Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

(*Z*)-1,2-Bis(4-nitrophenyl)ethene

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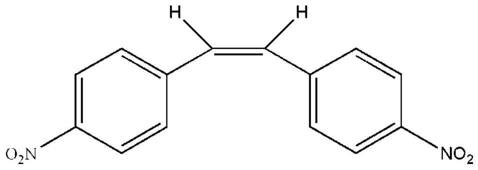
Received 23 August 2007; accepted 28 August 2007

Key indicators: single-crystal X-ray study; *T* = 298 K; mean σ(C–C) = 0.002 Å; *R* factor = 0.043; *wR* factor = 0.116; data-to-parameter ratio = 16.2.

The title compound, $C_{14}H_{10}N_2O_4$, is a *cis*-stilbene derivative with non-crystallographic twofold rotation axis. The two aryl groups reside on the same side of the olefinic bond, and the aryl groups and the olefinic bond are not in the same plane, so the molecule is a non-planar π-conjugate system. The molecules are linked by non-classical C—H$\cdots$O hydrogen bonds along the *b* and *c* directions of the unit cell to form sheets parallel to the *bc* plane.

Related literature

For the synthesis of geometrically pure (*cis* or *trans*) stilbenes, see: Cella & Stefani (2006); Ferré-Filmon *et al.* (2004); Jeffery & Ferber (2003); Shi & Xu (2002). For photophysical investigations on stilbenes and their derivatives, see: Albota *et al.* (1998); Reinhardt *et al.* (1998). For related *trans*-stilbene structures, see: Hulliger *et al.* (2002); De Borger *et al.* (2005); Zhang *et al.* (2005). For less common *cis*-stilbene structures, see: Traetteberg & Frantsen (1975); Tirado-Rives *et al.* (1984).



Experimental

Crystal data

$C_{14}H_{10}N_2O_4$
M_r = 270.24
Monoclinic, $P2_1/c$
a = 6.8922 (4) Å
b = 22.8669 (13) Å
c = 8.0727 (5) Å
β = 98.469 (2)°
V = 1258.41 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 298 (2) K
0.50 × 0.20 × 0.19 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.973, T_{max} = 0.981
9077 measured reflections
2951 independent reflections
2179 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.116
S = 1.05
2951 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Table 1
Selected torsion angles (°).

C3—C4—C13—C14	149.55 (16)	C9—C10—C14—C13	138.17 (17)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C2—H2*A*$\cdots$O3^{i}	0.93	2.45	3.3606 (18)	166
C9—H9*A*$\cdots$O4^{ii}	0.93	2.58	3.4381 (18)	153

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

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2003); software used to prepare material for publication: *SHELXTL*.

The authors are grateful for financial support of this work from the National Natural Science Foundation of China (NSFC) (grant No. 20472019) and the Natural Science Foundation of Hunan Province (NSFH) (grant No. 06 J J2002).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2032).

References

Albota, M., Beljonne, D., Brédas, J. L., Ehrlich, J. E., Fu, J.-Y., Heikal, A. A., Hess, S. E., Kogej, T., Levin, M. D., Marder, S. R., McCord-Maughon, D., Perry, J. W., Röckel, H., Rumi, M., Subramaniam, G., Webb, W. W., Wu, X.-L. & Xu, C. (1998). *Science*, **281**, 1653–1656.
Bruker (2003). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cella, R. & Stefani, H. A. (2006). *Tetrahedron*, **62**, 5656–5662.
De Borger, R., Vande Velde, C. M. L. & Blockhuys, F. (2005). *Acta Cryst.* E**61**, o819–o821.
Ferré-Filmon, K., Delaude, L., Demonceau, A. & Noels, A. F. (2004). *Coord. Chem. Rev.* **248**, 2323–2336.
Hulliger, J., Bebie, H., Kluge, S. & Quintel, A. (2002). *Chem. Mater.* **14**, 1523–1529.
Jeffery, T. & Ferber, B. (2003). *Tetrahedron Lett.* **44**, 193–197.
Reinhardt, B. A., Brott, L. L., Clarson, S. J., Dillard, A. G., Bhatt, J. C., Kannan, R., Yuan, L., He, G. S. & Prasad, P. N. (1998). *Chem. Mater.* **10**, 1863–1874.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2002). *SADABS*. Version 2.06. Bruker AXS Inc., Madison, Wisconsin, USA.

doi:10.1107/S1600536807042158

Shi, M. & Xu, B. (2002). *J. Org. Chem.* **67**, 294–297.

Tirado-Rives, J., Oliver, M. A., Fronczek, F. R. & Gandour, R. D. (1984). *J. Org. Chem.* **49**, 1627–1634.

Traetteberg, M. & Frantsen, E. B. (1975). *J. Mol. Struct.* **26**, 69–76.

Zhang, X., Yu, X. Q., Yu, W. T., He, W. & Jiang, M. H. (2005). *Chin. J. Struct. Chem.* **24**, 875–878.

supplementary materials

Acta Cryst. (2007). E**63**, o3999-o4000 [**doi:10.1107/S1600536807042158**]

(*Z*)-1,2-Bis(4-nitrophenyl)ethene

C. Chen and **C. Cao**

Comment

In recent years, the stilbene and its derivatives have been the subject of many photophysical investigations (Albota *et al.*, 1998; Reinhardt *et al.*, 1998). Many researches have been directed toward the synthesis of geometrically pure stilbenes, and many perfect methods have been developed (Cella *et al.*, 2006; Ferré-Filmon *et al.*, 2004; Jeffery *et al.*, 2003). Though a number of 4,4'-disubstituted stilbenes are obtained easily, and some *trans*-stilbene derivatives had been crystallographically characterized (Hulliger *et al.*, 2002; De Borger *et al.*, 2005; Zhang *et al.*, 2005), the crystal stuctures of *cis*-stilbene derivatives (Traetteberg *et al.*,1975; Tirado-Rives *et al.*, 1984) has been seldom reported up to the precent, and it is still a challenge topic.

The molecular structure of the title compound is illustrated in Fig. 1, where the molecule adopts a *cis* configuration with two aryl groups of *cis*-stilbene resideing on the same side. The bond angles (Table 1) <C(14)—C(13)—C(4) (129.41 (14)°) and <C(13)—C(14)—C(10) (128.71 (13)°) severely deviate from 120° due to the comparatively strong steric hindrance between the two aryl groups. There is a dihedral angle of 56.67° between two planes defined by N(1)/O(1)/O(2)/C(1)—C(6)/C(13) and N(2)/O(3)/O(4)/C(7)—C(12)/C(14). The torsion angles of C(3)—C(4)—C(13)—C(14) (149.55 (16)°) and C(9)—C(10)—C(14)—C(13) (138.17 (17)°) are also significantly deviated from 180°, which indicates that the whole molecule is non-coplanar.

Within the cell of the crystal structure, the molecules are held together by hydrogen bonding interactions (Fig. 2), where the phenyl groups donate hydrogen atoms (H(2) and H(9)) to the oxygen atoms (O(3) and O(4)) to form weak non-classical intermolecular C—H···O hydrogen bonds (Table 2).

Experimental

The title compound, (**I**) was synthesized starting from 4-nitrobenzyl(triphenyl) phosphonium chlorine (**II**) (2.2 mmol), which was obtained by reacting 4-nitrobenzyl chlorine with triphenylphosphite (Shi *et al.*, 2002), In compound (**II**), 4-nitrobenzaldehyde (2.0 mmol) and NaOH (3.0 mmol) were added to. The mixture was thoroughly ground in an open mortar at room temperature, next it was heated about 15 min at 45–50° C in an oven, and next it was ground again for 1–2 min. Above-mentioned procedure was repeated until the reaction was completed by TLC monitoring. After the mixture was cooled down to the room temperature, water (20 ml) was added to. Then the mixture was extracted with chloroform. The organic layer was dried over anhydrous magnesium sulfate. Subsequently it was filtered and concentrated. The yellow product was collected and then was purified by column chromatography on silica gel (petroleum ether/ethyl acetate, 40:1). Suitable crystals of the title compound were obtained by evaporation of an acetonitrile solution, yield: 7.5% (based on 4-nitrobenzaldehyde). IR (cm^{-1}, KBr, pellet): $\nu_{(C=C)}$ 3081(*m*), 1591(*s*), 1488(*s*), 715(*s*). ^{1}HNMR ($CDCl_3$)(400 MHz; TMS p.p.m.), δ(p.p.m.): 6.83(s, 2H, –C=C–), 7.24–7.35(m, 4H, Ar), 8.10–8.12(d, 4H, Ar).

Refinement

H atoms bonded to C were located geometrically; they were treated as riding, with distances C—H = 0.93 Å and U_{iso}(H)=1.2 times U_{eq}(C).

Figures

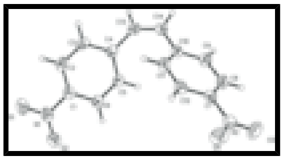


Fig. 1. The structure of the title compound, showing 30% probability ellipsoids and the atom-numbering scheme.

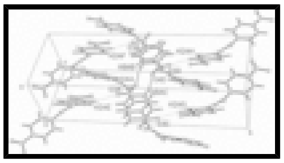


Fig. 2. A packing diagram for the title compound. Hydrogen bonds are indicated as dashed lines.

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Crystal data

$C_{14}H_{10}N_2O_4$

$M_r = 270.24$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 6.8922$ (4) Å

$b = 22.8669$ (13) Å

$c = 8.0727$ (5) Å

$\beta = 98.469$ (2)°

$V = 1258.41$ (13) Å^3

$Z = 4$

$F_{000} = 560$

$D_x = 1.426$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 195 reflections

$\theta = 2.0$–27.5°

$\mu = 0.11$ mm^{-1}

$T = 298$ (2) K

Block, yellow

0.50 × 0.20 × 0.19 mm

Data collection

Bruker SMART CCD APEXII diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 8.4 pixels mm^{-1}

$T = 298(2)$ K

ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 2002)

$T_{\min} = 0.973$, $T_{\max} = 0.981$

9077 measured reflections

2951 independent reflections

2179 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.019$

$\theta_{\max} = 27.8$°

$\theta_{\min} = 1.8$°

$h = -9 \rightarrow 8$

$k = -26 \rightarrow 29$

$l = -10 \rightarrow 9$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.043$	H-atom parameters constrained
$wR(F^2) = 0.116$	$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2 + 0.1997P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
2951 reflections	$\Delta\rho_{max} = 0.19$ e Å^{-3}
182 parameters	$\Delta\rho_{min} = -0.16$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2049 (2)	0.73977 (6)	0.61613 (16)	0.0503 (3)
N2	0.74204 (17)	0.46581 (6)	1.07266 (16)	0.0558 (3)
C12	0.7579 (2)	0.56150 (6)	0.93698 (17)	0.0509 (3)
H12A	0.7621	0.5794	1.0409	0.061*
C7	0.74826 (19)	0.50148 (6)	0.92206 (16)	0.0461 (3)
C6	0.2168 (2)	0.67990 (6)	0.63390 (18)	0.0511 (3)
H6A	0.1232	0.6594	0.6824	0.061*
N1	0.0403 (2)	0.77052 (6)	0.67462 (16)	0.0642 (4)
C2	0.3426 (2)	0.77145 (6)	0.54582 (18)	0.0576 (4)
H2A	0.3333	0.8119	0.5367	0.069*
C5	0.3704 (2)	0.65114 (6)	0.57828 (18)	0.0510 (3)
H5A	0.3801	0.6107	0.5900	0.061*
O2	−0.07476 (19)	0.74209 (6)	0.74400 (18)	0.0808 (4)
C10	0.75668 (19)	0.56807 (6)	0.63870 (17)	0.0467 (3)
C11	0.7613 (2)	0.59447 (6)	0.79455 (18)	0.0517 (3)
H11A	0.7667	0.6350	0.8027	0.062*
C4	0.5118 (2)	0.68122 (6)	0.50478 (16)	0.0479 (3)
O4	0.7539 (2)	0.49014 (6)	1.20713 (14)	0.0825 (4)

C9	0.7531 (2)	0.50730 (6)	0.63014 (18)	0.0553 (4)
H9A	0.7554	0.4890	0.5275	0.066*
C13	0.6705 (2)	0.65123 (7)	0.43457 (18)	0.0557 (4)
H13A	0.7087	0.6689	0.3407	0.067*
C8	0.7464 (2)	0.47360 (6)	0.77084 (19)	0.0558 (4)
H8A	0.7408	0.4330	0.7637	0.067*
C3	0.4939 (2)	0.74179 (6)	0.48956 (18)	0.0558 (4)
H3A	0.5863	0.7626	0.4403	0.067*
C14	0.7668 (2)	0.60270 (6)	0.48576 (18)	0.0547 (4)
H14A	0.8520	0.5886	0.4159	0.066*
O3	0.7226 (2)	0.41327 (5)	1.05662 (17)	0.0904 (5)
O1	0.0264 (3)	0.82307 (6)	0.6530 (2)	0.1119 (6)

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0558 (8)	0.0524 (8)	0.0401 (7)	0.0075 (6)	−0.0014 (6)	0.0029 (6)
N2	0.0534 (7)	0.0586 (8)	0.0569 (8)	0.0048 (6)	0.0129 (5)	0.0068 (6)
C12	0.0553 (8)	0.0506 (8)	0.0465 (7)	0.0015 (6)	0.0065 (6)	−0.0062 (6)
C7	0.0421 (7)	0.0482 (7)	0.0481 (7)	0.0033 (5)	0.0070 (5)	0.0044 (6)
C6	0.0507 (8)	0.0504 (8)	0.0512 (8)	−0.0043 (6)	0.0040 (6)	0.0036 (6)
N1	0.0750 (9)	0.0613 (8)	0.0553 (7)	0.0157 (7)	0.0059 (6)	0.0005 (6)
C2	0.0779 (11)	0.0422 (7)	0.0512 (8)	0.0033 (7)	0.0042 (7)	0.0103 (6)
C5	0.0537 (8)	0.0424 (7)	0.0559 (8)	−0.0028 (6)	0.0051 (6)	0.0042 (6)
O2	0.0701 (8)	0.0792 (8)	0.0976 (9)	0.0015 (7)	0.0268 (7)	−0.0105 (7)
C10	0.0443 (7)	0.0483 (7)	0.0476 (7)	0.0032 (6)	0.0072 (5)	−0.0004 (6)
C11	0.0595 (9)	0.0410 (7)	0.0545 (8)	0.0008 (6)	0.0074 (6)	−0.0025 (6)
C4	0.0526 (8)	0.0488 (7)	0.0406 (6)	−0.0002 (6)	0.0012 (5)	0.0073 (5)
O4	0.1144 (11)	0.0847 (9)	0.0501 (7)	−0.0059 (7)	0.0176 (6)	0.0030 (6)
C9	0.0694 (10)	0.0494 (8)	0.0475 (8)	0.0031 (7)	0.0096 (7)	−0.0072 (6)
C13	0.0613 (9)	0.0585 (9)	0.0491 (8)	−0.0027 (7)	0.0138 (6)	0.0099 (6)
C8	0.0693 (10)	0.0406 (7)	0.0576 (8)	0.0020 (6)	0.0101 (7)	−0.0024 (6)
C3	0.0639 (9)	0.0515 (8)	0.0515 (8)	−0.0042 (7)	0.0074 (6)	0.0155 (6)
C14	0.0574 (9)	0.0575 (9)	0.0514 (8)	0.0016 (7)	0.0157 (6)	0.0016 (6)
O3	0.1400 (13)	0.0519 (7)	0.0849 (9)	0.0025 (7)	0.0352 (8)	0.0156 (6)
O1	0.1440 (14)	0.0671 (8)	0.1377 (14)	0.0428 (9)	0.0643 (12)	0.0231 (8)

Geometric parameters (Å, °)

C1—C6	1.378 (2)	C5—C4	1.3948 (19)
C1—C2	1.381 (2)	C5—H5A	0.93
C1—N1	1.4709 (19)	C10—C9	1.3913 (19)
N2—O4	1.2119 (16)	C10—C11	1.3916 (19)
N2—O3	1.2135 (17)	C10—C14	1.477 (2)
N2—C7	1.4700 (18)	C11—H11A	0.93
C12—C11	1.378 (2)	C4—C3	1.394 (2)
C12—C7	1.3785 (19)	C4—C13	1.473 (2)
C12—H12A	0.93	C9—C8	1.379 (2)
C7—C8	1.376 (2)	C9—H9A	0.93

C6—C5	1.376 (2)	C13—C14	1.327 (2)
C6—H6A	0.93	C13—H13A	0.93
N1—O1	1.2158 (17)	C8—H8A	0.93
N1—O2	1.2231 (18)	C3—H3A	0.93
C2—C3	1.376 (2)	C14—H14A	0.93
C2—H2A	0.93		

C6—C1—C2	122.03 (14)	C9—C10—C11	118.43 (13)
C6—C1—N1	118.60 (13)	C9—C10—C14	119.78 (13)
C2—C1—N1	119.38 (13)	C11—C10—C14	121.70 (13)
O4—N2—O3	122.82 (13)	C12—C11—C10	121.08 (13)
O4—N2—C7	118.66 (13)	C12—C11—H11A	119.5
O3—N2—C7	118.51 (13)	C10—C11—H11A	119.5
C11—C12—C7	118.57 (13)	C3—C4—C5	117.97 (13)
C11—C12—H12A	120.7	C3—C4—C13	119.32 (13)
C7—C12—H12A	120.7	C5—C4—C13	122.61 (13)
C8—C7—C12	122.21 (13)	C8—C9—C10	121.31 (13)
C8—C7—N2	118.63 (13)	C8—C9—H9A	119.3
C12—C7—N2	119.16 (12)	C10—C9—H9A	119.3
C5—C6—C1	118.53 (13)	C14—C13—C4	129.41 (13)
C5—C6—H6A	120.7	C14—C13—H13A	115.3
C1—C6—H6A	120.7	C4—C13—H13A	115.3
O1—N1—O2	123.27 (15)	C7—C8—C9	118.35 (13)
O1—N1—C1	118.33 (15)	C7—C8—H8A	120.8
O2—N1—C1	118.40 (13)	C9—C8—H8A	120.8
C3—C2—C1	118.50 (13)	C2—C3—C4	121.48 (14)
C3—C2—H2A	120.8	C2—C3—H3A	119.3
C1—C2—H2A	120.8	C4—C3—H3A	119.3
C6—C5—C4	121.48 (13)	C13—C14—C10	128.73 (13)
C6—C5—H5A	119.3	C13—C14—H14A	115.6
C4—C5—H5A	119.3	C10—C14—H14A	115.6

C11—C12—C7—C8	1.5 (2)	C14—C10—C11—C12	−177.96 (13)
C11—C12—C7—N2	−179.22 (12)	C6—C5—C4—C3	0.3 (2)
O4—N2—C7—C8	176.23 (14)	C6—C5—C4—C13	−176.04 (13)
O3—N2—C7—C8	−4.7 (2)	C11—C10—C9—C8	2.5 (2)
O4—N2—C7—C12	−3.1 (2)	C14—C10—C9—C8	179.12 (14)
O3—N2—C7—C12	175.97 (14)	C3—C4—C13—C14	149.55 (16)
C2—C1—C6—C5	−0.5 (2)	C5—C4—C13—C14	−34.2 (2)
N1—C1—C6—C5	179.65 (12)	C12—C7—C8—C9	−0.5 (2)
C6—C1—N1—O1	−177.33 (16)	N2—C7—C8—C9	−179.73 (13)
C2—C1—N1—O1	2.8 (2)	C10—C9—C8—C7	−1.6 (2)
C6—C1—N1—O2	3.4 (2)	C1—C2—C3—C4	−1.1 (2)
C2—C1—N1—O2	−176.45 (14)	C5—C4—C3—C2	0.4 (2)
C6—C1—C2—C3	1.1 (2)	C13—C4—C3—C2	176.81 (14)
N1—C1—C2—C3	−179.03 (12)	C4—C13—C14—C10	−7.1 (3)
C1—C6—C5—C4	−0.2 (2)	C9—C10—C14—C13	138.17 (17)
C7—C12—C11—C10	−0.5 (2)	C11—C10—C14—C13	−45.4 (2)
C9—C10—C11—C12	−1.5 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2A···O3^{i}	0.93	2.45	3.3606 (18)	166
C9—H9A···O4^{ii}	0.93	2.58	3.4381 (18)	153

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2; (ii) *x*, *y*, *z*−1.

Fig. 1

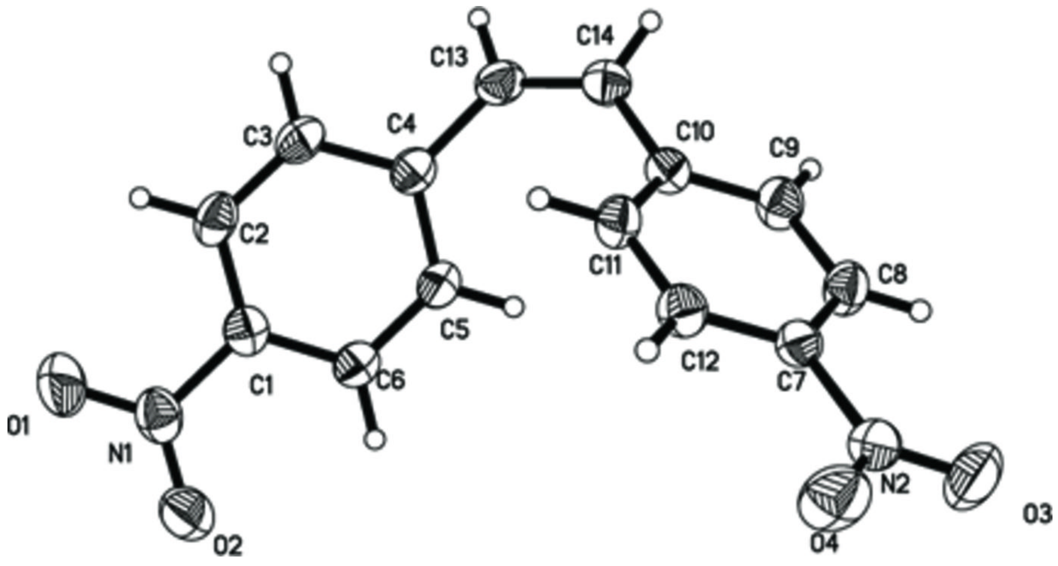
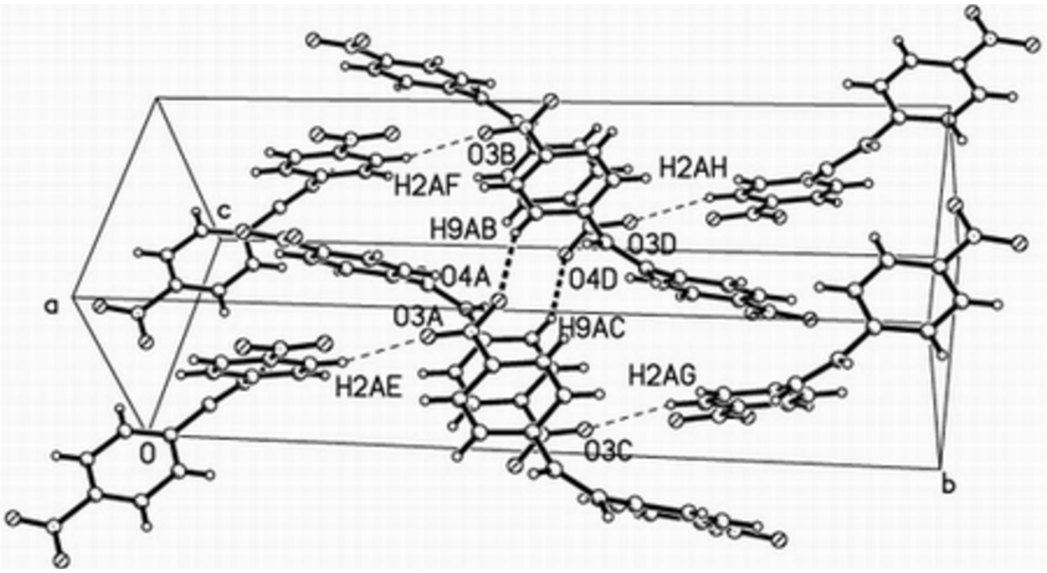


Fig. 2



Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

(*Z*)-1,2-Bis(4-nitrophenyl)ethene. Corrigendum

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Received 11 April 2008; accepted 11 April 2008

The name of the first author in the paper by Chen & Cao [*Acta Cryst.* (2007), E**63**, o3999] is corrected.

In the paper by Chen & Cao [*Acta Cryst.* (2007), E**63**, o3999], the name of the first author is incorrect. The correct name is given above.

doi:10.1107/S1600536808009999