

1-(1*H*-Benzimidazol-2-yl)ethanone

Xiao-Yan Yang, Ying Li, Yan Li,
Xue-Mei Li and Shu-Sheng
Zhang*

College of Chemistry and Molecular
Engineering, Qingdao University of Science and
Technology, 266042 Qingdao, Shandong,
People's Republic of China

Correspondence e-mail: shushzhang@126.com

Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.049
 wR factor = 0.142
Data-to-parameter ratio = 13.6

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

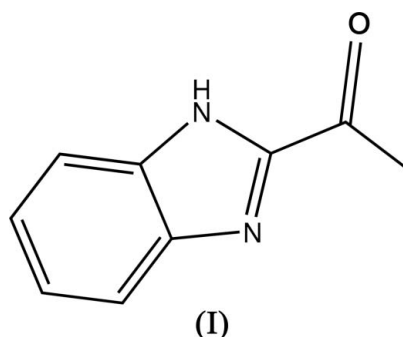
In the title compound, $\text{C}_9\text{H}_8\text{N}_2\text{O}$, all non-H atoms are essentially coplanar. $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds generate a centrosymmetric $R_2^2(10)$ dimer.

Received 10 April 2006

Accepted 13 April 2006

Comment

We have recently reported the synthesis and crystal structure of 2-(2-nitrophenyl)-1*H*-benzimidazole (Li *et al.*, 2005). In our ongoing studies of benzimidazole derivatives, the title compound, (I), was obtained as an intermediate.



In the molecule of (I) (Fig. 1), all non-H atoms are essentially coplanar, with a dihedral angle of $1.1(1)^\circ$ between the planes of the benzene and imidazole rings. The bond lengths in the benzimidazole ring system (Table 1) show a character intermediate between single and double bonds, comparable with those observed in 2-(2-nitrophenyl)-1*H*-benzimidazole (Li *et al.*, 2005). In the crystal structure, $\text{N1}-\text{H1A}\cdots\text{O1}$ hydrogen bonds (Table 2) link the molecules into centrosymmetric dimers (Fig. 2).

Experimental

Lactic acid (10 ml) was added to a solution of *o*-phenylenediamine (5.4 g, 0.05 mol) in hydrochloric acid (50 ml). The mixture was refluxed for 2 h and then filtered. On neutralization of the filtrate with sodium hydroxide (20%), 1-(1*H*-benzimidazol-2-yl)ethanol (3.2 g, 0.02 mol) was obtained. To a solution of this compound in glacial acetic acid (30 ml) was added a solution of CrO_3 (3.0 g, 0.03 mol) in water (10 ml). The mixture was reacted at 373 K for 1 h and then filtered. The filtrate was extracted with chloroform and dried. Single crystals of (I) suitable for X-ray diffraction analysis were obtained by slow evaporation of a toluene solution

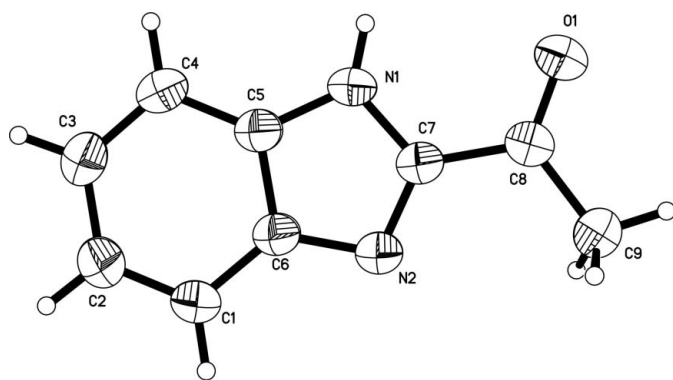


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering scheme.

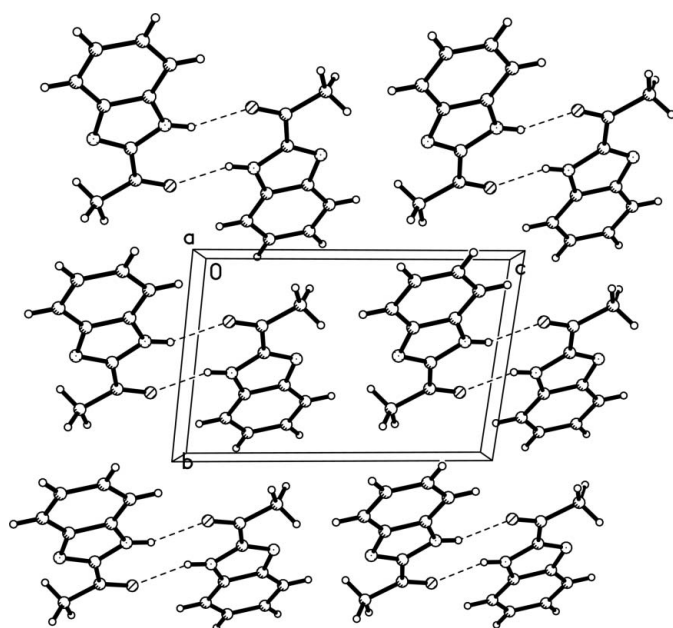


Figure 2
A view of the N—H...O hydrogen-bonded (dashed lines) dimers of (I).

Crystal data

$C_9H_8N_2O$
 $M_r = 160.17$
Triclinic, $P\bar{1}$
 $a = 5.7270$ (16) Å
 $b = 7.102$ (2) Å
 $c = 10.322$ (3) Å
 $\alpha = 95.493$ (4)°
 $\beta = 94.159$ (4)°
 $\gamma = 108.960$ (4)°

$V = 392.81$ (19) Å³
 $Z = 2$
 $D_x = 1.354$ Mg m⁻³
Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 293$ (2) K
Plate, colourless
 $0.46 \times 0.22 \times 0.08$ mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
 ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.959$, $T_{\max} = 0.993$

2230 measured reflections
1495 independent reflections
1194 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.013$
 $\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.050$
 $wR(F^2) = 0.142$
 $S = 1.00$
1495 reflections
110 parameters
H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0803P)^2 + 0.1068P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.21 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$

Table 1

Selected bond lengths (Å).

O1—C8	1.218 (2)	N2—C7	1.317 (2)
N1—C7	1.358 (2)	N2—C6	1.382 (3)
N1—C5	1.373 (2)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A...O1 ⁱ	0.86	2.05	2.868 (2)	158

Symmetry code: (i) $-x + 1, -y + 1, -z$.

After their location in a difference Fourier map, all H atoms were positioned geometrically (N—H = 0.86 Å and C—H = 0.93 or 0.96 Å) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2$ or 1.5 (methyl) times $U_{\text{eq}}(\text{parent atom})$.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 1997); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2003).

This project was supported by the Special Project of Qingdao for Leadership of Science and Technology (grant No. 05-2-JC-80) and the Outstanding Young Adult Scientific Research Encouraging Foundation of Shandong Province (grant No. 2005BS04007).

References

- Li, X.-M., Du, L.-P., Li, Y. & Zhang, S.-S. (2005). *Acta Cryst.* **E61**, o1902–o1903.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINTE*. Siemens Analytical X-Ray Instruments Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.