fact, as indicated in Table 3, each molecule in the crystal participates in two intermolecular hydrogen bonds: one with carboxylate as donor and chloroacetyl O of an adjacent molecule as acceptor and a second with N as donor and the carboxylate carbonyl O of a different adjacent molecule as acceptor. A similar intermolecular hydrogen-bonding network has been observed in crystalline *N*-acetylglycine (Levy, Peterson & Schomaker, 1957).

The observed *R* configuration of *N*-chloroacetyl-(+)-3,3,3-trifluoro-2-aminoisobutyric acid places the parent amino acid in the same stereochemical family as D-alanine, since both molecules have the same configuration of methyl, amino and carboxylate groups. This is relevant to the finding of Bailey, Chotamangsa & Vuttivej (1970) that D- and L-alanine are both substrates for the *P. cepacia* dialkylamino acid transaminase but are processed differently by the enzyme: D-alanine is decarboxylated and transaminated to acetaldehyde, but L-alanine is transaminated to pyruvate. Stereospecificity has also been observed in the reaction of the transaminase with the 3,3,3-trifluoro-2-aminoisobutyric acid enantiomers: the (+)-isomer (here shown to have the *R* configuration) causes rapid irreversible inactivation of the transaminase but the (−)-isomer (*S*) inactivates slowly or not at all (Keller, 1982). Also, inactivation of the transaminase by the racemic trifluoroamino acid is accompanied by decarboxylation (Keller & O'Leary, 1979). These facts suggest a similar mode of binding and processing for D-alanine and the *R* isomer of 3,3,3-trifluoro-2-aminoisobutyric acid by the dialkylamino acid transaminase.

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Structures of 3-(*p*-Ethoxyphenyl)sydnone (1), $C_{10}H_{10}N_2O_3$, and 3-(*p*-Tolyl)sydnone (2), $C_9H_8N_2O_2$

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Abstract. (1) $M_r = 206$, monoclinic, $P2_1/n$, $a =$ 7·609 (1), $b =$ 7·350 (1), $c =$ 17·567 (4) Å, $\beta =$ 94·93 (1)°, $V =$ 979·02 Å^3, $Z = 4$, $D_m =$ 1·4, $D_x =$ 1·399 g cm^{-3}, λ(Mo $K\alpha$) = 0·7093 Å, μ(Mo $K\alpha$) = 0·985 cm^{-1}, $F(000) =$ 431·92, $T = 298$ K, final $R =$ 0·051 for 1391 observed reflections. (2) $M_r = 176$, monoclinic, $P2_1/c$, $a =$ 3·853 (2), $b =$ 11·819 (3), $c =$ 18·249 (3) Å, $\beta =$ 92·22 (3)°, $V =$ 830·286 Å^3, $Z = 4$, $D_m =$ 1·4, $D_x =$ 1·41 g cm^{-3}, μ(Mo $K\alpha$) = 0·958 cm^{-1}, $F(000) =$ 367·92, $T = 298$ K, final $R =$

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Table 1. *Atomic positional parameters and equivalent isotropic temperature factors*

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

	x	y	z	B_{eq}(Å^2)
Compound (1)				
C(1)	0·0223 (3)	0·2583 (3)	0·5154 (1)	3·1 (1)
C(2)	0·0191 (3)	0·2743 (4)	0·4376 (1)	3·7 (1)
C(3)	0·8700 (3)	0·2179 (4)	0·3923 (1)	3·8 (2)
C(4)	0·7279 (3)	0·1470 (3)	0·4267 (1)	3·5 (1)
C(5)	0·7331 (3)	0·1340 (3)	0·5052 (1)	3·8 (1)
C(6)	0·8806 (3)	0·1891 (3)	0·5501 (1)	3·6 (1)
C(7)	0·3284 (3)	0·3783 (4)	0·5404 (1)	3·9 (2)
C(8)	0·4387 (3)	0·4138 (4)	0·6068 (1)	4·1 (2)
C(9)	0·5555 (3)	0·1037 (4)	0·3064 (1)	4·7 (2)
C(10)	0·3748 (4)	0·0307 (5)	0·2812 (1)	6·1 (2)
N(1)	0·1784 (2)	0·3127 (3)	0·5628 (1)	3·4 (2)
N(2)	0·1726 (3)	0·2976 (4)	0·6367 (1)	5·1 (2)
O(1)	0·3364 (2)	0·3600 (3)	0·6659 (1)	5·1 (1)
O(2)	0·5850 (2)	0·4754 (3)	0·6223 (1)	5·4 (1)
O(3)	0·5762 (2)	0·0851 (3)	0·3886 (1)	4·5 (1)
Compound (2)				
C(1)	0·3822 (10)	0·1255 (3)	0·8091 (2)	3·3 (2)
C(2)	0·3967 (12)	0·2058 (4)	0·7545 (2)	4·2 (3)
C(3)	0·2851 (12)	0·1770 (4)	0·6843 (2)	4·3 (3)
C(4)	0·1593 (11)	0·0703 (4)	0·6682 (2)	4·0 (3)
C(5)	0·1477 (11)	−0·0077 (4)	0·7242 (2)	4·0 (2)
C(6)	0·2582 (11)	0·0183 (4)	0·7950 (2)	3·9 (2)
C(7)	0·6617 (12)	0·0900 (3)	0·9323 (2)	3·9 (3)
C(8)	0·7242 (12)	0·1571 (4)	0·9949 (2)	4·5 (3)
C(9)	0·0420 (13)	0·0409 (4)	0·5916 (2)	5·3 (3)
N(1)	0·4981 (9)	0·1554 (3)	0·8828 (2)	3·7 (2)
N(2)	0·4379 (11)	0·2597 (3)	0·9037 (2)	5·3 (3)
O(1)	0·5785 (9)	0·2623 (3)	0·9746 (2)	5·6 (2)
O(2)	0·8604 (9)	0·1443 (3)	0·0556 (2)	5·7 (2)

0·055 for 763 observed reflections. The bond distances of the sydnone ring are similar in both structures but N(1)–C(7) of (1) and (2) and C(7)–C(8) of (1) are significantly shorter than comparable bonds in other 3-phenylsydnone derivatives. The dihedral angles between the sydnone ring and the phenyl ring are quite different [2° in (1) and 35° in (2)].

Introduction. There are a few studies on the unique aromaticity of the sydnone ring (Ohta & Kato, 1969; Stewart, 1964) and the syntheses of arylsydnone derivatives (Baker, Ollis & Poole, 1949; Yashunskii, Vasieva & Sheinker, 1959). The photochromic properties are particularly interesting. In order to correlate the variation of color and the structural conformation, the structure determinations of the title compounds were undertaken as part of a systematic study of a series of such compounds.

Experimental. Crystals of (1) and (2) obtained by slow evaporation of ethanol solutions.

(1) Crystal 0·3 × 0·4 × 0·6 mm. CAD-4 diffractometer. Unit cell: 24 reflections, 2θ range 20 to 30°. D_m by flotation (H_2O/CCl_4). No absorption correction. $2\theta_{max} = 60°$. Ranges of h, k, l: 0 to 12, 0 to 12, −26 to 26, respectively. Three standard reflections monitored every 2 h: variation <2%. 2851 unique reflections, 1391 observed with $I \geq 2\sigma(I)$. $R = 0·051$, $R_w = 0·032$, $S = 1·88$. Weighting scheme from counting statistics. Structure solved by direct method using the *MULTAN* program in the Enraf–Nonius (1979) *Structure Determination Package*, with 160 highest E's, 50 smallest E's and 900 $\sum_2$ relationships. H atoms found in difference Fourier map after isotropic refinement and then refined. $(\Delta/\sigma)_{max} = 0·32$. Peaks in final $\Delta\rho$ map +0·21 to −0·19 e Å^{-3}. Secondary-extinction coefficient 0·495 (length in µm). 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.*

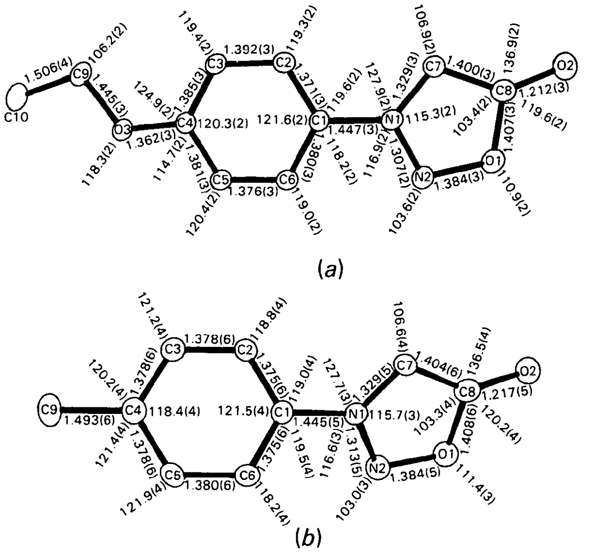

Fig. 1. Bond lengths (Å) and bond angles (°) of (*a*) compound (1), and (*b*) compound (2).

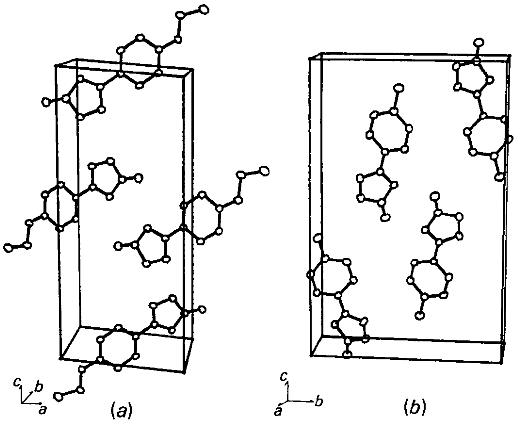

Fig. 2. Packing diagram of the unit cell. (*a*) Compound (1). (*b*) Compound (2).

Table 2. *Comparison of selected bond distances* (Å) *in the sydnone ring*

Compound (Reference)	O(1)—C(8)	O(1)—N(2)	N(2)—N(1)	N(1)—C(7)	C(7)—C(8)	C(8)—O(2)	Δ[O(2)]*	ω (°)	χ^2	Color
3-(*p*-Bromophenyl)-sydnone (*a*)	1·42 (1)	1·36 (1)	1·34 (1)	1·38 (1)	1·41 (1)	1·20 (1)	0·021	27·6		
3-Phenylsydnone (*b*)	1·411 (1)	1·373 (1)	1·313 (1)	1·347 (1)	1·413 (1)	1·221 (1)		30·0		
4-(3-Methyl-1-buten-2-yl)-3-phenylsydnone (*c*)	1·406 (3)	1·379 (2)	1·318 (2)	1·351 (2)	1·416 (2)	1·217 (2)	0·041 (2)	54·9	195·6	Transparent
4-(Cyclohexen-1-yl)-3-phenyl-sydnone (*d*)	1·400 (4)	1·384 (4)	1·325 (4)	1·350 (4)	1·418 (4)	1·205 (4)	0·013 (2)	63·8	21·1	Bright yellow
3-(*p*-Ethoxyphenyl)-sydnone (*e*)	1·407 (3)	1·384 (3)	1·307 (2)	1·329 (3)	1·400 (3)	1·212 (3)	0·030 (4)	2	4·1	Brown
3-(*p*-Tolyl)sydnone (*e*)	1·408 (6)	1·384 (5)	1·313 (5)	1·329 (5)	1·404 (6)	1·217 (5)	0·0019 (4)	35	3·4	Coated brown

References: (*a*) Bärnighausen, Jellinek, Munnik & Vos (1963); (*b*) Hope (1978); (*c*) Hašek, Obrda, Huml, Nešpůrek, Chojnacki & Šorm (1978); (*d*) Hašek, Obrda, Huml, Nešpůrek & Šorm (1979); (*e*) this work.

* Deviation (Å) of O(2) from the mean plane of the sydnone ring.

(2) Crystal 0·2 × 0·3 × 0·4 mm. Unit cell: 24 reflections, 2θ range 20 to 26°. $2\theta_{\max} = 60°$. 2424 unique reflections, 763 observed with $I \geq 2\sigma(I)$. Ranges of h, k, l: −5 to 5, 0 to 16, 0 to 25, respectively. Three standard reflections: variation <2%. $R = 0{\cdot}055$, $R_w = 0{\cdot}031$, $S = 1{\cdot}57$ based on F. Structure solved by direct method with 160 highest E's, 50 smallest E's and 1149 $\sum_2$ relationships. $(\Delta/\sigma)_{\max} = 0{\cdot}17$. Peaks in final $\Delta\rho$ map 0·2 to −0·22 e Å^{-3}. Extinction coefficient 0·065. Other details as for (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. The packing diagrams are given in Fig. 2.

The bond lengths of the sydnone ring are listed in Table 2 and compared with those from other 3-phenylsydnone derivatives (Nešpůrek, Hašek, Šorm, Kuml, Obrda, Lipinski & Chojnacki, 1982; Hope, 1978). N(1)—C(7) of (1) and (2) and C(7)—C(8) of (1) are significantly shorter than in the other derivatives. N(1)—N(2) is between a single (1·44 Å) and a double bond (1·24 Å).

In addition, the planarity of the sydnone ring is given in Table 2 as χ^2 which is defined as $\sum_{i=1}^{N} \Delta d_i^2/(N-3)$, where Δd_i is the distance of the atom i from the least-squares plane; N is the number of atoms to be considered in the plane. It is obvious that the two title compounds have better planarity. The large C(2)—C(1)—C(6) angle is similar to that of 3-phenylsydnone (122·6°) but less pronounced. The dihedral angles (ω) between the sydnone ring and the phenyl ring are also given in the table; these vary from 2 to 64°. The nearly coplanar one has the darkest color.

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39323 (38 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.