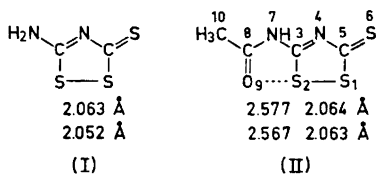


The Structure of 3-Acetamido-1,2,4-dithiazole-5-thione

GUNNAR EIDE, ASBJØRN HORDVIK and LEIF J. SÆTHRE

Chemical Institute, University of Bergen, N-5000 Bergen, Norway

Two independent structure studies of xanthan hydride (I) have been reported,^{1,2} and the lengths of the sulphur-sulphur bond in I from these studies are 2.063(5) and 2.052(4) Å, respectively.



We have carried out a structure investigation of the acetyl derivative of xanthan hydride, 3-acetamido-1,2,4-dithiazole-5-thione (II), in order to find out whether the O...S contact in II affects the sulphur-sulphur bond there. The preliminary results from this investigation are given.

The O...S contacts in the two crystallographically independent molecules of II are 2.577(3) and 2.567(3) Å, respectively, and the corresponding S-S bond lengths are 2.0644(15) and 2.0632(13) Å. Thus, when compared with I, the O...S contacts in II are seen to have no significant lengthening effect on the S-S bonds.

Other bond lengths in the two independent molecules of II, mentioned in the same order as above, are, S(2)-C(3) 1.758(3) and 1.752(3) Å, C(3)-N(4) 1.314(5) and 1.311(4) Å, N(4)-C(5) 1.350(5) and 1.347(5) Å, C(5)-S(6) 1.666(4) and 1.665(4) Å, C(5)-S(1) 1.753(3) and 1.752(4) Å, C(3)-N(7) 1.356(5) and 1.363(5) Å, N(7)-C(8) 1.381(5) and 1.390(5) Å, C(8)-C(10) 1.480(7) and 1.488(6) Å, and C(8)-O(9) 1.227(5) and 1.222(5) Å.

Crystals of II from 60% acetic acid are light yellow prisms and belong to the orthorhombic space group $P2_12_12_1$. The cell dimensions are $a=7.8275(5)$ Å, $b=32.975(1)$ Å, and $c=5.8320(3)$ Å. There

are eight molecules per unit cell; $D_c=1.697$ g cm⁻³, $D_m=1.694$ g cm⁻³.

The structure was solved by direct methods³ and refined by full matrix least squares. With anisotropic temperature factor coefficients for all atoms except hydrogen, the present R is 0.028.

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Received May 10, 1972.

The Structure of 2,5-Diphenyl-3,4-trimethylene-6a-thiathiophthene

BJØRN BIRKNES, ASBJØRN HORDVIK and LEIF J. SÆTHRE

Chemical Institute, University of Bergen, N-5000 Bergen, Norway

The results from the structure investigations of 6a-selenaselenophthene (I)¹ and 3,4-trimethylene-6a-selenaselenophthene (II)² show that the introduction of a 3,4-trimethylene bridge in (I) causes a decrease in the Se-Se distances; the sum of the Se-Se distances in II, 5.111(3) Å, is 0.054 Å smaller than the sum of the Se-Se distances in I, 5.165(3) Å.

An analysis of the structure of 2,5-diphenyl-3,4-trimethylene-6a-thiathiophthene (IV) has been carried out in order to find to which extent the 3,4-trimethylene bridge affects the sulphur-sulphur bonding there, and the preliminary results from this study are given.