Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(4-Hydroxyphenyl)acrylamide

Wei-Qiang Chen, Qi Ya and Xuan-Ming Duan*

Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, No. 2 Zhongguancunbeiyitiao, Haidian, Beijing 100180, People's Republic of China

Correspondence e-mail: xmduan@mail.ipc.ac.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.134
Data-to-parameter ratio = 13.7

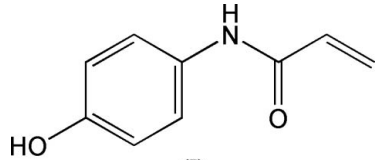
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 24 November 2005
Accepted 6 December 2005
Online 10 December 2005

In the title compound, $C_9H_9NO_2$, the mean planes of the acrylamide moiety and the benzene ring make a dihedral angle of 11.6 (2)°. In the crystal structure, intermolecular O—H···O and N—H···O hydrogen bonds link the molecules into two-dimensional corrugated sheets parallel to the *ac* plane.

Comment

The rational design of new materials in crystal engineering has been widely used (Desiraju, 1989; Thalladi *et al.*, 1998; Du *et al.*, 2005*a*). Recently, hydrogen bonding interactions have been widely used as the most successful strategy for engineering the structures of crystals to control molecular self-assembly in a helical structure (Gangopadhyay *et al.*, 2001; Anthony *et al.*, 2005; Du *et al.*, 2005*b*). Furthermore, intermolecular hydrogen-bonding interactions could provide precise topological control to design novel materials. The directional nature of hydrogen bonds is exploited in the organized self-assembly of molecules in the solid state (Steed & Atwood, 2000). Here we report the synthesis and X-ray crystal structure of the title compound, (I) (Fig. 1).



(I)

The N1—C7 bond length (Table 1) is significantly shorter than a typical single C—N bond (1.47 Å; Sasada, 1984) and very close to the C═N double-bond distance (1.28 Å; Wang *et al.*, 1998). It is indicative of the conjugation of atoms N1, C7, O2, C8 and C9, forming a π_5^6 configuration. The mean planes of the acrylamide moiety and the benzene ring make a dihedral angle of 11.6 (2)°. The crystal packing (Fig. 2) is characterized by the formation of two-dimensional corrugated sheets parallel to the *ac* plane *via* intermolecular O—H···O and N—H···O hydrogen bonds (Table 2).

Experimental

To a solution of 4-aminophenol (0.545 g, 5 mmol) and triethylamine (3.0 ml) in anhydrous tetrahydrofuran (15.0 ml), acrylic chloride in anhydrous tetrahydrofuran (5.0 ml) was added dropwise with stirring. After stirring for 24 h, ice water (20 ml) was added to the reaction mixture. The resulting mixture was extracted with chloroform. The organic layer was dried over magnesium sulfate, and the residue was recrystallized from ethyl acetate to give the title compound (I) (yield: 40%, 326 mg). ^{1}H NMR (300 MHz, $CDCl_3$): δ 5.72 (*m*, 1H), 6.30 (*m*,

2H), 6,72 (*d*, 2H), 7.40 (*d*, 2H). Crystals of (I) were obtained as blocks by recrystallization from an ethyl acetate solution.

Crystal data

$C_9H_9NO_2$
M_r = 163.17
Orthorhombic, *Pbca*
a = 12.787 (4) Å
b = 9.918 (3) Å
c = 13.524 (4) Å
V = 1715.0 (9) Å^3
Z = 8
D_x = 1.264 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2486 reflections
θ = 2.6–24.0°
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, colourless
0.38 × 0.30 × 0.24 mm

Data collection

Bruker APEX-II CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.814, T_{max} = 0.993
8550 measured reflections
1510 independent reflections
1195 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 25.0°
h = −11 → 15
k = −11 → 11
l = −16 → 15

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.134
S = 1.06
1510 reflections
110 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0742P)^2 + 0.3734P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C3	1.374 (2)	N1—C7	1.342 (2)
O2—C7	1.2339 (19)	N1—C6	1.420 (2)
C7—N1—C6	129.07 (14)	C1—C6—N1	117.51 (14)
O1—C3—C2	122.83 (15)	O2—C7—N1	123.18 (16)
O1—C3—C4	118.12 (14)	O2—C7—C8	122.02 (16)
C5—C6—N1	123.94 (15)	N1—C7—C8	114.81 (15)
C1—C2—C3—O1	178.68 (17)	C7—N1—C6—C1	168.01 (17)
O1—C3—C4—C5	−178.79 (17)	C6—N1—C7—O2	2.6 (3)
C4—C5—C6—N1	179.38 (17)	C6—N1—C7—C8	−177.74 (16)
C2—C1—C6—N1	−179.43 (16)	O2—C7—C8—C9	−3.9 (3)
C7—N1—C6—C5	−12.5 (3)	N1—C7—C8—C9	176.5 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.82	1.86	2.673 (2)	171
N1—H1*B*···O1^{ii}	0.86	2.09	2.916 (2)	161

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

All H atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å, N—H = 0.86 Å, O—H = 0.82 Å and U_{iso}(H) = 1.2U_{eq} of the parent atom.

Data collection: *APEXII* (Bruker, 2003); cell refinement: *APEXII* and *SAINT* (Bruker, 2001); 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, 2001) and *DIAMOND* (Brandenburg & Berndt, 1999); software used to prepare material for publication: *SHELXTL*.

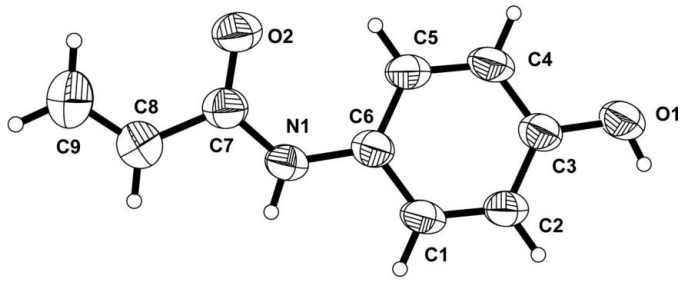


Figure 1
View of (I), with 30% probability displacement ellipsoids.

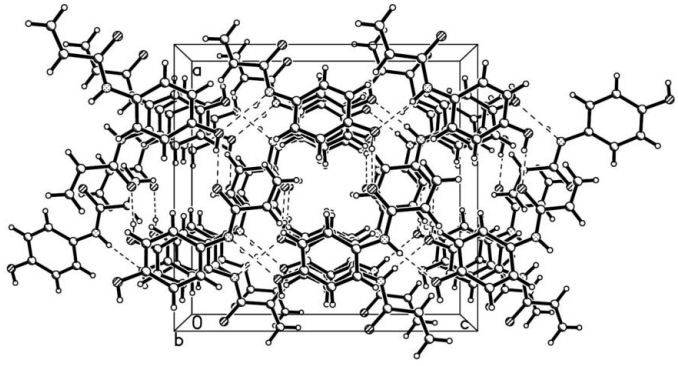


Figure 2
A perspective view of the crystal packing, showing the intermolecular hydrogen bonds (dashed lines).

This work was supported financially by the One Hundred Overseas Talents Program of the Chinese Academy of Sciences (CAS) and the Non-linear Nanophotonics Project of the Japan Science and Technology Agency (JST).

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