Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

Gallic acid monohydrate

Ren-Wang Jiang, Dong-Sheng Ming, Paul P. H. But and Thomas C. W. Mak*

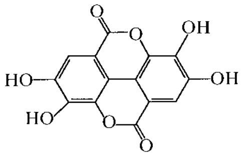
Department of Chemistry and Chinese Medicinal Material Research Centre, The Chinese University of Hong Kong, Hong Kong SAR, People's Republic of China
Correspondence e-mail: tcwmak@cuhk.edu.hk

Received 15 October 1999
Accepted 2 February 2000

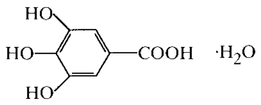
In the crystal structure of the title compound, 3,4,5-trihydroxybenzoic acid monohydrate, $C_7H_6O_5\cdot H_2O$, the gallic acid molecule has an intramolecular hydrogen bond involving a pair of hydroxyl groups, and it is also linked to a water molecule by a three-centre (bifurcated) O*W*—H···O hydrogen bond. The packing of the molecules is stabilized by intermolecular O—H···O and C—H···O hydrogen bonds.

Comment

Tannins are widely distributed in many edible and medicinal plants, and some with strong pharmacological activities have been used as hæmostatic and astringent agents. There are two kinds of tannins in nature: one is condensation tannin and the other is hydrolysable tannin. The basic units of hydrolysable tannins are ellagic acid, (I), and gallic acid. The crystal structure of the former was published over three decades ago (Mathieson & Poppleton, 1968). In the present paper, we report the crystal structure of gallic acid monohydrate, (II), which has been shown to exhibit antibacterial and antiviral activities (Jiang & Xiao, 1986).



(I)



(II)

The molecule of (II) is essentially planar. The mean deviation of the benzene ring is 0.0028 Å and its dihedral angle with the plane of the carboxyl group is 2.9°. The bond distances are all normal.

Within the asymmetric unit, there is an intramolecular hydrogen bond between O1 and O2. The water molecule is linked to the gallic acid by a three-centre (bifurcated) donor hydrogen bond to two acceptor hydroxyl groups, as represented by O*W*—HO*WB*···O2 and O*W*—HO*WB*···O3 (Fig. 1). These hydrogen bonds form two five-membered hydrogen-bonded rings. The intermolecular hydrogen bonds O3—H···O*W*, O2—H···O*W* and O*W*—HO*WA*···O2 link the asymmetric unit at the junction where the water molecules are spirally distributed, to form a channel running parallel to the *a* axis. The intermolecular hydrogen bond O4—H···O5 links the two adjacent channels and results in extended 'wavy' sheets parallel to the (200) plane. Adjacent sheets are linked by hydrogen bond O1—H···O5 and a weak C—H···O hydrogen bond between C6 and O1 to form a supramolecular assembly. Details of the hydrogen bonds are listed in Table 2. The crystal packing is shown in Fig. 2 in a projection along the short *b* axis.

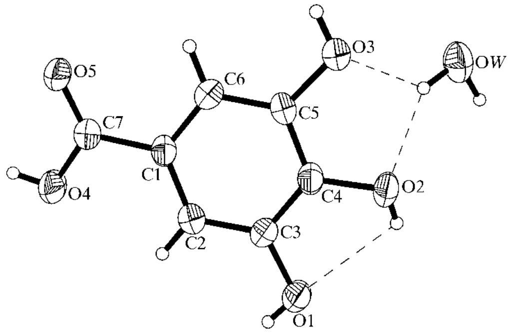


Figure 1
The molecular structure of (II) showing 50% probability displacement ellipsoids and the atom-numbering scheme; the hydrogen bonds in the asymmetric unit are indicated by dashed lines.

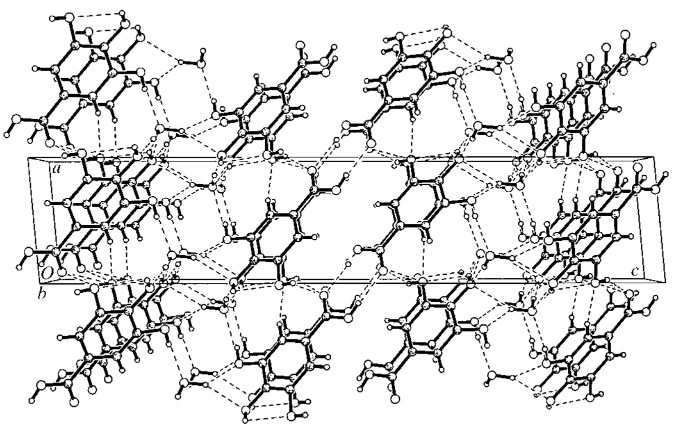


Figure 2
Packing diagram for (II) viewed down the *b* axis.

Experimental

A sample of compound (II) was extracted from the whole plant of *Geum japonicum*. The dried plant material (3 kg) was chopped into small pieces and extracted with 95% ethanol at room temperature. The extracted liquid was evaporated *in vacuo* to yield an ethanol extract (80 g), which was then suspended in distilled water and successively extracted with hexane, ethyl acetate and *n*-butanol. The *n*-butanol extract was subjected to Sephadex LH-20 column chromatography and eluted with EtOH–H_2O (4:1). The eluted liquid was condensed and allowed to stand at room temperature and yellow prismatic crystals of (II) (50 mg) were obtained.

Crystal data

$C_7H_6O_5{\cdot}H_2O$
$M_r = 188.13$
Monoclinic, $P2_1/c$
$a = 5.794\ (4)$ Å
$b = 4.719\ (5)$ Å
$c = 28.688\ (5)$ Å
$\beta = 95.08\ (3)^\circ$
$V = 781.4\ (3)$ Å^3
$Z = 4$

$D_x = 1.599$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 7.5$–12.5°
$\mu = 0.144$ mm^{-1}
$T = 293$ K
Prism, yellow
0.5 × 0.2 × 0.1 mm

Data collection

Rigaku AFC-7R diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (Rigaku, 1998)
$T_{\min} = 0.945$, $T_{\max} = 1.000$
1514 measured reflections
1369 independent reflections
907 reflections with $F > 4\sigma(F^2)$

$R_{\rm int} = 0.032$
$\theta_{\max} = 25^\circ$
$h = -1 \rightarrow 6$
$k = -1 \rightarrow 5$
$l = -34 \rightarrow 33$
3 standard reflections every 197 reflections intensity decay: none

Refinement

Refinement on F^2
$R(F) = 0.042$
$wR(F^2) = 0.127$
$S = 1.006$
1369 reflections
122 parameters

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0746P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.016$
$\Delta\rho_{\max} = 0.17$ e Å^{-3}
$\Delta\rho_{\min} = -0.25$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C3	1.371 (3)	C1—C6	1.390 (3)
O2—C4	1.375 (3)	C1—C7	1.474 (3)
O3—C5	1.371 (3)	C2—C3	1.385 (3)
O4—C7	1.315 (3)	C3—C4	1.380 (3)
O5—C7	1.229 (3)	C4—C5	1.383 (3)
C1—C2	1.390 (3)	C5—C6	1.381 (3)
C2—C1—C6	120.9 (2)	C3—C4—C5	120.2 (1)
C2—C1—C7	120.9 (2)	O3—C5—C6	123.7 (2)
C6—C1—C7	118.2 (2)	O3—C5—C4	115.9 (1)
C3—C2—C1	119.0 (2)	C6—C5—C4	120.3 (2)
O1—C3—C4	114.6 (2)	C5—C6—C1	119.2 (2)
O1—C3—C2	125.0 (2)	O5—C7—O4	121.1 (2)
C4—C3—C2	120.3 (2)	O5—C7—C1	123.9 (2)
O2—C4—C3	122.6 (2)	O4—C7—C1	115.0 (2)
O2—C4—C5	117.1 (1)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
OW—HOWA···O2$^{\rm i}$	1.01	1.90	2.906 (4)	174
OW—HOWB···O2	0.97	2.18	3.058 (4)	151
OW—HOWB···O3	0.97	2.19	2.944 (4)	134
O1—HO1···O5$^{\rm ii}$	0.82	2.06	2.796 (4)	150
O2—HO2···O1	0.82	2.33	2.693 (4)	108
O2—HO2···O$W^{\rm i}$	0.82	1.94	2.708 (4)	157
O3—HO3···O$W^{\rm iii}$	0.82	1.92	2.699 (4)	160
O4—HO4···O5$^{\rm iv}$	0.82	1.85	2.663 (4)	175
C6—H6···O1$^{\rm v}$	0.93	2.44	3.350 (5)	166

Symmetry codes: (i) $2-x, \frac{1}{2}+y, \frac{1}{2}-z$; (ii) $1+x, 1+y, z$; (iii) $1-x, y-\frac{1}{2}, \frac{1}{2}-z$; (iv) $-x, 1-y, -z$; (v) $x-1, y-1, z$.

H(—C) atoms were generated geometrically and treated with a riding model. H(—O) were located from difference maps and refined with isotropic displacement parameters.

Data collection: *Rigaku/AFC Diffractometer Control Software* (Rigaku, 1998); cell refinement: *Rigaku/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1998).

This work is supported by Hong Kong Research Grants Council Earmarked Grant CUHK 4206/99P and Industrial Support Fund AF/281/97.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: DE1123). Services for accessing these data are described at the back of the journal.

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