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Structure of Kojic Acid

BY J. LOKAJ

Department of Analytical Chemistry, Slovak Technical University, 812 37 *Bratislava, Czechoslovakia*

J. KOŽÍŠEK

Department of Inorganic Chemistry, Slovak Technical University, 812 37 *Bratislava, Czechoslovakia*

B. KOREŇ

Department of Physics, Slovak Technical University, 812 37 *Bratislava, Czechoslovakia*

M. UHER

Department of Organic Chemistry, Slovak Technical University, 812 37 *Bratislava, Czechoslovakia*

AND V. VRÁBEL

Department of Analytical Chemistry, Slovak Technical University, 812 37 *Bratislava, Czechoslovakia*

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Abstract. 5-Hydroxy-2-(hydroxymethyl)-4*H*-pyran-4-one, $C_6H_6O_4$, $M_r = 142{\cdot}1$, monoclinic, $P2_1/n$, $a = 3{\cdot}8323\ (8)$, $b = 18{\cdot}409\ (6)$, $c = 8{\cdot}505\ (4)$ Å, $\beta = 96{\cdot}56°$, $V = 596{\cdot}1$ Å^3, $Z = 4$, $D_x = 1{\cdot}58$, $D_m = 1{\cdot}57$ g cm^{-3}, λ(Cu $K\alpha$) = 1·54178 Å, $\mu = 10{\cdot}62$ cm^{-1}, $F(000) = 296$, $T = 300$ K, final $R = 0{\cdot}045$ for 676 observed reflections. The pyran ring is planar ($\chi^2 = 7{\cdot}81$). The molecules are linked by an O—H···O hydrogen bond [1·87 (3) and 2·08 (4) Å].

Experimental. A crystal of dimensions 0·1 × 0·15 × 0·15 mm was used; D_m by flotation in $CHBr_3/CCl_4$; Weissenberg photograph indicated a monoclinic lattice; Syntex $P2_1$ diffractometer, graphite monochromator, $\theta/2\theta$ scan. $2\theta_{max} = 110°$, time per reflection *ca* 60 s; two standard reflections ($0\bar{2}1$ and 121), variation 0·9 and 1·0%; 25 reflections with $7{\cdot}1 < 2\theta < 29{\cdot}5°$ used for refinement of lattice parameters; absorption correction was not applied; index range $-4 \le h \le 4$, $0 \le k \le 18$, $0 \le l \le 8$, 937 reflections measured, 741 unique, 676 [$I > 2{\cdot}449\sigma(I)$]. Choice of lattice parameters from program *UB* (Sivý, Sivý & Koreň, 1987). Data reduction carried out with program *XP*21 (Pavelčik, 1987). Positions of non-H atoms determined by direct methods in program *SHELXS*86 (Sheldrick, 1986). Anisotropic refinement by least squares (full matrix, F values). All H atoms were located from a difference Fourier map and refined isotropically. Scattering factors and f', f'' from *International Tables for X-ray Crystallography* (1974, Vol. IV, pp. 55, 99, 149). Maximum positive and maximum negative electron density in final difference Fourier synthesis 0·18 and 0·20 e Å^{-3}; final $R = 0{\cdot}045$, $wR = 0{\cdot}068$, $w = 1{\cdot}0/[\sigma^2(F_o) + 0{\cdot}005426F_o^2]$; $(\Delta/\sigma)_{max} = 0{\cdot}227$ in final refinement cycle (116 parameters). Calculations per-

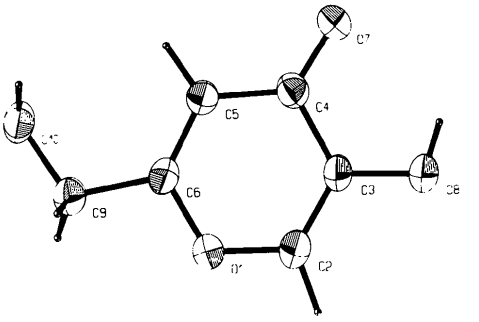

Fig. 1. A view of the molecule showing the atomic numbering.

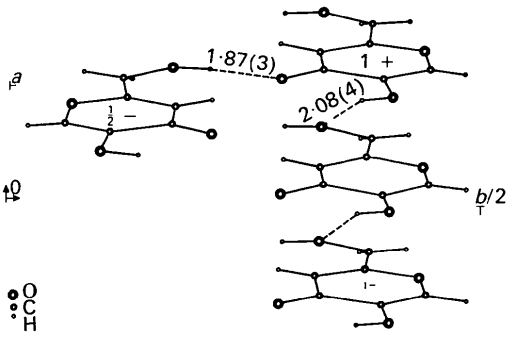

Fig. 2. Projection of the crystal structure down the x axis.

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Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* ($\times 10^4$) *of the non-H atoms*

$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i . \mathbf{a}_j$.

	x	y	z	U_{eq}(Å^2)
O(1)	1791 (5)	4447 (1)	3583 (2)	355 (7)
C(2)	1888 (8)	4525 (2)	1998 (3)	380 (9)
C(3)	3236 (8)	4013 (1)	1131 (3)	333 (9)
C(4)	4674 (7)	3351 (1)	1853 (3)	311 (9)
C(5)	4468 (7)	3296 (1)	3518 (3)	306 (9)
C(6)	3062 (7)	3833 (1)	4310 (3)	299 (9)
O(7)	5921 (6)	2886 (1)	1016 (2)	451 (8)
O(8)	3310 (7)	4118 (1)	−432 (2)	502 (9)
C(9)	2628 (9)	3867 (2)	6041 (3)	353 (11)
O(10)	4499 (6)	3324 (1)	6940 (2)	387 (8)

Table 2. *Interatomic distances* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

O(1)—C(2)	1·360 (1)	C(4)—O(7)	1·244 (1)
O(1)—C(6)	1·352 (1)	C(5)—C(4)	1·431 (2)
C(3)—C(2)	1·337 (2)	C(5)—C(6)	1·343 (2)
C(3)—O(8)	1·346 (2)	C(9)—C(6)	1·502 (2)
C(4)—C(3)	1·444 (2)	C(9)—O(10)	1·406 (2)
C(6)—O(6)—C(2)	119·4 (1)	O(7)—C(4)—C(3)	119·4 (1)
O(1)—C(2)—C(3)	121·9 (1)	C(4)—C(5)—C(6)	121·0 (1)
C(2)—C(3)—C(4)	120·8 (1)	O(1)—C(6)—C(9)	109·8 (1)
C(4)—C(3)—O(8)	119·4 (1)	C(9)—C(6)—C(5)	128·2 (1)
O(8)—C(3)—C(2)	119·7 (1)	C(5)—C(6)—O(1)	122·1 (1)
C(3)—C(4)—C(5)	114·8 (1)	C(6)—C(9)—O(10)	113·1 (1)
C(5)—C(4)—O(7)	125·9 (1)		

formed using an M4030-1 computer, Slovak Technical University, Bratislava, Czechoslovakia, with *SHELX*76 (Sheldrick, 1976). Structure and atomic numbering shown in Fig. 1* (drawn by use of *ORTEP;* Johnson, 1965). Projection of crystal structure in Fig. 2 (Pavelčík, Kettmann & Majer, 1985). Fractional atomic coordinates for non-H atoms are in Table 1; bond distances and angles are in Table 2.

Related literature. Kojic acid was prepared by transformation of saccharides with cultivated Aspergillus tamaril strain (Uher, 1987). Kojic acid can be isolated by thickening of the ultrafiltered medium, followed by crystallization from methanol, acetone or ethyl acetate.

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, bond lengths and angles and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53194 (10 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of a Phosphinohydrazone

BY HERMAN L. AMMON

Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742, *USA*

KARIMAT EL-SAYED

Physics Department, Ain Shams University, Cairo, Egypt

AND F. A. FOULI

Chemistry Department, Ain Shams University, Cairo, Egypt

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Abstract. $C_{27}H_{20}ClN_2O_3P$, $M_r = 486·9$, orthorhombic, $P2_12_12_1$, $a = 5·3832$ (4), $b = 15·884$ (2), $c = 27·67$ (1) Å, $V = 2366$ (1) Å^3, $Z = 4$, $D_x = 1·37$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å (graphite monochromator), $\mu = 23·3$ cm^{-1}, $F(000) = 1008$, $T = 293$ K, final $R = 0·042$ for 1911 reflections with $I >$

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