

Table 1. Atomic coordinates, in fractions of triclinic cell edges. Origin at a centre of symmetry.

| | <i>y</i> | <i>z</i> |
|----------------|----------|----------|
| S ₁ | 0.230 | 0.108 |
| S ₂ | 0.593 | 0.164 |
| C ₃ | 0.620 | 0.280 |
| C ₄ | 0.385 | 0.286 |
| C ₅ | 0.243 | 0.161 |
| C ₆ | 0.218 | 0.379 |
| O ₁ | 0.265 | 0.443 |
| O ₂ | 0.012 | 0.390 |

It is intended to refine the *a*-axis projection further, and to carry out a detailed structure analysis.

The work has been aided by a grant from *L. Meltzers Høyskolefond*.

1. Foss, O. *Acta Chem. Scand.* **10** (1956) 868.
2. Foss, O. and Schotte, L. *Acta Chem. Scand.* **11** (1957) 1424.
3. Foss, O. and Tjomsland, O. *Acta Chem. Scand.* **10** (1956) 869.
4. Foss, O. and Tjomsland, O. *To be published*.
5. Schotte, L. and Ström, H. *Acta Chem. Scand.* **10** (1956) 687.
6. Schotte, L. *Arkiv Kemi* **9** (1956) No. 37.

Received August 24, 1957.

Structure of Crystalline *Racem*-1,2-dithiane-3,6-dicarboxylic Acid

OLAV FOSS and TORBJØRN REISTAD

Chemical Institute, University of Bergen, Bergen, Norway

In two preceding notes^{1,2}, crystal data on some carboxylic acid derivatives of five-, six- and seven-membered cyclic disulphides, and preliminary results of a crystal structure determination of the five-membered one, 1,2-dithiolane-4-carboxylic acid, have been reported. A corresponding study of a six-membered representative, *racem*-1,2-dithiane-3,6-dicarboxylic acid³⁻⁶, has so far given the following results.

The crystals are monoclinic prismatic, with a four-molecule unit cell based on the space group C_{2h}^2-I2/c , and with the unit cell dimensions¹, $a = 9.62 \text{ \AA}$, $b = 9.26 \text{ \AA}$, $c = 9.70 \text{ \AA}$, $\beta = 102\frac{1}{2}^\circ$. The correctness of the centrosymmetric space group was first assumed, and confirmed through the subsequent work. The intensities of the $h0l$ reflections were estimated visually from Weissenberg photographs taken with CuK radiation; 51 reflections out of 57 attainable were recorded with measurable intensities. The position of the one sulphur atom of the asymmetric unit was derived

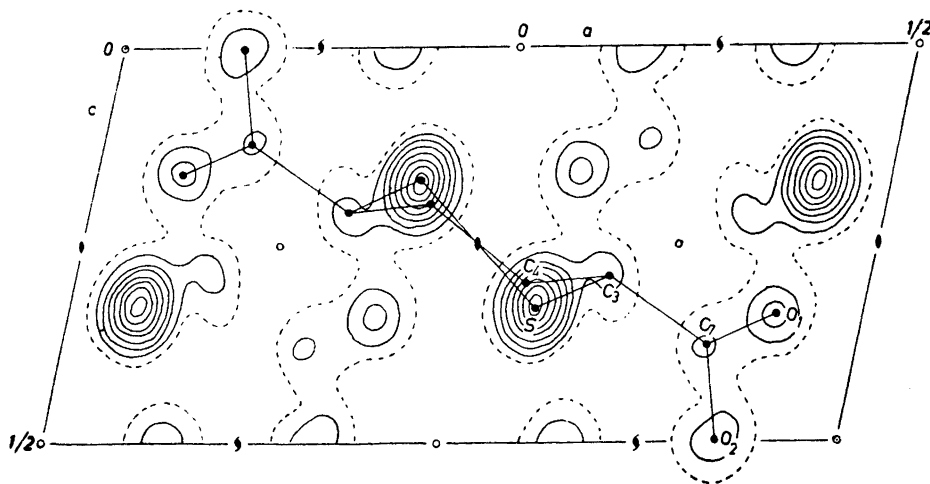


Fig. 1. Electron density projection of *racem*-1,2-dithiane-3,6-dicarboxylic acid along the *b* axis. Four asymmetric units (half a unit cell) are shown, and lines are drawn to indicate the outline of one molecule. Contours at intervals of $3 e \cdot \text{\AA}^{-2}$, beginning with $4 e \cdot \text{\AA}^{-2}$ (dashed).

from a F_0^2 synthesis of the $h0l$ data, and the sulphur atom then served as a heavy atom for the determination of the carbon and oxygen positions through F_0 syntheses. Refinement was carried out by means of successive ($F_0 - F_c$) syntheses, and led to a standard deviation in electron density of about $0.45 \text{ e} \cdot \text{\AA}^{-3}$ for the $h0l$ zone, and a corresponding reliability index R of 10.4 %.

The $h0l$ electron density map is shown in Fig. 1, and the x and z coordinates are listed in Table 1. They give a S—S bond length of 2.069 Å across the twofold axis, with an estimated standard deviation of about 0.014 Å.

Table 1. Atomic coordinates, in fractions of monoclinic cell edges. Origin at a centre of symmetry.

| | x | z |
|----------------|--------|--------|
| S | 0.0885 | 0.3325 |
| C ₃ | 0.173 | 0.292 |
| C ₄ | 0.070 | 0.302 |
| C ₇ | 0.313 | 0.379 |
| O ₁ | 0.393 | 0.342 |
| O ₂ | 0.348 | 0.499 |

The molecule possesses, by space group requirements, a twofold axis of symmetry. The 1,2-dithiane ring occurs in the chair form, and has the substituents in equatorial positions. The difference maps indicated a pronounced anisotropic thermal vibration for the sulphur atom. In the temperature factor $\exp[-B(\sin^2\theta/\lambda^2)]$ finally chosen B was 4.0 \AA^2 for the carbon and oxygen atoms and $(6.5 - 4.0 \sin^2\varphi) \text{ \AA}^2$ for the sulphur atom, where φ is the angle between the normal of the reflecting plane and the direction of maximum vibration of the atom. This direction lies about 16° from c in the acute angle, and is very close to the axial direction of the 1,2-dithiane ring, i. e., to the direction of movement of the atom for conversion of the ring.

The work will be continued, and details published later.

1. Foss, O. and Schotte, L. *Acta Chem. Scand.* **11** (1957) 1424.
2. Foss, O. and Tjomslund, O. *Acta Chem. Scand.* **11** (1957) 1426.
3. Fredga, A. *Ber.* **71** (1938) 289.
4. Fredga, A. *Arkiv Kemi, Mineral. Geol.* **12 A** (1938) No. 27.
5. Schotte, L. *Arkiv Kemi* **8** (1955) No. 56.
6. Schotte, L. *Arkiv Kemi* **9** (1956) No. 37.

Received August 24, 1957.

Aberrations Chromosomiques Produites dans des Graines par de Hautes Pressions d'Oxygène

L. EHRENBERG, J. MOUTSCHEN-DAHMEN*
et M. MOUTSCHEN-DAHMEN**

*Institut de chimie organique et de biochimie,
Université de Stockholm; Institut de recherche
forestière, Département de génétique,
Stockholm 51, Suède*

En 1951, Conger et Fairchild ont trouvé que l'oxygène pur produit des aberrations chromosomiques dans les microspores de *Tradescantia*¹.

Dans d'autres expériences, des résultats contradictoires ont été obtenus². Ceci peut indiquer que, alors que l'oxygène, sous certaines conditions, est capable de casser les chromosomes, le matériel biologique change dans son aptitude à résister à cet effet.

Dans une étude biochimique des mutations spontanées et de leurs mécanismes, nous nous sommes posé la question de savoir si l'oxygène peut produire des aberrations chromosomiques dans les graines de plantes supérieures.

Méthodes. Des graines sèches d'orge var. *Bonus*, dont la teneur en eau est de 11 %, ont été traitées pendant une ou deux semaines, respectivement, dans une bombe de fer sous 60 atmosphères de pression d'oxygène. Dans le but d'étudier l'effet d'une haute pression, *per se*, une expérience parallèle fût réalisée avec 60 atmosphères d'azote. Lors de ces traitements, on a pris soin de changer la pression très lentement afin d'éviter les effets thermiques.

Après une semaine de traitement, les graines sont mises à germer. Les pointes de racines sont fixées 30 à 90 h après la fin du traitement afin de pouvoir observer les successions des trois premières mitoses consécutives au traitement.

Après le traitement de deux semaines, nous avons attendu un délai de trois semaines avant de les mettre à germer.

* Chargé de recherche au *Fonds National belge de la Recherche Scientifique* (F.N.R.S.).

** Chargée de recherche à l'*Institut pour l'encouragement de la Recherche Scientifique dans l'Industrie et l'Agriculture* (I.R.S.I.A.).