Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Methanetrisamidines in Coordination Chemistry - Syntheses, Structures and CH-NH Tautomerism

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Crystallographic Data for

{$[C(C(NH\textit{i}\text{-}Pr)_2)_3]^{2+}[NiCl_4]^{2-}$} **2**

$[C(C(N(\textit{i}\text{-}Pr)CuCl)NH\textit{i}\text{-}Pr)_2(C(NH\textit{i}\text{-}Pr)_2)]$ **3**

fac-$[Cr(CO)_3CH(C(NHPh)NPh)_3]$ **4a**.

$\{[C(C(NHi\text{-}Pr)_2)_3]^{2+}[NiCl_4]^{2-}\}$ **2**

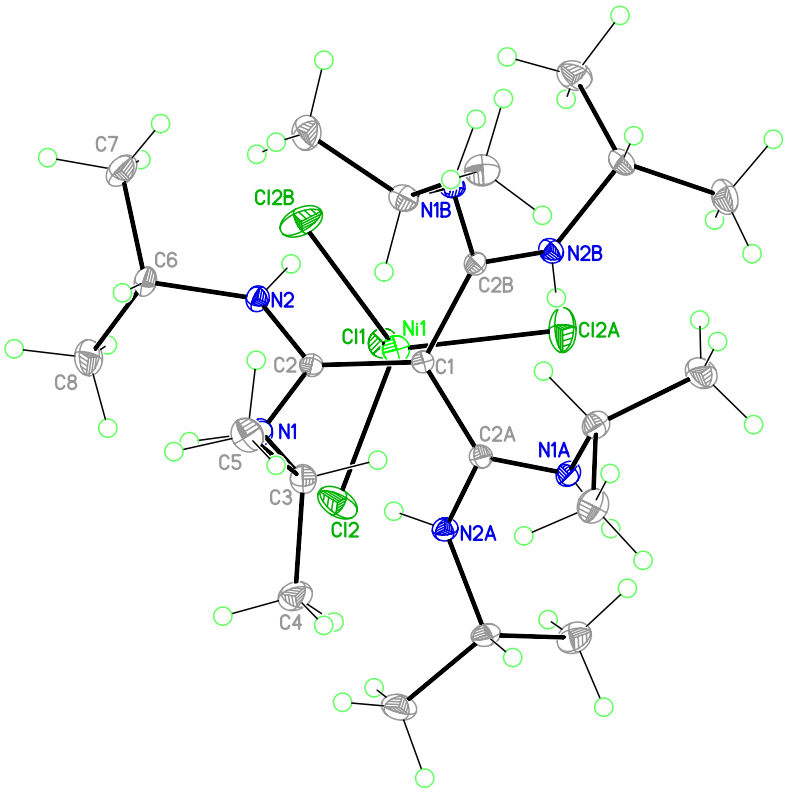


Table 1: Crystal structure data

Identification code	**bg_144m**
Empirical formula	$C_{22}H_{48}Cl_4N_6Ni$
Formula weight	597.17
Density (calculated)	1.236 $g \cdot cm^{-1}$
$F(000)$	2544
Temperature	100(1) K
Crystal size	0.18 × 0.16 × 0.12 mm
Crystal colour	pale blue
Crystal description	block
Wavelength	0.71073 Å
Crystal system	cubic
Space group	*Pa*-3
Unit cell dimensions	
a [Å]	18.5823(18)
b [Å]	18.5823(18)
c [Å]	18.5823(18)
α [°]	90
β [°]	90
γ [°]	90
Volume	6416.5(11) $Å^3$
Z	8
Cell measurement reflections used	9782
Cell measurement θ min/max	2.19°/29.18°
Diffractometer control software	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Diffractometer measurement device	Bruker D8 KAPPA series II with APEX II area detector system
Diffractometer measurement method	Data collection strategy APEX 2/COSMO
θ range for data collection	1.90°- 29.48°
Completeness to θ = 29.48°	99.0%
Index ranges	$-25 \le h \le 25$
	$-25 \le k \le 24$
	$-22 \le l \le 17$
Computing data reduction	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Absorption coefficient	0.958 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Computation absorption correction	BRUKER AXS SMART APEX 2 Vers. 3.0-

	2009
Max./min. Transmission	0.75/0.64
R_{merg} before/after correction	0.0524/ 0.0427
Computing structure solution	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Computing structure refinement	BRUKER AXS SHELXTL (c) 2008 / Vers. 2008/4
Refinement method	Full-matrix least-squares on F^2
Reflections collected	40041
Independent reflections	2961
R_{int}	0.0506
Data	2258
Restraints	0
Parameter	100
GooF	1.137
Weighting details	$w = 1/[\sigma^2(F_{obs}^2) + (0.0285P)^2 + 3.5033P]$ where $P = (F_{obs}^2 + 2F_{calc}^2)/3$
R_1 [$I > 2\sigma(I)$]	0.0296
wR_2 [$I > 2\sigma(I)$]	0.0665
R_1 [all data]	0.0534
wR_2 [all data]	0.0813
Largest diff. peak and hole	0.387/-0.255

Table 2: Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for bg_144m. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	U_{eq}
Ni(1)	7955(1)	2955(1)	2045(1)	23(1)
Cl(1)	8649(1)	3649(1)	1351(1)	26(1)
Cl(2)	8639(1)	2137(1)	2641(1)	37(1)
N(1)	6876(1)	243(1)	3336(1)	19(1)
H(1)	7121	-74	3006	22
N(2)	6653(1)	965(1)	2344(1)	18(1)
H(2)	6645	1450	2137	22
C(1)	6487(1)	1487(1)	3513(1)	15(1)
C(2)	6681(1)	882(1)	3059(1)	16(1)
C(3)	6668(1)	-29(1)	4053(1)	22(1)
H(3)	6415	366	4316	26
C(4)	7328(1)	-247(1)	4490(1)	32(1)
H(4A)	7590	-628	4234	48
H(4B)	7175	-426	4962	48
H(4C)	7643	171	4553	48
C(5)	6143(1)	-658(1)	3964(1)	29(1)
H(5A)	5718	-496	3698	44
H(5B)	5997	-834	4440	44
H(5C)	6379	-1048	3698	44
C(6)	6733(1)	384(1)	1806(1)	21(1)
H(6)	6535	-71	2013	26
C(7)	6302(1)	576(1)	1134(1)	30(1)
H(7A)	5800	664	1266	46
H(7B)	6327	178	789	46
H(7C)	6505	1011	913	46
C(8)	7528(1)	268(1)	1625(1)	31(1)
H(8A)	7722	702	1396	47
H(8B)	7576	-141	1296	47
H(8C)	7796	169	2069	47

Table 3: Anisotropic displacement parameters ($Å^2 \times 10^3$) for bg_144m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ni(1)	23(1)	23(1)	23(1)	-1(1)	-1(1)	1(1)
Cl(1)	26(1)	26(1)	26(1)	0(1)	0(1)	0(1)
Cl(2)	31(1)	48(1)	32(1)	16(1)	11(1)	16(1)
N(1)	23(1)	17(1)	16(1)	0(1)	1(1)	3(1)
N(2)	22(1)	17(1)	15(1)	-1(1)	1(1)	0(1)
C(1)	15(1)	15(1)	15(1)	-1(1)	-1(1)	1(1)
C(2)	12(1)	17(1)	17(1)	-1(1)	1(1)	-1(1)
C(3)	29(1)	19(1)	18(1)	2(1)	2(1)	2(1)
C(4)	42(1)	29(1)	24(1)	4(1)	-10(1)	1(1)
C(5)	32(1)	23(1)	32(1)	5(1)	4(1)	-1(1)
C(6)	26(1)	21(1)	17(1)	-4(1)	2(1)	0(1)
C(7)	40(1)	33(1)	19(1)	-3(1)	-5(1)	-2(1)
C(8)	31(1)	35(1)	27(1)	-5(1)	9(1)	3(1)

Table 4: Bond lengths [Å] for bg_144m.

Ni(1)-Cl(1)	2.2345(8)	N(1)-C(3)	1.4764(19)	C(1)-C(2)#1	1.4508(14)
Ni(1)-Cl(2)#1	2.2696(5)	N(2)-C(2)	1.3386(18)	C(3)-C(4)	1.526(2)
Ni(1)-Cl(2)#2	2.2696(5)	N(2)-C(6)	1.4780(19)	C(3)-C(5)	1.532(2)
Ni(1)-Cl(2)	2.2696(5)	C(1)-C(2)	1.4508(14)	C(6)-C(7)	1.526(2)
N(1)-C(2)	1.3449(19)	C(1)-C(2)#2	1.4508(14)	C(6)-C(8)	1.530(2)

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

Table 5: Bond angles [°] for bg_144m.

Cl(1)-Ni(1)-Cl(2)#1	110.194(14)	C(2)#2-C(1)-C(2)#1	119.892(12)
Cl(1)-Ni(1)-Cl(2)#2	110.194(14)	N(2)-C(2)-N(1)	119.42(13)
Cl(2)#1-Ni(1)-Cl(2)#2	108.739(14)	N(2)-C(2)-C(1)	118.68(13)
Cl(1)-Ni(1)-Cl(2)	110.195(14)	N(1)-C(2)-C(1)	121.89(13)
Cl(2)#1-Ni(1)-Cl(2)	108.737(14)	N(1)-C(3)-C(4)	111.15(13)
Cl(2)#2-Ni(1)-Cl(2)	108.740(14)	N(1)-C(3)-C(5)	109.31(13)
C(2)-N(1)-C(3)	125.26(12)	C(4)-C(3)-C(5)	111.48(13)
C(2)-N(2)-C(6)	125.75(13)	N(2)-C(6)-C(7)	109.30(13)
C(2)-C(1)-C(2)#2	119.893(12)	N(2)-C(6)-C(8)	110.36(13)
C(2)-C(1)-C(2)#1	119.892(12)	C(7)-C(6)-C(8)	111.11(14)

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

[C(C(N(*i*-Pr)CuCl)NH*i*-Pr)$_2$(C(NH*i*-Pr)$_2$)] **3**

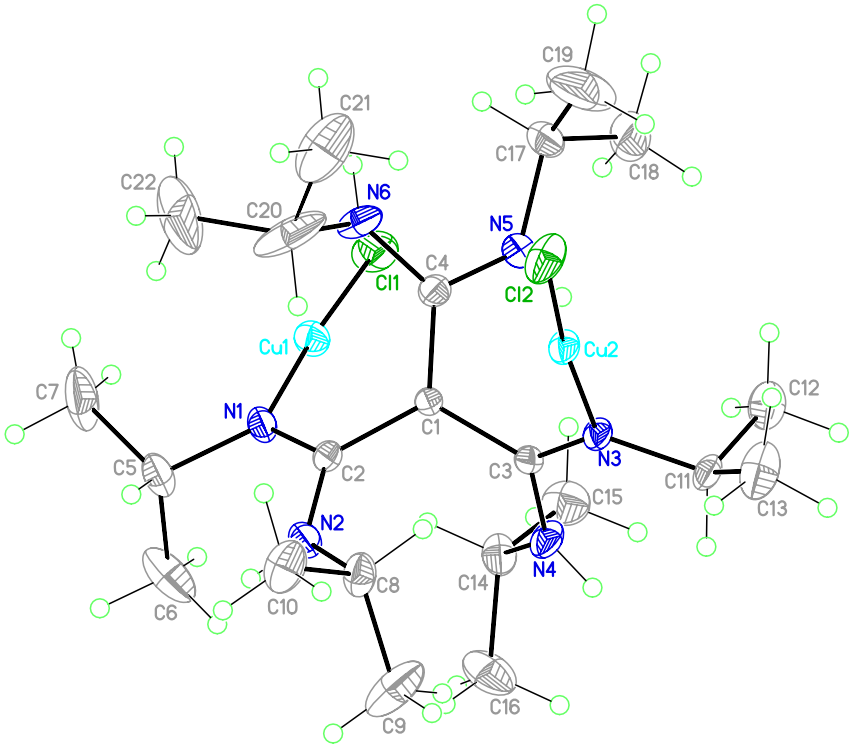


Table 1: Crystal structure data

Identification code	**bg_185m**
Empirical formula	$C_{26}H_{54}Cl_2Cu_2N_6O$
Formula weight	664.73
Density (calculated)	1.257 $g \cdot cm^{-1}$
$F(000)$	1408
Temperature	100(1) K
Crystal size	0.32 × 0.23 × 0.17 mm
Crystal colour	colourless
Crystal description	block
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	$P2_1/n$
Unit cell dimensions	
a [Å]	9.8688(3)
b [Å]	25.3571(7)
c [Å]	14.0716(4)
α [°]	90
β [°]	94.1590(10)
γ [°]	90
Volume	3512.06(18) $Å^3$
Z	4
Cell measurement reflections used	23976
Cell measurement θ min/max	2.22°/28.73°
Diffractometer control software	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Diffractometer measurement device	Bruker D8 KAPPA series II with APEX II area detector system
Diffractometer measurement method	Data collection strategy APEX 2/COSMO
θ range for data collection	1.61°- 28.73°
Completeness to θ = 27.00°	98.3%
Index ranges	$-13 \leq h \leq 13$
	$0 \leq k \leq 34$
	$0 \leq l \leq 18$
Computing data reduction	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Absorption coefficient	1.389 mm^{-1}

Absorption correction	Semi-empirical from equivalents
Computation absorption correction	BRUKER AXS SMART APEX 2 Vers. 3.0-2009
Max./min. Transmission	0.75/0.60
R_{merg} before/after correction	0.0565/ 0.0376
Computing structure solution	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Computing structure refinement	BRUKER AXS SHELXTL (c) 2008 / Vers. 2008/4
Refinement method	Full-matrix least-squares on F^2
Reflections collected	52732
Independent reflections	8868
R_{int}	0.0312
Data	7207
Restraints	0
Parameter	309
GooF	1.083
Weighting details	$w = 1/[\sigma^2(F_{obs}^2) + (0.0972P)^2 + 3.0578P]$
	where $P = (F_{obs}^2 + 2F_{calc}^2)/3$
R_1 [$I > 2\sigma(I)$]	0.0497
wR_2 [$I > 2\sigma(I)$]	0.1475
R_1 [all data]	0.0625
wR_2 [all data]	0.1560
Largest diff. peak and hole	1.442/-0.883

Table 2: Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for bg_185m. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	U_{eq}
Cu(1)	4776(1)	509(1)	6834(1)	22(1)
Cu(2)	6485(1)	2444(1)	4891(1)	19(1)
Cl(1)	5980(1)	-163(1)	6679(1)	34(1)
Cl(2)	5724(1)	2772(1)	3588(1)	32(1)
N(1)	3787(2)	1134(1)	7037(2)	20(1)
N(2)	3866(2)	2042(1)	7276(2)	22(1)
H(2)	3280	1997	7712	26
N(3)	7345(2)	2228(1)	6065(2)	18(1)
N(4)	7261(2)	1856(1)	7570(2)	24(1)
H(4)	7768	2115	7812	29
N(5)	6838(2)	1055(1)	5383(2)	28(1)
H(5)	7491	1107	5834	33
N(6)	4565(2)	1144(1)	4921(2)	26(1)
H(6)	4593	830	4657	31
C(1)	5525(2)	1628(1)	6313(2)	16(1)
C(2)	4338(2)	1597(1)	6886(2)	16(1)
C(3)	6764(2)	1914(1)	6656(2)	16(1)
C(4)	5621(3)	1281(1)	5524(2)	19(1)
C(5)	2562(3)	1098(1)	7570(2)	26(1)
H(5A)	1975	1412	7418	31
C(6)	2967(4)	1092(2)	8640(3)	43(1)
H(6A)	3558	789	8794	64
H(6B)	2149	1065	8993	64
H(6C)	3452	1418	8820	64
C(7)	1776(4)	602(1)	7278(4)	52(1)
H(7A)	1452	626	6605	78
H(7B)	998	565	7668	78
H(7C)	2372	294	7373	78
C(8)	4211(3)	2588(1)	7062(2)	26(1)
H(8)	4931	2594	6598	31
C(9)	4740(4)	2859(1)	7987(3)	50(1)
H(9A)	4034	2852	8442	75
H(9B)	4978	3225	7853	75

H(9C)	5547	2672	8259	75
C(10)	2946(3)	2874(1)	6633(3)	34(1)
H(10A)	2621	2702	6037	51
H(10B)	3174	3243	6504	51
H(10C)	2234	2863	7083	51
C(11)	8745(3)	2418(1)	6304(2)	21(1)
H(11)	8852	2499	7001	25
C(12)	9740(3)	1991(1)	6090(3)	36(1)
H(12A)	9545	1673	6450	54
H(12B)	10666	2111	6273	54
H(12C)	9655	1912	5406	54
C(13)	9003(3)	2922(1)	5751(3)	40(1)
H(13A)	9047	2838	5074	61
H(13B)	9865	3080	5997	61
H(13C)	8261	3173	5826	61
C(14)	7054(3)	1408(1)	8206(2)	25(1)
H(14)	6156	1241	8020	30
C(15)	8167(3)	1002(1)	8135(2)	35(1)
H(15A)	8129	860	7486	52
H(15B)	8038	715	8586	52
H(15C)	9053	1168	8286	52
C(16)	7039(4)	1622(2)	9217(2)	39(1)
H(16A)	7912	1791	9399	59
H(16B)	6889	1332	9656	59
H(16C)	6307	1882	9244	59
C(17)	7192(3)	735(1)	4569(3)	37(1)
H(17)	6484	456	4449	44
C(18)	8545(4)	470(2)	4863(4)	64(2)
H(18A)	9237	739	5015	97
H(18B)	8822	250	4337	97
H(18C)	8444	248	5424	97
C(19)	7249(6)	1065(2)	3680(3)	70(2)
H(19A)	6367	1235	3533	105
H(19B)	7464	839	3147	105
H(19C)	7954	1336	3784	105

C(20)	3379(4)	1466(2)	4665(3)	58(1)
H(20)	3389	1788	5077	69
C(21)	3483(5)	1629(2)	3590(4)	58(1)
H(21A)	4323	1829	3529	88
H(21B)	2701	1849	3380	88
H(21C)	3490	1312	3194	88
C(22)	2117(4)	1172(3)	4747(4)	72(2)
H(22A)	2145	844	4381	107
H(22B)	1345	1387	4498	107
H(22C)	2015	1089	5418	107
O(1)	9428(6)	-590(2)	7802(4)	105(2)
C(31)	10766(5)	-649(2)	8027(3)	54(1)
H(31A)	11301	-381	7706	65
H(31B)	11079	-1005	7856	65
C(32)	10854(8)	-578(3)	8987(5)	94(2)
H(32A)	10814	-197	9137	113
H(32B)	11728	-719	9268	113
C(33)	9670(6)	-866(2)	9406(4)	75(1)
H(33A)	9954	-1211	9684	90
H(33B)	9250	-651	9892	90
C(34)	8726(6)	-931(2)	8502(4)	75(1)
H(34A)	8673	-1303	8292	90
H(34B)	7800	-800	8596	90

Table 3: Anisotropic displacement parameters ($Å^2 \times 10^3$) for bg_185m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu(1)	21(1)	20(1)	25(1)	-3(1)	4(1)	2(1)
Cu(2)	16(1)	26(1)	14(1)	3(1)	-2(1)	-2(1)
Cl(1)	31(1)	28(1)	41(1)	-11(1)	-3(1)	7(1)
Cl(2)	30(1)	39(1)	26(1)	14(1)	-10(1)	-11(1)
N(1)	16(1)	20(1)	23(1)	-1(1)	6(1)	0(1)
N(2)	21(1)	20(1)	26(1)	-2(1)	8(1)	-1(1)
N(3)	14(1)	26(1)	14(1)	1(1)	-2(1)	-3(1)
N(4)	21(1)	35(1)	15(1)	3(1)	-4(1)	-10(1)
N(5)	20(1)	37(1)	27(1)	-11(1)	6(1)	-3(1)
N(6)	29(1)	23(1)	24(1)	-8(1)	-9(1)	2(1)
C(1)	13(1)	22(1)	12(1)	-2(1)	1(1)	-1(1)
C(2)	13(1)	20(1)	15(1)	-1(1)	-1(1)	0(1)
C(3)	13(1)	22(1)	14(1)	-3(1)	1(1)	0(1)
C(4)	20(1)	21(1)	15(1)	1(1)	2(1)	-4(1)
C(5)	22(1)	22(1)	37(2)	0(1)	14(1)	0(1)
C(6)	46(2)	49(2)	36(2)	15(2)	22(2)	19(2)
C(7)	31(2)	31(2)	97(3)	-10(2)	33(2)	-11(1)
C(8)	18(1)	18(1)	40(2)	-1(1)	4(1)	-1(1)
C(9)	48(2)	27(2)	70(3)	-10(2)	-29(2)	0(1)
C(10)	28(1)	28(2)	44(2)	7(1)	-7(1)	0(1)
C(11)	15(1)	27(1)	19(1)	0(1)	-3(1)	-7(1)
C(12)	21(1)	44(2)	41(2)	-4(1)	-1(1)	-1(1)
C(13)	29(2)	43(2)	48(2)	11(2)	-4(1)	-10(1)
C(14)	20(1)	38(2)	18(1)	8(1)	0(1)	-2(1)
C(15)	37(2)	36(2)	31(2)	1(1)	-1(1)	4(1)
C(16)	46(2)	52(2)	20(2)	7(1)	9(1)	12(2)
C(17)	32(2)	40(2)	41(2)	-21(1)	19(1)	-12(1)
C(18)	26(2)	71(3)	97(4)	-54(3)	17(2)	-4(2)
C(19)	108(4)	63(3)	45(3)	-16(2)	47(3)	-24(3)
C(20)	58(2)	38(2)	68(3)	-31(2)	-49(2)	27(2)
C(21)	51(2)	42(2)	78(3)	13(2)	-26(2)	-4(2)
C(22)	21(2)	120(4)	74(3)	21(3)	8(2)	24(2)

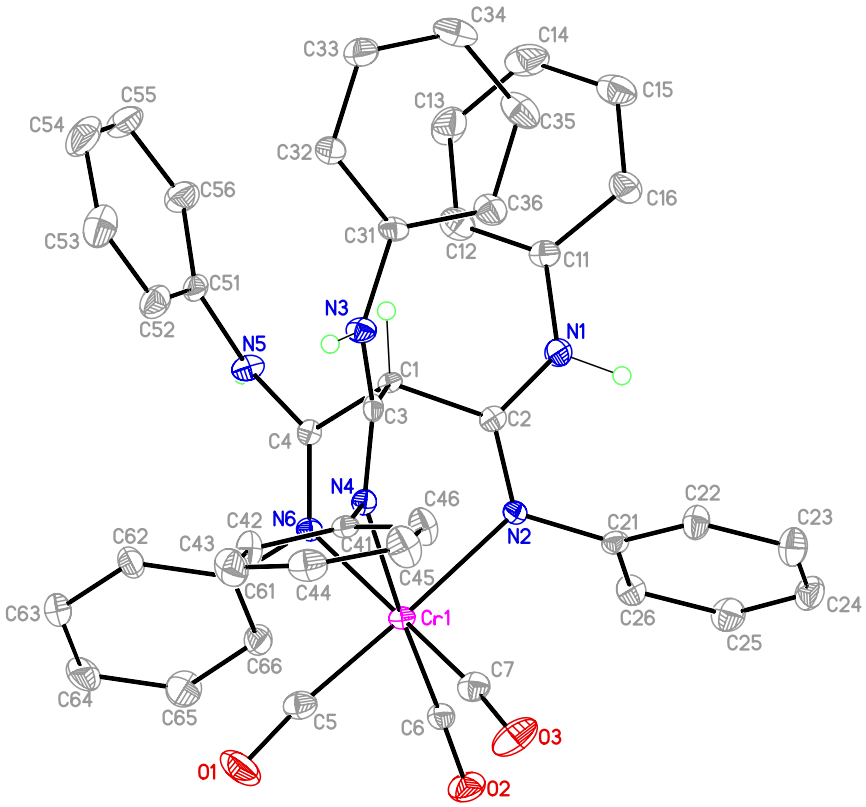
Table 4: Bond lengths [Å] for bg_185m.

Cu(1)-N(1)	1.894(2)	N(5)-C(4)	1.359(3)	C(11)-C(13)	1.527(4)
Cu(1)-Cl(1)	2.0993(8)	N(5)-C(17)	1.466(4)	C(14)-C(15)	1.514(4)
Cu(2)-N(3)	1.882(2)	N(6)-C(4)	1.342(3)	C(14)-C(16)	1.523(4)
Cu(2)-Cl(2)	2.1025(7)	N(6)-C(20)	1.451(4)	C(17)-C(19)	1.509(6)
N(1)-C(2)	1.317(3)	C(1)-C(4)	1.424(4)	C(17)-C(18)	1.526(6)
N(1)-C(5)	1.472(3)	C(1)-C(2)	1.472(3)	C(20)-C(22)	1.463(7)
N(2)-C(2)	1.352(3)	C(1)-C(3)	1.473(3)	C(20)-C(21)	1.579(7)
N(2)-C(8)	1.463(3)	C(5)-C(7)	1.519(4)	O(1)-C(31)	1.343(7)
N(3)-C(3)	1.314(3)	C(5)-C(6)	1.529(5)	O(1)-C(34)	1.515(8)
N(3)-C(11)	1.479(3)	C(8)-C(9)	1.529(5)	C(31)-C(32)	1.359(9)
N(4)-C(3)	1.350(3)	C(8)-C(10)	1.529(4)	C(32)-C(33)	1.531(9)
N(4)-C(14)	1.470(4)	C(11)-C(12)	1.506(4)	C(33)-C(34)	1.530(8)

Table 5: Bond angles [°] for bg_185m.

N(1)-Cu(1)-Cl(1)	175.95(7)	N(1)-C(5)-C(7)	109.6(2)
N(3)-Cu(2)-Cl(2)	171.92(7)	N(1)-C(5)-C(6)	109.7(2)
C(2)-N(1)-C(5)	120.1(2)	C(7)-C(5)-C(6)	110.5(3)
C(2)-N(1)-Cu(1)	119.89(17)	N(2)-C(8)-C(9)	108.6(3)
C(5)-N(1)-Cu(1)	118.39(17)	N(2)-C(8)-C(10)	109.6(2)
C(2)-N(2)-C(8)	127.9(2)	C(9)-C(8)-C(10)	110.0(3)
C(3)-N(3)-C(11)	119.8(2)	N(3)-C(11)-C(12)	109.4(2)
C(3)-N(3)-Cu(2)	122.84(17)	N(3)-C(11)-C(13)	110.1(2)
C(11)-N(3)-Cu(2)	117.37(17)	C(12)-C(11)-C(13)	111.4(3)
C(3)-N(4)-C(14)	127.4(2)	N(4)-C(14)-C(15)	110.6(2)
C(4)-N(5)-C(17)	127.6(3)	N(4)-C(14)-C(16)	107.7(3)
C(4)-N(6)-C(20)	125.8(2)	C(15)-C(14)-C(16)	111.2(3)
C(4)-C(1)-C(2)	119.7(2)	N(5)-C(17)-C(19)	111.5(3)
C(4)-C(1)-C(3)	117.4(2)	N(5)-C(17)-C(18)	106.6(3)
C(2)-C(1)-C(3)	121.4(2)	C(19)-C(17)-C(18)	112.6(4)
N(1)-C(2)-N(2)	121.3(2)	N(6)-C(20)-C(22)	111.6(4)
N(1)-C(2)-C(1)	119.3(2)	N(6)-C(20)-C(21)	106.1(4)
N(2)-C(2)-C(1)	119.3(2)	C(22)-C(20)-C(21)	108.9(3)
N(3)-C(3)-N(4)	121.6(2)	C(31)-O(1)-C(34)	105.7(5)
N(3)-C(3)-C(1)	118.8(2)	O(1)-C(31)-C(32)	102.1(5)
N(4)-C(3)-C(1)	119.6(2)	C(31)-C(32)-C(33)	108.9(6)
N(6)-C(4)-N(5)	116.9(2)	C(34)-C(33)-C(32)	99.6(5)
N(6)-C(4)-C(1)	124.2(2)	O(1)-C(34)-C(33)	101.5(5)
N(5)-C(4)-C(1)	118.9(2)		

fac-[Cr(CO)$_3$CH(C(NHPh)NPh)$_3$] **4a**.



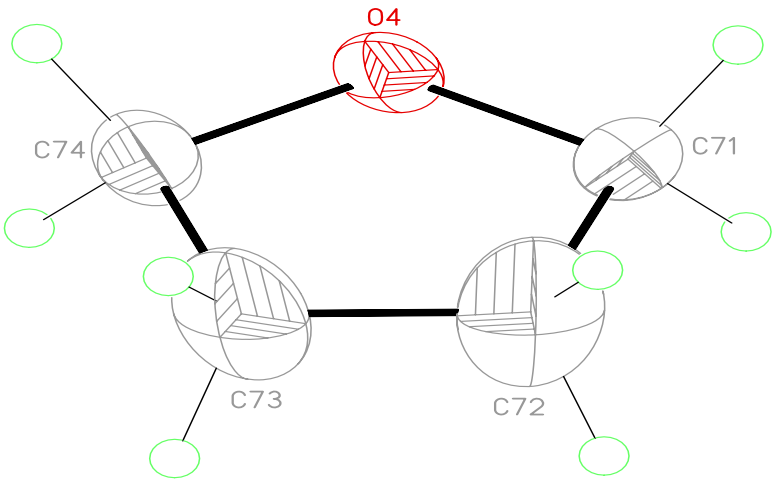


Table 1: Crystal structure data

Identification code	**bg_213x**
Empirical formula	$C_{47}H_{42}CrN_6O_4$
Formula weight	806.86
Density (calculated)	1.316 g · cm^{-1}
F(000)	1688
Temperature	180(1) K
Crystal size	0.150 × 0.120 × 0.030 mm
Crystal colour	orange
Crystal description	plate
Wavelength	0.71073 Å
Crystal system	orthorhombic
Space group	$Pna2_1$
Unit cell dimensions	
a [Å]	24.6646(14)
b [Å]	14.2926(7)
c [Å]	11.5541(7)
α [°]	90
β [°]	90
γ [°]	90
Volume	4073.1(4) $Å^3$
Z	4
Cell measurement reflections used	6062
Cell measurement *θ* min/max	2.42°/24.73°
Diffractometer control software	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Diffractometer measurement device	Bruker D8 KAPPA series II with APEX II area detector system
Diffractometer measurement method	Data collection strategy APEX 2/COSMO
θ range for data collection	1.651°- 27.169°
Completeness to *θ* = 25.242°	99.5%
Index ranges	$-31 \leq h \leq 31$
	$-18 \leq k \leq 12$
	$-14 \leq l \leq 14$
Computing data reduction	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Absorption coefficient	0.333 mm^{-1}

Absorption correction	Semi-empirical from equivalents
Computation absorption correction	BRUKER AXS SMART APEX 2 Vers. 3.0-2009
Max./min. Transmission	0.75/0.66
R_{merg} before/after correction	0.0672/ 0.0615
Computing structure solution	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Computing structure refinement	SHELXL-2013 (Sheldrick, 2013)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	32293
Independent reflections	8839
R_{int}	0.0607
Data	6082
Restraints	1
Parameter	523
GooF	0.999
Weighting details	$w = 1/[\sigma^2(F_{obs}^2) + (0.0401P)^2]$
	where $P = (F_{obs}^2 + 2F_{calc}^2)/3$
R_1 [$I > 2\sigma(I)$]	0.0441
wR_2 [$I > 2\sigma(I)$]	0.0826
R_1 [all data]	0.0859
wR_2 [all data]	0.0949
Absolute structure parameter	0.015(12)
Largest diff. peak and hole	0.305/-0.355

Table 2: Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for bg_213x. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	U_{eq}
Cr(1)	2522(1)	5727(1)	266(1)	18(1)
N(1)	3652(1)	7459(2)	2158(3)	29(1)
H(1)	3531	7392	2887	35
N(2)	2929(1)	6504(2)	1587(3)	18(1)
N(3)	2878(1)	8541(2)	-882(3)	23(1)
H(3)	2623	8680	-1412	27
N(4)	2500(1)	7051(2)	-584(3)	19(1)
N(5)	4101(1)	6500(2)	-1095(3)	22(1)
H(5)	4364	6087	-926	26
N(6)	3320(1)	5674(2)	-470(3)	18(1)
O(1)	2023(1)	4519(2)	-1554(3)	50(1)
O(2)	2464(1)	3913(2)	1548(3)	36(1)
O(3)	1371(1)	5888(2)	1055(3)	48(1)
C(1)	3411(1)	7297(2)	70(3)	17(1)
H(1A)	3684	7774	11	21
C(2)	3325(2)	7065(3)	1336(4)	19(1)
C(3)	2888(2)	7651(3)	-473(3)	18(1)
C(4)	3607(2)	6424(3)	-557(3)	18(1)
C(5)	2230(2)	5022(3)	-887(4)	28(1)
C(6)	2518(2)	4634(3)	1054(4)	23(1)
C(7)	1826(2)	5861(3)	775(4)	27(1)
C(11)	4145(2)	7961(3)	2071(4)	24(1)
C(12)	4538(2)	7751(3)	1259(4)	33(1)
H(12)	4485	7248	734	40
C(13)	5009(2)	8274(4)	1220(4)	42(1)
H(13)	5269	8148	635	50
C(14)	5102(2)	8965(4)	2002(5)	44(1)
H(14)	5430	9314	1966	53
C(15)	4723(2)	9158(3)	2852(4)	41(1)
H(15)	4790	9635	3405	49
C(16)	4241(2)	8658(3)	2885(4)	32(1)
H(16)	3980	8786	3468	38
C(21)	2844(2)	6337(3)	2801(4)	21(1)

C(22)	2559(2)	6983(3)	3460(4)	29(1)
H(22)	2406	7520	3104	35
C(23)	2502(2)	6844(3)	4638(4)	36(1)
H(23)	2309	7290	5088	43
C(24)	2716(2)	6059(3)	5164(4)	34(1)
H(24)	2680	5971	5975	40
C(25)	2988(2)	5414(3)	4496(4)	34(1)
H(25)	3127	4865	4851	40
C(26)	3057(2)	5539(3)	3324(4)	25(1)
H(26)	3249	5090	2879	30
C(31)	3233(2)	9279(3)	-546(4)	21(1)
C(32)	3455(2)	9855(3)	-1373(4)	29(1)
H(32)	3373	9755	-2165	35
C(33)	3792(2)	10578(3)	-1059(4)	36(1)
H(33)	3934	10987	-1631	43
C(34)	3919(2)	10712(3)	92(5)	40(1)
H(34)	4172	11182	305	48
C(35)	3687(2)	10158(3)	930(5)	39(1)
H(35)	3766	10268	1723	46
C(36)	3335(2)	9442(3)	618(4)	30(1)
H(36)	3167	9068	1195	36
C(41)	2011(2)	7368(3)	-1125(4)	19(1)
C(42)	1911(2)	7167(3)	-2270(4)	32(1)
H(42)	2156	6789	-2698	39
C(43)	1454(2)	7518(3)	-2795(4)	38(1)
H(43)	1390	7379	-3587	46
C(44)	1087(2)	8058(3)	-2199(4)	34(1)
H(44)	780	8310	-2585	40
C(45)	1175(2)	8226(3)	-1050(5)	39(1)
H(45)	917	8574	-617	47
C(46)	1638(2)	7892(3)	-512(4)	32(1)
H(46)	1700	8027	281	38
C(51)	4208(2)	7244(3)	-1894(4)	23(1)
C(52)	3814(2)	7549(3)	-2647(4)	32(1)
H(52)	3462	7281	-2612	39

C(53)	3926(2)	8233(3)	-3457(5)	43(1)
H(53)	3651	8460	-3958	51
C(54)	4444(2)	8601(3)	-3529(5)	53(2)
H(54)	4530	9047	-4109	64
C(55)	4838(2)	8301(4)	-2770(5)	52(2)
H(55)	5191	8567	-2807	62
C(56)	4721(2)	7630(3)	-1938(4)	37(1)
H(56)	4991	7429	-1405	45
C(61)	3494(2)	4855(3)	-1082(4)	21(1)
C(62)	3557(2)	4872(3)	-2276(4)	28(1)
H(62)	3486	5429	-2697	34
C(63)	3718(2)	4074(3)	-2851(4)	35(1)
H(63)	3770	4094	-3665	42
C(64)	3809(2)	3246(4)	-2261(5)	39(1)
H(64)	3914	2697	-2666	47
C(65)	3740(2)	3234(3)	-1081(5)	40(1)
H(65)	3801	2669	-668	47
C(66)	3591(2)	4036(3)	-487(4)	29(1)
H(66)	3550	4019	330	35
O(4)	4990(1)	5146(2)	-922(3)	48(1)
C(71)	4982(2)	5001(4)	288(5)	54(1)
H(71A)	5183	5504	689	65
H(71B)	4605	4993	577	65
C(72)	5240(4)	4099(5)	495(7)	135(4)
H(72A)	4985	3672	892	162
H(72B)	5562	4180	997	162
C(73)	5388(4)	3701(5)	-559(7)	100(3)
H(73A)	5786	3615	-579	120
H(73B)	5213	3084	-667	120
C(74)	5222(2)	4358(4)	-1481(6)	61(2)
H(74A)	4954	4056	-1997	73
H(74B)	5537	4556	-1950	73

Table 3: Anisotropic displacement parameters ($Å^2 \times 10^3$) for bg_213x. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cr(1)	19(1)	16(1)	21(1)	2(1)	0(1)	-2(1)
N(1)	31(2)	39(2)	18(2)	0(2)	-4(2)	-14(2)
N(2)	20(2)	16(2)	18(2)	-1(1)	0(1)	-1(1)
N(3)	26(2)	18(2)	24(2)	5(2)	-5(2)	-2(2)
N(4)	17(2)	21(2)	18(2)	0(1)	0(2)	0(2)
N(5)	16(2)	17(2)	33(2)	5(2)	2(2)	4(1)
N(6)	22(2)	13(2)	20(2)	1(2)	0(2)	0(1)
O(1)	58(2)	45(2)	47(2)	-15(2)	-17(2)	-16(2)
O(2)	44(2)	24(2)	40(2)	10(2)	4(2)	-3(2)
O(3)	21(2)	63(2)	59(2)	20(2)	11(2)	0(2)
C(1)	18(2)	16(2)	18(2)	1(2)	3(2)	-4(2)
C(2)	18(2)	17(2)	22(2)	2(2)	1(2)	3(2)
C(3)	24(2)	18(2)	13(2)	-1(2)	3(2)	3(2)
C(4)	17(2)	18(2)	18(2)	1(2)	0(2)	2(2)
C(5)	28(2)	26(2)	31(3)	6(2)	-3(2)	-3(2)
C(6)	22(2)	23(2)	24(2)	-2(2)	2(2)	-2(2)
C(7)	29(3)	24(2)	28(3)	6(2)	-4(2)	0(2)
C(11)	22(2)	23(2)	25(3)	5(2)	-6(2)	-2(2)
C(12)	27(2)	34(3)	37(3)	-3(2)	-6(2)	1(2)
C(13)	23(2)	65(4)	37(3)	-1(3)	3(2)	-6(2)
C(14)	27(2)	52(3)	53(4)	9(3)	-8(3)	-13(2)
C(15)	43(3)	36(3)	45(3)	-1(2)	-13(3)	-10(2)
C(16)	29(2)	35(3)	31(3)	-4(2)	-6(2)	-3(2)
C(21)	17(2)	23(2)	22(2)	1(2)	0(2)	-5(2)
C(22)	34(2)	29(2)	24(2)	0(2)	4(2)	6(2)
C(23)	36(3)	42(3)	30(3)	-4(2)	7(2)	6(2)
C(24)	34(2)	45(3)	21(3)	5(3)	-2(2)	-6(2)
C(25)	39(3)	32(3)	29(3)	8(2)	-6(2)	0(2)
C(26)	25(2)	23(2)	27(3)	-1(2)	-1(2)	4(2)
C(31)	23(2)	10(2)	29(3)	1(2)	0(2)	2(2)
C(32)	36(3)	21(2)	29(3)	-1(2)	3(2)	-4(2)
C(33)	41(3)	27(3)	40(3)	0(2)	9(2)	-8(2)
C(34)	33(2)	24(2)	62(4)	-6(3)	-7(3)	-5(2)

C(35)	53(3)	24(2)	40(3)	-1(2)	-19(3)	5(2)
C(36)	41(3)	19(2)	30(3)	3(2)	-5(2)	2(2)
C(41)	19(2)	17(2)	21(2)	3(2)	0(2)	-3(2)
C(42)	37(3)	38(3)	21(3)	-1(2)	1(2)	4(2)
C(43)	45(3)	43(3)	27(3)	2(2)	-14(2)	0(2)
C(44)	21(2)	37(3)	42(3)	7(2)	-11(2)	0(2)
C(45)	30(3)	46(3)	41(3)	-10(3)	-5(2)	13(2)
C(46)	27(2)	39(3)	28(3)	-8(2)	-4(2)	8(2)
C(51)	28(2)	18(2)	24(3)	-2(2)	11(2)	1(2)
C(52)	33(3)	30(3)	34(3)	2(2)	12(2)	4(2)
C(53)	53(3)	38(3)	37(3)	7(3)	9(3)	14(3)
C(54)	80(4)	34(3)	44(3)	12(3)	29(3)	1(3)
C(55)	59(3)	44(3)	51(4)	-2(3)	29(3)	-19(3)
C(56)	33(3)	36(3)	43(3)	-1(2)	13(2)	-6(2)
C(61)	19(2)	17(2)	27(3)	-4(2)	1(2)	-2(2)
C(62)	38(3)	25(2)	22(3)	-4(2)	-2(2)	-1(2)
C(63)	44(3)	35(3)	25(3)	-8(2)	6(2)	-6(2)
C(64)	46(3)	25(2)	47(3)	-15(2)	8(3)	1(2)
C(65)	52(3)	23(2)	44(3)	0(2)	10(3)	8(2)
C(66)	38(3)	22(2)	27(3)	-2(2)	7(2)	1(2)
O(4)	52(2)	44(2)	49(2)	9(2)	2(2)	17(2)
C(71)	54(3)	62(3)	46(4)	-4(4)	-7(3)	5(3)
C(72)	235(11)	101(6)	69(7)	27(5)	-10(6)	99(7)
C(73)	144(7)	67(5)	90(6)	11(4)	17(5)	53(5)
C(74)	64(4)	64(4)	55(4)	-2(3)	9(3)	15(3)

Table 4: Bond lengths [Å] for bg_213x.

Cr(1)-C(6)	1.808(4)	C(1)-C(3)	1.520(5)	C(42)-C(43)	1.374(6)
Cr(1)-C(5)	1.820(5)	C(1)-C(4)	1.523(5)	C(43)-C(44)	1.376(7)
Cr(1)-C(7)	1.823(4)	C(11)-C(12)	1.381(6)	C(44)-C(45)	1.367(6)
Cr(1)-N(4)	2.133(3)	C(11)-C(16)	1.391(6)	C(45)-C(46)	1.384(6)
Cr(1)-N(2)	2.138(3)	C(12)-C(13)	1.382(6)	C(51)-C(52)	1.377(6)
Cr(1)-N(6)	2.147(3)	C(13)-C(14)	1.358(7)	C(51)-C(56)	1.381(6)
N(1)-C(2)	1.368(5)	C(14)-C(15)	1.385(7)	C(52)-C(53)	1.381(6)
N(1)-C(11)	1.415(5)	C(15)-C(16)	1.388(6)	C(53)-C(54)	1.383(7)
N(2)-C(2)	1.296(5)	C(21)-C(22)	1.387(6)	C(54)-C(55)	1.379(7)
N(2)-C(21)	1.438(5)	C(21)-C(26)	1.393(6)	C(55)-C(56)	1.388(7)
N(3)-C(3)	1.358(5)	C(22)-C(23)	1.383(6)	C(61)-C(66)	1.379(6)
N(3)-C(31)	1.424(5)	C(23)-C(24)	1.381(6)	C(61)-C(62)	1.389(6)
N(4)-C(3)	1.290(5)	C(24)-C(25)	1.378(6)	C(62)-C(63)	1.378(6)
N(4)-C(41)	1.433(5)	C(25)-C(26)	1.377(6)	C(63)-C(64)	1.384(7)
N(5)-C(4)	1.370(5)	C(31)-C(32)	1.375(6)	C(64)-C(65)	1.374(6)
N(5)-C(51)	1.433(5)	C(31)-C(36)	1.388(6)	C(65)-C(66)	1.386(6)
N(6)-C(4)	1.289(5)	C(32)-C(33)	1.374(6)	O(4)-C(71)	1.413(7)
N(6)-C(61)	1.432(5)	C(33)-C(34)	1.380(7)	O(4)-C(74)	1.418(6)
O(1)-C(5)	1.169(5)	C(34)-C(35)	1.376(7)	C(71)-C(72)	1.458(8)
O(2)-C(6)	1.186(5)	C(35)-C(36)	1.390(6)	C(72)-C(73)	1.392(10)
O(3)-C(7)	1.168(5)	C(41)-C(42)	1.376(5)	C(73)-C(74)	1.479(8)
C(1)-C(2)	1.516(5)	C(41)-C(46)	1.382(6)		

Table 5: Bond angles [°] for bg_213x.

C(6)-Cr(1)-C(5)	83.58(19)	N(4)-C(3)-C(1)	116.7(3)
C(6)-Cr(1)-C(7)	85.64(19)	N(3)-C(3)-C(1)	118.0(3)
C(5)-Cr(1)-C(7)	85.52(19)	N(6)-C(4)-N(5)	126.1(3)
C(6)-Cr(1)-N(4)	176.74(16)	N(6)-C(4)-C(1)	118.0(3)
C(5)-Cr(1)-N(4)	98.29(16)	N(5)-C(4)-C(1)	115.7(3)
C(7)-Cr(1)-N(4)	91.83(15)	O(1)-C(5)-Cr(1)	174.1(4)
C(6)-Cr(1)-N(2)	95.26(16)	O(2)-C(6)-Cr(1)	173.7(4)
C(5)-Cr(1)-N(2)	175.18(16)	O(3)-C(7)-Cr(1)	174.9(4)
C(7)-Cr(1)-N(2)	99.07(16)	C(12)-C(11)-C(16)	119.7(4)
N(4)-Cr(1)-N(2)	83.10(12)	C(12)-C(11)-N(1)	122.7(4)
C(6)-Cr(1)-N(6)	100.00(15)	C(16)-C(11)-N(1)	117.4(4)
C(5)-Cr(1)-N(6)	93.06(16)	C(11)-C(12)-C(13)	119.6(4)
C(7)-Cr(1)-N(6)	174.01(17)	C(14)-C(13)-C(12)	121.0(5)
N(4)-Cr(1)-N(6)	82.61(12)	C(13)-C(14)-C(15)	120.1(4)
N(2)-Cr(1)-N(6)	82.52(12)	C(14)-C(15)-C(16)	119.8(5)
C(2)-N(1)-C(11)	131.8(4)	C(15)-C(16)-C(11)	119.7(4)
C(2)-N(2)-C(21)	115.5(3)	C(22)-C(21)-C(26)	119.8(4)
C(2)-N(2)-Cr(1)	121.0(3)	C(22)-C(21)-N(2)	119.9(4)
C(21)-N(2)-Cr(1)	122.8(2)	C(26)-C(21)-N(2)	120.2(4)
C(3)-N(3)-C(31)	126.0(3)	C(23)-C(22)-C(21)	119.8(4)
C(3)-N(4)-C(41)	117.2(3)	C(24)-C(23)-C(22)	120.7(4)
C(3)-N(4)-Cr(1)	121.7(3)	C(25)-C(24)-C(23)	118.9(5)
C(41)-N(4)-Cr(1)	120.2(2)	C(26)-C(25)-C(24)	121.6(4)
C(4)-N(5)-C(51)	121.0(3)	C(25)-C(26)-C(21)	119.1(4)
C(4)-N(6)-C(61)	118.5(3)	C(32)-C(31)-C(36)	120.0(4)
C(4)-N(6)-Cr(1)	120.4(3)	C(32)-C(31)-N(3)	119.9(4)
C(61)-N(6)-Cr(1)	119.9(2)	C(36)-C(31)-N(3)	120.0(4)
C(2)-C(1)-C(3)	110.6(3)	C(33)-C(32)-C(31)	120.5(4)
C(2)-C(1)-C(4)	108.9(3)	C(32)-C(33)-C(34)	119.7(4)
C(3)-C(1)-C(4)	110.3(3)	C(35)-C(34)-C(33)	120.3(4)
N(2)-C(2)-N(1)	123.0(4)	C(34)-C(35)-C(36)	120.1(5)
N(2)-C(2)-C(1)	117.2(3)	C(31)-C(36)-C(35)	119.2(4)
N(1)-C(2)-C(1)	119.8(3)	C(42)-C(41)-C(46)	119.1(4)
N(4)-C(3)-N(3)	125.1(3)	C(42)-C(41)-N(4)	120.3(4)

C(46)-C(41)-N(4)	120.6(4)	C(66)-C(61)-C(62)	119.3(4)
C(43)-C(42)-C(41)	119.6(4)	C(66)-C(61)-N(6)	120.0(4)
C(42)-C(43)-C(44)	121.6(5)	C(62)-C(61)-N(6)	120.7(4)
C(45)-C(44)-C(43)	118.7(4)	C(63)-C(62)-C(61)	119.8(4)
C(44)-C(45)-C(46)	120.4(4)	C(62)-C(63)-C(64)	121.1(5)
C(41)-C(46)-C(45)	120.4(4)	C(65)-C(64)-C(63)	118.7(5)
C(52)-C(51)-C(56)	119.9(4)	C(64)-C(65)-C(66)	120.9(5)
C(52)-C(51)-N(5)	120.7(4)	C(61)-C(66)-C(65)	120.1(4)
C(56)-C(51)-N(5)	119.3(4)	C(71)-O(4)-C(74)	109.9(4)
C(51)-C(52)-C(53)	120.6(4)	O(4)-C(71)-C(72)	106.6(5)
C(52)-C(53)-C(54)	119.7(5)	C(73)-C(72)-C(71)	109.4(6)
C(55)-C(54)-C(53)	119.7(5)	C(72)-C(73)-C(74)	107.4(5)
C(54)-C(55)-C(56)	120.5(5)	O(4)-C(74)-C(73)	106.7(5)
C(51)-C(56)-C(55)	119.5(5)		