[332]; the normal to the least-squares plane of the central ring has Miller indices 2·006, 2·189, 1·000; the six-membered rings have two alternating perpendicular distances: 3·518 Å (intra-'dimer' distance, *i.e.* distance between the two molecules which are related by the inversion center at $\frac{1}{2},\frac{1}{2},\frac{1}{2}$) and 3·385 Å (inter-'dimer' distance). Oddly, the inter-'dimer' distance is shorter than the intra-'dimer' distance.

Using the INDO atom-in-molecule charges (Pople & Beveridge, 1970),* the Madelung energy (Metzger, 1981) for AETCNQ, obtained by Ewald's method, is $E_M = -10·765$ kJ mol^{-1}. Using the non-bonded van der Waals and repulsion parameters of Williams and co-workers (Williams, 1981; Williams & Cox, 1984; Cox, Hsu & Williams, 1981), the dispersion and repulsion energies for AETCNQ are $E_d = -199·260$ and $E_r = 95·734$ kJ mol^{-1}, respectively, so that $E_M + E_d + E_r = -114·291$ kJ mol^{-1}, a value that should correlate with enthalpies of sublimation.

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* See deposition footnote.

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Structure of Methyl 4-(N,N-Dimethylamino)phenylcarbamate, DMAPCMe*

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Abstract. *Chemical Abstracts* name [4-(dimethyl-amino)phenyl]carbamic acid, methyl ester; registry number 78823-56-0; $C_{10}H_{14}N_2O_2$, $M_r = 194·23$, orthorhombic, *Pbca* (space group number 61), $a = 13·926$ (4), $b = 9·999$ (4), $c = 14·854$ (7) Å, $V = 2068·3$ Å^3, $Z = 8$, $D_x = 1·25$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0·53$ mm^{-1}, $F(000) = 832$, $T = 295$ (3) K, $R = 5·9\%$ for 786 observed reflections. The structure consists of flat molecules stacked along [001], with a large tilt, but no π–π perpendicular overlap. There is a significant quinoid distortion. The packing is controlled by intermolecular hydrogen bonding along [010]. This is supported by the infrared spectrum of the solid (N–H band at 3330 cm^{-1}). INDO and MINDO/3 calculations, and also the partial quinoid structure, suggest that DMAPCMe is a fairly strong electron

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donor; however, this is belied by electrochemical oxidation data. The lattice energy (Madelung + dispersion + repulsion) is -86.524 kJ mol^{-1}.

Introduction. The title compound (DMAPCMe) has been investigated as part of a systematic study of several molecules $D-\sigma-A$ (organic one-electron donor–sigma bridge–organic one-electron acceptor) whose potential electrical rectification properties may enable the assembly of ultra-thin $M_1|D-\sigma-A|M_2$ rectifiers, where M_1 and M_2 are metallic thin films (Metzger *et al.*, 1986). In particular, D would be a one-electron donor such as tetrathiafulvalene (TTF) or N,N,N',N'-tetramethyl-*para*-phenylenediamine (TMPD), σ would be a carbamate bridge, and A would be the excellent acceptor 7,7,8,8-tetracyanoquinodimethane (TCNQ) (Metzger & Panetta, 1983). Since several molecules of this type have been synthesized, it is of some interest to probe the molecular structure of the present molecule, which incorporates a donor similar to TMPD and the carbamate sigma bridge of other compounds studied previously, such as phenylcarbamate–TCNQ (Panetta, Baghdadchi & Metzger, 1984).

Crystal structures of urethanes and carbamates have been studied by other authors: ethyl carbamate or urethane, $NH_2.CO.O.C_2H_5$ (Bracher & Small, 1967), ammonium carbamate $NH_4{}^+NH_2.COO^-$ (Adams & Small, 1973), N-phenylurethane $C_6H_5.NH.CO.OC_2H_5$ (Ganis, Avitabile, Migdal & Goodman, 1971), bis(4-hydroxybutyl)-4,4'-methylenebis(phenylcarbamate), $(HO).C_4H_8.O.OC.NH.C_6H_4.NH.CO.O.C_4H_8.$-$(OH)$ (Forcier & Blackwell, 1981), cyclobisurethane $[CO.NH.C_6H_{12}.NH.CO.O.C_4H_8.O]$ (Beres & Alexander, 1976), and cyclotetraurethane $[CO.NH.C_6H_{12}.$-$NH.CO.O.C_4H_8.O]_2$ (Beres & Alexander, 1976).

A companion publication on DMAPCMe describes: (i) further theoretical calculations that elucidate its electron-donor properties, (ii) its cyclic voltammogram to measure its redox properties, (iii) IR spectra of its hydrogen-bonded association in solution, and (iv) a solution EPR spectrum of its radical cation (which also exhibits intermolecular hydrogen bonding at high concentration) (Laidlaw, Miura, Grant, Cooray, Clark, Kispert & Metzger, 1987).

Experimental. *Synthesis.* The title compound was first synthesized by Staudinger & Endle (1917) from 4-(N,N-dimethylamino)phenyl isocyanate and methanol in carbon disulfide; its melting temperature was determined as 374–376 K. DMAPCMe was prepared, following Staudinger & Endle, by the reaction of 4-(N,N-dimethylamino)phenyl isocyanate with a large excess of dry methanol, and separated by column chromatography; recrystallization from a benzene–hexane mixture and then from methanol–water gave pale yellow needles, melting temperature 373–375 K (uncorr.). Visible and ultraviolet spectra were measured

Table 1. *Summary of data collection and crystal structure determination*

Crystal color	Colorless
Crystal size	0.2 × 0.2 × 1.0 mm
Orientation matrix from	24 reflections, $\theta = 13$–$21°$
Scan mode	ω–2θ
Scan speed (° min^{-1})	0.60–21
Scan width parameters $\Delta\omega_a, \Delta\omega_b$ (°)	0.80, 0.20
Scan range (θ_{min} to θ_{max}) (°)	1–22
Index range	$h = 0$ to 10, $k = 0$ to 14, $l = 0$ to 15
Intensity control reflections	008, 222, 060
Fluctuation of control reflections	< 2%
Total reflections measured	1474
Reflections observed	786 $[F_{obs} > 1.67\sigma(F_{obs})]$
Number of parameters	141
Weighting scheme	Unit weights
R index (unweighted)	5.9%
Final maximum (shift/e.s.d.)	0.278
Final largest difference Fourier peak (e Å^{-3})	0.102

using a Cary 2200 spectrophotometer. The infrared spectrum of the solid, dispersed in a KBr pellet, was measured on a Jasco A-200 spectrophotometer. The ^{1}H NMR spectrum was measured on a Nicolet NT-200 spectrometer; the ^{13}C spectrum was measured on a Jeol FX-100 spectrometer.

X-ray diffraction data were obtained on an Enraf–Nonius CAD-4F automated kappa-geometry diffractometer at the University of Alabama, using graphite-monochromatized Mo $K\alpha$ radiation. Details about the data collection and refinement are given in Table 1. The data were corrected for Lorentz and polarization factors. The structure was solved by direct methods and refined on F by full-matrix least squares, using anisotropic thermal parameters for all non-hydrogen atoms, riding positions and variable isotropic thermal parameters for the H atoms, and unit weights, to a final unweighted R index of 5.9% (786 observations, 141 parameters). The programs used were *DATRDN* (Hunter, 1982), *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980), *SHELX*76 (Sheldrick, 1976), *ORTEP*II (Johnson, 1970*a*), *ORSBA* (Johnson, 1970*b*), and, for interplanar distances and lattice energies, programs *CELMAP* and *EWALD* (Metzger, 1976). Atomic scattering factors used were those of *SHELX*76.

Spectroscopic evidence for hydrogen bonding. The visible and ultraviolet absorption spectrum, measured for a 3.53×10^{-5} mol L^{-1} solution in acetonitrile, consists of peaks at 195 nm ($\log_{10}\varepsilon$ 4.44), 265 nm (4.38), 311 nm (3.55); there is evidence of formation of a complex (probably a H-bonded complex) because at higher concentrations (up to 1.41×10^{-4} mol L^{-1}) the molar absorptivities decrease by about 10%. The infrared spectrum of the solid dispersed in a KBr pellet gives evidence of hydrogen bonding: the bands are at 3330 (N—H), 3110 and 3060 (aromatic C—H), 3000–2800 (aliphatic C—H), and 1705 cm^{-1} (C=O); in fact the free N—H stretch frequency should be at

3340 cm^{-1} in the absence of hydrogen bonding. An IR study of the extent of hydrogen bonding as a function of solution concentration is described elsewhere (Laidlaw et al., 1987).

The ^{1}H NMR spectrum was measured in 99·9% acetone-d_6: it consists of singlet peaks at 2·86 (relative to Me$_4$Si: NMe$_2$ protons) and at 3·64 p.p.m. (OMe protons), two doublets at (7·36,7·32) and at (6·72, 6·68) p.p.m. due to the aromatic protons; the NH group proton was not observed. The ^{13}C NMR spectrum was measured in DCCl$_3$: 154·8 p.p.m. (relative to Me$_4$Si: C=O), singlets at 147·5 and 127·8 p.p.m. (aromatic carbons bonded to N), two doublets at 121·2 and 113·3 (other aromatic carbons), one quartet at 51·9 (O.CH$_3$ carbon), and one quartet at 40·9 p.p.m. (NMe$_2$ carbons). ^{13}C spectra have been observed for other urethanes (Krichendorf & Hull, 1981).

EPR spectra of the pink electrolytically generated DMAPCMe$^+$ radicals in concentrated solution also show evidence of intermolecular hydrogen bonding (Laidlaw et al., 1987).

Discussion. The final atom coordinates are given in Table 2. The molecular structure, with bond lengths and bond angles (uncorrected for thermal motion), is displayed in Fig. 1; the unit-cell packing and the hydrogen-bonding network can be seen in Fig. 2.

DMAPCMe has an extended conformation, but there is an 18·7° angle between the least-squares benzene plane and the least-squares plane through the carbamate moiety. The rigid-body analysis reveals that the molecule undergoes a translation motion with the smallest component approximately along the local y axis (i.e. along the H-bonding direction), and a libration motion with the largest component in the direction perpendicular to the benzene plane; this is in accordance with expectations. Except as discussed below, the bond lengths and bond angles resemble those of other carbamates.* The extended shape of the carbamic acid moiety resembles that of the trans form calculated to be lowest in energy by a geometry-minimized 4-21G level ab initio calculation (Van Alsenoy, Williams & Schaefer, 1981). There is a significant quinoid distortion of the benzene-ring bond distances: the bond lengths C5—C6 and C2—C3 [1·365 and 1·345 Å after correction for thermal motion] are shorter than the bond lengths C1—C6, C1—C2, C3—C4, and C4—C5

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* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, least-squares planes for selected groups within the molecule, rigid-body libration and translation tensors and a comparison of selected bond distances and bond angles between urethane structures have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44547 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$U_{eq} = \frac{1}{3}$(trace of orthogonalized **U** tensor).

|	x	y	z	U_{eq}
C1	0·4108 (5)	0·2186 (5)	1·0428 (4)	0·059 (5)
C2	0·3782 (5)	0·0924 (5)	1·0110 (4)	0·063 (5)
C3	0·3354 (5)	0·0782 (5)	0·9306 (4)	0·063 (5)
C4	0·3184 (4)	0·1840 (5)	0·8725 (4)	0·048 (3)
C5	0·3510 (4)	0·3114 (5)	0·9019 (4)	0·053 (4)
C6	0·3942 (5)	0·3262 (5)	0·9836 (4)	0·058 (4)
N7	0·2750 (4)	0·1605 (4)	0·7895 (3)	0·052 (3)
C8	0·2306 (4)	0·2483 (6)	0·7345 (4)	0·054 (4)
O9	0·2232 (3)	0·3699 (3)	0·7489 (3)	0·068 (3)
O10	0·1955 (3)	0·1892 (4)	0·6613 (3)	0·064 (3)
C11	0·1491 (6)	0·2707 (6)	0·5950 (5)	0·073 (5)
N12	0·4537 (5)	0·2325 (5)	1·1251 (4)	0·087 (5)
C13	0·4948 (7)	0·3595 (7)	1·1520 (5)	0·097 (6)
C14	0·4721 (6)	0·1182 (7)	1·1820 (4)	0·076 (5)
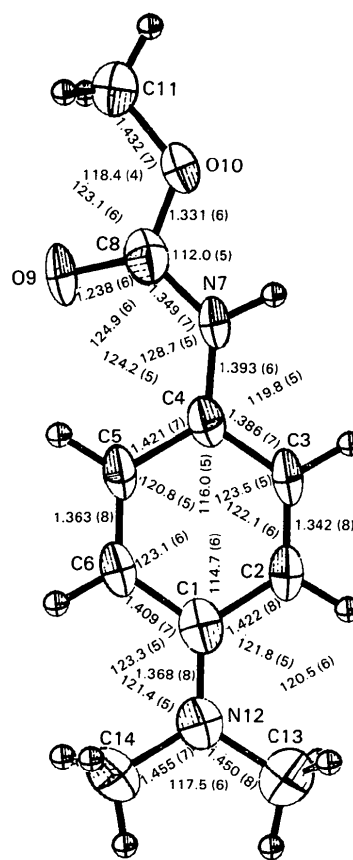
Fig. 1. *ORTEP*II drawing (Johnson, 1970a) of the molecule. The thermal ellipsoids of vibration are depicted at the 50% probability level; the bond lengths (Å) and bond angles (°) (uncorrected) for thermal motion) are given with their e.s.d.'s. The H—C bond distances are 1·000 Å, the N7—H7 bond distance is 0·942 Å.

[1·416, 1·432, 1·392, and 1·433 Å, respectively, after correction for thermal motion], and the C2—C1—C6 and C3—C4—C5 bond angles (115·05 and 116·32° after correction) are significantly less than 120°. This

$C_{10}H_{14}N_2O_2$

may be due to quinoid distortion, or to a large formal charge on atoms N7 and N12. The thermal ellipsoids of atoms C2, C3, C5, C6, N7, O9 and O10 indicate a significant librational mode along the long axis of the molecule, which is confirmed by the libration ellipsoid:* this effect has been noticed before, in the structure of ethyl carbamate, and attributed to the hydrogen-bonding network (Bracher & Small, 1967).

While there is no quinoid distortion in the phenyl ring of N-phenylurethane (Ganis, Avitabile, Migdal & Goodman, 1971), in ,DMAPCMe the C1—N12 and C4—N7 bond lengths are unusually short (1·370 and 1·396 Å after correction for thermal motion): they are shorter than the corresponding C—N distances in phenylcarbamate (Forcier & Blackwell, 1981) and in N-phenylurethane (Ganis, Avitable, Migdal & Goodman, 1971); they are also shorter than the aromatic ring-exocyclic nitrogen bond distances observed in neutral TMPD [1·420 (10) and 1·407 (10) Å] (Ikemoto, Katagiri, Nishimura, Yakushi & Kuroda, 1979); however, they are longer than the corresponding distances in the TMPD cation radical (Wurster's blue) salts (1·344 to 1·365 Å) [see Ikemoto et al. (1979) for a compilation].

The DMAPCMe molecules are tilted somewhat from the [001] axis, with no π–π overlap between nearest-neighbor DMAPCMe molecules (Fig. 2). Instead, there is intermolecular hydrogen bonding along [010], with a 2·968 Å distance between O9 of one molecule and N7 of the molecule related to it by a glide plane with translation b/2: this hydrogen bond is shown by thin lines in Fig. 2. The dihedral angle between the benzene-ring least-squares planes of the hydrogen-
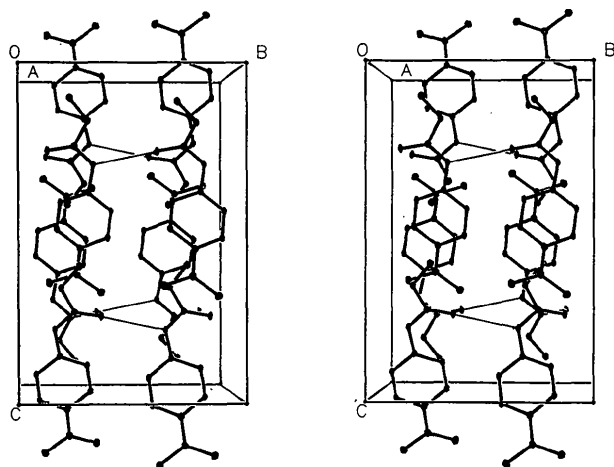
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* See deposition footnote.

Fig. 2. Stereoscopic ORTEPII drawing (Johnson, 1970a) of the molecular packing within the unit cell. H atoms are omitted for simplicity. Thin lines indicate intermolecular hydrogen bonds linking N7 and O9.

Table 3. INDO and MINDO/3 atom-in-molecule charges (|electrons|)

	INDO	MINDO/3		INDO	MINDO/3
C1	0·1337	0·1467	H2	−0·0161	0·0096
C2	−0·0345	−0·0857	H3	−0·0216	−0·0028
C3	−0·0010	−0·0086	H5	0·0048	0·0417
C4	0·1153	0·0840	H6	−0·0146	0·0117
C5	−0·0060	−0·0063	H7	0·1161	0·0960
C6	−0·0318	−0·0818	H111	−0·0279	−0·0278
N7	−0·2145	−0·1888	H112	−0·0270	−0·0328
C8	0·5856	0·8453	H113	−0·0270	−0·0322
O9	−0·4641	−0·6505	H131	−0·0274	−0·0105
O10	−0·3112	−0·5062	H132	−0·0325	−0·0139
C11	0·2541	0·3687	H133	−0·0365	−0·0217
N12	−0·1557	−0·1337	H141	−0·0275	−0·0101
C13	0·1684	0·1219	H142	−0·0372	−0·0224
C14	0·1709	0·1257	H143	−0·0345	−0·0167

bonded molecules is 54·4°. There is an infinite network of N7—H7—O9 hydrogen bonds along [010]. Thus, the stacking is controlled by intermolecular hydrogen bonding and totally ignores the possibility of inter-molecular π–π interactions.

Theoretical results. The INDO and MINDO/3 calculated dipole moments for DMAPCMe (2·78 and 3·02 D respectively)* are small; the atom-in-molecule charges are given in Table 3. The formal MINDO/3 charge of the dimethylamino group is only 0·0186 |electrons|; the charge of the N7-to-H113 group is −0·2233 |electrons|: thus, in its ground state, DMAPCMe does not have the zwitterionic character and large dipole moment of, say, P3CNQ (Metzger, Heimer & Ashwell, 1984).

The partial quinoid character is probably due to the two *para* nitrogen substituents. This raises the possibility that DMAPCMe may be a good one-electron donor like, say, TMPD. Using the fixed molecular geometries of the crystal structures of DMAPCMe and TMPD (Ikemoto et al., 1979), the MINDO/3 computed ionization potentials are 7·15 eV for DMAPCMe and 7·08 eV for TMPD [exp. = 6·25 eV (Batley & Lyons, 1968)]. However, AM1 calculations have recently corrected this misapprehension, and the cyclic voltammogram of DMAPCMe shows that DMPAPMe is a rather poor donor compared with TMPD (Laidlaw et al., 1987).

With the MINDO/3 charges of Table 3, the calculated Madelung energy of DMAPCMe is E_M = −12·922 kJ mol⁻¹; with the non-bonded van der Waals and repulsion parameters of Williams et al. [C, H: Williams (1981); N: Williams & Cox (1984); O: Cox, Hsu & Williams (1981)] the dispersion and repulsion energies are E_d = −154·689 and E_r = 81·087 kJ mol⁻¹: the net lattice energy is $E_M + E_d + E_r$ = −86·524 kJ mol⁻¹, a value that correlates well with typical enthalpies of sublimation (Metzger, 1981).

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* 1 D (debye) = 3·335 64 × 10⁻³⁰ C m.

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The Structure of (1,2-Benzisoxazol-3-yl)methanesulfonamide: A Novel Antiepileptic Drug

BY JOHN N. LISGARTEN AND REX A. PALMER*

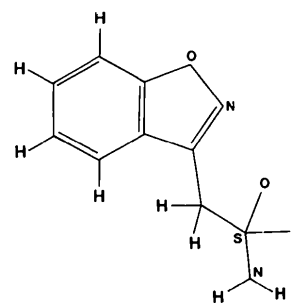*Department of Crystallography, Birkbeck College, University of London, Malet Street, London WC1E 7HX, England*

Abstract. $C_8H_8N_2O_3S$, $M_r = 212.54$, monoclinic, $P2_1/a$, $a = 7.347 (9)$, $b = 13.237 (4)$, $c = 10.128 (8)$ Å, $\beta = 108.916 (6)°$, $V = 931.9 (1)$ Å³, $Z = 4$, $D_m = 1.52 (4)$, $D_x = 1.514$ g cm⁻³, $\lambda(Cu K\alpha) = 1.54184$ Å, $\mu = 28.35$ cm⁻¹, $F(000) = 440$, room temperature, $R = 0.040$ for 1864 observed reflections. The sulfonamide N forms intermolecular hydrogen bonds with the benzisoxazole ring N and also with the O on the sulfonamide group. Centrosymmetrically related benzisoxazole ring pairs are π-bonded with a high degree of overlap.

Introduction. The title compound (zonisamide, I) is an experimental antiepileptic drug whose spectrum of activity in animals resembles that of phenytoin (one of the most extensively used drugs for the treatment of generalized seizures) but with a much higher ratio of

neurotoxic to effective anticonvulsant dose (Masuda, Utsui, Shiraishi, Karasawa, Yoshida & Shimizu, 1979). The structure analysis reported here was undertaken as part of a study of convulsant and anticonvulsant compounds.

(I)