Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Acetamidobenzonitrile

Burcu Arslan,[a]* Canan Kazak,[a] Cumhur Kirilmis,[b] Murat Koca[b] and Orhan Büyükgüngör[a]

[a]Department of Physics, Ondokuz Mayıs University, TR-55139, Samsun, Turkey, and [b]Department of Chemistry, Arts and Sciences Faculty, Fırat University, TR-23169, Elazığ, Turkey

Correspondence e-mail: nbarslan@ttnet.net.tr

Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.032
wR factor = 0.079
Data-to-parameter ratio = 7.4

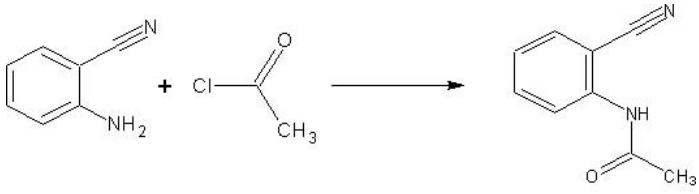
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 18 April 2005
Accepted 26 April 2005
Online 14 May 2005

The title compound, $C_9H_8N_2O$, was synthesized from 2-cyanoaniline and acetyl chloride in dry acetone. The crystal structure is stabilized by an intramolecular C—H···O hydrogen-bond contact, which forms a six-membered ring, and two intermolecular N—H···N and C—H···O hydrogen bonds.

Comment

Hydroxybenzonitriles, aminobenzonitriles and their derivatives are important starting materials in the synthesis of some heterocyclic molecules (Radl *et al.*, 2000; Arıcı *et al.*, 2004). Heterocyclic molecules play an important role in pharmaceutical research and development as a result of their desirable physical and chemical properties, and the solid-phase synthetic methodology has been developed for many types of ring systems (Franzen, 2000; Wilson, 2001). We present here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) (Fig. 1) shows normal bond lengths and angles (Table 1). The C≡N triple bond and C=O double bond lengths are 1.138 (3) and 1.210 (2) Å, respectively. The C6—N2—C7—O1 and C7—N2—C6—C1 torsion angles are 0.6 (4) and 142.9 (2)°, respectively.

The molecular structure of (I) is stabilized by a C—-H···O and N—-H···N hydrogen-bonding interaction. In the crystal structure, molecules are interlinked by N—H···N and C—H···O hydrogen bonds to form layers parallel to the *bc* plane (Table 2 and Fig. 2).

Experimental

A solution of 2-cyanoaniline (1.18 g, 10 mmol) in dry acetone (150 ml) was cooled to 278 K. Acetyl chloride (1.17 g, 15 mmol) was then added and the mixture was stirred for 8 h at room temperature. The reaction mixture was poured into water (500 ml) and the product precipitated twice from water. The resulting solid was filtered off and recrystallized from acetone–water (3:2) (yield 1.48 g, 92.50%).

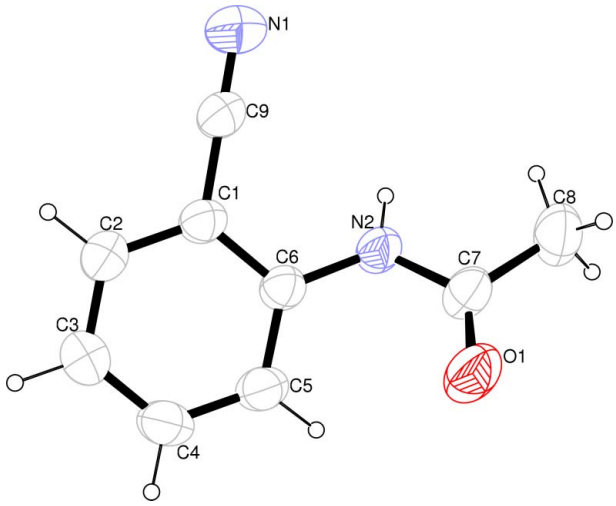


Figure 1
A view of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids.

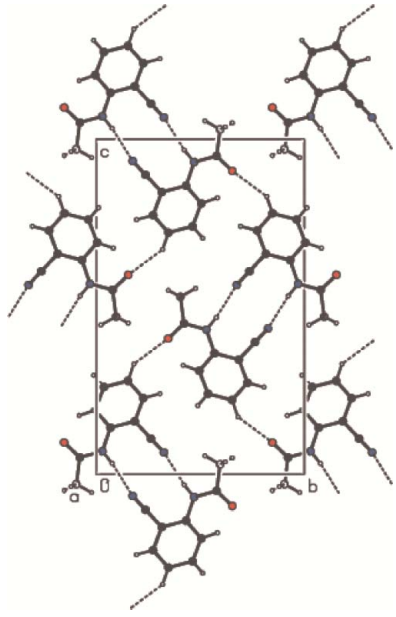


Figure 2
A molecular packing diagram of (I), viewed along the *a* axis. Dashed lines indicate intermolecular hydrogen bonds.

Crystal data

$C_9H_8N_2O$	Mo $K\alpha$ radiation
M_r = 160.17	Cell parameters from 1591 reflections
Orthorhombic, $P2_12_12_1$	θ = 1.8–27.8°
a = 3.8956 (3) Å	μ = 0.09 mm^{-1}
b = 11.3796 (14) Å	T = 296 K
c = 18.3249 (18) Å	Block, colourless
V = 812.35 (14) Å^3	0.60 × 0.36 × 0.10 mm
Z = 4	
D_x = 1.310 Mg m^{-3}	

Data collection

Stoe IPDS-II diffractometer	R_{int} = 0.031
ω scans	θ_{max} = 26.0°
1591 measured reflections	$h = -4 \rightarrow 4$
977 independent reflections	$k = 0 \rightarrow 14$
766 reflections with $I > 2\sigma(I)$	$l = 0 \rightarrow 22$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0515P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.032	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.079	$\Delta\rho_{max}$ = 0.12 e Å^{-3}
S = 0.92	$\Delta\rho_{min}$ = −0.12 e Å^{-3}
977 reflections	Extinction correction: *SHELXL97* (Sheldrick, 1997)
132 parameters	Extinction coefficient: 0.049 (7)
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.210 (2)	N2—C7	1.367 (3)
N1—C9	1.138 (3)	N2—C6	1.402 (2)
C7—N2—C6	125.69 (17)	O1—C7—C8	122.76 (19)
C5—C6—N2	122.50 (17)	N2—C7—C8	114.33 (18)
C1—C6—N2	119.23 (17)	N1—C9—C1	179.5 (3)
O1—C7—N2	122.91 (19)		
C7—N2—C6—C5	−37.9 (4)	C6—N2—C7—O1	0.6 (4)
C7—N2—C6—C1	142.9 (2)	C6—N2—C7—C8	−178.6 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H22···N1^{i}	0.85 (2)	2.26 (2)	3.081 (3)	163 (2)
C3—H3···O1^{ii}	0.98 (2)	2.47 (2)	3.270 (3)	139 (2)
C5—H5···O1	0.97 (2)	2.49 (3)	2.914 (3)	106 (2)

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, -z+1$; (ii) $-x, y-\frac{1}{2}, -z+\frac{3}{2}$.

The methyl H atoms were positioned geometrically and refined isotropically using a riding model [C—H = 0.96 Å and U_{iso} = $1.5U_{eq}$(C)]. The remaining H atoms were found in a difference Fourier map and refined isotropically. The C—H and N—H bond lengths are in the range 0.85 (2)–0.98 (2) Å. In the absence of significant anomalous scattering effects, Friedel pairs were merged.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

References

Arıcı, C., Ülkü, D., Kirilmiş, C., Koca, M. & Ahmedzade, M. (2004). *Acta Cryst.* E**60**, o1211–o1212.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Franzen, R. G. (2000). *J. Comb. Chem.* **2**, 195–214.
Radl, S., Hezky, P., Konvicka, P & Krejgi, J. (2000). *Collect. Czech. Chem. Commun.* **65**, 1093–1108.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Stoe & Cie (2002). *X-AREA* (Version 1.18) and *X-RED32* (Version 1.04). Stoe & Cie, Darmstadt, Germany.
Wilson, L. J. (2001). *Org. Lett.* **3**, 585–588.