The packing of the molecules of compound II in the crystal takes place at the usual
van der Waals distances, and there are no shortened intermolecular contacts.

Thus the change from a six-membered to a seven-membered lactam ring has no influence
on the strength of the Si-O interaction and leads to a slight decrease in the strength of
of the Si-Cl interaction, while the trigonal bipyramidal coordination of the Si atom and
the conformation of the Si-containing heterocyclic ring are preserved.

The authors thank V. A. Palyulin for assistance with the calculations.

LITERATURE CITED

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INFLUENCE OF HYDROGEN BONDS ON CONFORMATION OF PEROXIDES
OBTAINED FROM CYCLOHEXANONE. AN X-RAY STRUCTURAL STUDY
OF 1-HYDROXY-1'-HYDROPEROXYDICYCLOHEXYL PEROXIDE

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S. V. Lindeman, Yu. T. Struchkov,
I. P. Zyat'kov, and N. A. Turovskii

To investigate the influence of the mode of formation of hydrogen bonds in the
-crystal on the conformation of the central peroxide group in peroxides obtained
-from cyclohexanone, an X-ray structural study of 1-hydroxy-1'-hydroperoxydi-
cyclohexyl peroxide (I) has been carried out. The central peroxide group in
-compound I (O-O 1.478(1) Å) is oriented equatorially relative to the two cyclo-
-hexanone rings and has a conformation which is close to that found in 1,1'-di-
-hydroperoxydicyclohexyl peroxide (II) and which differs from that found in 1,1'-
dihydroxydicyclohexyl peroxide (III) (torsional angle COOC 120.5(2)° in compound
-I, 126.3(3)° in compound II, and 156.1(4)° in compound III). This is apparently
due to the different modes of formation of the H-bonds in the crystals of com-
-pounds I, II, and III (intramolecular H-bonds in compounds I and II, in contrast
to compound III).

Peroxides obtained from cyclohexanone form one of the basic classes of ketone peroxides
-used in the chemical industry and in laboratory practice as initiators of polymerization
-processes [1]. It is therefore of interest to investigate the influence of the substituents
-in these molecules on the structure of the central peroxide group and hence on the observed
physicochemical properties [1, 2], in particular the ability to undergo homolytic decompo-
sition.

1-Hydroxy-1'-hydroperoxydicyclohexyl peroxide (I) is "intermediate" between 1,1'-dihy-
-droperoxydicyclohexyl peroxide (II) and 1,1'-dihydroxydicyclohexyl peroxide (III), for
which the central peroxide groups were previously found to have different conformations
TABLE I. Coordinates ($10^3$, $10^3$ for the H atoms) and Temperature Factors $B_{eq}$ ($\overline{A}^2$) ($B_{iso}$ for the H atoms) of the Atoms of the Molecule of 1-Hydroxy-1'-hydroperoxydicyclohexyl Peroxide

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* The first figure in the numbering of this and subsequent H atoms is the number of the corresponding carbon atom.

Fig. 1. Structure of the molecule of compound I. The broken line indicates the intramolecular H-bond.

(torsional angle COOC ($\varphi$) of $126.3(3)^o$ in compound II [3] and $156.1(4)^o$ in compound III [4]) and different orientations relative to the cyclohexane rings (diequatorial in compound II and diaxial in compound III). It was suggested [4] that the observed differences are due to the interaction of a number of factors: the mode of formation of the hydrogen bonds in the crystal, the steric (and possibly electronic) influence of the substituents, and the conformational flexibility of the cyclohexane rings and the peroxide group. To investigate the role of these factors and to develop further the existing ideas on the structure of organic peroxides, an X-ray structural study of compound I was carried out.

**EXPERIMENTAL**

The unit cell parameters of the crystal of compound I and the intensities of 1935 independent reflections were measured at $-120^o$C on a Syntex P21 four-circle automatic diffractometer ($\lambda$MoKa, graphite monochromator, $\theta/2\theta$-scanning, $\sin \theta/\lambda_{max} = 0.683$). The crystals of compound I are monoclinic, space group $C2/c$, $a = 23.596(7)$, $b = 6.150(2)$, $c = 17.836(4)$ $\overline{\text{A}}$, $\beta = 98.10(2)^o$, $V = 2562(1)$ $\overline{\text{A}}^3$, $Z = 8$, $M = 246.30$, $d_{calc} = 1.277$ g/cm$^3$, $\mu$(MoKa) = 1.058 cm$^{-1}$.

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