
In the last case, steric structures with the same sign of charge at neighbouring atoms are preferred as opposed to Pauling's rule (Pauling: Proc. Nat. Acad. Sci. USA (1956) 58, 498). Special behaviour of the carboxyl group can be attributed to the presence of bond lengths and alteration of valence angles (Kulpe; Siedler; Dähne; Noth; J. prakt. Chem. (1978) 316, 316).

Typical polymethine radicals with branched polymethinic fragments are Wurster's coloured salts (cf. 11, ref.). NMR spectroscopy provides further experimental verification of the polymethinic electron system (Hagedoorn: Thesis, Univ. of Hull, Hull, England).

09.2-01 THE CRYSTAL AND MOLECULAR STRUCTURE OF 3'-FLUROBIPHENYL-4-CARBOXYLIC ACID. By A. Rawas and M.H. Sutherland, Physics Department, University of Hull, Hull, England.

3'-Fluorobiphenyl-4-carboxylic acid, C14H9O2F, is monoclinic, space group P21/c, with a = 3.82(1), b = 8.04(1), c = 32.52(2), β = 101.61(1), Z = 4, D = 1.42. The structure was solved by Patterson synthesis with Cuka x-ray data measured by densitometry and visually from equi inclination Weissenberg photographs. It was refined anisotropically by block diagonal least squares to R = 0.08 for 885 reflexions. The average C-C bond in the two phenyl rings is 1.39Å. The molecule is non planar; the two phenyl rings are rotated about the phenyl-phenyl bond by 36.5° and the acid group is rotated about its C-C bond by 3.4°. There is also distortion in the bond angle around C(3) with the internal angle of 124.5(1.2)°, the C-F bond is 1.33(1)Å and makes an angle of 27° with the phenyl plane.

Dimers formed from the molecules by an O-H...O bond of 2.62(5)Å, pack in a herring bone arrangement with the chlorine atoms lying in sheets parallel to (001).