The Crystal Structure of *p*-Coumaric Acid

Hiroyuki UTSUMI, Kazutoshi FUJII,*1 Hideo IRIE,*2 Akio FURUSAKI and Isamu NITTA

Faculty of Science, Kwansei Gakuin University, Nishinomiya,

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p-Coumaric acid, $C_6H_4(OH)CH{=}CHCOOH$, is a *p*-hydroxyl derivative of *trans*-cinnamic acid. Since the molecule has a hydroxyl, a carboxyl and an ethylenic group, polycondensation or polyaddition might occur in the solid phase if the arrangement of the molecules would be suitable to do so. Another problem of the coplanarity of the acrylic acid group with the benzene ring in the molecule may be interesting considering the conjugation between these groups as well as the repulsions between hydrogen atoms. In order to obtain information about these problems, the three-dimensional X-ray investigation has been performed.

The crystal of *p*-coumaric acid is monoclinic with the unit cell dimensions, $a=8.64\pm0.02$, $b=5.28\pm0.02$, $c=17.44\pm0.03$ Å and $\beta=100.0\pm0.3°$. The space group was found to be $P2_1/c$ from systematic absences. The unit cell contains four molecules, the calculated density being 1.42 $g\cdot cm^{-3}$. The three-dimensional data of intensities of 1376 reflections were measured visually from integrating Weissenberg photographs around the a and b axes taken with filtered Cu$K\alpha$ radiation.

The crystal structure was elucidated by means of the method of trial and error. The structure thus obtained was refined by the three-dimensional least squares method. The *R*-factor at the present stage is 16.8%, including hydrogen atoms. The crystal structure projected along the b axis is shown in Fig. 1.

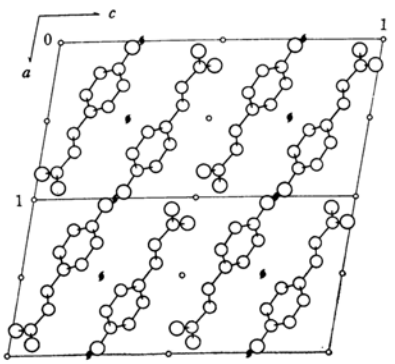

Fig. 1. Crystal structure projected along the b axis.

The molecule is almost planar, the angle between the plane-normal and the b axis being about 56°. The molecules are linked in dimers around a center of symmetry, by two O-H···O hydrogen bonds with a distance of 2.64 Å. The two molecules in a dimer are approximately coplanar.

The hydrogen bonds between phenolic hydroxyl groups form a kind of spiral running along the two-fold screw axis. The O-H···O distance is about 2.91 Å and seems to be weak. The crystal may be said to be composed of molecular layers parallel to (104), the angle between the plane of molecules and (104) being about 36°. Such molecular layers are 3.59 Å apart from one another and are attracted together mainly by weak van der Waals forces. In fact, the crystal shows perfect cleavage along the (104) plane.

*1 Present address: Central Research Laboratories, Sumitomo Bakelite Co., Ltd., Yokohama.
*2 Present address: Koyo Paint Mfg. Co., Ltd., Takatsuki.