

***N*-(3-Hydroxyphenyl)acetamide**Lars Kr. Hansen,<sup>a\*</sup> German L. Perlovich<sup>b,c</sup> and Annette Bauer-Brandl<sup>b</sup><sup>a</sup>Department of Chemistry, University of Tromsø, 9037 Tromsø, Norway, <sup>b</sup>Department of Pharmaceutics and Biopharmaceutics, University of Tromsø, 9037 Tromsø, Norway, and <sup>c</sup>Institute of Solution Chemistry, Russian Academy of Sciences, 153045 Ivanovo, Russian Federation

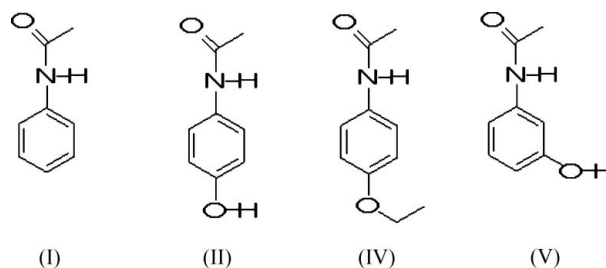
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**Key indicators**Single-crystal X-ray study  
*T* = 293 K  
Mean  $\sigma(C-C)$  = 0.003 Å  
*R* factor = 0.032  
*wR* factor = 0.093  
Data-to-parameter ratio = 9.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the crystal structure of the title compound, C<sub>8</sub>H<sub>9</sub>NO<sub>2</sub>, the topology of the hydrogen-bond network can be characterized by the graph-set *C*(6). The geometry of the hydrogen bonds in this compound is compared with the analogous parameters of similar compounds *viz.* acetanilide, paracetamol (forms I and II) and phenacetin.

**Comment**

Acetanilide derivatives show antipyretic and analgesic actions with undesirable side effects on the human body. The crystal structures of acetanilide, (I) (Johnson *et al.*, 1995), paracetamol (4-acetamidophenol), monoclinic form, (II) (Haisa *et al.*, 1976), paracetamol, orthorhombic form, (III) (Haisa *et al.*, 1974), and phenacetin (4-ethoxyacetanilide), (IV) (Patel *et al.*, 1983), have been reported, but the structure of the title compound, (V), remained unsolved: we report it here (Fig. 1). Its geometrical parameters are normal.



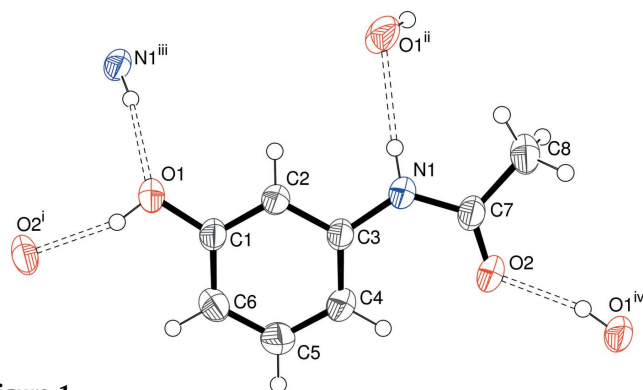
The hydrogen bonds for (V) are listed in Table 1. These result in a *C*(6) graph-set topology (Etter, 1990), as seen also for both forms of paracetamol (Haisa *et al.*, 1976; Haisa *et al.*, 1974). The packing of (V) is shown in Fig. 2.

It is interesting to compare the hydrogen bonds in (V) with the analogous parameters for the similar compounds (I)–(IV). In contrast to (V), molecules (I) and (IV) do not possess additional hydroxyl groups to create two more hydrogen bonds, therefore the hydrogen-bonding networks are formed only from N–H···O<sub>k</sub> (*k* = ketone) bonding and can be described by the graph-set assignment *C*(4).

Comparing the geometric parameters of the N–H···O<sub>h</sub> bonds (*h* = hydroxyl) of (II), (III) and (V) and the N–H···O<sub>k</sub> bonds of (I) and (IV), the *D*–H···*A* angles (°) can be arranged as follows: (III) [159 (4)] < (II) [165 (4)] < (V) [171] < (I) [172.3 (4)] < (IV) [180 (7)]. The *D*···*A* (Å) distances can be ordered as: (II) [2.934 (3)] < (I) [2.935 (3)] < (IV) [2.954 (9)] < (V) [2.963 (3)] < (III) [2.967 (5)].

The geometry of the O<sub>h</sub>–H···O<sub>k</sub> hydrogen bonds in (II), (III) and (V) can be described as follows: the *D*–H···*A* angles (°) are approximately the same within experimental

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**Figure 1**

View of (V) showing 50% displacement ellipsoids (arbitrary spheres for the H atoms). In addition, the appropriate atoms of nearby molecules involved in hydrogen bonding interactions are shown. Symmetry codes as in Table 1; additionally, (iii)  $1 - x, 1 - y, z + \frac{1}{2}$ ; (iv)  $\frac{1}{2} - x, \frac{1}{2} + y, z - \frac{1}{2}$ .

error: (V) [162] < (II) [165 (4)] < (III) [171 (5)]. However, the  $D \cdots A$  (Å) distances show a clear pattern: (V) [2.638 (2)] < (II) [2.663 (3)] < (III) [2.724 (5)]. It may therefore be supposed that the  $O_H - H \cdots O_k$  hydrogen-bond energy of (V) exceeds the analogous values for both (II) and (III) due to a more favourable conformation of the molecules in the crystal structure. It should be mentioned that in (V), a three-dimensional hydrogen-bond network arises; in contrast, in (III) the molecules form layers by means of the hydrogen bonds and these layers interact with each other only by van der Waals forces.

## Experimental

A commercial sample of 3-acetamidophenol (Sigma–Aldrich Co. Ltd, Gillingham, England) was used. Crystals of (I) were grown by slow evaporation of an ethanol solution.

### Crystal data

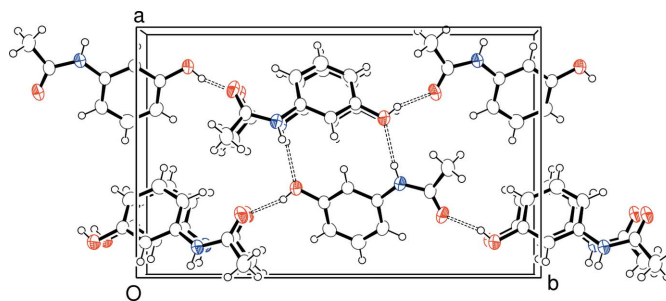
$C_8H_9NO_2$	$Z = 4$
$M_r = 151.16$	$D_x = 1.322 \text{ Mg m}^{-3}$
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation
$a = 10.5199$ (11) Å	$\mu = 0.10 \text{ mm}^{-1}$
$b = 17.0195$ (13) Å	$T = 293$ (2) K
$c = 4.2415$ (8) Å	Block, colourless
$V = 759.41$ (17) Å <sup>3</sup>	$0.40 \times 0.20 \times 0.15 \text{ mm}$

### Data collection

Enraf–Nonius CAD-4 diffractometer	946 measured reflections
$\omega$ –2 $\theta$ scans	946 independent reflections
Absorption correction: $\psi$ scan [ABSCALC in OSCAIL (McArdle & Daly, 1999; North et al., 1968)]	741 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.963, T_{\max} = 0.986$	$\theta_{\max} = 27.0^\circ$
	3 standard reflections
	frequency: 120 min
	intensity decay: 1%

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 0.0863P]$
$R[F^2 > 2\sigma(F^2)] = 0.032$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.093$	$(\Delta/\sigma)_{\max} < 0.001$
$S = 1.03$	$\Delta\rho_{\max} = 0.18 \text{ e \AA}^{-3}$
946 reflections	$\Delta\rho_{\min} = -0.14 \text{ e \AA}^{-3}$
102 parameters	
H-atom parameters constrained	


**Figure 2**

The packing for (I), viewed down [001], with hydrogen bonds indicated by dashed lines.

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O1-H1 \cdots O2^i$	0.82	1.85	2.638 (2)	162
$N1-H1A \cdots O1^{iii}$	0.86	2.11	2.963 (2)	171
$C4-H4 \cdots O2$	0.93	2.32	2.902 (3)	120

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

In the absence of significant anomalous scattering effects, Friedel pairs were averaged. The H atoms were placed in idealized locations ( $C-H = 0.93$ – $0.96$  Å,  $O-H = 0.82$  Å and  $N-H = 0.86$  Å) and refined as riding with  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C,N)$  or  $1.5U_{\text{eq}}(O, \text{methyl } C)$ . In addition, the methyl group was allowed to rotate but not to tip.

Data collection: *CAD-4-PC* (Enraf–Nonius, 1992); cell refinement: *CELDIM* in *CAD-4-PC* Software; data reduction: *XCAD4* (McArdle & Higgins, 1995); program(s) used to solve structure: *OSCAIL* (McArdle, 2005) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEK* (McArdle, 1993) and *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *OSCAIL*.

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