Structure of *cis*-Cyclobutane-1,3-dicarboxylic Acid. A Puckered Cyclobutane

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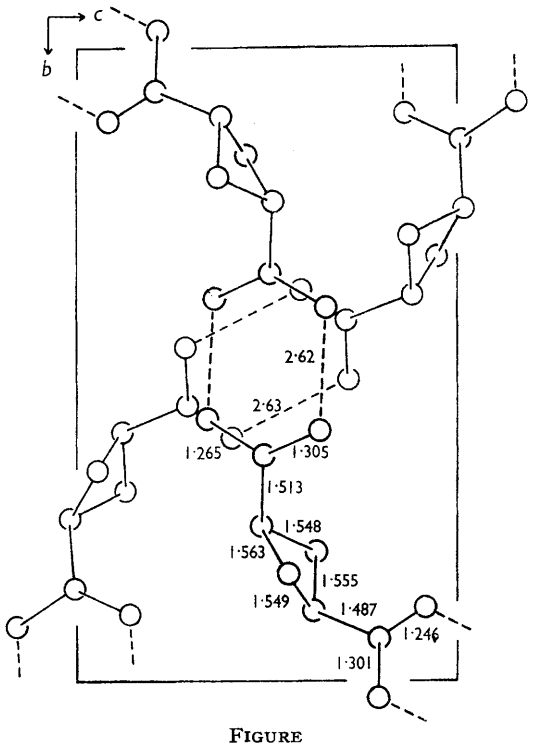
THE *trans*-isomer of cyclobutane-1,3-dicarboxylic acid has recently been shown to have a planar cyclobutane ring in the solid state.[1] We now present the results of a single-crystal *X*-ray diffraction study which show that the *cis*-isomer has a puckered cyclobutane ring.

Crystals of *cis*-cyclobutane-1,3-dicarboxylic acid, $C_6H_8O_4$ (m.p. 134°), are monoclinic, space group $P2_1/n$, $a = 6{\cdot}439$, $b = 13{\cdot}268$, $c = 8{\cdot}036$ Å; $\beta = 92{\cdot}84°$; $Z = 4$. The structure was determined from 427 independent reflections measured with a diffractometer. Refinement by least-squares reduced the *R*-factor to a final value of 0·057. Hydrogen atoms were refined with isotropic temperature factors; all other atoms were refined with anisotropic temperature factors.

The molecules, shown in the Figure, form hydrogen-bonded chains which cross in the region of hydrogen bonding. A difference map provides evidence of disorder in the hydrogen positions so that there may be weak hydrogen bonding between chains. The cyclobutane ring is puckered with a dihedral angle of 149°, consistent with values found in other compounds.[2] The carboxyl groups occupy positions analogous to the equatorial positions in cyclohexane. The average C–C single bond length within the ring is 1·554 Å (σ_{C-C} = 0·01 Å) somewhat longer than a normal C–C single bond (1·537 Å).[3]



FIGURE

(*Received, May 24th*, 1967; *Com.* 511.)

[1] T. N. Margulis and M. Fischer, *J. Amer. Chem. Soc.*, 1967, **89**, 223.
[2] S. Meiboom and L. C. Snyder, *J. Amer. Chem. Soc.*, 1967, **89**, 1038; I L. Karle, J. Karle, and K. Britts, *ibid.*, 1966, **88**, 2918.
[3] "Tables of Interatomic Distances", *Chem. Soc. Special Publ.*, 1965, *No.* 18, p. S145.