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4-Hydroxybenzamide

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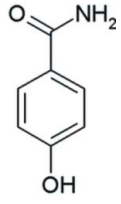
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.044; data-to-parameter ratio = 7.3.

The crystal structure of the title compound, $C_7H_7NO_2$, has not hitherto been published. The structure is stabilized by intermolecular O—H···O and N—H···O hydrogen bonds. The topology of the hydrogen-bond network can be characterized by the graph-set notation $R_4^4(20)$.

Related literature

For related literature, see: Kashino *et al.* (1991); Katsube *et al.* (1966); Pertlik (1990); Sasada *et al.* (1964); Etter (1990).



Experimental

Crystal data

$C_7H_7NO_2$
M_r = 137.14
Monoclinic, $P2_1/c$
a = 4.5828 (15) Å
b = 8.825 (3) Å
c = 15.888 (5) Å
β = 90.770 (7)°
V = 642.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293.1 K
0.30 × 0.20 × 0.20 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.905, T_{max} = 0.979
5970 measured reflections
1754 independent reflections
871 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.044
S = 5.41
871 reflections
119 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H5···O1^{i}	0.90 (3)	1.84 (3)	2.706 (2)	161 (2)
N3—H1···O2^{ii}	0.93 (3)	2.14 (3)	3.017 (3)	156 (2)
N3—H2···O1^{iii}	0.90 (3)	2.21 (3)	3.088 (3)	166 (2)

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2005); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEX* (McArdle, 1993) and *ORTEPIII* (Burnett & Johnson, (1996); software used to prepare material for publication: *CrystalStructure*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2135).

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  doi:10.1107/S160053680701793X

supplementary materials

Acta Cryst. (2007). E**63**, o2362 [**doi:10.1107/S160053680701793X**]

4-Hydroxybenzamide

L. K. Hansen, G. L. Perlovich and A. Bauer-Brandl

Comment

The molecular structure of the title compound, (III), is presented in Fig. 2. The geometric parameters of the hydrogen bonds are summarized in Table 1. The molecular packing is shown in Figs. 2 and 3.

The structure of its monohydrate was determined some years ago (Kashino *et al.*, 1991). The unit-cell volume of (III) is 642.5 (3) $Å^3$, whereas for the hydrate it is 746.7 (2) $Å^3$. In (III), there are two N—H···O and one O—H···O intermolecular hydrogen bonds. In the monohydrate, there are two N—H···O, two O(water)—H···O and one O—H···O(water) intermolecular hydrogen bonds.

The crystal structures of 2-hydroxybenzamide (salicylamide), (I) (Sasada *et al.*, 1964; Pertlik, 1990), and 3-hydroxybenzamide, (II) (Katsube *et al.*, 1966), have also been determined previously.

Experimental

A commercial sample of 4-hydroxybenzamide (Sigma-Aldrich Co. Ltd, St. Louis, USA) was used. Crystals of (III) were grown by slow evaporation of an acetone solution.

Refinement

The crystals were of poor quality and weakly diffracting, which accounts for the low fraction of measured reflections. The H atoms were placed in idealized locations, with C—H = 0.96 (2)–0.99 (2) Å, O—H = 0.90 (3) Å and N—H = 0.90 (3)–0.93 (3) Å, and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C,N)$ or $1.5U_{eq}(O,C\text{-methyl})$.

Figures

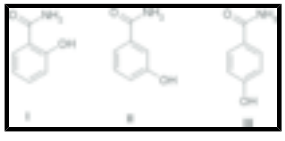


Fig. 1. Chemical schemes for compounds (I), (II) and (III).

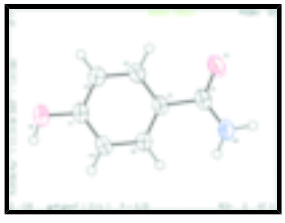


Fig. 2. The molecular structure of (III), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

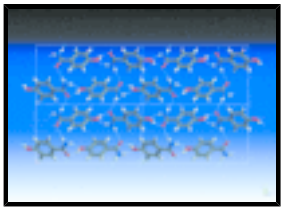


Fig. 3. Projection of the molecular packing of (III) along the a axis. Dashed lines indicate hydrogen bonds.

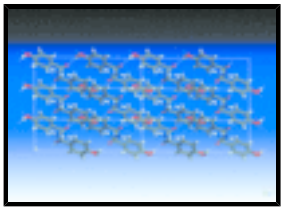


Fig. 4. Projection of the molecular packing of (III) along the b axis. Dashed lines indicate hydrogen bonds.

4-Hydroxybenzamide

Crystal data

$C_7H_7NO_2$	F_{000} = 288.00
M_r = 137.14	D_x = 1.418 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 433.1 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71070 Å
a = 4.5828 (15) Å	Cell parameters from 1110 reflections
b = 8.825 (3) Å	θ = 2.6–30.1°
c = 15.888 (5) Å	μ = 0.11 mm^{-1}
β = 90.770 (7)°	T = 293.1 K
V = 642.5 (3) Å^3	Prism, colourless
Z = 4	0.30 × 0.20 × 0.20 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer	871 reflections with $F^2 > 2\sigma(F^2)$
Detector resolution: 7.31 pixels mm^{-1}	R_{int} = 0.031
ω scans	θ_{max} = 30.6°
Absorption correction: multi-scan (Jacobson, 1998)	h = −6→6
T_{min} = 0.905, T_{max} = 0.979	k = −12→12
5970 measured reflections	l = −22→16
1754 independent reflections	

Refinement

Refinement on F	$(\Delta/\sigma)_{max}$ = 0.115
$R[F^2 > 2\sigma(F^2)]$ = 0.047	$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$wR(F^2)$ = 0.044	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
S = 5.41	Extinction correction: none

871 reflections
119 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2 + 0.3454P]$
where $P = (F_o^2 + 2F_c^2)/3$

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY

Refinement. Refinement using reflections with $F^2 > 2.0$ sigma(F^2). The weighted R-factor(wR), goodness of fit (S) and R-factor (gt) are based on F, with F set to zero for negative F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.7483 (4)	0.1346 (2)	0.30494 (11)	0.0527 (5)
O2	1.0947 (5)	0.2443 (2)	−0.07333 (11)	0.0543 (6)
N3	0.4860 (5)	0.3475 (3)	0.28422 (14)	0.0492 (7)
C4	0.6686 (5)	0.2409 (3)	0.25753 (13)	0.0398 (7)
C5	0.7782 (5)	0.2489 (3)	0.16993 (12)	0.0357 (6)
C6	0.9893 (6)	0.1458 (3)	0.14555 (16)	0.0431 (7)
C7	0.9875 (6)	0.2478 (3)	0.00638 (14)	0.0400 (7)
C8	1.0950 (6)	0.1447 (3)	0.06454 (16)	0.0461 (8)
C9	0.6756 (6)	0.3535 (3)	0.11146 (16)	0.0456 (7)
C10	0.7795 (6)	0.3522 (3)	0.02972 (16)	0.0460 (8)
H1	0.406 (6)	0.334 (3)	0.3373 (18)	0.054 (8)*
H2	0.421 (6)	0.422 (3)	0.250 (2)	0.065 (10)*
H3	0.527 (6)	0.429 (3)	0.1269 (18)	0.054 (8)*
H4	0.704 (6)	0.422 (3)	−0.0127 (19)	0.067 (9)*
H5	0.989 (8)	0.304 (4)	−0.108 (2)	0.098 (15)*
H6	1.243 (7)	0.075 (3)	0.048 (2)	0.074 (10)*
H7	1.054 (6)	0.073 (3)	0.1873 (18)	0.057 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0770 (15)	0.0490 (11)	0.0321 (8)	−0.0021 (11)	0.0042 (9)	0.0073 (9)
O2	0.0657 (14)	0.0658 (15)	0.0316 (9)	0.0105 (13)	0.0122 (9)	0.0015 (10)
N3	0.0632 (17)	0.0505 (16)	0.0343 (11)	0.0026 (14)	0.0132 (11)	0.0018 (12)
C4	0.0483 (16)	0.0407 (15)	0.0303 (11)	−0.0099 (15)	0.0013 (11)	−0.0005 (12)
C5	0.0420 (14)	0.0366 (14)	0.0285 (10)	−0.0048 (12)	0.0025 (10)	−0.0003 (10)
C6	0.0502 (16)	0.0447 (16)	0.0344 (12)	0.0017 (14)	0.0017 (11)	0.0031 (12)
C7	0.0449 (14)	0.0446 (16)	0.0305 (10)	−0.0048 (14)	0.0056 (10)	−0.0039 (12)
C8	0.0506 (17)	0.0485 (17)	0.0392 (13)	0.0070 (15)	0.0058 (12)	−0.0009 (13)
C9	0.0532 (17)	0.0488 (17)	0.0352 (12)	0.0103 (16)	0.0105 (11)	0.0039 (13)
C10	0.0555 (18)	0.0517 (18)	0.0310 (12)	0.0065 (16)	0.0071 (11)	0.0088 (13)

Geometric parameters (Å, °)

O1—C4	1.254 (3)	C9—C10	1.389 (3)
O2—C7	1.365 (3)	O2—H5	0.90 (3)
N3—C4	1.333 (3)	N3—H1	0.93 (3)
C4—C5	1.488 (3)	N3—H2	0.90 (3)
C5—C6	1.387 (4)	C6—H7	0.96 (2)
C5—C9	1.387 (3)	C8—H6	0.96 (3)
C6—C8	1.381 (3)	C9—H3	0.99 (2)
C7—C8	1.383 (4)	C10—H4	0.97 (3)
C7—C10	1.380 (4)		
O1—C4—N3	121.1 (2)	C7—O2—H5	111 (2)
O1—C4—C5	119.9 (2)	C4—N3—H1	116.8 (18)
N3—C4—C5	119.0 (2)	C4—N3—H2	122 (2)
C4—C5—C6	118.4 (2)	H1—N3—H2	121 (2)
C4—C5—C9	122.9 (2)	C5—C6—H7	116.9 (17)
C6—C5—C9	118.7 (2)	C8—C6—H7	121.8 (17)
C5—C6—C8	121.3 (2)	C6—C8—H6	121.2 (19)
O2—C7—C8	118.4 (2)	C7—C8—H6	119.4 (19)
O2—C7—C10	121.5 (2)	C5—C9—H3	120.8 (16)
C8—C7—C10	120.1 (2)	C10—C9—H3	119.0 (16)
C6—C8—C7	119.4 (2)	C7—C10—H4	118.6 (18)
C5—C9—C10	120.2 (2)	C9—C10—H4	121.2 (18)
C7—C10—C9	120.2 (2)		
O1—C4—C5—C6	−6.2 (4)	C9—C5—C6—C8	−0.8 (4)
O1—C4—C5—C9	172.9 (2)	C5—C6—C8—C7	−0.3 (4)
N3—C4—C5—C6	173.9 (2)	O2—C7—C8—C6	−179.8 (2)
N3—C4—C5—C9	−7.0 (4)	O2—C7—C10—C9	−179.7 (2)
C4—C5—C6—C8	178.4 (2)	C8—C7—C10—C9	−0.5 (4)
C4—C5—C9—C10	−177.9 (2)	C10—C7—C8—C6	0.9 (4)
C6—C5—C9—C10	1.2 (4)	C5—C9—C10—C7	−0.6 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H5···O1^{i}	0.90 (3)	1.84 (3)	2.706 (2)	161 (2)
N3—H1···O2^{ii}	0.93 (3)	2.14 (3)	3.017 (3)	156 (2)
N3—H2···O1^{iii}	0.90 (3)	2.21 (3)	3.088 (3)	166 (2)

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2; (ii) *x*−1, −*y*+1/2, *z*+1/2; (iii) −*x*+1, *y*+1/2, −*z*+1/2.

Fig. 1

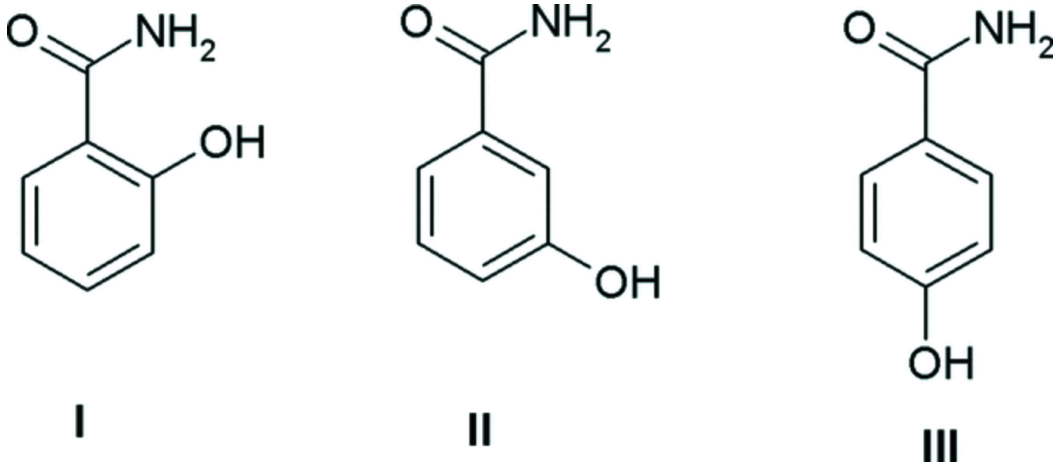
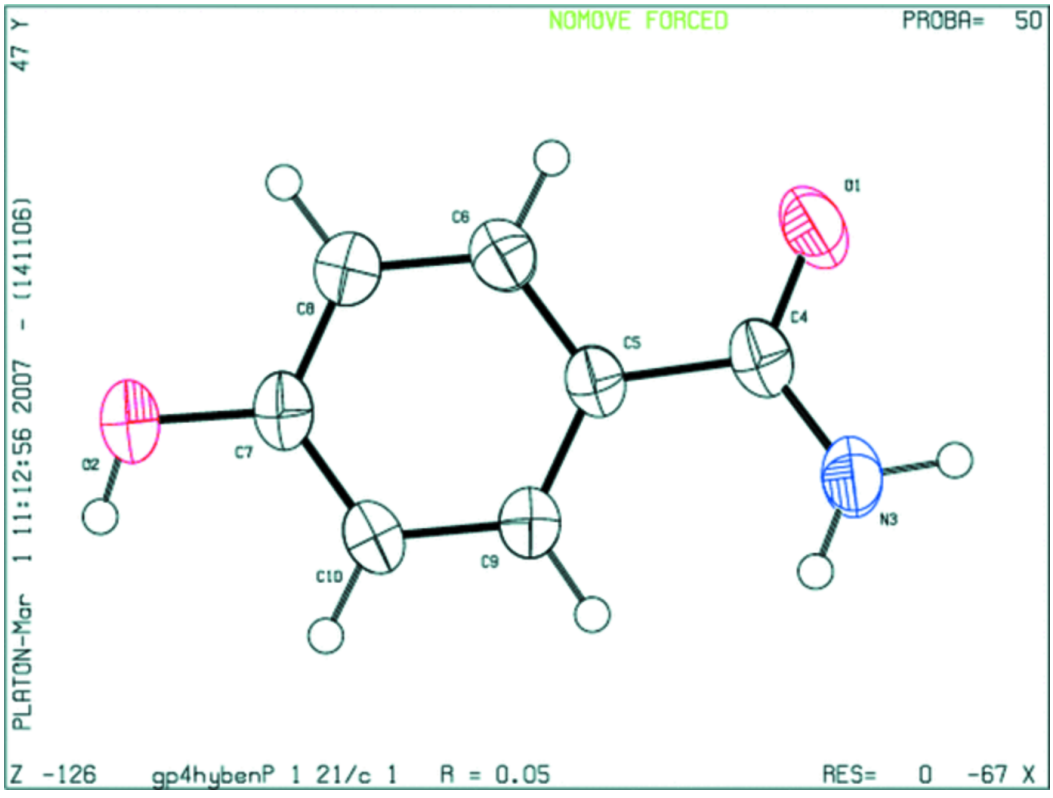


Fig. 2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C8
C4
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Fig. 3

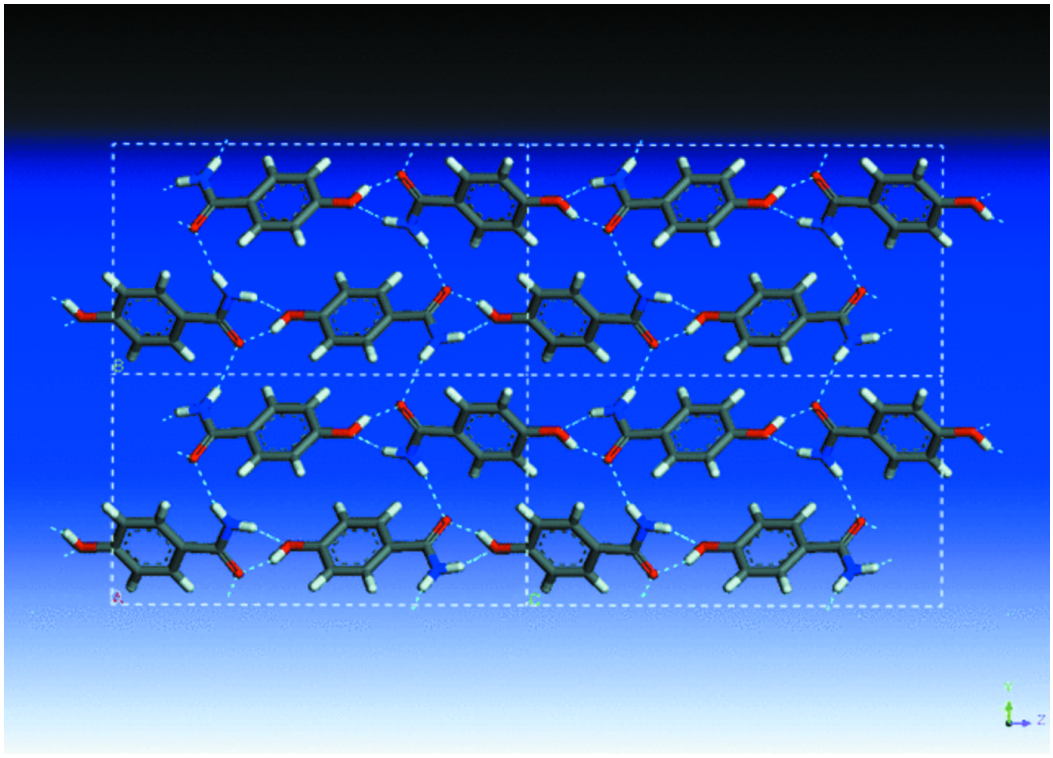

Fig. 4