

DTDD and BMDT in such a way that the shortest C<sub>sp<sup>2</sup></sub>—S bond is in a *trans* position to the O, S=C < fragment.

On the basis of the preceding considerations we suggest the existence of some intramolecular  $\pi$ -electron delocalization over the systems S(X3)=C(X3)—C(X4)=C(X9)—S(X8) (X=1;2) (DTDD) and O(Y5)=C(Y5)—C(Y4)=C(Y3)—S(Y3) (Y=0;1) (BMDT). These delocalizations of  $\pi$  electrons are probably responsible for a different pattern of S...S and S...O interactions in DTDD and BMDT compared to BTDTT and BTDTO. The two former structures have intermolecular S...S and S...O contacts involving the thione and carbonyl groups (Figs. 2 and 3), whereas this is not the case for the latter two structures.

The density of the DTDD crystals (1.79 g cm<sup>-3</sup>) is markedly higher than those of the related compounds (BMDT), (BTDTT) and (BTDTO) which all have a measured density of 1.62 g cm<sup>-3</sup>. The DTDD structure has five intermolecular S...S contact distances less than 3.7 Å. Two of them are rather short, S(13)...S(21; 1 + x, y, z) 3.359 (1), S(11)...S(28; 1 - x, -y, -z) 3.383 (1) Å. The remaining three are: S(15)...S(25; 2 - x, 0.5 + y, 0.5 - z) 3.453 (1), S(18)...S(21; 1 - x, 0.5 + y, 0.5 - z) 3.508 (1) and

S(11)...S(28; 1 - x, 0.5 + y, 0.5 - z) 3.670 (1) Å. The BMDT structure has four intermolecular S...O contact distances less than 3.25 Å with S(12)...O(5; x, 0.5 - y, 0.5 - z) 2.949 (1) Å as the strongest, S(1)...O(15) 3.071 (1), S(2)...O(15) 3.098 (1), S(11)...O(5; x, 0.5 - y, 0.5 + z) 3.225 (1) Å.

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## X-ray Study of 2-(3,5-Dimethylpyrazolyl)-1,3-benzothiazole

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**Abstract.** C<sub>12</sub>H<sub>11</sub>N<sub>3</sub>S, *M<sub>r</sub>* = 229.3, orthorhombic, *Pbca*, *a* = 16.841 (5), *b* = 12.189 (4), *c* = 10.842 (2) Å, *V* = 2225.6 (2) Å<sup>3</sup>, *Z* = 8, *D<sub>x</sub>* = 1.37, *D<sub>m</sub>* (floatation) = 1.43 g cm<sup>-3</sup>,  $\lambda(\text{Cu } K\alpha) = 1.54178 \text{ \AA}$ ,  $\mu = 23.77 \text{ cm}^{-1}$ , *F*(000) = 960, *R* = 0.038 for 1208 unique observed reflections [*I* > 2 $\sigma$ (*I*)]. The molecule consists of a five-membered dimethylpyrazole ring rather than a seven-membered ring. The S—C average bond distance, 1.746 Å, is shorter than for a single bond. The benzothiazole nucleus adopts an almost planar conformation with a dihedral angle between the mean planes of the two individual rings of 1.5°. The dimethylpyrazole ring does not deviate much from planarity and is inclined at an angle of 13° to

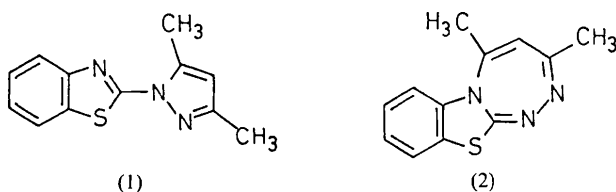
the benzothiazole ring. The molecules are well separated and stacked in parallel rows along the crystallographic axes.

**Introduction.** There has been considerable interest in studies of the structural configuration of the products obtained by the reaction of heterocyclic hydrazines with  $\beta$ -dicarbonyl compounds, and their biological activities. In the cases of 4-aryl-2-hydrazines (Singh, Vaid, Prakash & Prakash, 1986) and 2-hydrazinequinolines (Singh, Sehgal, Singh & Dhawan, 1987), a five-membered ring formation (1) of the pyrazole group has been suggested for the compounds obtained on treatment with pentane-2,4-dione. However, an isomeric seven-membered ring formation (2) has been proposed for the same compounds by other groups of workers (Mahajan,

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Sondhi & Rahlan, 1977; Alaka, Patnaik & Rout, 1982; Dhuri, Pradhan & Nayak, 1983; Surana, Tyagi & Jhoshi, 1972). The structure of the title compound, obtained by treating 2-hydrazinobenzothiazole with 2-substituted pentane-2,4-diones, has not yet been established and the pyrazole configuration has been proposed without evidence (Sawhney, Tomar, Prakash, Prakash & Singh, 1981). In order to remove the existing anomalies about the mode of pyrazole-ring formation and to establish its configuration in the dimethyl-substituted moiety, X-ray diffraction studies of 2-(3,5-dimethylpyrazolyl)-1,3-benzothiazole have been carried out. It is also interesting to establish the nature of the *N*-benzothiazole bond linkage because of the importance of the most characteristic properties of pyrazoles which is related to their *N*-substitution (Begtrup, Elguero, Faure, Camps, Estopa', Ilavsky', Fruchier, Marzin & Mendoza, 1988).



**Experimental.** A light-grey crystal of approximate dimensions  $0.14 \times 0.20 \times 0.18$  mm was mounted along its longer dimension on a syntax *P2*<sub>1</sub> diffractometer. Intensity data were collected using  $\theta:2\theta$  scans,  $2\theta_{\max} = 114.7^\circ$ , variable scan rate, graphite-monochromated  $\text{Cu K}\alpha$  radiation ( $\lambda = 1.54178 \text{ \AA}$ ), lattice parameters from the least-squares refinement of 15 reflections,  $10.62 \leq \theta \leq 28.02^\circ$ , systematic absences  $h = 2n + 1$  for  $hk0$ ,  $k = 2n + 1$  for  $0kl$ ,  $l = 2n + 1$  for  $h0l$  consistent with space group *Pbca*, monitored reflection (321) showed no intensity variation greater than 1.6%. 1511 unique reflections measured ( $0 \leq h \leq 17$ ,  $0 \leq k \leq 13$ ,  $0 \leq l \leq 11$ ) with 1208 intensities greater than  $2\sigma(I)$ . Consideration of the crystal shape and transmission factor enabled us to neglect absorption. Lorentz-polarization corrections, extinction corrections, real and imaginary contributions to anomalous dispersion applied (*International Tables for X-ray Crystallography*, 1974, Vol. IV); direct methods (*MULTAN78*; Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978) used to locate all the non-H atoms; least-squares refinement, isotropic followed by anisotropic was carried out; difference Fourier synthesis enabled location of H atoms. Combined refinement, isotropic for H and anisotropic for non-H atoms reduced  $R$  to 0.038,  $wR = 0.038$ ,  $S = 1.257$ .  $(\Delta/\sigma)_{\text{av}} = 0.0104$ ,  $(\Delta/\sigma)_{\text{max}} = 0.0434$ ; maximum electron density in the final difference Fourier map  $|0.19| \text{ e \AA}^{-3}$ ;  $w(F_o - F_c)^2$

minimized,  $w = 1/\sigma^2(F_o)$  from counting statistics, 146 parameters refined using 1208 reflections; all calculations carried out using *XRAY76* (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976), atomic scattering factors for C, N and S atoms from Cromer & Mann (1968), those for H atoms from Stewart, Davidson & Simpson (1965).

**Discussion.** Final atomic coordinates and equivalent isotropic thermal parameters are given in Table 1.\* The bond lengths and valence angles are given in Table 2. The atomic numbering scheme used in the crystal analysis and the molecular geometry is depicted in the *ORTEP* drawing (Johnson, 1971), Fig. 1.

Some of the atoms of the benzene ring have relatively large thermal parameters. The C(2)—C(3) bond distance [ $1.369(4) \text{ \AA}$ ] is significantly small. Although the mean value of the valence angles of the benzene ring is ideal, that of the bond lengths is shorter than the standard value. The C(1)—S(9) and C(8)—S(9) bond lengths of  $1.737(3)$  and  $1.754(3) \text{ \AA}$  respectively are shorter than the value reported for a  $\text{C}(sp^3)$ —S single bond of  $(1.8 \text{ \AA})$ ; Khan, Taylor, Lehn & Dietrich, 1988, and references therein) but considerably longer than the C—S double-bond length of  $1.61 \text{ \AA}$ . The shortening of the C—S bonds might be attributed to the difference between the  $sp^2$  and  $sp^3$  carbon rather than to the partial double-bond character of the C—S bonds. The difference of  $6\sigma$  between the two C—S bonds is not an uncommon phenomenon (Jain, 1987). The bond distances C(6)—N(7)  $1.391(4)$  and N(7)—C(8)  $1.280(1) \text{ \AA}$  are in agreement with those found in the related compounds. In majority of cases, the endocyclic C(1)—S(9)—C(8) angle in simple thiazoles is greater than  $90^\circ$ , but in the substituted thiazole compounds its value is less than  $90^\circ$  (Ruben, Kaplan, Zalkin & Templeton, 1974; Cameron & Hair, 1971; Smith, 1969; Laurent, Durant & Evrard, 1981). In the present molecule, the C—S—C angle is  $87.6(1)^\circ$ . The narrowing of the angle at S indicates extensive conjugation between the benzothiazole ring and the pyrazole rings which is evidenced by the shorter value of the exocyclic N(10)—C(8) bond length  $1.386(4) \text{ \AA}$ . A study of the N(10)—C(8) bond lengths in several substituted pyrazole compounds has revealed an interesting feature, namely that this bond length falls into two categories. In the first case, its value is  $\leq 1.40 \text{ \AA}$  when C(8) is part of an aromatic ring (Fronczek, Parodi, Fischer, Hsieh &

\* Lists of structure factors, anisotropic thermal parameters, least-squares planes and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53946 (19 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Fractional atomic coordinates ( $\times 10^4$ ) for non-H atoms and their equivalent isotropic thermal parameters ( $\text{\AA}^2 \times 10^3$ )

$$U_{eq} = (1/3)[U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aba^*b^*\cos\gamma + 2U_{13}aca^*c^*\cos\beta + U_{23}cb^*c^*\cos\alpha].$$

	x	y	z	$U_{eq}$
C(1)	2348 (2)	1321 (2)	2567 (3)	44 (2)
C(2)	1803 (2)	754 (2)	1839 (3)	53 (2)
C(3)	1379 (2)	1330 (3)	977 (3)	57 (2)
C(4)	1502 (2)	2455 (3)	796 (3)	60 (2)
C(5)	2039 (2)	3022 (2)	1525 (3)	54 (2)
C(6)	2467 (2)	2463 (2)	2425 (2)	42 (2)
N(7)	3023 (1)	2931 (2)	3213 (2)	45 (1)
C(8)	3314 (2)	2178 (2)	3910 (3)	41 (2)
S(9)	2981 (0)	826 (1)	3701 (1)	50 (0)
N(10)	3885 (1)	2443 (2)	4811 (2)	45 (1)
C(11)	4133 (2)	3992 (2)	5395 (3)	46 (2)
C(12)	4652 (2)	2966 (2)	6269 (3)	57 (2)
C(13)	4692 (2)	1814 (2)	6213 (3)	51 (2)
N(14)	4220 (1)	1424 (2)	5349 (2)	50 (2)
C(15)	5167 (2)	1047 (3)	7007 (3)	70 (2)
C(16)	3833 (2)	4415 (2)	5052 (3)	63 (2)

Table 2. Interatomic distances ( $\text{\AA}$ ) and angles ( $^\circ$ )

C(1)—C(2)	1.394 (4)	S(9)—C(8)	1.754 (3)
C(2)—C(3)	1.369 (4)	N(10)—C(8)	1.386 (4)
C(3)—C(4)	1.401 (5)	N(10)—C(11)	1.384 (4)
C(4)—C(5)	1.386 (4)	N(10)—N(14)	1.384 (3)
C(5)—C(6)	1.391 (4)	C(11)—C(12)	1.349 (4)
C(6)—C(1)	1.414 (4)	C(12)—C(13)	1.407 (4)
N(7)—C(6)	1.391 (4)	N(14)—C(13)	1.318 (4)
N(7)—C(8)	1.286 (4)	C(15)—C(13)	1.501 (5)
S(9)—C(1)	1.737 (3)	C(16)—C(11)	1.505 (4)
C(2)—C(1)—C(6)	121.3 (2)	S(9)—C(8)—N(10)	116.7 (2)
C(2)—C(1)—S(9)	129.3 (2)	C(1)—S(9)—C(8)	87.8 (1)
C(6)—C(1)—S(9)	109.4 (2)	C(8)—N(10)—C(11)	130.8 (2)
C(1)—C(2)—C(3)	118.4 (3)	C(8)—N(10)—N(14)	117.5 (2)
C(2)—C(3)—C(4)	121.3 (3)	C(11)—N(10)—N(14)	111.2 (2)
C(3)—C(4)—C(5)	120.3 (3)	N(10)—C(11)—C(12)	105.7 (2)
C(4)—C(5)—C(6)	119.6 (3)	N(10)—C(11)—C(16)	123.0 (2)
C(5)—C(6)—C(1)	119.0 (2)	C(16)—C(11)—C(12)	131.3 (3)
C(5)—C(6)—N(7)	125.3 (2)	C(11)—C(12)—C(13)	107.2 (3)
C(1)—C(6)—N(7)	115.6 (2)	C(12)—C(13)—N(14)	111.2 (3)
C(6)—N(7)—C(8)	108.9 (2)	C(12)—C(13)—C(15)	128.5 (3)
N(7)—C(8)—S(9)	118.3 (2)	N(14)—C(13)—C(15)	120.3 (3)
N(7)—C(8)—N(10)	125.0 (2)	N(10)—N(14)—C(13)	104.7 (2)

Chang, 1989; Galigne & Falgueirettes, 1969, 1970; De & Muhonen, 1989) or a group where some charge delocalization is possible (the title compound). In the second category, its value is  $> 1.40 \text{ \AA}$  when C(8) is part of an alkyl group (Conde & Conde, 1989). The shorter length in the first group might be due to the conjugation between the  $\pi$  orbitals of N(10) and the  $\pi$  orbitals of the benzothiazole moiety which consequently affects the geometry at the S atom. This trend is not possible for the second set of compounds.

The C(13)—N(14) bond length [ $1.318(4) \text{ \AA}$ ] is within the range of  $1.30(4) \text{ \AA}$  derived from theoretical considerations (Brown, Towns & Trefonas, 1970) and agrees well with the values reported for 1-(2,4-dinitrophenyl)pyrazole (Fronczek *et al.*, 1989), 1-(2,4-dinitrophenyl)-4-bromopyrazole (Galigne &

Falgueirettes, 1969), 1-(2,4-dinitrophenyl)-4-chloropyrazole (Galigne & Falgueirettes, 1970) and 1-amino-3-phenylpyrazole (Yamaguchi, Ohsawa, Kaihoh, Itoh, Okada, Kawabata & Igeta, 1989). The remaining bond distances of the pyrazole ring are in accordance with those obtained in the pyrazole compounds [references cited above, and Ehrlich (1960) and Conde & Conde (1989)]. The exocyclic C—C bond distances of the pyrazole ring are C(11)—C(16)  $1.505(4)$  and C(13)—C(15)  $1.501(5) \text{ \AA}$  and are similar to those found in the substituted pyrazole compounds (Cathy, Arcus, Wilkinson, Marks & Ibers 1976; Yamaguchi *et al.*, 1989).

The benzothiazole nucleus adopts an almost planar conformation with C(3) [ $-0.013(2) \text{ \AA}$ ] and C(4) [ $0.010(3) \text{ \AA}$ ] having maximum deviations from the mean plane. These atoms lie at the farthest end of the benzothiazole moiety. The benzene and the thiazole planes are approximately coplanar and have a small dihedral angle ( $\sim 1.5^\circ$ ). The pyrazole ring is planar with the largest displacement of any non-H atom from its plane being  $0.014 \text{ \AA}$  indicating extensive electron delocalization. The planar character of the pyrazole ring along with the observed similarity in bond lengths for C(8)—N(10)  $1.386(4)$ , N(10)—C(11)  $1.384(4)$  and N(10)—N(14)  $1.384(3) \text{ \AA}$  suggest that a significant mesomeric effect is operative along the fragment N(14)—N(10)—C(8) outside the pyrazole ring and also inside the ring along N(14)—N(10)—C(11). However, the C(11)—C(12) distance [ $1.349(4) \text{ \AA}$ ] indicates localized electron density on this bond compared to the adjacent bond C(12)—C(13) [ $1.407(4) \text{ \AA}$ ]. The pyrazole and the thiazole rings are twisted by  $13.3^\circ$ . The two methyl groups are oriented in the direction opposite to the benzothiazole moiety and lie in large thermal cavities. Since

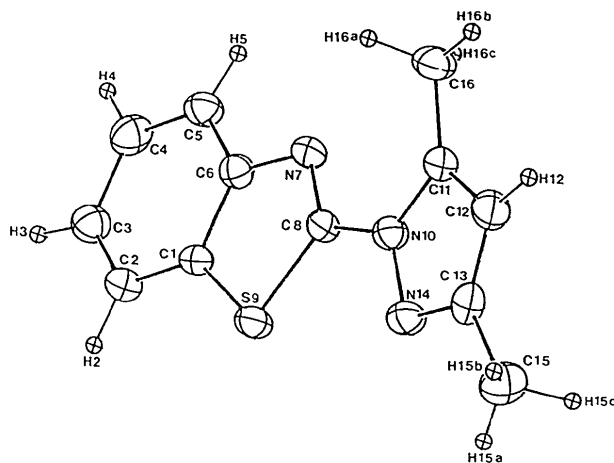


Fig. 1. ORTEP drawing of the title compound (relative configuration). Thermal ellipsoids are drawn at the 35% probability level. H atoms are drawn as spheres of arbitrary radius.

the structure consists of individual molecules stabilized in the crystal by van der Waals forces and there are no unusual short intermolecular contacts, the packing interactions do not influence the geometry of the molecule.

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## Structure of Isopropyl 2-Chloro-5-(2-methyl-1,4-oxathiin-3-ylcarbonylamino)-benzoate, Oxathiin Carboxanilide

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**Abstract.**  $C_{16}H_{18}ClNO_4S$ ,  $M_r = 355.8$ , monoclinic,  $P2_1/a$ ,  $a = 8.784(1)$ ,  $b = 20.342(1)$ ,  $c = 9.522(1)$  Å,  $\beta = 98.61(1)^\circ$ ,  $V = 1682.3$  Å<sup>3</sup>,  $Z = 4$ ,  $D_x = 1.404$  g cm<sup>-3</sup>,  $\lambda(\text{Cu } K\alpha) = 1.5418$  Å,  $\mu = 33.5$  cm<sup>-1</sup>,  $F(000) = 744$ ,  $T = 295$  K, final  $R = 0.044$  for 2156

observed reflections. The crystal structure and conformation are reported for this new potential AIDS drug whose mode of action differs from that of the dideoxynucleosides. The molecules are hydrogen bonded and form infinite chains along the  $a$  axis. The crystal packing leads to parallel stacking of the rings of the molecules.

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