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APPENDIX 1 : ADDITIONAL CRYSTALLOGRAPHIC DATA

$[CrCl_3(py)_3]$

Table A.1 **Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[CrCl_3(py)_3]$. U(eq) is defined as one-third of the trace of the orthogonalized U^{ij} tensor**

	x	y	z	U(eq)
Cr(1)	0	8137(1)	2500	30(1)
Cl(1)	572(1)	8198(1)	4675(1)	44(1)
Cl(2)	0	5993(1)	2500	44(1)
N(1)	1096(1)	8135(1)	2527(1)	37(1)
C(1)	1653(1)	7383(2)	3317(2)	45(1)
C(2)	2360(1)	7262(2)	3311(2)	58(1)
C(3)	2504(1)	7936(2)	2472(2)	67(1)
C(4)	1945(1)	8733(2)	1676(2)	63(1)
C(5)	1250(1)	8810(2)	1723(2)	48(1)
N(2)	0	10082(2)	2500	39(1)
C(6)	642(1)	10718(2)	3221(2)	52(1)
C(7)	661(2)	11989(2)	3228(3)	72(1)
C(8)	0	12632(3)	2500	83(1)
N(3)	2230(1)	5471(2)	189(2)	94(1)
C(9)	1717(1)	5385(2)	390(2)	63(1)
C(10)	1065(2)	5262(3)	656(3)	73(1)

Table A.2 Bond lengths [Å] and angles [°] for $[CrCl_3(py)_3]$

Cr(1)-N(2)	2.1037(17)	C(10)-H(10C)	0.87(4)
Cr(1)-N(1)#1	2.1040(13)	N(2)-Cr(1)-N(1)#1	90.06(3)
Cr(1)-N(1)	2.1040(13)	N(2)-Cr(1)-N(1)	90.06(3)
Cr(1)-Cl(2)	2.3196(6)	N(1)#1-Cr(1)-N(1)	179.88(6)
Cr(1)-Cl(1)#1	2.3304(4)	N(2)-Cr(1)-Cl(2)	180.0
Cr(1)-Cl(1)	2.3304(4)	N(1)#1-Cr(1)-Cl(2)	89.94(3)
N(1)-C(1)	1.344(2)	N(1)-Cr(1)-Cl(2)	89.94(3)
N(1)-C(5)	1.344(2)	N(2)-Cr(1)-Cl(1)#1	88.386(11)
C(1)-C(2)	1.376(2)	N(1)#1-Cr(1)-Cl(1)#1	90.64(4)
C(1)-H(1)	0.93(2)	N(1)-Cr(1)-Cl(1)#1	89.36(4)
C(2)-C(3)	1.367(3)	Cl(2)-Cr(1)-Cl(1)#1	91.614(11)
C(2)-H(2)	0.89(2)	N(2)-Cr(1)-Cl(1)	88.386(11)
C(3)-C(4)	1.378(3)	N(1)#1-Cr(1)-Cl(1)	89.36(4)
C(3)-H(3)	0.88(3)	N(1)-Cr(1)-Cl(1)	90.64(4)
C(4)-C(5)	1.373(3)	Cl(2)-Cr(1)-Cl(1)	91.614(11)
C(4)-H(4)	0.91(2)	Cl(1)#1-Cr(1)-Cl(1)	176.77(2)
C(5)-H(5)	0.98(2)	C(1)-N(1)-C(5)	117.90(14)
N(2)-C(6)	1.342(2)	C(1)-N(1)-Cr(1)	119.78(10)
N(2)-C(6)#1	1.342(2)	C(5)-N(1)-Cr(1)	122.18(11)
C(6)-C(7)	1.375(3)	N(1)-C(1)-C(2)	122.70(17)
C(6)-H(6)	0.952(18)	N(1)-C(1)-H(1)	116.5(12)
C(7)-C(8)	1.370(3)	C(2)-C(1)-H(1)	120.8(12)
C(7)-H(7)	0.89(2)	C(3)-C(2)-C(1)	118.86(19)
C(8)-C(7)#1	1.370(3)	C(3)-C(2)-H(2)	120.0(15)
C(8)-H(8)	1.03(5)	C(1)-C(2)-H(2)	121.0(15)
N(3)-C(9)	1.123(3)	C(2)-C(3)-C(4)	119.12(18)
C(9)-C(10)	1.439(3)	C(2)-C(3)-H(3)	117.8(16)
C(10)-H(10A)	1.00(3)	C(4)-C(3)-H(3)	123.0(16)
C(10)-H(10B)	0.91(3)	C(5)-C(4)-C(3)	119.29(19)

C(5)-C(4)-H(4)	117.8(14)	C(8)-C(7)-H(7)	124.6(17)
C(3)-C(4)-H(4)	122.9(14)	C(6)-C(7)-H(7)	116.1(17)
N(1)-C(5)-C(4)	122.10(18)	C(7)#1-C(8)-C(7)	119.0(3)
N(1)-C(5)-H(5)	113.9(11)	C(7)#1-C(8)-H(8)	120.48(14)
C(4)-C(5)-H(5)	123.9(11)	C(7)-C(8)-H(8)	120.48(14)
C(6)-N(2)-C(6)#1	118.2(2)	N(3)-C(9)-C(10)	179.4(3)
C(6)-N(2)-Cr(1)	120.90(10)	C(9)-C(10)-H(10A)	111.5(15)
C(6)#1-N(2)-Cr(1)	120.90(10)	C(9)-C(10)-H(10B)	107.0(19)
N(2)-C(6)-C(7)	122.1(2)	H(10A)-C(10)-H(10B)	108(3)
N(2)-C(6)-H(6)	117.8(11)	C(9)-C(10)-H(10C)	104(2)
C(7)-C(6)-H(6)	120.1(11)	H(10A)-C(10)-H(10C)	123(3)
C(8)-C(7)-C(6)	119.3(2)	H(10B)-C(10)-H(10C)	102(3)

Symmetry transformations used to generate equivalent atoms:

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

Table A.3 **Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[CrCl_3(py)_3]$. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	30(1)	27(1)	31(1)	0	12(1)	0
Cl(1)	43(1)	52(1)	33(1)	0(1)	13(1)	5(1)
Cl(2)	53(1)	27(1)	55(1)	0	26(1)	0
N(1)	35(1)	37(1)	38(1)	-1(1)	17(1)	-1(1)
C(1)	39(1)	46(1)	47(1)	-3(1)	16(1)	5(1)
C(2)	38(1)	65(1)	64(1)	-14(1)	16(1)	8(1)
C(3)	41(1)	88(2)	78(1)	-27(1)	33(1)	-9(1)
C(4)	58(1)	80(1)	63(1)	-11(1)	38(1)	-21(1)
C(5)	46(1)	52(1)	48(1)	-1(1)	23(1)	-7(1)

N(2)	44(1)	29(1)	45(1)	0	20(1)	0
C(6)	61(1)	41(1)	57(1)	-9(1)	28(1)	-11(1)
C(7)	104(2)	44(1)	79(2)	-18(1)	51(1)	-28(1)
C(8)	144(3)	33(1)	90(2)	0	68(2)	0
N(3)	102(2)	95(2)	117(2)	-1(1)	78(2)	-6(1)
C(9)	73(1)	57(1)	68(1)	-6(1)	38(1)	-3(1)
C(10)	70(1)	79(2)	80(2)	-22(1)	42(1)	-11(1)

Table A.4 **Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[CrCl_3(py)_3]$**

	x	y	z	U(eq)
H(1)	1537(12)	6932(16)	3869(19)	50(5)
H(2)	2730(14)	6790(20)	3870(20)	68(7)
H(3)	2951(14)	7820(20)	2450(20)	79(7)
H(4)	2011(12)	9210(20)	1110(20)	70(6)
H(5)	815(11)	9320(18)	1158(18)	52(5)
H(6)	1095(10)	10261(17)	3731(17)	47(5)
H(7)	1117(14)	12340(30)	3720(20)	78(7)
H(8)	0	13580(50)	2500	116(14)
H(10A)	759(16)	4500(30)	270(30)	90(8)
H(10B)	1255(17)	5190(30)	1500(30)	107(10)
H(10C)	860(20)	6000(40)	520(30)	128(13)

Table A.5 Torsion angles [°] for $[CrCl_3(py)_3]$

N(2)-Cr(1)-N(1)-C(1)	134.20(11)	Cr(1)-N(1)-C(5)-C(4)	-174.73(13)
Cl(2)-Cr(1)-N(1)-C(1)	-45.80(11)	C(3)-C(4)-C(5)-N(1)	0.4(3)
Cl(1)#1-Cr(1)-N(1)-C(1)	-137.42(11)	N(1)#1-Cr(1)-N(2)-C(6)	138.73(9)
Cl(1)-Cr(1)-N(1)-C(1)	45.81(11)	N(1)-Cr(1)-N(2)-C(6)	-41.27(9)
N(2)-Cr(1)-N(1)-C(5)	-50.02(12)	Cl(1)#1-Cr(1)-N(2)-C(6)	-130.63(9)
Cl(2)-Cr(1)-N(1)-C(5)	129.98(12)	Cl(1)-Cr(1)-N(2)-C(6)	49.37(9)
Cl(1)#1-Cr(1)-N(1)-C(5)	38.36(12)	N(1)#1-Cr(1)-N(2)-C(6)#1	-41.27(9)
Cl(1)-Cr(1)-N(1)-C(5)	-138.41(12)	N(1)-Cr(1)-N(2)-C(6)#1	138.73(9)
C(5)-N(1)-C(1)-C(2)	-1.5(2)	Cl(1)#1-Cr(1)-N(2)-C(6)#1	49.37(9)
Cr(1)-N(1)-C(1)-C(2)	174.50(13)	Cl(1)-Cr(1)-N(2)-C(6)#1	-130.63(9)
N(1)-C(1)-C(2)-C(3)	0.3(3)	C(6)#1-N(2)-C(6)-C(7)	-0.78(15)
C(1)-C(2)-C(3)-C(4)	1.3(3)	Cr(1)-N(2)-C(6)-C(7)	179.22(15)
C(2)-C(3)-C(4)-C(5)	-1.6(3)	N(2)-C(6)-C(7)-C(8)	1.5(3)
C(1)-N(1)-C(5)-C(4)	1.1(2)	C(6)-C(7)-C(8)-C(7)#1	-0.7(3)

Symmetry transformations used to generate equivalent atoms:

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

[Hpy][$CrCl_4(py)_2$]

Table A.6 **Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [Hpy][$CrCl_4(py)_2$]. U(eq) is defined as one-third of the trace of the orthogonalised U^{ij} tensor**

	x	y	z	U(eq)
Cr(1)	1842(1)	975(1)	2533(1)	36(1)
Cl(1)	1013(1)	1234(1)	372(1)	50(1)
Cl(2)	4224(1)	1552(1)	2392(1)	50(1)
Cl(3)	2614(1)	709(1)	4707(1)	53(1)
Cl(4)	-556(1)	401(1)	2705(1)	50(1)
N(1)	3099(3)	233(1)	1848(2)	39(1)
C(1)	2425(3)	-117(1)	900(3)	48(1)
C(2)	3234(4)	-595(1)	402(3)	56(1)
C(3)	4802(4)	-722(1)	881(3)	55(1)
C(4)	5499(4)	-378(1)	1865(3)	57(1)
C(5)	4629(3)	97(1)	2318(3)	49(1)
N(2)	561(3)	1720(1)	3209(2)	45(1)
C(6)	1253(4)	2087(1)	4111(3)	55(1)
C(7)	459(5)	2587(1)	4543(4)	69(1)
C(8)	-1089(5)	2711(1)	4052(4)	76(1)
C(9)	-1811(4)	2339(1)	3123(4)	75(1)
C(10)	-955(4)	1849(1)	2728(3)	59(1)
N(3)	1370(5)	-769(2)	3807(3)	74(1)
C(11)	636(5)	-1138(2)	2974(4)	82(1)
C(12)	1239(5)	-1684(2)	2815(4)	81(1)
C(13)	2617(5)	-1847(2)	3521(4)	78(1)
C(14)	3368(5)	-1456(2)	4376(4)	90(1)
C(15)	2703(6)	-907(2)	4485(4)	83(1)

Table A.7 **Bond lengths [Å] and angles [°] for [Hpy][$CrCl_4(py)_2$]**

Cr(1)-N(1)	2.097(2)	N(3)-C(15)	1.290(5)
Cr(1)-N(2)	2.109(2)	N(3)-C(11)	1.309(5)
Cr(1)-Cl(2)	2.3387(8)	N(3)-H(3N)	0.89(5)
Cr(1)-Cl(1)	2.3398(8)	C(11)-C(12)	1.336(5)
Cr(1)-Cl(3)	2.3451(8)	C(11)-H(11)	0.9300
Cr(1)-Cl(4)	2.3490(8)	C(12)-C(13)	1.347(5)
N(1)-C(1)	1.339(3)	C(12)-H(12)	0.9300
N(1)-C(5)	1.341(3)	C(13)-C(14)	1.362(5)
C(1)-C(2)	1.372(4)	C(13)-H(13)	0.9300
C(1)-H(1)	0.9300	C(14)-C(15)	1.356(6)
C(2)-C(3)	1.369(4)	C(14)-H(14)	0.9300
C(2)-H(2)	0.9300	C(15)-H(15)	0.9300
C(3)-C(4)	1.365(4)		
C(3)-H(3)	0.9300	N(1)-Cr(1)-N(2)	179.49(9)
C(4)-C(5)	1.374(4)	N(1)-Cr(1)-Cl(2)	90.36(6)
C(4)-H(4)	0.9300	N(2)-Cr(1)-Cl(2)	89.95(6)
C(5)-H(5)	0.9300	N(1)-Cr(1)-Cl(1)	90.43(6)
N(2)-C(10)	1.331(4)	N(2)-Cr(1)-Cl(1)	89.17(7)
N(2)-C(6)	1.337(3)	Cl(2)-Cr(1)-Cl(1)	90.05(3)
C(6)-C(7)	1.380(4)	N(1)-Cr(1)-Cl(3)	89.99(6)
C(6)-H(6)	0.9300	N(2)-Cr(1)-Cl(3)	90.41(7)
C(7)-C(8)	1.355(5)	Cl(2)-Cr(1)-Cl(3)	91.12(3)
C(7)-H(7)	0.9300	Cl(1)-Cr(1)-Cl(3)	178.75(3)
C(8)-C(9)	1.372(5)	N(1)-Cr(1)-Cl(4)	90.23(6)
C(8)-H(8)	0.9300	N(2)-Cr(1)-Cl(4)	89.46(6)
C(9)-C(10)	1.375(4)	Cl(2)-Cr(1)-Cl(4)	179.16(3)
C(9)-H(9)	0.9300	Cl(1)-Cr(1)-Cl(4)	90.54(3)
C(10)-H(10)	0.9300	Cl(3)-Cr(1)-Cl(4)	88.28(3)

C(1)-N(1)-C(5)	117.2(2)	C(7)-C(8)-C(9)	118.8(3)
C(1)-N(1)-Cr(1)	121.46(18)	C(7)-C(8)-H(8)	120.6
C(5)-N(1)-Cr(1)	121.31(18)	C(9)-C(8)-H(8)	120.6
N(1)-C(1)-C(2)	122.9(3)	C(8)-C(9)-C(10)	119.2(3)
N(1)-C(1)-H(1)	118.5	C(8)-C(9)-H(9)	120.4
C(2)-C(1)-H(1)	118.5	C(10)-C(9)-H(9)	120.4
C(3)-C(2)-C(1)	119.1(3)	N(2)-C(10)-C(9)	122.6(3)
C(3)-C(2)-H(2)	120.5	N(2)-C(10)-H(10)	118.7
C(1)-C(2)-H(2)	120.5	C(9)-C(10)-H(10)	118.7
C(4)-C(3)-C(2)	118.9(3)	C(15)-N(3)-C(11)	122.2(4)
C(4)-C(3)-H(3)	120.6	C(15)-N(3)-H(3N)	120(4)
C(2)-C(3)-H(3)	120.6	C(11)-N(3)-H(3N)	117(4)
C(3)-C(4)-C(5)	119.3(3)	N(3)-C(11)-C(12)	120.4(4)
C(3)-C(4)-H(4)	120.4	N(3)-C(11)-H(11)	119.8
C(5)-C(4)-H(4)	120.4	C(12)-C(11)-H(11)	119.8
N(1)-C(5)-C(4)	122.6(3)	C(11)-C(12)-C(13)	119.1(4)
N(1)-C(5)-H(5)	118.7	C(11)-C(12)-H(12)	120.5
C(4)-C(5)-H(5)	118.7	C(13)-C(12)-H(12)	120.5
C(10)-N(2)-C(6)	117.5(2)	C(12)-C(13)-C(14)	119.6(4)
C(10)-N(2)-Cr(1)	121.01(19)	C(12)-C(13)-H(13)	120.2
C(6)-N(2)-Cr(1)	121.4(2)	C(14)-C(13)-H(13)	120.2
N(2)-C(6)-C(7)	122.5(3)	C(15)-C(14)-C(13)	118.5(4)
N(2)-C(6)-H(6)	118.7	C(15)-C(14)-H(14)	120.8
C(7)-C(6)-H(6)	118.7	C(13)-C(14)-H(14)	120.8
C(8)-C(7)-C(6)	119.3(3)	N(3)-C(15)-C(14)	120.1(4)
C(8)-C(7)-H(7)	120.3	N(3)-C(15)-H(15)	119.9
C(6)-C(7)-H(7)	120.3	C(14)-C(15)-H(15)	119.9

Table A.8 **Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[Hpy][CrCl_4(py)_2]$. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	35(1)	36(1)	38(1)	-1(1)	3(1)	-3(1)
Cl(1)	47(1)	59(1)	45(1)	7(1)	-3(1)	-3(1)
Cl(2)	44(1)	51(1)	56(1)	1(1)	2(1)	-14(1)
Cl(3)	62(1)	58(1)	39(1)	3(1)	2(1)	0(1)
Cl(4)	39(1)	44(1)	66(1)	-1(1)	9(1)	-6(1)
N(1)	35(1)	41(1)	40(1)	-1(1)	2(1)	-2(1)
C(1)	41(2)	48(2)	54(2)	-10(1)	0(1)	-3(1)
C(2)	60(2)	46(2)	62(2)	-13(1)	5(2)	-4(1)
C(3)	58(2)	39(2)	69(2)	-1(1)	17(2)	6(1)
C(4)	42(2)	57(2)	71(2)	1(2)	4(2)	11(1)
C(5)	41(2)	52(2)	54(2)	-4(1)	-2(1)	-1(1)
N(2)	48(1)	39(1)	49(1)	-4(1)	9(1)	-3(1)
C(6)	62(2)	49(2)	55(2)	-9(1)	3(2)	0(1)
C(7)	77(3)	54(2)	76(2)	-21(2)	19(2)	-6(2)
C(8)	73(2)	44(2)	114(3)	-18(2)	34(2)	2(2)
C(9)	52(2)	51(2)	124(3)	-14(2)	14(2)	8(2)
C(10)	46(2)	47(2)	83(2)	-12(2)	2(2)	3(1)
N(3)	93(3)	63(2)	68(2)	3(2)	19(2)	14(2)
C(11)	64(2)	98(3)	82(3)	9(2)	-10(2)	5(2)
C(12)	90(3)	73(2)	78(3)	-14(2)	-5(2)	-23(2)
C(13)	95(3)	58(2)	82(3)	2(2)	14(2)	14(2)
C(14)	72(3)	100(3)	94(3)	7(2)	-21(2)	7(2)
C(15)	105(3)	76(3)	67(2)	-12(2)	-8(2)	-22(2)

Table A.9 **Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for [Hpy][$CrCl_4(py)_2$]**

	x	y	z	U(eq)
H(1)	1362	-32	565	57
H(2)	2723	-829	-253	67
H(3)	5384	-1038	543	65
H(4)	6550	-463	2224	68
H(5)	5120	333	2977	59
H(6)	2310	2003	4461	66
H(7)	980	2835	5164	82
H(8)	-1651	3042	4340	91
H(9)	-2868	2417	2765	90
H(10)	-1454	1598	2101	70
H(3N)	1010(70)	-390(20)	3790(50)	89
H(11)	-312	-1020	2489	98
H(12)	715	-1947	2226	97
H(13)	3052	-2226	3424	94
H(14)	4317	-1562	4875	108
H(15)	3209	-630	5050	100

Table A.10 Torsion angles [°] for [Hpy][$CrCl_4(py)_2$]

Cl(2)-Cr(1)-N(1)-C(1)	-133.5(2)	Cl(4)-Cr(1)-N(2)-C(10)	-45.6(2)
Cl(1)-Cr(1)-N(1)-C(1)	-43.4(2)	Cl(2)-Cr(1)-N(2)-C(6)	-43.4(2)
Cl(3)-Cr(1)-N(1)-C(1)	135.4(2)	Cl(1)-Cr(1)-N(2)-C(6)	-133.5(2)
Cl(4)-Cr(1)-N(1)-C(1)	47.1(2)	Cl(3)-Cr(1)-N(2)-C(6)	47.7(2)
Cl(2)-Cr(1)-N(1)-C(5)	44.9(2)	Cl(4)-Cr(1)-N(2)-C(6)	136.0(2)
Cl(1)-Cr(1)-N(1)-C(5)	134.9(2)	C(10)-N(2)-C(6)-C(7)	-0.3(4)
Cl(3)-Cr(1)-N(1)-C(5)	-46.3(2)	Cr(1)-N(2)-C(6)-C(7)	178.2(2)
Cl(4)-Cr(1)-N(1)-C(5)	-134.5(2)	N(2)-C(6)-C(7)-C(8)	0.7(5)
C(5)-N(1)-C(1)-C(2)	-0.5(4)	C(6)-C(7)-C(8)-C(9)	-0.9(6)
Cr(1)-N(1)-C(1)-C(2)	177.9(2)	C(7)-C(8)-C(9)-C(10)	0.7(6)
N(1)-C(1)-C(2)-C(3)	-0.4(5)	C(6)-N(2)-C(10)-C(9)	0.0(5)
C(1)-C(2)-C(3)-C(4)	1.6(5)	Cr(1)-N(2)-C(10)-C(9)	-178.4(3)
C(2)-C(3)-C(4)-C(5)	-1.9(4)	C(8)-C(9)-C(10)-N(2)	-0.2(6)
C(1)-N(1)-C(5)-C(4)	0.1(4)	C(15)-N(3)-C(11)-C(12)	1.2(6)
Cr(1)-N(1)-C(5)-C(4)	-178.3(2)	N(3)-C(11)-C(12)-C(13)	-0.3(6)
C(3)-C(4)-C(5)-N(1)	1.1(5)	C(11)-C(12)-C(13)-C(14)	-0.1(6)
Cl(2)-Cr(1)-N(2)-C(10)	135.0(2)	C(12)-C(13)-C(14)-C(15)	-0.4(6)
Cl(1)-Cr(1)-N(2)-C(10)	44.9(2)	C(11)-N(3)-C(15)-C(14)	-1.8(6)
Cl(3)-Cr(1)-N(2)-C(10)	-133.9(2)	C(13)-C(14)-C(15)-N(3)	1.3(6)

Table A.11 Hydrogen bonds for [Hpy][$CrCl_4(py)_2$] [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(3)-H(3N)...Cl(4)	0.89(5)	2.43(5)	3.235(4)	150(5)
N(3)-H(3N)...Cl(3)	0.89(5)	2.94(5)	3.586(4)	131(4)

$[CrCl_3(py)_2(DMF)]$

Table A.12 **Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[CrCl_3(py)_2(DMF)]$. U(eq) is defined as one-third of the trace of the orthogonalised U^{ij} tensor**

	x	y	z	U(eq)
Cr(1)	3856(1)	9243(1)	3357(1)	34(1)
Cl(1)	3988(1)	10037(1)	1097(1)	51(1)
Cl(2)	2058(1)	8139(1)	2288(1)	47(1)
Cl(3)	5605(1)	10338(1)	4523(1)	54(1)
N(1)	2108(3)	10180(2)	3978(3)	40(1)
C(1)	2092(4)	11171(3)	3715(4)	51(1)
C(2)	960(5)	11789(3)	4101(4)	62(1)
C(3)	-222(5)	11385(4)	4795(4)	67(1)
C(4)	-236(4)	10377(4)	5080(4)	60(1)
C(5)	943(4)	9795(3)	4653(4)	49(1)
N(2)	5604(3)	8252(2)	2890(2)	39(1)
C(6)	5425(4)	7259(3)	2972(3)	45(1)
C(7)	6491(5)	6580(3)	2586(4)	64(1)
C(8)	7797(5)	6934(4)	2119(4)	72(1)
C(9)	8025(4)	7949(4)	2033(4)	64(1)
C(10)	6903(4)	8578(3)	2425(3)	51(1)
O(1)	3685(2)	8522(2)	5281(2)	44(1)
N(3)	4421(3)	8025(2)	7596(3)	44(1)
C(11)	4693(4)	8393(3)	6327(3)	42(1)
C(12)	2939(5)	7703(5)	7924(5)	94(2)
C(13)	5620(5)	7871(3)	8776(4)	60(1)
O(2)	839(5)	3826(3)	2134(4)	93(1)
N(4)	1039(4)	5140(3)	594(3)	56(1)
C(14)	355(6)	4351(3)	1113(4)	69(1)
C(15)	2507(5)	5459(3)	1202(5)	69(1)
C(16)	362(6)	5697(4)	-639(5)	84(1)

Table A.13 **Bond lengths [Å] and angles [°] for $[CrCl_3(py)_2(DMF)]$**

Cr(1)-O(1)	2.003(2)	N(3)-C(13)	1.465(4)
Cr(1)-N(1)	2.102(3)	C(11)-H(11)	0.9300
Cr(1)-N(2)	2.106(3)	C(12)-H(12A)	0.9600
Cr(1)-Cl(1)	2.3120(9)	C(12)-H(12B)	0.9600
Cr(1)-Cl(3)	2.3268(9)	C(12)-H(12C)	0.9600
Cr(1)-Cl(2)	2.3277(9)	C(13)-H(13A)	0.9600
N(1)-C(1)	1.343(5)	C(13)-H(13B)	0.9600
N(1)-C(5)	1.343(4)	C(13)-H(13C)	0.9600
C(1)-C(2)	1.365(6)	O(2)-C(14)	1.212(5)
C(1)-H(1)	0.9300	N(4)-C(14)	1.318(5)
C(2)-C(3)	1.373(6)	N(4)-C(16)	1.434(5)
C(2)-H(2)	0.9300	N(4)-C(15)	1.442(5)
C(3)-C(4)	1.367(7)	C(14)-H(14)	0.9300
C(3)-H(3)	0.9300	C(15)-H(15A)	0.9600
C(4)-C(5)	1.382(5)	C(15)-H(15B)	0.9600
C(4)-H(4)	0.9300	C(15)-H(15C)	0.9600
C(5)-H(5)	0.9300	C(16)-H(16A)	0.9600
N(2)-C(10)	1.331(4)	C(16)-H(16B)	0.9600
N(2)-C(6)	1.336(5)	C(16)-H(16C)	0.9600
C(6)-C(7)	1.374(5)		
C(6)-H(6)	0.9300	O(1)-Cr(1)-N(1)	86.98(10)
C(7)-C(8)	1.350(7)	O(1)-Cr(1)-N(2)	88.77(10)
C(7)-H(7)	0.9300	N(1)-Cr(1)-N(2)	175.74(10)
C(8)-C(9)	1.370(8)	O(1)-Cr(1)-Cl(1)	177.96(7)
C(8)-H(8)	0.9300	N(1)-Cr(1)-Cl(1)	92.93(7)
C(9)-C(10)	1.370(6)	N(2)-Cr(1)-Cl(1)	91.33(7)
C(9)-H(9)	0.9300	O(1)-Cr(1)-Cl(3)	89.91(7)
C(10)-H(10)	0.9300	N(1)-Cr(1)-Cl(3)	89.32(8)
O(1)-C(11)	1.265(4)	N(2)-Cr(1)-Cl(3)	90.36(8)
N(3)-C(11)	1.287(4)	Cl(1)-Cr(1)-Cl(3)	92.12(4)
N(3)-C(12)	1.437(5)	O(1)-Cr(1)-Cl(2)	87.90(7)

N(1)-Cr(1)-Cl(2)	89.34(8)	C(9)-C(8)-H(8)	120.1
N(2)-Cr(1)-Cl(2)	90.83(8)	C(10)-C(9)-C(8)	118.4(4)
Cl(1)-Cr(1)-Cl(2)	90.06(3)	C(10)-C(9)-H(9)	120.8
Cl(3)-Cr(1)-Cl(2)	177.49(4)	C(8)-C(9)-H(9)	120.8
C(1)-N(1)-C(5)	117.2(3)	N(2)-C(10)-C(9)	123.2(4)
C(1)-N(1)-Cr(1)	122.4(2)	N(2)-C(10)-H(10)	118.4
C(5)-N(1)-Cr(1)	120.3(2)	C(9)-C(10)-H(10)	118.4
N(1)-C(1)-C(2)	123.1(4)	C(11)-O(1)-Cr(1)	128.2(2)
N(1)-C(1)-H(1)	118.4	C(11)-N(3)-C(12)	122.3(3)
C(2)-C(1)-H(1)	118.4	C(11)-N(3)-C(13)	121.9(3)
C(1)-C(2)-C(3)	119.0(4)	C(12)-N(3)-C(13)	115.8(3)
C(1)-C(2)-H(2)	120.5	O(1)-C(11)-N(3)	123.2(3)
C(3)-C(2)-H(2)	120.5	O(1)-C(11)-H(11)	118.4
C(4)-C(3)-C(2)	119.3(4)	N(3)-C(11)-H(11)	118.4
C(4)-C(3)-H(3)	120.4	N(3)-C(12)-H(12A)	109.5
C(2)-C(3)-H(3)	120.4	N(3)-C(12)-H(12B)	109.5
C(3)-C(4)-C(5)	118.7(4)	H(12A)-C(12)-H(12B)	109.5
C(3)-C(4)-H(4)	120.6	N(3)-C(12)-H(12C)	109.5
C(5)-C(4)-H(4)	120.6	H(12A)-C(12)-H(12C)	109.5
N(1)-C(5)-C(4)	122.7(4)	H(12B)-C(12)-H(12C)	109.5
N(1)-C(5)-H(5)	118.7	N(3)-C(13)-H(13A)	109.5
C(4)-C(5)-H(5)	118.7	N(3)-C(13)-H(13B)	109.5
C(10)-N(2)-C(6)	116.8(3)	H(13A)-C(13)-H(13B)	109.5
C(10)-N(2)-Cr(1)	122.0(2)	N(3)-C(13)-H(13C)	109.5
C(6)-N(2)-Cr(1)	121.1(2)	H(13A)-C(13)-H(13C)	109.5
N(2)-C(6)-C(7)	123.4(4)	H(13B)-C(13)-H(13C)	109.5
N(2)-C(6)-H(6)	118.3	C(14)-N(4)-C(16)	120.8(4)
C(7)-C(6)-H(6)	118.3	C(14)-N(4)-C(15)	121.9(4)
C(8)-C(7)-C(6)	118.4(4)	C(16)-N(4)-C(15)	117.3(4)
C(8)-C(7)-H(7)	120.8	O(2)-C(14)-N(4)	125.8(5)
C(6)-C(7)-H(7)	120.8	O(2)-C(14)-H(14)	117.1
C(7)-C(8)-C(9)	119.8(4)	N(4)-C(14)-H(14)	117.1
C(7)-C(8)-H(8)	120.1	N(4)-C(15)-H(15A)	109.5

N(4)-C(15)-H(15B)	109.5	N(4)-C(16)-H(16B)	109.5
H(15A)-C(15)-H(15B)	109.5	H(16A)-C(16)-H(16B)	109.5
N(4)-C(15)-H(15C)	109.5	N(4)-C(16)-H(16C)	109.5
H(15A)-C(15)-H(15C)	109.5	H(16A)-C(16)-H(16C)	109.5
H(15B)-C(15)-H(15C)	109.5	H(16B)-C(16)-H(16C)	109.5
N(4)-C(16)-H(16A)	109.5		

Table A.14 **Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[CrCl_3(py)_2(DMF)]$. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	31(1)	38(1)	32(1)	3(1)	4(1)	0(1)
Cl(1)	62(1)	52(1)	41(1)	12(1)	15(1)	7(1)
Cl(2)	36(1)	49(1)	54(1)	-4(1)	-3(1)	-4(1)
Cl(3)	47(1)	56(1)	59(1)	-11(1)	2(1)	-12(1)
N(1)	39(1)	44(2)	39(1)	3(1)	6(1)	4(1)
C(1)	60(2)	50(2)	41(2)	4(2)	7(2)	6(2)
C(2)	78(3)	54(2)	54(2)	0(2)	2(2)	26(2)
C(3)	65(3)	86(3)	49(2)	-3(2)	5(2)	34(3)
C(4)	47(2)	82(3)	51(2)	5(2)	12(2)	17(2)
C(5)	44(2)	58(2)	47(2)	8(2)	10(2)	6(2)
N(2)	33(1)	50(2)	34(1)	3(1)	2(1)	2(1)
C(6)	40(2)	52(2)	43(2)	6(2)	2(1)	9(2)
C(7)	74(3)	64(3)	53(2)	1(2)	1(2)	25(2)
C(8)	59(3)	106(4)	50(2)	9(2)	9(2)	45(3)
C(9)	38(2)	98(4)	56(2)	9(2)	10(2)	14(2)
C(10)	36(2)	68(3)	48(2)	7(2)	6(1)	0(2)
O(1)	38(1)	58(1)	35(1)	8(1)	2(1)	2(1)
N(3)	48(2)	53(2)	31(1)	1(1)	1(1)	-1(1)
C(11)	42(2)	46(2)	39(2)	3(1)	3(1)	6(2)

C(12)	67(3)	165(6)	50(2)	27(3)	10(2)	-24(3)
C(13)	73(3)	62(2)	44(2)	5(2)	-10(2)	9(2)
O(2)	122(3)	70(2)	90(2)	21(2)	22(2)	0(2)
N(4)	60(2)	59(2)	48(2)	1(1)	3(1)	-10(2)
C(14)	88(3)	64(3)	57(2)	-1(2)	14(2)	-13(3)
C(15)	65(3)	61(3)	80(3)	-6(2)	-1(2)	-5(2)
C(16)	86(3)	101(4)	63(3)	20(3)	4(2)	-4(3)

Table A.15 **Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for $[CrCl_3(py)_2(DMF)]$**

	x	y	z	U(eq)
H(1)	2890	11451	3247	61
H(2)	989	12472	3897	75
H(3)	-1004	11792	5068	80
H(4)	-1024	10090	5553	72
H(5)	929	9109	4841	59
H(6)	4532	7014	3309	54
H(7)	6317	5894	2644	76
H(8)	8540	6491	1856	86
H(9)	8921	8204	1717	76
H(10)	7056	9266	2363	61
H(11)	5680	8572	6170	51
H(12A)	2196	8055	7298	141
H(12B)	2791	7844	8944	141
H(12C)	2841	6995	7750	141
H(13A)	5722	7167	8985	90
H(13B)	5368	8218	9654	90
H(13C)	6554	8126	8462	90
H(14)	-583	4183	655	83

H(15A)	2737	5139	2143	104
H(15B)	2509	6174	1332	104
H(15C)	3253	5277	535	104
H(16A)	-640	5450	-889	125
H(16B)	956	5620	-1476	125
H(16C)	315	6394	-378	125

Table A.16 Torsion angles [°] for [$CrCl_3(py)_2(DMF)$]

O(1)-Cr(1)-N(1)-C(1)	140.8(2)	Cl(1)-Cr(1)-N(2)-C(6)	-126.2(2)
Cl(1)-Cr(1)-N(1)-C(1)	-41.2(2)	Cl(3)-Cr(1)-N(2)-C(6)	141.7(2)
Cl(3)-Cr(1)-N(1)-C(1)	50.9(2)	Cl(2)-Cr(1)-N(2)-C(6)	-36.1(2)
Cl(2)-Cr(1)-N(1)-C(1)	-131.3(2)	C(10)-N(2)-C(6)-C(7)	-1.0(5)
O(1)-Cr(1)-N(1)-C(5)	-39.7(2)	Cr(1)-N(2)-C(6)-C(7)	175.6(3)
Cl(1)-Cr(1)-N(1)-C(5)	138.2(2)	N(2)-C(6)-C(7)-C(8)	1.0(5)
Cl(3)-Cr(1)-N(1)-C(5)	-129.7(2)	C(6)-C(7)-C(8)-C(9)	-0.4(6)
Cl(2)-Cr(1)-N(1)-C(5)	48.2(2)	C(7)-C(8)-C(9)-C(10)	-0.2(6)
C(5)-N(1)-C(1)-C(2)	0.0(5)	C(6)-N(2)-C(10)-C(9)	0.3(5)
Cr(1)-N(1)-C(1)-C(2)	179.5(3)	Cr(1)-N(2)-C(10)-C(9)	-176.2(3)
N(1)-C(1)-C(2)-C(3)	0.2(6)	C(8)-C(9)-C(10)-N(2)	0.3(5)
C(1)-C(2)-C(3)-C(4)	-0.1(6)	N(1)-Cr(1)-O(1)-C(11)	-121.5(3)
C(2)-C(3)-C(4)-C(5)	-0.2(6)	N(2)-Cr(1)-O(1)-C(11)	58.1(3)
C(1)-N(1)-C(5)-C(4)	-0.3(5)	Cl(3)-Cr(1)-O(1)-C(11)	-32.2(3)
Cr(1)-N(1)-C(5)-C(4)	-179.8(3)	Cl(2)-Cr(1)-O(1)-C(11)	149.0(3)
C(3)-C(4)-C(5)-N(1)	0.4(6)	Cr(1)-O(1)-C(11)-N(3)	171.1(3)
O(1)-Cr(1)-N(2)-C(10)	-131.9(2)	C(12)-N(3)-C(11)-O(1)	1.7(6)
Cl(1)-Cr(1)-N(2)-C(10)	50.2(2)	C(13)-N(3)-C(11)-O(1)	179.0(3)
Cl(3)-Cr(1)-N(2)-C(10)	-42.0(2)	C(16)-N(4)-C(14)-O(2)	179.1(5)
Cl(2)-Cr(1)-N(2)-C(10)	140.2(2)	C(15)-N(4)-C(14)-O(2)	1.1(7)
O(1)-Cr(1)-N(2)-C(6)	51.8(2)		

[$CrCl_3(pytb)_3$]

Table A.17 **Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [$CrCl_3(pytb)_3$]. U(eq) is defined as one-third of the trace of the orthogonalised U^{ij} tensor**

	x	y	z	U(eq)
Cr(1)	8089(1)	511(1)	3464(1)	47(1)
Cl(1)	7480(1)	89(1)	2524(1)	64(1)
Cl(2)	8604(1)	930(1)	2390(1)	84(1)
Cl(3)	8641(1)	897(1)	4523(1)	68(1)
N(1)	8288(1)	4(1)	3358(2)	51(1)
C(1)	8734(1)	127(1)	3339(3)	71(1)
C(2)	8885(1)	-187(1)	3282(3)	80(1)
C(3)	8578(1)	-655(1)	3255(2)	60(1)
C(4)	8115(1)	-782(1)	3281(2)	62(1)
C(5)	7988(1)	-449(1)	3326(2)	55(1)
C(6)	8745(1)	-1007(1)	3211(3)	77(1)
C(7)	8949(2)	-1012(2)	4085(3)	108(2)
C(8)	8350(2)	-1493(2)	3011(4)	111(2)
C(9)	9111(2)	-866(2)	2505(3)	99(2)
N(11)	7633(1)	109(1)	4467(1)	46(1)
C(11)	7745(1)	-121(1)	5034(2)	51(1)
C(12)	7456(1)	-391(1)	5673(2)	54(1)
C(13)	7030(1)	-422(1)	5800(2)	48(1)
C(14)	6923(1)	-173(1)	5230(2)	55(1)
C(15)	7219(1)	73(1)	4575(2)	54(1)
C(16)	6717(1)	-696(1)	6536(2)	69(1)
C(17)	6984(2)	-450(2)	7373(3)	141(2)
C(18)	6277(2)	-679(2)	6561(3)	121(2)
C(19)	6632(2)	-1177(2)	6541(5)	165(3)

N(21)	7876(1)	1008(1)	3541(1)	49(1)
C(21)	7787(1)	1153(1)	4278(2)	57(1)
C(22)	7604(1)	1440(1)	4317(2)	59(1)
C(23)	7508(1)	1608(1)	3576(2)	51(1)
C(24)	7619(1)	1471(1)	2821(2)	56(1)
C(25)	7792(1)	1175(1)	2827(2)	57(1)
C(26)	7309(1)	1933(1)	3609(2)	64(1)
C(27)	7688(2)	2400(2)	3879(6)	193(4)
C(28)	7112(2)	1961(2)	2752(3)	135(2)
C(29)	6913(2)	1757(2)	4242(3)	105(2)
O(31)	4990(4)	191(3)	270(6)	128(3)
C(31)	5777(10)	279(11)	220(30)	188(16)
C(32)	5520(20)	188(19)	703(18)	290(30)
C(33)	4730(11)	-79(12)	-160(30)	260(20)
C(34)	4412(19)	-133(16)	-100(20)	230(20)
C(41)	7101(18)	3670(30)	3810(40)	380(30)
C(42)	7020(30)	3630(30)	2980(40)	390(30)

Table A.18 **Bond lengths [Å] and angles [°] for $[CrCl_3(pytb)_3]$**

Cr(1)-N(1)	2.105(2)	C(1)-H(1)	0.9300
Cr(1)-N(21)	2.105(2)	C(2)-C(3)	1.375(5)
Cr(1)-N(11)	2.130(2)	C(2)-H(2)	0.9300
Cr(1)-Cl(2)	2.3056(9)	C(3)-C(4)	1.379(4)
Cr(1)-Cl(1)	2.3248(9)	C(3)-C(6)	1.530(5)
Cr(1)-Cl(3)	2.3263(9)	C(4)-C(5)	1.375(4)
N(1)-C(5)	1.332(4)	C(4)-H(4)	0.9300
N(1)-C(1)	1.332(4)	C(5)-H(5)	0.9300
C(1)-C(2)	1.368(5)	C(6)-C(8)	1.525(6)

C(6)-C(7)	1.532(6)	C(19)-H(19A)	0.9600
C(6)-C(9)	1.534(5)	C(19)-H(19B)	0.9600
C(7)-H(7A)	0.9600	C(19)-H(19C)	0.9600
C(7)-H(7B)	0.9600	N(21)-C(25)	1.338(4)
C(7)-H(7C)	0.9600	N(21)-C(21)	1.341(4)
C(8)-H(8A)	0.9600	C(21)-C(22)	1.369(4)
C(8)-H(8B)	0.9600	C(21)-H(21)	0.9300
C(8)-H(8C)	0.9600	C(22)-C(23)	1.391(4)
C(9)-H(9A)	0.9600	C(22)-H(22)	0.9300
C(9)-H(9B)	0.9600	C(23)-C(24)	1.381(4)
C(9)-H(9C)	0.9600	C(23)-C(26)	1.528(4)
N(11)-C(15)	1.331(4)	C(24)-C(25)	1.370(4)
N(11)-C(11)	1.342(4)	C(24)-H(24)	0.9300
C(11)-C(12)	1.369(4)	C(25)-H(25)	0.9300
C(11)-H(11)	0.9300	C(26)-C(27)	1.493(6)
C(12)-C(13)	1.386(4)	C(26)-C(29)	1.513(5)
C(12)-H(12)	0.9300	C(26)-C(28)	1.517(6)
C(13)-C(14)	1.380(4)	C(27)-H(27A)	0.9600
C(13)-C(16)	1.516(4)	C(27)-H(27B)	0.9600
C(14)-C(15)	1.374(4)	C(27)-H(27C)	0.9600
C(14)-H(14)	0.9300	C(28)-H(28A)	0.9600
C(15)-H(15)	0.9300	C(28)-H(28B)	0.9600
C(16)-C(19)	1.480(6)	C(28)-H(28C)	0.9600
C(16)-C(18)	1.497(6)	C(29)-H(29A)	0.9600
C(16)-C(17)	1.564(7)	C(29)-H(29B)	0.9600
C(17)-H(17A)	0.9600	C(29)-H(29C)	0.9600
C(17)-H(17B)	0.9600	O(31)-C(33)	1.11(3)
C(17)-H(17C)	0.9600	O(31)-C(32)	1.90(5)
C(18)-H(18A)	0.9600	C(31)-C(32)	1.07(5)
C(18)-H(18B)	0.9600	C(31)-H(31A)	0.9600
C(18)-H(18C)	0.9600	C(31)-H(31B)	0.9600

C(31)-H(31C)	0.9600	C(2)-C(1)-H(1)	118.4
C(32)-H(32A)	0.9700	C(1)-C(2)-C(3)	121.4(3)
C(32)-H(32B)	0.9700	C(1)-C(2)-H(2)	119.3
C(33)-C(34)	0.99(4)	C(3)-C(2)-H(2)	119.3
C(33)-H(33A)	0.9700	C(2)-C(3)-C(4)	115.5(3)
C(33)-H(33B)	0.9700	C(2)-C(3)-C(6)	121.5(3)
C(34)-H(34A)	0.9600	C(4)-C(3)-C(6)	123.1(3)
C(34)-H(34B)	0.9600	C(5)-C(4)-C(3)	120.2(3)
C(34)-H(34C)	0.9600	C(5)-C(4)-H(4)	119.9
C(41)-C(42)#1	1.18(7)	C(3)-C(4)-H(4)	119.9
C(41)-C(42)#2	1.29(7)	N(1)-C(5)-C(4)	123.9(3)
N(1)-Cr(1)-N(21)	178.27(10)	N(1)-C(5)-H(5)	118.0
N(1)-Cr(1)-N(11)	88.03(9)	C(4)-C(5)-H(5)	118.0
N(21)-Cr(1)-N(11)	92.08(9)	C(8)-C(6)-C(3)	111.8(3)
N(1)-Cr(1)-Cl(2)	89.49(7)	C(8)-C(6)-C(7)	108.8(4)
N(21)-Cr(1)-Cl(2)	90.44(7)	C(3)-C(6)-C(7)	107.6(3)
N(11)-Cr(1)-Cl(2)	177.30(7)	C(8)-C(6)-C(9)	108.0(4)
N(1)-Cr(1)-Cl(1)	89.70(7)	C(3)-C(6)-C(9)	109.7(3)
N(21)-Cr(1)-Cl(1)	88.57(7)	C(7)-C(6)-C(9)	111.0(4)
N(11)-Cr(1)-Cl(1)	87.32(7)	C(6)-C(7)-H(7A)	109.5
Cl(2)-Cr(1)-Cl(1)	93.73(4)	C(6)-C(7)-H(7B)	109.5
N(1)-Cr(1)-Cl(3)	91.18(7)	H(7A)-C(7)-H(7B)	109.5
N(21)-Cr(1)-Cl(3)	90.55(7)	C(6)-C(7)-H(7C)	109.5
N(11)-Cr(1)-Cl(3)	86.58(7)	H(7A)-C(7)-H(7C)	109.5
Cl(2)-Cr(1)-Cl(3)	92.41(4)	H(7B)-C(7)-H(7C)	109.5
Cl(1)-Cr(1)-Cl(3)	173.80(4)	C(6)-C(8)-H(8A)	109.5
C(5)-N(1)-C(1)	115.8(3)	C(6)-C(8)-H(8B)	109.5
C(5)-N(1)-Cr(1)	123.7(2)	H(8A)-C(8)-H(8B)	109.5
C(1)-N(1)-Cr(1)	120.5(2)	C(6)-C(8)-H(8C)	109.5
N(1)-C(1)-C(2)	123.2(3)	H(8A)-C(8)-H(8C)	109.5
N(1)-C(1)-H(1)	118.4	H(8B)-C(8)-H(8C)	109.5

C(6)-C(9)-H(9A)	109.5	C(16)-C(17)-H(17B)	109.5
C(6)-C(9)-H(9B)	109.5	H(17A)-C(17)-H(17B)	109.5
H(9A)-C(9)-H(9B)	109.5	C(16)-C(17)-H(17C)	109.5
C(6)-C(9)-H(9C)	109.5	H(17A)-C(17)-H(17C)	109.5
H(9A)-C(9)-H(9C)	109.5	H(17B)-C(17)-H(17C)	109.5
H(9B)-C(9)-H(9C)	109.5	C(16)-C(18)-H(18A)	109.5
C(15)-N(11)-C(11)	115.9(2)	C(16)-C(18)-H(18B)	109.5
C(15)-N(11)-Cr(1)	122.07(19)	H(18A)-C(18)-H(18B)	109.5
C(11)-N(11)-Cr(1)	122.06(18)	C(16)-C(18)-H(18C)	109.5
N(11)-C(11)-C(12)	123.6(3)	H(18A)-C(18)-H(18C)	109.5
N(11)-C(11)-H(11)	118.2	H(18B)-C(18)-H(18C)	109.5
C(12)-C(11)-H(11)	118.2	C(16)-C(19)-H(19A)	109.5
C(11)-C(12)-C(13)	120.7(3)	C(16)-C(19)-H(19B)	109.5
C(11)-C(12)-H(12)	119.7	H(19A)-C(19)-H(19B)	109.5
C(13)-C(12)-H(12)	119.7	C(16)-C(19)-H(19C)	109.5
C(14)-C(13)-C(12)	115.2(3)	H(19A)-C(19)-H(19C)	109.5
C(14)-C(13)-C(16)	123.2(3)	H(19B)-C(19)-H(19C)	109.5
C(12)-C(13)-C(16)	121.5(3)	C(25)-N(21)-C(21)	116.0(3)
C(15)-C(14)-C(13)	121.1(3)	C(25)-N(21)-Cr(1)	120.1(2)
C(15)-C(14)-H(14)	119.4	C(21)-N(21)-Cr(1)	123.7(2)
C(13)-C(14)-H(14)	119.4	N(21)-C(21)-C(22)	123.1(3)
N(11)-C(15)-C(14)	123.4(3)	N(21)-C(21)-H(21)	118.4
N(11)-C(15)-H(15)	118.3	C(22)-C(21)-H(21)	118.4
C(14)-C(15)-H(15)	118.3	C(21)-C(22)-C(23)	121.1(3)
C(19)-C(16)-C(18)	112.3(4)	C(21)-C(22)-H(22)	119.5
C(19)-C(16)-C(13)	111.0(3)	C(23)-C(22)-H(22)	119.5
C(18)-C(16)-C(13)	112.8(3)	C(24)-C(23)-C(22)	115.3(3)
C(19)-C(16)-C(17)	108.4(5)	C(24)-C(23)-C(26)	123.1(3)
C(18)-C(16)-C(17)	105.5(4)	C(22)-C(23)-C(26)	121.6(3)
C(13)-C(16)-C(17)	106.3(3)	C(25)-C(24)-C(23)	120.7(3)
C(16)-C(17)-H(17A)	109.5	C(25)-C(24)-H(24)	119.7

C(23)-C(24)-H(24)	119.7	C(33)-O(31)-C(32)	124(2)
N(21)-C(25)-C(24)	123.8(3)	C(32)-C(31)-H(31A)	109.5
N(21)-C(25)-H(25)	118.1	C(32)-C(31)-H(31B)	109.5
C(24)-C(25)-H(25)	118.1	H(31A)-C(31)-H(31B)	109.5
C(27)-C(26)-C(29)	109.8(5)	C(32)-C(31)-H(31C)	109.5
C(27)-C(26)-C(28)	110.7(5)	H(31A)-C(31)-H(31C)	109.5
C(29)-C(26)-C(28)	106.4(4)	H(31B)-C(31)-H(31C)	109.5
C(27)-C(26)-C(23)	107.7(3)	C(31)-C(32)-O(31)	111(3)
C(29)-C(26)-C(23)	110.6(3)	C(31)-C(32)-H(32A)	109.4
C(28)-C(26)-C(23)	111.6(3)	O(31)-C(32)-H(32A)	109.4
C(26)-C(27)-H(27A)	109.5	C(31)-C(32)-H(32B)	109.4
C(26)-C(27)-H(27B)	109.5	O(31)-C(32)-H(32B)	109.4
H(27A)-C(27)-H(27B)	109.5	H(32A)-C(32)-H(32B)	108.0
C(26)-C(27)-H(27C)	109.5	C(34)-C(33)-O(31)	115(3)
H(27A)-C(27)-H(27C)	109.5	C(34)-C(33)-H(33A)	108.6
H(27B)-C(27)-H(27C)	109.5	O(31)-C(33)-H(33A)	108.6
C(26)-C(28)-H(28A)	109.5	C(34)-C(33)-H(33B)	108.6
C(26)-C(28)-H(28B)	109.5	O(31)-C(33)-H(33B)	108.6
H(28A)-C(28)-H(28B)	109.5	H(33A)-C(33)-H(33B)	107.6
C(26)-C(28)-H(28C)	109.5	C(33)-C(34)-H(34A)	109.5
H(28A)-C(28)-H(28C)	109.5	C(33)-C(34)-H(34B)	109.5
H(28B)-C(28)-H(28C)	109.5	H(34A)-C(34)-H(34B)	109.5
C(26)-C(29)-H(29A)	109.5	C(33)-C(34)-H(34C)	109.5
C(26)-C(29)-H(29B)	109.5	H(34A)-C(34)-H(34C)	109.5
H(29A)-C(29)-H(29B)	109.5	H(34B)-C(34)-H(34C)	109.5
C(26)-C(29)-H(29C)	109.5	C(42)#1-C(41)-C(42)#2	101(6)
H(29A)-C(29)-H(29C)	109.5	C(41)#2-C(42)-C(41)#1	134(9)
H(29B)-C(29)-H(29C)	109.5		

Symmetry transformations used to generate equivalent atoms:

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

Table A.19 **Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[CrCl_3(pytb)_3]$. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	45(1)	48(1)	47(1)	5(1)	5(1)	23(1)
Cl(1)	74(1)	70(1)	56(1)	-10(1)	-16(1)	43(1)
Cl(2)	93(1)	81(1)	87(1)	34(1)	45(1)	49(1)
Cl(3)	53(1)	59(1)	83(1)	-5(1)	-14(1)	21(1)
N(1)	42(1)	54(2)	58(1)	4(1)	8(1)	24(1)
C(1)	44(2)	55(2)	107(3)	9(2)	12(2)	20(2)
C(2)	47(2)	76(3)	121(3)	9(2)	14(2)	33(2)
C(3)	62(2)	69(2)	63(2)	14(2)	14(2)	43(2)
C(4)	63(2)	50(2)	74(2)	8(2)	13(2)	29(2)
C(5)	44(2)	57(2)	64(2)	2(2)	5(1)	26(2)
C(6)	86(3)	88(3)	83(2)	23(2)	18(2)	63(2)
C(7)	141(4)	139(4)	95(3)	25(3)	8(3)	108(4)
C(8)	122(4)	82(3)	153(5)	19(3)	24(3)	70(3)
C(9)	112(4)	126(4)	100(3)	22(3)	34(3)	91(3)
N(11)	40(1)	52(1)	47(1)	2(1)	0(1)	23(1)
C(11)	44(2)	64(2)	51(2)	4(1)	1(1)	32(2)
C(12)	62(2)	59(2)	50(2)	6(1)	1(1)	37(2)
C(13)	51(2)	41(2)	54(2)	-1(1)	6(1)	24(1)
C(14)	46(2)	59(2)	67(2)	11(2)	9(1)	32(2)
C(15)	48(2)	56(2)	64(2)	12(1)	1(1)	30(2)
C(16)	68(2)	63(2)	79(2)	21(2)	27(2)	35(2)
C(17)	150(5)	160(5)	65(3)	19(3)	31(3)	42(4)
C(18)	105(4)	135(4)	136(4)	54(4)	70(3)	69(3)
C(19)	183(6)	64(3)	248(8)	69(4)	132(6)	61(4)
N(21)	53(1)	46(1)	45(1)	3(1)	2(1)	23(1)

C(21)	69(2)	58(2)	43(2)	5(1)	1(1)	32(2)
C(22)	75(2)	58(2)	49(2)	3(1)	8(2)	37(2)
C(23)	46(2)	44(2)	56(2)	6(1)	4(1)	18(1)
C(24)	67(2)	57(2)	46(2)	7(1)	-2(1)	33(2)
C(25)	72(2)	61(2)	42(2)	-1(1)	1(1)	36(2)
C(26)	67(2)	58(2)	72(2)	9(2)	8(2)	36(2)
C(27)	111(4)	60(3)	418(14)	-43(5)	-47(6)	50(3)
C(28)	192(6)	219(7)	92(3)	37(4)	23(4)	176(6)
C(29)	120(4)	137(4)	97(3)	29(3)	35(3)	95(4)
O(31)	170(9)	125(7)	112(6)	8(5)	0(6)	91(7)
C(31)	119(13)	210(20)	200(30)	80(20)	-32(15)	60(13)
C(32)	520(70)	350(50)	140(20)	150(30)	160(40)	330(50)
C(33)	160(20)	250(30)	390(50)	-200(30)	10(20)	100(20)
C(34)	320(70)	280(40)	160(20)	-80(30)	-30(30)	210(50)
C(41)	410(60)	400(90)	410(80)	220(60)	230(50)	260(60)
C(42)	510(90)	360(70)	370(60)	240(60)	290(60)	260(50)

Table A.20 **Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[CrCl_3(pytb)_3]$**

	x	y	z	U(eq)
H(1)	8954	440	3366	85
H(2)	9201	-80	3262	96
H(4)	7889	-1094	3269	74
H(5)	7673	-546	3335	66
H(7A)	9229	-723	4176	162
H(7B)	9016	-1261	4104	162
H(7C)	8729	-1057	4524	162

H(8A)	8110	-1583	3430	166
H(8B)	8464	-1707	3024	166
H(8C)	8228	-1497	2454	166
H(9A)	8992	-816	1981	148
H(9B)	9183	-1109	2424	148
H(9C)	9386	-586	2667	148
H(11)	8035	-95	4989	61
H(12)	7546	-557	6026	64
H(14)	6647	-171	5291	66
H(15)	7126	221	4186	65
H(17A)	6776	-566	7850	211
H(17B)	7106	-122	7321	211
H(17C)	7234	-510	7460	211
H(18A)	6095	-829	6063	181
H(18B)	6349	-361	6572	181
H(18C)	6104	-834	7065	181
H(19A)	6483	-1328	6017	248
H(19B)	6435	-1343	7014	248
H(19C)	6921	-1172	6594	248
H(21)	7852	1054	4788	68
H(22)	7542	1525	4846	71
H(24)	7575	1581	2304	67
H(25)	7855	1085	2305	68
H(27A)	7565	2603	3962	289
H(27B)	7923	2524	3444	289
H(27C)	7822	2372	4404	289
H(28A)	6897	1654	2555	203
H(28B)	7359	2112	2346	203
H(28C)	6954	2135	2812	203
H(29A)	7022	1736	4798	157
H(29B)	6670	1457	4067	157

H(29C)	6796	1968	4262	157
H(31A)	5662	44	-216	282
H(31B)	6053	306	466	282
H(31C)	5848	571	-32	282
H(32A)	5649	406	1173	350
H(32B)	5429	-119	921	350
H(33A)	4830	10	-748	316
H(33B)	4726	-368	-54	316
H(34A)	4414	96	274	340
H(34B)	4215	-436	133	340
H(34C)	4296	-112	-651	340

Table A.21 Torsion angles [°] for $[CrCl_3(pytb)_3]$

N(11)-Cr(1)-N(1)-C(5)	47.5(2)	Cr(1)-N(1)-C(5)-C(4)	-178.1(2)
Cl(2)-Cr(1)-N(1)-C(5)	-133.5(2)	C(3)-C(4)-C(5)-N(1)	-0.9(5)
Cl(1)-Cr(1)-N(1)-C(5)	-39.8(2)	C(2)-C(3)-C(6)-C(8)	-168.8(4)
Cl(3)-Cr(1)-N(1)-C(5)	134.1(2)	C(4)-C(3)-C(6)-C(8)	12.1(5)
N(11)-Cr(1)-N(1)-C(1)	-130.8(3)	C(2)-C(3)-C(6)-C(7)	71.8(5)
Cl(2)-Cr(1)-N(1)-C(1)	48.1(3)	C(4)-C(3)-C(6)-C(7)	-107.3(4)
Cl(1)-Cr(1)-N(1)-C(1)	141.9(3)	C(2)-C(3)-C(6)-C(9)	-49.1(5)
Cl(3)-Cr(1)-N(1)-C(1)	-44.3(3)	C(4)-C(3)-C(6)-C(9)	131.8(4)
C(5)-N(1)-C(1)-C(2)	0.7(5)	N(1)-Cr(1)-N(11)-C(15)	-143.5(2)
Cr(1)-N(1)-C(1)-C(2)	179.1(3)	N(21)-Cr(1)-N(11)-C(15)	34.8(2)
N(1)-C(1)-C(2)-C(3)	-1.1(7)	Cl(1)-Cr(1)-N(11)-C(15)	-53.7(2)
C(1)-C(2)-C(3)-C(4)	0.5(6)	Cl(3)-Cr(1)-N(11)-C(15)	125.2(2)
C(1)-C(2)-C(3)-C(6)	-178.7(4)	N(1)-Cr(1)-N(11)-C(11)	36.9(2)
C(2)-C(3)-C(4)-C(5)	0.4(5)	N(21)-Cr(1)-N(11)-C(11)	-144.9(2)
C(6)-C(3)-C(4)-C(5)	179.6(3)	Cl(1)-Cr(1)-N(11)-C(11)	126.7(2)
C(1)-N(1)-C(5)-C(4)	0.3(5)	Cl(3)-Cr(1)-N(11)-C(11)	-54.4(2)

C(15)-N(11)-C(11)-C(12)	2.0(4)	N(11)-Cr(1)-N(21)-C(21)	39.0(2)
Cr(1)-N(11)-C(11)-C(12)	-178.3(2)	Cl(2)-Cr(1)-N(21)-C(21)	-140.0(2)
N(11)-C(11)-C(12)-C(13)	-3.6(5)	Cl(1)-Cr(1)-N(21)-C(21)	126.3(2)
C(11)-C(12)-C(13)-C(14)	1.5(4)	Cl(3)-Cr(1)-N(21)-C(21)	-47.5(2)
C(11)-C(12)-C(13)-C(16)	-176.3(3)	C(25)-N(21)-C(21)-C(22)	2.5(5)
C(12)-C(13)-C(14)-C(15)	1.9(5)	Cr(1)-N(21)-C(21)-C(22)	-173.2(2)
C(16)-C(13)-C(14)-C(15)	179.7(3)	N(21)-C(21)-C(22)-C(23)	-1.4(5)
C(11)-N(11)-C(15)-C(14)	1.6(4)	C(21)-C(22)-C(23)-C(24)	-1.1(5)
Cr(1)-N(11)-C(15)-C(14)	-178.1(2)	C(21)-C(22)-C(23)-C(26)	-179.4(3)
C(13)-C(14)-C(15)-N(11)	-3.7(5)	C(22)-C(23)-C(24)-C(25)	2.6(5)
C(14)-C(13)-C(16)-C(19)	128.8(5)	C(26)-C(23)-C(24)-C(25)	-179.2(3)
C(12)-C(13)-C(16)-C(19)	-53.6(5)	C(21)-N(21)-C(25)-C(24)	-1.0(5)
C(14)-C(13)-C(16)-C(18)	1.7(5)	Cr(1)-N(21)-C(25)-C(24)	174.9(3)
C(12)-C(13)-C(16)-C(18)	179.3(4)	C(23)-C(24)-C(25)-N(21)	-1.6(5)
C(14)-C(13)-C(16)-C(17)	-113.5(4)	C(24)-C(23)-C(26)-C(27)	-104.0(5)
C(12)-C(13)-C(16)-C(17)	64.2(4)	C(22)-C(23)-C(26)-C(27)	74.2(5)
N(11)-Cr(1)-N(21)-C(25)	-136.5(2)	C(24)-C(23)-C(26)-C(29)	136.0(4)
Cl(2)-Cr(1)-N(21)-C(25)	44.5(2)	C(22)-C(23)-C(26)-C(29)	-45.9(5)
Cl(1)-Cr(1)-N(21)-C(25)	-49.2(2)	C(24)-C(23)-C(26)-C(28)	17.8(5)
Cl(3)-Cr(1)-N(21)-C(25)	136.9(2)	C(22)-C(23)-C(26)-C(28)	-164.1(4)

Symmetry transformations used to generate equivalent atoms:

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

[$CrCl_3(bipy)(H_2O)$]

Table A.22 **Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [$CrCl_3(bipy)(H_2O)$]. U(eq) is defined as one-third of the trace of the orthogonalised U^{ij} tensor**

	x	y	z	U(eq)
Cr(1)	8853(1)	1809(1)	8330(1)	34(1)
Cl(1)	9614(1)	1872(1)	9761(1)	51(1)
Cl(2)	8148(1)	1943(1)	6740(1)	44(1)
Cl(3)	8699(1)	-360(1)	8875(1)	57(1)
N(1)	8973(1)	3795(2)	8041(2)	36(1)
N(2)	8460(1)	2637(2)	9782(2)	36(1)
C(1)	8733(1)	4622(3)	8802(3)	40(1)
C(2)	8810(1)	5977(3)	8774(3)	49(1)
C(3)	9132(1)	6471(3)	7918(4)	58(1)
C(4)	9368(1)	5619(3)	7126(3)	54(1)
C(5)	9284(1)	4277(3)	7222(3)	46(1)
C(6)	8412(1)	3967(3)	9704(3)	39(1)
C(7)	8092(1)	4634(3)	10455(3)	50(1)
C(8)	7838(1)	3935(3)	11342(3)	55(1)
C(9)	7907(1)	2605(3)	11469(3)	52(1)
C(10)	8216(1)	1970(3)	10664(3)	43(1)
O(1)	9231(1)	1302(2)	6791(2)	46(1)
O(2)	10000	-352(3)	7500	49(1)

Table A.23 Bond lengths [Å] and angles [°] for [$CrCl_3$(bipy)(H_2O)]

Cr(1)-O(1)	2.003(2)	O(2)-H(2A)	0.84(3)
Cr(1)-N(1)	2.059(2)	O(1)-Cr(1)-N(1)	92.28(9)
Cr(1)-N(2)	2.066(2)	O(1)-Cr(1)-N(2)	170.71(9)
Cr(1)-Cl(3)	2.3083(8)	N(1)-Cr(1)-N(2)	78.79(9)
Cr(1)-Cl(2)	2.3114(8)	O(1)-Cr(1)-Cl(3)	93.31(7)
Cr(1)-Cl(1)	2.3435(8)	N(1)-Cr(1)-Cl(3)	174.10(6)
N(1)-C(5)	1.331(4)	N(2)-Cr(1)-Cl(3)	95.70(7)
N(1)-C(1)	1.345(3)	O(1)-Cr(1)-Cl(2)	87.50(7)
N(2)-C(10)	1.341(3)	N(1)-Cr(1)-Cl(2)	88.83(6)
N(2)-C(6)	1.353(4)	N(2)-Cr(1)-Cl(2)	89.74(6)
C(1)-C(2)	1.386(4)	Cl(3)-Cr(1)-Cl(2)	93.26(3)
C(1)-C(6)	1.476(4)	O(1)-Cr(1)-Cl(1)	88.28(7)
C(2)-C(3)	1.382(5)	N(1)-Cr(1)-Cl(1)	85.16(6)
C(2)-H(2)	0.9300	N(2)-Cr(1)-Cl(1)	93.46(6)
C(3)-C(4)	1.374(5)	Cl(3)-Cr(1)-Cl(1)	93.16(3)
C(3)-H(3)	0.9300	Cl(2)-Cr(1)-Cl(1)	172.51(3)
C(4)-C(5)	1.381(4)	C(5)-N(1)-C(1)	119.9(2)
C(4)-H(4)	0.9300	C(5)-N(1)-Cr(1)	124.3(2)
C(5)-H(5)	0.9300	C(1)-N(1)-Cr(1)	115.63(18)
C(6)-C(7)	1.384(4)	C(10)-N(2)-C(6)	119.0(2)
C(7)-C(8)	1.376(5)	C(10)-N(2)-Cr(1)	125.93(19)
C(7)-H(7)	0.9300	C(6)-N(2)-Cr(1)	114.66(17)
C(8)-C(9)	1.361(5)	N(1)-C(1)-C(2)	121.3(3)
C(8)-H(8)	0.9300	N(1)-C(1)-C(6)	114.9(2)
C(9)-C(10)	1.382(4)	C(2)-C(1)-C(6)	123.8(3)
C(9)-H(9)	0.9300	C(3)-C(2)-C(1)	118.5(3)
C(10)-H(10)	0.9300	C(3)-C(2)-H(2)	120.8
O(1)-H(1A)	0.80(3)	C(1)-C(2)-H(2)	120.8
O(1)-H(1B)	0.72(4)	C(4)-C(3)-C(2)	119.8(3)

C(4)-C(3)-H(3)	120.1	C(6)-C(7)-H(7)	120.4
C(2)-C(3)-H(3)	120.1	C(9)-C(8)-C(7)	119.4(3)
C(3)-C(4)-C(5)	119.0(3)	C(9)-C(8)-H(8)	120.3
C(3)-C(4)-H(4)	120.5	C(7)-C(8)-H(8)	120.3
C(5)-C(4)-H(4)	120.5	C(8)-C(9)-C(10)	119.5(3)
N(1)-C(5)-C(4)	121.6(3)	C(8)-C(9)-H(9)	120.2
N(1)-C(5)-H(5)	119.2	C(10)-C(9)-H(9)	120.2
C(4)-C(5)-H(5)	119.2	N(2)-C(10)-C(9)	121.6(3)
N(2)-C(6)-C(7)	121.0(3)	N(2)-C(10)-H(10)	119.2
N(2)-C(6)-C(1)	114.9(2)	C(9)-C(10)-H(10)	119.2
C(7)-C(6)-C(1)	124.1(3)	Cr(1)-O(1)-H(1A)	122(2)
C(8)-C(7)-C(6)	119.3(3)	Cr(1)-O(1)-H(1B)	111(3)
C(8)-C(7)-H(7)	120.4	H(1A)-O(1)-H(1B)	111(4)

Table A.24 **Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[CrCl_3(bipy)(H_2O)]$. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	46(1)	28(1)	28(1)	0(1)	5(1)	5(1)
Cl(1)	59(1)	53(1)	38(1)	-4(1)	-6(1)	17(1)
Cl(2)	46(1)	46(1)	38(1)	-2(1)	3(1)	1(1)
Cl(3)	98(1)	29(1)	43(1)	3(1)	8(1)	0(1)
N(1)	42(1)	32(1)	34(1)	4(1)	1(1)	1(1)
N(2)	44(1)	34(1)	32(1)	-2(1)	3(1)	2(1)
C(1)	45(2)	32(1)	39(1)	0(1)	-7(1)	3(1)
C(2)	58(2)	30(1)	55(2)	0(1)	-6(1)	2(1)
C(3)	61(2)	36(2)	71(2)	12(2)	-13(2)	-6(1)
C(4)	49(2)	52(2)	58(2)	21(2)	-5(1)	-10(1)

C(5)	42(2)	49(2)	46(2)	9(1)	0(1)	1(1)
C(6)	43(1)	36(1)	36(1)	-7(1)	-1(1)	2(1)
C(7)	52(2)	43(2)	53(2)	-16(1)	0(1)	5(1)
C(8)	46(2)	67(2)	52(2)	-21(2)	10(1)	3(2)
C(9)	49(2)	66(2)	41(2)	-7(1)	9(1)	-7(2)
C(10)	47(2)	46(2)	36(2)	-2(1)	4(1)	-4(1)
O(1)	50(1)	50(1)	36(1)	-7(1)	4(1)	10(1)
O(2)	62(2)	44(2)	39(2)	0	4(1)	0

Table A.25 **Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for [$CrCl_3$(bipy)(H_2O)]**

	x	y	z	U(eq)
H(2)	8648	6541	9319	58
H(3)	9188	7376	7878	69
H(4)	9581	5941	6536	65
H(5)	9448	3696	6701	55
H(7)	8050	5544	10362	59
H(8)	7620	4368	11850	66
H(9)	7748	2127	12093	62
H(10)	8254	1057	10736	52
H(1A)	9095(12)	1030(30)	6080(40)	55
H(1B)	9441(13)	890(40)	7030(40)	55
H(2A)	9985(13)	-870(30)	6830(30)	59

Table A.26 Torsion angles [°] for [$CrCl_3(bipy)(H_2O)$]

O(1)-Cr(1)-N(1)-C(5)	-10.0(2)	Cr(1)-N(1)-C(1)-C(6)	-1.3(3)
N(2)-Cr(1)-N(1)-C(5)	172.6(2)	N(1)-C(1)-C(2)-C(3)	1.5(4)
Cl(3)-Cr(1)-N(1)-C(5)	151.6(6)	C(6)-C(1)-C(2)-C(3)	177.9(3)
Cl(2)-Cr(1)-N(1)-C(5)	-97.5(2)	C(1)-C(2)-C(3)-C(4)	-0.3(4)
Cl(1)-Cr(1)-N(1)-C(5)	78.1(2)	C(2)-C(3)-C(4)-C(5)	-1.0(5)
O(1)-Cr(1)-N(1)-C(1)	173.47(18)	C(1)-N(1)-C(5)-C(4)	-0.1(4)
N(2)-Cr(1)-N(1)-C(1)	-3.95(18)	Cr(1)-N(1)-C(5)-C(4)	-176.5(2)
Cl(3)-Cr(1)-N(1)-C(1)	-24.9(8)	C(3)-C(4)-C(5)-N(1)	1.3(4)
Cl(2)-Cr(1)-N(1)-C(1)	86.02(17)	C(10)-N(2)-C(6)-C(7)	-4.0(4)
Cl(1)-Cr(1)-N(1)-C(1)	-98.46(18)	Cr(1)-N(2)-C(6)-C(7)	169.3(2)
O(1)-Cr(1)-N(2)-C(10)	165.6(5)	C(10)-N(2)-C(6)-C(1)	174.4(2)
N(1)-Cr(1)-N(2)-C(10)	-178.3(2)	Cr(1)-N(2)-C(6)-C(1)	-12.3(3)
Cl(3)-Cr(1)-N(2)-C(10)	-0.4(2)	N(1)-C(1)-C(6)-N(2)	9.0(3)
Cl(2)-Cr(1)-N(2)-C(10)	92.9(2)	C(2)-C(1)-C(6)-N(2)	-167.6(2)
Cl(1)-Cr(1)-N(2)-C(10)	-93.9(2)	N(1)-C(1)-C(6)-C(7)	-172.6(2)
O(1)-Cr(1)-N(2)-C(6)	-7.2(7)	C(2)-C(1)-C(6)-C(7)	10.8(4)
N(1)-Cr(1)-N(2)-C(6)	8.99(18)	N(2)-C(6)-C(7)-C(8)	3.0(4)
Cl(3)-Cr(1)-N(2)-C(6)	-173.12(17)	C(1)-C(6)-C(7)-C(8)	-175.2(3)
Cl(2)-Cr(1)-N(2)-C(6)	-79.87(17)	C(6)-C(7)-C(8)-C(9)	0.4(4)
Cl(1)-Cr(1)-N(2)-C(6)	93.35(17)	C(7)-C(8)-C(9)-C(10)	-2.7(5)
C(5)-N(1)-C(1)-C(2)	-1.3(4)	C(6)-N(2)-C(10)-C(9)	1.6(4)
Cr(1)-N(1)-C(1)-C(2)	175.4(2)	Cr(1)-N(2)-C(10)-C(9)	-170.9(2)
C(5)-N(1)-C(1)-C(6)	-178.0(2)	C(8)-C(9)-C(10)-N(2)	1.8(4)

Table A.27 Hydrogen bonds for [$CrCl_3$(bipy)(H_2O)] [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1B)...O(2)	0.72(4)	1.98(4)	2.690(3)	173(4)
O(1)-H(1A)...Cl(3)#1	0.80(3)	2.40(4)	3.192(2)	176(3)
O(2)-H(2A)...Cl(1)#1	0.84(3)	2.39(3)	3.1671(17)	156(3)

Symmetry transformations used to generate equivalent atoms:

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

[$HpyNH_2$][$CrCl_4$(bipy)]

Table A.28 **Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [$HpyNH_2$][$CrCl_4$(bipy)]. U(eq) is defined as one-third of the trace of the orthogonalised U^{ij} tensor**

	x	y	z	U(eq)
Cr(1)	2303(1)	2244(1)	5000	33(1)
Cl(1)	4444(1)	2771(1)	5000	46(1)
Cl(2)	255(1)	1482(1)	5000	40(1)
Cl(3)	1754(1)	3416(1)	3976(1)	50(1)
N(1)	2854(2)	1042(2)	4203(2)	36(1)
C(1)	3152(3)	109(2)	4551(2)	36(1)
C(2)	3473(3)	-767(3)	4094(2)	49(1)
C(3)	3490(4)	-691(3)	3260(2)	55(1)
C(4)	3209(4)	266(3)	2907(2)	53(1)
C(5)	2896(3)	1115(3)	3387(2)	43(1)
N(2)	5000	5000	1603(3)	53(1)
C(6)	4807(4)	4087(3)	1999(2)	53(1)
C(7)	4794(4)	4061(3)	2814(2)	55(1)
C(8)	5000	5000	3254(3)	60(1)
N(3)	5000	5000	4043(3)	125(4)
Cl(4)	2165(3)	6616(2)	4095(2)	166(1)
C(9)	1356(6)	6046(5)	5000	65(2)

Table A.29 Bond lengths [Å] and angles [°] for $[HpyNH_2][CrCl_4(bipy)]$

Cr(1)-N(1)	2.088(3)	C(9)-H(9A)	0.90(7)
Cr(1)-N(1)#1	2.088(3)	C(9)-H(9B)	0.97(7)
Cr(1)-Cl(3)#1	2.3172(9)		
Cr(1)-Cl(3)	2.3172(9)	N(1)-Cr(1)-N(1)#1	78.02(14)
Cr(1)-Cl(1)	2.3415(13)	N(1)-Cr(1)-Cl(3)#1	172.25(7)
Cr(1)-Cl(2)	2.3515(12)	N(1)#1-Cr(1)-Cl(3)#1	94.23(7)
N(1)-C(1)	1.347(4)	N(1)-Cr(1)-Cl(3)	94.23(7)
N(1)-C(5)	1.348(4)	N(1)#1-Cr(1)-Cl(3)	172.25(7)
C(1)-C(2)	1.381(4)	Cl(3)#1-Cr(1)-Cl(3)	93.52(5)
C(1)-C(1)#1	1.479(6)	N(1)-Cr(1)-Cl(1)	86.63(7)
C(2)-C(3)	1.378(5)	N(1)#1-Cr(1)-Cl(1)	86.63(7)
C(2)-H(2)	0.94(4)	Cl(3)#1-Cr(1)-Cl(1)	93.22(4)
C(3)-C(4)	1.374(6)	Cl(3)-Cr(1)-Cl(1)	93.22(4)
C(3)-H(3)	0.94(4)	N(1)-Cr(1)-Cl(2)	87.46(7)
C(4)-C(5)	1.372(5)	N(1)#1-Cr(1)-Cl(2)	87.46(7)
C(4)-H(4)	0.88(5)	Cl(3)#1-Cr(1)-Cl(2)	91.99(4)
C(5)-H(5)	0.93(4)	Cl(3)-Cr(1)-Cl(2)	91.99(4)
N(2)-C(6)#2	1.340(4)	Cl(1)-Cr(1)-Cl(2)	172.39(5)
N(2)-C(6)	1.340(4)	C(1)-N(1)-C(5)	118.5(3)
N(2)-H(2N)	0.76(7)	C(1)-N(1)-Cr(1)	115.5(2)
C(6)-C(7)	1.344(5)	C(5)-N(1)-Cr(1)	126.0(2)
C(6)-H(6)	0.94(4)	N(1)-C(1)-C(2)	121.6(3)
C(7)-C(8)	1.406(4)	N(1)-C(1)-C(1)#1	115.26(16)
C(7)-H(7)	0.80(4)	C(2)-C(1)-C(1)#1	123.1(2)
C(8)-N(3)	1.300(7)	C(3)-C(2)-C(1)	119.5(3)
C(8)-C(7)#2	1.406(4)	C(3)-C(2)-H(2)	123(3)
N(3)-H(3N)	0.96(7)	C(1)-C(2)-H(2)	118(3)
Cl(4)-C(9)	1.861(5)	C(4)-C(3)-C(2)	118.8(3)
C(9)-Cl(4)#1	1.861(5)	C(4)-C(3)-H(3)	120(2)

C(2)-C(3)-H(3)	121(2)	C(6)-C(7)-C(8)	119.6(4)
C(5)-C(4)-C(3)	119.6(3)	C(6)-C(7)-H(7)	122(3)
C(5)-C(4)-H(4)	116(3)	C(8)-C(7)-H(7)	119(3)
C(3)-C(4)-H(4)	124(3)	N(3)-C(8)-C(7)	121.1(2)
N(1)-C(5)-C(4)	122.1(3)	N(3)-C(8)-C(7)#2	121.1(2)
N(1)-C(5)-H(5)	118(2)	C(7)-C(8)-C(7)#2	117.9(5)
C(4)-C(5)-H(5)	120(2)	C(8)-N(3)-H(3N)	112(4)
C(6)#2-N(2)-C(6)	121.7(5)	Cl(4)#1-C(9)-Cl(4)	106.6(3)
C(6)#2-N(2)-H(2N)	119.2(2)	Cl(4)#1-C(9)-H(9A)	109(2)
C(6)-N(2)-H(2N)	119.2(2)	Cl(4)-C(9)-H(9A)	109(2)
N(2)-C(6)-C(7)	120.6(4)	Cl(4)#1-C(9)-H(9B)	115(2)
N(2)-C(6)-H(6)	120(2)	Cl(4)-C(9)-H(9B)	115(2)
C(7)-C(6)-H(6)	119(2)	H(9A)-C(9)-H(9B)	102(6)

Symmetry transformations used to generate equivalent atoms:

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

Table A.30 **Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[HpyNH_2][CrCl_4(bipy)]$. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	39(1)	25(1)	35(1)	0	0	2(1)
Cl(1)	42(1)	34(1)	63(1)	0	0	-3(1)
Cl(2)	44(1)	38(1)	39(1)	0	0	-2(1)
Cl(3)	62(1)	39(1)	50(1)	14(1)	3(1)	8(1)
N(1)	39(1)	32(1)	36(1)	0(1)	0(1)	0(1)
C(1)	36(1)	31(1)	41(2)	-2(1)	0(1)	-1(1)
C(2)	55(2)	32(2)	59(2)	-10(2)	-4(2)	6(1)
C(3)	60(2)	50(2)	54(2)	-21(2)	-2(2)	8(2)

C(4)	54(2)	65(2)	40(2)	-9(2)	2(2)	-1(2)
C(5)	49(2)	44(2)	37(2)	1(1)	2(1)	3(1)
N(2)	53(2)	70(3)	36(2)	0	0	2(2)
C(6)	53(2)	57(2)	49(2)	-11(2)	0(2)	-2(2)
C(7)	74(2)	44(2)	47(2)	-2(2)	4(2)	-10(2)
C(8)	97(4)	46(3)	36(2)	0	0	-12(3)
N(3)	281(12)	54(3)	39(3)	0	0	-37(5)
Cl(4)	157(2)	126(2)	217(3)	-73(2)	11(2)	-15(1)
C(9)	55(3)	43(3)	97(5)	0	0	-4(2)

Table A.31 **Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[HpyNH_2][CrCl_4(bipy)]$**

	x	y	z	U(eq)
H(2)	3620(40)	-1400(30)	4370(30)	60(11)
H(3)	3710(40)	-1280(30)	2940(20)	55(10)
H(4)	3210(40)	380(40)	2380(30)	70(13)
H(5)	2740(30)	1770(30)	3150(20)	42(9)
H(2N)	5000	5000	1140(40)	56(17)
H(6)	4690(40)	3450(30)	1710(30)	53(11)
H(7)	4650(40)	3520(30)	3060(30)	58(12)
H(3N)	5490(70)	4430(60)	4260(40)	150
H(9A)	1460(70)	5340(60)	5000	78
H(9B)	430(70)	6120(50)	5000	78

Table A.32 Torsion angles [°] for [HpyNH$_2$][CrCl$_4$(bipy)]

N(1)#1-Cr(1)-N(1)-C(1)	6.0(2)
Cl(1)-Cr(1)-N(1)-C(1)	93.3(2)
Cl(2)-Cr(1)-N(1)-C(1)	-81.9(2)
N(1)#1-Cr(1)-N(1)-C(5)	-176.1(2)
Cl(3)-Cr(1)-N(1)-C(5)	4.1(3)
Cl(1)-Cr(1)-N(1)-C(5)	-88.8(3)
Cl(2)-Cr(1)-N(1)-C(5)	95.9(3)
C(5)-N(1)-C(1)-C(2)	-1.2(4)
Cr(1)-N(1)-C(1)-C(2)	176.8(2)
C(5)-N(1)-C(1)-C(1)#1	176.8(2)
Cr(1)-N(1)-C(1)-C(1)#1	-5.2(2)
N(1)-C(1)-C(2)-C(3)	0.0(5)
C(1)#1-C(1)-C(2)-C(3)	-177.8(3)
C(1)-C(2)-C(3)-C(4)	1.2(6)
C(2)-C(3)-C(4)-C(5)	-1.2(6)
C(1)-N(1)-C(5)-C(4)	1.2(5)
Cr(1)-N(1)-C(5)-C(4)	-176.6(3)
C(3)-C(4)-C(5)-N(1)	0.0(6)
C(6)#2-N(2)-C(6)-C(7)	0.4(3)
N(2)-C(6)-C(7)-C(8)	-0.7(6)
C(6)-C(7)-C(8)-N(3)	-179.6(3)
C(6)-C(7)-C(8)-C(7)#2	0.4(3)

Symmetry transformations used to generate equivalent atoms:

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

Table A.33 Hydrogen bonds for $[HpyNH_2][CrCl_4(bipy)]$ [Å and º]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2N)...Cl(2)#3	0.76(7)	2.67(5)	3.250(4)	134.9(10)
N(3)-H(3N)...Cl(1)	0.96(7)	2.66(8)	3.278(3)	123(6)
N(3)-H(3N)...Cl(4)#2	0.96(7)	2.80(7)	3.605(3)	142(6)

Symmetry transformations used to generate equivalent atoms:

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

$[CrCl_2(bipy)_2][Cl]\cdot H_2O$

Table A.34 **Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[CrCl_2(bipy)_2][Cl]\cdot H_2O$. U(eq) is defined as one-third of the trace of the orthogonalised U^{ij} tensor**

	x	y	z	U(eq)
Cr(1)	2223(1)	416(1)	533(1)	73(1)
Cl(1)	3202(1)	995(1)	197(1)	97(1)
Cl(2)	541(1)	644(1)	249(1)	86(1)
N(1)	1359(4)	-65(2)	907(2)	77(1)
N(2)	1979(5)	770(2)	1132(2)	87(2)
N(3)	3665(4)	105(2)	759(2)	80(2)
N(4)	2554(4)	-32(2)	7(2)	73(1)
C(1)	983(7)	90(3)	1307(3)	95(2)
C(2)	277(9)	-177(4)	1577(3)	131(3)
C(3)	-40(10)	-597(4)	1408(4)	143(4)
C(4)	371(8)	-763(3)	1020(3)	114(3)
C(5)	1079(6)	-485(3)	767(3)	89(2)
C(6)	1356(7)	547(3)	1441(3)	96(2)
C(7)	1150(9)	759(5)	1859(4)	147(4)
C(8)	1555(12)	1184(5)	1955(4)	148(4)
C(9)	2189(9)	1391(4)	1663(4)	128(4)
C(10)	2378(7)	1186(3)	1232(3)	106(3)
C(11)	4081(5)	-229(2)	478(2)	76(2)
C(12)	5021(6)	-475(3)	605(3)	96(2)
C(13)	5538(7)	-375(4)	1001(4)	116(3)
C(14)	5147(7)	-30(3)	1284(3)	112(3)
C(15)	4198(7)	205(3)	1148(3)	106(2)
C(16)	3463(5)	-306(2)	62(2)	75(2)

C(17)	3748(7)	-627(2)	-260(3)	93(2)
C(18)	3130(8)	-677(3)	-637(3)	103(2)
C(19)	2228(7)	-398(3)	-697(3)	103(2)
C(20)	1956(6)	-82(3)	-367(3)	91(2)
Cr(2)	2036(1)	2963(1)	537(1)	79(1)
Cl(3)	3180(2)	3482(1)	194(1)	102(1)
Cl(4)	416(2)	3305(1)	311(1)	100(1)
N(5)	1063(5)	2446(2)	811(2)	79(1)
N(6)	1972(4)	2518(2)	7(2)	80(2)
N(7)	3384(5)	2632(2)	825(2)	83(2)
N(8)	2201(5)	3307(2)	1133(2)	89(2)
C(21)	847(6)	2098(2)	525(3)	82(2)
C(22)	146(7)	1743(3)	649(3)	97(2)
C(23)	-359(7)	1760(3)	1078(4)	110(3)
C(24)	-108(7)	2109(3)	1364(3)	107(2)
C(25)	586(7)	2452(3)	1218(3)	99(2)
C(26)	1378(5)	2128(2)	74(2)	78(2)
C(27)	1292(7)	1789(3)	-254(3)	105(2)
C(28)	1834(9)	1841(4)	-659(3)	120(3)
C(29)	2405(8)	2241(4)	-734(3)	116(3)
C(30)	2465(7)	2565(3)	-391(3)	102(2)
C(31)	3653(6)	2783(3)	1227(3)	90(2)
C(32)	4532(9)	2553(4)	1474(3)	131(3)
C(33)	5067(9)	2207(4)	1287(5)	142(4)
C(34)	4786(8)	2060(4)	865(4)	127(3)
C(35)	3927(6)	2281(3)	631(3)	100(2)
C(36)	3036(7)	3174(3)	1396(3)	94(2)
C(37)	3287(9)	3406(4)	1803(3)	129(3)
C(38)	2659(13)	3784(5)	1912(4)	148(4)
C(39)	1823(12)	3927(4)	1642(4)	145(4)
C(40)	1610(9)	3670(3)	1254(3)	120(3)

Cl(5)	8871(13)	120(5)	2664(3)	293(6)
Cl(6)	4814(13)	980(5)	1997(5)	380(10)
Cl(7)	7750(20)	6179(10)	1740(5)	530(20)
Cl(8)	9180(20)	1837(8)	2547(6)	486(16)
O(1)	252(18)	2982(10)	2305(5)	468(18)
O(2)	7390(30)	8686(12)	1741(6)	630(30)
O(3)	50(30)	4107(19)	2471(9)	1040(60)
O(4)	1480(40)	2393(8)	2445(8)	660(40)
O(5)	7960(20)	4680(10)	2130(8)	548(19)

Table A.35 Bond lengths [Å] and angles [°] for $[CrCl_2(bipy)_2][Cl]\cdot H_2O$

Cr(1)-N(1)	2.063(6)	C(2)-H(2)	0.9300
Cr(1)-N(2)	2.065(6)	C(3)-C(4)	1.335(13)
Cr(1)-N(4)	2.065(6)	C(3)-H(3)	0.9300
Cr(1)-N(3)	2.068(5)	C(4)-C(5)	1.391(10)
Cr(1)-Cl(1)	2.285(2)	C(4)-H(4)	0.9300
Cr(1)-Cl(2)	2.2906(18)	C(5)-H(5)	0.9300
N(1)-C(5)	1.336(8)	C(6)-C(7)	1.401(12)
N(1)-C(1)	1.342(9)	C(7)-C(8)	1.359(15)
N(2)-C(10)	1.337(9)	C(7)-H(7)	0.9300
N(2)-C(6)	1.345(10)	C(8)-C(9)	1.298(14)
N(3)-C(15)	1.346(9)	C(8)-H(8)	0.9300
N(3)-C(11)	1.372(8)	C(9)-C(10)	1.423(12)
N(4)-C(20)	1.324(9)	C(9)-H(9)	0.9300
N(4)-C(16)	1.365(8)	C(10)-H(10)	0.9300
C(1)-C(2)	1.401(12)	C(11)-C(12)	1.393(10)
C(1)-C(6)	1.459(11)	C(11)-C(16)	1.450(9)
C(2)-C(3)	1.375(13)	C(12)-C(13)	1.356(12)

C(12)-H(12)	0.9300	C(22)-H(22)	0.9300
C(13)-C(14)	1.389(12)	C(23)-C(24)	1.355(12)
C(13)-H(13)	0.9300	C(23)-H(23)	0.9300
C(14)-C(15)	1.392(11)	C(24)-C(25)	1.374(11)
C(14)-H(14)	0.9300	C(24)-H(24)	0.9300
C(15)-H(15)	0.9300	C(25)-H(25)	0.9300
C(16)-C(17)	1.376(9)	C(26)-C(27)	1.386(10)
C(17)-C(18)	1.344(11)	C(27)-C(28)	1.370(12)
C(17)-H(17)	0.9300	C(27)-H(27)	0.9300
C(18)-C(19)	1.369(12)	C(28)-C(29)	1.370(13)
C(18)-H(18)	0.9300	C(28)-H(28)	0.9300
C(19)-C(20)	1.378(11)	C(29)-C(30)	1.385(11)
C(19)-H(19)	0.9300	C(29)-H(29)	0.9300
C(20)-H(20)	0.9300	C(30)-H(30)	0.9300
Cr(2)-N(8)	2.030(6)	C(31)-C(36)	1.448(11)
Cr(2)-N(6)	2.031(6)	C(31)-C(32)	1.449(12)
Cr(2)-N(7)	2.072(6)	C(32)-C(33)	1.320(14)
Cr(2)-N(5)	2.075(6)	C(32)-H(32)	0.9300
Cr(2)-Cl(3)	2.281(2)	C(33)-C(34)	1.356(14)
Cr(2)-Cl(4)	2.290(2)	C(33)-H(33)	0.9300
N(5)-C(25)	1.328(9)	C(34)-C(35)	1.401(12)
N(5)-C(21)	1.344(8)	C(34)-H(34)	0.9300
N(6)-C(30)	1.321(9)	C(35)-H(35)	0.9300
N(6)-C(26)	1.357(9)	C(36)-C(37)	1.410(12)
N(7)-C(31)	1.305(9)	C(37)-C(38)	1.373(15)
N(7)-C(35)	1.342(9)	C(37)-H(37)	0.9300
N(8)-C(40)	1.324(10)	C(38)-C(39)	1.350(16)
N(8)-C(36)	1.328(10)	C(38)-H(38)	0.9300
C(21)-C(22)	1.385(10)	C(39)-C(40)	1.390(13)
C(21)-C(26)	1.476(10)	C(39)-H(39)	0.9300
C(22)-C(23)	1.402(12)	C(40)-H(40)	0.9300

		C(3)-C(2)-C(1)	117.3(9)
N(1)-Cr(1)-N(2)	79.1(3)	C(3)-C(2)-H(2)	121.3
N(1)-Cr(1)-N(4)	94.0(2)	C(1)-C(2)-H(2)	121.4
N(2)-Cr(1)-N(4)	170.0(2)	C(4)-C(3)-C(2)	121.9(9)
N(1)-Cr(1)-N(3)	87.5(2)	C(4)-C(3)-H(3)	119.0
N(2)-Cr(1)-N(3)	93.7(2)	C(2)-C(3)-H(3)	119.0
N(4)-Cr(1)-N(3)	78.6(2)	C(3)-C(4)-C(5)	118.3(9)
N(1)-Cr(1)-Cl(1)	173.21(18)	C(3)-C(4)-H(4)	120.8
N(2)-Cr(1)-Cl(1)	94.2(2)	C(5)-C(4)-H(4)	120.9
N(4)-Cr(1)-Cl(1)	92.42(16)	N(1)-C(5)-C(4)	121.6(8)
N(3)-Cr(1)-Cl(1)	91.63(16)	N(1)-C(5)-H(5)	119.2
N(1)-Cr(1)-Cl(2)	86.92(15)	C(4)-C(5)-H(5)	119.2
N(2)-Cr(1)-Cl(2)	92.36(16)	N(2)-C(6)-C(7)	118.7(9)
N(4)-Cr(1)-Cl(2)	94.57(16)	N(2)-C(6)-C(1)	115.4(7)
N(3)-Cr(1)-Cl(2)	170.85(18)	C(7)-C(6)-C(1)	125.8(9)
Cl(1)-Cr(1)-Cl(2)	94.79(8)	C(8)-C(7)-C(6)	121.3(11)
C(5)-N(1)-C(1)	119.6(6)	C(8)-C(7)-H(7)	119.2
C(5)-N(1)-Cr(1)	125.9(5)	C(6)-C(7)-H(7)	119.4
C(1)-N(1)-Cr(1)	114.2(5)	C(9)-C(8)-C(7)	119.8(11)
C(10)-N(2)-C(6)	119.3(7)	C(9)-C(8)-H(8)	120.0
C(10)-N(2)-Cr(1)	126.1(6)	C(7)-C(8)-H(8)	120.2
C(6)-N(2)-Cr(1)	114.6(5)	C(8)-C(9)-C(10)	119.3(11)
C(15)-N(3)-C(11)	119.6(6)	C(8)-C(9)-H(9)	120.5
C(15)-N(3)-Cr(1)	125.4(5)	C(10)-C(9)-H(9)	120.2
C(11)-N(3)-Cr(1)	115.0(4)	N(2)-C(10)-C(9)	121.3(9)
C(20)-N(4)-C(16)	118.2(6)	N(2)-C(10)-H(10)	119.3
C(20)-N(4)-Cr(1)	126.0(5)	C(9)-C(10)-H(10)	119.4
C(16)-N(4)-Cr(1)	115.8(5)	N(3)-C(11)-C(12)	120.1(7)
N(1)-C(1)-C(2)	121.0(8)	N(3)-C(11)-C(16)	115.6(6)
N(1)-C(1)-C(6)	116.1(7)	C(12)-C(11)-C(16)	124.3(7)
C(2)-C(1)-C(6)	122.9(8)	C(13)-C(12)-C(11)	119.6(8)

C(13)-C(12)-H(12)	120.2	N(7)-Cr(2)-N(5)	86.8(2)
C(11)-C(12)-H(12)	120.2	N(8)-Cr(2)-Cl(3)	89.75(18)
C(12)-C(13)-C(14)	121.1(8)	N(6)-Cr(2)-Cl(3)	96.10(18)
C(12)-C(13)-H(13)	119.5	N(7)-Cr(2)-Cl(3)	90.97(17)
C(14)-C(13)-H(13)	119.4	N(5)-Cr(2)-Cl(3)	174.70(18)
C(15)-C(14)-C(13)	117.6(8)	N(8)-Cr(2)-Cl(4)	96.9(2)
C(15)-C(14)-H(14)	121.2	N(6)-Cr(2)-Cl(4)	91.30(17)
C(13)-C(14)-H(14)	121.2	N(7)-Cr(2)-Cl(4)	171.92(18)
N(3)-C(15)-C(14)	122.0(8)	N(5)-Cr(2)-Cl(4)	87.05(16)
N(3)-C(15)-H(15)	119.0	Cl(3)-Cr(2)-Cl(4)	95.61(9)
C(14)-C(15)-H(15)	119.0	C(25)-N(5)-C(21)	119.6(7)
N(4)-C(16)-C(17)	121.0(7)	C(25)-N(5)-Cr(2)	125.8(5)
N(4)-C(16)-C(11)	114.9(6)	C(21)-N(5)-Cr(2)	114.4(5)
C(17)-C(16)-C(11)	124.0(7)	C(30)-N(6)-C(26)	116.9(7)
C(18)-C(17)-C(16)	120.3(8)	C(30)-N(6)-Cr(2)	126.8(5)
C(18)-C(17)-H(17)	119.8	C(26)-N(6)-Cr(2)	116.3(5)
C(16)-C(17)-H(17)	119.9	C(31)-N(7)-C(35)	121.6(7)
C(17)-C(18)-C(19)	118.8(7)	C(31)-N(7)-Cr(2)	114.1(5)
C(17)-C(18)-H(18)	120.6	C(35)-N(7)-Cr(2)	124.2(5)
C(19)-C(18)-H(18)	120.6	C(40)-N(8)-C(36)	118.9(7)
C(18)-C(19)-C(20)	119.7(8)	C(40)-N(8)-Cr(2)	125.1(6)
C(18)-C(19)-H(19)	120.2	C(36)-N(8)-Cr(2)	115.7(5)
C(20)-C(19)-H(19)	120.1	N(5)-C(21)-C(22)	121.0(7)
N(4)-C(20)-C(19)	122.0(7)	N(5)-C(21)-C(26)	115.8(6)
N(4)-C(20)-H(20)	119.0	C(22)-C(21)-C(26)	123.2(7)
C(19)-C(20)-H(20)	119.0	C(21)-C(22)-C(23)	118.5(8)
N(8)-Cr(2)-N(6)	169.4(3)	C(21)-C(22)-H(22)	120.8
N(8)-Cr(2)-N(7)	78.4(3)	C(23)-C(22)-H(22)	120.8
N(6)-Cr(2)-N(7)	92.7(2)	C(24)-C(23)-C(22)	119.4(8)
N(8)-Cr(2)-N(5)	94.5(2)	C(24)-C(23)-H(23)	120.3
N(6)-Cr(2)-N(5)	79.2(2)	C(22)-C(23)-H(23)	120.3

C(23)-C(24)-C(25)	119.1(9)	C(31)-C(32)-H(32)	119.9
C(23)-C(24)-H(24)	120.4	C(32)-C(33)-C(34)	120.2(10)
C(25)-C(24)-H(24)	120.4	C(32)-C(33)-H(33)	119.9
N(5)-C(25)-C(24)	122.3(8)	C(34)-C(33)-H(33)	119.9
N(5)-C(25)-H(25)	118.8	C(33)-C(34)-C(35)	119.3(10)
C(24)-C(25)-H(25)	118.8	C(33)-C(34)-H(34)	120.3
N(6)-C(26)-C(27)	122.4(7)	C(35)-C(34)-H(34)	120.3
N(6)-C(26)-C(21)	114.2(6)	N(7)-C(35)-C(34)	120.0(9)
C(27)-C(26)-C(21)	123.4(7)	N(7)-C(35)-H(35)	120.0
C(28)-C(27)-C(26)	119.5(8)	C(34)-C(35)-H(35)	120.0
C(28)-C(27)-H(27)	120.3	N(8)-C(36)-C(37)	121.2(9)
C(26)-C(27)-H(27)	120.3	N(8)-C(36)-C(31)	114.8(7)
C(27)-C(28)-C(29)	118.2(9)	C(37)-C(36)-C(31)	124.0(9)
C(27)-C(28)-H(28)	120.9	C(38)-C(37)-C(36)	117.7(10)
C(29)-C(28)-H(28)	120.9	C(38)-C(37)-H(37)	121.1
C(28)-C(29)-C(30)	119.4(9)	C(36)-C(37)-H(37)	121.1
C(28)-C(29)-H(29)	120.3	C(39)-C(38)-C(37)	121.4(10)
C(30)-C(29)-H(29)	120.4	C(39)-C(38)-H(38)	119.3
N(6)-C(30)-C(29)	123.5(8)	C(37)-C(38)-H(38)	119.3
N(6)-C(30)-H(30)	118.3	C(38)-C(39)-C(40)	117.1(11)
C(29)-C(30)-H(30)	118.2	C(38)-C(39)-H(39)	121.5
N(7)-C(31)-C(36)	116.7(7)	C(40)-C(39)-H(39)	121.4
N(7)-C(31)-C(32)	118.7(8)	N(8)-C(40)-C(39)	123.5(10)
C(36)-C(31)-C(32)	124.5(8)	N(8)-C(40)-H(40)	118.1
C(33)-C(32)-C(31)	120.0(10)	C(39)-C(40)-H(40)	118.4
C(33)-C(32)-H(32)	120.0		

Table A.36 **Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[CrCl_2(bipy)_2][Cl]\cdot H_2O$. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	57(1)	76(1)	87(1)	-6(1)	0(1)	2(1)
Cl(1)	72(1)	88(1)	129(2)	6(1)	9(1)	-7(1)
Cl(2)	62(1)	81(1)	114(1)	-7(1)	-8(1)	5(1)
N(1)	66(3)	84(4)	80(4)	-3(3)	6(3)	5(3)
N(2)	73(3)	88(4)	99(4)	-19(4)	-7(3)	8(3)
N(3)	65(3)	92(4)	83(4)	-1(3)	-8(3)	0(3)
N(4)	63(3)	81(3)	76(3)	2(3)	4(3)	-3(3)
C(1)	95(5)	100(6)	89(5)	-1(5)	7(4)	4(4)
C(2)	161(9)	128(8)	105(7)	-5(6)	39(6)	-7(7)
C(3)	153(9)	144(9)	134(8)	1(8)	60(7)	-30(8)
C(4)	122(6)	99(6)	122(7)	25(5)	12(6)	-10(5)
C(5)	78(4)	96(5)	94(5)	4(4)	2(4)	-5(4)
C(6)	97(5)	109(6)	81(5)	-14(5)	6(4)	10(5)
C(7)	151(9)	180(12)	109(8)	-22(8)	30(6)	14(9)
C(8)	195(12)	131(10)	118(9)	-39(8)	21(8)	8(9)
C(9)	125(8)	120(8)	140(9)	-56(7)	-32(7)	21(6)
C(10)	86(5)	97(6)	135(7)	-20(5)	-12(5)	2(4)
C(11)	63(4)	66(4)	100(5)	7(4)	4(4)	5(3)
C(12)	77(4)	82(5)	128(7)	16(5)	11(5)	17(4)
C(13)	74(5)	133(8)	140(8)	40(7)	-12(5)	13(5)
C(14)	81(5)	135(7)	120(7)	15(6)	-27(5)	13(5)
C(15)	89(5)	125(6)	103(6)	-10(5)	-10(5)	5(5)
C(16)	65(4)	66(4)	92(5)	5(4)	16(3)	-2(3)
C(17)	98(5)	75(5)	105(6)	-4(4)	23(5)	10(4)
C(18)	113(6)	92(6)	103(6)	-30(5)	17(5)	2(5)
C(19)	93(5)	122(7)	96(6)	-20(5)	-1(4)	-13(5)

C(20)	71(4)	102(6)	100(6)	-14(5)	8(4)	0(4)
Cr(2)	84(1)	75(1)	79(1)	-2(1)	-8(1)	-3(1)
Cl(3)	112(1)	94(1)	99(1)	4(1)	-3(1)	-23(1)
Cl(4)	98(1)	87(1)	114(2)	4(1)	-19(1)	8(1)
N(5)	85(4)	76(4)	74(4)	-3(3)	-2(3)	6(3)
N(6)	80(3)	92(4)	69(4)	-1(3)	-3(3)	-2(3)
N(7)	82(4)	89(4)	79(4)	2(3)	-9(3)	-5(3)
N(8)	100(4)	78(4)	89(4)	-3(3)	-14(4)	-1(3)
C(21)	74(4)	71(4)	102(6)	2(4)	-9(4)	11(3)
C(22)	88(5)	79(5)	124(7)	2(5)	-7(5)	2(4)
C(23)	98(6)	97(6)	135(8)	5(6)	11(6)	-11(5)
C(24)	110(6)	110(6)	100(6)	15(5)	16(5)	-11(5)
C(25)	105(6)	88(5)	102(6)	2(5)	3(5)	6(5)
C(26)	71(4)	75(4)	88(5)	1(4)	-6(4)	5(3)
C(27)	108(6)	88(5)	120(7)	-20(5)	-1(5)	-7(5)
C(28)	129(7)	130(8)	102(7)	-30(6)	5(6)	-17(6)
C(29)	110(6)	152(8)	87(6)	-11(6)	10(5)	-11(6)
C(30)	102(5)	118(7)	87(5)	-8(5)	1(5)	-20(5)
C(31)	88(5)	107(6)	76(5)	7(4)	-3(4)	-8(4)
C(32)	119(7)	180(10)	96(7)	15(7)	-16(6)	2(7)
C(33)	103(7)	178(11)	144(10)	28(9)	-15(7)	34(7)
C(34)	97(6)	130(8)	154(10)	21(7)	-12(6)	11(6)
C(35)	84(5)	104(6)	112(6)	-1(5)	1(4)	12(4)
C(36)	101(5)	107(6)	75(5)	-6(4)	1(4)	-15(5)
C(37)	119(7)	182(10)	87(6)	-18(7)	-10(5)	-8(7)
C(38)	190(12)	169(11)	87(7)	-47(7)	10(8)	-22(10)
C(39)	203(12)	124(8)	109(8)	-35(7)	3(8)	14(8)
C(40)	156(8)	103(6)	100(7)	-13(5)	-11(6)	15(6)
Cl(5)	335(15)	391(16)	153(7)	0(9)	23(8)	29(13)
Cl(6)	363(16)	369(17)	409(18)	-189(15)	-235(15)	124(15)
Cl(7)	560(30)	840(50)	208(11)	-163(19)	-121(16)	380(30)

Cl(8)	560(30)	610(30)	283(15)	143(18)	230(20)	100(30)
O(1)	430(30)	740(40)	234(15)	-210(20)	189(17)	-310(30)
O(2)	880(50)	780(60)	230(15)	-40(20)	210(30)	-460(50)
O(3)	720(50)	1880(120)	500(30)	-770(60)	520(40)	-880(70)
O(4)	1210(100)	390(20)	380(30)	-260(20)	180(40)	-300(40)
O(5)	490(40)	620(40)	540(30)	170(30)	300(30)	-40(30)

Table A.37 **Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for $[CrCl_2(bipy)_2][Cl]\cdot H_2O$**

	x	y	z	U(eq)
H(2)	33	-75	1859	157
H(3)	-556	-771	1568	172
H(4)	189	-1056	921	137
H(5)	1364	-595	495	107
H(7)	727	607	2076	176
H(8)	1378	1326	2228	177
H(9)	2517	1670	1736	154
H(10)	2787	1344	1014	127
H(12)	5293	-707	418	115
H(13)	6165	-541	1086	139
H(14)	5506	42	1555	134
H(15)	3923	439	1332	127
H(17)	4371	-810	-217	111
H(18)	3311	-897	-853	123
H(19)	1801	-421	-959	124
H(20)	1333	102	-409	109
H(22)	12	1499	453	116

H(23)	-861	1534	1165	132
H(24)	-402	2115	1656	128
H(25)	727	2698	1411	118
H(27)	870	1528	-199	126
H(28)	1815	1612	-878	144
H(29)	2750	2293	-1011	140
H(30)	2874	2831	-444	123
H(32)	4720	2650	1765	158
H(33)	5638	2062	1444	170
H(34)	5159	1815	733	152
H(35)	3734	2185	340	120
H(37)	3858	3307	1992	155
H(38)	2814	3944	2178	178
H(39)	1408	4186	1713	174
H(40)	1020	3757	1070	144

Table A.38 Torsion angles [°] for $[CrCl_2(bipy)_2][Cl]\cdot H_2O$

N(2)-Cr(1)-N(1)-C(5)	-179.7(6)	N(4)-Cr(1)-N(2)-C(10)	128.5(13)
N(4)-Cr(1)-N(1)-C(5)	-7.1(6)	N(3)-Cr(1)-N(2)-C(10)	89.0(6)
N(3)-Cr(1)-N(1)-C(5)	-85.5(6)	Cl(1)-Cr(1)-N(2)-C(10)	-2.9(6)
Cl(1)-Cr(1)-N(1)-C(5)	-167.9(11)	Cl(2)-Cr(1)-N(2)-C(10)	-97.9(6)
Cl(2)-Cr(1)-N(1)-C(5)	87.3(5)	N(1)-Cr(1)-N(2)-C(6)	-4.2(5)
N(2)-Cr(1)-N(1)-C(1)	6.3(5)	N(4)-Cr(1)-N(2)-C(6)	-51.5(15)
N(4)-Cr(1)-N(1)-C(1)	179.0(5)	N(3)-Cr(1)-N(2)-C(6)	-90.9(5)
N(3)-Cr(1)-N(1)-C(1)	100.6(5)	Cl(1)-Cr(1)-N(2)-C(6)	177.2(5)
Cl(1)-Cr(1)-N(1)-C(1)	18.1(17)	Cl(2)-Cr(1)-N(2)-C(6)	82.2(5)
Cl(2)-Cr(1)-N(1)-C(1)	-86.7(5)	N(1)-Cr(1)-N(3)-C(15)	-87.0(6)
N(1)-Cr(1)-N(2)-C(10)	175.7(6)	N(2)-Cr(1)-N(3)-C(15)	-8.1(6)

N(4)-Cr(1)-N(3)-C(15)	178.4(6)	C(10)-N(2)-C(6)-C(1)	-178.3(7)
Cl(1)-Cr(1)-N(3)-C(15)	86.2(6)	Cr(1)-N(2)-C(6)-C(1)	1.6(8)
Cl(2)-Cr(1)-N(3)-C(15)	-139.2(10)	N(1)-C(1)-C(6)-N(2)	3.9(10)
N(1)-Cr(1)-N(3)-C(11)	92.7(5)	C(2)-C(1)-C(6)-N(2)	-176.3(8)
N(2)-Cr(1)-N(3)-C(11)	171.6(5)	N(1)-C(1)-C(6)-C(7)	-174.0(8)
N(4)-Cr(1)-N(3)-C(11)	-1.9(4)	C(2)-C(1)-C(6)-C(7)	5.9(14)
Cl(1)-Cr(1)-N(3)-C(11)	-94.0(4)	N(2)-C(6)-C(7)-C(8)	0.7(15)
Cl(2)-Cr(1)-N(3)-C(11)	40.5(14)	C(1)-C(6)-C(7)-C(8)	178.5(10)
N(1)-Cr(1)-N(4)-C(20)	93.8(6)	C(6)-C(7)-C(8)-C(9)	-3(2)
N(2)-Cr(1)-N(4)-C(20)	140.2(12)	C(7)-C(8)-C(9)-C(10)	5.1(19)
N(3)-Cr(1)-N(4)-C(20)	-179.5(6)	C(6)-N(2)-C(10)-C(9)	2.2(11)
Cl(1)-Cr(1)-N(4)-C(20)	-88.4(6)	Cr(1)-N(2)-C(10)-C(9)	-177.7(6)
Cl(2)-Cr(1)-N(4)-C(20)	6.6(6)	C(8)-C(9)-C(10)-N(2)	-4.7(15)
N(1)-Cr(1)-N(4)-C(16)	-84.5(4)	C(15)-N(3)-C(11)-C(12)	2.6(10)
N(2)-Cr(1)-N(4)-C(16)	-38.2(15)	Cr(1)-N(3)-C(11)-C(12)	-177.1(5)
N(3)-Cr(1)-N(4)-C(16)	2.1(4)	C(15)-N(3)-C(11)-C(16)	-178.8(6)
Cl(1)-Cr(1)-N(4)-C(16)	93.3(4)	Cr(1)-N(3)-C(11)-C(16)	1.4(7)
Cl(2)-Cr(1)-N(4)-C(16)	-171.7(4)	N(3)-C(11)-C(12)-C(13)	-1.6(11)
C(5)-N(1)-C(1)-C(2)	-1.6(11)	C(16)-C(11)-C(12)-C(13)	180.0(7)
Cr(1)-N(1)-C(1)-C(2)	172.7(7)	C(11)-C(12)-C(13)-C(14)	-0.1(13)
C(5)-N(1)-C(1)-C(6)	178.2(6)	C(12)-C(13)-C(14)-C(15)	0.8(13)
Cr(1)-N(1)-C(1)-C(6)	-7.5(9)	C(11)-N(3)-C(15)-C(14)	-2.0(12)
N(1)-C(1)-C(2)-C(3)	-2.0(15)	Cr(1)-N(3)-C(15)-C(14)	177.8(6)
C(6)-C(1)-C(2)-C(3)	178.2(10)	C(13)-C(14)-C(15)-N(3)	0.2(13)
C(1)-C(2)-C(3)-C(4)	5.2(18)	C(20)-N(4)-C(16)-C(17)	-0.4(9)
C(2)-C(3)-C(4)-C(5)	-4.7(17)	Cr(1)-N(4)-C(16)-C(17)	178.1(5)
C(1)-N(1)-C(5)-C(4)	2.3(11)	C(20)-N(4)-C(16)-C(11)	179.5(6)
Cr(1)-N(1)-C(5)-C(4)	-171.4(6)	Cr(1)-N(4)-C(16)-C(11)	-2.0(7)
C(3)-C(4)-C(5)-N(1)	0.8(13)	N(3)-C(11)-C(16)-N(4)	0.4(8)
C(10)-N(2)-C(6)-C(7)	-0.3(11)	C(12)-C(11)-C(16)-N(4)	178.9(6)
Cr(1)-N(2)-C(6)-C(7)	179.7(7)	N(3)-C(11)-C(16)-C(17)	-179.7(6)

C(12)-C(11)-C(16)-C(17)	-1.3(11)	Cl(3)-Cr(2)-N(7)-C(31)	91.2(5)
N(4)-C(16)-C(17)-C(18)	-0.1(11)	Cl(4)-Cr(2)-N(7)-C(31)	-53.3(16)
C(11)-C(16)-C(17)-C(18)	180.0(7)	N(8)-Cr(2)-N(7)-C(35)	179.7(6)
C(16)-C(17)-C(18)-C(19)	1.2(12)	N(6)-Cr(2)-N(7)-C(35)	5.4(6)
C(17)-C(18)-C(19)-C(20)	-1.8(13)	N(5)-Cr(2)-N(7)-C(35)	84.5(6)
C(16)-N(4)-C(20)-C(19)	-0.2(10)	Cl(3)-Cr(2)-N(7)-C(35)	-90.7(6)
Cr(1)-N(4)-C(20)-C(19)	-178.5(6)	Cl(4)-Cr(2)-N(7)-C(35)	124.7(13)
C(18)-C(19)-C(20)-N(4)	1.3(13)	N(6)-Cr(2)-N(8)-C(40)	-151.9(13)
N(8)-Cr(2)-N(5)-C(25)	12.5(6)	N(7)-Cr(2)-N(8)-C(40)	175.3(7)
N(6)-Cr(2)-N(5)-C(25)	-176.1(6)	N(5)-Cr(2)-N(8)-C(40)	-98.9(7)
N(7)-Cr(2)-N(5)-C(25)	90.6(6)	Cl(3)-Cr(2)-N(8)-C(40)	84.3(7)
Cl(3)-Cr(2)-N(5)-C(25)	155.5(16)	Cl(4)-Cr(2)-N(8)-C(40)	-11.3(7)
Cl(4)-Cr(2)-N(5)-C(25)	-84.2(6)	N(6)-Cr(2)-N(8)-C(36)	34.1(17)
N(8)-Cr(2)-N(5)-C(21)	-173.1(5)	N(7)-Cr(2)-N(8)-C(36)	1.3(5)
N(6)-Cr(2)-N(5)-C(21)	-1.7(5)	N(5)-Cr(2)-N(8)-C(36)	87.1(6)
N(7)-Cr(2)-N(5)-C(21)	-95.0(5)	Cl(3)-Cr(2)-N(8)-C(36)	-89.7(5)
Cl(3)-Cr(2)-N(5)-C(21)	-30(2)	Cl(4)-Cr(2)-N(8)-C(36)	174.6(5)
Cl(4)-Cr(2)-N(5)-C(21)	90.2(4)	C(25)-N(5)-C(21)-C(22)	-0.8(10)
N(8)-Cr(2)-N(6)-C(30)	-124.4(14)	Cr(2)-N(5)-C(21)-C(22)	-175.5(5)
N(7)-Cr(2)-N(6)-C(30)	-92.3(6)	C(25)-N(5)-C(21)-C(26)	177.6(6)
N(5)-Cr(2)-N(6)-C(30)	-178.5(7)	Cr(2)-N(5)-C(21)-C(26)	2.9(7)
Cl(3)-Cr(2)-N(6)-C(30)	-1.0(6)	N(5)-C(21)-C(22)-C(23)	1.5(11)
Cl(4)-Cr(2)-N(6)-C(30)	94.7(6)	C(26)-C(21)-C(22)-C(23)	-176.8(7)
N(8)-Cr(2)-N(6)-C(26)	54.3(15)	C(21)-C(22)-C(23)-C(24)	-3.1(12)
N(7)-Cr(2)-N(6)-C(26)	86.3(5)	C(22)-C(23)-C(24)-C(25)	3.8(13)
N(5)-Cr(2)-N(6)-C(26)	0.1(5)	C(21)-N(5)-C(25)-C(24)	1.5(11)
Cl(3)-Cr(2)-N(6)-C(26)	177.6(4)	Cr(2)-N(5)-C(25)-C(24)	175.6(6)
Cl(4)-Cr(2)-N(6)-C(26)	-86.6(5)	C(23)-C(24)-C(25)-N(5)	-3.1(13)
N(8)-Cr(2)-N(7)-C(31)	1.7(5)	C(30)-N(6)-C(26)-C(27)	0.7(10)
N(6)-Cr(2)-N(7)-C(31)	-172.6(5)	Cr(2)-N(6)-C(26)-C(27)	-178.0(6)
N(5)-Cr(2)-N(7)-C(31)	-93.6(5)	C(30)-N(6)-C(26)-C(21)	-179.9(6)

Cr(2)-N(6)-C(26)-C(21)	1.3(7)	C(32)-C(33)-C(34)-C(35)	0.3(17)
N(5)-C(21)-C(26)-N(6)	-2.8(8)	C(31)-N(7)-C(35)-C(34)	1.9(11)
C(22)-C(21)-C(26)-N(6)	175.6(6)	Cr(2)-N(7)-C(35)-C(34)	-175.9(6)
N(5)-C(21)-C(26)-C(27)	176.5(7)	C(33)-C(34)-C(35)-N(7)	-0.7(14)
C(22)-C(21)-C(26)-C(27)	-5.1(11)	C(40)-N(8)-C(36)-C(37)	1.2(12)
N(6)-C(26)-C(27)-C(28)	0.9(12)	Cr(2)-N(8)-C(36)-C(37)	175.6(7)
C(21)-C(26)-C(27)-C(28)	-178.4(8)	C(40)-N(8)-C(36)-C(31)	-178.2(7)
C(26)-C(27)-C(28)-C(29)	-2.9(14)	Cr(2)-N(8)-C(36)-C(31)	-3.8(9)
C(27)-C(28)-C(29)-C(30)	3.4(15)	N(7)-C(31)-C(36)-N(8)	5.4(10)
C(26)-N(6)-C(30)-C(29)	-0.3(12)	C(32)-C(31)-C(36)-N(8)	-174.4(8)
Cr(2)-N(6)-C(30)-C(29)	178.4(7)	N(7)-C(31)-C(36)-C(37)	-174.0(8)
C(28)-C(29)-C(30)-N(6)	-1.8(15)	C(32)-C(31)-C(36)-C(37)	6.3(13)
C(35)-N(7)-C(31)-C(36)	177.7(7)	N(8)-C(36)-C(37)-C(38)	-1.9(14)
Cr(2)-N(7)-C(31)-C(36)	-4.2(8)	C(31)-C(36)-C(37)-C(38)	177.4(9)
C(35)-N(7)-C(31)-C(32)	-2.5(11)	C(36)-C(37)-C(38)-C(39)	0.6(18)
Cr(2)-N(7)-C(31)-C(32)	175.6(6)	C(37)-C(38)-C(39)-C(40)	1.4(19)
N(7)-C(31)-C(32)-C(33)	2.0(14)	C(36)-N(8)-C(40)-C(39)	1.0(14)
C(36)-C(31)-C(32)-C(33)	-178.2(9)	Cr(2)-N(8)-C(40)-C(39)	-172.9(8)
C(31)-C(32)-C(33)-C(34)	-0.9(17)	C(38)-C(39)-C(40)-N(8)	-2.3(17)

[Hpyphenyl][$CrCl_4$(dppe)]

Table A.39 **Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [Hpyphenyl][$CrCl_4$(dppe)]. U(eq) is defined as one-third of the trace of the orthogonalised U^{ij} tensor**

	x	y	z	U(eq)
Cr(1)	8697(1)	3680(1)	1508(1)	39(1)
Cl(1)	9169(2)	3834(1)	489(1)	52(1)
Cl(2)	8754(2)	5093(1)	1638(1)	53(1)
Cl(3)	10867(2)	3491(1)	1668(1)	50(1)
Cl(4)	6477(2)	3647(1)	1453(1)	52(1)
P(1)	8318(2)	3361(1)	2589(1)	47(1)
P(2)	8482(2)	2162(1)	1490(1)	49(1)
C(1)	8434(9)	2247(5)	2683(3)	71(2)
C(2)	7763(9)	1839(5)	2231(3)	71(2)
C(11)	6797(7)	3669(5)	2942(3)	57(2)
C(12)	6111(9)	3182(7)	3368(4)	100(3)
C(13)	4965(12)	3506(10)	3661(5)	130(5)
C(14)	4569(12)	4271(12)	3512(6)	135(6)
C(15)	5243(11)	4743(8)	3107(5)	103(4)
C(16)	6353(8)	4447(6)	2813(4)	76(3)
C(21)	9424(7)	3711(5)	3102(3)	58(2)
C(22)	9396(9)	3370(7)	3672(4)	99(3)
C(23)	10194(12)	3664(9)	4070(4)	120(4)
C(24)	10975(10)	4328(8)	3917(5)	106(4)
C(25)	11037(9)	4683(6)	3362(4)	82(3)
C(26)	10244(8)	4357(5)	2962(3)	65(2)
C(31)	9954(7)	1568(4)	1367(3)	55(2)
C(32)	10751(8)	1778(5)	880(4)	73(2)

C(33)	11860(10)	1325(7)	729(5)	101(3)
C(34)	12131(10)	663(7)	1100(6)	105(4)
C(35)	11347(10)	461(6)	1599(5)	100(3)
C(36)	10247(8)	898(5)	1736(4)	72(2)
C(41)	7403(7)	1704(4)	1003(4)	56(2)
C(42)	7151(9)	2091(6)	489(4)	84(3)
C(43)	6378(11)	1721(7)	101(4)	101(3)
C(44)	5870(12)	973(8)	248(7)	126(5)
C(45)	6123(15)	598(8)	752(7)	157(6)
C(46)	6868(12)	950(6)	1154(5)	116(4)
N(1)	12323(7)	3906(4)	407(3)	67(2)
C(52)	13471(9)	3679(5)	577(3)	72(2)
C(53)	14563(8)	3767(5)	201(3)	68(2)
C(54)	14484(6)	4099(4)	-368(3)	46(2)
C(55)	13269(7)	4343(5)	-515(4)	66(2)
C(56)	12198(8)	4232(5)	-130(4)	72(2)
C(57)	15631(7)	4216(4)	-784(3)	51(2)
C(58)	16864(7)	4048(5)	-612(3)	58(2)
C(59)	17945(8)	4149(5)	-1014(4)	71(2)
C(60)	17813(9)	4433(5)	-1562(4)	75(2)
C(61)	16585(10)	4631(6)	-1742(4)	81(3)
C(62)	15503(7)	4523(5)	-1354(3)	63(2)
Cr(2)	1659(1)	1461(1)	6796(1)	50(1)
Cl(5)	1047(2)	1130(1)	5864(1)	75(1)
Cl(6)	2332(2)	150(1)	7088(1)	71(1)
Cl(7)	-415(2)	1209(1)	7239(1)	64(1)
Cl(8)	3714(2)	1891(1)	6437(1)	64(1)
P(3)	2346(2)	2056(1)	7704(1)	49(1)
P(4)	860(2)	2891(1)	6600(1)	49(1)
C(3)	2245(7)	3169(4)	7550(3)	51(2)
C(4)	961(7)	3385(4)	7292(3)	51(2)

C(71)	3990(7)	1894(4)	7924(3)	55(2)
C(72)	4691(10)	1198(6)	7789(4)	94(3)
C(73)	5915(10)	1088(7)	7964(5)	107(4)
C(74)	6490(10)	1619(7)	8275(4)	90(3)
C(75)	5849(10)	2327(7)	8389(5)	102(3)
C(76)	4607(9)	2449(5)	8223(4)	86(3)
C(81)	1341(7)	1836(5)	8389(3)	58(2)
C(82)	1224(11)	1035(5)	8592(4)	95(3)
C(83)	516(12)	817(6)	9119(4)	111(4)
C(84)	-97(10)	1388(7)	9438(4)	95(3)
C(85)	17(11)	2186(7)	9233(4)	114(4)
C(86)	755(10)	2423(6)	8723(3)	92(3)
C(91)	-790(7)	3084(4)	6415(3)	55(2)
C(92)	-1077(8)	3361(5)	5861(4)	67(2)
C(93)	-2357(10)	3495(6)	5721(5)	87(3)
C(94)	-3350(10)	3361(6)	6142(6)	96(3)
C(95)	-3081(9)	3098(6)	6699(5)	87(3)
C(96)	-1831(8)	2942(5)	6833(4)	71(2)
C(101)	1824(7)	3522(4)	6049(3)	51(2)
C(102)	2087(8)	4346(5)	6121(4)	72(2)
C(103)	2821(10)	4806(6)	5692(4)	93(3)
C(104)	3307(9)	4448(7)	5190(4)	91(3)
C(105)	3031(10)	3643(7)	5121(4)	91(3)
C(106)	2314(9)	3177(5)	5543(3)	79(3)
N(2)	-1916(9)	532(5)	6124(4)	102(3)
C(112)	-1662(12)	-8(8)	5717(5)	122(4)
C(113)	-2663(11)	-435(7)	5520(5)	107(4)
C(114)	-3910(9)	-338(5)	5751(4)	69(2)
C(115)	-4121(10)	241(6)	6163(4)	91(3)
C(116)	-3126(12)	658(7)	6340(5)	106(4)
C(117)	-5003(9)	-817(5)	5560(3)	67(2)

C(118)	-4796(10)	-1382(6)	5135(4)	90(3)
C(119)	-5789(13)	-1839(7)	4966(5)	116(4)
C(120)	-7037(12)	-1742(7)	5205(5)	103(3)
C(121)	-7272(11)	-1177(8)	5621(5)	106(3)
C(122)	-6251(11)	-729(6)	5796(4)	95(3)
O(1S)	2758(17)	1391(11)	2992(8)	162(6)
C(1S)	3850(20)	1284(13)	2586(10)	125(7)
C(2S)	3780(20)	2019(13)	2182(9)	114(6)
C(3S)	3410(20)	2523(15)	2469(11)	134(8)
C(4S)	2600(20)	2244(14)	2897(10)	133(8)
O(2S)	90(20)	925(15)	3463(11)	102(8)

Table A.40 Bond lengths [Å] and angles [°] for [Hpyphenyl][$CrCl_4$(dppe)]

Cr(1)-Cl(4)	2.310(2)	C(2)-H(2A)	0.9700
Cr(1)-Cl(3)	2.319(2)	C(2)-H(2B)	0.9700
Cr(1)-Cl(1)	2.3401(19)	C(11)-C(12)	1.372(11)
Cr(1)-Cl(2)	2.3450(19)	C(11)-C(16)	1.374(11)
Cr(1)-P(2)	2.492(2)	C(12)-C(13)	1.432(14)
Cr(1)-P(1)	2.494(2)	C(12)-H(12)	0.9300
P(1)-C(11)	1.797(7)	C(13)-C(14)	1.347(17)
P(1)-C(21)	1.817(8)	C(13)-H(13)	0.9300
P(1)-C(1)	1.824(8)	C(14)-C(15)	1.323(17)
P(2)-C(31)	1.817(7)	C(14)-H(14)	0.9300
P(2)-C(41)	1.828(8)	C(15)-C(16)	1.386(12)
P(2)-C(2)	1.843(8)	C(15)-H(15)	0.9300
C(1)-C(2)	1.480(11)	C(16)-H(16)	0.9300
C(1)-H(1A)	0.9700	C(21)-C(26)	1.361(11)
C(1)-H(1B)	0.9700	C(21)-C(22)	1.385(11)

C(22)-C(23)	1.382(13)	N(1)-C(52)	1.323(10)
C(22)-H(22)	0.9300	N(1)-C(56)	1.325(9)
C(23)-C(24)	1.364(15)	N(1)-H(1)	0.8600
C(23)-H(23)	0.9300	C(52)-C(53)	1.366(10)
C(24)-C(25)	1.360(13)	C(52)-H(52)	0.9300
C(24)-H(24)	0.9300	C(53)-C(54)	1.387(9)
C(25)-C(26)	1.402(11)	C(53)-H(53)	0.9300
C(25)-H(25)	0.9300	C(54)-C(55)	1.379(9)
C(26)-H(26)	0.9300	C(54)-C(57)	1.467(9)
C(31)-C(32)	1.360(11)	C(55)-C(56)	1.364(10)
C(31)-C(36)	1.389(10)	C(55)-H(55)	0.9300
C(32)-C(33)	1.395(12)	C(56)-H(56)	0.9300
C(32)-H(32)	0.9300	C(57)-C(58)	1.384(9)
C(33)-C(34)	1.376(14)	C(57)-C(62)	1.386(10)
C(33)-H(33)	0.9300	C(58)-C(59)	1.393(10)
C(34)-C(35)	1.371(14)	C(58)-H(58)	0.9300
C(34)-H(34)	0.9300	C(59)-C(60)	1.328(11)
C(35)-C(36)	1.368(11)	C(59)-H(59)	0.9300
C(35)-H(35)	0.9300	C(60)-C(61)	1.396(11)
C(36)-H(36)	0.9300	C(60)-H(60)	0.9300
C(41)-C(42)	1.343(11)	C(61)-C(62)	1.376(11)
C(41)-C(46)	1.364(12)	C(61)-H(61)	0.9300
C(42)-C(43)	1.402(12)	C(62)-H(62)	0.9300
C(42)-H(42)	0.9300	Cr(2)-Cl(8)	2.312(2)
C(43)-C(44)	1.343(14)	Cr(2)-Cl(6)	2.326(2)
C(43)-H(43)	0.9300	Cr(2)-Cl(7)	2.326(2)
C(44)-C(45)	1.316(16)	Cr(2)-Cl(5)	2.361(2)
C(44)-H(44)	0.9300	Cr(2)-P(3)	2.496(2)
C(45)-C(46)	1.395(15)	Cr(2)-P(4)	2.502(2)
C(45)-H(45)	0.9300	P(3)-C(71)	1.825(8)
C(46)-H(46)	0.9300	P(3)-C(81)	1.827(7)

P(3)-C(3)	1.835(7)	C(91)-C(92)	1.372(10)
P(4)-C(91)	1.813(8)	C(91)-C(96)	1.393(10)
P(4)-C(101)	1.815(7)	C(92)-C(93)	1.399(11)
P(4)-C(4)	1.829(6)	C(92)-H(92)	0.9300
C(3)-C(4)	1.528(9)	C(93)-C(94)	1.359(13)
C(3)-H(3A)	0.9700	C(93)-H(93)	0.9300
C(3)-H(3B)	0.9700	C(94)-C(95)	1.370(13)
C(4)-H(4A)	0.9700	C(94)-H(94)	0.9300
C(4)-H(4B)	0.9700	C(95)-C(96)	1.371(11)
C(71)-C(76)	1.358(10)	C(95)-H(95)	0.9300
C(71)-C(72)	1.383(10)	C(96)-H(96)	0.9300
C(72)-C(73)	1.364(12)	C(101)-C(106)	1.376(10)
C(72)-H(72)	0.9300	C(101)-C(102)	1.394(10)
C(73)-C(74)	1.323(13)	C(102)-C(103)	1.379(11)
C(73)-H(73)	0.9300	C(102)-H(102)	0.9300
C(74)-C(75)	1.360(12)	C(103)-C(104)	1.378(13)
C(74)-H(74)	0.9300	C(103)-H(103)	0.9300
C(75)-C(76)	1.377(12)	C(104)-C(105)	1.368(13)
C(75)-H(75)	0.9300	C(104)-H(104)	0.9300
C(76)-H(76)	0.9300	C(105)-C(106)	1.365(11)
C(81)-C(82)	1.363(11)	C(105)-H(105)	0.9300
C(81)-C(86)	1.372(10)	C(106)-H(106)	0.9300
C(82)-C(83)	1.386(12)	N(2)-C(116)	1.330(12)
C(82)-H(82)	0.9300	N(2)-C(112)	1.330(12)
C(83)-C(84)	1.346(13)	N(2)-H(2)	0.8600
C(83)-H(83)	0.9300	C(112)-C(113)	1.367(14)
C(84)-C(85)	1.359(13)	C(112)-H(112)	0.9300
C(84)-H(84)	0.9300	C(113)-C(114)	1.367(12)
C(85)-C(86)	1.379(12)	C(113)-H(113)	0.9300
C(85)-H(85)	0.9300	C(114)-C(115)	1.379(11)
C(86)-H(86)	0.9300	C(114)-C(117)	1.483(12)

C(115)-C(116)	1.337(13)	Cl(4)-Cr(1)-Cl(2)	93.96(7)
C(115)-H(115)	0.9300	Cl(3)-Cr(1)-Cl(2)	93.87(7)
C(116)-H(116)	0.9300	Cl(1)-Cr(1)-Cl(2)	94.17(7)
C(117)-C(122)	1.370(12)	Cl(4)-Cr(1)-P(2)	83.19(7)
C(117)-C(118)	1.383(11)	Cl(3)-Cr(1)-P(2)	88.22(7)
C(118)-C(119)	1.364(13)	Cl(1)-Cr(1)-P(2)	92.52(7)
C(118)-H(118)	0.9300	Cl(2)-Cr(1)-P(2)	172.92(8)
C(119)-C(120)	1.375(14)	Cl(4)-Cr(1)-P(1)	88.20(7)
C(119)-H(119)	0.9300	Cl(3)-Cr(1)-P(1)	84.57(7)
C(120)-C(121)	1.371(14)	Cl(1)-Cr(1)-P(1)	173.48(8)
C(120)-H(120)	0.9300	Cl(2)-Cr(1)-P(1)	91.53(7)
C(121)-C(122)	1.383(13)	P(2)-Cr(1)-P(1)	81.93(7)
C(121)-H(121)	0.9300	C(11)-P(1)-C(21)	100.1(3)
C(122)-H(122)	0.9300	C(11)-P(1)-C(1)	108.2(4)
O(1S)-C(4S)	1.41(2)	C(21)-P(1)-C(1)	102.9(4)
O(1S)-C(1S)	1.42(2)	C(11)-P(1)-Cr(1)	117.6(3)
C(1S)-C(2S)	1.47(2)	C(21)-P(1)-Cr(1)	121.7(3)
C(1S)-H(1SA)	0.9700	C(1)-P(1)-Cr(1)	105.0(2)
C(1S)-H(1SB)	0.9700	C(31)-P(2)-C(41)	102.0(3)
C(2S)-C(3S)	1.13(2)	C(31)-P(2)-C(2)	106.9(4)
C(2S)-H(2SA)	0.9700	C(41)-P(2)-C(2)	103.4(4)
C(2S)-H(2SB)	0.9700	C(31)-P(2)-Cr(1)	117.9(3)
C(3S)-C(4S)	1.30(3)	C(41)-P(2)-Cr(1)	120.9(2)
C(3S)-H(3SA)	0.9700	C(2)-P(2)-Cr(1)	104.2(3)
C(3S)-H(3SB)	0.9700	C(2)-C(1)-P(1)	111.4(6)
C(4S)-H(4SA)	0.9700	C(2)-C(1)-H(1A)	109.3
C(4S)-H(4SB)	0.9700	P(1)-C(1)-H(1A)	109.3
		C(2)-C(1)-H(1B)	109.3
Cl(4)-Cr(1)-Cl(3)	169.48(8)	P(1)-C(1)-H(1B)	109.3
Cl(4)-Cr(1)-Cl(1)	94.54(7)	H(1A)-C(1)-H(1B)	108.0
Cl(3)-Cr(1)-Cl(1)	91.88(7)	C(1)-C(2)-P(2)	110.4(6)

C(1)-C(2)-H(2A)	109.6	C(22)-C(23)-H(23)	119.8
P(2)-C(2)-H(2A)	109.6	C(25)-C(24)-C(23)	120.8(10)
C(1)-C(2)-H(2B)	109.6	C(25)-C(24)-H(24)	119.6
P(2)-C(2)-H(2B)	109.6	C(23)-C(24)-H(24)	119.6
H(2A)-C(2)-H(2B)	108.1	C(24)-C(25)-C(26)	117.6(10)
C(12)-C(11)-C(16)	118.6(8)	C(24)-C(25)-H(25)	121.2
C(12)-C(11)-P(1)	122.7(7)	C(26)-C(25)-H(25)	121.2
C(16)-C(11)-P(1)	118.5(6)	C(21)-C(26)-C(25)	123.5(8)
C(11)-C(12)-C(13)	118.8(11)	C(21)-C(26)-H(26)	118.3
C(11)-C(12)-H(12)	120.6	C(25)-C(26)-H(26)	118.3
C(13)-C(12)-H(12)	120.6	C(32)-C(31)-C(36)	120.2(7)
C(14)-C(13)-C(12)	120.0(12)	C(32)-C(31)-P(2)	117.6(6)
C(14)-C(13)-H(13)	120.0	C(36)-C(31)-P(2)	122.2(6)
C(12)-C(13)-H(13)	120.0	C(31)-C(32)-C(33)	121.6(9)
C(15)-C(14)-C(13)	121.0(12)	C(31)-C(32)-H(32)	119.2
C(15)-C(14)-H(14)	119.5	C(33)-C(32)-H(32)	119.2
C(13)-C(14)-H(14)	119.5	C(34)-C(33)-C(32)	117.3(10)
C(14)-C(15)-C(16)	120.4(12)	C(34)-C(33)-H(33)	121.4
C(14)-C(15)-H(15)	119.8	C(32)-C(33)-H(33)	121.4
C(16)-C(15)-H(15)	119.8	C(35)-C(34)-C(33)	121.3(9)
C(11)-C(16)-C(15)	121.1(10)	C(35)-C(34)-H(34)	119.3
C(11)-C(16)-H(16)	119.4	C(33)-C(34)-H(34)	119.3
C(15)-C(16)-H(16)	119.4	C(36)-C(35)-C(34)	120.9(9)
C(26)-C(21)-C(22)	116.8(8)	C(36)-C(35)-H(35)	119.5
C(26)-C(21)-P(1)	122.0(6)	C(34)-C(35)-H(35)	119.5
C(22)-C(21)-P(1)	121.0(7)	C(35)-C(36)-C(31)	118.6(9)
C(23)-C(22)-C(21)	120.9(10)	C(35)-C(36)-H(36)	120.7
C(23)-C(22)-H(22)	119.5	C(31)-C(36)-H(36)	120.7
C(21)-C(22)-H(22)	119.5	C(42)-C(41)-C(46)	119.3(8)
C(24)-C(23)-C(22)	120.3(10)	C(42)-C(41)-P(2)	120.9(6)
C(24)-C(23)-H(23)	119.8	C(46)-C(41)-P(2)	119.8(7)

C(41)-C(42)-C(43)	120.9(9)	N(1)-C(56)-H(56)	120.1
C(41)-C(42)-H(42)	119.6	C(55)-C(56)-H(56)	120.1
C(43)-C(42)-H(42)	119.6	C(58)-C(57)-C(62)	118.5(7)
C(44)-C(43)-C(42)	119.6(10)	C(58)-C(57)-C(54)	121.1(6)
C(44)-C(43)-H(43)	120.2	C(62)-C(57)-C(54)	120.3(7)
C(42)-C(43)-H(43)	120.2	C(57)-C(58)-C(59)	120.7(7)
C(45)-C(44)-C(43)	119.1(11)	C(57)-C(58)-H(58)	119.7
C(45)-C(44)-H(44)	120.4	C(59)-C(58)-H(58)	119.7
C(43)-C(44)-H(44)	120.4	C(60)-C(59)-C(58)	120.4(8)
C(44)-C(45)-C(46)	123.1(11)	C(60)-C(59)-H(59)	119.8
C(44)-C(45)-H(45)	118.4	C(58)-C(59)-H(59)	119.8
C(46)-C(45)-H(45)	118.4	C(59)-C(60)-C(61)	120.1(8)
C(41)-C(46)-C(45)	117.9(10)	C(59)-C(60)-H(60)	119.9
C(41)-C(46)-H(46)	121.0	C(61)-C(60)-H(60)	119.9
C(45)-C(46)-H(46)	121.0	C(62)-C(61)-C(60)	120.3(8)
C(52)-N(1)-C(56)	121.1(7)	C(62)-C(61)-H(61)	119.8
C(52)-N(1)-H(1)	119.5	C(60)-C(61)-H(61)	119.8
C(56)-N(1)-H(1)	119.5	C(61)-C(62)-C(57)	119.9(7)
N(1)-C(52)-C(53)	121.0(7)	C(61)-C(62)-H(62)	120.1
N(1)-C(52)-H(52)	119.5	C(57)-C(62)-H(62)	120.1
C(53)-C(52)-H(52)	119.5	Cl(8)-Cr(2)-Cl(6)	94.03(8)
C(52)-C(53)-C(54)	120.3(7)	Cl(8)-Cr(2)-Cl(7)	171.18(8)
C(52)-C(53)-H(53)	119.9	Cl(6)-Cr(2)-Cl(7)	91.38(8)
C(54)-C(53)-H(53)	119.9	Cl(8)-Cr(2)-Cl(5)	93.70(8)
C(55)-C(54)-C(53)	116.2(7)	Cl(6)-Cr(2)-Cl(5)	96.27(8)
C(55)-C(54)-C(57)	121.6(6)	Cl(7)-Cr(2)-Cl(5)	92.63(8)
C(53)-C(54)-C(57)	122.2(6)	Cl(8)-Cr(2)-P(3)	81.76(8)
C(56)-C(55)-C(54)	121.7(7)	Cl(6)-Cr(2)-P(3)	92.70(8)
C(56)-C(55)-H(55)	119.1	Cl(7)-Cr(2)-P(3)	91.03(7)
C(54)-C(55)-H(55)	119.1	Cl(5)-Cr(2)-P(3)	170.22(8)
N(1)-C(56)-C(55)	119.7(8)	Cl(8)-Cr(2)-P(4)	89.00(8)

Cl(6)-Cr(2)-P(4)	173.62(8)	C(73)-C(72)-C(71)	120.8(9)
Cl(7)-Cr(2)-P(4)	84.96(8)	C(73)-C(72)-H(72)	119.6
Cl(5)-Cr(2)-P(4)	89.13(8)	C(71)-C(72)-H(72)	119.6
P(3)-Cr(2)-P(4)	82.16(7)	C(74)-C(73)-C(72)	123.0(9)
C(71)-P(3)-C(81)	103.1(3)	C(74)-C(73)-H(73)	118.5
C(71)-P(3)-C(3)	104.2(3)	C(72)-C(73)-H(73)	118.5
C(81)-P(3)-C(3)	105.6(3)	C(73)-C(74)-C(75)	117.5(9)
C(71)-P(3)-Cr(2)	120.2(2)	C(73)-C(74)-H(74)	121.3
C(81)-P(3)-Cr(2)	117.8(3)	C(75)-C(74)-H(74)	121.3
C(3)-P(3)-Cr(2)	104.3(2)	C(74)-C(75)-C(76)	120.6(9)
C(91)-P(4)-C(101)	103.3(3)	C(74)-C(75)-H(75)	119.7
C(91)-P(4)-C(4)	103.9(3)	C(76)-C(75)-H(75)	119.7
C(101)-P(4)-C(4)	105.9(3)	C(71)-C(76)-C(75)	122.2(8)
C(91)-P(4)-Cr(2)	121.2(2)	C(71)-C(76)-H(76)	118.9
C(101)-P(4)-Cr(2)	116.0(2)	C(75)-C(76)-H(76)	118.9
C(4)-P(4)-Cr(2)	105.0(2)	C(82)-C(81)-C(86)	118.2(7)
C(4)-C(3)-P(3)	109.9(5)	C(82)-C(81)-P(3)	117.3(6)
C(4)-C(3)-H(3A)	109.7	C(86)-C(81)-P(3)	124.4(6)
P(3)-C(3)-H(3A)	109.7	C(81)-C(82)-C(83)	121.0(8)
C(4)-C(3)-H(3B)	109.7	C(81)-C(82)-H(82)	119.5
P(3)-C(3)-H(3B)	109.7	C(83)-C(82)-H(82)	119.5
H(3A)-C(3)-H(3B)	108.2	C(84)-C(83)-C(82)	120.9(9)
C(3)-C(4)-P(4)	109.9(4)	C(84)-C(83)-H(83)	119.5
C(3)-C(4)-H(4A)	109.7	C(82)-C(83)-H(83)	119.5
P(4)-C(4)-H(4A)	109.7	C(83)-C(84)-C(85)	118.0(9)
C(3)-C(4)-H(4B)	109.7	C(83)-C(84)-H(84)	121.0
P(4)-C(4)-H(4B)	109.7	C(85)-C(84)-H(84)	121.0
H(4A)-C(4)-H(4B)	108.2	C(84)-C(85)-C(86)	122.3(9)
C(76)-C(71)-C(72)	115.8(8)	C(84)-C(85)-H(85)	118.9
C(76)-C(71)-P(3)	122.2(6)	C(86)-C(85)-H(85)	118.9
C(72)-C(71)-P(3)	121.9(6)	C(81)-C(86)-C(85)	119.5(9)

C(81)-C(86)-H(86)	120.3	C(103)-C(104)-H(104)	120.4
C(85)-C(86)-H(86)	120.3	C(106)-C(105)-C(104)	121.7(9)
C(92)-C(91)-C(96)	117.1(8)	C(106)-C(105)-H(105)	119.2
C(92)-C(91)-P(4)	122.2(6)	C(104)-C(105)-H(105)	119.2
C(96)-C(91)-P(4)	120.7(6)	C(105)-C(106)-C(101)	119.9(8)
C(91)-C(92)-C(93)	121.6(9)	C(105)-C(106)-H(106)	120.0
C(91)-C(92)-H(92)	119.2	C(101)-C(106)-H(106)	120.0
C(93)-C(92)-H(92)	119.2	C(116)-N(2)-C(112)	120.8(10)
C(94)-C(93)-C(92)	119.9(9)	C(116)-N(2)-H(2)	119.6
C(94)-C(93)-H(93)	120.0	C(112)-N(2)-H(2)	119.6
C(92)-C(93)-H(93)	120.0	N(2)-C(112)-C(113)	119.3(11)
C(93)-C(94)-C(95)	119.3(9)	N(2)-C(112)-H(112)	120.4
C(93)-C(94)-H(94)	120.4	C(113)-C(112)-H(112)	120.4
C(95)-C(94)-H(94)	120.4	C(112)-C(113)-C(114)	121.1(9)
C(94)-C(95)-C(96)	121.0(10)	C(112)-C(113)-H(113)	119.5
C(94)-C(95)-H(95)	119.5	C(114)-C(113)-H(113)	119.5
C(96)-C(95)-H(95)	119.5	C(113)-C(114)-C(115)	117.2(9)
C(95)-C(96)-C(91)	121.1(8)	C(113)-C(114)-C(117)	122.0(8)
C(95)-C(96)-H(96)	119.5	C(115)-C(114)-C(117)	120.8(8)
C(91)-C(96)-H(96)	119.5	C(116)-C(115)-C(114)	120.3(10)
C(106)-C(101)-C(102)	118.9(7)	C(116)-C(115)-H(115)	119.8
C(106)-C(101)-P(4)	119.0(6)	C(114)-C(115)-H(115)	119.8
C(102)-C(101)-P(4)	122.1(6)	N(2)-C(116)-C(115)	121.3(10)
C(103)-C(102)-C(101)	120.4(8)	N(2)-C(116)-H(116)	119.4
C(103)-C(102)-H(102)	119.8	C(115)-C(116)-H(116)	119.4
C(101)-C(102)-H(102)	119.8	C(122)-C(117)-C(118)	117.1(9)
C(104)-C(103)-C(102)	119.8(9)	C(122)-C(117)-C(114)	122.1(8)
C(104)-C(103)-H(103)	120.1	C(118)-C(117)-C(114)	120.8(8)
C(102)-C(103)-H(103)	120.1	C(119)-C(118)-C(117)	121.4(10)
C(105)-C(104)-C(103)	119.2(8)	C(119)-C(118)-H(118)	119.3
C(105)-C(104)-H(104)	120.4	C(117)-C(118)-H(118)	119.3

C(118)-C(119)-C(120)	120.9(10)	C(1S)-C(2S)-H(2SA)	110.7
C(118)-C(119)-H(119)	119.6	C(4S)-C(2S)-H(2SA)	141.6
C(120)-C(119)-H(119)	119.6	C(3S)-C(2S)-H(2SB)	110.7
C(121)-C(120)-C(119)	118.9(11)	C(1S)-C(2S)-H(2SB)	110.7
C(121)-C(120)-H(120)	120.5	C(4S)-C(2S)-H(2SB)	104.0
C(119)-C(120)-H(120)	120.5	H(2SA)-C(2S)-H(2SB)	108.8
C(120)-C(121)-C(122)	119.5(10)	C(2S)-C(3S)-C(4S)	112(3)
C(120)-C(121)-H(121)	120.3	C(2S)-C(3S)-H(3SA)	109.3
C(122)-C(121)-H(121)	120.3	C(4S)-C(3S)-H(3SA)	109.3
C(117)-C(122)-C(121)	122.2(9)	C(2S)-C(3S)-H(3SB)	109.3
C(117)-C(122)-H(122)	118.9	C(4S)-C(3S)-H(3SB)	109.3
C(121)-C(122)-H(122)	118.9	H(3SA)-C(3S)-H(3SB)	107.9
C(4S)-O(1S)-C(1S)	98.9(18)	C(3S)-C(4S)-O(1S)	110(2)
O(1S)-C(1S)-C(2S)	102.1(17)	O(1S)-C(4S)-C(2S)	80.1(14)
O(1S)-C(1S)-H(1SA)	111.4	C(3S)-C(4S)-H(4SA)	109.7
C(2S)-C(1S)-H(1SA)	111.4	O(1S)-C(4S)-H(4SA)	109.7
O(1S)-C(1S)-H(1SB)	111.4	C(2S)-C(4S)-H(4SA)	112.3
C(2S)-C(1S)-H(1SB)	111.4	C(3S)-C(4S)-H(4SB)	109.7
H(1SA)-C(1S)-H(1SB)	109.2	O(1S)-C(4S)-H(4SB)	109.7
C(3S)-C(2S)-C(1S)	105(2)	C(2S)-C(4S)-H(4SB)	131.8
C(1S)-C(2S)-C(4S)	74.2(14)	H(4SA)-C(4S)-H(4SB)	108.2
C(3S)-C(2S)-H(2SA)	110.7		

Table A.41 **Anisotropic displacement parameters ($Å^2 x\ 10^3$) for [Hpyphenyl][$CrCl_4$(dppe)]. The anisotropic displacement factor exponent takes the form:**

$2p^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	44(1)	37(1)	36(1)	-6(1)	-3(1)	5(1)
Cl(1)	58(1)	60(1)	38(1)	-2(1)	-3(1)	3(1)
Cl(2)	66(1)	38(1)	57(1)	-11(1)	-13(1)	6(1)
Cl(3)	45(1)	58(1)	47(1)	-6(1)	-2(1)	7(1)
Cl(4)	44(1)	58(1)	54(1)	-10(1)	-8(1)	6(1)
P(1)	50(1)	53(1)	36(1)	-6(1)	0(1)	6(1)
P(2)	62(1)	38(1)	48(1)	-8(1)	-3(1)	4(1)
C(1)	105(7)	61(5)	42(4)	12(4)	9(4)	13(5)
C(2)	92(6)	57(5)	62(5)	-7(4)	12(5)	-7(4)
C(11)	56(5)	78(6)	38(4)	-18(4)	3(3)	3(4)
C(12)	72(7)	138(9)	85(7)	3(7)	25(6)	3(6)
C(13)	90(9)	202(15)	91(8)	-13(9)	48(7)	-11(9)
C(14)	74(8)	243(19)	90(9)	-34(11)	7(7)	55(10)
C(15)	89(8)	157(11)	69(6)	-33(7)	-16(6)	43(7)
C(16)	64(6)	104(7)	62(5)	-23(5)	1(4)	29(5)
C(21)	51(5)	76(6)	46(4)	-9(4)	-1(4)	8(4)
C(22)	85(7)	163(10)	49(5)	21(6)	-16(5)	-29(7)
C(23)	115(10)	193(13)	51(6)	21(7)	-31(6)	-16(9)
C(24)	80(8)	168(12)	78(8)	-44(8)	-25(6)	10(7)
C(25)	85(7)	91(7)	74(6)	-21(5)	-25(5)	3(5)
C(26)	73(6)	69(5)	57(5)	-22(4)	-17(4)	18(5)
C(31)	57(5)	50(4)	59(5)	-14(4)	-11(4)	5(4)
C(32)	76(6)	68(6)	76(6)	-18(5)	-8(5)	20(5)
C(33)	88(8)	104(8)	110(8)	-24(7)	13(6)	20(6)
C(34)	85(8)	81(7)	146(10)	-13(7)	15(7)	35(6)

C(35)	72(7)	83(7)	140(10)	23(7)	1(7)	20(5)
C(36)	63(6)	60(5)	92(6)	6(5)	-10(5)	17(4)
C(41)	58(5)	37(4)	74(5)	-12(4)	-8(4)	5(3)
C(42)	111(8)	75(6)	70(6)	-11(5)	-23(5)	-18(5)
C(43)	144(10)	90(8)	78(7)	-27(6)	-42(6)	-17(7)
C(44)	138(11)	95(9)	160(13)	-42(9)	-74(10)	-19(8)
C(45)	208(16)	85(9)	188(15)	6(9)	-99(13)	-64(9)
C(46)	150(10)	72(7)	132(10)	9(6)	-65(8)	-31(7)
N(1)	61(5)	70(5)	65(4)	-1(4)	19(4)	-1(4)
C(52)	75(6)	91(7)	48(5)	1(4)	2(4)	10(5)
C(53)	64(5)	90(6)	48(5)	9(4)	-2(4)	17(4)
C(54)	41(4)	47(4)	52(4)	-8(3)	-7(3)	3(3)
C(55)	56(5)	78(6)	62(5)	11(4)	-2(4)	-7(4)
C(56)	53(5)	79(6)	81(6)	17(5)	-1(5)	3(4)
C(57)	53(5)	50(4)	52(4)	-11(3)	-4(4)	-2(3)
C(58)	48(5)	70(5)	57(5)	2(4)	-7(4)	4(4)
C(59)	47(5)	89(6)	78(6)	-5(5)	-5(4)	-5(4)
C(60)	64(6)	89(7)	72(6)	-16(5)	9(5)	-9(5)
C(61)	93(7)	94(7)	54(5)	4(5)	3(5)	6(6)
C(62)	50(5)	87(6)	51(5)	0(4)	3(4)	12(4)
Cr(2)	66(1)	41(1)	41(1)	-10(1)	5(1)	6(1)
Cl(5)	98(2)	77(1)	51(1)	-23(1)	2(1)	-4(1)
Cl(6)	105(2)	40(1)	64(1)	-5(1)	9(1)	12(1)
Cl(7)	70(1)	67(1)	55(1)	-10(1)	6(1)	-4(1)
Cl(8)	62(1)	64(1)	62(1)	-3(1)	10(1)	10(1)
P(3)	64(1)	41(1)	43(1)	-10(1)	-1(1)	11(1)
P(4)	61(1)	46(1)	40(1)	-7(1)	0(1)	8(1)
C(3)	68(5)	40(4)	44(4)	-8(3)	-4(4)	4(3)
C(4)	64(5)	47(4)	42(4)	-11(3)	-3(3)	13(4)
C(71)	66(5)	51(5)	47(4)	-6(3)	-3(4)	13(4)
C(72)	102(8)	78(6)	111(8)	-34(6)	-51(6)	37(6)

C(73)	102(8)	104(8)	126(9)	-46(7)	-47(7)	51(7)
C(74)	84(7)	95(8)	97(7)	-16(6)	-35(6)	22(6)
C(75)	95(8)	96(8)	123(9)	-36(7)	-49(7)	11(6)
C(76)	90(7)	64(6)	112(8)	-42(5)	-38(6)	14(5)
C(81)	74(5)	60(5)	41(4)	-5(4)	0(4)	3(4)
C(82)	156(10)	50(5)	74(6)	-16(5)	37(6)	3(6)
C(83)	177(11)	74(7)	74(7)	-1(5)	30(7)	-17(7)
C(84)	131(9)	94(8)	54(5)	-5(5)	29(6)	-9(7)
C(85)	159(11)	102(9)	73(7)	-19(6)	43(7)	29(8)
C(86)	149(9)	68(6)	52(5)	-4(4)	33(6)	29(6)
C(91)	62(5)	52(4)	51(4)	-6(4)	-2(4)	7(4)
C(92)	76(6)	67(5)	59(5)	-11(4)	-9(4)	0(4)
C(93)	88(8)	98(8)	82(7)	-11(6)	-36(6)	19(6)
C(94)	72(7)	86(7)	137(10)	-46(7)	-35(7)	16(6)
C(95)	69(7)	97(7)	96(8)	-24(6)	-1(6)	12(5)
C(96)	68(6)	72(6)	74(6)	-12(4)	-11(5)	11(4)
C(101)	62(5)	51(5)	40(4)	-1(3)	-6(3)	9(4)
C(102)	80(6)	74(6)	62(5)	-10(4)	3(4)	-16(5)
C(103)	119(8)	85(7)	74(6)	-1(5)	9(6)	-43(6)
C(104)	87(7)	107(9)	73(7)	32(6)	2(5)	-22(6)
C(105)	121(8)	89(7)	55(5)	14(5)	23(5)	19(6)
C(106)	123(8)	57(5)	53(5)	2(4)	20(5)	15(5)
N(2)	92(7)	97(6)	122(7)	-29(6)	-31(6)	-6(5)
C(112)	100(9)	148(11)	122(9)	-67(9)	7(7)	-6(8)
C(113)	96(8)	117(9)	111(8)	-64(7)	7(7)	-5(7)
C(114)	79(6)	72(6)	59(5)	-18(4)	-7(5)	3(5)
C(115)	95(7)	84(7)	102(7)	-50(6)	-22(6)	12(6)
C(116)	114(10)	95(8)	116(9)	-48(7)	-24(8)	6(7)
C(117)	85(6)	65(5)	54(5)	-14(4)	-1(4)	10(5)
C(118)	101(8)	78(7)	92(7)	-38(5)	12(6)	10(6)
C(119)	132(11)	97(8)	123(10)	-56(7)	-1(8)	-19(8)

C(120)	121(10)	94(8)	93(8)	-17(6)	-4(7)	-31(7)
C(121)	84(8)	132(10)	100(8)	-16(7)	12(6)	-12(7)
C(122)	103(8)	101(8)	82(7)	-42(6)	10(6)	3(6)

Table A.42 **Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for [Hpyphenyl][$CrCl_4$(dppe)]**

	x	y	z	U(eq)
H(1A)	9341	2089	2658	85
H(1B)	8052	2065	3070	85
H(2A)	6850	1981	2263	85
H(2B)	7834	1249	2294	85
H(12)	6386	2652	3464	120
H(13)	4494	3188	3954	156
H(14)	3809	4471	3696	162
H(15)	4971	5276	3020	124
H(16)	6804	4781	2522	92
H(22)	8833	2937	3789	119
H(23)	10199	3409	4445	144
H(24)	11471	4540	4195	128
H(25)	11585	5126	3251	98
H(26)	10281	4594	2581	78
H(32)	10553	2234	641	87
H(33)	12394	1465	392	121
H(34)	12859	347	1011	126
H(35)	11567	20	1848	120
H(36)	9707	751	2070	86
H(42)	7494	2611	390	101

H(43)	6217	1991	-255	121
H(44)	5346	724	-3	151
H(45)	5789	73	844	188
H(46)	6997	680	1515	139
H(1)	11648	3840	649	80
H(52)	13536	3457	958	86
H(53)	15362	3603	328	82
H(55)	13176	4591	-886	79
H(56)	11384	4385	-244	87
H(58)	16971	3867	-226	70
H(59)	18765	4015	-897	86
H(60)	18539	4501	-1827	90
H(61)	16498	4837	-2125	98
H(62)	14687	4656	-1476	76
H(3A)	2308	3447	7910	61
H(3B)	2962	3352	7274	61
H(4A)	899	3976	7223	61
H(4B)	245	3203	7568	61
H(72)	4324	801	7578	112
H(73)	6365	619	7859	128
H(74)	7302	1512	8410	108
H(75)	6252	2731	8580	122
H(76)	4177	2929	8320	103
H(82)	1625	629	8375	114
H(83)	463	268	9253	133
H(84)	-583	1242	9788	114
H(85)	-418	2585	9445	136
H(86)	855	2976	8606	110
H(92)	-404	3461	5571	81
H(93)	-2528	3675	5342	105
H(94)	-4203	3447	6052	115

H(95)	-3755	3024	6991	104
H(96)	-1675	2738	7210	85
H(102)	1766	4586	6461	86
H(103)	2988	5356	5741	112
H(104)	3816	4752	4901	109
H(105)	3340	3406	4777	109
H(106)	2156	2627	5490	95
H(2)	-1289	802	6248	122
H(112)	-813	-95	5568	146
H(113)	-2492	-797	5225	128
H(115)	-4960	341	6319	109
H(116)	-3282	1045	6620	127
H(118)	-3962	-1451	4962	108
H(119)	-5620	-2222	4684	139
H(120)	-7710	-2055	5088	123
H(121)	-8111	-1096	5784	127
H(122)	-6417	-355	6084	114
H(1SA)	3770	785	2381	150
H(1SB)	4649	1270	2780	150
H(2SA)	4632	2157	1993	137
H(2SB)	3193	1929	1881	137
H(3SA)	2985	2938	2231	161
H(3SB)	4138	2781	2630	161
H(4SA)	1717	2361	2800	160
H(4SB)	2749	2514	3252	160

Table A.43 Torsion angles [°] for [Hpyphenyl][$CrCl_4$(dppe)]

Cl(4)-Cr(1)-P(1)-C(11)	-26.7(3)	C(41)-P(2)-C(2)-C(1)	-173.0(6)
Cl(3)-Cr(1)-P(1)-C(11)	161.0(3)	Cr(1)-P(2)-C(2)-C(1)	-45.8(6)
Cl(2)-Cr(1)-P(1)-C(11)	67.2(3)	C(21)-P(1)-C(11)-C(12)	-87.0(8)
P(2)-Cr(1)-P(1)-C(11)	-110.0(3)	C(1)-P(1)-C(11)-C(12)	20.3(8)
Cl(4)-Cr(1)-P(1)-C(21)	-150.4(3)	Cr(1)-P(1)-C(11)-C(12)	139.0(7)
Cl(3)-Cr(1)-P(1)-C(21)	37.3(3)	C(21)-P(1)-C(11)-C(16)	88.1(7)
Cl(2)-Cr(1)-P(1)-C(21)	-56.5(3)	C(1)-P(1)-C(11)-C(16)	-164.6(6)
P(2)-Cr(1)-P(1)-C(21)	126.3(3)	Cr(1)-P(1)-C(11)-C(16)	-46.0(7)
Cl(4)-Cr(1)-P(1)-C(1)	93.7(3)	C(16)-C(11)-C(12)-C(13)	-0.3(14)
Cl(3)-Cr(1)-P(1)-C(1)	-78.6(3)	P(1)-C(11)-C(12)-C(13)	174.8(8)
Cl(2)-Cr(1)-P(1)-C(1)	-172.4(3)	C(11)-C(12)-C(13)-C(14)	0.8(19)
P(2)-Cr(1)-P(1)-C(1)	10.3(3)	C(12)-C(13)-C(14)-C(15)	-2(2)
Cl(4)-Cr(1)-P(2)-C(31)	167.4(3)	C(13)-C(14)-C(15)-C(16)	2(2)
Cl(3)-Cr(1)-P(2)-C(31)	-18.7(3)	C(12)-C(11)-C(16)-C(15)	0.7(13)
Cl(1)-Cr(1)-P(2)-C(31)	73.1(3)	P(1)-C(11)-C(16)-C(15)	-174.6(7)
P(1)-Cr(1)-P(2)-C(31)	-103.4(3)	C(14)-C(15)-C(16)-C(11)	-1.6(15)
Cl(4)-Cr(1)-P(2)-C(41)	41.2(3)	C(11)-P(1)-C(21)-C(26)	-110.2(7)
Cl(3)-Cr(1)-P(2)-C(41)	-144.9(3)	C(1)-P(1)-C(21)-C(26)	138.3(7)
Cl(1)-Cr(1)-P(2)-C(41)	-53.1(3)	Cr(1)-P(1)-C(21)-C(26)	21.3(8)
P(1)-Cr(1)-P(2)-C(41)	130.4(3)	C(11)-P(1)-C(21)-C(22)	64.8(8)
Cl(4)-Cr(1)-P(2)-C(2)	-74.3(3)	C(1)-P(1)-C(21)-C(22)	-46.8(8)
Cl(3)-Cr(1)-P(2)-C(2)	99.6(3)	Cr(1)-P(1)-C(21)-C(22)	-163.7(7)
Cl(1)-Cr(1)-P(2)-C(2)	-168.6(3)	C(26)-C(21)-C(22)-C(23)	-1.6(15)
P(1)-Cr(1)-P(2)-C(2)	14.8(3)	P(1)-C(21)-C(22)-C(23)	-176.8(9)
C(11)-P(1)-C(1)-C(2)	84.0(6)	C(21)-C(22)-C(23)-C(24)	3.6(19)
C(21)-P(1)-C(1)-C(2)	-170.7(6)	C(22)-C(23)-C(24)-C(25)	-3.7(19)
Cr(1)-P(1)-C(1)-C(2)	-42.4(6)	C(23)-C(24)-C(25)-C(26)	1.8(16)
P(1)-C(1)-C(2)-P(2)	59.8(7)	C(22)-C(21)-C(26)-C(25)	-0.3(12)
C(31)-P(2)-C(2)-C(1)	79.8(6)	P(1)-C(21)-C(26)-C(25)	174.9(6)

C(24)-C(25)-C(26)-C(21)	0.2(13)	C(52)-C(53)-C(54)-C(55)	1.5(12)
C(41)-P(2)-C(31)-C(32)	80.6(7)	C(52)-C(53)-C(54)-C(57)	179.1(7)
C(2)-P(2)-C(31)-C(32)	-171.2(6)	C(53)-C(54)-C(55)-C(56)	-2.7(12)
Cr(1)-P(2)-C(31)-C(32)	-54.4(7)	C(57)-C(54)-C(55)-C(56)	179.7(7)
C(41)-P(2)-C(31)-C(36)	-96.7(7)	C(52)-N(1)-C(56)-C(55)	-0.5(13)
C(2)-P(2)-C(31)-C(36)	11.5(7)	C(54)-C(55)-C(56)-N(1)	2.3(13)
Cr(1)-P(2)-C(31)-C(36)	128.3(6)	C(55)-C(54)-C(57)-C(58)	173.1(7)
C(36)-C(31)-C(32)-C(33)	1.4(13)	C(53)-C(54)-C(57)-C(58)	-4.3(11)
P(2)-C(31)-C(32)-C(33)	-176.0(7)	C(55)-C(54)-C(57)-C(62)	-4.8(11)
C(31)-C(32)-C(33)-C(34)	-1.2(15)	C(53)-C(54)-C(57)-C(62)	177.8(7)
C(32)-C(33)-C(34)-C(35)	-0.5(17)	C(62)-C(57)-C(58)-C(59)	-3.1(11)
C(33)-C(34)-C(35)-C(36)	1.9(18)	C(54)-C(57)-C(58)-C(59)	178.9(7)
C(34)-C(35)-C(36)-C(31)	-1.6(16)	C(57)-C(58)-C(59)-C(60)	2.3(13)
C(32)-C(31)-C(36)-C(35)	0.0(13)	C(58)-C(59)-C(60)-C(61)	-0.3(13)
P(2)-C(31)-C(36)-C(35)	177.2(7)	C(59)-C(60)-C(61)-C(62)	-0.8(14)
C(31)-P(2)-C(41)-C(42)	-103.9(7)	C(60)-C(61)-C(62)-C(57)	-0.1(13)
C(2)-P(2)-C(41)-C(42)	145.2(7)	C(58)-C(57)-C(62)-C(61)	2.0(11)
Cr(1)-P(2)-C(41)-C(42)	29.3(8)	C(54)-C(57)-C(62)-C(61)	180.0(7)
C(31)-P(2)-C(41)-C(46)	74.5(9)	Cl(8)-Cr(2)-P(3)-C(71)	-41.0(3)
C(2)-P(2)-C(41)-C(46)	-36.3(9)	Cl(6)-Cr(2)-P(3)-C(71)	52.7(3)
Cr(1)-P(2)-C(41)-C(46)	-152.3(7)	Cl(7)-Cr(2)-P(3)-C(71)	144.1(3)
C(46)-C(41)-C(42)-C(43)	-1.8(15)	P(4)-Cr(2)-P(3)-C(71)	-131.1(3)
P(2)-C(41)-C(42)-C(43)	176.6(8)	Cl(8)-Cr(2)-P(3)-C(81)	-168.2(3)
C(41)-C(42)-C(43)-C(44)	0.8(17)	Cl(6)-Cr(2)-P(3)-C(81)	-74.5(3)
C(42)-C(43)-C(44)-C(45)	-1(2)	Cl(7)-Cr(2)-P(3)-C(81)	16.9(3)
C(43)-C(44)-C(45)-C(46)	2(3)	P(4)-Cr(2)-P(3)-C(81)	101.7(3)
C(42)-C(41)-C(46)-C(45)	2.8(17)	Cl(8)-Cr(2)-P(3)-C(3)	75.2(2)
P(2)-C(41)-C(46)-C(45)	-175.6(10)	Cl(6)-Cr(2)-P(3)-C(3)	168.8(2)
C(44)-C(45)-C(46)-C(41)	-3(2)	Cl(7)-Cr(2)-P(3)-C(3)	-99.7(2)
C(56)-N(1)-C(52)-C(53)	-0.7(13)	P(4)-Cr(2)-P(3)-C(3)	-15.0(2)
N(1)-C(52)-C(53)-C(54)	0.1(13)	Cl(8)-Cr(2)-P(4)-C(91)	149.6(3)

Cl(7)-Cr(2)-P(4)-C(91)	-36.8(3)	C(74)-C(75)-C(76)-C(71)	-2.5(17)
Cl(5)-Cr(2)-P(4)-C(91)	55.9(3)	C(71)-P(3)-C(81)-C(82)	-72.7(8)
P(3)-Cr(2)-P(4)-C(91)	-128.6(3)	C(3)-P(3)-C(81)-C(82)	178.2(7)
Cl(8)-Cr(2)-P(4)-C(101)	23.0(3)	Cr(2)-P(3)-C(81)-C(82)	62.3(8)
Cl(7)-Cr(2)-P(4)-C(101)	-163.5(3)	C(71)-P(3)-C(81)-C(86)	103.9(8)
Cl(5)-Cr(2)-P(4)-C(101)	-70.7(3)	C(3)-P(3)-C(81)-C(86)	-5.2(9)
P(3)-Cr(2)-P(4)-C(101)	104.8(3)	Cr(2)-P(3)-C(81)-C(86)	-121.1(7)
Cl(8)-Cr(2)-P(4)-C(4)	-93.4(3)	C(86)-C(81)-C(82)-C(83)	0.9(16)
Cl(7)-Cr(2)-P(4)-C(4)	80.1(3)	P(3)-C(81)-C(82)-C(83)	177.8(9)
Cl(5)-Cr(2)-P(4)-C(4)	172.8(3)	C(81)-C(82)-C(83)-C(84)	1.3(19)
P(3)-Cr(2)-P(4)-C(4)	-11.6(3)	C(82)-C(83)-C(84)-C(85)	-1.0(18)
C(71)-P(3)-C(3)-C(4)	173.5(5)	C(83)-C(84)-C(85)-C(86)	-1.5(19)
C(81)-P(3)-C(3)-C(4)	-78.2(5)	C(82)-C(81)-C(86)-C(85)	-3.3(15)
Cr(2)-P(3)-C(3)-C(4)	46.6(5)	P(3)-C(81)-C(86)-C(85)	-179.9(8)
P(3)-C(3)-C(4)-P(4)	-61.2(6)	C(84)-C(85)-C(86)-C(81)	3.7(18)
C(91)-P(4)-C(4)-C(3)	171.9(5)	C(101)-P(4)-C(91)-C(92)	22.9(7)
C(101)-P(4)-C(4)-C(3)	-79.6(5)	C(4)-P(4)-C(91)-C(92)	133.3(6)
Cr(2)-P(4)-C(4)-C(3)	43.6(5)	Cr(2)-P(4)-C(91)-C(92)	-109.3(6)
C(81)-P(3)-C(71)-C(76)	-76.6(8)	C(101)-P(4)-C(91)-C(96)	-158.2(6)
C(3)-P(3)-C(71)-C(76)	33.6(8)	C(4)-P(4)-C(91)-C(96)	-47.8(7)
Cr(2)-P(3)-C(71)-C(76)	149.8(7)	Cr(2)-P(4)-C(91)-C(96)	69.6(7)
C(81)-P(3)-C(71)-C(72)	104.0(8)	C(96)-C(91)-C(92)-C(93)	0.0(12)
C(3)-P(3)-C(71)-C(72)	-145.8(7)	P(4)-C(91)-C(92)-C(93)	178.9(6)
Cr(2)-P(3)-C(71)-C(72)	-29.6(8)	C(91)-C(92)-C(93)-C(94)	0.9(14)
C(76)-C(71)-C(72)-C(73)	1.2(15)	C(92)-C(93)-C(94)-C(95)	0.2(15)
P(3)-C(71)-C(72)-C(73)	-179.4(8)	C(93)-C(94)-C(95)-C(96)	-2.2(15)
C(71)-C(72)-C(73)-C(74)	1.3(18)	C(94)-C(95)-C(96)-C(91)	3.2(14)
C(72)-C(73)-C(74)-C(75)	-4.3(18)	C(92)-C(91)-C(96)-C(95)	-2.0(12)
C(73)-C(74)-C(75)-C(76)	4.9(18)	P(4)-C(91)-C(96)-C(95)	179.1(6)
C(72)-C(71)-C(76)-C(75)	-0.6(14)	C(91)-P(4)-C(101)-C(106)	-93.9(7)
P(3)-C(71)-C(76)-C(75)	-180.0(8)	C(4)-P(4)-C(101)-C(106)	157.1(6)

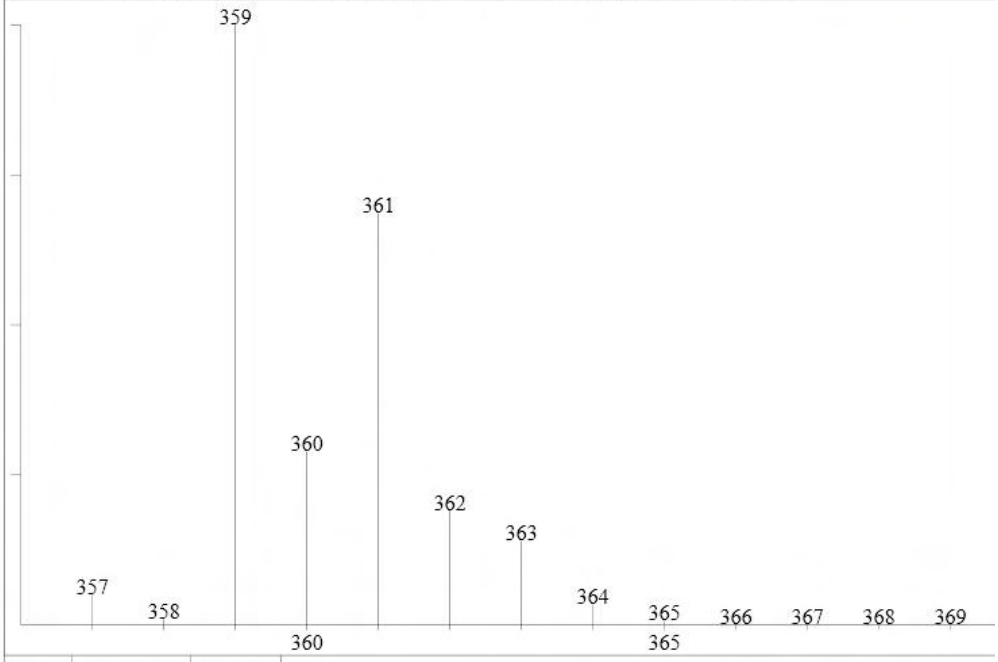
Cr(2)-P(4)-C(101)-C(106) 41.2(7)	C(115)-C(114)-C(117)-C(122)-2.3(14)
C(91)-P(4)-C(101)-C(102) 86.3(7)	C(113)-C(114)-C(117)-C(118)-0.3(14)
C(4)-P(4)-C(101)-C(102) -22.7(7)	C(115)-C(114)-C(117)-C(118)178.3(9)
Cr(2)-P(4)-C(101)-C(102) -138.6(6)	C(122)-C(117)-C(118)-C(119)-0.9(15)
C(106)-C(101)-C(102)-C(103) 0.3(13)	C(114)-C(117)-C(118)-C(119)178.5(10)
P(4)-C(101)-C(102)-C(103)-179.9(7)	C(117)-C(118)-C(119)-C(120) 1.2(18)
C(101)-C(102)-C(103)-C(104)-0.5(15)	C(118)-C(119)-C(120)-C(121)-0.1(19)
C(102)-C(103)-C(104)-C(105) 1.2(16)	C(119)-C(120)-C(121)-C(122)-1.0(17)
C(103)-C(104)-C(105)-C(106)-1.7(16)	C(118)-C(117)-C(122)-C(121)-0.3(15)
C(104)-C(105)-C(106)-C(101) 1.5(15)	C(114)-C(117)-C(122)-C(121)-179.7(9)
C(102)-C(101)-C(106)-C(105)-0.8(13)	C(120)-C(121)-C(122)-C(117) 1.3(17)
P(4)-C(101)-C(106)-C(105) 179.4(7)	C(4S)-O(1S)-C(1S)-C(2S) -21(2)
C(116)-N(2)-C(112)-C(113) 0.1(19)	O(1S)-C(1S)-C(2S)-C(3S) 35(3)
N(2)-C(112)-C(113)-C(114) -3(2)	O(1S)-C(1S)-C(2S)-C(4S) 15.0(16)
C(112)-C(113)-C(114)-C(115) 3.7(17)	C(1S)-C(2S)-C(3S)-C(4S) -34(3)
C(112)-C(113)-C(114)-C(117)-177.7(10)	C(2S)-C(3S)-C(4S)-O(1S) 20(3)
C(113)-C(114)-C(115)-C(116)-2.6(15)	C(1S)-O(1S)-C(4S)-C(3S) 5(3)
C(117)-C(114)-C(115)-C(116)178.8(10)	C(1S)-O(1S)-C(4S)-C(2S) 15.2(15)
C(112)-N(2)-C(116)-C(115) 1.0(18)	C(1S)-C(2S)-C(4S)-C(3S) 146(3)
C(114)-C(115)-C(116)-N(2) 0.3(17)	C(3S)-C(2S)-C(4S)-O(1S) -161(3)
C(113)-C(114)-C(117)-C(122)179.1(10)	C(1S)-C(2S)-C(4S)-O(1S) -15.0(16)

Table A.44 Hydrogen bonds for [Hpyphenyl][$CrCl_4$(dppe)] [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...Cl(1)	0.86	2.62	3.255(7)	131.9
N(1)-H(1)...Cl(3)	0.86	2.44	3.183(6)	145.1
N(2)-H(2)...Cl(5)	0.86	2.55	3.217(10)	134.8
N(2)-H(2)...Cl(7)	0.86	2.62	3.330(9)	140.0

APPENDIX 2 : CALCULATED MS DISTRIBUTION PATTERNS

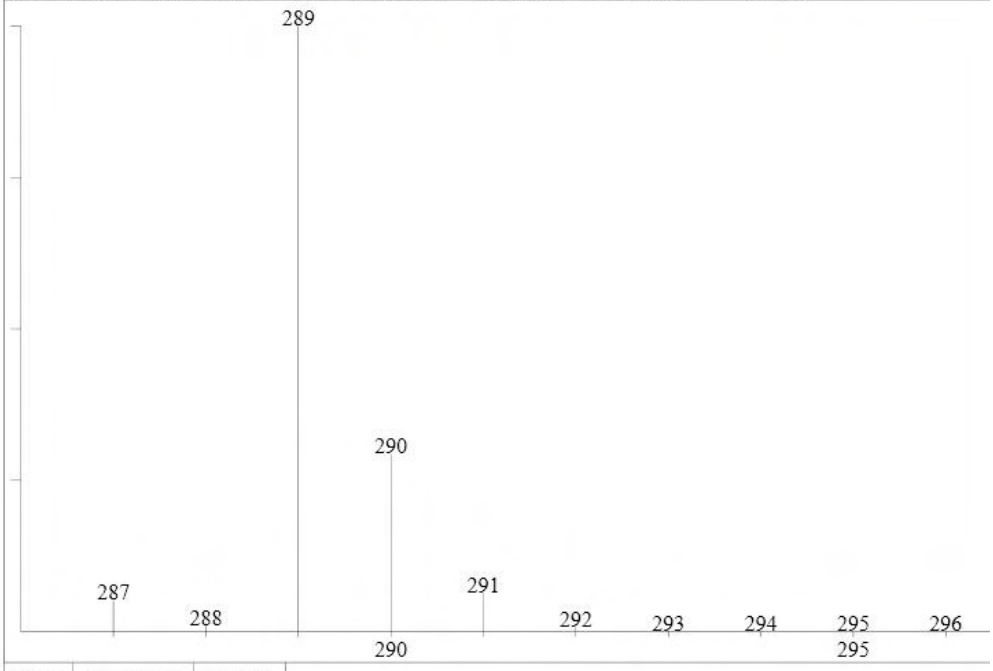
DISTRIBUTION OF ISOTOPES CALCULATED BY 'ISOFORM' PROGRAM FOR
Formula : CrCl2C15H15N3
Factor : 100 Nominal MW = 359 Exact MW = 359.00479 Average MW = 360.21



Mass	Abundance	*Factor
357	4.95391	4.95
358	0.89096	0.89
359	100.00000	100.00
360	28.90886	28.91
361	68.60853	68.61
362	18.95201	18.95
363	13.90177	13.90
364	3.37117	3.37
365	0.66502	0.67
366	0.07687	0.08
367	0.00551	0.01
368	0.00027	0.00
369	0.00001	0.00

Figure B1 Calculated isotopic distribution pattern for $[CrCl_2(py)_3]$

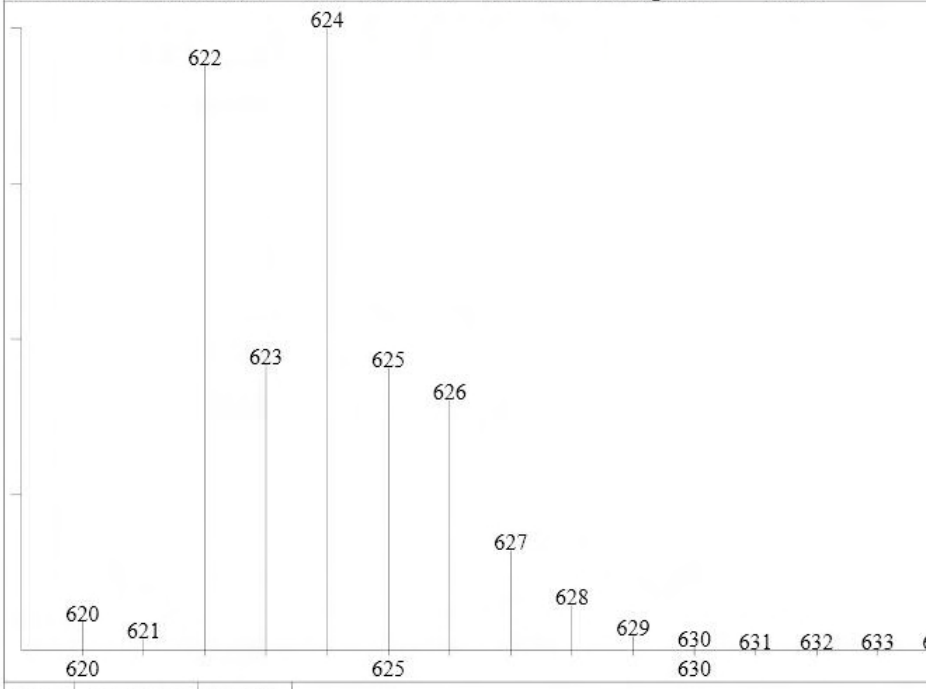
DISTRIBUTION OF ISOTOPES CALCULATED BY 'ISOFORM' PROGRAM FOR
Formula : CrC15H15N3
Factor : 100 Nominal MW = 289 Exact MW = 289.06708 Average MW = 289.30



Mass	Abundance	*Factor
287	5.11601	5.12
288	0.92011	0.92
289	100.00000	100.00
290	29.26631	29.27
291	6.37031	6.37
292	0.75932	0.76
293	0.05501	0.06
294	0.00269	0.00
295	0.00010	0.00
296	0.00000	0.00

Figure B2 Calculated distribution pattern for $[Cr(py)_3]$

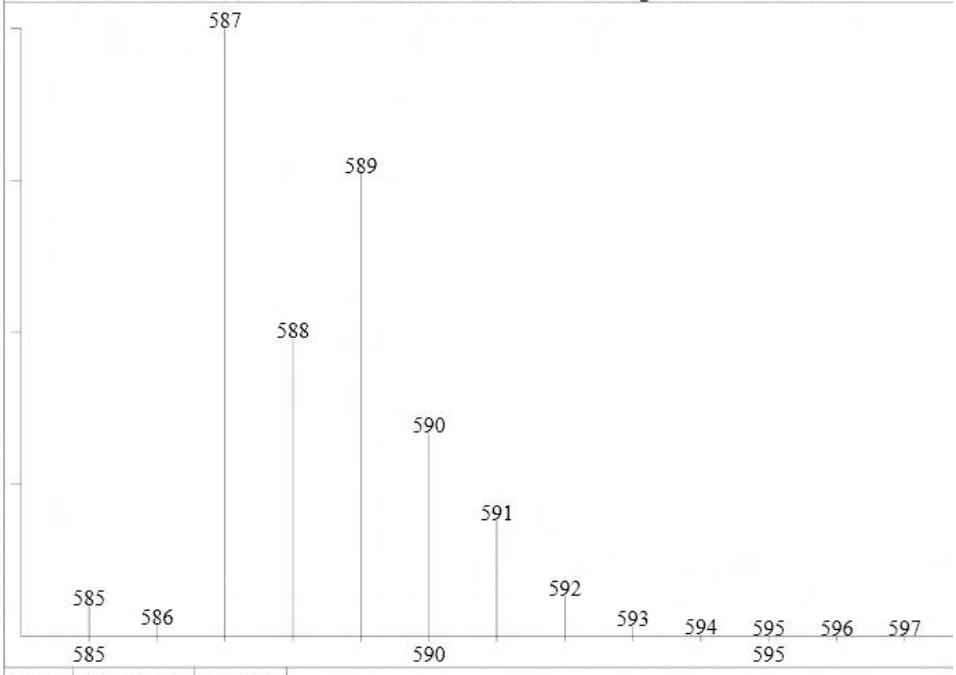
DISTRIBUTION OF ISOTOPES CALCULATED BY 'ISOFORM' PROGRAM FOR
Formula : CrCl3C33H27N3
Factor : 100 Nominal MW = 622 Exact MW = 622.06757 Average MW = 623.96



Mass	Abundance	*Factor
620	4.56889	4.57
621	1.74280	1.74
622	93.94258	93.94
623	45.83363	45.83
624	100.00000	100.00
625	45.33328	45.33
626	40.11766	40.12
627	15.97106	15.97
628	7.13687	7.14
629	2.22202	2.22
630	0.51818	0.52
631	0.08985	0.09
632	0.01159	0.01
633	0.00114	0.00

Figure B3 Calculated isotopic distribution pattern for [$CrCl_3$(pyphenyl)$_3$]

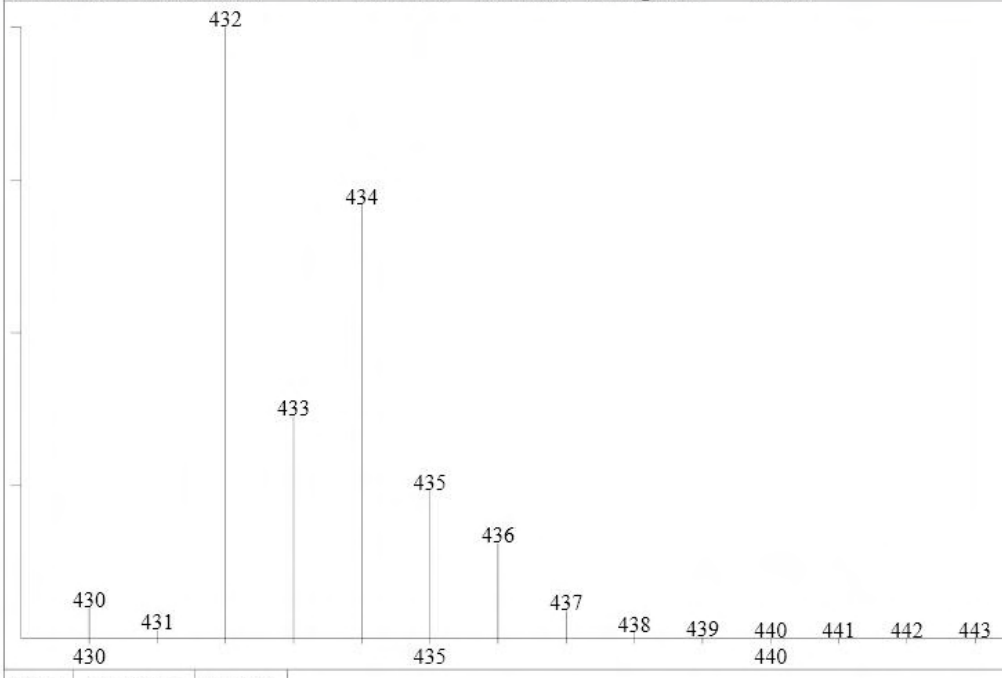
DISTRIBUTION OF ISOTOPES CALCULATED BY 'ISOFORM' PROGRAM FOR
Formula : CrCl2C33H27N3
Factor : 100 Nominal MW = 587 Exact MW = 587.09869 Average MW = 588.50



Mass	Abundance	*Factor
585	4.94033	4.94
586	1.88449	1.88
587	100.00000	100.00
588	48.95714	48.96
589	76.14979	76.15
590	33.36229	33.36
591	19.02644	19.03
592	6.60021	6.60
593	1.63242	1.63
594	0.29192	0.29
595	0.03826	0.04
596	0.00380	0.00
597	0.00029	0.00

Figure B4 Calculated isotopic distribution pattern for [$CrCl_2$(pyphenyl)$_3$]

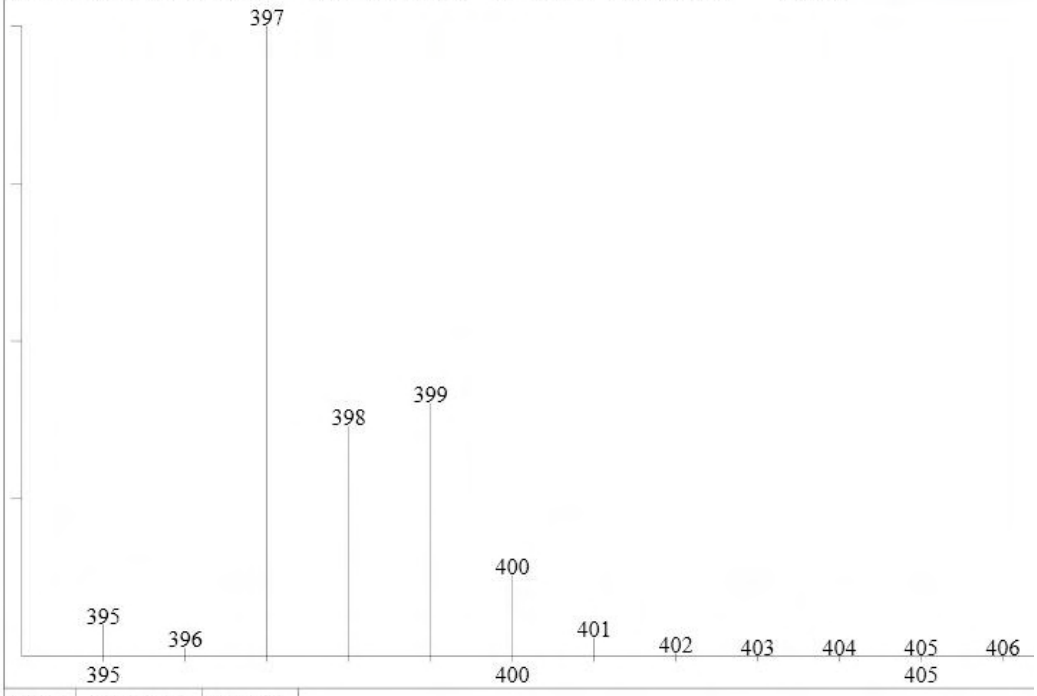
DISTRIBUTION OF ISOTOPES CALCULATED BY 'ISOFORM' PROGRAM FOR
Formula : CrCl2C22H18N2
Factor : 100 Nominal MW = 432 Exact MW = 432.02518 Average MW = 433.30



Mass	Abundance	*Factor
430	4.95005	4.95
431	1.25880	1.26
432	100.00000	100.00
433	36.32783	36.33
434	70.94023	70.94
435	24.11300	24.11
436	15.46292	15.46
437	4.44995	4.45
438	0.94869	0.95
439	0.13475	0.13
440	0.01292	0.01
441	0.00089	0.00
442	0.00005	0.00
443	0.00000	0.00

Figure B5 Calculated isotopic distribution pattern for [$CrCl_2$(pyphenyl)$_2$]

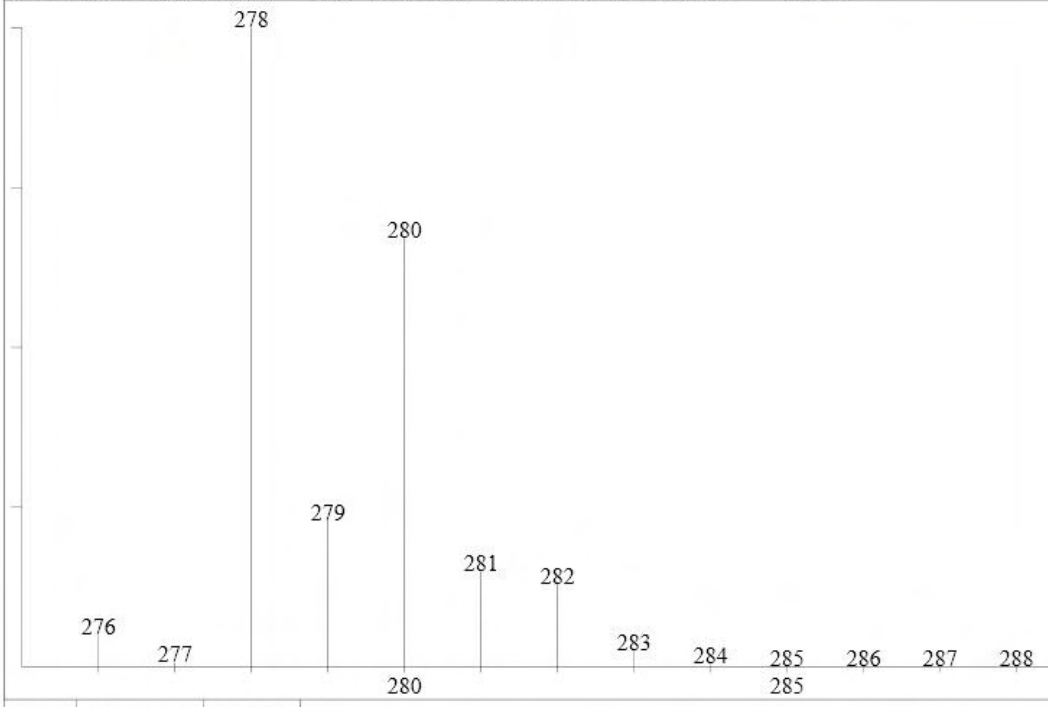
DISTRIBUTION OF ISOTOPES CALCULATED BY 'ISOFORM' PROGRAM FOR
Formula : CrClC22H18N2
Factor : 100 Nominal MW = 397 Exact MW = 397.05630 Average MW = 397.85



Mass	Abundance	*Factor
395	5.02967	5.03
396	1.27905	1.28
397	100.00000	100.00
398	36.50312	36.50
399	40.10129	40.10
400	12.82716	12.83
401	2.88725	2.89
402	0.41940	0.42
403	0.04060	0.04
404	0.00280	0.00
405	0.00014	0.00
406	0.00001	0.00

Figure B6 Calculated isotopic distribution pattern for [CrCl(pyphenyl)$_2$]

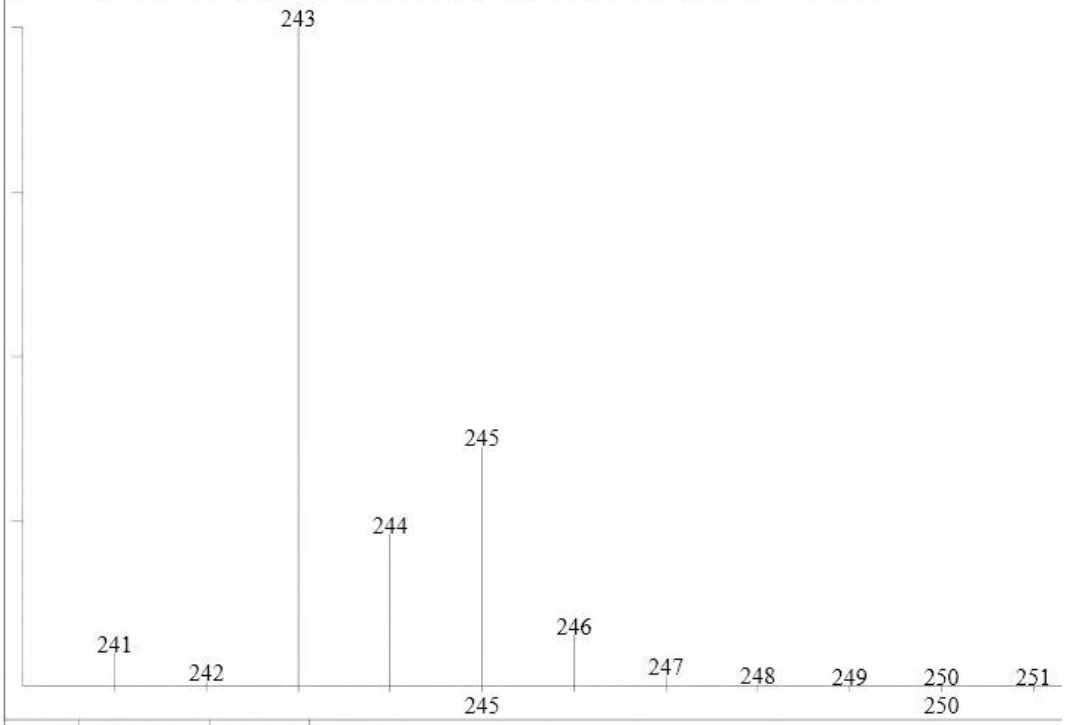
DISTRIBUTION OF ISOTOPES CALCULATED BY 'ISOFORM' PROGRAM FOR
Formula : CrCl2C10H8N2
Factor : 100 Nominal MW = 278 Exact MW = 277.94693 Average MW = 279.09



Mass	Abundance	*Factor
276	4.95605	4.96
277	0.59274	0.59
278	100.00000	100.00
279	22.89535	22.90
280	67.10867	67.11
281	14.88057	14.88
282	12.91008	12.91
283	2.57114	2.57
284	0.49073	0.49
285	0.04322	0.04
286	0.00212	0.00
287	0.00007	0.00
288	0.00000	0.00

Figure B7 Calculated isotopic distribution pattern for [$CrCl_2$(bipy)]

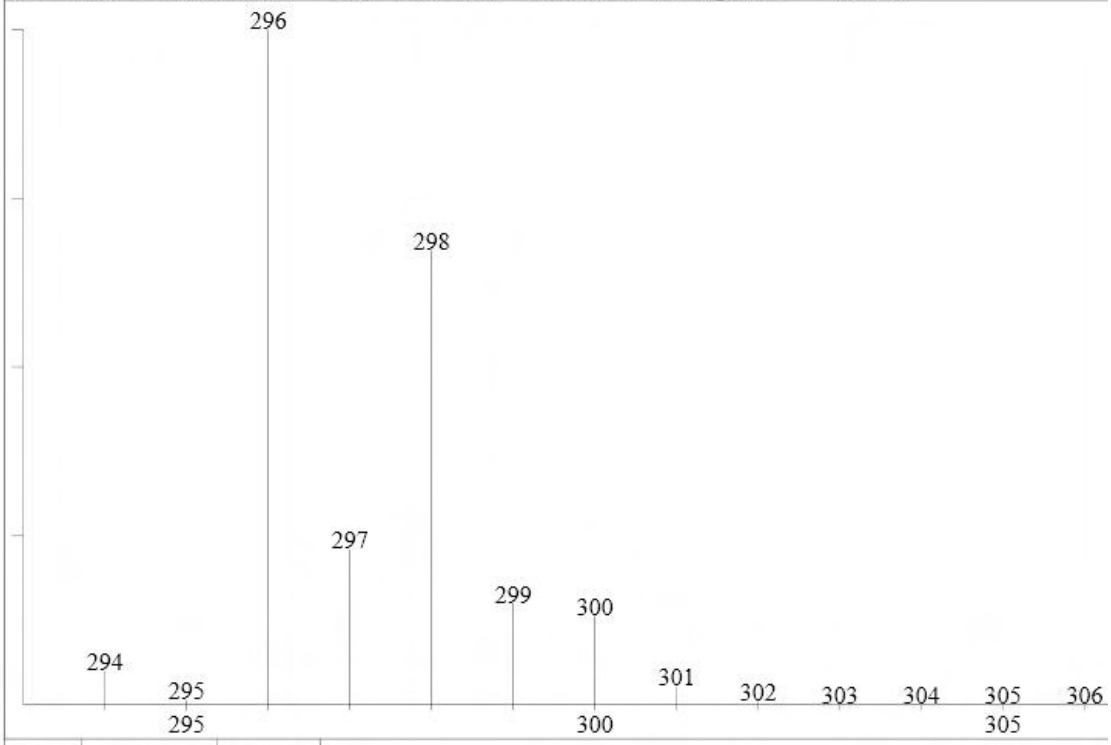
DISTRIBUTION OF ISOTOPES CALCULATED BY 'ISOFORM' PROGRAM FOR
Formula : CrClC10H8N2
Factor : 100 Nominal MW = 243 Exact MW = 242.97810 Average MW = 243.64



Mass	Abundance	*Factor
241	5.03586	5.04
242	0.60229	0.60
243	100.00000	100.00
244	23.07146	23.07
245	36.20943	36.21
246	7.74196	7.74
247	1.53822	1.54
248	0.13667	0.14
249	0.00671	0.01
250	0.00021	0.00
251	0.00000	0.00

Figure B8 Calculated isotopic distribution pattern for [CrCl(bipy)]

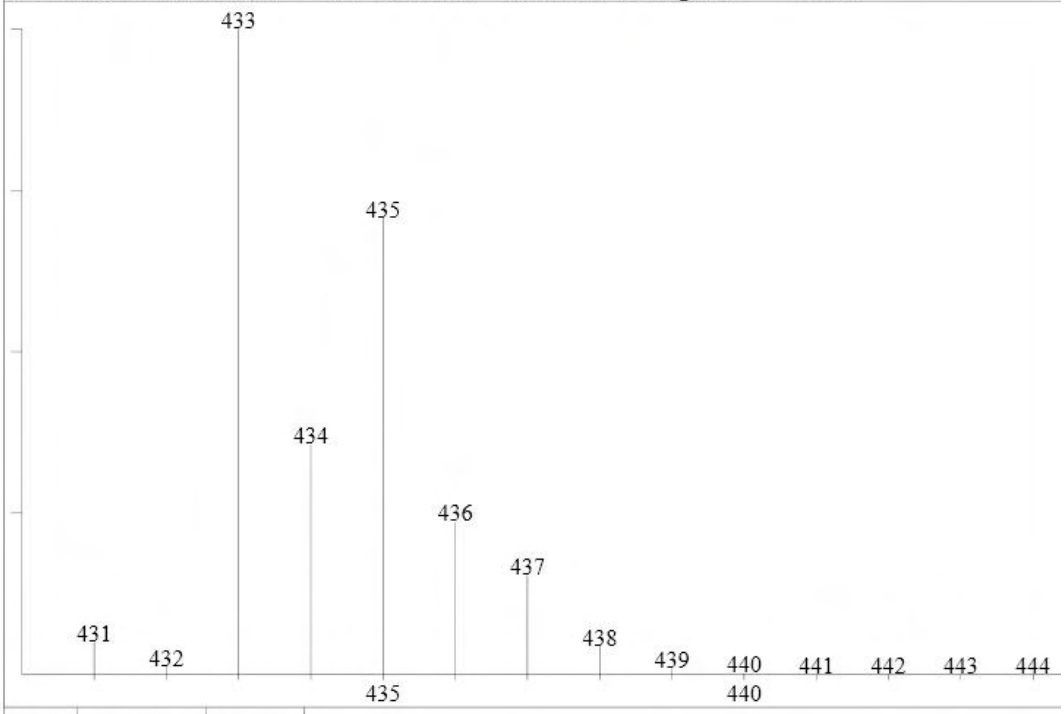
DISTRIBUTION OF ISOTOPES CALCULATED BY 'ISOFORM' PROGRAM FOR
Formula : CrCl2C10H10N2O
Factor : 100 Nominal MW = 296 Exact MW = 295.95749 Average MW = 297.11



Mass	Abundance	*Factor
294	4.95553	4.96
295	0.59611	0.60
296	100.00000	100.00
297	22.96326	22.96
298	67.31802	67.32
299	14.97135	14.97
300	13.05357	13.05
301	2.60966	2.61
302	0.51834	0.52
303	0.04872	0.05
304	0.00313	0.00
305	0.00015	0.00
306	0.00001	0.00

Figure B9 Calculated isotopic distribution pattern for [$CrCl_2$(bipy)(H_2O)]

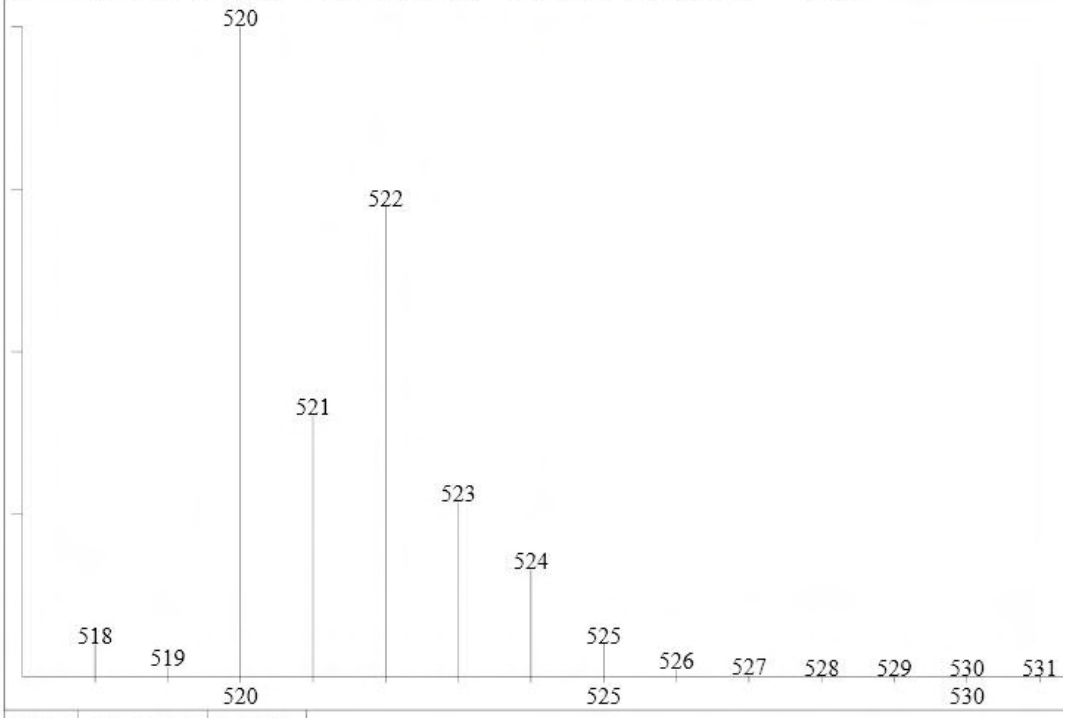
DISTRIBUTION OF ISOTOPES CALCULATED BY 'ISOFORM' PROGRAM FOR
Formula : CrCl2C21H17N3
Factor : 100 Nominal MW = 433 Exact MW = 433.02045 Average MW = 434.29



Mass	Abundance	*Factor
431	4.95050	4.95
432	1.22154	1.22
433	100.00000	100.00
434	35.57617	35.58
435	70.68070	70.68
436	23.58248	23.58
437	15.28814	15.29
438	4.33554	4.34
439	0.91644	0.92
440	0.12796	0.13
441	0.01198	0.01
442	0.00080	0.00
443	0.00004	0.00
444	0.00000	0.00

Figure B10 Calculated isotopic distribution pattern for [$CrCl_2$(bipy)(pyphenyl)]

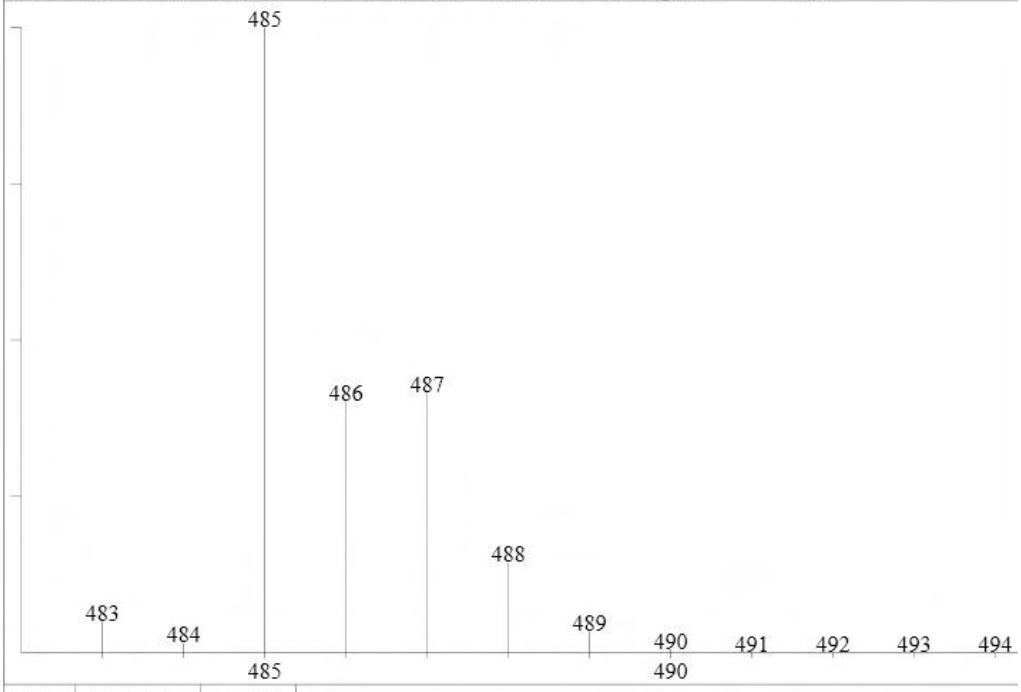
DISTRIBUTION OF ISOTOPES CALCULATED BY 'ISOFORM' PROGRAM FOR
Formula : CrCl2C26H24P2
Factor : 100 Nominal MW = 520 Exact MW = 520.01355 Average MW = 521.33



Mass	Abundance	*Factor
518	4.94757	4.95
519	1.44568	1.45
520	100.00000	100.00
521	40.09836	40.10
522	72.32935	72.33
523	26.80604	26.81
524	16.40310	16.40
525	5.04531	5.05
526	1.12433	1.12
527	0.17281	0.17
528	0.01849	0.02
529	0.00144	0.00
530	0.00009	0.00
531	0.00000	0.00

Figure B11 Calculated isotopic distribution pattern for [$CrCl_2$(dppe)]

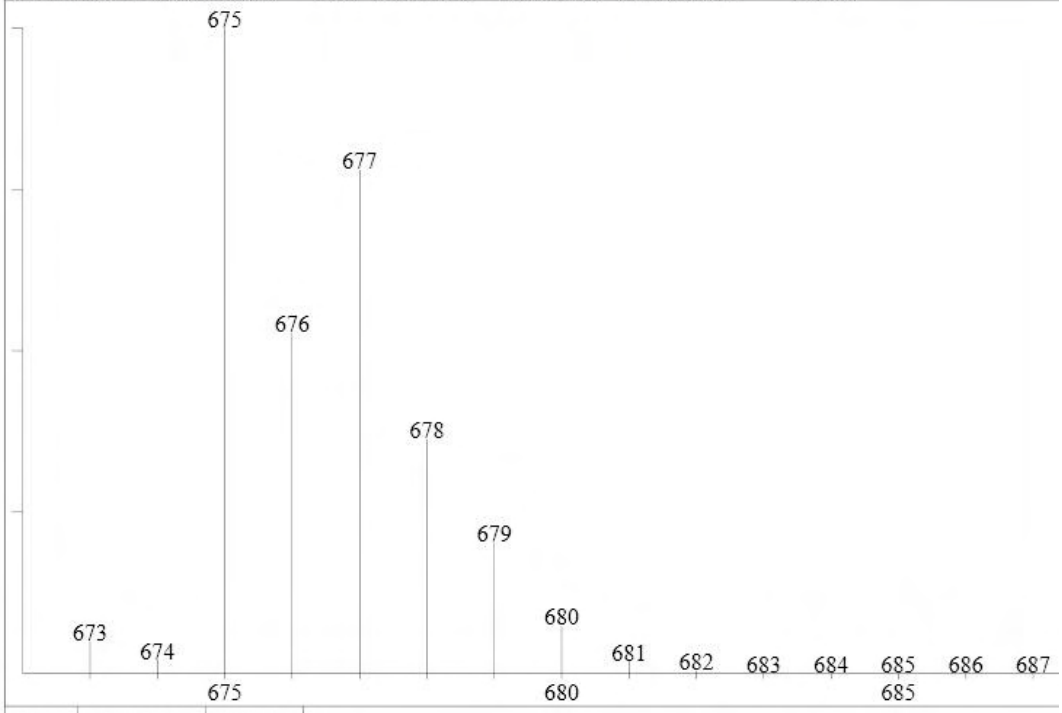
DISTRIBUTION OF ISOTOPES CALCULATED BY 'ISOFORM' PROGRAM FOR
Formula : CrClC26H24P2
Factor : 100 Nominal MW = 485 Exact MW = 485.04468 Average MW = 485.87



Mass	Abundance	*Factor
483	5.02711	5.03
484	1.46892	1.47
485	100.00000	100.00
486	40.27325	40.27
487	41.51217	41.51
488	14.35761	14.36
489	3.39121	3.39
490	0.53486	0.53
491	0.05790	0.06
492	0.00454	0.00
493	0.00027	0.00
494	0.00001	0.00

Figure B12 Calculated isotopic distribution pattern for [CrCl(dppe)]

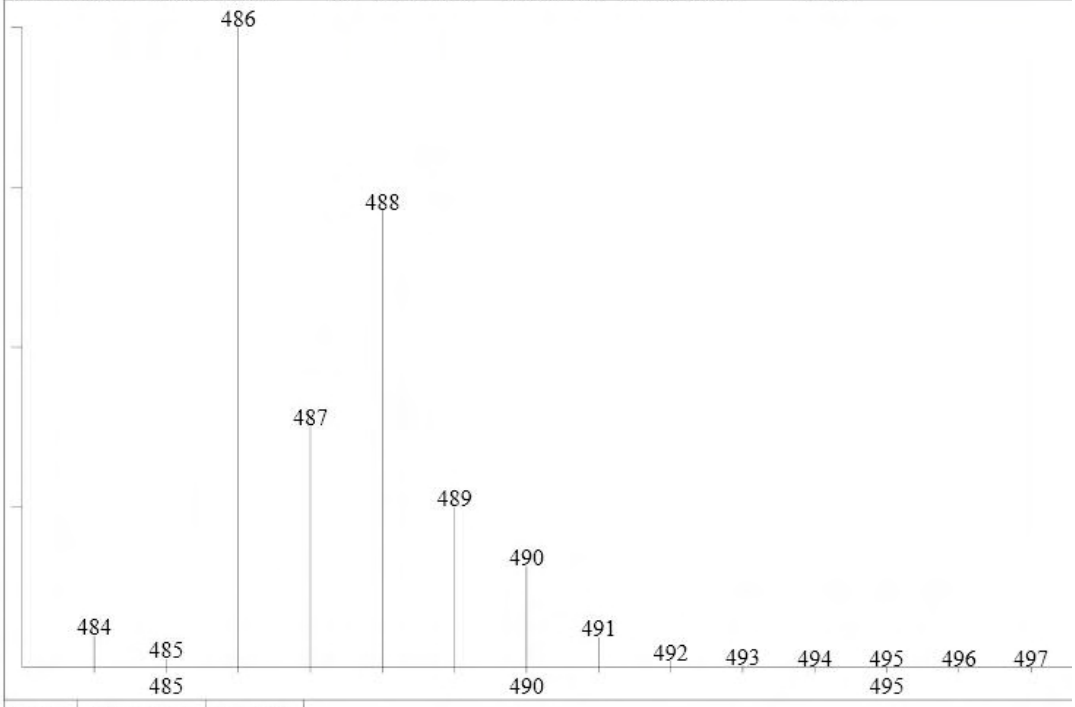
DISTRIBUTION OF ISOTOPES CALCULATED BY 'ISOFORM' PROGRAM FOR
Formula : CrCl2C37H33NP2
Factor : 100 Nominal MW = 675 Exact MW = 675.08698 Average MW = 676.53



Mass	Abundance	*Factor
673	4.93669	4.94
674	2.07020	2.07
675	100.00000	100.00
676	52.70916	52.71
677	77.99624	78.00
678	36.24558	36.25
679	20.31294	20.31
680	7.33225	7.33
681	1.89048	1.89
682	0.35676	0.36
683	0.05009	0.05
684	0.00539	0.01
685	0.00046	0.00
686	0.00003	0.00
687	0.00000	0.00

Figure B13 Calculated isotopic distribution pattern for [$CrCl_2$(dppe)(pyphenyl)]

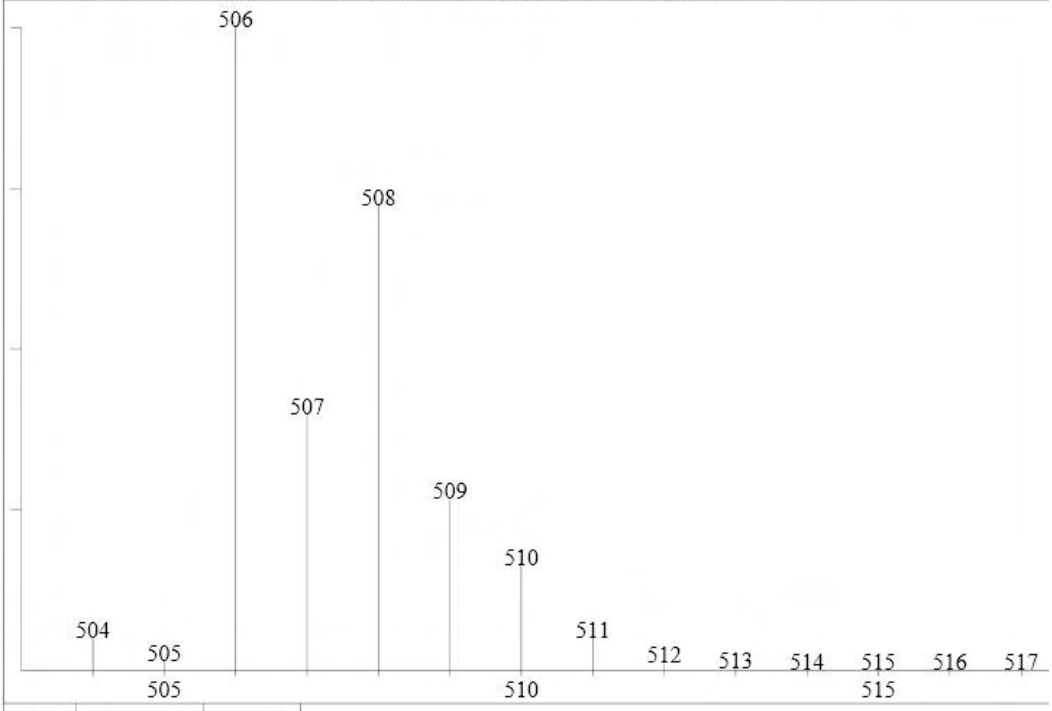
DISTRIBUTION OF ISOTOPES CALCULATED BY 'ISOFORM' PROGRAM FOR
Formula : CrCl2C23H29N2P
Factor : 100 Nominal MW = 486 Exact MW = 486.08502 Average MW = 487.37



Mass	Abundance	*Factor
484	4.94925	4.95
485	1.32170	1.32
486	100.00000	100.00
487	37.59678	37.60
488	71.39383	71.39
489	25.01416	25.01
490	15.76921	15.77
491	4.64682	4.65
492	1.00556	1.01
493	0.14691	0.15
494	0.01466	0.01
495	0.00105	0.00
496	0.00006	0.00
497	0.00000	0.00

Figure B14 Calculated isotopic distribution pattern for [$CrCl_2$(dppea)(pytb)]

DISTRIBUTION OF ISOTOPES CALCULATED BY 'ISOFORM' PROGRAM FOR
Formula : CrCl2C25H25N2P
Factor : 100 Nominal MW = 506 Exact MW = 506.05371 Average MW = 507.36



Mass	Abundance	*Factor
504	4.94781	4.95
505	1.42819	1.43
506	100.00000	100.00
507	39.74537	39.75
508	72.19593	72.20
509	26.55268	26.55
510	16.31263	16.31
511	4.98874	4.99
512	1.10735	1.11
513	0.16910	0.17
514	0.01793	0.02
515	0.00139	0.00
516	0.00008	0.00
517	0.00000	0.00

Figure B15 Calculated isotopic distribution pattern for [$CrCl_2$(dppea)(pyphenyl)]