

Xiao-Ru Zhang, Shu-Sheng
Zhang,* Min-Hua Xu and
Xue-Mei LiCollege 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 $\sigma(C-C) = 0.004$ Å
 R factor = 0.053
 wR factor = 0.142
Data-to-parameter ratio = 13.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

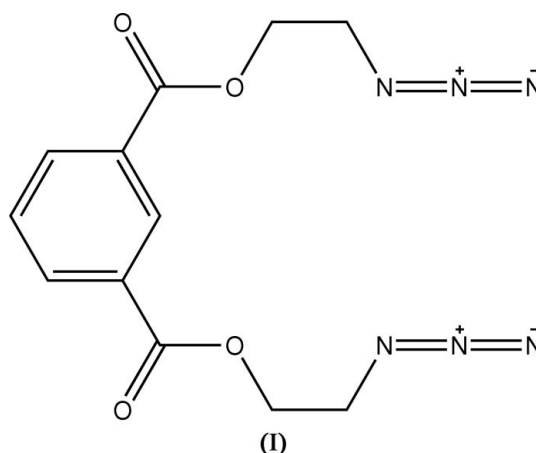
Bis(2-azidoethyl) isophthalate

In the non-planar molecule of the title compound, $C_{12}H_{12}N_6O_4$, one azide group lies almost in the plane of the benzene ring, while the other is inclined above this plane. In the crystal structure, the molecules are linked into chains along the a axis by $C-H \cdots N$ hydrogen bonds. The packing is further stabilized by dipole-dipole and van der Waals interactions.

Received 21 December 2005
Accepted 9 February 2006

Comment

We have reported recently the structure of bis(2-azidoethyl) pyridine-2,6-dicarboxylate, (II) (Du *et al.*, 2006). In our ongoing studies, the title compound, (I), was obtained in the reaction of isophthalic acid and 2-azidoethanol. Its crystal structure is presented here.



Bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987), and comparable to those in (II). In the non-planar molecule of (I), the N4/N5/N6 azide group lies almost in the plane of the benzene ring [maximum displacement of 0.305 (4) Å from the mean plane for N6], while the N1/N2/N3 azide group is inclined above this plane with displacements ranging from 1.910 (2) to 2.578 (3) Å for N3 and N1, respectively. In the crystal structure, the molecules are linked into chains along the a axis (Fig. 2) by weak $C-H \cdots N$ hydrogen bonds (Table 2). The packing is further stabilized by dipole-dipole and van der Waals interactions.

Experimental

The title compound was obtained according to the method of Du *et al.* (2006). Colourless single crystals suitable for X-ray crystallographic analysis were grown by slow evaporation of an ethyl acetate solution.

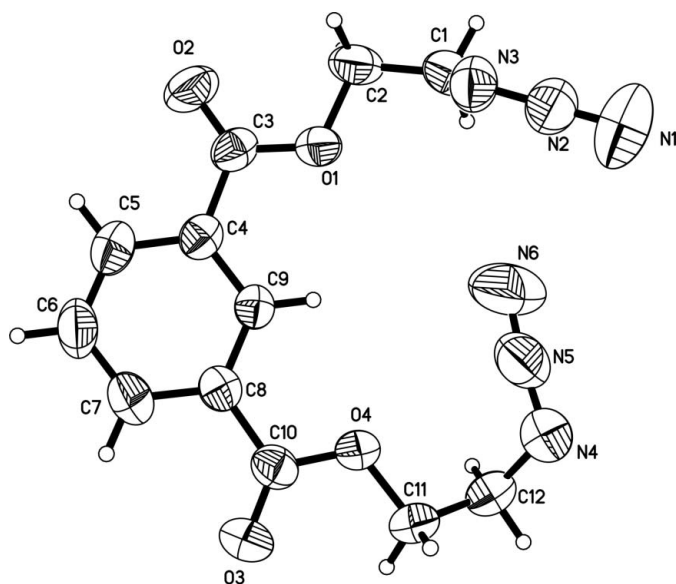


Figure 1
The structure of compound (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

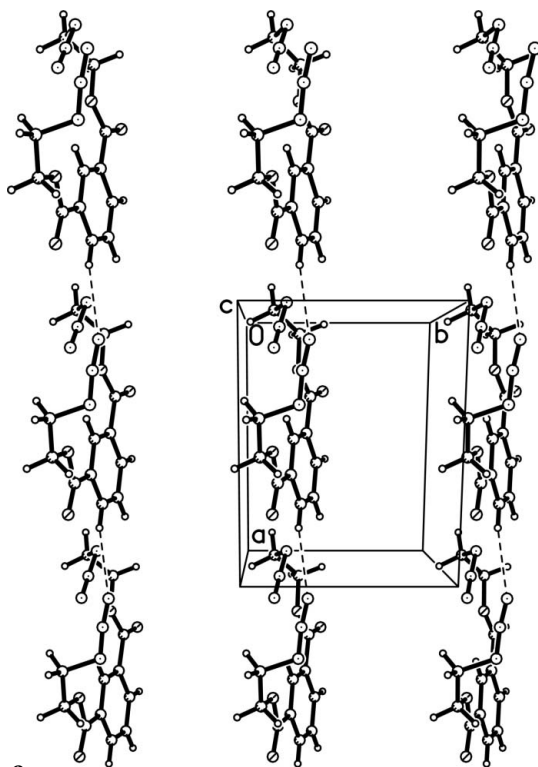


Figure 2
A view of (I) down the *c* axis, showing the chains along the *a* axis. Hydrogen bonds are indicated by dashed lines.

Crystal data

$C_{12}H_{12}N_6O_4$
 $M_r = 304.28$
 Monoclinic, $P2_1/c$
 $a = 10.616$ (3) Å
 $b = 7.2262$ (19) Å
 $c = 21.640$ (5) Å
 $\beta = 119.164$ (10)°
 $V = 1449.6$ (7) Å³
 $Z = 4$

$D_x = 1.394$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 1426 reflections
 $\theta = 3.0$ – 21.4 °
 $\mu = 0.11$ mm⁻¹
 $T = 293$ (2) K
 Needle, colourless
 $0.30 \times 0.06 \times 0.06$ mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.968$, $T_{\max} = 0.994$
 8307 measured reflections

2756 independent reflections
 1767 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$
 $\theta_{\max} = 25.8$ °
 $h = -10 \rightarrow 12$
 $k = -7 \rightarrow 8$
 $l = -26 \rightarrow 26$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.142$
 $S = 1.02$
 2756 reflections
 211 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0614P)^2 + 0.2657P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.16$ e Å⁻³
 $\Delta\rho_{\min} = -0.17$ e Å⁻³

Table 1

Selected bond lengths (Å).

O1—C3	1.330 (3)	O4—C11	1.445 (3)
O1—C2	1.446 (3)	N1—N2	1.123 (3)
O2—C3	1.206 (3)	N2—N3	1.215 (3)
O3—C10	1.206 (2)	N4—N5	1.226 (3)
O4—C10	1.333 (3)	N5—N6	1.141 (4)

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C5—H5A···N1 ⁱ	0.93	2.58	3.459 (5)	157

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

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

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 Project of Educational Administration of Shandong Province (No. J04B12) and the Outstanding Adult-Young 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.
 Du, P., Zhang, X.-R., Xu, M.-H. & Zhang, S.-S. (2006). *Acta Cryst. E* **62**, o300–o302.
 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.