Table 2. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

In(1)–Te(1)	2·819 (1)	Te(1)–In(1)–Te(8)	113·73 (2)
Te(1)–Te(4₁)	4·721 (1)	Te(1)–In(1)–Te(5₁)	101·26 (1)
Te(1)–Te(8)	4·721 (1)	Te(1)–In(2)–Te(2)	66·59 (2)
Te(1)–Te(5₁)	4·358 (1)	Te(2)–In(2)–Te(3)	82·61 (2)
Te(1)–In(2)	3·576 (1)	Te(1)–In(2)–Te(3)	75·52 (2)
Te(1)–Te(2)	3·926 (1)	Te(2)–In(2)–Te(4)	75·52 (2)
Te(2)–Te(3)	4·721 (1)	Te(1)–In(2)–Te(5)	120·00 (2)
Te(1)–Te(3)	4·379 (1)		
Te(1)–Te(4)	6·454 (1)		

Discussion. Since there is no evidence of polyionic formation in InTe, valence saturation rules give rise to an extreme ionic formulation $(In^{3+})(In^+)_2(Te^{2-})$. The structure contains two different In atom sites as suggested by this formula. In(1) exists, on a covalent model, in a state of sp^3 hybridization, being surrounded by four Te atoms forming a tetrahedron slightly foreshortened along c. The In–Te bond of 2·819 (1) Å compares favourably with that of 2·86 Å in In_4Te_3 where the tetrahedron has three Te and one In atom. In In_2Te_5 (Sutherland, Hogg & Walton, 1976) the tetrahedrally coordinated In has three In–Te bonds of 2·86 Å and one of 2·73 Å to the end member of a $(Te_3)^{2-}$ polyanion.

The environment of In(2) is consistent with the extreme ionic formulation In^+ for this atom. It is surrounded by a cage-like system of eight Te atoms in a distorted square anti-prismatic arrangement, again fore-shortened along c, with In–Te distances of 3·576 (1) Å. The cage is completed by two In atoms sym-metrically disposed along c, also at distances of 3·576 (1) Å. These distances are comparable with those around In(4) in In_4Te_3 which is surrounded by seven Te atoms with an average In–Te distance of 3·49 Å and one In atom at 3·45 Å. The thermal parameters of In(2) were found to be significantly greater than those of In(1) and Te(1) and to be highly anisotropic with the maximum of the vibration ellipsoid occurring in the c direction towards the neighbouring In atoms.

The shortest Te–Te distance of 3·926 (1) Å [Te(1)–Te(2)] is comparable to that of 4·072 (2) Å found in In_4Te_3 and on average the Te atoms appear to have approximately the diameter of the Te^{2-} ion (4·44 Å) in both compounds.

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8-Quinolyl Cyanomethyl Sulfone

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Abstract. $C_{11}H_8N_2O_2S$, $M=232·26$, monoclinic, $P2_1/c$ (No. 14), $Z=4$. At $-40°C$, $a=7·419$ (1), $b=7·968$ (1), $c=17·636$ (2) Å, $\beta=100·20$ (1)°, $V=1026·1$ Å³, $D_c=1·503$ g cm⁻³. Mo $K\alpha$ radiation, $\lambda=0·71069$ Å, $\mu=1·98$ cm⁻¹. Syntex diffractometer, 2066 reflections, 177 variables refined by full-matrix least squares, $R=0·033$. NMR evidence for a possible C–H···N intramolecular interaction (between the methylene group and the N atom of the quinolyl moiety) is contradicted by the rather long H···N distance, 2·59 (2) Å, found in the crystal structure.

Introduction. Colorless crystals of the title compound were grown by sublimation. The crystal used in this investigation was a parallelepiped with dimensions $0·32 \times 0·32 \times 0·28$ mm perpendicular to (001), (10$\bar{2}$), and (011) respectively. The space group and approximate unit-cell parameters were obtained from oscillation and Weissenberg photographs. The crystal was mounted on a Syntex $P2_1$ diffractometer (Mo $K\alpha$ radiation, monochromated with a graphite crystal) equipped with a low-temperature apparatus which kept the crystal cooled to $-40°C$. The unit-cell dimen-

sions at this temperature were refined by least squares using the Bragg angles of 73 reflections.

Intensity data for 2364 unique reflections ($4 < 2\theta < 55°$) were collected with the ω-scan technique. Scans of $1\cdot0°$ were employed with scan rates which ranged from $1\cdot0$ to $5\cdot0°$ min^{-1} depending on the number of counts accumulated in a rapid preliminary scan. Background measurements were taken at both ends of the scan with ω displaced by $1\cdot0°$ from the $K\alpha$ peak; each measurement was made for one-half of the scan time. The intensities of four standard reflections were monitored after every 96 reflections; only statistical variations were noted. The intensities were corrected for Lorentz and polarization effects but not for absorption.

The structure was solved by direct methods (*MUL-TAN*); the H atoms were located from a difference map. Refinement of the structure by full-matrix least squares was carried out with only those 2066 reflections for which $I > 2\sigma(I)$. The refinement of all positional and thermal (anisotropic for the non-hydrogen atoms; isotropic for the H atoms) parameters converged at a conventional R of $0\cdot033$. The largest shift in any parameter during the final cycle of refinement was $0\cdot18\sigma$. The largest peak in the final difference map had a magnitude of $0\cdot27$ e Å^{-3} and was located between S(1) and

C(4). The final positional and thermal parameters are given in Table 1.* The mathematical and computational details are noted elsewhere (Harlow, Loghry, Williams & Simonsen, 1975).

Discussion. This is the fourth crystal-structure investigation of a cyanomethyl sulfone derivative (Loghry & Simonsen, 1976; Sammes, Harlow & Simonsen, 1976; Harlow, Sammes & Simonsen, 1974). This series of compounds, where the C–H bonds of the methylene group are polarized by the neighboring sulfonyl and cyano functions, was designed to study C–H$\cdots$X (X=N,O,F) intramolecular interactions by both crystallographic and spectroscopic methods. For the title compound, a ^{1}H NMR study showed a strong low-field shift in the –CH$_2$– protons relative to a reference compound in which no intramolecular interaction could occur. This suggested the existence of a significant C–H$\cdots$N interaction between the methylene
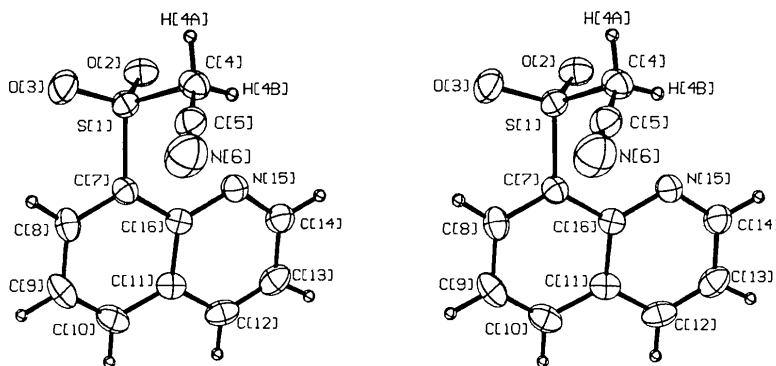
Fig. 1. Atom-numbering scheme and general conformation of the molecule.

Table 1. *Final positional and thermal parameters*

(a) Non-hydrogen atoms. The anisotropic thermal parameters are $\times 10^4$ and are in the form $\exp[-2\pi^2(h^2a^{*2}U_{11} + \ldots + klb^*c^*U_{23})]$.

	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S(1)	0·01739 (5)	0·77435 (5)	0·33533 (2)	353 (2)	269 (2)	304 (2)	17 (2)	53 (1)	39 (2)
O(2)	−0·1317 (2)	0·6650 (2)	0·3062 (1)	393 (6)	450 (7)	426 (7)	−51 (5)	11 (5)	66 (5)
O(3)	−0·0182 (2)	0·9491 (2)	0·3457 (1)	560 (8)	317 (6)	503 (5)	100 (5)	116 (6)	55 (5)
C(4)	0·1727 (3)	0·7616 (2)	0·2685 (1)	464 (10)	334 (9)	295 (8)	−22 (7)	68 (7)	23 (5)
C(5)	0·3411 (2)	0·8545 (2)	0·2943 (1)	412 (9)	363 (9)	363 (9)	69 (8)	80 (7)	49 (7)
N(6)	0·4711 (2)	0·9284 (2)	0·3156 (1)	422 (9)	591 (11)	711 (12)	−2 (8)	41 (8)	−36 (9)
C(7)	0·1335 (2)	0·6978 (2)	0·4249 (1)	327 (8)	299 (8)	279 (7)	−20 (6)	76 (6)	10 (6)
C(8)	0·1454 (2)	0·8024 (2)	0·4870 (1)	411 (9)	318 (9)	373 (9)	−28 (7)	161 (7)	−36 (7)
C(9)	0·2185 (3)	0·7443 (2)	0·5615 (1)	510 (10)	489 (11)	295 (8)	−103 (9)	145 (7)	−88 (8)
C(10)	0·2749 (3)	0·5831 (2)	0·5721 (1)	415 (9)	521 (11)	269 (8)	−98 (8)	75 (7)	34 (7)
C(11)	0·2680 (2)	0·4719 (2)	0·5089 (2)	284 (7)	370 (9)	312 (7)	−63 (6)	59 (6)	61 (6)
C(12)	0·3306 (2)	0·3040 (2)	0·5169 (1)	318 (8)	432 (10)	424 (9)	−30 (7)	14 (7)	152 (8)
C(13)	0·3281 (2)	0·2097 (2)	0·4529 (1)	373 (9)	289 (9)	586 (11)	21 (7)	30 (8)	60 (8)
C(14)	0·2612 (3)	0·2794 (2)	0·3803 (1)	432 (9)	309 (8)	455 (10)	26 (7)	6 (8)	−47 (8)
N(15)	0·1960 (2)	0·4328 (2)	0·3694 (1)	409 (7)	311 (7)	342 (7)	20 (6)	25 (6)	−33 (6)
C(16)	0·1987 (2)	0·5296 (1)	0·4334 (1)	284 (7)	288 (8)	295 (7)	−35 (6)	56 (6)	14 (6)

A C 32B – 10*

Table 1 (cont.)

(b) Hydrogen atoms

	x	y	z	U_{iso}
H(4A)	0·106 (3)	0·810 (3)	0·224 (1)	0·050 (6)
H(4B)	0·192 (3)	0·654 (3)	0·261 (1)	0·043 (5)
H(8)	0·101 (3)	0·912 (2)	0·478 (1)	0·034 (5)
H(9)	0·229 (3)	0·821 (2)	0·605 (1)	0·052 (6)
H(10)	0·325 (3)	0·542 (2)	0·623 (1)	0·047 (5)
H(12)	0·380 (3)	0·264 (2)	0·567 (1)	0·045 (5)
H(13)	0·372 (3)	0·098 (3)	0·455 (1)	0·054 (6)
H(14)	0·269 (3)	0·216 (2)	0·333 (1)	0·040 (5)

group and the quinolyl N atom (Sammes & Harlow, 1976).

The conformation and atom-numbering scheme for the title compound are shown in Fig. 1; the quinolyl H atoms are numbered in accord with the C atom to which each is attached. The bond distances and angles are displayed in Fig. 2 and are found to be in reasonable agreement with reported values [for the cyanomethyl sulfone moiety, see the three references listed above; for aromatic sulfone parameters, see Sime & Woodhouse (1974) and Harlow, Simonsen, Pfluger & Sammes (1974); for the quinolyl moiety, see Sax & Desiderato (1967) and Castellano & Prout (1971)]. Fig. 3 lists the deviations of the atoms from the least-squares mean plane of the quinolyl ring system. No unusually short intermolecular contacts were noted; a packing diagram is shown in Fig. 4. The quinolyl rings are parallel to each other across centers of symmetry, the closest contacts being between C(9) and C(13), 3·438 (3) Å, and between C(10) and C(13), 3·473 (3) Å.

The molecular geometry can be characterized as follows: (1) The closest intramolecular C–H···N contact of interest involves atom H(4B). The H(4B)···N(15) distance of 2·59 (2) Å can hardly be described as a significant interaction, and thus cannot be used to explain the unusual NMR results for the –CH₂– protons. (2) The quinolyl ring system is not perfectly planar. The deviations from the plane arise from a folding about the C(11)–C(16) bond axis and a twisting about the C(8)···C(13) axis. (3) A conformation in which the methylene group, rather than the sulfonyl O atoms, most closely approaches the ring N atom is not surprising since a strong repulsion between a N lone-pair and an electronegative O atom has been clearly demonstrated in a derivative of 8-nitroquinoline where the nitro group was rotated 59·2° out of the quinolyl plane (Sax & Desiderato, 1967). The fact that the S atom deviates markedly (−0·260 Å) from the quinolyl plane might also be attributed to the repulsion between O(2) and N(15). (4) A large increase in the S(1)–C(7)–C(16) angle to relieve this repulsion is not possible because it would bring about an even closer contact between O(3) and H(8), a contact which is already uncomfortably short, 2·37 (2) Å. (5) When viewed along the S(1)–C(4) bond, the quinolyl and cyano substituents are staggered in a gauche, rather than an anti, conformation. The repulsion between
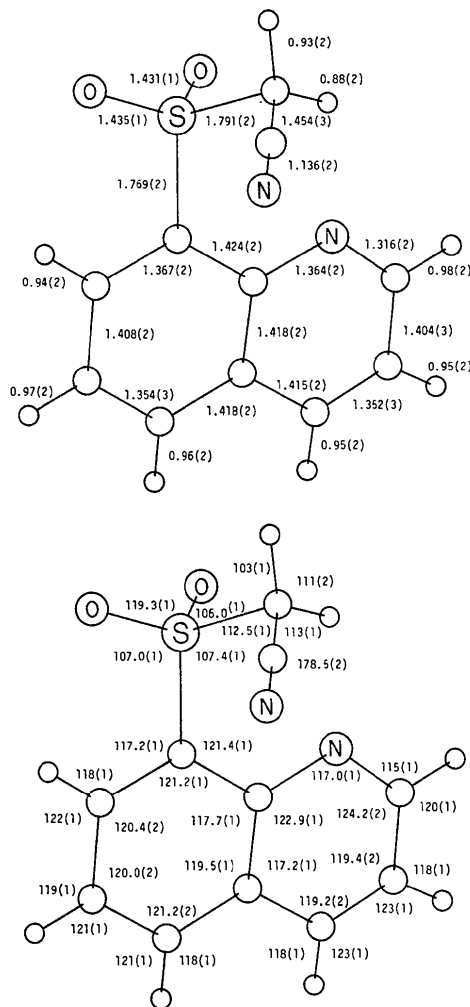

Fig. 2. Interatomic bond distances and angles with estimated standard deviations in parentheses. The view is identical with that in Fig. 1.
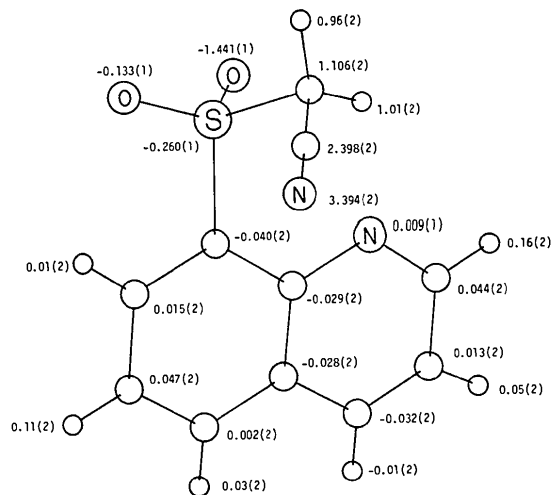

Fig. 3. Deviations of the atoms from the least-squares mean plane calculated for the quinolyl moiety.
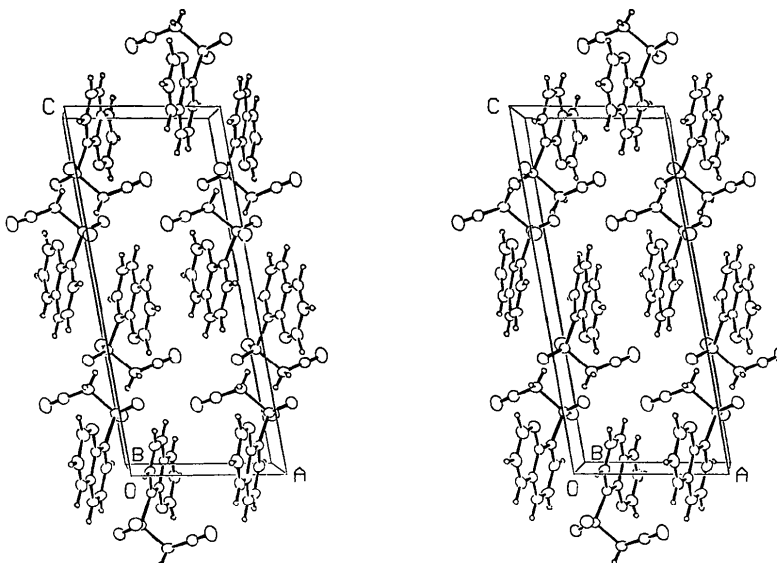
Fig. 4. Packing diagram for 8-quinolyl cyanomethyl sulfone.

these two groups would explain the larger C–S–C angle, 107·4°, than is generally found for acyclic sulfones, 102–105°.

In summation, it appears that the general conformation of the molecule can be better explained as a balance of repulsive forces rather than in terms of an attractive C–H···N force.

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Refinement of the Structure of 1-Methyl-2-(9'-fluorenylidene)-1,2-dihydropyridine. A Crowded Fulvalene

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Abstract. $C_{19}H_{15}N$; orthorhombic, Pbca; $a=16\cdot674$ (2), $b=17\cdot328$ (2), $c=9\cdot525$ (1) Å; $Z=8$; $R=0\cdot042$. Intramolecular nonbonded contacts are responsible for a 35·7° twist of the exocyclic C=C. Bond lengths in the five-ring and heterocyclic six-ring show the effect of π-electron delocalization, indicating that a dipolar resonance form makes a substantial contribution to the ground-state hybrid.

Introduction. A $0\cdot1 \times 0\cdot1 \times 0\cdot2$ mm crystal was used to measure the lattice constants and intensities on a Picker FACS-I diffractometer equipped with a graphite monochromator and Mo X-ray source ($K\alpha, \lambda = 0\cdot71069$ Å). The cell parameters were determined by the least-squares method from 13 Bragg angles measured manually at $\pm 2\theta$ (average $|2\theta_o - 2\theta_c| = 0\cdot004°$). The intensities were measured with the θ–2θ scan