Les paramètres atomique sont rassemblés dans le Tableau 1, les distances et les angles dans le Tableau 2. La Fig. 1 montre la molécule et la Fig. 2 l'empilement moléculaire. La molécule représentée en Fig. 1 se caractérise par la planéité du cycle pentagonal dans lequel l'azote N3 a un net caractère sp^2 favorable à une conjugaison partielle du système O1C2O2N3. Celle-ci se traduit par une diminution des longueurs de liaisons autour de C2 par rapport aux valeurs standards (*Tables of Interatomic Distances and Configuration in Molecules and Ions*, 1958). Nous devons aussi noter une différence notable entre les liaisons S—N3 et S—N' [$\Delta l = 0{,}066$ (3) Å] et la valeur de 68,9 (8)° de l'angle dièdre N3SN'C1'.

Nous devons enfin signaler l'existence d'une forte liaison hydrogène intermoléculaire entre l'hydrogène H' d'une molécule et l'oxygène O2 de la molécule inverse. La distance entre ces deux atomes est de 2,21 (3) Å.

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Acta Cryst. (1987). C**43**, 2468–2469

Structure of 1,3,2-Dithiazole-4-thione

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(*Received* 13 *July* 1987; *accepted* 30 *July* 1987)

Abstract. C_2HNS_3, $M_r = 135{\cdot}2$, monoclinic, $P2_1/m$, $a = 5{\cdot}990$ (1), $b = 6{\cdot}422$ (1), $c = 6{\cdot}058$ (1) Å, $\beta = 100{\cdot}79$ (1)°, $V = 228{\cdot}9$ (1) Å^3, $Z = 2$, $D_x = 1{\cdot}96$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 13{\cdot}8$ cm^{-1}, $F(000) = 136$, $T = 293$ K, $R = 0{\cdot}039$ for 534 unique observed reflections. All of the atoms of the molecule lie on a mirror plane of the lattice. The five-membered —SNSCC— ring has SN, SC, and CC bond distances of 1·588 (4) and 1·621 (4), 1·648 (5) and 1·717 (4), and 1·420 (5) Å, respectively. The *exo* CS bond is 1·668 (4) Å.

Experimental. Compound prepared by the reaction of S_4N_4 with $SiMe_3CCSiMe_3$. The intense-blue crystal used for data collection was obtained by sublimation *in vacuo*. Data crystal 0·11 × 0·19 × 0·25 mm mounted on a glass fiber. Intensities measured with an Enraf–Nonius CAD-4 diffractometer using ω–2θ scans of 4 to 16°min^{-1} in θ. Unit cell determined from least-squares analysis of angle data for 25 reflections with $17 < 2\theta < 24°$. Absorption correction based on φ scans varied from 0·94 to 1·00. Data collected to (sin θ)/λ of 0·75 Å^{-1}, $-9 < h < 9$, $-10 < k < 0$, $0 < l < 9$. Three standard reflections ($20\bar{3}$, $\bar{1}30$, 202) decreased less than 0·7% over 8·0 h of data collection. 916 reflections measured, 848 unique ($R_{int} = 0{\cdot}01$), 314 reflections with $I < 3\sigma(I)$ considered unobserved. Solved by Patterson and Fourier methods. Full-matrix least squares minimized $\sum w(\Delta F)^2$. H atom refined isotropically and other atoms anisotropically for a total of 40 variables. $R = 0{\cdot}039$, $wR = 0{\cdot}055$, $S = 1{\cdot}53$, where

Table 1. *Fractional atomic coordinates and isotropic thermal parameters* (Å^2)

	x	z	B or B_{eq}
S(1)	0·2406 (2)	−0·2081 (2)	3·32 (2)
S(2)	0·1822 (2)	0·2206 (2)	3·51 (3)
S(3)	0·6701 (2)	0·4313 (2)	3·26 (2)
N	0·0636 (8)	−0·0429 (8)	4·0 (1)
C(1)	0·4650 (7)	0·2034 (7)	2·38 (8)
C(2)	0·4830 (8)	−0·0270 (8)	2·87 (9)
H	0·650 (9)	−0·05 (1)	4 (1)

The H atom was refined isotropically. All atoms have y coordinates of 0·25 (mirror plane). Equivalent isotropic thermal parameter defined as: $B_{eq} = \frac{4}{3}[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ac(\cos\beta)B(1,3)]$.

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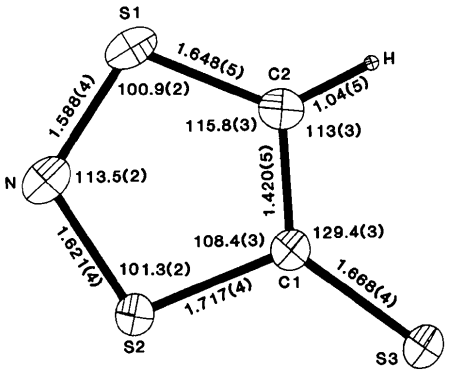

Fig. 1. *ORTEP*II diagram (Johnson, 1976), atom-numbering scheme, bond distances (Å), and bond angles (°). Non-H ellipsoids at 30% probability level, H atom given arbitrary radius.

non-Poisson $w^{-1} = [\sigma^2(I) + 0{\cdot}0025I^2]/4F^2$. Final $(\Delta/\sigma)_{max} < 0{\cdot}001$, $\Delta\rho_{max} = 0{\cdot}66$ (4) and $\Delta\rho_{min} = -0{\cdot}38$ (4) e Å^{-3} on final difference map. Atomic scattering factors and anomalous-dispersion correction from *International Tables for X-ray Crystallography* (1974) and programs used were those of Enraf–Nonius (1982) *SDP*.* Table 1 gives the atom coordinates and Fig. 1 shows the molecule with the numbering scheme, bond distances, and bond angles.

Related literature. There are no structural reports of direct analogs of the title compound. Related structures include the CN_2S_2 ring of 1,3,2,4-dithiadiazol-5-one (Roesky, Wehner, Zehnder, Deiseroth & Simon, 1978), the CN_2S_2 ring of the $CN_2S_2SBr^+$ cation (Wolmershauser, Kruger & Tsay, 1982), and the C_2NS_2 ring of the 1,3,2-benzodithiazolyl group (Awere *et al.*, 1987).

We thank the National Science Foundation, the State of Arkansas, the Research Corporation, and the Natural Sciences and Engineering Research Council of Canada for financial support.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44292 (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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SHORT COMMUNICATIONS

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Acta Cryst. (1987). C**43**, 2469

Structure du chloro-3 méthyl-2 4*H*-pyrazino[1,2-*a*]pyrimidinone-4. Erratum. Par C. SABLAYROLLES et J. P. CHAPAT, *Laboratoire de Chimie Pharmaceutique UA CNRS n° 1111, Faculté de Pharmacie, 15 avenue Charles Flahaut,* 34060 *Montpellier CEDEX, France* et BERNARD DUCOURANT et ROBERT FOURCADE, *Laboratoire des Acides Minéraux UA n° 79, Université des Sciences et Techniques du Languedoc, place Eugène Bataillon,* 34060 *Montpellier CEDEX, France*

(*Reçu le* 28 *septembre* 1987)

Abstract

The *Abstract* of the paper by Sablayrolles, Chapat, Ducourant & Fourcade [*Acta Cryst.* (1987), C**43**, 1173–1174] contains a printer's error. The correct chemical formula is $C_8H_6ClN_3O$.

Le résumé contient tous les détails pertinents.

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