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3-(Acetylamino)benzoic acid

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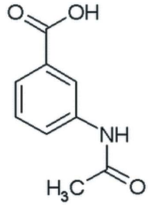
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.052; wR factor = 0.037; data-to-parameter ratio = 7.8.

The title compound, $C_9H_9NO_3$, was crystallized from methanol. The monoclinic structure features one molecule in the asymmetric unit. The topology of the O—H···O and N—H···O hydrogen-bond network can be characterized by the graph-set assignments $C(9)$ and $R_2^2(14)$.

Related literature

For the crystal structures of the *ortho*- and *para*-isomers of the title compound, see: Feeder & Jones (1992); Kashino *et al.* (1986); Kovalevsky (1999); Mascarenhas *et al.* (1980); Rajnikant & Deshmukh (2004).

For related literature, see: Etter (1990).



Experimental

Crystal data

$C_9H_9NO_3$
M_r = 179.17
Monoclinic, $P2_1/n$
a = 3.9522 (15) Å
b = 10.699 (4) Å
c = 19.831 (7) Å
β = 93.393 (8)°
V = 837.1 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293.1 K
0.60 × 0.10 × 0.05 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.937, T_{max} = 0.995
9339 measured reflections
2325 independent reflections
1168 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.037
S = 1.50
1168 reflections
152 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H7···O1^{i}	1.02 (3)	1.71 (3)	2.714 (2)	164 (2)
N1—H1···O2^{ii}	1.02 (2)	2.01 (2)	3.022 (2)	173.3 (18)

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku, 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: *CrystalStructure*; 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: HB2363).

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