

Inorganic Chemistry

including bioinorganic chemistry

Inorg. Chem., 1997, 36(21), 4875-4882, DOI:[10.1021/ic961247t](https://doi.org/10.1021/ic961247t)

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Table S1. Data collection for Complex 1.

Diffractometer Used	Siemens SMART CCD System
Radiation Source	MoK α (λ = 0.71073 Å)
Temperature (K)	296
Monochromator	Highly oriented graphite crystal
2 θ Range	1.7 to 25.0°
Scan Type	ω
Scan Speed	10 seconds/frame
Frame Width (ω)	0.3°
Decay	0 % (First 50 frames recollected and relative intensities determined)
Index Ranges	-24 $\leq$ h $\leq$ 25, -32 $\leq$ k $\leq$ 31 -21 $\leq$ l $\leq$ 12
Reflections collected	13501
Independent Reflections	5746 (R_{int} = 5.76%)
Observed Reflections	4378 ($> 2\sigma$)
Absorption Correction	empirical
Min./Max. Transmission	0.8526/0.9021

Table S2. Structure determination summary for Complex 1.

<u>Crystal Data</u>	<u>Compound 1</u>
Empirical formula	$C_{42}H_{35}Cl_2Cr_2N_8O_{14}$
Color; Habit	Red irregular
Crystal size (mm)	0.45 x 0.27 x 0.17
Crystal system	Monoclinic
Space group	Cc
Unit Cell Dimensions	$a = 16.8259(8) \text{ \AA}$ $b = 21.9622(11) \text{ \AA}$ $c = 14.6056(8) \text{ \AA}$ $\beta = 122.1830(10)^\circ$
Volume	$4568.0(4) \text{ \AA}^3$
Z	4
Formula weight	1015.4
Density(calc.)	1.476 g/cm^3
Absorption coefficient	6.68 cm^{-1}
F(000)	2008

Table S3. Solution and refinement for Complex 1.

Structure Solution	Heavy Atom Methods using Siemens SHELXTL PLUS (PC Version)
Refinement method	Full-matrix least-squares on F^2 using SHELXL-93
Hydrogen Atoms	Riding model with refined isotropic U
Weighting Scheme	$w=1/[\sigma^2(F_o^2)+(0.0094P)^2+30.5189P]$ where $P=(F_o^2+2F_c^2)/3$
Number of Parameters Refined	667
Final R indices [$I>2\sigma(I)$]	R1 = 7.21%, wR2 = 13.05%
R indices (all data)	R1 = 10.87%, wR2 = 15.80%
Goodness-of-fit on F^2	1.168
Data-to-parameter Ratio	8.5:1
Largest diff. peak and hole	0.571 and -0.387 $e\text{\AA}^{-3}$

Table S4. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for Complex 1.

	x	y	z	U(eq)	S5
Cr(1)	0	376(1)	0	38(1)	
Cr(2)	1293(1)	66(1)	-705(2)	34(1)	
Cl(1)	129(2)	-2535(1)	-3598(3)	67(1)	
Cl(2)	377(4)	-2918(2)	1900(5)	105(1)	
O(1)	-44(4)	84(3)	-1328(6)	36(2)	
O(2)	1234(4)	16(3)	586(6)	38(2)	
O(3)	203(5)	602(3)	1374(6)	45(2)	
O(4)	1161(5)	115(3)	-2127(6)	43(2)	
O(5)	407(5)	1202(3)	-146(6)	48(2)	
O(6)	1443(4)	960(3)	-589(6)	44(2)	
O(11)*	-306(25)	-2758(18)	-4696(23)	122(16)	
O(11A)**	37(33)	-2866(23)	-4429(43)	170(26)	
O(12)	183(9)	-2962(5)	-2885(11)	117(4)	
O(13)*	-348(15)	-1984(10)	-3658(17)	102(7)	
O(13A)**	-755(28)	-2397(25)	-3832(59)	296(40)	
O(14)#	1119(10)	-2356(7)	-3123(15)	83(5)	
O(14A)##	709(35)	-2018(14)	-3185(38)	118(19)	
O(21)*	132(26)	-2966(17)	796(26)	139(17)	
O(21A)**	-342(38)	-3076(23)	1013(45)	188(24)	
O(22)	761(9)	-3443(6)	2517(12)	143(5)	
O(23)	-126(12)	-2604(8)	2178(16)	200(8)	
O(24)	1104(19)	-2551(9)	2124(25)	282(13)	
N(1)	-1386(6)	640(4)	-781(8)	48(2)	
N(2)	-653(7)	-421(4)	-70(8)	51(2)	
N(3)	1414(6)	-862(3)	-696(7)	40(2)	
N(4)	2752(6)	-23(4)	111(8)	46(2)	
C(1)	-1667(7)	1227(6)	-994(9)	60(3)	
C(2)	-2619(8)	1379(8)	-1486(11)	83(5)	
C(3)	-3247(9)	946(9)	-1701(13)	96(5)	
C(4)	-2948(8)	326(8)	-1456(11)	77(4)	
C(5)	-2005(8)	194(6)	-1010(10)	59(3)	
C(6)	-1595(8)	-413(5)	-673(10)	49(3)	
C(7)	-2142(11)	-940(7)	-1011(13)	83(5)	
C(8)	-1696(13)	-1465(7)	-654(15)	96(5)	
C(9)	-733(12)	-1498(6)	32(14)	82(4)	
C(10)	-234(9)	-945(6)	302(11)	62(3)	
C(11)	702(9)	-1248(5)	-1104(11)	62(3)	
C(12)	832(12)	-1869(6)	-980(14)	86(4)	
C(13)	1713(15)	-2088(6)	-492(15)	100(6)	
C(14)	2447(12)	-1709(7)	-122(14)	95(5)	
C(15)	2294(9)	-1064(6)	-227(11)	63(3)	
C(16)	3072(8)	-592(6)	197(10)	57(3)	
C(17)	4020(9)	-718(8)	619(12)	86(5)	
C(18)	4604(8)	-237(10)	937(12)	99(6)	
C(19)	4321(9)	343(9)	907(12)	85(5)	
C(20)	3357(7)	427(6)	438(10)	60(3)	
C(21)	1027(7)	1347(4)	-352(9)	47(3)	
C(22)	1256(9)	1996(4)	-325(13)	77(4)	
N(1S)	-1755(8)	554(5)	1469(10)	78(3)	
N(2S)	-1422(6)	-708(4)	1846(8)	48(2)	
N(3S)	7617(7)	4307(5)	2857(9)	66(3)	
N(4S)	7711(6)	5507(5)	2496(8)	62(3)	
C(1S)	-1984(10)	1172(6)	1385(12)	74(4)	
C(2S)	-2857(9)	1351(6)	1108(13)	74(4)	

C(3S)	-3507(9)	910(6)	923(12)	75(4)
C(4S)	-3343(6)	328(5)	967(9)	45(3)
C(5S)	-2476(7)	151(5)	1258(9)	48(3)
C(6S)	-2313(7)	-517(5)	1329(9)	48(3)
C(7S)	-3054(8)	-944(6)	888(12)	69(4)
C(8S)	-2871(9)	-1545(6)	962(13)	79(4)
C(9S)	-1967(9)	-1727(6)	1461(12)	72(4)
C(10S)	-1279(9)	-1312(6)	1900(10)	66(3)
C(11S)	7511(11)	3722(7)	2860(13)	90(4)
C(12S)	8192(16)	3307(9)	2976(17)	130(8)
C(13S)	8997(18)	3533(12)	3123(20)	155(11)
C(14S)	9157(13)	4147(11)	3165(16)	127(8)
C(15S)	8434(8)	4529(7)	2999(10)	68(4)
C(16S)	8526(8)	5185(7)	2997(10)	64(4)
C(17S)	9383(10)	5486(10)	3482(13)	98(6)
C(18S)	9419(12)	6074(12)	3463(16)	124(8)
C(19S)	8617(15)	6424(9)	2989(14)	126(8)
C(20S)	7767(10)	6097(7)	2528(12)	83(4)

S6

U(eq) is defined as one third of the trace
of the orthogonalized U_{ij} tensor.

* site occupancy factor (s.o.f.) = 55%

** s.o.f. = 45%

s.o.f. = 70%

s.o.f. = 30%

Table S5. Bond lengths [Å] for Complex 1.

S7

Cr(1)-O(3)	1.912(7)	Cr(1)-O(2)	1.944(6)
Cr(1)-O(5)	1.989(7)	Cr(1)-O(1)	2.007(7)
Cr(1)-N(2)	2.041(8)	Cr(1)-N(1)	2.060(8)
Cr(1)-Cr(2)	2.940(2)	Cr(2)-O(1)	1.925(6)
Cr(2)-O(2)	1.943(7)	Cr(2)-O(4)	1.972(7)
Cr(2)-O(6)	1.976(6)	Cr(2)-N(3)	2.048(7)
Cr(2)-N(4)	2.089(9)	Cl(1)-O(11A)	1.35(4)
Cl(1)-O(12)	1.369(11)	Cl(1)-O(13A)	1.37(4)
Cl(1)-O(14A)	1.41(3)	Cl(1)-O(13)	1.43(2)
Cl(1)-O(11)	1.45(3)	Cl(1)-O(14)	1.475(13)
Cl(2)-O(21A)	1.26(5)	Cl(2)-O(23)	1.312(13)
Cl(2)-O(24)	1.35(2)	Cl(2)-O(22)	1.391(13)
Cl(2)-O(21)	1.44(3)	O(5)-C(21)	1.270(10)
O(6)-C(21)	1.261(11)	N(1)-C(5)	1.337(14)
N(1)-C(1)	1.351(14)	N(2)-C(10)	1.307(14)
N(2)-C(6)	1.341(13)	N(3)-C(11)	1.322(13)
N(3)-C(15)	1.334(14)	N(4)-C(20)	1.311(14)
N(4)-C(16)	1.340(14)	C(1)-C(2)	1.40(2)
C(2)-C(3)	1.33(2)	C(3)-C(4)	1.43(2)
C(4)-C(5)	1.39(2)	C(5)-C(6)	1.46(2)
C(6)-C(7)	1.40(2)	C(7)-C(8)	1.32(2)
C(8)-C(9)	1.38(2)	C(9)-C(10)	1.41(2)
C(11)-C(12)	1.38(2)	C(12)-C(13)	1.35(2)
C(13)-C(14)	1.34(2)	C(14)-C(15)	1.43(2)
C(15)-C(16)	1.52(2)	C(16)-C(17)	1.40(2)
C(17)-C(18)	1.35(2)	C(18)-C(19)	1.35(2)
C(19)-C(20)	1.40(2)	C(21)-C(22)	1.473(13)
N(1S)-C(5S)	1.397(14)	N(1S)-C(1S)	1.40(2)
N(2S)-C(6S)	1.338(13)	N(2S)-C(10S)	1.34(2)
N(3S)-C(11S)	1.30(2)	N(3S)-C(15S)	1.37(2)
N(4S)-C(20S)	1.30(2)	N(4S)-C(16S)	1.36(2)
C(1S)-C(2S)	1.36(2)	C(2S)-C(3S)	1.38(2)
C(3S)-C(4S)	1.30(2)	C(4S)-C(5S)	1.341(13)
C(5S)-C(6S)	1.485(14)	C(6S)-C(7S)	1.413(14)
C(7S)-C(8S)	1.34(2)	C(8S)-C(9S)	1.35(2)
C(9S)-C(10S)	1.34(2)	C(11S)-C(12S)	1.40(2)
C(12S)-C(13S)	1.35(3)	C(13S)-C(14S)	1.37(3)
C(14S)-C(15S)	1.39(2)	C(15S)-C(16S)	1.45(2)
C(16S)-C(17S)	1.39(2)	C(17S)-C(18S)	1.30(2)
C(18S)-C(19S)	1.38(3)	C(19S)-C(20S)	1.41(2)

Table S6. Bond angles [°] for Complex 1.

O(3)-Cr(1)-O(2)	95.2(3)	O(3)-Cr(1)-O(5)	89.9(3)
O(2)-Cr(1)-O(5)	94.0(3)	O(3)-Cr(1)-O(1)	172.3(3)
O(2)-Cr(1)-O(1)	77.1(3)	O(5)-Cr(1)-O(1)	91.4(3)
O(3)-Cr(1)-N(2)	93.7(3)	O(2)-Cr(1)-N(2)	95.3(3)
O(5)-Cr(1)-N(2)	169.6(3)	O(1)-Cr(1)-N(2)	86.3(3)
O(3)-Cr(1)-N(1)	91.4(3)	O(2)-Cr(1)-N(1)	170.9(3)
O(5)-Cr(1)-N(1)	92.1(3)	O(1)-Cr(1)-N(1)	96.2(3)
N(2)-Cr(1)-N(1)	78.1(4)	O(3)-Cr(1)-Cr(2)	132.5(2)
O(2)-Cr(1)-Cr(2)	40.8(2)	O(5)-Cr(1)-Cr(2)	79.2(2)
O(1)-Cr(1)-Cr(2)	40.6(2)	N(2)-Cr(1)-Cr(2)	105.2(3)
N(1)-Cr(1)-Cr(2)	134.6(3)	O(1)-Cr(2)-O(2)	79.1(3)
O(1)-Cr(2)-O(4)	93.0(3)	O(2)-Cr(2)-O(4)	172.1(3)
O(1)-Cr(2)-O(6)	94.8(3)	O(2)-Cr(2)-O(6)	92.5(3)
O(4)-Cr(2)-O(6)	88.4(3)	O(1)-Cr(2)-N(3)	96.4(3)
O(2)-Cr(2)-N(3)	89.7(3)	O(4)-Cr(2)-N(3)	90.9(3)
O(6)-Cr(2)-N(3)	168.8(3)	O(1)-Cr(2)-N(4)	173.2(4)
O(2)-Cr(2)-N(4)	95.3(3)	O(4)-Cr(2)-N(4)	92.5(3)
O(6)-Cr(2)-N(4)	89.2(3)	N(3)-Cr(2)-N(4)	79.7(3)
O(1)-Cr(2)-Cr(1)	42.7(2)	O(2)-Cr(2)-Cr(1)	40.9(2)
O(4)-Cr(2)-Cr(1)	131.9(2)	O(6)-Cr(2)-Cr(1)	79.9(2)
N(3)-Cr(2)-Cr(1)	108.6(2)	N(4)-Cr(2)-Cr(1)	133.3(3)
O(11A)-Cl(1)-O(12)	104(3)	O(11A)-Cl(1)-O(13A)	108(3)
O(12)-Cl(1)-O(13A)	88(3)	O(11A)-Cl(1)-O(14A)	123(3)
O(12)-Cl(1)-O(14A)	119(2)	O(13A)-Cl(1)-O(14A)	110(3)
O(11A)-Cl(1)-O(13)	128(3)	O(12)-Cl(1)-O(13)	115.7(11)
O(14A)-Cl(1)-O(13)	65(2)	O(12)-Cl(1)-O(11)	114(2)
O(13A)-Cl(1)-O(11)	88(3)	O(14A)-Cl(1)-O(11)	125(2)
O(13)-Cl(1)-O(11)	106(2)	O(11A)-Cl(1)-O(14)	97(2)
O(12)-Cl(1)-O(14)	102.9(9)	O(13A)-Cl(1)-O(14)	150(2)
O(13)-Cl(1)-O(14)	105.1(12)	O(11)-Cl(1)-O(14)	113(2)
O(21A)-Cl(2)-O(23)	92(3)	O(21A)-Cl(2)-O(24)	131(3)
O(23)-Cl(2)-O(24)	105.1(14)	O(21A)-Cl(2)-O(22)	107(3)
O(23)-Cl(2)-O(22)	112.9(11)	O(24)-Cl(2)-O(22)	106.8(13)
O(23)-Cl(2)-O(21)	122.6(14)	O(24)-Cl(2)-O(21)	90(2)
O(22)-Cl(2)-O(21)	115(2)	Cr(2)-O(1)-Cr(1)	96.7(3)
Cr(2)-O(2)-Cr(1)	98.3(3)	C(21)-O(5)-Cr(1)	128.8(6)
C(21)-O(6)-Cr(2)	128.8(6)	C(5)-N(1)-C(1)	120.8(10)
C(5)-N(1)-Cr(1)	115.7(8)	C(1)-N(1)-Cr(1)	123.4(7)
C(10)-N(2)-C(6)	118.2(10)	C(10)-N(2)-Cr(1)	125.3(8)
C(6)-N(2)-Cr(1)	115.9(7)	C(11)-N(3)-C(15)	120.7(10)
C(11)-N(3)-Cr(2)	124.9(7)	C(15)-N(3)-Cr(2)	114.4(8)
C(20)-N(4)-C(16)	118.1(10)	C(20)-N(4)-Cr(2)	125.9(8)
C(16)-N(4)-Cr(2)	115.6(8)	N(1)-C(1)-C(2)	120.6(12)
C(3)-C(2)-C(1)	120(2)	C(2)-C(3)-C(4)	119.5(12)
C(5)-C(4)-C(3)	118.6(14)	N(1)-C(5)-C(4)	120.5(13)
N(1)-C(5)-C(6)	114.8(10)	C(4)-C(5)-C(6)	124.5(12)
N(2)-C(6)-C(7)	123.1(12)	N(2)-C(6)-C(5)	114.5(10)
C(7)-C(6)-C(5)	122.2(12)	C(8)-C(7)-C(6)	117.0(14)
C(7)-C(8)-C(9)	122.2(13)	C(8)-C(9)-C(10)	116.9(13)
N(2)-C(10)-C(9)	122.3(13)	N(3)-C(11)-C(12)	122.3(12)
C(13)-C(12)-C(11)	118.4(14)	C(14)-C(13)-C(12)	120.7(13)
C(13)-C(14)-C(15)	119.7(14)	N(3)-C(15)-C(14)	118.1(13)
N(3)-C(15)-C(16)	117.5(10)	C(14)-C(15)-C(16)	124.4(12)
N(4)-C(16)-C(17)	122.3(13)	N(4)-C(16)-C(15)	112.5(10)
C(17)-C(16)-C(15)	125.2(12)	C(18)-C(17)-C(16)	116.6(14)
C(17)-C(18)-C(19)	123.3(12)	C(18)-C(19)-C(20)	116(2)

N(4)-C(20)-C(19)	123.6(14)	O(6)-C(21)-O(5)	122.9(9)
O(6)-C(21)-C(22)	118.9(9)	O(5)-C(21)-C(22)	118.2(9)
C(5S)-N(1S)-C(1S)	115.4(10)	C(6S)-N(2S)-C(10S)	117.1(9)
C(11S)-N(3S)-C(15S)	118.8(12)	C(20S)-N(4S)-C(16S)	117.9(11)
C(2S)-C(1S)-N(1S)	120.7(12)	C(1S)-C(2S)-C(3S)	118.4(11)
C(4S)-C(3S)-C(2S)	123.8(11)	C(3S)-C(4S)-C(5S)	117.8(10)
C(4S)-C(5S)-N(1S)	123.8(10)	C(4S)-C(5S)-C(6S)	115.9(9)
N(1S)-C(5S)-C(6S)	120.3(9)	N(2S)-C(6S)-C(7S)	120.0(10)
N(2S)-C(6S)-C(5S)	117.4(9)	C(7S)-C(6S)-C(5S)	122.7(10)
C(8S)-C(7S)-C(6S)	120.4(11)	C(7S)-C(8S)-C(9S)	118.6(11)
C(10S)-C(9S)-C(8S)	119.6(13)	C(9S)-C(10S)-N(2S)	124.2(12)
N(3S)-C(11S)-C(12S)	123(2)	C(13S)-C(12S)-C(11S)	118(2)
C(12S)-C(13S)-C(14S)	122(2)	C(13S)-C(14S)-C(15S)	117(2)
N(3S)-C(15S)-C(14S)	122(2)	N(3S)-C(15S)-C(16S)	117.0(10)
C(14S)-C(15S)-C(16S)	121(2)	N(4S)-C(16S)-C(17S)	120(2)
N(4S)-C(16S)-C(15S)	116.1(10)	C(17S)-C(16S)-C(15S)	123.6(14)
C(18S)-C(17S)-C(16S)	121(2)	C(17S)-C(18S)-C(19S)	122(2)
C(18S)-C(19S)-C(20S)	116(2)	N(4S)-C(20S)-C(19S)	124(2)

Table S7. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for Complex 1.

S10

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cr(1)	34(1)	46(1)	35(1)	3(1)	19(1)	2(1)
Cr(2)	28(1)	40(1)	33(1)	-4(1)	16(1)	0(1)
Cl(1)	74(2)	60(2)	71(2)	-4(2)	40(2)	-9(2)
Cl(2)	116(3)	76(3)	131(4)	-2(3)	71(3)	25(3)
O(1)	26(3)	50(4)	30(4)	-4(3)	13(3)	-7(3)
O(2)	36(3)	40(4)	42(4)	4(3)	23(3)	5(3)
O(3)	57(4)	48(4)	40(4)	4(4)	31(4)	7(3)
O(4)	41(3)	61(4)	30(4)	2(4)	22(3)	-2(3)
O(5)	60(4)	38(4)	51(5)	-3(4)	33(4)	3(3)
O(6)	47(4)	42(3)	49(5)	-14(4)	29(4)	-8(3)
O(11)	131(30)	181(30)	43(11)	-14(15)	40(15)	-77(22)
O(11A)	101(28)	175(34)	256(58)	-182(39)	111(35)	-85(24)
O(12)	151(11)	84(7)	124(10)	32(7)	78(9)	-20(7)
O(13)	95(14)	123(17)	91(15)	48(14)	50(13)	90(13)
O(13A)	133(31)	264(56)	513(105)	-169(64)	188(50)	-65(35)
O(14)	73(10)	76(10)	92(12)	-4(11)	39(9)	-32(8)
O(14A)	162(46)	36(18)	103(31)	22(24)	33(32)	-34(21)
O(21)	186(35)	149(31)	64(16)	14(17)	54(20)	103(29)
O(21A)	189(47)	142(32)	132(44)	-42(31)	17(34)	-27(32)
O(22)	124(10)	132(11)	171(15)	47(10)	76(10)	50(8)
O(23)	199(15)	182(15)	260(23)	26(15)	150(16)	110(13)
O(24)	353(29)	204(19)	383(41)	-24(22)	259(30)	-109(20)
N(1)	48(5)	59(6)	40(6)	3(5)	26(5)	3(5)
N(2)	72(6)	36(5)	50(6)	14(5)	37(5)	8(4)
N(3)	39(4)	41(4)	39(5)	2(5)	20(4)	4(4)
N(4)	36(5)	67(6)	37(6)	-2(5)	22(4)	4(4)
C(1)	50(6)	89(9)	45(7)	-1(7)	28(6)	16(6)
C(2)	48(7)	131(13)	65(10)	-13(9)	27(7)	23(8)
C(3)	35(7)	177(17)	75(11)	19(12)	28(7)	14(9)
C(4)	28(6)	140(13)	45(8)	-9(9)	6(6)	4(7)
C(5)	47(7)	98(10)	38(7)	2(7)	26(6)	-13(6)
C(6)	53(6)	61(7)	35(6)	3(6)	24(6)	-8(6)
C(7)	104(11)	84(10)	84(11)	-18(9)	66(10)	-52(9)
C(8)	147(15)	63(9)	105(14)	-30(10)	87(13)	-57(10)
C(9)	128(13)	49(7)	107(13)	1(8)	88(12)	-16(8)
C(10)	67(7)	75(9)	52(8)	0(7)	36(6)	2(6)
C(11)	80(8)	54(7)	67(9)	-3(7)	49(7)	-5(6)
C(12)	122(12)	61(9)	102(13)	-6(9)	77(11)	-15(9)
C(13)	169(17)	35(7)	109(15)	-5(9)	82(15)	3(9)
C(14)	116(12)	78(10)	99(13)	26(10)	61(11)	59(10)
C(15)	86(9)	67(8)	62(8)	17(7)	56(8)	26(7)
C(16)	57(7)	68(8)	43(7)	1(7)	24(6)	3(6)
C(17)	54(8)	132(13)	77(11)	35(10)	39(8)	54(8)
C(18)	25(6)	197(20)	61(10)	12(12)	13(7)	12(9)
C(19)	47(8)	162(16)	53(9)	-8(10)	32(7)	-17(9)
C(20)	31(5)	103(10)	42(7)	1(7)	17(5)	-9(6)
C(21)	52(6)	42(6)	56(7)	1(5)	36(6)	1(4)
C(22)	107(9)	38(6)	119(13)	-6(7)	83(10)	-15(6)
N(1S)	82(8)	89(8)	70(8)	15(7)	46(7)	8(6)
N(2S)	43(5)	51(5)	47(6)	-9(5)	22(5)	-3(4)
N(3S)	66(6)	71(7)	64(7)	11(6)	36(6)	13(5)
N(4S)	57(6)	75(7)	45(6)	3(6)	20(5)	-14(5)
C(1S)	83(9)	58(8)	77(11)	5(8)	40(8)	-12(7)
C(2S)	87(10)	48(7)	104(12)	15(8)	62(9)	22(7)
C(3S)	65(8)	79(9)	92(11)	-5(9)	50(8)	5(7)

C(4S)	32(5)	46(6)	66(8)	0(6)	32(5)	1(4)	S11
C(5S)	40(6)	67(7)	38(7)	-7(6)	22(5)	-19(5)	
C(6S)	50(6)	52(6)	40(7)	-14(6)	23(6)	-8(5)	
C(7S)	51(7)	69(8)	72(10)	-20(8)	23(7)	-11(6)	
C(8S)	64(8)	63(8)	114(13)	-12(9)	51(9)	-20(7)	
C(9S)	79(8)	58(7)	95(11)	-19(8)	58(9)	-21(7)	
C(10S)	63(8)	87(10)	40(7)	-6(7)	23(6)	7(7)	
C(11S)	102(11)	91(11)	77(11)	11(10)	48(9)	26(9)	
C(12S)	190(21)	114(15)	116(17)	31(13)	101(18)	81(16)	
C(13S)	191(24)	163(22)	158(23)	62(19)	124(21)	132(21)	
C(14S)	121(14)	187(21)	117(16)	78(16)	93(14)	92(15)	
C(15S)	49(7)	106(11)	42(8)	11(8)	19(6)	30(7)	
C(16S)	44(7)	103(10)	37(8)	3(7)	17(6)	-7(7)	
C(17S)	54(8)	165(18)	57(10)	11(11)	18(7)	-25(10)	
C(18S)	75(11)	188(23)	85(15)	25(15)	27(10)	-58(14)	
C(19S)	150(17)	124(15)	52(11)	-6(11)	20(12)	-78(14)	
C(20S)	88(10)	78(10)	73(11)	-13(9)	36(9)	-26(8)	

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(ha^*)^2 U_{11} + \dots + 2hka^* b^* U_{12}]$$

Table S8. Hydrogen coordinates [$\times 10^4$] and isotropic displacement parameters [$\text{\AA}^2 \times 10^3$].

	x	y	z	U
H(1A)	-1225(7)	1533(6)	-814(9)	72
H(2A)	-2810(8)	1782(8)	-1662(11)	100
H(3B)	-3877(9)	1045(9)	-2008(13)	116
H(4B)	-3376(8)	17(8)	-1592(11)	93
H(7A)	-2792(11)	-923(7)	-1467(13)	99
H(8A)	-2042(13)	-1824(7)	-873(15)	115
H(9A)	-428(12)	-1868(6)	303(14)	98
H(10A)	416(9)	-953(6)	761(11)	75
H(11B)	93(9)	-1095(5)	-1489(11)	75
H(12B)	322(12)	-2131(6)	-1227(14)	103
H(13A)	1814(15)	-2506(6)	-410(15)	121
H(14B)	3053(12)	-1864(7)	201(14)	115
H(17A)	4236(9)	-1115(8)	678(12)	103
H(18A)	5233(8)	-306(10)	1189(12)	119
H(19A)	4742(9)	667(9)	1182(12)	102
H(20A)	3131(7)	822(6)	354(10)	72
H(22B)	886(9)	2234(4)	-134(13)	116
H(22C)	1120(9)	2119(4)	-1025(13)	116
H(22D)	1911(9)	2059(4)	201(13)	116
H(1SB)	-1533(10)	1464(6)	1520(12)	88
H(2SB)	-3012(9)	1762(6)	1046(13)	89
H(3SB)	-4098(9)	1035(6)	757(12)	90
H(4SB)	-3811(6)	44(5)	801(9)	54
H(7SA)	-3672(8)	-810(6)	545(12)	82
H(8SA)	-3356(9)	-1828(6)	676(13)	94
H(9SA)	-1823(9)	-2139(6)	1499(12)	86
H(10B)	-662(9)	-1451(6)	2267(10)	79
H(11A)	6962(11)	3572(7)	2783(13)	108
H(12A)	8092(16)	2889(9)	2953(17)	156
H(13B)	9456(18)	3265(12)	3197(20)	186
H(14A)	9724(13)	4301(11)	3298(16)	152
H(17B)	9937(10)	5261(10)	3823(13)	118
H(18B)	10001(12)	6265(12)	3778(16)	149
H(19B)	8634(15)	6847(9)	2973(14)	151
H(20B)	7211(10)	6318(7)	2229(12)	99

Figure S1. Labelling scheme for atoms other than in cation for Complex 1.

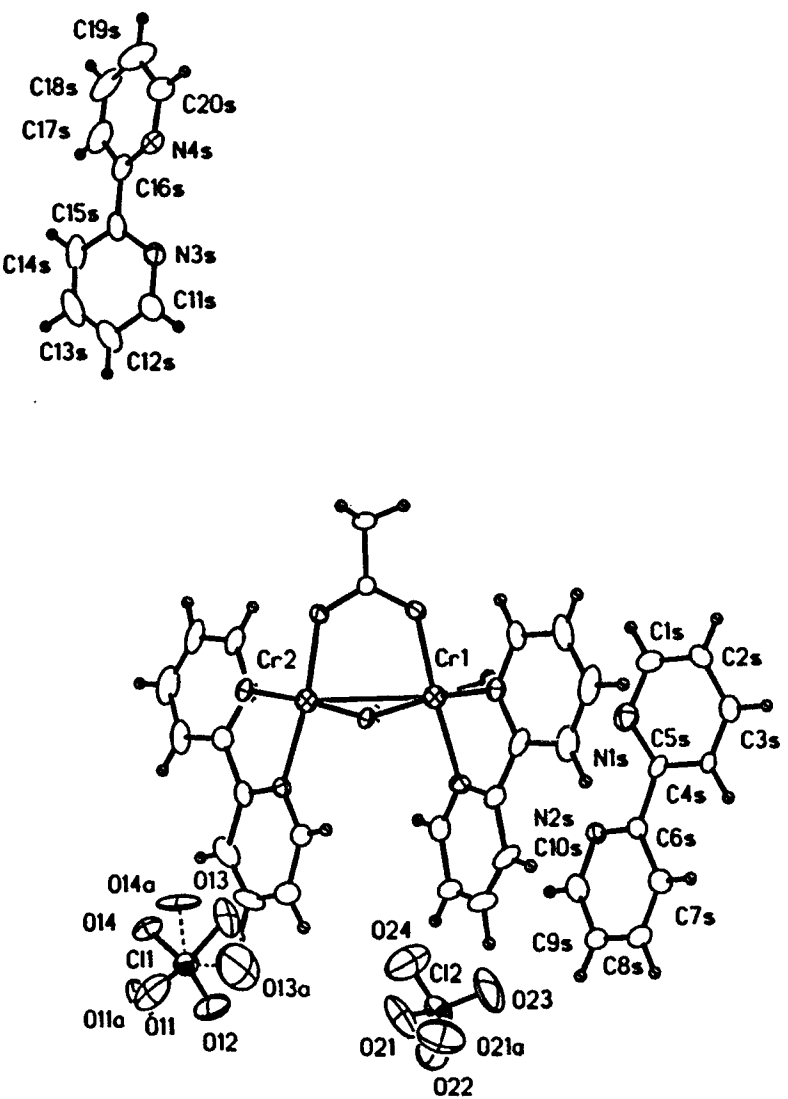


Table S9. Crystal data for Complex 2.

Empirical Formula:	$\text{Cr}_3\text{C}_{37}\text{H}_{41}\text{N}_4\text{O}_{18}\text{Cl}_{16}$
Color of Crystal:	purple
Crystal Dimensions were:	.45 x .35 x .40 mm.
Space Group:	$\bar{P}1$
Cell Dimensions (at -175. C; 43 reflections)	
a =	16.104(5)
b =	17.623(5)
c =	12.236(3)
alpha =	93.33(1)
beta =	92.81(1)
gamma =	64.84(1)
Z (Molecules/cell):	2
Volume:	3136.68
Calculated Density:	1.644
Wavelength:	.71069
Molecular Weight:	1552.98
Linear Absorption Coefficient:	12.487

Table S10. Data collection for Complex 2.

The diffractometer utilized for data collection was designed and constructed locally. A Picker four-circle goniostat equipped with a Furnas Monochromator (HOG crystal) and Picker X-ray generator is interfaced to a Z80 microprocessor which is controlled by an RS232 Serial port on an IBM PC microcomputer. Motors are Slo-Syn stepping motors, and a special top/bottom-left right slit assembly is used to align the crystal. All computations are performed on IBM compatible microcomputer systems using DOS or OS/2 operating systems.

Detector to sample distance =	22.5 cm.
Sample to source distance =	23.5 cm.
Take off angle =	2.0 deg.
Average omega scan width at half height =	.25 deg.

Data collection performed using standard moving crystal-moving detector technique with the following values:

Scan speed =	10.0 deg/min
Scan width =	2.0 + dispersion
Single background time at extremes of scan =	3 sec.
Aperture size =	3.0 x 4.0 mm.

Limits of data collection were:

Minimum two-theta =	6 deg.
Maximum two-theta =	45 deg.

Total number of reflections collected =	8373
Number of unique intensities =	8184
Number with $F > 0.0$ =	7778
Number with $F > 2.33\sigma(F)$ =	6732
R for Averaging =	.050

Final residuals are:

R(F) =	.0602
Rw(F) =	.0616

Goodness of Fit for the last cycle =	1.572
Maximum delta/sigma for last cycle =	.07

Table S11. Fractional coordinates and isotropic thermal parameters for Complex 2.

Atom	x	y	z	Biso
CR(1)	431(1)	1823(1)	4056(1)	14
CR(2)	-570(1)	3861(1)	3452(1)	15
CR(3)	2526(1)	276(1)	3615(1)	14
N(4)	-1207(4)	4031(3)	1932(4)	20
C(5)	-998(6)	3444(4)	1115(6)	31
C(6)	-1441(7)	3595(5)	120(7)	43
C(7)	-2137(7)	4380(5)	-59(7)	44
C(8)	-2366(6)	4987(5)	772(6)	32
C(9)	-1893(5)	4795(4)	1774(6)	23
C(10)	-2088(5)	5400(4)	2727(6)	19
C(11)	-2760(5)	6212(4)	2727(6)	25
C(12)	-2888(5)	6715(4)	3666(7)	28
C(13)	-2333(5)	6400(4)	4567(6)	25
C(14)	-1669(5)	5598(4)	4525(6)	21
N(15)	-1538(4)	5097(3)	3618(4)	17
N(16)	3461(4)	-922(3)	3129(4)	16
C(17)	3488(5)	-1634(4)	3486(5)	19
C(18)	4087(5)	-2408(4)	3044(6)	22
C(19)	4661(5)	-2445(4)	2255(6)	25
C(20)	4650(5)	-1722(5)	1900(6)	25
C(21)	4045(4)	-959(4)	2355(5)	17
C(22)	3990(4)	-129(4)	2057(5)	16
C(23)	4611(5)	-32(5)	1410(6)	24
C(24)	4520(5)	782(5)	1259(6)	26
C(25)	3804(5)	1455(5)	1729(6)	23
C(26)	3208(5)	1306(4)	2363(6)	21
N(27)	3301(4)	539(3)	2543(4)	16
O(28)	233(3)	2716(3)	3103(4)	16
O(29)	1735(3)	1431(3)	3906(3)	16
O(30)	479(3)	2498(2)	5386(3)	16
C(31)	276(4)	3269(4)	5612(5)	16
O(32)	-98(3)	3855(3)	4966(4)	18
C(33)	526(5)	3472(4)	6755(6)	20
O(34)	-904(3)	2195(3)	4254(4)	18
C(35)	-1587(4)	2893(4)	4191(5)	16
O(36)	-1547(3)	3570(3)	3938(4)	18
C(37)	-2509(5)	2942(4)	4403(6)	22
O(38)	276(3)	4301(3)	2950(4)	20
C(39)	1105(5)	3923(4)	2655(6)	23
O(40)	1552(4)	3150(3)	2614(5)	39
C(41)	1553(6)	4469(5)	2337(8)	37
O(42)	329(3)	1126(3)	2774(3)	16
C(43)	896(4)	569(4)	2168(5)	17
O(44)	1750(3)	195(3)	2357(3)	16
C(45)	532(5)	311(5)	1118(6)	23
O(46)	599(3)	917(3)	5084(4)	17
C(47)	1226(4)	188(4)	5189(5)	16
O(48)	1925(3)	-151(2)	4621(3)	16

S17

Atom	x	y	z	Biso
C(49)	1120(5)	-316(4)	6065(6)	22
O(50)	3414(3)	246(3)	4778(3)	18
C(51)	3424(5)	842(4)	5431(6)	21
O(52)	2873(4)	1579(3)	5388(5)	35
C(53)	4194(6)	565(5)	6275(6)	30
CL(54)	4408(1)	3109(1)	644(1)	26
O(55)	5127(3)	2308(3)	857(4)	29
O(56)	4707(7)	3632(4)	165(7)	86
O(57)	3769(5)	2965(4)	-124(5)	66
O(58)	3932(4)	3488(3)	1617(4)	34
C(59)	9309(5)	1982(4)	7027(6)	25
CL(60)	8486(1)	3043(1)	7132(2)	29
CL(61)	10052(1)	1737(1)	8180(2)	38
CL(62)	8741(1)	1322(1)	6898(2)	31
C(63)	5140(5)	2288(5)	3587(6)	26
CL(64)	5143(1)	3219(1)	4216(2)	36
CL(65)	6268(1)	1521(1)	3442(2)	37
CL(66)	4512(1)	1923(1)	4375(2)	34
C(67)	4668(8)	4966(6)	2506(8)	56
CL(68)	4412(3)	5583(2)	1394(2)	74
CL(69)	5454(3)	5077(2)	3414(3)	80
CL(70)	3617(3)	5338(2)	3293(3)	99
C(71)	1956(11)	2379(10)	9779(11)	97
CL(72)	1111(3)	3387(2)	9592(3)	51
CL(73)	2586(3)	1913(2)	8615(3)	60
CL(74)	1553(3)	1741(2)	10377(3)	43
C(75)	7236(11)	1689(10)	687(13)	31
CL(76)	8118(2)	1787(1)	1655(2)	44
CL(77)	7398(2)	2079(2)	-548(2)	63
CL(78)	7273(3)	642(3)	635(4)	53
C(75)'	7149(11)	2384(10)	937(14)	35
CL(78)'	6699(3)	3463(3)	1326(4)	40
CL(A)	6156(16)	4179(15)	1909(19)	104(9)
CL(B)	2171(15)	951(14)	7392(18)	89(8)
CL(C)	2056(20)	1129(19)	9772(24)	98(12)
CL(D)	4577(23)	5291(20)	3731(26)	35(11)
CL(E)	2806(14)	363(13)	9151(17)	59
H(1)	-58(4)	294(4)	128(5)	19(13)
H(2)	-124(5)	316(4)	-49(6)	29(15)
H(3)	-245(5)	452(4)	-78(6)	32(16)
H(4)	-285(4)	559(4)	73(5)	22(14)
H(5)	-315(4)	639(4)	206(5)	23(14)
H(6)	-331(5)	725(5)	363(6)	41(17)
H(7)	-240(4)	668(4)	516(6)	22(14)
H(8)	-127(5)	536(4)	514(6)	29(15)
H(9)	312(4)	-156(4)	403(5)	12(13)
H(10)	408(5)	-274(5)	336(6)	37(17)
H(11)	506(5)	-295(5)	192(6)	30(15)
H(12)	503(5)	-174(4)	135(5)	21(14)

Atom	x	y	z	Biso
H(13)	510(5)	-49(5)	112(6)	35(16)
H(14)	496(4)	82(4)	82(5)	20(14)
H(15)	371(5)	195(5)	160(6)	30(16)
H(16)	269(4)	173(3)	271(4)	0(11)
H(17)	66(4)	274(4)	289(5)	12(13)
H(18)	192(6)	153(5)	433(7)	44(19)
H(19)	117(5)	312(5)	684(6)	34(16)
H(20)	38(5)	401(5)	682(6)	27(15)
H(21)	23(5)	334(5)	720(6)	30(16)
H(22)	-290(7)	341(7)	471(9)	70(21)
H(23)	-273(8)	295(7)	388(9)	82(21)
H(24)	-257(8)	265(7)	488(10)	87(21)
H(25)	219(6)	415(5)	212(6)	41(17)
H(26)	126(8)	471(7)	177(9)	96(22)
H(27)	153(7)	485(6)	299(9)	77(21)
H(28)	8(6)	22(5)	131(6)	45(17)
H(29)	18(5)	77(4)	69(6)	22(14)
H(30)	97(6)	-8(5)	74(7)	45(18)
H(31)	114(7)	-79(7)	576(9)	92(22)
H(32)	158(7)	-49(6)	646(8)	67(20)
H(33)	60(7)	-2(6)	640(8)	67(20)
H(34)	425(6)	5(6)	666(8)	68(20)
H(35)	476(6)	46(5)	588(7)	44(17)
H(36)	405(5)	102(5)	681(6)	35(16)
H(37)	963(4)	192(4)	633(5)	19(13)
H(38)	482(5)	247(4)	295(6)	33(16)
H(39)	482(6)	441(6)	234(7)	60(20)
H(40)	215(10)	312(9)	992(12)	109(27)

Notes:

- 1) Fractional coordinates are X 10**4 for non-hydrogen atoms and X 10**3 for hydrogen atoms. Biso values are X 10.
- 2) Isotropic values for those atoms refined anisotropically are calculated using the formula given by W. C. Hamilton, Acta Cryst., 12,609 (1959)
- 3) Parameters marked by an asterisk (*) were not varied.

Table S12. Anisotropic thermal parameters for Complex 2 (bij form).

Atom	b11	b22	b33	b12	b13	b23
CR(1)	18(1)	10.0(4)	29(1)	-7.3(4)	-4(1)	1.1(4)
CR(2)	22(1)	9.6(4)	27(1)	-6.8(4)	-6(1)	0.8(4)
CR(3)	18(1)	10.2(4)	26(1)	-6.8(4)	-4.9(5)	0.5(4)
N(4)	31(3)	13(3)	34(5)	-9(2)	-4(3)	1(3)
C(5)	50(5)	12(3)	41(6)	-1(3)	-7(4)	-2(3)
C(6)	71(6)	25(4)	44(7)	-4(4)	-22(5)	-8(4)
C(7)	66(6)	35(4)	47(7)	-12(4)	-31(5)	-2(4)
C(8)	41(5)	25(4)	45(6)	-5(3)	-19(4)	4(4)
C(9)	33(4)	16(3)	33(5)	-6(3)	-6(4)	1(3)
C(10)	26(4)	13(3)	40(6)	-10(3)	-8(4)	5(3)
C(11)	24(4)	19(3)	48(6)	-1(3)	-9(4)	3(4)
C(12)	29(4)	16(3)	64(7)	-5(3)	-8(4)	-1(4)
C(13)	33(4)	17(3)	42(6)	-8(3)	-1(4)	-7(3)
C(14)	30(4)	19(3)	33(5)	-13(3)	-5(4)	-2(3)
N(15)	24(3)	12(2)	33(5)	-8(2)	-2(3)	0(3)
N(16)	23(3)	12(2)	23(4)	-7(2)	-10(3)	-2(2)
C(17)	27(4)	15(3)	29(5)	-7(3)	-10(3)	1(3)
C(18)	30(4)	14(3)	40(6)	-7(3)	-12(4)	-2(3)
C(19)	28(4)	16(3)	52(6)	-6(3)	-4(4)	-8(3)
C(20)	25(4)	25(4)	41(6)	-7(3)	-3(4)	-10(4)
C(21)	18(3)	23(3)	22(5)	-10(3)	-3(3)	-4(3)
C(22)	20(4)	17(3)	23(5)	-8(3)	-10(3)	2(3)
C(23)	28(4)	26(3)	27(5)	-8(3)	0(4)	-4(3)
C(24)	41(5)	38(4)	20(5)	-25(4)	4(4)	0(4)
C(25)	35(4)	29(4)	31(5)	-22(3)	-4(4)	5(3)
C(26)	25(4)	19(3)	38(5)	-10(3)	-11(4)	4(3)
N(27)	22(3)	13(2)	30(4)	-10(2)	-7(3)	3(3)
O(28)	22(2)	10(2)	31(3)	-7(2)	-3(2)	0(2)
O(29)	21(2)	12(2)	30(3)	-9(2)	-7(2)	-2(2)
O(30)	28(3)	9(2)	27(3)	-9(2)	-1(2)	0(2)
C(31)	14(3)	21(3)	31(5)	-10(3)	-4(3)	5(3)
O(32)	26(3)	14(2)	31(4)	-9(2)	-9(2)	1(2)
C(33)	30(4)	17(3)	33(5)	-13(3)	-9(4)	0(3)
O(34)	20(3)	14(2)	43(4)	-8(2)	-2(2)	-1(2)
C(35)	21(4)	18(3)	21(5)	-9(3)	-6(3)	-4(3)
O(36)	22(2)	13(2)	37(4)	-7(2)	-5(2)	3(2)
C(37)	20(4)	17(3)	56(6)	-8(3)	-3(4)	1(3)
O(38)	27(3)	12(2)	44(4)	-9(2)	-1(3)	3(2)
C(39)	32(4)	16(3)	45(6)	-11(3)	-6(4)	4(3)
O(40)	27(3)	18(3)	127(7)	-7(2)	9(3)	15(3)
C(41)	44(5)	25(4)	88(8)	-20(4)	1(5)	10(4)
O(42)	18(2)	12(2)	35(4)	-7(2)	-3(2)	-5(2)
C(43)	23(4)	14(3)	32(5)	-10(3)	-3(4)	5(3)

Atom	b11	b22	b33	b12	b13	b23
O(44)	21(3)	18(2)	25(3)	-10(2)	-5(2)	0(2)
C(45)	26(4)	26(3)	31(5)	-12(3)	-10(4)	-3(3)
O(46)	24(3)	12(2)	35(4)	-9(2)	-3(2)	1(2)
C(47)	22(4)	11(3)	33(5)	-10(3)	-4(4)	-7(3)
O(48)	22(3)	9(2)	32(3)	-6(2)	-1(2)	-1(2)
C(49)	30(4)	17(3)	37(6)	-8(3)	-3(4)	9(3)
O(50)	26(3)	12(2)	31(3)	-8(2)	-8(2)	-3(2)
C(51)	24(4)	20(3)	38(6)	-10(3)	-11(4)	4(3)
O(52)	40(3)	16(2)	79(5)	-6(2)	-35(3)	-6(3)
C(53)	41(5)	23(3)	51(6)	-14(3)	-20(4)	-3(4)
CL(54)	43(1)	17(1)	36(1)	-9(1)	4(1)	3(1)
O(55)	25(3)	25(2)	58(4)	-2(2)	-8(3)	13(3)
O(56)	150(8)	40(4)	175(10)	-47(5)	96(7)	-9(5)
O(57)	66(5)	59(4)	73(6)	7(3)	-47(4)	-15(4)
O(58)	38(3)	33(3)	51(4)	-7(2)	7(3)	-4(3)
C(59)	29(4)	22(3)	52(6)	-16(3)	-3(4)	1(3)
CL(60)	39(1)	21(1)	45(1)	-9(1)	-8(1)	-2(1)
CL(61)	45(1)	27(1)	76(2)	-15(1)	-29(1)	5(1)
CL(62)	38(1)	28(1)	67(2)	-23(1)	-5(1)	0(1)
C(63)	33(4)	24(3)	43(6)	-13(3)	-4(4)	3(3)
CL(64)	52(1)	25(1)	70(2)	-19(1)	-16(1)	7(1)
CL(65)	33(1)	35(1)	78(2)	-13(1)	-2(1)	3(1)
CL(66)	49(1)	40(1)	52(2)	-30(1)	7(1)	-5(1)
C(67)	104(9)	41(5)	74(8)	-36(5)	-29(7)	12(5)
CL(68)	184(3)	39(1)	67(2)	-61(2)	-36(2)	17(1)
CL(69)	128(3)	44(1)	146(3)	-40(2)	-66(2)	14(2)
CL(70)	113(3)	59(2)	164(4)	11(2)	34(3)	-4(2)
C(71)	165(14)	110(10)	130(14)	-97(10)	-83(11)	80(10)
CL(72)	67(2)	50(2)	52(2)	-12(2)	-13(2)	4(2)
CL(73)	81(3)	48(2)	97(3)	-22(2)	29(2)	5(2)
CL(74)	65(2)	58(2)	53(3)	-43(2)	-18(2)	15(2)
C(75)	35(9)	34(8)	53(13)	-20(7)	-7(8)	-5(8)
CL(76)	42(1)	50(1)	50(2)	-3(1)	-5(1)	15(1)
CL(77)	54(2)	113(2)	52(2)	-37(2)	-16(1)	32(2)
CL(78)	61(3)	48(2)	90(4)	-18(2)	16(3)	-11(2)
C(75)'	33(9)	34(8)	61(14)	-10(7)	-9(9)	2(9)
CL(78)'	35(2)	34(2)	85(4)	-11(2)	-5(2)	10(2)

Form of the anisotropic thermal parameter:

$$\exp[-(h^*2b_{11}+\dots+2hkb_{12}+\dots)]$$

All values are X 10**4.

Table S13. Bond lengths [Å] for Complex 2.

A	B	Distance	A	B	Distance
CR(1)	O(28)	1.921(5)	CL(C)	CL(E)	1.56(3)
CR(1)	O(29)	1.926(5)	CL(C)	C(71)	2.14(3)
CR(1)	O(30)	1.977(4)	CL(C)	C(71)	2.14(3)
CR(1)	O(34)	1.987(4)	CL(D)	C(67)	1.56(3)
CR(1)	O(42)	1.980(4)	O(30)	C(31)	1.271(7)
CR(1)	O(46)	2.009(4)	O(32)	C(31)	1.254(7)
CR(2)	O(28)	1.913(5)	O(34)	C(35)	1.257(7)
CR(2)	O(32)	1.967(4)	O(36)	C(35)	1.279(8)
CR(2)	O(36)	1.975(4)	O(38)	C(39)	1.272(8)
CR(2)	O(38)	1.969(5)	O(40)	C(39)	1.241(8)
CR(2)	N(4)	2.053(5)	O(42)	C(43)	1.251(7)
CR(2)	N(15)	2.076(5)	O(44)	C(43)	1.263(7)
CR(3)	O(29)	1.909(5)	O(46)	C(47)	1.261(7)
CR(3)	O(44)	1.973(4)	O(48)	C(47)	1.251(7)
CR(3)	O(48)	1.965(4)	O(50)	C(51)	1.288(8)
CR(3)	O(50)	1.953(4)	O(52)	C(51)	1.225(8)
CR(3)	N(16)	2.078(5)	N(4)	C(5)	1.341(9)
CR(3)	N(27)	2.052(5)	N(4)	C(9)	1.348(8)
CL(54)	O(55)	1.423(5)	N(15)	C(10)	1.352(8)
CL(54)	O(56)	1.375(7)	N(15)	C(14)	1.344(8)
CL(54)	O(57)	1.452(6)	N(16)	C(17)	1.335(8)
CL(54)	O(58)	1.418(5)	N(16)	C(21)	1.347(8)
CL(60)	C(59)	1.775(7)	N(27)	C(22)	1.359(8)
CL(61)	C(59)	1.754(8)	N(27)	C(26)	1.326(8)
CL(62)	C(59)	1.757(7)	C(5)	C(6)	1.362(11)
CL(64)	C(63)	1.772(7)	C(6)	C(7)	1.383(12)
CL(65)	C(63)	1.752(8)	C(7)	C(8)	1.375(11)
CL(66)	C(63)	1.758(8)	C(8)	C(9)	1.391(10)
CL(68)	C(67)	1.714(10)	C(9)	C(10)	1.485(9)
CL(69)	CL(A)	2.349(24)	C(10)	C(11)	1.379(9)
CL(69)	CL(D)	1.37(3)	C(11)	C(12)	1.378(11)
CL(69)	C(67)	1.710(11)	C(12)	C(13)	1.369(11)
CL(70)	CL(D)	1.58(3)	C(13)	C(14)	1.362(10)
CL(70)	C(67)	1.834(13)	C(17)	C(18)	1.390(10)
CL(72)	C(71)	1.737(16)	C(18)	C(19)	1.350(11)
CL(73)	CL(B)	2.476(22)	C(19)	C(20)	1.363(11)
CL(73)	CL(C)	2.45(3)	C(20)	C(21)	1.386(10)
CL(73)	C(71)	1.740(18)	C(21)	C(22)	1.493(9)
CL(74)	CL(C)	1.26(3)	C(22)	C(23)	1.376(10)
CL(74)	C(71)	1.727(13)	C(23)	C(24)	1.401(10)
CL(76)	C(75)	1.864(15)	C(24)	C(25)	1.374(11)
CL(76)	C(75)'	1.700(16)	C(25)	C(26)	1.379(10)
CL(77)	C(75)	1.772(16)	C(31)	C(33)	1.502(9)
CL(77)	C(75)'	1.878(17)	C(35)	C(37)	1.483(10)
CL(78)	CL(E)	1.864(20)	C(39)	C(41)	1.502(11)
CL(78)	C(75)	1.816(16)	C(43)	C(45)	1.513(9)
CL(78)'	CL(A)	1.372(23)	C(47)	C(49)	1.491(10)
CL(78)'	C(75)'	1.768(17)	C(51)	C(53)	1.504(10)
CL(A)	C(67)	2.330(26)	C(75)	C(75)'	1.197(21)
CL(B)	CL(E)	2.43(3)			

A	B	Distance
CL(72)	H(40)	1.58(14)
O(28)	H(17)	.77(6)
O(29)	H(18)	.64(8)
C(5)	H(1)	.88(6)
C(6)	H(2)	1.00(7)
C(7)	H(3)	.99(7)
C(8)	H(4)	1.02(6)
C(11)	H(5)	.98(6)
C(12)	H(6)	.90(8)
C(13)	H(7)	.84(7)
C(14)	H(8)	.95(7)
C(17)	H(9)	.88(6)
C(18)	H(10)	.71(7)
C(19)	H(11)	.94(7)
C(20)	H(12)	.93(7)
C(23)	H(13)	.92(7)
C(24)	H(14)	.94(6)
C(25)	H(15)	.84(7)
C(26)	H(16)	.95(5)
C(33)	H(19)	.96(8)
C(33)	H(20)	.87(7)
C(33)	H(21)	.85(8)
C(37)	H(22)	.87(11)
C(37)	H(23)	.71(11)
C(37)	H(24)	.84(12)
C(41)	H(25)	.97(8)
C(41)	H(26)	.85(12)
C(41)	H(27)	1.01(11)
C(45)	H(28)	.86(8)
C(45)	H(29)	.93(7)
C(45)	H(30)	.87(9)
C(49)	H(31)	.88(11)
C(49)	H(32)	.82(10)
C(49)	H(33)	.89(10)
C(53)	H(34)	1.02(10)
C(53)	H(35)	.99(8)
C(53)	H(36)	.96(8)
C(59)	H(37)	1.00(6)
C(63)	H(38)	.91(7)
C(67)	H(39)	.92(9)
C(71)	H(40)	1.47(14)

Table S14. Bond angles [°] for Complex 2.

A	B	C	Angle
O(28)	CR(1)	O(29)	89.34(20)
O(28)	CR(1)	O(30)	92.97(18)
O(28)	CR(1)	O(34)	92.79(19)
O(28)	CR(1)	O(42)	89.52(18)
O(28)	CR(1)	O(46)	177.90(19)
O(29)	CR(1)	O(30)	90.16(19)
O(29)	CR(1)	O(34)	177.85(19)
O(29)	CR(1)	O(42)	92.59(18)
O(29)	CR(1)	O(46)	92.38(19)
O(30)	CR(1)	O(34)	89.48(18)
O(30)	CR(1)	O(42)	176.31(18)
O(30)	CR(1)	O(46)	85.82(17)
O(34)	CR(1)	O(42)	87.68(17)
O(34)	CR(1)	O(46)	85.49(18)
O(42)	CR(1)	O(46)	91.61(18)
O(28)	CR(2)	O(32)	95.00(18)
O(28)	CR(2)	O(36)	93.06(21)
O(28)	CR(2)	O(38)	94.08(20)
O(28)	CR(2)	N(4)	93.01(20)
O(28)	CR(2)	N(15)	171.77(20)
O(32)	CR(2)	O(36)	91.03(19)
O(32)	CR(2)	O(38)	90.74(19)
O(32)	CR(2)	N(4)	171.88(20)
O(32)	CR(2)	N(15)	93.11(20)
O(36)	CR(2)	O(38)	172.47(19)
O(36)	CR(2)	N(4)	87.25(20)
O(36)	CR(2)	N(15)	85.38(19)
O(38)	CR(2)	N(4)	89.98(21)
O(38)	CR(2)	N(15)	87.22(20)
N(4)	CR(2)	N(15)	78.86(21)
O(29)	CR(3)	O(44)	92.10(19)
O(29)	CR(3)	O(48)	95.02(19)
O(29)	CR(3)	O(50)	94.06(19)
O(29)	CR(3)	N(16)	172.03(22)
O(29)	CR(3)	N(27)	93.56(21)
O(44)	CR(3)	O(48)	92.53(18)
O(44)	CR(3)	O(50)	173.23(18)
O(44)	CR(3)	N(16)	86.50(19)
O(44)	CR(3)	N(27)	88.35(19)
O(48)	CR(3)	O(50)	89.73(19)
O(48)	CR(3)	N(16)	92.88(19)
O(48)	CR(3)	N(27)	171.34(19)
O(50)	CR(3)	N(16)	87.01(19)
O(50)	CR(3)	N(27)	88.47(20)
N(16)	CR(3)	N(27)	78.57(21)
O(55)	CL(54)	O(56)	113.0(5)
O(55)	CL(54)	O(57)	106.7(4)
O(55)	CL(54)	O(58)	110.4(3)
O(56)	CL(54)	O(57)	107.4(6)
O(56)	CL(54)	O(58)	111.3(4)

A	B	C	Angle
O(57)	CL(54)	O(58)	107.8(4)
CL(A)	CL(69)	CL(D)	125.1(15)
CL(A)	CL(69)	C(67)	68.0(7)
CL(D)	CL(69)	C(67)	59.9(14)
CL(D)	CL(70)	C(67)	53.9(12)
CL(B)	CL(73)	CL(C)	72.7(9)
CL(B)	CL(73)	C(71)	120.1(7)
CL(C)	CL(73)	C(71)	58.6(8)
CL(C)	CL(74)	C(71)	90.1(15)
C(75)	CL(76)	C(75)'	38.9(7)
C(75)	CL(77)	C(75)'	38.1(7)
CL(E)	CL(78)	C(75)	168.5(8)
CL(A)	CL(78)'	C(75)'	155.5(12)
CL(69)	CL(A)	CL(78)'	159.6(15)
CL(69)	CL(A)	C(67)	42.9(5)
CL(78)'	CL(A)	C(67)	143.5(15)
CL(73)	CL(B)	CL(E)	67.3(8)
CL(73)	CL(C)	CL(74)	97.2(16)
CL(73)	CL(C)	CL(E)	82.1(14)
CL(73)	CL(C)	C(71)	43.9(7)
CL(74)	CL(C)	CL(E)	170.9(25)
CL(74)	CL(C)	C(71)	53.8(12)
CL(E)	CL(C)	C(71)	123.8(19)
CL(69)	CL(D)	CL(70)	142.3(24)
CL(69)	CL(D)	C(67)	71.0(16)
CL(70)	CL(D)	C(67)	71.3(15)
CL(78)	CL(E)	CL(B)	113.3(11)
CL(78)	CL(E)	CL(C)	112.7(16)
CL(B)	CL(E)	CL(C)	91.3(15)
CR(1)	O(28)	CR(2)	122.64(26)
CR(1)	O(29)	CR(3)	122.35(24)
CR(1)	O(30)	C(31)	135.7(4)
CR(2)	O(32)	C(31)	131.2(4)
CR(1)	O(34)	C(35)	133.4(4)
CR(2)	O(36)	C(35)	135.0(4)
CR(2)	O(38)	C(39)	130.8(4)
CR(1)	O(42)	C(43)	134.4(4)
CR(3)	O(44)	C(43)	131.6(4)
CR(1)	O(46)	C(47)	131.9(4)
CR(3)	O(48)	C(47)	133.7(4)
CR(3)	O(50)	C(51)	129.4(4)
CR(2)	N(4)	C(5)	125.1(5)
CR(2)	N(4)	C(9)	115.8(4)
C(5)	N(4)	C(9)	119.1(6)
CR(2)	N(15)	C(10)	115.4(4)
CR(2)	N(15)	C(14)	125.9(5)
C(10)	N(15)	C(14)	118.7(6)
CR(3)	N(16)	C(17)	125.0(5)
CR(3)	N(16)	C(21)	115.6(4)
C(17)	N(16)	C(21)	119.3(6)

S25

A	B	C	Angle
CR(3)	N(27)	C(22)	116.7(4)
CR(3)	N(27)	C(26)	124.2(5)
C(22)	N(27)	C(26)	119.0(6)
N(4)	C(5)	C(6)	122.5(7)
C(5)	C(6)	C(7)	119.1(8)
C(6)	C(7)	C(8)	119.2(8)
C(7)	C(8)	C(9)	119.2(7)
N(4)	C(9)	C(8)	121.0(6)
N(4)	C(9)	C(10)	115.4(6)
C(8)	C(9)	C(10)	123.6(6)
N(15)	C(10)	C(9)	114.4(6)
N(15)	C(10)	C(11)	121.4(6)
C(9)	C(10)	C(11)	124.1(6)
C(10)	C(11)	C(12)	119.0(7)
C(11)	C(12)	C(13)	119.1(7)
C(12)	C(13)	C(14)	119.8(7)
N(15)	C(14)	C(13)	121.9(7)
N(16)	C(17)	C(18)	121.0(7)
C(17)	C(18)	C(19)	119.7(7)
C(18)	C(19)	C(20)	119.7(7)
C(19)	C(20)	C(21)	119.3(7)
N(16)	C(21)	C(20)	121.0(6)
N(16)	C(21)	C(22)	114.9(6)
C(20)	C(21)	C(22)	124.1(6)
N(27)	C(22)	C(21)	113.9(6)
N(27)	C(22)	C(23)	121.8(6)
C(21)	C(22)	C(23)	124.1(6)
C(22)	C(23)	C(24)	118.3(7)
C(23)	C(24)	C(25)	119.4(7)
C(24)	C(25)	C(26)	118.8(7)
N(27)	C(26)	C(25)	122.6(7)
O(30)	C(31)	O(32)	125.7(6)
O(30)	C(31)	C(33)	115.6(6)
O(32)	C(31)	C(33)	118.7(6)
O(34)	C(35)	O(36)	124.3(6)
O(34)	C(35)	C(37)	118.7(6)
O(36)	C(35)	C(37)	117.0(6)
O(38)	C(39)	O(40)	124.5(6)
O(38)	C(39)	C(41)	116.3(6)
O(40)	C(39)	C(41)	119.2(7)
O(42)	C(43)	O(44)	125.8(6)
O(42)	C(43)	C(45)	117.6(6)
O(44)	C(43)	C(45)	116.6(6)
O(46)	C(47)	O(48)	125.8(6)
O(46)	C(47)	C(49)	117.0(6)
O(48)	C(47)	C(49)	117.2(6)
O(50)	C(51)	O(52)	124.8(6)
O(50)	C(51)	C(53)	114.1(6)
O(52)	C(51)	C(53)	121.0(6)
CL(60)	CL(59)	CL(61)	110.4(4)

A	B	C	Angle
CL(60)	C(59)	CL(62)	109.3(4)
CL(61)	C(59)	CL(62)	110.4(4)
CL(64)	C(63)	CL(65)	110.2(4)
CL(64)	C(63)	CL(66)	109.7(4)
CL(65)	C(63)	CL(66)	110.5(4)
CL(68)	C(67)	CL(69)	114.6(6)
CL(68)	C(67)	CL(70)	106.6(6)
CL(68)	C(67)	CL(A)	91.0(8)
CL(68)	C(67)	CL(D)	125.4(14)
CL(69)	C(67)	CL(70)	103.9(6)
CL(69)	C(67)	CL(A)	69.2(7)
CL(69)	C(67)	CL(D)	49.1(12)
CL(70)	C(67)	CL(A)	162.2(8)
CL(70)	C(67)	CL(D)	54.8(13)
CL(A)	C(67)	CL(D)	116.1(15)
CL(72)	C(71)	CL(73)	113.7(7)
CL(72)	C(71)	CL(74)	113.0(10)
CL(72)	C(71)	CL(C)	138.0(12)
CL(73)	C(71)	CL(74)	113.0(9)
CL(73)	C(71)	CL(C)	77.5(10)
CL(74)	C(71)	CL(C)	36.1(8)
CL(76)	C(75)	CL(77)	104.1(8)
CL(76)	C(75)	CL(78)	112.4(8)
CL(76)	C(75)	C(75)'	63.1(10)
CL(77)	C(75)	CL(78)	117.8(9)
CL(77)	C(75)	C(75)'	75.8(12)
CL(78)	C(75)	C(75)'	166.3(15)
CL(76)	C(75)'	CL(77)	106.4(9)
CL(76)	C(75)'	CL(78)'	113.5(9)
CL(76)	C(75)'	C(75)	78.0(11)
CL(77)	C(75)'	CL(78)'	117.7(9)
CL(77)	C(75)'	C(75)	66.1(11)
CL(78)'	C(75)'	C(75)	164.1(15)

A	B	C	Angle
C(71)	CL(72)	H(40)	52.(5)
CR(1)	O(28)	H(17)	117.(5)
CR(2)	O(28)	H(17)	104.(5)
CR(1)	O(29)	H(18)	111.(8)
CR(3)	O(29)	H(18)	104.(8)
N(4)	C(5)	H(1)	115.(4)
C(6)	C(5)	H(1)	122.(4)
C(5)	C(6)	H(2)	121.(4)
C(7)	C(6)	H(2)	120.(4)
C(6)	C(7)	H(3)	121.(4)
C(8)	C(7)	H(3)	120.(4)
C(7)	C(8)	H(4)	127.(4)
C(9)	C(8)	H(4)	114.(4)
C(10)	C(11)	H(5)	118.(4)
C(12)	C(11)	H(5)	123.(4)
C(11)	C(12)	H(6)	117.(5)
C(13)	C(12)	H(6)	124.(5)
C(12)	C(13)	H(7)	122.(5)
C(14)	C(13)	H(7)	118.(5)
N(15)	C(14)	H(8)	116.(4)
C(13)	C(14)	H(8)	122.(4)
N(16)	C(17)	H(9)	114.(4)
C(18)	C(17)	H(9)	125.(4)
C(17)	C(18)	H(10)	110.(6)
C(19)	C(18)	H(10)	130.(6)
C(18)	C(19)	H(11)	123.(4)
C(20)	C(19)	H(11)	117.(4)
C(19)	C(20)	H(12)	120.(4)
C(21)	C(20)	H(12)	120.(4)
C(22)	C(23)	H(13)	121.(5)
C(24)	C(23)	H(13)	121.(5)
C(23)	C(24)	H(14)	115.(4)
C(25)	C(24)	H(14)	125.(4)
C(24)	C(25)	H(15)	121.(5)
C(26)	C(25)	H(15)	120.(5)
N(27)	C(26)	H(16)	113.(3)
C(25)	C(26)	H(16)	124.(3)
C(31)	C(33)	H(19)	105.(4)
C(31)	C(33)	H(20)	109.(5)
C(31)	C(33)	H(21)	108.(5)
H(19)	C(33)	H(20)	115.(6)
H(19)	C(33)	H(21)	110.(6)
H(20)	C(33)	H(21)	111.(6)
C(35)	C(37)	H(22)	117.(7)
C(35)	C(37)	H(23)	107.(9)
C(35)	C(37)	H(24)	120.(8)
H(22)	C(37)	H(23)	100.(10)
H(22)	C(37)	H(24)	93.(9)
H(23)	C(37)	H(24)	118.(11)
C(39)	C(41)	H(25)	113.(5)

A	B	C	Angle
C(39)	C(41)	H(26)	106.(8)
C(39)	C(41)	H(27)	107.(6)
H(25)	C(41)	H(26)	106.(9)
H(25)	C(41)	H(27)	110.(7)
H(26)	C(41)	H(27)	115.(9)
C(43)	C(45)	H(28)	105.(5)
C(43)	C(45)	H(29)	113.(4)
C(43)	C(45)	H(30)	112.(5)
H(28)	C(45)	H(29)	96.(6)
H(28)	C(45)	H(30)	119.(7)
H(29)	C(45)	H(30)	111.(6)
C(47)	C(49)	H(31)	108.(7)
C(47)	C(49)	H(32)	109.(7)
C(47)	C(49)	H(33)	109.(6)
H(31)	C(49)	H(32)	102.(9)
H(31)	C(49)	H(33)	112.(9)
H(32)	C(49)	H(33)	116.(9)
C(51)	C(53)	H(34)	112.(5)
C(51)	C(53)	H(35)	106.(5)
C(51)	C(53)	H(36)	107.(5)
H(34)	C(53)	H(35)	111.(7)
H(34)	C(53)	H(36)	109.(7)
H(35)	C(53)	H(36)	111.(6)
CL(60)	C(59)	H(37)	106.(4)
CL(61)	C(59)	H(37)	113.(4)
CL(62)	C(59)	H(37)	108.(4)
CL(64)	C(63)	H(38)	103.(5)
CL(65)	C(63)	H(38)	115.(5)
CL(66)	C(63)	H(38)	108.(5)
CL(68)	C(67)	H(39)	115.(6)
CL(69)	C(67)	H(39)	111.(6)
CL(70)	C(67)	H(39)	105.(6)
CL(A)	C(67)	H(39)	65.(6)
CL(D)	C(67)	H(39)	119.(6)
CL(72)	C(71)	H(40)	58.(6)
CL(73)	C(71)	H(40)	99.(6)
CL(74)	C(71)	H(40)	146.(6)
CL(C)	C(71)	H(40)	164.(6)
CL(72)	H(40)	C(71)	69.(6)