r(C aromatique) = 1,77, r(—S—) = 1,80 Å, on observe que les distances interatomiques intermoléculaires indiquées ci-après sont voisines de la somme des rayons des atomes concernés. Il s'agit de C(1)—C(7^{ii}) [3,55 (2)] [(ii): $2-x$, $1-y$, $1-z$], de C(3)—C(7^{ii}) [3,38 (1)], de C(5)—S(9^{ii}) [3,535 (9)] et de C(7)—C(12^{iii}) [3,44 (1) Å] [(iii): $\frac{3}{2}-x$, $\frac{1}{2}-y$, $1-z$].

La Fig. 2 montre que les molécules sont distribuées le long des plans $x=0$, $x=\frac{1}{2}$ et $z=\pm\frac{1}{4}$. La cohésion intermoléculaire est due uniquement aux interactions de van der Waals.

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Acta Cryst. (1987). C**43**, 1171–1173

Structure of 4,4′-Dimethyl-2,2′-bithiazole

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(*Received* 4 *October* 1986; *accepted* 26 *January* 1987)

Abstract. 4,4′-Dimethyl-2,2′-bithiazole, $C_8H_8N_2S_2$, M_r = 196·26, monoclinic, $P2_1/a$, a = 7·693 (8), b = 12·139 (10), c = 5·241 (8) Å, β = 108·2 (1)°, V = 464·9 (9) Å^3, D_x = 1·40 g cm^{-3}, Z = 2, λ(Cu $K\alpha$) = 1·5418 Å, μ(Cu $K\alpha$) = 46·7 cm^{-1}, $F(000)$ = 204, T = 293 K, R = 5·9% based on 719 independent reflections. The structure consists of the packing of planar dimers placed on inversion centers. Bond distances and angles are as expected; a short packing contact (N···H—C 2·59 Å) indicates some acid character of this hydrogen.

Introduction. In the last decade many efforts have been devoted to producing polymers with electroconducting properties after the discovery of the metallic-like behaviour of doped polyacetylene (hereafter referred to as PA) (Shirakawa, Louis, MacDiarmid, Chiang & Heeger, 1977). More recently polyheterocyclic systems have attracted the attention of many researchers with the aim of overcoming the drawbacks of PA, namely lack of air stability and processability. Moreover, the conduction models proposed for these materials require further elucidation in order to be commonly accepted and to encourage potential applicative developments. In particular, the nature of charge carriers, their number, the mobility in the system, the overlap of delocalized orbitals, *i.e.* the lateral packing, the band gap, the ionization potentials, the electronic affinities and so on, play a decisive role in understanding the complex phenomena occurring in the conduction process. From this point of view we are interested in polythiazole systems and we prepared 4,4′-dimethyl-2,2′-bithiazole as a model compound in order to obtain precise intercycle geometric parameters for *ab initio* calculations on this polymer. Here we present the crystal and molecular structures of this compound, and relate them to those of known thiazole derivatives.

Experimental. The synthesis of the title compound was carried out by cyclization of dithiooxamide and chloroacetone (Karrer, Leiser & Graf, 1944). Crystals suitable for X-ray analysis were obtained from a cold benzene/petroleum ether mixture. In Table 1 experimental details are summarized. Intensity data were collected on a Philips PW 1100 computer-controlled diffractometer with a randomly oriented crystal. Unit-cell parameters and their e.s.d.'s were determined by accurate centring of 24 strong reflections (θ range 7–16°) and then refined by least squares. The structure was solved by the Patterson method; a subsequent

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0108-2701/87/061171-03$01.50

electron density map revealed the positions of all atoms. The positional and thermal parameters were refined, using a block-diagonal-matrix least-squares method, with unit weight factors, minimizing $\sum (F_o-F_c)^2$. After a difference Fourier map, which allowed the location of all H atoms, four least-squares cycles were carried out, refining the positional and thermal (isotropic) parameters of the H atoms also, to yield a conventional R value equal to 0·059 (final shift-to-e.s.d. ratio for 71 refined variables was <0·10). Both the real and imaginary components of the anomalous dispersion were included in the atomic-scattering-factor calculations (*International Tables for X-ray Crystallography*, 1974). In Table 2, the fractional coordinates and equivalent isotropic thermal parameters are given.* All the computer programs used are part of the crystallographic set written by A. Immirzi. No corrections were made for absorption or secondary extinction.

Discussion. Fig. 1 gives an *ORTEP* (Johnson, 1976) drawing of the molecule, while interatomic distances and angles are reported in Table 3. The dimer lies on an inversion center, at the middle point of the C1—C1′ bond, and in a plane of equation: $-0{\cdot}7568x - 0{\cdot}0857y + 0{\cdot}6480z = 1{\cdot}1770$, referred to orthogonal axes,† the mean square displacement being 0·006 Å. A comparison between this structure and those of known thiazole derivatives (Caranoni & Reboul, 1982; Nygaard *et al.*, 1971) reveals no significant differences, either in bond distances or in bond angles. In fact, the N—C2 and N—C1 distances [1·395 (6) and 1·332 (6) Å, respectively; see Table 3] differ from the corresponding ones in thiazole [1·372 (1) and 1·367 (1) Å] by 4σ, thereby constituting too feeble evidence for assessing a possibly increased 'quinoidic' character in the dimer with respect to the monomer (for confirmation see other distances and angles in the two compounds).

The packing distances in the crystal are comparable with the sum of van der Waals radii, except for a contact between N and H related to H3 by a glide plane (2·59 Å), thus determining the intermolecular cohesion. Such short distances have been found in structures of compounds containing a thiazole moiety (Caranoni & Reboul, 1982), but implying hydrogen-bond formation. This case concerns a relatively strong C—H···N interaction, comparable to those attributed to hydrogen bonds, 2·3–2·6 Å (Taylor & Kennard, 1982); therefore one has to admit a certain acidic character of hydrogen H3.

Table 1. *Experimental data*

Scan mode	θ–2θ
Scan speed (° min^{-1})	3·0
Scan width (°)	2·0
θ range (°); $d_{\min}$ (Å)	2–60; 0·89
Measured reflections	$\pm h, +k, +l$ ($-8\rightarrow8, 0\rightarrow13, 0\rightarrow5$)
Number of independent collected reflections	719
Number of observed reflections (with $I > 2{\cdot}0\,\sigma$)*	536
Standard reflections (measured every 80 refls)	211, $2\bar{1}1$, $\bar{2}1\bar{1}$†
Wavelength (Å) (Cu $K\bar{\alpha}$ graphite-monochromated radiation)	1·5418
μ(Cu $K\alpha$) (cm^{-1})‡	46·7
Temperature (K)	293
Approximate crystal size (mm) (roughly cubic)	0·1 × 0·12 × 0·1 mm

* $\sigma(I)$ = peak counts + total background counts.

† The intensity variation of the standard reflections during the collection was less than 2·5%.

‡ The variation in transmittance was estimated at ±3·5%.

Table 2. *Atomic fractional coordinates* (× 10^4; × 10^3 *for* H) *and thermal parameters* (Å^2 × 10) *with e.s.d.'s in parentheses*

	x	y	z	B_{eq}/B_{iso}
S	1898 (2)	4387 (1)	8783 (3)	37 (1)*
N	−74 (6)	3500 (3)	4373 (8)	34 (2)*
C1	359 (6)	4468 (3)	5606 (10)	29 (2)*
C2	838 (6)	2643 (3)	6023 (10)	31 (2)*
C3	1947 (7)	2961 (4)	8413 (11)	36 (2)*
C4	503 (8)	1454 (4)	4988 (12)	39 (3)*
H3	287 (8)	250 (5)	1016 (13)	59 (14)
H4	110 (8)	117 (5)	609 (13)	64 (15)
H4′	62 (11)	132 (6)	334 (16)	88 (20)
H4″	−71 (8)	133 (5)	464 (13)	62 (15)

* B_{eq} = (trace of diagonalized B)/3.

Table 3. *Selected interatomic distances* (Å) *and angles* (°) *in the molecule, with e.s.d.'s in parentheses*

S—C1	1·718 (5)	N—C2	1·395 (6)
S—C3	1·744 (5)	C2—C3	1·334 (7)
N—C1	1·332 (6)	C2—C4	1·535 (6)
C1—C1′	1·468 (6)	C4—H4$_{avg}$*	1·00 (6)
C3—H3	1·11 (5)		
C1—S—C3	89·0 (2)	N—C2—C3	114·5 (5)
S—C1—N	114·3 (5)	C2—C3—S	111·2 (5)
C1—N—C2	110·9 (5)	S—C1—C1′	121·4 (2)
N—C2—C4	119·2 (5)	N—C1—C1′	124·3 (5)

* The C—H distances were corrected for thermal motion in the independent-motion approximation (Johnson, 1970).

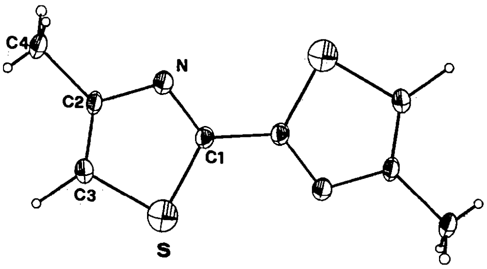

Fig. 1. Molecule viewed normally to the dimer plane, at 50% probability level of the thermal ellipsoids.

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43746 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

† The orthogonalization matrix is: a, 0, $c\cos\beta$ / 0, b, 0 / 0, 0, $c\sin\beta$.

This research was partially supported by the 'Progetto strategico materiali' of CNR. The helpful suggestions of the referees are acknowledged.

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Acta Cryst. (1987). C**43**, 1173–1174

Structure du Chloro-3 Méthyl-2 4*H*-Pyrazino[1,2-*a*]pyrimidinone-4

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(*Reçu le* 4 *juin* 1986; *accepté le* 27 *janvier* 1987)

Abstract. $C_8H_6ClN_3$, $M_r = 195\cdot6$, monoclinic, $P2_1/c$, $Z = 4$, $a = 3\cdot783$ (2), $b = 9\cdot099$ (3), $c = 23\cdot41$ (1) Å, $\beta = 83\cdot66$ (3)°, $V = 800\cdot9$ Å^3, $D_x = 1\cdot62$, $D_m = 1\cdot62$ g cm^{-3}, Mo $K\alpha_1$ radiation, $\lambda = 0\cdot70926$ Å, $\mu = 4\cdot1$ cm^{-1}, $F(000) = 400$, $R = 0\cdot055$ for 1110 reflections. Confirmation is obtained of the structure proposed by Abignente, Arena, Caprariis, Patscot, Marmo, Lampa & Rossi [*Eur. J. Med. Chem. Chim. Ther.* (1985). **20**(1), 79–85].

Introduction. Au cours de la synthèse de la méthyl-2 imidazo[1,2-*a*]pyrazinecarboxylate-3 d'éthyle, la condensation de l'amino-2 pyrazine avec le chloro-2 acetylacetate d'éthyle fournit deux produits secondaires dont l'un avait été décrit par nous-mêmes (Sablayrolles, Cros, Milhavet, Rechenq, Chapat, Boucard, Serrano & McNeill, 1984) comme la chloro-2 (oxo-1 éthyl)-3 imidazo[1,2-*a*]pyrazine. Cette structure a été refutée par les travaux de Abignente, Arena, Caprariis, Patscot, Marmo, Lampa & Rossi (1985). Afin de trancher entre les deux hypothèses formulées à la suite d'études par RMN, nous avons entrepris la résolution de la structure cristalline.

Partie expérimentale. Composé préparé par condensation du chloro-2 acetylacetate d'éthyle (Sablayrolles *et al.*, 1984) sans réarrangement de type DIMROTH (Guerret, Jacquier & Maury, 1971). Cristaux jaunes, stables à l'air, p.f. = 447 K. Monocristaux obtenus par recristallisation dans l'éthanol à 293 K, saturation puis évaporation contrôlée. Monocristal, fragment d'une aiguille ($L = 0{,}8$ cm) ($0{,}6 \times 0{,}1 \times 0{,}07$ mm). Densité mesurée par picnométrie dans le tétrachlorure de carbone préalablement saturé. Diffractomètre CAD-4 Enraf–Nonius. Rayonnement $K\alpha_1$ du molybdène isolé par monochromateur à lame de graphite. 1761 réflexions mesurées à $T = 293$ K pour $2° < \theta < 25°$ ($0 \leq h \leq 4$, $0 \leq k \leq 10$, $-27 \leq l \leq 27$); mode de balayage ω–$\frac{1}{3}\theta$; vitesse maximale de comptage.

Trois réflexions standard ($\bar{2}27$, $0\bar{2}7$, $11\bar{5}$) mesurées tous les 50 enregistrements. Variation des intensités inférieures à 3%. Paramètres de maille déterminés à partir de 20 réflexions soigneusement corrigées puis affinées à partir des données du diffractogramme de poudre (Norbert & Maurin, 1969). Données corrigées de Lorentz et polarization mais non de l'absorption.

Structure résolue par la méthode de l'atome lourd. Affinement de la structure par *LINUS* (Busing, Martin & Levy, 1962) en matrice complète [$\sum(\Delta F)^2$]. Affinements en agitation anisotrope ($R = 0{,}055$ pour les 1110 réflexions non nulles) soit 9,5 données par paramètres. Sélection avec $\sigma(I)/(I) < 0{,}3$. Facteurs de diffusion de

0108-2701/87/061173-02$01.50