Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Carbamoyl-3-nitrobenzoic acid

Xue-Mei Li, Shan-Shan Gu, Qiang Xu 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 σ(C–C) = 0.004 Å
R factor = 0.057
wR factor = 0.170
Data-to-parameter ratio = 11.8

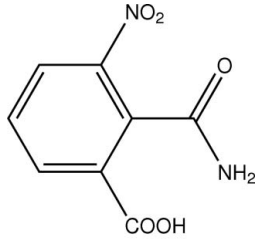
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 15 May 2006
Accepted 22 May 2006

In the title compound, $C_8H_6N_2O_5$, molecules are linked into ribbons along the b axis by N—H···O hydrogen bonds. The ribbons are interlinked into a three-dimensional framework.

Comment

We have previously reported the 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.



(I)

The bond lengths and angles in (I) show normal values (Allen *et al.*, 1987). The benzene ring, nitro and carboxyl groups are essentially coplanar, while atoms O3 and N2 lie above and below the molecular plane, with dihedral angles of 6.9 (2), 5.6 (1) and 84.5 (2)° between the C1–C6 ring plane and the mean planes through the C8/O4/O5, N1/O1/O2 and and C7/N2/O3 groups, respectively. An intramolecular C4—H4*A*···O5 hydrogen bond forms a five-membered ring and contributes to the planarity of the molecule.

Molecules of (I) are linked into ribbons along the b axis (Fig. 2) *via* N—H···O and C—H···O hydrogen bonds. These ribbons are further interlinked into a three-dimensional framework by O5—H5*A*···O4 and C2—H2*C*···O2 hydrogen bonds (Table 1).

Experimental

Compound (I) was synthesized according to the method of Chapman & Stephen (1925). Single crystals were obtained by slow evaporation of an aqueous solution at room temperature over a period of 2 d.

Crystal data

$C_8H_6N_2O_5$
M_r = 210.15
Monoclinic, $P2_1/c$
a = 9.6080 (12) Å
b = 6.8998 (9) Å
c = 15.3291 (14) Å
β = 125.755 (5)°
V = 824.68 (17) Å^3
Z = 4
D_x = 1.693 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 293 (2) K
Plate, yellow
0.25 × 0.20 × 0.06 mm

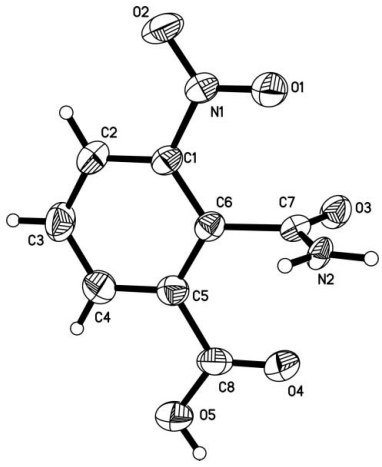


Figure 1
The structure of the compound (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.965, T_{max} = 0.991
4196 measured reflections
1606 independent reflections
1368 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.170
S = 1.07
1606 reflections
136 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0923P)^2 + 0.663P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O3^{i}	0.86	1.99	2.697 (3)	138
O5—H5A···O4^{ii}	0.82	1.90	2.716 (3)	172
C2—H2C···O2^{iii}	0.93	2.48	3.323 (4)	150
C4—H4A···O5	0.93	2.41	2.733 (4)	100

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

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms with C—H = 0.93 Å, O—H = 0.82 Å and N—H = 0.86 Å, and with U_{iso}(H) = 1.2U_{eq}(C,N) and 1.5 U_{eq}(O).

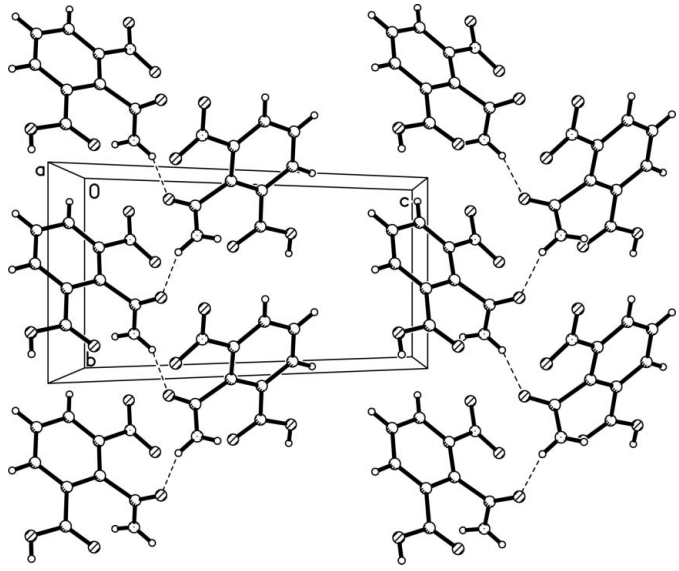


Figure 2
The packing of (I), showing ribbons running along the *b* axis. Hydrogen bonds are indicated by dashed lines.

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*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Chapman, E. & Stephen, H. (1925). *J. Chem. Soc.* **127**, 1791–1797.
Li, X.-M., Du, L.-P., Li, Y. & Zhang, S.-S. (2005). *Acta Cryst.* E**61**, o1902–o1903.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.