C(14)-N(3)-Ni	130.92(11)
C(21)-N(3)-Ni	120.34(10)
C(7)-N(4)-C(8)	113.45(13)
C(7)-N(4)-Ni	124.51(11)
C(8)-N(4)-Ni	120.27(10)
C(29)-N(5)-C(2)	107.71(13)
C(29)-N(5)-C(30)	129.1(2)
C(2)-N(5)-C(30)	123.15(14)
C(14)-N(6)-C(16)	107.75(13)
C(14)-N(6)-C(15)	129.1(2)
C(16)-N(6)-C(15)	123.14(14)
N(1)-C(1)-C(6)	128.44(14)
N(1)-C(1)-C(2)	109.04(14)
C(6)-C(1)-C(2)	122.5(2)
N(5)-C(2)-C(3)	133.0(2)
N(5)-C(2)-C(1)	105.85(14)
C(3)-C(2)-C(1)	121.2(2)
C(4)-C(3)-C(2)	116.7(2)
C(3)-C(4)-C(5)	122.0(2)
C(6)-C(5)-C(4)	121.6(2)
C(5)-C(6)-C(1)	116.0(2)
C(5)-C(6)-C(7)	121.6(2)
C(1)-C(6)-C(7)	121.78(14)
O(2)-C(7)-N(4)	124.6(2)
O(2)-C(7)-C(6)	119.3(2)
N(4)-C(7)-C(6)	116.06(14)
C(9)-C(8)-C(13)	117.79(14)
C(9)-C(8)-N(4)	119.25(14)
C(13)-C(8)-N(4)	122.94(14)
O(3)-C(9)-C(10)	122.5(2)
O(3)-C(9)-C(8)	116.20(14)
C(10)-C(9)-C(8)	121.3(2)
C(11)-C(10)-C(9)	119.5(2)
C(12)-C(11)-C(10)	120.7(2)
C(11)-C(12)-C(13)	120.3(2)
C(12)-C(13)-C(8)	120.1(2)
C(12)-C(13)-C(14)	122.0(2)
C(8)-C(13)-C(14)	117.90(14)
N(3)-C(14)-N(6)	110.20(14)
N(3)-C(14)-C(13)	121.73(14)
N(6)-C(14)-C(13)	128.08(14)
N(6)-C(16)-C(21)	106.01(14)
N(6)-C(16)-C(17)	132.9(2)
C(21)-C(16)-C(17)	121.1(2)
C(18)-C(17)-C(16)	116.7(2)
C(17)-C(18)-C(19)	122.1(2)
C(20)-C(19)-C(18)	121.7(2)

C(19)-C(20)-C(21)	115.8(2)
C(19)-C(20)-C(22)	121.9(2)
C(21)-C(20)-C(22)	121.73(14)
N(3)-C(21)-C(16)	108.94(14)
N(3)-C(21)-C(20)	128.34(14)
C(16)-C(21)-C(20)	122.7(2)
O(1)-C(22)-N(2)	124.4(2)
O(1)-C(22)-C(20)	118.8(2)
N(2)-C(22)-C(20)	116.65(14)
C(28)-C(23)-C(24)	117.4(2)
C(28)-C(23)-N(2)	123.2(2)
C(24)-C(23)-N(2)	119.36(14)
O(4)-C(24)-C(25)	122.6(2)
O(4)-C(24)-C(23)	116.29(14)
C(25)-C(24)-C(23)	121.1(2)
C(26)-C(25)-C(24)	119.7(2)
C(27)-C(26)-C(25)	120.7(2)
C(26)-C(27)-C(28)	120.1(2)
C(27)-C(28)-C(23)	120.5(2)
C(27)-C(28)-C(29)	121.7(2)
C(23)-C(28)-C(29)	117.79(14)
N(1)-C(29)-N(5)	110.23(14)
N(1)-C(29)-C(28)	121.81(14)
N(5)-C(29)-C(28)	127.96(14)

Table S14. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for the Ni(II) Complex (26).[6]

	U11	U22	U33	U23	U13	U12
Ni	22(1)	13(1)	11(1)	-1(1)	1(1)	-3(1)
O(1)	34(1)	21(1)	24(1)	-5(1)	-1(1)	4(1)
O(2)	48(1)	20(1)	24(1)	-5(1)	6(1)	-14(1)
O(3)	40(1)	24(1)	18(1)	-2(1)	-1(1)	7(1)
O(4)	50(1)	26(1)	18(1)	-3(1)	4(1)	-20(1)
N(1)	23(1)	15(1)	14(1)	-1(1)	1(1)	-2(1)
N(2)	23(1)	14(1)	13(1)	-2(1)	-1(1)	-3(1)
N(3)	22(1)	15(1)	15(1)	-1(1)	1(1)	-5(1)
N(4)	25(1)	14(1)	13(1)	-2(1)	3(1)	-3(1)
N(5)	27(1)	22(1)	13(1)	-2(1)	1(1)	-3(1)
N(6)	27(1)	21(1)	13(1)	-3(1)	-1(1)	-9(1)
C(1)	20(1)	19(1)	15(1)	1(1)	1(1)	-2(1)
C(2)	22(1)	22(1)	16(1)	0(1)	0(1)	-2(1)
C(3)	30(1)	29(1)	15(1)	2(1)	5(1)	-2(1)
C(4)	29(1)	26(1)	24(1)	7(1)	6(1)	-5(1)
C(5)	27(1)	21(1)	24(1)	2(1)	1(1)	-6(1)
C(6)	22(1)	18(1)	17(1)	1(1)	1(1)	-3(1)
C(7)	23(1)	16(1)	17(1)	1(1)	-2(1)	-2(1)
C(8)	24(1)	15(1)	17(1)	-5(1)	2(1)	-6(1)
C(9)	30(1)	18(1)	17(1)	-3(1)	1(1)	-5(1)
C(10)	26(1)	17(1)	24(1)	-6(1)	2(1)	-2(1)
C(11)	29(1)	22(1)	22(1)	-9(1)	8(1)	-8(1)
C(12)	29(1)	22(1)	16(1)	-5(1)	5(1)	-11(1)
C(13)	23(1)	18(1)	17(1)	-5(1)	2(1)	-8(1)
C(14)	23(1)	19(1)	13(1)	-2(1)	2(1)	-10(1)
C(15)	36(1)	32(1)	16(1)	-7(1)	1(1)	-12(1)
C(16)	24(1)	21(1)	17(1)	0(1)	-1(1)	-9(1)
C(17)	31(1)	31(1)	17(1)	1(1)	-6(1)	-12(1)
C(18)	26(1)	30(1)	24(1)	5(1)	-7(1)	-7(1)
C(19)	22(1)	22(1)	24(1)	2(1)	-2(1)	-3(1)
C(20)	21(1)	20(1)	17(1)	1(1)	0(1)	-6(1)
C(21)	21(1)	19(1)	15(1)	2(1)	-1(1)	-7(1)
C(22)	22(1)	17(1)	16(1)	1(1)	3(1)	-3(1)
C(23)	21(1)	15(1)	17(1)	-5(1)	1(1)	-1(1)
C(24)	29(1)	19(1)	18(1)	-3(1)	2(1)	-4(1)
C(25)	34(1)	19(1)	26(1)	-6(1)	1(1)	-9(1)
C(26)	31(1)	22(1)	24(1)	-9(1)	-2(1)	-5(1)
C(27)	27(1)	23(1)	16(1)	-5(1)	-2(1)	-2(1)
C(28)	22(1)	18(1)	17(1)	-4(1)	1(1)	-1(1)
C(29)	20(1)	19(1)	13(1)	-2(1)	0(1)	-1(1)
C(30)	34(1)	32(1)	16(1)	-8(1)	4(1)	-6(1)

C(31)	66(2)	43(1)	24(1)	-4(1)	-9(1)	28(1)
C(32)	61(1)	30(1)	26(1)	-5(1)	9(1)	-26(1)

Table S15. Calculated Hydrogen Coordinates ($\times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for the Ni(II) Complex (26).

	x	y	z	U(eq)
H(3)	3733(2)	6238(2)	-1630(1)	32
H(4)	4116(2)	7934(2)	-1066(1)	33
H(5)	3399(2)	8411(2)	509(1)	30
H(10)	-3333(2)	9523(2)	3364(1)	28
H(11)	-2854(2)	8892(2)	5019(1)	28
H(12)	-740(2)	7140(2)	5529(1)	26
H(15A)	3210(6)	5605(8)	6654(4)	41
H(15B)	1178(11)	5748(10)	6605(5)	41
H(15C)	1901(17)	6752(2)	6078(1)	41
H(17)	4942(2)	3613(2)	6590(1)	31
H(18)	6741(2)	1883(2)	6018(1)	33
H(19)	6408(2)	1416(2)	4451(1)	29
H(25)	569(2)	416(2)	1675(1)	31
H(26)	441(2)	1065(2)	21(1)	31
H(27)	1025(2)	2804(2)	-502(1)	28
H(30A)	3659(13)	4275(9)	-1690(4)	41
H(30B)	1736(4)	4167(10)	-1599(5)	41
H(30C)	3345(16)	3139(2)	-1102(1)	41
H(31A)	-3318(12)	9421(12)	896(2)	81
H(31B)	-3196(10)	10119(4)	1811(12)	81
H(31C)	-4177(4)	9136(8)	1902(11)	81
H(32A)	402(17)	568(10)	4147(2)	54
H(32B)	1026(11)	-135(4)	3214(9)	54
H(32C)	-743(6)	934(7)	3163(9)	54

3.4. Ni(II) Complex (62).

The data collection crystal was an orange plate with an approximately triangular circumference. Examination of the diffraction pattern on a Nonius Kappa CCD diffractometer indicated a triclinic crystal system. All work was done at 150 K using an Oxford Cryosystems Cryostream Cooler. The data collection strategy was set up to measure a hemisphere of reciprocal space with a redundancy factor of 2.2, which means that 90% of the reflections were measured at least 2.2 times. A combination of phi and omega scans with a frame width of 1.0° was used. Data integration was done with Denzo,[1] and scaling and merging of the data was done with Scalepack.[1] Merging the data and averaging the symmetry equivalent reflections resulted in an R(int) value of 0.038. The teXsan package indicated the space group to be $P\bar{1}$, based on the intensity statistics.[2]

The structure was solved by the Patterson method in SHELXS-86,[3] and expanded with DIRDIF92.[10] The remaining non-hydrogen atoms were located by standard Fourier methods. The asymmetric unit consists of two molecules of the Ni complex, three molecules of CH_2Cl_2, and one molecule of MeOH. Full-matrix least-squares refinements based on F^2 were performed in SHELXL-97.[11] The hydrocarbon chain of one of the Ni complexes is disordered, with two of the carbon atoms each disordered over two sites. The occupancy factors for C(38A) and C(39A) refined to 0.70(1), while those for C(38C) and C(39C) were restricted to 0.30(1). All disordered carbon atoms were kept isotropic. A carbon atom for one of the CH_2Cl_2 molecules was also kept isotropic, as was the MeOH molecule. Besides these two slightly ill-behaved solvent molecules, there is also a region of disordered solvent which was very difficult to model. The SQUEEZE option of PLATON was used to deal with this region of electron density.[8,12] This program modifies the observed structure factors by subtracting away the contributions to them of the electron density in the disordered regions. This region occupies a total of 149 $Å^3$ per unit cell, and the electron density removed by this SQUEEZE procedure amounts to 29 electrons/unit cell.

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[10] DIRDIF92: Beurskens, P. T.; Admiraal, G.; Beurskens, G.; Bosman, W. P.; Garcia-Granda, S.; Smits, J. M. M.; Smykalla, C. The DIRDIF program system, 1992, *Technical Report of the Crystallography Laboratory*, University of Nijmegen, The Netherlands.

[11] SHELXL-97: Sheldrick, G. M. Universität Göttingen, Germany, 1997.

[12] PLATON: *A Multipurpose Crystallographic Tool*, 2001; Spek, A. L.; Utrecht University, Utrecht, The Netherlands.

The hydrogen atoms were included in the model at calculated positions using a riding model with U(H) = 1.2 × Ueq (bonded C atom). No hydrogen atoms were added to the MeOH solvent molecule. The final refinement cycle was based on 19460 intensities and 1110 variables and resulted in agreement factors of $R_1(F) = 0.086$ and $wR_2(F^2) = 0.204$. For the subset of data with $I > 2\sigma(I)$, the $R_1(F)$ value is 0.063 for 14511 reflections. The final difference electron density map contains maximum and minimum peak heights of 2.52 and -1.26 e/Å^3. The largest peaks in the map are near the ill-behaved solvent molecules. Neutral atom scattering factors were used and include terms for anomalous dispersion.[5]

Table S16. Crystal Data Collection and Refinement Parameters for the Ni(II) complex (62).

Empirical formula	$2(C_{46}H_{34}N_6NiO_4)+3CH_2Cl_2+CH_3OH$
Formula weight	1873.82
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 14.0172(1) Å
	b = 15.0853(1) Å
	c = 21.7777(2) Å
	α = 99.550(1)°
	β = 108.700(1)°
	γ = 93.394(1)°
Volume	4270.17(6) $Å^3$
Z	2
Density (calculated)	1.457 Mg/m^3
Absorption coefficient	0.697 mm^{-1}
F(000)	1936
Crystal size	0.12 × 0.38 × 0.38 mm
Theta range for data collection	2.06 to 27.45°
Index ranges	$0 \le h \le 18$, $-19 \le k \le 19$, $-28 \le l \le 26$
Reflections collected	82309
Independent reflections	19460 [R(int) = 0.038]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	19460 / 0 / 1110
Goodness-of-fit on F^2	1.099
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0634, wR_2 = 0.1919
R indices (all data)	R_1 = 0.0862, wR_2 = 0.2042
Largest diff. peak and hole	2.515 and -1.261 e/A^3

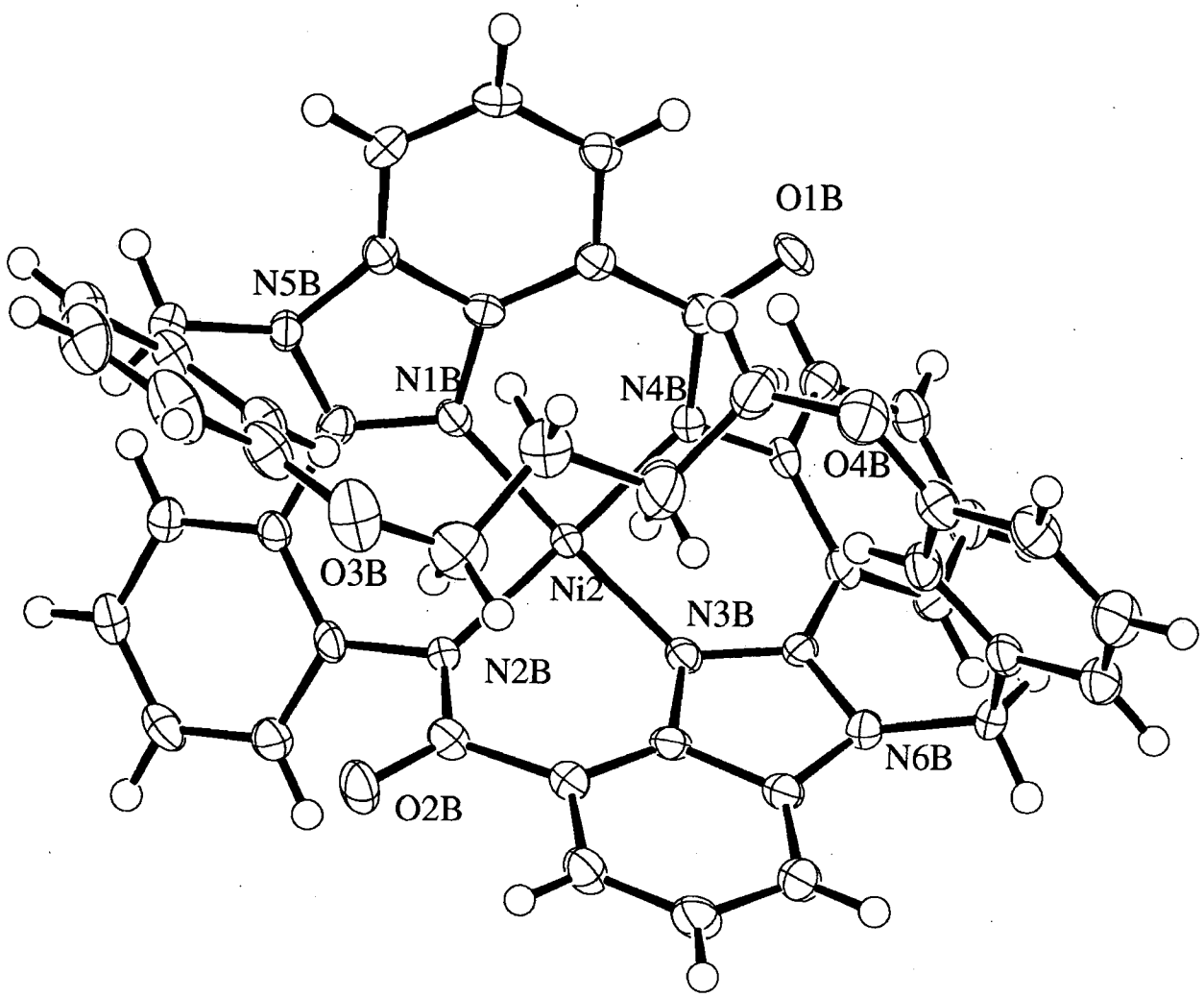


Figure S18. ORTEP drawing (50% probability thermal ellipsoids) of the molecular structure of the Ni(II) complex **62**.

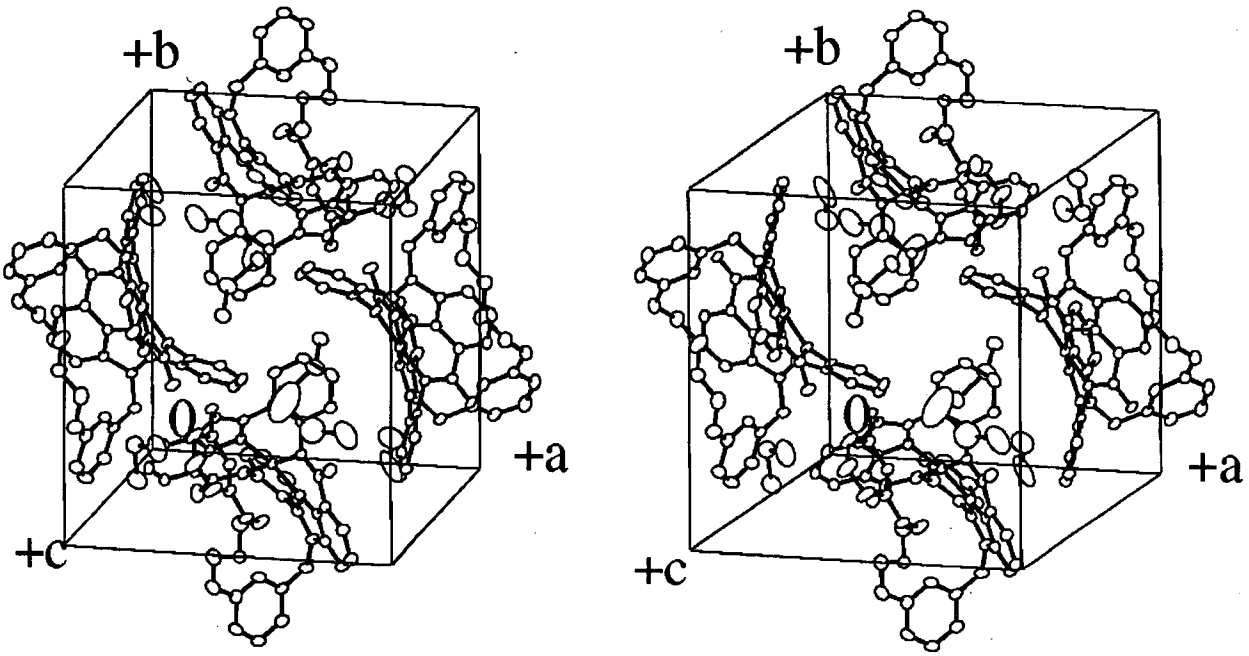


Figure S19. Packing diagram of the Ni(II) complex **62**.

Table S17. Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for the Ni(II) Complex (62).

	x	y	z	U(eq)
Ni(1)	4184(1)	343(1)	1893(1)	19(1)
O(1A)	1518(2)	-991(2)	531(2)	47(1)
O(2A)	6429(2)	760(2)	3704(1)	30(1)
O(3A)	4041(2)	-527(2)	4360(1)	32(1)
O(4A)	2361(2)	-3238(2)	1915(1)	38(1)
N(1A)	3303(2)	1032(2)	2188(1)	20(1)
N(2A)	5274(2)	869(2)	2698(1)	21(1)
N(3A)	4957(2)	-551(2)	1679(1)	22(1)
N(4A)	3091(2)	-179(2)	1101(1)	26(1)
N(5A)	2733(2)	1795(2)	2935(1)	22(1)
N(6A)	5214(2)	-1909(2)	1232(2)	26(1)
C(1A)	2324(2)	650(2)	2073(2)	23(1)
C(2A)	1965(2)	1107(2)	2546(2)	23(1)
C(3A)	1022(3)	824(2)	2578(2)	31(1)
C(4A)	465(3)	84(3)	2109(2)	34(1)
C(5A)	812(3)	-353(2)	1611(2)	34(1)
C(6A)	1757(2)	-74(2)	1583(2)	28(1)
C(7A)	2117(3)	-457(2)	1031(2)	31(1)
C(8A)	3357(3)	-397(2)	520(2)	26(1)
C(9A)	2911(3)	-4(2)	-28(2)	35(1)
C(10A)	3214(3)	-172(3)	-578(2)	37(1)
C(11A)	3938(3)	-755(3)	-608(2)	36(1)
C(12A)	4386(3)	-1139(2)	-74(2)	32(1)
C(13A)	4120(3)	-955(2)	501(2)	25(1)
C(14A)	4737(2)	-1165(2)	1124(2)	24(1)
C(15A)	4915(3)	-2818(2)	815(2)	33(1)
C(16A)	5778(3)	-1761(2)	1906(2)	26(1)
C(17A)	6403(3)	-2283(2)	2299(2)	34(1)
C(18A)	6853(3)	-1895(3)	2960(2)	36(1)
C(19A)	6688(3)	-1033(2)	3228(2)	31(1)
C(20A)	6050(2)	-511(2)	2838(2)	23(1)
C(21A)	5609(2)	-904(2)	2176(2)	23(1)
C(22A)	5927(2)	430(2)	3118(2)	22(1)
C(23A)	5361(2)	1824(2)	2937(2)	20(1)
C(24A)	6301(3)	2349(2)	3147(2)	26(1)
C(25A)	6393(3)	3271(2)	3369(2)	30(1)
C(26A)	5541(3)	3707(2)	3372(2)	29(1)
C(27A)	4599(3)	3198(2)	3155(2)	27(1)
C(28A)	4503(2)	2258(2)	2953(2)	21(1)
C(29A)	3524(2)	1708(2)	2701(2)	21(1)

C(30A)	2790(3)	2249(2)	3595(2)	25(1)
C(31A)	2933(2)	1580(2)	4061(2)	24(1)
C(32A)	2529(3)	1722(3)	4569(2)	39(1)
C(33A)	2669(4)	1118(3)	5003(2)	55(1)
C(34A)	3194(3)	384(3)	4927(2)	43(1)
C(35A)	3571(3)	238(2)	4414(2)	27(1)
C(36A)	3451(3)	839(2)	3983(2)	25(1)
C(37A)	4317(3)	-791(3)	3786(2)	40(1)
C(38A)	3540(6)	-1041(5)	3139(3)	48(2)*
C(39A)	3424(4)	-2041(4)	2833(3)	29(2)*
C(38C)	3195(8)	-1306(7)	3224(5)	14(3)*
C(39C)	3333(12)	-1728(12)	2578(9)	51(5)*
C(40A)	2460(3)	-2286(3)	2166(2)	45(1)
C(41A)	2965(3)	-3558(2)	1567(2)	29(1)
C(42A)	2912(3)	-4496(2)	1405(2)	32(1)
C(43A)	3511(3)	-4878(2)	1066(2)	34(1)
C(44A)	4179(3)	-4337(2)	884(2)	29(1)
C(45A)	4220(3)	-3404(2)	1041(2)	26(1)
C(46A)	3614(3)	-3016(2)	1375(2)	31(1)
Cl(1)	5377(1)	3591(1)	922(1)	39(1)
Cl(2)	4385(1)	2088(1)	1256(1)	43(1)
Cl(3)	8186(1)	8472(1)	1591(1)	75(1)
Cl(4)	7224(1)	7233(1)	335(1)	77(1)
Cl(5)	2619(2)	7765(2)	4580(2)	153(1)
Cl(6)	4574(3)	7057(3)	4912(2)	202(2)
O(5)	168(4)	7458(3)	675(2)	92(1)**
C(47)	5384(4)	2957(3)	1532(2)	51(1)
C(48)	8135(4)	7391(3)	1138(2)	50(1)
C(49)	3810(6)	7863(6)	5141(4)	112(3)**
C(50)	215(6)	6627(6)	506(4)	101(2)**
Ni(2)	1649(1)	5925(1)	7074(1)	17(1)
O(1B)	-815(2)	7048(2)	6038(1)	27(1)
O(2B)	2877(2)	4148(2)	8260(1)	31(1)
O(3B)	-365(2)	2572(2)	7384(2)	46(1)
O(4B)	-2072(2)	6044(2)	7588(1)	36(1)
N(1B)	1227(2)	5058(2)	6294(1)	18(1)
N(2B)	2511(2)	5097(2)	7509(1)	20(1)
N(3B)	1864(2)	6690(2)	7881(1)	20(1)
N(4B)	759(2)	6726(2)	6635(1)	19(1)
N(5B)	912(2)	3670(2)	5679(1)	19(1)
N(6B)	1532(2)	7731(2)	8613(1)	22(1)
C(1B)	227(2)	4930(2)	5892(2)	19(1)
C(2B)	-3(2)	4057(2)	5510(2)	19(1)
C(3B)	-982(2)	3729(2)	5090(2)	25(1)
C(4B)	-1707(2)	4319(2)	5062(2)	25(1)
C(5B)	-1471(2)	5211(2)	5419(2)	22(1)
C(6B)	-489(2)	5534(2)	5850(2)	19(1)

C(7B)	-194(2)	6498(2)	6189(2)	20(1)
C(8B)	1064(2)	7684(2)	6839(2)	19(1)
C(9B)	1002(2)	8226(2)	6368(2)	24(1)
C(10B)	1322(3)	9144(2)	6558(2)	27(1)
C(11B)	1701(3)	9551(2)	7220(2)	26(1)
C(12B)	1768(2)	9023(2)	7689(2)	24(1)
C(13B)	1453(2)	8096(2)	7508(2)	21(1)
C(14B)	1596(2)	7524(2)	7996(2)	19(1)
C(15B)	892(2)	8380(2)	8824(2)	24(1)
C(16B)	1772(2)	6983(2)	8909(2)	23(1)
C(17B)	1798(3)	6813(3)	9526(2)	30(1)
C(18B)	2037(3)	5958(3)	9638(2)	34(1)
C(19B)	2250(3)	5323(3)	9178(2)	29(1)
C(20B)	2216(2)	5492(2)	8561(2)	23(1)
C(21B)	1968(2)	6338(2)	8445(2)	21(1)
C(22B)	2552(2)	4853(2)	8092(2)	23(1)
C(23B)	3092(2)	4605(2)	7167(2)	20(1)
C(24B)	4116(2)	4540(2)	7493(2)	25(1)
C(25B)	4696(3)	4091(2)	7160(2)	29(1)
C(26B)	4283(3)	3717(2)	6494(2)	29(1)
C(27B)	3272(2)	3775(2)	6157(2)	23(1)
C(28B)	2669(2)	4204(2)	6494(2)	20(1)
C(29B)	1616(2)	4296(2)	6156(2)	20(1)
C(30B)	958(3)	2695(2)	5541(2)	24(1)
C(31B)	417(2)	2194(2)	5908(2)	26(1)
C(32B)	56(3)	1292(2)	5670(2)	38(1)
C(33B)	-420(3)	828(3)	6014(3)	48(1)
C(34B)	-548(3)	1266(3)	6585(2)	46(1)
C(35B)	-193(3)	2188(3)	6824(2)	35(1)
C(36B)	297(3)	2647(2)	6487(2)	29(1)
C(37B)	-140(3)	3531(3)	7617(2)	41(1)
C(38B)	-918(3)	4060(3)	7225(2)	38(1)
C(39B)	-761(4)	5039(3)	7537(3)	63(2)
C(40B)	-1545(3)	5605(3)	7181(2)	38(1)
C(41B)	-1571(3)	6771(2)	8081(2)	28(1)
C(42B)	-2103(3)	7113(3)	8494(2)	34(1)
C(43B)	-1665(3)	7842(3)	8998(2)	38(1)
C(44B)	-691(3)	8236(3)	9120(2)	31(1)
C(45B)	-157(2)	7913(2)	8706(2)	24(1)
C(46B)	-598(2)	7181(2)	8189(2)	26(1)

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.
*The occupancy factors for C(38A) and C(39A) are 0.70(1), while those for C(38C) and C(39C) are 0.30(1). All four atoms were kept isotropic.
**Refined isotropically.

Table S18. Bond Lengths [Å] and Angles [°] for the Ni(II) Complex (62).

Ni(1)-N(1A)	1.859(3)
Ni(1)-N(3A)	1.870(3)
Ni(1)-N(4A)	1.912(3)
Ni(1)-N(2A)	1.927(3)
O(1A)-C(7A)	1.258(4)
O(2A)-C(22A)	1.242(4)
O(3A)-C(35A)	1.369(4)
O(3A)-C(37A)	1.427(4)
O(4A)-C(41A)	1.365(4)
O(4A)-C(40A)	1.431(5)
N(1A)-C(29A)	1.322(4)
N(1A)-C(1A)	1.384(4)
N(2A)-C(22A)	1.360(4)
N(2A)-C(23A)	1.433(4)
N(3A)-C(14A)	1.331(4)
N(3A)-C(21A)	1.380(4)
N(4A)-C(7A)	1.355(4)
N(4A)-C(8A)	1.425(4)
N(5A)-C(29A)	1.364(4)
N(5A)-C(2A)	1.395(4)
N(5A)-C(30A)	1.463(4)
N(6A)-C(14A)	1.355(4)
N(6A)-C(16A)	1.398(5)
N(6A)-C(15A)	1.469(4)
C(1A)-C(6A)	1.389(5)
C(1A)-C(2A)	1.389(5)
C(2A)-C(3A)	1.391(5)
C(3A)-C(4A)	1.381(5)
C(3A)-H(3A)	0.95
C(4A)-C(5A)	1.409(6)
C(4A)-H(4A)	0.95
C(5A)-C(6A)	1.389(5)
C(5A)-H(5A)	0.95
C(6A)-C(7A)	1.493(5)
C(8A)-C(9A)	1.402(5)
C(8A)-C(13A)	1.406(5)
C(9A)-C(10A)	1.385(6)
C(9A)-H(9A)	0.95
C(10A)-C(11A)	1.391(6)
C(10A)-H(10A)	0.95
C(11A)-C(12A)	1.372(5)
C(11A)-H(11A)	0.95
C(12A)-C(13A)	1.408(5)
C(12A)-H(12A)	0.95
C(13A)-C(14A)	1.454(5)

C(15A)-C(45A)	1.523(5)
C(15A)-H(15A)	0.99
C(15A)-H(15B)	0.99
C(16A)-C(17A)	1.394(5)
C(16A)-C(21A)	1.395(5)
C(17A)-C(18A)	1.381(6)
C(17A)-H(17A)	0.95
C(18A)-C(19A)	1.398(5)
C(18A)-H(18A)	0.95
C(19A)-C(20A)	1.400(5)
C(19A)-H(19A)	0.95
C(20A)-C(21A)	1.383(5)
C(20A)-C(22A)	1.492(5)
C(23A)-C(24A)	1.394(5)
C(23A)-C(28A)	1.409(4)
C(24A)-C(25A)	1.378(5)
C(24A)-H(24A)	0.95
C(25A)-C(26A)	1.399(5)
C(25A)-H(25A)	0.95
C(26A)-C(27A)	1.383(5)
C(26A)-H(26A)	0.95
C(27A)-C(28A)	1.398(4)
C(27A)-H(27A)	0.95
C(28A)-C(29A)	1.451(4)
C(30A)-C(31A)	1.524(4)
C(30A)-H(30A)	0.99
C(30A)-H(30B)	0.99
C(31A)-C(36A)	1.385(5)
C(31A)-C(32A)	1.387(5)
C(32A)-C(33A)	1.395(6)
C(32A)-H(32A)	0.95
C(33A)-C(34A)	1.382(6)
C(33A)-H(33A)	0.95
C(34A)-C(35A)	1.374(5)
C(34A)-H(34A)	0.95
C(35A)-C(36A)	1.390(5)
C(36A)-H(36A)	0.95
C(37A)-C(38A)	1.452(8)
C(37A)-C(38C)	1.697(11)
C(37A)-H(37A)	0.99
C(37A)-H(37B)	0.99
C(37A)-H(37C)	0.99
C(37A)-H(37D)	0.99
C(38A)-C(39A)	1.520(9)
C(38A)-H(38A)	0.99
C(38A)-H(38B)	0.99
C(39A)-C(40A)	1.606(7)

C(39A)-H(39A)	0.99
C(39A)-H(39B)	0.99
C(38C)-C(39C)	1.52(2)
C(38C)-H(38C)	0.99
C(38C)-H(38D)	0.99
C(39C)-C(40A)	1.39(2)
C(39C)-H(39C)	0.99
C(39C)-H(39D)	0.99
C(40A)-H(40A)	0.99
C(40A)-H(40B)	0.99
C(40A)-H(40C)	0.99
C(40A)-H(40D)	0.99
C(41A)-C(42A)	1.392(5)
C(41A)-C(46A)	1.392(5)
C(42A)-C(43A)	1.377(5)
C(42A)-H(42A)	0.95
C(43A)-C(44A)	1.398(5)
C(43A)-H(43A)	0.95
C(44A)-C(45A)	1.385(5)
C(44A)-H(44A)	0.95
C(45A)-C(46A)	1.382(5)
C(46A)-H(46A)	0.95
Cl(1)-C(47)	1.760(4)
Cl(2)-C(47)	1.738(5)
Cl(3)-C(48)	1.745(5)
Cl(4)-C(48)	1.772(5)
Cl(5)-C(49)	1.705(9)
Cl(6)-C(49)	1.780(9)
O(5)-C(50)	1.258(9)
C(47)-H(47A)	0.99
C(47)-H(47B)	0.99
C(48)-H(48A)	0.99
C(48)-H(48B)	0.99
C(49)-H(49A)	0.99
C(49)-H(49B)	0.99
Ni(2)-N(3B)	1.861(3)
Ni(2)-N(1B)	1.863(3)
Ni(2)-N(4B)	1.931(3)
Ni(2)-N(2B)	1.938(3)
O(1B)-C(7B)	1.243(4)
O(2B)-C(22B)	1.245(4)
O(3B)-C(35B)	1.360(5)
O(3B)-C(37B)	1.431(5)
O(4B)-C(41B)	1.371(4)
O(4B)-C(40B)	1.432(5)
N(1B)-C(29B)	1.332(4)
N(1B)-C(1B)	1.376(4)

N(2B)-C(22B)	1.365(4)
N(2B)-C(23B)	1.430(4)
N(3B)-C(14B)	1.342(4)
N(3B)-C(21B)	1.385(4)
N(4B)-C(7B)	1.360(4)
N(4B)-C(8B)	1.434(4)
N(5B)-C(29B)	1.360(4)
N(5B)-C(2B)	1.406(4)
N(5B)-C(30B)	1.462(4)
N(6B)-C(14B)	1.361(4)
N(6B)-C(16B)	1.396(4)
N(6B)-C(15B)	1.480(4)
C(1B)-C(6B)	1.387(4)
C(1B)-C(2B)	1.395(4)
C(2B)-C(3B)	1.389(4)
C(3B)-C(4B)	1.384(5)
C(3B)-H(3B)	0.95
C(4B)-C(5B)	1.400(5)
C(4B)-H(4B)	0.95
C(5B)-C(6B)	1.398(4)
C(5B)-H(5B)	0.95
C(6B)-C(7B)	1.485(4)
C(8B)-C(13B)	1.399(5)
C(8B)-C(9B)	1.399(4)
C(9B)-C(10B)	1.381(5)
C(9B)-H(9B)	0.95
C(10B)-C(11B)	1.383(5)
C(10B)-H(10B)	0.95
C(11B)-C(12B)	1.380(5)
C(11B)-H(11B)	0.95
C(12B)-C(13B)	1.393(5)
C(12B)-H(12B)	0.95
C(13B)-C(14B)	1.450(4)
C(15B)-C(45B)	1.516(5)
C(15B)-H(15C)	0.99
C(15B)-H(15D)	0.99
C(16B)-C(21B)	1.388(4)
C(16B)-C(17B)	1.399(5)
C(17B)-C(18B)	1.391(5)
C(17B)-H(17B)	0.95
C(18B)-C(19B)	1.384(5)
C(18B)-H(18B)	0.95
C(19B)-C(20B)	1.397(5)
C(19B)-H(19B)	0.95
C(20B)-C(21B)	1.384(5)
C(20B)-C(22B)	1.493(5)
C(23B)-C(24B)	1.401(4)

C(23B)-C(28B)	1.404(4)
C(24B)-C(25B)	1.388(5)
C(24B)-H(24B)	0.95
C(25B)-C(26B)	1.381(5)
C(25B)-H(25B)	0.95
C(26B)-C(27B)	1.387(5)
C(26B)-H(26B)	0.95
C(27B)-C(28B)	1.406(4)
C(27B)-H(27B)	0.95
C(28B)-C(29B)	1.450(4)
C(30B)-C(31B)	1.519(5)
C(30B)-H(30C)	0.99
C(30B)-H(30D)	0.99
C(31B)-C(32B)	1.375(5)
C(31B)-C(36B)	1.396(5)
C(32B)-C(33B)	1.390(6)
C(32B)-H(32B)	0.95
C(33B)-C(34B)	1.379(7)
C(33B)-H(33B)	0.95
C(34B)-C(35B)	1.401(6)
C(34B)-H(34B)	0.95
C(35B)-C(36B)	1.388(5)
C(36B)-H(36B)	0.95
C(37B)-C(38B)	1.511(6)
C(37B)-H(37E)	0.99
C(37B)-H(37F)	0.99
C(38B)-C(39B)	1.492(6)
C(38B)-H(38E)	0.99
C(38B)-H(38F)	0.99
C(39B)-C(40B)	1.524(6)
C(39B)-H(39E)	0.99
C(39B)-H(39F)	0.99
C(40B)-H(40E)	0.99
C(40B)-H(40F)	0.99
C(41B)-C(46B)	1.395(5)
C(41B)-C(42B)	1.398(5)
C(42B)-C(43B)	1.370(6)
C(42B)-H(42B)	0.95
C(43B)-C(44B)	1.380(5)
C(43B)-H(43B)	0.95
C(44B)-C(45B)	1.393(5)
C(44B)-H(44B)	0.95
C(45B)-C(46B)	1.390(5)
C(46B)-H(46B)	0.95

N(1A)-Ni(1)-N(3A)	166.98(11)
N(1A)-Ni(1)-N(4A)	89.73(12)

N(3A)-Ni(1)-N(4A)	89.09(12)
N(1A)-Ni(1)-N(2A)	89.68(11)
N(3A)-Ni(1)-N(2A)	91.37(11)
N(4A)-Ni(1)-N(2A)	179.26(11)
C(35A)-O(3A)-C(37A)	118.6(3)
C(41A)-O(4A)-C(40A)	119.0(3)
C(29A)-N(1A)-C(1A)	107.0(3)
C(29A)-N(1A)-Ni(1)	128.5(2)
C(1A)-N(1A)-Ni(1)	119.4(2)
C(22A)-N(2A)-C(23A)	113.9(3)
C(22A)-N(2A)-Ni(1)	127.7(2)
C(23A)-N(2A)-Ni(1)	118.0(2)
C(14A)-N(3A)-C(21A)	106.9(3)
C(14A)-N(3A)-Ni(1)	128.4(2)
C(21A)-N(3A)-Ni(1)	119.5(2)
C(7A)-N(4A)-C(8A)	115.4(3)
C(7A)-N(4A)-Ni(1)	128.5(2)
C(8A)-N(4A)-Ni(1)	115.7(2)
C(29A)-N(5A)-C(2A)	106.8(3)
C(29A)-N(5A)-C(30A)	126.5(3)
C(2A)-N(5A)-C(30A)	122.7(3)
C(14A)-N(6A)-C(16A)	107.1(3)
C(14A)-N(6A)-C(15A)	126.4(3)
C(16A)-N(6A)-C(15A)	122.6(3)
N(1A)-C(1A)-C(6A)	128.3(3)
N(1A)-C(1A)-C(2A)	108.6(3)
C(6A)-C(1A)-C(2A)	123.1(3)
C(1A)-C(2A)-C(3A)	121.1(3)
C(1A)-C(2A)-N(5A)	106.1(3)
C(3A)-C(2A)-N(5A)	132.7(3)
C(4A)-C(3A)-C(2A)	116.4(3)
C(3A)-C(4A)-C(5A)	122.3(3)
C(6A)-C(5A)-C(4A)	121.1(3)
C(1A)-C(6A)-C(5A)	115.8(3)
C(1A)-C(6A)-C(7A)	120.9(3)
C(5A)-C(6A)-C(7A)	123.0(3)
O(1A)-C(7A)-N(4A)	123.9(3)
O(1A)-C(7A)-C(6A)	119.8(3)
N(4A)-C(7A)-C(6A)	116.3(3)
C(9A)-C(8A)-C(13A)	118.8(3)
C(9A)-C(8A)-N(4A)	120.2(3)
C(13A)-C(8A)-N(4A)	120.8(3)
C(10A)-C(9A)-C(8A)	120.3(4)
C(9A)-C(10A)-C(11A)	121.0(4)
C(12A)-C(11A)-C(10A)	119.4(4)
C(11A)-C(12A)-C(13A)	120.8(4)
C(8A)-C(13A)-C(12A)	119.6(3)

C(8A)-C(13A)-C(14A)	117.2(3)
C(12A)-C(13A)-C(14A)	122.0(3)
N(3A)-C(14A)-N(6A)	111.5(3)
N(3A)-C(14A)-C(13A)	119.6(3)
N(6A)-C(14A)-C(13A)	128.7(3)
N(6A)-C(15A)-C(45A)	111.9(3)
C(17A)-C(16A)-C(21A)	121.3(3)
C(17A)-C(16A)-N(6A)	132.9(3)
C(21A)-C(16A)-N(6A)	105.8(3)
C(18A)-C(17A)-C(16A)	116.2(3)
C(17A)-C(18A)-C(19A)	122.5(3)
C(18A)-C(19A)-C(20A)	121.6(4)
C(21A)-C(20A)-C(19A)	115.5(3)
C(21A)-C(20A)-C(22A)	123.1(3)
C(19A)-C(20A)-C(22A)	121.3(3)
N(3A)-C(21A)-C(20A)	128.3(3)
N(3A)-C(21A)-C(16A)	108.7(3)
C(20A)-C(21A)-C(16A)	123.0(3)
O(2A)-C(22A)-N(2A)	124.9(3)
O(2A)-C(22A)-C(20A)	118.8(3)
N(2A)-C(22A)-C(20A)	116.4(3)
C(24A)-C(23A)-C(28A)	118.5(3)
C(24A)-C(23A)-N(2A)	120.3(3)
C(28A)-C(23A)-N(2A)	121.3(3)
C(25A)-C(24A)-C(23A)	120.9(3)
C(24A)-C(25A)-C(26A)	120.8(3)
C(27A)-C(26A)-C(25A)	119.1(3)
C(26A)-C(27A)-C(28A)	120.5(3)
C(27A)-C(28A)-C(23A)	120.1(3)
C(27A)-C(28A)-C(29A)	121.9(3)
C(23A)-C(28A)-C(29A)	117.7(3)
N(1A)-C(29A)-N(5A)	111.5(3)
N(1A)-C(29A)-C(28A)	121.2(3)
N(5A)-C(29A)-C(28A)	127.4(3)
N(5A)-C(30A)-C(31A)	110.7(3)
C(36A)-C(31A)-C(32A)	120.1(3)
C(36A)-C(31A)-C(30A)	121.1(3)
C(32A)-C(31A)-C(30A)	118.8(3)
C(31A)-C(32A)-C(33A)	119.1(3)
C(34A)-C(33A)-C(32A)	120.8(4)
C(35A)-C(34A)-C(33A)	119.6(3)
O(3A)-C(35A)-C(34A)	115.6(3)
O(3A)-C(35A)-C(36A)	124.0(3)
C(34A)-C(35A)-C(36A)	120.4(3)
C(31A)-C(36A)-C(35A)	120.0(3)
O(3A)-C(37A)-C(38A)	120.2(4)
O(3A)-C(37A)-C(38C)	101.7(4)

C(37A)-C(38A)-C(39A)	113.6(5)
C(38A)-C(39A)-C(40A)	110.4(5)
C(39C)-C(38C)-C(37A)	110.8(9)
C(40A)-C(39C)-C(38C)	110.4(12)
C(39C)-C(40A)-O(4A)	127.6(8)
O(4A)-C(40A)-C(39A)	108.1(4)
O(4A)-C(41A)-C(42A)	115.8(3)
O(4A)-C(41A)-C(46A)	124.6(3)
C(42A)-C(41A)-C(46A)	119.6(3)
C(43A)-C(42A)-C(41A)	119.7(3)
C(42A)-C(43A)-C(44A)	121.0(3)
C(45A)-C(44A)-C(43A)	119.0(3)
C(46A)-C(45A)-C(44A)	120.3(3)
C(46A)-C(45A)-C(15A)	120.8(3)
C(44A)-C(45A)-C(15A)	118.8(3)
C(45A)-C(46A)-C(41A)	120.4(3)
Cl(2)-C(47)-Cl(1)	112.2(2)
Cl(3)-C(48)-Cl(4)	111.3(3)
Cl(5)-C(49)-Cl(6)	113.7(5)
N(3B)-Ni(2)-N(1B)	169.26(11)
N(3B)-Ni(2)-N(4B)	89.51(11)
N(1B)-Ni(2)-N(4B)	90.03(11)
N(3B)-Ni(2)-N(2B)	90.98(11)
N(1B)-Ni(2)-N(2B)	89.22(11)
N(4B)-Ni(2)-N(2B)	178.49(11)
C(35B)-O(3B)-C(37B)	119.8(3)
C(41B)-O(4B)-C(40B)	119.0(3)
C(29B)-N(1B)-C(1B)	106.7(3)
C(29B)-N(1B)-Ni(2)	128.5(2)
C(1B)-N(1B)-Ni(2)	119.9(2)
C(22B)-N(2B)-C(23B)	114.6(3)
C(22B)-N(2B)-Ni(2)	126.5(2)
C(23B)-N(2B)-Ni(2)	118.5(2)
C(14B)-N(3B)-C(21B)	106.8(3)
C(14B)-N(3B)-Ni(2)	128.6(2)
C(21B)-N(3B)-Ni(2)	120.5(2)
C(7B)-N(4B)-C(8B)	114.1(2)
C(7B)-N(4B)-Ni(2)	127.3(2)
C(8B)-N(4B)-Ni(2)	118.3(2)
C(29B)-N(5B)-C(2B)	107.0(2)
C(29B)-N(5B)-C(30B)	126.4(3)
C(2B)-N(5B)-C(30B)	123.1(3)
C(14B)-N(6B)-C(16B)	107.2(3)
C(14B)-N(6B)-C(15B)	125.9(3)
C(16B)-N(6B)-C(15B)	121.3(3)
N(1B)-C(1B)-C(6B)	128.3(3)
N(1B)-C(1B)-C(2B)	109.4(3)

C(6B)-C(1B)-C(2B)	122.3(3)
C(3B)-C(2B)-C(1B)	121.4(3)
C(3B)-C(2B)-N(5B)	133.3(3)
C(1B)-C(2B)-N(5B)	105.3(3)
C(4B)-C(3B)-C(2B)	116.5(3)
C(3B)-C(4B)-C(5B)	122.4(3)
C(6B)-C(5B)-C(4B)	120.9(3)
C(1B)-C(6B)-C(5B)	116.4(3)
C(1B)-C(6B)-C(7B)	121.2(3)
C(5B)-C(6B)-C(7B)	122.1(3)
O(1B)-C(7B)-N(4B)	124.0(3)
O(1B)-C(7B)-C(6B)	118.7(3)
N(4B)-C(7B)-C(6B)	117.3(3)
C(13B)-C(8B)-C(9B)	118.3(3)
C(13B)-C(8B)-N(4B)	121.3(3)
C(9B)-C(8B)-N(4B)	120.3(3)
C(10B)-C(9B)-C(8B)	121.0(3)
C(9B)-C(10B)-C(11B)	120.6(3)
C(12B)-C(11B)-C(10B)	118.9(3)
C(11B)-C(12B)-C(13B)	121.4(3)
C(12B)-C(13B)-C(8B)	119.8(3)
C(12B)-C(13B)-C(14B)	121.7(3)
C(8B)-C(13B)-C(14B)	118.3(3)
N(3B)-C(14B)-N(6B)	110.9(3)
N(3B)-C(14B)-C(13B)	121.0(3)
N(6B)-C(14B)-C(13B)	128.0(3)
N(6B)-C(15B)-C(45B)	110.8(3)
C(21B)-C(16B)-N(6B)	106.3(3)
C(21B)-C(16B)-C(17B)	121.9(3)
N(6B)-C(16B)-C(17B)	131.8(3)
C(18B)-C(17B)-C(16B)	115.2(3)
C(19B)-C(18B)-C(17B)	122.8(3)
C(18B)-C(19B)-C(20B)	121.9(3)
C(21B)-C(20B)-C(19B)	115.5(3)
C(21B)-C(20B)-C(22B)	121.9(3)
C(19B)-C(20B)-C(22B)	122.1(3)
C(20B)-C(21B)-N(3B)	128.5(3)
C(20B)-C(21B)-C(16B)	122.8(3)
N(3B)-C(21B)-C(16B)	108.7(3)
O(2B)-C(22B)-N(2B)	124.0(3)
O(2B)-C(22B)-C(20B)	118.8(3)
N(2B)-C(22B)-C(20B)	117.2(3)
C(24B)-C(23B)-C(28B)	118.2(3)
C(24B)-C(23B)-N(2B)	120.3(3)
C(28B)-C(23B)-N(2B)	121.5(3)
C(25B)-C(24B)-C(23B)	120.8(3)
C(26B)-C(25B)-C(24B)	120.8(3)

C(25B)-C(26B)-C(27B)	119.7(3)
C(26B)-C(27B)-C(28B)	120.0(3)
C(23B)-C(28B)-C(27B)	120.5(3)
C(23B)-C(28B)-C(29B)	117.8(3)
C(27B)-C(28B)-C(29B)	121.7(3)
N(1B)-C(29B)-N(5B)	111.5(3)
N(1B)-C(29B)-C(28B)	121.0(3)
N(5B)-C(29B)-C(28B)	127.5(3)
N(5B)-C(30B)-C(31B)	111.9(3)
C(32B)-C(31B)-C(36B)	120.4(3)
C(32B)-C(31B)-C(30B)	119.7(3)
C(36B)-C(31B)-C(30B)	120.0(3)
C(31B)-C(32B)-C(33B)	119.7(4)
C(34B)-C(33B)-C(32B)	120.7(4)
C(33B)-C(34B)-C(35B)	119.8(4)
O(3B)-C(35B)-C(36B)	124.4(4)
O(3B)-C(35B)-C(34B)	116.1(3)
C(36B)-C(35B)-C(34B)	119.5(4)
C(35B)-C(36B)-C(31B)	120.0(3)
O(3B)-C(37B)-C(38B)	113.3(4)
C(39B)-C(38B)-C(37B)	112.5(4)
C(38B)-C(39B)-C(40B)	115.1(4)
O(4B)-C(40B)-C(39B)	113.1(4)
O(4B)-C(41B)-C(46B)	125.1(3)
O(4B)-C(41B)-C(42B)	115.8(3)
C(46B)-C(41B)-C(42B)	119.1(3)
C(43B)-C(42B)-C(41B)	119.9(3)
C(42B)-C(43B)-C(44B)	121.4(3)
C(43B)-C(44B)-C(45B)	119.5(3)
C(46B)-C(45B)-C(44B)	119.6(3)
C(46B)-C(45B)-C(15B)	121.2(3)
C(44B)-C(45B)-C(15B)	119.1(3)
C(45B)-C(46B)-C(41B)	120.5(3)

Table S19. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for the Ni(II) Complex (62).[6]

	U11	U22	U33	U23	U13	U12
Ni(1)	18(1)	20(1)	21(1)	3(1)	7(1)	5(1)
O(1A)	30(1)	53(2)	43(2)	-16(1)	5(1)	-3(1)
O(2A)	32(1)	34(1)	24(1)	9(1)	7(1)	11(1)
O(3A)	42(1)	26(1)	37(1)	12(1)	20(1)	16(1)
O(4A)	42(2)	34(1)	43(2)	2(1)	27(1)	-1(1)
N(1A)	19(1)	21(1)	22(1)	7(1)	8(1)	7(1)
N(2A)	19(1)	21(1)	23(1)	3(1)	7(1)	6(1)
N(3A)	22(1)	21(1)	26(1)	4(1)	10(1)	3(1)
N(4A)	25(1)	25(1)	24(2)	0(1)	6(1)	7(1)
N(5A)	23(1)	24(1)	26(2)	9(1)	13(1)	10(1)
N(6A)	32(2)	21(1)	33(2)	6(1)	20(1)	9(1)
C(1A)	19(2)	24(2)	29(2)	13(1)	9(1)	9(1)
C(2A)	22(2)	24(2)	27(2)	11(1)	10(1)	9(1)
C(3A)	26(2)	36(2)	40(2)	16(2)	18(2)	12(2)
C(4A)	20(2)	33(2)	54(2)	17(2)	15(2)	7(1)
C(5A)	21(2)	27(2)	52(2)	9(2)	8(2)	2(1)
C(6A)	21(2)	26(2)	35(2)	7(2)	5(1)	4(1)
C(7A)	22(2)	29(2)	34(2)	1(2)	2(1)	4(1)
C(8A)	29(2)	25(2)	22(2)	0(1)	6(1)	2(1)
C(9A)	36(2)	28(2)	28(2)	-2(2)	0(2)	2(2)
C(10A)	49(2)	32(2)	20(2)	1(2)	1(2)	-4(2)
C(11A)	54(2)	30(2)	22(2)	-3(2)	13(2)	-8(2)
C(12A)	39(2)	24(2)	31(2)	-2(2)	17(2)	-2(2)
C(13A)	29(2)	21(2)	24(2)	0(1)	9(1)	-1(1)
C(14A)	26(2)	22(2)	29(2)	3(1)	17(1)	2(1)
C(15A)	44(2)	23(2)	40(2)	2(2)	27(2)	8(2)
C(16A)	27(2)	21(2)	37(2)	9(1)	18(2)	5(1)
C(17A)	37(2)	26(2)	49(2)	15(2)	23(2)	13(2)
C(18A)	37(2)	33(2)	46(2)	21(2)	15(2)	15(2)
C(19A)	31(2)	33(2)	36(2)	17(2)	15(2)	12(2)
C(20A)	22(2)	25(2)	28(2)	13(1)	12(1)	7(1)
C(21A)	20(2)	24(2)	31(2)	11(1)	16(1)	5(1)
C(22A)	17(1)	28(2)	25(2)	6(1)	11(1)	5(1)
C(23A)	23(2)	21(2)	17(2)	4(1)	7(1)	4(1)
C(24A)	25(2)	30(2)	25(2)	7(1)	10(1)	5(1)
C(25A)	31(2)	33(2)	23(2)	4(2)	8(1)	-6(2)
C(26A)	37(2)	20(2)	30(2)	2(1)	13(2)	0(1)
C(27A)	34(2)	23(2)	29(2)	7(1)	16(2)	10(1)
C(28A)	24(2)	22(2)	18(2)	4(1)	8(1)	3(1)
C(29A)	22(2)	22(2)	23(2)	10(1)	10(1)	8(1)
C(30A)	32(2)	23(2)	30(2)	7(1)	20(2)	13(1)

C(31A)	23(2)	26(2)	23(2)	6(1)	7(1)	8(1)
C(32A)	54(2)	48(2)	28(2)	16(2)	22(2)	35(2)
C(33A)	80(3)	73(3)	35(2)	27(2)	39(2)	47(3)
C(34A)	65(3)	50(2)	29(2)	22(2)	23(2)	36(2)
C(35A)	27(2)	27(2)	29(2)	7(1)	9(1)	12(1)
C(36A)	29(2)	24(2)	26(2)	4(1)	14(1)	7(1)
C(37A)	53(2)	38(2)	38(2)	10(2)	24(2)	24(2)
C(40A)	44(2)	35(2)	63(3)	-5(2)	34(2)	1(2)
C(41A)	31(2)	32(2)	27(2)	4(2)	11(2)	3(2)
C(42A)	34(2)	27(2)	36(2)	13(2)	10(2)	0(2)
C(43A)	40(2)	22(2)	36(2)	7(2)	7(2)	4(2)
C(44A)	35(2)	23(2)	29(2)	5(1)	9(2)	9(1)
C(45A)	31(2)	23(2)	24(2)	4(1)	9(1)	7(1)
C(46A)	41(2)	23(2)	31(2)	4(1)	17(2)	5(2)
Cl(1)	45(1)	34(1)	40(1)	6(1)	17(1)	2(1)
Cl(2)	42(1)	48(1)	47(1)	15(1)	23(1)	3(1)
Cl(3)	70(1)	52(1)	97(1)	-6(1)	32(1)	-7(1)
Cl(4)	65(1)	112(1)	48(1)	14(1)	17(1)	-10(1)
Cl(5)	85(1)	155(2)	217(3)	108(2)	16(2)	-20(1)
Cl(6)	165(3)	266(4)	146(3)	-34(3)	36(2)	102(3)
C(47)	59(3)	52(3)	33(2)	12(2)	4(2)	-6(2)
C(48)	54(3)	47(3)	54(3)	16(2)	20(2)	10(2)
Ni(2)	18(1)	18(1)	16(1)	3(1)	5(1)	6(1)
O(1B)	19(1)	25(1)	34(1)	7(1)	4(1)	11(1)
O(2B)	43(1)	25(1)	31(1)	13(1)	16(1)	15(1)
O(3B)	59(2)	44(2)	60(2)	29(2)	43(2)	19(1)
O(4B)	26(1)	36(1)	44(2)	0(1)	13(1)	-1(1)
N(1B)	18(1)	20(1)	18(1)	5(1)	6(1)	6(1)
N(2B)	21(1)	21(1)	17(1)	3(1)	5(1)	9(1)
N(3B)	16(1)	23(1)	20(1)	5(1)	6(1)	6(1)
N(4B)	19(1)	16(1)	21(1)	3(1)	6(1)	5(1)
N(5B)	21(1)	17(1)	20(1)	4(1)	8(1)	5(1)
N(6B)	19(1)	23(1)	21(1)	1(1)	5(1)	6(1)
C(1B)	20(1)	21(2)	17(2)	7(1)	6(1)	3(1)
C(2B)	22(2)	22(2)	18(2)	6(1)	9(1)	6(1)
C(3B)	26(2)	26(2)	21(2)	0(1)	8(1)	0(1)
C(4B)	19(2)	31(2)	19(2)	4(1)	2(1)	-1(1)
C(5B)	18(1)	29(2)	21(2)	7(1)	7(1)	5(1)
C(6B)	20(1)	25(2)	15(1)	5(1)	8(1)	4(1)
C(7B)	22(2)	22(2)	19(2)	6(1)	9(1)	6(1)
C(8B)	16(1)	18(2)	24(2)	4(1)	8(1)	7(1)
C(9B)	27(2)	26(2)	23(2)	6(1)	12(1)	8(1)
C(10B)	31(2)	24(2)	34(2)	12(2)	16(2)	9(1)
C(11B)	27(2)	21(2)	33(2)	4(1)	12(1)	3(1)
C(12B)	22(2)	25(2)	25(2)	2(1)	8(1)	2(1)
C(13B)	16(1)	22(2)	25(2)	4(1)	8(1)	6(1)
C(14B)	16(1)	21(2)	17(2)	1(1)	5(1)	4(1)

C(15B)	25(2)	23(2)	24(2)	0(1)	9(1)	8(1)
C(16B)	20(2)	29(2)	20(2)	5(1)	6(1)	6(1)
C(17B)	31(2)	42(2)	21(2)	7(2)	11(1)	16(2)
C(18B)	39(2)	48(2)	21(2)	14(2)	12(2)	17(2)
C(19B)	30(2)	35(2)	28(2)	14(2)	12(2)	13(2)
C(20B)	22(2)	26(2)	21(2)	7(1)	6(1)	8(1)
C(21B)	18(1)	28(2)	17(2)	4(1)	5(1)	6(1)
C(22B)	23(2)	24(2)	24(2)	7(1)	8(1)	6(1)
C(23B)	24(2)	16(1)	23(2)	7(1)	9(1)	9(1)
C(24B)	26(2)	21(2)	27(2)	6(1)	6(1)	6(1)
C(25B)	20(2)	28(2)	37(2)	9(2)	7(1)	10(1)
C(26B)	28(2)	26(2)	38(2)	8(2)	17(2)	12(1)
C(27B)	28(2)	20(2)	24(2)	4(1)	12(1)	6(1)
C(28B)	24(2)	17(1)	22(2)	7(1)	9(1)	7(1)
C(29B)	26(2)	20(2)	19(2)	5(1)	11(1)	5(1)
C(30B)	28(2)	19(2)	24(2)	1(1)	9(1)	6(1)
C(31B)	23(2)	25(2)	31(2)	10(1)	8(1)	9(1)
C(32B)	39(2)	24(2)	50(2)	7(2)	15(2)	6(2)
C(33B)	48(2)	22(2)	78(3)	14(2)	23(2)	1(2)
C(34B)	44(2)	36(2)	77(3)	33(2)	31(2)	12(2)
C(35B)	33(2)	35(2)	46(2)	21(2)	19(2)	13(2)
C(36B)	29(2)	24(2)	35(2)	10(2)	12(2)	5(1)
C(37B)	49(2)	51(3)	37(2)	18(2)	27(2)	14(2)
C(38B)	43(2)	36(2)	40(2)	11(2)	19(2)	6(2)
C(39B)	45(3)	46(3)	68(3)	-21(2)	-8(2)	14(2)
C(40B)	33(2)	38(2)	38(2)	-7(2)	10(2)	4(2)
C(41B)	23(2)	30(2)	33(2)	11(2)	10(1)	7(1)
C(42B)	27(2)	39(2)	41(2)	11(2)	16(2)	7(2)
C(43B)	36(2)	47(2)	38(2)	8(2)	24(2)	13(2)
C(44B)	31(2)	35(2)	28(2)	4(2)	14(2)	11(2)
C(45B)	26(2)	26(2)	23(2)	7(1)	11(1)	11(1)
C(46B)	24(2)	28(2)	31(2)	6(1)	13(1)	10(1)

Table S20. Calculated Hydrogen Coordinates ($\times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for the Ni(II) Complex (62).

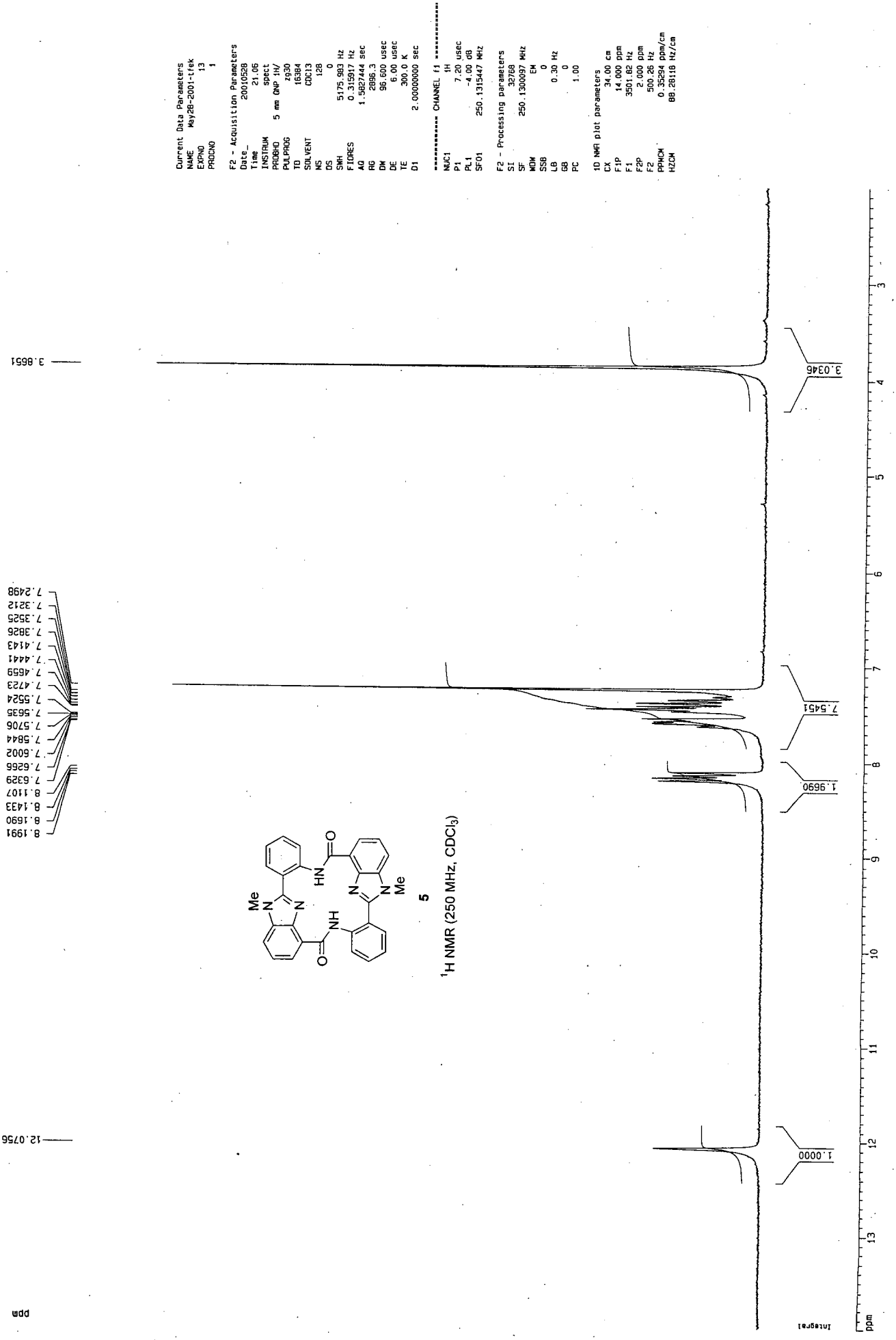
	x	y	z	U(eq)
H(3A)	774(3)	1124(2)	2905(2)	37
H(4A)	-174(3)	-140(3)	2123(2)	40
H(5A)	392(3)	-846(2)	1288(2)	41
H(9A)	2398(3)	379(2)	-22(2)	41
H(10A)	2925(3)	116(3)	-939(2)	45
H(11A)	4119(3)	-886(3)	-995(2)	44
H(12A)	4883(3)	-1535(2)	-93(2)	38
H(15A)	5530(3)	-3115(2)	829(2)	39
H(15B)	4561(3)	-2765(2)	352(2)	39
H(17A)	6513(3)	-2872(2)	2122(2)	41
H(18A)	7292(3)	-2225(3)	3243(2)	43
H(19A)	7015(3)	-797(2)	3686(2)	37
H(24A)	6886(3)	2068(2)	3138(2)	32
H(25A)	7043(3)	3614(2)	3521(2)	36
H(26A)	5608(3)	4343(2)	3522(2)	35
H(27A)	4013(3)	3490(2)	3142(2)	32
H(30A)	2159(3)	2527(2)	3569(2)	30
H(30B)	3366(3)	2739(2)	3771(2)	30
H(32A)	2162(3)	2223(3)	4620(2)	47
H(33A)	2401(4)	1214(3)	5354(2)	65
H(34A)	3294(3)	-19(3)	5229(2)	52
H(36A)	3725(3)	742(2)	3634(2)	30
H(37A)	4711(3)	-1311(3)	3855(2)	47
H(37B)	4786(3)	-285(3)	3769(2)	47
H(37C)	4837(3)	-1215(3)	3861(2)	47
H(37D)	4573(3)	-259(3)	3647(2)	47
H(38A)	3707(6)	-680(5)	2839(3)	57
H(38B)	2882(6)	-886(5)	3177(3)	57
H(39A)	3338(4)	-2410(4)	3152(3)	35
H(39B)	4045(4)	-2186(4)	2733(3)	35
H(38C)	2916(8)	-1783(7)	3404(5)	16
H(38D)	2705(8)	-858(7)	3141(5)	16
H(39C)	3482(12)	-1243(12)	2354(9)	61
H(39D)	3915(12)	-2086(12)	2670(9)	61
H(40A)	1839(3)	-2123(3)	2259(2)	54
H(40B)	2557(3)	-1943(3)	1836(2)	54
H(40C)	2209(3)	-2009(3)	1771(2)	54
H(40D)	1958(3)	-2207(3)	2397(2)	54
H(42A)	2464(3)	-4872(2)	1529(2)	38

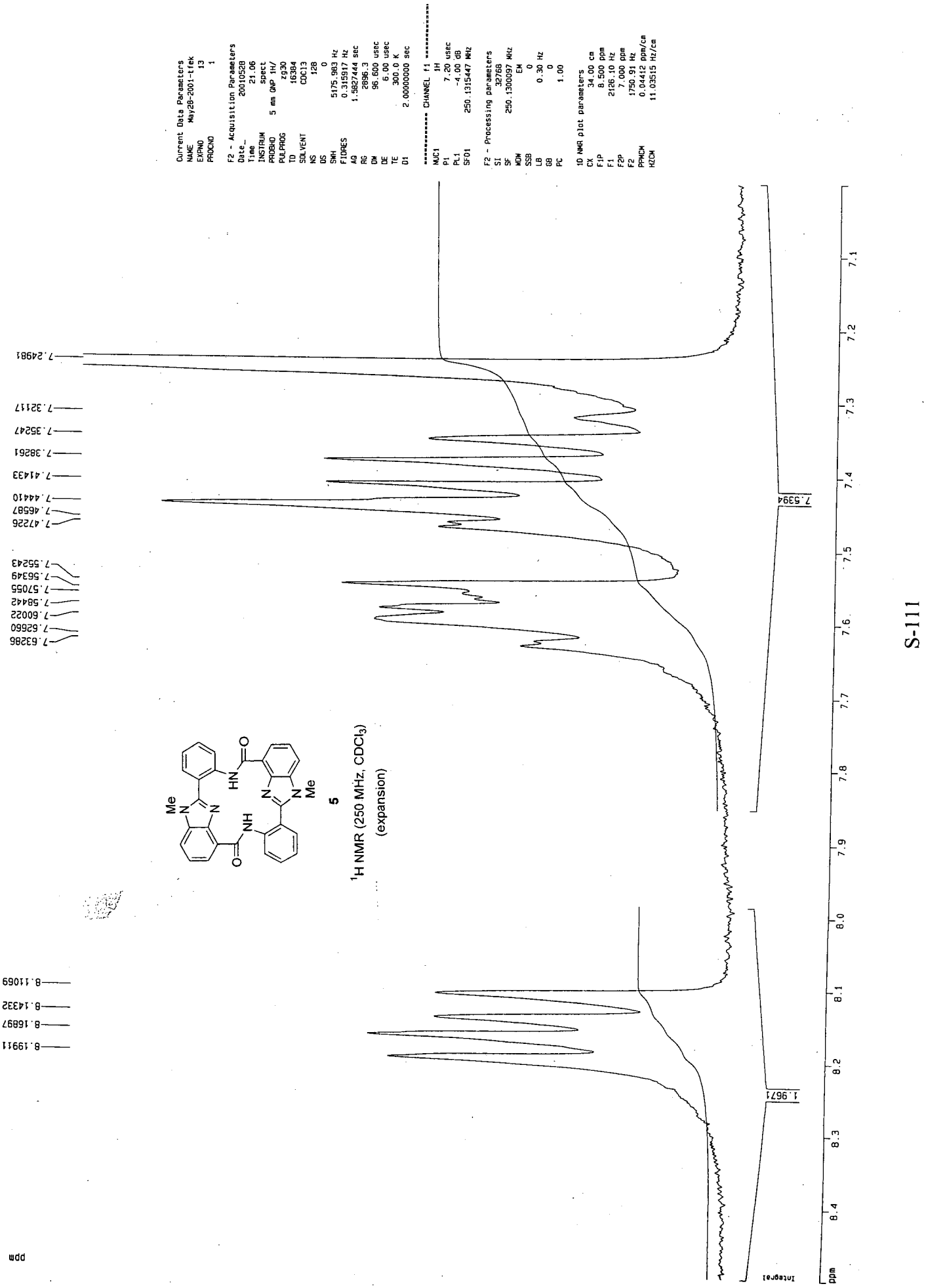
H(43A)	3470(3)	-5519(2)	954(2)	41
H(44A)	4598(3)	-4605(2)	657(2)	35
H(46A)	3640(3)	-2376(2)	1476(2)	37
H(47A)	6034(4)	2695(3)	1667(2)	61
H(47B)	5340(4)	3364(3)	1926(2)	61
H(48A)	7960(4)	6932(3)	1373(2)	60
H(48B)	8811(4)	7302(3)	1102(2)	60
H(49A)	3758(6)	7791(6)	5573(4)	134
H(49B)	4151(6)	8479(6)	5197(4)	134
H(3B)	-1145(2)	3131(2)	4834(2)	30
H(4B)	-2389(2)	4111(2)	4792(2)	30
H(5B)	-1986(2)	5603(2)	5367(2)	27
H(9B)	736(2)	7959(2)	5912(2)	29
H(10B)	1281(3)	9499(2)	6231(2)	33
H(11B)	1912(3)	10184(2)	7349(2)	32
H(12B)	2035(2)	9298(2)	8144(2)	29
H(15C)	833(2)	8876(2)	8573(2)	29
H(15D)	1217(2)	8648(2)	9299(2)	29
H(17B)	1663(3)	7249(3)	9846(2)	36
H(18B)	2055(3)	5804(3)	10046(2)	41
H(19B)	2425(3)	4756(3)	9286(2)	35
H(24B)	4417(2)	4806(2)	7949(2)	30
H(25B)	5385(3)	4041(2)	7392(2)	34
H(26B)	4690(3)	3422(2)	6269(2)	34
H(27B)	2988(2)	3525(2)	5698(2)	28
H(30C)	1677(3)	2579(2)	5673(2)	29
H(30D)	643(3)	2459(2)	5060(2)	29
H(32B)	131(3)	987(2)	5273(2)	45
H(33B)	-659(3)	203(3)	5853(3)	58
H(34B)	-876(3)	944(3)	6816(2)	56
H(36B)	550(3)	3269(2)	6650(2)	34
H(37E)	533(3)	3730(3)	7597(2)	50
H(37F)	-101(3)	3671(3)	8086(2)	50
H(38E)	-880(3)	4000(3)	6774(2)	45
H(38F)	-1604(3)	3798(3)	7185(2)	45
H(39E)	-81(4)	5300(3)	7563(3)	76
H(39F)	-765(4)	5090(3)	7996(3)	76
H(40E)	-1201(3)	6071(3)	7027(2)	46
H(40F)	-2045(3)	5209(3)	6787(2)	46
H(42B)	-2767(3)	6841(3)	8426(2)	41
H(43B)	-2039(3)	8082(3)	9268(2)	45
H(44B)	-388(3)	8724(3)	9484(2)	37
H(46B)	-235(2)	6959(2)	7907(2)	32

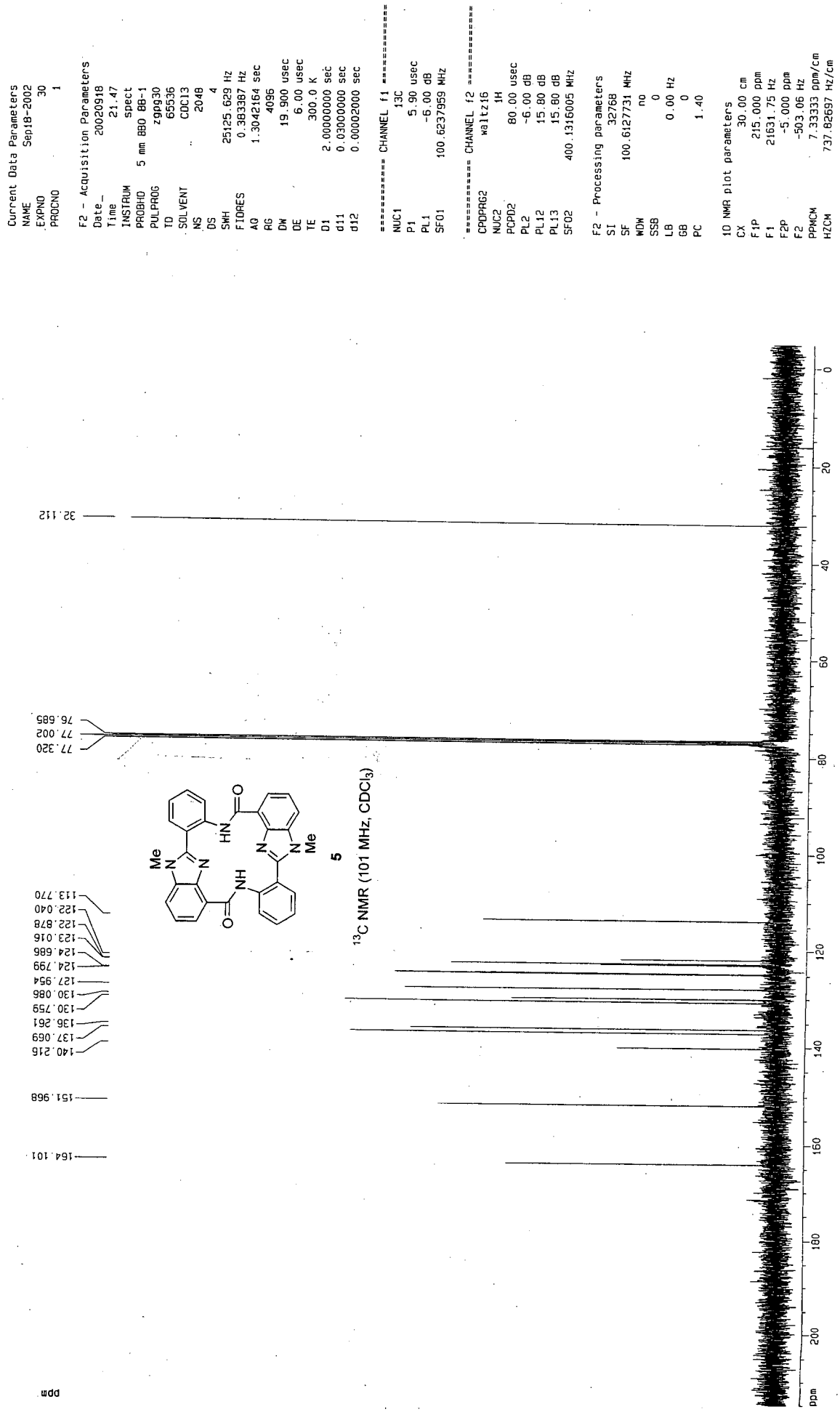
Table S21. Deviation (Å) from Planarity Relative to the Mean 4N-Plane for the Core Sixteen Atoms in (5), (25), (26), (62), Senge's Porphyrin,[a] and Kobayashi's Phthalocyanine.[b]

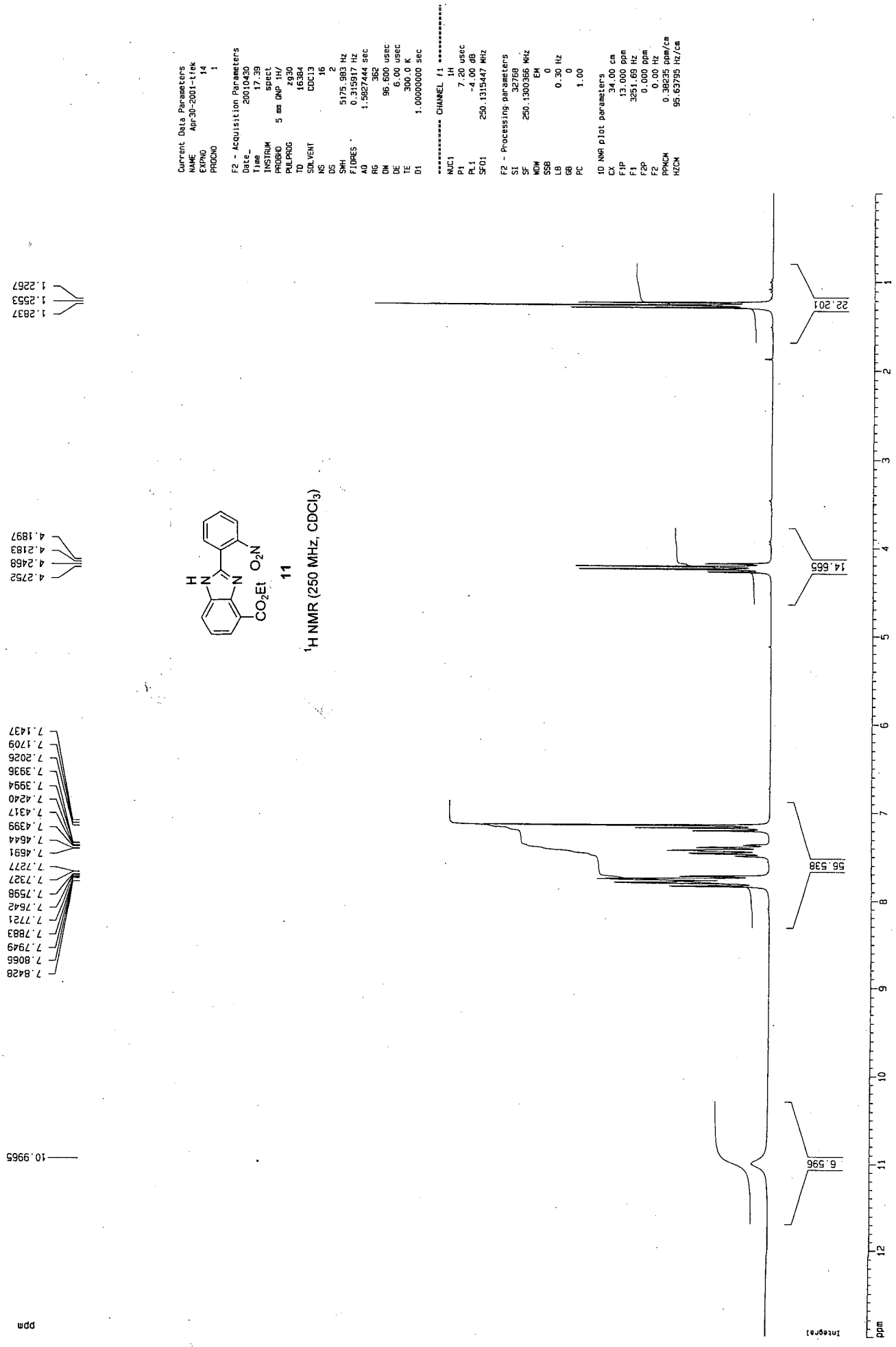
	Deviation/Å						
Atom No[c]	**5**	**25**	**26**		**62**[d]	Senge's porphyrin[a]	**2** (R = Ph)[b]
1	-0.060	-0.072	-0.088	-0.099	-0.073	0.02	-0.120
2	-0.057	0.063	0.122	-0.005	0.048	-0.31	-0.414
3	0.741	0.817	0.811	0.805	0.852	-0.77	-0.070
4	0.762	0.827	0.813	0.852	0.841	-0.43	0.309
5	0.060	0.073	0.083	0.097	0.076	-0.02	0.120
6	-0.647	-0.712	-0.785	-0.663	-0.715	0.49	0.367
7	-1.285	-1.277	-1.240	-1.214	-1.238	1.00	0.027
8	-0.955	-0.880	-0.799	-0.887	-0.839	0.63	-0.326
9	-0.051	-0.073	-0.088	-0.103	-0.076	0.02	-0.120
10	-0.166	0.066	0.125	-0.060	0.023	-0.35	-0.303
11	0.592	0.864	0.820	0.780	0.798	-0.82	0.067
12	0.627	0.827	0.822	0.925	0.838	-0.45	0.403
13	0.059	0.076	0.089	0.105	0.076	-0.02	0.120
14	-0.649	-0.732	-0.801	-0.679	-0.695	0.49	0.372
15	-1.147	-1.174	-1.249	-1.323	-1.292	1.01	0.012
16	-0.854	-0.789	-0.797	-0.933	-0.885	0.63	-0.368
SUA/Å[e]	8.712	9.322	9.532	9.530	9.365	7.46	3.518
SUM/Å[f]	3.765	4.132	4.120	4.122	4.180	3.60	0.176
AVA/Å[g]	0.545	0.583	0.596	0.596	0.585	0.47	0.220
AVM/Å[h]	0.941	1.033	1.030	1.031	1.045	0.90	0.044

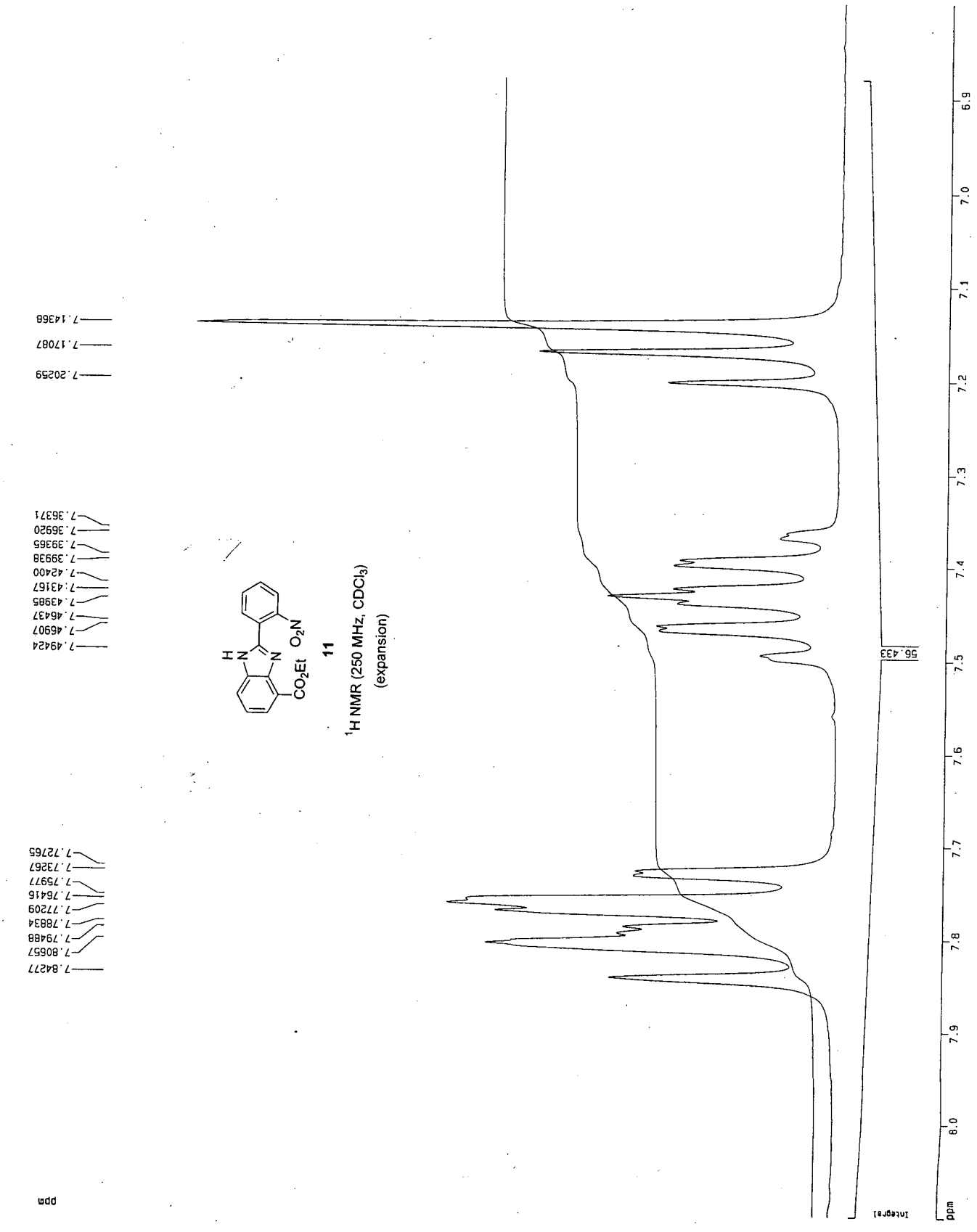
[a] Senge's porphyrin: Zn(II)·H_2**1**·(pyridine) (R = H, R^1 = ^{t}Bu). Senge, M. O.; Ema, T.; Smith, K. M. *J. Chem. Soc., Chem. Commun.* **1995**, 733-734. [b] Kobayashi's phthalocyanine: **2** (R = Ph). Kobayashi, N.; Fukuda, T.; Ueno, K.; Ogino, H. *J. Am. Chem. Soc.* **2001**, *123*, 10740-10741. [c] For numbering system, see Main Manuscript, Figure 7. [c] Two sets of data for two distinct molecules of **62** present in the cell. [e] SUA - the sum of the absolute distortions for the sixteen core atoms. [f] SUM – the sum of the absolute distortions for the meso atoms (atoms 3, 7, 11, and 15). [g] AVA – the average absolute distortion for the sixteen core atoms (SUA/16). [h] AVM – the average absolute distortion for the meso atoms (SUM/16).

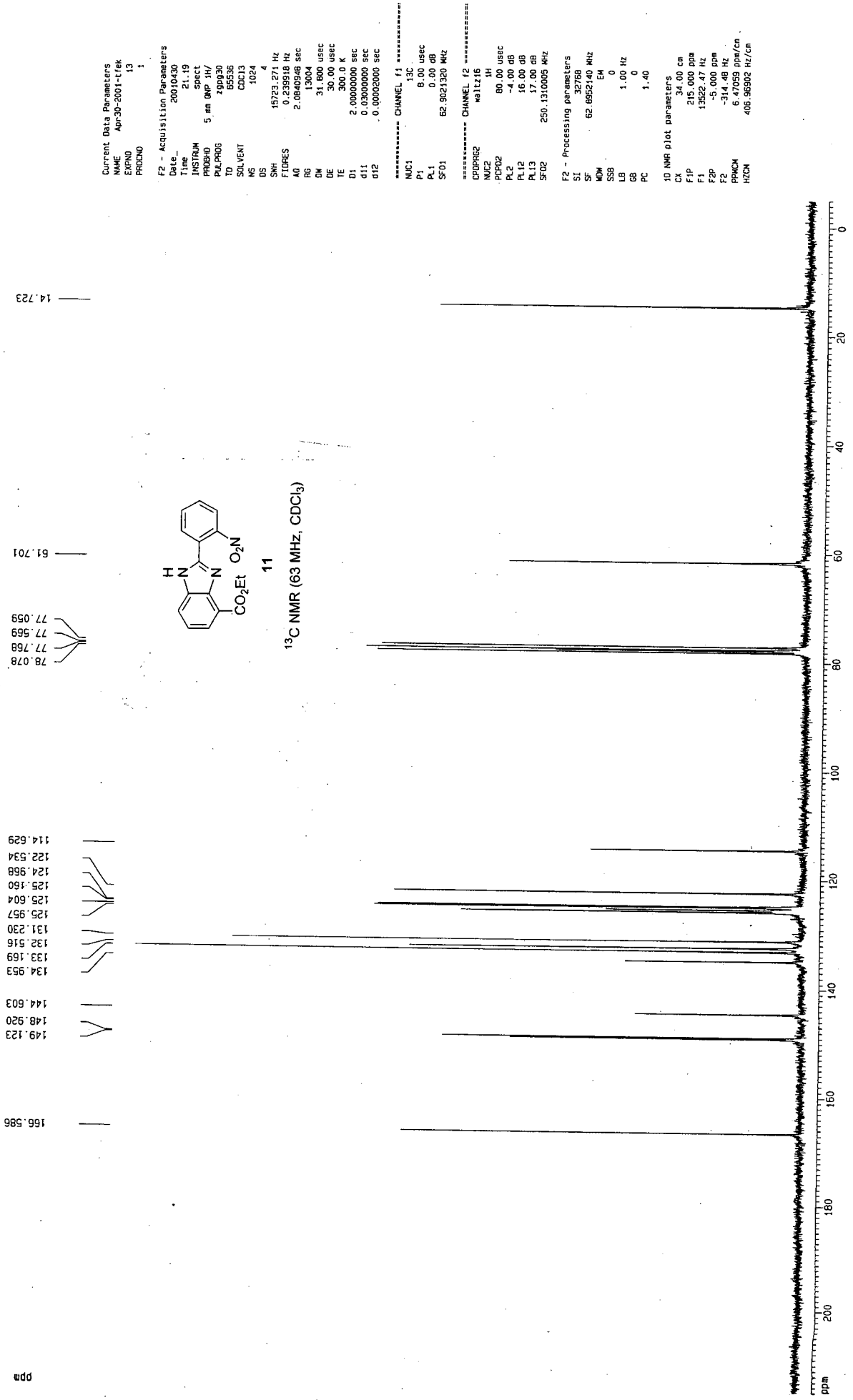


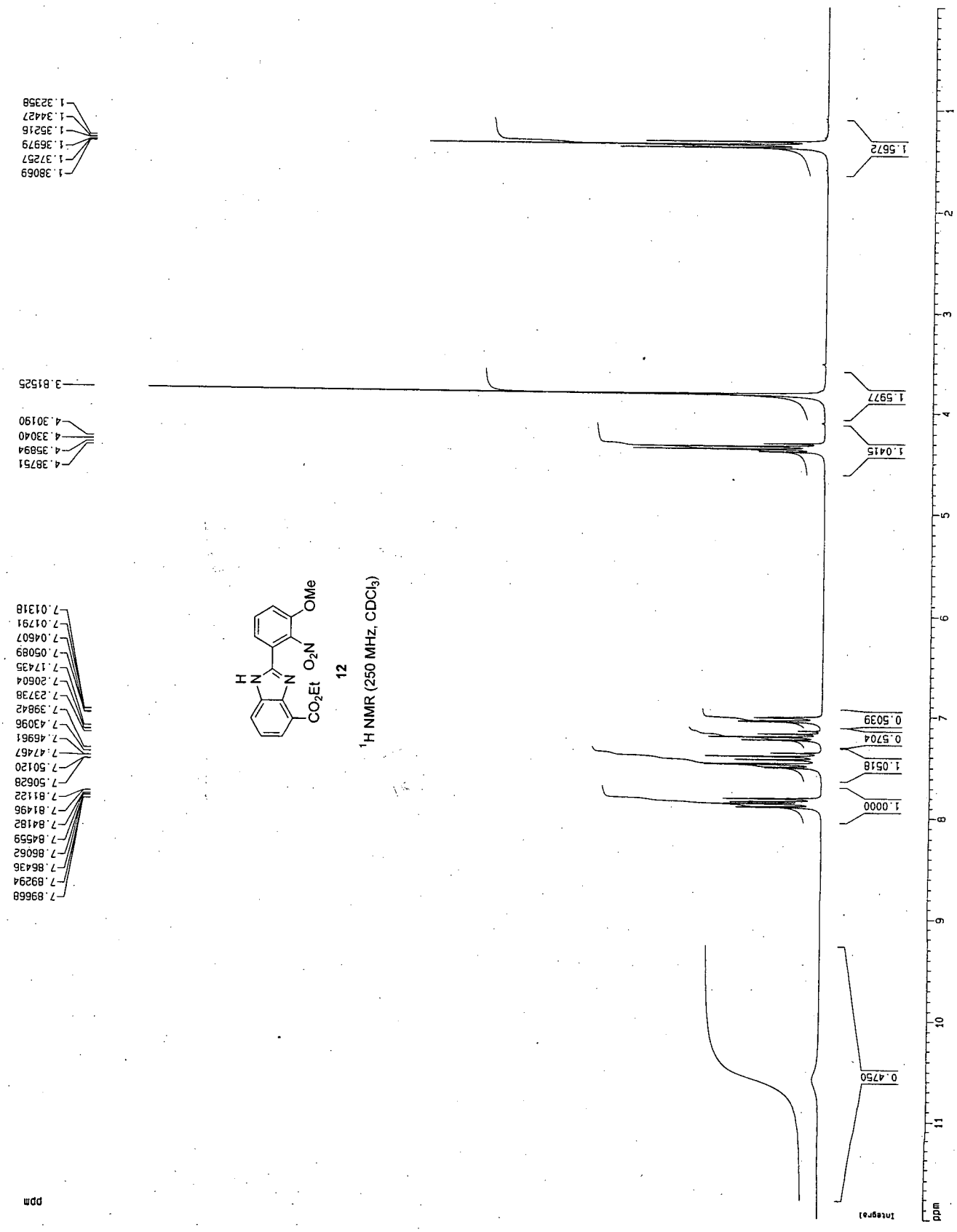






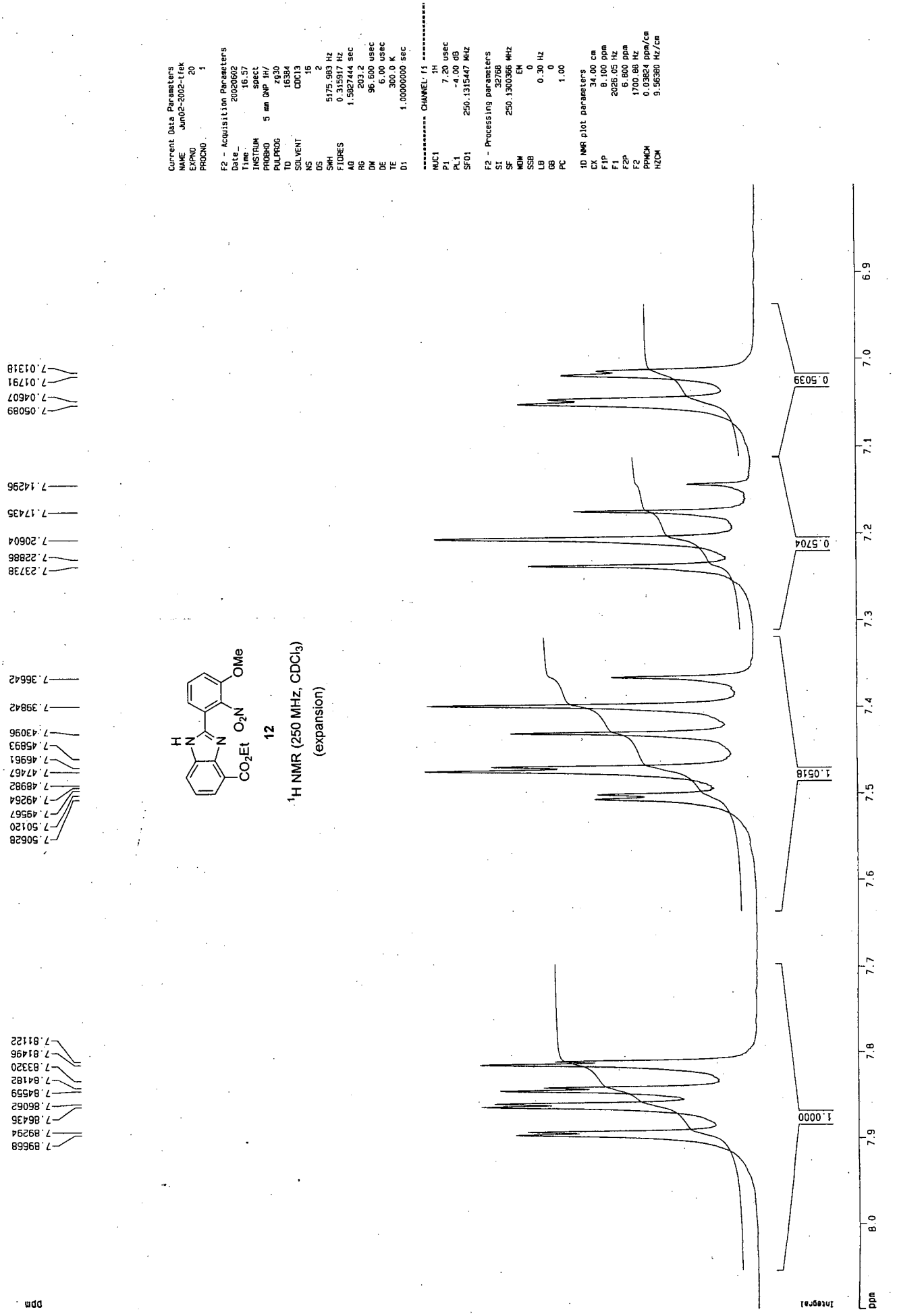


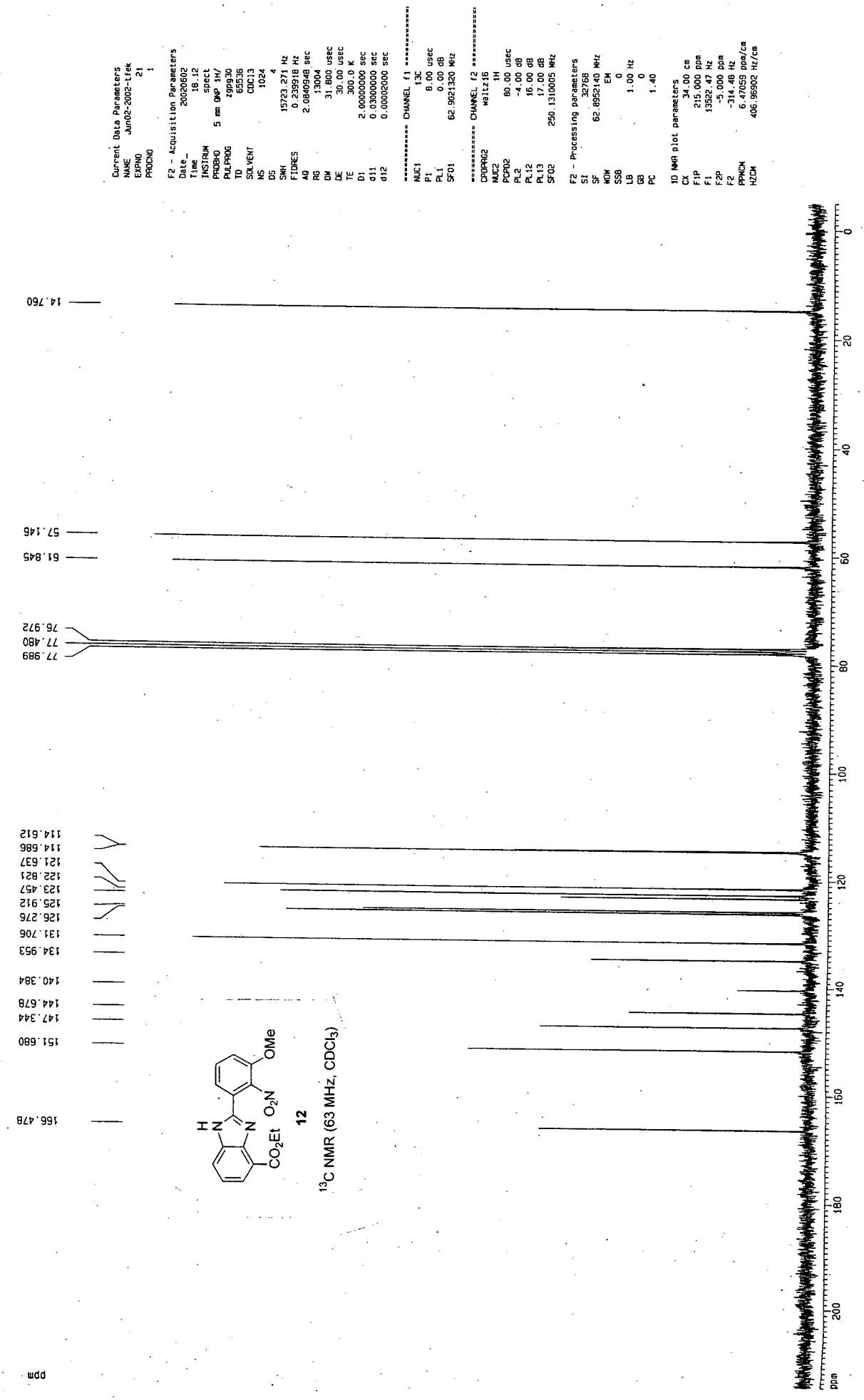


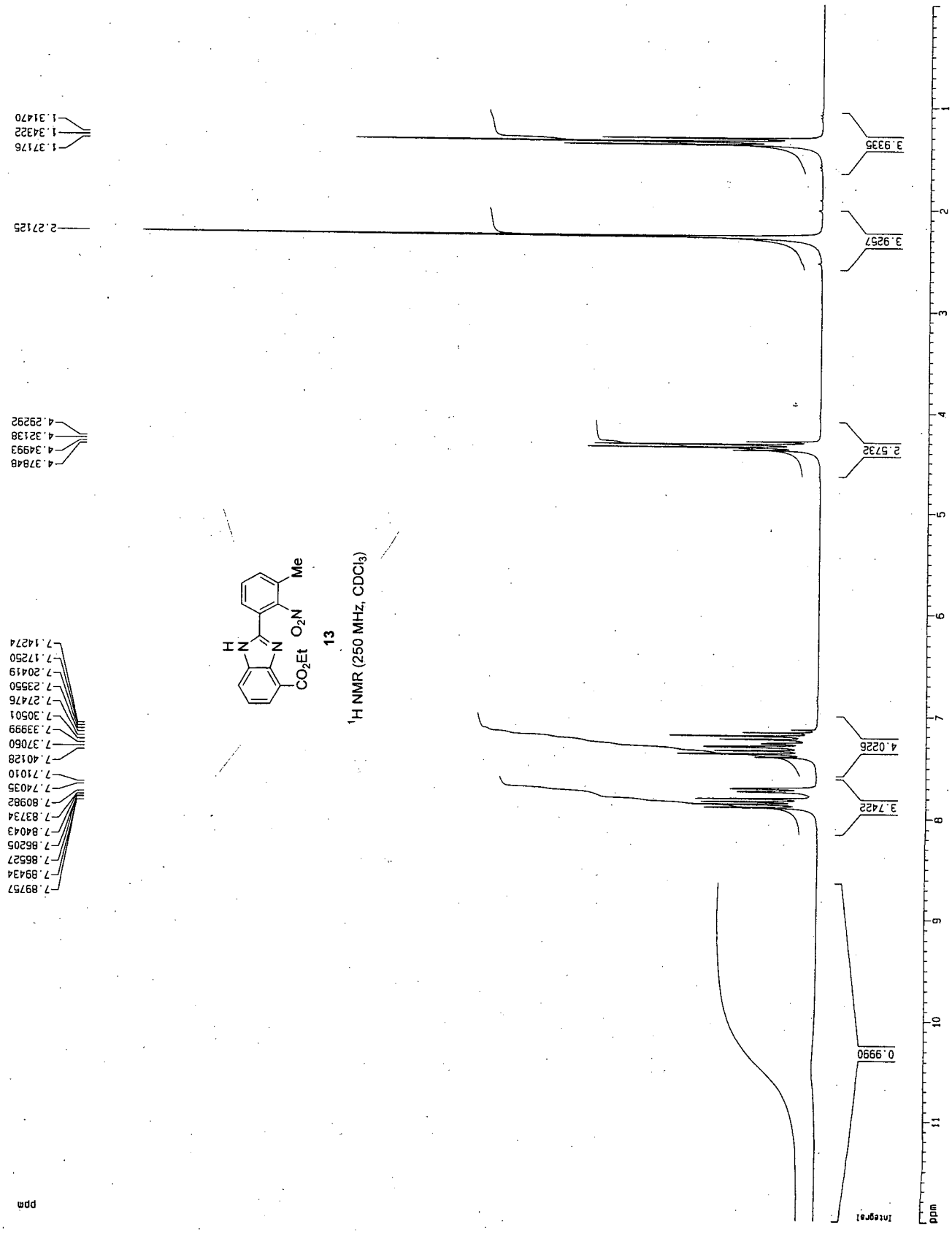


12

^{1}H NMR (250 MHz, $CDCl_3$)







13

^{1}H NMR (250 MHz, $CDCl_3$)