Supporting Information

Oxidation Reactivity Channels for 2-(Pyridin-2-yl)-N,N-diphenylacetamides

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X-ray crystallography – general experimental summary

Single crystals of each compound were obtained from the purification procedures described n the synthesis sections. Crystals were selected by microscopic examination, mounted on a glass fiber, placed on a goniometer and centered on a four-circle automated X-ray diffractometer and determinations of crystal class, orientation matrix and unit cell parameters were performed in standard fashion.[1] Data were collected by using graphite-monochromated MoK_α radiation. The data collection for **1** and **4** were done at 20 °C and 19 °C, respectively while the data sets for the remaining compounds were done at low temperatures. Data collections and reductions used SAINT.[2]

The structure solution for **1** used the SHELXTL-NT structure determination package.[3] Absorption correction used XPREP, Version 5.03.[4] The structure was solved by direct methods. Non-hydrogen atoms were refined anisotropically and the hydrogen atoms were refined with variable isotropic thermal paraters. The absorption corrections for the remaining compounds were accomplished with SADABS[5], the structure solved by direct methods using SHELX97[6] and all non-hydrogen atoms refined anisotropically. H-atoms were generally located in these refinements but they were placed in calculated positions by applying the riding model. Exceptions are noted in specific molecule comments below. The structure Figures are drawn with 25% thermal ellipsoids unless noted otherwise.

Summary Table of Crystallographic Data For **1**, **2**, **4**, **6**, **7**, (**9 + 11**), **12** and **14**.

	1	**2**	**4**	**6**	**7**	**9 + 11**	**12**	**14**
Compound ID#	rtp044	rtp05k	rtp055	rtp05n	rps19a	rtp5jp	rtp05l	rtp05al
Empirical formula	$C_{19}N_{16}N_2O$	$C_{20}H_{18}N_2O$	$C_{33}H_{27}N_3O_2$	$C_{20}H_{16}N_2O_2$	$C_{19}H_{16}N_2O_2$	$C_{38}H_{32}N_4O_5$	$C_{20}H_{18}N_2O_3$	$C_{33}H_{27}N_3O_3$
Formula weight	288.34	302.36	497.58	316.35	304.34	624.68	334.36	513.58
Crystal system	monoclinic	monoclinic	monoclinic	orthorhombic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	P2(1)/n	C2/c	Pc(1)/n	P2(1)2(1)2(1)	P2(1)/n	Pc	P2(1)/c	P2(1)/n
Crystal size [mm]	0.34 x 0.21 x 0.21	0.32 x 0.15 x 0.06	0.55 x 0.30 x 0.15	0.26 x 0.20 x 0.1	0.45 x 0.44 x 0.18	0.16 x 0.12 x 0.08	0.30 x 0.10 x 0.01	0.36 x 0.30 x 0.07
a [Å]	10.1537(10)	15.9783(16)	9.7206(10)	9.6324(2)	16.2324(11)	6.1070(3)	10.7259(6)	9.8097(11)
b [Å]	11.5135(13)	6.2843(7)	16.6521(11)	12.4812(3)	5.6544(4)	16.1821(8)	18.5233(10)	16.7962(18)
c [Å]	12.8787(12)	32.0443(3)	17.1319(14)	14.0456(3)	18.3459(12)	15.2318(7)	17.1998(9)	17.0633(19)
α [°]	90	90	90	90	90	90	90	90
β [°]	98.021(9)	101.218(5)	104.408(9)	90	115.587(3)	92.612(2)	94.687(3)	105.000(6)
γ [°]	90	90	90	90	90	90	90	90
V [Å^3]	1490.9(3)	3156.2(6)	2685.9(4)	1688.62(16)	1518.73(18)	1503.70(13)	3405.8(3)	2715.6(5)
Z	4	8	4	4	4	2	8	4
T [°C]	20	-40	19	-40	-50	-50	-50	-65
Density (calcd) [gcm^{-3}]	1.285	1.273	1.230	1.244	1.331	1.380	1.304	1.256
Absorption Coeff [mm^{-1}]	0.081	0.079	0.077	0.082	0.088	0.093	0.089	0.081
Absorption correction	Gaussian	semi-emp	psi-scan	semi-emp	semi-emp	semi-emp	semi-emp	semi-emp
Transmission: min/max	0.979/0.980	0.976/0.995	0.962/0.985	0.960/0.992	0.960/0.980	0.9500/0.9900	0.806/0.999	0.907/0.998
F(000)	608	1280	1048	664	640	656	1408	1080
Index range	-12≤h≤12 -13≤k≤13 -15≤l≤15	-22≤h≤21 -9≤k≤8 -41≤l≤46	0≤h≤12 -20≤k≤13 -20≤l≤15	-10≤h≤14 -18≤k≤19 -21≤l≤21	-24≤h≤24 -8≤k≤4 -28≤l≤28	-8≤h≤7 -21≤k≤20 -20≤l≤20	-10≤h≤14 -25≤k≤21 -23≤l≤23	-17≤h≤15 -26≤k≤29 -27≤l≤29
2θ max		61.2		65.5	69.2			
Refl. collected	10805	23523	10410	29190	20730	16827	44612	47241
Refln independent	2776	4852	4994	3486	6003	3601	8814	14367
R_{int}	0.0447	0.0235	0.0312	0.0204	0.0202	0.0238	0.0540	0.0559
No. of variables	265	276	348	218	209	425	465	460
GooF	1.020	1.043	1.018	1.062	0.945	1.069	1.033	0.998
Final R [I≥2σ(I)]	0.0372	0.050	0.0426	0.0392	0.0439	0.0536	0.0573	0.0546
Final ωR2	0.0786	0.1233	0.0979	0.1031	0.0925	0.1445	0.1487	0.1314
Largest resid peak [e/Å^3]	0.133	0.259	0.110	0.277	0.340	0.638	0.344	0.350

X-ray Crystallographic data for **1** (rtp044)

Compound 1. The molecule crystallized in the monoclinic space group $P2_1/n$. There are four molecules in the unit cell with no unusually close approaches between molecules. The N1 geometry is planar (sum of angles 359.87°) and the N1-C1 bond length [1.362(2) Å] is shorter than the N1-C8 [1.444(2) Å] and N1-C14 [1.449(2) Å] bond lengths. This difference is typical of N,N-diarylamide units found in the Cambridge Crystallographic database.[7] Small bond length and bond angle variations in the pyridine ring are also typical of those found in many substituted pyridines: N2-C3 [1.329(2) Å], N2-C7 [1.343(3) Å], C3-N2-C7 [117.35(17)°], C3-C4 [1.382(3) Å], C4-C5 [1.376(3) Å], C5-C6 [1.365(3) Å], C6-C7 [1.364(3) Å]. The carbonyl bond length C1-O [1.2201(19) Å] is typical.

Table 1. Crystal data and structure refinement for rtp044.

Identification code	rtp044	
Empirical formula	C19 H16 N2 O	
Formula weight	288.34	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 10.1537(10) Å	α= 90°.
	b = 11.5135(13) Å	β= 98.021(9)°.
	c = 12.8787(12) Å	γ = 90°.
Volume	1490.9(3) $Å^3$	
Z	4	
Density (calculated)	1.285 Mg/m^3	
Absorption coefficient	0.081 mm^{-1}	
F(000)	608	
Crystal size	.34 x .21 x .21 mm^3	
Theta range for data collection	2.38 to 25.50°.	
Index ranges	-12<=h<=12, -13<=k<=13, -15<=l<=15	
Reflections collected	10805	
Independent reflections	2776 [R(int) = 0.0447]	
Completeness to theta = 25.50°	100.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.980 and 0.979	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2776 / 0 / 265	
Goodness-of-fit on F^2	1.020	
Final R indices [I>2sigma(I)]	R1 = 0.0372, wR2 = 0.0786	
R indices (all data)	R1 = 0.0655, wR2 = 0.0963	
Largest diff. peak and hole	0.133 and -0.108 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for rtp044. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O	3299(1)	671(1)	6217(1)	66(1)
N(1)	4607(1)	2215(1)	6692(1)	48(1)
N(2)	3678(2)	-931(1)	8656(1)	61(1)
C(1)	3853(2)	1293(2)	6911(1)	49(1)
C(2)	3724(2)	1048(2)	8048(2)	55(1)
C(3)	4438(2)	-40(2)	8460(1)	48(1)
C(4)	5808(2)	-87(2)	8673(2)	65(1)
C(5)	6416(2)	-1080(2)	9099(2)	73(1)
C(6)	5640(2)	-1997(2)	9303(2)	69(1)
C(7)	4294(3)	-1889(2)	9073(2)	69(1)
C(8)	5184(2)	3049(1)	7461(1)	45(1)
C(9)	6535(2)	3030(2)	7791(2)	55(1)
C(10)	7089(2)	3826(2)	8527(2)	65(1)
C(11)	6305(2)	4635(2)	8924(2)	62(1)
C(12)	4961(2)	4664(2)	8583(1)	58(1)
C(13)	4389(2)	3870(2)	7849(1)	52(1)
C(14)	4801(2)	2455(1)	5620(1)	46(1)
C(15)	4266(2)	3447(2)	5136(1)	55(1)
C(16)	4493(2)	3708(2)	4126(2)	60(1)
C(17)	5243(2)	2972(2)	3608(2)	63(1)
C(18)	5767(2)	1976(2)	4091(2)	64(1)
C(19)	5548(2)	1710(2)	5099(2)	55(1)

Table 3. Bond lengths [Å] and angles [°] for rtp044.

O-C(1)	1.2201(19)
N(1)-C(1)	1.362(2)
N(1)-C(8)	1.444(2)
N(1)-C(14)	1.448(2)
N(2)-C(3)	1.329(2)
N(2)-C(7)	1.343(2)
C(1)-C(2)	1.514(2)
C(2)-C(3)	1.506(2)
C(2)-H(2A)	0.982(19)
C(2)-H(2B)	0.96(2)
C(3)-C(4)	1.382(3)
C(4)-C(5)	1.376(3)
C(4)-H(4)	0.96(2)
C(5)-C(6)	1.365(3)
C(5)-H(5)	0.99(2)
C(6)-C(7)	1.364(3)
C(6)-H(6)	0.96(2)
C(7)-H(7)	0.98(2)
C(8)-C(9)	1.378(2)
C(8)-C(13)	1.380(2)
C(9)-C(10)	1.381(3)
C(9)-H(9)	0.975(18)
C(10)-C(11)	1.370(3)
C(10)-H(10)	0.97(2)
C(11)-C(12)	1.375(3)
C(11)-H(11)	0.95(2)
C(12)-C(13)	1.383(2)
C(12)-H(12)	0.97(2)
C(13)-H(13)	0.981(18)
C(14)-C(15)	1.376(2)

C(14)-C(19)	1.380(2)
C(15)-C(16)	1.385(3)
C(15)-H(15)	0.967(19)
C(16)-C(17)	1.373(3)
C(16)-H(16)	1.00(2)
C(17)-C(18)	1.377(3)
C(17)-H(17)	0.98(2)
C(18)-C(19)	1.382(3)
C(18)-H(18)	0.93(2)
C(19)-H(19)	0.957(19)
C(1)-N(1)-C(8)	124.23(14)
C(1)-N(1)-C(14)	120.11(13)
C(8)-N(1)-C(14)	115.53(13)
C(3)-N(2)-C(7)	117.35(17)
O-C(1)-N(1)	121.38(16)
O-C(1)-C(2)	120.40(17)
N(1)-C(1)-C(2)	118.22(16)
C(3)-C(2)-C(1)	113.19(15)
C(3)-C(2)-H(2A)	107.9(11)
C(1)-C(2)-H(2A)	111.7(11)
C(3)-C(2)-H(2B)	107.9(12)
C(1)-C(2)-H(2B)	107.9(12)
H(2A)-C(2)-H(2B)	108.1(16)
N(2)-C(3)-C(4)	121.84(17)
N(2)-C(3)-C(2)	116.43(16)
C(4)-C(3)-C(2)	121.66(17)
C(5)-C(4)-C(3)	119.7(2)
C(5)-C(4)-H(4)	120.6(13)
C(3)-C(4)-H(4)	119.7(13)
C(6)-C(5)-C(4)	118.7(2)
C(6)-C(5)-H(5)	122.0(13)

C(4)-C(5)-H(5)	119.2(14)
C(7)-C(6)-C(5)	118.4(2)
C(7)-C(6)-H(6)	121.0(12)
C(5)-C(6)-H(6)	120.6(12)
N(2)-C(7)-C(6)	124.0(2)
N(2)-C(7)-H(7)	114.6(13)
C(6)-C(7)-H(7)	121.4(13)
C(9)-C(8)-C(13)	120.45(16)
C(9)-C(8)-N(1)	119.44(15)
C(13)-C(8)-N(1)	120.11(15)
C(8)-C(9)-C(10)	119.56(18)
C(8)-C(9)-H(9)	118.8(10)
C(10)-C(9)-H(9)	121.6(10)
C(11)-C(10)-C(9)	120.38(19)
C(11)-C(10)-H(10)	119.9(12)
C(9)-C(10)-H(10)	119.7(12)
C(10)-C(11)-C(12)	119.96(19)
C(10)-C(11)-H(11)	119.2(13)
C(12)-C(11)-H(11)	120.8(13)
C(11)-C(12)-C(13)	120.39(19)
C(11)-C(12)-H(12)	123.4(12)
C(13)-C(12)-H(12)	116.2(12)
C(8)-C(13)-C(12)	119.25(18)
C(8)-C(13)-H(13)	120.1(10)
C(12)-C(13)-H(13)	120.6(10)
C(15)-C(14)-C(19)	120.33(17)
C(15)-C(14)-N(1)	119.53(15)
C(19)-C(14)-N(1)	120.12(15)
C(14)-C(15)-C(16)	119.90(18)
C(14)-C(15)-H(15)	120.3(11)
C(16)-C(15)-H(15)	119.8(11)

C(17)-C(16)-C(15)	119.94(19)
C(17)-C(16)-H(16)	120.2(12)
C(15)-C(16)-H(16)	119.9(12)
C(16)-C(17)-C(18)	120.04(19)
C(16)-C(17)-H(17)	118.6(12)
C(18)-C(17)-H(17)	121.4(12)
C(17)-C(18)-C(19)	120.41(19)
C(17)-C(18)-H(18)	120.1(12)
C(19)-C(18)-H(18)	119.4(12)
C(14)-C(19)-C(18)	119.37(19)
C(14)-C(19)-H(19)	119.3(11)
C(18)-C(19)-H(19)	121.3(11)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for rtp044. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O	77(1)	61(1)	56(1)	-3(1)	-2(1)	-17(1)
N(1)	53(1)	48(1)	41(1)	-2(1)	5(1)	-4(1)
N(2)	63(1)	58(1)	59(1)	7(1)	0(1)	-9(1)
C(1)	49(1)	48(1)	48(1)	3(1)	2(1)	2(1)
C(2)	61(1)	54(1)	51(1)	5(1)	12(1)	1(1)
C(3)	54(1)	51(1)	39(1)	0(1)	6(1)	-3(1)
C(4)	58(1)	68(2)	69(2)	7(1)	10(1)	-3(1)
C(5)	63(2)	83(2)	70(2)	5(1)	4(1)	15(1)
C(6)	93(2)	56(1)	54(1)	-1(1)	-3(1)	15(1)
C(7)	87(2)	54(1)	62(1)	6(1)	-2(1)	-10(1)
C(8)	48(1)	47(1)	40(1)	-1(1)	2(1)	0(1)
C(9)	49(1)	59(1)	55(1)	-5(1)	6(1)	5(1)
C(10)	49(1)	74(2)	67(2)	-8(1)	-7(1)	-3(1)
C(11)	69(2)	61(1)	53(1)	-12(1)	-5(1)	-5(1)
C(12)	67(2)	55(1)	52(1)	-9(1)	5(1)	6(1)
C(13)	49(1)	55(1)	49(1)	-1(1)	1(1)	2(1)
C(14)	49(1)	48(1)	42(1)	-5(1)	4(1)	-5(1)
C(15)	63(1)	50(1)	52(1)	-2(1)	10(1)	5(1)
C(16)	73(2)	56(1)	52(1)	5(1)	7(1)	-5(1)
C(17)	68(2)	74(2)	48(1)	-2(1)	13(1)	-15(1)
C(18)	64(1)	72(2)	59(1)	-16(1)	20(1)	-3(1)
C(19)	56(1)	54(1)	55(1)	-7(1)	6(1)	3(1)

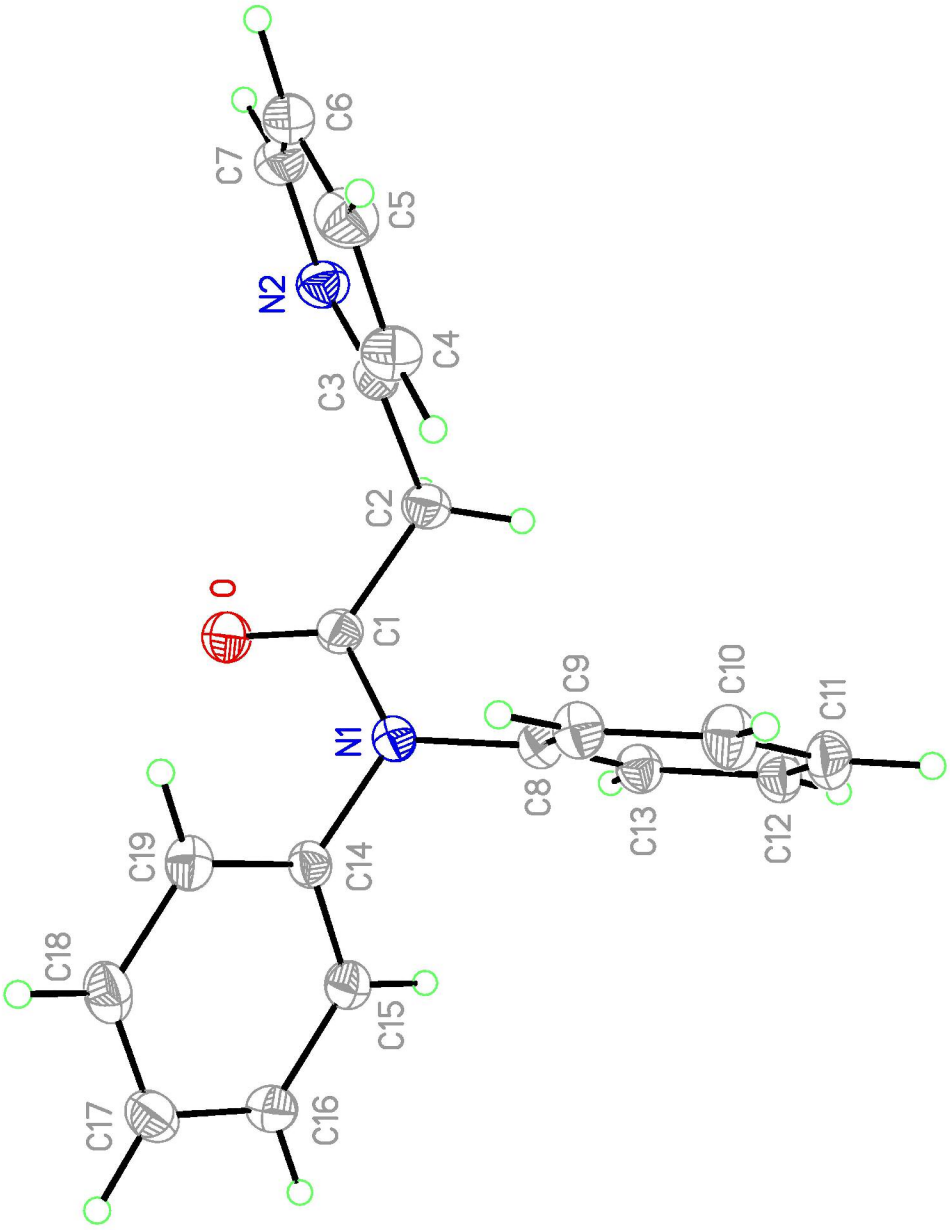
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for rtp044.

	x	y	z	U(eq)
H(2A)	4063(18)	1694(17)	8507(15)	66(6)
H(2B)	2800(20)	951(17)	8101(16)	78(7)
H(4)	6330(20)	570(20)	8515(16)	87(7)
H(5)	7400(20)	-1101(19)	9263(17)	93(7)
H(6)	6040(20)	-2696(18)	9621(16)	73(6)
H(7)	3700(20)	-2530(20)	9201(17)	90(7)
H(9)	7077(18)	2455(16)	7491(14)	60(5)
H(10)	8040(20)	3820(17)	8752(15)	78(6)
H(11)	6700(20)	5180(18)	9422(16)	77(6)
H(12)	4360(20)	5226(18)	8828(15)	76(6)
H(13)	3437(19)	3910(14)	7581(13)	58(5)
H(15)	3737(18)	3966(16)	5499(14)	63(5)
H(16)	4110(20)	4428(18)	3777(16)	78(6)
H(17)	5410(19)	3183(17)	2901(17)	78(6)
H(18)	6263(19)	1467(18)	3734(15)	73(6)
H(19)	5912(19)	1023(17)	5446(14)	67(6)

Table 6. Torsion angles [°] for rtp044.

C(8)-N(1)-C(1)-O	173.88(16)
C(14)-N(1)-C(1)-O	-1.9(2)
C(8)-N(1)-C(1)-C(2)	-6.7(2)
C(14)-N(1)-C(1)-C(2)	177.56(15)
O-C(1)-C(2)-C(3)	69.4(2)
N(1)-C(1)-C(2)-C(3)	-110.08(19)
C(7)-N(2)-C(3)-C(4)	0.0(3)
C(7)-N(2)-C(3)-C(2)	-176.78(16)
C(1)-C(2)-C(3)-N(2)	-110.11(19)
C(1)-C(2)-C(3)-C(4)	73.1(2)
N(2)-C(3)-C(4)-C(5)	0.1(3)
C(2)-C(3)-C(4)-C(5)	176.69(18)
C(3)-C(4)-C(5)-C(6)	-0.1(3)
C(4)-C(5)-C(6)-C(7)	0.1(3)
C(3)-N(2)-C(7)-C(6)	0.0(3)
C(5)-C(6)-C(7)-N(2)	0.0(3)
C(1)-N(1)-C(8)-C(9)	107.1(2)
C(14)-N(1)-C(8)-C(9)	-77.00(19)
C(1)-N(1)-C(8)-C(13)	-74.0(2)
C(14)-N(1)-C(8)-C(13)	101.98(18)
C(13)-C(8)-C(9)-C(10)	1.1(3)
N(1)-C(8)-C(9)-C(10)	-179.95(17)
C(8)-C(9)-C(10)-C(11)	-0.3(3)
C(9)-C(10)-C(11)-C(12)	-0.6(3)
C(10)-C(11)-C(12)-C(13)	0.8(3)
C(9)-C(8)-C(13)-C(12)	-0.9(3)
N(1)-C(8)-C(13)-C(12)	-179.84(16)
C(11)-C(12)-C(13)-C(8)	-0.1(3)
C(1)-N(1)-C(14)-C(15)	113.16(18)
C(8)-N(1)-C(14)-C(15)	-63.0(2)
C(1)-N(1)-C(14)-C(19)	-68.6(2)
C(8)-N(1)-C(14)-C(19)	115.26(18)
C(19)-C(14)-C(15)-C(16)	-0.9(3)

N(1)-C(14)-C(15)-C(16)	177.31(16)
C(14)-C(15)-C(16)-C(17)	0.5(3)
C(15)-C(16)-C(17)-C(18)	0.0(3)
C(16)-C(17)-C(18)-C(19)	-0.2(3)
C(15)-C(14)-C(19)-C(18)	0.8(3)
N(1)-C(14)-C(19)-C(18)	-177.44(16)
C(17)-C(18)-C(19)-C(14)	-0.2(3)


C6
C7
C5
N2
C4
C3
C2
O
C1
C9
C10
C11
N1
C8
C13
C12
C19
C14
C18
C15
C17
C16

X-ray Crystallographic data for **2** (rtp05k)

Compound 2. The molecule crystallized in the monoclinic space group C2/c. There are eight molecules in the unit cell with no unusual close approaches. All non-hydrogen atoms were refined anisotropicaly and H-atoms were included and refined in position with isotopic Us. The geometries of H12 and $H20_{abc}$ deviated from expected and these were fixed in ideal positions. The N2 geometry is planar (sum of angles 359.83°) and the N2-C7 bond length [1.3691(15) Å] is shorter than N2-C8 [1.4374(14) Å] and N2-C14 [1.4446(15) Å]. These compare favorably with the data for **1**. The pertinent data for the pyridine ring are N1-C5 [1.3361(16) Å], N1-C1 [1.3413(15) Å], C1-N1-C_5 [118.22(10)°], C1-C2 [1.3860(18) Å], C2-C3 [1.375(2) Å], C3-C4 [1.3835(18) Å], C4-C5 [1.3813(18) Å] and the carbonyl group C7-O bond length [1.2133(14) Å] is shorter than that in **1** as expected with the 6-Me substitution.

Table 1. Crystal data and structure refinement for rtp05k.

Identification code	rtp05k	
Empirical formula	C20 H18 N2 O	
Formula weight	302.36	
Temperature	233(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 15.9783(16) Å	α= 90°.
	b = 6.2843(7) Å	β= 101.218(5)°.
	c = 32.044(3) Å	γ = 90°.
Volume	3156.2(6) $Å^3$	
Z	8	
Density (calculated)	1.273 Mg/m^3	
Absorption coefficient	0.079 mm^{-1}	
F(000)	1280	
Crystal size	0.32 x 0.15 x 0.06 mm^3	
Theta range for data collection	2.60 to 30.80°.	
Index ranges	-22<=h<=21, -9<=k<=8, -41<=l<=46	
Reflections collected	23523	
Independent reflections	4852 [R(int) = 0.0235]	
Completeness to theta = 30.80°	98.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.976 and 0.995	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4852 / 0 / 276	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.0500, wR2 = 0.1233	
R indices (all data)	R1 = 0.0652, wR2 = 0.1320	
Largest diff. peak and hole	0.259 and -0.186 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for rtp05k. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O	1222(1)	3458(2)	1042(1)	47(1)
N(1)	1089(1)	1991(2)	-13(1)	30(1)
N(2)	2174(1)	1072(2)	1369(1)	32(1)
C(1)	581(1)	2984(2)	-338(1)	30(1)
C(2)	633(1)	5155(2)	-404(1)	34(1)
C(3)	1241(1)	6328(2)	-139(1)	36(1)
C(4)	1774(1)	5304(2)	193(1)	34(1)
C(5)	1664(1)	3150(2)	250(1)	29(1)
C(6)	2179(1)	1972(2)	622(1)	34(1)
C(7)	1810(1)	2261(2)	1023(1)	30(1)
C(8)	2933(1)	-182(2)	1388(1)	29(1)
C(9)	2879(1)	-2248(2)	1241(1)	37(1)
C(10)	3622(1)	-3421(3)	1259(1)	48(1)
C(11)	4400(1)	-2551(3)	1426(1)	50(1)
C(12)	4451(1)	-509(3)	1579(1)	50(1)
C(13)	3715(1)	691(2)	1562(1)	40(1)
C(14)	1826(1)	1175(2)	1753(1)	36(1)
C(15)	1920(1)	2998(3)	1998(1)	51(1)
C(16)	1586(1)	3042(4)	2369(1)	71(1)
C(17)	1172(1)	1299(5)	2490(1)	77(1)
C(18)	1087(1)	-501(4)	2245(1)	69(1)
C(19)	1413(1)	-585(3)	1871(1)	49(1)
C(20)	-61(1)	1640(3)	-621(1)	46(1)

Table 3. Bond lengths [Å] and angles [°] for rtp05k.

O-C(7)	1.2133(14)
N(1)-C(5)	1.3361(16)
N(1)-C(1)	1.3413(15)
N(2)-C(7)	1.3691(15)
N(2)-C(8)	1.4374(14)
N(2)-C(14)	1.4446(15)
C(1)-C(2)	1.3860(18)
C(1)-C(20)	1.4930(19)
C(2)-C(3)	1.375(2)
C(2)-H(2)	0.976317)
C(3)-C(4)	1.3835(18)
C(3)-H(3)	0.973(18)
C(4)-C(5)	1.3813(18)
C(4)-H(4)	0.963(17)
C(5)-C(6)	1.5060(16)
C(6)-C(7)	1.5264(16)
C(6)-H(6A)	0.988(17)
C(6)-H(6B)	1.004(18)
C(8)-C(9)	1.3783(19)
C(8)-C(13)	1.3793(18)
C(9)-C(10)	1.3900(19)
C(9)-H(9)	0.965(17)
C(10)-C(11)	1.367(3)
C(10)-H(10)	1.02(2)
C(11)-C(12)	1.370(3)
C(11)-H(11)	0.99(2)
C(12)-C(13)	1.389(2)
C(12)-H(12)	0.9400
C(13)-H(13)	0.978(18)

C(14)-C(19)	1.379(2)
C(14)-C(15)	1.381(2)
C(15)-C(16)	1.395(2)
C(15)-H(15)	1.00(2)
C(16)-C(17)	1.375(4)
C(16)-H(16)	0.98(3)
C(17)-C(18)	1.368(4)
C(17)-H(17)	0.95(3)
C(18)-C(19)	1.397(2)
C(18)-H(18)	0.99(2)
C(19)-H(19)	0.99(2)
C(20)-H(20A)	0.93(3)
C(20)-H(20B)	1.00(3)
C(20)-H(20C)	0.94(3)

C(5)-N(1)-C(1)	118.22(10)
C(7)-N(2)-C(8)	123.73(9)
C(7)-N(2)-C(14)	119.37(10)
C(8)-N(2)-C(14)	116.73(9)
N(1)-C(1)-C(2)	122.13(11)
N(1)-C(1)-C(20)	116.66(12)
C(2)-C(1)-C(20)	121.19(12)
C(3)-C(2)-C(1)	119.30(11)
C(3)-C(2)-H(2)	121.9(10)
C(1)-C(2)-H(2)	118.8(10)
C(2)-C(3)-C(4)	118.70(12)
C(2)-C(3)-H(3)	121.6(10)
C(4)-C(3)-H(3)	118.8(10)
C(5)-C(4)-C(3)	118.70(12)
C(5)-C(4)-H(4)	121.6(10)
C(3)-C(4)-H(4)	119.6(10)

N(1)-C(5)-C(4)	122.72(11)
N(1)-C(5)-C(6)	115.74(11)
C(4)-C(5)-C(6)	121.52(12)
C(5)-C(6)-C(7)	111.64(10)
C(5)-C(6)-H(6A)	111.9(10)
C(7)-C(6)-H(6A)	108.9(10)
C(5)-C(6)-H(6B)	108.0(10)
C(7)-C(6)-H(6B)	108.3(10)
H(6A)-C(6)-H(6B)	107.9(14)
O-C(7)-N(2)	120.69(11)
O-C(7)-C(6)	122.96(11)
N(2)-C(7)-C(6)	116.34(10)
C(9)-C(8)-C(13)	120.27(12)
C(9)-C(8)-N(2)	120.39(11)
C(13)-C(8)-N(2)	119.33(12)
C(8)-C(9)-C(10)	119.27(14)
C(8)-C(9)-H(9)	119.8(10)
C(10)-C(9)-H(9)	120.9(10)
C(11)-C(10)-C(9)	120.61(15)
C(11)-C(10)-H(10)	120.8(12)
C(9)-C(10)-H(10)	118.6(12)
C(10)-C(11)-C(12)	120.02(13)
C(10)-C(11)-H(11)	122.2(12)
C(12)-C(11)-H(11)	117.8(12)
C(11)-C(12)-C(13)	120.21(14)
C(11)-C(12)-H(12)	119.9
C(13)-C(12)-H(12)	119.9
C(8)-C(13)-C(12)	119.60(15)
C(8)-C(13)-H(13)	121.0(10)
C(12)-C(13)-H(13)	119.4(10)
C(19)-C(14)-C(15)	120.87(14)

C(19)-C(14)-N(2)	118.85(13)
C(15)-C(14)-N(2)	120.28(14)
C(14)-C(15)-C(16)	119.0(2)
C(14)-C(15)-H(15)	120.4(13)
C(16)-C(15)-H(15)	120.6(13)
C(17)-C(16)-C(15)	120.7(2)
C(17)-C(16)-H(16)	121.6(14)
C(15)-C(16)-H(16)	117.7(15)
C(18)-C(17)-C(16)	119.73(16)
C(18)-C(17)-H(17)	118.5(15)
C(16)-C(17)-H(17)	121.8(15)
C(17)-C(18)-C(19)	120.7(2)
C(17)-C(18)-H(18)	121.0(14)
C(19)-C(18)-H(18)	118.3(15)
C(14)-C(19)-C(18)	119.00(18)
C(14)-C(19)-H(19)	119.1(11)
C(18)-C(19)-H(19)	121.9(11)
C(1)-C(20)-H(20A)	110.3(16
C(1)-C(20)-H(20B)	112.7(15)
H(20A)-C(20)-H(20B)	100(2)
C(1)-C(20)-H(20C)	113.5(16)
H(20A)-C(20)-H(20C)	115(2)
H(20B)-C(20)-H(20C)	104(2)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for rtp05k. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O	41(1)	65(1)	35(1)	11(1)	10(1)	28(1)
N(1)	31(1)	29(1)	30(1)	3(1)	8(1)	5(1)
N(2)	31(1)	42(1)	24(1)	4(1)	6(1)	13(1)
C(1)	28(1)	35(1)	28(1)	1(1)	8(1)	5(1)
C(2)	35(1)	37(1)	29(1)	9(1)	8(1)	11(1)
C(3)	45(1)	29(1)	37(1)	6(1)	13(1)	4(1)
C(4)	37(1)	35(1)	31(1)	0(1)	6(1)	-2(1)
C(5)	28(1)	33(1)	26(1)	5(1)	8(1)	7(1)
C(6)	31(1)	45(1)	27(1)	8(1)	7(1)	12(1)
C(7)	26(1)	36(1)	27(1)	3(1)	3(1)	6(1)
C(8)	28(1)	36(1)	22(1)	6(1)	4(1)	9(1)
C(9)	39(1)	39(1)	34(1)	0(1)	7(1)	6(1)
C(10)	59(1)	42(1)	44(1)	6(1)	16(1)	20(1)
C(11)	44(1)	65(1)	42(1)	17(1)	15(1)	28(1)
C(12)	28(1)	74(1)	48(1)	13(1)	3(1)	4(1)
C(13)	34(1)	44(1)	39(1)	4(1)	3(1)	1(1)
C(14)	30(1)	53(1)	23(1)	3(1)	3(1)	14(1)
C(15)	47(1)	68(1)	36(1)	-12(1)	1(1)	13(1)
C(16)	62(1)	114(2)	35(1)	-22(1)	2(1)	31(1)
C(17)	61(1)	144(2)	31(1)	11(1)	18(1)	43(1)
C(18)	56(1)	105(2)	53(1)	28(1)	28(1)	22(1)
C(19)	44(1)	63(1)	41(1)	12(1)	15(1)	14(1)
C(20)	40(1)	51(1)	43(1)	-8(1)	2(1)	-1(1)

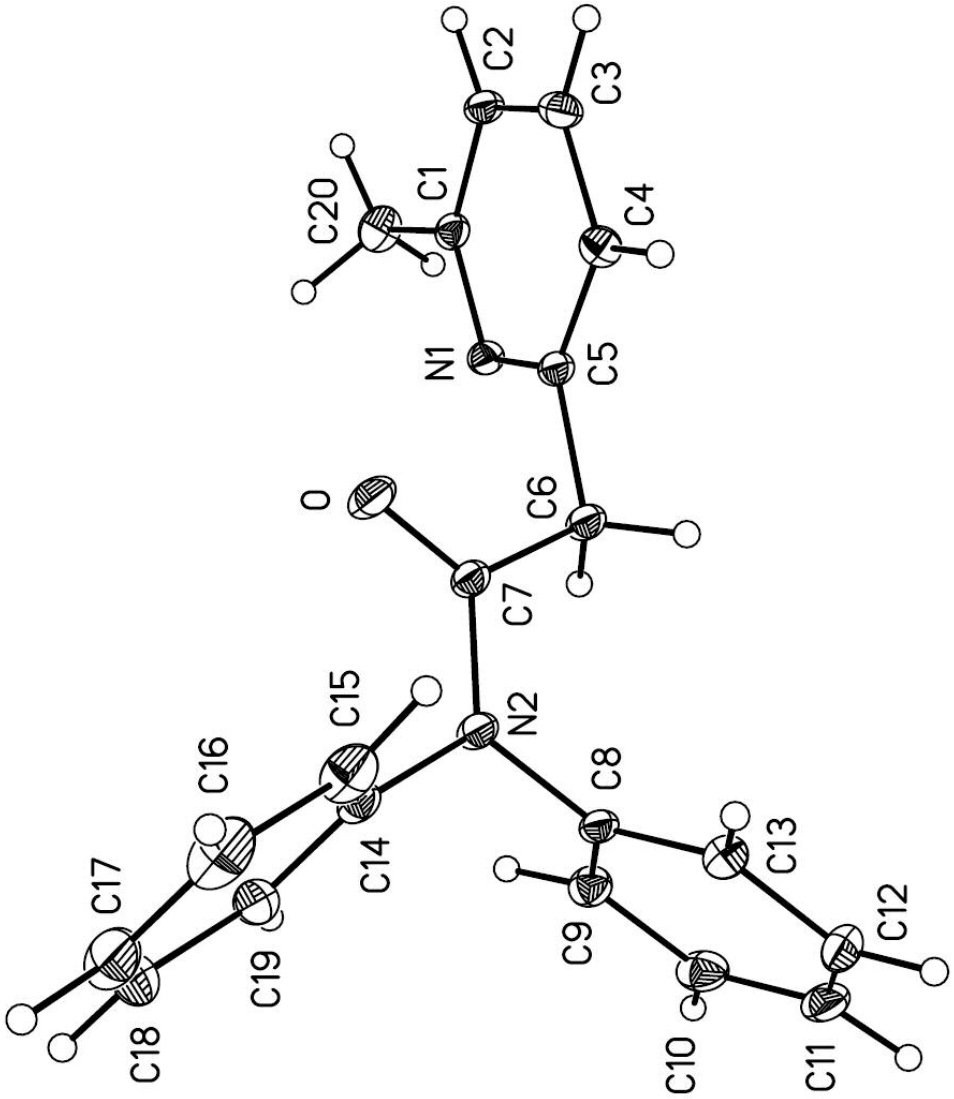
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for rtp05k.

	x	y	z	U(eq)
H(2)	238(11)	5800(30)	-639(5)	48(4)
H(3)	1291(10)	7860(30)	-172(5)	48(4)
H(4)	2205(11)	6100(30)	380(5)	48(4)
H(6A)	2782(11)	2430(30)	682(5)	51(5)
H(6B)	2163(11)	420(30)	550(6)	53(5)
H(9)	2327(11)	-2870(30)	1132(6)	50(5)
H(10)	3575(13)	-4940(40)	1144(7)	75(6)
H(11)	4938(13)	-3320(30)	1428(6)	66(6)
H(12)	4986	81	1695	65
H(13)	3759(11)	2130(30)	1680(6)	52(5)
H(15)	2197(14)	4300(40)	1902(7)	78(7)
H(16)	1653(15)	4360(40)	2536(8)	88(7)
H(17)	951(15)	1290(40)	2744(8)	95(8)
H(18)	781(16)	-1770(40)	2325(8)	90(8)
H(19)	1361(12)	-1880(30)	1691(6)	59(5)
H(20A)	211(17)	620(40)	-758(8)	100(8)
H(20B)	-387(17)	700(40)	-460(9)	103(8)
H(20C)	-484(17)	2440(40)	-802(9)	99(8)

Table 6. Torsion angles [°] for rtp05k.

C(5)-N(1)-C(1)-C(2)	-0.53(17)
C(5)-N(1)-C(1)-C(20)	-179.33(11)
N(1)-C(1)-C(2)-C(3)	2.13(18)
C(20)-C(1)-C(2)-C(3)	-179.14(12)
C(1)-C(2)-C(3)-C(4)	-1.16(18)
C(2)-C(3)-C(4)-C(5)	-1.24(19)
C(1)-N(1)-C(5)-C(4)	-2.03(17)
C(1)-N(1)-C(5)-C(6)	176.46(10)
C(3)-C(4)-C(5)-N(1)	2.94(18)
C(3)-C(4)-C(5)-C(6)	-175.47(11)
N(1)-C(5)-C(6)-C(7)	-97.15(13)
C(4)-C(5)-C(6)-C(7)	81.36(15)
C(8)-N(2)-C(7)-O	-172.33(13)
C(14)-N(2)-C(7)-O	2.88(19)
C(8)-N(2)-C(7)-C(6)	8.20(18)
C(14)-N(2)-C(7)-C(6)	-176.59(12)
C(5)-C(6)-C(7)-O	-6.28(19)
C(5)-C(6)-C(7)-N(2)	173.18(11)
C(7)-N(2)-C(8)-C(9)	-87.42(16)
C(14)-N(2)-C(8)-C(9)	97.26(14)
C(7)-N(2)-C(8)-C(13)	93.69(15)
C(14)-N(2)-C(8)-C(13)	-81.64(15)
C(13)-C(8)-C(9)-C(10)	-1.65(19)
N(2)-C(8)-C(9)-C(10)	179.46(11)
C(8)-C(9)-C(10)-C(11)	0.7(2)
C(9)-C(10)-C(11)-C(12)	0.4(2)
C(10)-C(11)-C(12)-C(13)	-0.6(2)
C(9)-C(8)-C(13)-C(12)	1.4(2)
N(2)-C(8)-C(13)-C(12)	-179.66(12)
C(11)-C(12)-C(13)-C(8)	-0.3(2)
C(7)-N(2)-C(14)-C(19)	110.98(14)
C(8)-N(2)-C(14)-C(19)	-73.48(15)
C(7)-N(2)-C(14)-C(15)	-69.96(16)

C(8)-N(2)-C(14)-C(15)	105.58(14)
C(19)-C(14)-C(15)-C(16)	-0.2(2)
N(2)-C(14)-C(15)-C(16)	-179.24(13)
C(14)-C(15)-C(16)-C(17)	0.1(3)
C(15)-C(16)-C(17)-C(18)	0.2(3)
C(16)-C(17)-C(18)-C(19)	-0.4(3)
C(15)-C(14)-C(19)-C(18)	0.0(2)
N(2)-C(14)-C(19)-C(18)	179.07(13)
C(17)-C(18)-C(19)-C(14)	0.3(3)


C2
C3
C20
C1
C4
N1
C5
O
C6
C7
C15
N2
C16
C8
C14
C13
C17
C9
C12
C19
C18
C10
C11

X-ray Crystallographic data and crystal packing for **4** (rtp055)

Compound 4. The molecule crystallized in the monoclinic space group $P2_1/n$. There are four molecules in the unit cell with no unusual intermolecular contacts. The non-hydrogen atoms were refined anisotropically. The H-atoms on C6 were allowed to vary in position as well as U_{iso}. The H-atoms on the phenyl rings and pyridine ring were placed in ideal positions [riding model] with fixed U's set to 1.2U (equiv) of the parent atom. The H-atoms on C9 were disordered over two sites with occupancies 63.3% and 36.7%. The amido N atoms, N2 and N3, are planar (sums of angles: N2, 359.98°; N3, 359.61°). The N2-C7 [1.5122(1)] and N3-C8 [1.3753(19) Å] are shorter than respective N-C (phyenyl) bond lengths: N2-C10 [1.440(2) Å], N2-C16 [1.4405(19) Å], N3-C28 [1.4404(19) Å], N3-C22 [1.441(2) Å]. The carbonyl bond lengths C7-O1 [1.2147(17) Å] and C8-O2 [1.2140(17) Å] compare favorably with the related distance in **2**.

Table 1. Crystal data and structure refinement for rtp055.

Identification code	rtp055	
Empirical formula	C33 H27 N3 O2	
Formula weight	497.58	
Temperature	292(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 9.7206(10) Å	α= 90°.
	b = 16.6521(11) Å	β= 104.408(9)°.
	c = 17.1319(14) Å	γ = 90°.
Volume	2685.9(4) $Å^3$	
Z	4	
Density (calculated)	1.230 Mg/m^3	
Absorption coefficient	0.077 mm^{-1}	
F(000)	1048	
Crystal size	0.55 x 0.30 x 0.15 mm^3	
Theta range for data collection	1.73 to 25.50°.	
Index ranges	0<=h<=11, -20<=k<=20, -20<=l<=20	
Reflections collected	10410	
Independent reflections	4994 [R(int) = 0.0312]	
Completeness to theta = 25.50°	100.0 %	
Absorption correction	Psi-scan	
Max. and min. transmission	0.9851 and 0.9616	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4994 / 0 / 348	
Goodness-of-fit on F^2	1.018	
Final R indices [I>2sigma(I)]	R1 = 0.0426, wR2 = 0.0979	
R indices (all data)	R1 = 0.0705, wR2 = 0.1096	
Largest diff. peak and hole	0.110 and -0.150 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for rtp055. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4067(1)	1767(1)	3890(1)	60(1)
O(2)	4719(1)	1686(1)	2180(1)	48(1)
N(1)	3097(1)	3625(1)	1807(1)	48(1)
N(2)	3075(1)	2966(1)	4073(1)	43(1)
N(3)	6571(1)	2171(1)	3144(1)	42(1)
C(1)	1992(2)	3832(1)	1197(1)	62(1)
C(2)	736(2)	3413(1)	1030(1)	74(1)
C(3)	592(2)	2764(1)	1494(1)	73(1)
C(4)	1715(2)	2548(1)	2126(1)	55(1)
C(5)	2946(2)	2996(1)	2263(1)	39(1)
C(6)	4222(2)	2804(1)	2944(1)	37(1)
C(7)	3803(2)	2460(1)	3686(1)	42(1)
C(8)	5178(2)	2175(1)	2705(1)	38(1)
C(9)	2186(3)	4556(2)	717(2)	109(1)
C(10)	2948(2)	3807(1)	3874(1)	43(1)
C(11)	4125(2)	4297(1)	4069(1)	54(1)
C(12)	3997(2)	5094(1)	3837(1)	70(1)
C(13)	2707(3)	5394(1)	3437(1)	76(1)
C(14)	1526(2)	4912(1)	3266(1)	69(1)
C(15)	1643(2)	4114(1)	3481(1)	54(1)
C(16)	2391(2)	2677(1)	4674(1)	44(1)
C(17)	2304(2)	3177(1)	5305(1)	55(1)
C(18)	1601(2)	2921(2)	5871(1)	67(1)
C(19)	1005(2)	2173(2)	5818(1)	75(1)
C(20)	1085(2)	1679(1)	5188(1)	73(1)
C(21)	1775(2)	1928(1)	4617(1)	58(1)
C(22)	7190(2)	2815(1)	3679(1)	45(1)
C(23)	7461(2)	2714(1)	4500(1)	62(1)
C(24)	8033(2)	3345(2)	5005(1)	80(1)
C(25)	8315(2)	4059(2)	4692(2)	86(1)

C(26)	8056(2)	4161(1)	3876(2)	79(1)
C(27)	7503(2)	3531(1)	3363(1)	60(1)
C(28)	7400(2)	1455(1)	3141(1)	45(1)
C(29)	8677(2)	1494(1)	2939(1)	62(1)
C(30)	9465(2)	799(1)	2944(1)	77(1)
C(31)	8987(2)	83(1)	3150(1)	80(1)
C(32)	7710(3)	43(1)	3352(1)	80(1)
C(33)	6911(2)	730(1)	3348(1)	61(1)

Table 3. Bond lengths [Å] and angles [°] for rtp055.

O(1)-C(7)	1.2147(17)	C(12)-H(12)	0.9300
O(2)-C(8)	1.2140(17)	C(13)-C(14)	1.372(3)
N(1)-C(5)	1.3350(19)	C(13)-H(13)	0.9300
N(1)-C(1)	1.344(2)	C(14)-C(15)	1.375(2)
N(2)-C(7)	1.3722(19)	C(14)-H(14)	0.9300
N(2)-C(10)	1.440(2)	C(15)-H(15)	0.9300
N(2)-C(16)	1.4405(19)	C(16)-C(21)	1.375(2)
N(3)-C(8)	1.3753(19)	C(16)-C(17)	1.384(2)
N(3)-C(28)	1.4404(19)	C(17)-C(18)	1.385(3)
N(3)-C(22)	1.441(2)	C(17)-H(17)	0.9300
C(1)-C(2)	1.374(3)	C(18)-C(19)	1.367(3)
C(1)-C(9)	1.497(3)	C(18)-H(18)	0.9300
C(2)-C(3)	1.369(3)	C(19)-C(20)	1.375(3)
C(2)-H(2)	0.9300	C(19)-H(19)	0.9300
C(3)-C(4)	1.380(3)	C(20)-C(21)	1.380(3)
C(3)-H(3)	0.9300	C(20)-H(20)	0.9300
C(4)-C(5)	1.380(2)	C(21)-H(21)	0.9300
C(4)-H(4)	0.9300	C(22)-C(27)	1.374(2)
C(5)-C(6)	1.511(2)	C(22)-C(23)	1.377(2)
C(6)-C(8)	1.524(2)	C(23)-C(24)	1.386(3)
C(6)-C(7)	1.539(2)	C(23)-H(23)	0.9300
C(6)-H(6)	0.958(14)	C(24)-C(25)	1.361(3)
C(9)-H(9A)	0.9600	C(24)-H(24)	0.9300
C(9)-H(9B)	0.9600	C(25)-C(26)	1.367(3)
C(9)-H(9C)	0.9600	C(25)-H(25)	0.9300
C(9)-H(9D)	0.9600	C(26)-C(27)	1.388(3)
C(9)-H(9E)	0.9600	C(26)-H(26)	0.9300
C(9)-H(9F)	0.9600	C(27)-H(27)	0.9300
C(10)-C(11)	1.377(2)	C(28)-C(29)	1.370(2)
C(10)-C(15)	1.378(2)	C(28)-C(33)	1.376(2)
C(11)-C(12)	1.381(3)	C(29)-C(30)	1.387(3)
C(11)-H(11)	0.9300	C(29)-H(29)	0.9300
C(12)-C(13)	1.366(3)	C(30)-C(31)	1.358(3)

C(30)-H(30)	0.9300	C(32)-C(33)	1.381(3)
C(31)-C(32)	1.371(3)	C(32)-H(32)	0.9300
C(31)-H(31)	0.9300	C(33)-H(33)	0.9300

C(5)-N(1)-C(1)	118.25(15)	O(2)-C(8)-C(6)	121.64(14)
C(7)-N(2)-C(10)	120.46(12)	N(3)-C(8)-C(6)	116.11(13)
C(7)-N(2)-C(16)	121.65(13)	C(1)-C(9)-H(9A)	109.5
C(10)-N(2)-C(16)	117.87(12)	C(1)-C(9)-H(9B)	109.5
C(8)-N(3)-C(28)	118.50(13)	H(9A)-C(9)-H(9B)	109.5
C(8)-N(3)-C(22)	122.86(12)	C(1)-C(9)-H(9C)	109.5
C(28)-N(3)-C(22)	118.25(12)	H(9A)-C(9)-H(9C)	109.5
N(1)-C(1)-C(2)	121.87(18)	H(9B)-C(9)-H(9C)	109.5
N(1)-C(1)-C(9)	116.67(18)	C(1)-C(9)-H(9D)	109.5
C(2)-C(1)-C(9)	121.45(19)	H(9A)-C(9)-H(9D)	54.6
C(3)-C(2)-C(1)	119.64(18)	H(9B)-C(9)-H(9D)	57.9
C(3)-C(2)-H(2)	120.2	H(9C)-C(9)-H(9D)	141.0
C(1)-C(2)-H(2)	120.2	C(1)-C(9)-H(9E)	109.5
C(2)-C(3)-C(4)	119.07(18)	H(9A)-C(9)-H(9E)	141.0
C(2)-C(3)-H(3)	120.5	H(9B)-C(9)-H(9E)	54.6
C(4)-C(3)-H(3)	120.5	H(9C)-C(9)-H(9E)	57.9
C(5)-C(4)-C(3)	118.40(18)	H(9D)-C(9)-H(9E)	109.5
C(5)-C(4)-H(4)	120.8	C(1)-C(9)-H(9F)	109.5
C(3)-C(4)-H(4)	120.8	H(9A)-C(9)-H(9F)	57.9
N(1)-C(5)-C(4)	122.77(15)	H(9B)-C(9)-H(9F)	141.0
N(1)-C(5)-C(6)	115.39(13)	H(9C)-C(9)-H(9F)	54.6
C(4)-C(5)-C(6)	121.83(15)	H(9D)-C(9)-H(9F)	109.5
C(5)-C(6)-C(8)	112.12(12)	H(9E)-C(9)-H(9F)	109.5
C(5)-C(6)-C(7)	112.47(12)	C(11)-C(10)-C(15)	120.45(16)
C(8)-C(6)-C(7)	105.70(12)	C(11)-C(10)-N(2)	120.13(15)
C(5)-C(6)-H(6)	106.4(9)	C(15)-C(10)-N(2)	119.42(15)
C(8)-C(6)-H(6)	110.8(9)	C(10)-C(11)-C(12)	119.31(18)
C(7)-C(6)-H(6)	109.4(9)	C(10)-C(11)-H(11)	120.3
O(1)-C(7)-N(2)	122.88(14)	C(12)-C(11)-H(11)	120.3
O(1)-C(7)-C(6)	120.67(14)	C(13)-C(12)-C(11)	120.1(2)
N(2)-C(7)-C(6)	116.39(13)	C(13)-C(12)-H(12)	119.9
O(2)-C(8)-N(3)	122.19(14)	C(11)-C(12)-H(12)	119.9

C(12)-C(13)-C(14)	120.51(19)	C(24)-C(25)-C(26)	120.4(2)
C(12)-C(13)-H(13)	119.7	C(24)-C(25)-H(25)	119.8
C(14)-C(13)-H(13)	119.7	C(26)-C(25)-H(25)	119.8
C(13)-C(14)-C(15)	119.95(19)	C(25)-C(26)-C(27)	119.9(2)
C(13)-C(14)-H(14)	120.0	C(25)-C(26)-H(26)	120.1
C(15)-C(14)-H(14)	120.0	C(27)-C(26)-H(26)	120.1
C(14)-C(15)-C(10)	119.61(18)	C(22)-C(27)-C(26)	119.68(19)
C(14)-C(15)-H(15)	120.2	C(22)-C(27)-H(27)	120.2
C(10)-C(15)-H(15)	120.2	C(26)-C(27)-H(27)	120.2
C(21)-C(16)-C(17)	119.40(16)	C(29)-C(28)-C(33)	120.02(16)
C(21)-C(16)-N(2)	121.53(15)	C(29)-C(28)-N(3)	120.25(16)
C(17)-C(16)-N(2)	119.02(15)	C(33)-C(28)-N(3)	119.72(15)
C(16)-C(17)-C(18)	119.89(19)	C(28)-C(29)-C(30)	119.47(19)
C(16)-C(17)-H(17)	120.1	C(28)-C(29)-H(29)	120.3
C(18)-C(17)-H(17)	120.1	C(30)-C(29)-H(29)	120.3
C(19)-C(18)-C(17)	120.55(19)	C(31)-C(30)-C(29)	120.7(2)
C(19)-C(18)-H(18)	119.7	C(31)-C(30)-H(30)	119.7
C(17)-C(18)-H(18)	119.7	C(29)-C(30)-H(30)	119.7
C(18)-C(19)-C(20)	119.43(18)	C(30)-C(31)-C(32)	119.84(19)
C(18)-C(19)-H(19)	120.3	C(30)-C(31)-H(31)	120.1
C(20)-C(19)-H(19)	120.3	C(32)-C(31)-H(31)	120.1
C(19)-C(20)-C(21)	120.6(2)	C(31)-C(32)-C(33)	120.2(2)
C(19)-C(20)-H(20)	119.7	C(31)-C(32)-H(32)	119.9
C(21)-C(20)-H(20)	119.7	C(33)-C(32)-H(32)	119.9
C(16)-C(21)-C(20)	120.10(18)	C(28)-C(33)-C(32)	119.82(18)
C(16)-C(21)-H(21)	120.0	C(28)-C(33)-H(33)	120.1
C(20)-C(21)-H(21)	120.0	C(32)-C(33)-H(33)	120.1
C(27)-C(22)-C(23)	120.25(17)		
C(27)-C(22)-N(3)	119.58(15)		
C(23)-C(22)-N(3)	120.16(16)		
C(22)-C(23)-C(24)	119.3(2)		
C(22)-C(23)-H(23)	120.3		
C(24)-C(23)-H(23)	120.3		
C(25)-C(24)-C(23)	120.4(2)		
C(25)-C(24)-H(24)	119.8		
C(23)-C(24)-H(24)	119.8		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for rtp055. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	74(1)	48(1)	72(1)	16(1)	42(1)	19(1)
O(2)	46(1)	49(1)	51(1)	-10(1)	15(1)	-2(1)
N(1)	44(1)	53(1)	46(1)	7(1)	9(1)	0(1)
N(2)	43(1)	45(1)	44(1)	3(1)	19(1)	7(1)
N(3)	36(1)	43(1)	49(1)	-3(1)	12(1)	4(1)
C(1)	57(1)	72(1)	52(1)	10(1)	2(1)	5(1)
C(2)	52(1)	97(2)	60(1)	-2(1)	-7(1)	6(1)
C(3)	44(1)	93(2)	76(1)	-15(1)	4(1)	-18(1)
C(4)	46(1)	59(1)	59(1)	-4(1)	12(1)	-12(1)
C(5)	35(1)	42(1)	42(1)	-4(1)	14(1)	0(1)
C(6)	35(1)	37(1)	41(1)	-2(1)	12(1)	-1(1)
C(7)	41(1)	42(1)	46(1)	3(1)	17(1)	5(1)
C(8)	37(1)	41(1)	41(1)	1(1)	16(1)	-1(1)
C(9)	107(2)	115(2)	88(2)	51(2)	-9(2)	-3(2)
C(10)	45(1)	43(1)	43(1)	-2(1)	17(1)	7(1)
C(11)	50(1)	55(1)	59(1)	-11(1)	15(1)	1(1)
C(12)	77(2)	50(1)	92(2)	-13(1)	36(1)	-12(1)
C(13)	94(2)	48(1)	96(2)	11(1)	44(1)	13(1)
C(14)	68(1)	60(1)	80(1)	12(1)	23(1)	25(1)
C(15)	47(1)	55(1)	60(1)	3(1)	17(1)	11(1)
C(16)	36(1)	58(1)	40(1)	7(1)	12(1)	11(1)
C(17)	47(1)	72(1)	48(1)	-2(1)	16(1)	10(1)
C(18)	56(1)	102(2)	47(1)	3(1)	23(1)	20(1)
C(19)	65(1)	103(2)	68(1)	26(1)	38(1)	18(1)
C(20)	71(1)	77(1)	85(2)	19(1)	43(1)	4(1)
C(21)	61(1)	60(1)	60(1)	4(1)	28(1)	2(1)
C(22)	34(1)	49(1)	52(1)	-6(1)	9(1)	6(1)
C(23)	64(1)	67(1)	52(1)	-1(1)	6(1)	16(1)
C(24)	69(1)	98(2)	62(1)	-24(1)	-6(1)	23(1)
C(25)	52(1)	90(2)	107(2)	-43(2)	3(1)	-5(1)

C(26)	60(1)	67(1)	113(2)	-21(1)	28(1)	-20(1)
C(27)	51(1)	60(1)	72(1)	-6(1)	21(1)	-9(1)
C(28)	44(1)	48(1)	44(1)	-2(1)	13(1)	10(1)
C(29)	50(1)	62(1)	79(1)	-6(1)	25(1)	6(1)
C(30)	53(1)	83(2)	99(2)	-20(1)	24(1)	16(1)
C(31)	65(1)	66(1)	103(2)	-23(1)	6(1)	26(1)
C(32)	84(2)	51(1)	101(2)	6(1)	18(1)	15(1)
C(33)	61(1)	54(1)	73(1)	8(1)	24(1)	12(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for rtp055.

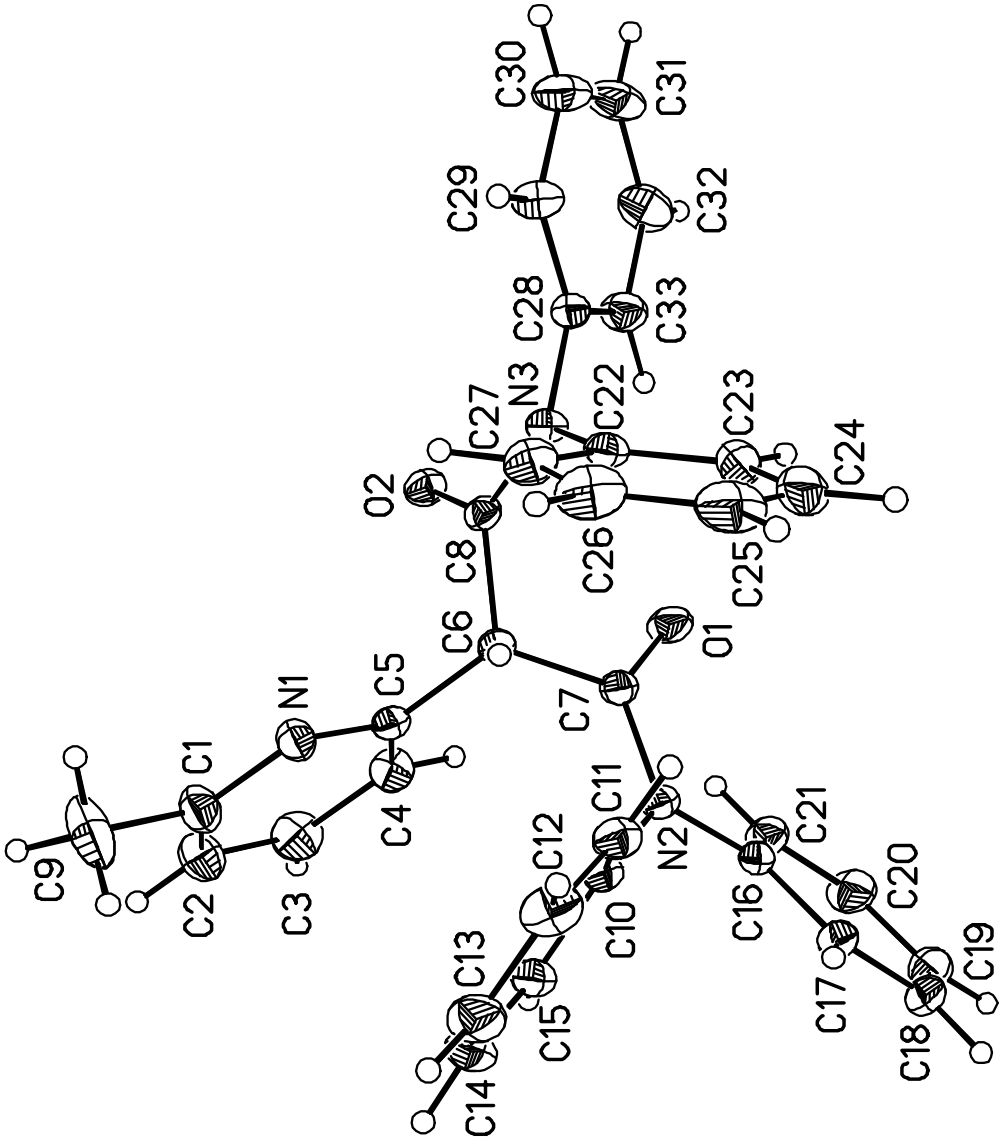
	x	y	z	U(eq)
H(2)	-12	3569	604	88
H(3)	-251	2473	1385	87
H(4)	1643	2111	2451	66
H(6)	4722(16)	3300(9)	3087(9)	37(4)
H(9A)	1546	4527	192	108(7)
H(9B)	3146	4574	666	108(7)
H(9C)	1990	5032	987	108(7)
H(9D)	2436	4389	234	108(7)
H(9E)	2930	4887	1032	108(7)
H(9F)	1317	4857	579	108(7)
H(11)	4997	4094	4353	65
H(12)	4791	5426	3954	84
H(13)	2628	5930	3279	91
H(14)	647	5124	3005	82
H(15)	846	3784	3362	64
H(17)	2716	3684	5349	66
H(18)	1534	3261	6291	80
H(19)	550	2000	6206	90
H(20)	670	1173	5146	88
H(21)	1824	1589	4193	70
H(23)	7262	2227	4715	75
H(24)	8224	3279	5560	96
H(25)	8688	4481	5035	103
H(26)	8250	4651	3665	95
H(27)	7344	3593	2808	72
H(29)	9013	1983	2800	74
H(30)	10330	824	2804	93
H(31)	9525	-380	3153	96
H(32)	7381	-447	3492	95
H(33)	6045	702	3485	74

Table 6. Torsion angles [°] for rtp055.

C(5)-N(1)-C(1)-C(2)	-0.7(3)
C(5)-N(1)-C(1)-C(9)	178.02(19)
N(1)-C(1)-C(2)-C(3)	0.1(3)
C(9)-C(1)-C(2)-C(3)	-178.6(2)
C(1)-C(2)-C(3)-C(4)	0.4(3)
C(2)-C(3)-C(4)-C(5)	-0.2(3)
C(1)-N(1)-C(5)-C(4)	0.9(2)
C(1)-N(1)-C(5)-C(6)	-179.15(15)
C(3)-C(4)-C(5)-N(1)	-0.5(3)
C(3)-C(4)-C(5)-C(6)	179.63(16)
N(1)-C(5)-C(6)-C(8)	-93.91(16)
C(4)-C(5)-C(6)-C(8)	86.01(18)
N(1)-C(5)-C(6)-C(7)	147.13(13)
C(4)-C(5)-C(6)-C(7)	-32.9(2)
C(10)-N(2)-C(7)-O(1)	172.06(15)
C(16)-N(2)-C(7)-O(1)	-9.4(2)
C(10)-N(2)-C(7)-C(6)	-10.6(2)
C(16)-N(2)-C(7)-C(6)	167.96(13)
C(5)-C(6)-C(7)-O(1)	112.34(17)
C(8)-C(6)-C(7)-O(1)	-10.3(2)
C(5)-C(6)-C(7)-N(2)	-65.05(18)
C(8)-C(6)-C(7)-N(2)	172.30(13)
C(28)-N(3)-C(8)-O(2)	-17.3(2)
C(22)-N(3)-C(8)-O(2)	170.04(15)
C(28)-N(3)-C(8)-C(6)	159.77(13)
C(22)-N(3)-C(8)-C(6)	-12.9(2)
C(5)-C(6)-C(8)-O(2)	-26.1(2)
C(7)-C(6)-C(8)-O(2)	96.77(16)
C(5)-C(6)-C(8)-N(3)	156.83(13)
C(7)-C(6)-C(8)-N(3)	-80.29(15)
C(7)-N(2)-C(10)-C(11)	-68.7(2)
C(16)-N(2)-C(10)-C(11)	112.65(17)
C(7)-N(2)-C(10)-C(15)	110.69(17)

C(16)-N(2)-C(10)-C(15)	-67.94(19)
C(15)-C(10)-C(11)-C(12)	-2.6(3)
N(2)-C(10)-C(11)-C(12)	176.80(15)
C(10)-C(11)-C(12)-C(13)	1.6(3)
C(11)-C(12)-C(13)-C(14)	0.4(3)
C(12)-C(13)-C(14)-C(15)	-1.6(3)
C(13)-C(14)-C(15)-C(10)	0.6(3)
C(11)-C(10)-C(15)-C(14)	1.5(3)
N(2)-C(10)-C(15)-C(14)	-177.90(16)
C(7)-N(2)-C(16)-C(21)	-34.6(2)
C(10)-N(2)-C(16)-C(21)	144.06(16)
C(7)-N(2)-C(16)-C(17)	148.02(15)
C(10)-N(2)-C(16)-C(17)	-33.4(2)
C(21)-C(16)-C(17)-C(18)	0.0(2)
N(2)-C(16)-C(17)-C(18)	177.49(15)
C(16)-C(17)-C(18)-C(19)	0.8(3)
C(17)-C(18)-C(19)-C(20)	-1.2(3)
C(18)-C(19)-C(20)-C(21)	0.9(3)
C(17)-C(16)-C(21)-C(20)	-0.4(3)
N(2)-C(16)-C(21)-C(20)	-177.79(16)
C(19)-C(20)-C(21)-C(16)	-0.1(3)
C(8)-N(3)-C(22)-C(27)	-73.9(2)
C(28)-N(3)-C(22)-C(27)	113.43(17)
C(8)-N(3)-C(22)-C(23)	105.89(18)
C(28)-N(3)-C(22)-C(23)	-66.8(2)
C(27)-C(22)-C(23)-C(24)	0.9(3)
N(3)-C(22)-C(23)-C(24)	-178.84(16)
C(22)-C(23)-C(24)-C(25)	0.4(3)
C(23)-C(24)-C(25)-C(26)	-0.8(3)
C(24)-C(25)-C(26)-C(27)	-0.1(3)
C(23)-C(22)-C(27)-C(26)	-1.8(3)
N(3)-C(22)-C(27)-C(26)	177.92(16)
C(25)-C(26)-C(27)-C(22)	1.4(3)
C(8)-N(3)-C(28)-C(29)	126.53(17)
C(22)-N(3)-C(28)-C(29)	-60.4(2)
C(8)-N(3)-C(28)-C(33)	-54.1(2)

C(22)-N(3)-C(28)-C(33)	118.94(18)
C(33)-C(28)-C(29)-C(30)	0.2(3)
N(3)-C(28)-C(29)-C(30)	179.61(17)
C(28)-C(29)-C(30)-C(31)	-0.3(3)
C(29)-C(30)-C(31)-C(32)	0.3(4)
C(30)-C(31)-C(32)-C(33)	-0.1(4)
C(29)-C(28)-C(33)-C(32)	-0.1(3)
N(3)-C(28)-C(33)-C(32)	-179.44(17)
C(31)-C(32)-C(33)-C(28)	0.0(3)


C30
C31
C29
C32
C28
C33
N3
C27
C22
C23
C24
O2
C26
C25
C8
C6
O1
C5
N1
C7
C1
C4
C11
C12
N2
C21
C9
C2
C3
C10
C16
C20
C13
C17
C19
C15
C18
C14

X-ray Crystallographic data and crystal packing for **6** (rtp05n)

Compound 6. The molecule crystallized in the orthorhombic space group P2(1)2(1)2(1). There are four molecules in the unit cell with no unusual intermolecular distances. Integration of the data yielded 29369 reflections to a maximum $2\theta = 65.36°$ of which 6235 were independent with 5272 with $2\sigma(I)$. Averaging Friedel pairs gave 3486 independent reflections with 2948 with $2\sigma(I)$. The absolute configuration was not determined. The final cell constants listed in the summary table were based on the xyz centroids of 7040 reflections above $10\sigma(I)$. All non-hydrogen atoms were refined anisotropically. H-atoms were included in ideal positions with fixed $U_{iso} = 1.3$ U (equiv) of the parent atom for phenyl C atoms and $U_{iso} = 1.5$ U (equiv) for hydrogen atoms on C20. The N2-C7 bond length [1.3618(16) Å] is shorter than N2-C8 [1.4344(17) Å] and N2-C14 [1.4353(17) Å] and the N2 atom is planar (sum of angles, 359.77°). The carbonyl bond lengths are C_6-O1 [1.2084(16) Å] and C7-O2 [1.2199(17)Å] with the shorter being adjacent to the pyridine ring. The carbonyl C = O vectors are twisted relative to each other by 68.4° and the N1-C5-C6-O1 torsion angle is -171.6°.

Table 1. Crystal data and structure refinement for rtp05n.

Identification code	rtp05n	
Empirical formula	C20 H16 N2 O2	
Formula weight	316.35	
Temperature	233(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 9.6324(2) Å	α= 90°.
	b = 12.4812(3) Å	β= 90°.
	c = 14.0456(3) Å	γ = 90°.
Volume	1688.62(6) $Å^3$	
Z	4	
Density (calculated)	1.244 Mg/m^3	
Absorption coefficient	0.082 mm^{-1}	
F(000)	664	
Crystal size	0.26 x 0.20 x 0.10 mm^3	
Theta range for data collection	2.56 to 32.76°.	
Index ranges	-10<=h<=14, -18<=k<=19, -21<=l<=21	
Reflections collected	29190	
Independent reflections	3486 [R(int) = 0.0204]	
Completeness to theta = 32.76°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.992 and 0.960	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3486 / 0 / 218	
Goodness-of-fit on F^2	1.062	
Final R indices [I>2sigma(I)]	R1 = 0.0392, wR2 = 0.1031	
R indices (all data)	R1 = 0.0513, wR2 = 0.1131	
Largest diff. peak and hole	0.277 and -0.158 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for rtp05n. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	2821(2)	3830(1)	-1666(1)	49(1)
O(2)	5109(1)	5201(1)	-935(1)	39(1)
N(1)	1903(1)	5879(1)	-80(1)	36(1)
N(2)	4326(1)	4368(1)	410(1)	29(1)
C(1)	851(2)	6463(1)	257(1)	44(1)
C(2)	-502(2)	6304(2)	-61(2)	62(1)
C(3)	-783(2)	5532(2)	-726(2)	71(1)
C(4)	303(2)	4910(2)	-1077(1)	55(1)
C(5)	1618(2)	5118(1)	-726(1)	36(1)
C(6)	2834(2)	4470(1)	-1020(1)	33(1)
C(7)	4202(2)	4722(1)	-503(1)	29(1)
C(8)	3237(1)	3754(1)	844(1)	29(1)
C(9)	2934(2)	2738(1)	507(1)	37(1)
C(10)	1835(2)	2177(1)	905(1)	44(1)
C(11)	1059(2)	2620(2)	1628(1)	46(1)
C(12)	1399(2)	3623(1)	1983(1)	43(1)
C(13)	2489(2)	4193(1)	1594(1)	36(1)
C(14)	5489(2)	4680(1)	986(1)	32(1)
C(15)	5746(2)	5757(1)	1156(1)	42(1)
C(16)	6870(2)	6038(2)	1729(1)	56(1)
C(17)	7710(2)	5263(2)	2114(1)	59(1)
C(18)	7438(2)	4198(2)	1949(1)	54(1)
C(19)	6318(2)	3899(1)	1387(1)	42(1)
C(20)	1197(3)	7264(2)	1021(2)	61(1)

Table 3. Bond lengths [Å] and angles [°] for rtp05n.

O(1)-C(6)	1.2084(16)
O(2)-C(7)	1.2199(17)
N(1)-C(1)	1.335(2)
N(1)-C(5)	1.3418(19)
N(2)-C(7)	1.3618(16)
N(2)-C(8)	1.4344(17)
N(2)-C(14)	1.4353(17)
C(1)-C(2)	1.393(3)
C(1)-C(20)	1.504(3)
C(2)-C(3)	1.369(4)
C(2)-H(2)	0.9400
C(3)-C(4)	1.392(3)
C(3)-H(3)	0.9400
C(4)-C(5)	1.383(2)
C(4)-H(4)	0.9400
C(5)-C(6)	1.483(2)
C(6)-C(7)	1.537(2)
C(8)-C(9)	1.3847(19)
C(8)-C(13)	1.3891(19)
C(9)-C(10)	1.387(2)
C(9)-H(9)	0.9400
C(10)-C(11)	1.377(3)
C(10)-H(10)	0.9400
C(11)-C(12)	1.387(3)
C(11)-H(11)	0.9400
C(12)-C(13)	1.381(2)
C(12)-H(12)	0.9400
C(13)-H(13)	0.9400
C(14)-C(19)	1.380(2)
C(14)-C(15)	1.386(2)
C(15)-C(16)	1.394(3)
C(15)-H(15)	0.9400
C(16)-C(17)	1.372(3)

C(16)-H(16)	0.9400
C(17)-C(18)	1.375(3)
C(17)-H(17)	0.9400
C(18)-C(19)	1.388(2)
C(18)-H(18)	0.9400
C(19)-H(19)	0.9400
C(20)-H(20A)	0.9700
C(20)-H(20B)	0.9700
C(20)-H(20C)	0.9700

C(1)-N(1)-C(5)	118.14(14)
C(7)-N(2)-C(8)	120.59(12)
C(7)-N(2)-C(14)	120.75(12)
C(8)-N(2)-C(14)	118.43(11)
N(1)-C(1)-C(2)	121.18(17)
N(1)-C(1)-C(20)	116.66(17)
C(2)-C(1)-C(20)	122.11(17)
C(3)-C(2)-C(1)	120.34(19)
C(3)-C(2)-H(2)	119.8
C(1)-C(2)-H(2)	119.8
C(2)-C(3)-C(4)	119.0(2)
C(2)-C(3)-H(3)	120.5
C(4)-C(3)-H(3)	120.5
C(5)-C(4)-C(3)	117.21(19)
C(5)-C(4)-H(4)	121.4
C(3)-C(4)-H(4)	121.4
N(1)-C(5)-C(4)	124.10(15)
N(1)-C(5)-C(6)	114.39(13)
C(4)-C(5)-C(6)	121.47(15)
O(1)-C(6)-C(5)	124.13(14)
O(1)-C(6)-C(7)	119.96(14)
C(5)-C(6)-C(7)	115.71(11)
O(2)-C(7)-N(2)	124.37(13)
O(2)-C(7)-C(6)	118.61(12)
N(2)-C(7)-C(6)	117.00(12)
C(9)-C(8)-C(13)	120.71(13)

C(9)-C(8)-N(2)	119.92(12)
C(13)-C(8)-N(2)	119.37(12)
C(8)-C(9)-C(10)	119.10(14)
C(8)-C(9)-H(9)	120.5
C(10)-C(9)-H(9)	120.5
C(11)-C(10)-C(9)	120.55(14)
C(11)-C(10)-H(10)	119.7
C(9)-C(10)-H(10)	119.7
C(10)-C(11)-C(12)	119.98(15)
C(10)-C(11)-H(11)	120.0
C(12)-C(11)-H(11)	120.0
C(13)-C(12)-C(11)	120.16(15)
C(13)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9
C(12)-C(13)-C(8)	119.43(14)
C(12)-C(13)-H(13)	120.3
C(8)-C(13)-H(13)	120.3
C(19)-C(14)-C(15)	120.72(14)
C(19)-C(14)-N(2)	119.32(13)
C(15)-C(14)-N(2)	119.94(13)
C(14)-C(15)-C(16)	118.82(16)
C(14)-C(15)-H(15)	120.6
C(16)-C(15)-H(15)	120.6
C(17)-C(16)-C(15)	120.53(17)
C(17)-C(16)-H(16)	119.7
C(15)-C(16)-H(16)	119.7
C(16)-C(17)-C(18)	120.21(17)
C(16)-C(17)-H(17)	119.9
C(18)-C(17)-H(17)	119.9
C(17)-C(18)-C(19)	120.22(18)
C(17)-C(18)-H(18)	119.9
C(19)-C(18)-H(18)	119.9
C(14)-C(19)-C(18)	119.49(16)
C(14)-C(19)-H(19)	120.3
C(18)-C(19)-H(19)	120.3
C(1)-C(20)-H(20A)	109.5

C(1)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(1)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for rtp05n. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	59(1)	50(1)	37(1)	-14(1)	-10(1)	10(1)
O(2)	41(1)	41(1)	35(1)	4(1)	5(1)	-1(1)
N(1)	39(1)	36(1)	32(1)	1(1)	0(1)	8(1)
N(2)	28(1)	33(1)	27(1)	1(1)	-1(1)	-2(1)
C(1)	51(1)	43(1)	37(1)	6(1)	7(1)	17(1)
C(2)	47(1)	83(1)	55(1)	3(1)	6(1)	27(1)
C(3)	36(1)	106(2)	72(1)	-4(1)	-10(1)	13(1)
C(4)	42(1)	73(1)	51(1)	-10(1)	-13(1)	5(1)
C(5)	35(1)	42(1)	30(1)	1(1)	-4(1)	5(1)
C(6)	38(1)	36(1)	26(1)	0(1)	-4(1)	3(1)
C(7)	32(1)	28(1)	27(1)	-2(1)	1(1)	5(1)
C(8)	27(1)	33(1)	26(1)	2(1)	-2(1)	-1(1)
C(9)	41(1)	37(1)	33(1)	-4(1)	1(1)	-3(1)
C(10)	49(1)	42(1)	42(1)	-2(1)	-3(1)	-16(1)
C(11)	37(1)	58(1)	42(1)	8(1)	2(1)	-12(1)
C(12)	39(1)	55(1)	36(1)	1(1)	8(1)	0(1)
C(13)	38(1)	38(1)	32(1)	-3(1)	3(1)	0(1)
C(14)	28(1)	39(1)	28(1)	-1(1)	-1(1)	-1(1)
C(15)	45(1)	41(1)	42(1)	-1(1)	-5(1)	-6(1)
C(16)	55(1)	60(1)	53(1)	-6(1)	-9(1)	-21(1)
C(17)	42(1)	88(1)	47(1)	-3(1)	-13(1)	-13(1)
C(18)	39(1)	77(1)	47(1)	6(1)	-11(1)	8(1)
C(19)	39(1)	47(1)	40(1)	1(1)	-6(1)	6(1)
C(20)	79(1)	49(1)	54(1)	-10(1)	11(1)	19(1)

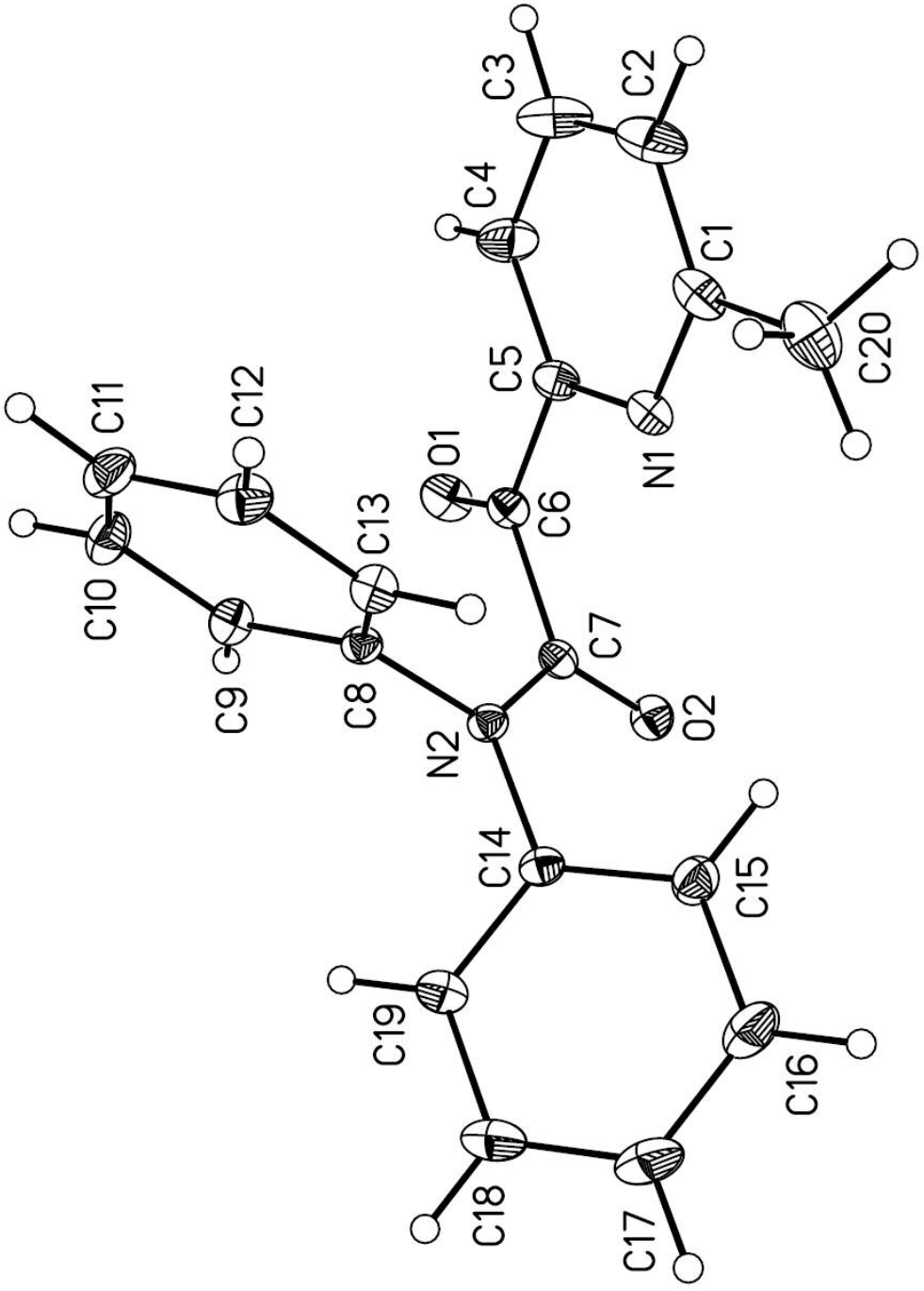
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for rtp05n.

	x	y	z	U(eq)
H(2)	-1226	6728	181	80
H(3)	-1695	5423	-943	93
H(4)	149	4372	-1533	72
H(9)	3466	2433	16	48
H(10)	1618	1488	679	58
H(11)	299	2243	1881	59
H(12)	886	3916	2489	56
H(13)	2723	4872	1835	47
H(15)	5172	6287	889	55
H(16)	7053	6764	1853	73
H(17)	8474	5461	2491	76
H(18)	8012	3669	2219	70
H(19)	6126	3171	1280	54
H(20A)	927	6980	1637	91
H(20B)	699	7926	901	91
H(20C)	2188	7403	1018	91

Table 6. Torsion angles [°] for rtp05n.

C(5)-N(1)-C(1)-C(2)	-1.1(2)
C(5)-N(1)-C(1)-C(20)	176.59(15)
N(1)-C(1)-C(2)-C(3)	0.6(3)
C(20)-C(1)-C(2)-C(3)	-177.0(2)
C(1)-C(2)-C(3)-C(4)	0.1(4)
C(2)-C(3)-C(4)-C(5)	-0.2(4)
C(1)-N(1)-C(5)-C(4)	1.0(2)
C(1)-N(1)-C(5)-C(6)	-176.72(13)
C(3)-C(4)-C(5)-N(1)	-0.4(3)
C(3)-C(4)-C(5)-C(6)	177.19(19)
N(1)-C(5)-C(6)-O(1)	-171.55(14)
C(4)-C(5)-C(6)-O(1)	10.7(3)
N(1)-C(5)-C(6)-C(7)	3.36(19)
C(4)-C(5)-C(6)-C(7)	-174.42(16)
C(8)-N(2)-C(7)-O(2)	-176.21(13)
C(14)-N(2)-C(7)-O(2)	9.3(2)
C(8)-N(2)-C(7)-C(6)	2.30(17)
C(14)-N(2)-C(7)-C(6)	-172.17(12)
O(1)-C(6)-C(7)-O(2)	68.35(18)
C(5)-C(6)-C(7)-O(2)	-106.78(15)
O(1)-C(6)-C(7)-N(2)	-110.25(15)
C(5)-C(6)-C(7)-N(2)	74.62(16)
C(7)-N(2)-C(8)-C(9)	66.54(17)
C(14)-N(2)-C(8)-C(9)	-118.87(14)
C(7)-N(2)-C(8)-C(13)	-112.88(14)
C(14)-N(2)-C(8)-C(13)	61.71(17)
C(13)-C(8)-C(9)-C(10)	2.5(2)
N(2)-C(8)-C(9)-C(10)	-176.94(14)
C(8)-C(9)-C(10)-C(11)	-0.3(2)
C(9)-C(10)-C(11)-C(12)	-1.8(3)
C(10)-C(11)-C(12)-C(13)	1.9(3)
C(11)-C(12)-C(13)-C(8)	0.2(2)
C(9)-C(8)-C(13)-C(12)	-2.4(2)

N(2)-C(8)-C(13)-C(12)	177.00(14)
C(7)-N(2)-C(14)-C(19)	-123.46(15)
C(8)-N(2)-C(14)-C(19)	61.96(17)
C(7)-N(2)-C(14)-C(15)	58.27(18)
C(8)-N(2)-C(14)-C(15)	-116.32(15)
C(19)-C(14)-C(15)-C(16)	0.8(2)
N(2)-C(14)-C(15)-C(16)	179.09(15)
C(14)-C(15)-C(16)-C(17)	0.3(3)
C(15)-C(16)-C(17)-C(18)	-1.0(3)
C(16)-C(17)-C(18)-C(19)	0.5(3)
C(15)-C(14)-C(19)-C(18)	-1.3(2)
N(2)-C(14)-C(19)-C(18)	-179.59(15)
C(17)-C(18)-C(19)-C(14)	0.7(3)


C3
C2
C4
C1
C5
C20
N1
C11
C12
O1
C6
C13
C10
C7
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C8
O2
N2
C14
C15
C19
C16
C18
C17

X-ray Crystallographic data and crystal packing for **7** (rps19a)

Compound 7. The molecule crystallized in the monoclinic space group P2(1)/n with four molecules per unit cell. The integration of data gave 21675 reflections out to a maximum of 2θ = 69.09° of which 11,249 were independent in the triclinic space group. The final triclinic cell constants were based on the xyz cetroids of 5410 reflections above 10σ(I). After full data collection the true cell was found to be monoclinic. The data were merged on all Friedel pairs. Non-hydrogen atoms were refined anisotropically and H-atoms were included in idealized positions with fixed isotropic U's [U_{iso} = 1.2 Uequiv on aromatic C and 1.5 Uequiv on hydroxyl H]. There are weak hydrogen bonds in the crystal that link O1-H1 [x,y,z] to O2=C [1-x, -y, -z] resulting dimmers. The N2-C7 bond length [1.3638(11) Å] is short compared to N2-C8 [1.4448(11) Å] and N2-C14 [1.4415(11) Å] bond length and N2 is planar (sum of angles 359.86°). The carbonyl bond length C7-O2 [1.2209(11) Å] is not significantly affected by the H-bonding. The HC-OH bond length [1.4146(11) Å] is typical of alcohols. The H-bonded dimmer displays O1-H1•••O2A 2.087 Å and O1-H1•••O2 2.138 Å

Table 1. Crystal data and structure refinement for rpsl9a.

Peak and hole Identification code	rpsl9a	
Empirical formula	C19 H16 N2 O2	
Formula weight	304.34	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 16.2324(11) Å	α= 90°.
	b = 5.6544(4) Å	β= 115.587(3)°.
	c = 18.3459(12) Å	γ = 90°.
Volume	1518.73(18) $Å^3$	
Z	4	
Density (calculated)	1.331 Mg/m^3	
Absorption coefficient	0.088 mm^{-1}	
F(000)	640	
Crystal size	0.45 x 0.44 x 0.18 mm^3	
Theta range for data collection	3.34 to 34.61°.	
Index ranges	-24<=h<=24, -8<=k<=4, -28<=l<=24	
Reflections collected	20730	
Independent reflections	6003 [R(int) = 0.0202]	
Completeness to theta = 34.61°	92.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.980 and 0.960	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6003 / 0 / 209	
Goodness-of-fit on F^2	0.945	
Final R indices [I>2sigma(I)]	R1 = 0.0439, wR2 = 0.0925	
R indices (all data)	R1 = 0.0608, wR2 = 0.1018	
Largest diff. p	0.340 and -0.199 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for rpsl9a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	3697(1)	-1567(1)	16(1)	34(1)
O(2)	4922(1)	1827(1)	546(1)	35(1)
N(1)	2195(1)	-252(2)	570(1)	36(1)
N(2)	4777(1)	2542(1)	1705(1)	24(1)
C(1)	1353(1)	672(3)	280(1)	45(1)
C(2)	1107(1)	2774(2)	-132(1)	44(1)
C(3)	1764(1)	4041(2)	-250(1)	41(1)
C(4)	2639(1)	3127(2)	38(1)	34(1)
C(5)	2821(1)	965(2)	436(1)	25(1)
C(6)	3731(1)	-280(2)	690(1)	25(1)
C(7)	4536(1)	1455(2)	978(1)	25(1)
C(8)	4362(1)	1902(2)	2233(1)	23(1)
C(9)	4611(1)	-181(2)	2673(1)	29(1)
C(10)	4238(1)	-711(2)	3209(1)	35(1)
C(11)	3638(1)	845(2)	3311(1)	37(1)
C(12)	3396(1)	2922(2)	2872(1)	36(1)
C(13)	3753(1)	3453(2)	2326(1)	29(1)
C(14)	5502(1)	4265(2)	2011(1)	23(1)
C(15)	5622(1)	5939(2)	1510(1)	27(1)
C(16)	6310(1)	7615(2)	1840(1)	33(1)
C(17)	6876(1)	7645(2)	2663(1)	35(1)
C(18)	6755(1)	5975(2)	3157(1)	33(1)
C(19)	6072(1)			

Table 3. Bond distances [Å] and angles [°] for rpsl9a.

O(1)-C(6)	1.4146(11)
O(1)-H(1)	0.8300
O(2)-C(7)	1.2209(11)
N(1)-C(5)	1.3351(12)
N(1)-C(1)	1.3405(15)
N(2)-C(7)	1.3638(11)
N(2)-C(14)	1.4415(11)
N(2)-C(8)	1.4448(11)
C(1)-C(2)	1.3715(19)
C(1)-H(1A)	0.9400
C(2)-C(3)	1.3779(18)
C(2)-H(2)	0.9400
C(3)-C(4)	1.3840(16)
C(3)-H(3)	0.9400
C(4)-C(5)	1.3888(14)
C(4)-H(4)	0.9400
C(5)-C(6)	1.5168(13)
C(6)-C(7)	1.5345(13)
C(6)-H(6)	0.9900
C(8)-C(9)	1.3859(13)
C(8)-C(13)	1.3860(13)
C(9)-C(10)	1.3921(14)
C(9)-H(9)	0.9400
C(10)-C(11)	1.3833(16)
C(10)-H(10)	0.9400
C(11)-C(12)	1.3816(17)
C(11)-H(11)	0.9400
C(12)-C(13)	1.3892(14)
C(12)-H(12)	0.9400
C(13)-H(13)	0.9400
C(14)-C(19)	1.3914(12)
C(14)-C(15)	1.3917(12)
C(15)-C(16)	1.3887(14)

C(15)-H(15)	0.9400
C(16)-C(17)	1.3876(15)
C(16)-H(16)	0.9400
C(17)-C(18)	1.3803(15)
C(17)-H(17)	0.9400
C(18)-C(19)	1.3882(14)
C(18)-H(18)	0.9400
C(19)-H(19)	0.9400

C(6)-O(1)-H(1)	109.5
C(5)-N(1)-C(1)	116.90(10)
C(7)-N(2)-C(14)	121.74(7)
C(7)-N(2)-C(8)	121.59(7)
C(14)-N(2)-C(8)	116.53(7)
N(1)-C(1)-C(2)	124.09(11)
N(1)-C(1)-H(1A)	118.0
C(2)-C(1)-H(1A)	118.0
C(1)-C(2)-C(3)	118.46(11)
C(1)-C(2)-H(2)	120.8
C(3)-C(2)-H(2)	120.8
C(2)-C(3)-C(4)	118.86(11)
C(2)-C(3)-H(3)	120.6
C(4)-C(3)-H(3)	120.6
C(3)-C(4)-C(5)	118.61(10)
C(3)-C(4)-H(4)	120.7
C(5)-C(4)-H(4)	120.7
N(1)-C(5)-C(4)	123.05(9)
N(1)-C(5)-C(6)	114.97(8)
C(4)-C(5)-C(6)	121.79(9)
O(1)-C(6)-C(5)	107.81(7)
O(1)-C(6)-C(7)	109.62(7)
C(5)-C(6)-C(7)	112.40(8)
O(1)-C(6)-H(6)	109.0
C(5)-C(6)-H(6)	109.0
C(7)-C(6)-H(6)	109.0
O(2)-C(7)-N(2)	123.14(9)

O(2)-C(7)-C(6)	119.07(8)
N(2)-C(7)-C(6)	117.79(8)
C(9)-C(8)-C(13)	120.66(8)
C(9)-C(8)-N(2)	120.06(8)
C(13)-C(8)-N(2)	119.18(8)
C(8)-C(9)-C(10)	119.23(9)
C(8)-C(9)-H(9)	120.4
C(10)-C(9)-H(9)	120.4
C(11)-C(10)-C(9)	120.30(10)
C(11)-C(10)-H(10)	119.8
C(9)-C(10)-H(10)	119.8
C(12)-C(11)-C(10)	120.07(9)
C(12)-C(11)-H(11)	120.0
C(10)-C(11)-H(11)	120.0
C(11)-C(12)-C(13)	120.16(10)
C(11)-C(12)-H(12)	119.9
C(13)-C(12)-H(12)	119.9
C(8)-C(13)-C(12)	119.55(9)
C(8)-C(13)-H(13)	120.2
C(12)-C(13)-H(13)	120.2
C(19)-C(14)-C(15)	119.73(8)
C(19)-C(14)-N(2)	118.48(8)
C(15)-C(14)-N(2)	121.75(8)
C(16)-C(15)-C(14)	119.43(9)
C(16)-C(15)-H(15)	120.3
C(14)-C(15)-H(15)	120.3
C(17)-C(16)-C(15)	120.90(9)
C(17)-C(16)-H(16)	119.5
C(15)-C(16)-H(16)	119.5
C(18)-C(17)-C(16)	119.40(9)
C(18)-C(17)-H(17)	120.3
C(16)-C(17)-H(17)	120.3
C(17)-C(18)-C(19)	120.40(9)
C(17)-C(18)-H(18)	119.8
C(19)-C(18)-H(18)	119.8
C(18)-C(19)-C(14)	120.13(9)

C(18)-C(19)-H(19)	119.9
C(14)-C(19)-H(19)	119.9

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for rpsl9a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	32(1)	37(1)	34(1)	-14(1)	16(1)	-5(1)
O(2)	41(1)	39(1)	34(1)	-9(1)	25(1)	-9(1)
N(1)	31(1)	39(1)	39(1)	4(1)	17(1)	-3(1)
N(2)	24(1)	27(1)	23(1)	-3(1)	12(1)	-4(1)
C(1)	30(1)	59(1)	48(1)	4(1)	19(1)	0(1)
C(2)	33(1)	58(1)	37(1)	-2(1)	12(1)	12(1)
C(3)	46(1)	37(1)	35(1)	2(1)	12(1)	10(1)
C(4)	36(1)	30(1)	36(1)	2(1)	14(1)	-1(1)
C(5)	27(1)	27(1)	23(1)	-3(1)	10(1)	-2(1)
C(6)	27(1)	25(1)	24(1)	-3(1)	11(1)	-2(1)
C(7)	25(1)	26(1)	25(1)	-3(1)	11(1)	-1(1)
C(8)	25(1)	25(1)	22(1)	-3(1)	11(1)	-3(1)
C(9)	35(1)	26(1)	29(1)	-1(1)	15(1)	0(1)
C(10)	44(1)	32(1)	30(1)	2(1)	17(1)	-8(1)
C(11)	34(1)	50(1)	29(1)	-2(1)	17(1)	-11(1)
C(12)	29(1)	48(1)	34(1)	-4(1)	17(1)	2(1)
C(13)	30(1)	30(1)	29(1)	-1(1)	14(1)	3(1)
C(14)	21(1)	23(1)	25(1)	-1(1)	10(1)	0(1)
C(15)	26(1)	27(1)	27(1)	4(1)	11(1)	1(1)
C(16)	31(1)	28(1)	41(1)	5(1)	16(1)	-2(1)
C(17)	27(1)	31(1)	44(1)	-5(1)	13(1)	-6(1)
C(18)	27(1)	37(1)	30(1)	-5(1)	7(1)	-3(1)
C(19)	28(1)	31(1)	25(1)	0(1)	9(1)	-3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for rpsl9a.

	x	y	z	U(eq)
H(1)	4133	-1175	-80	51
H(1A)	902	-173	364	54
H(2)	504	3337	-329	53
H(3)	1621	5501	-521	49
H(4)	3101	3952	-35	41
H(6)	3820	-1398	1133	30
H(9)	5027	-1224	2611	35
H(10)	4394	-2132	3504	42
H(11)	3393	488	3678	44
H(12)	2990	3979	2943	43
H(13)	3582	4855	2021	35
H(15)	5241	5937	952	33
H(16)	6394	8744	1502	40
H(17)	7337	8793	2882	42
H(18)	7138	5983	3715	40
H(19)	5996	3147	3175	35

Table 6. Torsion angles [°] for rpsl9a.

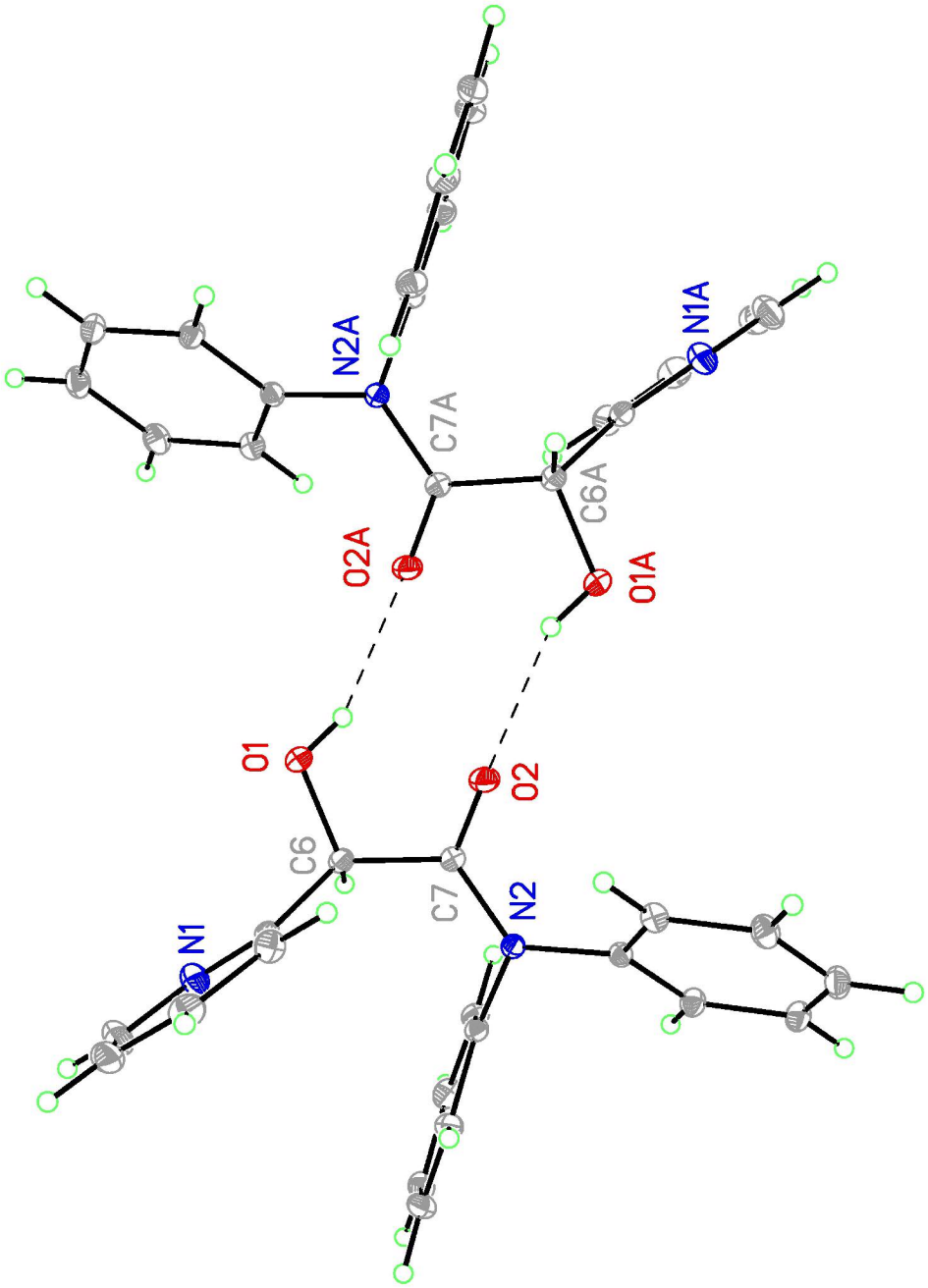
C(5)-N(1)-C(1)-C(2)	-0.70(18)
N(1)-C(1)-C(2)-C(3)	-0.8(2)
C(1)-C(2)-C(3)-C(4)	1.12(18)
C(2)-C(3)-C(4)-C(5)	-0.09(16)
C(1)-N(1)-C(5)-C(4)	1.82(15)
C(1)-N(1)-C(5)-C(6)	-173.28(9)
C(3)-C(4)-C(5)-N(1)	-1.45(15)
C(3)-C(4)-C(5)-C(6)	173.33(9)
N(1)-C(5)-C(6)-O(1)	91.36(10)
C(4)-C(5)-C(6)-O(1)	-83.81(11)
N(1)-C(5)-C(6)-C(7)	-147.72(8)
C(4)-C(5)-C(6)-C(7)	37.11(12)
C(14)-N(2)-C(7)-O(2)	1.25(14)
C(8)-N(2)-C(7)-O(2)	-174.26(9)
C(14)-N(2)-C(7)-C(6)	-177.63(8)
C(8)-N(2)-C(7)-C(6)	6.85(13)
O(1)-C(6)-C(7)-O(2)	12.59(12)
C(5)-C(6)-C(7)-O(2)	-107.29(10)
O(1)-C(6)-C(7)-N(2)	-168.48(8)
C(5)-C(6)-C(7)-N(2)	71.64(10)
C(7)-N(2)-C(8)-C(9)	75.33(12)
C(14)-N(2)-C(8)-C(9)	-100.41(10)
C(7)-N(2)-C(8)-C(13)	-108.17(10)
C(14)-N(2)-C(8)-C(13)	76.09(11)
C(13)-C(8)-C(9)-C(10)	0.35(14)
N(2)-C(8)-C(9)-C(10)	176.80(9)
C(8)-C(9)-C(10)-C(11)	-1.08(15)
C(9)-C(10)-C(11)-C(12)	0.78(16)
C(10)-C(11)-C(12)-C(13)	0.24(16)
C(9)-C(8)-C(13)-C(12)	0.66(14)
N(2)-C(8)-C(13)-C(12)	-175.82(9)
C(11)-C(12)-C(13)-C(8)	-0.96(15)
C(7)-N(2)-C(14)-C(19)	-142.21(9)

C(8)-N(2)-C(14)-C(19)	33.52(12)
C(7)-N(2)-C(14)-C(15)	39.94(13)
C(8)-N(2)-C(14)-C(15)	-144.33(9)
C(19)-C(14)-C(15)-C(16)	-0.21(14)
N(2)-C(14)-C(15)-C(16)	177.61(9)
C(14)-C(15)-C(16)-C(17)	-0.23(15)
C(15)-C(16)-C(17)-C(18)	0.43(16)
C(16)-C(17)-C(18)-C(19)	-0.20(16)
C(17)-C(18)-C(19)-C(14)	-0.24(16)
C(15)-C(14)-C(19)-C(18)	0.45(14)
N(2)-C(14)-C(19)-C(18)	-177.45(9)

Table 7. Hydrogen bonds for rpsl9a [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(2)#1	0.83	2.09	2.8476(10)	152.3

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z


N2A
C7A
N1A
C6A
O2A
O1A
O1
O2
C6
C7
N2
N1

X-ray Crystallographic data and crystal packing for **9/11** mixture (rtp5jp)

Compound Mixture 9 + 11. The compound crystallized in the monoclinic space group Pc with two molecules per unit cell. The asymmetric unit contained two molecules of **11** and one of **9**. The Friedel pairs were merged and averaged. If the substituents on C6 and C25 are ignored there is a non-crystallographic center of symmetry. The OH on C6 and H on C25 negates the center. All non-hydrogen atoms were refined anisotropically and the H-atoms were included in idealized positions with fixed isotropic U's = 1.2 U(equiv) except for H3 for which U = 1.5 U(equiv) [O3]. There appears to be no chemical hydrogen bonding in the molecule. Both N2 and N4 are in planar environments (sum of angles N2 3.59.9°, N4 360.0°). The N2-C7 [1.349(7) Å] and N4-C26 [1.371(7) Å] are short compared to the N-Ph bond lengths N2-C8 [1.446(6) Å], N2-C14 [1.420(7)Å], N4-C27 [1.449(7) Å] and N4-C33 [1.457(7) Å]. The carbonyl distances C7-O2 [1.225(6) Å], C26-O5 [1.214(6) Å], the alcohol distances C6-O3 [1.450(8) Å] and the N-oxide distances N1-O1 [1.290(6) Å] and N3-O4 [1.316(6) Å] are typical.

Table 1. Crystal data and structure refinement for rtp5jp.

Identification code	rtp5jp	
Empirical formula	C38 H32 N4 O5	
Formula weight	624.68	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	Pc	
Unit cell dimensions	a = 6.1070(3) Å	α= 90°.
	b = 16.1821(8) Å	β= 92.612(2)°.
	c = 15.2318(7) Å	γ = 90°.
Volume	1503.70(13) $Å^3$	
Z	2	
Density (calculated)	1.380 Mg/m^3	
Absorption coefficient	0.093 mm^{-1}	
F(000)	656	
Crystal size	0.16 x 0.12 x 0.08 mm^3	
Theta range for data collection	2.68 to 27.94°.	
Index ranges	-8<=h<=7, -21<=k<=20, -20<=l<=20	
Reflections collected	16827	
Independent reflections	3601 [R(int) = 0.0238]	
Completeness to theta = 27.94°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9900 and 0.9500	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3601 / 2 / 425	
Goodness-of-fit on F^2	1.069	
Final R indices [I>2sigma(I)]	R1 = 0.0536, wR2 = 0.1445	
R indices (all data)	R1 = 0.0685, wR2 = 0.1610	
Largest diff. peak and hole	0.638 and -0.527 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for rtp5jp. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	5531(7)	1841(3)	2655(3)	48(1)
O(2)	10168(7)	963(2)	2263(3)	37(1)
O(3)	11748(11)	2365(4)	3549(4)	114(2)
N(1)	6211(8)	1499(3)	3383(4)	36(1)
N(2)	10516(8)	2187(3)	1576(3)	30(1)
C(1)	4878(10)	980(4)	3848(4)	42(2)
C(2)	5496(11)	652(5)	4585(4)	49(2)
C(3)	7637(11)	795(4)	4965(4)	44(2)
C(4)	9029(11)	1313(4)	4494(4)	39(1)
C(5)	8298(10)	1642(3)	3711(4)	31(1)
C(6)	9642(9)	2174(3)	3119(4)	33(1)
C(7)	10098(9)	1719(3)	2282(4)	29(1)
C(8)	10499(9)	3080(3)	1598(3)	28(1)
C(9)	12296(11)	3499(3)	1915(4)	33(1)
C(10)	12223(12)	4387(3)	1924(4)	43(2)
C(11)	10405(12)	4794(3)	1613(4)	40(1)
C(12)	8617(11)	4349(4)	1281(4)	40(1)
C(13)	8662(10)	3493(3)	1287(4)	34(1)
C(14)	11024(9)	1798(3)	774(4)	31(1)
C(15)	9434(13)	1372(4)	290(5)	48(2)
C(16)	9818(16)	1042(5)	-543(5)	61(2)
C(17)	11913(14)	1110(4)	-854(4)	50(2)
C(18)	13502(14)	1518(5)	-362(6)	64(2)
C(19)	13084(11)	1847(4)	444(5)	48(2)
O(4)	9564(8)	3146(3)	5915(3)	53(1)
O(5)	4899(8)	4046(2)	6304(3)	39(1)
N(3)	8828(8)	3496(3)	5180(3)	34(1)
N(4)	4509(8)	2815(3)	6994(3)	30(1)
C(20)	10169(11)	3991(4)	4772(5)	47(2)
C(21)	9419(13)	4351(4)	3937(4)	51(2)

C(22)	7412(14)	4178(4)	3613(5)	54(2)
C(23)	6043(10)	3698(4)	4078(4)	35(1)
C(24)	6731(9)	3342(3)	4875(3)	29(1)
C(25)	5362(10)	2827(3)	5420(3)	30(1)
C(26)	4928(9)	3296(3)	6281(4)	28(1)
C(27)	4560(9)	1920(3)	6983(3)	30(1)
C(28)	2737(11)	1468(4)	6639(4)	37(1)
C(29)	2782(10)	635(4)	6642(4)	40(1)
C(30)	4668(12)	209(4)	6958(4)	45(2)
C(31)	6465(11)	638(4)	7281(4)	44(2)
C(32)	6424(10)	1501(4)	7322(4)	39(1)
C(33)	4049(10)	3198(3)	7831(3)	32(1)
C(34)	5686(12)	3601(5)	8301(5)	51(2)
C(35)	5181(14)	3940(5)	9099(4)	55(2)
C(36)	3192(15)	3856(4)	9442(5)	54(2)
C(37)	1542(14)	3451(5)	8965(5)	56(2)
C(38)	1983(12)	3109(5)	8142(4)	52(2)

Table 3. Bond lengths [Å] and angles [°] for rtp5jp.

O(1)-N(1)	1.290(6)
O(2)-C(7)	1.225(6)
O(3)-C(6)	1.450(8)
O(3)-H(3)	0.8300
N(1)-C(5)	1.367(7)
N(1)-C(1)	1.386(8)
N(2)-C(7)	1.349(7)
N(2)-C(14)	1.420(7)
N(2)-C(8)	1.446(6)
C(1)-C(2)	1.283(9)
C(1)-H(1A)	0.9400
C(2)-C(3)	1.425(9)
C(2)-H(2)	0.9400
C(3)-C(4)	1.412(8)
C(3)-H(3A)	0.9400
C(4)-C(5)	1.363(8)
C(4)-H(4)	0.9400
C(5)-C(6)	1.515(8)
C(6)-C(7)	1.509(8)
C(6)-H(6)	0.9900
C(8)-C(9)	1.360(8)
C(8)-C(13)	1.371(8)
C(9)-C(10)	1.437(7)
C(9)-H(9)	0.9400
C(10)-C(11)	1.358(9)
C(10)-H(10)	0.9400
C(11)-C(12)	1.385(9)
C(11)-H(11)	0.9400
C(12)-C(13)	1.386(8)
C(12)-H(12)	0.9400
C(13)-H(13)	0.9400
C(14)-C(19)	1.378(9)
C(14)-C(15)	1.378(9)

C(15)-C(16)	1.405(11)
C(15)-H(15)	0.9400
C(16)-C(17)	1.389(11)
C(16)-H(16)	0.9400
C(17)-C(18)	1.368(12)
C(17)-H(17)	0.9400
C(18)-C(19)	1.373(10)
C(18)-H(18)	0.9400
C(19)-H(19)	0.9400
O(4)-N(3)	1.316(6)
O(5)-C(26)	1.214(6)
N(3)-C(20)	1.321(8)
N(3)-C(24)	1.364(7)
N(4)-C(26)	1.371(7)
N(4)-C(27)	1.449(7)
N(4)-C(33)	1.457(7)
C(20)-C(21)	1.453(10)
C(20)-H(20)	0.9400
C(21)-C(22)	1.330(10)
C(21)-H(21)	0.9400
C(22)-C(23)	1.363(10)
C(22)-H(22)	0.9400
C(23)-C(24)	1.392(8)
C(23)-H(23)	0.9400
C(24)-C(25)	1.465(8)
C(25)-C(26)	1.549(7)
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(27)-C(32)	1.404(8)
C(27)-C(28)	1.412(8)
C(28)-C(29)	1.349(8)
C(28)-H(28)	0.9400
C(29)-C(30)	1.408(9)
C(29)-H(29)	0.9400
C(30)-C(31)	1.371(9)
C(30)-H(30)	0.9400

C(31)-C(32)	1.397(8)
C(31)-H(31)	0.9400
C(32)-H(32)	0.9400
C(33)-C(34)	1.369(8)
C(33)-C(38)	1.375(9)
C(34)-C(35)	1.381(10)
C(34)-H(34)	0.9400
C(35)-C(36)	1.350(11)
C(35)-H(35)	0.9400
C(36)-C(37)	1.380(12)
C(36)-H(36)	0.9400
C(37)-C(38)	1.408(9)
C(37)-H(37)	0.9400
C(38)-H(38)	0.9400

C(6)-O(3)-H(3)	109.5
O(1)-N(1)-C(5)	120.0(5)
O(1)-N(1)-C(1)	121.6(5)
C(5)-N(1)-C(1)	118.4(5)
C(7)-N(2)-C(14)	119.6(4)
C(7)-N(2)-C(8)	122.7(5)
C(14)-N(2)-C(8)	117.6(4)
C(2)-C(1)-N(1)	122.7(6)
C(2)-C(1)-H(1A)	118.6
N(1)-C(1)-H(1A)	118.6
C(1)-C(2)-C(3)	121.1(6)
C(1)-C(2)-H(2)	119.5
C(3)-C(2)-H(2)	119.5
C(4)-C(3)-C(2)	117.0(6)
C(4)-C(3)-H(3A)	121.5
C(2)-C(3)-H(3A)	121.5
C(5)-C(4)-C(3)	119.7(6)
C(5)-C(4)-H(4)	120.2
C(3)-C(4)-H(4)	120.2
C(4)-C(5)-N(1)	121.1(5)
C(4)-C(5)-C(6)	125.3(6)

N(1)-C(5)-C(6)	113.6(5)
O(3)-C(6)-C(7)	106.9(5)
O(3)-C(6)-C(5)	110.3(5)
C(7)-C(6)-C(5)	110.6(4)
O(3)-C(6)-H(6)	109.7
C(7)-C(6)-H(6)	109.7
C(5)-C(6)-H(6)	109.7
O(2)-C(7)-N(2)	122.2(5)
O(2)-C(7)-C(6)	121.1(5)
N(2)-C(7)-C(6)	116.7(4)
C(9)-C(8)-C(13)	121.0(5)
C(9)-C(8)-N(2)	120.0(5)
C(13)-C(8)-N(2)	119.0(5)
C(8)-C(9)-C(10)	118.5(5)
C(8)-C(9)-H(9)	120.8
C(10)-C(9)-H(9)	120.8
C(11)-C(10)-C(9)	120.5(6)
C(11)-C(10)-H(10)	119.8
C(9)-C(10)-H(10)	119.8
C(10)-C(11)-C(12)	119.6(5)
C(10)-C(11)-H(11)	120.2
C(12)-C(11)-H(11)	120.2
C(11)-C(12)-C(13)	120.2(5)
C(11)-C(12)-H(12)	119.9
C(13)-C(12)-H(12)	119.9
C(8)-C(13)-C(12)	120.3(5)
C(8)-C(13)-H(13)	119.8
C(12)-C(13)-H(13)	119.8
C(19)-C(14)-C(15)	117.8(6)
C(19)-C(14)-N(2)	121.8(6)
C(15)-C(14)-N(2)	120.4(6)
C(14)-C(15)-C(16)	122.1(7)
C(14)-C(15)-H(15)	119.0
C(16)-C(15)-H(15)	119.0
C(17)-C(16)-C(15)	118.2(7)
C(17)-C(16)-H(16)	120.9

C(15)-C(16)-H(16)	120.9
C(18)-C(17)-C(16)	119.5(7)
C(18)-C(17)-H(17)	120.3
C(16)-C(17)-H(17)	120.3
C(17)-C(18)-C(19)	121.4(8)
C(17)-C(18)-H(18)	119.3
C(19)-C(18)-H(18)	119.3
C(18)-C(19)-C(14)	120.9(7)
C(18)-C(19)-H(19)	119.5
C(14)-C(19)-H(19)	119.5
O(4)-N(3)-C(20)	117.8(6)
O(4)-N(3)-C(24)	119.4(5)
C(20)-N(3)-C(24)	122.9(6)
C(26)-N(4)-C(27)	123.7(5)
C(26)-N(4)-C(33)	120.2(4)
C(27)-N(4)-C(33)	116.1(4)
N(3)-C(20)-C(21)	118.5(6)
N(3)-C(20)-H(20)	120.8
C(21)-C(20)-H(20)	120.8
C(22)-C(21)-C(20)	119.3(7)
C(22)-C(21)-H(21)	120.4
C(20)-C(21)-H(21)	120.4
C(21)-C(22)-C(23)	120.2(7)
C(21)-C(22)-H(22)	119.9
C(23)-C(22)-H(22)	119.9
C(22)-C(23)-C(24)	121.4(6)
C(22)-C(23)-H(23)	119.3
C(24)-C(23)-H(23)	119.3
N(3)-C(24)-C(23)	117.6(5)
N(3)-C(24)-C(25)	117.5(5)
C(23)-C(24)-C(25)	124.9(5)
C(24)-C(25)-C(26)	108.9(4)
C(24)-C(25)-H(25A)	109.9
C(26)-C(25)-H(25A)	109.9
C(24)-C(25)-H(25B)	109.9
C(26)-C(25)-H(25B)	109.9

H(25A)-C(25)-H(25B)	108.3
O(5)-C(26)-N(4)	122.8(5)
O(5)-C(26)-C(25)	121.2(5)
N(4)-C(26)-C(25)	116.0(4)
C(32)-C(27)-C(28)	119.9(5)
C(32)-C(27)-N(4)	119.8(5)
C(28)-C(27)-N(4)	120.3(5)
C(29)-C(28)-C(27)	120.1(5)
C(29)-C(28)-H(28)	120.0
C(27)-C(28)-H(28)	120.0
C(28)-C(29)-C(30)	120.4(5)
C(28)-C(29)-H(29)	119.8
C(30)-C(29)-H(29)	119.8
C(31)-C(30)-C(29)	120.3(5)
C(31)-C(30)-H(30)	119.8
C(29)-C(30)-H(30)	119.8
C(30)-C(31)-C(32)	120.4(6)
C(30)-C(31)-H(31)	119.8
C(32)-C(31)-H(31)	119.8
C(31)-C(32)-C(27)	118.8(5)
C(31)-C(32)-H(32)	120.6
C(27)-C(32)-H(32)	120.6
C(34)-C(33)-C(38)	122.0(6)
C(34)-C(33)-N(4)	119.7(6)
C(38)-C(33)-N(4)	118.3(5)
C(33)-C(34)-C(35)	117.6(7)
C(33)-C(34)-H(34)	121.2
C(35)-C(34)-H(34)	121.2
C(36)-C(35)-C(34)	122.8(7)
C(36)-C(35)-H(35)	118.6
C(34)-C(35)-H(35)	118.6
C(35)-C(36)-C(37)	119.5(7)
C(35)-C(36)-H(36)	120.2
C(37)-C(36)-H(36)	120.2
C(36)-C(37)-C(38)	119.3(8)
C(36)-C(37)-H(37)	120.3

C(38)-C(37)-H(37)	120.3
C(33)-C(38)-C(37)	118.8(7)
C(33)-C(38)-H(38)	120.6
C(37)-C(38)-H(38)	120.6

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for rtp5jp. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	49(3)	46(3)	49(3)	2(2)	-12(2)	5(2)
O(2)	46(2)	21(2)	44(2)	1(2)	8(2)	2(2)
O(3)	118(4)	116(5)	107(4)	-16(4)	3(3)	-5(4)
N(1)	36(3)	26(2)	45(3)	-12(2)	3(2)	4(2)
N(2)	37(2)	22(2)	32(2)	2(2)	1(2)	-1(2)
C(1)	39(3)	42(3)	45(4)	-12(3)	15(3)	-9(3)
C(2)	49(3)	49(4)	51(4)	-11(3)	26(3)	-11(3)
C(3)	60(4)	43(3)	31(3)	6(3)	18(3)	-7(3)
C(4)	45(4)	35(3)	36(3)	-3(3)	9(3)	6(3)
C(5)	38(3)	22(2)	33(3)	-3(2)	10(2)	-1(2)
C(6)	34(3)	29(3)	38(3)	3(2)	6(2)	-1(2)
C(7)	32(3)	21(2)	34(3)	-2(2)	1(2)	0(2)
C(8)	37(3)	18(2)	28(2)	3(2)	4(2)	-2(2)
C(9)	41(3)	23(2)	36(3)	2(2)	6(2)	-1(2)
C(10)	67(4)	24(3)	39(3)	3(2)	9(3)	-18(3)
C(11)	74(4)	19(2)	27(3)	6(2)	10(3)	3(3)
C(12)	49(4)	35(3)	38(3)	8(3)	8(3)	8(3)
C(13)	40(3)	30(3)	32(3)	-1(2)	-3(2)	2(3)
C(14)	36(3)	26(2)	31(3)	3(2)	3(2)	7(2)
C(15)	55(4)	49(4)	40(4)	-5(3)	4(3)	-13(3)
C(16)	84(6)	56(5)	44(4)	-16(3)	1(4)	-22(4)
C(17)	78(5)	45(4)	26(3)	-5(3)	7(3)	14(3)
C(18)	52(5)	73(5)	67(5)	-21(4)	18(4)	9(4)
C(19)	36(3)	50(4)	56(4)	-7(3)	-6(3)	2(3)
O(4)	51(3)	44(3)	62(3)	6(2)	-20(2)	9(2)
O(5)	57(3)	23(2)	39(2)	-2(2)	12(2)	2(2)
N(3)	32(3)	35(3)	35(3)	-1(2)	4(2)	5(2)
N(4)	38(2)	23(2)	29(2)	-5(2)	7(2)	0(2)
C(20)	41(4)	44(4)	57(4)	-19(3)	17(3)	-3(3)
C(21)	73(5)	39(3)	43(3)	-7(3)	25(3)	-15(3)

C(22)	85(6)	44(4)	34(3)	-3(3)	3(3)	10(4)
C(23)	40(4)	39(3)	27(3)	-1(2)	0(2)	0(3)
C(24)	31(3)	26(3)	30(3)	-6(2)	0(2)	6(2)
C(25)	44(3)	20(2)	27(2)	-7(2)	1(2)	0(2)
C(26)	26(3)	24(2)	34(3)	2(2)	4(2)	1(2)
C(27)	33(3)	26(3)	30(3)	-1(2)	4(2)	-1(2)
C(28)	36(3)	38(3)	34(3)	-1(2)	-4(2)	-8(3)
C(29)	46(3)	38(3)	36(3)	-6(3)	0(2)	-10(3)
C(30)	68(4)	28(3)	40(3)	0(3)	10(3)	-6(3)
C(31)	58(4)	34(3)	40(3)	4(3)	0(3)	13(3)
C(32)	34(3)	36(3)	48(4)	4(3)	0(2)	0(3)
C(33)	42(3)	24(2)	28(3)	-4(2)	1(2)	-3(2)
C(34)	44(4)	66(5)	41(4)	-12(3)	4(3)	-16(3)
C(35)	73(5)	57(5)	35(4)	-8(3)	-6(3)	-15(4)
C(36)	85(6)	36(3)	41(4)	-2(3)	8(4)	7(4)
C(37)	58(5)	74(5)	38(4)	-3(3)	15(3)	12(4)
C(38)	47(4)	68(5)	45(3)	-22(3)	21(3)	-8(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for rtp5jp.

	x	y	z	U(eq)
H(3)	11556	2601	4023	170
H(1A)	3462	862	3612	50
H(2)	4519	313	4880	59
H(3A)	8102	556	5504	53
H(4)	10453	1430	4720	46
H(6)	8842	2693	2977	40
H(9)	13557	3214	2123	40
H(10)	13443	4687	2146	52
H(11)	10360	5375	1624	48
H(12)	7369	4628	1050	48
H(13)	7427	3193	1077	41
H(15)	8049	1299	524	58
H(16)	8687	783	-880	74
H(17)	12237	877	-1398	60
H(18)	14909	1574	-581	76
H(19)	14219	2109	775	57
H(20)	11576	4108	5016	56
H(21)	10341	4702	3630	61
H(22)	6937	4387	3060	65
H(23)	4603	3605	3855	42
H(25A)	6108	2303	5556	36
H(25B)	3969	2704	5101	36
H(28)	1491	1748	6409	44
H(29)	1547	336	6431	48
H(30)	4696	-371	6948	54
H(31)	7733	351	7477	53
H(32)	7624	1795	7573	47
H(34)	7102	3646	8089	61
H(35)	6266	4242	9416	66
H(36)	2934	4072	10000	65

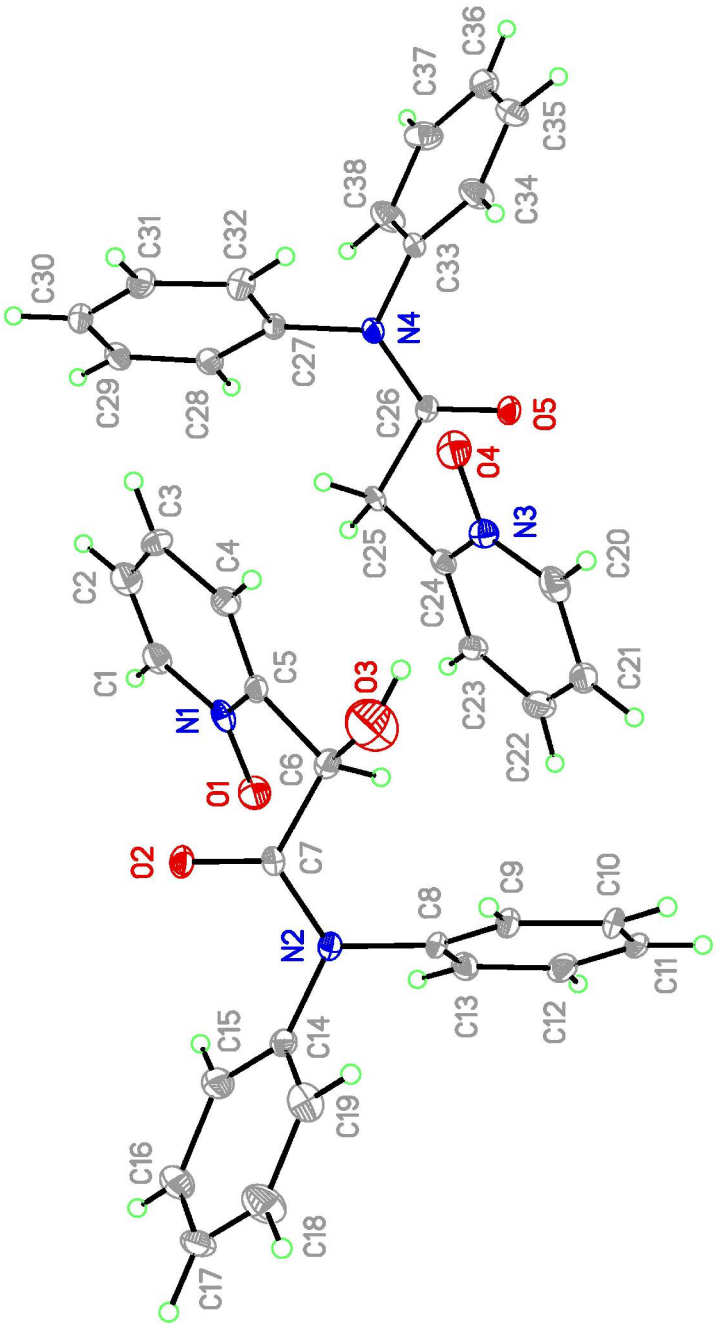
H(37)	138	3403	9189	68
H(38)	885	2826	7811	63

Table 6. Torsion angles [°] for rtp5jp.

O(1)-N(1)-C(1)-C(2)	-177.9(6)
C(5)-N(1)-C(1)-C(2)	2.5(9)
N(1)-C(1)-C(2)-C(3)	-1.2(10)
C(1)-C(2)-C(3)-C(4)	0.2(10)
C(2)-C(3)-C(4)-C(5)	-0.6(9)
C(3)-C(4)-C(5)-N(1)	2.0(9)
C(3)-C(4)-C(5)-C(6)	-177.2(5)
O(1)-N(1)-C(5)-C(4)	177.6(5)
C(1)-N(1)-C(5)-C(4)	-2.9(8)
O(1)-N(1)-C(5)-C(6)	-3.2(7)
C(1)-N(1)-C(5)-C(6)	176.3(5)
C(4)-C(5)-C(6)-O(3)	-6.5(8)
N(1)-C(5)-C(6)-O(3)	174.3(5)
C(4)-C(5)-C(6)-C(7)	111.5(6)
N(1)-C(5)-C(6)-C(7)	-67.7(6)
C(14)-N(2)-C(7)-O(2)	1.0(8)
C(8)-N(2)-C(7)-O(2)	-178.2(5)
C(14)-N(2)-C(7)-C(6)	178.1(5)
C(8)-N(2)-C(7)-C(6)	-1.1(8)
O(3)-C(6)-C(7)-O(2)	93.0(7)
C(5)-C(6)-C(7)-O(2)	-27.1(7)
O(3)-C(6)-C(7)-N(2)	-84.2(6)
C(5)-C(6)-C(7)-N(2)	155.8(5)
C(7)-N(2)-C(8)-C(9)	82.5(7)
C(14)-N(2)-C(8)-C(9)	-96.7(7)
C(7)-N(2)-C(8)-C(13)	-98.1(7)
C(14)-N(2)-C(8)-C(13)	82.6(7)
C(13)-C(8)-C(9)-C(10)	0.5(9)
N(2)-C(8)-C(9)-C(10)	179.8(5)
C(8)-C(9)-C(10)-C(11)	-0.7(9)
C(9)-C(10)-C(11)-C(12)	-0.4(10)
C(10)-C(11)-C(12)-C(13)	1.8(10)
C(9)-C(8)-C(13)-C(12)	0.8(9)

N(2)-C(8)-C(13)-C(12)	-178.5(5)
C(11)-C(12)-C(13)-C(8)	-2.0(9)
C(7)-N(2)-C(14)-C(19)	-111.6(7)
C(8)-N(2)-C(14)-C(19)	67.7(7)
C(7)-N(2)-C(14)-C(15)	69.8(7)
C(8)-N(2)-C(14)-C(15)	-110.9(6)
C(19)-C(14)-C(15)-C(16)	-4.4(11)
N(2)-C(14)-C(15)-C(16)	174.2(6)
C(14)-C(15)-C(16)-C(17)	4.0(12)
C(15)-C(16)-C(17)-C(18)	-2.5(12)
C(16)-C(17)-C(18)-C(19)	1.5(12)
C(17)-C(18)-C(19)-C(14)	-1.9(12)
C(15)-C(14)-C(19)-C(18)	3.3(10)
N(2)-C(14)-C(19)-C(18)	-175.3(6)
O(4)-N(3)-C(20)-C(21)	177.1(5)
C(24)-N(3)-C(20)-C(21)	-3.5(9)
N(3)-C(20)-C(21)-C(22)	0.5(10)
C(20)-C(21)-C(22)-C(23)	2.9(11)
C(21)-C(22)-C(23)-C(24)	-3.4(10)
O(4)-N(3)-C(24)-C(23)	-177.5(5)
C(20)-N(3)-C(24)-C(23)	3.1(8)
O(4)-N(3)-C(24)-C(25)	3.5(7)
C(20)-N(3)-C(24)-C(25)	-175.9(5)
C(22)-C(23)-C(24)-N(3)	0.4(9)
C(22)-C(23)-C(24)-C(25)	179.4(5)
N(3)-C(24)-C(25)-C(26)	66.6(6)
C(23)-C(24)-C(25)-C(26)	-112.3(6)
C(27)-N(4)-C(26)-O(5)	-179.3(5)
C(33)-N(4)-C(26)-O(5)	-1.4(8)
C(27)-N(4)-C(26)-C(25)	3.0(8)
C(33)-N(4)-C(26)-C(25)	-179.1(5)
C(24)-C(25)-C(26)-O(5)	28.5(7)
C(24)-C(25)-C(26)-N(4)	-153.7(5)
C(26)-N(4)-C(27)-C(32)	99.1(7)
C(33)-N(4)-C(27)-C(32)	-78.9(7)
C(26)-N(4)-C(27)-C(28)	-81.5(7)

C(33)-N(4)-C(27)-C(28)	100.6(7)
C(32)-C(27)-C(28)-C(29)	0.4(9)
N(4)-C(27)-C(28)-C(29)	-179.1(5)
C(27)-C(28)-C(29)-C(30)	-2.2(10)
C(28)-C(29)-C(30)-C(31)	1.1(11)
C(29)-C(30)-C(31)-C(32)	1.7(11)
C(30)-C(31)-C(32)-C(27)	-3.5(10)
C(28)-C(27)-C(32)-C(31)	2.4(9)
N(4)-C(27)-C(32)-C(31)	-178.1(6)
C(26)-N(4)-C(33)-C(34)	-69.4(8)
C(27)-N(4)-C(33)-C(34)	108.6(6)
C(26)-N(4)-C(33)-C(38)	113.4(7)
C(27)-N(4)-C(33)-C(38)	-68.6(7)
C(38)-C(33)-C(34)-C(35)	-1.7(11)
N(4)-C(33)-C(34)-C(35)	-178.8(6)
C(33)-C(34)-C(35)-C(36)	3.1(12)
C(34)-C(35)-C(36)-C(37)	-3.3(13)
C(35)-C(36)-C(37)-C(38)	2.0(12)
C(34)-C(33)-C(38)-C(37)	0.6(11)
N(4)-C(33)-C(38)-C(37)	177.7(6)
C(36)-C(37)-C(38)-C(33)	-0.7(11)


C36
C37
C35
C38
C34
C33
C31
C32
C30
N4
C27
C29
C28
C26
O5
O4
C3
N3
C25
C20
C2
C4
C24
C1
C5
C21
O3
C23
N1
C22
C6
O1
O2
C7
C8
C9
C10
N2
C11
C13
C12
C15
C14
C19
C16
C18
C17

X-ray Crystallographic data and crystal packing for **12** (rtp05l)

Compound 12. The molecule crystallized in the monoclinic space group P2(1)/c with two molecules in the asymmetric unit and eight molecules in the unit cell. Integration of the data gave 45,394 reflections of which 9096 were independent and 2099 had $I \geq 2\sigma(I)$. All non0-hydrogen atoms were refined anisotropically. The atoms on the phenyl ring C28-C33 showed large anisotropic displacements and a simple positional disorder model could not be implemented. The H-atoms were included: aromatic H-atoms in ideal positions, U_{oso} = 1.3 U equiv of the parent atom; terminal methyl H0atoms in ideal positions U_{iso} = 1.5 U equiv of the parent atom and the remaining H-atoms wer found in difference maps. They were well behaved except for the H on O2. The large isotropic U is consistent with the H-atom being somewhere between O2 and O4 [x – 1, y, z]. Hydrogen bonding is apparent between O2-H(0s)•••O4 [1.546(4) Å] and O5-H(O5)•••O1 [1.84(3) Å]. The N4 is planar (sum of angles 359.98 (N2), 3.59.97° (N4) and N2-C7 [1.360(2) Å] is short compared to N2-C8 1.443(2) Å and N2-C(14) 1.441(2) Å. The carabonyl distance C7-O3 [1.215(2) Å], N-oxide distances N1-O1 [1.3180(19) Å] and alcohol distance C6-O2 [1.447(3) Å] are all typical.[7]

Table 1. Crystal data and structure refinement for rtp05l.

Identification code	rtp05l	
Empirical formula	C20 H18 N2 O3	
Formula weight	334.36	
Temperature	233(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 10.7259(6) Å	α= 90°.
	b = 18.5233(10) Å	β= 94.687(3)°.
	c = 17.1998(9) Å	γ = 90°.
Volume	3405.8(3) $Å^3$	
Z	8	
Density (calculated)	1.304 Mg/m^3	
Absorption coefficient	0.089 mm^{-1}	
F(000)	1408	
Crystal size	0.30 x 0.10 x 0.01 mm^3	
Theta range for data collection	2.38 to 28.74°.	
Index ranges	-10<=h<=14, -25<=k<=21, -23<=l<=23	
Reflections collected	44612	
Independent reflections	8814 [R(int) = 0.0540]	
Completeness to theta = 28.74°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	.999 and .806	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8814 / 0 / 465	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0573, wR2 = 0.1487	
R indices (all data)	R1 = 0.1130, wR2 = 0.1791	
Largest diff. peak and hole	0.344 and -0.412 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for rtp05l. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	2215(1)	1423(1)	1004(1)	50(1)
O(2)	-944(2)	1565(1)	2141(1)	84(1)
O(3)	1528(1)	1827(1)	3096(1)	56(1)
N(1)	1648(2)	2050(1)	1064(1)	41(1)
N(2)	1152(2)	626(1)	2986(1)	45(1)
C(1)	1998(2)	2615(1)	625(1)	63(1)
C(2)	1405(3)	3262(1)	704(2)	85(1)
C(3)	515(3)	3352(1)	1205(2)	90(1)
C(4)	157(2)	2767(1)	1631(2)	68(1)
C(5)	720(2)	2108(1)	1548(1)	42(1)
C(6)	320(2)	1440(1)	1937(1)	46(1)
C(7)	1077(2)	1319(1)	2724(1)	43(1)
C(8)	1823(2)	454(1)	3724(1)	46(1)
C(9)	1233(2)	46(1)	4251(1)	62(1)
C(10)	1871(3)	-165(1)	4945(1)	69(1)
C(11)	3081(3)	53(1)	5119(1)	67(1)
C(12)	3659(2)	476(1)	4603(1)	66(1)
C(13)	3042(2)	671(1)	3893(1)	54(1)
C(14)	607(2)	27(1)	2544(1)	50(1)
C(15)	-675(2)	-75(1)	2472(2)	68(1)
C(16)	-1157(3)	-662(2)	2044(2)	95(1)
C(17)	-374(5)	-1137(2)	1712(2)	105(1)
C(18)	893(4)	-1039(1)	1800(2)	90(1)
C(19)	1399(3)	-453(1)	2218(1)	63(1)
C(20)	3000(3)	2483(2)	101(2)	106(1)
O(4)	7184(1)	1206(1)	1181(1)	54(1)

O(5)	3886(1)	859(1)	2075(1)	51(1)
O(6)	6418(1)	627(1)	2955(1)	52(1)
N(3)	6646(2)	578(1)	1035(1)	43(1)
N(4)	5996(2)	1823(1)	2889(1)	41(1)
C(21)	7131(2)	110(1)	529(1)	56(1)
C(22)	6540(3)	-543(1)	393(1)	66(1)
C(23)	5500(2)	-723(1)	760(1)	66(1)
C(24)	5014(2)	-232(1)	1254(1)	53(1)
C(25)	5584(2)	425(1)	1380(1)	39(1)
C(26)	5089(2)	1027(1)	1852(1)	38(1)
C(27)	5919(2)	1135(1)	2611(1)	38(1)
C(28)	5462(2)	2446(1)	2490(1)	44(1)
C(29)	6223(3)	2891(1)	2106(2)	76(1)
C(30)	5729(5)	3530(2)	1782(2)	120(2)
C(31)	4496(6)	3696(2)	1848(2)	129(2)
C(32)	3748(4)	3239(2)	2214(2)	107(1)
C(33)	4222(2)	2614(1)	2546(1)	66(1)
C(34)	6683(2)	1983(1)	3622(1)	49(1)
C(35)	7950(2)	1922(1)	3708(2)	70(1)
C(36)	8567(3)	2146(2)	4416(2)	104(1)
C(37)	7911(5)	2416(2)	5000(2)	138(2)
C(38)	6671(5)	2457(2)	4900(2)	155(2)
C(39)	6044(3)	2244(2)	4214(1)	102(1)
C(40)	8266(3)	341(2)	161(2)	85(1)

Table 3. Bond lengths [Å] and angles [°] for rtp05l.

O(1)-N(1)	1.3180(19)
O(2)-C(6)	1.447(3)
O(2)-H(2O)	1.1005(18)
O(3)-C(7)	1.215(2)
N(1)-C(5)	1.354(2)
N(1)-C(1)	1.362(3)
N(2)-C(7)	1.360(2)
N(2)-C(14)	1.441(2)
N(2)-C(8)	1.443(2)
C(1)-C(2)	1.369(4)
C(1)-C(20)	1.478(4)
C(2)-C(3)	1.347(4)
C(2)-H(2)	0.9400
C(3)-C(4)	1.380(4)
C(3)-H(3)	0.9400
C(4)-C(5)	1.373(3)
C(4)-H(4)	0.9400
C(5)-C(6)	1.487(3)
C(6)-C(7)	1.537(3)
C(6)-H(6)	0.953(19)
C(8)-C(9)	1.374(3)
C(8)-C(13)	1.377(3)
C(9)-C(10)	1.383(3)
C(9)-H(9)	0.9400
C(10)-C(11)	1.368(4)
C(10)-H(10)	0.9400
C(11)-C(12)	1.370(3)
C(11)-H(11)	0.9400
C(12)-C(13)	1.389(3)

C(12)-H(12)	0.9400
C(13)-H(13)	0.9400
C(14)-C(19)	1.381(3)
C(14)-C(15)	1.383(3)
C(15)-C(16)	1.389(4)
C(15)-H(15)	0.9400
C(16)-C(17)	1.372(5)
C(16)-H(16)	0.9400
C(17)-C(18)	1.367(5)
C(17)-H(17)	0.9400
C(18)-C(19)	1.388(3)
C(18)-H(18)	0.9400
C(19)-H(19)	0.9400
C(20)-H(20A)	0.9700
C(20)-H(20B)	0.9700
C(20)-H(20C)	0.9700
O(4)-N(3)	1.312(2)
O(5)-C(26)	1.410(2)
O(5)-H(5O)	0.84(2)
O(6)-C(27)	1.213(2)
N(3)-C(25)	1.357(2)
N(3)-C(21)	1.362(3)
N(4)-C(27)	1.361(2)
N(4)-C(28)	1.437(2)
N(4)-C(34)	1.439(2)
C(21)-C(22)	1.377(3)
C(21)-C(40)	1.479(3)
C(22)-C(23)	1.367(3)
C(22)-H(22)	0.9400
C(23)-C(24)	1.375(3)
C(23)-H(23)	0.9400

C(24)-C(25)	1.371(3)
C(24)-H(24)	0.9400
C(25)-C(26)	1.502(3)
C(26)-C(27)	1.532(2)
C(26)-H(26)	0.989(18)
C(28)-C(29)	1.367(3)
C(28)-C(33)	1.378(3)
C(29)-C(30)	1.393(4)
C(29)-H(29)	0.9400
C(30)-C(31)	1.372(6)
C(30)-H(30)	0.9400
C(31)-C(32)	1.357(6)
C(31)-H(31)	0.9400
C(32)-C(33)	1.369(4)
C(32)-H(32)	0.9400
C(33)-H(33)	0.9400
C(34)-C(35)	1.360(3)
C(34)-C(39)	1.362(3)
C(35)-C(36)	1.400(4)
C(35)-H(35)	0.9400
C(36)-C(37)	1.367(5)
C(36)-H(36)	0.9400
C(37)-C(38)	1.330(6)
C(37)-H(37)	0.9400
C(38)-C(39)	1.369(4)
C(38)-H(38)	0.9400
C(39)-H(39)	0.9400
C(40)-H(40A)	0.9700
C(40)-H(40B)	0.9700
C(40)-H(40C)	0.9700

C(6)-O(2)-H(2O)	105.30(15)
O(1)-N(1)-C(5)	119.07(15)
O(1)-N(1)-C(1)	118.98(18)
C(5)-N(1)-C(1)	121.94(18)
C(7)-N(2)-C(14)	122.82(16)
C(7)-N(2)-C(8)	120.78(16)
C(14)-N(2)-C(8)	116.38(15)
N(1)-C(1)-C(2)	117.9(3)
N(1)-C(1)-C(20)	117.2(2)
C(2)-C(1)-C(20)	124.9(3)
C(3)-C(2)-C(1)	122.0(3)
C(3)-C(2)-H(2)	119.0
C(1)-C(2)-H(2)	119.0
C(2)-C(3)-C(4)	119.0(2)
C(2)-C(3)-H(3)	120.5
C(4)-C(3)-H(3)	120.5
C(5)-C(4)-C(3)	119.9(3)
C(5)-C(4)-H(4)	120.0
C(3)-C(4)-H(4)	120.0
N(1)-C(5)-C(4)	119.1(2)
N(1)-C(5)-C(6)	117.57(16)
C(4)-C(5)-C(6)	123.2(2)
O(2)-C(6)-C(5)	106.62(17)
O(2)-C(6)-C(7)	104.33(16)
C(5)-C(6)-C(7)	111.48(16)
O(2)-C(6)-H(6)	116.5(11)
C(5)-C(6)-H(6)	108.4(11)
C(7)-C(6)-H(6)	109.5(11)
O(3)-C(7)-N(2)	123.09(18)
O(3)-C(7)-C(6)	120.68(18)
N(2)-C(7)-C(6)	116.16(17)

C(9)-C(8)-C(13)	120.2(2)
C(9)-C(8)-N(2)	118.64(19)
C(13)-C(8)-N(2)	121.16(18)
C(8)-C(9)-C(10)	120.2(2)
C(8)-C(9)-H(9)	119.9
C(10)-C(9)-H(9)	119.9
C(11)-C(10)-C(9)	119.9(2)
C(11)-C(10)-H(10)	120.1
C(9)-C(10)-H(10)	120.1
C(10)-C(11)-C(12)	120.0(2)
C(10)-C(11)-H(11)	120.0
C(12)-C(11)-H(11)	120.0
C(11)-C(12)-C(13)	120.6(2)
C(11)-C(12)-H(12)	119.7
C(13)-C(12)-H(12)	119.7
C(8)-C(13)-C(12)	119.1(2)
C(8)-C(13)-H(13)	120.5
C(12)-C(13)-H(13)	120.5
C(19)-C(14)-C(15)	121.0(2)
C(19)-C(14)-N(2)	118.24(19)
C(15)-C(14)-N(2)	120.7(2)
C(14)-C(15)-C(16)	118.7(3)
C(14)-C(15)-H(15)	120.7
C(16)-C(15)-H(15)	120.7
C(17)-C(16)-C(15)	120.5(3)
C(17)-C(16)-H(16)	119.7
C(15)-C(16)-H(16)	119.7
C(18)-C(17)-C(16)	120.3(3)
C(18)-C(17)-H(17)	119.8
C(16)-C(17)-H(17)	119.8
C(17)-C(18)-C(19)	120.3(3)

C(17)-C(18)-H(18)	119.8
C(19)-C(18)-H(18)	119.8
C(14)-C(19)-C(18)	119.1(3)
C(14)-C(19)-H(19)	120.4
C(18)-C(19)-H(19)	120.4
C(1)-C(20)-H(20A)	109.5
C(1)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(1)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(26)-O(5)-H(5O)	106.4(17)
O(4)-N(3)-C(25)	118.27(15)
O(4)-N(3)-C(21)	120.09(17)
C(25)-N(3)-C(21)	121.61(18)
C(27)-N(4)-C(28)	125.03(15)
C(27)-N(4)-C(34)	120.80(15)
C(28)-N(4)-C(34)	114.14(15)
N(3)-C(21)-C(22)	118.2(2)
N(3)-C(21)-C(40)	117.4(2)
C(22)-C(21)-C(40)	124.4(2)
C(23)-C(22)-C(21)	121.2(2)
C(23)-C(22)-H(22)	119.4
C(21)-C(22)-H(22)	119.4
C(22)-C(23)-C(24)	119.3(2)
C(22)-C(23)-H(23)	120.4
C(24)-C(23)-H(23)	120.4
C(25)-C(24)-C(23)	119.9(2)
C(25)-C(24)-H(24)	120.1
C(23)-C(24)-H(24)	120.1
N(3)-C(25)-C(24)	119.77(17)

N(3)-C(25)-C(26)	115.28(16)
C(24)-C(25)-C(26)	124.89(17)
O(5)-C(26)-C(25)	110.81(15)
O(5)-C(26)-C(27)	106.12(14)
C(25)-C(26)-C(27)	110.60(15)
O(5)-C(26)-H(26)	109.3(10)
C(25)-C(26)-H(26)	108.1(10)
C(27)-C(26)-H(26)	111.9(10)
O(6)-C(27)-N(4)	122.92(16)
O(6)-C(27)-C(26)	121.14(17)
N(4)-C(27)-C(26)	115.84(16)
C(29)-C(28)-C(33)	121.0(2)
C(29)-C(28)-N(4)	119.0(2)
C(33)-C(28)-N(4)	119.8(2)
C(28)-C(29)-C(30)	118.8(3)
C(28)-C(29)-H(29)	120.6
C(30)-C(29)-H(29)	120.6
C(31)-C(30)-C(29)	119.7(3)
C(31)-C(30)-H(30)	120.1
C(29)-C(30)-H(30)	120.1
C(32)-C(31)-C(30)	120.5(3)
C(32)-C(31)-H(31)	119.7
C(30)-C(31)-H(31)	119.7
C(31)-C(32)-C(33)	120.5(4)
C(31)-C(32)-H(32)	119.7
C(33)-C(32)-H(32)	119.7
C(32)-C(33)-C(28)	119.3(3)
C(32)-C(33)-H(33)	120.3
C(28)-C(33)-H(33)	120.3
C(35)-C(34)-C(39)	120.5(2)
C(35)-C(34)-N(4)	120.96(19)

C(39)-C(34)-N(4)	118.4(2)
C(34)-C(35)-C(36)	117.9(3)
C(34)-C(35)-H(35)	121.1
C(36)-C(35)-H(35)	121.1
C(37)-C(36)-C(35)	120.8(3)
C(37)-C(36)-H(36)	119.6
C(35)-C(36)-H(36)	119.6
C(38)-C(37)-C(36)	119.8(3)
C(38)-C(37)-H(37)	120.1
C(36)-C(37)-H(37)	120.1
C(37)-C(38)-C(39)	120.7(4)
C(37)-C(38)-H(38)	119.7
C(39)-C(38)-H(38)	119.7
C(34)-C(39)-C(38)	120.4(3)
C(34)-C(39)-H(39)	119.8
C(38)-C(39)-H(39)	119.8
C(21)-C(40)-H(40A)	109.5
C(21)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(21)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for rtp05l. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	48(1)	41(1)	61(1)	-4(1)	7(1)	10(1)
O(2)	54(1)	119(2)	78(1)	-11(1)	5(1)	6(1)
O(3)	65(1)	47(1)	53(1)	-6(1)	-14(1)	2(1)
N(1)	47(1)	32(1)	44(1)	0(1)	-6(1)	0(1)
N(2)	45(1)	43(1)	46(1)	-1(1)	-2(1)	-2(1)
C(1)	81(2)	48(1)	57(1)	12(1)	-12(1)	-20(1)
C(2)	124(3)	37(1)	84(2)	14(1)	-43(2)	-11(2)
C(3)	119(3)	36(1)	105(2)	-13(2)	-53(2)	27(2)
C(4)	68(2)	60(2)	71(2)	-21(1)	-20(1)	27(1)
C(5)	40(1)	41(1)	42(1)	-7(1)	-8(1)	8(1)
C(6)	40(1)	55(1)	43(1)	-4(1)	2(1)	-2(1)
C(7)	35(1)	49(1)	45(1)	-4(1)	3(1)	3(1)
C(8)	54(1)	40(1)	43(1)	-3(1)	1(1)	3(1)
C(9)	80(2)	48(1)	57(1)	-1(1)	4(1)	-14(1)
C(10)	109(2)	48(1)	52(1)	5(1)	10(1)	-2(1)
C(11)	96(2)	56(1)	47(1)	3(1)	-3(1)	27(1)
C(12)	58(1)	77(2)	60(1)	4(1)	-8(1)	21(1)
C(13)	46(1)	64(1)	50(1)	6(1)	3(1)	10(1)
C(14)	54(1)	47(1)	46(1)	3(1)	-1(1)	-13(1)
C(15)	58(1)	70(2)	73(2)	23(1)	-12(1)	-20(1)
C(16)	100(2)	85(2)	91(2)	41(2)	-46(2)	-54(2)
C(17)	170(4)	69(2)	68(2)	12(2)	-38(2)	-56(2)
C(18)	163(3)	53(2)	55(2)	-5(1)	10(2)	-21(2)
C(19)	83(2)	50(1)	56(1)	-5(1)	14(1)	-10(1)
C(20)	126(3)	104(2)	93(2)	26(2)	39(2)	-35(2)
O(4)	45(1)	58(1)	58(1)	6(1)	4(1)	-7(1)

O(5)	39(1)	65(1)	50(1)	-1(1)	7(1)	1(1)
O(6)	71(1)	44(1)	40(1)	2(1)	-9(1)	7(1)
N(3)	43(1)	55(1)	30(1)	2(1)	1(1)	4(1)
N(4)	47(1)	41(1)	34(1)	-3(1)	-5(1)	5(1)
C(21)	56(1)	76(2)	35(1)	-3(1)	7(1)	15(1)
C(22)	78(2)	76(2)	45(1)	-20(1)	1(1)	18(1)
C(23)	75(2)	59(1)	62(1)	-21(1)	-3(1)	-2(1)
C(24)	55(1)	54(1)	49(1)	-9(1)	3(1)	-6(1)
C(25)	39(1)	50(1)	28(1)	-1(1)	0(1)	1(1)
C(26)	37(1)	43(1)	34(1)	0(1)	2(1)	0(1)
C(27)	40(1)	43(1)	31(1)	0(1)	4(1)	2(1)
C(28)	49(1)	40(1)	42(1)	-4(1)	-11(1)	5(1)
C(29)	81(2)	71(2)	72(2)	23(1)	-16(1)	-18(1)
C(30)	178(4)	72(2)	98(2)	39(2)	-53(3)	-35(2)
C(31)	202(5)	56(2)	111(3)	-7(2)	-91(3)	36(3)
C(32)	119(3)	87(2)	104(2)	-40(2)	-57(2)	59(2)
C(33)	61(2)	66(2)	67(1)	-22(1)	-14(1)	20(1)
C(34)	66(1)	41(1)	36(1)	-4(1)	-11(1)	7(1)
C(35)	67(2)	75(2)	64(1)	9(1)	-21(1)	-5(1)
C(36)	105(2)	83(2)	110(3)	16(2)	-66(2)	-8(2)
C(37)	219(5)	83(2)	95(3)	-43(2)	-94(3)	45(3)
C(38)	218(5)	172(4)	62(2)	-59(2)	-57(3)	109(4)
C(39)	124(3)	128(3)	49(1)	-31(2)	-16(2)	62(2)
C(40)	77(2)	114(2)	67(2)	3(2)	36(1)	15(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for rtp05l.

	x	y	z	U(eq)
H(2O)	-1552	1323	1664	125
H(2)	1625	3656	399	110
H(3)	144	3806	1264	117
H(4)	-472	2819	1977	88
H(6)	439(17)	1041(10)	1601(11)	40(5)
H(9)	393	-90	4140	80
H(10)	1474	-458	5298	90
H(11)	3515	-88	5591	87
H(12)	4482	636	4731	85
H(13)	3452	947	3532	70
H(15)	-1208	246	2707	88
H(16)	-2027	-735	1982	124
H(17)	-710	-1531	1422	136
H(18)	1424	-1370	1577	117
H(19)	2270	-383	2277	81
H(20A)	3758	2337	408	159
H(20B)	3159	2922	-182	159
H(20C)	2742	2103	-266	159
H(5O)	3370(20)	1076(13)	1760(14)	67(8)
H(22)	6857	-871	42	86
H(23)	5120	-1176	675	85
H(24)	4294	-347	1505	68
H(26)	5043(16)	1468(10)	1527(10)	33(5)
H(29)	7064	2769	2061	99
H(30)	6239	3845	1520	156
H(31)	4166	4131	1638	167

H(32)	2897	3351	2240	139
H(33)	3706	2304	2809	86
H(35)	8398	1736	3305	91
H(36)	9443	2110	4490	134
H(37)	8336	2572	5469	180
H(38)	6220	2634	5306	201
H(39)	5167	2277	4151	132
H(40A)	8129	815	-69	127
H(40B)	8443	-2	-242	127
H(40C)	8969	359	553	127

Table 6. Torsion angles [°] for rtp05l.

O(1)-N(1)-C(1)-C(2)	-179.30(19)
C(5)-N(1)-C(1)-C(2)	2.0(3)
O(1)-N(1)-C(1)-C(20)	0.3(3)
C(5)-N(1)-C(1)-C(20)	-178.4(2)
N(1)-C(1)-C(2)-C(3)	1.0(4)
C(20)-C(1)-C(2)-C(3)	-178.5(3)
C(1)-C(2)-C(3)-C(4)	-2.5(4)
C(2)-C(3)-C(4)-C(5)	1.0(4)
O(1)-N(1)-C(5)-C(4)	177.87(17)
C(1)-N(1)-C(5)-C(4)	-3.4(3)
O(1)-N(1)-C(5)-C(6)	-5.0(2)
C(1)-N(1)-C(5)-C(6)	173.67(17)
C(3)-C(4)-C(5)-N(1)	1.9(3)
C(3)-C(4)-C(5)-C(6)	-175.0(2)
N(1)-C(5)-C(6)-O(2)	-156.81(16)
C(4)-C(5)-C(6)-O(2)	20.1(3)
N(1)-C(5)-C(6)-C(7)	89.9(2)
C(4)-C(5)-C(6)-C(7)	-93.1(2)
C(14)-N(2)-C(7)-O(3)	179.50(19)
C(8)-N(2)-C(7)-O(3)	-2.1(3)
C(14)-N(2)-C(7)-C(6)	2.6(3)
C(8)-N(2)-C(7)-C(6)	-179.00(16)
O(2)-C(6)-C(7)-O(3)	-87.5(2)
C(5)-C(6)-C(7)-O(3)	27.2(3)
O(2)-C(6)-C(7)-N(2)	89.5(2)
C(5)-C(6)-C(7)-N(2)	-155.78(17)
C(7)-N(2)-C(8)-C(9)	128.9(2)
C(14)-N(2)-C(8)-C(9)	-52.6(2)
C(7)-N(2)-C(8)-C(13)	-53.1(3)

C(14)-N(2)-C(8)-C(13)	125.4(2)
C(13)-C(8)-C(9)-C(10)	-1.7(3)
N(2)-C(8)-C(9)-C(10)	176.2(2)
C(8)-C(9)-C(10)-C(11)	2.1(4)
C(9)-C(10)-C(11)-C(12)	-0.3(4)
C(10)-C(11)-C(12)-C(13)	-1.9(4)
C(9)-C(8)-C(13)-C(12)	-0.5(3)
N(2)-C(8)-C(13)-C(12)	-178.36(19)
C(11)-C(12)-C(13)-C(8)	2.3(3)
C(7)-N(2)-C(14)-C(19)	108.8(2)
C(8)-N(2)-C(14)-C(19)	-69.7(2)
C(7)-N(2)-C(14)-C(15)	-73.2(3)
C(8)-N(2)-C(14)-C(15)	108.3(2)
C(19)-C(14)-C(15)-C(16)	-1.7(3)
N(2)-C(14)-C(15)-C(16)	-179.7(2)
C(14)-C(15)-C(16)-C(17)	1.1(4)
C(15)-C(16)-C(17)-C(18)	0.2(4)
C(16)-C(17)-C(18)-C(19)	-0.9(4)
C(15)-C(14)-C(19)-C(18)	1.1(3)
N(2)-C(14)-C(19)-C(18)	179.1(2)
C(17)-C(18)-C(19)-C(14)	0.3(4)
O(4)-N(3)-C(21)-C(22)	179.88(18)
C(25)-N(3)-C(21)-C(22)	-2.4(3)
O(4)-N(3)-C(21)-C(40)	0.0(3)
C(25)-N(3)-C(21)-C(40)	177.7(2)
N(3)-C(21)-C(22)-C(23)	-0.6(3)
C(40)-C(21)-C(22)-C(23)	179.4(2)
C(21)-C(22)-C(23)-C(24)	2.1(4)
C(22)-C(23)-C(24)-C(25)	-0.8(3)
O(4)-N(3)-C(25)-C(24)	-178.53(17)
C(21)-N(3)-C(25)-C(24)	3.7(3)

O(4)-N(3)-C(25)-C(26)	4.3(2)
C(21)-N(3)-C(25)-C(26)	-173.44(16)
C(23)-C(24)-C(25)-N(3)	-2.1(3)
C(23)-C(24)-C(25)-C(26)	174.77(19)
N(3)-C(25)-C(26)-O(5)	170.17(15)
C(24)-C(25)-C(26)-O(5)	-6.8(3)
N(3)-C(25)-C(26)-C(27)	-72.4(2)
C(24)-C(25)-C(26)-C(27)	110.6(2)
C(28)-N(4)-C(27)-O(6)	177.46(18)
C(34)-N(4)-C(27)-O(6)	-0.4(3)
C(28)-N(4)-C(27)-C(26)	-6.1(3)
C(34)-N(4)-C(27)-C(26)	176.06(16)
O(5)-C(26)-C(27)-O(6)	85.1(2)
C(25)-C(26)-C(27)-O(6)	-35.1(2)
O(5)-C(26)-C(27)-N(4)	-91.35(19)
C(25)-C(26)-C(27)-N(4)	148.42(16)
C(27)-N(4)-C(28)-C(29)	-101.1(2)
C(34)-N(4)-C(28)-C(29)	76.8(2)
C(27)-N(4)-C(28)-C(33)	83.5(2)
C(34)-N(4)-C(28)-C(33)	-98.5(2)
C(33)-C(28)-C(29)-C(30)	1.3(4)
N(4)-C(28)-C(29)-C(30)	-174.0(2)
C(28)-C(29)-C(30)-C(31)	-0.6(5)
C(29)-C(30)-C(31)-C(32)	-1.1(5)
C(30)-C(31)-C(32)-C(33)	2.1(5)
C(31)-C(32)-C(33)-C(28)	-1.4(4)
C(29)-C(28)-C(33)-C(32)	-0.3(3)
N(4)-C(28)-C(33)-C(32)	175.0(2)
C(27)-N(4)-C(34)-C(35)	68.4(3)
C(28)-N(4)-C(34)-C(35)	-109.7(2)
C(27)-N(4)-C(34)-C(39)	-116.0(3)

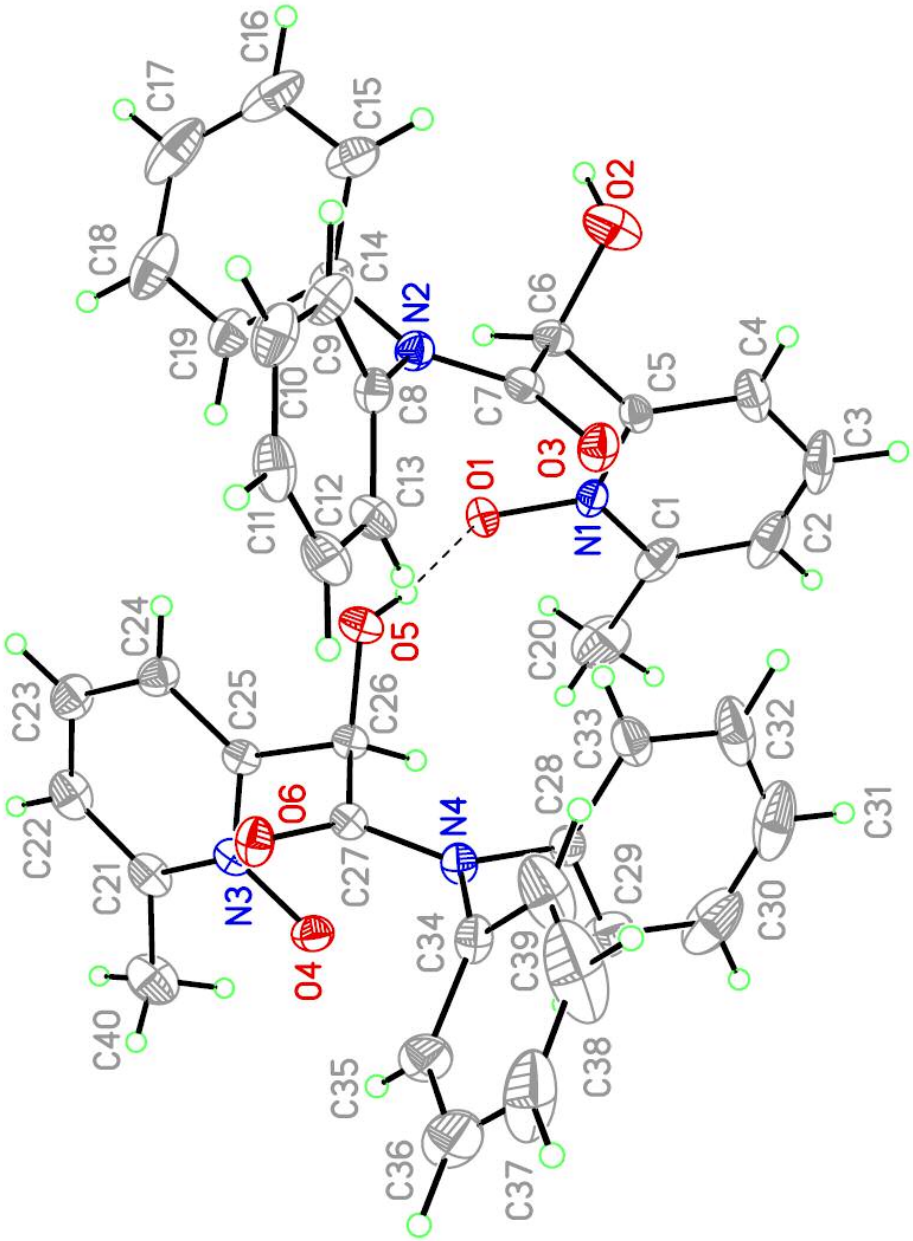
C(28)-N(4)-C(34)-C(39)	66.0(3)
C(39)-C(34)-C(35)-C(36)	-1.0(4)
N(4)-C(34)-C(35)-C(36)	174.6(2)
C(34)-C(35)-C(36)-C(37)	0.0(4)
C(35)-C(36)-C(37)-C(38)	1.1(6)
C(36)-C(37)-C(38)-C(39)	-1.2(7)
C(35)-C(34)-C(39)-C(38)	0.9(5)
N(4)-C(34)-C(39)-C(38)	-174.8(3)
C(37)-C(38)-C(39)-C(34)	0.2(7)

Table 7. Hydrogen bonds for rtp05l [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2O)...O(4)#1	1.1005(18)	1.5466(14)	2.580(2)	153.83(11)
O(5)-H(5O)...O(1)	0.84(2)	1.84(3)	2.675(2)	172(2)

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z


C16
C17
C15
C18
C14
O2
C6
N2
C19
C9
C10
C8
C7
C4
C5
C3
O3
O1
C12
C13
C11
N1
C1
C2
C24
O5
C20
C23
C25
C26
C33
C32
C28
O6
N4
C22
C21
N3
C27
C29
C31
C30
C34
C39
O4
C40
C35
C38
C36
C37

X-ray Crystallographic data and crystal packing for **14** (rtp05al)

Compound 14. The molecule crystallized in the monoclinic space group P2(1)/n with four molecules per unit cell. The integration of the data gave 47,241 reflections of which 14,367 were independent and 7021 were greater than $2\sigma(I)$. The non-hydrogen atoms were refined anisotropically and H-atoms were included and their positions and U_{iso}'s allowed to vary. The N atoms are planar (sum of angles 359.98° (N2) and 3.59.90° (N3)) and the bonding parameters in the malonamide chain closely resemble those in **4**.

Table 1. Crystal data and structure refinement for rtp05a1.

Identification code	rtp05a1	
Empirical formula	C33 H27 N3 O3	
Formula weight	513.58	
Temperature	208(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 9.8097(11) Å	α= 90°.
	b = 16.7962(18) Å	β= 105.000(6)°.
	c = 17.0633(19) Å	γ = 90°.
Volume	2715.6(5) $Å^3$	
Z	4	
Density (calculated)	1.256 Mg/m^3	
Absorption coefficient	0.081 mm^{-1}	
F(000)	1080	
Crystal size	0.36 x 0.30 x 0.07 mm^3	
Theta range for data collection	1.73 to 38.69°.	
Index ranges	-17<=h<=15, -26<=k<=29, -27<=l<=29	
Reflections collected	47241	
Independent reflections	14367 [R(int) = 0.0559]	
Completeness to theta = 38.69°	92.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.907 and 0.998	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14367 / 0 / 460	
Goodness-of-fit on F^2	0.998	
Final R indices [I>2sigma(I)]	R1 = 0.0546, wR2 = 0.1314	
R indices (all data)	R1 = 0.1278, wR2 = 0.1624	
Largest diff. peak and hole	0.350 and -0.197 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for rtp05a1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	994(1)	3854(1)	8085(1)	55(1)
O(2)	1074(1)	1802(1)	5954(1)	45(1)
O(3)	468(1)	1669(1)	7708(1)	39(1)
N(1)	2180(1)	3491(1)	8163(1)	35(1)
N(2)	2034(1)	3012(1)	5823(1)	33(1)
N(3)	-1366(1)	2175(1)	6748(1)	32(1)
C(1)	3319(1)	3698(1)	8780(1)	52(1)
C(2)	4553(1)	3288(1)	8875(1)	63(1)
C(3)	4671(1)	2685(1)	8360(1)	65(1)
C(4)	3517(1)	2499(1)	7726(1)	47(1)
C(5)	2278(1)	2910(1)	7627(1)	30(1)
C(6)	974(1)	2780(1)	6957(1)	27(1)
C(7)	1342(1)	2480(1)	6190(1)	31(1)
C(8)	10(1)	2163(1)	7189(1)	29(1)
C(9)	3095(3)	4362(2)	9305(1)	92(1)
C(10)	2129(1)	3838(1)	6058(1)	33(1)
C(11)	924(1)	4300(1)	5888(1)	41(1)
C(12)	1006(2)	5078(1)	6168(1)	54(1)
C(13)	2282(2)	5388(1)	6590(1)	56(1)
C(14)	3483(1)	4934(1)	6732(1)	52(1)
C(15)	3423(1)	4151(1)	6470(1)	41(1)
C(16)	2708(1)	2768(1)	5211(1)	37(1)
C(17)	2772(1)	3299(1)	4599(1)	46(1)
C(18)	3462(1)	3072(1)	4017(1)	60(1)
C(19)	4063(2)	2336(1)	4040(1)	66(1)
C(20)	4005(2)	1818(1)	4649(1)	62(1)
C(21)	3336(1)	2030(1)	5240(1)	47(1)
C(22)	-1992(1)	2847(1)	6264(1)	34(1)
C(23)	-2383(1)	2787(1)	5430(1)	48(1)
C(24)	-2987(2)	3441(1)	4971(1)	63(1)

C(25)	-3188(1)	4138(1)	5341(1)	65(1)
C(26)	-2804(1)	4196(1)	6172(1)	61(1)
C(27)	-2210(1)	3545(1)	6642(1)	46(1)
C(28)	-2206(1)	1474(1)	6728(1)	35(1)
C(29)	-3506(1)	1519(1)	6887(1)	50(1)
C(30)	-4297(2)	828(1)	6861(1)	63(1)
C(31)	-3798(2)	112(1)	6672(1)	65(1)
C(32)	-2498(2)	71(1)	6517(1)	66(1)
C(33)	-1694(1)	751(1)	6543(1)	49(1)

Table 3. Bond lengths [Å] and angles [°] for rtp05a1.

O(1)-N(1)	1.2893(11)
O(2)-C(7)	1.2147(11)
O(3)-C(8)	1.2110(11)
N(1)-C(5)	1.3578(12)
N(1)-C(1)	1.3674(14)
N(2)-C(7)	1.3683(12)
N(2)-C(16)	1.4328(12)
N(2)-C(10)	1.4406(12)
N(3)-C(8)	1.3652(12)
N(3)-C(28)	1.4330(12)
N(3)-C(22)	1.4388(12)
C(1)-C(2)	1.365(2)
C(1)-C(9)	1.483(2)
C(2)-C(3)	1.366(2)
C(2)-H(2)	0.94(2)
C(3)-C(4)	1.3838(19)
C(3)-H(3)	0.96(2)
C(4)-C(5)	1.3691(14)
C(4)-H(4)	0.992(16)
C(5)-C(6)	1.4947(12)
C(6)-C(8)	1.5234(12)
C(6)-C(7)	1.5299(12)
C(6)-H(6)	0.978(10)
C(9)-H(9A)	0.946(19)
C(9)-H(9B)	1.00(3)
C(9)-H(9C)	0.94(3)
C(10)-C(11)	1.3807(15)
C(10)-C(15)	1.3853(14)
C(11)-C(12)	1.3862(16)
C(11)-H(11)	0.983(15)
C(12)-C(13)	1.375(2)
C(12)-H(12)	1.006(17)
C(13)-C(14)	1.372(2)

C(13)-H(13)	0.989(15)
C(14)-C(15)	1.3847(16)
C(14)-H(14)	0.982(17)
C(15)-H(15)	0.989(14)
C(16)-C(21)	1.3796(17)
C(16)-C(17)	1.3860(15)
C(17)-C(18)	1.3930(18)
C(17)-H(17)	0.936(15)
C(18)-C(19)	1.366(3)
C(18)-H(18)	0.946(19)
C(19)-C(20)	1.368(2)
C(19)-H(19)	0.97(2)
C(20)-C(21)	1.3833(17)
C(20)-H(20)	0.938(18)
C(21)-H(21)	0.942(15)
C(22)-C(23)	1.3797(16)
C(22)-C(27)	1.3805(15)
C(23)-C(24)	1.3887(18)
C(23)-H(23)	0.986(15)
C(24)-C(25)	1.369(2)
C(24)-H(24)	0.98(2)
C(25)-C(26)	1.373(2)
C(25)-H(25)	1.014(16)
C(26)-C(27)	1.3924(17)
C(26)-H(26)	0.998(18)
C(27)-H(27)	0.981(15)
C(28)-C(29)	1.3727(16)
C(28)-C(33)	1.3812(15)
C(29)-C(30)	1.3920(17)
C(29)-H(29)	1.021(16)
C(30)-C(31)	1.367(2)
C(30)-H(30)	0.990(18)
C(31)-C(32)	1.370(2)
C(31)-H(31)	0.970(19)
C(32)-C(33)	1.3822(17)
C(32)-H(32)	1.033(18)

C(33)-H(33)	0.975(18)
O(1)-N(1)-C(5)	119.36(8)
O(1)-N(1)-C(1)	119.61(9)
C(5)-N(1)-C(1)	121.03(9)
C(7)-N(2)-C(16)	121.60(8)
C(7)-N(2)-C(10)	120.36(8)
C(16)-N(2)-C(10)	118.02(7)
C(8)-N(3)-C(28)	118.76(7)
C(8)-N(3)-C(22)	122.85(7)
C(28)-N(3)-C(22)	118.29(7)
C(2)-C(1)-N(1)	119.08(12)
C(2)-C(1)-C(9)	124.95(15)
N(1)-C(1)-C(9)	115.97(14)
C(1)-C(2)-C(3)	121.17(12)
C(1)-C(2)-H(2)	114.8(13)
C(3)-C(2)-H(2)	123.9(13)
C(2)-C(3)-C(4)	118.80(12)
C(2)-C(3)-H(3)	119.4(12)
C(4)-C(3)-H(3)	121.8(12)
C(5)-C(4)-C(3)	120.23(12)
C(5)-C(4)-H(4)	119.4(9)
C(3)-C(4)-H(4)	120.4(9)
N(1)-C(5)-C(4)	119.61(9)
N(1)-C(5)-C(6)	115.05(8)
C(4)-C(5)-C(6)	125.34(9)
C(5)-C(6)-C(8)	111.45(7)
C(5)-C(6)-C(7)	110.93(7)
C(8)-C(6)-C(7)	107.33(7)
C(5)-C(6)-H(6)	106.8(6)
C(8)-C(6)-H(6)	109.3(6)
C(7)-C(6)-H(6)	111.1(6)
O(2)-C(7)-N(2)	123.47(9)
O(2)-C(7)-C(6)	120.92(8)
N(2)-C(7)-C(6)	115.55(7)
O(3)-C(8)-N(3)	122.66(8)

O(3)-C(8)-C(6)	121.26(8)
N(3)-C(8)-C(6)	115.98(7)
C(1)-C(9)-H(9A)	107.8(11)
C(1)-C(9)-H(9B)	108.7(14)
H(9A)-C(9)-H(9B)	114(2)
C(1)-C(9)-H(9C)	110.8(16)
H(9A)-C(9)-H(9C)	113.8(19)
H(9B)-C(9)-H(9C)	101(2)
C(11)-C(10)-C(15)	121.06(9)
C(11)-C(10)-N(2)	119.49(9)
C(15)-C(10)-N(2)	119.43(9)
C(10)-C(11)-C(12)	119.14(11)
C(10)-C(11)-H(11)	120.0(8)
C(12)-C(11)-H(11)	120.8(8)
C(13)-C(12)-C(11)	120.09(12)
C(13)-C(12)-H(12)	120.5(9)
C(11)-C(12)-H(12)	119.4(9)
C(14)-C(13)-C(12)	120.37(11)
C(14)-C(13)-H(13)	118.8(9)
C(12)-C(13)-H(13)	120.8(9)
C(13)-C(14)-C(15)	120.55(12)
C(13)-C(14)-H(14)	120.8(9)
C(15)-C(14)-H(14)	118.6(9)
C(14)-C(15)-C(10)	118.73(11)
C(14)-C(15)-H(15)	123.5(8)
C(10)-C(15)-H(15)	117.8(8)
C(21)-C(16)-C(17)	119.88(10)
C(21)-C(16)-N(2)	121.16(9)
C(17)-C(16)-N(2)	118.92(10)
C(16)-C(17)-C(18)	119.07(13)
C(16)-C(17)-H(17)	117.1(9)
C(18)-C(17)-H(17)	123.8(9)
C(19)-C(18)-C(17)	120.91(14)
C(19)-C(18)-H(18)	122.9(12)
C(17)-C(18)-H(18)	116.1(12)
C(18)-C(19)-C(20)	119.60(13)

C(18)-C(19)-H(19)	121.1(10)
C(20)-C(19)-H(19)	119.3(10)
C(19)-C(20)-C(21)	120.76(15)
C(19)-C(20)-H(20)	120.7(11)
C(21)-C(20)-H(20)	118.6(12)
C(16)-C(21)-C(20)	119.78(13)
C(16)-C(21)-H(21)	118.9(9)
C(20)-C(21)-H(21)	121.2(9)
C(23)-C(22)-C(27)	120.60(10)
C(23)-C(22)-N(3)	119.88(9)
C(27)-C(22)-N(3)	119.52(9)
C(22)-C(23)-C(24)	119.16(13)
C(22)-C(23)-H(23)	116.4(9)
C(24)-C(23)-H(23)	124.3(9)
C(25)-C(24)-C(23)	120.59(13)
C(25)-C(24)-H(24)	121.4(10)
C(23)-C(24)-H(24)	118.0(11)
C(24)-C(25)-C(26)	120.17(12)
C(24)-C(25)-H(25)	120.3(9)
C(26)-C(25)-H(25)	119.5(9)
C(25)-C(26)-C(27)	120.11(13)
C(25)-C(26)-H(26)	121.2(10)
C(27)-C(26)-H(26)	118.6(10)
C(22)-C(27)-C(26)	119.35(12)
C(22)-C(27)-H(27)	119.6(8)
C(26)-C(27)-H(27)	121.0(8)
C(29)-C(28)-C(33)	120.41(10)
C(29)-C(28)-N(3)	120.42(9)
C(33)-C(28)-N(3)	119.17(9)
C(28)-C(29)-C(30)	119.06(12)
C(28)-C(29)-H(29)	119.8(9)
C(30)-C(29)-H(29)	121.1(9)
C(31)-C(30)-C(29)	120.70(13)
C(31)-C(30)-H(30)	121.0(9)
C(29)-C(30)-H(30)	118.3(9)
C(30)-C(31)-C(32)	119.86(11)

C(30)-C(31)-H(31)	120.1(11)
C(32)-C(31)-H(31)	120.0(11)
C(31)-C(32)-C(33)	120.31(14)
C(31)-C(32)-H(32)	120.4(10)
C(33)-C(32)-H(32)	119.3(10)
C(28)-C(33)-C(32)	119.65(12)
C(28)-C(33)-H(33)	118.4(9)
C(32)-C(33)-H(33)	121.8(9)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for rtp05a1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2} U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	46(1)	66(1)	51(1)	-20(1)	10(1)	17(1)
O(2)	59(1)	36(1)	49(1)	-12(1)	29(1)	-14(1)
O(3)	38(1)	38(1)	40(1)	12(1)	12(1)	3(1)
N(1)	32(1)	44(1)	30(1)	-3(1)	7(1)	0(1)
N(2)	36(1)	34(1)	30(1)	-3(1)	13(1)	-8(1)
N(3)	30(1)	31(1)	36(1)	4(1)	8(1)	-3(1)
C(1)	51(1)	67(1)	34(1)	-6(1)	1(1)	-12(1)
C(2)	41(1)	97(1)	41(1)	8(1)	-6(1)	-9(1)
C(3)	32(1)	101(1)	57(1)	18(1)	3(1)	18(1)
C(4)	38(1)	59(1)	45(1)	6(1)	10(1)	16(1)
C(5)	27(1)	34(1)	28(1)	3(1)	9(1)	1(1)
C(6)	28(1)	28(1)	27(1)	1(1)	8(1)	0(1)
C(7)	33(1)	33(1)	31(1)	-2(1)	11(1)	-5(1)
C(8)	31(1)	29(1)	30(1)	1(1)	12(1)	2(1)
C(9)	107(2)	96(2)	59(1)	-38(1)	-3(1)	-12(1)
C(10)	38(1)	32(1)	31(1)	2(1)	10(1)	-8(1)
C(11)	39(1)	38(1)	45(1)	8(1)	7(1)	-5(1)
C(12)	56(1)	36(1)	71(1)	10(1)	19(1)	2(1)
C(13)	69(1)	34(1)	66(1)	-4(1)	21(1)	-10(1)
C(14)	55(1)	44(1)	55(1)	-6(1)	8(1)	-19(1)
C(15)	37(1)	40(1)	43(1)	-1(1)	7(1)	-10(1)
C(16)	32(1)	51(1)	28(1)	-9(1)	10(1)	-14(1)
C(17)	39(1)	67(1)	33(1)	1(1)	11(1)	-15(1)
C(18)	50(1)	100(1)	33(1)	-4(1)	16(1)	-27(1)
C(19)	54(1)	104(1)	49(1)	-30(1)	29(1)	-28(1)
C(20)	55(1)	73(1)	66(1)	-29(1)	32(1)	-14(1)
C(21)	47(1)	53(1)	48(1)	-12(1)	23(1)	-8(1)
C(22)	27(1)	34(1)	39(1)	7(1)	5(1)	-3(1)
C(23)	52(1)	47(1)	40(1)	6(1)	0(1)	-15(1)
C(24)	56(1)	67(1)	51(1)	24(1)	-14(1)	-22(1)

C(25)	41(1)	58(1)	84(1)	33(1)	-5(1)	1(1)
C(26)	50(1)	45(1)	86(1)	14(1)	16(1)	13(1)
C(27)	40(1)	43(1)	54(1)	4(1)	12(1)	9(1)
C(28)	35(1)	35(1)	34(1)	3(1)	9(1)	-7(1)
C(29)	39(1)	50(1)	65(1)	4(1)	20(1)	-7(1)
C(30)	45(1)	67(1)	79(1)	12(1)	22(1)	-17(1)
C(31)	61(1)	52(1)	77(1)	15(1)	11(1)	-24(1)
C(32)	69(1)	40(1)	88(1)	-4(1)	20(1)	-15(1)
C(33)	50(1)	39(1)	62(1)	-6(1)	21(1)	-9(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for rtp05a1.

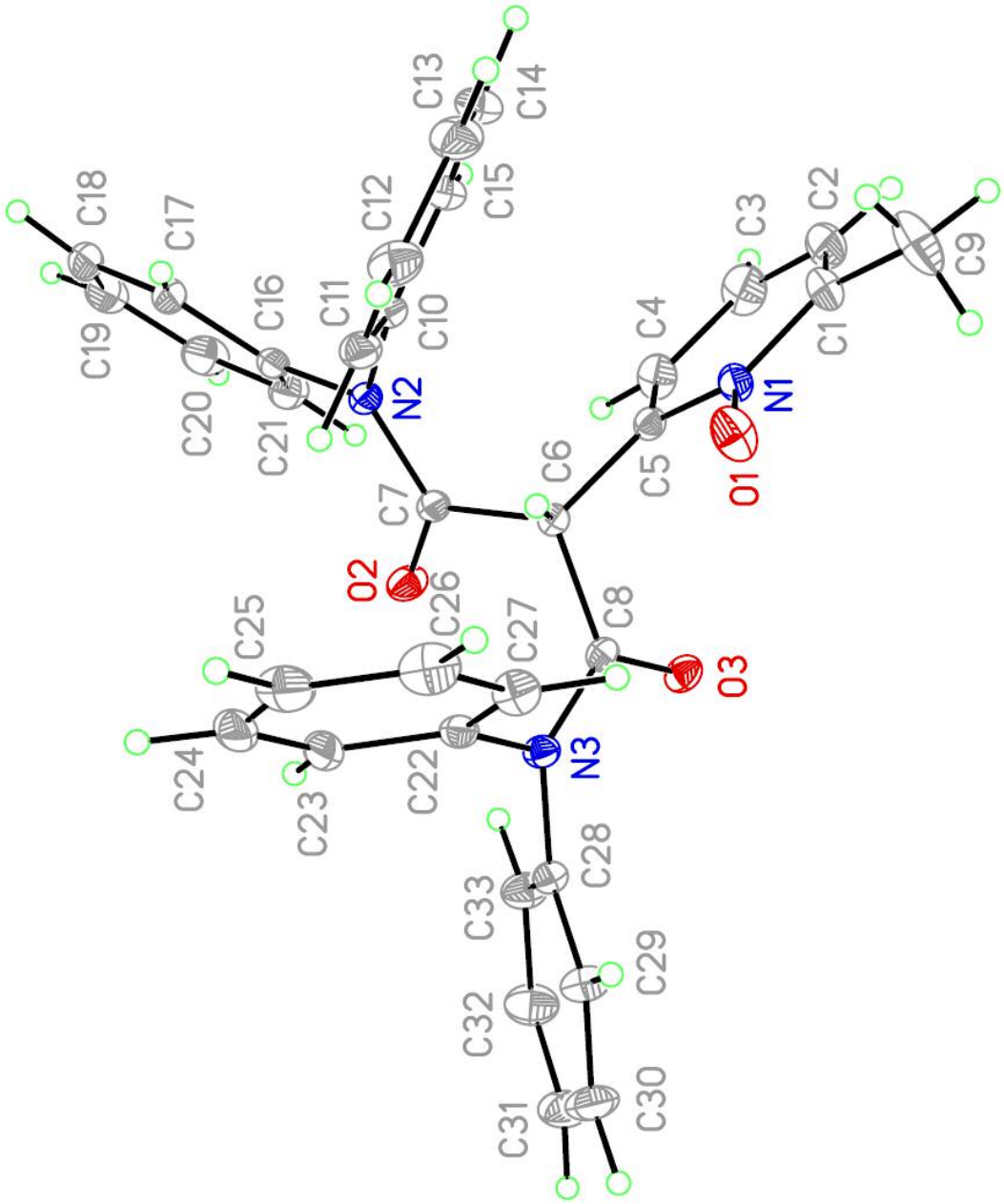
	x	y	z	U(eq)
H(2)	5270(20)	3435(11)	9332(13)	94(6)
H(3)	5550(20)	2400(11)	8446(12)	90(6)
H(4)	3571(16)	2058(9)	7348(9)	59(4)
H(6)	481(12)	3292(6)	6859(6)	27(2)
H(9A)	2930(20)	4830(11)	8986(12)	75(5)
H(9B)	2310(30)	4217(14)	9550(15)	114(8)
H(9C)	3860(30)	4403(14)	9771(18)	120(8)
H(11)	13(16)	4068(8)	5596(9)	50(3)
H(12)	119(18)	5405(9)	6077(10)	67(4)
H(13)	2351(17)	5939(9)	6800(9)	63(4)
H(14)	4407(18)	5161(9)	7005(10)	64(4)
H(15)	4256(15)	3798(8)	6566(8)	47(3)
H(17)	2372(16)	3802(9)	4618(9)	55(4)
H(18)	3520(20)	3463(11)	3629(12)	79(5)
H(19)	4520(20)	2169(10)	3624(12)	80(5)
H(20)	4420(20)	1313(11)	4677(11)	76(5)
H(21)	3270(16)	1672(8)	5653(10)	55(4)
H(23)	-2171(16)	2278(9)	5199(9)	56(4)
H(24)	-3230(20)	3392(10)	4377(13)	84(5)
H(25)	-3621(18)	4616(9)	5004(10)	71(4)
H(26)	-2979(19)	4693(10)	6451(10)	73(5)
H(27)	-1911(16)	3582(8)	7236(10)	53(4)
H(29)	-3857(17)	2053(9)	7046(10)	63(4)
H(30)	-5230(19)	868(9)	6980(10)	68(4)
H(31)	-4360(20)	-365(11)	6646(11)	84(5)
H(32)	-2106(19)	-469(10)	6383(11)	75(5)
H(33)	-785(19)	741(9)	6409(10)	65(4)

Table 6. Torsion angles [°] for rtp05a1.

O(1)-N(1)-C(1)-C(2)	177.44(12)
C(5)-N(1)-C(1)-C(2)	-2.79(17)
O(1)-N(1)-C(1)-C(9)	-2.1(2)
C(5)-N(1)-C(1)-C(9)	177.66(16)
N(1)-C(1)-C(2)-C(3)	0.8(2)
C(9)-C(1)-C(2)-C(3)	-179.73(19)
C(1)-C(2)-C(3)-C(4)	0.9(2)
C(2)-C(3)-C(4)-C(5)	-0.7(2)
O(1)-N(1)-C(5)-C(4)	-177.20(10)
C(1)-N(1)-C(5)-C(4)	3.04(15)
O(1)-N(1)-C(5)-C(6)	3.18(13)
C(1)-N(1)-C(5)-C(6)	-176.59(9)
C(3)-C(4)-C(5)-N(1)	-1.26(17)
C(3)-C(4)-C(5)-C(6)	178.32(11)
N(1)-C(5)-C(6)-C(8)	-90.15(9)
C(4)-C(5)-C(6)-C(8)	90.25(11)
N(1)-C(5)-C(6)-C(7)	150.32(8)
C(4)-C(5)-C(6)-C(7)	-29.29(12)
C(16)-N(2)-C(7)-O(2)	-10.77(15)
C(10)-N(2)-C(7)-O(2)	170.65(9)
C(16)-N(2)-C(7)-C(6)	166.41(8)
C(10)-N(2)-C(7)-C(6)	-12.17(12)
C(5)-C(6)-C(7)-O(2)	110.05(10)
C(8)-C(6)-C(7)-O(2)	-11.92(12)
C(5)-C(6)-C(7)-N(2)	-67.20(10)
C(8)-C(6)-C(7)-N(2)	170.83(8)
C(28)-N(3)-C(8)-O(3)	-17.74(13)
C(22)-N(3)-C(8)-O(3)	165.92(9)
C(28)-N(3)-C(8)-C(6)	158.72(8)
C(22)-N(3)-C(8)-C(6)	-17.62(12)
C(5)-C(6)-C(8)-O(3)	-23.16(11)
C(7)-C(6)-C(8)-O(3)	98.49(10)
C(5)-C(6)-C(8)-N(3)	160.33(8)

C(7)-C(6)-C(8)-N(3)	-78.03(9)
C(7)-N(2)-C(10)-C(11)	-67.66(12)
C(16)-N(2)-C(10)-C(11)	113.70(10)
C(7)-N(2)-C(10)-C(15)	110.65(11)
C(16)-N(2)-C(10)-C(15)	-67.99(12)
C(15)-C(10)-C(11)-C(12)	-2.93(16)
N(2)-C(10)-C(11)-C(12)	175.36(10)
C(10)-C(11)-C(12)-C(13)	1.72(19)
C(11)-C(12)-C(13)-C(14)	0.5(2)
C(12)-C(13)-C(14)-C(15)	-1.5(2)
C(13)-C(14)-C(15)-C(10)	0.35(18)
C(11)-C(10)-C(15)-C(14)	1.90(16)
N(2)-C(10)-C(15)-C(14)	-176.39(10)
C(7)-N(2)-C(16)-C(21)	-33.94(14)
C(10)-N(2)-C(16)-C(21)	144.68(10)
C(7)-N(2)-C(16)-C(17)	148.53(9)
C(10)-N(2)-C(16)-C(17)	-32.85(12)
C(21)-C(16)-C(17)-C(18)	0.66(15)
N(2)-C(16)-C(17)-C(18)	178.22(10)
C(16)-C(17)-C(18)-C(19)	0.35(17)
C(17)-C(18)-C(19)-C(20)	-0.9(2)
C(18)-C(19)-C(20)-C(21)	0.4(2)
C(17)-C(16)-C(21)-C(20)	-1.10(17)
N(2)-C(16)-C(21)-C(20)	-178.61(10)
C(19)-C(20)-C(21)-C(16)	0.6(2)
C(8)-N(3)-C(22)-C(23)	111.63(11)
C(28)-N(3)-C(22)-C(23)	-64.73(13)
C(8)-N(3)-C(22)-C(27)	-69.07(13)
C(28)-N(3)-C(22)-C(27)	114.58(11)
C(27)-C(22)-C(23)-C(24)	0.66(17)
N(3)-C(22)-C(23)-C(24)	179.95(10)
C(22)-C(23)-C(24)-C(25)	0.3(2)
C(23)-C(24)-C(25)-C(26)	-0.5(2)
C(24)-C(25)-C(26)-C(27)	-0.1(2)
C(23)-C(22)-C(27)-C(26)	-1.26(17)
N(3)-C(22)-C(27)-C(26)	179.44(10)

C(25)-C(26)-C(27)-C(22)	0.97(19)
C(8)-N(3)-C(28)-C(29)	129.95(11)
C(22)-N(3)-C(28)-C(29)	-53.55(13)
C(8)-N(3)-C(28)-C(33)	-50.36(13)
C(22)-N(3)-C(28)-C(33)	126.14(11)
C(33)-C(28)-C(29)-C(30)	0.20(19)
N(3)-C(28)-C(29)-C(30)	179.88(11)
C(28)-C(29)-C(30)-C(31)	-0.7(2)
C(29)-C(30)-C(31)-C(32)	0.9(2)
C(30)-C(31)-C(32)-C(33)	-0.7(2)
C(29)-C(28)-C(33)-C(32)	0.02(19)
N(3)-C(28)-C(33)-C(32)	-179.67(12)
C(31)-C(32)-C(33)-C(28)	0.2(2)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C26
C25
C27
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1. Data collection, cell refinement and data reduction uses XSCANS, Version 2.10 [Siemens, 1994].
2. SMART and SAINT software, Bruker Analytical Instruments, Madison, Version 5.1.
3. Structure solution, structure refinement and final table preparation software uses SHELXTL-NT, Version 5.10 [Bruker, 1999].
4. Absorption correction uses XPREP, Version 5.03. [Siemens, 1994].
5. SADABS absorption correction software, Bruker Analytical Instruments, Madison, Version 5.1
6. SHELX97, Version 6.12 Sheldrick, G.W., Bruker Analytical Instruments, Madison 2001.
7. Allen, F. H. Cambridge Structural Database, *Acta. Crystallogr.* **2002**, *B58*, 380.

Additional Experimental Procedures and Data

Procedures: Reactions were generally carried out under dry nitrogen in order to minimize contact of sensitive reagents with water unless noted otherwise. Standard methods were used to dry solvents. TLC methods using silica gel plates were used to monitor reaction progress and product purities. Silica gel (70 – 230 mesh, 60 Å) packed (3 cm x 40 cm) in a glass column was used for chromatographic separations. NMR spectra were recorded on 250 MHz or 500 MHz instruments and denterated solvents were employed. Me_4Si was employed as the internal reference. FT-IR were recorded using KBr pellets. The high resolution mass spectra were recorded using a ESI-MS TOF spectrometer. The low resolution mass spectrum of **1** was recorded by FAB methods.

Reagents. Commercial organic reagents were used as received from suppliers. Solvents were dried and distilled prior to use.

Infrared Spectroscopic Data for 1-4, **13**, **14**

Compound 1. IR (KBr, cm^{-1}):3061, 3039, 2927, 2854, 1674 (CO), 1592, 1491, 1452, 1436, 1355, 1276, 1216, 1157, 1134, 1075, 1037, 996, 928, 847, 797, 756, 702, 639, 579, 551, 511, 463.

Compound 2. IR (KBr, cm^{-1}):3448; 3060; 2924; 2856; 1675 (CO); 1588; 1491; 1455; 1351; 1296; 1156; 1079; 1032; 995; 762; 698; 581; 510.

Compound 3. IR (KBr, cm^{-1}): 3058, 2923, 2856, 1735, 1682 (ν_{co}), 1589, 1487, 1462, 1349, 1298, 1238, 1148, 1077, 1032, 1016, 996, 907, 873, 838, 756, 698, 626, 595, 578, 564, 515.

Compound 4. IR (KBr, cm^{-1}): 3060-2924, 1687 (CO), 1587, 1489, 1453, 1344, 1154, 1073, 1027, 866, 757, 696, 628, 562, 508.

Compound 13. IR (KBr, cm^{-1}): 3447, 3059, 2925, 2854, 2492, 2349, 1959, 1681 (ν_{co}), 1589, 1489, 1436, 1351, 1279, 1236, 1154, 1073, 1033, 994, 919, 844, 757, 697, 627, 587.

Compound 14. IR (KBr, cm^{-1}): 3360, 3082, 3019, 2922, 1990, 1800, 1681, 1589, 1489, 1450, 1390, 1347, 1293, 1157, 1079, 1028, 839, 759, 691.

Specific Oxidation Procedures and Characterization Data

Compound 5. **1** (0.2 g; 0.87 mmol) in CH_2Cl_2 (10 mL) was combined with *m*CPBA (0.18 g, 0.87 mmol) and the mixture heated (50-60 °C, 12h). The resulting mixture was flash chromatographed on silica gel using ethyl acetate ($R_f = 0.6$) or CH_2Cl_2/MeOH 99/1 ($R_f = 0.63$) as the elution solvent. Compound **5** was obtained as colorless crystals. Yield: 0.017 g, 6.5%. IR(KBr, cm^{-1}): 3412, 3057, 2925, 1704, 1663 (ν_{co}), 1586, 1488, 1448, 1377, 1267, 1225, 1164, 1079, 1010, 940, 763, 751, 694, 659, 578, 516, 464.

Compound 7. **1** (1.1 g, 3.81 mmol) in CH_2Cl_2 (20 mL) was combined with *m*CPBA (1.0 g, 4.6 mmol). The mixture was heated (50-60 °C, 12h). The resulting mixture was flash chromatographed on silica gel using ethyl acetate ($R_f = 0.36$) or CH_2Cl_2/MeOH 99/1 ($R_f = 0.39$) as eluants. The product **7** was recovered as analytically pure colorless crystals after recrystallization from MeOH. Yield: 0.81 g, 70%. IR(KBr, cm^{-1}): 3412, 3057, 2925, 1668

(ν_{co}), 1589, 1489, 1441, 1347, 1299, 1191, 1073, 991, 896, 832, 757, 698, 664, 634, 591, 519. Anal. Calcd for $C_{19}H_{16}N_2O$: C 74.98, H 5.30, N 9.20. Found: C 75.05, H 5.60, N 9.08.

Compound 9. **1** (0.2 g, 0.87 mmol) in CH_2Cl_2 (10 mL) was combined with *m*CPBA (0.18 g, 1 mmol). The mixture was stirred at 23 °C (12h) and the resulting mixture flash chromatographed on silica gel using ethyl acetate (R_f = 0.36) or CH_2Cl_2/MeOH 99/1 (R_f = 0.31) as eluants until **5** and **7** were removed and the retained **9** was eluted with CH_2Cl_2/MeOH (98/2). Yield: 0.044 g, 16%. IR (KBr, cm^{-1}): 3057, 1670 (ν_{co}), 1590, 1489, 1439, 1372, 1320, 1259, 1211, 1167, 1098, 1027, 914, 853, 802, 760, 591, 552, 517, 478. Anal. Calcd for $C_{19}H_{16}N_2O_2$: C 74.98, H 5.30, N 9.20. Found: 70.58, H 5.10, N 8.66. Compound **11** may be a trace containment in this sample.

Compound 11. **1** (0.331 g, 1.45 mmol) in CH_2Cl_2 (10 mL) was combined with *m*CPBA (0.75 g, 4.35 mmol). The mixture was heated (50-60 °C, 12h) and the residue flash chromatographed on silica gel using CH_2Cl_2/MeOH 99/1 (R_f = 0.21) as the eluant. Yield: 0.287 g, 62%. The white powder was further purified by recrystallization from MeOH. IR (KBr, cm^{-1}): 3063, 1672 (ν_{co}), 1592, 1491, 1436, 1399, 1360, 1298, 1236, 1190, 1113, 1069, 1034, 991, 982, 900, 839, 861, 769, 699, 646, 560. Anal. Calcd for $C_{19}H_{16}N_2O_3$: C 71.24, H 5.03, N 8.74. Found: C 72.99, H 5.21, N 8.78.

Compound 6. **2** (0.66 g, 2.18 mmol) in CH_2Cl_2 (10 mL) was combined with *m*CPBA (0.452 g, 1.95 mmol) and the mixture heated (55 °C, 12h). The resulting mixture was flash chromatographed on silica gel using ethyl acetate (R_f = 0.84) or CH_2Cl_2/MeOH 99/1 (R_f = 0.63) as the eluant. **6** was recovered as a colorless solid. Yield: 0.054 g, 7.8%; m.p. 148-150. IR (KBr, cm^{-1}): 2925, 2858, 1701, (ν_{co} ketone), 1660 (ν_{co} amide), 1589, 1489, 1456, 1372, 1288, 1225,

1161, 1075, 1030, 952, 837, 761, 695. Anal. Calcd for $C_{20}H_{16}N_2O_2$: C 75.93, H 5.10, N 8.85. Found: C 73.03, H 5.10, N 8.85.

Compound 8. **2** (0.66 g, 2.18 mmol) in CH_2Cl_2 (10 mL) was combined with *m*CPBA (0.452 g, 1.95 mmol) and the mixture heated (55 °C, 12h). The resulting mixture was flash chromatographed on silica gel using ethyl acetate ($R_f = 0.62$) or CH_2Cl_2/MeOH 99/1 ($R_f = 0.28$) as the eluants. This fraction provided a white solid. Yield: 0.35 g, 50%; m.p. 86-88 °C. IR(KBr, cm^{-1}): 3417, 3062, 3038, 1669 (ν_{co}), 1593, 1491, 1455, 1343, 1307, 1194, 1156, 1074, 1030, 1003, 980, 802, 757, 701, 611, 508. Anal. Calcd for $C_{20}H_{16}N_2O_2$: C 75.45, H 5.70, N 8.80. Found: C 75.13, H 5.68, N 8.81.

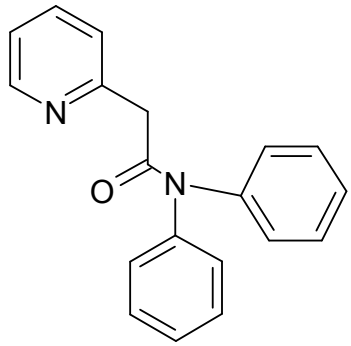
Compound 10. **2** (0.66 g, 2.18 mmol) in CH_2Cl_2 (10 mL) was combined with *m*CPBA (0.452 g, 1.95 mmol) and the mixture heated (55 °C, 12h). The resulting mixture was flash chromatographed on silica gel using as the eluant ethyl acetate ($R_f = 0.11$) or CH_2Cl_2/MeOH 99/1 ($R_f = 0.12$). This fraction containing **2** provided a white solid. Yield: 0.255 g, 36%; m.p. 178-180 °C. IR(KBr, cm^{-1}): 3054, 1673 (ν_{co}), 1589, 1491, 1449, 1364, 1291, 1250, 1166, 1081, 1031, 989, 968, 842, 762, 697, 624, 573, 530, 497.

Compound 12. **8** (0.2 g, 0.62 mmol) in CH_2Cl_2 (10 mL) was combined with *m*CPBA (0.195 g, 0.84 mmol) and the mixture heated (50 °C, 12h). The resulting mixture was flash chromatographed with ethyl acetate ($R_f = 0.4$) or CH_2Cl_2/MeOH 99/1 ($R_f = 0.17$) providing a white solid. Yield: 0.12 g, 57%; m.p. 168-170 °C. IR(KBr, cm^{-1}): 3425, 1678 (ν_{co}), 1641, 1630, 1620, 1591, 1493, 1462, 1451, 1425, 1402, 1304, 1258, 1211, 1161, 1077, 1029. Anal. Calcd for $C_{20}H_{18}N_2O_3$ C 71.84, H 5.43, N 8.38. Found: C 71.84, H 5.71, N 7.88.

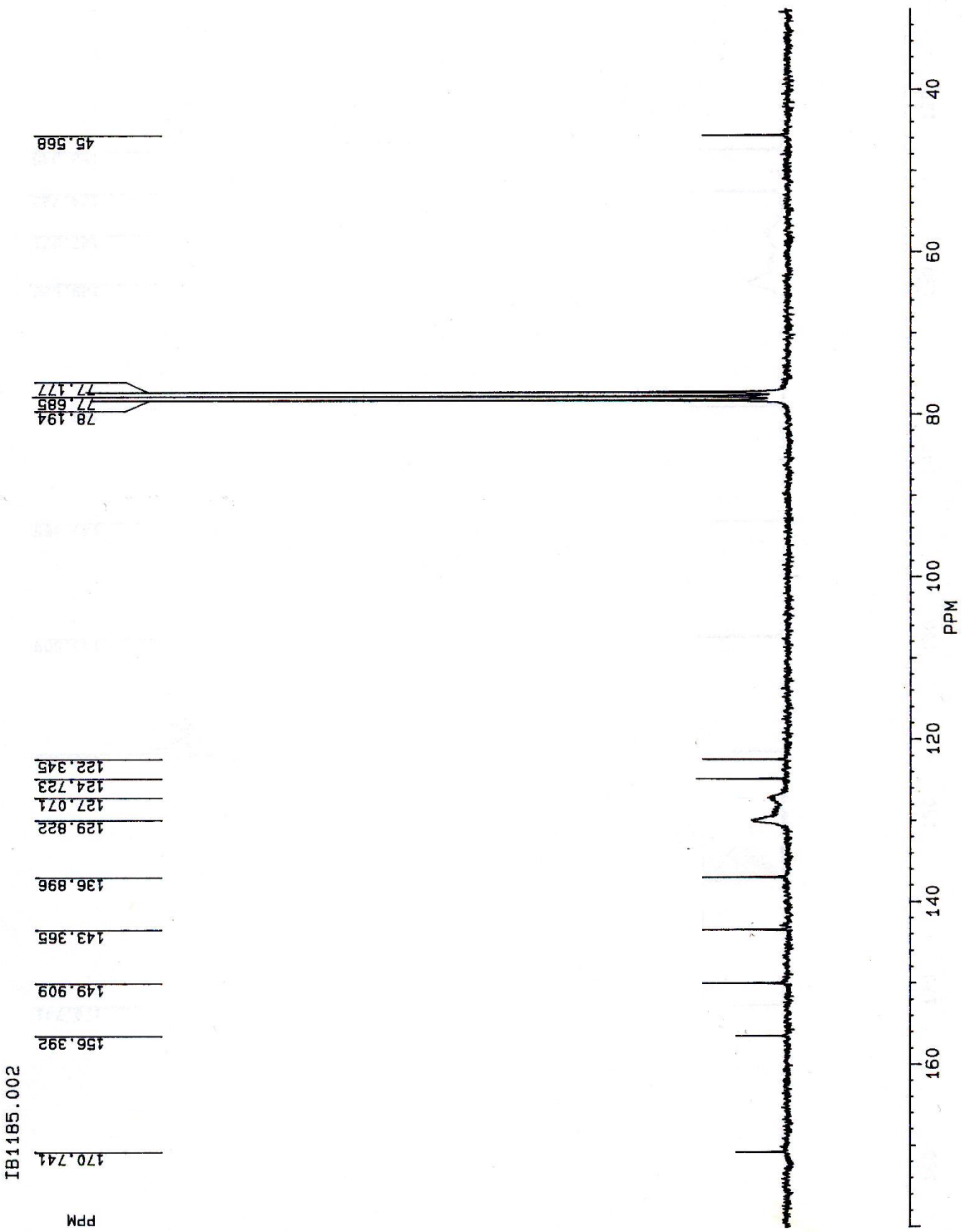
Proton-1 and Carbon-13 NMR Spectra

^{1}H and ^{13}C NMR Spectra for Compounds **1 - 14**

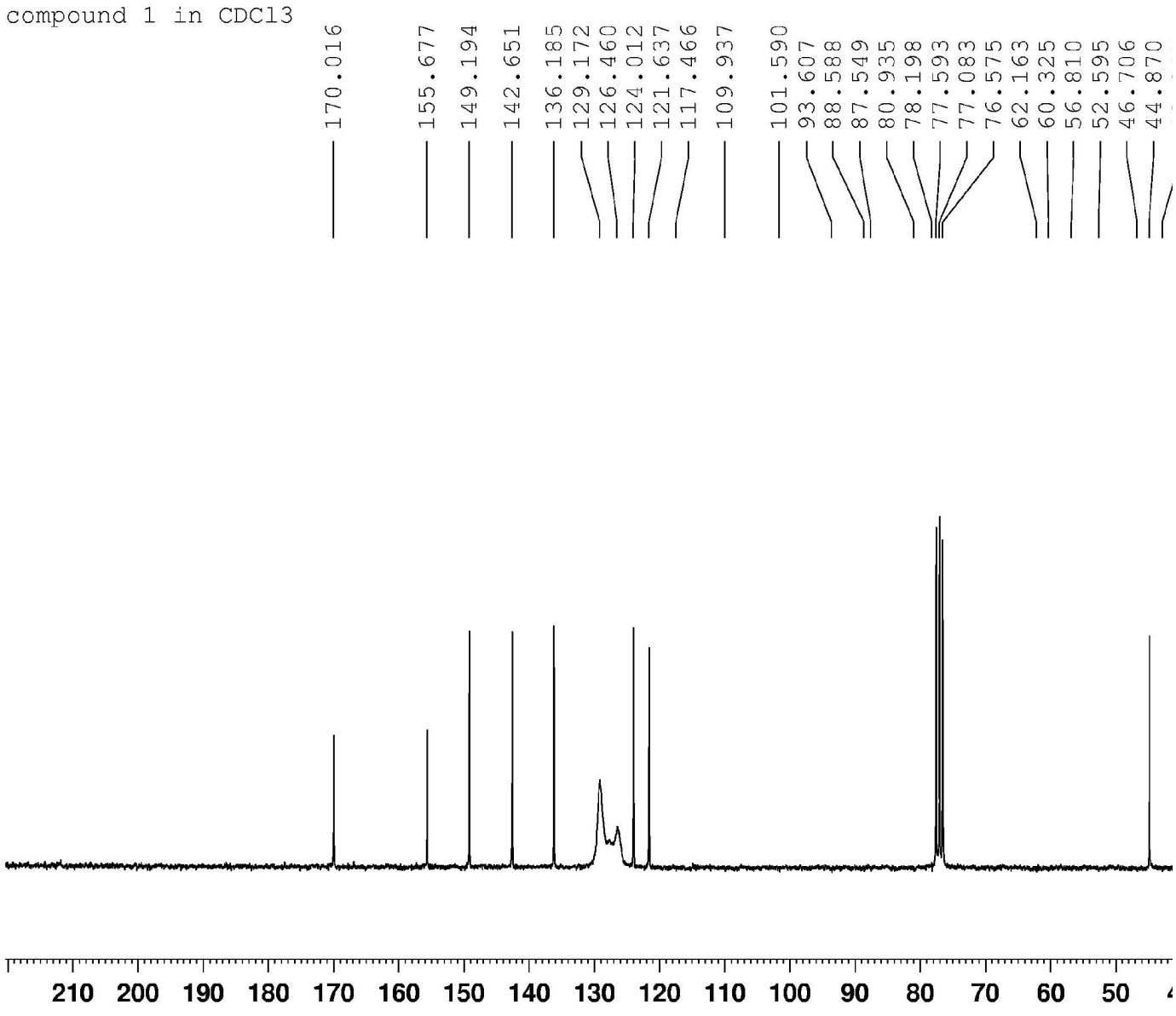
compound 1 N,N-Diphenyl-2-pyridin-2-yl-acetamide



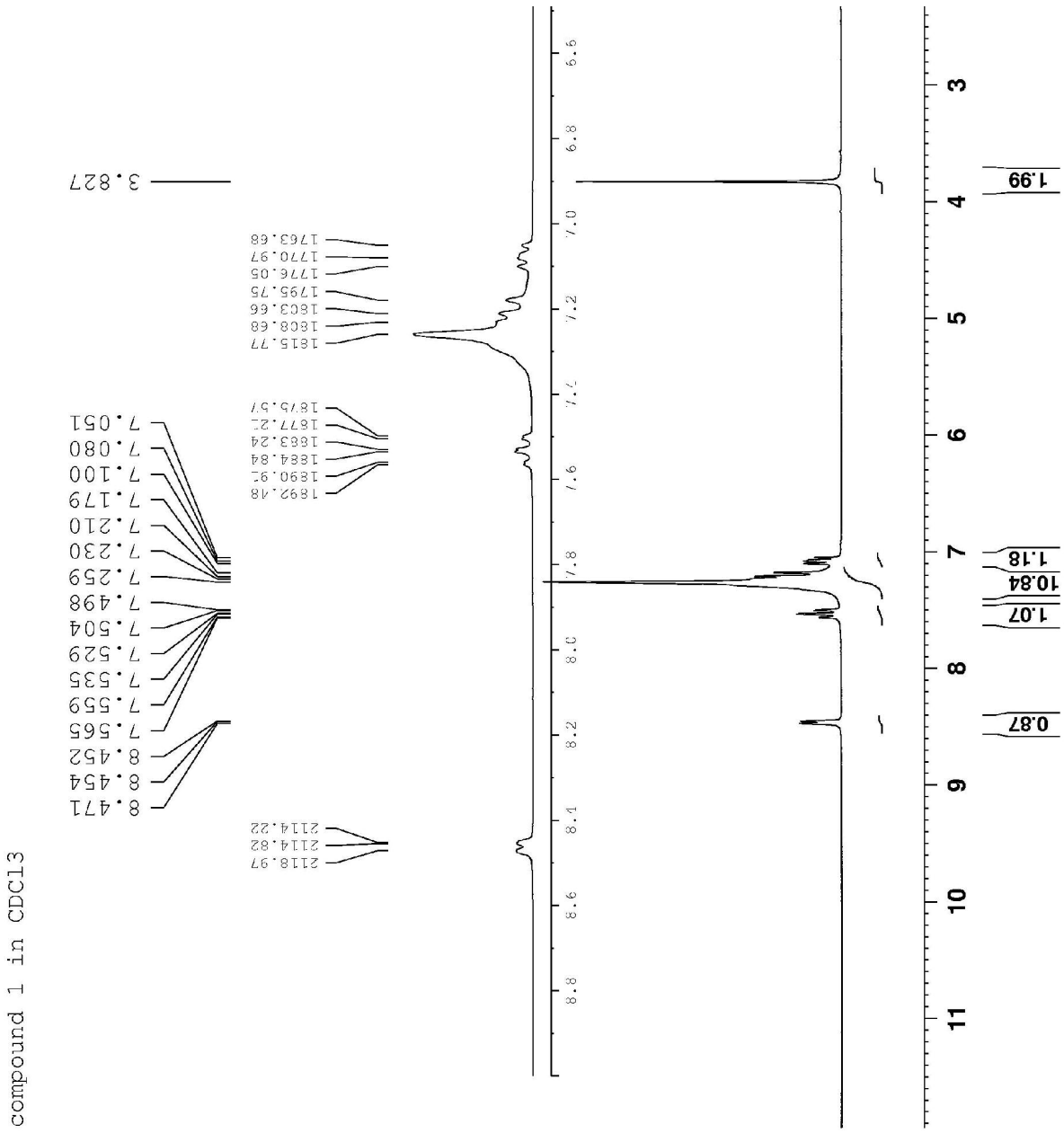
^{13}C $\{^{1}H\}$ NMR; compound 1, $CDCl_3$



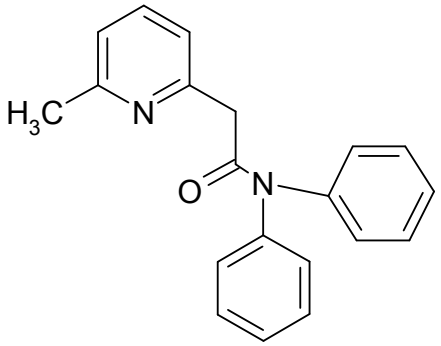
^{13}C {^{1}H} NMR; compound 1, $CDCl_3$



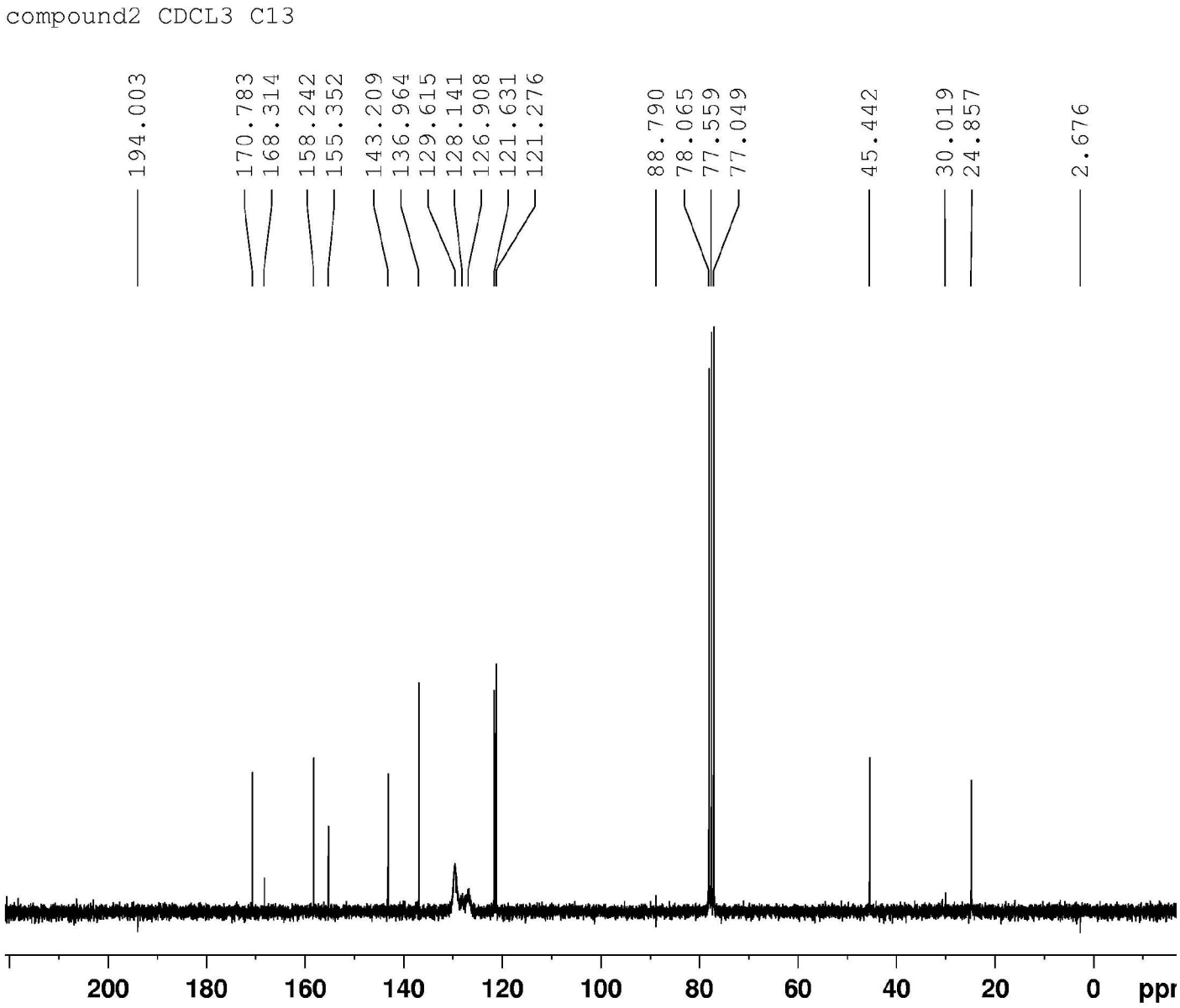
^{1}H NMR; compound 1, $CDCl_3$



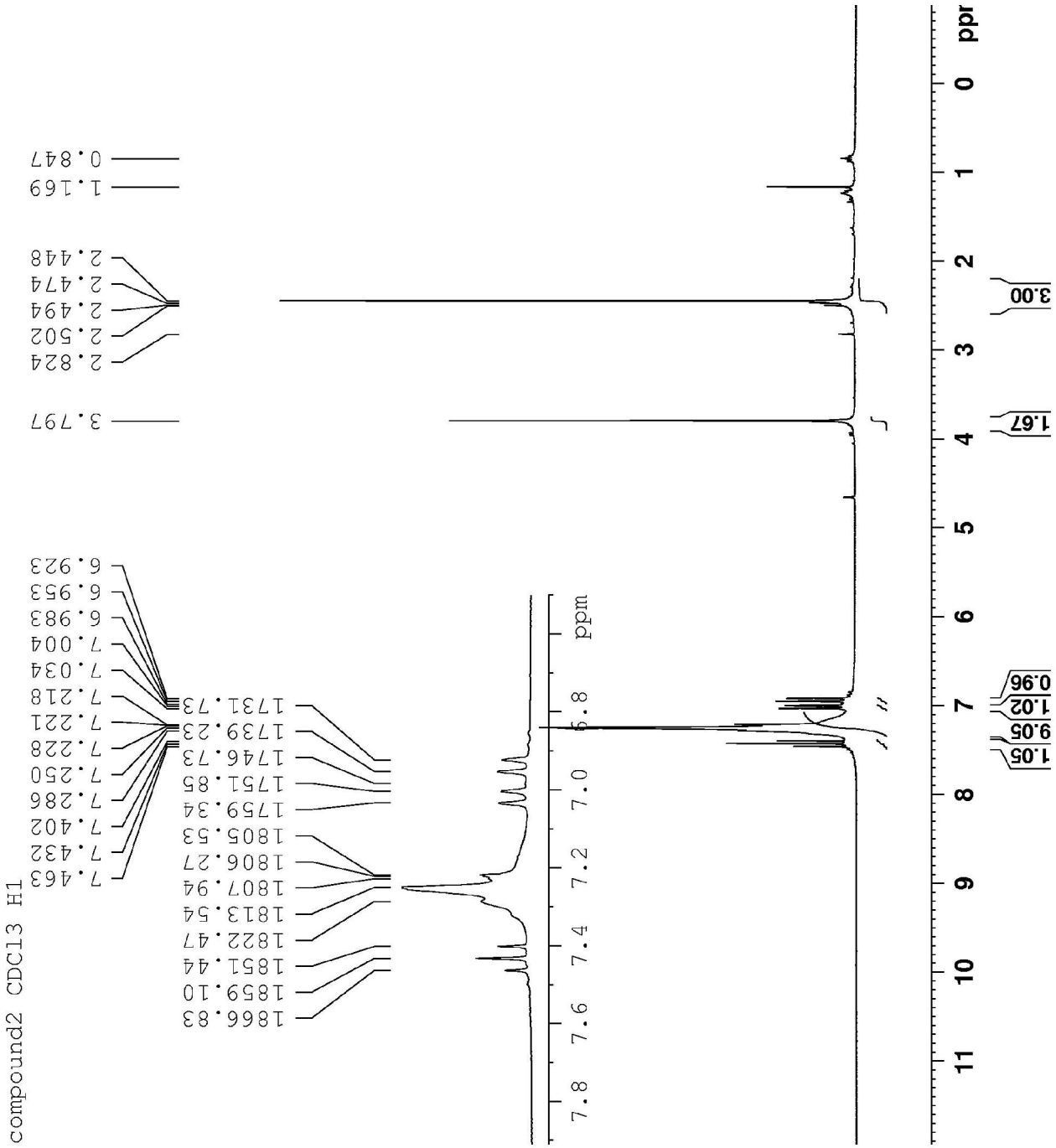
compound 2 2-(6-Methyl-pyridin-2-yl)-N,N-diphenyl-acetamide



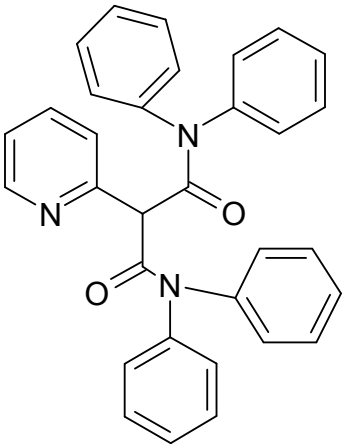
^{13}C {^{1}H}NMR; compound 2, $CDCl_3$



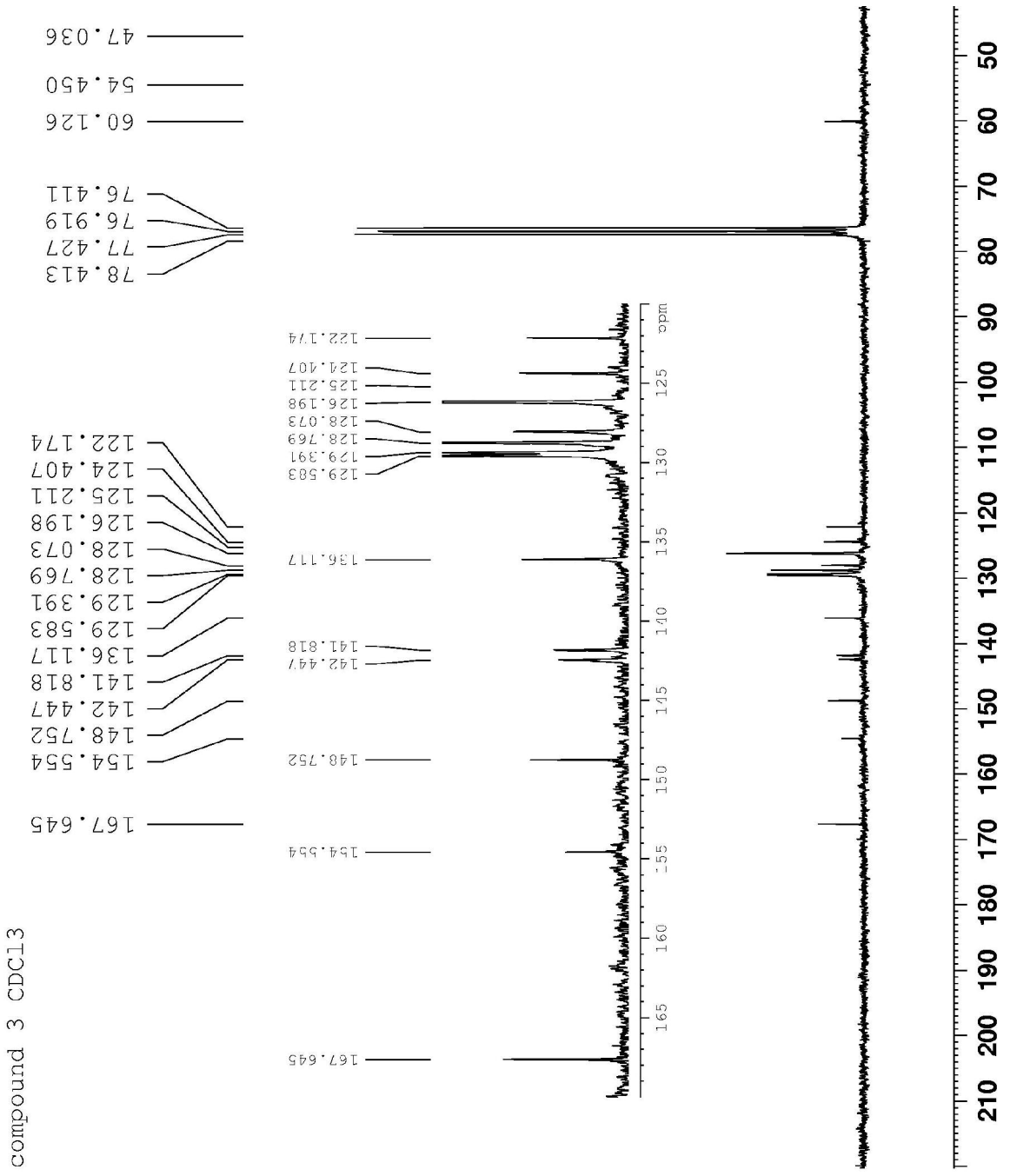
^{1}H NMR; compound 2, $CDCl_3$



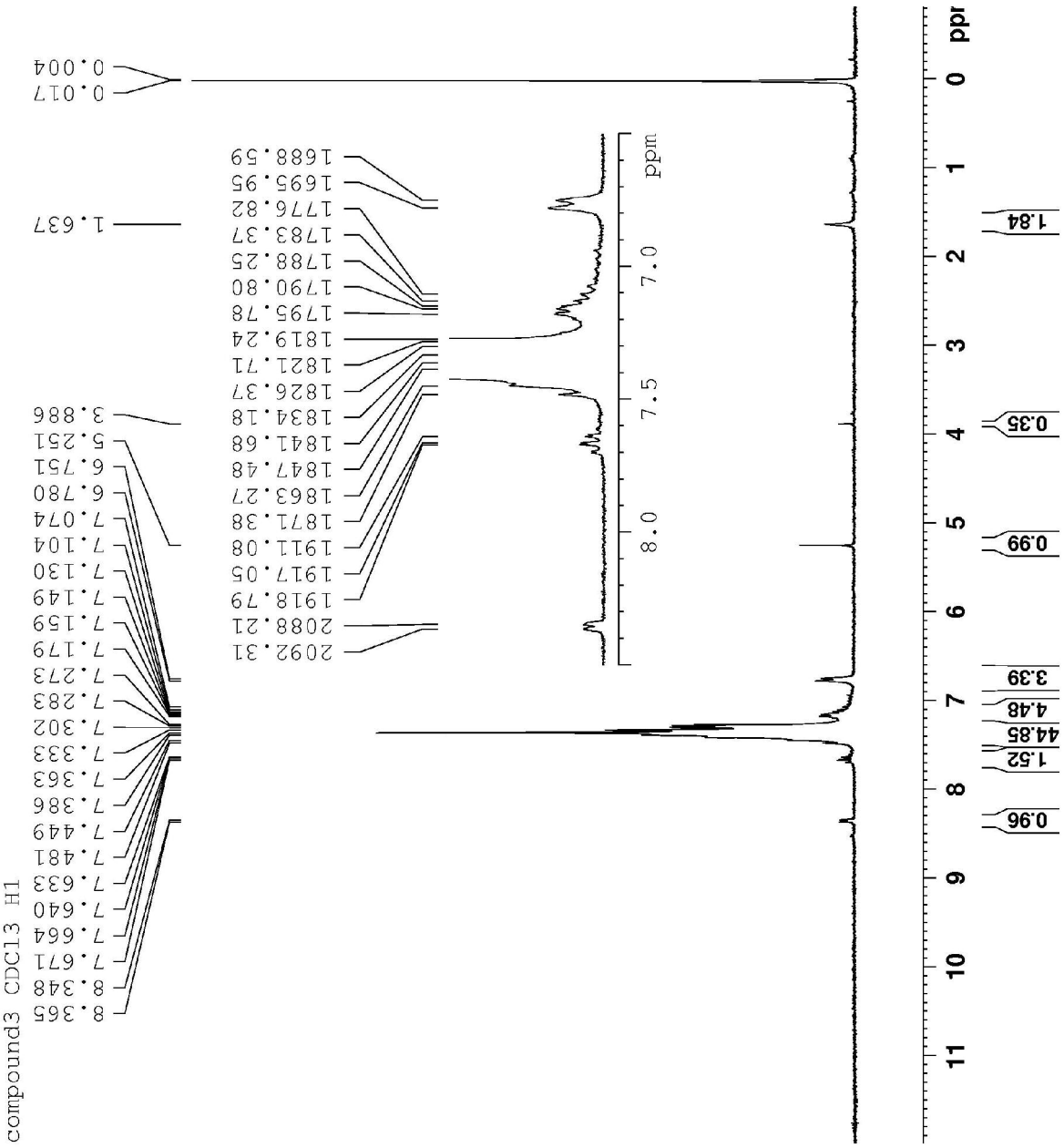
compound 3 N,N,N',N'-Tetraphenyl-2-pyridin-2-yl-malonamide



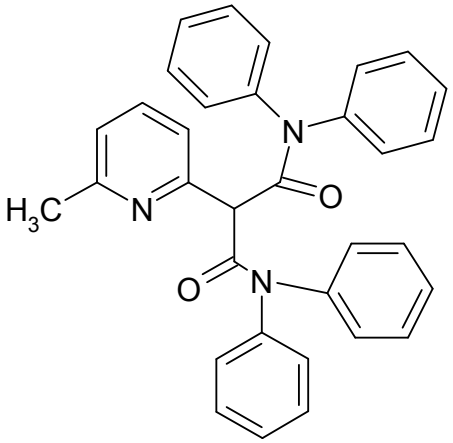
$^{13}C\ \{^{1}H\}$ NMR; compound 3, $CDCl_3$



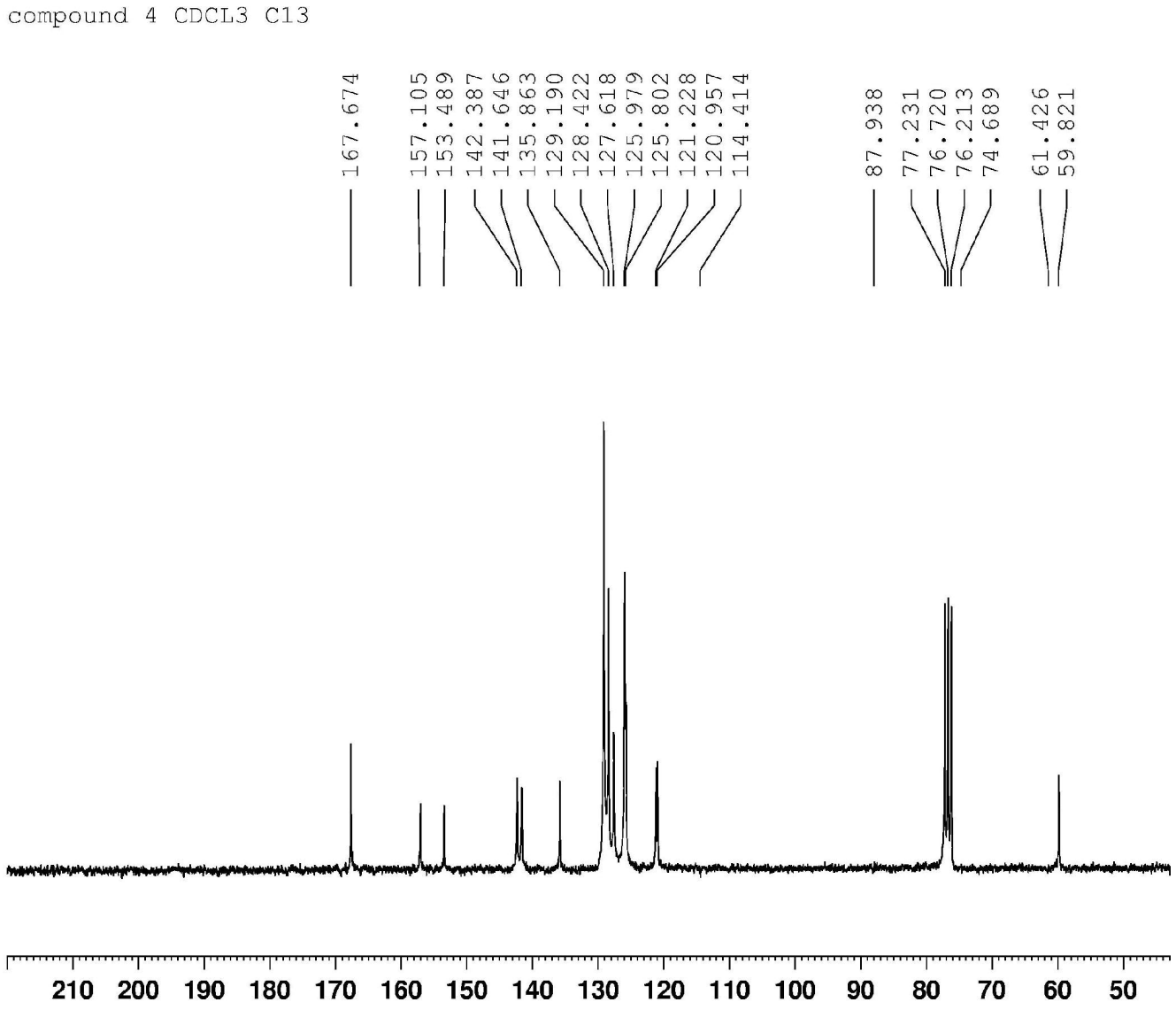
^{1}H NMR; compound 3, $CDCl_3$



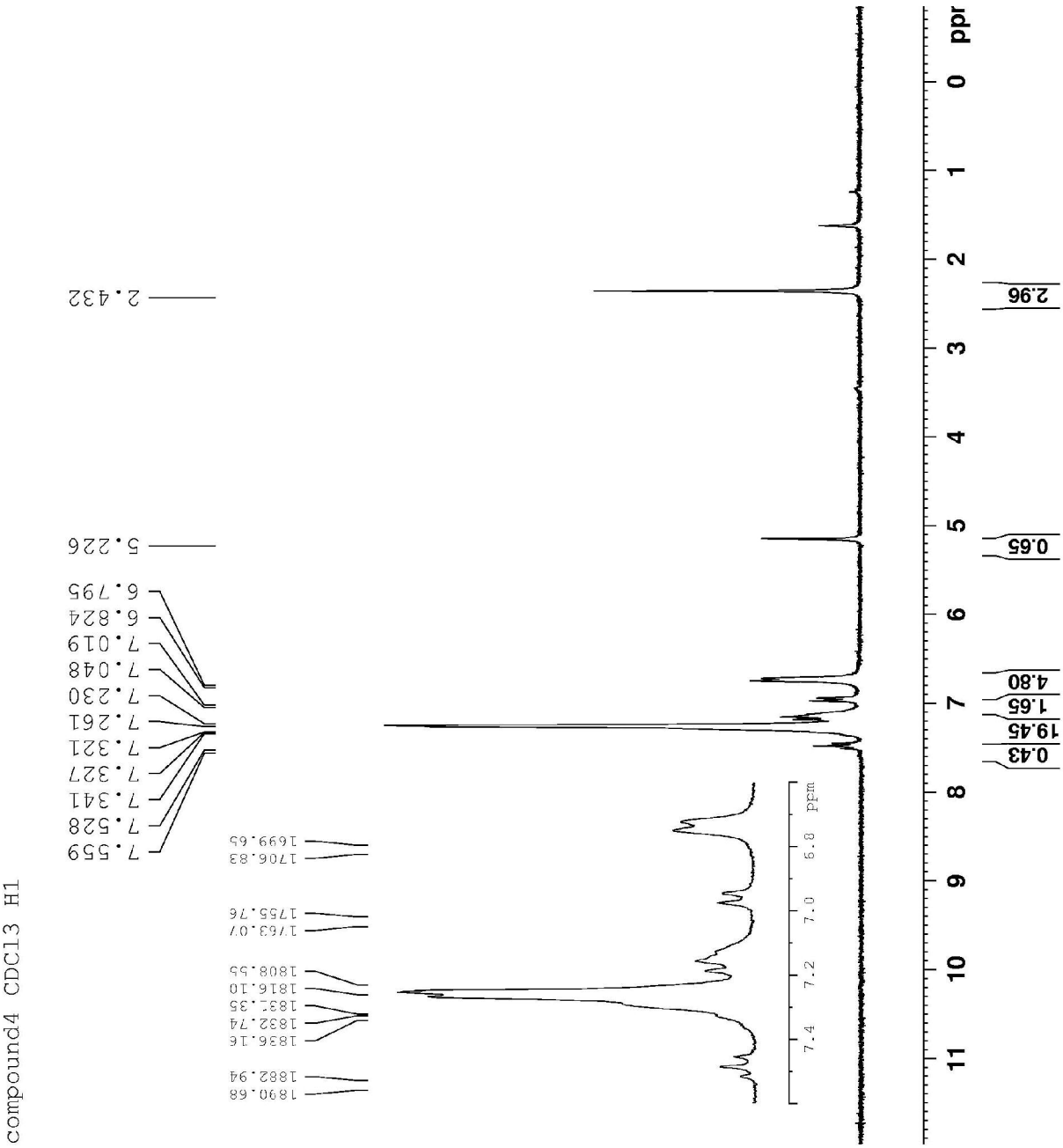
compound 4 2-(6-Methyl-pyridin-2-yl)-N,N,N',N'-tetraphenyl-malonamide



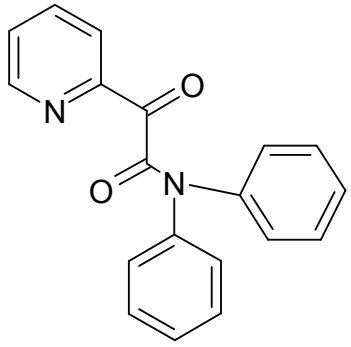
^{13}C {^{1}H} NMR; compound 4, $CDCl_3$



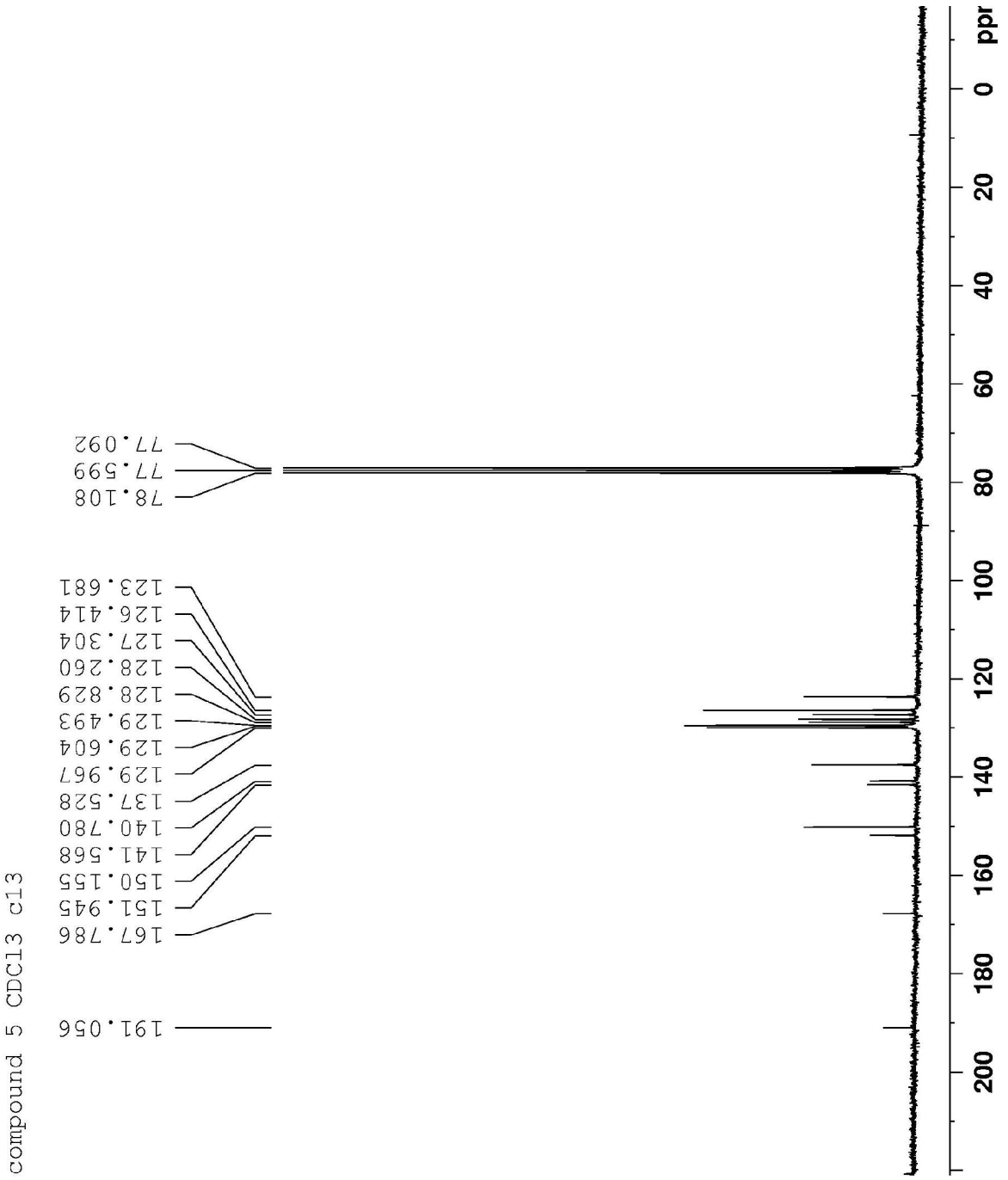
^{1}H NMR; compound 4, $CDCl_3$



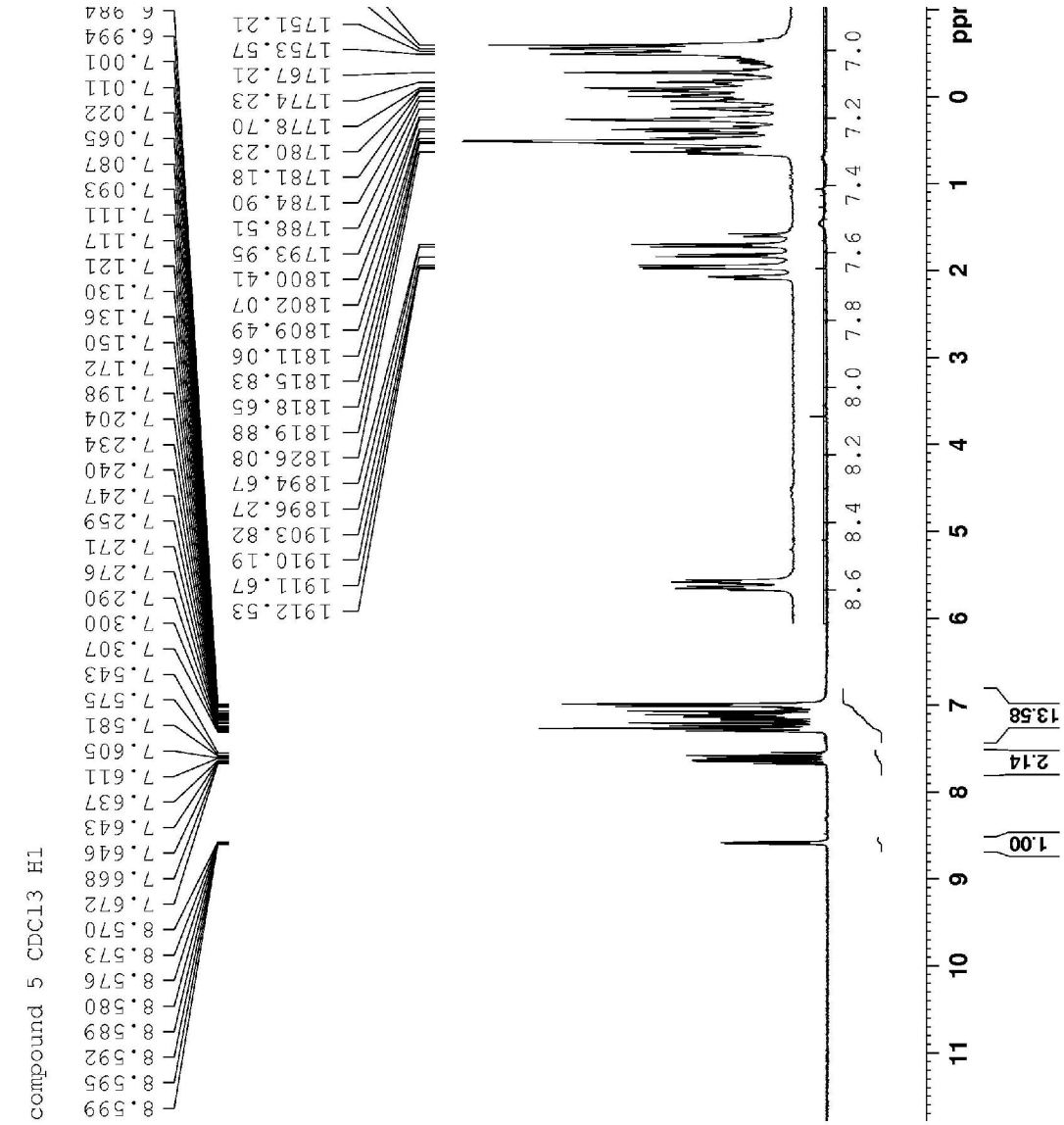
compound 5 2-Oxo-N,N-diphenyl-2-pyridin-2-yl-acetamide



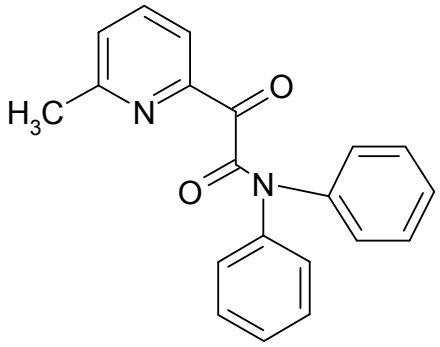
^{13}C {^{1}H} NMR; compound 5, $CDCl_3$



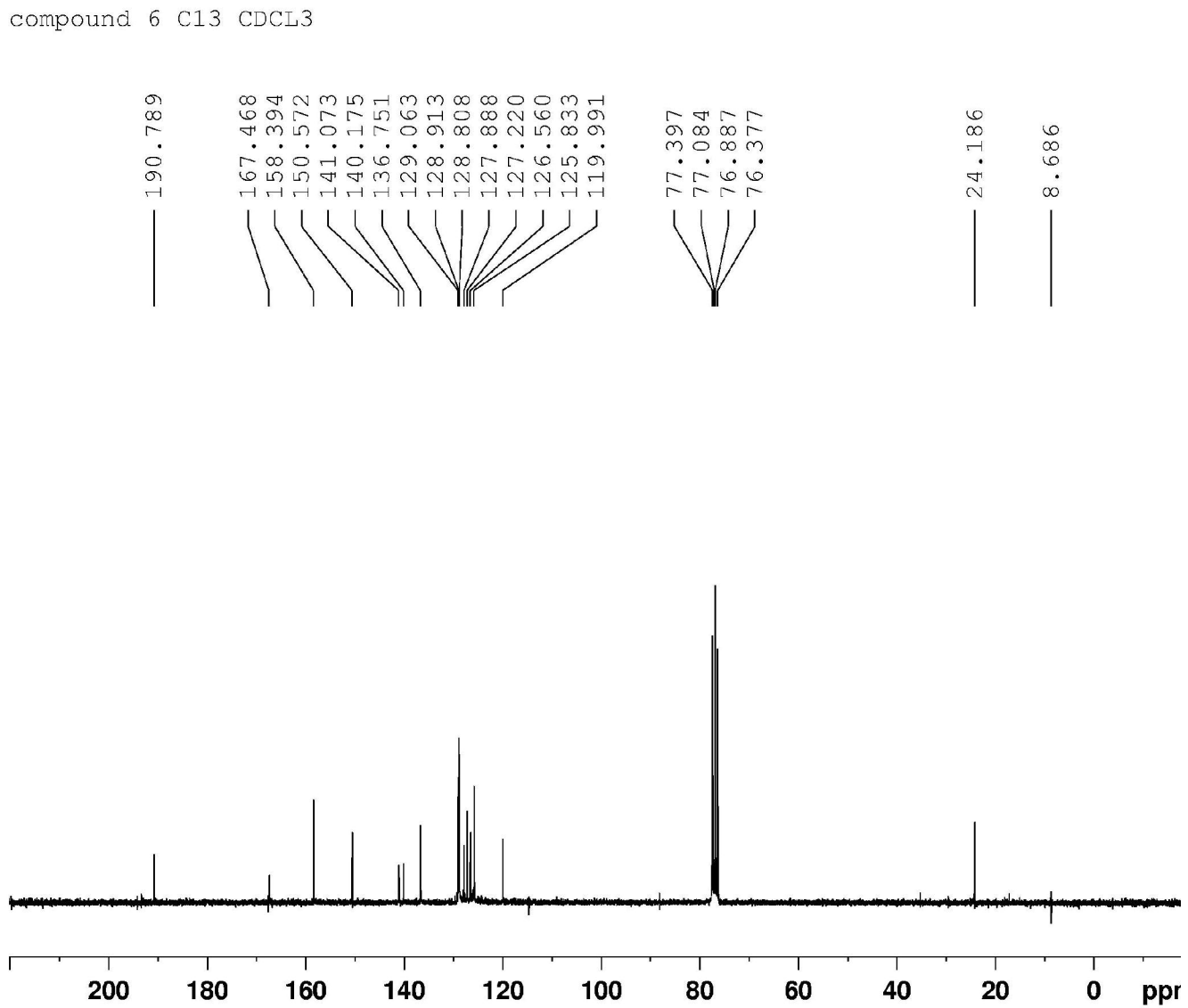
^{1}H NMR; compound 5, $CDCl_3$



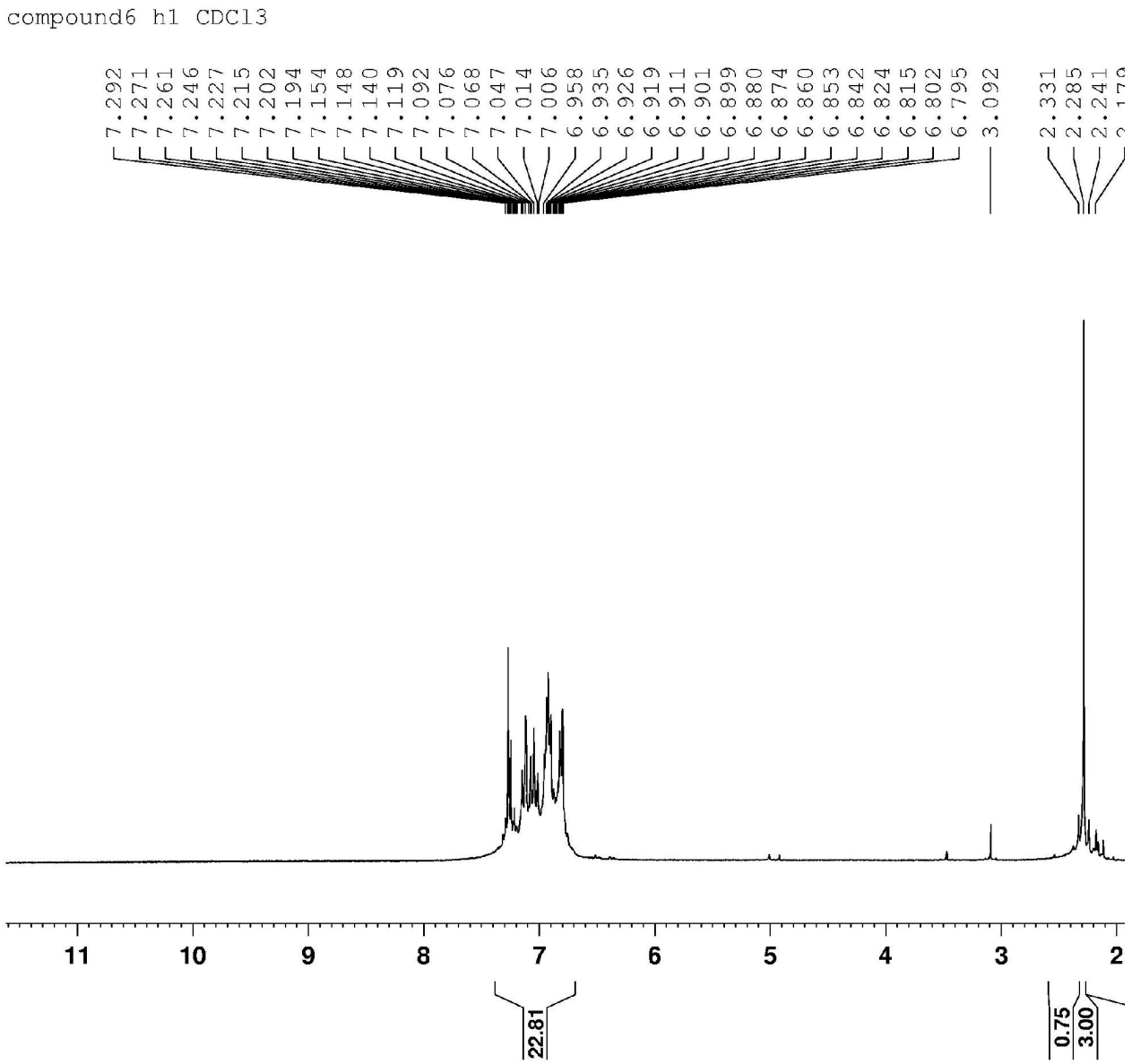
compound 6



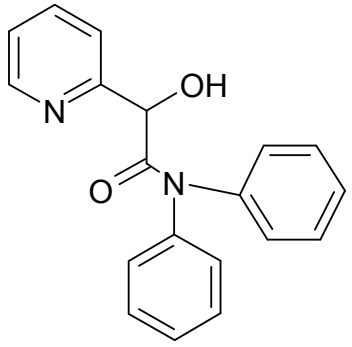
^{13}C {^{1}H} NMR; compound 6, $CDCl_3$



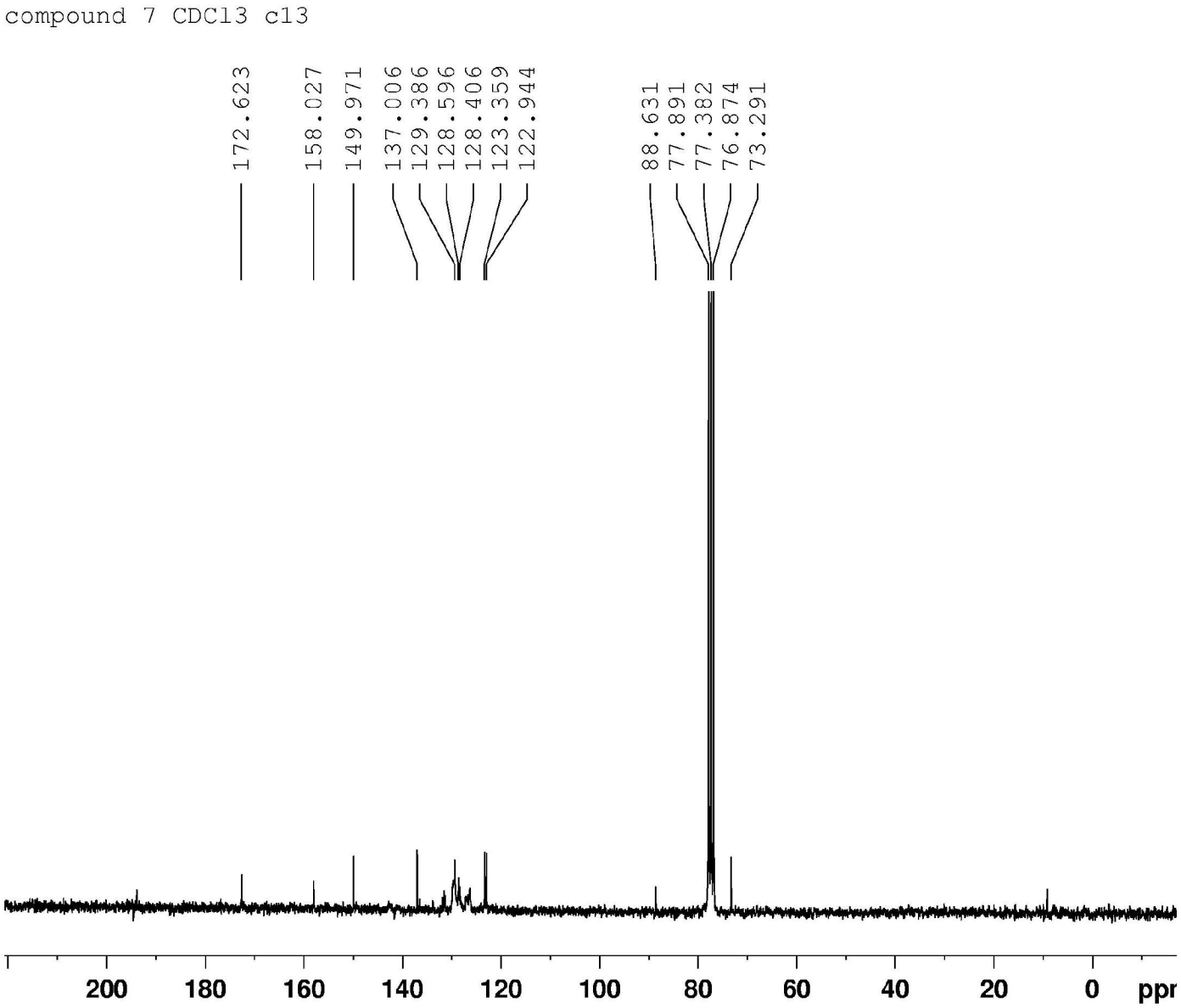
^{1}H NMR: compound 6, $CDCl_3$



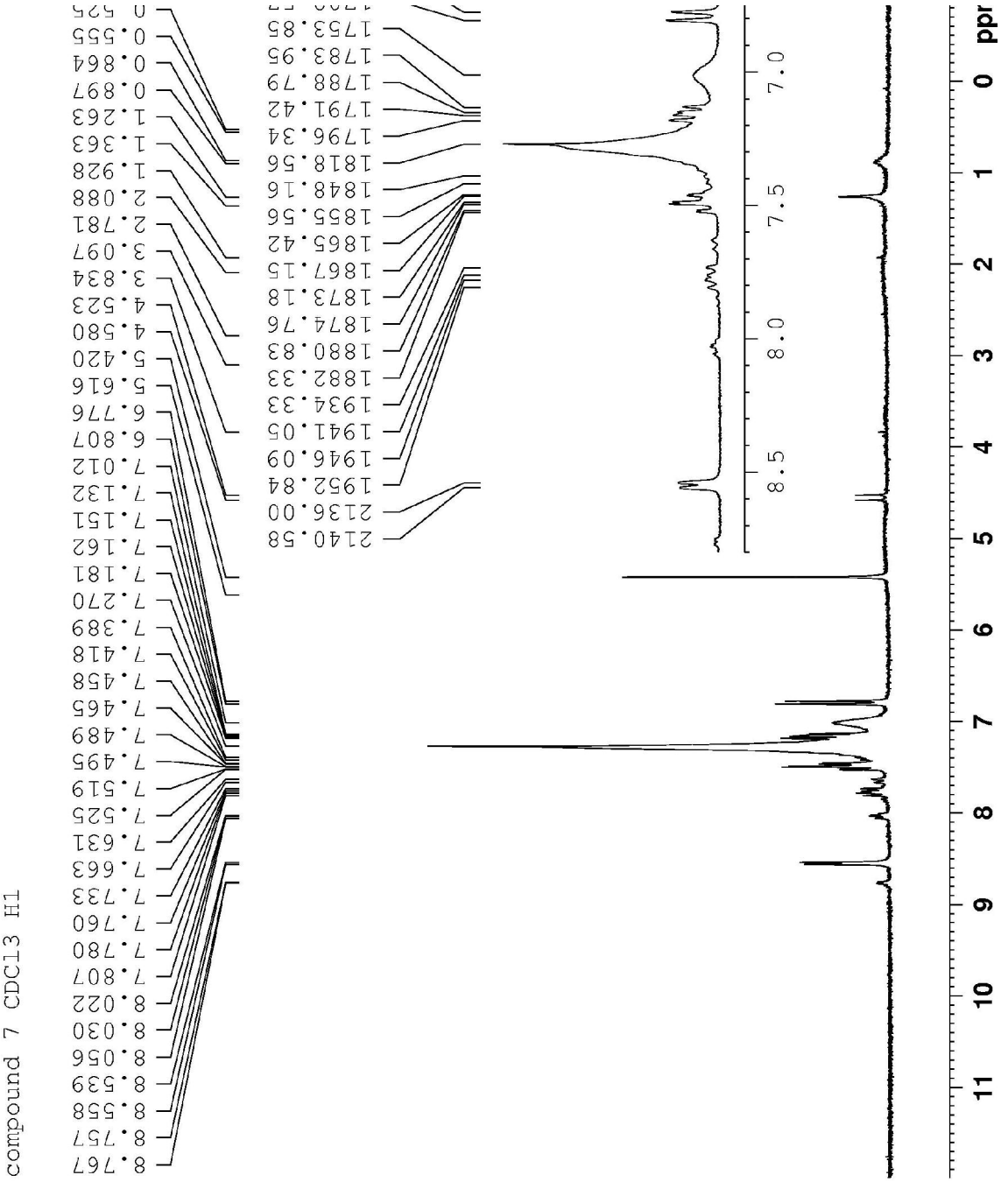
compound 7 2-Hydroxy-N,N-diphenyl-2-pyridin-2-yl-acetamide



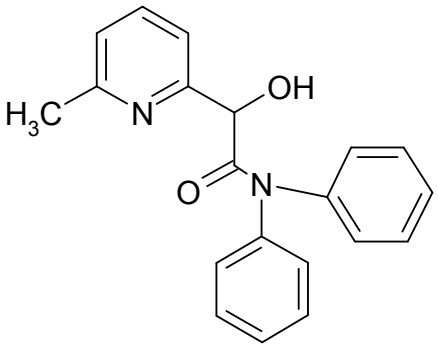
^{13}C {^{1}H} NMR; compound 7, $CDCl_3$



^{1}H NMR: compound 7. $CDCl_3$

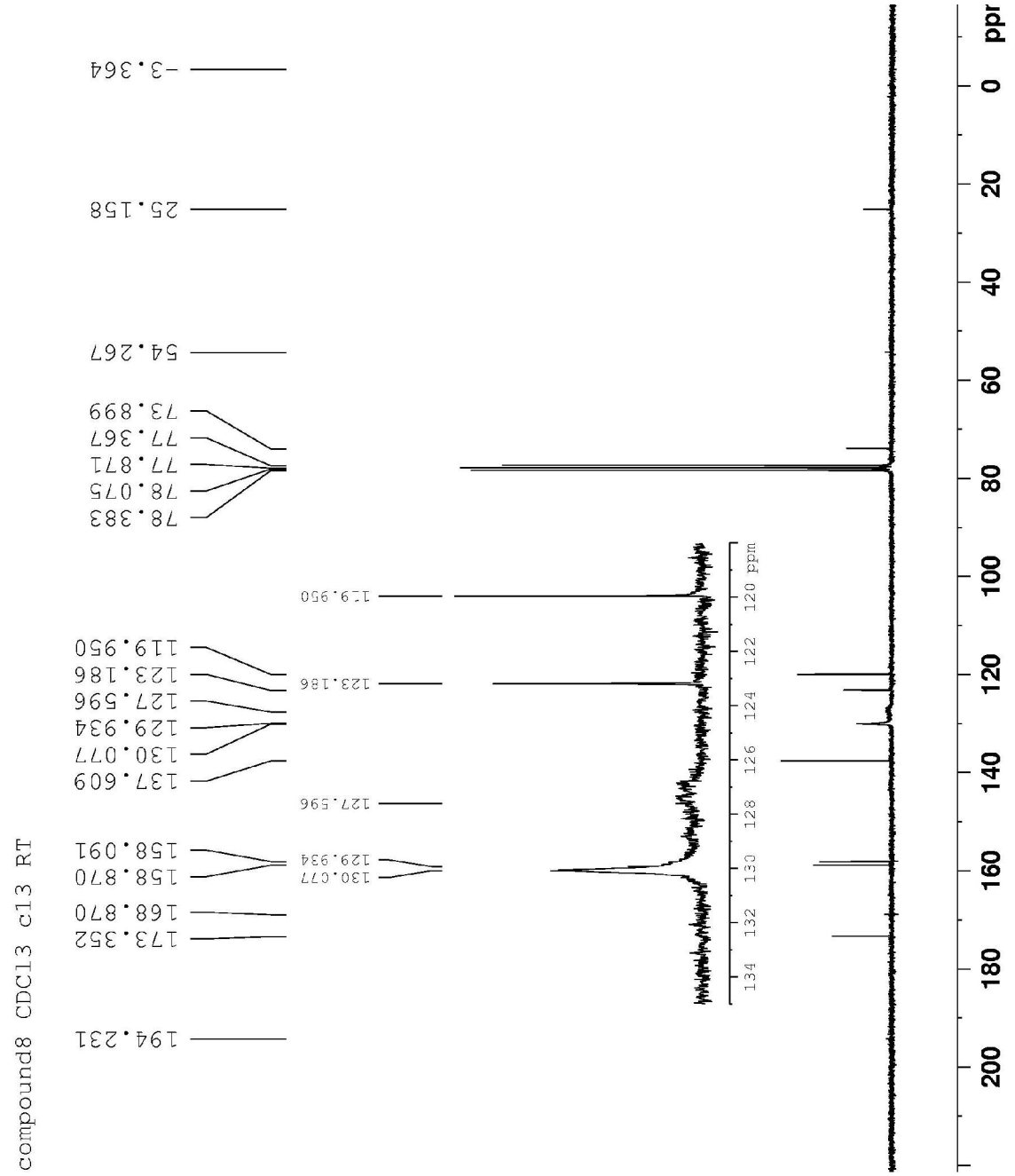


compound 8 2-Hydroxy-2-(6-methyl-pyridin-2-yl)
-N,N-diphenyl-acetamide

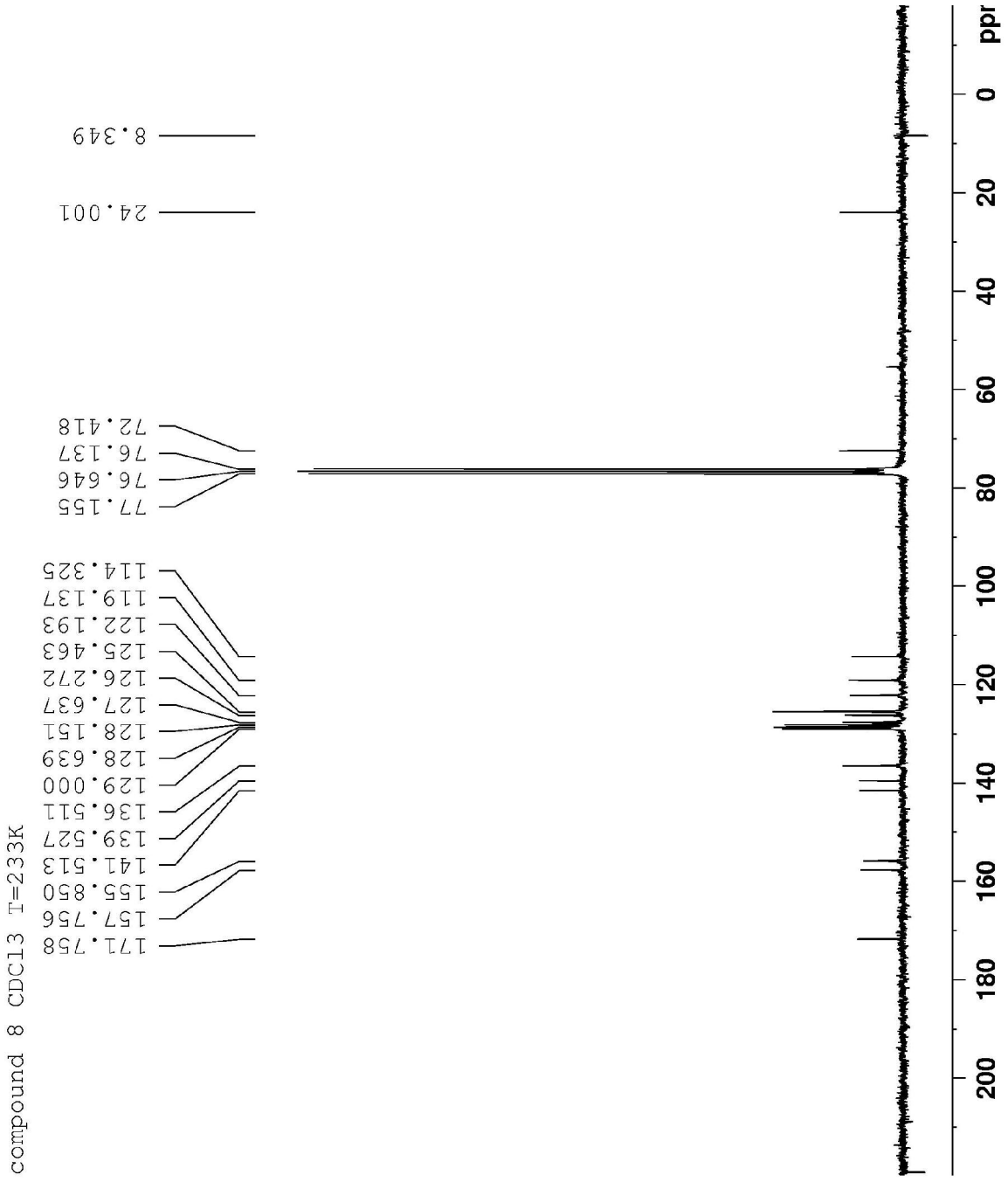


^{13}C {^{1}H} NMR; compound 8, $CDCl_3$,

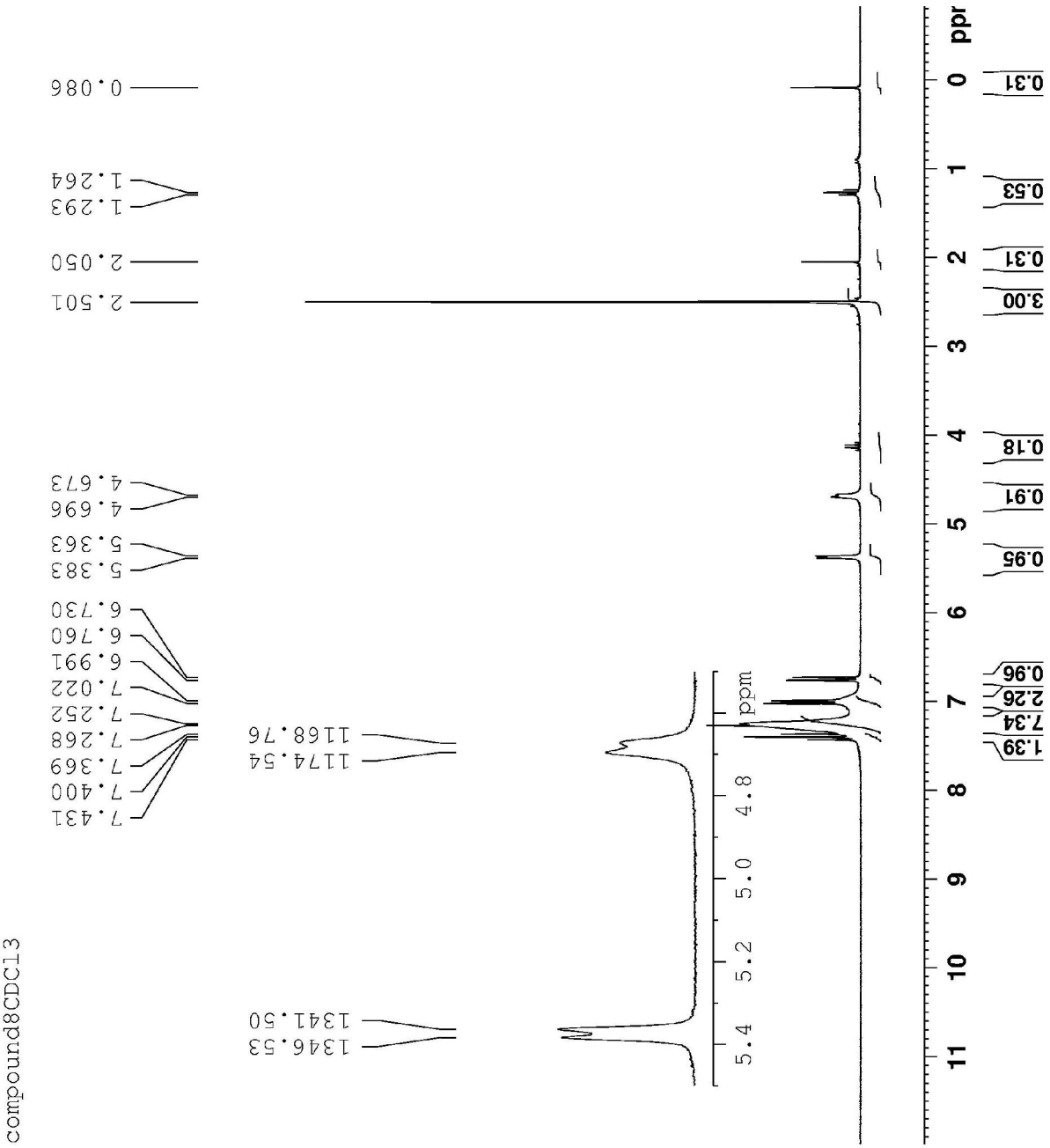
21°C



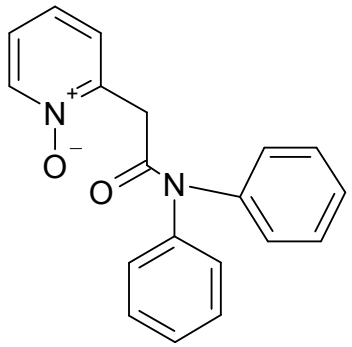
^{13}C $\{^{1}H\}$ NMR; compound 8, $CDCl_3$, T=233K



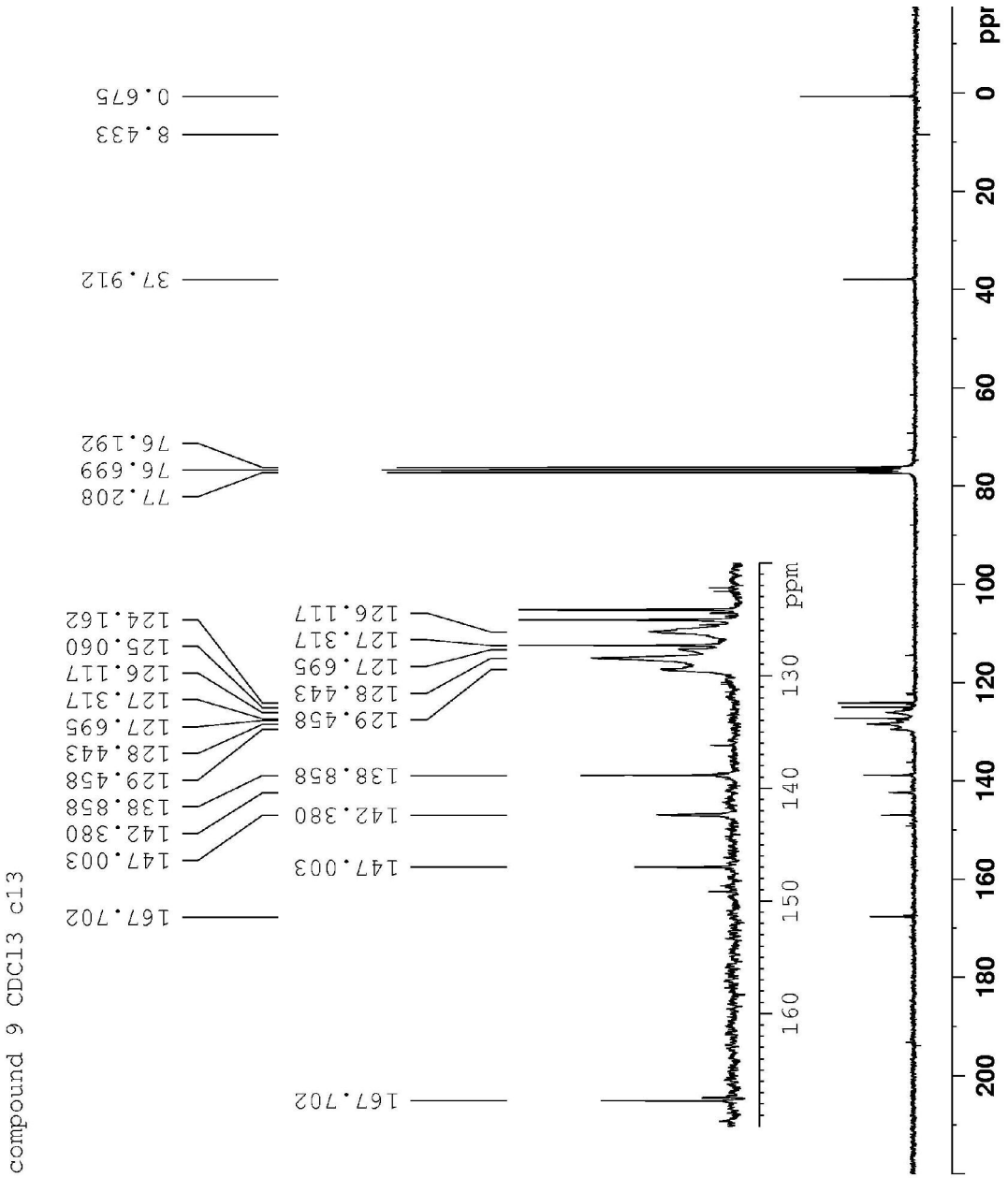
^{1}H NMR; compound 8, $CDCl_3$



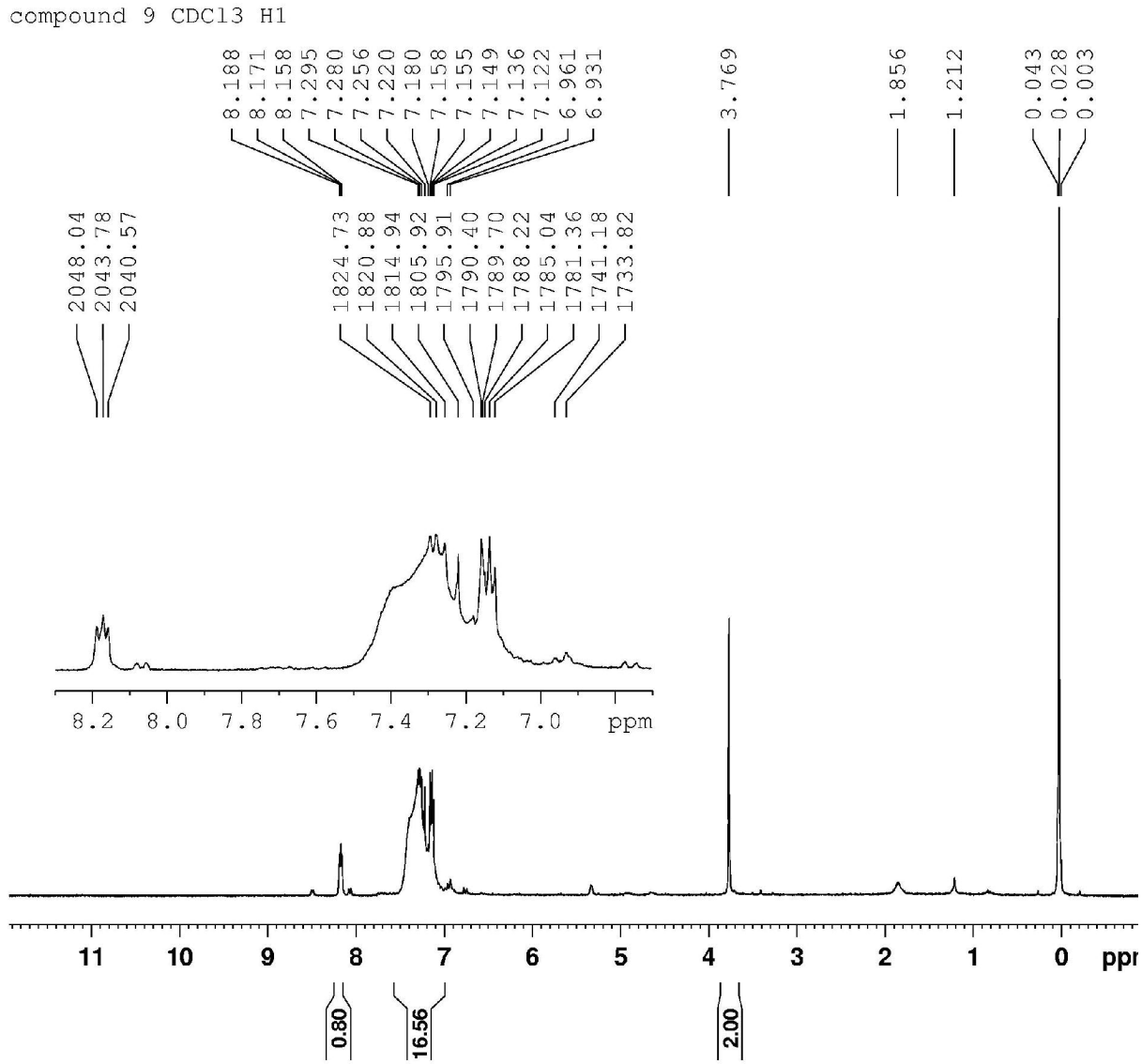
compound 9 2-(1-Oxy-pyridin-2-yl)-N,N-diphenyl -acetamide



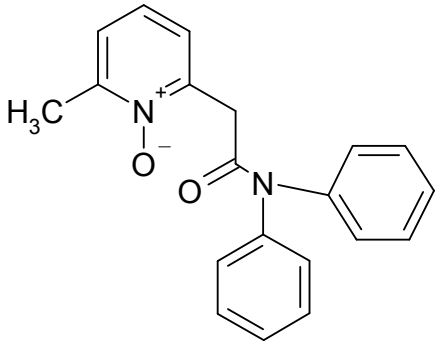
^{13}C $\{^{1}H\}$ NMR; compound 9, $CDCl_3$



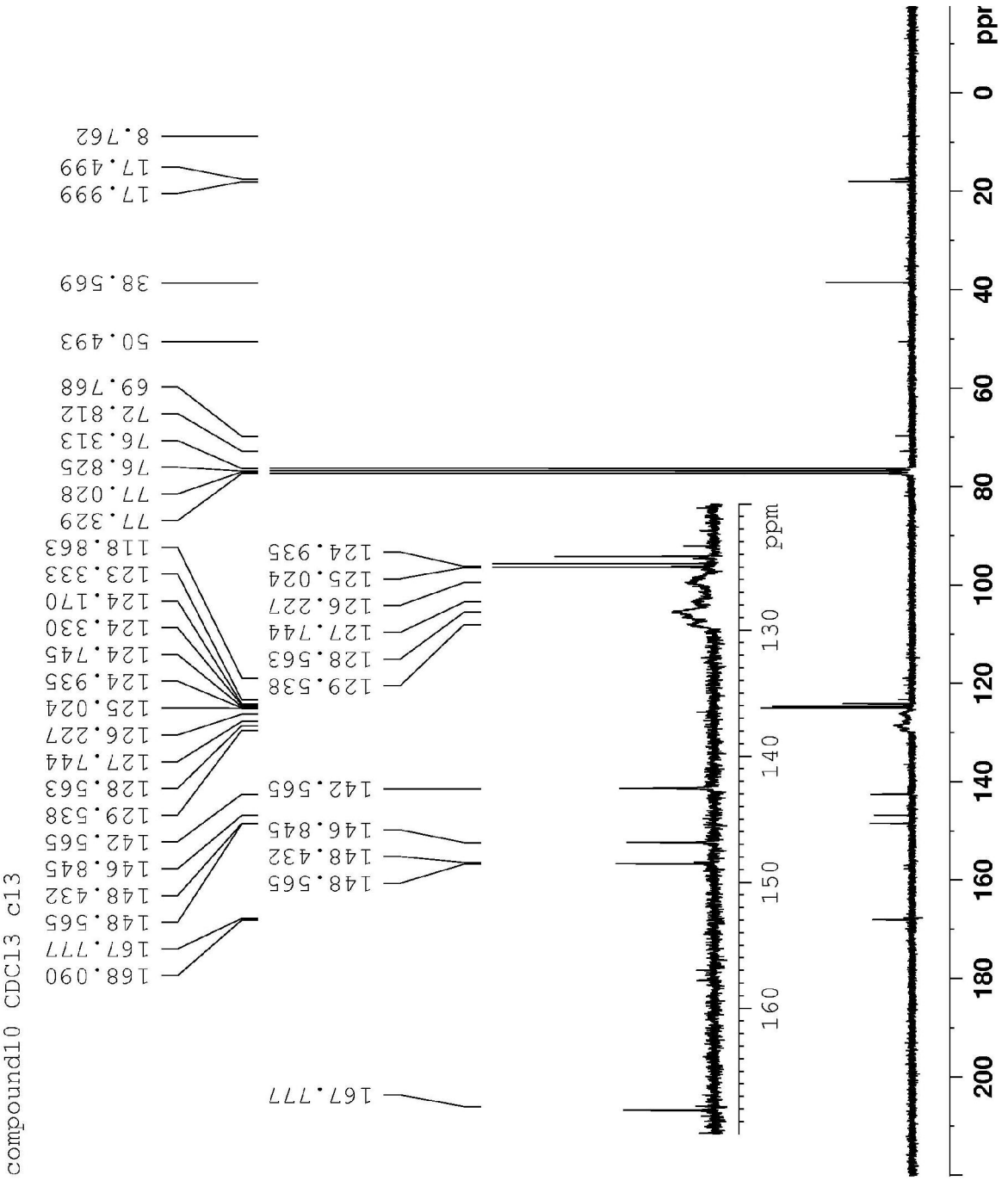
^{1}H NMR; compound 9, $CDCl_3$



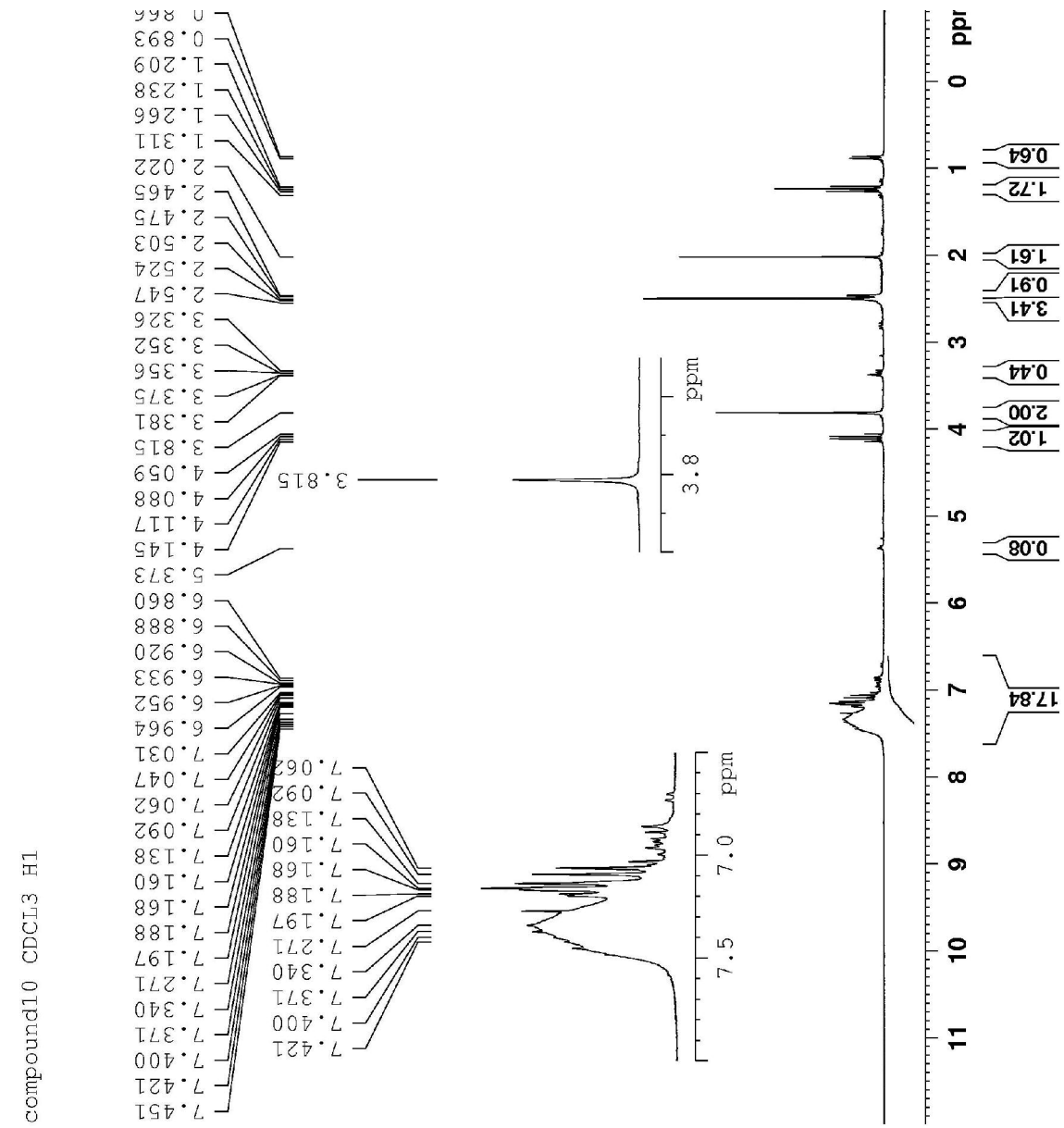
compound 10 2-(6-Methyl-1-oxy-pyridin-2-yl)-N,N -diphenyl-acetamide



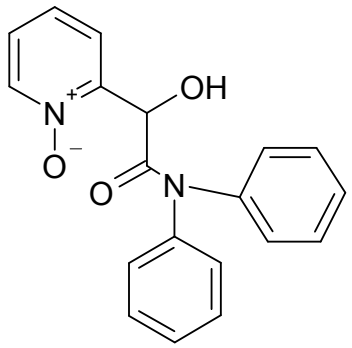
^{13}C {^{1}H} NMR; compound 10, $CDCl_3$



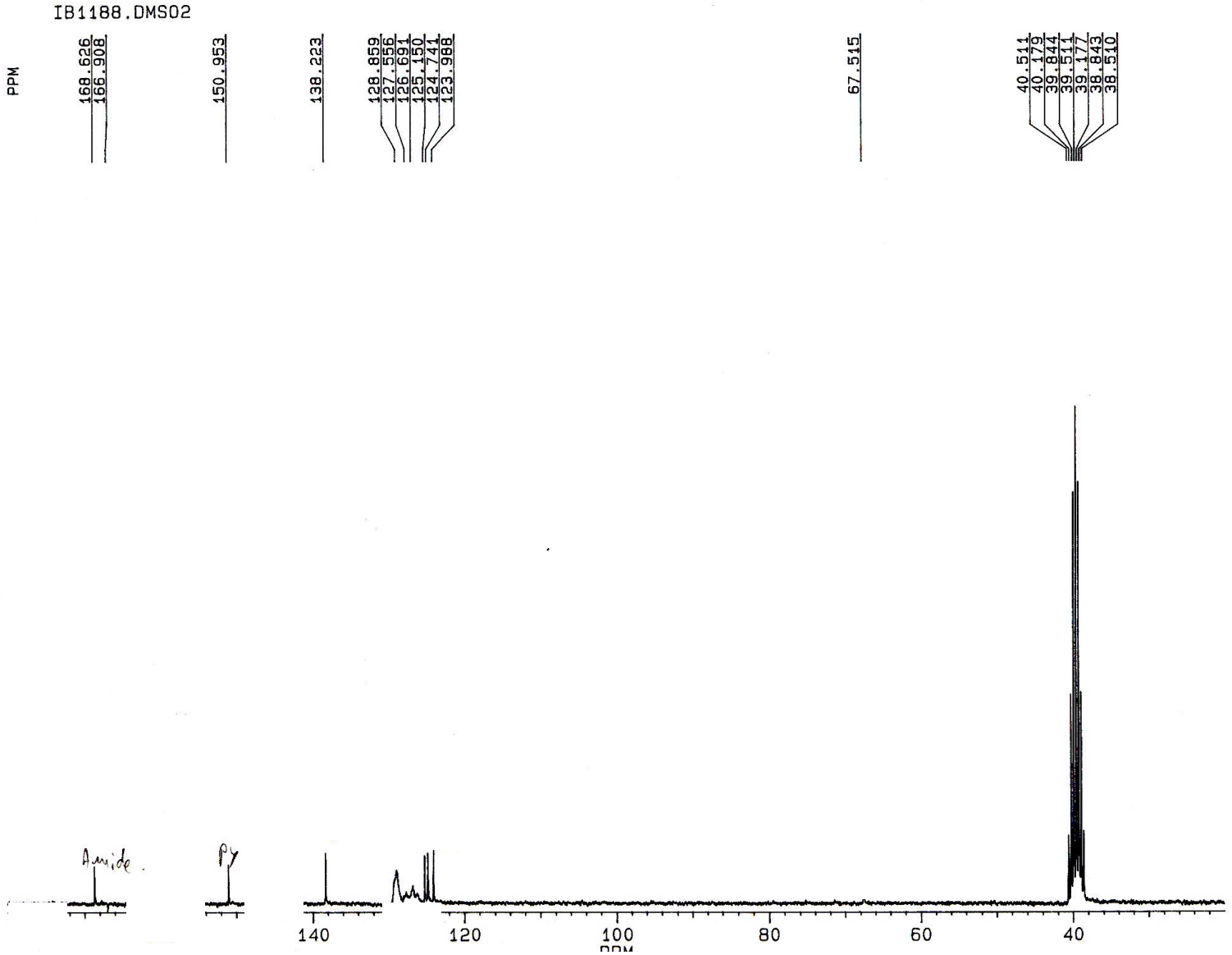
^{1}H NMR; compound 10, $CDCl_3$



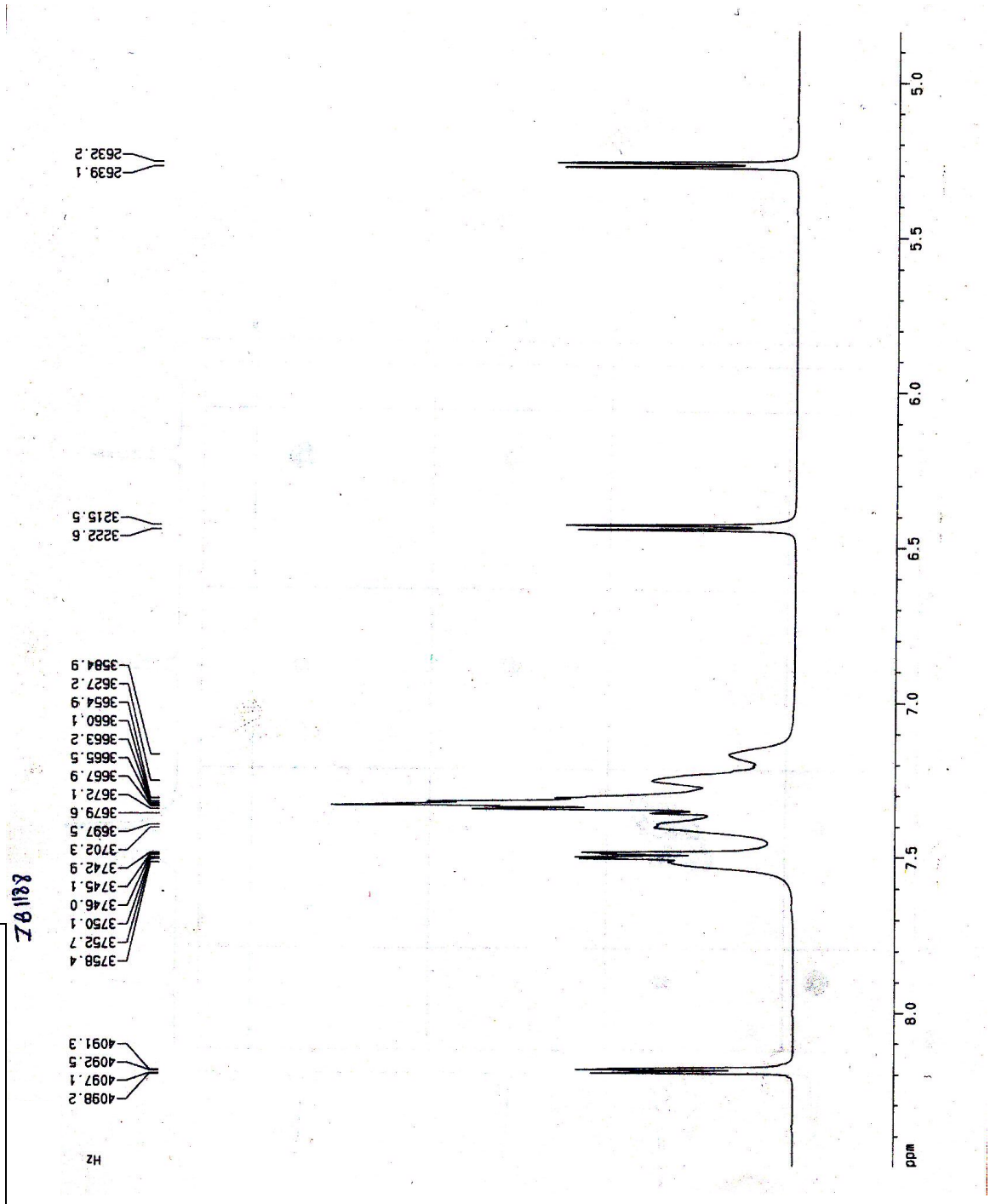
compound 11 2-Hydroxy-2-(1-oxy-pyridin-2-yl)-N, N-diphenyl-acetamide



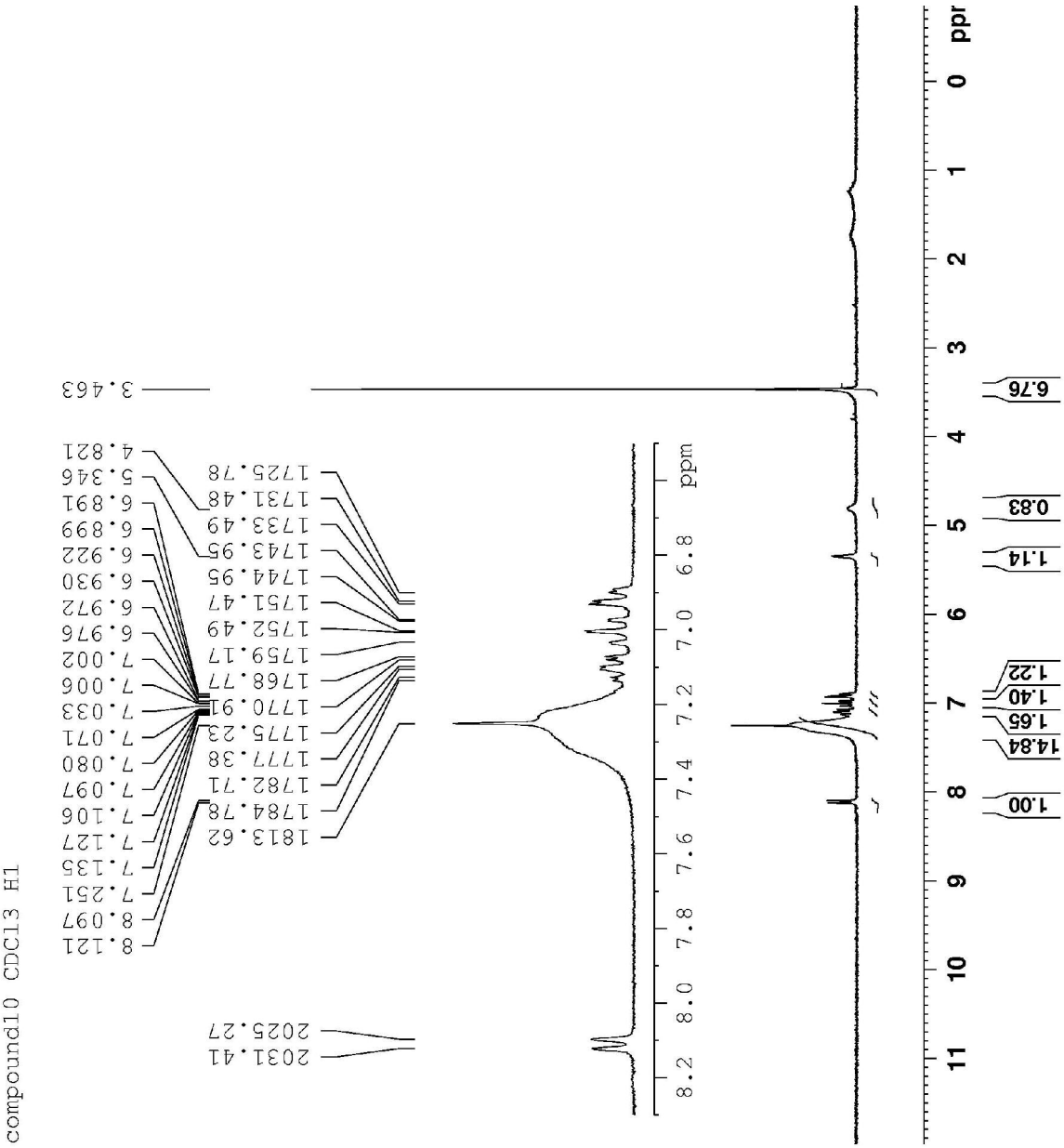
^{13}C {^{1}H} NMR; compound 11, DMSO



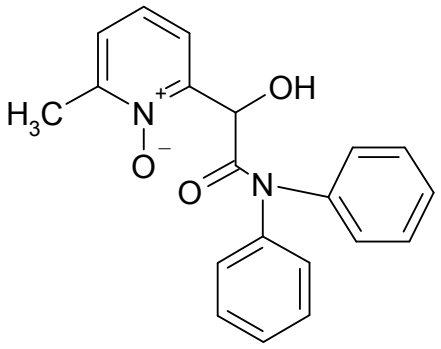
^{1}H NMR; compound 11, $CDCl_3$



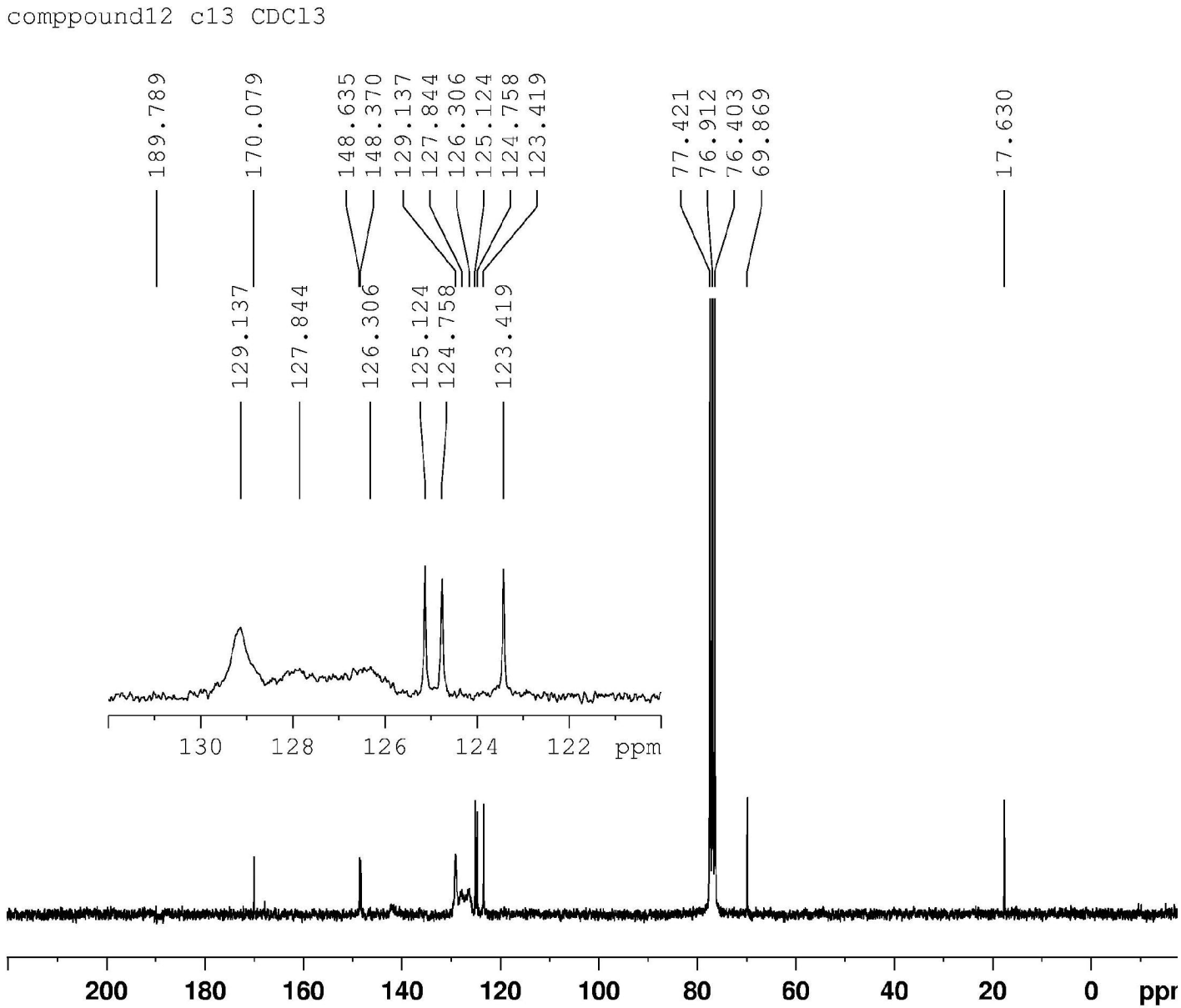
^{1}H NMR; compound 11, $CDCl_3$



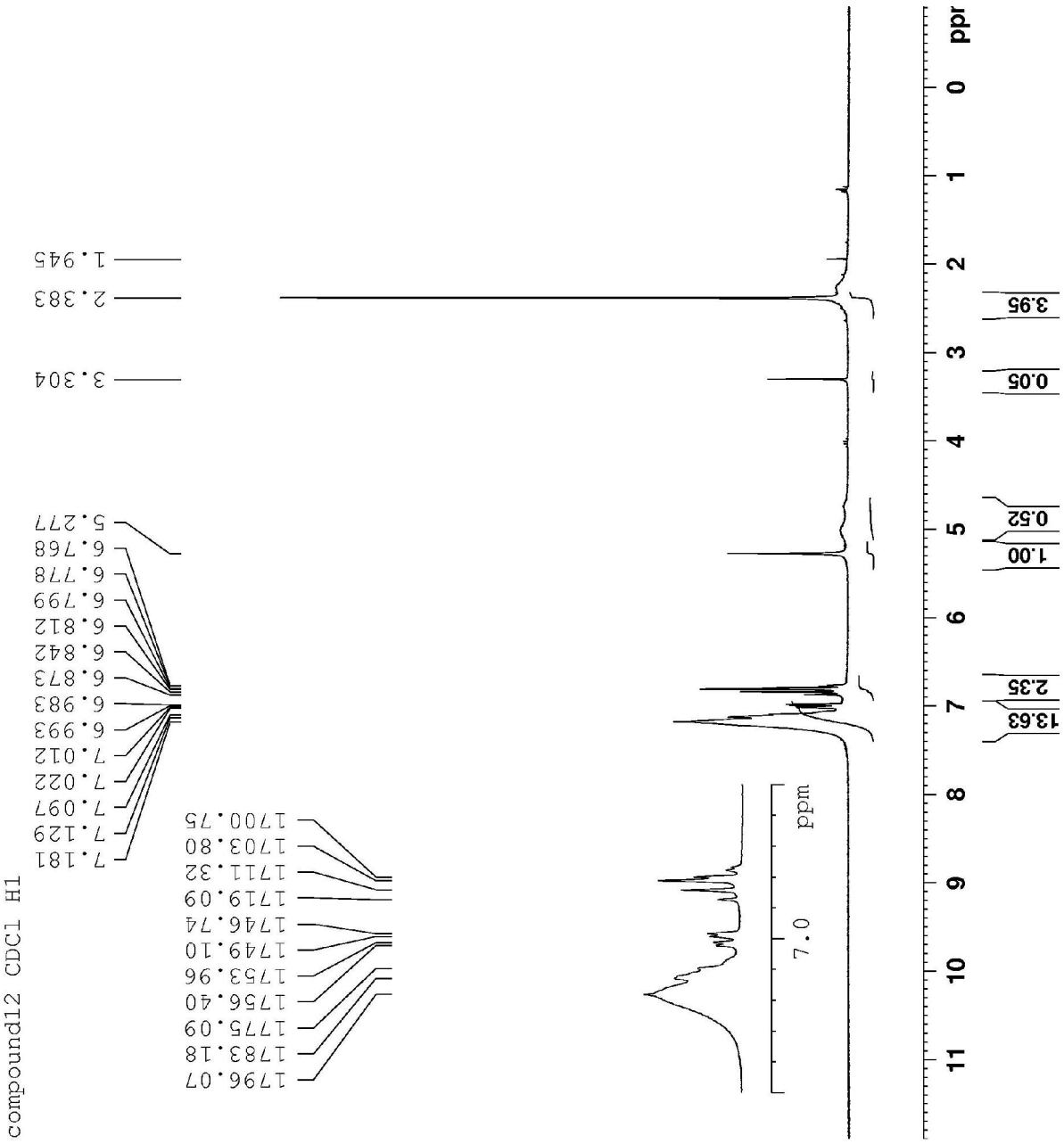
compound 12 2-Hydroxy-2-(6-methyl-1-oxy-pyridin-2-yl)-N,N-diphenyl-acetamide



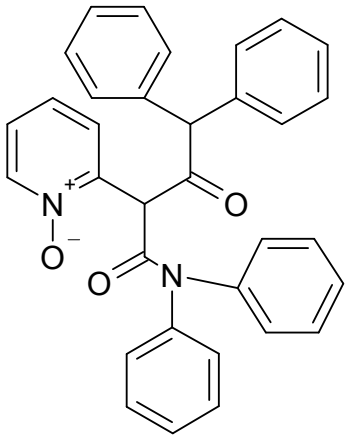
^{13}C {^{1}H} NMR; compound 12, $CDCl_3$



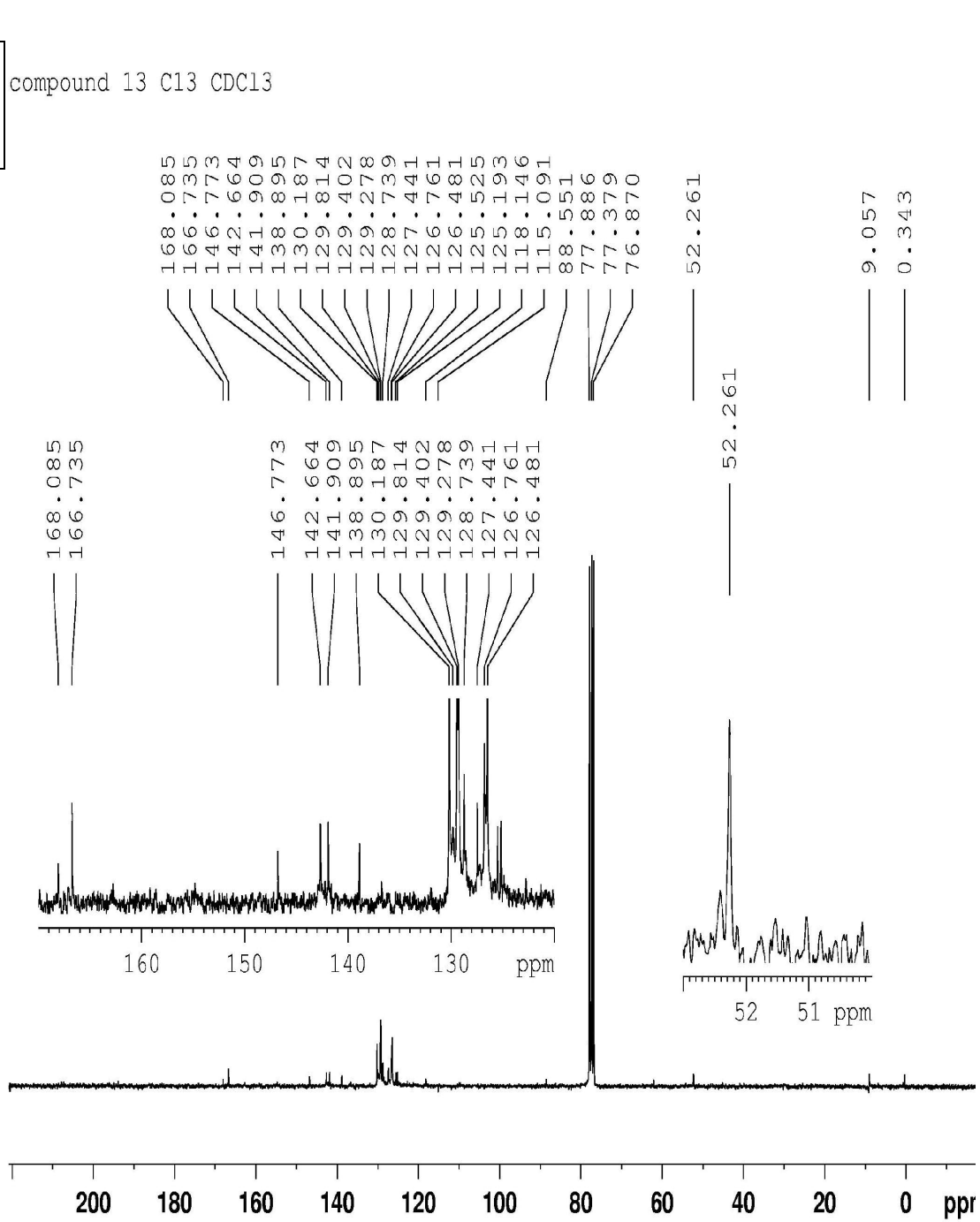
^{1}H NMR; compound 12, $CDCl_3$



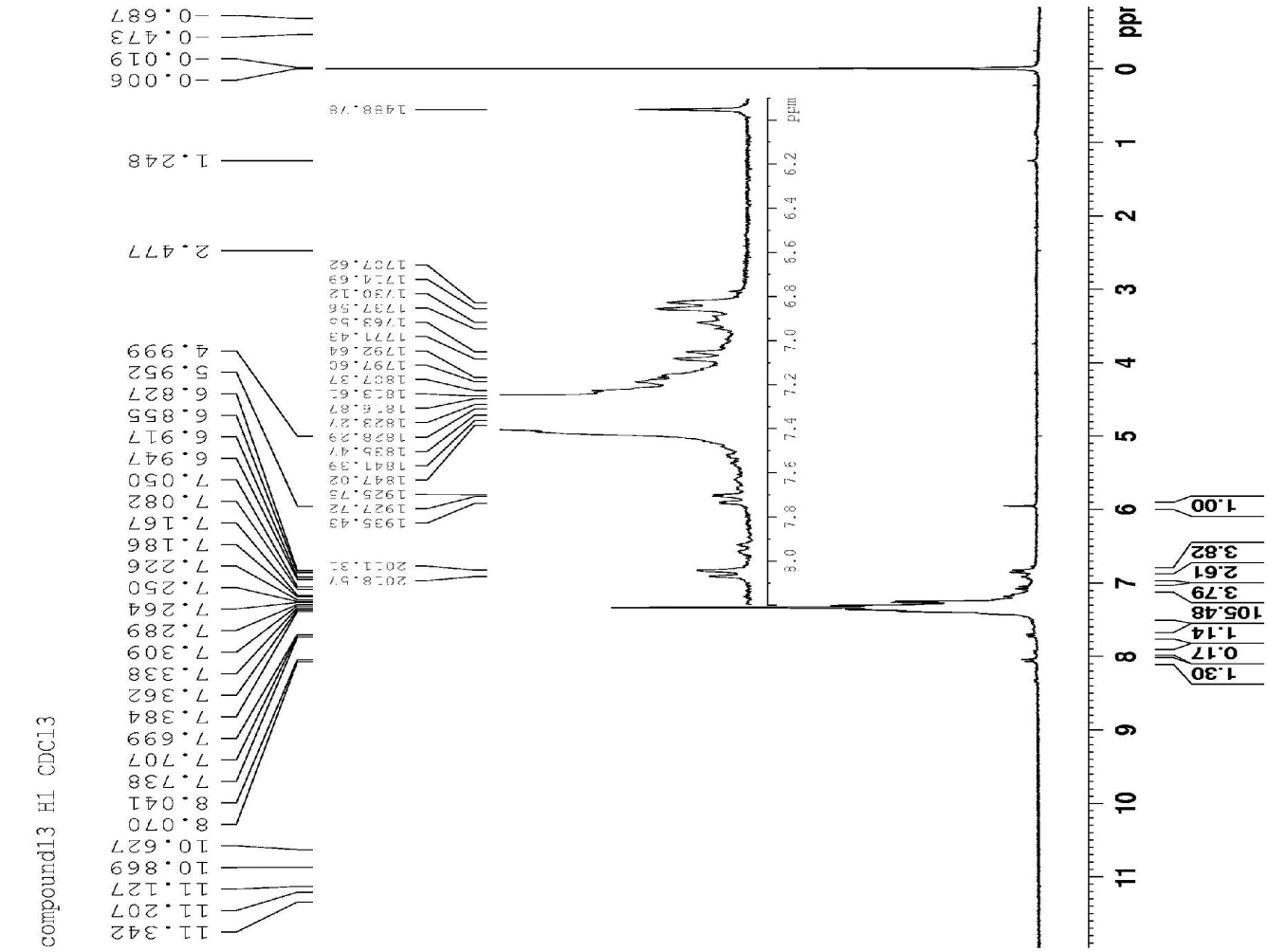
compound 13 3-Oxo-2-(1-oxy-pyridin-2-yl)-4,4,N, N-tetraphenyl-butyramide



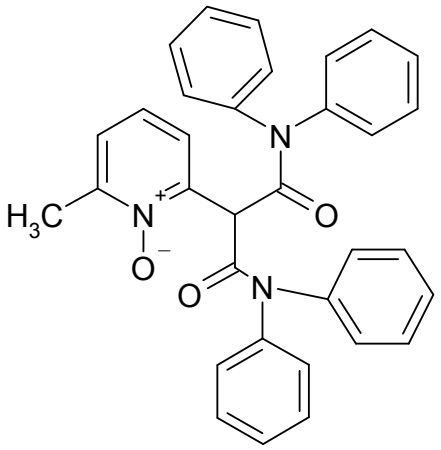
^{13}C {^{1}H} NMR; compound 13, $CDCl_3$



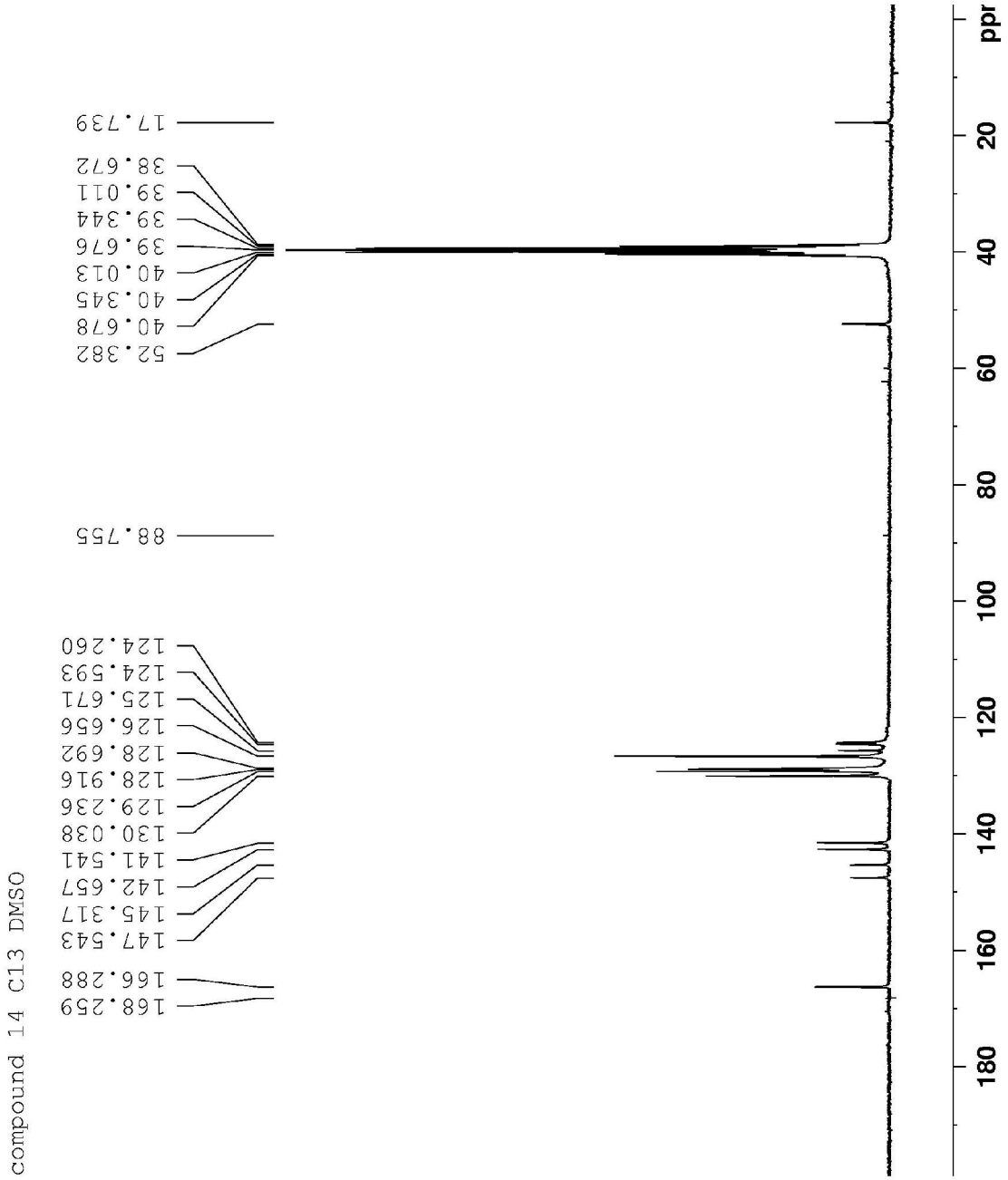
^{1}H NMR; compound 13, $CDCl_3$



compound 14



^{13}C {^{1}H} NMR; compound 14, DMSO



^{1}H NMR; compound 14, DMSO