to the more strongly bonded square plane. A tabulation (Table 4) of comparable distances in the two complexes shows a marked similarity.

The bridging (μ_3) oxygen atom is 0·7 Å out of the plane of the equilateral triangle of copper(II) atoms so that the Cu–O–Cu angles [110·9 (4)°] are near tetrahedral. Bond distances and angles within the amine-oxime ligands (Fig. 1 and Table 3) are similar to those previously observed (Schlemper, 1968). The difference in Cu–N(oxime) and Cu–N(amine) distances of 0·07 Å is comparable to that difference in Ni–N distances of 0·05 Å. The square planar coordination about each copper is not perfect, with the maximum deviation of 0·25 (1) Å from the least-squares coordination plane exhibited by N(1) (see Fig. 2).

There is considerable intermolecular hydrogen bonding between the disordered perchlorate oxygen [O(11)], the noncoordinated waters [O(7) and O(8)], the coordinated water [O(4)], the oxime oxygen [O(2)], and the amine nitrogen [N(2)] as shown in Table 5. The shortest bond (2·54 Å) is between the disordered perchlorate oxygen [O(11)] and the noncoordinated water

on the threefold axis [O(7)]. There is also an apparent intra-ionic hydrogen bond between the amine nitrogen [N(2)] and the oxime oxygen [O(2)].

Table 5. *Probable hydrogen-bond distances*

O(7)···O(11)	2·54 (3) Å	O(8)···O(8)	2·77 (2) Å
O(1)···O(21)	2·75 (2)	O(4)···O(7)	2·90 (1)
O(4)···O(8)	2·75 (1)	O(2)···N(2)	2·99 (1)
O(2)···O(8)	2·77 (1)	O(4)···O(8)	3·39 (1)
		N(2)···O(8)	3·37 (1)

The magnetic properties (Young & Murmann, 1963) have been confirmed by Gary Long (private communication) and are easily interpreted on the basis of this structure and electron pairing through magnetic exchange leaving a single unpaired electron per trimer.

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2,3,6,7-Tetrahydro-4H-thiazolo[3,2-a]s-triazin-2-on-4-thione, C5H5S2N3O

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Abstract. $C_5H_5S_2N_3O$, orthorhombic, *Pbca*, $a = 8\cdot234$ (8), $b = 14\cdot579$ (15), $c = 12\cdot459$ (13) Å, $Z = 8$, $D_x = 1\cdot66$ g cm^{-3}. The molecule is planar to within $\pm 0\cdot016$ Å. The structure shows hydrogen bonding and short S···(triazine ring) intermolecular approaches.

Experimental. The exo- and endocyclic nitrogen atoms of 2-amino-2-thiazoline exhibit different nucleophilic character and this difference has been the subject of many studies. The reaction of this molecule with carbethoxy isothiocyanate (C_2H_5O–C–NCS) could lead to either or both of two possible products (A or B).
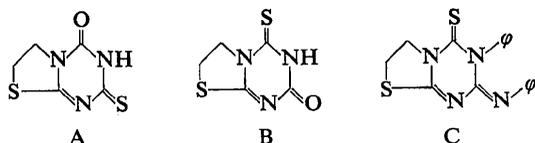
However, only a single isomer was produced in the reaction and this X-ray study established that the reaction product has the structure B. A detailed study of the chemistry of these compounds will be published (Klayman, Woods & Flippen, 1974). Crystals were
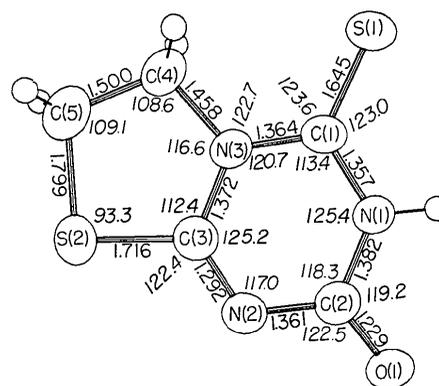

Fig. 1. Bond distances and angles. Based solely on least-squares parameters, standard deviations are on the order of 0·005 Å for bond lengths and 0·3° for angles.

Table 1. *Fractional coordinates and thermal parameters with standard deviations*

The thermal parameters are of the form

$$T = \exp\left[-\tfrac{1}{4}(B_{11}h^2a^{*2} + B_{22}k^2b^{*2} + B_{33}l^2c^{*2} + 2B_{12}hka^*b^* + 2B_{13}hla^*c^* + 2B_{23}klb^*c^*)\right].$$

Standard deviations are based solely on least-squares parameters.

	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
S(1)	0·2054 (1)	0·1315 (1)	0·2437 (1)	4·54 (5)	4·16 (5)	4·27 (6)	−0·06 (5)	1·89 (5)	−0·03 (4)
S(2)	−0·0915 (2)	0·3966 (1)	0·4437 (1)	7·53 (8)	3·04 (5)	5·49 (6)	0·13 (5)	2·14 (6)	−0·22 (4)
O(1)	−0·1106 (4)	0·0776 (2)	0·5698 (2)	6·48 (17)	3·70 (14)	3·39 (13)	0·06 (12)	1·68 (12)	0·62 (11)
N(1)	0·0329 (4)	0·1100 (2)	0·4207 (2)	3·65 (15)	3·01 (14)	2·71 (14)	0·08 (12)	0·53 (13)	0·31 (12)
N(2)	−0·1067 (4)	0·2259 (2)	0·5145 (2)	5·12 (18)	3·40 (17)	3·21 (16)	−0·12 (13)	1·05 (14)	−0·07 (13)
N(3)	0·0451 (3)	0·2561 (2)	0·3573 (2)	2·84 (14)	2·92 (14)	2·70 (13)	−0·44 (12)	0·14 (12)	0·18 (11)
C(1)	0·0911 (4)	0·1670 (3)	0·3436 (3)	2·71 (17)	3·73 (19)	2·69 (16)	−0·17 (14)	0·23 (14)	0·02 (15)
C(2)	−0·0658 (5)	0·1359 (3)	0·5051 (3)	4·71 (22)	3·44 (19)	2·69 (17)	−0·21 (17)	−0·12 (16)	−0·03 (15)
C(3)	−0·0512 (5)	0·2812 (3)	0·4422 (3)	4·03 (19)	3·36 (18)	3·28 (17)	−0·34 (15)	0·19 (17)	−0·35 (16)
C(4)	0·0935 (6)	0·3291 (3)	0·2840 (4)	4·91 (24)	3·33 (19)	3·72 (20)	−0·31 (17)	0·15 (18)	0·67 (15)
C(5)	0·0257 (6)	0·4181 (3)	0·3245 (4)	5·34 (26)	3·70 (21)	5·19 (25)	−0·24 (19)	0·23 (20)	0·84 (18)
H−N(1)	0·059 (5)	0·048 (3)	0·414 (3)						
H−C(4A)	0·052 (6)	0·312 (3)	0·218 (4)						
H−C(4B)	0·224 (6)	0·333 (3)	0·289 (3)						
H−C(5A)	−0·041 (6)	0·445 (3)	0·282 (4)						
H−C(5B)	0·108 (6)	0·461 (3)	0·339 (4)						

provided by Dr D. L. Klayman of the Walter Reed Army Medical Center. The 1039 independent reflections were collected from a thin colorless plate ($\sim 0.97 \times 0.65 \times 0.12$ mm) on an automatic diffractometer using Mo $K\alpha$ radiation ($\lambda = 0.71069$, Zr filter). The θ–2θ scan mode of data collection was used (maximum $\sin \theta / \lambda = 0.538$).

The structure was solved by routine application of the symbolic addition procedure for centrosymmetric crystals (Karle & Karle, 1966) using programs written by R. D. Gilardi and S. A. Brenner of this laboratory and the structure was refined using full-matrix least-squares methods (Busing *et al.*, 1971). No absorption corrections were applied ($\mu_R = 0.612$). Atomic scattering factors used were those listed in *International Tables for X-ray Crystallography* (1962) and the function minimized was $\sum W(|F_o| - |F_c|)^2$. Weights (W) were calculated according to a procedure outlined by Gilardi (1973). The final R index is 0·056 ($R_W = 0.050$). Hydrogen atoms were located in a difference map and their positional parameters were included in the refinement. Table 1 lists the final coordinates and thermal factors. Bond distances and angles are illustrated in Fig. 1. A

comparison of observed and calculated structure factors is obtainable.*

Discussion. Fig. 1 was drawn by program *ORTEP* (Johnson, 1965). The atoms are located at their final refined coordinates with anisotropic thermal parameters for the heavy atoms and arbitrary isotropic parameters for the hydrogen atoms. The entire molecule (excluding hydrogen atoms) is planar to within ±0·016 Å. It (B) is quite similar to the fused ring portion of an anti-radiation compound (C) studied earlier (Karle, Flippen & Karle, 1967). In C the fused ring moiety is planar to within ±0·26 Å. The larger deviations from planarity may be a consequence of the repulsive forces in effect between the bulky substituent groups. The most striking similarity between the two molecules is the strong intermolecular force existing between the doubly bonded sulfur of one molecule and the triazine ring of a neighboring molecule. In C the sulfur atom is at a distance of 3·24 Å from the best plane through the triazine ring. In B this distance is 3·42 Å (van der Waals separations would be 3·60 Å for S···C and 3·42 Å for S···N). Closest atom–atom approaches between the sulfur atom and its neighboring triazine ring are S···N at 3·37 Å for molecule C and an S···N and S···C approach of 3·40 Å for molecule B. The C=S bond is at an angle of 56·8° to the best plane through the triazine ring of the nearest molecule in the present study (B) and at an angle of 58·5° in molecule C. The packing of molecule B is also influenced by the presence of a N(1)−H···O(1) intermolecular hydrogen bond which links the molecules in pairs across a center of symmetry [N(1)···O(1) = 2·81, H(N1)···O(1) = 1·89 Å]. The hydrogen bonds are illustrated in the middle of the cell in
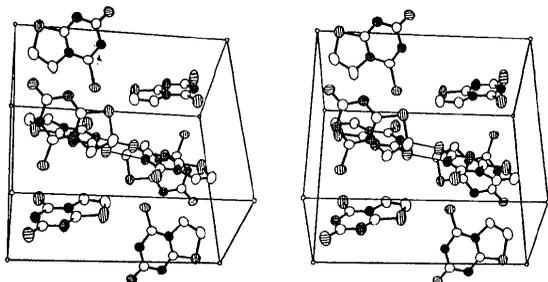

Fig. 2. The contents of one unit cell. The projection is drawn with **a** pointing into the paper, **b** horizontal and pointing to the left, and **c** vertical and pointing upwards. A pair of NH···O hydrogen bonds around the center of symmetry at ½,½,½ are indicated.

Fig. 2. Aside from the distances discussed above the only intermolecular approach less than van der Waals separations is S(2)$\cdots$S(2)' at 3·65 Å.

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Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England).

Current awareness service

The Crystallographic Data Centre, Cambridge, is now able to offer an alerting service which aims at providing rapid references to recent structure determinations of organic and organometallic compounds. The service is intended to bridge the gap between the annual bibliographic volumes published in the *Molecular Structures and Dimensions* series (Crystallographic Data Centre and International Union of Crystallography; Utrecht: Oosthoek, 1970, 1971, 1973, 1974). The majority of references are selected by direct scanning of 10 journals and the remainder are obtained from about 250 journals searched in collaboration with the Centre de Documentation, Centre National de la Recherche Scientifique, Paris. Major crystallographic meetings, such as those of the International Union of Crystallography, the American Crystallographic Association, the European Crystallographic Committee and the Italian Crystallographic Association, are covered directly.

The citations are provided as computer listings with entries grouped, by molecular formula, in 86 chemical classes. For each entry the formula and name of the compound and the full bibliographic reference are listed. Supplementary information may be given, *e. g.* the temperature of the study, an indication that the absolute configuration was determined, *etc.*

Listings are mailed at about 6-weekly intervals, each batch containing approximately 300 entries. The cost is £15 ($36) per annum for 1974 (all postage extra). Orders can be placed with Dr D. G. Watson, Crystallographic Data Centre, University Chemical Laboratory, Cambridge CB2 1EW, England.

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (M.M. Woolfson, Physics Department, University of York, Heslington, York YO1 5DD, England). As far as practicable books will be reviewed in a country different from that of publication.

The Raman effect. Vol. 2. Applications. Edited by ANTHONY ANDERSON. Pp.xi + 1033. Figs. 124. Tables 69. New York: Marcel Dekker, 1973. Price $45.00.

This second, final volume of *The Raman Effect* contains five reviews covering the application of the phenomenon to inorganic chemistry, molecular, ionic, covalent and metallic crystals, electronic transitions and high-resolution studies of gases. It complements the first volume (published in 1971) which reviewed general principles, instrumental methods and developments and included sections on the stimulated effect and Brillouin scattering.

The entries in the present volume are mainly well supported by references – if one excludes that quoted (p. 755) claiming that the *Journal of Chemical Physics* was in print in 1670. Three of the articles contain no references later than early 1970, the remaining two apparently dating from the following year despite the 1973 publication date. The last two years have seen an enormous growth of interest in resonance effects in Raman spectroscopy and applications to the study of rapid reactions and molecules of biological interest. These important areas find no place in the present volume and this omission reduces significantly the value of the work. No doubt all research groups in this field will feel obliged to obtain these highly priced volumes for their virtues of inclusion rather than their sins of omission.

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