Supplementary data

Crystallographic data for compound **2c**

The structure was solved by direct methods, SHELXS-86,[1] and refined to a final *R* value of 0.0540 for I>2s(I) by full matrix least squares analysis on $|F|^2$ (236 parameters) using SHELXL-93.[2] All the non-hydrogen atoms were refined anisotropically. The hydrogens, with the exception of the hydroxyl hydrogen which was located from the difference map, were fixed geometrically and those in similar environments were given common temperature factors (CH 0.03651, CH_2 0.3295, CH_3 0.07375). The hydroxyl hydrogen was isotropically refined with an independent temperature factor. All calculations were carried out using a VAX-1 mainframe computer. Figures were drawn using SCHAKAL.[3]

1. G. M. Sheldrick, *Acta Cryst.*, 1990, **A46**, 467.
2. G. M. Sheldrick, *SHELXL-93, A computer programme for crystal structure determination*, University of Gottingen, 1993.
3. E. Keller, University of Freiburg, Germany.

Table 1. Crystal data and structure refinement for **2c**

Identification code	TS1
Empirical formula	C_{16} H_{25} N O
Formula weight	247.37
Temperature	293(2) K
Wavelength	0.71703 Å
Crystal system	monoclinic
Space group	$P2_1$
Unit cell dimensions	a = 10.460(2) Å alpha = 90 °. b = 5.5610(4) Å beta = 110.951(7) °. c = 13.412(2) Å gamma = 90 °.
Volume	728.5(2) $Å^3$
Z	2
Density (calculated)	1.128 Mg/m^3
Absorption coefficient	0.069 mm^-1

F(000)	272
Crystal size	0.5 x 0.5 x 0.15 mm
Theta range for data collection	1.64 to 25.21 deg.
Index ranges	-12<=h<=11, 0<=k<=6, 0<=l<=14
Reflections collected	1476
Independent reflections	1413 [R(int) = 0.0392]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1413 / 6 / 263
Goodness-of-fit on *F*2	1.056
Final *R* indices [I>2sigma(I)]	R_1 = 0.0406, wR_2 = 0.0882
R indices (all data)	R_1 = 0.1141, wR_2 = 0.1101
Largest diff. peak and hole	0.175 and -0.180 e.Å^{-3}

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

	x	y	z	U(eq)
N	2173(3)	6562(6)	5233(3)	46(1)
O	-507(3)	5049(6)	4236(2)	52(1)
C(1)	3418(4)	6784(9)	5974(3)	49(1)
C(2)	4448(5)	5093(10)	6172(4)	54(1)
C(3)	4151(5)	3020(9)	5572(3)	53(1)
C(4)	2873(5)	2745(9)	4822(3)	48(1)
C(5)	1904(4)	4532(7)	4652(3)	40(1)
C(6)	492(4)	4363(7)	3805(3)	41(1)
C(7)	317(4)	6049(8)	2841(3)	41(1)
C(8)	1626(4)	6390(8)	2594(4)	43(1)
C(9)	2062(4)	4194(9)	2104(3)	45(1)
C(10)	3319(5)	4733(15)	1825(5)	70(2)
C(11)	873(4)	3353(10)	1130(3)	49(1)
C(12)	-436(5)	3049(9)	1339(4)	49(1)
C(13)	-843(4)	5327(8)	1802(3)	41(1)
C(14)	-2283(4)	5189(10)	1852(4)	52(1)
C(15)	-3368(6)	4437(18)	788(5)	78(2)
C(16)	-2693(6)	7548(12)	2221(6)	73(2)

Table 3. Bond lengths [Å] and angles [°] for **2c**

N-C(1)	1.333(5)
N-C(5)	1.342(5)
O-C(6)	1.415(5)
C(1)-C(2)	1.382(7)
C(2)-C(3)	1.377(7)
C(3)-C(4)	1.363(6)
C(4)-C(5)	1.379(6)
C(5)-C(6)	1.511(5)
C(6)-C(7)	1.554(6)
C(7)-C(8)	1.531(6)
C(7)-C(13)	1.538(6)
C(8)-C(9)	1.531(6)
C(9)-C(11)	1.520(6)
C(9)-C(10)	1.521(6)
C(11)-C(12)	1.502(6)
C(12)-C(13)	1.536(6)
C(13)-C(14)	1.534(6)
C(14)-C(16)	1.518(7)
C(14)-C(15)	1.531(7)
C(1)-N-C(5)	117.2(4)
N-C(1)-C(2)	124.5(5)
C(3)-C(2)-C(1)	117.4(4)
C(4)-C(3)-C(2)	118.8(5)
C(3)-C(4)-C(5)	120.7(5)
N-C(5)-C(4)	121.4(4)
N-C(5)-C(6)	115.7(3)
C(4)-C(5)-C(6)	122.9(4)
O-C(6)-C(5)	110.0(3)
O-C(6)-C(7)	107.0(3)
C(5)-C(6)-C(7)	112.4(3)
C(8)-C(7)-C(13)	108.3(3)
C(8)-C(7)-C(6)	114.0(3)
C(13)-C(7)-C(6)	114.6(3)
C(9)-C(8)-C(7)	114.8(4)
C(11)-C(9)-C(10)	111.3(4)
C(11)-C(9)-C(8)	109.7(4)
C(10)-C(9)-C(8)	111.4(5)
C(12)-C(11)-C(9)	113.2(3)
C(11)-C(12)-C(13)	112.6(4)
C(14)-C(13)-C(12)	113.3(4)
C(14)-C(13)-C(7)	116.2(3)
C(12)-C(13)-C(7)	109.8(3)
C(16)-C(14)-C(15)	109.8(5)
C(16)-C(14)-C(13)	111.6(4)

C(15)-C(14)-C(13)	112.6(4)

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for **2c**.
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}
N	55(2)	32(2)	50(2)	-4(2)	17(2)	0(2)
O	62(2)	50(2)	51(2)	6(2)	29(2)	-6(2)
C(1)	57(3)	40(3)	54(2)	-2(2)	23(2)	-8(2)
C(2)	50(3)	62(3)	50(2)	7(3)	19(2)	-5(3)
C(3)	61(3)	51(3)	52(3)	8(3)	29(3)	11(3)
C(4)	66(3)	37(3)	40(2)	-4(2)	18(2)	1(3)
C(5)	56(2)	26(2)	42(2)	3(2)	23(2)	-1(2)
C(6)	57(2)	28(2)	42(2)	0(2)	23(2)	-7(2)
C(7)	57(3)	27(2)	44(2)	-1(2)	23(2)	0(2)
C(8)	48(3)	42(3)	41(2)	7(2)	17(2)	-4(2)
C(9)	49(2)	48(3)	40(2)	9(2)	18(2)	7(2)
C(10)	53(3)	103(5)	61(3)	2(4)	27(3)	6(4)
C(11)	55(3)	59(3)	38(2)	-1(2)	21(2)	9(2)
C(12)	58(3)	46(3)	42(2)	-6(2)	17(2)	0(2)
C(13)	50(2)	35(2)	38(2)	6(2)	16(2)	3(2)
C(14)	51(3)	59(3)	50(3)	2(3)	23(2)	1(3)
C(15)	51(3)	111(6)	69(4)	-2(4)	17(3)	2(4)
C(16)	63(4)	73(4)	91(5)	3(4)	37(3)	17(3)

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

	x	y	z	U(eq)
H(1A)	-587(54)	4057(138)	4610(42)	105(26)
H(1)	3639(41)	8421(96)	6446(28)	69(14)
H(2)	5415(46)	5546(90)	6750(34)	78(14)
H(3)	4872(47)	1803(99)	5672(30)	78(16)
H(4)	2583(40)	1501(88)	4464(30)	46(13)
H(6)	354(34)	2473(79)	3530(27)	41(10)
H(7)	179(40)	7504(86)	3165(32)	53(12)
H(8A)	2405(35)	6936(74)	3228(27)	37(10)
H(8B)	1509(34)	7536(81)	2022(29)	43(11)
H(9)	2339(40)	2762(99)	2662(32)	63(13)
H(10A)	4181(50)	5287(108)	2466(43)	85(16)
H(10B)	3591(45)	3545(94)	1535(33)	54(16)
H(10C)	3029(60)	6230(150)	1193(50)	137(25)
H(11A)	1157(43)	1980(103)	812(33)	61(13)
H(11B)	735(27)	4493(64)	539(24)	17(8)
H(12A)	-369(35)	1853(79)	1844(29)	41(11)
H(12B)	-1140(37)	2682(83)	643(31)	56(12)
H(13)	-908(30)	6675(70)	1252(26)	26(9)
H(14)	-2263(37)	4078(82)	2355(31)	41(12)
H(15A)	-3354(47)	5557(103)	230(40)	70(16)
H(15B)	-4323(46)	4709(103)	814(34)	73(14)
H(15C)	-3205(68)	2802(160)	544(59)	137(29)
H(16A)	-2066(58)	7876(145)	2990(48)	114(22)
H(16B)	-2806(59)	8715(123)	1694(48)	106(24)
H(16C)	-3716(51)	7410(112)	2182(34)	87(16)

Crystallographic data for compound **6**

The structure was solved by direct methods, SHELXS-86[1], and refined by full matrix least squares using SHELXL-93[2]. Data were corrected for Lorentz and polarization effects but not for absorption. Hydrogen atoms were included in calculated positions with thermal parameters 30% larger than the atom to which they were attached. The non-hydrogen atoms were refined anisotropically. All calculations were performed on a Silicon Graphics R4000 computer. The ORTEX program was used to obtain the drawings [3].

1. G.M. Sheldrick, Acta.Cryst.,(1990).A46,467.
2. G.M. Sheldrick, SHELXL-93 a computer program for crystal structure determination, University of Gottingen 1993.
3. P. McArdle J. Appl.Cryst.(1995),28,65.

Table 1. Crystal data and structure refinement for **6**

Identification code	cs1
Empirical formula	$C_{17}H_{27}NO$
Formula weight	261.40
Temperature	293(2) K
Wavelength	0.71069 Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 10.8957(10)Å
	b = 11.2627(9)Å
	c = 13.3035(10)Å
Volume	1632.5(2) $Å^3$
Z	4
Density (calculated)	1.064 Mg/m^3
Absorption coefficient	0.065 mm^{-1}
F(000)	576
Crystal size	0.5 x 0.5 x 0.5 mm
Theta range for data collection	2.37 to 25.96 °.
Index ranges	0<=h<=13; 0<=k<=13; 0<=l<=16
Reflections collected	1904
Independent reflections	1838 [R(int) = 0.0168]
Reflections observed (>2σ)	1523
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1838 / 0 / 176
Goodness-of-fit on F^2	0.925
Final R indices [I>2σ(I)]	R_1 = 0.0350 wR_2 = 0.1081
R indices (all data)	R_1 = 0.0434 wR_2 = 0.1155
Absolute structure parameter	2(2)
Largest diff. peak and hole	0.150 and -0.089 e.$Å^{-3}$

R indices ; $R_1 = [\Sigma\,||F_o| - |F_c||]/\Sigma|F_o|$ (based on F),

$wR_2 = [[\Sigma_w (|F_o - F_c|)^2]/[\Sigma_w (|F_o|)^2]]^{1/2}$ (based on F^2).

$w = q/[(\sigma F_o)^2 + (a*P)^2 + b*P + d + e*\sin(\theta)]$.

Goodness-of-fit = $[\Sigma_w (|F_o^2| - |F_c^2|)^2/(\text{Nobs-Nparameters})]^{1/2}$.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **6**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
N(1)	1124(1)	6647(1)	4649(1)	56(1)
O(1)	-661(1)	9297(1)	4585(1)	62(1)
C(1)	-2246(2)	7909(2)	1924(2)	73(1)
C(2)	-1454(3)	7114(2)	1268(2)	85(1)
C(3)	-118(3)	7470(2)	1284(2)	78(1)
C(4)	425(2)	7506(2)	2349(1)	57(1)
C(5)	-366(2)	8327(2)	3010(1)	51(1)
C(6)	-1713(2)	7953(2)	2978(2)	60(1)
C(7)	-3582(3)	7529(3)	1944(2)	99(1)
C(8)	1810(2)	7791(2)	2358(2)	70(1)
C(9)	2116(3)	8970(2)	1855(2)	97(1)
C(10)	2557(3)	6793(3)	1886(3)	119(1)
C(11)	88(2)	8429(2)	4102(1)	50(1)
C(12)	-176(3)	9691(2)	5516(2)	86(1)
C(13)	81(2)	7263(2)	4674(1)	48(1)
C(14)	1145(2)	5597(2)	5124(2)	63(1)
C(15)	166(2)	5134(2)	5625(2)	68(1)
C(16)	-907(2)	5780(2)	5657(2)	69(1)
C(17)	-952(2)	6863(2)	5180(1)	60(1)

Table 3. Bond lengths [Å] and angles [°] for **6**

N(1)-C(13)	1.331(2)
N(1)-C(14)	1.341(3)
O(1)-C(12)	1.418(3)
O(1)-C(11)	1.426(2)
C(1)-C(7)	1.517(3)
C(1)-C(6)	1.518(3)
C(1)-C(2)	1.519(4)
C(2)-C(3)	1.509(4)
C(3)-C(4)	1.536(3)
C(4)-C(5)	1.540(2)
C(4)-C(8)	1.542(3)
C(5)-C(6)	1.527(3)
C(5)-C(11)	1.539(2)
C(8)-C(9)	1.524(3)
C(8)-C(10)	1.524(4)
C(11)-C(13)	1.519(2)
C(13)-C(17)	1.386(3)
C(14)-C(15)	1.361(3)
C(15)-C(16)	1.377(3)
C(16)-C(17)	1.376(3)
C(13)-N(1)-C(14)	117.5(2)
C(12)-O(1)-C(11)	113.3(2)
C(7)-C(1)-C(6)	111.1(2)
C(7)-C(1)-C(2)	112.9(2)
C(6)-C(1)-C(2)	109.4(2)
C(3)-C(2)-C(1)	112.5(2)
C(2)-C(3)-C(4)	113.1(2)
C(3)-C(4)-C(5)	109.1(2)
C(3)-C(4)-C(8)	113.0(2)
C(5)-C(4)-C(8)	114.7(2)
C(6)-C(5)-C(11)	110.9(2)
C(6)-C(5)-C(4)	110.9(2)
C(11)-C(5)-C(4)	113.8(2)
C(1)-C(6)-C(5)	113.7(2)
C(9)-C(8)-C(10)	110.1(2)
C(9)-C(8)-C(4)	113.1(2)
C(10)-C(8)-C(4)	111.4(2)
O(1)-C(11)-C(13)	111.33(13)
O(1)-C(11)-C(5)	107.05(14)
C(13)-C(11)-C(5)	113.97(13)
N(1)-C(13)-C(17)	122.4(2)
N(1)-C(13)-C(11)	115.7(2)
C(17)-C(13)-C(11)	121.9(2)
N(1)-C(14)-C(15)	123.7(2)

C(14)-C(15)-C(16)	118.5(2)
C(17)-C(16)-C(15)	118.9(2)
C(16)-C(17)-C(13)	118.9(2)

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for **6**. The anisotropic displacement
factor exponent takes the form: $-2\pi^2$ [h^2 a^{*2} U11 + ... + 2 h k a* b* U

Atom	U11	U22	U33	U23	U13	U12
N(1)	47(1)	60(1)	62(1)	3(1)	-1(1)	3(1)
O(1)	75(1)	52(1)	59(1)	-10(1)	-2(1)	8(1)
C(1)	85(1)	61(1)	73(1)	9(1)	-29(1)	-4(1)
C(2)	115(2)	78(1)	62(1)	-5(1)	-29(1)	-10(1)
C(3)	112(2)	72(1)	51(1)	-5(1)	-1(1)	-1(2)
C(4)	72(1)	49(1)	50(1)	-1(1)	2(1)	-1(1)
C(5)	60(1)	44(1)	50(1)	2(1)	-2(1)	-1(1)
C(6)	61(1)	59(1)	60(1)	0(1)	-9(1)	1(1)
C(7)	89(2)	94(2)	113(2)	9(2)	-46(2)	-14(2)
C(8)	73(1)	71(1)	67(1)	-5(1)	20(1)	1(1)
C(9)	102(2)	91(2)	98(2)	2(2)	28(2)	-25(2)
C(10)	97(2)	105(2)	155(3)	-29(2)	37(2)	16(2)
C(11)	52(1)	46(1)	51(1)	-3(1)	0(1)	-2(1)
C(12)	120(2)	71(1)	67(1)	-20(1)	-6(1)	7(2)
C(13)	47(1)	51(1)	46(1)	-2(1)	-2(1)	-1(1)
C(14)	57(1)	60(1)	73(1)	5(1)	-6(1)	10(1)
C(15)	73(1)	57(1)	74(1)	16(1)	-7(1)	0(1)
C(16)	61(1)	72(1)	73(1)	18(1)	7(1)	-6(1)
C(17)	50(1)	65(1)	64(1)	7(1)	3(1)	7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **6**

Atom	x	y	z	U(eq)
H(1)	-2211(2)	8714(2)	1645(2)	95
H(2A)	-1528(3)	6301(2)	1500(2)	111
H(2B)	-1753(3)	7146(2)	582(2)	111
H(3A)	-34(3)	8248(2)	979(2)	102
H(3B)	348(3)	6912(2)	881(2)	102
H(4)	338(2)	6704(2)	2625(1)	74
H(5)	-319(2)	9123(2)	2716(1)	67
H(6A)	-1792(2)	7174(2)	3282(2)	78
H(6B)	-2190(2)	8505(2)	3378(2)	78
H(7A)	-3896(7)	7505(20)	1270(3)	138
H(7B)	-4049(4)	8087(12)	2333(15)	138
H(7C)	-3646(3)	6755(9)	2241(16)	138
H(8)	2062(2)	7853(2)	3063(2)	91
H(9A)	2976(5)	9131(10)	1930(15)	136
H(9B)	1650(16)	9594(4)	2164(12)	136
H(9C)	1916(20)	8926(7)	1153(4)	136
H(10A)	2378(20)	6059(5)	2223(15)	166
H(10B)	3416(3)	6968(12)	1949(19)	166
H(10C)	2348(19)	6722(17)	1187(6)	166
H(11)	933(2)	8728(2)	4088(1)	65
H(12A)	-699(12)	10296(14)	5791(8)	121
H(12B)	631(9)	10010(18)	5412(3)	121
H(12C)	-132(19)	9035(5)	5975(6)	121
H(14)	1869(2)	5161(2)	5110(2)	82
H(15)	221(2)	4399(2)	5939(2)	88
H(16)	-1590(2)	5488(2)	5996(2)	89
H(17)	-1663(2)	7319(2)	5196(1)	78