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CONFORMATION OF THE CYCLOHEXANE-1.4-DIONE MOLECULE IN AN ADDITION COMPOUND

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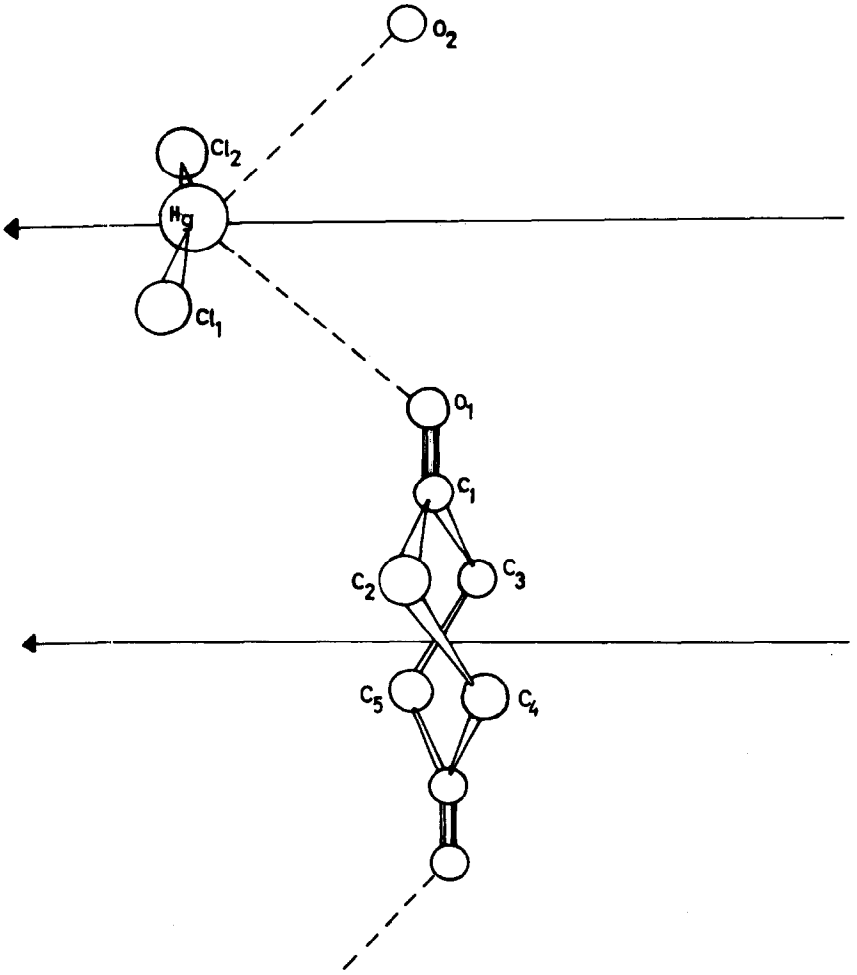
Two recent investigations of the crystal structure of cyclohexane-1.4-dione (1,2) are in very good agreement and demonstrate that, in the crystalline form stable at room temperature and lower temperature, the molecule is present in a "twisted boat" form having at least very nearly the symmetry C_2. If the molecule retains this conformation in solution the finding (3) is explained in a natural way that the substances has an electric dipole moment. In order to test the rigidity of the molecule electron diffraction investigation of the vapour was started in our laboratory and at the same time some new addition compounds prepared, the crystal structure of which we wanted to investigate. One of the latter investigations, that of a monoclinic 1:1 compound formed with mercury chloride, has been carried out and it was found that in the crystal both the dione and the mercury chloride molecules are situated on two-fold symmetry axes. Both kinds of molecules must therefore have the symmetry C_2. The atomic distances and angles resulting


O2
Cl2
Hg
Cl1
O1
C1
C2
C3
C5
C4

from the (two-dimensional) X-ray analysis are listed in Table 1.

In the figure the arrangements of the molecule is visualized.

TABLE 1

Interatomic distances

Hg-Cl	2.30 Å	C_1-C_2	1.45 Å
Hg····O	2.79 Å	C_1-C_3	1.47 Å
C_1-O	2.26 Å	C_2-C_4	1.53 Å

Angles

Cl_1-Hg-Cl_2	173°	O_1-C_1-C_2	119°
O_1-Hg-O_2	86°	O_1-C_1-C_3	122°
O_1-Hg-Cl_1	96°	C_2-C_1-C_3	117°
O_1-Hg-Cl_2	89°	C_1-C_2-C_4	111°
Hg-O_1-C_1	124°	C_1-C_3-C_5	111°

A comparison of the structure found for the dione molecule in the present compound and in the dione crystal shows that although the general form is not much altered, the angle between the two C-O directions (175°) is about 20° greater in the addition compound. Besides this change it appears probable that the increase in the C-O bond length (about 0.05 Å) is significant. These findings make us look forward to the results of the electron diffraction investigation of the dione vapour and the X-ray investigation of its crystalline modification stable above 47° C which will give some indications regarding the rigidity of the

molecule. Further details will be published in Acta Chemica Scandinavica. Here we may add that the space group of the addition compound is C2/c and that the unit cell containing four formula units has the parameters:

$$a = 7.57 \text{ Å} ; b = 17.11 \text{ Å} ; c = 7.56 \text{ Å} ; \beta = 108^{\circ}5$$

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