Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

1,2-Bis(2,4-dinitrophenoxy)ethane

P. G. Aravindan,[a]
S. Selvanayagam,[a]
D. Velmurugan,[a]*
K. Ravikumar,[b]
S. Saravanan[c] and
P. C. Srinivasan[c]

[a]Department of Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India, [b]Laboratory of X-ray Crystallography, Indian Institute of Chemical Technology, Hyderabad 500 007, India, and [c]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India

Correspondence e-mail: d_velu@yahoo.com

Received 7 October 2004
Accepted 11 October 2004
Online 22 October 2004

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.048
wR factor = 0.148
Data-to-parameter ratio = 14.1

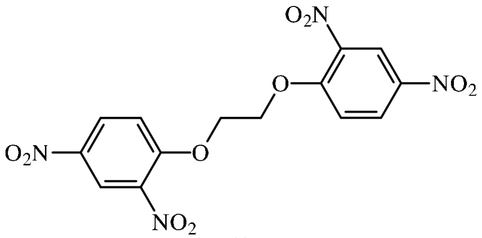
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

© 2004 International Union of Crystallography
All rights reserved

The title compound, $C_{14}H_{10}N_4O_{10}$, crystallizes in the monoclinic space group *C*2/*c* with the molecule on an inversion centre. The nitro groups are slightly twisted away from the planes of the benzene rings. In the crystal structure, weak intermolecular C—H···O interactions link the molecules into layers which can be describedby an $R_2^2(10)$ ring and a *C*(6) chain.

Comment

Nitro-substituted aromatic compounds are well known for their uses as dyes, battery intermediates and explosives (Sivasamy *et al.*, 1988; Renuka *et al.*, 2001). 1,3-Dinitrobenzene has been found to function as an organic cathode material in batteries. These derivatives promote specific irreversible inhibition of human thioredoxin reductase (Arnér *et al.*, 1995). The X-ray crystal structure analysis of the title compound, (I), was carried out as part of our studies on substitution of the nitro group.



(I)

Molecules of (I) lie across crystallographic inversion centres and the asymmetric unit therefore contains one-half molecule. The mid-point of the C7—C7^i bond [symmetry code: (i) $1 - x$, $1 - y$, $-z$] lies on the centre of inversion (Fig. 1). The bond lengths and angles (Table 1) in the structure are comparable with those observed in related structures (Bailey *et al.*, 1989; Aravindan *et al.*, 2003). The molecule adopts a *trans* configuration about the ethylene C7—C7^i bond [O5—C7—C7^i—O5^i = 180°]. The orientation of the two nitro groups on the benzene ring is consistent with the achievement of minimum steric interactions. The nitro groups are slightly twisted away from the benzene ring by 3.6 (1) and 8.6 (1)° for nitro groups at C2 and C4, respectively. The average N—O distance [1.212 (2) Å] is comparable with the mean value of 1.217 (11) Å reported by Allen *et al.* (1987). Due to the close approach of atoms H6 and H7*A* (H6···H7*A* = 2.30 Å), the angle C6—C1—O5 [123.6 (1)°] is larger than C2—C1—O5 [118.7 (1)°].

doi: 10.1107/S1600536804025577

In the crystal structure, weak intermolecular C—H···O interactions (Table 2) link the molecules into a two-dimensional network that can be described by an $R_2^2(10)$ ring and *C*(6) chain (Bernstein *et al.*, 1995). The two-dimensional networks are parallel to the (202) planes.

Experimental

The title compound was prepared by the reaction of ethylene glycol (10 mmol), 2,4-dinitrochlorobenzene (20 mmol) and sodium hydride (20 mmol) in boiling tetrahydrofuran over a period of 2 h. The solvent was completely removed and the residue was carefully digested with ice-cold water; the precipitated solid was dried over anhydrous calcium chloride. Crystals were obtained from acetone by slow evaporation of the solvent.

Crystal data

$C_{14}H_{10}N_4O_{10}$
$M_r = 394.26$
Monoclinic, $C2/c$
$a = 6.8876$ (1) Å
$b = 13.9289$ (1) Å
$c = 16.5396$ (5) Å
$\beta = 95.146$ (3)°
$V = 1580.36$ (5) Å^3
$Z = 4$
$D_x = 1.657$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2638 reflections
$\theta = 2.5$–27.9°
$\mu = 0.14$ mm^{-1}
$T = 293$ (2) K
Block, yellow
0.26 × 0.20 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: none
4664 measured reflections
1792 independent reflections
1542 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.015$
$\theta_{\rm max} = 28.0°$
$h = -6 \rightarrow 9$
$k = -15 \rightarrow 17$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.148$
$S = 1.01$
1792 reflections
127 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0894P)^2 + 0.878P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.38$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.25$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—N1	1.205 (2)	O4—N2	1.217 (2)
O2—N1	1.209 (2)	C7—C7$^{\rm i}$	1.506 (3)
O3—N2	1.217 (2)		
C1—O5—C7	118.9 (1)	C6—C1—C2	117.7 (1)
O1—N1—O2	122.4 (1)	C3—C2—N1	116.2 (1)
O3—N2—O4	123.6 (2)	C1—C2—N1	122.4 (1)
O5—C1—C6	123.6 (1)	O5—C7—C7$^{\rm i}$	104.4 (2)
C7—O5—C1—C6	−1.4 (2)	C1—O5—C7—C7$^{\rm i}$	179.55 (16)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O2$^{\rm ii}$	0.93	2.48	3.404 (2)	176
C6—H6···O3$^{\rm iii}$	0.93	2.54	3.337 (2)	144

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

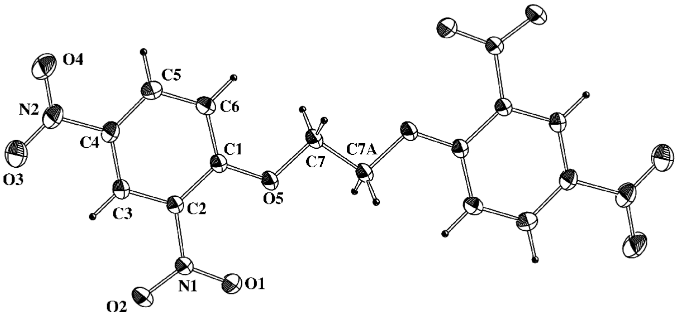


Figure 1
The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. C7A and unlabelled atoms are related to labelled atoms by $1 - x$, $1 - y$, $-z$.

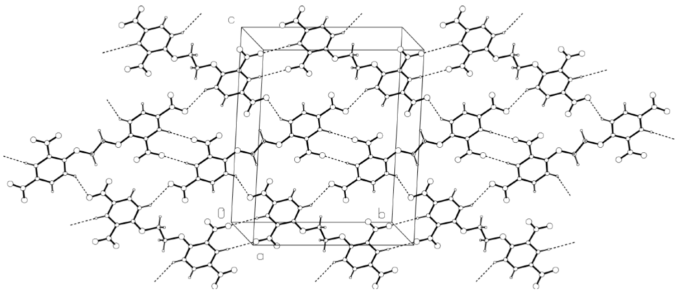


Figure 2
The molecular packing of the title compound, viewed approximately down the *a* axis.

All H atoms were positioned geometrically and allowed to ride on their parent C atoms, with aromatic C—H distances of 0.93 Å and methylene C—H distances of 0.97 Å, and with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(parent C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ZORTEP* (Zsolnai, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL*97 and *PARST* (Nardelli, 1995).

DV, PGA and SSN thank the Council of Scientific Industrial Research (CSIR), Government of India, for financial support. The Department of Science & Technology (DST) and the University Grants Commission (UGC), Government of India, are gratefully acknowledged for providing funds to the department through FIST and SAP.

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.

Aravindan, P. G., Yogavel, M., Thirumavalavan, M., Akilan, P., Velmurugan, D., Kandaswamy, M., Shamuga Sundara Raj, S. & Fun, H.-K. (2003). *Acta Cryst.* E**59**, o806–o807.

Arnér, E. S. J., Björnstedt, M. & Holmgren, A. (1995). *J. Biol. Chem.* **270**, 3479–3482.

Bailey, N. A., Fenton, D. E., Williams, M. G. & Winter, D. J. (1989). *Acta Cryst.* C**45**, 1778–1780.

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.

Bruker (2001). *SMART* (Version 5.625) and *SAINT* (Version 6.28*a*). Bruker AXS Inc., Madison, Wisconsin, USA.

Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.

Renuka, D. N., John Fredrick, V., Saravanan, S. & Srinivasan, P. C. (2001). *Indian J. Chem. Sect. A*, **40**, 175–181.

Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.

Sivasamy, K., Rajeswari, S. & Dakshinamoorthy, K. J. (1988). *J. Electrochem. Soc. India*, **37**, 343–347.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

Zsolnai, L. (1997). *ZORTEP*. University of Heidelberg, Germany.