C(6)–S bond length may be interpreted in terms of π bonding between a $p\pi$ orbital of the C atom and $3d$ orbitals of the S atom (McDowell, 1975; Hosoya, 1966). Empirical calculations (Pauling, 1960) show that the bond order of this bond is about 1·25. The S–C(8) bond distance of 1·798 (9) Å agrees well with the normal S–C(sp^3) distance (Talberg, 1974).

The mean-plane calculations (Ahmed, Hall, Pippy & Huber, 1973) indicate that the S–C(6)–C(5)–N(4) segment of the thiazine moiety is planar (Table 3) within the limits of experimental error. The C(5)–N(4) bond distance of 1·428 (9) Å is significantly shorter than C(9)–N(4) and C(9)–N(1) because of the smaller radius of the sp^2-hybridized C(5) atom.

In the imidazole ring system N(1)–C(2)–C(3), 104·9 (6)°, and C(2)–C(3)–N(4), 101·7 (7)°, are comparable to the 102·5° observed in ethylenethiourea (Wheatley, 1956).

The structure analysis has confirmed that this ring system is imidazo[2,1-*c*][1,4]thiazine with the methyl group attached at carbon atom 2.

Intensity measurements were carried out for us at Twente University of Technology by Ing G. J. Van Hummel and Dr Sybolt Harkema with the permission of Dr D. Feil. One of us (MSH) is grateful to CSIR, India, for a Junior Research Fellowship.

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Format for Papers to be Published in *Acta Crystallographica*, Section C

Publication of Section C of *Acta Cryst.* will commence 15 January 1983. Details of the division into three new sections are given on page 1 of Volumes A**38** and B**38**. Section C will include all papers concerned with the straightforward determination and refinement of crystal structures such as are now published in Section B and in *Crystal Structure Communications* (*CSC*). The overall format of papers in Section C will resemble that used for Short Structural Papers (SSP) but without the present restriction on length. The *Introduction* section, which in SSP's contains the experimental details, will be replaced by a new *Introduction* (analogous to the *Preliminary Information* in *CSC*) and an *Experimental* section, the latter giving the essential experimental information in an abbreviated telegraphic form similar to that used for the crystal data in the *Abstract*.

Analysis of the types of information presented in SSP's, dealing with a single material at one temperature, in the first half of 1981 shows that a typical paper includes (1) a table of atomic coordinates and isotropic or equivalent isotropic thermal parameters, (2) a table of intramolecular bond distances and angles, (3) one figure showing a projection of the molecule with thermal ellipsoids and atomic numbering and (4) one figure showing the packing, either as a stereoview or as a projection. Most papers will be expected to conform to this 'typical' pattern, with additional tables and figures deposited as a Supplementary Publication. Papers on more than one material, or on materials at more than one temperature or pressure, may be appropriately scaled in content. All duplicated information within the paper will be deleted. A significant reduction in the resulting length of papers is expected from the new format without loss of vital information but with easier access to the information presented.

Papers submitted for consideration in *Acta Cryst.*, Section C must hence conform with the following arrangement:

The *Title* will consist of the name of the substance and the chemical formula; a qualification such as 'Structure of ...', 'New Form of ...', 'from Minas Gerais' *etc.* may be added.

The *Abstract* will consist (preferably in the order given here) of the formula weight, space group, unit-cell dimensions with an indication of accuracy (normally the estimated standard deviation in units of the last quoted decimal place enclosed in parentheses),* volume (Å^3), Z, measured and calculated density, radiation and wavelength, linear absorption coefficient, measurement temperature, the final value of R (see below for definition) and number of unique

* All primary measured and derived quantities given in the paper must be accompanied by their e.s.d.'s.

reflections, source of the material, and such other information (especially structural) as can be conveyed in approximately 50 further words.

The *Introduction* will briefly state the reason for undertaking the structure determination and its chemical, physical, biological or other interest. If organic, or containing complicated organic ligands, a display of the structural formula of the material studied should be given, in accordance with IUPAC convention.

The *Experimental* section will give the source of the material, the method of measuring D_m, the crystal shape and size, the diffractometer used, the reflections used for measuring the lattice parameters, the systematic absences, the absorption correction applied (with maximum and minimum values), the maximum value of 2θ reached in the intensity measurements, the range of hkl measured, the standard reflections and their intensity variation throughout the experiment with their overall e.s.d.'s, the number of reflections measured, the number of unique reflections, the value of $R_{\rm int}$ (from merging equivalent reflections), the number of unobserved reflections, the criterion for recognizing unobserved reflections, the method used to solve the structure, the use of F or F^2 magnitudes in least-squares refinement, the methods of locating and refining hydrogen-atom coordinates (if applicable and if by methods other than least squares), the parameters refined, the final $R\ [=\sum(||F_o| - |F_c||)/\sum F_o]$ given only in the *Abstract*, $wR\ \{=[\sum w(|F_o| - |F_c|)^2/\sum wF_o^2]^{1/2}\}$, $S\ \{=[\sum w(|F_o| - |F_c|)^2/(m - n)]^{1/2}\}$ [where w is the weight, m is the number of observations, n is the number of variables, F_o is the observed and F_c is the calculated value of $F(hkl)$], the method used to evaluate w, the ratio of maximum least-squares shift to error in the final refinement cycle, the average ratio of shift to error, the maximum and minimum height in the final difference Fourier synthesis, the secondary-extinction value (if used), $F(000)$, the source of atomic scattering factors and (if used) anomalous-dispersion corrections, and all computer programs used.

The *Discussion* will generally include two tables [as in (1) and (2) above] and two figures [as in (3) and (4) above]. Additional tables and figures may be deposited. If the table of bond distances and angles is very long, this will be deposited and unusual values only given for publication. Comment should be made on any unusual features of coordination, bonding, bond lengths, bond angles, thermal vibrations, *etc.*

Any nonroutine measurement of physical properties (magnetic susceptibility, dielectric permittivity, elastic moduli, *etc.*) should be mentioned in the *Abstract* and the numerical values quoted there if possible. If the numerical values are too lengthy to be given in the *Abstract*, they should be given in a suitably headed paragraph in the paper, normally preceding the *Discussion*.

Tables of structure factors, anisotropic thermal parameters, least-squares planes and hydrogen-atom coordinates if not refined must be submitted in duplicate with the paper, but will not normally be published. After acceptance of the paper they will be deposited along with any other extensive tables or figures, in accordance with the Union's procedures.

The requirements regarding figures and references remain unchanged. Acknowledgements may be included at the end of the text.

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Commission on Journals
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Authors are reminded that chemical formulae and nomenclature in papers submitted to *Acta Crystallographica* and *Journal of Applied Crystallography* should conform to the rules of nomenclature established by the International Union of Pure and Applied Chemistry (IUPAC), the International Union of Biochemistry (IUB) and other appropriate bodies. As far as possible the crystallographic nomenclature should correspond to the systematic name. A structural formula should generally be given for all organic and organometallic compounds.

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