The sum (360·0°) of the angles at N(1) indicates that it adopts a planar configuration. The second N atom in (—)-cytisine, N(12), and its three substituents, C(11), C(13) and H(12), form a flattened pyramid with the N lone pair axial relative to ring *C*. A similar conformation exists for C(11), C(13), and C(14) around N(12) in (—)-*N*-methylcytisine. The sum of the three bond angles around N(12) is 331·9° for (—)-*N*-methylcytisine indicating that hybridization of the N atom is close to tetrahedral. A similar situation is observed for (—)-cytisine. The essentially identical conformations adopted by both molecules in the crystal are not consistent with the difference observed in the proton NMR spectra of both alkaloids. The axial protons at positions C(11) and C(13) in *N*-methylcytisine are shielded (δ 1·62 and 1·70) compared with the equatorial protons (δ 2·29 and 2·42). This shielding is due to a well documented combination of effects of the antiperiplanar N lone pair (Hamlow, Okuda & Nakagawa, 1964) and the equatorial methyl substituent (Booth, 1966). However, in cytisine, this axial shielding is absent, all four protons having chemical shifts in the range δ2·31–2·49. This suggests that, in solution, the conformation of ring *C* of cytisine is not rigidly chair-form.

The packing arrangement of the cytisine molecule, with two molecules in the asymmetric unit, leads to a hydrogen-bonding network between N(12)···O(2′) of neighbouring molecules. These are weak interactions with O(2)···N(12′) and N(12)···O(2′) distances 3·186 (5) and 3·244 (5) Å. Respective hydrogen bonds O(2)···H(12′), 2·55 (5) Å, and O(2′)···H(12), 2·44 (4) Å, subtend intermolecular bond angles of 144 (4) and 146(5)°. *N*-Methylcytisine has no similar intermolecular network.

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Structures of 4-Acetyl-3-(*p*-tolyl)sydnone (1) and 4-Acetyl-3-phenylsydnone Oxime (2)

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Abstract. (1) $C_{11}H_{10}N_2O_3$, $M_r = 218\cdot2$, orthorhombic, $P2_12_12_1$, $a = 10\cdot995$ (4), $b = 15\cdot158$ (2), $c = 6\cdot530$ (3) Å, $V = 1088\cdot3$ (7) Å^3, $Z = 4$, $D_m = 1\cdot3$ (1), $D_x = 1\cdot33$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·7093 Å, μ(Mo $K\alpha$) = 0·093 mm^{-1}, $F(000) = 456$, $T = 298$ K, final $R = 0\cdot038$ for 855 observed reflections. (2) $C_{10}H_9N_3O_3$, $M_r = 219\cdot2$, monoclinic, $P2_1/n$, $a = 7\cdot871$ (1), $b = 7\cdot741$ (2), $c = 16\cdot880$ (5) Å, $\beta = 96\cdot20$ (2)°, $V = 1022$ (2) Å^3, $Z = 4$, $D_m = 1\cdot4$ (1), $D_x = 1\cdot42$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, μ(Cu $K\alpha$) = 0·87 mm^{-1}, $F(000) = 456$, $T = 298$ K, final $R = 0\cdot041$ for 1553 observed reflections. The bond lengths of the sydnone ring are similar in both structures. The bond lengths N(1)—C(7) and C(7)—C(8) of 3,4-disubstituted sydnone derivatives are longer than the corresponding bond lengths in 3-substituted sydnone derivatives, and the dihedral angles between the sydnone ring and the phenyl ring of (1) and (2) [68·4 (2) and 78·6 (1)° respectively] are larger than those of 3-substituted sydnone derivatives. This may be attributed to steric effects.

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Introduction. Crystal structures of four 3-substituted sydnone derivatives have been published recently (Wang, Lee & Yeh, 1984; Ueng, Lee, Wang & Yeh, 1985) and the sydnone ring has been most satisfactorily described as a cyclic resonance-stabilized azomethine–imine type of bonding according to the bond lengths obtained so far. In order to understand the effect on bond lengths of the sydnone ring when the 4-H atom in the sydnone ring is substituted by an electron-withdrawing group, the structure determinations of the title compounds were undertaken.

Experimental. (1) Crystal 0·4 × 0·5 × 0·6 mm. CAD-4 diffractometer. Unit cell: 25 reflections, 2θ range 22 to 27°. D_m by flotation (C_6H_6/CCl_4). $2\theta_{max} = 60°$. Ranges of h, k, l: 0 to 15, 0 to 21, 0 to 9, respectively. Three standard reflections monitored every 2 h: variation on $I < 2\%$. 1833 unique reflections, 855 observed with $I \geq 2\sigma(I)$. $R(F) = 0·038$, $wR = 0·026$, $S = 2·10$. Weighting scheme from counting statistics. Structure solved by direct method using *MULTAN* with 154 highest E's, 67 smallest E's and 1623 $\sum_2$ relationships. H atoms found in difference Fourier map after isotropic refinement and then refined. $(\Delta/\sigma)_{max} = 0·30$. Peaks in final ΔF map 0·14 to $-0·20$ e Å^{-3}. Secondary-extinction coefficient 0·62 (3) (length in μm). The maximum extinction correction is 1·239 for 010. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Computing programs: NRCC *SDP PDP*-11 package (Gabe & Lee, 1981), *MULTAN* and *ORTEP* from Enraf–Nonius (1979) *Structure Determination Package*. (2) Crystal 0·3 × 0·4 × 0·4 mm. Unit cell: 25 reflections, 2θ range 33 to 69°. D_m by flotation ($CH_2Cl_2/CHCl_3$). $2\theta_{max} = 155°$. Ranges of h, k, l: 0 to 9, 0 to 9, −21 to 21, respectively. Three standard reflections monitored every 2 h: variation on $I < 4\%$. 2118 unique reflections, 1553 observed with $I \geq 2\sigma(I)$. $R(F) = 0·041$, $wR = 0·030$, $S = 3·09$. Structure solved by direct method with 214 highest E's, 49 smallest E's and 1974 $\sum_2$ relationships. H atoms found in difference Fourier map after isotropic refinement and then refined. $(\Delta/\sigma)_{max} = 0·24$. Peaks in final ΔF map 0·22 to $-0·14$ e Å^{-3}. Secondary-extinction coefficient 0·43 (2) (length in μm). The maximum extinction correction is 1·288 for $\bar{1}01$. Other details as in (1).

Discussion. Atomic positional parameters and equivalent isotropic temperature factors are listed in Table 1.* The bond lengths and angles are shown in Fig. 1 and Table 2 respectively.

Table 1. *Atomic positional parameters and equivalent isotropic temperature factors* (Å^2) *for* (1) *and* (2)

$$B_{eq} = \tfrac{8}{3}\pi^2 \textstyle\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i . \mathbf{a}_j.$$

Compound (1)

	x	y	z	B_{eq}
C(1)	0·4584 (2)	0·0797 (2)	0·0954 (5)	4·2 (2)
C(2)	0·3923 (3)	0·0647 (2)	0·2696 (5)	4·8 (2)
C(3)	0·2690 (3)	0·0897 (2)	0·2695 (6)	4·8 (2)
C(4)	0·2194 (2)	0·1285 (2)	0·0975 (5)	4·5 (2)
C(5)	0·2903 (3)	0·1425 (2)	−0·0738 (5)	5·1 (2)
C(6)	0·4124 (2)	0·1180 (2)	−0·0751 (5)	4·8 ([illegible]
C(7)	0·6418 (2)	−0·0228 (2)	0·1042 (5)	4·3 ([illegible]
C(8)	0·7682 (3)	−0·0059 (2)	0·1028 (5)	5·2 (2)
C(9)	0·5782 (3)	−0·1069 (2)	0·0989 (5)	4·9 (2)
C(10)	0·0869 (2)	0·1570 (2)	0·1017 (6)	5·8 (2)
C(11)	0·6572 (3)	−0·1879 (2)	0·0982 (7)	7·9 (3)
N(1)	0·5881 (2)	0·0572 (1)	0·0999 (4)	4·3 (1)
N(2)	0·6607 (2)	0·1245 (2)	0·0953 (5)	5·9 (2)
O(1)	0·7753 (2)	0·0875 (2)	0·0988 (4)	6·3 (1)
O(2)	0·8603 (2)	−0·0481 (2)	0·1040 (4)	7·1 (2)
O(3)	0·4680 (2)	−0·1114 (1)	0·0936 (4)	6·2 (2)

Compound (2)

	x	y	z	B_{eq}
C(1)	0·6827 (2)	0·5953 (2)	0·3252 (1)	3·5 (1)
C(2)	0·6041 (3)	0·7283 (3)	0·3606 (1)	4·5 (1)
C(3)	0·4478 (3)	0·7853 (3)	0·3251 (1)	5·3 (1)
C(4)	0·3765 (3)	0·7097 (3)	0·2552 (1)	5·1 (1)
C(5)	0·4585 (3)	0·5782 (3)	0·2210 (1)	5·1 (1)
C(6)	0·6146 (3)	0·5200 (3)	0·2558 (1)	4·6 (1)
N(1)	0·8511 (2)	0·5401 (2)	0·3603 (1)	3·7 (1)
C(7)	0·8997 (2)	0·3995 (2)	0·4045 (1)	3·3 (1)
N(2)	0·9747 (2)	0·6432 (2)	0·3443 (1)	5·0 (1)
O(1)	1·1209 (2)	0·5657 (2)	0·3806 (1)	5·0 (1)
C(8)	1·0805 (2)	0·4124 (3)	0·4182 (1)	3·8 (1)
O(2)	1·1946 (2)	0·3280 (2)	0·4533 (1)	4·7 (1)
C(9)	0·7942 (2)	0·2680 (2)	0·4351 (1)	3·5 (1)
N(3)	0·8820 (2)	0·1394 (2)	0·4653 (1)	3·9 (1)
O(3)	0·7807 (2)	0·0161 (2)	0·4987 (1)	4·7 (1)
C(10)	0·6051 (3)	0·2853 (3)	0·4350 (1)	6·6 (2)

Table 2. *Bond angles* (°) *of* (1) *and* (2)

Compound (1)

C(2)–C(1)–C(6)	123·8 (2)	C(2)–C(1)–N(1)	117·4 (2)
C(6)–C(1)–N(1)	118·6 (2)	C(1)–C(2)–C(3)	117·8 (2)
C(2)–C(3)–C(4)	119·7 (2)	C(3)–C(4)–C(5)	120·1 (2)
C(3)–C(4)–C(10)	119·0 (2)	C(5)–C(4)–C(10)	120·9 (2)
C(4)–C(5)–C(6)	120·6 (2)	C(1)–C(6)–C(5)	118·0 (2)
C(8)–C(7)–C(9)	129·2 (2)	C(8)–C(7)–N(1)	105·5 (2)
C(9)–C(7)–N(1)	125·2 (2)	C(7)–C(8)–O(1)	103·6 (2)
C(7)–C(8)–O(2)	137·3 (3)	O(1)–C(8)–O(2)	119·1 (2)
C(7)–C(9)–C(11)	116·0 (2)	C(7)–C(9)–O(3)	122·1 (2)
C(11)–C(9)–O(3)	121·9 (2)	C(1)–N(1)–C(7)	129·4 (2)
C(1)–N(1)–N(2)	114·6 (2)	C(7)–N(1)–N(2)	116·0 (2)
N(1)–N(2)–O(1)	104·1 (2)	C(8)–O(1)–N(2)	110·8 (2)

Compound (2)

C(2)–C(1)–C(6)	122·8 (1)	C(2)–C(1)–N(1)	118·5 (1)
C(6)–C(1)–N(1)	118·6 (1)	C(1)–C(2)–C(3)	118·2 (1)
C(2)–C(3)–C(4)	119·8 (1)	C(3)–C(4)–C(5)	120·7 (1)
C(4)–C(5)–C(6)	120·2 (1)	C(1)–C(6)–C(5)	118·3 (1)
C(1)–N(1)–C(7)	130·7 (1)	C(1)–N(1)–N(2)	113·7 (1)
C(7)–N(1)–N(2)	115·6 (1)	N(1)–C(7)–C(8)	104·6 (1)
N(1)–C(7)–C(9)	128·7 (1)	C(8)–C(7)–C(9)	126·6 (1)
N(1)–N(2)–O(1)	104·2 (1)	N(2)–O(1)–C(8)	110·5 (1)
C(7)–C(8)–O(1)	105·0 (1)	C(7)–C(8)–O(2)	135·9 (1)
O(1)–C(8)–O(2)	119·1 (1)	C(7)–C(9)–N(3)	112·5 (1)
C(7)–C(9)–C(10)	123·2 (1)	N(3)–C(9)–C(10)	124·2 (1)
C(9)–N(3)–O(3)	112·5 (1)		

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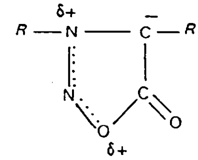
* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43663 (34 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

The bond lengths of the sydnone ring are listed in Table 3 and compared with those from other sydnone derivatives. The bond distances of the sydnone ring are similar in both title structures and similar to those of 4-(3-methyl-1-buten-2-yl)-3-phenylsydnone (Hašek, Obrda, Huml, Nešpůrek, Chojnacki & Šorm, 1978) and 4-(cyclohexen-1-yl)-3-phenylsydnone (Hašek, Obrda, Huml, Nešpůrek & Šorm, 1979). The O(1)—C(8), O(1)—N(2), N(1)—N(2) and C(8)—O(2) bond lengths of the four 3,4-disubstituted sydnone derivatives are comparable with the corresponding ones of the 3-substituted sydnone derivatives. The C(7)—C(8) bonds of the former compounds (1)–(4) [1·413 (4)–1·420 (3) Å] are slightly longer than those of the latter compounds (5)–(8) [1·400 (3)–1·404 (6) Å]. A similar effect was observed with the N(1)—C(7) bond length [1·350 (4)–1·352 (2) *vs* 1·329 (5)–1·334 (2) Å]. Basically the bond patterns of the sydnone ring for both types are essentially the same except for the minor differences in the N(1)—C(7) and C(7)—C(8) bond lengths. Therefore the azomethine–imine type proposed previously (Ueng, Lee, Wang & Yeh, 1985) can still be satisfactorily applied to the 3,4-disubstituted sydnone derivatives. The substituents of the 4-position may contribute to the resonance form,  , more than in the 3-substituted compounds. This is consistent with the ^{13}C NMR study of such sydnone derivatives (Ma & Yeh, 1985). It shows that there is higher electron density at the C(7) atom of the 3-substituted than at most of the aromatic carbon atoms and the chemical shift of C(7) undergoes a downfield shift of about 12–14 p.p.m. when 4-H is replaced by an electron-withdrawing substituent such as formyl, acetyl or cyano groups.

The dihedral angles between the sydnone ring and the phenyl ring of 3,4-disubstituted sydnone derivatives are given in Table 3. They vary from 2 to 79°. From Table 3, it is obvious that the dihedral angles of the

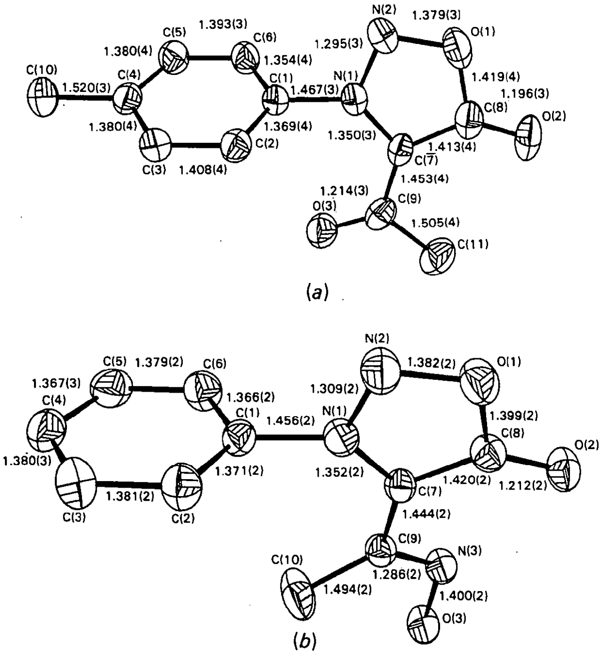


Fig. 1. Bond lengths (Å) of (*a*) 4-acetyl-3-(*p*-tolyl)sydnone and (*b*) 4-acetyl-3-phenylsydnone oxime. Thermal-motion ellipsoids of 30% probability.

Table 3. *Comparison of selected bond distances* (Å) *in the sydnone ring*

	(1)[a]	(2)[a]	(3)[b]	(4)[c]	(5)[d]	(6)[d]	(7)[e]	(8)[e]*
O(1)—C(8)	1·419 (4)	1·399 (2)	1·406 (3)	1·400 (4)	1·408 (6)	1·407 (3)	1·412 (2)	1·420 (3)
O(1)—N(2)	1·379 (3)	1·382 (2)	1·379 (2)	1·380 (4)	1·384 (5)	1·384 (3)	1·382 (1)	1·384 (2)
N(2)—N(1)	1·295 (3)	1·309 (2)	1·318 (2)	1·325 (4)	1·313 (5)	1·307 (2)	1·312 (2)	1·316 (2)
N(1)—C(7)	1·350 (3)	1·352 (2)	1·351 (2)	1·350 (4)	1·329 (5)	1·329 (3)	1·334 (2)	1·334 (2)
C(7)—C(8)	1·413 (4)	1·420 (3)	1·416 (2)	1·418 (4)	1·404 (6)	1·400 (3)	1·404 (3)	1·400 (2)
C(8)—O(2)	1·196 (3)	1·212 (2)	1·217 (2)	1·205 (4)	1·217 (5)	1·212 (3)	1·206 (2)	1·211 (2)
Δ[O(2)]†	0·011 (6)	0·001 (3)	0·041 (2)	0·013 (2)	0·019 (4)	0·030 (4)	0·005 (3)	0·038 (2)
ω(°)	68·4 (2)	78·6 (1)	54·9	63·8	35	2	39·1 (1)	24·4 (1)
χ^2‡	5·4	16·4	70·3	6·8	3·4	4·1	4·9	22·6

References: (*a*) This work; (*b*) Hašek, Obrda, Huml, Nešpůrek, Chojnacki & Šorm (1978); (*c*) Hašek, Obrda, Huml, Nešpůrek & Šorm (1979); (*d*) Wang, Lee & Yeh (1984); (*e*) Ueng, Lee, Wang & Yeh (1985).

* (1) 4-Acetyl-3-(*p*-tolyl)sydnone; (2) 4-acetyl-3-phenylsydnone oxime; (3) 4-(3-methyl-1-buten-2-yl)-3-phenylsydnone; (4) 4-(cyclohexen-1-yl)-3-phenylsydnone; (5) 3-(*p*-tolyl)sydnone; (6) 3-(*p*-ethoxyphenyl)sydnone; (7) 3-(*p*-benzyloxyphenyl)sydnone; (8) 3-(*p*-isopropoxyphenyl)sydnone.

† Deviation (Å) of the exocyclic oxygen atom O(2) from the mean plane of the sydnone ring.

‡ χ^2 is defined as $\sum_{i=1}^{n} \Delta d_i^2/(\sigma_{x_i}^2 + \sigma_{y_i}^2 + \sigma_{z_i}^2)$, where Δd_i is the distance from the least-squares plane; σ_{x_i}, σ_{y_i} and σ_{z_i} are the standard deviations of coordinates x, y and z in atom i. χ^2 of compounds (3) and (4) are recalculated by our definition. The maximum deviation distance from the mean plane of compound (1) is Δ[N(2)] [0·007 (5) Å], that of compound (2) is Δ[C(8)] [0·007 (2) Å].

3,4-disubstituted sydnone derivatives (55–79°) are larger than those of the 3-substituted sydnone derivatives (2–39°). This dihedral angle can also be described as the torsional angle of C(1)—N(1) and C(7)—C(9). The larger torsional angle of 3,4-disubstituted sydnone derivatives can be understood as the steric effect from these two bulky groups on the neighboring atoms of the sydnone ring, namely N(1) and C(7).

The C(7)—C(9) bond lengths of compounds (1) and (2) [1·444 (2) and 1·453 (4) Å] are shorter than those of compounds (3) and (4) [1·465 (3) and 1·464 (4) Å]. The dihedral angles between the sydnone ring and the plane of the sp^2 orbitals of the double bond on the 4-substituent of the compounds (1) and (2) [sydnone ring and —C(7)—C(9)—O(3)—C(11)—, 2·5 (2)°; sydnone ring and —C(7)—C(9)—C(10)—N(3)—O(3)—, 12·7 (1)°] are also smaller than the corresponding angles of compounds (3) and (4) (49·8 and 28·0°).

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(±)-(5α,8α,9α)-2-Chloro-5,8,9,10-tetrahydro-5,9-methanobenzocycloocten-8-amine Hydrochloride Sesquihydrate

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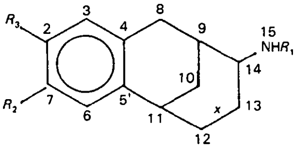
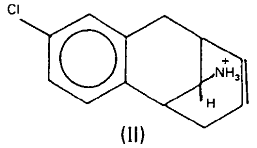
Abstract. $C_{13}H_{15}ClN^+.Cl^-.1·5H_2O$, $M_r = 283·20$, triclinic, $P\bar{1}$, $a = 19·329 (4)$, $b = 10·316 (2)$, $c = 7·410 (4)$ Å, $\alpha = 98·803 (4)$, $\beta = 100·091 (4)$, $\gamma = 87·034 (2)$°, $U = 1437·1$ Å^3, $Z = 4$, $D_x = 1·309$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0·71069$ Å, $\mu = 0·391$ mm^{-1}, $F(000) = 596$, $T = 293$ K, $R = 0·051$ for 3325 reflexions. There are two independent cations in the asymmetric unit with very similar dimensions. The bicyclo[3.3.1]nonane system adopts a distorted sofa–sofa conformation. The structure contains hydrophobic and hydrophilic regions. In the latter there is extensive hydrogen bonding connecting the R—NH_3^+ groups, the anions and the water molecules.

Introduction. The title compound, known by the number Org 6997 (Savage, Sleigh & Clark, 1980), is of pharmacological interest in that it shows activity in animal models which are believed to be predictive for the treatment of disorders of the central nervous system. In particular it could be a useful agent for the treatment of depression.





(II)

(I) $R_1 = H_2^+ (Cl^-)$, $R_2 = H$, $R_3 = Cl$, $x = C{=}C$.
(III) $R_1 = COMe$, $R_2 = OMe$, $R_3 = H$, $x = C{-}C$.

The sesquihydrate reported here has proved to be more suitable for drug formulation than the anhydrous material which was the subject of an earlier structure determination (Jones & Sheldrick, 1982). Structures have now been reported for the title cation (I), the isomer (II) (Jones, Kennard & Horn, 1979) and the related compound (III) (Murray-Rust, Murray-Rust & Middlemiss, 1982).

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