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Supplementary Table 1. Atomic Coordinates, Thermal Parameters, and Complete Bond Distances and Bond Angles for Compound 4

(Atomic Coordinates and Equivalent Isotropic Thermal Parameters)

Atom	x	y	z	B_{eq}
Cr(1)	0.52851(10)	0.1816(1)	0.17843(9)	3.85(3)
Cr(2)	0.91260(9)	0.2452(1)	0.16213(8)	3.75(3)
O(1)	0.3491(6)	0.2525(8)	0.2290(7)	10.9(3)
O(2)	0.6195(10)	0.1773(9)	0.3604(5)	14.2(4)
O(3)	0.5771(7)	0.4162(6)	0.1766(6)	9.2(3)
O(4)	1.0999(5)	0.3567(9)	0.2122(5)	10.3(3)
O(5)	1.0124(5)	0.0319(7)	0.1656(6)	8.3(2)
O(6)	0.9335(5)	0.2745(7)	-0.0182(4)	7.0(2)
C(1)	0.5104(5)	0.1613(7)	0.0392(5)	3.7(2)
C(2)	0.4416(6)	0.1010(8)	0.0683(6)	4.6(2)
C(3)	0.4685(7)	0.0233(8)	0.1352(6)	5.1(3)
C(4)	0.5623(7)	0.0075(8)	0.1697(6)	4.2(2)
C(4a)	0.6338(5)	0.0659(6)	0.1409(5)	3.4(2)
C(5)	0.8395(6)	0.1905(8)	0.2656(5)	4.1(2)
C(6)	0.8685(6)	0.3005(8)	0.2785(6)	4.6(2)
C(7)	0.8382(6)	0.3781(7)	0.2144(6)	4.3(2)
C(8)	0.7838(6)	0.3482(6)	0.1374(6)	3.5(2)
C(8a)	0.7547(5)	0.2379(6)	0.1245(5)	3.3(2)
C(9)	0.6903(5)	0.1929(6)	0.0443(5)	3.0(2)
C(9a)	0.6067(5)	0.1438(6)	0.0740(5)	3.2(2)
C(10)	0.7397(6)	0.0488(6)	0.1627(5)	3.5(2)
C(10a)	0.7841(5)	0.1610(6)	0.1859(5)	3.2(2)
C(11)	0.7661(5)	0.0175(6)	0.0792(5)	3.6(2)
C(12)	0.7405(5)	0.0948(6)	0.0157(5)	3.3(2)
C(13)	0.7581(6)	0.0782(7)	-0.0652(6)	4.0(2)
C(14)	0.8013(6)	-0.0198(9)	-0.0824(7)	5.3(3)
C(15)	0.8277(8)	-0.0946(9)	-0.0193(8)	6.0(3)
C(16)	0.8112(7)	-0.0786(7)	0.0628(8)	5.1(3)
C(17)	0.4185(8)	0.2248(9)	0.2083(7)	6.3(3)
C(18)	0.5843(9)	0.1801(9)	0.2890(7)	6.6(3)
C(19)	0.5585(8)	0.3242(9)	0.1767(7)	5.9(3)
C(20)	1.0269(7)	0.3186(9)	0.1935(6)	6.3(3)
C(21)	0.9743(6)	0.1164(9)	0.1639(6)	5.8(3)
C(22)	0.9256(6)	0.2624(8)	0.0515(6)	4.5(2)

C(23)	0.323(2)	0.082(2)	0.512(2)	13.7(9)
C(24)	0.311(2)	0.118(2)	0.428(2)	12.2(8)
C(25)	0.223(2)	0.138(1)	0.368(1)	10.3(6)
C(26)	0.147(2)	0.122(1)	0.418(2)	10.5(7)
C(27)	0.158(2)	0.087(2)	0.498(2)	12.4(9)
C(28)	0.241(3)	0.065(2)	0.545(1)	13.4(9)
H(1)	0.491(6)	0.217(7)	−0.008(5)	5(2)
H(2)	0.386(5)	0.109(5)	0.048(4)	1(1)
H(3)	0.416(6)	−0.007(7)	0.162(5)	4(1)
H(4)	0.579(6)	−0.035(7)	0.209(5)	4(2)
H(5)	0.873(5)	0.137(6)	0.307(4)	3(1)
H(6)	0.907(5)	0.317(6)	0.334(5)	3(1)
H(7)	0.866(7)	0.456(9)	0.219(7)	8(3)
H(8)	0.763(6)	0.400(7)	0.094(6)	5(2)
H(9)	0.671(5)	0.250(6)	0.005(4)	3(1)
H(10)	0.763(6)	0.002(7)	0.199(5)	4(2)
H(11)	0.733(7)	0.132(8)	−0.112(6)	7(2)
H(12)	0.814(5)	−0.036(6)	−0.147(5)	4(1)
H(13)	0.859(6)	−0.161(8)	−0.026(6)	5(2)
H(14)	0.836(6)	−0.129(7)	0.104(5)	4(1)
H(15)	0.3871	0.0693	0.5433	15.6
H(16)	0.3640	0.1284	0.3999	14.9
H(17)	0.2156	0.1675	0.3286	12.0
H(18)	0.0838	0.1331	0.3841	12.5
H(19)	0.1053	0.0764	0.5259	14.6
H(20)	0.2536	0.0381	0.6018	15.1

(Anisotropic Thermal Parameters)

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Cr(1)	0.0486(8)	0.0440(8)	0.0520(8)	-0.0110(7)	0.0060(6)	-0.0102(7)
Cr(2)	0.0380(7)	0.0525(9)	0.0465(8)	-0.0065(7)	-0.0055(5)	0.0041(7)
O(1)	0.099(6)	0.137(8)	0.20(1)	-0.018(6)	0.085(7)	-0.057(8)
O(2)	0.31(2)	0.146(9)	0.050(5)	-0.024(10)	-0.045(7)	-0.023(6)
O(3)	0.145(8)	0.047(5)	0.180(9)	-0.017(5)	0.084(7)	-0.024(5)
O(4)	0.074(5)	0.20(1)	0.112(7)	-0.079(6)	0.012(5)	-0.043(7)
O(5)	0.076(5)	0.096(6)	0.149(8)	0.054(5)	0.031(5)	0.050(6)
O(6)	0.099(5)	0.113(6)	0.054(4)	-0.031(5)	0.013(4)	-0.006(4)
C(1)	0.037(4)	0.048(5)	0.050(5)	-0.007(4)	-0.007(4)	-0.008(4)
C(2)	0.031(5)	0.068(7)	0.070(6)	-0.005(5)	-0.009(5)	-0.017(5)
C(3)	0.063(6)	0.061(6)	0.066(6)	-0.024(5)	0.006(5)	-0.009(5)
C(4)	0.060(6)	0.048(6)	0.048(5)	-0.019(5)	0.006(5)	0.001(5)
C(4a)	0.043(4)	0.038(5)	0.043(4)	-0.002(4)	-0.001(4)	-0.002(4)
C(5)	0.036(4)	0.065(6)	0.050(5)	-0.002(4)	-0.001(4)	0.007(5)
C(6)	0.049(5)	0.070(6)	0.049(5)	-0.024(5)	-0.010(4)	-0.006(5)
C(7)	0.054(5)	0.045(5)	0.061(6)	-0.008(4)	0.002(4)	-0.003(5)
C(8)	0.044(5)	0.031(4)	0.055(5)	-0.006(4)	0.002(4)	0.000(4)
C(8a)	0.030(4)	0.043(5)	0.050(5)	-0.005(4)	-0.001(3)	-0.004(4)
C(9)	0.034(4)	0.029(4)	0.045(4)	0.002(3)	-0.005(3)	0.003(4)
C(9a)	0.040(4)	0.035(4)	0.043(4)	-0.004(3)	-0.002(3)	-0.001(4)
C(10)	0.050(5)	0.025(4)	0.051(5)	-0.001(4)	-0.009(4)	0.015(4)
C(10a)	0.034(4)	0.045(5)	0.038(4)	-0.001(3)	-0.007(3)	0.002(4)
C(11)	0.039(4)	0.043(5)	0.052(5)	0.001(4)	0.004(4)	0.004(4)
C(12)	0.037(4)	0.037(5)	0.051(5)	0.001(3)	0.004(4)	-0.001(4)

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(13)	0.039(5)	0.050(6)	0.061(6)	-0.001(4)	0.008(4)	0.000(5)
C(14)	0.050(6)	0.071(7)	0.082(8)	0.007(5)	0.019(5)	-0.007(6)
C(15)	0.067(7)	0.056(7)	0.11(1)	0.018(5)	0.029(7)	0.000(7)
C(16)	0.057(6)	0.039(5)	0.093(8)	0.011(4)	0.008(6)	0.010(6)
C(17)	0.071(7)	0.086(8)	0.087(8)	-0.017(6)	0.027(6)	-0.017(6)
C(18)	0.119(9)	0.068(7)	0.058(7)	-0.014(7)	0.004(6)	-0.016(6)
C(19)	0.091(8)	0.060(7)	0.082(7)	-0.021(6)	0.037(6)	-0.032(6)
C(20)	0.070(7)	0.097(8)	0.064(6)	-0.030(6)	-0.003(5)	0.003(6)
C(21)	0.047(5)	0.095(8)	0.074(7)	0.026(6)	0.004(5)	0.038(6)
C(22)	0.055(5)	0.057(6)	0.053(6)	-0.006(5)	-0.006(4)	-0.005(5)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

(Bond Distances)

atom	atom	distance	atom	atom	distance
Cr(1)	C(1)	2.207(8)	Cr(1)	C(2)	2.189(9)
Cr(1)	C(3)	2.186(9)	Cr(1)	C(4)	2.207(10)
Cr(1)	C(4a)	2.245(8)	Cr(1)	C(9a)	2.240(8)
Cr(1)	C(17)	1.82(1)	Cr(1)	C(18)	1.79(1)
Cr(1)	C(19)	1.81(1)	Cr(2)	C(5)	2.233(9)
Cr(2)	C(6)	2.192(10)	Cr(2)	C(7)	2.207(9)
Cr(2)	C(8)	2.217(8)	Cr(2)	C(8a)	2.236(7)
Cr(2)	C(10a)	2.217(8)	Cr(2)	C(20)	1.83(1)
Cr(2)	C(21)	1.81(1)	Cr(2)	C(22)	1.829(10)
O(1)	C(17)	1.16(1)	O(2)	C(18)	1.16(1)
O(3)	C(19)	1.16(1)	O(4)	C(20)	1.16(1)
O(5)	C(21)	1.17(1)	O(6)	C(22)	1.153(10)
C(1)	C(2)	1.39(1)	C(1)	C(9a)	1.41(1)
C(2)	C(3)	1.43(1)	C(3)	C(4)	1.37(1)
C(4)	C(4a)	1.41(1)	C(4a)	C(9a)	1.43(1)
C(4a)	C(10)	1.51(1)	C(5)	C(6)	1.42(1)
C(5)	C(10a)	1.41(1)	C(6)	C(7)	1.41(1)
C(7)	C(8)	1.37(1)	C(8)	C(8a)	1.42(1)
C(8a)	C(9)	1.532(10)	C(8a)	C(10a)	1.37(1)
C(9)	C(9a)	1.50(1)	C(9)	C(12)	1.52(1)
C(10)	C(10a)	1.54(1)	C(10)	C(11)	1.51(1)
C(11)	C(12)	1.39(1)	C(11)	C(16)	1.40(1)
C(12)	C(13)	1.38(1)	C(13)	C(14)	1.41(1)
C(14)	C(15)	1.36(1)	C(15)	C(16)	1.39(1)
C(23)	C(24)	1.33(3)	C(23)	C(28)	1.40(3)
C(24)	C(25)	1.32(2)	C(25)	C(26)	1.33(3)
C(26)	C(27)	1.31(3)	C(27)	C(28)	1.40(3)

(Bond Angles)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	Cr(1)	C(2)	36.8(3)	C(1)	Cr(1)	C(3)	67.6(4)
C(1)	Cr(1)	C(4)	79.1(3)	C(1)	Cr(1)	C(4a)	67.1(3)
C(1)	Cr(1)	C(9a)	36.8(3)	C(1)	Cr(1)	C(17)	111.2(4)
C(1)	Cr(1)	C(18)	159.5(4)	C(1)	Cr(1)	C(19)	94.3(4)
C(2)	Cr(1)	C(3)	38.2(3)	C(2)	Cr(1)	C(4)	66.9(4)
C(2)	Cr(1)	C(4a)	78.8(3)	C(2)	Cr(1)	C(9a)	66.2(3)
C(2)	Cr(1)	C(17)	87.5(4)	C(2)	Cr(1)	C(18)	149.8(4)
C(2)	Cr(1)	C(19)	121.8(5)	C(3)	Cr(1)	C(4)	36.3(3)
C(3)	Cr(1)	C(4a)	66.2(3)	C(3)	Cr(1)	C(9a)	78.7(3)
C(3)	Cr(1)	C(17)	91.9(4)	C(3)	Cr(1)	C(18)	112.1(4)
C(3)	Cr(1)	C(19)	160.0(5)	C(4)	Cr(1)	C(4a)	36.8(3)
C(4)	Cr(1)	C(9a)	66.5(3)	C(4)	Cr(1)	C(17)	120.9(4)
C(4)	Cr(1)	C(18)	89.5(4)	C(4)	Cr(1)	C(19)	152.2(4)
C(4a)	Cr(1)	C(9a)	37.3(3)	C(4a)	Cr(1)	C(17)	157.4(4)
C(4a)	Cr(1)	C(18)	93.6(4)	C(4a)	Cr(1)	C(19)	115.8(4)
C(9a)	Cr(1)	C(17)	147.9(4)	C(9a)	Cr(1)	C(18)	122.8(4)
C(9a)	Cr(1)	C(19)	91.9(4)	C(17)	Cr(1)	C(18)	89.3(5)
C(17)	Cr(1)	C(19)	86.7(5)	C(18)	Cr(1)	C(19)	87.9(5)
C(5)	Cr(2)	C(6)	37.4(3)	C(5)	Cr(2)	C(7)	66.9(3)
C(5)	Cr(2)	C(8)	78.8(3)	C(5)	Cr(2)	C(8a)	65.5(3)
C(5)	Cr(2)	C(10a)	37.0(3)	C(5)	Cr(2)	C(20)	117.7(4)
C(5)	Cr(2)	C(21)	91.5(4)	C(5)	Cr(2)	C(22)	154.9(3)
C(6)	Cr(2)	C(7)	37.3(3)	C(6)	Cr(2)	C(8)	66.6(3)
C(6)	Cr(2)	C(8a)	78.0(3)	C(6)	Cr(2)	C(10a)	66.9(3)

atom	atom	atom	angle	atom	atom	atom	angle
C(6)	Cr(2)	C(20)	91.1(4)	C(6)	Cr(2)	C(21)	118.7(4)
C(6)	Cr(2)	C(22)	152.8(4)	C(7)	Cr(2)	C(8)	36.2(3)
C(7)	Cr(2)	C(8a)	65.7(3)	C(7)	Cr(2)	C(10a)	78.3(3)
C(7)	Cr(2)	C(20)	91.8(4)	C(7)	Cr(2)	C(21)	156.0(4)
C(7)	Cr(2)	C(22)	115.5(4)	C(8)	Cr(2)	C(8a)	37.3(3)
C(8)	Cr(2)	C(10a)	66.5(3)	C(8)	Cr(2)	C(20)	117.5(4)
C(8)	Cr(2)	C(21)	153.2(4)	C(8)	Cr(2)	C(22)	90.1(4)
C(8a)	Cr(2)	C(10a)	35.8(3)	C(8a)	Cr(2)	C(20)	154.8(4)
C(8a)	Cr(2)	C(21)	116.0(4)	C(8a)	Cr(2)	C(22)	92.1(3)
C(10a)	Cr(2)	C(20)	154.7(4)	C(10a)	Cr(2)	C(21)	90.7(4)
C(10a)	Cr(2)	C(22)	117.9(3)	C(20)	Cr(2)	C(21)	89.2(5)
C(20)	Cr(2)	C(22)	87.4(4)	C(21)	Cr(2)	C(22)	88.5(4)
Cr(1)	C(1)	C(2)	70.9(5)	Cr(1)	C(1)	C(9a)	72.9(5)
C(2)	C(1)	C(9a)	119.9(8)	Cr(1)	C(2)	C(1)	72.3(5)
Cr(1)	C(2)	C(3)	70.8(5)	C(1)	C(2)	C(3)	120.2(8)
Cr(1)	C(3)	C(2)	71.0(5)	Cr(1)	C(3)	C(4)	72.6(5)
C(2)	C(3)	C(4)	119.8(9)	Cr(1)	C(4)	C(3)	71.0(6)
Cr(1)	C(4)	C(4a)	73.1(5)	C(3)	C(4)	C(4a)	121.6(9)
Cr(1)	C(4a)	C(4)	70.1(5)	Cr(1)	C(4a)	C(9a)	71.2(4)
Cr(1)	C(4a)	C(10)	136.9(5)	C(4)	C(4a)	C(9a)	118.5(7)
C(4)	C(4a)	C(10)	128.6(8)	C(9a)	C(4a)	C(10)	112.3(7)
Cr(2)	C(5)	C(6)	69.7(5)	Cr(2)	C(5)	C(10a)	70.9(5)
C(6)	C(5)	C(10a)	118.3(8)	Cr(2)	C(6)	C(5)	72.9(5)
Cr(2)	C(6)	C(7)	71.9(5)	C(5)	C(6)	C(7)	120.0(8)

atom	atom	atom	angle	atom	atom	atom	angle
Cr(2)	C(7)	C(6)	70.8(5)	Cr(2)	C(7)	C(8)	72.3(5)
C(6)	C(7)	C(8)	120.9(8)	Cr(2)	C(8)	C(7)	71.5(5)
Cr(2)	C(8)	C(8a)	72.1(4)	C(7)	C(8)	C(8a)	119.0(8)
Cr(2)	C(8a)	C(8)	70.6(4)	Cr(2)	C(8a)	C(9)	130.9(5)
Cr(2)	C(8a)	C(10a)	71.3(4)	C(8)	C(8a)	C(9)	125.3(7)
C(8)	C(8a)	C(10a)	120.9(7)	C(9)	C(8a)	C(10a)	113.8(7)
C(8a)	C(9)	C(9a)	105.6(6)	C(8a)	C(9)	C(12)	107.1(6)
C(9a)	C(9)	C(12)	103.5(6)	Cr(1)	C(9a)	C(1)	70.3(5)
Cr(1)	C(9a)	C(4a)	71.5(4)	Cr(1)	C(9a)	C(9)	134.7(5)
C(1)	C(9a)	C(4a)	120.1(7)	C(1)	C(9a)	C(9)	126.9(7)
C(4a)	C(9a)	C(9)	112.8(6)	C(4a)	C(10)	C(10a)	106.5(6)
C(4a)	C(10)	C(11)	104.4(6)	C(10a)	C(10)	C(11)	106.2(7)
Cr(2)	C(10a)	C(5)	72.1(5)	Cr(2)	C(10a)	C(8a)	72.9(4)
Cr(2)	C(10a)	C(10)	134.4(6)	C(5)	C(10a)	C(8a)	120.7(7)
C(5)	C(10a)	C(10)	125.7(7)	C(8a)	C(10a)	C(10)	113.0(6)
C(10)	C(11)	C(12)	113.4(7)	C(10)	C(11)	C(16)	126.1(8)
C(12)	C(11)	C(16)	120.5(8)	C(9)	C(12)	C(11)	113.3(7)
C(9)	C(12)	C(13)	125.8(7)	C(11)	C(12)	C(13)	120.9(8)
C(12)	C(13)	C(14)	118.7(9)	C(13)	C(14)	C(15)	120(1)
C(14)	C(15)	C(16)	121(1)	C(11)	C(16)	C(15)	117.9(10)
Cr(1)	C(17)	O(1)	178(1)	Cr(1)	C(18)	O(2)	178(1)
Cr(1)	C(19)	O(3)	178.9(9)	Cr(2)	C(20)	O(4)	178.9(10)
Cr(2)	C(21)	O(5)	178.4(9)	Cr(2)	C(22)	O(6)	179.2(9)
C(24)	C(23)	C(28)	117(2)	C(23)	C(24)	C(25)	123(2)
C(24)	C(25)	C(26)	118(2)	C(25)	C(26)	C(27)	122(2)
C(26)	C(27)	C(28)	119(2)	C(23)	C(28)	C(27)	117(2)

Supplementary Table 2. Atomic Coordinates, Thermal Parameters, and Complete Bond Distances and Bond Angles for Compound 5

atom	x	y	z	B _{eq}
Cr(1)	0.2452(1)	0.94018(10)	0.01515(6)	3.10(3)
Cr(2)	0.2712(1)	0.55182(9)	0.03571(6)	2.97(3)
Cr(3)	0.4819(1)	0.77339(8)	0.24517(6)	2.78(3)
O(1)	-0.0077(6)	0.8476(5)	-0.0374(3)	5.9(2)
O(2)	0.3383(7)	0.8551(5)	-0.0970(3)	5.5(2)
O(3)	0.1680(9)	1.1065(6)	-0.0704(4)	8.7(3)
O(4)	0.2588(8)	0.3640(5)	-0.0289(3)	7.5(2)
O(5)	0.5297(6)	0.4906(4)	0.1075(3)	5.0(2)
O(6)	0.1632(7)	0.4642(6)	0.1429(3)	6.5(2)
O(7)	0.6128(7)	0.7824(5)	0.3829(3)	6.5(2)
O(8)	0.2882(6)	0.9168(5)	0.2706(3)	5.6(2)
O(9)	0.6583(6)	0.9208(4)	0.2090(3)	5.5(2)
C(1)	0.2032(8)	0.9403(7)	0.1135(4)	3.4(2)
C(2)	0.2608(10)	1.0249(7)	0.1033(4)	4.2(2)
C(3)	0.3802(8)	1.0274(6)	0.0831(4)	3.2(2)
C(4)	0.4421(8)	0.9430(6)	0.0732(4)	3.0(2)
C(4a)	0.3853(7)	0.8566(5)	0.0841(3)	2.3(2)
C(5)	0.3476(9)	0.6601(6)	-0.0228(4)	3.2(2)
C(6)	0.2414(8)	0.6174(6)	-0.0601(4)	3.8(2)
C(7)	0.1243(9)	0.6164(7)	-0.0378(4)	4.4(2)
C(8)	0.1090(8)	0.6566(6)	0.0210(4)	3.7(2)
C(8a)	0.2206(7)	0.6995(5)	0.0575(3)	2.6(2)
C(9)	0.2223(7)	0.7554(6)	0.1196(3)	2.8(2)
C(9a)	0.2635(7)	0.8538(5)	0.1051(3)	2.6(2)

atom	x	y	z	B _{eq}
C(10)	0.4405(7)	0.7587(5)	0.0793(3)	2.1(2)
C(10a)	0.3373(6)	0.7010(5)	0.0356(3)	2.2(2)
C(11)	0.4536(7)	0.7144(5)	0.1457(3)	2.4(2)
C(12)	0.3341(8)	0.7124(5)	0.1680(3)	2.9(2)
C(13)	0.3241(10)	0.6675(6)	0.2268(4)	3.8(2)
C(14)	0.436(1)	0.6250(6)	0.2613(4)	4.3(2)
C(15)	0.553(1)	0.6280(5)	0.2392(4)	3.9(2)
C(16)	0.5637(8)	0.6738(5)	0.1829(4)	2.9(2)
C(17)	0.0876(9)	0.8848(7)	-0.0165(4)	4.2(2)
C(18)	0.3035(8)	0.8870(6)	-0.0537(4)	3.8(2)
C(19)	0.1963(10)	1.0429(7)	-0.0368(4)	5.0(2)
C(20)	0.2624(9)	0.4368(7)	-0.0030(4)	4.4(2)
C(21)	0.4314(8)	0.5151(5)	0.0793(4)	3.1(2)
C(22)	0.2048(9)	0.4983(6)	0.1017(5)	4.2(2)
C(23)	0.5608(9)	0.7793(6)	0.3294(4)	4.3(2)
C(24)	0.3650(8)	0.8636(6)	0.2612(4)	3.5(2)
C(25)	0.5899(9)	0.8644(6)	0.2240(4)	3.5(2)
C(26)	0.056(2)	0.274(1)	0.255(2)	14.0(10)
C(27)	0.086(1)	0.219(2)	0.3085(10)	9.1(5)
C(28)	0.070(1)	0.128(2)	0.3079(7)	8.5(5)
C(29)	0.021(1)	0.081(1)	0.2561(9)	8.5(4)
C(30)	-0.011(2)	0.128(2)	0.2023(7)	10.3(6)
C(31)	0.008(2)	0.219(2)	0.201(1)	13.3(9)
H(1)	0.144(7)	0.937(6)	0.127(4)	3(1)

atom	x	y	z	B _{eq}
H(2)	0.222(7)	1.071(5)	0.109(3)	2(1)
H(3)	0.416(7)	1.091(5)	0.076(3)	2(1)
H(4)	0.510(6)	0.945(5)	0.058(3)	1(1)
H(5)	0.412(6)	0.657(4)	-0.033(3)	0(1)
H(6)	0.254(8)	0.580(6)	-0.101(4)	4(1)
H(7)	0.058(6)	0.587(4)	-0.058(3)	1(1)
H(8)	0.02(1)	0.649(8)	0.036(5)	9(1)
H(9)	0.155(7)	0.761(6)	0.135(4)	3(1)
H(10)	0.512(6)	0.756(4)	0.066(3)	0(1)
H(11)	0.241(7)	0.669(5)	0.238(3)	3(1)
H(12)	0.426(8)	0.593(6)	0.295(4)	4(1)
H(13)	0.625(8)	0.599(6)	0.266(4)	4(1)
H(14)	0.641(7)	0.674(5)	0.167(3)	2(1)
H(15)	0.0689	0.3402	0.2576	17.6342
H(16)	0.1219	0.2480	0.3496	10.1819
H(17)	0.096(7)	0.103(5)	0.336(3)	1(1)
H(18)	0.0088	0.0148	0.2580	10.2376
H(19)	-0.0493	0.0961	0.1634	16.5403
H(20)	-0.0114	0.2526	0.1623	16.9924

$$B_{eq} = \frac{8}{3} \pi^2 (U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^* \cos \gamma + 2U_{13}aa^*cc^* \cos \beta + 2U_{23}bb^*cc^* \cos \alpha)$$

(Anisotropic Thermal Parameters)

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Cr(1)	0.0405(8)	0.0455(8)	0.0297(6)	0.0154(7)	0.0000(5)	0.0038(6)
Cr(2)	0.0382(7)	0.0401(7)	0.0320(7)	-0.0069(6)	-0.0011(5)	-0.0065(6)
Cr(3)	0.0483(8)	0.0281(6)	0.0259(6)	-0.0009(6)	-0.0022(5)	-0.0019(5)
O(1)	0.042(4)	0.101(6)	0.072(4)	0.015(4)	-0.017(3)	-0.012(4)
O(2)	0.079(5)	0.084(5)	0.050(4)	0.009(4)	0.026(3)	-0.009(4)
O(3)	0.149(8)	0.101(6)	0.080(5)	0.056(6)	0.020(5)	0.053(5)
O(4)	0.141(7)	0.064(5)	0.070(5)	-0.011(5)	-0.015(5)	-0.024(4)
O(5)	0.060(4)	0.057(4)	0.064(4)	0.019(3)	-0.012(3)	-0.014(3)
O(6)	0.079(5)	0.101(6)	0.072(5)	-0.023(4)	0.022(4)	0.016(4)
O(7)	0.115(6)	0.073(5)	0.044(4)	0.002(4)	-0.022(4)	-0.008(4)
O(8)	0.069(5)	0.074(5)	0.070(4)	0.022(4)	0.013(4)	-0.018(4)
O(9)	0.071(5)	0.046(4)	0.091(5)	-0.010(3)	0.014(4)	0.001(4)
C(1)	0.038(5)	0.063(6)	0.028(4)	0.017(5)	0.009(4)	-0.010(4)
C(2)	0.072(7)	0.037(5)	0.044(5)	0.024(5)	-0.002(5)	-0.005(4)
C(3)	0.046(5)	0.035(5)	0.042(5)	0.003(4)	0.005(4)	0.003(4)
C(4)	0.036(5)	0.042(5)	0.035(4)	0.001(4)	0.004(4)	0.008(4)
C(4a)	0.030(4)	0.034(4)	0.020(3)	0.005(3)	0.001(3)	0.001(3)
C(5)	0.040(5)	0.052(5)	0.033(4)	0.010(4)	0.014(4)	-0.001(4)
C(6)	0.047(6)	0.058(6)	0.034(5)	-0.001(4)	-0.006(4)	-0.005(4)
C(7)	0.041(6)	0.062(6)	0.051(6)	-0.008(5)	-0.021(5)	-0.010(5)
C(8)	0.029(4)	0.056(5)	0.049(5)	-0.003(4)	-0.010(4)	-0.004(4)
C(8a)	0.025(4)	0.044(5)	0.029(4)	0.001(3)	0.001(3)	-0.002(3)
C(9)	0.024(4)	0.048(5)	0.035(4)	-0.002(4)	0.011(3)	-0.006(4)
C(9a)	0.030(4)	0.043(5)	0.026(4)	0.002(4)	0.002(3)	-0.003(3)

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(10)	0.019(4)	0.035(4)	0.027(4)	0.003(3)	0.005(3)	-0.001(3)
C(10a)	0.029(4)	0.029(4)	0.023(4)	0.005(3)	0.003(3)	0.002(3)
C(11)	0.035(4)	0.032(4)	0.025(4)	-0.002(3)	0.005(3)	0.000(3)
C(12)	0.052(5)	0.029(4)	0.028(4)	-0.005(4)	0.006(4)	0.000(3)
C(13)	0.064(6)	0.042(5)	0.043(5)	-0.018(5)	0.021(5)	-0.002(4)
C(14)	0.098(9)	0.033(5)	0.032(5)	-0.010(5)	0.010(5)	0.001(4)
C(15)	0.078(7)	0.023(4)	0.038(5)	0.008(4)	-0.016(5)	0.000(4)
C(16)	0.045(5)	0.028(4)	0.036(4)	0.008(4)	-0.002(4)	-0.009(3)
C(17)	0.039(5)	0.077(7)	0.039(5)	0.026(5)	-0.007(4)	-0.002(5)
C(18)	0.047(5)	0.054(5)	0.045(5)	0.004(4)	0.011(4)	0.000(4)
C(19)	0.077(7)	0.072(7)	0.044(5)	0.028(6)	0.014(5)	0.015(5)
C(20)	0.065(6)	0.050(6)	0.046(5)	-0.014(5)	-0.007(4)	-0.018(5)
C(21)	0.048(5)	0.033(4)	0.036(4)	-0.006(4)	0.006(4)	-0.006(4)
C(22)	0.050(6)	0.047(6)	0.058(6)	-0.007(4)	-0.004(5)	0.011(4)
C(23)	0.074(6)	0.043(5)	0.040(5)	0.004(5)	-0.003(5)	-0.007(4)
C(24)	0.047(5)	0.045(5)	0.037(4)	-0.007(4)	0.002(4)	-0.009(4)
C(25)	0.055(5)	0.030(5)	0.045(5)	-0.002(4)	0.000(4)	-0.002(4)
C(26)	0.13(2)	0.07(1)	0.35(4)	-0.01(1)	0.11(2)	0.01(2)
C(27)	0.042(7)	0.13(1)	0.18(2)	-0.014(9)	0.029(9)	-0.08(1)
C(28)	0.064(9)	0.19(2)	0.069(10)	0.03(1)	-0.001(7)	0.03(1)
C(29)	0.09(1)	0.11(1)	0.12(1)	0.018(9)	0.013(9)	-0.02(1)
C(30)	0.10(1)	0.22(2)	0.066(9)	0.04(1)	0.011(8)	-0.01(1)
C(31)	0.18(2)	0.15(2)	0.18(2)	0.04(2)	0.05(2)	0.10(2)

(Bond Distances)

atom	atom	distance	atom	atom	distance
Cr(1)	C(1)	2.202(8)	Cr(1)	C(2)	2.199(9)
Cr(1)	C(3)	2.207(8)	Cr(1)	C(4)	2.207(8)
Cr(1)	C(4a)	2.219(7)	Cr(1)	C(9a)	2.242(7)
Cr(1)	C(17)	1.844(10)	Cr(1)	C(18)	1.838(9)
Cr(1)	C(19)	1.841(9)	Cr(2)	C(5)	2.207(9)
Cr(2)	C(6)	2.201(8)	Cr(2)	C(7)	2.186(9)
Cr(2)	C(8)	2.236(9)	Cr(2)	C(8a)	2.225(8)
Cr(2)	C(10a)	2.223(7)	Cr(2)	C(20)	1.817(9)
Cr(2)	C(21)	1.842(9)	Cr(2)	C(22)	1.831(10)
Cr(3)	C(11)	2.235(7)	Cr(3)	C(12)	2.217(7)
Cr(3)	C(13)	2.215(9)	Cr(3)	C(14)	2.195(9)
Cr(3)	C(15)	2.198(8)	Cr(3)	C(16)	2.203(8)
Cr(3)	C(23)	1.829(8)	Cr(3)	C(24)	1.842(9)
Cr(3)	C(25)	1.822(9)	O(1)	C(17)	1.15(1)
O(2)	C(18)	1.138(9)	O(3)	C(19)	1.15(1)
O(4)	C(20)	1.17(1)	O(5)	C(21)	1.150(9)
O(6)	C(22)	1.15(1)	O(7)	C(23)	1.167(9)
O(8)	C(24)	1.145(9)	O(9)	C(25)	1.155(9)
C(1)	C(2)	1.38(1)	C(1)	C(9a)	1.40(1)
C(2)	C(3)	1.39(1)	C(3)	C(4)	1.39(1)
C(4)	C(4a)	1.40(1)	C(4a)	C(9a)	1.424(10)
C(4a)	C(10)	1.513(10)	C(5)	C(6)	1.38(1)
C(5)	C(10a)	1.39(1)	C(6)	C(7)	1.39(1)
C(7)	C(8)	1.40(1)	C(8)	C(8a)	1.42(1)

atom	atom	distance
C(8a)	C(9)	1.530(10)
C(9)	C(9a)	1.50(1)
C(10)	C(10a)	1.529(9)
C(11)	C(12)	1.41(1)
C(12)	C(13)	1.42(1)
C(14)	C(15)	1.39(1)
C(26)	C(27)	1.36(3)
C(27)	C(28)	1.31(2)
C(29)	C(30)	1.30(2)

atom	atom	distance
C(8a)	C(10a)	1.383(9)
C(9)	C(12)	1.54(1)
C(10)	C(11)	1.521(9)
C(11)	C(16)	1.401(10)
C(13)	C(14)	1.40(1)
C(15)	C(16)	1.38(1)
C(26)	C(31)	1.40(3)
C(28)	C(29)	1.30(2)
C(30)	C(31)	1.31(3)

(Bond Angles)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	Cr(1)	C(2)	36.4(3)	C(1)	Cr(1)	C(3)	66.2(3)
C(1)	Cr(1)	C(4)	78.3(3)	C(1)	Cr(1)	C(4a)	66.3(3)
C(1)	Cr(1)	C(9a)	36.8(3)	C(1)	Cr(1)	C(17)	91.6(4)
C(1)	Cr(1)	C(18)	154.1(4)	C(1)	Cr(1)	C(19)	118.9(4)
C(2)	Cr(1)	C(3)	36.8(3)	C(2)	Cr(1)	C(4)	66.2(3)
C(2)	Cr(1)	C(4a)	78.0(3)	C(2)	Cr(1)	C(9a)	66.1(3)
C(2)	Cr(1)	C(17)	117.9(4)	C(2)	Cr(1)	C(18)	155.6(4)
C(2)	Cr(1)	C(19)	92.7(4)	C(3)	Cr(1)	C(4)	36.8(3)
C(3)	Cr(1)	C(4a)	66.2(3)	C(3)	Cr(1)	C(9a)	78.7(3)
C(3)	Cr(1)	C(17)	154.7(4)	C(3)	Cr(1)	C(18)	118.8(4)
C(3)	Cr(1)	C(19)	91.5(4)	C(4)	Cr(1)	C(4a)	36.8(3)
C(4)	Cr(1)	C(9a)	66.8(3)	C(4)	Cr(1)	C(17)	154.0(4)
C(4)	Cr(1)	C(18)	92.3(3)	C(4)	Cr(1)	C(19)	116.9(4)
C(4a)	Cr(1)	C(9a)	37.2(3)	C(4a)	Cr(1)	C(17)	117.3(3)
C(4a)	Cr(1)	C(18)	91.7(3)	C(4a)	Cr(1)	C(19)	153.6(4)
C(9a)	Cr(1)	C(17)	90.8(3)	C(9a)	Cr(1)	C(18)	117.3(3)
C(9a)	Cr(1)	C(19)	155.7(3)	C(17)	Cr(1)	C(18)	86.5(4)
C(17)	Cr(1)	C(19)	88.9(4)	C(18)	Cr(1)	C(19)	86.9(4)
C(5)	Cr(2)	C(6)	36.6(3)	C(5)	Cr(2)	C(7)	65.8(4)
C(5)	Cr(2)	C(8)	78.7(3)	C(5)	Cr(2)	C(8a)	65.6(3)
C(5)	Cr(2)	C(10a)	36.5(3)	C(5)	Cr(2)	C(20)	111.3(4)
C(5)	Cr(2)	C(21)	95.0(3)	C(5)	Cr(2)	C(22)	160.0(4)
C(6)	Cr(2)	C(7)	37.0(3)	C(6)	Cr(2)	C(8)	67.2(3)
C(6)	Cr(2)	C(8a)	78.2(3)	C(6)	Cr(2)	C(10a)	65.9(3)

atom	atom	atom	angle	atom	atom	atom	angle
C(6)	Cr(2)	C(20)	88.6(4)	C(6)	Cr(2)	C(21)	123.2(3)
C(6)	Cr(2)	C(22)	150.0(4)	C(7)	Cr(2)	C(8)	37.0(3)
C(7)	Cr(2)	C(8a)	65.9(3)	C(7)	Cr(2)	C(10a)	77.4(3)
C(7)	Cr(2)	C(20)	94.6(4)	C(7)	Cr(2)	C(21)	159.9(4)
C(7)	Cr(2)	C(22)	113.7(4)	C(8)	Cr(2)	C(8a)	37.1(3)
C(8)	Cr(2)	C(10a)	66.4(3)	C(8)	Cr(2)	C(20)	123.7(3)
C(8)	Cr(2)	C(21)	149.3(3)	C(8)	Cr(2)	C(22)	89.9(4)
C(8a)	Cr(2)	C(10a)	36.2(2)	C(8a)	Cr(2)	C(20)	160.1(3)
C(8a)	Cr(2)	C(21)	113.0(3)	C(8a)	Cr(2)	C(22)	95.4(3)
C(10a)	Cr(2)	C(20)	147.3(3)	C(10a)	Cr(2)	C(21)	90.7(3)
C(10a)	Cr(2)	C(22)	123.7(3)	C(20)	Cr(2)	C(21)	86.7(4)
C(20)	Cr(2)	C(22)	88.7(4)	C(21)	Cr(2)	C(22)	86.4(4)
C(11)	Cr(3)	C(12)	37.1(3)	C(11)	Cr(3)	C(13)	67.1(3)
C(11)	Cr(3)	C(14)	78.0(3)	C(11)	Cr(3)	C(15)	65.6(3)
C(11)	Cr(3)	C(16)	36.8(3)	C(11)	Cr(3)	C(23)	153.7(3)
C(11)	Cr(3)	C(24)	116.8(3)	C(11)	Cr(3)	C(25)	91.0(3)
C(12)	Cr(3)	C(13)	37.3(3)	C(12)	Cr(3)	C(14)	66.2(3)
C(12)	Cr(3)	C(15)	78.0(3)	C(12)	Cr(3)	C(16)	66.8(3)
C(12)	Cr(3)	C(23)	150.7(4)	C(12)	Cr(3)	C(24)	90.3(3)
C(12)	Cr(3)	C(25)	118.6(3)	C(13)	Cr(3)	C(14)	37.0(3)
C(13)	Cr(3)	C(15)	66.7(4)	C(13)	Cr(3)	C(16)	79.6(3)
C(13)	Cr(3)	C(23)	113.4(4)	C(13)	Cr(3)	C(24)	90.1(4)
C(13)	Cr(3)	C(25)	155.8(3)	C(14)	Cr(3)	C(15)	36.8(3)
C(14)	Cr(3)	C(16)	66.4(4)	C(14)	Cr(3)	C(23)	88.1(4)

atom	atom	atom	angle	atom	atom	atom	angle
C(14)	Cr(3)	C(24)	117.6(4)	C(14)	Cr(3)	C(25)	151.4(4)
C(15)	Cr(3)	C(16)	36.5(3)	C(15)	Cr(3)	C(23)	90.0(3)
C(15)	Cr(3)	C(24)	154.4(4)	C(15)	Cr(3)	C(25)	114.7(4)
C(16)	Cr(3)	C(23)	117.1(3)	C(16)	Cr(3)	C(24)	153.5(3)
C(16)	Cr(3)	C(25)	88.9(3)	C(23)	Cr(3)	C(24)	89.4(4)
C(23)	Cr(3)	C(25)	90.8(4)	C(24)	Cr(3)	C(25)	91.0(4)
Cr(1)	C(1)	C(2)	71.7(5)	Cr(1)	C(1)	C(9a)	73.2(4)
C(2)	C(1)	C(9a)	121.3(8)	Cr(1)	C(2)	C(1)	71.9(5)
Cr(1)	C(2)	C(3)	71.9(5)	C(1)	C(2)	C(3)	120.9(9)
Cr(1)	C(3)	C(2)	71.2(5)	Cr(1)	C(3)	C(4)	71.6(5)
C(2)	C(3)	C(4)	119.5(8)	Cr(1)	C(4)	C(3)	71.6(5)
Cr(1)	C(4)	C(4a)	72.1(4)	C(3)	C(4)	C(4a)	120.2(7)
Cr(1)	C(4a)	C(4)	71.1(4)	Cr(1)	C(4a)	C(9a)	72.3(4)
Cr(1)	C(4a)	C(10)	131.4(5)	C(4)	C(4a)	C(9a)	120.5(7)
C(4)	C(4a)	C(10)	127.7(6)	C(9a)	C(4a)	C(10)	111.7(6)
Cr(2)	C(5)	C(6)	71.5(5)	Cr(2)	C(5)	C(10a)	72.4(5)
C(6)	C(5)	C(10a)	120.7(8)	Cr(2)	C(6)	C(5)	71.9(5)
Cr(2)	C(6)	C(7)	70.9(5)	C(5)	C(6)	C(7)	118.7(8)
Cr(2)	C(7)	C(6)	72.1(5)	Cr(2)	C(7)	C(8)	73.4(5)
C(6)	C(7)	C(8)	122.8(8)	Cr(2)	C(8)	C(7)	69.6(5)
Cr(2)	C(8)	C(8a)	71.0(4)	C(7)	C(8)	C(8a)	116.4(8)
Cr(2)	C(8a)	C(8)	71.9(5)	Cr(2)	C(8a)	C(9)	134.2(5)
Cr(2)	C(8a)	C(10a)	71.8(4)	C(8)	C(8a)	C(9)	124.9(7)
C(8)	C(8a)	C(10a)	121.1(7)	C(9)	C(8a)	C(10a)	113.8(6)

atom	atom	atom	angle	atom	atom	atom	angle
C(8a)	C(9)	C(9a)	105.3(6)	C(8a)	C(9)	C(12)	105.0(6)
C(9a)	C(9)	C(12)	106.8(6)	Cr(1)	C(9a)	C(1)	70.0(5)
Cr(1)	C(9a)	C(4a)	70.5(4)	Cr(1)	C(9a)	C(9)	133.9(5)
C(1)	C(9a)	C(4a)	117.6(7)	C(1)	C(9a)	C(9)	129.0(7)
C(4a)	C(9a)	C(9)	113.3(6)	C(4a)	C(10)	C(10a)	107.0(5)
C(4a)	C(10)	C(11)	106.8(6)	C(10a)	C(10)	C(11)	106.1(6)
Cr(2)	C(10a)	C(5)	71.2(5)	Cr(2)	C(10a)	C(8a)	72.0(4)
Cr(2)	C(10a)	C(10)	134.0(5)	C(5)	C(10a)	C(8a)	120.4(7)
C(5)	C(10a)	C(10)	127.2(7)	C(8a)	C(10a)	C(10)	112.2(6)
Cr(3)	C(11)	C(10)	133.7(5)	Cr(3)	C(11)	C(12)	70.8(4)
Cr(3)	C(11)	C(16)	70.4(4)	C(10)	C(11)	C(12)	112.1(6)
C(10)	C(11)	C(16)	128.3(7)	C(12)	C(11)	C(16)	119.5(7)
Cr(3)	C(12)	C(9)	133.3(5)	Cr(3)	C(12)	C(11)	72.2(4)
Cr(3)	C(12)	C(13)	71.3(5)	C(9)	C(12)	C(11)	112.5(6)
C(9)	C(12)	C(13)	126.6(7)	C(11)	C(12)	C(13)	120.7(7)
Cr(3)	C(13)	C(12)	71.5(5)	Cr(3)	C(13)	C(14)	70.7(5)
C(12)	C(13)	C(14)	117.8(9)	Cr(3)	C(14)	C(13)	72.3(5)
Cr(3)	C(14)	C(15)	71.7(5)	C(13)	C(14)	C(15)	121.2(8)
Cr(3)	C(15)	C(14)	71.5(6)	Cr(3)	C(15)	C(16)	72.0(5)
C(14)	C(15)	C(16)	121.3(8)	Cr(3)	C(16)	C(11)	72.9(4)
Cr(3)	C(16)	C(15)	71.6(5)	C(11)	C(16)	C(15)	119.5(8)
Cr(1)	C(17)	O(1)	177.2(8)	Cr(1)	C(18)	O(2)	178.8(8)
Cr(1)	C(19)	O(3)	178.1(9)	Cr(2)	C(20)	O(4)	178.2(9)
Cr(2)	C(21)	O(5)	178.1(7)	Cr(2)	C(22)	O(6)	179.5(9)
Cr(3)	C(23)	O(7)	179.0(8)	Cr(3)	C(24)	O(8)	177.0(7)
Cr(3)	C(25)	O(9)	178.1(7)	C(27)	C(26)	C(31)	110(1)
C(26)	C(27)	C(28)	123(1)	C(27)	C(28)	C(29)	122(1)
C(28)	C(29)	C(30)	118(1)	C(29)	C(30)	C(31)	119(1)
C(26)	C(31)	C(30)	125(2)				