Crystal Structure of 3,6-Spirodicycloheptyliden-1,2,4,5-tetraoxa-cycloheptan ("Dimeric Cycloheptanone Peroxide")

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Crystals of "dimeric cycloheptanone peroxide", prepared by T. Ledaal (to be published), belong to the monoclinic

$$\begin{array}{c} \mathsf{CH_2} - \mathsf{CH_2} \\ \mathsf{CH_2} \\ \mathsf{CH_2} \\ \mathsf{CH_2} - \mathsf{CH_2} \\ \mathsf{CH_2} - \mathsf{CH_2} \end{array} 0 - 0 \\ \mathsf{CH_2} - \mathsf{CH_2} \\ \mathsf{CH_2} - \mathsf{CH_2} \\ \mathsf{CH_2} - \mathsf{CH_2} \\ \end{array}$$

system. The space group is $P2_1/c$ and the unit cell, containing two molecules, has the following parameters:

$$a = 9.39 \text{ Å}, b = 6.37 \text{ Å}, c = 11.51 \text{ Å}, \beta = 102^{\circ}$$

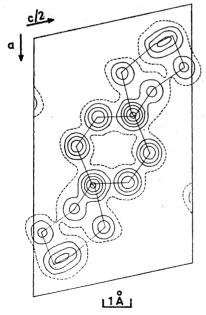


Fig. 1. Fourier projection along b-axis.

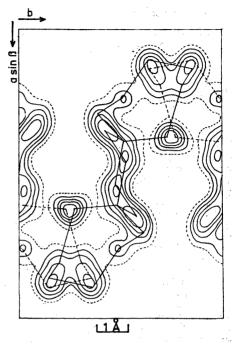


Fig. 2. Fourier projection along c-axis.

Fourier maps for the h0l- and hk0-projections were obtained by a computer procedure based on the Cochran-Douglas method. The maps could easily be interpreted and least squares refinements gave the following R-values: $R_{h0l} = 10$ %, $R_{hk0} = 12$ %.

The final electron density maps (Figs. 1 and 2) show considerable overlapping. The publication of interatomic distances and angles will therefore be postponed until the threedimensional analysis, now in progress, has been finished. It may be stated, however, that the centre chair-formed ring corresponds roughly to that found in "dimeric eyclohexanone peroxide".²

- Cochran, W. and Douglas, A. S. Proc. Roy. Soc. (London) 227 (1954) 486; 243 (1958) 281.
- 2. Groth, P. Acta Chem. Scand. 18 (1964) 1301.

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