe(1)-C(27)-C(26)	-83.5(11)
Re(4)-C(20)-C(26)-Fe(1)	-111.7(12)	C(23)-Fe(1)-C(27)-C(26)	76.8(13)
C(22)-Fe(1)-C(26)-C(27)	-163.4(10)	C(24)-Fe(1)-C(27)-C(26)	119.2(11)
C(25)-Fe(1)-C(26)-C(27)	-45(2)	C(28)-Fe(1)-C(27)-C(26)	-121.3(17)
C(30)-Fe(1)-C(26)-C(27)	117.2(13)	C(22)-Fe(1)-C(27)-C(28)	163(2)
C(21)-Fe(1)-C(26)-C(27)	162.1(15)	C(25)-Fe(1)-C(27)-C(28)	-77.5(15)
C(29)-Fe(1)-C(26)-C(27)	79.2(12)	C(30)-Fe(1)-C(27)-C(28)	81.5(14)

C(21)-Fe(1)-C(27)-C(28)	-41(3)	C(25)-Fe(1)-C(29)-C(30)	-163.0(10)
C(26)-Fe(1)-C(27)-C(28)	121.3(17)	C(27)-Fe(1)-C(29)-C(30)	83.6(12)
C(29)-Fe(1)-C(27)-C(28)	37.8(13)	C(21)-Fe(1)-C(29)-C(30)	-118.1(11)
C(23)-Fe(1)-C(27)-C(28)	-161.9(14)	C(26)-Fe(1)-C(29)-C(30)	39.7(11)
C(24)-Fe(1)-C(27)-C(28)	-119.4(14)	C(23)-Fe(1)-C(29)-C(30)	-39(3)
C(26)-C(27)-C(28)-C(29)	2(2)	C(24)-Fe(1)-C(29)-C(30)	161.9(17)
Fe(1)-C(27)-C(28)-C(29)	-57.7(13)	C(28)-Fe(1)-C(29)-C(30)	122.9(16)
C(26)-C(27)-C(28)-Fe(1)	59.2(12)	C(28)-C(29)-C(30)-C(26)	1(2)
C(22)-Fe(1)-C(28)-C(29)	-46(3)	Fe(1)-C(29)-C(30)-C(26)	-59.8(11)
C(25)-Fe(1)-C(28)-C(29)	-122.7(11)	C(28)-C(29)-C(30)-Fe(1)	60.3(15)
C(30)-Fe(1)-C(28)-C(29)	35.7(11)	C(27)-C(26)-C(30)-C(29)	0.5(18)
C(27)-Fe(1)-C(28)-C(29)	117.4(18)	C(20)-C(26)-C(30)-C(29)	175.0(14)
C(21)-Fe(1)-C(28)-C(29)	-78.6(13)	Fe(1)-C(26)-C(30)-C(29)	60.5(12)
C(26)-Fe(1)-C(28)-C(29)	81.0(12)	C(27)-C(26)-C(30)-Fe(1)	-60.1(11)
C(23)-Fe(1)-C(28)-C(29)	163(2)	C(20)-C(26)-C(30)-Fe(1)	114.5(14)
C(24)-Fe(1)-C(28)-C(29)	-163.7(11)	C(22)-Fe(1)-C(30)-C(29)	122.8(12)
C(22)-Fe(1)-C(28)-C(27)	-163.3(19)	C(25)-Fe(1)-C(30)-C(29)	43(3)
C(25)-Fe(1)-C(28)-C(27)	119.8(13)	C(27)-Fe(1)-C(30)-C(29)	-79.2(12)
C(30)-Fe(1)-C(28)-C(27)	-81.7(13)	C(21)-Fe(1)-C(30)-C(29)	79.9(14)
C(21)-Fe(1)-C(28)-C(27)	164.0(12)	C(26)-Fe(1)-C(30)-C(29)	-117.6(16)
C(26)-Fe(1)-C(28)-C(27)	-36.4(12)	C(23)-Fe(1)-C(30)-C(29)	165.3(12)
C(29)-Fe(1)-C(28)-C(27)	-117.4(18)	C(24)-Fe(1)-C(30)-C(29)	-160(2)
C(23)-Fe(1)-C(28)-C(27)	46(3)	C(28)-Fe(1)-C(30)-C(29)	-35.0(11)
C(24)-Fe(1)-C(28)-C(27)	78.9(14)	C(22)-Fe(1)-C(30)-C(26)	-119.6(9)
C(27)-C(28)-C(29)-C(30)	-1(2)	C(25)-Fe(1)-C(30)-C(26)	160.6(19)
Fe(1)-C(28)-C(29)-C(30)	-58.3(13)	C(27)-Fe(1)-C(30)-C(26)	38.4(9)
C(27)-C(28)-C(29)-Fe(1)	57.0(13)	C(21)-Fe(1)-C(30)-C(26)	-162.6(9)
C(22)-Fe(1)-C(29)-C(28)	161.6(10)	C(29)-Fe(1)-C(30)-C(26)	117.6(16)
C(25)-Fe(1)-C(29)-C(28)	74.1(13)	C(23)-Fe(1)-C(30)-C(26)	-77.1(12)
C(30)-Fe(1)-C(29)-C(28)	-122.9(16)	C(24)-Fe(1)-C(30)-C(26)	-43(3)
C(27)-Fe(1)-C(29)-C(28)	-39.3(11)	C(28)-Fe(1)-C(30)-C(26)	82.6(10)
C(21)-Fe(1)-C(29)-C(28)	119.0(11)	C(10)-O(10)-C(31)-C(32)	178.7(14)
C(26)-Fe(1)-C(29)-C(28)	-83.2(12)	C(20)-O(20)-C(33)-C(34)	165.7(16)
C(23)-Fe(1)-C(29)-C(28)	-161.9(19)	C(45)-Re(41)-Re(42)-C(49)	134.3(7)
C(24)-Fe(1)-C(29)-C(28)	39(2)	C(44)-Re(41)-Re(42)-C(49)	-135.3(7)
C(22)-Fe(1)-C(29)-C(30)	-75.5(12)	C(43)-Re(41)-Re(42)-C(49)	-45.7(7)

C(42)-Re(41)-Re(42)-C(49)	44.4(6)	C(52)-Re(43)-Re(44)-C(60)	-24.7(6)
C(45)-Re(41)-Re(42)-C(47)	-54.5(7)	C(53)-Re(43)-Re(44)-C(60)	62.9(7)
C(44)-Re(41)-Re(42)-C(47)	35.8(7)	C(54)-Re(43)-Re(44)-C(60)	150.7(6)
C(43)-Re(41)-Re(42)-C(47)	125.5(7)	C(56)-Re(44)-C(60)-O(60)	-90.3(15)
C(42)-Re(41)-Re(42)-C(47)	-144.5(7)	C(59)-Re(44)-C(60)-O(60)	173.9(15)
C(45)-Re(41)-Re(42)-C(48)	-137.7(7)	C(57)-Re(44)-C(60)-O(60)	2.7(15)
C(44)-Re(41)-Re(42)-C(48)	-47.4(7)	Re(43)-Re(44)-C(60)-O(60)	94.7(14)
C(43)-Re(41)-Re(42)-C(48)	42.2(7)	C(56)-Re(44)-C(60)-C(66)	87.5(13)
C(42)-Re(41)-Re(42)-C(48)	132.3(7)	C(59)-Re(44)-C(60)-C(66)	-8.3(13)
C(45)-Re(41)-Re(42)-C(50)	42.8(7)	C(57)-Re(44)-C(60)-C(66)	-179.5(13)
C(44)-Re(41)-Re(42)-C(50)	133.1(7)	Re(43)-Re(44)-C(60)-C(66)	-87.5(12)
C(43)-Re(41)-Re(42)-C(50)	-137.2(7)	C(66)-C(60)-O(60)-C(73)	-177.1(14)
C(42)-Re(41)-Re(42)-C(50)	-47.2(6)	Re(44)-C(60)-O(60)-C(73)	1(2)
C(46)-Re(42)-C(50)-O(50)	100.6(14)	O(50)-C(50)-C(61)-C(62)	27(2)
C(49)-Re(42)-C(50)-O(50)	-163.6(14)	Re(42)-C(50)-C(61)-C(62)	-150.7(14)
C(47)-Re(42)-C(50)-O(50)	7.6(15)	O(50)-C(50)-C(61)-C(65)	-149.5(18)
Re(41)-Re(42)-C(50)-O(50)	-82.8(13)	Re(42)-C(50)-C(61)-C(65)	33(2)
C(46)-Re(42)-C(50)-C(61)	-82.2(14)	O(50)-C(50)-C(61)-Fe(41)	-61.8(16)
C(49)-Re(42)-C(50)-C(61)	13.6(14)	Re(42)-C(50)-C(61)-Fe(41)	120.4(11)
C(47)-Re(42)-C(50)-C(61)	-175.2(13)	C(67)-Fe(41)-C(61)-C(62)	-77.3(12)
Re(41)-Re(42)-C(50)-C(61)	94.5(13)	C(70)-Fe(41)-C(61)-C(62)	170.6(19)
C(61)-C(50)-O(50)-C(71)	168.4(14)	C(65)-Fe(41)-C(61)-C(62)	116.7(16)
Re(42)-C(50)-O(50)-C(71)	-14(2)	C(69)-Fe(41)-C(61)-C(62)	-159.2(13)
C(55)-Re(43)-Re(44)-C(59)	149.9(7)	C(63)-Fe(41)-C(61)-C(62)	36.7(12)
C(52)-Re(43)-Re(44)-C(59)	-119.6(7)	C(66)-Fe(41)-C(61)-C(62)	-48(2)
C(53)-Re(43)-Re(44)-C(59)	-32.0(7)	C(64)-Fe(41)-C(61)-C(62)	80.0(13)
C(54)-Re(43)-Re(44)-C(59)	55.9(6)	C(68)-Fe(41)-C(61)-C(62)	-119.0(12)
C(55)-Re(43)-Re(44)-C(58)	66.9(8)	C(67)-Fe(41)-C(61)-C(50)	44.7(17)
C(52)-Re(43)-Re(44)-C(58)	157.5(8)	C(70)-Fe(41)-C(61)-C(50)	-67(3)
C(53)-Re(43)-Re(44)-C(58)	-114.9(8)	C(65)-Fe(41)-C(61)-C(50)	-121(2)
C(54)-Re(43)-Re(44)-C(58)	-27.1(7)	C(69)-Fe(41)-C(61)-C(50)	-37.1(19)
C(55)-Re(43)-Re(44)-C(57)	-17.7(8)	C(62)-Fe(41)-C(61)-C(50)	122.1(18)
C(52)-Re(43)-Re(44)-C(57)	72.8(7)	C(63)-Fe(41)-C(61)-C(50)	158.8(17)
C(53)-Re(43)-Re(44)-C(57)	160.4(8)	C(66)-Fe(41)-C(61)-C(50)	74(3)
C(54)-Re(43)-Re(44)-C(57)	-111.8(7)	C(64)-Fe(41)-C(61)-C(50)	-158.0(18)
C(55)-Re(43)-Re(44)-C(60)	-115.3(7)	C(68)-Fe(41)-C(61)-C(50)	3.0(17)

C(67)-Fe(41)-C(61)-C(65)	166.0(11)	C(62)-Fe(41)-C(63)-C(64)	120.6(16)
C(70)-Fe(41)-C(61)-C(65)	54(2)	C(66)-Fe(41)-C(63)-C(64)	-117.5(11)
C(69)-Fe(41)-C(61)-C(65)	84.1(16)	C(68)-Fe(41)-C(63)-C(64)	166.8(16)
C(62)-Fe(41)-C(61)-C(65)	-116.7(16)	C(61)-Fe(41)-C(63)-C(64)	83.6(11)
C(63)-Fe(41)-C(61)-C(65)	-79.9(13)	C(67)-Fe(41)-C(63)-C(62)	79.6(13)
C(66)-Fe(41)-C(61)-C(65)	-165.0(18)	C(70)-Fe(41)-C(63)-C(62)	162.7(12)
C(64)-Fe(41)-C(61)-C(65)	-36.7(14)	C(65)-Fe(41)-C(63)-C(62)	-82.1(12)
C(68)-Fe(41)-C(61)-C(65)	124.3(13)	C(69)-Fe(41)-C(63)-C(62)	-168(2)
C(50)-C(61)-C(62)-C(63)	-177.4(16)	C(66)-Fe(41)-C(63)-C(62)	121.9(12)
C(65)-C(61)-C(62)-C(63)	-0.1(19)	C(64)-Fe(41)-C(63)-C(62)	-120.6(16)
Fe(41)-C(61)-C(62)-C(63)	-58.9(12)	C(68)-Fe(41)-C(63)-C(62)	46(2)
C(50)-C(61)-C(62)-Fe(41)	-118.6(18)	C(61)-Fe(41)-C(63)-C(62)	-37.0(11)
C(65)-C(61)-C(62)-Fe(41)	58.7(12)	C(62)-C(63)-C(64)-C(65)	0(2)
C(67)-Fe(41)-C(62)-C(63)	-118.1(13)	Fe(41)-C(63)-C(64)-C(65)	-59.1(15)
C(70)-Fe(41)-C(62)-C(63)	-48(3)	C(62)-C(63)-C(64)-Fe(41)	58.6(13)
C(65)-Fe(41)-C(62)-C(63)	81.0(13)	C(67)-Fe(41)-C(64)-C(63)	46(3)
C(69)-Fe(41)-C(62)-C(63)	171(2)	C(70)-Fe(41)-C(64)-C(63)	122.9(11)
C(66)-Fe(41)-C(62)-C(63)	-77.2(14)	C(65)-Fe(41)-C(64)-C(63)	-118.4(17)
C(64)-Fe(41)-C(62)-C(63)	36.8(12)	C(69)-Fe(41)-C(64)-C(63)	163.5(11)
C(68)-Fe(41)-C(62)-C(63)	-160.4(13)	C(62)-Fe(41)-C(64)-C(63)	-37.0(10)
C(61)-Fe(41)-C(62)-C(63)	120.9(17)	C(66)-Fe(41)-C(64)-C(63)	80.8(13)
C(67)-Fe(41)-C(62)-C(61)	121.0(10)	C(68)-Fe(41)-C(64)-C(63)	-163(2)
C(70)-Fe(41)-C(62)-C(61)	-169(2)	C(61)-Fe(41)-C(64)-C(63)	-80.9(11)
C(65)-Fe(41)-C(62)-C(61)	-39.9(10)	C(67)-Fe(41)-C(64)-C(65)	164.8(18)
C(69)-Fe(41)-C(62)-C(61)	50(3)	C(70)-Fe(41)-C(64)-C(65)	-118.7(13)
C(63)-Fe(41)-C(62)-C(61)	-120.9(17)	C(69)-Fe(41)-C(64)-C(65)	-78.1(15)
C(66)-Fe(41)-C(62)-C(61)	162.0(10)	C(62)-Fe(41)-C(64)-C(65)	81.4(13)
C(64)-Fe(41)-C(62)-C(61)	-84.0(12)	C(63)-Fe(41)-C(64)-C(65)	118.4(17)
C(68)-Fe(41)-C(62)-C(61)	78.7(12)	C(66)-Fe(41)-C(64)-C(65)	-160.8(12)
C(61)-C(62)-C(63)-C(64)	0(2)	C(68)-Fe(41)-C(64)-C(65)	-45(3)
Fe(41)-C(62)-C(63)-C(64)	-58.9(14)	C(61)-Fe(41)-C(64)-C(65)	37.5(12)
C(61)-C(62)-C(63)-Fe(41)	59.3(12)	C(63)-C(64)-C(65)-C(61)	0(2)
C(67)-Fe(41)-C(63)-C(64)	-159.9(10)	Fe(41)-C(64)-C(65)-C(61)	-59.1(14)
C(70)-Fe(41)-C(63)-C(64)	-76.8(14)	C(63)-C(64)-C(65)-Fe(41)	59.5(14)
C(65)-Fe(41)-C(63)-C(64)	38.4(10)	C(62)-C(61)-C(65)-C(64)	0(2)
C(69)-Fe(41)-C(63)-C(64)	-48(3)	C(50)-C(61)-C(65)-C(64)	177.2(17)

Fe(41)-C(61)-C(65)-C(64)	59.0(14)	C(62)-Fe(41)-C(66)-C(67)	-75.1(12)
C(62)-C(61)-C(65)-Fe(41)	-59.2(11)	C(63)-Fe(41)-C(66)-C(67)	-117.0(12)
C(50)-C(61)-C(65)-Fe(41)	118.2(18)	C(64)-Fe(41)-C(66)-C(67)	-159.2(13)
C(67)-Fe(41)-C(65)-C(64)	-160(2)	C(68)-Fe(41)-C(66)-C(67)	38.6(12)
C(70)-Fe(41)-C(65)-C(64)	80.6(17)	C(61)-Fe(41)-C(66)-C(67)	-39(2)
C(69)-Fe(41)-C(65)-C(64)	122.8(16)	C(67)-Fe(41)-C(66)-C(60)	121(2)
C(62)-Fe(41)-C(65)-C(64)	-81.9(15)	C(70)-Fe(41)-C(66)-C(60)	-119(2)
C(63)-Fe(41)-C(65)-C(64)	-38.0(13)	C(65)-Fe(41)-C(66)-C(60)	-71(3)
C(66)-Fe(41)-C(65)-C(64)	46(3)	C(69)-Fe(41)-C(66)-C(60)	-157.2(19)
C(68)-Fe(41)-C(65)-C(64)	164.3(16)	C(62)-Fe(41)-C(66)-C(60)	46.2(18)
C(61)-Fe(41)-C(65)-C(64)	-120.9(19)	C(63)-Fe(41)-C(66)-C(60)	4.4(18)
C(67)-Fe(41)-C(65)-C(61)	-40(3)	C(64)-Fe(41)-C(66)-C(60)	-38(2)
C(70)-Fe(41)-C(65)-C(61)	-158.5(11)	C(68)-Fe(41)-C(66)-C(60)	159.9(19)
C(69)-Fe(41)-C(65)-C(61)	-116.3(13)	C(61)-Fe(41)-C(66)-C(60)	82(2)
C(62)-Fe(41)-C(65)-C(61)	39.0(11)	C(70)-C(66)-C(67)-C(68)	-4.8(19)
C(63)-Fe(41)-C(65)-C(61)	82.9(12)	C(60)-C(66)-C(67)-C(68)	178.8(15)
C(66)-Fe(41)-C(65)-C(61)	166.8(16)	Fe(41)-C(66)-C(67)-C(68)	-62.8(12)
C(64)-Fe(41)-C(65)-C(61)	120.9(19)	C(70)-C(66)-C(67)-Fe(41)	58.0(12)
C(68)-Fe(41)-C(65)-C(61)	-74.8(16)	C(60)-C(66)-C(67)-Fe(41)	-118.5(16)
O(60)-C(60)-C(66)-C(70)	-31(2)	C(70)-Fe(41)-C(67)-C(66)	-37.3(10)
Re(44)-C(60)-C(66)-C(70)	150.5(15)	C(65)-Fe(41)-C(67)-C(66)	-165(2)
O(60)-C(60)-C(66)-C(67)	144.5(16)	C(69)-Fe(41)-C(67)-C(66)	-80.6(12)
Re(44)-C(60)-C(66)-C(67)	-34(2)	C(62)-Fe(41)-C(67)-C(66)	123.2(10)
O(60)-C(60)-C(66)-Fe(41)	56.6(18)	C(63)-Fe(41)-C(67)-C(66)	81.2(12)
Re(44)-C(60)-C(66)-Fe(41)	-121.6(12)	C(64)-Fe(41)-C(67)-C(66)	48(3)
C(67)-Fe(41)-C(66)-C(70)	-119.2(15)	C(68)-Fe(41)-C(67)-C(66)	-118.2(17)
C(65)-Fe(41)-C(66)-C(70)	48(2)	C(61)-Fe(41)-C(67)-C(66)	165.1(10)
C(69)-Fe(41)-C(66)-C(70)	-37.7(13)	C(70)-Fe(41)-C(67)-C(68)	80.8(13)
C(62)-Fe(41)-C(66)-C(70)	165.7(11)	C(65)-Fe(41)-C(67)-C(68)	-46(3)
C(63)-Fe(41)-C(66)-C(70)	123.8(12)	C(69)-Fe(41)-C(67)-C(68)	37.6(12)
C(64)-Fe(41)-C(66)-C(70)	81.6(15)	C(62)-Fe(41)-C(67)-C(68)	-118.6(13)
C(68)-Fe(41)-C(66)-C(70)	-80.6(13)	C(63)-Fe(41)-C(67)-C(68)	-160.6(13)
C(61)-Fe(41)-C(66)-C(70)	-158.1(19)	C(66)-Fe(41)-C(67)-C(68)	118.2(17)
C(70)-Fe(41)-C(66)-C(67)	119.2(15)	C(64)-Fe(41)-C(67)-C(68)	166(2)
C(65)-Fe(41)-C(66)-C(67)	167.4(19)	C(61)-Fe(41)-C(67)-C(68)	-76.7(15)
C(69)-Fe(41)-C(66)-C(67)	81.5(13)	C(66)-C(67)-C(68)-C(69)	4(2)

Fe(41)-C(67)-C(68)-C(69)	-58.9(16)	C(61)-Fe(41)-C(69)-C(68)	76.5(14)
C(66)-C(67)-C(68)-Fe(41)	62.5(12)	C(68)-C(69)-C(70)-C(66)	-2(3)
C(67)-Fe(41)-C(68)-C(69)	117.9(17)	Fe(41)-C(69)-C(70)-C(66)	-61.6(14)
C(70)-Fe(41)-C(68)-C(69)	36.4(12)	C(68)-C(69)-C(70)-Fe(41)	59.6(17)
C(65)-Fe(41)-C(68)-C(69)	-78.4(14)	C(67)-C(66)-C(70)-C(69)	4(2)
C(62)-Fe(41)-C(68)-C(69)	-162.7(11)	C(60)-C(66)-C(70)-C(69)	-179.3(17)
C(63)-Fe(41)-C(68)-C(69)	163.9(16)	Fe(41)-C(66)-C(70)-C(69)	61.6(16)
C(66)-Fe(41)-C(68)-C(69)	79.8(13)	C(67)-C(66)-C(70)-Fe(41)	-57.4(11)
C(64)-Fe(41)-C(68)-C(69)	-44(3)	C(60)-C(66)-C(70)-Fe(41)	119.1(16)
C(61)-Fe(41)-C(68)-C(69)	-120.6(12)	C(67)-Fe(41)-C(70)-C(69)	-80.7(15)
C(70)-Fe(41)-C(68)-C(67)	-81.5(12)	C(65)-Fe(41)-C(70)-C(69)	81.7(17)
C(65)-Fe(41)-C(68)-C(67)	163.7(11)	C(62)-Fe(41)-C(70)-C(69)	-157(2)
C(69)-Fe(41)-C(68)-C(67)	-117.9(17)	C(63)-Fe(41)-C(70)-C(69)	166.4(16)
C(62)-Fe(41)-C(68)-C(67)	79.4(13)	C(66)-Fe(41)-C(70)-C(69)	-118(2)
C(63)-Fe(41)-C(68)-C(67)	46(2)	C(64)-Fe(41)-C(70)-C(69)	124.7(17)
C(66)-Fe(41)-C(68)-C(67)	-38.1(11)	C(68)-Fe(41)-C(70)-C(69)	-36.2(15)
C(64)-Fe(41)-C(68)-C(67)	-162(2)	C(61)-Fe(41)-C(70)-C(69)	42(3)
C(61)-Fe(41)-C(68)-C(67)	121.4(12)	C(67)-Fe(41)-C(70)-C(66)	37.8(10)
C(67)-C(68)-C(69)-C(70)	-1(3)	C(65)-Fe(41)-C(70)-C(66)	-159.8(11)
Fe(41)-C(68)-C(69)-C(70)	-58.3(17)	C(69)-Fe(41)-C(70)-C(66)	118(2)
C(67)-C(68)-C(69)-Fe(41)	57.4(13)	C(62)-Fe(41)-C(70)-C(66)	-39(3)
C(67)-Fe(41)-C(69)-C(70)	82.1(14)	C(63)-Fe(41)-C(70)-C(66)	-75.1(15)
C(65)-Fe(41)-C(69)-C(70)	-117.6(14)	C(64)-Fe(41)-C(70)-C(66)	-116.8(13)
C(62)-Fe(41)-C(69)-C(70)	161.2(18)	C(68)-Fe(41)-C(70)-C(66)	82.3(12)
C(63)-Fe(41)-C(69)-C(70)	-38(4)	C(61)-Fe(41)-C(70)-C(66)	160.4(17)
C(66)-Fe(41)-C(69)-C(70)	37.9(13)	C(50)-O(50)-C(71)-C(72)	-176.9(15)
C(64)-Fe(41)-C(69)-C(70)	-74.7(16)	C(60)-O(60)-C(73)-C(74)	178.2(18)
C(68)-Fe(41)-C(69)-C(70)	121(2)		
C(61)-Fe(41)-C(69)-C(70)	-162.5(13)		
C(67)-Fe(41)-C(69)-C(68)	-38.9(11)		
C(70)-Fe(41)-C(69)-C(68)	-121(2)		
C(65)-Fe(41)-C(69)-C(68)	121.3(12)		
C(62)-Fe(41)-C(69)-C(68)	40(3)		
C(63)-Fe(41)-C(69)-C(68)	-159(3)		
C(66)-Fe(41)-C(69)-C(68)	-83.1(13)		
C(64)-Fe(41)-C(69)-C(68)	164.3(11)		

Appendix 9

Crystallographic data of Complex 28

Table 1. Crystal data and structure refinement for Complex **28**.

Identification code	db61a3_c2c	
Empirical formula	$C_{32.50}$ H_{29} Cl_3 Fe_2 O_8 Re_2	
Formula weight	1138.01	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 22.2670(16) Å	a= 90°.
	b = 15.2017(11) Å	b= 100.1860(10)°.
	c = 21.6438(15) Å	g = 90°.
Volume	7210.9(9) $Å^3$	
Z	8	
Density (calculated)	2.097 Mg/m^3	
Absorption coefficient	7.751 mm^{-1}	
F(000)	4328	
Crystal size	0.40 x 0.36 x 0.26 mm^3	
Theta range for data collection	2.38 to 26.25°.	
Index ranges	-27<=h<=16, -12<=k<=18, -23<=l<=26	
Reflections collected	18498	
Independent reflections	6671 [R(int) = 0.0367]	
Completeness to theta = 25.00°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.133 and 0.069	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6671 / 0 / 431	
Goodness-of-fit on F^2	1.156	
Final R indices [I>2σ(I)]	R1 = 0.0346, wR2 = 0.0885	
R indices (all data)	R1 = 0.0386, wR2 = 0.0927	
Extinction coefficient	0	
Largest diff. peak and hole	2.194 and -0.856 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Complex **28**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Re(1)	1923(1)	4253(1)	503(1)	41(1)
Re(2)	561(1)	2891(1)	-405(1)	43(1)
Cl(1)	790(1)	4375(1)	106(1)	48(1)
Cl(2)	1700(1)	2769(1)	-14(1)	47(1)
C(1)	2066(3)	4734(5)	-295(4)	63(2)
O(1)	2152(3)	5031(5)	-755(3)	100(2)
C(2)	2778(3)	4114(4)	737(3)	51(2)
O(2)	3302(2)	4083(3)	863(3)	66(1)
C(3)	2045(3)	5377(5)	869(3)	54(2)
O(3)	2135(2)	6074(4)	1086(3)	80(2)
C(4)	1727(3)	3645(4)	1353(3)	45(1)
O(4)	1333(2)	3916(3)	1703(2)	62(1)
C(5)	737(4)	3363(6)	-1196(4)	74(2)
O(5)	834(4)	3650(6)	-1650(3)	131(3)
C(6)	404(3)	1793(5)	-808(3)	61(2)
O(6)	282(3)	1144(4)	-1075(3)	98(2)
C(7)	-273(3)	3150(5)	-693(3)	54(2)
O(7)	-765(2)	3323(4)	-901(3)	73(1)
C(8)	410(3)	2416(4)	499(3)	42(1)
O(8)	643(2)	1699(3)	796(2)	62(1)
Fe(1)	2703(1)	2856(1)	2307(1)	58(1)
C(9)	1968(3)	2817(4)	1602(3)	46(1)
C(10)	1834(4)	2406(5)	2161(3)	62(2)
C(11)	2235(4)	1693(5)	2311(4)	67(2)
C(12)	2626(3)	1653(4)	1872(4)	62(2)
C(13)	2469(3)	2333(4)	1429(3)	50(1)
C(14)	3042(7)	4096(7)	2442(5)	107(4)
C(15)	2789(6)	3809(8)	2982(5)	109(4)
C(16)	3139(7)	3065(8)	3203(5)	111(4)
C(17)	3568(6)	2904(8)	2815(6)	110(4)
C(18)	3498(5)	3541(9)	2361(6)	107(4)
Fe(2)	-836(1)	2488(1)	860(1)	56(1)
C(19)	46(3)	2850(4)	895(3)	42(1)
C(20)	-354(3)	3590(4)	735(3)	48(1)
C(21)	-669(3)	3726(5)	1231(3)	60(2)
C(22)	-491(3)	3082(5)	1696(3)	64(2)
C(23)	-50(3)	2537(5)	1497(3)	53(2)

C(24)	-1129(6)	1670(9)	133(5)	111(4)
C(25)	-1526(6)	2362(10)	98(6)	113(4)
C(26)	-1760(4)	2332(10)	644(8)	121(4)
C(27)	-1500(5)	1655(10)	1033(6)	116(4)
C(28)	-1093(5)	1213(7)	695(6)	102(3)
C(29)	1028(5)	4762(6)	1635(4)	85(3)
C(30)	833(9)	5005(8)	2168(6)	177(8)
C(31)	998(5)	1047(6)	522(5)	91(3)
C(32)	1155(7)	346(7)	947(6)	125(4)
Cl(3)	645(3)	605(4)	2546(3)	187(2)
C(33)	0	-75(18)	2500	250(20)

Table 3. Bond lengths [Å] and angles [°] for Complex **28**.

Re(1)-C(3)	1.882(7)
Re(1)-C(2)	1.894(7)
Re(1)-C(1)	1.953(7)
Re(1)-C(4)	2.171(6)
Re(1)-Cl(1)	2.5252(15)
Re(1)-Cl(2)	2.5289(15)
Re(2)-C(6)	1.887(8)
Re(2)-C(7)	1.892(7)
Re(2)-C(5)	1.959(8)
Re(2)-C(8)	2.166(6)
Re(2)-Cl(1)	2.5249(15)
Re(2)-Cl(2)	2.5351(15)
C(1)-O(1)	1.140(8)
C(2)-O(2)	1.150(8)
C(3)-O(3)	1.162(8)
C(4)-O(4)	1.321(7)
C(4)-C(9)	1.437(9)
O(4)-C(29)	1.451(9)
C(5)-O(5)	1.131(9)
C(6)-O(6)	1.151(9)
C(7)-O(7)	1.140(8)
C(8)-O(8)	1.324(7)
C(8)-C(19)	1.441(8)
O(8)-C(31)	1.457(9)
Fe(1)-C(10)	2.024(8)
Fe(1)-C(9)	2.030(6)
Fe(1)-C(14)	2.032(9)
Fe(1)-C(16)	2.035(9)
Fe(1)-C(18)	2.039(10)
Fe(1)-C(13)	2.040(6)
Fe(1)-C(15)	2.043(9)
Fe(1)-C(17)	2.044(11)
Fe(1)-C(12)	2.050(7)
Fe(1)-C(11)	2.054(8)
C(9)-C(10)	1.440(9)
C(9)-C(13)	1.440(9)
C(10)-C(11)	1.405(10)
C(10)-H(10)	0.9800
C(11)-C(12)	1.400(10)

C(11)-H(11)	0.9800
C(12)-C(13)	1.410(9)
C(12)-H(12)	0.9800
C(13)-H(13)	0.9800
C(14)-C(18)	1.354(16)
C(14)-C(15)	1.453(16)
C(14)-H(14)	0.9800
C(15)-C(16)	1.408(16)
C(15)-H(15)	0.9800
C(16)-C(17)	1.400(17)
C(16)-H(16)	0.9800
C(17)-C(18)	1.369(16)
C(17)-H(17)	0.9800
C(18)-H(18)	0.9800
Fe(2)-C(24)	2.022(10)
Fe(2)-C(19)	2.027(6)
Fe(2)-C(23)	2.027(7)
Fe(2)-C(27)	2.032(8)
Fe(2)-C(20)	2.033(6)
Fe(2)-C(28)	2.035(9)
Fe(2)-C(26)	2.042(9)
Fe(2)-C(22)	2.046(8)
Fe(2)-C(21)	2.054(7)
Fe(2)-C(25)	2.055(10)
C(19)-C(23)	1.437(8)
C(19)-C(20)	1.438(8)
C(20)-C(21)	1.399(9)
C(20)-H(20)	0.9800
C(21)-C(22)	1.410(11)
C(21)-H(21)	0.9800
C(22)-C(23)	1.408(10)
C(22)-H(22)	0.9800
C(23)-H(23)	0.9800
C(24)-C(25)	1.367(18)
C(24)-C(28)	1.391(15)
C(24)-H(24)	0.9800
C(25)-C(26)	1.373(18)
C(25)-H(25)	0.9800
C(26)-C(27)	1.388(17)
C(26)-H(26)	0.9800

C(27)-C(28)	1.429(17)
C(27)-H(27)	0.9800
C(28)-H(28)	0.9800
C(29)-C(30)	1.355(12)
C(29)-H(29A)	0.9700
C(29)-H(29B)	0.9700
C(30)-H(30A)	0.9600
C(30)-H(30B)	0.9600
C(30)-H(30C)	0.9600
C(31)-C(32)	1.411(13)
C(31)-H(31A)	0.9700
C(31)-H(31B)	0.9700
C(32)-H(32A)	0.9600
C(32)-H(32B)	0.9600
C(32)-H(32C)	0.9600
Cl(3)-C(33)	1.758(16)
C(33)-Cl(3)#1	1.758(16)
C(33)-H(33A)	0.9700
C(33)-H(33B)	0.9700

C(3)-Re(1)-C(2)	85.8(3)
C(3)-Re(1)-C(1)	90.0(3)
C(2)-Re(1)-C(1)	88.0(3)
C(3)-Re(1)-C(4)	93.7(3)
C(2)-Re(1)-C(4)	94.0(3)
C(1)-Re(1)-C(4)	175.9(3)
C(3)-Re(1)-Cl(1)	97.90(19)
C(2)-Re(1)-Cl(1)	175.2(2)
C(1)-Re(1)-Cl(1)	88.9(2)
C(4)-Re(1)-Cl(1)	88.90(16)
C(3)-Re(1)-Cl(2)	176.8(2)
C(2)-Re(1)-Cl(2)	97.3(2)
C(1)-Re(1)-Cl(2)	89.6(2)
C(4)-Re(1)-Cl(2)	86.67(16)
Cl(1)-Re(1)-Cl(2)	78.97(5)
C(6)-Re(2)-C(7)	86.6(3)
C(6)-Re(2)-C(5)	88.2(4)
C(7)-Re(2)-C(5)	88.4(3)
C(6)-Re(2)-C(8)	94.4(3)
C(7)-Re(2)-C(8)	93.9(2)

C(5)-Re(2)-C(8)	176.6(3)
C(6)-Re(2)-Cl(1)	178.1(2)
C(7)-Re(2)-Cl(1)	93.9(2)
C(5)-Re(2)-Cl(1)	89.9(3)
C(8)-Re(2)-Cl(1)	87.38(16)
C(6)-Re(2)-Cl(2)	100.5(2)
C(7)-Re(2)-Cl(2)	172.2(2)
C(5)-Re(2)-Cl(2)	88.6(2)
C(8)-Re(2)-Cl(2)	88.88(15)
Cl(1)-Re(2)-Cl(2)	78.86(5)
Re(2)-Cl(1)-Re(1)	101.28(5)
Re(1)-Cl(2)-Re(2)	100.90(5)
O(1)-C(1)-Re(1)	178.5(8)
O(2)-C(2)-Re(1)	175.5(6)
O(3)-C(3)-Re(1)	177.8(6)
O(4)-C(4)-C(9)	107.4(5)
O(4)-C(4)-Re(1)	127.4(4)
C(9)-C(4)-Re(1)	125.0(4)
C(4)-O(4)-C(29)	124.3(5)
O(5)-C(5)-Re(2)	178.7(9)
O(6)-C(6)-Re(2)	176.2(7)
O(7)-C(7)-Re(2)	175.9(6)
O(8)-C(8)-C(19)	107.6(5)
O(8)-C(8)-Re(2)	127.1(4)
C(19)-C(8)-Re(2)	125.3(4)
C(8)-O(8)-C(31)	123.8(5)
C(10)-Fe(1)-C(9)	41.6(3)
C(10)-Fe(1)-C(14)	131.1(5)
C(9)-Fe(1)-C(14)	111.4(4)
C(10)-Fe(1)-C(16)	118.8(5)
C(9)-Fe(1)-C(16)	154.9(5)
C(14)-Fe(1)-C(16)	67.4(4)
C(10)-Fe(1)-C(18)	168.0(5)
C(9)-Fe(1)-C(18)	129.4(4)
C(14)-Fe(1)-C(18)	38.9(5)
C(16)-Fe(1)-C(18)	66.6(5)
C(10)-Fe(1)-C(13)	69.2(3)
C(9)-Fe(1)-C(13)	41.4(2)
C(14)-Fe(1)-C(13)	121.5(4)
C(16)-Fe(1)-C(13)	161.5(5)

C(18)-Fe(1)-C(13)	109.2(4)
C(10)-Fe(1)-C(15)	108.5(4)
C(9)-Fe(1)-C(15)	121.3(4)
C(14)-Fe(1)-C(15)	41.8(5)
C(16)-Fe(1)-C(15)	40.4(4)
C(18)-Fe(1)-C(15)	68.1(5)
C(13)-Fe(1)-C(15)	156.8(4)
C(10)-Fe(1)-C(17)	151.6(4)
C(9)-Fe(1)-C(17)	164.3(5)
C(14)-Fe(1)-C(17)	66.3(5)
C(16)-Fe(1)-C(17)	40.2(5)
C(18)-Fe(1)-C(17)	39.2(5)
C(13)-Fe(1)-C(17)	125.2(5)
C(15)-Fe(1)-C(17)	68.2(5)
C(10)-Fe(1)-C(12)	68.1(3)
C(9)-Fe(1)-C(12)	68.8(3)
C(14)-Fe(1)-C(12)	153.2(5)
C(16)-Fe(1)-C(12)	124.3(4)
C(18)-Fe(1)-C(12)	118.9(5)
C(13)-Fe(1)-C(12)	40.3(3)
C(15)-Fe(1)-C(12)	161.9(4)
C(17)-Fe(1)-C(12)	105.9(4)
C(10)-Fe(1)-C(11)	40.3(3)
C(9)-Fe(1)-C(11)	68.7(3)
C(14)-Fe(1)-C(11)	166.9(5)
C(16)-Fe(1)-C(11)	106.6(4)
C(18)-Fe(1)-C(11)	151.1(5)
C(13)-Fe(1)-C(11)	67.8(3)
C(15)-Fe(1)-C(11)	126.2(5)
C(17)-Fe(1)-C(11)	117.3(4)
C(12)-Fe(1)-C(11)	39.9(3)
C(4)-C(9)-C(10)	125.2(6)
C(4)-C(9)-C(13)	127.3(6)
C(10)-C(9)-C(13)	106.4(6)
C(4)-C(9)-Fe(1)	117.0(4)
C(10)-C(9)-Fe(1)	68.9(4)
C(13)-C(9)-Fe(1)	69.6(4)
C(11)-C(10)-C(9)	108.1(6)
C(11)-C(10)-Fe(1)	71.0(5)
C(9)-C(10)-Fe(1)	69.4(4)

C(11)-C(10)-H(10)	125.9
C(9)-C(10)-H(10)	125.9
Fe(1)-C(10)-H(10)	125.9
C(12)-C(11)-C(10)	108.8(6)
C(12)-C(11)-Fe(1)	69.9(4)
C(10)-C(11)-Fe(1)	68.7(4)
C(12)-C(11)-H(11)	125.6
C(10)-C(11)-H(11)	125.6
Fe(1)-C(11)-H(11)	125.6
C(11)-C(12)-C(13)	108.8(6)
C(11)-C(12)-Fe(1)	70.2(4)
C(13)-C(12)-Fe(1)	69.4(4)
C(11)-C(12)-H(12)	125.6
C(13)-C(12)-H(12)	125.6
Fe(1)-C(12)-H(12)	125.6
C(12)-C(13)-C(9)	107.9(6)
C(12)-C(13)-Fe(1)	70.2(4)
C(9)-C(13)-Fe(1)	68.9(4)
C(12)-C(13)-H(13)	126.0
C(9)-C(13)-H(13)	126.0
Fe(1)-C(13)-H(13)	126.0
C(18)-C(14)-C(15)	108.9(11)
C(18)-C(14)-Fe(1)	70.8(6)
C(15)-C(14)-Fe(1)	69.5(6)
C(18)-C(14)-H(14)	125.5
C(15)-C(14)-H(14)	125.5
Fe(1)-C(14)-H(14)	125.5
C(16)-C(15)-C(14)	104.1(11)
C(16)-C(15)-Fe(1)	69.5(6)
C(14)-C(15)-Fe(1)	68.7(5)
C(16)-C(15)-H(15)	127.9
C(14)-C(15)-H(15)	127.9
Fe(1)-C(15)-H(15)	127.9
C(17)-C(16)-C(15)	109.4(11)
C(17)-C(16)-Fe(1)	70.3(6)
C(15)-C(16)-Fe(1)	70.1(5)
C(17)-C(16)-H(16)	125.3
C(15)-C(16)-H(16)	125.3
Fe(1)-C(16)-H(16)	125.3
C(18)-C(17)-C(16)	107.7(12)

C(18)-C(17)-Fe(1)	70.2(6)
C(16)-C(17)-Fe(1)	69.5(7)
C(18)-C(17)-H(17)	126.2
C(16)-C(17)-H(17)	126.2
Fe(1)-C(17)-H(17)	126.2
C(14)-C(18)-C(17)	109.9(12)
C(14)-C(18)-Fe(1)	70.3(6)
C(17)-C(18)-Fe(1)	70.6(7)
C(14)-C(18)-H(18)	125.1
C(17)-C(18)-H(18)	125.1
Fe(1)-C(18)-H(18)	125.1
C(24)-Fe(2)-C(19)	112.0(4)
C(24)-Fe(2)-C(23)	132.3(5)
C(19)-Fe(2)-C(23)	41.5(2)
C(24)-Fe(2)-C(27)	67.3(5)
C(19)-Fe(2)-C(27)	153.4(5)
C(23)-Fe(2)-C(27)	117.8(4)
C(24)-Fe(2)-C(20)	120.6(4)
C(19)-Fe(2)-C(20)	41.5(2)
C(23)-Fe(2)-C(20)	69.4(3)
C(27)-Fe(2)-C(20)	163.0(5)
C(24)-Fe(2)-C(28)	40.1(4)
C(19)-Fe(2)-C(28)	120.4(4)
C(23)-Fe(2)-C(28)	109.7(4)
C(27)-Fe(2)-C(28)	41.1(5)
C(20)-Fe(2)-C(28)	154.2(4)
C(24)-Fe(2)-C(26)	64.9(6)
C(19)-Fe(2)-C(26)	166.0(5)
C(23)-Fe(2)-C(26)	150.8(5)
C(27)-Fe(2)-C(26)	39.8(5)
C(20)-Fe(2)-C(26)	126.8(5)
C(28)-Fe(2)-C(26)	66.9(5)
C(24)-Fe(2)-C(22)	168.2(5)
C(19)-Fe(2)-C(22)	68.8(3)
C(23)-Fe(2)-C(22)	40.4(3)
C(27)-Fe(2)-C(22)	106.5(4)
C(20)-Fe(2)-C(22)	68.3(3)
C(28)-Fe(2)-C(22)	128.7(4)
C(26)-Fe(2)-C(22)	117.3(5)
C(24)-Fe(2)-C(21)	151.6(5)

C(19)-Fe(2)-C(21)	68.3(2)
C(23)-Fe(2)-C(21)	68.0(3)
C(27)-Fe(2)-C(21)	125.9(5)
C(20)-Fe(2)-C(21)	40.0(2)
C(28)-Fe(2)-C(21)	165.3(4)
C(26)-Fe(2)-C(21)	107.5(5)
C(22)-Fe(2)-C(21)	40.2(3)
C(24)-Fe(2)-C(25)	39.2(5)
C(19)-Fe(2)-C(25)	129.6(4)
C(23)-Fe(2)-C(25)	169.1(5)
C(27)-Fe(2)-C(25)	67.8(5)
C(20)-Fe(2)-C(25)	107.9(4)
C(28)-Fe(2)-C(25)	67.8(5)
C(26)-Fe(2)-C(25)	39.2(5)
C(22)-Fe(2)-C(25)	149.5(6)
C(21)-Fe(2)-C(25)	117.2(5)
C(23)-C(19)-C(20)	107.0(5)
C(23)-C(19)-C(8)	125.3(5)
C(20)-C(19)-C(8)	127.2(5)
C(23)-C(19)-Fe(2)	69.3(3)
C(20)-C(19)-Fe(2)	69.5(3)
C(8)-C(19)-Fe(2)	119.7(4)
C(21)-C(20)-C(19)	107.7(6)
C(21)-C(20)-Fe(2)	70.8(4)
C(19)-C(20)-Fe(2)	69.0(3)
C(21)-C(20)-H(20)	126.2
C(19)-C(20)-H(20)	126.2
Fe(2)-C(20)-H(20)	126.2
C(20)-C(21)-C(22)	109.2(6)
C(20)-C(21)-Fe(2)	69.2(4)
C(22)-C(21)-Fe(2)	69.6(4)
C(20)-C(21)-H(21)	125.4
C(22)-C(21)-H(21)	125.4
Fe(2)-C(21)-H(21)	125.4
C(23)-C(22)-C(21)	108.3(6)
C(23)-C(22)-Fe(2)	69.1(4)
C(21)-C(22)-Fe(2)	70.2(4)
C(23)-C(22)-H(22)	125.9
C(21)-C(22)-H(22)	125.9
Fe(2)-C(22)-H(22)	125.9

C(22)-C(23)-C(19)	107.8(6)
C(22)-C(23)-Fe(2)	70.5(4)
C(19)-C(23)-Fe(2)	69.2(3)
C(22)-C(23)-H(23)	126.1
C(19)-C(23)-H(23)	126.1
Fe(2)-C(23)-H(23)	126.1
C(25)-C(24)-C(28)	111.7(12)
C(25)-C(24)-Fe(2)	71.7(7)
C(28)-C(24)-Fe(2)	70.5(6)
C(25)-C(24)-H(24)	124.2
C(28)-C(24)-H(24)	124.2
Fe(2)-C(24)-H(24)	124.2
C(24)-C(25)-C(26)	105.5(12)
C(24)-C(25)-Fe(2)	69.1(6)
C(26)-C(25)-Fe(2)	69.9(6)
C(24)-C(25)-H(25)	127.2
C(26)-C(25)-H(25)	127.2
Fe(2)-C(25)-H(25)	127.2
C(25)-C(26)-C(27)	111.4(13)
C(25)-C(26)-Fe(2)	70.9(6)
C(27)-C(26)-Fe(2)	69.7(6)
C(25)-C(26)-H(26)	124.3
C(27)-C(26)-H(26)	124.3
Fe(2)-C(26)-H(26)	124.3
C(26)-C(27)-C(28)	105.9(11)
C(26)-C(27)-Fe(2)	70.5(6)
C(28)-C(27)-Fe(2)	69.5(5)
C(26)-C(27)-H(27)	127.0
C(28)-C(27)-H(27)	127.0
Fe(2)-C(27)-H(27)	127.0
C(24)-C(28)-C(27)	105.5(11)
C(24)-C(28)-Fe(2)	69.4(6)
C(27)-C(28)-Fe(2)	69.3(6)
C(24)-C(28)-H(28)	127.2
C(27)-C(28)-H(28)	127.2
Fe(2)-C(28)-H(28)	127.2
C(30)-C(29)-O(4)	111.7(8)
C(30)-C(29)-H(29A)	109.3
O(4)-C(29)-H(29A)	109.3
C(30)-C(29)-H(29B)	109.3

O(4)-C(29)-H(29B)	109.3
H(29A)-C(29)-H(29B)	107.9
C(29)-C(30)-H(30A)	109.5
C(29)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(29)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(32)-C(31)-O(8)	109.8(8)
C(32)-C(31)-H(31A)	109.7
O(8)-C(31)-H(31A)	109.7
C(32)-C(31)-H(31B)	109.7
O(8)-C(31)-H(31B)	109.7
H(31A)-C(31)-H(31B)	108.2
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
Cl(3)-C(33)-Cl(3)#1	108.0(15)
Cl(3)-C(33)-H(33A)	110.1
Cl(3)#1-C(33)-H(33A)	110.1
Cl(3)-C(33)-H(33B)	110.1
Cl(3)#1-C(33)-H(33B)	110.1
H(33A)-C(33)-H(33B)	108.4

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Complex **28**. 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}
Re(1)	39(1)	43(1)	42(1)	1(1)	14(1)	-2(1)
Re(2)	42(1)	53(1)	36(1)	1(1)	11(1)	-3(1)
Cl(1)	44(1)	43(1)	59(1)	4(1)	10(1)	2(1)
Cl(2)	44(1)	51(1)	47(1)	-7(1)	13(1)	3(1)
C(1)	57(4)	72(5)	63(5)	14(4)	18(3)	-2(3)
O(1)	119(5)	120(5)	71(4)	39(4)	46(4)	1(4)
C(2)	48(4)	54(4)	55(4)	-5(3)	20(3)	-4(3)
O(2)	45(3)	75(3)	81(4)	-5(3)	18(2)	-1(2)
C(3)	43(3)	57(4)	64(4)	4(3)	14(3)	-1(3)
O(3)	59(3)	68(3)	116(5)	-30(3)	26(3)	-11(3)
C(4)	49(3)	51(3)	40(3)	-6(3)	18(3)	-1(3)
O(4)	67(3)	69(3)	60(3)	8(2)	35(2)	15(2)
C(5)	62(4)	103(6)	58(5)	16(4)	16(4)	2(4)
O(5)	143(7)	186(9)	74(4)	62(5)	49(4)	10(6)
C(6)	46(3)	79(5)	59(4)	-15(4)	9(3)	-3(3)
O(6)	90(4)	90(4)	111(5)	-54(4)	10(4)	-7(3)
C(7)	52(4)	64(4)	46(4)	-2(3)	10(3)	-4(3)
O(7)	48(3)	98(4)	68(3)	3(3)	-5(2)	3(3)
C(8)	45(3)	39(3)	42(3)	4(2)	12(2)	-2(2)
O(8)	76(3)	56(3)	62(3)	18(2)	33(2)	20(2)
Fe(1)	75(1)	53(1)	45(1)	3(1)	4(1)	-1(1)
C(9)	46(3)	49(3)	43(3)	-2(3)	12(3)	-2(2)
C(10)	74(5)	59(4)	60(4)	10(3)	31(4)	-1(3)
C(11)	95(6)	49(4)	59(4)	10(3)	17(4)	1(4)
C(12)	69(4)	44(3)	71(5)	6(3)	11(4)	7(3)
C(13)	59(4)	47(3)	46(3)	-1(3)	13(3)	4(3)
C(14)	151(11)	68(6)	82(7)	-3(5)	-32(7)	-34(6)
C(15)	139(10)	101(8)	80(7)	-48(6)	0(7)	-9(7)
C(16)	161(12)	101(8)	54(6)	5(5)	-24(7)	-17(8)
C(17)	109(9)	116(9)	87(8)	9(7)	-29(7)	-11(6)
C(18)	89(7)	129(10)	97(8)	-11(7)	1(6)	-40(7)
Fe(2)	47(1)	67(1)	56(1)	3(1)	17(1)	-11(1)
C(19)	38(3)	45(3)	43(3)	2(2)	10(2)	-3(2)
C(20)	47(3)	49(3)	48(3)	-8(3)	11(3)	-1(3)
C(21)	58(4)	63(4)	62(4)	-12(3)	23(3)	7(3)
C(22)	67(4)	78(5)	52(4)	-3(3)	26(3)	-3(4)
C(23)	60(4)	59(4)	41(3)	5(3)	15(3)	-3(3)

C(24)	116(9)	134(10)	86(7)	-35(7)	22(6)	-79(8)
C(25)	81(7)	143(11)	103(9)	27(8)	-19(6)	-48(7)
C(26)	52(5)	141(11)	167(13)	18(10)	11(7)	-25(6)
C(27)	90(7)	164(12)	96(8)	21(8)	22(6)	-73(8)
C(28)	103(8)	72(6)	124(9)	1(6)	1(7)	-44(5)
C(29)	106(6)	79(5)	85(6)	15(5)	57(5)	41(5)
C(30)	350(20)	96(8)	106(9)	3(7)	105(12)	100(12)
C(31)	119(7)	60(5)	109(7)	22(5)	64(6)	39(5)
C(32)	184(13)	71(6)	127(10)	15(6)	49(9)	50(7)
Cl(3)	205(5)	171(4)	184(4)	9(3)	30(4)	84(4)
C(33)	350(50)	130(20)	220(30)	0	-110(30)	0

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Complex **28**.

	x	y	z	U(eq)
H(10)	1514	2586	2393	75
H(11)	2249	1302	2674	81
H(12)	2957	1229	1875	74
H(13)	2668	2457	1069	60
H(14)	2905	4607	2178	128
H(15)	2464	4089	3166	131
H(16)	3086	2710	3568	133
H(17)	3868	2426	2863	131
H(18)	3738	3585	2024	128
H(20)	-395	3941	350	57
H(21)	-979	4181	1245	72
H(22)	-650	3019	2088	77
H(23)	156	2037	1728	63
H(24)	-893	1522	-194	134
H(25)	-1634	2776	-250	136
H(26)	-2056	2754	755	145
H(27)	-1594	1494	1443	139
H(28)	-850	686	826	122
H(29A)	1307	5204	1528	102
H(29B)	682	4732	1294	102
H(30A)	585	4545	2295	213
H(30B)	597	5534	2094	213
H(30C)	1179	5106	2494	213
H(31A)	761	826	133	109
H(31B)	1365	1318	426	109
H(32A)	1309	578	1357	187
H(32B)	1463	-9	810	187
H(32C)	801	-6	963	187
H(33A)	39	-448	2869	304
H(33B)	-39	-448	2131	304

Table 6. Torsion angles [°] for Complex **28**.

C(7)-Re(2)-Cl(1)-Re(1)	-177.3(2)
C(5)-Re(2)-Cl(1)-Re(1)	-89.0(2)
C(8)-Re(2)-Cl(1)-Re(1)	88.97(16)
Cl(2)-Re(2)-Cl(1)-Re(1)	-0.40(5)
C(3)-Re(1)-Cl(1)-Re(2)	180.0(2)
C(1)-Re(1)-Cl(1)-Re(2)	90.2(2)
C(4)-Re(1)-Cl(1)-Re(2)	-86.42(16)
Cl(2)-Re(1)-Cl(1)-Re(2)	0.40(5)
C(2)-Re(1)-Cl(2)-Re(2)	-177.3(2)
C(1)-Re(1)-Cl(2)-Re(2)	-89.4(2)
C(4)-Re(1)-Cl(2)-Re(2)	89.12(16)
Cl(1)-Re(1)-Cl(2)-Re(2)	-0.40(5)
C(6)-Re(2)-Cl(2)-Re(1)	178.5(2)
C(7)-Re(2)-Cl(2)-Re(1)	23.6(15)
C(5)-Re(2)-Cl(2)-Re(1)	90.6(3)
C(8)-Re(2)-Cl(2)-Re(1)	-87.15(16)
Cl(1)-Re(2)-Cl(2)-Re(1)	0.40(5)
C(6)-Re(2)-C(8)-O(8)	48.6(6)
C(7)-Re(2)-C(8)-O(8)	135.5(6)
Cl(1)-Re(2)-C(8)-O(8)	-130.7(5)
Cl(2)-Re(2)-C(8)-O(8)	-51.8(5)
C(6)-Re(2)-C(8)-C(19)	-133.4(5)
C(7)-Re(2)-C(8)-C(19)	-46.5(5)
Cl(1)-Re(2)-C(8)-C(19)	47.3(5)
Cl(2)-Re(2)-C(8)-C(19)	126.2(5)
C(19)-C(8)-O(8)-C(31)	174.8(7)
Re(2)-C(8)-O(8)-C(31)	-6.9(10)
O(4)-C(4)-C(9)-C(10)	-4.4(9)
Re(1)-C(4)-C(9)-C(10)	-179.3(5)
O(4)-C(4)-C(9)-C(13)	-170.8(6)
Re(1)-C(4)-C(9)-C(13)	14.3(9)
O(4)-C(4)-C(9)-Fe(1)	-86.7(6)
Re(1)-C(4)-C(9)-Fe(1)	98.4(5)
C(10)-Fe(1)-C(9)-C(4)	119.8(6)
C(14)-Fe(1)-C(9)-C(4)	-8.6(7)
C(16)-Fe(1)-C(9)-C(4)	73.6(10)
C(18)-Fe(1)-C(9)-C(4)	-49.1(8)
C(13)-Fe(1)-C(9)-C(4)	-122.5(6)
C(15)-Fe(1)-C(9)-C(4)	37.0(7)

C(17)-Fe(1)-C(9)-C(4)	-87.1(15)
C(12)-Fe(1)-C(9)-C(4)	-159.7(5)
C(11)-Fe(1)-C(9)-C(4)	157.3(5)
C(14)-Fe(1)-C(9)-C(10)	-128.4(6)
C(16)-Fe(1)-C(9)-C(10)	-46.2(10)
C(18)-Fe(1)-C(9)-C(10)	-168.9(6)
C(13)-Fe(1)-C(9)-C(10)	117.8(5)
C(15)-Fe(1)-C(9)-C(10)	-82.7(6)
C(17)-Fe(1)-C(9)-C(10)	153.1(14)
C(12)-Fe(1)-C(9)-C(10)	80.5(4)
C(11)-Fe(1)-C(9)-C(10)	37.5(4)
C(10)-Fe(1)-C(9)-C(13)	-117.8(5)
C(14)-Fe(1)-C(9)-C(13)	113.9(6)
C(16)-Fe(1)-C(9)-C(13)	-164.0(9)
C(18)-Fe(1)-C(9)-C(13)	73.3(7)
C(15)-Fe(1)-C(9)-C(13)	159.5(6)
C(17)-Fe(1)-C(9)-C(13)	35.4(16)
C(12)-Fe(1)-C(9)-C(13)	-37.3(4)
C(11)-Fe(1)-C(9)-C(13)	-80.2(4)
C(4)-C(9)-C(10)-C(11)	-169.7(6)
C(13)-C(9)-C(10)-C(11)	-0.9(8)
Fe(1)-C(9)-C(10)-C(11)	-60.8(6)
C(4)-C(9)-C(10)-Fe(1)	-108.9(6)
C(13)-C(9)-C(10)-Fe(1)	59.9(4)
C(9)-Fe(1)-C(10)-C(11)	118.7(6)
C(14)-Fe(1)-C(10)-C(11)	-165.8(6)
C(16)-Fe(1)-C(10)-C(11)	-81.7(6)
C(18)-Fe(1)-C(10)-C(11)	164.2(19)
C(13)-Fe(1)-C(10)-C(11)	79.9(5)
C(15)-Fe(1)-C(10)-C(11)	-124.6(6)
C(17)-Fe(1)-C(10)-C(11)	-46.4(11)
C(12)-Fe(1)-C(10)-C(11)	36.5(4)
C(14)-Fe(1)-C(10)-C(9)	75.4(6)
C(16)-Fe(1)-C(10)-C(9)	159.6(5)
C(18)-Fe(1)-C(10)-C(9)	45(2)
C(13)-Fe(1)-C(10)-C(9)	-38.8(4)
C(15)-Fe(1)-C(10)-C(9)	116.7(5)
C(17)-Fe(1)-C(10)-C(9)	-165.1(9)
C(12)-Fe(1)-C(10)-C(9)	-82.2(4)
C(11)-Fe(1)-C(10)-C(9)	-118.7(6)

C(9)-C(10)-C(11)-C(12)	1.2(9)
Fe(1)-C(10)-C(11)-C(12)	-58.5(6)
C(9)-C(10)-C(11)-Fe(1)	59.8(5)
C(10)-Fe(1)-C(11)-C(12)	120.7(6)
C(9)-Fe(1)-C(11)-C(12)	82.0(5)
C(14)-Fe(1)-C(11)-C(12)	175.0(16)
C(16)-Fe(1)-C(11)-C(12)	-124.1(6)
C(18)-Fe(1)-C(11)-C(12)	-52.5(10)
C(13)-Fe(1)-C(11)-C(12)	37.2(4)
C(15)-Fe(1)-C(11)-C(12)	-164.1(6)
C(17)-Fe(1)-C(11)-C(12)	-82.1(6)
C(9)-Fe(1)-C(11)-C(10)	-38.7(4)
C(14)-Fe(1)-C(11)-C(10)	54.3(18)
C(16)-Fe(1)-C(11)-C(10)	115.2(6)
C(18)-Fe(1)-C(11)-C(10)	-173.2(8)
C(13)-Fe(1)-C(11)-C(10)	-83.5(5)
C(15)-Fe(1)-C(11)-C(10)	75.2(6)
C(17)-Fe(1)-C(11)-C(10)	157.2(6)
C(12)-Fe(1)-C(11)-C(10)	-120.7(6)
C(10)-C(11)-C(12)-C(13)	-1.1(9)
Fe(1)-C(11)-C(12)-C(13)	-58.9(5)
C(10)-C(11)-C(12)-Fe(1)	57.8(6)
C(10)-Fe(1)-C(12)-C(11)	-36.8(4)
C(9)-Fe(1)-C(12)-C(11)	-81.7(5)
C(14)-Fe(1)-C(12)-C(11)	-177.5(8)
C(16)-Fe(1)-C(12)-C(11)	74.0(7)
C(18)-Fe(1)-C(12)-C(11)	154.0(6)
C(13)-Fe(1)-C(12)-C(11)	-120.0(6)
C(15)-Fe(1)-C(12)-C(11)	45.6(15)
C(17)-Fe(1)-C(12)-C(11)	113.8(6)
C(10)-Fe(1)-C(12)-C(13)	83.2(4)
C(9)-Fe(1)-C(12)-C(13)	38.3(4)
C(14)-Fe(1)-C(12)-C(13)	-57.5(10)
C(16)-Fe(1)-C(12)-C(13)	-166.0(6)
C(18)-Fe(1)-C(12)-C(13)	-85.9(6)
C(15)-Fe(1)-C(12)-C(13)	165.6(13)
C(17)-Fe(1)-C(12)-C(13)	-126.2(6)
C(11)-Fe(1)-C(12)-C(13)	120.0(6)
C(11)-C(12)-C(13)-C(9)	0.5(8)
Fe(1)-C(12)-C(13)-C(9)	-58.8(4)

C(11)-C(12)-C(13)-Fe(1)	59.3(5)
C(4)-C(9)-C(13)-C(12)	168.7(6)
C(10)-C(9)-C(13)-C(12)	0.2(8)
Fe(1)-C(9)-C(13)-C(12)	59.6(5)
C(4)-C(9)-C(13)-Fe(1)	109.0(6)
C(10)-C(9)-C(13)-Fe(1)	-59.4(5)
C(10)-Fe(1)-C(13)-C(12)	-80.3(5)
C(9)-Fe(1)-C(13)-C(12)	-119.2(6)
C(14)-Fe(1)-C(13)-C(12)	153.5(6)
C(16)-Fe(1)-C(13)-C(12)	39.1(15)
C(18)-Fe(1)-C(13)-C(12)	112.4(6)
C(15)-Fe(1)-C(13)-C(12)	-168.7(11)
C(17)-Fe(1)-C(13)-C(12)	71.8(6)
C(11)-Fe(1)-C(13)-C(12)	-36.9(4)
C(10)-Fe(1)-C(13)-C(9)	39.0(4)
C(14)-Fe(1)-C(13)-C(9)	-87.3(6)
C(16)-Fe(1)-C(13)-C(9)	158.3(13)
C(18)-Fe(1)-C(13)-C(9)	-128.4(5)
C(15)-Fe(1)-C(13)-C(9)	-49.5(12)
C(17)-Fe(1)-C(13)-C(9)	-169.0(5)
C(12)-Fe(1)-C(13)-C(9)	119.2(6)
C(11)-Fe(1)-C(13)-C(9)	82.4(4)
C(10)-Fe(1)-C(14)-C(18)	-170.4(6)
C(9)-Fe(1)-C(14)-C(18)	-126.8(7)
C(16)-Fe(1)-C(14)-C(18)	80.3(8)
C(13)-Fe(1)-C(14)-C(18)	-81.5(8)
C(15)-Fe(1)-C(14)-C(18)	119.8(10)
C(17)-Fe(1)-C(14)-C(18)	36.4(8)
C(12)-Fe(1)-C(14)-C(18)	-41.7(12)
C(11)-Fe(1)-C(14)-C(18)	145.4(16)
C(10)-Fe(1)-C(14)-C(15)	69.8(8)
C(9)-Fe(1)-C(14)-C(15)	113.5(7)
C(16)-Fe(1)-C(14)-C(15)	-39.5(7)
C(18)-Fe(1)-C(14)-C(15)	-119.8(10)
C(13)-Fe(1)-C(14)-C(15)	158.7(6)
C(17)-Fe(1)-C(14)-C(15)	-83.3(8)
C(12)-Fe(1)-C(14)-C(15)	-161.5(8)
C(11)-Fe(1)-C(14)-C(15)	26(2)
C(18)-C(14)-C(15)-C(16)	0.8(11)
Fe(1)-C(14)-C(15)-C(16)	60.9(7)

C(18)-C(14)-C(15)-Fe(1)	-60.1(7)
C(10)-Fe(1)-C(15)-C(16)	113.1(8)
C(9)-Fe(1)-C(15)-C(16)	157.1(7)
C(14)-Fe(1)-C(15)-C(16)	-115.1(11)
C(18)-Fe(1)-C(15)-C(16)	-79.2(9)
C(13)-Fe(1)-C(15)-C(16)	-166.8(9)
C(17)-Fe(1)-C(15)-C(16)	-36.8(8)
C(12)-Fe(1)-C(15)-C(16)	37.3(18)
C(11)-Fe(1)-C(15)-C(16)	71.9(9)
C(10)-Fe(1)-C(15)-C(14)	-131.8(7)
C(9)-Fe(1)-C(15)-C(14)	-87.8(8)
C(16)-Fe(1)-C(15)-C(14)	115.1(11)
C(18)-Fe(1)-C(15)-C(14)	36.0(7)
C(13)-Fe(1)-C(15)-C(14)	-51.7(14)
C(17)-Fe(1)-C(15)-C(14)	78.3(8)
C(12)-Fe(1)-C(15)-C(14)	152.4(12)
C(11)-Fe(1)-C(15)-C(14)	-173.0(7)
C(14)-C(15)-C(16)-C(17)	-0.9(12)
Fe(1)-C(15)-C(16)-C(17)	59.5(8)
C(14)-C(15)-C(16)-Fe(1)	-60.4(6)
C(10)-Fe(1)-C(16)-C(17)	154.8(7)
C(9)-Fe(1)-C(16)-C(17)	-172.0(7)
C(14)-Fe(1)-C(16)-C(17)	-79.5(8)
C(18)-Fe(1)-C(16)-C(17)	-37.2(8)
C(13)-Fe(1)-C(16)-C(17)	43.2(17)
C(15)-Fe(1)-C(16)-C(17)	-120.3(11)
C(12)-Fe(1)-C(16)-C(17)	72.8(8)
C(11)-Fe(1)-C(16)-C(17)	112.9(7)
C(10)-Fe(1)-C(16)-C(15)	-84.9(8)
C(9)-Fe(1)-C(16)-C(15)	-51.7(13)
C(14)-Fe(1)-C(16)-C(15)	40.8(8)
C(18)-Fe(1)-C(16)-C(15)	83.1(9)
C(13)-Fe(1)-C(16)-C(15)	163.6(11)
C(17)-Fe(1)-C(16)-C(15)	120.3(11)
C(12)-Fe(1)-C(16)-C(15)	-166.9(7)
C(11)-Fe(1)-C(16)-C(15)	-126.8(8)
C(15)-C(16)-C(17)-C(18)	0.7(13)
Fe(1)-C(16)-C(17)-C(18)	60.1(7)
C(15)-C(16)-C(17)-Fe(1)	-59.4(7)
C(10)-Fe(1)-C(17)-C(18)	-170.3(8)

C(9)-Fe(1)-C(17)-C(18)	48.8(19)
C(14)-Fe(1)-C(17)-C(18)	-36.2(8)
C(16)-Fe(1)-C(17)-C(18)	-118.6(12)
C(13)-Fe(1)-C(17)-C(18)	76.8(9)
C(15)-Fe(1)-C(17)-C(18)	-81.6(9)
C(12)-Fe(1)-C(17)-C(18)	116.5(8)
C(11)-Fe(1)-C(17)-C(18)	157.8(8)
C(10)-Fe(1)-C(17)-C(16)	-51.7(13)
C(9)-Fe(1)-C(17)-C(16)	167.4(12)
C(14)-Fe(1)-C(17)-C(16)	82.5(8)
C(18)-Fe(1)-C(17)-C(16)	118.6(12)
C(13)-Fe(1)-C(17)-C(16)	-164.6(6)
C(15)-Fe(1)-C(17)-C(16)	37.0(7)
C(12)-Fe(1)-C(17)-C(16)	-124.9(7)
C(11)-Fe(1)-C(17)-C(16)	-83.5(8)
C(15)-C(14)-C(18)-C(17)	-0.5(12)
Fe(1)-C(14)-C(18)-C(17)	-59.7(8)
C(15)-C(14)-C(18)-Fe(1)	59.3(7)
C(16)-C(17)-C(18)-C(14)	-0.1(13)
Fe(1)-C(17)-C(18)-C(14)	59.6(8)
C(16)-C(17)-C(18)-Fe(1)	-59.7(8)
C(10)-Fe(1)-C(18)-C(14)	37(2)
C(9)-Fe(1)-C(18)-C(14)	74.7(8)
C(16)-Fe(1)-C(18)-C(14)	-82.5(8)
C(13)-Fe(1)-C(18)-C(14)	116.8(7)
C(15)-Fe(1)-C(18)-C(14)	-38.5(7)
C(17)-Fe(1)-C(18)-C(14)	-120.6(12)
C(12)-Fe(1)-C(18)-C(14)	159.9(6)
C(11)-Fe(1)-C(18)-C(14)	-164.5(7)
C(10)-Fe(1)-C(18)-C(17)	157.5(18)
C(9)-Fe(1)-C(18)-C(17)	-164.8(7)
C(14)-Fe(1)-C(18)-C(17)	120.6(12)
C(16)-Fe(1)-C(18)-C(17)	38.1(8)
C(13)-Fe(1)-C(18)-C(17)	-122.6(8)
C(15)-Fe(1)-C(18)-C(17)	82.0(9)
C(12)-Fe(1)-C(18)-C(17)	-79.5(9)
C(11)-Fe(1)-C(18)-C(17)	-43.9(13)
O(8)-C(8)-C(19)-C(23)	-1.2(8)
Re(2)-C(8)-C(19)-C(23)	-179.5(5)
O(8)-C(8)-C(19)-C(20)	-171.5(6)

Re(2)-C(8)-C(19)-C(20)	10.2(9)
O(8)-C(8)-C(19)-Fe(2)	-85.7(6)
Re(2)-C(8)-C(19)-Fe(2)	96.0(5)
C(24)-Fe(2)-C(19)-C(23)	-129.7(6)
C(27)-Fe(2)-C(19)-C(23)	-46.9(10)
C(20)-Fe(2)-C(19)-C(23)	118.4(5)
C(28)-Fe(2)-C(19)-C(23)	-85.7(6)
C(26)-Fe(2)-C(19)-C(23)	156(2)
C(22)-Fe(2)-C(19)-C(23)	37.6(4)
C(21)-Fe(2)-C(19)-C(23)	81.0(4)
C(25)-Fe(2)-C(19)-C(23)	-171.0(7)
C(24)-Fe(2)-C(19)-C(20)	111.9(6)
C(23)-Fe(2)-C(19)-C(20)	-118.4(5)
C(27)-Fe(2)-C(19)-C(20)	-165.3(9)
C(28)-Fe(2)-C(19)-C(20)	155.8(5)
C(26)-Fe(2)-C(19)-C(20)	37(2)
C(22)-Fe(2)-C(19)-C(20)	-80.8(4)
C(21)-Fe(2)-C(19)-C(20)	-37.5(4)
C(25)-Fe(2)-C(19)-C(20)	70.5(7)
C(24)-Fe(2)-C(19)-C(8)	-10.1(7)
C(23)-Fe(2)-C(19)-C(8)	119.6(6)
C(27)-Fe(2)-C(19)-C(8)	72.8(11)
C(20)-Fe(2)-C(19)-C(8)	-121.9(6)
C(28)-Fe(2)-C(19)-C(8)	33.9(7)
C(26)-Fe(2)-C(19)-C(8)	-84(2)
C(22)-Fe(2)-C(19)-C(8)	157.2(6)
C(21)-Fe(2)-C(19)-C(8)	-159.4(5)
C(25)-Fe(2)-C(19)-C(8)	-51.4(8)
C(23)-C(19)-C(20)-C(21)	1.2(7)
C(8)-C(19)-C(20)-C(21)	173.0(6)
Fe(2)-C(19)-C(20)-C(21)	60.6(5)
C(23)-C(19)-C(20)-Fe(2)	-59.3(4)
C(8)-C(19)-C(20)-Fe(2)	112.4(6)
C(24)-Fe(2)-C(20)-C(21)	152.2(7)
C(19)-Fe(2)-C(20)-C(21)	-118.5(6)
C(23)-Fe(2)-C(20)-C(21)	-80.0(4)
C(27)-Fe(2)-C(20)-C(21)	38.6(14)
C(28)-Fe(2)-C(20)-C(21)	-172.8(8)
C(26)-Fe(2)-C(20)-C(21)	72.1(7)
C(22)-Fe(2)-C(20)-C(21)	-36.5(4)

C(25)-Fe(2)-C(20)-C(21)	111.2(6)
C(24)-Fe(2)-C(20)-C(19)	-89.3(7)
C(23)-Fe(2)-C(20)-C(19)	38.5(4)
C(27)-Fe(2)-C(20)-C(19)	157.1(12)
C(28)-Fe(2)-C(20)-C(19)	-54.3(10)
C(26)-Fe(2)-C(20)-C(19)	-169.4(6)
C(22)-Fe(2)-C(20)-C(19)	82.0(4)
C(21)-Fe(2)-C(20)-C(19)	118.5(6)
C(25)-Fe(2)-C(20)-C(19)	-130.3(6)
C(19)-C(20)-C(21)-C(22)	-1.3(8)
Fe(2)-C(20)-C(21)-C(22)	58.1(5)
C(19)-C(20)-C(21)-Fe(2)	-59.4(4)
C(24)-Fe(2)-C(21)-C(20)	-57.5(10)
C(19)-Fe(2)-C(21)-C(20)	38.8(4)
C(23)-Fe(2)-C(21)-C(20)	83.7(4)
C(27)-Fe(2)-C(21)-C(20)	-167.0(6)
C(28)-Fe(2)-C(21)-C(20)	167.6(15)
C(26)-Fe(2)-C(21)-C(20)	-127.0(6)
C(22)-Fe(2)-C(21)-C(20)	121.2(6)
C(25)-Fe(2)-C(21)-C(20)	-85.7(6)
C(24)-Fe(2)-C(21)-C(22)	-178.7(8)
C(19)-Fe(2)-C(21)-C(22)	-82.4(4)
C(23)-Fe(2)-C(21)-C(22)	-37.4(4)
C(27)-Fe(2)-C(21)-C(22)	71.8(6)
C(20)-Fe(2)-C(21)-C(22)	-121.2(6)
C(28)-Fe(2)-C(21)-C(22)	46.4(16)
C(26)-Fe(2)-C(21)-C(22)	111.8(6)
C(25)-Fe(2)-C(21)-C(22)	153.1(6)
C(20)-C(21)-C(22)-C(23)	0.9(8)
Fe(2)-C(21)-C(22)-C(23)	58.8(5)
C(20)-C(21)-C(22)-Fe(2)	-57.9(5)
C(24)-Fe(2)-C(22)-C(23)	57(2)
C(19)-Fe(2)-C(22)-C(23)	-38.6(4)
C(27)-Fe(2)-C(22)-C(23)	113.8(6)
C(20)-Fe(2)-C(22)-C(23)	-83.3(4)
C(28)-Fe(2)-C(22)-C(23)	74.0(6)
C(26)-Fe(2)-C(22)-C(23)	155.3(6)
C(21)-Fe(2)-C(22)-C(23)	-119.6(6)
C(25)-Fe(2)-C(22)-C(23)	-172.0(7)
C(24)-Fe(2)-C(22)-C(21)	176.9(19)

C(19)-Fe(2)-C(22)-C(21)	81.1(4)
C(23)-Fe(2)-C(22)-C(21)	119.6(6)
C(27)-Fe(2)-C(22)-C(21)	-126.6(6)
C(20)-Fe(2)-C(22)-C(21)	36.3(4)
C(28)-Fe(2)-C(22)-C(21)	-166.3(6)
C(26)-Fe(2)-C(22)-C(21)	-85.0(6)
C(25)-Fe(2)-C(22)-C(21)	-52.4(9)
C(21)-C(22)-C(23)-C(19)	-0.1(8)
Fe(2)-C(22)-C(23)-C(19)	59.4(4)
C(21)-C(22)-C(23)-Fe(2)	-59.5(5)
C(20)-C(19)-C(23)-C(22)	-0.7(7)
C(8)-C(19)-C(23)-C(22)	-172.6(6)
Fe(2)-C(19)-C(23)-C(22)	-60.2(5)
C(20)-C(19)-C(23)-Fe(2)	59.5(4)
C(8)-C(19)-C(23)-Fe(2)	-112.5(6)
C(24)-Fe(2)-C(23)-C(22)	-166.5(6)
C(19)-Fe(2)-C(23)-C(22)	118.8(6)
C(27)-Fe(2)-C(23)-C(22)	-82.8(7)
C(20)-Fe(2)-C(23)-C(22)	80.3(4)
C(28)-Fe(2)-C(23)-C(22)	-127.1(6)
C(26)-Fe(2)-C(23)-C(22)	-49.5(11)
C(21)-Fe(2)-C(23)-C(22)	37.3(4)
C(25)-Fe(2)-C(23)-C(22)	158(2)
C(24)-Fe(2)-C(23)-C(19)	74.7(6)
C(27)-Fe(2)-C(23)-C(19)	158.3(6)
C(20)-Fe(2)-C(23)-C(19)	-38.5(3)
C(28)-Fe(2)-C(23)-C(19)	114.0(5)
C(26)-Fe(2)-C(23)-C(19)	-168.3(9)
C(22)-Fe(2)-C(23)-C(19)	-118.8(6)
C(21)-Fe(2)-C(23)-C(19)	-81.6(4)
C(25)-Fe(2)-C(23)-C(19)	39(2)
C(19)-Fe(2)-C(24)-C(25)	-126.4(7)
C(23)-Fe(2)-C(24)-C(25)	-170.0(6)
C(27)-Fe(2)-C(24)-C(25)	82.3(8)
C(20)-Fe(2)-C(24)-C(25)	-80.8(8)
C(28)-Fe(2)-C(24)-C(25)	122.0(11)
C(26)-Fe(2)-C(24)-C(25)	38.7(7)
C(22)-Fe(2)-C(24)-C(25)	142.4(19)
C(21)-Fe(2)-C(24)-C(25)	-41.7(12)
C(19)-Fe(2)-C(24)-C(28)	111.6(7)

C(23)-Fe(2)-C(24)-C(28)	68.0(9)
C(27)-Fe(2)-C(24)-C(28)	-39.6(7)
C(20)-Fe(2)-C(24)-C(28)	157.2(7)
C(26)-Fe(2)-C(24)-C(28)	-83.3(8)
C(22)-Fe(2)-C(24)-C(28)	20(2)
C(21)-Fe(2)-C(24)-C(28)	-163.7(7)
C(25)-Fe(2)-C(24)-C(28)	-122.0(11)
C(28)-C(24)-C(25)-C(26)	-1.5(12)
Fe(2)-C(24)-C(25)-C(26)	-60.8(8)
C(28)-C(24)-C(25)-Fe(2)	59.3(7)
C(19)-Fe(2)-C(25)-C(24)	75.7(8)
C(23)-Fe(2)-C(25)-C(24)	43(3)
C(27)-Fe(2)-C(25)-C(24)	-80.7(8)
C(20)-Fe(2)-C(25)-C(24)	116.7(7)
C(28)-Fe(2)-C(25)-C(24)	-36.1(7)
C(26)-Fe(2)-C(25)-C(24)	-116.4(11)
C(22)-Fe(2)-C(25)-C(24)	-165.7(7)
C(21)-Fe(2)-C(25)-C(24)	159.1(6)
C(24)-Fe(2)-C(25)-C(26)	116.4(11)
C(19)-Fe(2)-C(25)-C(26)	-167.9(7)
C(23)-Fe(2)-C(25)-C(26)	159.0(19)
C(27)-Fe(2)-C(25)-C(26)	35.6(9)
C(20)-Fe(2)-C(25)-C(26)	-126.9(8)
C(28)-Fe(2)-C(25)-C(26)	80.2(9)
C(22)-Fe(2)-C(25)-C(26)	-49.4(13)
C(21)-Fe(2)-C(25)-C(26)	-84.5(9)
C(24)-C(25)-C(26)-C(27)	2.3(13)
Fe(2)-C(25)-C(26)-C(27)	-58.0(8)
C(24)-C(25)-C(26)-Fe(2)	60.3(7)
C(24)-Fe(2)-C(26)-C(25)	-38.7(8)
C(19)-Fe(2)-C(26)-C(25)	42(2)
C(23)-Fe(2)-C(26)-C(25)	-172.0(8)
C(27)-Fe(2)-C(26)-C(25)	-122.6(13)
C(20)-Fe(2)-C(26)-C(25)	71.9(10)
C(28)-Fe(2)-C(26)-C(25)	-82.7(9)
C(22)-Fe(2)-C(26)-C(25)	154.3(8)
C(21)-Fe(2)-C(26)-C(25)	111.8(9)
C(24)-Fe(2)-C(26)-C(27)	84.0(9)
C(19)-Fe(2)-C(26)-C(27)	164.3(16)
C(23)-Fe(2)-C(26)-C(27)	-49.4(14)

C(20)-Fe(2)-C(26)-C(27)	-165.4(7)
C(28)-Fe(2)-C(26)-C(27)	39.9(8)
C(22)-Fe(2)-C(26)-C(27)	-83.1(9)
C(21)-Fe(2)-C(26)-C(27)	-125.5(9)
C(25)-Fe(2)-C(26)-C(27)	122.6(13)
C(25)-C(26)-C(27)-C(28)	-2.2(13)
Fe(2)-C(26)-C(27)-C(28)	-60.9(7)
C(25)-C(26)-C(27)-Fe(2)	58.7(8)
C(24)-Fe(2)-C(27)-C(26)	-77.6(9)
C(19)-Fe(2)-C(27)-C(26)	-171.6(9)
C(23)-Fe(2)-C(27)-C(26)	155.2(8)
C(20)-Fe(2)-C(27)-C(26)	43.6(17)
C(28)-Fe(2)-C(27)-C(26)	-116.2(11)
C(22)-Fe(2)-C(27)-C(26)	113.1(9)
C(21)-Fe(2)-C(27)-C(26)	73.3(10)
C(25)-Fe(2)-C(27)-C(26)	-35.1(9)
C(24)-Fe(2)-C(27)-C(28)	38.7(7)
C(19)-Fe(2)-C(27)-C(28)	-55.3(12)
C(23)-Fe(2)-C(27)-C(28)	-88.5(7)
C(20)-Fe(2)-C(27)-C(28)	159.9(11)
C(26)-Fe(2)-C(27)-C(28)	116.2(11)
C(22)-Fe(2)-C(27)-C(28)	-130.7(7)
C(21)-Fe(2)-C(27)-C(28)	-170.5(6)
C(25)-Fe(2)-C(27)-C(28)	81.2(8)
C(25)-C(24)-C(28)-C(27)	0.2(11)
Fe(2)-C(24)-C(28)-C(27)	60.3(7)
C(25)-C(24)-C(28)-Fe(2)	-60.0(8)
C(26)-C(27)-C(28)-C(24)	1.2(11)
Fe(2)-C(27)-C(28)-C(24)	-60.4(6)
C(26)-C(27)-C(28)-Fe(2)	61.5(7)
C(19)-Fe(2)-C(28)-C(24)	-88.7(8)
C(23)-Fe(2)-C(28)-C(24)	-133.3(8)
C(27)-Fe(2)-C(28)-C(24)	116.6(11)
C(20)-Fe(2)-C(28)-C(24)	-50.1(13)
C(26)-Fe(2)-C(28)-C(24)	77.9(8)
C(22)-Fe(2)-C(28)-C(24)	-174.7(7)
C(21)-Fe(2)-C(28)-C(24)	148.4(14)
C(25)-Fe(2)-C(28)-C(24)	35.4(8)
C(24)-Fe(2)-C(28)-C(27)	-116.6(11)
C(19)-Fe(2)-C(28)-C(27)	154.8(6)

C(23)-Fe(2)-C(28)-C(27)	110.2(7)
C(20)-Fe(2)-C(28)-C(27)	-166.7(8)
C(26)-Fe(2)-C(28)-C(27)	-38.6(7)
C(22)-Fe(2)-C(28)-C(27)	68.7(8)
C(21)-Fe(2)-C(28)-C(27)	31.9(19)
C(25)-Fe(2)-C(28)-C(27)	-81.2(8)
C(4)-O(4)-C(29)-C(30)	-157.8(11)
C(8)-O(8)-C(31)-C(32)	-177.4(9)

Appendix 10

Crystallographic data of Complex 33

Table 1. Crystal data and structure refinement for Complex **33**.

Identification code	db55a3a_abs	
Empirical formula	C_{40} H_{22} Fe O_{22} Re_4 Ti	
Formula weight	1703.13	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P $\bar{1}$	
Unit cell dimensions	a = 10.7406(7) Å	a= 90.9060(10)°.
	b = 12.1924(8) Å	b= 94.7320(10)°.
	c = 18.4356(12) Å	g = 95.6650(10)°.
Volume	2393.5(3) $Å^3$	
Z	2	
Density (calculated)	2.363 Mg/m^3	
Absorption coefficient	10.607 mm^{-1}	
F(000)	1572	
Crystal size	0.17 x 0.17 x 0.01 mm^3	
Theta range for data collection	2.41 to 26.33°.	
Index ranges	-13<=h<=5, -14<=k<=13, -21<=l<=22	
Reflections collected	12826	
Independent reflections	8569 [R(int) = 0.0308]	
Completeness to theta = 25.00°	97.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.727 and 0.215	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8569 / 0 / 608	
Goodness-of-fit on F^2	1.025	
Final R indices [I>2sigma(I)]	R1 = 0.0503, wR2 = 0.1319	
R indices (all data)	R1 = 0.0778, wR2 = 0.1520	
Extinction coefficient	0.00036(10)	
Largest diff. peak and hole	3.273 and -1.699 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Complex **33**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	2508(1)	8347(1)	-291(1)	45(1)
Re(2)	2014(1)	7706(1)	1271(1)	44(1)
Re(3)	8470(1)	2372(1)	4638(1)	62(1)
Re(4)	6893(1)	3587(1)	3518(1)	46(1)
Fe(1)	3470(2)	4021(1)	1560(1)	40(1)
Ti(1)	5958(2)	6973(2)	2524(1)	38(1)
C(1)	2876(15)	8806(12)	-1244(9)	60(4)
O(1)	3129(13)	9049(10)	-1824(7)	85(4)
C(2)	2566(12)	6755(11)	-514(8)	50(3)
O(2)	2549(12)	5873(9)	-691(7)	75(3)
C(3)	669(15)	8112(13)	-566(10)	67(4)
O(3)	-366(10)	7975(12)	-768(9)	103(5)
C(4)	2327(16)	9851(13)	60(10)	70(5)
O(4)	2261(13)	10736(9)	266(8)	91(4)
C(5)	4269(14)	8509(12)	116(9)	57(4)
O(5)	5290(10)	8622(10)	366(8)	87(4)
C(6)	1575(14)	7272(15)	2215(11)	69(5)
O(6)	1305(12)	7038(14)	2775(8)	101(5)
C(7)	700(12)	6645(12)	785(9)	54(4)
O(7)	-132(10)	6105(10)	506(8)	90(4)
C(8)	870(20)	8825(14)	1210(8)	91(8)
O(8)	-41(11)	9337(10)	1165(8)	87(4)
C(9)	3316(15)	8954(13)	1565(9)	60(4)
O(9)	4011(12)	9683(10)	1728(8)	86(4)
C(10)	3505(10)	6617(10)	1393(6)	35(3)
O(10)	4543(7)	6928(6)	1772(5)	42(2)
C(11)	9543(19)	1747(15)	5365(11)	86(6)
O(11)	10214(16)	1371(15)	5786(11)	142(7)
C(12)	8492(15)	1241(14)	3886(11)	70(5)
O(12)	8444(14)	587(11)	3431(10)	107(5)
C(13)	6870(19)	1610(14)	4923(11)	79(5)
O(13)	5963(15)	1160(12)	5092(8)	104(5)
C(14)	8200(20)	3605(18)	5320(10)	83(6)
O(14)	7967(18)	4285(14)	5703(9)	122(6)
C(15)	9900(17)	3206(14)	4193(12)	80(5)
O(15)	10656(14)	3685(12)	3927(10)	113(5)
C(16)	6062(13)	2065(12)	3327(8)	50(3)

O(16)	5589(10)	1201(8)	3228(7)	69(3)
C(17)	5717(19)	3751(14)	4248(10)	72(5)
O(17)	5007(17)	3852(13)	4645(9)	119(6)
C(18)	7950(17)	4939(14)	3862(10)	70(4)
O(18)	8589(14)	5689(10)	4110(8)	96(4)
C(19)	8014(14)	3469(13)	2824(9)	66(5)
O(19)	8722(13)	3305(13)	2341(8)	102(5)
C(20)	5707(13)	4386(9)	2820(7)	42(3)
O(20)	5833(7)	5407(6)	2681(4)	39(2)
C(21)	3482(11)	5526(10)	1068(7)	42(3)
C(22)	4573(12)	4980(11)	933(7)	43(3)
C(23)	4168(13)	3959(11)	570(7)	48(3)
C(24)	2871(13)	3834(11)	480(8)	51(3)
C(25)	2412(12)	4764(11)	795(8)	49(3)
C(26)	4472(12)	3829(10)	2532(7)	44(3)
C(27)	4222(14)	2800(12)	2140(8)	59(4)
C(28)	2872(17)	2562(14)	1998(10)	76(5)
C(29)	2296(14)	3412(15)	2318(9)	68(5)
C(30)	3256(14)	4211(13)	2622(8)	56(4)
C(31)	7000(14)	7108(15)	1423(9)	67(5)
C(32)	7621(15)	6427(14)	1866(11)	71(5)
C(33)	8156(14)	7032(19)	2480(10)	78(5)
C(34)	7891(16)	8081(15)	2399(11)	75(5)
C(35)	7127(15)	8138(13)	1773(11)	71(5)
C(36)	4557(18)	7016(17)	3455(11)	86(7)
C(37)	5770(20)	6912(18)	3790(9)	89(7)
C(38)	6463(18)	7850(20)	3677(11)	84(6)
C(39)	5720(20)	8507(14)	3263(11)	80(5)
C(40)	4600(9)	7991(7)	3162(5)	79(5)
O(21)	1887(9)	112(7)	3125(5)	127(7)
O(22)	2301(9)	1241(7)	4453(5)	127(6)

Table 3. Bond lengths [Å] and angles [°] for Complex **33**.

O(5)-C(5)	1.149(18)	Ti(1)-C(37)	2.361(17)
Re(1)-C(1)	1.912(17)	Ti(1)-C(32)	2.381(15)
Re(1)-C(5)	1.967(15)	Ti(1)-C(36)	2.377(15)
Re(1)-C(4)	1.968(17)	Ti(1)-C(40)	2.376(8)
Re(1)-C(2)	1.985(14)	Ti(1)-C(34)	2.392(14)
Re(1)-C(3)	1.989(17)	Ti(1)-C(31)	2.398(16)
Re(1)-Re(2)	3.0712(8)	C(1)-O(1)	1.161(18)
Re(2)-C(6)	1.909(19)	C(2)-O(2)	1.117(16)
Re(2)-C(8)	1.923(14)	C(3)-O(3)	1.138(19)
Re(2)-C(7)	1.965(15)	C(4)-O(4)	1.150(18)
Re(2)-C(9)	1.999(17)	C(6)-O(6)	1.129(19)
Re(2)-C(10)	2.178(11)	C(7)-O(7)	1.138(17)
Re(3)-C(11)	1.912(18)	C(8)-O(8)	1.209(18)
Re(3)-C(12)	1.94(2)	C(9)-O(9)	1.123(18)
Re(3)-C(13)	1.98(2)	C(10)-O(10)	1.286(14)
Re(3)-C(15)	1.999(19)	C(10)-C(21)	1.448(17)
Re(3)-C(14)	2.00(2)	C(11)-O(11)	1.15(2)
Re(3)-Re(4)	3.0569(8)	C(12)-O(12)	1.14(2)
Re(4)-C(19)	1.84(2)	C(13)-O(13)	1.14(2)
Re(4)-C(17)	1.941(18)	C(14)-O(14)	1.14(2)
Re(4)-C(18)	1.972(18)	C(15)-O(15)	1.11(2)
Re(4)-C(16)	1.991(15)	C(16)-O(16)	1.129(16)
Re(4)-C(20)	2.059(13)	C(17)-O(17)	1.11(2)
Fe(1)-C(30)	2.003(14)	C(18)-O(18)	1.151(19)
Fe(1)-C(25)	2.019(13)	C(19)-O(19)	1.24(2)
Fe(1)-C(22)	2.025(12)	C(20)-O(20)	1.272(14)
Fe(1)-C(28)	2.033(15)	C(20)-C(26)	1.481(18)
Fe(1)-C(23)	2.032(13)	C(21)-C(22)	1.440(17)
Fe(1)-C(26)	2.043(13)	C(21)-C(25)	1.454(17)
Fe(1)-C(24)	2.043(14)	C(22)-C(23)	1.416(18)
Fe(1)-C(27)	2.038(14)	C(22)-H(22)	0.9300
Fe(1)-C(29)	2.058(15)	C(23)-C(24)	1.382(19)
Fe(1)-C(21)	2.059(12)	C(23)-H(23)	0.9300
Ti(1)-O(20)	1.929(8)	C(24)-C(25)	1.417(19)
Ti(1)-O(10)	1.968(9)	C(24)-H(24)	0.9300
Ti(1)-C(39)	2.343(16)	C(25)-H(25)	0.9300
Ti(1)-C(35)	2.347(14)	C(26)-C(27)	1.430(19)
Ti(1)-C(33)	2.363(15)	C(26)-C(30)	1.45(2)
Ti(1)-C(38)	2.363(17)	C(27)-C(28)	1.45(2)

C(27)-H(27)	0.9300	C(2)-Re(1)-Re(2)	87.6(4)
C(28)-C(29)	1.40(2)	C(3)-Re(1)-Re(2)	89.0(5)
C(28)-H(28)	0.9300	C(6)-Re(2)-C(8)	93.2(6)
C(29)-C(30)	1.42(2)	C(6)-Re(2)-C(7)	92.2(7)
C(29)-H(29)	0.9300	C(8)-Re(2)-C(7)	89.8(8)
C(30)-H(30)	0.9300	C(6)-Re(2)-C(9)	98.9(7)
C(31)-C(32)	1.36(2)	C(8)-Re(2)-C(9)	84.7(9)
C(31)-C(35)	1.39(2)	C(7)-Re(2)-C(9)	167.8(6)
C(31)-H(31)	0.9300	C(6)-Re(2)-C(10)	87.6(5)
C(32)-C(33)	1.39(2)	C(8)-Re(2)-C(10)	172.2(8)
C(32)-H(32)	0.9300	C(7)-Re(2)-C(10)	98.0(5)
C(33)-C(34)	1.35(2)	C(9)-Re(2)-C(10)	87.5(5)
C(33)-H(33)	0.9300	C(6)-Re(2)-Re(1)	175.5(5)
C(34)-C(35)	1.37(2)	C(8)-Re(2)-Re(1)	84.7(4)
C(34)-H(34)	0.9300	C(7)-Re(2)-Re(1)	83.8(5)
C(35)-H(35)	0.9300	C(9)-Re(2)-Re(1)	84.8(5)
C(36)-C(40)	1.31(2)	C(10)-Re(2)-Re(1)	95.0(3)
C(36)-C(37)	1.41(3)	C(11)-Re(3)-C(12)	97.4(8)
C(36)-H(36)	0.9300	C(11)-Re(3)-C(13)	96.5(8)
C(37)-C(38)	1.34(3)	C(12)-Re(3)-C(13)	88.9(8)
C(37)-H(37)	0.9300	C(11)-Re(3)-C(15)	93.4(8)
C(38)-C(39)	1.37(3)	C(12)-Re(3)-C(15)	87.6(8)
C(38)-H(38)	0.9300	C(13)-Re(3)-C(15)	169.9(8)
C(39)-C(40)	1.30(2)	C(11)-Re(3)-C(14)	91.4(8)
C(39)-H(39)	0.9300	C(12)-Re(3)-C(14)	170.8(7)
C(40)-H(40)	0.9300	C(13)-Re(3)-C(14)	87.4(8)
		C(15)-Re(3)-C(14)	94.6(8)
C(1)-Re(1)-C(5)	94.9(7)	C(11)-Re(3)-Re(4)	174.5(6)
C(1)-Re(1)-C(4)	93.9(6)	C(12)-Re(3)-Re(4)	86.7(5)
C(5)-Re(1)-C(4)	89.6(7)	C(13)-Re(3)-Re(4)	87.3(5)
C(1)-Re(1)-C(2)	94.5(6)	C(15)-Re(3)-Re(4)	83.0(5)
C(5)-Re(1)-C(2)	91.9(6)	C(14)-Re(3)-Re(4)	84.8(5)
C(4)-Re(1)-C(2)	171.4(6)	C(19)-Re(4)-C(17)	178.6(7)
C(1)-Re(1)-C(3)	93.1(7)	C(19)-Re(4)-C(18)	86.4(7)
C(5)-Re(1)-C(3)	171.9(7)	C(17)-Re(4)-C(18)	92.5(8)
C(4)-Re(1)-C(3)	90.1(7)	C(19)-Re(4)-C(16)	93.9(7)
C(2)-Re(1)-C(3)	87.3(6)	C(17)-Re(4)-C(16)	87.4(7)
C(1)-Re(1)-Re(2)	177.1(5)	C(18)-Re(4)-C(16)	167.6(6)
C(5)-Re(1)-Re(2)	82.9(5)	C(19)-Re(4)-C(20)	92.3(5)
C(4)-Re(1)-Re(2)	84.2(5)	C(17)-Re(4)-C(20)	87.0(6)

C(18)-Re(4)-C(20)	94.9(6)	C(26)-Fe(1)-C(29)	69.7(6)
C(16)-Re(4)-C(20)	97.4(5)	C(24)-Fe(1)-C(29)	118.9(6)
C(19)-Re(4)-Re(3)	92.5(4)	C(27)-Fe(1)-C(29)	68.8(7)
C(17)-Re(4)-Re(3)	88.3(5)	C(30)-Fe(1)-C(21)	109.6(6)
C(18)-Re(4)-Re(3)	86.6(5)	C(25)-Fe(1)-C(21)	41.8(5)
C(16)-Re(4)-Re(3)	81.1(4)	C(22)-Fe(1)-C(21)	41.3(5)
C(20)-Re(4)-Re(3)	175.1(3)	C(28)-Fe(1)-C(21)	162.1(6)
C(30)-Fe(1)-C(25)	121.4(6)	C(23)-Fe(1)-C(21)	69.0(5)
C(30)-Fe(1)-C(22)	128.2(6)	C(26)-Fe(1)-C(21)	121.7(5)
C(25)-Fe(1)-C(22)	69.4(5)	C(24)-Fe(1)-C(21)	69.1(5)
C(30)-Fe(1)-C(28)	68.9(7)	C(27)-Fe(1)-C(21)	155.8(5)
C(25)-Fe(1)-C(28)	122.6(6)	C(29)-Fe(1)-C(21)	127.2(7)
C(22)-Fe(1)-C(28)	153.4(7)	O(20)-Ti(1)-O(10)	96.1(3)
C(30)-Fe(1)-C(23)	164.8(6)	O(20)-Ti(1)-C(39)	133.5(6)
C(25)-Fe(1)-C(23)	68.3(6)	O(10)-Ti(1)-C(39)	104.4(6)
C(22)-Fe(1)-C(23)	40.8(5)	O(20)-Ti(1)-C(35)	133.6(5)
C(28)-Fe(1)-C(23)	117.3(7)	O(10)-Ti(1)-C(35)	88.1(5)
C(30)-Fe(1)-C(26)	42.0(6)	C(39)-Ti(1)-C(35)	89.0(7)
C(25)-Fe(1)-C(26)	157.9(6)	O(20)-Ti(1)-C(33)	91.2(6)
C(22)-Fe(1)-C(26)	108.0(5)	O(10)-Ti(1)-C(33)	133.4(5)
C(28)-Fe(1)-C(26)	70.0(6)	C(39)-Ti(1)-C(33)	103.3(8)
C(23)-Fe(1)-C(26)	124.9(6)	C(35)-Ti(1)-C(33)	55.8(6)
C(30)-Fe(1)-C(24)	155.1(6)	O(20)-Ti(1)-C(38)	106.9(7)
C(25)-Fe(1)-C(24)	40.8(5)	O(10)-Ti(1)-C(38)	135.4(6)
C(22)-Fe(1)-C(24)	68.2(6)	C(39)-Ti(1)-C(38)	34.0(7)
C(28)-Fe(1)-C(24)	104.4(6)	C(35)-Ti(1)-C(38)	101.7(8)
C(23)-Fe(1)-C(24)	39.7(6)	C(33)-Ti(1)-C(38)	84.7(7)
C(26)-Fe(1)-C(24)	160.3(6)	O(20)-Ti(1)-C(37)	78.5(6)
C(30)-Fe(1)-C(27)	69.3(7)	O(10)-Ti(1)-C(37)	125.0(7)
C(25)-Fe(1)-C(27)	160.0(6)	C(39)-Ti(1)-C(37)	55.5(7)
C(22)-Fe(1)-C(27)	119.2(6)	C(35)-Ti(1)-C(37)	134.4(9)
C(28)-Fe(1)-C(27)	41.8(6)	C(33)-Ti(1)-C(37)	101.6(8)
C(23)-Fe(1)-C(27)	105.5(6)	C(38)-Ti(1)-C(37)	32.8(7)
C(26)-Fe(1)-C(27)	41.0(5)	O(20)-Ti(1)-C(32)	78.5(5)
C(24)-Fe(1)-C(27)	122.5(6)	O(10)-Ti(1)-C(32)	102.9(6)
C(30)-Fe(1)-C(29)	40.9(6)	C(39)-Ti(1)-C(32)	133.9(7)
C(25)-Fe(1)-C(29)	107.3(6)	C(35)-Ti(1)-C(32)	55.7(6)
C(22)-Fe(1)-C(29)	165.9(7)	C(33)-Ti(1)-C(32)	34.1(6)
C(28)-Fe(1)-C(29)	40.1(7)	C(38)-Ti(1)-C(32)	118.6(7)
C(23)-Fe(1)-C(29)	152.0(6)	C(37)-Ti(1)-C(32)	128.4(7)

O(20)-Ti(1)-C(36)	84.7(6)	O(3)-C(3)-Re(1)	175.6(17)
O(10)-Ti(1)-C(36)	90.6(6)	O(4)-C(4)-Re(1)	177.9(15)
C(39)-Ti(1)-C(36)	54.3(6)	O(5)-C(5)-Re(1)	178.3(14)
C(35)-Ti(1)-C(36)	141.6(7)	O(6)-C(6)-Re(2)	178.5(17)
C(33)-Ti(1)-C(36)	136.0(7)	O(7)-C(7)-Re(2)	173.7(12)
C(38)-Ti(1)-C(36)	55.3(6)	O(8)-C(8)-Re(2)	166.0(19)
C(37)-Ti(1)-C(36)	34.7(7)	O(9)-C(9)-Re(2)	177.3(14)
C(32)-Ti(1)-C(36)	159.4(8)	O(10)-C(10)-C(21)	113.0(10)
O(20)-Ti(1)-C(40)	116.1(4)	O(10)-C(10)-Re(2)	120.6(8)
O(10)-Ti(1)-C(40)	81.3(4)	C(21)-C(10)-Re(2)	126.4(8)
C(39)-Ti(1)-C(40)	32.1(5)	C(10)-O(10)-Ti(1)	161.3(8)
C(35)-Ti(1)-C(40)	110.3(5)	O(11)-C(11)-Re(3)	178(2)
C(33)-Ti(1)-C(40)	135.0(6)	O(12)-C(12)-Re(3)	176.5(15)
C(38)-Ti(1)-C(40)	54.4(6)	O(13)-C(13)-Re(3)	178.9(18)
C(37)-Ti(1)-C(40)	55.0(5)	O(14)-C(14)-Re(3)	175.5(19)
C(32)-Ti(1)-C(40)	164.6(5)	O(15)-C(15)-Re(3)	177.1(18)
C(36)-Ti(1)-C(40)	32.0(6)	O(16)-C(16)-Re(4)	179.2(13)
O(20)-Ti(1)-C(34)	124.0(6)	O(17)-C(17)-Re(4)	177.2(19)
O(10)-Ti(1)-C(34)	121.5(6)	O(18)-C(18)-Re(4)	175.0(16)
C(39)-Ti(1)-C(34)	78.9(6)	O(19)-C(19)-Re(4)	174.8(14)
C(35)-Ti(1)-C(34)	33.5(6)	O(20)-C(20)-C(26)	112.8(11)
C(33)-Ti(1)-C(34)	32.9(6)	O(20)-C(20)-Re(4)	125.7(10)
C(38)-Ti(1)-C(34)	75.7(7)	C(26)-C(20)-Re(4)	120.6(8)
C(37)-Ti(1)-C(34)	105.1(8)	C(20)-O(20)-Ti(1)	176.2(8)
C(32)-Ti(1)-C(34)	55.2(6)	C(22)-C(21)-C(10)	125.3(11)
C(36)-Ti(1)-C(34)	129.5(6)	C(22)-C(21)-C(25)	105.4(11)
C(40)-Ti(1)-C(34)	109.9(5)	C(10)-C(21)-C(25)	129.3(11)
O(20)-Ti(1)-C(31)	101.9(5)	C(22)-C(21)-Fe(1)	68.1(7)
O(10)-Ti(1)-C(31)	77.6(5)	C(10)-C(21)-Fe(1)	129.4(9)
C(39)-Ti(1)-C(31)	122.9(6)	C(25)-C(21)-Fe(1)	67.6(7)
C(35)-Ti(1)-C(31)	34.1(6)	C(23)-C(22)-C(21)	108.5(11)
C(33)-Ti(1)-C(31)	55.9(6)	C(23)-C(22)-Fe(1)	69.9(7)
C(38)-Ti(1)-C(31)	131.2(6)	C(21)-C(22)-Fe(1)	70.6(7)
C(37)-Ti(1)-C(31)	157.4(8)	C(23)-C(22)-H(22)	125.8
C(32)-Ti(1)-C(31)	33.0(6)	C(21)-C(22)-H(22)	125.8
C(36)-Ti(1)-C(31)	167.0(8)	Fe(1)-C(22)-H(22)	125.3
C(40)-Ti(1)-C(31)	138.2(6)	C(24)-C(23)-C(22)	109.1(12)
C(34)-Ti(1)-C(31)	55.6(6)	C(24)-C(23)-Fe(1)	70.6(8)
O(1)-C(1)-Re(1)	177.3(14)	C(22)-C(23)-Fe(1)	69.3(7)
O(2)-C(2)-Re(1)	174.5(14)	C(24)-C(23)-H(23)	125.4

C(22)-C(23)-H(23)	125.4	C(26)-C(30)-Fe(1)	70.5(8)
Fe(1)-C(23)-H(23)	126.2	C(29)-C(30)-H(30)	125.3
C(23)-C(24)-C(25)	108.7(12)	C(26)-C(30)-H(30)	125.3
C(23)-C(24)-Fe(1)	69.7(8)	Fe(1)-C(30)-H(30)	124.2
C(25)-C(24)-Fe(1)	68.7(8)	C(32)-C(31)-C(35)	106.8(16)
C(23)-C(24)-H(24)	125.6	C(32)-C(31)-Ti(1)	72.8(10)
C(25)-C(24)-H(24)	125.6	C(35)-C(31)-Ti(1)	70.9(9)
Fe(1)-C(24)-H(24)	127.5	C(32)-C(31)-H(31)	126.6
C(24)-C(25)-C(21)	108.2(11)	C(35)-C(31)-H(31)	126.6
C(24)-C(25)-Fe(1)	70.5(8)	Ti(1)-C(31)-H(31)	121.5
C(21)-C(25)-Fe(1)	70.6(7)	C(31)-C(32)-C(33)	108.5(16)
C(24)-C(25)-H(25)	125.9	C(31)-C(32)-Ti(1)	74.2(9)
C(21)-C(25)-H(25)	125.9	C(33)-C(32)-Ti(1)	72.2(9)
Fe(1)-C(25)-H(25)	124.6	C(31)-C(32)-H(32)	125.8
C(27)-C(26)-C(30)	105.9(12)	C(33)-C(32)-H(32)	125.8
C(27)-C(26)-C(20)	127.9(13)	Ti(1)-C(32)-H(32)	119.7
C(30)-C(26)-C(20)	126.2(12)	C(34)-C(33)-C(32)	107.8(16)
C(27)-C(26)-Fe(1)	69.3(8)	C(34)-C(33)-Ti(1)	74.7(9)
C(30)-C(26)-Fe(1)	67.5(8)	C(32)-C(33)-Ti(1)	73.7(9)
C(20)-C(26)-Fe(1)	129.3(9)	C(34)-C(33)-H(33)	126.1
C(26)-C(27)-C(28)	108.4(15)	C(32)-C(33)-H(33)	126.1
C(26)-C(27)-Fe(1)	69.7(8)	Ti(1)-C(33)-H(33)	117.5
C(28)-C(27)-Fe(1)	68.9(8)	C(33)-C(34)-C(35)	108.6(15)
C(26)-C(27)-H(27)	125.8	C(33)-C(34)-Ti(1)	72.4(9)
C(28)-C(27)-H(27)	125.8	C(35)-C(34)-Ti(1)	71.4(8)
Fe(1)-C(27)-H(27)	127.2	C(33)-C(34)-H(34)	125.7
C(29)-C(28)-C(27)	108.2(14)	C(35)-C(34)-H(34)	125.7
C(29)-C(28)-Fe(1)	70.9(9)	Ti(1)-C(34)-H(34)	122.1
C(27)-C(28)-Fe(1)	69.3(8)	C(34)-C(35)-C(31)	108.1(16)
C(29)-C(28)-H(28)	125.9	C(34)-C(35)-Ti(1)	75.1(9)
C(27)-C(28)-H(28)	125.9	C(31)-C(35)-Ti(1)	75.0(8)
Fe(1)-C(28)-H(28)	125.5	C(34)-C(35)-H(35)	125.9
C(28)-C(29)-C(30)	108.0(14)	C(31)-C(35)-H(35)	125.9
C(28)-C(29)-Fe(1)	69.0(9)	Ti(1)-C(35)-H(35)	116.1
C(30)-C(29)-Fe(1)	67.5(8)	C(40)-C(36)-C(37)	106.7(16)
C(28)-C(29)-H(29)	126.0	C(40)-C(36)-Ti(1)	73.9(8)
C(30)-C(29)-H(29)	126.0	C(37)-C(36)-Ti(1)	72.0(10)
Fe(1)-C(29)-H(29)	129.1	C(40)-C(36)-H(36)	126.6
C(29)-C(30)-C(26)	109.4(14)	C(37)-C(36)-H(36)	126.6
C(29)-C(30)-Fe(1)	71.7(9)	Ti(1)-C(36)-H(36)	119.4

C(38)-C(37)-C(36)	106.4(17)	C(40)-C(39)-C(38)	108.0(16)
C(38)-C(37)-Ti(1)	73.7(11)	C(40)-C(39)-Ti(1)	75.4(8)
C(36)-C(37)-Ti(1)	73.3(10)	C(38)-C(39)-Ti(1)	73.8(10)
C(38)-C(37)-H(37)	126.8	C(40)-C(39)-H(39)	126.0
C(36)-C(37)-H(37)	126.8	C(38)-C(39)-H(39)	126.0
Ti(1)-C(37)-H(37)	118.3	Ti(1)-C(39)-H(39)	116.8
C(37)-C(38)-C(39)	107.9(18)	C(36)-C(40)-C(39)	111.0(15)
C(37)-C(38)-Ti(1)	73.5(11)	C(36)-C(40)-Ti(1)	74.0(8)
C(39)-C(38)-Ti(1)	72.2(10)	C(39)-C(40)-Ti(1)	72.6(8)
C(37)-C(38)-H(38)	126.1	C(36)-C(40)-H(40)	124.5
C(39)-C(38)-H(38)	126.1	C(39)-C(40)-H(40)	124.5
Ti(1)-C(38)-H(38)	120.0	Ti(1)-C(40)-H(40)	120.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for Complex **33**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(5)	47(6)	87(9)	122(11)	0(8)	0(7)	-5(6)
Re(1)	40(1)	38(1)	57(1)	0(1)	4(1)	8(1)
Re(2)	33(1)	43(1)	56(1)	1(1)	3(1)	9(1)
Re(3)	62(1)	48(1)	71(1)	11(1)	-23(1)	1(1)
Re(4)	50(1)	37(1)	48(1)	1(1)	-8(1)	5(1)
Fe(1)	38(1)	34(1)	45(1)	0(1)	-4(1)	2(1)
Ti(1)	37(1)	29(1)	46(1)	-4(1)	-1(1)	3(1)
C(1)	74(10)	45(8)	61(11)	-2(7)	6(8)	10(7)
O(1)	110(10)	87(9)	60(8)	16(7)	30(7)	0(7)
C(2)	51(8)	38(8)	62(10)	10(7)	13(7)	7(6)
O(2)	93(8)	45(6)	90(9)	2(6)	9(7)	10(6)
C(3)	61(10)	53(9)	89(13)	-3(8)	9(9)	18(7)
O(3)	36(6)	109(11)	156(14)	3(9)	-20(7)	-2(6)
C(4)	77(11)	50(9)	92(13)	21(9)	38(10)	23(8)
O(4)	104(10)	45(7)	129(12)	-11(7)	28(9)	12(6)
C(5)	46(8)	62(9)	67(11)	-5(8)	12(7)	10(7)
C(6)	47(8)	89(12)	76(13)	14(10)	13(8)	21(8)
O(6)	73(8)	166(15)	68(9)	26(9)	24(7)	17(8)
C(7)	36(7)	49(8)	76(11)	5(7)	-10(7)	10(6)
O(7)	49(6)	69(7)	145(13)	-10(8)	-27(7)	7(6)
C(8)	180(19)	88(12)	35(9)	38(8)	70(11)	101(13)
O(8)	71(7)	75(8)	124(11)	13(7)	21(7)	41(6)
C(9)	62(9)	55(9)	66(11)	-3(8)	13(8)	18(8)
O(9)	83(8)	60(7)	107(11)	-14(7)	-18(7)	-13(6)
C(10)	31(6)	40(6)	31(7)	2(5)	-2(5)	0(5)
O(10)	39(4)	32(4)	52(6)	-7(4)	-4(4)	1(3)
C(11)	90(13)	71(12)	92(15)	26(11)	-29(11)	8(10)
O(11)	115(12)	127(13)	170(17)	74(13)	-63(12)	-9(10)
C(12)	54(9)	57(10)	96(14)	6(10)	-22(9)	11(7)
O(12)	108(11)	67(8)	144(14)	-34(9)	-20(10)	25(8)
C(13)	93(13)	55(10)	83(14)	18(9)	-13(11)	-4(9)
O(13)	107(11)	92(10)	106(12)	21(9)	7(9)	-18(9)
C(14)	104(14)	93(14)	42(10)	13(10)	-13(10)	-22(11)
O(14)	162(16)	107(12)	86(11)	-34(9)	6(11)	-27(11)
C(15)	62(10)	57(10)	114(16)	8(10)	-8(10)	-6(8)
O(15)	92(10)	96(11)	144(15)	13(10)	10(10)	-20(8)
C(16)	52(8)	51(9)	45(8)	5(7)	-8(6)	5(6)

O(16)	71(7)	42(6)	90(9)	-4(5)	-12(6)	-5(5)
C(17)	97(13)	66(11)	59(11)	9(8)	23(10)	20(9)
O(17)	156(15)	113(12)	99(12)	-1(9)	54(11)	34(11)
C(18)	86(12)	57(10)	66(11)	0(8)	-2(9)	10(9)
O(18)	119(11)	50(7)	106(11)	-1(7)	-43(9)	-13(7)
C(19)	52(8)	70(10)	67(11)	45(9)	-28(8)	-18(7)
O(19)	87(9)	129(12)	92(11)	1(9)	26(8)	2(8)
C(20)	68(8)	29(6)	29(7)	0(5)	12(6)	5(6)
O(20)	47(5)	36(5)	31(5)	-8(4)	-2(4)	-1(4)
C(21)	39(6)	43(7)	40(8)	3(6)	-8(5)	0(5)
C(22)	44(7)	49(7)	38(7)	5(6)	8(6)	9(6)
C(23)	56(8)	42(7)	46(8)	-11(6)	7(6)	-3(6)
C(24)	60(8)	40(7)	50(9)	-11(6)	-9(7)	-1(6)
C(25)	36(6)	50(8)	59(9)	6(7)	-12(6)	1(6)
C(26)	55(8)	35(7)	39(8)	2(6)	-1(6)	-5(5)
C(27)	67(9)	47(8)	57(10)	6(7)	-29(8)	1(7)
C(28)	85(12)	58(10)	72(12)	17(9)	-32(10)	-32(9)
C(29)	42(8)	93(13)	62(11)	8(9)	4(7)	-22(8)
C(30)	65(9)	63(9)	38(8)	-6(7)	4(7)	-3(7)
C(31)	49(8)	85(12)	60(11)	-14(9)	10(8)	-32(8)
C(32)	57(9)	62(10)	100(15)	-3(10)	31(10)	7(8)
C(33)	45(8)	124(17)	66(12)	19(12)	0(8)	18(10)
C(34)	60(10)	75(12)	83(13)	-28(10)	16(9)	-29(9)
C(35)	52(9)	52(9)	110(15)	33(10)	17(10)	-4(7)
C(36)	76(12)	106(15)	74(13)	-52(12)	42(11)	-26(11)
C(37)	150(20)	90(14)	37(10)	4(9)	8(11)	67(15)
C(38)	74(12)	113(17)	62(12)	-39(12)	1(10)	1(12)
C(39)	107(15)	43(9)	89(14)	-18(9)	23(12)	-1(9)
C(40)	71(11)	91(14)	82(14)	-21(11)	13(10)	42(11)
O(21)	176(15)	86(10)	121(13)	-48(9)	95(12)	-29(9)
O(22)	172(16)	101(11)	110(12)	-37(9)	-41(11)	71(11)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Complex **33**.

	x	y	z	U(eq)
H(22)	5402	5252	1062	51
H(23)	4692	3454	416	58
H(24)	2381	3236	250	62
H(25)	1572	4870	824	59
H(27)	4822	2358	1999	71
H(28)	2460	1952	1740	91
H(29)	1436	3445	2329	81
H(30)	3125	4876	2843	67
H(31)	6572	6922	972	81
H(32)	7679	5682	1775	86
H(33)	8615	6760	2875	93
H(34)	8178	8669	2717	90
H(35)	6757	8757	1610	86
H(36)	3863	6494	3444	103
H(37)	6030	6308	4041	106
H(38)	7298	8036	3847	101
H(39)	5981	9196	3087	95
H(40)	3918	8276	2914	95

Table 6. Torsion angles [°] for Complex **33**.

C(5)-Re(1)-Re(2)-C(8)	127.0(9)	Re(1)-Re(2)-C(10)-C(21)	-74.7(10)
C(4)-Re(1)-Re(2)-C(8)	36.7(9)	C(19)-Re(4)-C(20)-C(26)	110.1(11)
C(2)-Re(1)-Re(2)-C(8)	-140.8(9)	C(17)-Re(4)-C(20)-C(26)	-71.2(11)
C(3)-Re(1)-Re(2)-C(8)	-53.4(9)	C(18)-Re(4)-C(20)-C(26)	-163.4(11)
C(5)-Re(1)-Re(2)-C(7)	-142.7(6)	C(16)-Re(4)-C(20)-C(26)	15.9(11)
C(4)-Re(1)-Re(2)-C(7)	127.1(7)	O(10)-C(10)-C(21)-C(22)	-21.8(18)
C(2)-Re(1)-Re(2)-C(7)	-50.5(6)	Re(2)-C(10)-C(21)-C(22)	156.8(10)
C(3)-Re(1)-Re(2)-C(7)	36.9(6)	O(10)-C(10)-C(21)-C(25)	159.8(13)
C(5)-Re(1)-Re(2)-C(9)	41.9(6)	Re(2)-C(10)-C(21)-C(25)	-21.6(19)
C(4)-Re(1)-Re(2)-C(9)	-48.4(7)	O(10)-C(10)-C(21)-Fe(1)	67.7(14)
C(2)-Re(1)-Re(2)-C(9)	134.1(6)	Re(2)-C(10)-C(21)-Fe(1)	-113.7(10)
C(3)-Re(1)-Re(2)-C(9)	-138.6(6)	C(10)-C(21)-C(22)-C(23)	-176.5(12)
C(5)-Re(1)-Re(2)-C(10)	-45.1(5)	C(25)-C(21)-C(22)-C(23)	2.3(14)
C(4)-Re(1)-Re(2)-C(10)	-135.4(6)	C(21)-C(22)-C(23)-C(24)	-0.8(16)
C(2)-Re(1)-Re(2)-C(10)	47.1(5)	C(22)-C(23)-C(24)-C(25)	-1.0(17)
C(3)-Re(1)-Re(2)-C(10)	134.4(5)	C(23)-C(24)-C(25)-C(21)	2.5(16)
C(12)-Re(3)-Re(4)-C(19)	-50.6(7)	C(22)-C(21)-C(25)-C(24)	-2.9(15)
C(13)-Re(3)-Re(4)-C(19)	-139.7(8)	C(10)-C(21)-C(25)-C(24)	175.8(13)
C(15)-Re(3)-Re(4)-C(19)	37.4(8)	O(20)-C(20)-C(26)-C(27)	134.1(14)
C(14)-Re(3)-Re(4)-C(19)	132.7(7)	Re(4)-C(20)-C(26)-C(27)	-56.0(17)
C(12)-Re(3)-Re(4)-C(17)	130.6(8)	O(20)-C(20)-C(26)-C(30)	-48.6(17)
C(13)-Re(3)-Re(4)-C(17)	41.6(8)	Re(4)-C(20)-C(26)-C(30)	121.3(13)
C(15)-Re(3)-Re(4)-C(17)	-141.4(8)	C(26)-C(27)-C(28)-C(29)	-1.9(18)
C(14)-Re(3)-Re(4)-C(17)	-46.0(8)	C(27)-C(28)-C(29)-C(30)	3.3(19)
C(12)-Re(3)-Re(4)-C(18)	-136.8(7)	C(28)-C(29)-C(30)-C(26)	-3.6(18)
C(13)-Re(3)-Re(4)-C(18)	134.1(8)	C(27)-C(26)-C(30)-C(29)	2.4(16)
C(15)-Re(3)-Re(4)-C(18)	-48.8(8)	C(20)-C(26)-C(30)-C(29)	-175.4(13)
C(14)-Re(3)-Re(4)-C(18)	46.5(8)	C(31)-C(32)-C(33)-C(34)	-1.7(19)
C(12)-Re(3)-Re(4)-C(16)	42.9(7)	C(32)-C(31)-C(35)-C(34)	3.9(17)
C(13)-Re(3)-Re(4)-C(16)	-46.1(7)	C(40)-C(36)-C(37)-C(38)	0.4(18)
C(15)-Re(3)-Re(4)-C(16)	130.9(7)	C(36)-C(37)-C(38)-C(39)	-2(2)
C(14)-Re(3)-Re(4)-C(16)	-133.7(7)	C(37)-C(38)-C(39)-C(40)	3(2)
C(6)-Re(2)-C(10)-O(10)	-79.8(11)	C(37)-C(36)-C(40)-C(39)	1.4(17)
C(7)-Re(2)-C(10)-O(10)	-171.7(10)	C(38)-C(39)-C(40)-C(36)	-2.7(18)
C(9)-Re(2)-C(10)-O(10)	19.3(10)		
Re(1)-Re(2)-C(10)-O(10)	103.8(9)		
C(6)-Re(2)-C(10)-C(21)	101.7(12)		
C(7)-Re(2)-C(10)-C(21)	9.8(12)		
C(9)-Re(2)-C(10)-C(21)	-159.2(11)		

Table 7. Selected least-squares planes and deviations from the planes (Åx10^3) for Complex **33**.

Plane 1	4.491(33)x + 4.487(62)y - 15.695(65)z = 2.365(59)					
Atoms *	Re(2)	C(10)	O(10)	C(21)	rms	[Ti(1)]
Deviations	2(3)	-8(10)	3(4)	3(3)	5	[-552(18)]
Plane 2	-5.907(49)x + 3.672(59)y + 15.374(29)z = 2.637(59)					
Atoms *	Re(4)	C(20)	O(20)	C(26)	rms	[Ti(1)]
Deviations	17(3)	-62(10)	25(4)	20(3)	36	[285(17)]
Plane 3	0.523(76)x + 5.578(76)y - 16.520(57)z = 1.485(45)					
Atoms *	C(21)	C(22)	C(23)	C(24)	C(25)	rms	[Fe(1)]
Deviations	15(8)	-10(8)	0(9)	10(9)	-16(9)	12	[-1638(6)]
Plane 4	-0.492(80)x - 6.016(84)y + 16.178(70)z = 1.563(49)					
Atoms *	C(26)	C(27)	C(28)	C(29)	C(30)	rms	[Fe(1)]
Deviations	8(9)	4(9)	-15(10)	20(10)	-17(9)	14	[-1631(6)]
Plane 5	9.090(45)x + 1.928(94)y - 10.101(120) z = 6.282(77)					
Atoms *	C(31)	C(32)	C(33)	C(34)	C(35)	rms	[Ti(1)]
Deviations	15(9)	1(10)	-16(10)	26(10)	-25(9)	19	[-2071(7)]
Plane 6	-4.011 (78)x + 5.098(98)y + 15.916(675)5 z = 7.250(82)					
Atoms *	C(36)	C(37)	C(38)	C(39)	C(40)	rms	[Ti(1)]
Deviations	-2(9)	-7(11)	14(11)	-15(10)	11(9)	11	[-2068(7)]

Dihedral angles between planes (º):

Planes 1 and 2:	39.3(4)	Planes 3 and 4:	2.4(9)
Planes 1 and 3:	21.9(7)	Planes 5 and 6	51.4(7)
Planes 2 and 4:	53.8(4)		

* rms = root mean square deviation from the plane;
atoms not involved in calculating the plane are shown in brackets [ ].