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Gallic acid monohydrate

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Key indicators

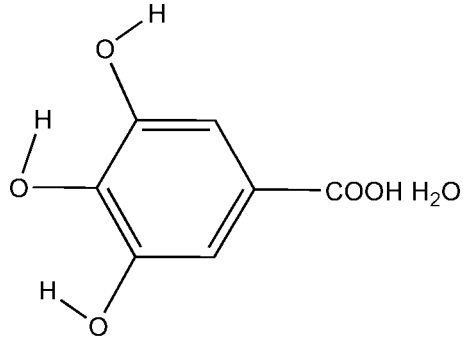
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.005 Å
R factor = 0.049
wR factor = 0.188
Data-to-parameter ratio = 15.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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 is essentially planar and has two intramolecular hydrogen bonds between hydroxyl groups. The H atoms of the three hydroxyl groups are oriented in the same direction around the ring, and form intra- and intermolecular hydrogen bonds. The crystal structure is stabilized by all available intermolecular hydrogen bonds, including also those involving the water molecule.

Comment

Gallic acid, 3,4,5-trihydroxybenzoic acid, is a naturally occurring plant phenol which has antitumor and anti-oxidative activity. It induces apotosis in the human myelogenous leukemic cell line (Sakaguchi *et al.*, 1999; Satoh & Sakagami, 1997). Therefore the determination of its crystal structure is important for the structural clarification of its biological function. Recently the crystal structure was determined in a monohydrate form by Jiang *et al.* (2000). We have now determined its structure as a different monohydrated form, (I).



(I)

The molecular structure of (I) is essentially planar, as shown in Fig. 1. In the molecule, all the H atoms of the three hydroxyl groups are oriented in the same direction around the ring, forming two intramolecular hydrogen bonds between a pair of hydroxyl groups at positions 3 and 4, and at positions 4 and 5. The hydroxyl groups at positions 3 and 4 are also linked to the water-O atom and to the hydroxyl-O atom of a neighbouring molecule by a bifurcated hydrogen bond. This hydrogen-bonding scheme is different from that reported by Jiang *et al.* (2000), in which only one intramolecular hydrogen bond is present, and one of the three H atoms of the hydroxyl groups is oriented in the reverse direction to the others. Furthermore, a hydrogen bond is formed between the carboxyl groups in the

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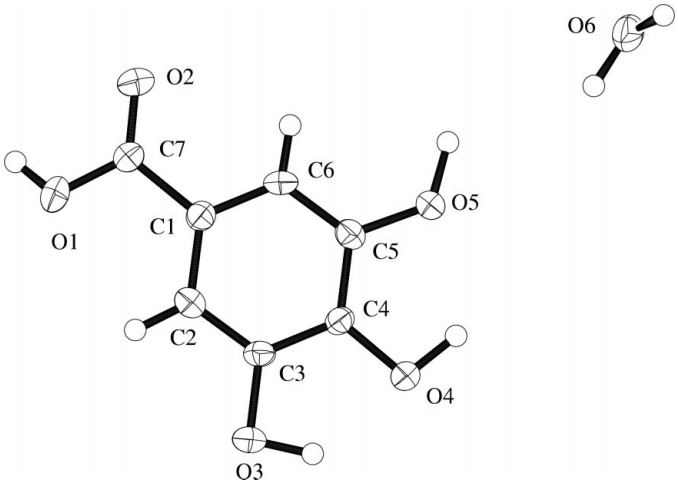

Figure 1
*ORTEP*II (Johnson, 1976) drawing of the title compound with the atomic numbering scheme. Ellipsoids for non-H atoms correspond to 50% probability.

previous structure, but this interaction is not present in the structure reported here. All of the possible hydrogen bonds are present as either intra- or intermolecular interactions, as shown in Table 2. The two different crystal structures and hydrogen-bonding schemes observed for gallic acid monohydrate may have a role in the biological function of this compound.

Experimental

The crystal was obtained by slow evaporation of an ethanol solution.

Crystal data

$C_7H_6O_5\cdot H_2O$
M_r = 188.13
Monoclinic, $P2/n$
a = 14.15 (1) Å
b = 3.622 (9) Å
c = 15.028 (10) Å
β = 97.52 (7)°
V = 764 (1) Å^3
Z = 4
D_x = 1.636 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 18 reflections
θ = 10.0–14.3°
μ = 0.15 mm^{-1}
T = 296.2 K
Needle, colorless
0.50 × 0.10 × 0.03 mm

Data collection

Rigaku AFC-5*R* diffractometer
ω–2θ scans
Absorption correction: none
2109 measured reflections
1766 independent reflections
764 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 27.5°
$h = 0 \rightarrow 18$
$k = -4 \rightarrow 0$
$l = -19 \rightarrow 19$
3 standard reflections
every 150 reflections
intensity decay: 0.1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.188
S = 0.91
1766 reflections
118 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.317 (5)	C1—C6	1.380 (5)
O2—C7	1.203 (5)	C1—C7	1.487 (5)
O3—C3	1.373 (4)	C2—C3	1.376 (4)
O4—C4	1.370 (4)	C3—C4	1.391 (5)
O5—C5	1.372 (4)	C4—C5	1.390 (5)
C1—C2	1.396 (5)	C5—C6	1.377 (4)
C2—C1—C6	119.7 (3)	C3—C4—C5	119.3 (3)
C2—C1—C7	122.2 (3)	O5—C5—C4	116.8 (3)
C6—C1—C7	118.0 (3)	O5—C5—C6	124.0 (3)
C1—C2—C3	119.3 (3)	C4—C5—C6	119.6 (3)
O3—C3—C2	119.8 (3)	C1—C6—C5	121.0 (3)
O3—C3—C4	119.2 (3)	O1—C7—O2	122.6 (3)
C2—C3—C4	121.0 (3)	O1—C7—C1	113.5 (3)
O4—C4—C3	117.4 (3)	O2—C7—C1	123.8 (3)
O4—C4—C5	123.2 (3)		
O1—C7—C1—C2	2.7 (5)	O5—C5—C4—C3	−178.9 (3)
O1—C7—C1—C6	178.6 (3)	O5—C5—C6—C1	177.2 (3)
O2—C7—C1—C2	−175.3 (4)	C1—C2—C3—C4	−1.9 (6)
O2—C7—C1—C6	0.2 (6)	C1—C6—C5—C4	−1.5 (6)
O3—C3—C2—C1	−179.0 (3)	C2—C1—C6—C5	1.4 (6)
O3—C3—C4—O4	−0.2 (5)	C2—C3—C4—C5	1.8 (6)
O3—C3—C4—C5	179.0 (3)	C3—C2—C1—C6	0.3 (6)
O4—C4—C3—C2	−177.3 (3)	C3—C2—C1—C7	175.7 (4)
O4—C4—C5—O5	0.9 (5)	C3—C4—C5—C6	−0.1 (6)
O4—C4—C5—C6	178.9 (4)	C5—C6—C1—C7	−174.2 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O4	0.850	2.328	2.692 (8)	106.3
O4—H4···O5	0.945	2.306	2.752 (8)	108.9
O3—H3···O6^{i}	0.850	1.949	2.770 (4)	161.6
O4—H4···O5^{ii}	0.945	1.907	2.767 (8)	150.0
O5—H5···O2^{iii}	0.851	1.878	2.729 (4)	177.7
O6—H7···O4^{ii}	0.820	2.182	2.977 (4)	163.8
O6—H8···O3^{iv}	0.812	1.941	2.747 (4)	170.9
O1—H1···O6^{iii}	0.830	1.859	2.686 (4)	174.2

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

All H atoms were located from difference Fourier maps and were not refined.

Data collection: *MSC /AFC Diffractometer Control Software* (Molecular Structure Corporation & Rigaku Corporation, 1999); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation & Rigaku Corporation, 1999); program(s) used to solve structure: *SIR*88 (Burla *et al.*, 1989) and *DIRDIF* (Beurskens *et al.*, 1992); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *TEXSAN*.

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