peak 0·23, min. −0·26 e Å^{-3}. Other programs used: *XANADU* (Roberts & Sheldrick, 1975) and *PLUTO* (Motherwell & Clegg, 1978). Scattering factors from *International Tables for X-ray Crystallography* (1974). No correction for secondary extinction.

Discussion. Atomic coordinates are given in Table 1,* with bond lengths and angles in Table 2. The atom numbering is shown in Fig. 1. The bond lengths and angles show no unusual features. The dimensions of the 3-[1-hydroxy-1-(4-methylphenyl)ethyl]-1,2,4,5-tetrazine moiety in the molecule agree well with those reported for (*R,R*)-(+)-3,6-bis[1-hydroxy-1-(4-methylphenyl)ethyl]-1,2,4,5-tetrazine (Low, Neilson & Scrimgeour, 1986). The phenyl and tetrazine rings are planar within experimental error [max. deviations: phenyl *A* 0·01 (2), phenyl *B* 0·01 (2), tetrazine 0·02 (2) Å]. The angles between the normals to the planes of these rings are 83 (1) and 17 (1)° for tetrazine/phenyl *A* and tetrazine/phenyl *B* respectively. The phenyl *A*/phenyl *B* angle is 67 (1)°. There is one hydrogen bond in the structure, O1*A*···N5(x,1+y,z), 3·06 (1) Å, with O1*A*—HO1 1·11, HO1···N5 1·99 Å, angle at H = 158°.

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* Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51794 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of 1,3-Dimethylimidazolium-2-dithiocarboxylate

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Abstract. $C_6H_8N_2S_2$, $M_r = 172{\cdot}24$, monoclinic, $P2_1/n$, $a = 7{\cdot}117$ (1), $b = 10{\cdot}572$ (2), $c = 10{\cdot}739$ (3) Å, $\beta = 99{\cdot}66$ (1)°, $Z = 4$, $V = 796{\cdot}5$ (2) Å^3, D_x(130 K) = 1·44 g cm^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å, $\mu = 5{\cdot}7$ cm^{-1}, $F(000) = 360$, $T = 130$ K, $R = 0{\cdot}029$, 1201 unique reflections with $I > 3\sigma(I)$. The molecule consists of a planar imidazolium ring with the C atoms of the two methyl groups and the dithiocarboxylate group lying within the plane of the ring. The CS_2 group is nearly perpendicular to the ring, with a torsion angle of 71·7°.

Introduction. We report the structure of a heterocyclic dithiocarboxylate zwitterion. Metal complexes of 1,1-dithiolate ligands have been of interest for a long time. We have recently reported complexes of this zwitterionic dithiocarboxylate ligand with nickel triad metals (Borer, Kong & Sinn, 1986) and other soft acid metals (Borer, Kong, Keihl & Forkey, 1987).

Experimental. 1,3-Dimethylimidazolium-2-dithiocarboxylate obtained as prisms from water according to the procedures of Keihl & Borer (1984), crystal dimensions 0·18 × 0·30 × 0·40 mm, Syntex $P2_1$ diffractometer (UC, Davis), locally modified LT-1 apparatus, $T = 130$ K, Mo $K\alpha$ radiation, graphite monochromator, cell dimensions from least-squares fit

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Table 1. *Atomic coordinates* ($\times 10^4$) *and thermal parameters* ($Å^2 \times 10^3$)

Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U
S(1)	2867 (1)	2141 (1)	9160 (1)	19 (1)
S(2)	3402 (1)	1658 (1)	11972 (1)	19 (1)
N(1)	7475 (2)	2503 (2)	10425 (2)	15 (1)
N(2)	6236 (2)	4070 (2)	11304 (2)	13 (1)
C(1)	4029 (3)	2222 (2)	10646 (2)	14 (1)
C(4)	8874 (3)	3412 (2)	10701 (2)	18 (1)
C(3)	8112 (3)	4385 (2)	11251 (2)	16 (1)
C(2)	5879 (3)	2909 (2)	10800 (2)	13 (1)
C(5)	7694 (3)	1292 (2)	9794 (2)	22 (1)
C(6)	4895 (3)	4841 (2)	11865 (2)	17 (1)

of 22 reflections with $35 < 2\theta < 40°$; space group $P2_1/n$ (No. 14) based on absences $h0l$, $h+l = 2n+1$; $0k0$, $k = 2n+1$, data collected to $2\theta_{max} = 50°$ with hkl ranges 0 to 14, 0 to 14, 0 to 8, respectively; scans, 0·9° range, 60° min^{-1} speed (Hope & Nichols, 1981), ±0·9° offset for background, two check reflections monitored every 200 reflections showed no decay; 1646 reflections measured, 1400 unique data, $R_{int} = 0·028$, 1201 observed [$I > 3\sigma(I)$] used in the solution and refinement (based on F); structure solved by direct methods; absorption correction [program *XABS*, a method which obtains an absorption tensor from $F_o - F_c$ differences (Hope & Moezzi, 1987)] applied, full-matrix least-squares refinement, 98 parameters; range of absorption-correction factors 1·09–1·18, all non-H atoms with anisotropic thermal parameters, isotropic thermal parameters of H atoms set equal to 1·2 times the equivalent isotropic thermal parameter of the bonded C atom. H atoms included using a riding model with C–H distance 0·96 Å, $R = 0·029$, $wR = 0·033$, quantity minimized $\sum w(F_o - F_c)^2$, $w = 1/[\sigma^2(F_o)]$, $S = 1·045$, $(\Delta/\sigma)_{max} = 0·15$; $\Delta\rho$ excursions 0·32 and −0·34 e $Å^{-3}$; atomic scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974); computer programs from the *SHELXTL* package (version 3; Sheldrick, 1981). The final atomic coordinates and isotropic thermal parameters are given in Table 1.*

Discussion. Bond lengths and angles for 1,3-dimethylimidazolium-2-dithiocarboxylate are given in Table 2. The structure (Fig. 1) consists of an essentially planar imidazolium ring with the C atoms of the methyls and dithiocarboxylate group lying within the plane of the ring. The CS_2 group is nearly perpendicular to the ring with a torsion angle of 71·7°. The C–S distances are

Table 2. *Bond distances* (Å) *and angles* (°)

S(1)–C(1)	1·672 (2)	S(2)–C(1)	1·672 (2)
N(1)–C(4)	1·380 (3)	N(1)–C(2)	1·338 (3)
N(1)–C(5)	1·469 (3)	N(2)–C(3)	1·387 (3)
N(2)–C(2)	1·349 (3)	N(2)–C(6)	1·459 (3)
C(1)–C(2)	1·498 (3)	C(4)–C(3)	1·345 (3)
C(4)–N(1)–C(2)	109·3 (2)	C(4)–N(1)–C(5)	125·3 (2)
C(2)–N(1)–C(5)	125·4 (2)	C(3)–N(2)–C(2)	108·6 (2)
C(3)–N(2)–C(6)	125·7 (2)	C(2)–N(2)–C(6)	125·6 (2)
S(1)–C(1)–S(2)	129·4 (1)	S(1)–C(1)–C(2)	114·7 (2)
S(2)–C(1)–C(2)	115·9 (1)	N(1)–C(4)–C(3)	107·3 (2)
N(2)–C(3)–C(4)	107·3 (2)	N(1)–C(2)–N(2)	107·5 (2)
N(1)–C(2)–C(1)	126·2 (2)	N(2)–C(2)–C(1)	126·3 (2)

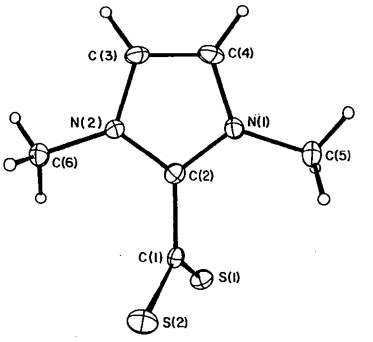

Fig. 1. A computer-generated drawing of 1,3-dimethylimidazolium-2-dithiocarboxylate showing the numbering scheme and anisotropic thermal ellipsoids at 50% probability level.

equal, indicating that the negative charge is equally spread over the S atoms. Within the ring, the C(3)–C(4) bond distance of 1·345 (3) Å is consistent with double-bond character and compares with the value 1·31 Å found in 1,3-dimethyl-2(3*H*)-imidazolethione which contains a single S atom in place of the CS_2 group (Ansell, Forkey & Moore, 1970). Neither molecule contains an aromatic ring. The bond distances, N(2)–C(2) and N(1)–C(2), are nearly equal (1·344 Å) and indicate significant C–N double-bond character. This suggests conjugation of the three atoms, N(1)–C(2)–N(2).

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