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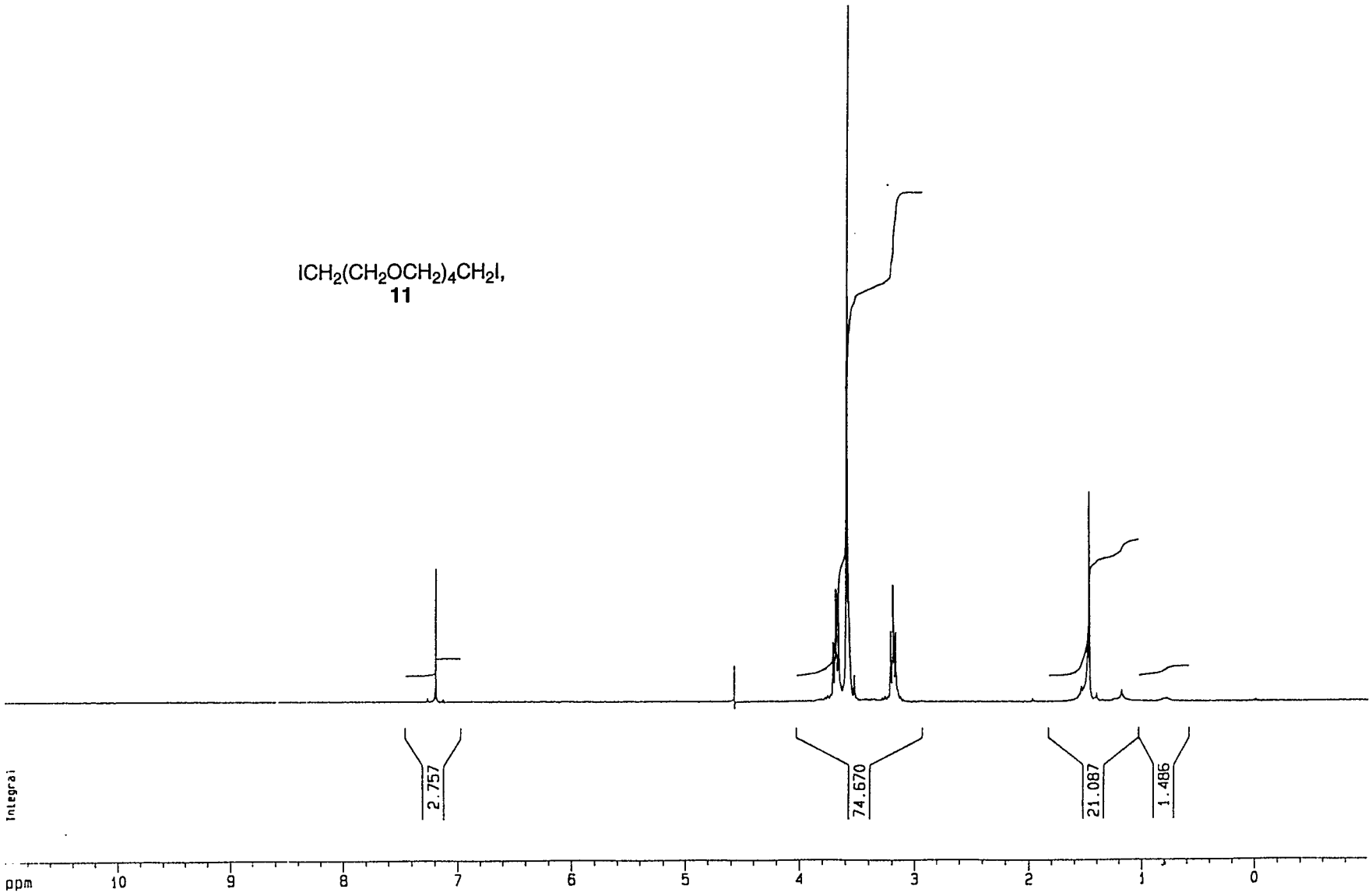
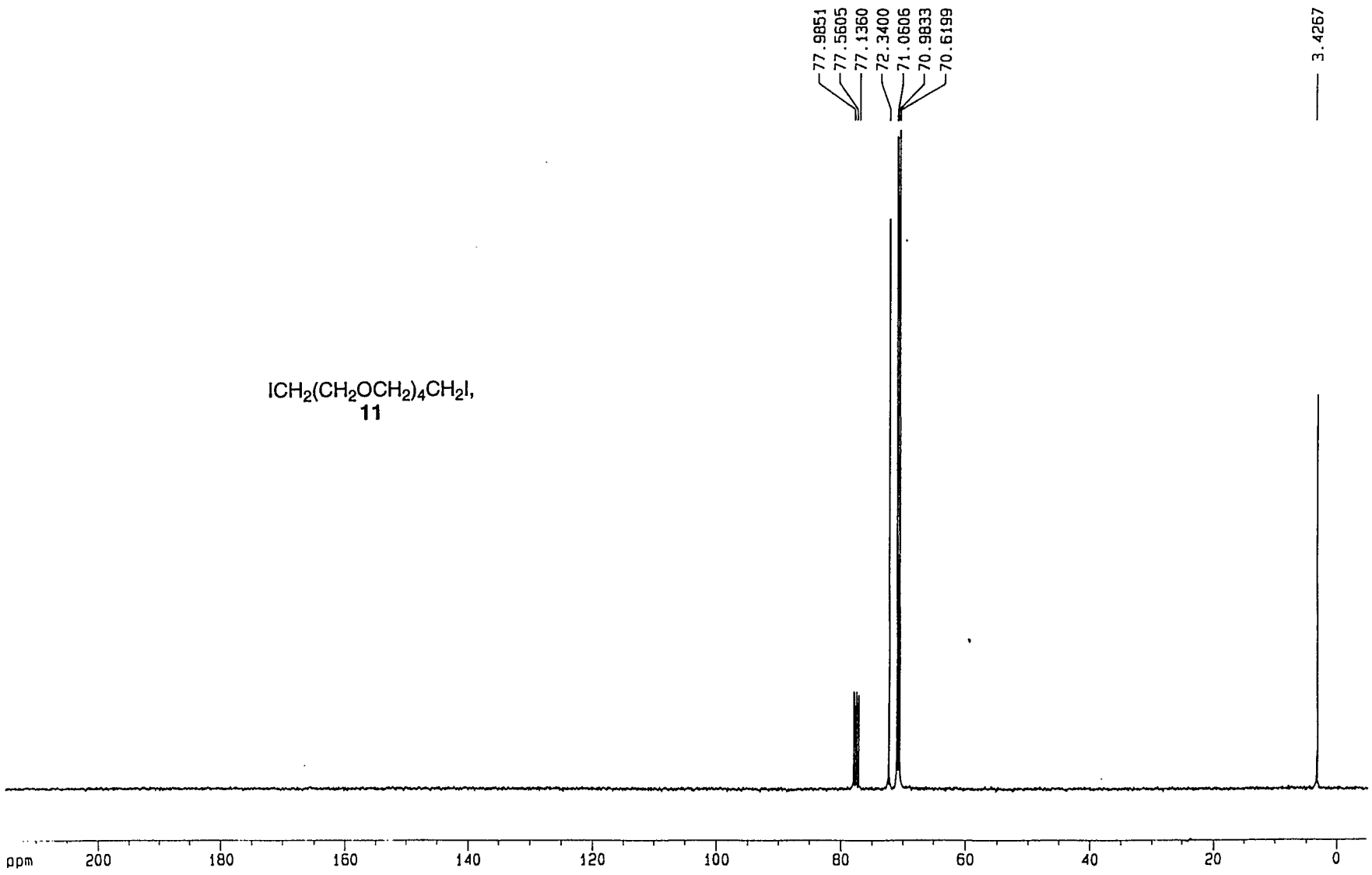
$ICH_2(CH_2OCH_2)_4CH_2I$,
11





$ICH_2(CH_2OCH_2)_4CH_2I$,
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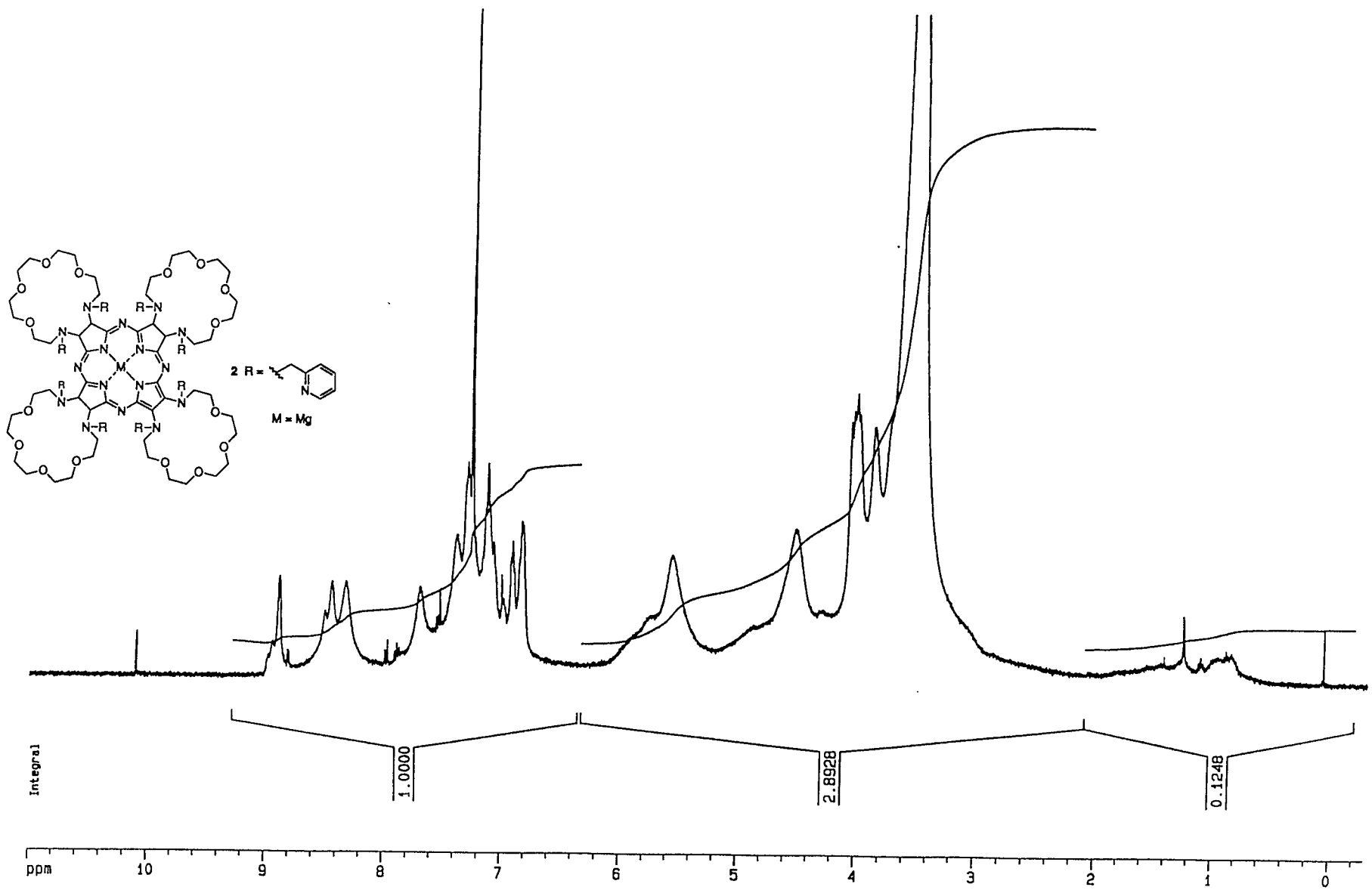
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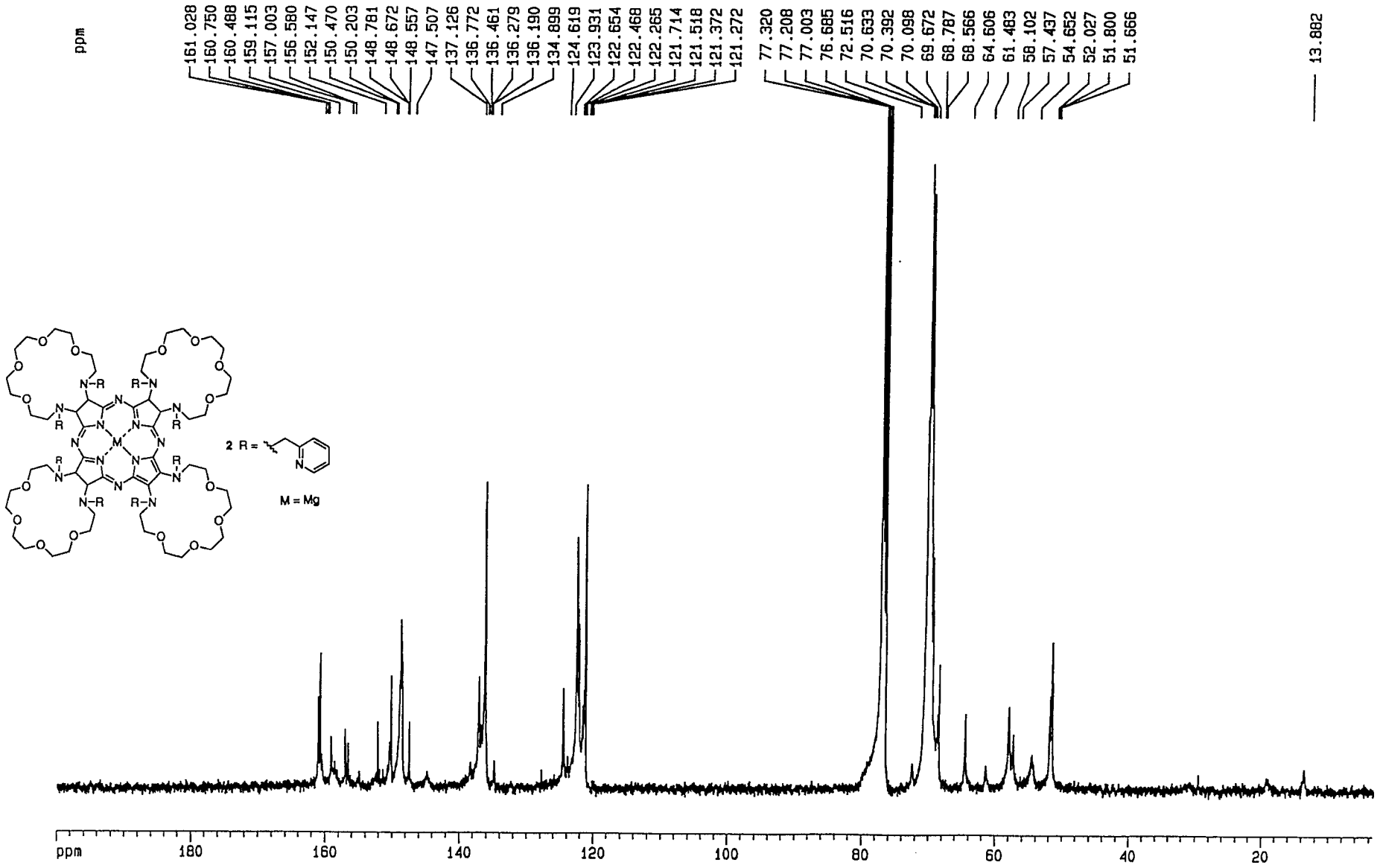
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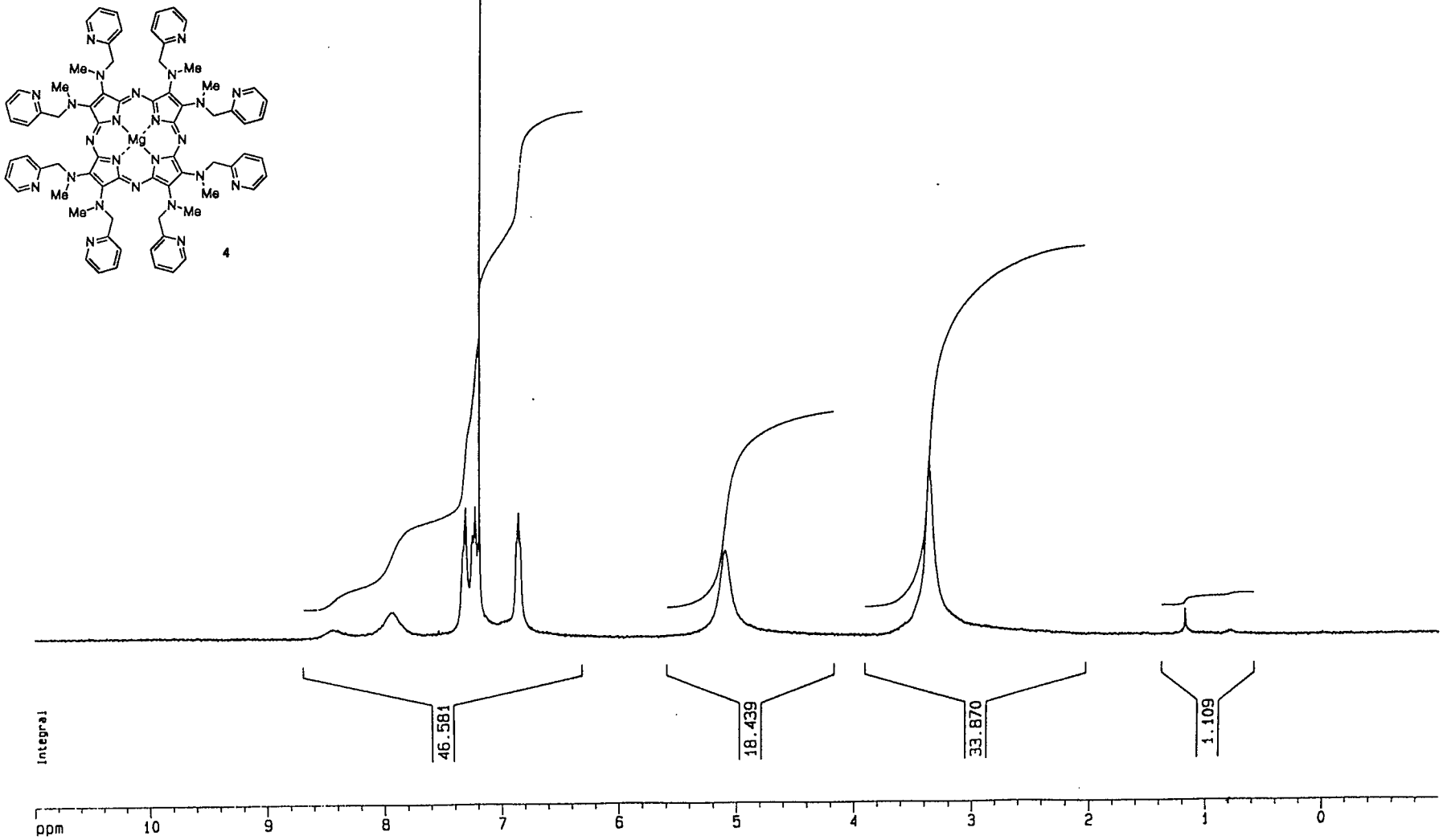
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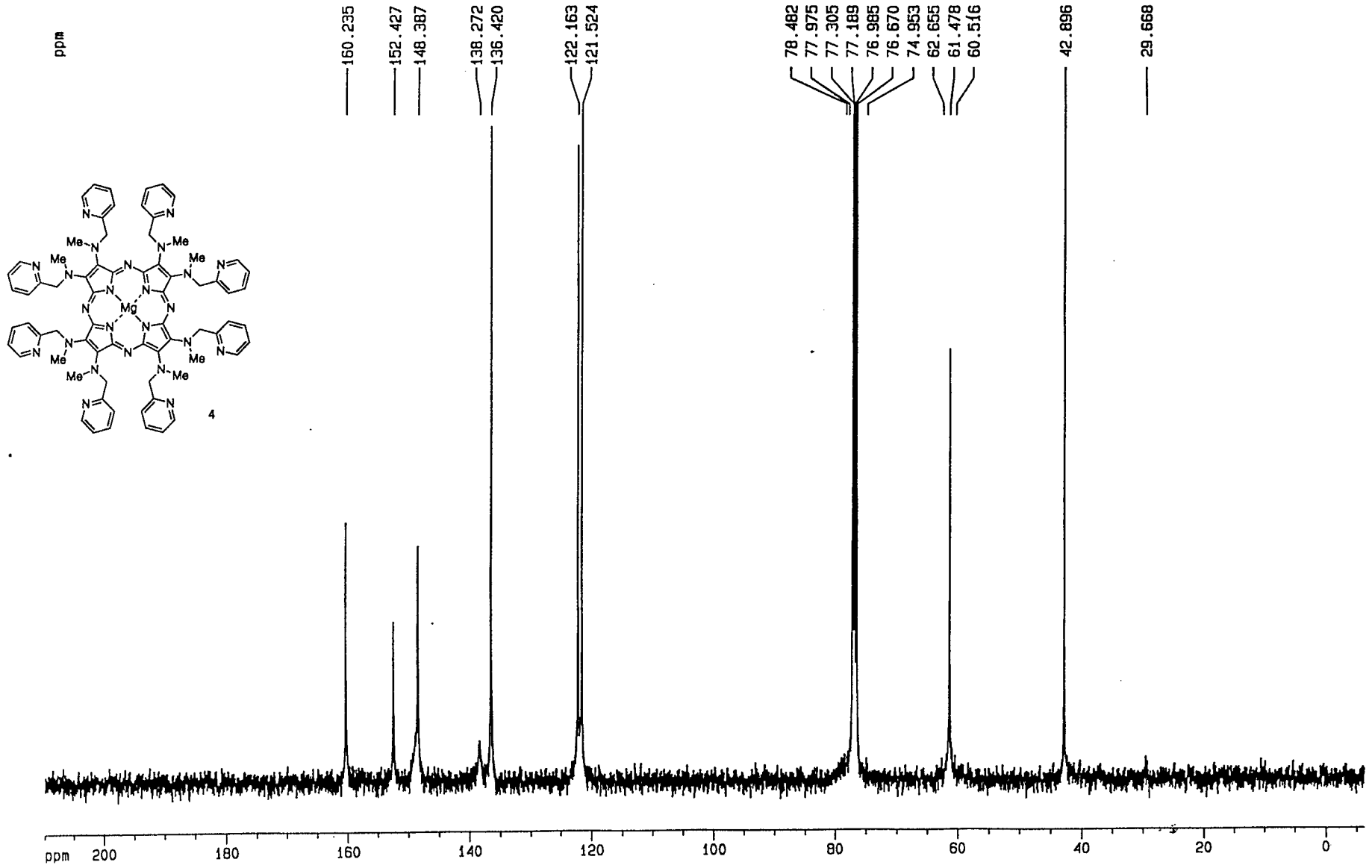
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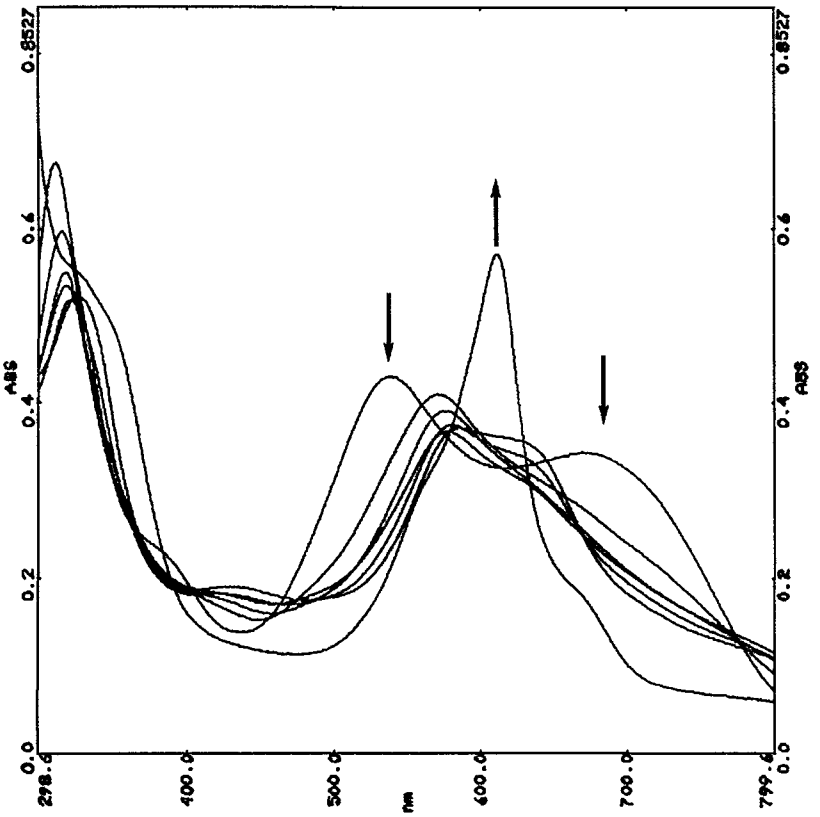


Figure 1: Porphyrazine **1** (M = Ni) titrated with $Hg(ClO_4)_2$ (0, 2, 4, 8, 20, 40, >100 equiv).

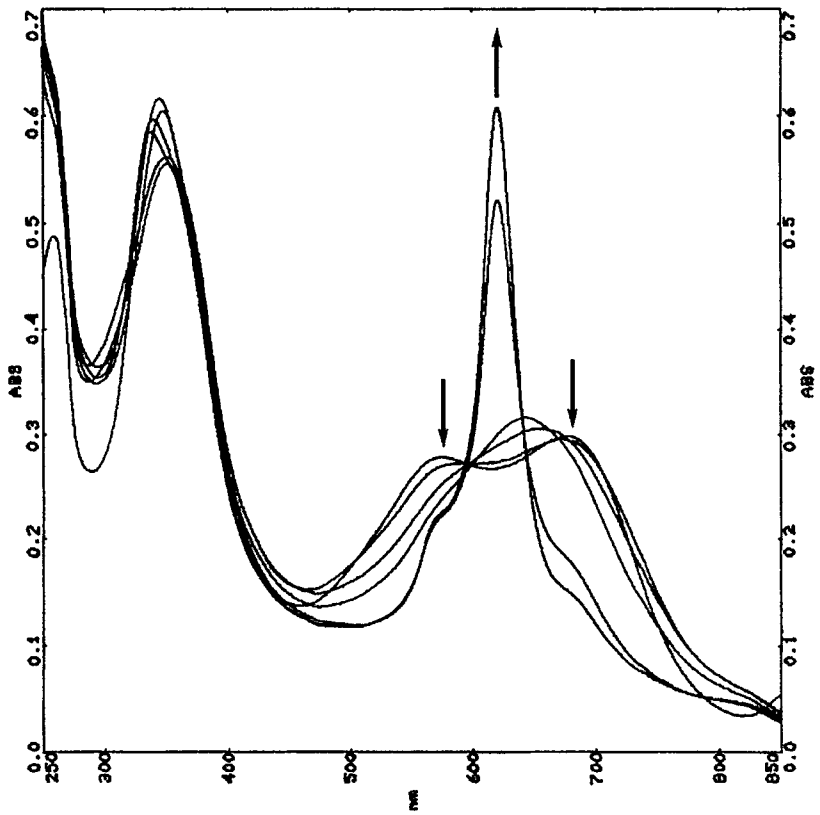


Figure 2: Porphyrazine **2** titrated with $AgBF_4$ (0, 1, 2, 3, 4, 6 equiv).

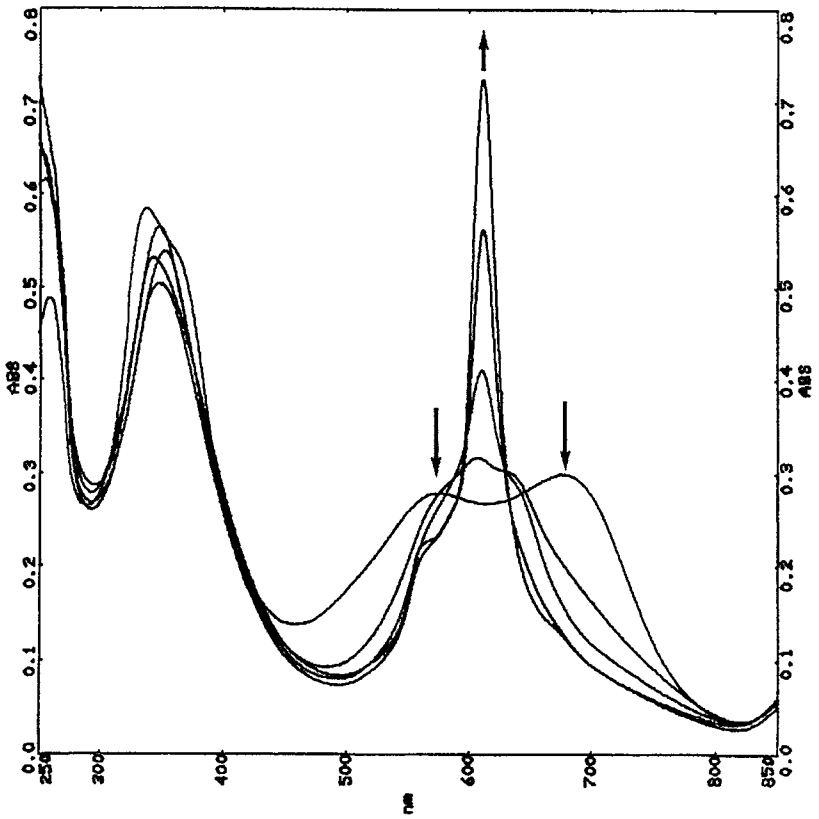


Figure 3: Porphyrazine **2** titrated with $Pb(NO_3)_2$ (0, 2, 4, 6, 8 equiv).

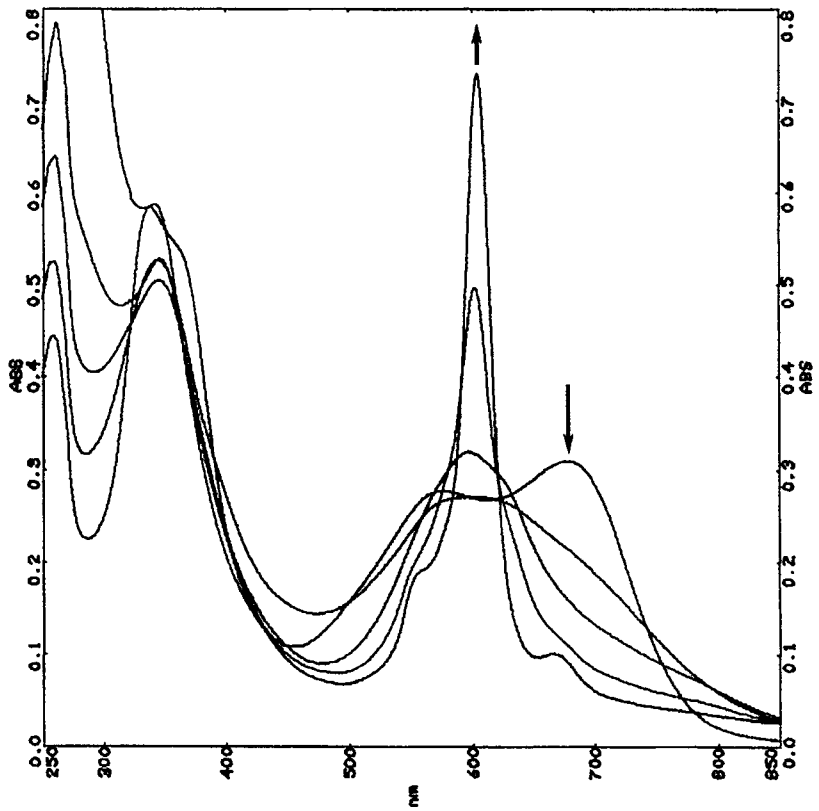


Figure 4: Porphyrazine **2** titrated with $CuCl_2$ (0, 2, 4, 8, 20 equiv).

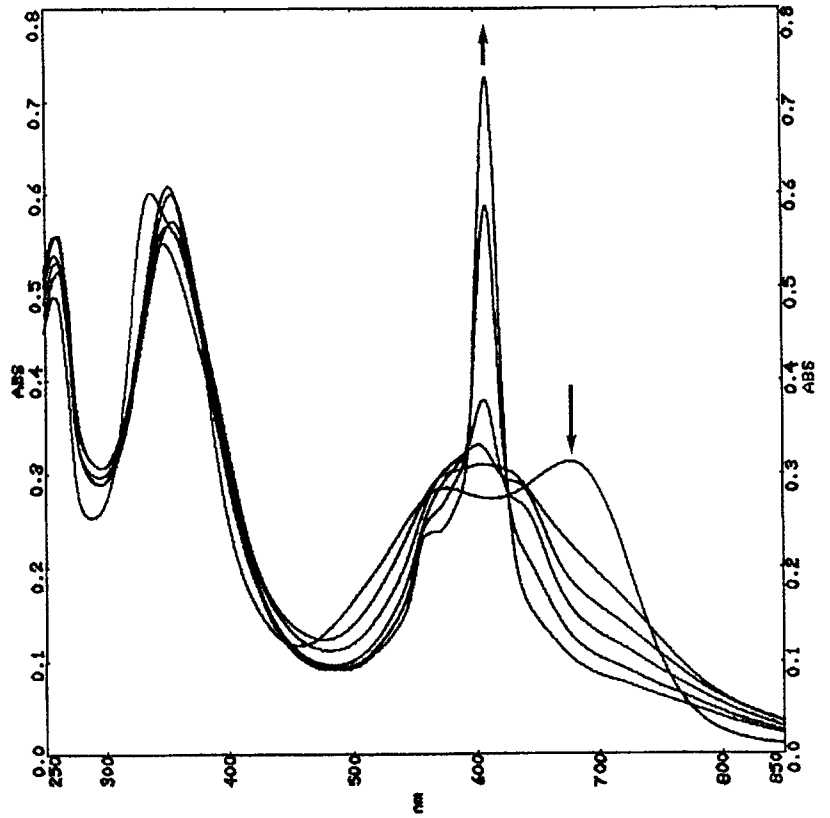


Figure 5: Porphyrazine **2** titrated with $CoCl_2$ (0, 2, 4, 8, 20, 40 equiv).

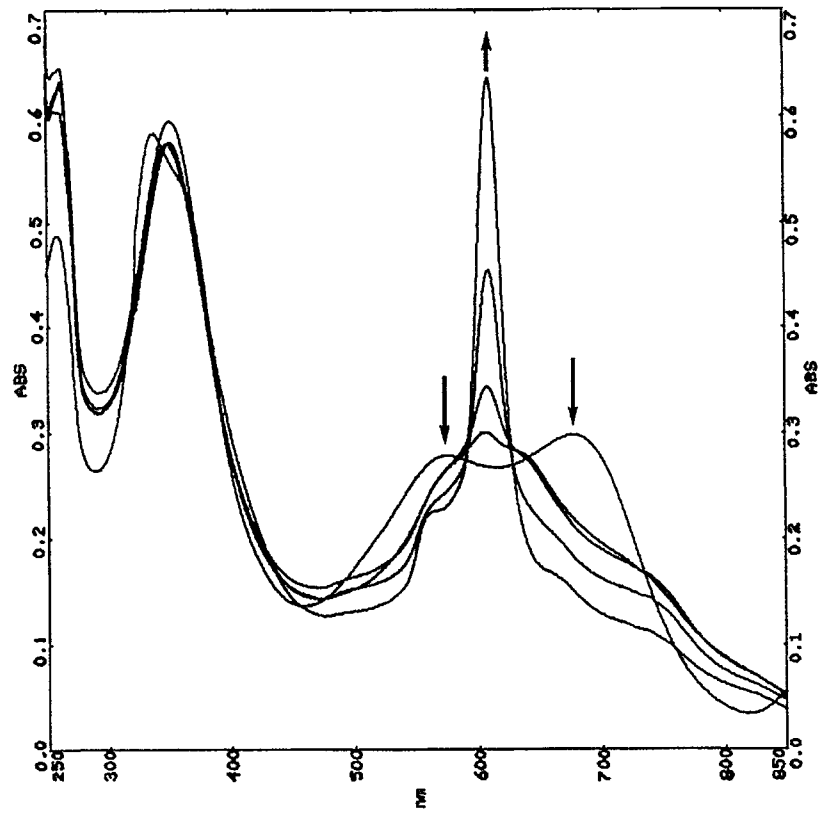


Figure 6: Porphyrazine **2** titrated with $Zn(ClO_4)_2$ (0, 4, 8, 20, 40 equiv).

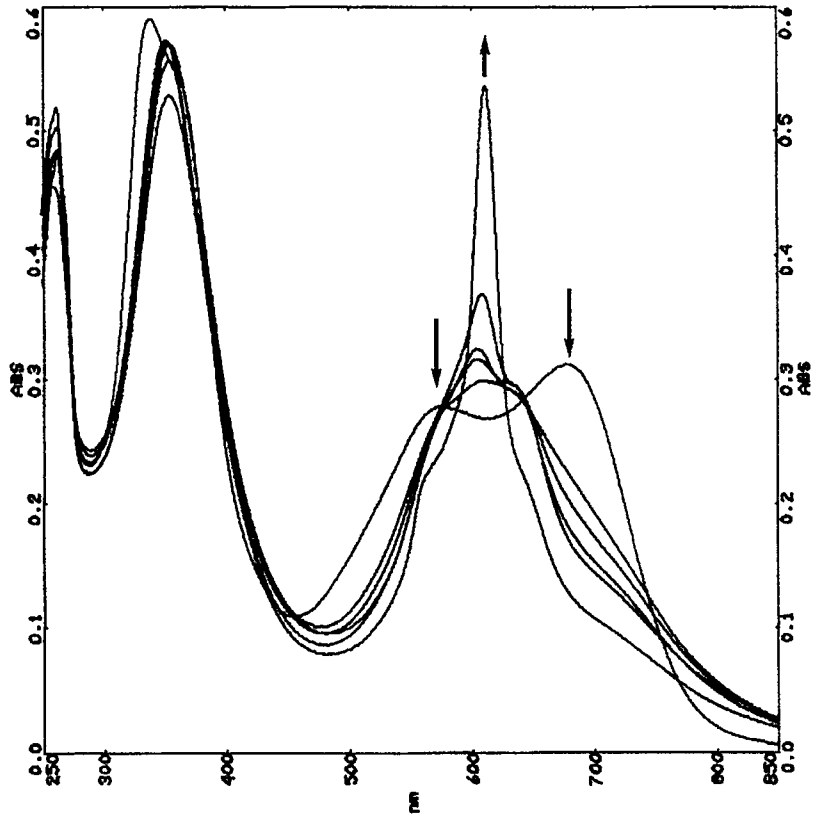


Figure 7: Porphyrazine **2** titrated with $CdCl_2$ (0, 2, 4, 8, 20, 40 equiv).

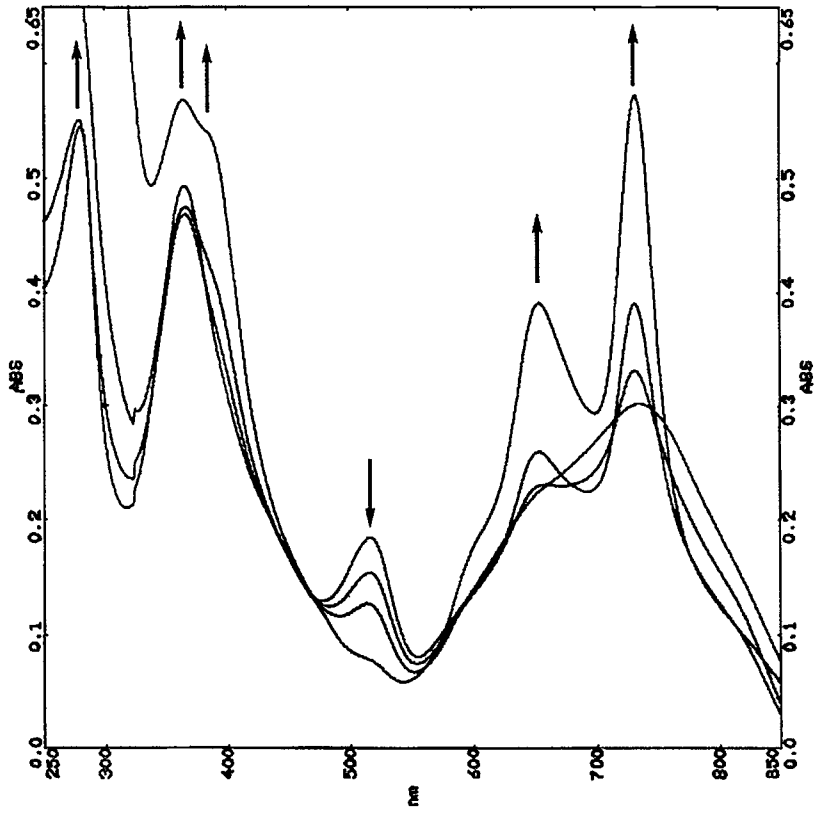


Figure 8: Norphthalocyanine **3** titrated with $Cu(OAc)_2$ (0, 2, 10, 100 equiv).

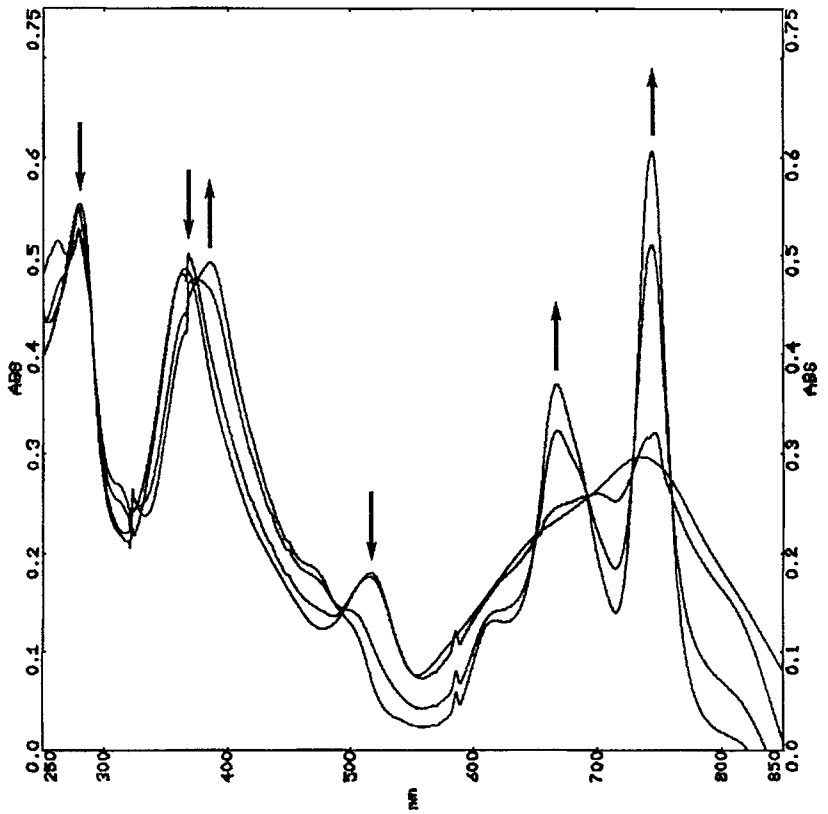


Figure 9: Norphthalocyanine **3** titrated with $Hg(ClO_4)_2 \cdot 3H_2O$ (0, 1, 2, 10 equiv).

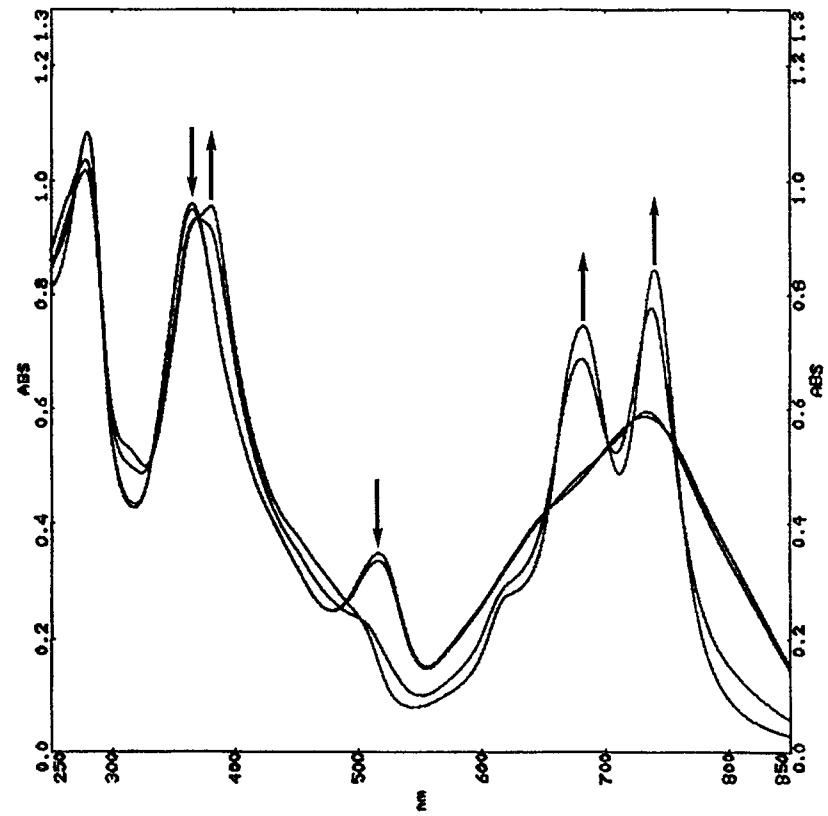


Figure 10: Norphthalocyanine **3** titrated with $AgBF_4$ (0, 1, 2, 4 equiv).

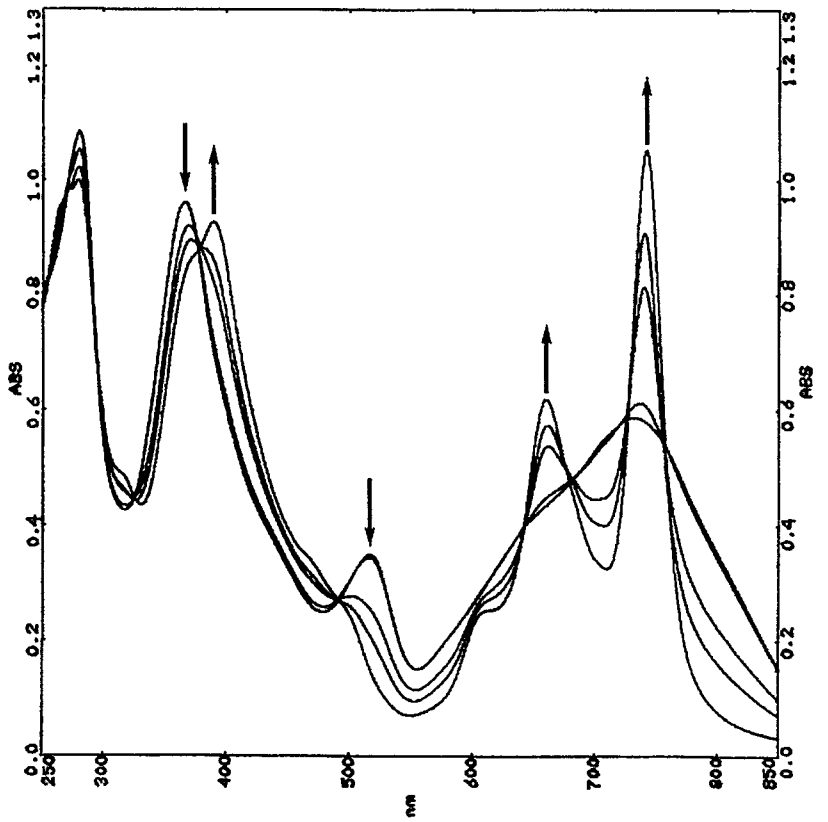


Figure 11: Norphthalocyanine **3** titrated with $Zn(ClO_4)_2 \cdot 6H_2O$ (0, 2, 4, 10, 100 equiv).

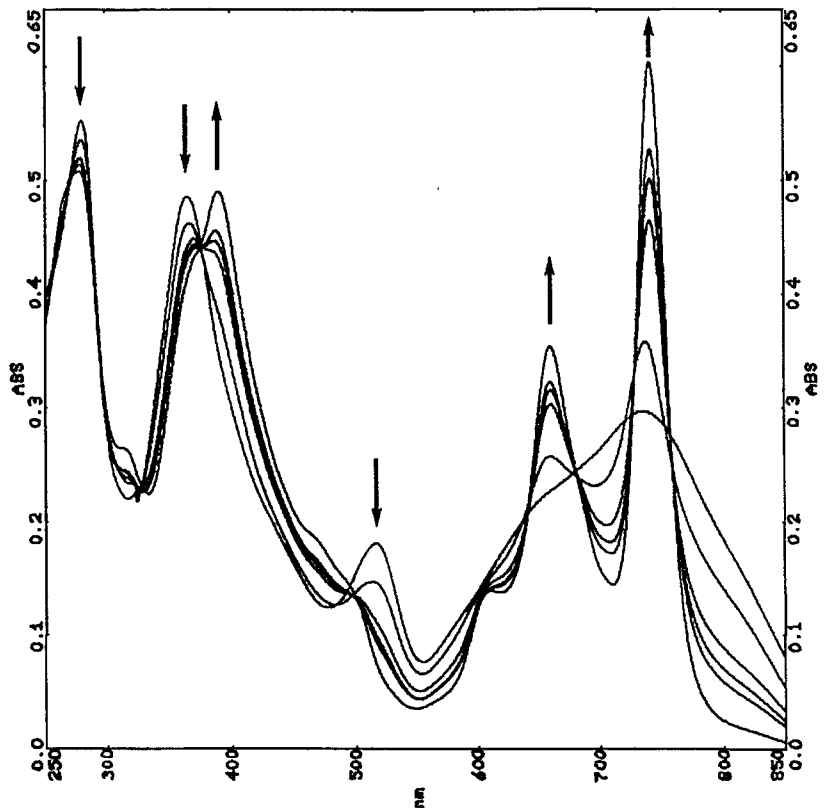


Figure 12: Norphthalocyanine **3** titrated with $Co(BF_4)_2$ (0, 1, 2, 4, 10, 100 equiv).

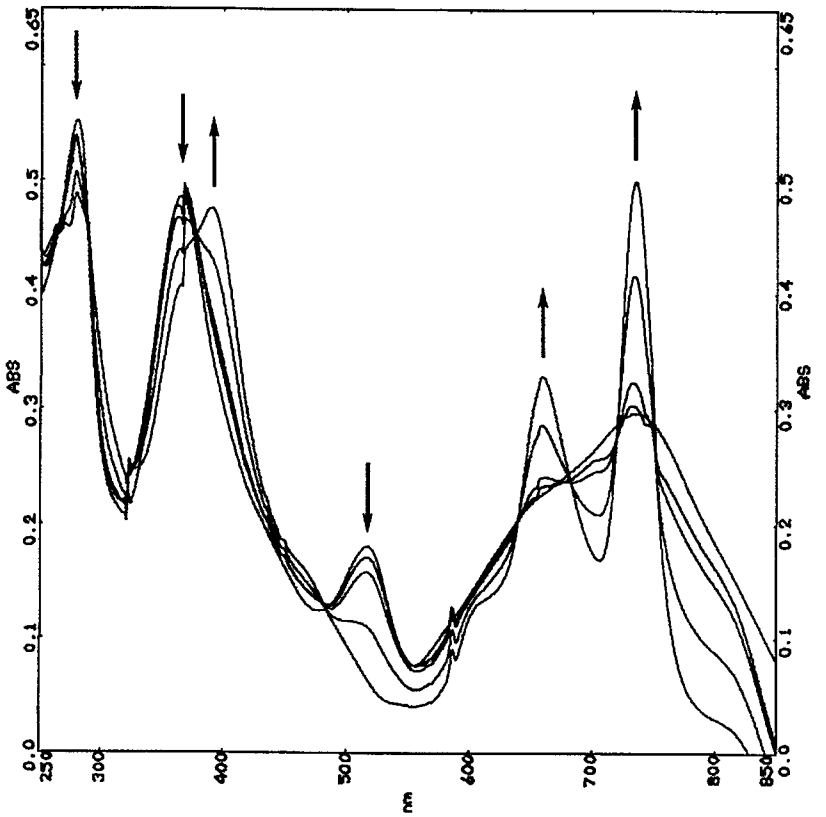


Figure 13: Norphthalocyanine **3** titrated with $CdCl_2$ (0, 1, 2, 10, 100 equiv).

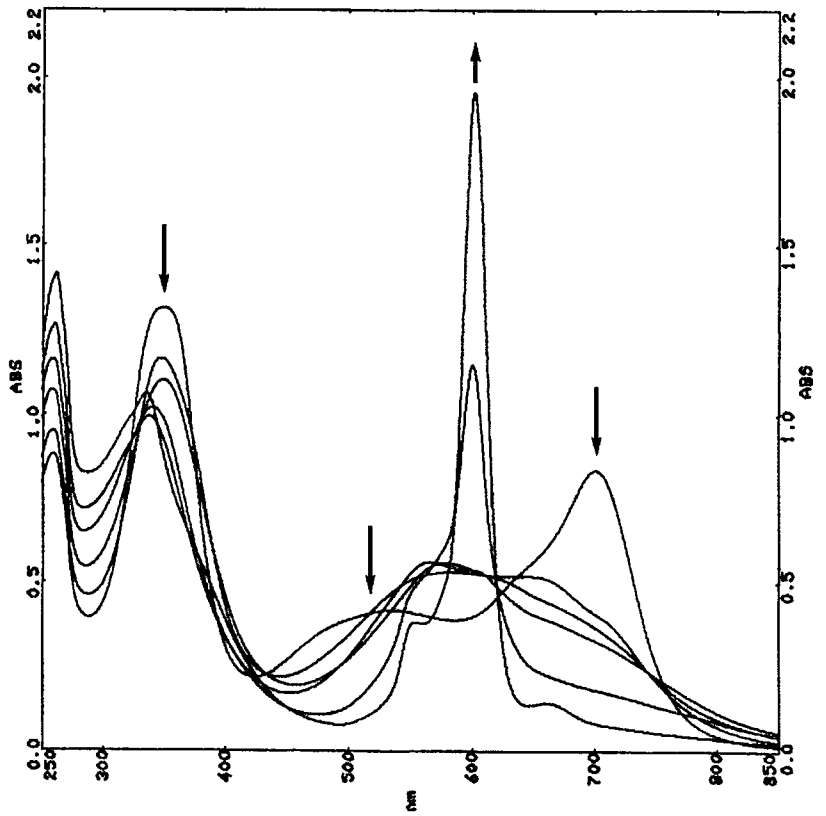


Figure 14: Porphyrazine **4** titrated with $CuCl_2$ (0, 1, 2, 3, 4, 6 equiv).

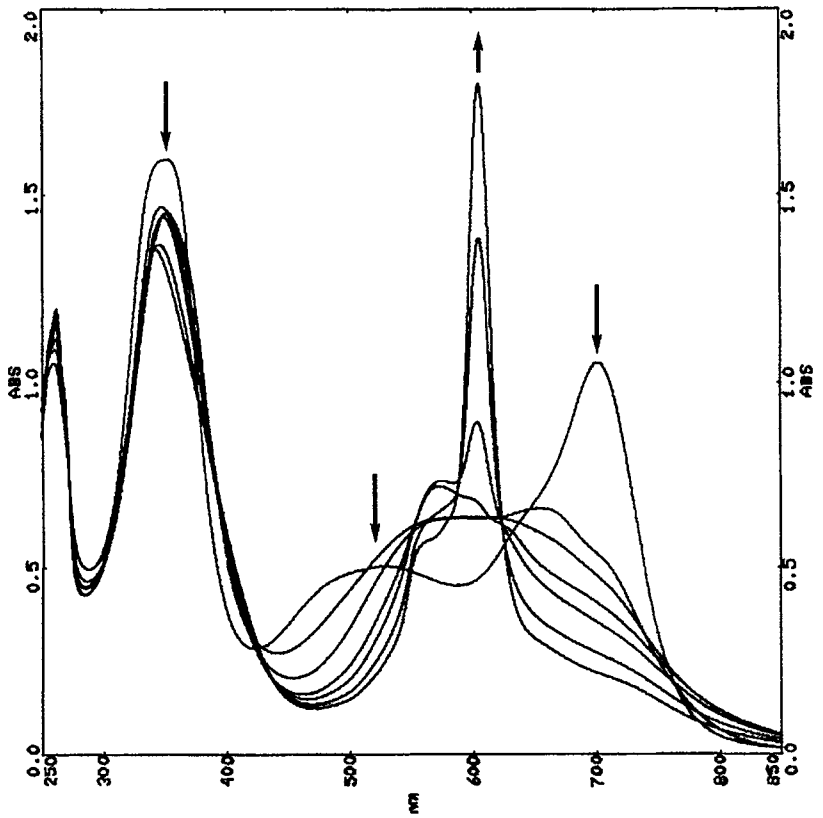


Figure 15: Porphyrazine **4** titrated with $Zn(ClO_4)_2$ (0, 1, 2, 3, 4, 6, 8 equiv).

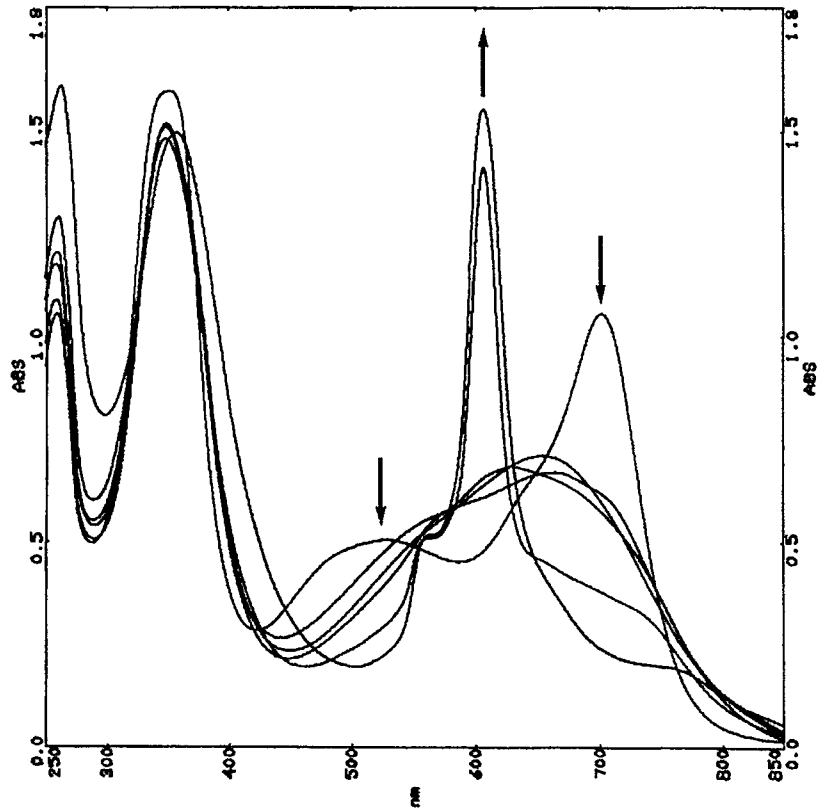


Figure 16: Porphyrazine **4** titrated with $Hg(ClO_4)_2$ (0, 1, 2, 3, 4, 6 equiv).

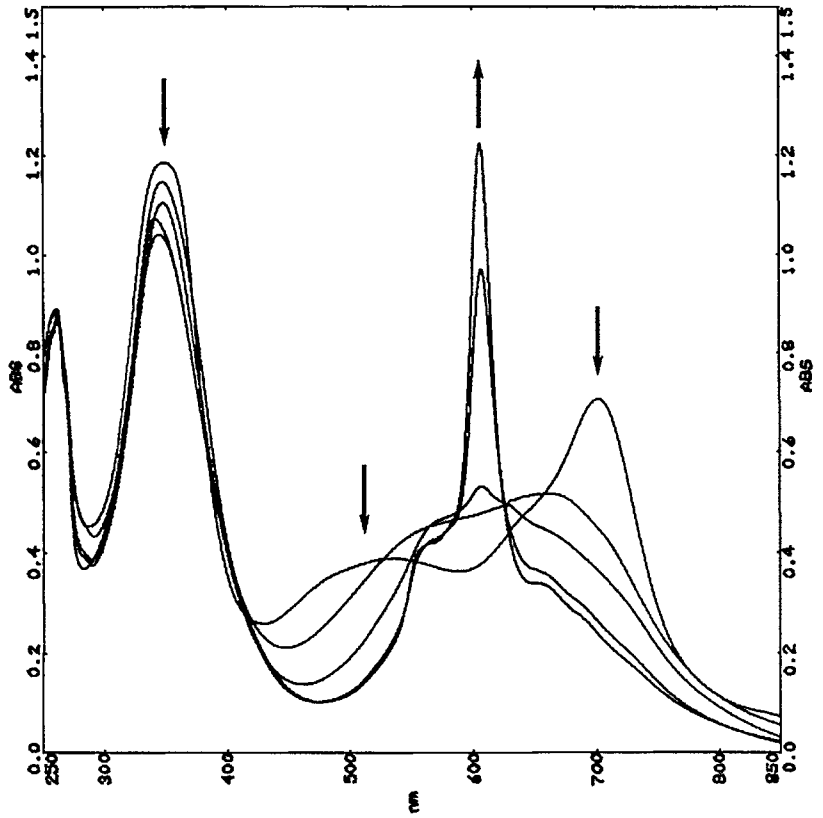


Figure 17: Porphyrazine **4** titrated with $CdCl_2$ (0, 1, 2, 3, 4 equiv).

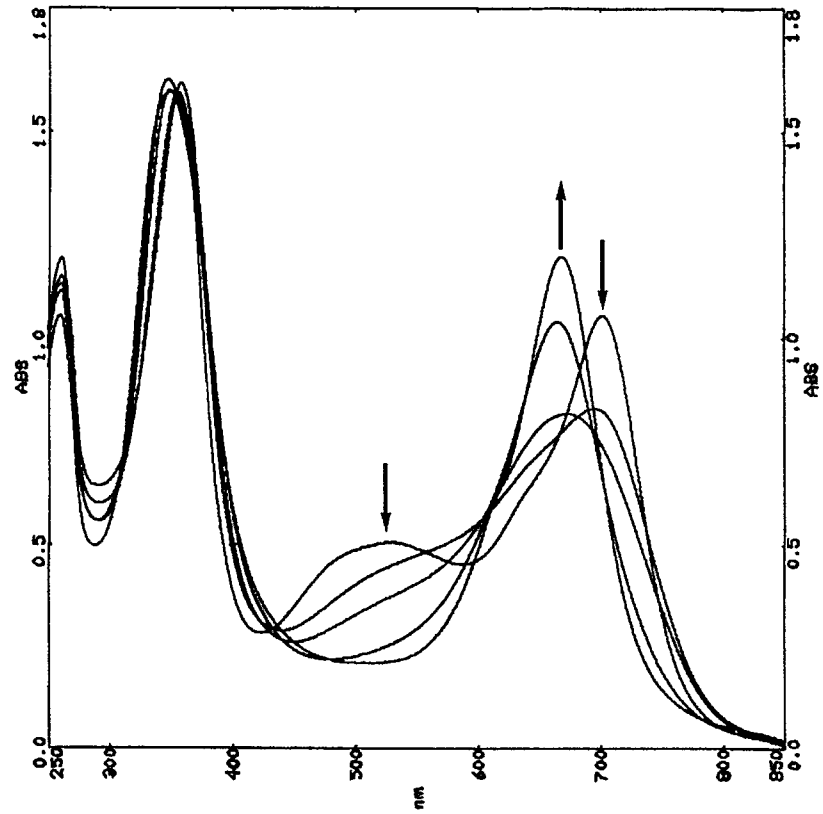


Figure 18: Porphyrazine **4** titrated with $AgBF_4$ (0, 1, 2, 4, 6 equiv).

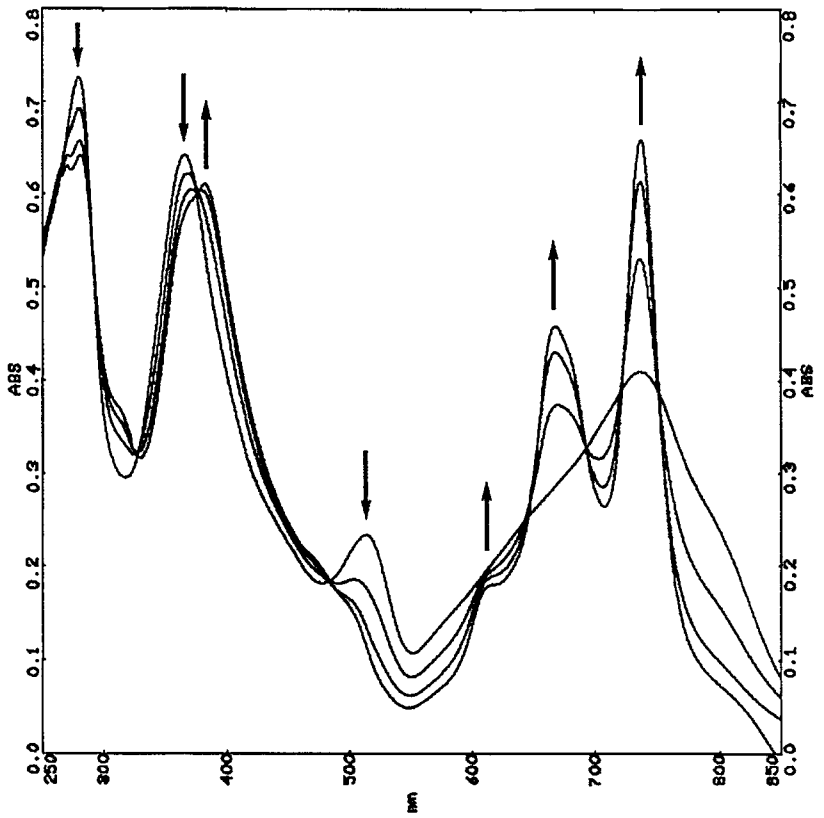


Figure 19: Norphthalocyanine **5** titrated with $CdCl_2$ (0.0, 0.25, 0.50, 1.0 equiv).

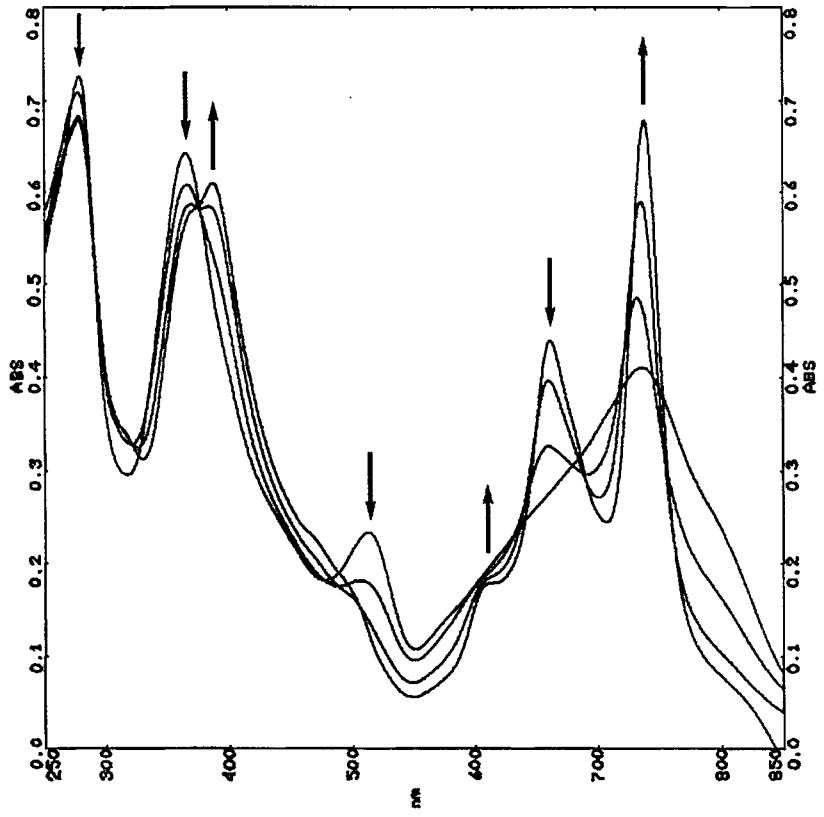


Figure 20: Norphthalocyanine **5** titrated with $Co(BF_4)_2$ (0.0, 0.25, 0.50, 1.0 equiv).

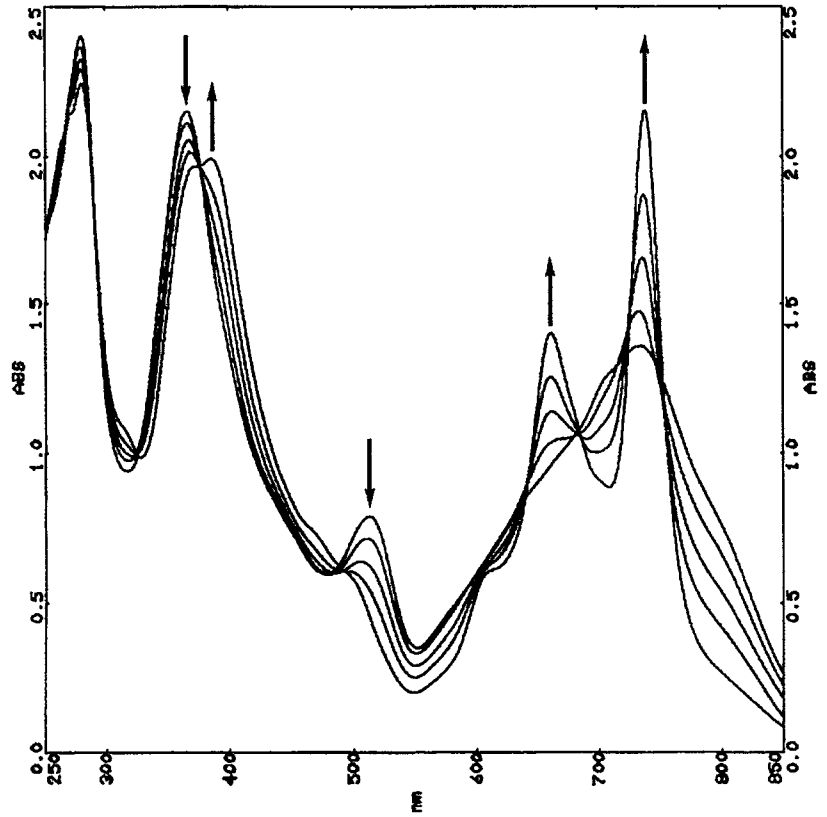


Figure 21: Norphthalocyanine **5** titrated with $Zn(ClO_4)_2$ (0.0, 0.50, 1.0, 1.5, 2.0 equiv).

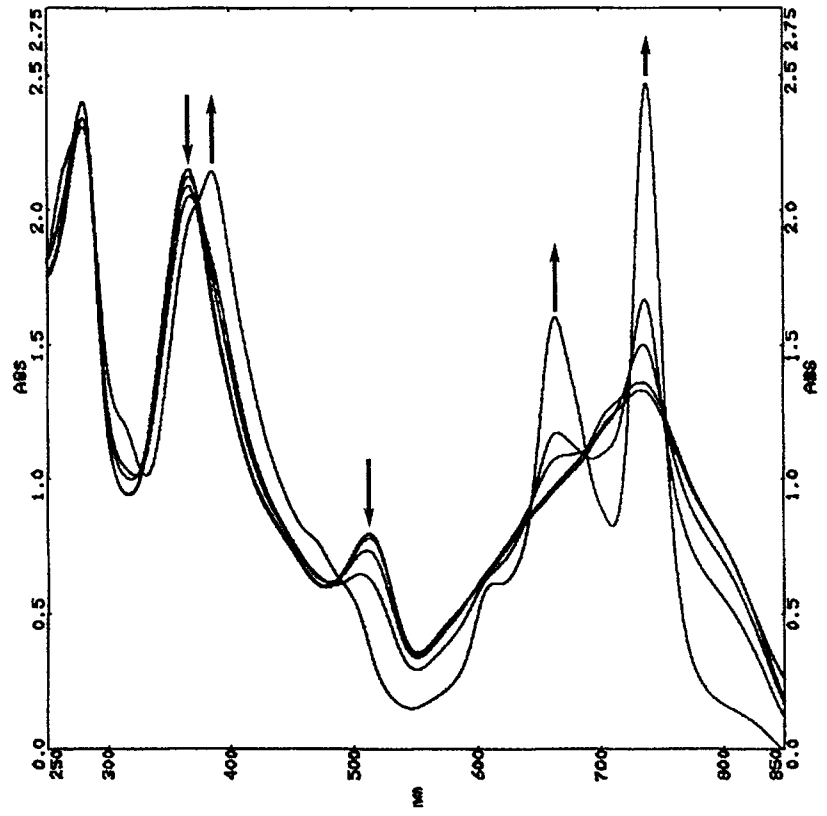
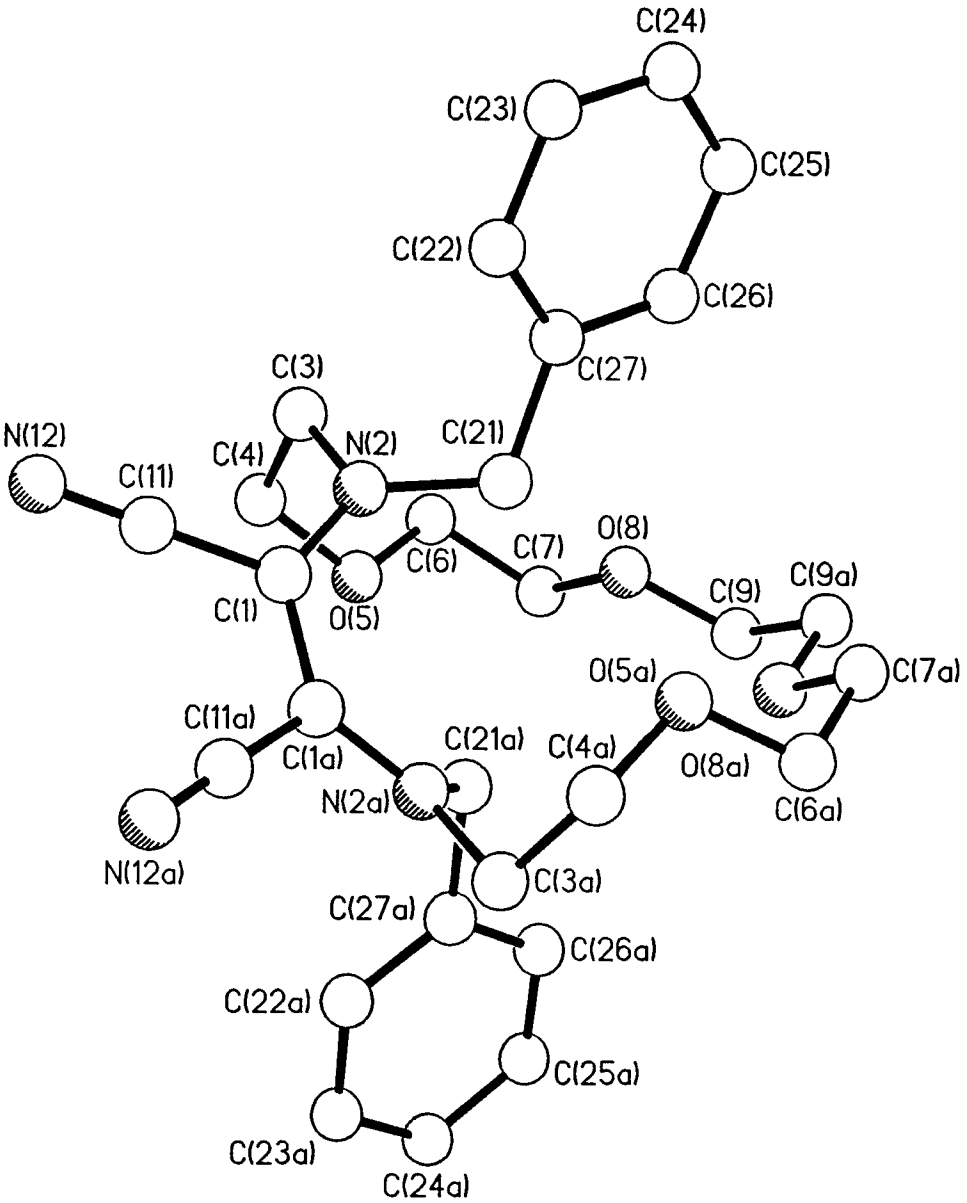


Figure 22: Norphthalocyanine **5** titrated with $Hg(ClO_4)_2$ (0.0, 0.50, 1.0, 1.5, 2.0 equiv).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C(23)
C(25)
C(22)
C(26)
C(27)
C(3)
N(12)
C(4)
N(2)
C(21)
C(11)
C(6)
C(7)
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C(3a)
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C(24a)

Table 1. Crystal data and structure refinement for 1.

Identification code	AGMB19
Empirical formula	$C_{28}H_{34}N_4O_4$
Formula weight	490.59
Temperature	293(2) K
Diffractometer Used	Siemens P4/PC
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 14.203(3) Å alpha = 90° b = 11.753(3) Å beta = 112.13(2)° c = 16.923(5) Å gamma = 90°
Volume, Z	2616.9(12) $Å^3$, 4
Density (calculated)	1.245 Mg/m^3
Absorption coefficient	0.680 mm^{-1}
F(000)	1048
Crystal colour/morphology	Yellow cubes
Crystal size	0.37 x 0.33 x 0.33 mm
θ range for data collection	5.05 to 62.49°
Limiting indices	$-16 \leq h \leq 15$, $0 \leq k \leq 13$, $0 \leq l \leq 19$
Scan type	ω-scans
Reflections collected	2097
Independent reflections	2097 (R_{int} = 0.0000)
Observed reflections [F>4σ(F)]	1799
Absorption correction	None
Structure solution method	Direct
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2050 / 0 / 152
Goodness-of-fit on F^2	1.058
Final R indices [F>4σ(F)]	R1 = 0.0928, wR2 = 0.2550
R indices (all data)	R1 = 0.1012, wR2 = 0.2888
Extinction coefficient	0.0035(8)
Largest diff. peak and hole	0.507 and -0.439 $eÅ^{-3}$
Mean and maximum shift/error	0.000 and 0.000

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

	x	y	z	U(eq)	sof
C(1)	502(2)	2538(2)	2528(2)	34(1)	1
N(2)	1147(2)	1630(2)	2641(1)	39(1)	1
C(3)	1840(2)	1568(3)	2183(2)	54(1)	1
C(4)	1294(3)	1361(4)	1244(2)	75(1)	1
O(5)	667(2)	387(3)	1072(1)	78(1)	1
C(6)	1156(3)	-661(5)	1049(3)	97(2)	1
C(7)	508(4)	-1621(5)	1098(3)	104(2)	1
O(8)	552(2)	-1729(2)	1946(2)	90(1)	1
C(9)	-6(4)	-2679(3)	2066(3)	115(2)	1
C(11)	908(2)	3630(2)	2442(2)	47(1)	1
N(12)	1232(2)	4491(2)	2367(3)	77(1)	1
C(21)	1117(2)	656(2)	3164(2)	39(1)	1
C(22)	2677(2)	1361(1)	4385(1)	65(1)	1
C(23)	3555(2)	1147(2)	5095(1)	86(1)	1
C(24)	3858(2)	33(2)	5333(1)	82(1)	1
C(25)	3283(2)	-867(2)	4862(2)	88(1)	1
C(26)	2405(2)	-654(1)	4152(1)	67(1)	1
C(27)	2102(1)	461(2)	3914(1)	38(1)	1

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

C(1)-N(2)	1.373(3)	C(1)-C(1)#1	1.394(5)
C(1)-C(11)	1.436(4)	N(2)-C(21)	1.457(3)
N(2)-C(3)	1.465(3)	C(3)-C(4)	1.503(5)
C(4)-O(5)	1.412(5)	O(5)-C(6)	1.421(5)
C(6)-C(7)	1.478(7)	C(7)-O(8)	1.418(6)
O(8)-C(9)	1.428(6)	C(9)-C(9)#1	1.461(12)
C(11)-N(12)	1.138(4)	C(21)-C(27)	1.511(3)

N(2)-C(1)-C(1)#1	128.42(14)	N(2)-C(1)-C(11)	115.9(2)
C(1)#1-C(1)-C(11)	115.67(14)	C(1)-N(2)-C(21)	121.7(2)
C(1)-N(2)-C(3)	120.7(2)	C(21)-N(2)-C(3)	117.5(2)
N(2)-C(3)-C(4)	112.7(3)	O(5)-C(4)-C(3)	112.5(3)
C(4)-O(5)-C(6)	115.6(3)	O(5)-C(6)-C(7)	109.8(3)
O(8)-C(7)-C(6)	109.5(3)	C(7)-O(8)-C(9)	113.5(3)
O(8)-C(9)-C(9)#1	110.3(3)	N(12)-C(11)-C(1)	179.3(4)
N(2)-C(21)-C(27)	113.6(2)	C(26)-C(27)-C(21)	118.3(2)
C(22)-C(27)-C(21)	121.6(2)		

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 1.

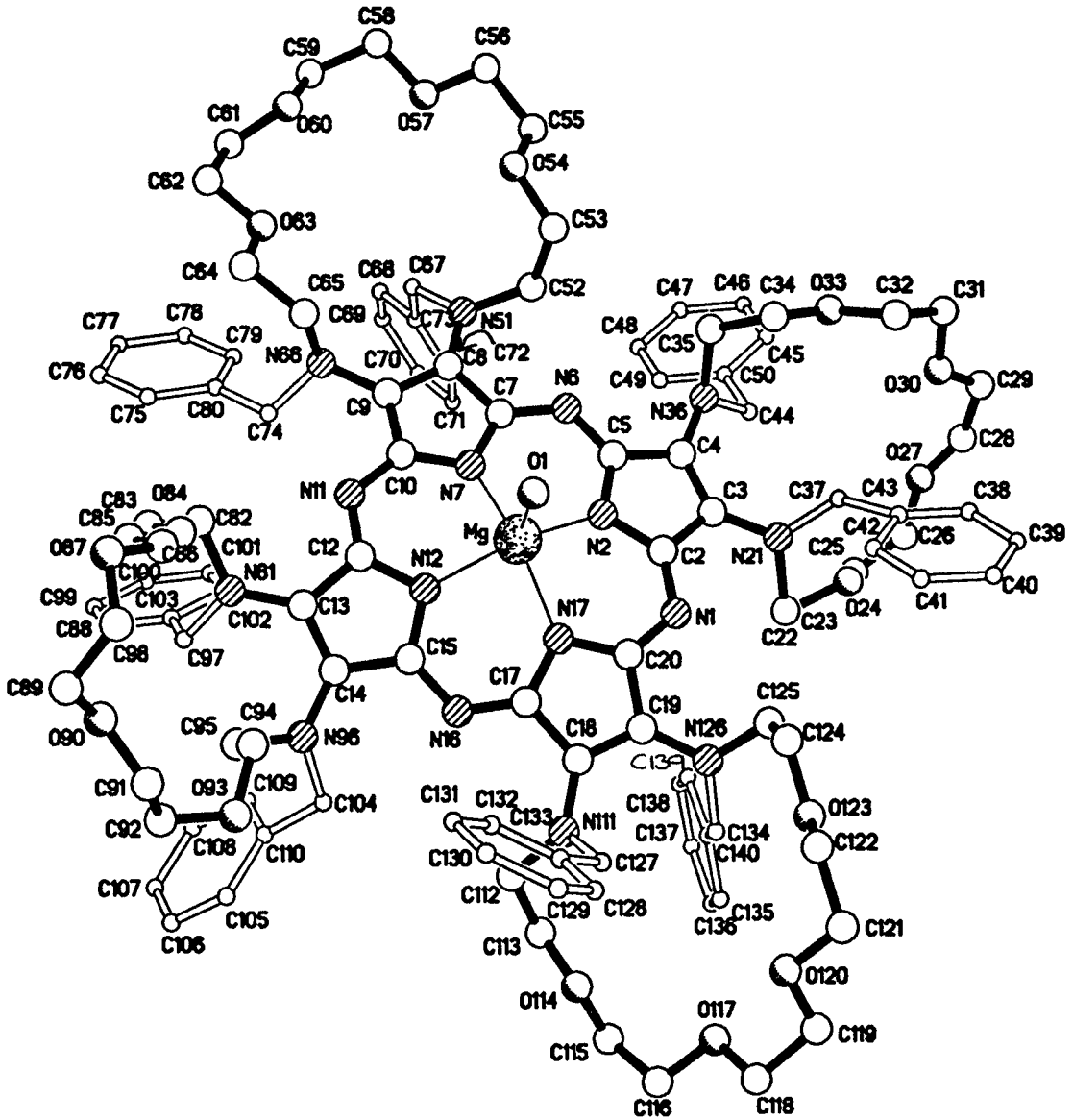
The anisotropic displacement factor exponent takes the form:

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

	U11	U22	U33	U23	U13	U12
C(1)	28(1)	35(1)	33(1)	2(1)	4(1)	0(1)
N(2)	34(1)	45(1)	38(1)	7(1)	14(1)	10(1)
C(3)	43(2)	71(2)	54(2)	11(2)	25(1)	14(1)
C(4)	69(2)	113(3)	51(2)	16(2)	30(2)	26(2)
O(5)	57(2)	122(2)	49(1)	-19(1)	13(1)	30(2)
C(6)	65(3)	139(4)	75(3)	-48(3)	14(2)	32(3)
C(7)	74(3)	131(4)	82(3)	-66(3)	2(2)	23(3)
O(8)	92(2)	66(2)	75(2)	-28(1)	-13(2)	11(1)
C(9)	112(4)	51(2)	112(4)	-21(2)	-36(3)	15(2)
C(11)	26(1)	47(2)	58(2)	8(1)	6(1)	-1(1)
N(12)	49(2)	52(2)	122(3)	18(2)	23(2)	-12(1)
C(21)	34(1)	37(1)	39(1)	3(1)	6(1)	1(1)
C(22)	60(2)	60(2)	52(2)	8(2)	-6(2)	-11(2)
C(23)	63(2)	108(3)	57(2)	10(2)	-11(2)	-28(2)
C(24)	56(2)	119(4)	53(2)	24(2)	-2(2)	22(2)
C(25)	87(3)	84(3)	64(2)	15(2)	-2(2)	39(2)
C(26)	72(2)	54(2)	57(2)	3(2)	4(2)	19(2)
C(27)	34(1)	44(1)	32(1)	3(1)	10(1)	3(1)

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

	x	y	z	U(eq)	sof
H(3A)	2325(2)	960(3)	2424(2)	65	1
H(3B)	2216(2)	2276(3)	2265(2)	65	1
H(4A)	880(3)	2020(4)	988(2)	90	1
H(4B)	1790(3)	1271(4)	982(2)	90	1
H(6A)	1805(3)	-697(5)	1524(3)	116	1
H(6B)	1280(3)	-711(5)	524(3)	116	1
H(7A)	-188(4)	-1488(5)	713(3)	125	1
H(7B)	742(4)	-2319(5)	926(3)	125	1
H(9A)	293(4)	-3379(3)	1966(3)	137	1
H(9B)	-702(4)	-2641(3)	1660(3)	137	1
H(21A)	956(2)	-21(2)	2810(2)	47	1
H(21B)	576(2)	769(2)	3374(2)	47	1
H(22A)	2474(2)	2107(1)	4226(1)	78	1
H(23A)	3939(2)	1749(3)	5410(2)	103	1
H(24A)	4445(2)	-110(3)	5808(2)	99	1
H(25A)	3486(3)	-1613(2)	5021(2)	105	1
H(26A)	2020(2)	-1256(2)	3837(2)	80	1


C58
C59
C56
C61
O60
O57
C55
C62
O54
O63
C53
C64
C65
C68
C67
C52
C47
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N51
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C35
C45
C76
N66
C70
C8
C72
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C50
O30
C29
C75
C80
C74
C9
C71
C7
N6
N36
C44
C5
C4
C28
O27
O1
N11
C10
N7
C3
C37
C43
C38
C83
O84
C85
C82
C42
C26
C39
O87
C86
C101
C12
Mg
N2
C2
N21
C25
C100
N61
N12
C99
C103
C13
N17
N1
C41
C40
C88
C102
C22
C23
O24
C98
C97
C15
C20
C89
C14
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C125
C95
C94
N96
N16
C18
N126
C124
O90
C139
C91
O93
C109
C104
C131
C132
C133
N111
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O123
C92
C108
C110
C130
C127
C137
C134
C122
C107
C112
C129
C128
C140
C135
C136
C121
C105
C113
O120
C106
O114
O117
C119
C115
C116
C118

Table 1. Crystal data and structure refinement for 1.

Identification code	AB9521
Empirical formula	$C_{112}H_{136}N_{16}O_{17}Mg$. $0.75MeCO_2Et$
Formula weight	2068.76
Temperature	203(2) K
Diffractometer Used	Siemens P4/PC
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	*a* = 24.419(9) Å alpha = 90° *b* = 17.824(8) Å beta = 99.43(3)° *c* = 25.512(10) Å gamma = 90°
Volume, Z	10954(7) $Å^3$, 4
Density (calculated)	1.254 Mg/m^3
Absorption coefficient	0.746 mm^{-1}
F(000)	4416
Crystal colour/morphology	Deep red blocks
Crystal size	0.43 x 0.33 x 0.27 mm
θ range for data collection	2.32 to 56.08°
Limiting indices	$0 \leq h \leq 26$, $0 \leq k \leq 19$, $-27 \leq l \leq 27$
Scan type	ω-scans
Reflections collected	14673
Independent reflections	14288 (R_{int} = 0.0692)
Observed reflections [F>4σ(F)]	7682
Absorption correction	None
Structure solution method	Direct
Refinement method	Full-matrix-block least-squares on F^2
Data / restraints / parameters	12172 / 673 / 1328
Goodness-of-fit on F^2	1.042
Final R indices [F>4σ(F)]	R1 = 0.1481, wR2 = 0.4019
R indices (all data)	R1 = 0.2208, wR2 = 0.5143
Extinction coefficient	0.00045(13)
Largest diff. peak and hole	0.848 and -0.578 $eÅ^{-3}$
Mean and maximum shift/error	0.118 and -0.738

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

	x	y	z	U(eq)	sof
Mg	8833(1)	5075(2)	1066(1)	52(1)	1
O(1)	8820(2)	6000(4)	615(2)	70(2)	1
N(1)	8933(3)	5872(4)	2290(3)	61(2)	1
C(2)	9401(4)	5623(5)	2147(3)	62(2)	1
N(2)	9450(3)	5251(4)	1691(2)	56(2)	1
C(3)	9955(4)	5708(6)	2480(3)	73(3)	1
C(4)	10312(4)	5410(6)	2195(3)	72(3)	1
C(5)	9996(4)	5113(5)	1707(3)	62(2)	1
N(6)	10226(3)	4707(4)	1360(3)	63(2)	1
C(7)	9937(3)	4334(5)	947(3)	57(2)	1
N(7)	9378(3)	4352(4)	803(2)	54(2)	1
C(8)	10188(3)	3813(5)	597(4)	60(2)	1
C(9)	9736(3)	3525(5)	256(3)	55(2)	1
C(10)	9246(4)	3868(5)	385(3)	59(2)	1
N(11)	8727(3)	3715(4)	117(3)	57(2)	1
C(12)	8267(3)	3954(5)	259(3)	54(2)	1
N(12)	8224(3)	4424(4)	685(2)	52(2)	1
C(13)	7713(3)	3690(5)	11(3)	62(2)	1
C(14)	7349(3)	3971(6)	327(4)	71(3)	1
C(15)	7666(3)	4427(5)	733(3)	58(2)	1
N(16)	7439(3)	4788(4)	1110(3)	58(2)	1
C(17)	7732(3)	5194(4)	1495(3)	54(2)	1
N(17)	8305(3)	5296(4)	1577(3)	57(2)	1
C(18)	7484(4)	5586(5)	1899(3)	58(2)	1
C(19)	7915(4)	5945(5)	2218(3)	63(2)	1
C(20)	8424(4)	5735(5)	2023(3)	59(2)	1
N(21)	10026(4)	6077(6)	2977(3)	98(3)	1
C(22)	9689(5)	5805(10)	3405(5)	123(5)	1
C(23)	9962(7)	5179(9)	3769(6)	131(5)	1
O(24)	10423(8)	5610(11)	4096(8)	237(7)	1
C(25)	10778(14)	5134(21)	4435(15)	336(24)	1
C(26)	11215(14)	5514(18)	4639(12)	242(14)	1
O(27)	11507(9)	5977(12)	4360(8)	261(11)	1
C(28)	11909(12)	6361(18)	4464(12)	234(12)	1
C(29)	12122(8)	6898(11)	4162(7)	149(6)	1
O(30)	11885(7)	6959(11)	3645(5)	225(8)	1
C(31)	12118(10)	7347(15)	3292(7)	234(14)	1
C(32)	11683(10)	7436(14)	2759(8)	212(10)	1
O(33)	11690(4)	6671(7)	2548(4)	147(4)	1
C(34)	11299(5)	6582(9)	2077(4)	105(4)	1
C(35)	11231(4)	5736(8)	1972(4)	90(3)	1
N(36)	10910(3)	5330(6)	2314(3)	96(3)	1
C(37)	10452(8)	6571(10)	3185(6)	153(7)	1
C(38)	10566(6)	7843(9)	3728(5)	249(13)	1
C(39)	10311(9)	8510(7)	3835(6)	243(14)	1
C(40)	9805(9)	8712(8)	3536(9)	349(24)	1
C(41)	9553(6)	8246(11)	3130(9)	358(26)	1
C(42)	9807(7)	7579(9)	3022(6)	250(14)	1
C(43)	10314(7)	7377(7)	3321(5)	155(7)	1
C(44)	11179(6)	5224(8)	2859(5)	116(4)	1
C(45)	12142(5)	4716(8)	3126(5)	220(11)	1
C(46)	12532(4)	4148(12)	3123(7)	237(11)	1
C(47)	12382(7)	3482(10)	2854(8)	293(17)	1

C(48)	11842(8)	3384(7)	2588(7)	258(14)	1
C(49)	11453(5)	3952(8)	2591(5)	204(10)	1
C(50)	11603(5)	4619(7)	2860(5)	126(5)	1
N(51)	10746(3)	3640(4)	655(3)	60(2)	1
C(52)	11197(4)	4041(6)	1040(4)	87(3)	1
C(53)	11449(5)	4655(7)	780(4)	90(3)	1
O(54)	11754(3)	4410(4)	366(3)	88(2)	1
C(55)	12303(4)	4147(7)	560(5)	98(4)	1
C(56)	12572(4)	3854(7)	91(5)	91(3)	1
O(57)	12273(3)	3236(4)	-119(3)	87(2)	1
C(58)	12458(4)	2974(7)	-576(5)	94(3)	1
C(59)	12118(5)	2293(8)	-803(5)	111(4)	1
O(60)	11587(3)	2560(5)	-1015(3)	102(2)	1
C(61)	11216(5)	1974(7)	-1176(5)	98(4)	1
C(62)	10650(4)	2330(6)	-1391(4)	85(3)	1
O(63)	10484(2)	2728(4)	-964(2)	71(2)	1
C(64)	9955(4)	3039(5)	-1125(3)	65(2)	1
C(65)	9794(4)	3474(5)	-669(3)	68(2)	1
N(66)	9759(3)	3034(4)	-191(3)	61(2)	1
C(67)	10934(4)	2939(5)	451(4)	63(2)	1
C(68)	11290(3)	1680(4)	736(2)	94(3)	1
C(69)	11375(3)	1093(3)	1099(3)	113(4)	1
C(70)	11181(4)	1147(4)	1580(3)	97(3)	1
C(71)	10901(3)	1789(4)	1699(2)	94(3)	1
C(72)	10816(3)	2376(3)	1336(3)	86(3)	1
C(73)	11010(3)	2321(3)	855(2)	57(2)	1
C(74)	9333(4)	2454(5)	-264(5)	86(3)	1
C(75)	9154(3)	1418(5)	-925(3)	108(4)	1
C(76)	9291(5)	742(5)	-1142(3)	144(6)	1
C(77)	9777(5)	372(4)	-927(5)	160(8)	1
C(78)	10126(4)	678(5)	-494(6)	227(14)	1
C(79)	9989(3)	1354(5)	-277(4)	149(7)	1
C(80)	9503(3)	1724(3)	-492(3)	79(3)	1
N(81)	7599(3)	3194(4)	-423(3)	75(2)	1
C(82)	7857(3)	3289(6)	-901(3)	77(3)	1
C(83)	7469(5)	3492(6)	-1381(4)	112(4)	1
O(84)	7318(4)	4236(5)	-1415(4)	127(3)	1
C(85)	6936(7)	4416(8)	-1869(6)	167(8)	1
C(86)	6776(8)	5194(9)	-1913(6)	225(12)	1
O(87)	6404(5)	5363(7)	-2368(4)	176(5)	1
C(88)	5912(7)	5663(10)	-2253(9)	212(9)	1
C(89)	5490(8)	5094(16)	-2234(10)	335(9)	1
O(90)	5587(14)	4720(19)	-1756(13)	337(9)	0.50
C(91)	5327(27)	5005(29)	-1361(12)	335(9)	0.50
C(92)	5345(17)	4459(28)	-937(12)	337(9)	0.50
O(93)	5650(20)	4700(24)	-466(11)	336(9)	0.50
C(94)	6210(17)	4596(29)	-453(21)	336(9)	0.50
C(95)	6387(22)	3861(25)	-256(14)	334(9)	0.50
O(90')	5661(12)	4572(21)	-1846(16)	338(9)	0.50
C(91')	5219(17)	4179(25)	-1708(12)	333(9)	0.50
C(92')	5267(13)	4164(32)	-1135(12)	336(9)	0.50
O(93')	5753(16)	3819(21)	-912(14)	336(9)	0.50
C(94')	5954(19)	4127(40)	-419(16)	338(9)	0.50
C(95')	6547(14)	4002(46)	-310(8)	334(9)	0.50
N(96)	6765(4)	3894(8)	261(4)	151(6)	1
C(97)	7269(4)	2524(6)	-391(4)	84(3)	1
C(98)	7416(4)	1158(5)	-527(4)	177(8)	1
C(99)	7714(5)	496(4)	-417(5)	197(10)	1
C(100)	8194(4)	490(5)	-40(4)	132(5)	1
C(101)	8377(3)	1146(6)	228(3)	108(4)	1
C(102)	8079(4)	1808(4)	118(3)	97(4)	1
C(103)	7599(3)	1814(4)	-259(3)	89(3)	1

C(104)	6544(7)	3624(11)	736(7)	196(10)	1
C(105)	5692(4)	2826(8)	517(7)	281(16)	1
C(106)	5458(5)	2116(11)	434(8)	270(15)	1
C(107)	5797(9)	1485(8)	480(6)	248(16)	1
C(108)	6370(8)	1564(8)	609(5)	245(17)	1
C(109)	6604(4)	2274(11)	691(4)	164(9)	1
C(110)	6265(5)	2905(8)	645(5)	131(5)	1
N(111)	6922(3)	5616(4)	1933(3)	64(2)	1
C(112)	6600(4)	4949(5)	1929(4)	71(3)	1
C(113)	6456(4)	4727(6)	2464(4)	79(3)	1
O(114)	6101(3)	5260(4)	2633(3)	83(2)	1
C(115)	5971(5)	5117(7)	3147(5)	101(4)	1
C(116)	5709(6)	5800(8)	3316(5)	106(4)	1
O(117)	6080(4)	6394(5)	3397(3)	106(2)	1
C(118)	5790(8)	7086(9)	3450(6)	138(6)	1
C(119)	6195(8)	7731(10)	3493(6)	143(6)	1
O(120)	6369(4)	7824(5)	3005(3)	104(2)	1
C(121)	6678(6)	8501(7)	2998(6)	120(5)	1
C(122)	7087(6)	8409(6)	2646(6)	105(4)	1
O(123)	7484(3)	7856(4)	2856(3)	102(2)	1
C(124)	7895(5)	7740(6)	2544(6)	105(4)	1
C(125)	8214(4)	7059(6)	2751(5)	93(3)	1
N(126)	7910(4)	6363(4)	2676(3)	78(2)	1
C(127)	6653(4)	6339(5)	1948(4)	80(3)	1
C(128)	6071(4)	7296(4)	1404(4)	144(7)	1
C(129)	5793(4)	7580(4)	926(5)	191(11)	1
C(130)	5791(4)	7182(6)	457(4)	161(8)	1
C(131)	6068(4)	6500(6)	466(3)	121(5)	1
C(132)	6347(3)	6216(4)	944(4)	106(4)	1
C(133)	6348(3)	6614(4)	1413(3)	91(3)	1
C(134)	7571(5)	6145(6)	3056(4)	91(3)	1
C(135)	7499(3)	5261(4)	3804(3)	96(3)	1
C(136)	7668(3)	4634(5)	4112(3)	126(5)	1
C(137)	8120(3)	4216(4)	4013(3)	99(4)	1
C(138)	8404(3)	4424(4)	3606(3)	86(3)	1
C(139)	8235(3)	5051(4)	3298(2)	85(3)	1
C(140)	7783(3)	5470(3)	3396(2)	77(3)	1
C(141)	4194(10)	8156(16)	807(14)	207(13)	0.75
C(142)	4168(11)	8084(19)	1369(9)	180(13)	0.75
O(143)	4615(7)	8371(9)	1693(6)	148(5)	0.75
C(144)	4832(11)	8163(13)	2143(11)	145(9)	0.75
O(145)	4713(10)	7552(12)	2301(7)	209(8)	0.75
C(146)	5206(10)	8656(12)	2481(9)	162(10)	0.75

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

Mg-N(12)	2.008(7)	Mg-O(1)	2.006(7)
Mg-N(17)	2.017(7)	Mg-N(2)	2.031(7)
Mg-N(7)	2.042(7)	N(1)-C(2)	1.331(11)
N(1)-C(20)	1.337(11)	C(2)-N(2)	1.361(11)
C(2)-C(3)	1.483(12)	N(2)-C(5)	1.352(11)
C(3)-C(4)	1.334(13)	C(3)-N(21)	1.413(9)
C(4)-N(36)	1.449(9)	C(4)-C(5)	1.452(12)
C(5)-N(6)	1.336(11)	N(6)-C(7)	1.344(11)
C(7)-N(7)	1.354(10)	C(7)-C(8)	1.489(12)
N(7)-C(10)	1.368(11)	C(8)-N(51)	1.382(8)
C(8)-C(9)	1.386(12)	C(9)-C(10)	1.430(11)
C(9)-N(66)	1.446(8)	C(10)-N(11)	1.367(11)
N(11)-C(12)	1.307(10)	C(12)-N(12)	1.390(10)
C(12)-C(13)	1.475(11)	N(12)-C(15)	1.386(10)
C(13)-C(14)	1.386(11)	C(13)-N(81)	1.408(9)
C(14)-N(96)	1.416(9)	C(14)-C(15)	1.438(12)
C(15)-N(16)	1.350(10)	N(16)-C(17)	1.331(10)
C(17)-N(17)	1.391(10)	C(17)-C(18)	1.457(11)
N(17)-C(20)	1.373(10)	C(18)-C(19)	1.377(12)
C(18)-N(111)	1.390(8)	C(19)-N(126)	1.387(8)
C(19)-C(20)	1.462(12)	N(21)-C(37)	1.40(2)
N(21)-C(22)	1.55(2)	C(22)-C(23)	1.53(2)
C(23)-O(24)	1.50(2)	O(24)-C(25)	1.40(3)
C(25)-C(26)	1.30(4)	C(26)-O(27)	1.36(3)
O(27)-C(28)	1.19(3)	C(28)-C(29)	1.39(3)
C(29)-O(30)	1.35(2)	O(30)-C(31)	1.33(2)
C(31)-C(32)	1.59(3)	C(32)-O(33)	1.47(2)
O(33)-C(34)	1.418(13)	C(34)-C(35)	1.54(2)
C(35)-N(36)	1.456(13)	N(36)-C(44)	1.450(14)
C(37)-C(43)	1.53(2)	C(44)-C(50)	1.50(2)
N(51)-C(67)	1.455(11)	N(51)-C(52)	1.527(12)
C(52)-C(53)	1.47(2)	C(53)-O(54)	1.457(12)
O(54)-C(55)	1.428(11)	C(55)-C(56)	1.55(2)
C(56)-O(57)	1.379(12)	O(57)-C(58)	1.398(13)
C(58)-C(59)	1.53(2)	C(59)-O(60)	1.403(12)
O(60)-C(61)	1.400(13)	C(61)-C(62)	1.54(2)
C(62)-O(63)	1.413(11)	O(63)-C(64)	1.403(10)
C(64)-C(65)	1.505(12)	C(65)-N(66)	1.465(11)
N(66)-C(74)	1.456(11)	C(67)-C(73)	1.498(10)
C(74)-C(80)	1.511(11)	N(81)-C(97)	1.450(12)
N(81)-C(82)	1.472(8)	C(82)-C(83)	1.467(8)
C(83)-O(84)	1.375(8)	O(84)-C(85)	1.400(9)
C(85)-C(86)	1.440(10)	C(86)-O(87)	1.384(9)
O(87)-C(88)	1.390(9)	C(88)-C(89)	1.453(10)
C(89)-O(90')	1.373(11)	C(89)-O(90)	1.377(10)
O(90)-C(91)	1.374(10)	C(91)-C(92)	1.451(10)
C(92)-O(93)	1.376(10)	O(93)-C(94)	1.374(11)
C(94)-C(95)	1.443(11)	C(95)-N(96)	1.480(10)
O(90')-C(91')	1.379(10)	C(91')-C(92')	1.448(10)
C(92')-O(93')	1.375(10)	O(93')-C(94')	1.386(10)
C(94')-C(95')	1.447(11)	C(95')-N(96)	1.479(10)
N(96)-C(104)	1.49(2)	C(97)-C(103)	1.510(13)
C(104)-C(110)	1.45(2)	N(111)-C(112)	1.424(11)
N(111)-C(127)	1.450(11)	C(112)-C(113)	1.517(13)
C(113)-O(114)	1.400(11)	O(114)-C(115)	1.423(12)
C(115)-C(116)	1.47(2)	C(116)-O(117)	1.389(14)
O(117)-C(118)	1.44(2)	C(118)-C(119)	1.51(2)
C(119)-O(120)	1.39(2)	O(120)-C(121)	1.42(2)
C(121)-C(122)	1.46(2)	C(122)-O(123)	1.423(13)

O(123)-C(124)	1.395(13)	C(124)-C(125)	1.49(2)
C(125)-N(126)	1.442(13)	N(126)-C(134)	1.428(13)
C(127)-C(133)	1.525(12)	C(134)-C(140)	1.525(12)

N(12)-Mg-O(1)	104.9(3)	N(12)-Mg-N(17)	85.6(3)
O(1)-Mg-N(17)	105.0(3)	N(12)-Mg-N(2)	149.9(3)
O(1)-Mg-N(2)	105.2(3)	N(17)-Mg-N(2)	86.1(3)
N(12)-Mg-N(7)	87.0(3)	O(1)-Mg-N(7)	106.3(3)
N(17)-Mg-N(7)	148.7(3)	N(2)-Mg-N(7)	85.2(3)
C(2)-N(1)-C(20)	124.5(7)	N(1)-C(2)-N(2)	126.6(8)
N(1)-C(2)-C(3)	123.6(8)	N(2)-C(2)-C(3)	109.8(8)
C(5)-N(2)-C(2)	106.7(7)	C(5)-N(2)-Mg	126.7(6)
C(2)-N(2)-Mg	126.1(6)	C(4)-C(3)-N(21)	132.8(8)
C(4)-C(3)-C(2)	105.3(8)	N(21)-C(3)-C(2)	121.8(8)
C(3)-C(4)-N(36)	130.7(8)	C(3)-C(4)-C(5)	108.0(8)
N(36)-C(4)-C(5)	121.3(8)	N(6)-C(5)-N(2)	126.7(8)
N(6)-C(5)-C(4)	123.0(8)	N(2)-C(5)-C(4)	110.1(8)
C(5)-N(6)-C(7)	124.3(7)	N(7)-C(7)-N(6)	125.2(8)
N(7)-C(7)-C(8)	110.4(8)	N(6)-C(7)-C(8)	124.3(8)
C(7)-N(7)-C(10)	107.1(7)	C(7)-N(7)-Mg	127.5(6)
C(10)-N(7)-Mg	124.8(5)	N(51)-C(8)-C(9)	130.8(8)
N(51)-C(8)-C(7)	124.8(8)	C(9)-C(8)-C(7)	104.1(7)
C(8)-C(9)-C(10)	107.9(7)	C(8)-C(9)-N(66)	126.1(7)
C(10)-C(9)-N(66)	125.7(7)	N(11)-C(10)-N(7)	126.7(7)
N(11)-C(10)-C(9)	122.8(8)	N(7)-C(10)-C(9)	110.6(8)
C(12)-N(11)-C(10)	124.3(7)	N(11)-C(12)-N(12)	126.4(7)
N(11)-C(12)-C(13)	123.2(8)	N(12)-C(12)-C(13)	110.1(7)
C(12)-N(12)-C(15)	105.9(6)	C(12)-N(12)-Mg	125.5(5)
C(15)-N(12)-Mg	128.0(5)	C(14)-C(13)-N(81)	128.4(7)
C(14)-C(13)-C(12)	105.4(7)	N(81)-C(13)-C(12)	125.9(7)
C(13)-C(14)-N(96)	128.6(7)	C(13)-C(14)-C(15)	107.6(7)
N(96)-C(14)-C(15)	123.6(7)	N(16)-C(15)-N(12)	126.0(7)
N(16)-C(15)-C(14)	123.2(8)	N(12)-C(15)-C(14)	110.8(7)
C(17)-N(16)-C(15)	123.5(7)	N(16)-C(17)-N(17)	125.9(7)
N(16)-C(17)-C(18)	123.2(7)	N(17)-C(17)-C(18)	110.9(7)
C(20)-N(17)-C(17)	105.7(7)	C(20)-N(17)-Mg	125.1(6)
C(17)-N(17)-Mg	127.7(5)	C(19)-C(18)-N(111)	127.8(7)
C(19)-C(18)-C(17)	105.9(7)	N(111)-C(18)-C(17)	126.3(7)
C(18)-C(19)-N(126)	129.4(7)	C(18)-C(19)-C(20)	106.9(7)
N(126)-C(19)-C(20)	123.4(8)	N(1)-C(20)-N(17)	125.5(8)
N(1)-C(20)-C(19)	123.3(8)	N(17)-C(20)-C(19)	110.6(8)
C(37)-N(21)-C(3)	127.3(9)	C(37)-N(21)-C(22)	112.2(10)
C(3)-N(21)-C(22)	119.1(8)	C(23)-C(22)-N(21)	115.2(12)
O(24)-C(23)-C(22)	100.2(14)	C(25)-O(24)-C(23)	111(2)
O(24)-C(25)-C(26)	108(4)	O(27)-C(26)-C(25)	125(4)
C(28)-O(27)-C(26)	136(3)	O(27)-C(28)-C(29)	130(3)
O(30)-C(29)-C(28)	117(2)	C(29)-O(30)-C(31)	123(2)
O(30)-C(31)-C(32)	109(2)	O(33)-C(32)-C(31)	100(2)
C(34)-O(33)-C(32)	111.6(14)	O(33)-C(34)-C(35)	107.2(12)
N(36)-C(35)-C(34)	116.0(10)	C(44)-N(36)-C(4)	119.7(8)
C(44)-N(36)-C(35)	115.9(9)	C(4)-N(36)-C(35)	116.7(7)
N(21)-C(37)-C(43)	120(2)	C(42)-C(43)-C(37)	109.2(14)
C(38)-C(43)-C(37)	130.0(13)	N(36)-C(44)-C(50)	107.5(11)
C(49)-C(50)-C(44)	119.3(10)	C(45)-C(50)-C(44)	120.7(10)
C(8)-N(51)-C(67)	121.0(6)	C(8)-N(51)-C(52)	123.9(6)
C(67)-N(51)-C(52)	113.4(7)	C(53)-C(52)-N(51)	111.8(9)
O(54)-C(53)-C(52)	114.0(10)	C(55)-O(54)-C(53)	114.2(8)
O(54)-C(55)-C(56)	109.6(9)	O(57)-C(56)-C(55)	107.8(9)
C(56)-O(57)-C(58)	111.6(9)	O(57)-C(58)-C(59)	110.6(9)
O(60)-C(59)-C(58)	106.6(10)	C(61)-O(60)-C(59)	111.9(10)
O(60)-C(61)-C(62)	107.3(9)	O(63)-C(62)-C(61)	106.7(8)
C(62)-O(63)-C(64)	109.8(7)	O(63)-C(64)-C(65)	108.9(7)

N(66)-C(65)-C(64)	115.2(7)	C(9)-N(66)-C(74)	114.3(6)
C(9)-N(66)-C(65)	110.2(6)	C(74)-N(66)-C(65)	114.2(8)
N(51)-C(67)-C(73)	113.4(7)	C(72)-C(73)-C(67)	122.2(5)
C(68)-C(73)-C(67)	117.8(5)	N(66)-C(74)-C(80)	115.1(7)
C(79)-C(80)-C(74)	121.8(8)	C(75)-C(80)-C(74)	118.2(8)
C(13)-N(81)-C(97)	120.9(6)	C(13)-N(81)-C(82)	121.6(6)
C(97)-N(81)-C(82)	117.2(8)	C(83)-C(82)-N(81)	114.6(8)
O(84)-C(83)-C(82)	114.8(9)	C(83)-O(84)-C(85)	114.1(9)
O(84)-C(85)-C(86)	114.9(11)	O(87)-C(86)-C(85)	114.0(12)
C(86)-O(87)-C(88)	112.1(12)	O(87)-C(88)-C(89)	112.4(13)
O(90')-C(89)-C(88)	111(2)	O(90)-C(89)-C(88)	110(2)
C(91)-O(90)-C(89)	116(2)	O(90)-C(91)-C(92)	110(2)
O(93)-C(92)-C(91)	113(2)	C(94)-O(93)-C(92)	112(2)
O(93)-C(94)-C(95)	112(2)	C(94)-C(95)-N(96)	113(2)
C(89)-O(90')-C(91')	112(2)	O(90')-C(91')-C(92')	109(2)
O(93')-C(92')-C(91')	110(2)	C(92')-O(93')-C(94')	111(2)
O(93')-C(94')-C(95')	108(2)	C(94')-C(95')-N(96)	113(2)
C(14)-N(96)-C(95)	125(3)	C(14)-N(96)-C(95')	107(2)
C(14)-N(96)-C(104)	115.3(11)	C(95)-N(96)-C(104)	117(3)
C(95')-N(96)-C(104)	137(2)	N(81)-C(97)-C(103)	115.0(8)
C(102)-C(103)-C(97)	121.3(7)	C(98)-C(103)-C(97)	118.7(7)
C(110)-C(104)-N(96)	112.3(11)	C(109)-C(110)-C(104)	116.3(13)
C(105)-C(110)-C(104)	123.7(13)	C(18)-N(111)-C(112)	121.2(6)
C(18)-N(111)-C(127)	119.4(7)	C(112)-N(111)-C(127)	119.3(7)
N(111)-C(112)-C(113)	114.9(8)	O(114)-C(113)-C(112)	110.2(8)
C(113)-O(114)-C(115)	113.9(8)	O(114)-C(115)-C(116)	107.2(9)
O(117)-C(116)-C(115)	111.6(10)	C(116)-O(117)-C(118)	110.3(12)
O(117)-C(118)-C(119)	109.4(14)	O(120)-C(119)-C(118)	108.6(12)
C(119)-O(120)-C(121)	110.6(12)	O(120)-C(121)-C(122)	109.3(10)
O(123)-C(122)-C(121)	109.7(12)	C(124)-O(123)-C(122)	113.3(11)
O(123)-C(124)-C(125)	107.6(10)	N(126)-C(125)-C(124)	115.1(9)
C(19)-N(126)-C(134)	120.8(7)	C(19)-N(126)-C(125)	119.9(8)
C(134)-N(126)-C(125)	119.1(8)	N(111)-C(127)-C(133)	114.8(8)
C(132)-C(133)-C(127)	122.5(7)	C(128)-C(133)-C(127)	117.5(7)
N(126)-C(134)-C(140)	114.9(8)	C(139)-C(140)-C(134)	121.7(6)
C(135)-C(140)-C(134)	118.2(6)		

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 1.

The anisotropic displacement factor exponent takes the form:

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

	U11	U22	U33	U23	U13	U12
Mg	48(1)	63(2)	46(1)	1(1)	7(1)	3(1)
O(1)	59(4)	81(4)	69(4)	13(3)	4(3)	-2(3)
N(1)	63(5)	58(4)	60(4)	-4(3)	4(4)	0(4)
C(2)	58(5)	71(6)	53(5)	-2(5)	2(4)	-9(5)
N(2)	48(4)	72(5)	48(4)	6(3)	5(3)	-3(3)
C(3)	86(7)	78(6)	49(5)	8(5)	-4(5)	-3(5)
C(4)	65(6)	104(8)	45(5)	5(5)	-1(4)	1(5)
C(5)	59(6)	67(6)	58(5)	5(4)	5(4)	3(5)
N(6)	55(4)	88(5)	44(4)	13(4)	5(3)	8(4)
C(7)	49(5)	69(6)	56(5)	13(4)	17(4)	6(4)
N(7)	48(4)	68(5)	46(4)	2(3)	10(3)	6(3)
C(8)	57(5)	51(5)	75(6)	21(4)	21(5)	6(4)
C(9)	51(5)	61(5)	58(5)	1(4)	26(4)	5(4)
C(10)	64(6)	65(6)	52(5)	8(4)	17(4)	4(4)
N(11)	57(4)	66(5)	52(4)	-1(3)	19(3)	10(4)
C(12)	49(5)	60(5)	55(5)	-1(4)	13(4)	7(4)
N(12)	45(4)	63(4)	48(4)	-3(3)	11(3)	-2(3)
C(13)	55(5)	69(6)	63(5)	-9(4)	12(4)	-8(4)
C(14)	47(5)	99(7)	70(6)	-32(5)	26(4)	-19(5)
C(15)	61(5)	60(5)	53(5)	-3(4)	7(4)	-2(4)
N(16)	50(4)	62(4)	64(4)	-12(4)	15(3)	-3(3)
C(17)	56(5)	50(5)	60(5)	2(4)	25(4)	5(4)
N(17)	66(5)	54(4)	52(4)	-3(3)	13(3)	6(3)
C(18)	68(6)	56(5)	52(5)	-1(4)	20(4)	4(4)
C(19)	78(6)	59(5)	56(5)	-7(4)	21(5)	5(5)
C(20)	68(6)	58(5)	50(5)	-1(4)	11(4)	-1(4)
N(21)	96(6)	138(8)	53(5)	-13(5)	-14(4)	-42(6)
C(22)	105(10)	178(15)	83(8)	-19(9)	6(7)	-16(10)
C(23)	153(14)	125(12)	112(10)	12(9)	11(10)	6(11)
O(24)	219(10)	235(10)	247(10)	48(8)	12(8)	-13(8)
C(25)	242(31)	279(36)	415(46)	-37(33)	-163(32)	128(28)
C(26)	260(32)	225(29)	241(30)	92(24)	49(26)	-44(24)
O(27)	249(20)	265(20)	218(17)	54(15)	-110(16)	-112(17)
C(28)	198(26)	226(29)	250(32)	8(25)	-47(23)	-40(22)
C(29)	164(13)	133(12)	132(12)	-21(10)	-32(10)	-34(11)
O(30)	232(14)	342(21)	103(9)	-82(11)	30(9)	-138(14)
C(31)	276(26)	336(32)	87(11)	-44(15)	22(14)	-211(25)
C(32)	245(24)	227(24)	146(16)	-76(17)	-23(15)	-72(20)
O(33)	128(7)	213(12)	96(6)	-31(7)	5(5)	-49(8)
C(34)	78(7)	171(14)	59(6)	-38(7)	-5(5)	-23(8)
C(35)	60(6)	149(11)	58(6)	-1(7)	2(5)	-1(7)
N(36)	57(5)	183(10)	43(4)	8(5)	-11(4)	-9(5)
C(37)	193(17)	164(15)	113(11)	-57(11)	55(11)	-25(13)
C(38)	324(33)	188(24)	233(28)	33(21)	46(25)	111(24)
C(39)	407(43)	88(12)	257(27)	-25(15)	122(29)	25(19)
C(40)	324(38)	219(29)	507(56)	155(36)	82(39)	185(29)
C(41)	353(27)	359(27)	359(27)	0(10)	53(11)	-5(10)
C(42)	237(24)	170(20)	283(27)	63(19)	-134(22)	12(18)
C(43)	262(22)	124(12)	74(8)	-23(8)	15(11)	85(13)
C(44)	117(10)	118(10)	106(9)	-14(8)	0(8)	-7(8)
C(45)	130(15)	305(30)	201(20)	-40(20)	-44(14)	88(18)
C(46)	179(15)	265(19)	239(17)	4(16)	-47(13)	50(15)
C(47)	290(19)	289(19)	295(19)	-4(10)	36(10)	20(10)

C(48)	324(41)	174(22)	288(31)	-70(22)	90(30)	64(23)
C(49)	277(27)	108(13)	230(22)	-56(14)	46(19)	33(16)
C(50)	100(10)	164(14)	104(10)	-5(9)	-14(8)	46(10)
N(51)	43(4)	57(4)	78(5)	-7(4)	9(3)	-2(3)
C(52)	69(6)	96(8)	94(8)	1(6)	8(6)	6(6)
C(53)	89(7)	116(9)	69(7)	9(6)	21(6)	1(7)
O(54)	72(4)	101(5)	83(5)	16(4)	-12(4)	-2(4)
C(55)	69(7)	112(9)	104(8)	-19(7)	-15(6)	21(6)
C(56)	62(6)	103(9)	102(8)	18(7)	-5(6)	-5(6)
O(57)	75(4)	82(5)	103(5)	-2(4)	11(4)	3(4)
C(58)	65(7)	101(9)	112(9)	10(7)	5(6)	2(6)
C(59)	77(8)	129(11)	128(10)	-2(9)	21(7)	42(8)
O(60)	72(5)	104(6)	129(6)	-23(5)	12(4)	12(4)
C(61)	88(8)	103(9)	109(9)	-34(7)	30(7)	18(7)
C(62)	83(7)	89(7)	82(7)	-19(6)	16(6)	-11(6)
O(63)	66(4)	84(4)	65(4)	-11(3)	15(3)	-5(3)
C(64)	65(6)	76(6)	54(5)	8(5)	7(4)	0(5)
C(65)	71(6)	66(6)	65(6)	6(5)	2(5)	6(5)
N(66)	59(4)	61(4)	65(4)	6(4)	18(3)	0(4)
C(67)	51(5)	65(6)	74(6)	3(5)	12(4)	1(4)
C(68)	108(9)	87(8)	93(8)	15(6)	35(7)	28(7)
C(69)	161(12)	66(7)	118(10)	25(7)	43(9)	33(7)
C(70)	115(9)	71(8)	100(9)	27(6)	-1(7)	4(7)
C(71)	120(9)	85(8)	83(7)	30(6)	33(7)	-6(7)
C(72)	96(8)	81(7)	84(7)	-4(6)	22(6)	-6(6)
C(73)	45(4)	56(5)	70(6)	0(4)	14(4)	-4(4)
C(74)	78(7)	66(6)	126(9)	-10(6)	50(6)	-1(5)
C(75)	119(10)	79(8)	128(10)	-32(8)	26(8)	-15(7)
C(76)	182(17)	119(12)	146(13)	-55(11)	68(12)	-40(12)
C(77)	112(12)	105(12)	289(24)	-70(14)	108(15)	-12(10)
C(78)	113(13)	78(11)	510(45)	-55(17)	108(20)	5(9)
C(79)	98(10)	66(8)	273(21)	2(10)	1(11)	-10(7)
C(80)	78(7)	72(7)	101(8)	3(6)	55(6)	-3(6)
N(81)	71(5)	83(5)	79(5)	-31(4)	31(4)	-19(4)
C(82)	65(6)	90(7)	77(6)	-17(5)	19(5)	8(5)
C(83)	121(10)	122(11)	88(8)	9(8)	0(7)	31(9)
O(84)	125(7)	124(7)	134(8)	10(6)	23(6)	-3(6)
C(85)	184(17)	180(17)	128(13)	67(12)	-2(12)	69(14)
C(86)	185(19)	361(36)	108(13)	52(18)	-35(13)	93(21)
O(87)	158(10)	196(12)	161(10)	-36(9)	-12(8)	19(9)
C(88)	186(15)	200(16)	253(17)	-19(14)	50(14)	19(14)
C(89)	328(11)	325(12)	349(11)	19(9)	45(8)	-7(9)
O(90)	329(12)	322(13)	355(13)	25(11)	42(11)	-6(11)
C(91)	327(13)	321(13)	353(13)	24(11)	41(11)	-8(11)
C(92)	328(13)	322(13)	355(13)	23(11)	41(11)	-10(11)
O(93)	329(13)	320(13)	355(13)	24(11)	40(11)	-5(11)
C(94)	328(13)	321(13)	354(13)	24(11)	42(11)	-12(11)
C(95)	325(13)	321(13)	354(13)	23(11)	42(11)	-8(11)
O(90')	331(12)	322(13)	357(13)	26(11)	41(11)	-7(11)
C(91')	324(13)	319(13)	353(13)	24(11)	44(11)	-11(11)
C(92')	326(13)	321(13)	355(13)	24(11)	41(11)	-10(11)
O(93')	331(12)	320(13)	354(13)	23(11)	42(11)	-10(11)
C(94')	330(13)	323(13)	355(13)	24(11)	40(11)	-9(11)
C(95')	324(13)	320(13)	354(13)	23(11)	43(11)	-8(11)
N(96)	81(6)	258(15)	124(8)	-117(10)	50(6)	-73(8)
C(97)	67(6)	87(8)	100(8)	-32(6)	19(5)	-13(6)
C(98)	186(17)	127(13)	187(17)	-71(12)	-58(13)	49(12)
C(99)	195(19)	116(13)	248(23)	-67(14)	-58(17)	24(13)
C(100)	133(13)	120(13)	150(13)	4(11)	47(11)	26(10)
C(101)	129(11)	76(8)	129(11)	5(8)	47(8)	-24(8)
C(102)	125(10)	85(8)	86(8)	-7(6)	30(7)	-42(8)
C(103)	90(8)	90(8)	92(8)	-37(6)	34(6)	-36(7)

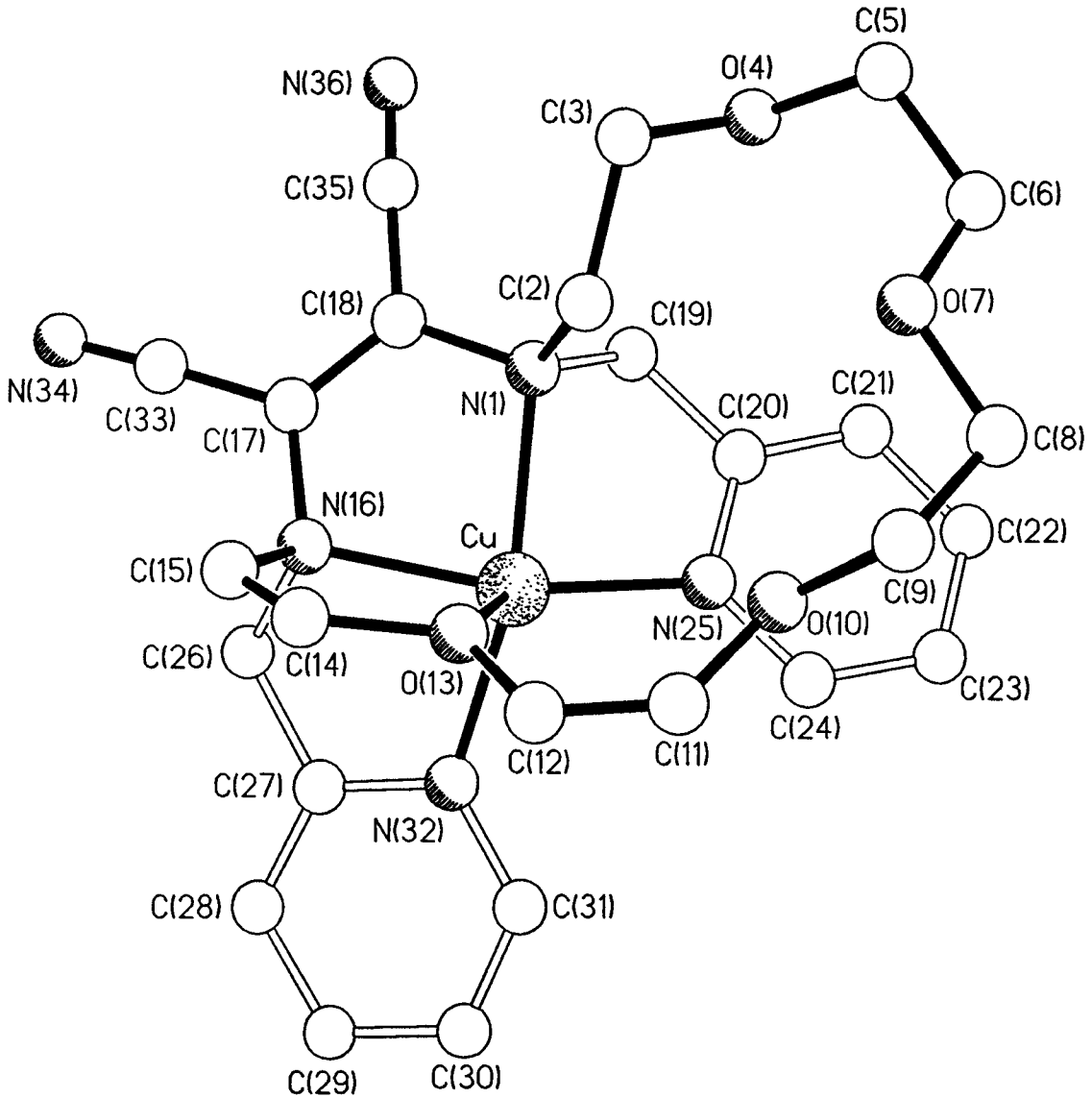
C(104)	149(13)	273(21)	202(16)	-165(16)	138(13)	-145(15)
C(105)	113(14)	179(20)	508(45)	56(25)	-76(20)	-54(14)
C(106)	267(17)	262(17)	272(17)	6(10)	19(10)	-1(10)
C(107)	351(40)	173(23)	195(22)	-22(19)	-31(26)	-49(27)
C(108)	393(44)	264(32)	110(16)	113(20)	132(22)	151(28)
C(109)	111(11)	286(27)	99(11)	50(16)	32(9)	30(17)
C(110)	74(9)	187(16)	128(11)	-45(11)	7(8)	5(10)
N(111)	63(4)	55(4)	79(5)	-8(4)	26(4)	5(4)
C(112)	62(6)	74(6)	80(6)	-26(5)	22(5)	2(5)
C(113)	81(7)	71(6)	89(7)	-14(5)	23(6)	3(5)
O(114)	79(4)	83(5)	93(5)	-6(4)	36(4)	7(4)
C(115)	114(9)	101(9)	105(8)	17(7)	67(8)	0(7)
C(116)	112(9)	115(10)	104(9)	-10(8)	58(8)	-15(9)
O(117)	140(7)	96(6)	92(5)	-14(4)	43(5)	10(6)
C(118)	197(17)	124(12)	109(11)	-18(9)	67(11)	46(13)
C(119)	214(18)	118(12)	92(10)	-29(9)	10(11)	49(13)
O(120)	122(6)	89(6)	102(6)	-22(5)	14(5)	22(5)
C(121)	119(11)	61(8)	172(14)	-41(8)	-4(10)	3(7)
C(122)	118(10)	54(7)	132(11)	-23(7)	-14(8)	3(7)
O(123)	103(6)	67(5)	132(7)	-21(4)	9(5)	17(4)
C(124)	115(9)	49(6)	158(12)	-19(7)	41(9)	-2(6)
C(125)	79(7)	85(8)	117(9)	-33(7)	19(6)	-2(6)
N(126)	99(6)	58(5)	79(5)	-21(4)	25(5)	2(4)
C(127)	80(7)	64(6)	104(8)	8(6)	43(6)	12(5)
C(128)	88(9)	93(9)	222(18)	-19(10)	-58(10)	30(8)
C(129)	109(12)	82(10)	338(30)	-2(14)	-92(16)	-6(9)
C(130)	80(9)	136(14)	245(23)	86(15)	-42(11)	-20(10)
C(131)	87(9)	145(13)	128(11)	50(10)	13(8)	1(9)
C(132)	90(8)	119(10)	111(10)	19(9)	25(7)	17(8)
C(133)	54(6)	61(7)	154(11)	15(7)	10(7)	-6(5)
C(134)	124(9)	81(7)	72(7)	-14(6)	30(6)	34(7)
C(135)	86(8)	118(10)	86(8)	10(7)	24(6)	6(7)
C(136)	123(11)	136(12)	133(11)	39(10)	59(9)	12(10)
C(137)	91(8)	78(8)	129(10)	16(7)	22(7)	-8(6)
C(138)	101(8)	70(7)	84(7)	-5(6)	3(6)	0(6)
C(139)	110(8)	86(8)	62(6)	-19(6)	20(6)	0(6)
C(140)	86(7)	83(7)	62(6)	-29(5)	16(5)	8(6)
C(141)	129(20)	198(27)	288(40)	7(27)	12(22)	-57(19)
C(142)	176(23)	288(36)	82(14)	-27(18)	37(15)	-77(23)
O(143)	180(14)	151(12)	111(10)	26(10)	16(10)	-42(11)
C(144)	173(21)	111(16)	148(21)	78(16)	15(17)	19(15)
O(145)	294(24)	180(17)	150(14)	19(14)	25(14)	-22(17)
C(146)	164(19)	114(15)	175(21)	-36(15)	-67(17)	19(14)

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

	x	y	z	U(eq)	sof
H(22A)	9624(5)	6230(10)	3623(5)	148	1
H(22B)	9330(5)	5628(10)	3228(5)	148	1
H(23A)	9709(7)	4970(9)	3985(6)	157	1
H(23B)	10103(7)	4781(9)	3568(6)	157	1
H(25A)	10885(14)	4710(21)	4236(15)	404	1
H(25B)	10590(14)	4947(21)	4715(15)	404	1
H(26A)	11105(14)	5818(18)	4919(12)	290	1
H(26B)	11480(14)	5150(18)	4813(12)	290	1
H(28A)	12211(12)	6010(18)	4565(12)	281	1
H(28B)	11861(12)	6619(18)	4788(12)	281	1
H(29A)	12094(8)	7382(11)	4329(7)	179	1
H(29B)	12514(8)	6794(11)	4174(7)	179	1
H(31A)	12446(10)	7087(15)	3218(7)	281	1
H(31B)	12230(10)	7838(15)	3435(7)	281	1
H(32A)	11317(10)	7574(14)	2830(8)	255	1
H(32B)	11805(10)	7801(14)	2521(8)	255	1
H(34A)	11431(5)	6826(9)	1781(4)	126	1
H(34B)	10946(5)	6804(9)	2119(4)	126	1
H(35A)	11055(4)	5665(8)	1606(4)	108	1
H(35B)	11597(4)	5512(8)	2011(4)	108	1
H(37A)	10708(8)	6596(10)	2932(6)	184	1
H(37B)	10652(8)	6344(10)	3506(6)	184	1
H(38A)	10905(6)	7708(9)	3928(5)	298	1
H(39A)	10480(13)	8821(11)	4107(8)	292	1
H(40A)	9634(13)	9158(10)	3608(12)	418	1
H(41A)	9214(8)	8382(17)	2929(12)	429	1
H(42A)	9639(11)	7268(13)	2750(8)	300	1
H(44A)	10908(6)	5079(8)	3079(5)	139	1
H(44B)	11356(6)	5686(8)	2999(5)	139	1
H(45A)	12243(5)	5162(8)	3306(5)	264	1
H(46A)	12892(5)	4213(16)	3302(10)	284	1
H(47A)	12642(10)	3101(12)	2853(11)	351	1
H(48A)	11742(12)	2938(8)	2408(10)	309	1
H(49A)	11092(6)	3887(12)	2413(8)	245	1
H(52A)	11036(4)	4240(6)	1334(4)	104	1
H(52B)	11482(4)	3684(6)	1181(4)	104	1
H(53A)	11159(5)	4999(7)	626(4)	109	1
H(53B)	11700(5)	4929(7)	1047(4)	109	1
H(55A)	12288(4)	3748(7)	815(5)	118	1
H(55B)	12525(4)	4553(7)	737(5)	118	1
H(56A)	12564(4)	4240(7)	-178(5)	109	1
H(56B)	12955(4)	3715(7)	215(5)	109	1
H(58A)	12846(4)	2835(7)	-490(5)	113	1
H(58B)	12424(4)	3369(7)	-840(5)	113	1
H(59A)	12289(5)	2057(8)	-1079(5)	133	1
H(59B)	12096(5)	1928(8)	-526(5)	133	1
H(61A)	11186(5)	1648(7)	-878(5)	118	1
H(61B)	11346(5)	1679(7)	-1451(5)	118	1
H(62A)	10682(4)	2668(6)	-1683(4)	102	1
H(62B)	10381(4)	1944(6)	-1518(4)	102	1
H(64A)	9688(4)	2643(5)	-1231(3)	78	1
H(64B)	9960(4)	3368(5)	-1427(3)	78	1
H(65A)	10062(4)	3874(5)	-575(3)	82	1
H(65B)	9435(4)	3707(5)	-787(3)	82	1
H(67A)	11283(4)	3027(5)	327(4)	76	1

H(67B)	10665(4)	2780(5)	148(4)	76	1
H(68A)	11420(3)	1643(4)	414(2)	113	1
H(69A)	11562(5)	664(4)	1020(5)	135	1
H(70A)	11238(5)	755(5)	1823(4)	117	1
H(71A)	10771(5)	1825(6)	2021(3)	113	1
H(72A)	10629(4)	2805(4)	1415(4)	103	1
H(74A)	9011(4)	2649(5)	-498(5)	104	1
H(74B)	9222(4)	2351(5)	77(5)	104	1
H(75A)	8829(3)	1666(5)	-1069(3)	129	1
H(76A)	9058(7)	538(8)	-1431(4)	173	1
H(77A)	9869(7)	-80(5)	-1072(7)	192	1
H(78A)	10451(5)	430(7)	-350(8)	273	1
H(79A)	10222(5)	1559(7)	12(5)	179	1
H(82A)	8139(3)	3676(6)	-832(3)	92	1
H(82B)	8041(3)	2825(6)	-967(3)	92	1
H(83A)	7637(5)	3365(6)	-1689(4)	135	1
H(83B)	7136(5)	3190(6)	-1397(4)	135	1
H(85A)	6605(7)	4114(8)	-1872(6)	200	1
H(85B)	7096(7)	4281(8)	-2180(6)	200	1
H(86A)	6610(8)	5329(9)	-1605(6)	270	1
H(86B)	7106(8)	5498(9)	-1906(6)	270	1
H(88A)	5773(7)	6032(10)	-2521(9)	254	1
H(88B)	5987(7)	5918(10)	-1912(9)	254	1
H(89A)	5126(8)	5328(16)	-2280(10)	402	0.50
H(89B)	5493(8)	4740(16)	-2522(10)	402	0.50
H(89C)	5291(8)	5031(16)	-2589(10)	402	0.50
H(89D)	5233(8)	5317(16)	-2032(10)	402	0.50
H(91A)	4944(27)	5125(29)	-1504(12)	403	0.50
H(91B)	5510(27)	5464(29)	-1222(12)	403	0.50
H(92A)	4969(17)	4351(28)	-882(12)	404	0.50
H(92B)	5504(17)	3996(28)	-1044(12)	404	0.50
H(94A)	6413(17)	4975(29)	-228(21)	403	0.50
H(94B)	6296(17)	4657(29)	-809(21)	403	0.50
H(95A)	6575(22)	3612(25)	-514(14)	401	0.50
H(95B)	6064(22)	3565(25)	-216(14)	401	0.50
H(91C)	5218(17)	3671(25)	-1844(12)	400	0.50
H(91D)	4873(17)	4418(25)	-1863(12)	400	0.50
H(92C)	5260(13)	4672(32)	-1001(12)	403	0.50
H(92D)	4954(13)	3894(32)	-1036(12)	403	0.50
H(94C)	5778(19)	3891(40)	-148(16)	405	0.50
H(94D)	5875(19)	4660(40)	-421(16)	405	0.50
H(95C)	6733(14)	4428(46)	-440(8)	401	0.50
H(95D)	6635(14)	3562(46)	-505(8)	401	0.50
H(97A)	7027(4)	2456(6)	-729(4)	101	1
H(97B)	7035(4)	2602(6)	-123(4)	101	1
H(98A)	7095(4)	1162(5)	-779(4)	212	1
H(99A)	7592(7)	57(5)	-596(6)	236	1
H(10A)	8393(6)	47(6)	34(6)	158	1
H(10B)	8698(4)	1142(8)	480(4)	130	1
H(10C)	8201(5)	2246(5)	297(5)	116	1
H(10D)	6847(7)	3578(11)	1031(7)	235	1
H(10E)	6285(7)	3992(11)	833(7)	235	1
H(10F)	5466(4)	3249(8)	486(7)	337	1
H(10G)	5075(5)	2064(15)	348(11)	324	1
H(10H)	5641(13)	1010(9)	425(9)	298	1
H(10I)	6597(12)	1142(10)	639(8)	295	1
H(10J)	6987(4)	2327(15)	777(7)	196	1
H(11A)	6802(4)	4540(5)	1799(4)	85	1
H(11B)	6257(4)	5016(5)	1681(4)	85	1
H(11C)	6277(4)	4239(6)	2436(4)	95	1
H(11D)	6793(4)	4689(6)	2723(4)	95	1
H(11E)	6306(5)	5002(7)	3395(5)	122	1

H(11F)	5720(5)	4694(7)	3136(5)	122	1
H(11G)	5397(6)	5937(8)	3046(5)	127	1
H(11H)	5567(6)	5698(8)	3642(5)	127	1
H(11I)	5615(8)	7067(9)	3765(6)	166	1
H(11J)	5503(8)	7157(9)	3143(6)	166	1
H(11K)	6018(8)	8186(10)	3590(6)	172	1
H(11L)	6512(8)	7626(10)	3766(6)	172	1
H(12A)	6864(6)	8618(7)	3355(6)	144	1
H(12B)	6429(6)	8911(7)	2875(6)	144	1
H(12C)	6903(6)	8256(6)	2296(6)	126	1
H(12D)	7273(6)	8883(6)	2610(6)	126	1
H(12E)	8139(5)	8172(6)	2565(6)	126	1
H(12F)	7728(5)	7667(6)	2176(6)	126	1
H(12G)	8539(4)	7019(6)	2578(5)	112	1
H(12H)	8345(4)	7126(6)	3128(5)	112	1
H(12I)	6932(4)	6708(5)	2086(4)	95	1
H(12J)	6390(4)	6309(5)	2193(4)	95	1
H(12K)	6072(4)	7563(4)	1717(4)	173	1
H(12L)	5607(5)	8037(5)	920(7)	229	1
H(13A)	5605(5)	7372(9)	138(5)	193	1
H(13B)	6067(6)	6233(9)	153(4)	145	1
H(13C)	6532(5)	5759(5)	950(5)	127	1
H(13D)	7201(5)	6032(6)	2869(4)	109	1
H(13E)	7539(5)	6568(6)	3288(4)	109	1
H(13F)	7196(3)	5541(4)	3870(3)	115	1
H(13G)	7478(5)	4495(7)	4384(4)	152	1
H(13H)	8233(5)	3796(5)	4220(4)	119	1
H(13I)	8707(3)	4144(5)	3540(4)	103	1
H(13J)	8425(4)	5191(6)	3025(3)	103	1
H(14A)	3864(10)	7949(16)	603(14)	311	0.75
H(14B)	4513(10)	7890(16)	728(14)	311	0.75
H(14C)	4224(10)	8676(16)	720(14)	311	0.75
H(14D)	3836(11)	8337(19)	1442(9)	216	0.75
H(14E)	4133(11)	7557(19)	1453(9)	216	0.75
H(14F)	5252(10)	9112(12)	2294(9)	243	0.75
H(14G)	5559(10)	8414(12)	2578(9)	243	0.75
H(14H)	5053(10)	8768(12)	2796(9)	243	0.75


C(5)
O(4)
N(36)
C(3)
C(35)
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C(18)
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O(7)
C(19)
N(34)
C(33)
N(1)
C(20)
C(21)
C(17)
C(8)
N(16)
Cu
C(22)
C(15)
C(9)
N(25)
O(10)
C(26)
C(14)
O(13)
C(23)
C(24)
C(12)
C(11)
C(27)
N(32)
C(28)
C(31)
C(29)
C(30)

Table 1. Crystal data and structure refinement for 1.

Identification code	AGMB22
Empirical formula	$C_{26}H_{32}N_6O_4Cu \cdot 2BF_4$
Formula weight	729.74
Temperature	293(2) K
Diffractometer Used	Siemens P4/PC
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	a = 8.082(3) Å alpha = 90° b = 9.797(3) Å beta = 96.84(4)° c = 20.206(11) Å gamma = 90°
Volume, Z	1588.6(12) $Å^3$, 2
Density (calculated)	1.526 Mg/m^3
Absorption coefficient	1.781 mm^{-1}
F(000)	746
Crystal colour/morphology	Deep blue plates
Crystal size	0.40 x 0.37 x 0.20 mm
θ range for data collection	2.20 to 62.54°
Limiting indices	$-8 \leq h \leq 9$, $-11 \leq k \leq 9$, $-23 \leq l \leq 23$
Scan type	ω-scans
Reflections collected	2893
Independent reflections	2801 (R_{int} = 0.0786)
Observed reflections [F>4σ(F)]	2717
Absorption correction	Face-indexed numerical
Max. and min. transmission	0.7116 and 0.5191
Structure solution method	Direct
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2788 / 1 / 425
Goodness-of-fit on F^2	1.060
Final R indices [F>4σ(F)]	R1 = 0.0549, wR2 = 0.1497
R indices (all data)	R1 = 0.0565, wR2 = 0.1888
Absolute structure parameter	0.04(6)
Extinction coefficient	0.0033(6)
Largest diff. peak and hole	0.575 and -0.571 $eÅ^{-3}$
Mean and maximum shift/error	0.000 and 0.000

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

	x	y	z	U(eq)	sof
Cu	2829(1)	4596(1)	2157(1)	42(1)	1
N(1)	3762(6)	2630(6)	2178(2)	46(1)	1
C(2)	5411(8)	2596(8)	2595(4)	52(2)	1
C(3)	6175(11)	1203(9)	2762(4)	71(2)	1
O(4)	5315(9)	451(7)	3213(3)	87(2)	1
C(5)	6167(17)	352(13)	3872(5)	104(4)	1
C(6)	5836(23)	1430(14)	4316(5)	124(5)	1
O(7)	6203(16)	2697(11)	4127(4)	138(4)	1
C(8)	5840(18)	3748(17)	4552(5)	112(4)	1
C(9)	6440(14)	5036(15)	4278(6)	104(4)	1
O(10)	5428(8)	5374(8)	3694(3)	90(2)	1
C(11)	5935(25)	6543(15)	3389(7)	153(7)	1
C(12)	5883(31)	6784(17)	2792(7)	192(11)	1
O(13)	5230(7)	5905(6)	2288(3)	67(1)	1
C(14)	5708(19)	6102(21)	1666(5)	178(10)	1
C(15)	5003(16)	5434(14)	1168(6)	118(5)	1
N(16)	3464(6)	4631(8)	1207(2)	52(1)	1
C(17)	3696(9)	3225(8)	1028(3)	55(2)	1
C(18)	3818(8)	2262(8)	1495(3)	54(2)	1
C(19)	2430(8)	1848(7)	2469(4)	54(2)	1
C(20)	1907(8)	2644(7)	3042(3)	47(1)	1
C(21)	1324(10)	2018(9)	3573(4)	66(2)	1
C(22)	888(11)	2809(10)	4091(4)	74(2)	1
C(23)	1015(10)	4213(8)	4055(3)	62(2)	1
C(24)	1590(8)	4783(9)	3496(3)	53(2)	1
N(25)	2012(6)	4018(6)	2994(3)	44(1)	1
C(26)	1963(12)	5241(9)	788(3)	71(2)	1
C(27)	1281(10)	6377(8)	1180(3)	59(2)	1
C(28)	501(15)	7478(10)	871(4)	84(3)	1
C(29)	-191(13)	8443(9)	1243(4)	76(2)	1
C(30)	-3(10)	8309(8)	1919(4)	64(2)	1
C(31)	826(9)	7209(8)	2201(3)	60(2)	1
N(32)	1475(7)	6223(6)	1842(2)	49(1)	1
C(33)	3729(10)	2923(10)	337(4)	69(2)	1
N(34)	3670(12)	2727(12)	-225(3)	101(3)	1
C(35)	3955(11)	839(10)	1331(4)	72(2)	1
N(36)	3993(13)	-298(14)	1226(5)	110(3)	1
B(1)	-1272(10)	2521(12)	1111(4)	66(2)	1
F(11)	-40(8)	1893(9)	834(4)	110(2)	1
F(12)	-611(18)	3403(12)	1570(5)	196(5)	1
F(13)	-2268(13)	3199(18)	688(5)	232(7)	1
F(14)	-1959(18)	1657(17)	1480(8)	257(8)	1
B(2)	456(12)	8416(9)	4023(4)	61(2)	1
F(21)	389(7)	9470(7)	4441(2)	85(1)	1
F(22)	2019(7)	8283(9)	3817(3)	119(2)	1
F(23)	-597(8)	8635(10)	3442(3)	123(3)	1
F(24)	29(15)	7259(7)	4316(5)	156(4)	1