Inorganic Chemistry
including bioinorganic chemistry
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Identification code	w436
Empirical formula	$C_{31}H_{64}Cl_2Cr_2CuN_{12}O_{15}$
Formula weight	1083.38
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 29.029(7) Å α = 90° b = 12.239(4) Å β = 118.90(2)° c = 14.850(4) Å γ = 90°
Volume	4619(2) $Å^3$
Z	4
Density (calculated)	1.558 Mg/m^3
Absorption coefficient	1.110 mm^{-1}
F(000)	2260
Crystal size	0.86 x 0.42 x 0.40 mm
θ range for data collection	2.92 to 27.56°
Index ranges	$0 \leq h \leq 37$, $-4 \leq k \leq 15$, $-19 \leq \ell \leq 16$
Reflections collected	7333
Independent reflections	5287 (R_{int} = 0.0216)
Absorption correction	Semi-empirical from ψ-scans
Max. and min. transmission	0.862 and 0.809
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5287 / 0 / 296
Goodness-of-fit on F^2	1.046
Final R indices [$I>2\sigma(I)$]	R1 = 0.0686, wR2 = 0.1504
R indices (all data)	R1 = 0.1093, wR2 = 0.1771
Largest diff. peak and hole	1.313 and -1.805 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^{4}] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cu(1)	5000	1410(1)	2500	65(1)
Cr(1)	3893(1)	1535(1)	2945(1)	32(1)
O(1)	4148(1)	192(3)	2682(3)	47(1)
O(2)	3889(1)	2386(3)	1858(3)	47(1)
O(3)	4551(1)	2077(3)	4027(3)	45(1)
N(1)	4586(1)	148(3)	2585(3)	32(1)
N(2)	4290(2)	2331(3)	1633(3)	34(1)
N(3)	4960(1)	2161(3)	3829(3)	35(1)
N(4)	3496(2)	2811(4)	3258(4)	51(1)
N(5)	3743(2)	672(4)	4020(3)	47(1)
N(6)	3108(2)	1027(4)	1911(3)	51(1)
C(1)	4762(2)	-811(3)	2553(4)	33(1)
C(2)	4513(3)	-1838(5)	2635(7)	78(2)
C(3)	4234(2)	2905(4)	862(4)	36(1)
C(4)	3764(2)	3603(7)	252(5)	81(2)
C(5)	5327(2)	2839(4)	4378(3)	34(1)
C(6)	5328(2)	3565(5)	5182(5)	59(2)
C(7)	3584(4)	2575(6)	4308(6)	93(3)
C(8)	3544(3)	1451(7)	4519(6)	84(2)
C(9)	3330(3)	-148(6)	3383(6)	78(2)
C(10)	2926(3)	242(7)	2429(6)	92(3)
C(11)	2801(3)	2063(8)	1662(6)	98(3)
C(12)	2934(3)	2780(7)	2497(7)	94(3)
C(13)	3718(3)	3903(5)	3272(7)	79(2)
C(14)	4212(3)	86(6)	4797(5)	74(2)
C(15)	3049(3)	556(7)	936(5)	76(2)
Cl(1)	3210(1)	6537(2)	1682(1)	63(1)
O(11)	2813(2)	5765(6)	1365(6)	124(2)
O(12)	3678(3)	6109(6)	1843(9)	183(5)
O(13)	3097(4)	7480(8)	1142(8)	200(5)
O(14)	3303(4)	6851(9)	2651(6)	179(4)
C(20)	5000	5191(11)	2500	118(5)
O(20)	4563(5)	5715(11)	1516(11)	108(4)

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

Cu(1)-N(1)#1	1.997(4)	Cu(1)-N(1)	1.997(4)
Cu(1)-N(2)	2.147(4)	Cu(1)-N(2)#1	2.148(4)
Cu(1)-N(3)	2.229(4)	Cu(1)-N(3)#1	2.229(4)
Cr(1)-O(2)	1.916(3)	Cr(1)-O(1)	1.919(3)
Cr(1)-O(3)	1.925(3)	Cr(1)-N(4)	2.122(4)
Cr(1)-N(5)	2.129(4)	Cr(1)-N(6)	2.134(4)
O(1)-N(1)	1.348(4)	O(2)-N(2)	1.358(5)
O(3)-N(3)	1.359(5)	N(1)-C(1)	1.290(5)
N(2)-C(3)	1.284(6)	N(3)-C(5)	1.283(6)
N(4)-C(12)	1.469(8)	N(4)-C(13)	1.480(8)
N(4)-C(7)	1.482(8)	N(5)-C(14)	1.478(8)
N(5)-C(8)	1.486(8)	N(5)-C(9)	1.498(8)
N(6)-C(10)	1.479(8)	N(6)-C(15)	1.489(7)
N(6)-C(11)	1.491(9)	C(1)-C(1)#1	1.464(8)
C(1)-C(2)	1.484(7)	C(3)-C(5)#1	1.484(6)
C(3)-C(4)	1.489(7)	C(5)-C(3)#1	1.484(6)
C(5)-C(6)	1.488(7)	C(7)-C(8)	1.428(10)
C(9)-C(10)	1.416(10)	C(11)-C(12)	1.413(11)
Cl(1)-O(13)	1.353(8)	Cl(1)-O(12)	1.364(6)
Cl(1)-O(14)	1.384(7)	Cl(1)-O(11)	1.386(6)
C(20)-O(20)	1.538(14)		

N(1)#1-Cu(1)-N(1)	78.7(2)	N(1)#1-Cu(1)-N(2)	143.2(2)
N(1)-Cu(1)-N(2)	90.7(2)	N(1)#1-Cu(1)-N(2)#1	90.7(2)
N(1)-Cu(1)-N(2)#1	143.2(2)	N(2)-Cu(1)-N(2)#1	116.6(2)
N(1)#1-Cu(1)-N(3)	131.6(2)	N(1)-Cu(1)-N(3)	88.46(14)
N(2)-Cu(1)-N(3)	82.47(14)	N(2)#1-Cu(1)-N(3)	72.43(14)
N(1)#1-Cu(1)-N(3)#1	88.46(14)	N(1)-Cu(1)-N(3)#1	131.6(2)
N(2)-Cu(1)-N(3)#1	72.43(14)	N(2)#1-Cu(1)-N(3)#1	82.47(14)
N(3)-Cu(1)-N(3)#1	131.3(2)	O(2)-Cr(1)-O(1)	98.1(2)
O(2)-Cr(1)-O(3)	96.6(2)	O(1)-Cr(1)-O(3)	98.1(2)
O(2)-Cr(1)-N(4)	90.1(2)	O(1)-Cr(1)-N(4)	168.2(2)
O(3)-Cr(1)-N(4)	89.3(2)	O(2)-Cr(1)-N(5)	169.0(2)
O(1)-Cr(1)-N(5)	88.1(2)	O(3)-Cr(1)-N(5)	91.4(2)
N(4)-Cr(1)-N(5)	82.6(2)	O(2)-Cr(1)-N(6)	89.0(2)
O(1)-Cr(1)-N(6)	89.2(2)	O(3)-Cr(1)-N(6)	170.0(2)
N(4)-Cr(1)-N(6)	82.4(2)	N(5)-Cr(1)-N(6)	82.0(2)
N(1)-O(1)-Cr(1)	122.1(3)	N(2)-O(2)-Cr(1)	121.5(3)
N(3)-O(3)-Cr(1)	117.6(3)	C(1)-N(1)-O(1)	116.7(4)
C(1)-N(1)-Cu(1)	116.2(3)	O(1)-N(1)-Cu(1)	127.1(3)
C(3)-N(2)-O(2)	115.9(4)	C(3)-N(2)-Cu(1)	119.5(3)
O(2)-N(2)-Cu(1)	124.5(3)	C(5)-N(3)-O(3)	117.0(4)
C(5)-N(3)-Cu(1)	116.6(3)	O(3)-N(3)-Cu(1)	125.8(3)
C(12)-N(4)-C(13)	110.4(6)	C(12)-N(4)-C(7)	111.5(6)
C(13)-N(4)-C(7)	108.0(6)	C(12)-N(4)-Cr(1)	109.4(4)
C(13)-N(4)-Cr(1)	112.9(3)	C(7)-N(4)-Cr(1)	104.6(4)
C(14)-N(5)-C(8)	110.9(5)	C(14)-N(5)-C(9)	108.9(5)
C(8)-N(5)-C(9)	111.0(5)	C(14)-N(5)-Cr(1)	112.4(3)
C(8)-N(5)-Cr(1)	109.0(4)	C(9)-N(5)-Cr(1)	104.5(4)
C(10)-N(6)-C(15)	110.6(5)	C(10)-N(6)-C(11)	111.0(6)
C(15)-N(6)-C(11)	108.3(6)	C(10)-N(6)-Cr(1)	109.9(4)
C(15)-N(6)-Cr(1)	113.2(3)	C(11)-N(6)-Cr(1)	103.5(4)
N(1)-C(1)-C(1)#1	114.5(2)	N(1)-C(1)-C(2)	123.4(4)
C(1)#1-C(1)-C(2)	122.1(3)	N(2)-C(3)-C(5)#1	115.5(4)
N(2)-C(3)-C(4)	122.7(4)	C(5)#1-C(3)-C(4)	121.7(4)
N(3)-C(5)-C(3)#1	115.3(4)	N(3)-C(5)-C(6)	125.2(4)
C(3)#1-C(5)-C(6)	119.5(4)	C(8)-C(7)-N(4)	115.3(6)
C(7)-C(8)-N(5)	114.6(5)	C(10)-C(9)-N(5)	115.4(6)
C(9)-C(10)-N(6)	114.1(6)	C(12)-C(11)-N(6)	115.7(6)

C(11)-C(12)-N(4)	115.0(6)	O(13)-Cl(1)-O(12)	111.6(6)
O(13)-Cl(1)-O(14)	104.4(7)	O(12)-Cl(1)-O(14)	104.3(7)
O(13)-Cl(1)-O(11)	117.1(5)	O(12)-Cl(1)-O(11)	113.1(4)
O(14)-Cl(1)-O(11)	104.7(5)		

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters [A^2 x 10^3] for 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
Cu(1)	65(1)	24(1)	148(1)	0	85(1)	0
Cr(1)	27(1)	37(1)	38(1)	0(1)	21(1)	0(1)
O(1)	41(2)	38(2)	79(3)	-5(2)	43(2)	-5(2)
O(2)	41(2)	56(2)	54(2)	17(2)	32(2)	12(2)
O(3)	38(2)	58(2)	48(2)	-9(2)	26(2)	-12(2)
N(1)	32(2)	29(2)	41(2)	-3(2)	22(2)	-2(2)
N(2)	36(2)	33(2)	40(2)	2(2)	24(2)	3(2)
N(3)	31(2)	35(2)	39(2)	-5(2)	17(2)	-1(2)
N(4)	49(3)	47(3)	70(3)	-5(2)	40(2)	5(2)
N(5)	45(2)	57(3)	46(2)	5(2)	28(2)	-5(2)
N(6)	32(2)	76(3)	48(3)	-7(2)	22(2)	-7(2)
C(1)	36(2)	22(2)	44(3)	1(2)	22(2)	0(2)
C(2)	75(5)	32(3)	153(7)	1(4)	75(5)	-9(3)
C(3)	34(2)	42(3)	34(2)	8(2)	17(2)	6(2)
C(4)	55(4)	123(6)	75(4)	52(5)	39(3)	41(4)
C(5)	36(2)	34(2)	32(2)	-4(2)	18(2)	-1(2)
C(6)	64(4)	65(4)	63(4)	-28(3)	42(3)	-19(3)
C(7)	157(8)	76(5)	97(6)	-17(5)	101(6)	-3(5)
C(8)	113(6)	104(6)	68(4)	8(4)	68(5)	15(5)
C(9)	66(4)	71(5)	95(5)	15(4)	37(4)	-25(4)
C(10)	86(5)	121(7)	77(5)	-25(5)	44(4)	-65(5)
C(11)	42(3)	140(8)	82(5)	-13(5)	5(3)	35(4)
C(12)	53(4)	81(5)	139(8)	-2(5)	39(5)	24(4)
C(13)	86(5)	43(3)	130(7)	-11(4)	68(5)	8(3)
C(14)	65(4)	94(5)	61(4)	32(4)	30(3)	2(4)
C(15)	57(4)	116(6)	53(4)	-24(4)	25(3)	-19(4)
Cl(1)	49(1)	76(1)	69(1)	11(1)	32(1)	-5(1)
O(11)	74(4)	148(6)	150(6)	-33(5)	55(4)	-49(4)
O(12)	120(6)	98(5)	399(15)	-32(7)	178(8)	-20(4)
O(13)	181(8)	161(8)	182(9)	99(7)	27(7)	2(7)
O(14)	217(10)	233(10)	106(6)	-39(6)	94(6)	-55(8)
C(20)	129(12)	69(8)	126(12)	0	39(10)	0
O(20)	105(9)	99(9)	134(11)	-11(8)	70(8)	-8(7)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(2A)	4742(9)	-2443(7)	2727(41)	118
H(2B)	4185(10)	-1943(22)	2018(17)	118
H(2C)	4451(19)	-1793(18)	3213(24)	118
H(4A)	3600(12)	3389(29)	-458(9)	121
H(4B)	3870(4)	4354(8)	314(34)	121
H(4C)	3518(10)	3517(35)	506(28)	121
H(6A)	5314(17)	4314(5)	4978(16)	89
H(6B)	5643(9)	3445(26)	5822(9)	89
H(6C)	5027(10)	3405(25)	5266(24)	89
H(7A)	3931(4)	2836(6)	4800(6)	112
H(7B)	3330(4)	2988(6)	4417(6)	112
H(8A)	3177(3)	1284(7)	4294(6)	101
H(8B)	3738(3)	1339(7)	5257(6)	101
H(9A)	3500(3)	-763(6)	3252(6)	94
H(9B)	3169(3)	-417(6)	3782(6)	94
H(10A)	2658(3)	592(7)	2541(6)	111
H(10B)	2764(3)	-376(7)	1975(6)	111
H(11A)	2846(3)	2448(8)	1139(6)	117
H(11B)	2431(3)	1879(8)	1366(6)	117
H(12A)	2738(3)	2568(7)	2844(7)	113
H(12B)	2823(3)	3512(7)	2229(7)	113
H(13A)	4087(6)	3906(14)	3761(29)	119
H(13B)	3541(15)	4442(8)	3463(41)	119
H(13C)	3671(19)	4069(19)	2601(12)	119
H(14A)	4323(12)	-439(28)	4461(6)	110
H(14B)	4128(6)	-282(34)	5270(24)	110
H(14C)	4491(7)	600(8)	5166(26)	110
H(15A)	3173(19)	1071(18)	615(20)	114
H(15B)	2685(4)	398(40)	481(17)	114
H(15C)	3250(16)	-106(23)	1083(7)	114

Table 1. Crystal data and structure refinement for 2583. $Cr^{III}Ni^{II}Cr^{III}$

Identification code	2583
Empirical formula	$C_{30}H_{60}Cl_2Cr_2N_{12}NiO_{14}$
Formula weight	1046.51
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions, l.s. on	6359 Reflections a = 32.333(6) Å alpha = 90° b = 8.772(2) Å beta = 109.51(3)° c = 16.716(3) Å gamma = 90°
Volume, Z	4469(2) $Å^3$, 4
Density (calculated)	1.555 Mg/m^3
Absorption coefficient	1.088 mm^{-1}
F(000)	2184
Crystal size	0.35 x 0.42 x 0.48 mm
Diffractometer used	Siemens SMART
θ range for data collection	1.34 to 30.00°
Limiting indices	$-46 \le h \le 49$, $-11 \le k \le 13$, $-25 \le l \le 21$
Reflections collected	21944
Independent reflections	6394 (R_{int} = 0.0382)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5987 / 0 / 282
Goodness-of-fit on F^2	1.041
Final R indices [I>2σ(I)]	R1 = 0.0398, wR2 = 0.0865
R indices (all data)	R1 = 0.0648, wR2 = 0.1011
Largest diff. peak and hole	0.438 and -0.693 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 2583. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ni(1)	5000	5284(1)	2500	12(1)
Cr(1)	6158(1)	5250(1)	3171(1)	13(1)
O(1)	5843(1)	3498(2)	3381(1)	19(1)
O(2)	5857(1)	6767(2)	3624(1)	18(1)
O(3)	5817(1)	5545(2)	1979(1)	18(1)
N(4)	6612(1)	6927(2)	3069(1)	17(1)
N(5)	6580(1)	3766(2)	2800(1)	18(1)
N(6)	6634(1)	4930(2)	4389(1)	16(1)
N(1)	5405(1)	3426(2)	2945(1)	16(1)
N(2)	5423(1)	6525(2)	3493(1)	15(1)
N(3)	5380(1)	5854(2)	1773(1)	15(1)
C(7)	6776(1)	6327(3)	2395(1)	21(1)
C(8)	6920(1)	4678(3)	2577(1)	20(1)
C(9)	6785(1)	2788(2)	3562(1)	20(1)
C(10)	6970(1)	3769(2)	4347(1)	18(1)
C(11)	6835(1)	6467(2)	4618(1)	20(1)
C(12)	6978(1)	7091(2)	3905(1)	20(1)
C(13)	6404(1)	8441(2)	2807(2)	23(1)
C(14)	6335(1)	2784(3)	2071(1)	24(1)
C(15)	6436(1)	4457(3)	5035(1)	22(1)
C(1)	5236(1)	2087(2)	2756(2)	22(1)
C(2)	5488(1)	632(3)	3025(2)	41(1)
C(3)	5271(1)	6980(2)	4078(1)	17(1)
C(4)	5539(1)	7785(3)	4875(1)	28(1)
C(5)	5199(1)	6637(2)	1091(1)	18(1)
C(6)	5436(1)	7152(3)	507(2)	30(1)
Cl	6813(1)	281(1)	5750(1)	20(1)
O(10)	6771(1)	136(2)	4871(1)	47(1)
O(11)	6390(1)	486(2)	5835(1)	42(1)
O(12)	7086(1)	1588(2)	6101(1)	26(1)
O(13)	7018(1)	-1072(2)	6202(1)	31(1)

O(11)-Cl-O(13)	109.72(11)	O(10)-Cl-O(13)	109.45(12)
O(11)-Cl-O(12)	109.46(11)	O(10)-Cl-O(12)	108.80(11)
O(13)-Cl-O(12)	109.21(11)		

Symmetry transformations used to generate equivalent atoms:

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

Table 3. Bond lengths [Å] and angles [°] for 2583.

Ni(1)-N(3)	2.058(2)	Ni(1)-N(3)#1	2.058(2)
Ni(1)-N(1)#1	2.067(2)	Ni(1)-N(1)	2.067(2)
Ni(1)-N(2)#1	2.072(2)	Ni(1)-N(2)	2.072(2)
Cr(1)-O(1)	1.940(2)	Cr(1)-O(3)	1.945(2)
Cr(1)-O(2)	1.9458(14)	Cr(1)-N(6)	2.121(2)
Cr(1)-N(5)	2.122(2)	Cr(1)-N(4)	2.126(2)
O(1)-N(1)	1.361(2)	O(2)-N(2)	1.362(2)
O(3)-N(3)	1.364(2)	N(4)-C(13)	1.487(3)
N(4)-C(7)	1.492(3)	N(4)-C(12)	1.506(3)
N(5)-C(14)	1.487(3)	N(5)-C(9)	1.495(3)
N(5)-C(8)	1.504(3)	N(6)-C(15)	1.485(3)
N(6)-C(11)	1.491(3)	N(6)-C(10)	1.507(3)
N(1)-C(1)	1.288(3)	N(2)-C(3)	1.296(3)
N(3)-C(5)	1.292(3)	C(7)-C(8)	1.519(3)
C(9)-C(10)	1.515(3)	C(11)-C(12)	1.518(3)
C(1)-C(1)#1	1.482(4)	C(1)-C(2)	1.500(3)
C(3)-C(5)#1	1.479(3)	C(3)-C(4)	1.501(3)
C(5)-C(3)#1	1.479(3)	C(5)-C(6)	1.500(3)
Cl-O(11)	1.432(2)	Cl-O(10)	1.436(2)
Cl-O(13)	1.443(2)	Cl-O(12)	1.446(2)

N(3)-Ni(1)-N(3)#1	151.91(10)	N(3)-Ni(1)-N(1)#1	114.20(7)
N(3)#1-Ni(1)-N(1)#1	88.44(7)	N(3)-Ni(1)-N(1)	88.44(7)
N(3)#1-Ni(1)-N(1)	114.20(7)	N(1)#1-Ni(1)-N(1)	75.90(9)
N(3)-Ni(1)-N(2)#1	76.36(7)	N(3)#1-Ni(1)-N(2)#1	88.91(7)
N(1)#1-Ni(1)-N(2)#1	87.50(7)	N(1)-Ni(1)-N(2)#1	150.65(7)
N(3)-Ni(1)-N(2)	88.91(7)	N(3)#1-Ni(1)-N(2)	76.36(7)
N(1)#1-Ni(1)-N(2)	150.65(7)	N(1)-Ni(1)-N(2)	87.50(7)
N(2)#1-Ni(1)-N(2)	116.65(10)	O(1)-Cr(1)-O(3)	97.95(6)
O(1)-Cr(1)-O(2)	96.30(6)	O(3)-Cr(1)-O(2)	96.98(6)
O(1)-Cr(1)-N(6)	88.71(6)	O(3)-Cr(1)-N(6)	169.15(6)
O(2)-Cr(1)-N(6)	90.75(6)	O(1)-Cr(1)-N(5)	89.70(7)
O(3)-Cr(1)-N(5)	89.03(6)	O(2)-Cr(1)-N(5)	170.82(6)
N(6)-Cr(1)-N(5)	82.41(7)	O(1)-Cr(1)-N(4)	169.03(6)
O(3)-Cr(1)-N(4)	89.83(7)	O(2)-Cr(1)-N(4)	90.38(7)
N(6)-Cr(1)-N(4)	82.49(7)	N(5)-Cr(1)-N(4)	82.68(7)
N(1)-O(1)-Cr(1)	117.11(11)	N(2)-O(2)-Cr(1)	116.91(11)
N(3)-O(3)-Cr(1)	118.10(11)	C(13)-N(4)-C(7)	109.4(2)
C(13)-N(4)-C(12)	109.0(2)	C(7)-N(4)-C(12)	111.6(2)
C(13)-N(4)-Cr(1)	112.63(13)	C(7)-N(4)-Cr(1)	104.20(13)
C(12)-N(4)-Cr(1)	109.98(12)	C(14)-N(5)-C(9)	109.2(2)
C(14)-N(5)-C(8)	109.7(2)	C(9)-N(5)-C(8)	111.3(2)
C(14)-N(5)-Cr(1)	112.15(13)	C(9)-N(5)-Cr(1)	104.46(12)
C(8)-N(5)-Cr(1)	109.90(13)	C(15)-N(6)-C(11)	108.8(2)
C(15)-N(6)-C(10)	109.6(2)	C(11)-N(6)-C(10)	111.3(2)
C(15)-N(6)-Cr(1)	112.64(13)	C(11)-N(6)-Cr(1)	104.00(12)
C(10)-N(6)-Cr(1)	110.35(12)	C(1)-N(1)-O(1)	116.9(2)
C(1)-N(1)-Ni(1)	117.73(14)	O(1)-N(1)-Ni(1)	125.21(12)
C(3)-N(2)-O(2)	117.4(2)	C(3)-N(2)-Ni(1)	116.77(13)
O(2)-N(2)-Ni(1)	125.44(12)	C(5)-N(3)-O(3)	117.1(2)
C(5)-N(3)-Ni(1)	117.72(13)	O(3)-N(3)-Ni(1)	125.04(12)
N(4)-C(7)-C(8)	110.3(2)	N(5)-C(8)-C(7)	110.9(2)
N(5)-C(9)-C(10)	110.3(2)	N(6)-C(10)-C(9)	110.1(2)
N(6)-C(11)-C(12)	110.2(2)	N(4)-C(12)-C(11)	110.1(2)
N(1)-C(1)-C(1)#1	114.31(12)	N(1)-C(1)-C(2)	124.0(2)
C(1)#1-C(1)-C(2)	121.67(13)	N(2)-C(3)-C(5)#1	114.7(2)
N(2)-C(3)-C(4)	124.2(2)	C(5)#1-C(3)-C(4)	121.1(2)
N(3)-C(5)-C(3)#1	114.3(2)	N(3)-C(5)-C(6)	123.6(2)
C(3)#1-C(5)-C(6)	122.1(2)	O(11)-Cl-O(10)	110.18(14)

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 2583.

The anisotropic displacement factor exponent takes the form:

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

	U11	U22	U33	U23	U13	U12
Ni(1)	12(1)	11(1)	13(1)	0	3(1)	0
Cr(1)	12(1)	13(1)	13(1)	0(1)	4(1)	1(1)
O(1)	12(1)	17(1)	25(1)	4(1)	3(1)	1(1)
O(2)	12(1)	17(1)	23(1)	-3(1)	5(1)	-1(1)
O(3)	12(1)	26(1)	16(1)	1(1)	3(1)	3(1)
N(4)	17(1)	15(1)	19(1)	3(1)	6(1)	2(1)
N(5)	18(1)	18(1)	16(1)	-1(1)	5(1)	2(1)
N(6)	15(1)	18(1)	16(1)	0(1)	6(1)	1(1)
N(1)	14(1)	15(1)	19(1)	2(1)	5(1)	0(1)
N(2)	12(1)	14(1)	18(1)	0(1)	4(1)	0(1)
N(3)	13(1)	16(1)	15(1)	-1(1)	3(1)	0(1)
C(7)	20(1)	26(1)	20(1)	3(1)	10(1)	1(1)
C(8)	17(1)	27(1)	18(1)	1(1)	8(1)	3(1)
C(9)	21(1)	17(1)	21(1)	4(1)	7(1)	6(1)
C(10)	16(1)	19(1)	19(1)	5(1)	6(1)	5(1)
C(11)	17(1)	21(1)	19(1)	-4(1)	4(1)	-2(1)
C(12)	17(1)	18(1)	22(1)	-2(1)	5(1)	-1(1)
C(13)	22(1)	17(1)	31(1)	5(1)	9(1)	2(1)
C(14)	23(1)	26(1)	22(1)	-9(1)	5(1)	1(1)
C(15)	21(1)	29(1)	17(1)	4(1)	9(1)	3(1)
C(1)	17(1)	15(1)	32(1)	3(1)	8(1)	2(1)
C(2)	23(1)	16(1)	76(2)	8(1)	8(1)	4(1)
C(3)	16(1)	18(1)	15(1)	-2(1)	3(1)	1(1)
C(4)	19(1)	42(2)	22(1)	-13(1)	4(1)	-2(1)
C(5)	16(1)	21(1)	16(1)	1(1)	5(1)	-1(1)
C(6)	20(1)	48(2)	24(1)	14(1)	9(1)	4(1)
Cl	24(1)	18(1)	20(1)	0(1)	9(1)	1(1)
O(10)	93(2)	28(1)	23(1)	-6(1)	23(1)	-11(1)
O(11)	21(1)	42(1)	63(1)	4(1)	14(1)	4(1)
O(12)	29(1)	21(1)	27(1)	-3(1)	7(1)	-1(1)
O(13)	33(1)	21(1)	42(1)	11(1)	16(1)	7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 2583.

	x	y	z	U(eq)
H(7A)	7027(1)	6952(3)	2372(1)	25
H(7B)	6541(1)	6398(3)	1836(1)	25
H(8A)	6967(1)	4227(3)	2071(1)	24
H(8B)	7201(1)	4637(3)	3053(1)	24
H(9A)	7024(1)	2173(2)	3476(1)	24
H(9B)	6563(1)	2080(2)	3639(1)	24
H(10A)	7051(1)	3117(2)	4860(1)	22
H(10B)	7237(1)	4295(2)	4331(1)	22
H(11A)	7092(1)	6394(2)	5144(1)	23
H(11B)	6620(1)	7169(2)	4726(1)	23
H(12A)	7058(1)	8180(2)	4012(1)	24
H(12B)	7240(1)	6529(2)	3884(1)	24
H(13A)	6312(5)	8862(8)	3263(4)	35
H(13B)	6148(3)	8326(4)	2293(6)	35
H(13C)	6616(2)	9132(6)	2693(10)	35
H(14A)	6221(5)	3410(4)	1559(3)	37
H(14B)	6091(3)	2288(15)	2191(4)	37
H(14C)	6533(2)	2005(12)	1982(7)	37
H(15A)	6316(5)	3425(7)	4906(6)	33
H(15B)	6201(4)	5166(11)	5026(7)	33
H(15C)	6662(1)	4468(18)	5598(2)	33
H(2A)	5766(3)	848(4)	3476(9)	61
H(2B)	5547(6)	179(12)	2539(4)	61
H(2C)	5315(3)	-80(9)	3237(12)	61
H(4A)	5837(2)	7945(18)	4866(5)	42
H(4B)	5550(5)	7162(9)	5369(2)	42
H(4C)	5405(3)	8772(9)	4911(6)	42
H(6A)	5742(2)	6811(18)	729(6)	45
H(6B)	5427(5)	8267(3)	468(9)	45
H(6C)	5295(4)	6715(17)	-58(3)	45

Table 1. Crystal data and structure refinement for 2150. $Cr^{II}Fe^{II}Cr^{III}$

Identification code	2150
Empirical formula	$C_{30}H_{62}Cl_2Cr_2FeN_{12}O_{15}$
Formula weight	1061.65
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions, l.s. on	52 Reflections
	a = 30.941(6) Å alpha = 90°
	b = 8.777(2) Å beta = 96.22(3)°
	c = 16.801(3) Å gamma = 90°
Volume, Z	4536(2) $Å^3$, 4
Density (calculated)	1.552 Mg/m^3
Absorption coefficient	0.980 mm^{-1}
F(000)	2216
Crystal size	0.32 x 0.35 x 0.46 mm
Diffractometer used	Enraf-Nonius CAD4
θ range for data collection	2.44 to 26.33°
Limiting indices	$0 \le h \le 38$, $0 \le k \le 10$, $-20 \le l \le 20$
Reflections collected	4693
Independent reflections	4605 (R_{int} = 0.0153)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4601 / 0 / 285
Goodness-of-fit on F^2	1.058
Final R indices [I>2σ(I)]	R1 = 0.0442, wR2 = 0.1125
R indices (all data)	R1 = 0.0782, wR2 = 0.1357
Largest diff. peak and hole	0.618 and -0.570 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 2150. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	0	216(1)	2500	24(1)
Cr(1)	1125(1)	169(1)	2837(1)	28(1)
O(1)	811(1)	1829(3)	2267(1)	33(1)
O(2)	803(1)	-1385(3)	2208(2)	37(1)
O(3)	759(1)	155(3)	3704(1)	33(1)
N(1)	392(1)	1508(3)	1972(2)	29(1)
N(2)	375(1)	-1491(3)	2325(2)	31(1)
N(3)	338(1)	588(3)	3515(2)	29(1)
N(4)	1534(1)	-1448(3)	3489(2)	34(1)
N(5)	1564(1)	1743(3)	3445(2)	34(1)
N(6)	1614(1)	56(4)	2045(2)	37(1)
C(1)	268(1)	1919(4)	1236(2)	33(1)
C(2)	546(1)	2778(5)	710(2)	50(1)
C(3)	223(1)	-2855(4)	2404(3)	42(1)
C(4)	471(2)	-4300(5)	2294(4)	71(2)
C(5)	167(1)	1436(4)	4040(2)	33(1)
C(6)	395(1)	1841(6)	4845(2)	51(1)
C(7)	1853(2)	-638(5)	4066(3)	51(1)
C(8)	1724(2)	955(5)	4200(2)	50(1)
C(9)	1929(1)	2050(5)	2945(3)	53(1)
C(10)	1825(2)	1572(5)	2115(3)	53(1)
C(11)	1928(1)	-1196(5)	2301(3)	51(1)
C(12)	1752(2)	-2267(5)	2866(3)	53(1)
C(13)	1286(1)	-2581(5)	3916(3)	56(1)
C(14)	1355(2)	3184(5)	3636(3)	58(1)
C(15)	1434(2)	-203(7)	1202(2)	60(1)
Cl	3128(1)	176(1)	4102(1)	57(1)
O(11)	2913(2)	1399(5)	4430(3)	99(1)
O(12)	3563(1)	453(8)	4180(4)	152(2)
O(13)	3037(2)	-1168(5)	4493(3)	125(2)
O(14)	2952(1)	44(4)	3288(2)	73(1)
O(20)	2543(3)	126(17)	828(6)	156(6)

O(12)-Cl-O(11)	109.4(4)	O(13)-Cl-O(11)	109.3(3)
O(12)-Cl-O(14)	112.3(4)	O(13)-Cl-O(14)	108.0(3)
O(11)-Cl-O(14)	106.9(2)		

Symmetry transformations used to generate equivalent atoms:

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

Table 3. Bond lengths [Å] and angles [°] for 2150.

Fe(1)-N(3)	1.929(3)	Fe(1)-N(3)#1	1.929(3)
Fe(1)-N(2)	1.937(3)	Fe(1)-N(2)#1	1.937(3)
Fe(1)-N(1)	1.943(3)	Fe(1)-N(1)#1	1.943(3)
Cr(1)-O(2)	1.934(2)	Cr(1)-O(3)	1.940(2)
Cr(1)-O(1)	1.945(2)	Cr(1)-N(5)	2.119(3)
Cr(1)-N(6)	2.121(3)	Cr(1)-N(4)	2.124(3)
O(1)-N(1)	1.368(3)	O(2)-N(2)	1.365(3)
O(3)-N(3)	1.361(3)	N(1)-C(1)	1.305(4)
N(2)-C(3)	1.297(5)	N(3)-C(5)	1.310(4)
N(4)-C(13)	1.487(5)	N(4)-C(7)	1.489(5)
N(4)-C(12)	1.490(5)	N(5)-C(14)	1.470(5)
N(5)-C(8)	1.482(5)	N(5)-C(9)	1.505(5)
N(6)-C(10)	1.481(5)	N(6)-C(15)	1.483(5)
N(6)-C(11)	1.499(5)	C(1)-C(5)#1	1.439(5)
C(1)-C(2)	1.502(5)	C(3)-C(3)#1	1.452(7)
C(3)-C(4)	1.504(5)	C(5)-C(1)#1	1.439(5)
C(5)-C(6)	1.498(5)	C(7)-C(8)	1.478(6)
C(9)-C(10)	1.459(6)	C(11)-C(12)	1.480(6)
Cl-O(12)	1.359(5)	Cl-O(13)	1.395(4)
Cl-O(11)	1.408(4)	Cl-O(14)	1.420(4)

N(3)-Fe(1)-N(3)#1	160.5(2)	N(3)-Fe(1)-N(2)	89.34(12)
N(3)#1-Fe(1)-N(2)	105.86(12)	N(3)-Fe(1)-N(2)#1	105.86(12)
N(3)#1-Fe(1)-N(2)#1	89.34(12)	N(2)-Fe(1)-N(2)#1	78.6(2)
N(3)-Fe(1)-N(1)	89.94(12)	N(3)#1-Fe(1)-N(1)	78.68(12)
N(2)-Fe(1)-N(1)	88.21(12)	N(2)#1-Fe(1)-N(1)	159.13(12)
N(3)-Fe(1)-N(1)#1	78.68(11)	N(3)#1-Fe(1)-N(1)#1	89.94(12)
N(2)-Fe(1)-N(1)#1	159.13(12)	N(2)#1-Fe(1)-N(1)#1	88.21(12)
N(1)-Fe(1)-N(1)#1	108.6(2)	O(2)-Cr(1)-O(3)	95.60(10)
O(2)-Cr(1)-O(1)	93.41(11)	O(3)-Cr(1)-O(1)	94.20(10)
O(2)-Cr(1)-N(5)	171.10(11)	O(3)-Cr(1)-N(5)	92.10(11)
O(1)-Cr(1)-N(5)	90.46(11)	O(2)-Cr(1)-N(6)	89.12(11)
O(3)-Cr(1)-N(6)	169.84(11)	O(1)-Cr(1)-N(6)	94.49(11)
N(5)-Cr(1)-N(6)	82.58(12)	O(2)-Cr(1)-N(4)	93.03(12)
O(3)-Cr(1)-N(4)	88.36(11)	O(1)-Cr(1)-N(4)	172.80(11)
N(5)-Cr(1)-N(4)	82.72(12)	N(6)-Cr(1)-N(4)	82.40(12)
N(1)-O(1)-Cr(1)	115.3(2)	N(2)-O(2)-Cr(1)	114.9(2)
N(3)-O(3)-Cr(1)	116.4(2)	C(1)-N(1)-O(1)	117.1(3)
C(1)-N(1)-Fe(1)	117.4(2)	O(1)-N(1)-Fe(1)	124.8(2)
C(3)-N(2)-O(2)	116.4(3)	C(3)-N(2)-Fe(1)	118.0(2)
O(2)-N(2)-Fe(1)	125.2(2)	C(5)-N(3)-O(3)	116.6(3)
C(5)-N(3)-Fe(1)	118.1(2)	O(3)-N(3)-Fe(1)	125.0(2)
C(13)-N(4)-C(7)	110.2(3)	C(13)-N(4)-C(12)	108.2(3)
C(7)-N(4)-C(12)	111.6(3)	C(13)-N(4)-Cr(1)	112.8(2)
C(7)-N(4)-Cr(1)	109.5(2)	C(12)-N(4)-Cr(1)	104.5(2)
C(14)-N(5)-C(8)	109.2(3)	C(14)-N(5)-C(9)	110.0(3)
C(8)-N(5)-C(9)	111.0(3)	C(14)-N(5)-Cr(1)	113.2(2)
C(8)-N(5)-Cr(1)	104.2(2)	C(9)-N(5)-Cr(1)	109.1(2)
C(10)-N(6)-C(15)	109.3(3)	C(10)-N(6)-C(11)	111.7(3)
C(15)-N(6)-C(11)	109.1(3)	C(10)-N(6)-Cr(1)	104.2(2)
C(15)-N(6)-Cr(1)	112.7(2)	C(11)-N(6)-Cr(1)	109.8(2)
N(1)-C(1)-C(5)#1	113.1(3)	N(1)-C(1)-C(2)	124.6(3)
C(5)#1-C(1)-C(2)	122.2(3)	N(2)-C(3)-C(3)#1	112.7(2)
N(2)-C(3)-C(4)	124.8(4)	C(3)#1-C(3)-C(4)	122.5(2)
N(3)-C(5)-C(1)#1	112.5(3)	N(3)-C(5)-C(6)	123.9(3)
C(1)#1-C(5)-C(6)	123.6(3)	C(8)-C(7)-N(4)	112.3(3)
C(7)-C(8)-N(5)	112.5(3)	C(10)-C(9)-N(5)	112.3(3)
C(9)-C(10)-N(6)	112.6(3)	C(12)-C(11)-N(6)	112.2(3)
C(11)-C(12)-N(4)	111.7(3)	O(12)-Cl-O(13)	110.9(4)

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 2150.

The anisotropic displacement factor exponent takes the form:

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

	U11	U22	U33	U23	U13	U12
Fe(1)	26(1)	22(1)	24(1)	0	4(1)	0
Cr(1)	27(1)	29(1)	27(1)	-1(1)	4(1)	1(1)
O(1)	26(1)	35(1)	37(1)	6(1)	0(1)	-4(1)
O(2)	28(1)	37(1)	46(2)	-14(1)	7(1)	0(1)
O(3)	29(1)	43(1)	28(1)	3(1)	3(1)	7(1)
N(1)	27(1)	26(1)	33(2)	-1(1)	3(1)	-1(1)
N(2)	28(2)	29(2)	37(2)	-6(1)	5(1)	1(1)
N(3)	29(1)	29(2)	28(1)	4(1)	4(1)	2(1)
N(4)	35(2)	33(2)	34(2)	0(1)	4(1)	4(1)
N(5)	36(2)	31(2)	35(2)	-3(1)	0(1)	1(1)
N(6)	31(2)	49(2)	30(2)	-1(1)	6(1)	1(1)
C(1)	33(2)	33(2)	32(2)	6(2)	7(1)	-1(1)
C(2)	44(2)	60(3)	45(2)	18(2)	8(2)	-9(2)
C(3)	36(2)	27(2)	61(3)	-5(2)	2(2)	1(2)
C(4)	54(3)	31(2)	127(5)	-24(3)	5(3)	8(2)
C(5)	36(2)	39(2)	25(2)	-2(1)	4(1)	1(2)
C(6)	45(2)	74(3)	34(2)	-14(2)	-2(2)	11(2)
C(7)	64(3)	47(2)	39(2)	3(2)	-13(2)	6(2)
C(8)	63(3)	44(2)	39(2)	-4(2)	-14(2)	3(2)
C(9)	52(3)	52(3)	55(3)	-3(2)	9(2)	-18(2)
C(10)	52(3)	56(3)	55(3)	6(2)	24(2)	-10(2)
C(11)	49(2)	54(3)	51(3)	-5(2)	16(2)	14(2)
C(12)	57(3)	49(3)	52(3)	-1(2)	13(2)	21(2)
C(13)	56(3)	44(2)	69(3)	21(2)	8(2)	3(2)
C(14)	59(3)	34(2)	76(3)	-16(2)	-11(2)	8(2)
C(15)	48(2)	106(4)	27(2)	-5(2)	5(2)	2(3)
Cl	63(1)	51(1)	54(1)	-3(1)	-5(1)	5(1)
O(11)	116(3)	89(3)	89(3)	-39(2)	4(3)	20(3)
O(12)	49(3)	219(7)	182(6)	-6(5)	-14(3)	-2(3)
O(13)	218(6)	76(3)	76(3)	31(2)	-3(3)	-7(3)
O(14)	98(3)	67(2)	50(2)	-2(2)	-7(2)	8(2)
O(20)	79(6)	324(20)	64(5)	-12(8)	6(5)	17(8)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 2150.

	x	y	z	U(eq)
H(2A)	823(1)	2994(5)	1003(2)	74
H(2B)	405(1)	3717(5)	542(2)	74
H(2C)	587(1)	2174(5)	248(2)	74
H(4A)	759(2)	-4053(5)	2171(4)	107
H(4B)	323(2)	-4879(5)	1862(4)	107
H(4C)	489(2)	-4889(5)	2778(4)	107
H(6A)	680(1)	1401(6)	4903(2)	77
H(6B)	232(1)	1453(6)	5256(2)	77
H(6C)	417(1)	2929(6)	4892(2)	77
H(7A)	1881(2)	-1178(5)	4573(3)	61
H(7B)	2135(2)	-645(5)	3864(3)	61
H(8A)	1972(2)	1507(5)	4460(2)	60
H(8B)	1498(2)	964(5)	4557(2)	60
H(9A)	1994(1)	3132(5)	2959(3)	64
H(9B)	2187(1)	1514(5)	3175(3)	64
H(10A)	2090(2)	1543(5)	1855(3)	64
H(10B)	1632(2)	2319(5)	1837(3)	64
H(11A)	1996(1)	-1754(5)	1833(3)	61
H(11B)	2196(1)	-754(5)	2555(3)	61
H(12A)	1987(2)	-2882(5)	3125(3)	63
H(12B)	1545(2)	-2945(5)	2571(3)	63
H(13A)	1081(1)	-3096(5)	3539(3)	84
H(13B)	1134(1)	-2069(5)	4306(3)	84
H(13C)	1484(1)	-3310(5)	4180(3)	84
H(14A)	1251(2)	3698(5)	3149(3)	86
H(14B)	1563(2)	3818(5)	3946(3)	86
H(14C)	1116(2)	2976(5)	3939(3)	86
H(15A)	1297(2)	-1186(7)	1155(2)	91
H(15B)	1665(2)	-164(7)	864(2)	91
H(15C)	1223(2)	572(7)	1041(2)	91