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2-Hydroxy-3-methoxybenzoic acid

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Key indicators

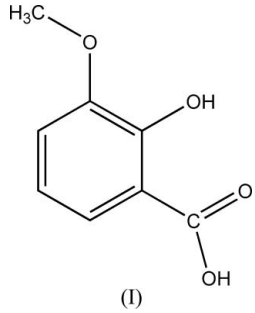
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.116
Data-to-parameter ratio = 12.0

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

The title compound, $C_8H_8O_4$, has an intramolecular O—H···O hydrogen bond. Intermolecular O—H···O hydrogen bonding gives rise to a dimeric structure, which is further extended into infinite stacks parallel to the *a* axis *via* π–π interactions between the aromatic rings of neigboring molecules.

Comment

Hydrogen-bonding interactions between ligands are specific and directional. When present in metal complexes they are usually not dependent on the properties of the metal ions, but they play a critical role in the overall structures and functions of the complexes and the way in which they pack in the solid state. In this sense, 2-hydroxy-3-methoxybenzoic acid is an excellent candidate for the construction of supramolecular complexes, since it not only has multiple coordination modes but can also form regular hydrogen bonds, functioning as both a hydrogen-bond donor and acceptor (Moncol *et al.*, 2006; Kozlevcar *et al.*, 2006). In this context we report here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) is depicted in Fig. 1. The C—O and C—C distances show no remarkable features, with C—O distances in the range 1.237 (2)–1.426 (2) Å. The title molecule acts as both a hydrogen-bond donor and acceptor, forming dimers with neighboring molecules through O—H···O hydrogen bonding (Table 1), while π–π interactions between the dimers lead to the formation of infinite stacks of the molecules along the *a* axis (Fig. 2). The centroid-to-centroid and interplanar distances between adjacent aromatic rings (symmetry code: $x-1, y, z$) are 3.867 (4) and 3.528 (3) Å, respectively.

Experimental

2-Hydroxy-3-methoxybenzoic acid was dissolved in hot methanol with stirring. Yellow single crystals suitable for X-ray diffraction were

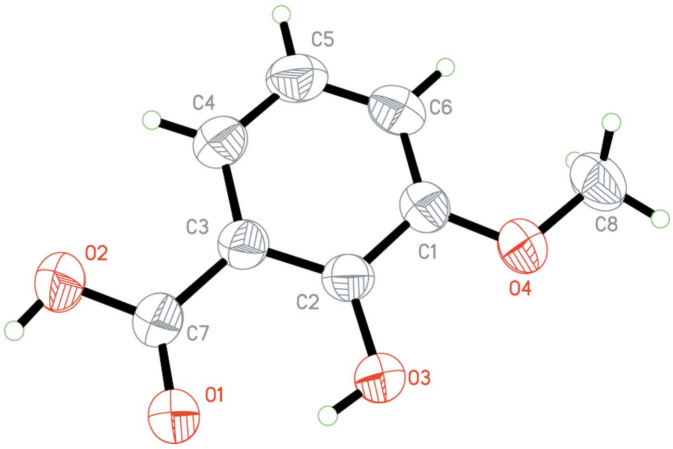


Figure 1
The molecular structure of (I), showing the atomic numbering scheme. Non-H atoms are shown with 50% probability displacement ellipsoids.

obtained at room temperature by slow evaporation of the solvent over a period of several days.

Crystal data

$C_8H_8O_4$
M_r = 168.14
Monoclinic, $P2_1/n$
a = 3.8668 (2) Å
b = 27.9090 (11) Å
c = 7.0885 (3) Å
β = 94.319 (2)°
V = 762.81 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 293 (2) K
0.20 × 0.18 × 0.15 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: none
4322 measured reflections
1346 independent reflections
1051 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.116
S = 1.05
1346 reflections
112 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.82	1.85	2.6703 (15)	176
O3—H3···O1	0.82	1.90	2.6169 (14)	145

Symmetry code: (i) $-x, -y, -z+1$.

All H atoms were placed in calculated positions (C—H = 0.93 or 0.96 Å; O—H = 0.82 Å) and were refined using a riding model, with

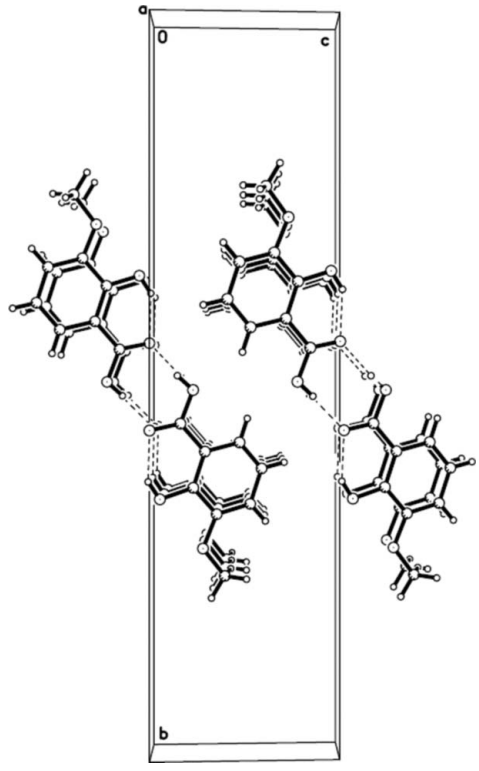


Figure 2
The molecular packing of (I), showing the intra- and intermolecular hydrogen bonding and π–π interactions. The view is along the a axis and hydrogen-bonding interactions are shown as dashed lines.

U_{iso}(H) = 1.2U_{eq}(C) for H atoms of the aromatic ring and 1.5U_{eq}(C,O) for methyl and hydroxyl H atoms.

Data collection: *APEXII* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

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