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The planarity of the dicarboxylic acid dimer configuration.

By G. A. JEFFREY and M. SAX, *The Crystallography Laboratory, The University of Pittsburgh, Pittsburgh* 13, *Pa, U.S.A.*

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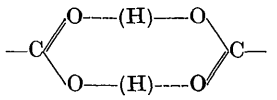
When two carboxylic acid groups are hydrogen-bonded across a center of symmetry in a crystal structure, it would appear natural to expect that the resulting six-membered ring, I, would be planar. So much so that this stereochemical feature is seldom described from this point of view, although, of course, its planarity can be deduced from the atomic parameters of the particular structure. We have examined the planarity of this con-



I

figuration in twelve recent analyses involving carboxylic acids dimerized across a center of symmetry. The results are shown in Table 1. The carbon and oxygen atoms of each carboxylic acid group define a plane, and because of the center of symmetry, the two planes must be parallel. The orientation of these planes varies from coplanar, within experimental error, to a separation of 0·5 Å. One can conclude that, while the planar configuration may well be that of lowest energy, significant departures from planarity can be incurred by the steric packing requirements of the remainder of the molecule, and that coplanarity of the two carbon and four oxygen atoms is the exception rather than the rule.

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Table 1

Carboxylic acid structure	Separation of planes	Estimated mean standard deviation	
β-Ionylidene crotonic	0·011 Å	0·01 Å	Eichhorn, MacGillavry (1959)
Anhydrous citric	0·016	0·007	Nordman, Weldon & Patterson (1961)
Benzoic	0·057	0·01	Sim, Robertson & Goodwin (1955)
β-Succinic	0·082	0·005	Broadley, J. S., Cruickshank, D. W. J., Morrison, J. D., Robertson, J. M. & Shearer, H. M. M. (1959)
Malonic	0·084 0·549		Goedkoop & MacGillavry (1957)
α-Thiophenic	0·096	0·006	Nardelli, Fava & Giraldi (1962)
Tiglic	0·10	0·007	Porte, A. L. & Robertson, J. M. (1959)
2-Naphthoic	0·136	0·01	Trotter (1961)
α-Selenophenic	0·163	0·009	Nardelli, Fava & Giraldi (1962)
Dihydromalvalic	0·212	0·003	Jeffrey & Sax (1963)
α-Pimelic	0·304 0·465	0·01	Kay & Katz (1958)
1-Naphthoic	0·375	0·009	Trotter (1960)