Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

(*E*)-2-Methyl-4-(phenyldiazenyl)phenol

Çiğdem Albayrak,[a]* İsmail Erdem Gümrükçüoğlu,[a] Mustafa Odabaşoğlu[a] and Orhan Büyükgüngör[b]

[a]Department of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayıs University, TR-55139 Kurupelit Samsun, Turkey, and [b]Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, TR-55139 Kurupelit Samsun, Turkey
Correspondence e-mail: cigdema@omu.edu.tr

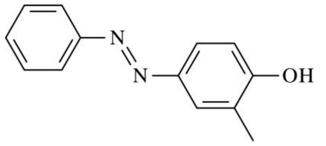
Received 26 June 2007; accepted 25 July 2007

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.051; wR factor = 0.152; data-to-parameter ratio = 13.0.

In the molecule of the title compound, $C_{13}H_{12}N_2O$, all atoms except for the methyl H atoms are coplanar and the dihedral angle between the aromatic rings is 1.38 (7)°. In the crystal structure, intermolecular O—H···N and C—H···O hydrogen bonds link the molecules to form two edge-fused $R_2^2(6)$ motifs. They are also connected by C—H···π and π–π interactions between phenyldiazenyl rings [centroid-to-centroid distance and plane-to-plane separation 3.708 (1) and 3.418 Å, respectively] to form a three-dimensional network. The two N atoms are disordered over two positions, the site-occupancy ratio being 3:2.

Related literature

For general background, see: Stenhouse (1868); Mohlau (1883); Witt (1909); Elion (1923*a*,*b*); Fuchs (1923); Knecht (1924); Venkataraman (1970); Egli *et al.* (1991); Marmion (1991); Garg & Sharma (1996); Modest *et al.* (1957); Ravindranath *et al.* (1983); Etter (1990). For related literature, see: Odabaşoğlu *et al.* (2003, 2007); Ersanlı, Albayrak *et al.* (2004); Ersanlı, Odabaşoğlu *et al.* (2004); Çakır *et al.* (2005); Şahin *et al.* (2005*a*,*b*,*c*,*d*,*e*). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{13}H_{12}N_2O$
M_r = 212.25
Monoclinic, $P2_1/c$
a = 9.0537 (6) Å
b = 10.5716 (9) Å
c = 12.0287 (7) Å
β = 108.952 (4)°
V = 1088.88 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
0.66 × 0.48 × 0.14 mm

Data collection

Stoe IPDS2 diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.747, T_{max} = 0.949
15802 measured reflections
2131 independent reflections
1457 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.152
S = 1.05
2131 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

*Cg*2 is the centroid of the phenyldiazenyl ring.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2B^{i}	0.82	2.10	2.904 (8)	168
O1—H1···N1A^{i}	0.82	2.08	2.891 (6)	172
C2—H2···O1^{ii}	0.93	2.65	3.427 (3)	142
C12—H12···O1^{ii}	0.93	2.57	3.367 (2)	144
C13—H13*B*···*Cg*2	0.96	2.81	3.495 (3)	130

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for the use of the Stoe IPDSII diffractometer (purchased under grant No. F279 of the University Research Fund).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2282).

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.
Çakır, S., Biçer, E., Odabaşoğlu, M. & Albayrak, Ç. (2005). *J. Braz. Chem. Soc.* **16**, 711–717.
Egli, R., Peter, A. P. & Freeman, H. S. (1991). Editors. *Colour Chemistry: The Design and Synthesis of Organic Dyes and Pigments*, ch. VII. London: Elsevier.
Elion, L. (1923*a*). *Recl Trav. Chim. Pays Bas*, **42**, 145–183.
Elion, L. (1923*b*). *Recl Trav. Chim. Pays Bas*, **42**, 513–515.
Ersanlı, C. C., Albayrak, Ç., Odabaşoğlu, M., Kazak, C. & Erdömez, A. (2004). *Acta Cryst.* C**60**, o455–o457.
Ersanlı, C. C., Odabaşoğlu, M., Albayrak, Ç. & Erdömez, A. (2004). *Acta Cryst.* E**60**, o230–o231.
Etter, M. C. (1990). *Acc. Chem. Res.* **23**, 120–126.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Fuchs, W. (1923). *Recl Trav. Chim. Pays Bas*, **42**, 511–512.
Garg, H. G. & Sharma, R. A. (1996). *J. Med. Chem.* **12**, 1122–1126.
Knecht, E. (1924). *J. Chem. Soc.* pp. 1538–1539.
Marmion, D. M. (1991). *Handbook of US Colorants*, 3rd ed., p. 23. New York: Wiley.
Modest, E. J., Schlein, H. N. & Foley, G. E. (1957). *J. Pharmacol.* **9**, 68–71.
Mohlau, R. (1883). *Berichte*, **16**, 30–80.

© 2007 International Union of Crystallography doi:10.1107/S1600536807036501

Odabaşoğlu, M., Albayrak, Ç., Büyükgüngör, O. & Goesmann, H. (2003). *Acta Cryst.* C**59**, o234–o236.

Odabaşoğlu, M., Albayrak, Ç., Özkanca, R., Aykan, F. Z. & Lönnecke, P. (2007). *J. Mol. Struct.* In the press.

Ravindranath, L. K., Ramadas, S. R. & Rao, S. B. (1983). *Electrochim. Acta*, **28**, 601–610.

Şahin, O., Albayrak, Ç., Odabaşoğlu, M. & Büyükgüngör, O. (2005*a*). *Acta Cryst.* E**61**, o4149–o4150.

Şahin, O., Albayrak, Ç., Odabaşoğlu, M. & Büyükgüngör, O. (2005*b*). *Acta Cryst.* E**61**, o4151–o4153.

Şahin, O., Albayrak, Ç., Odabaşoğlu, M. & Büyükgüngör, O. (2005*c*). *Acta Cryst.* E**61**, o4154–o4155.

Şahin, O., Albayrak, Ç., Odabaşoğlu, M. & Büyükgüngör, O. (2005*d*). *Acta Cryst.* E**61**, E61, o4276–o4278.

Şahin, O., Albayrak, Ç., Odabaşoğlu, M. & Büyükgüngör, O. (2005*e*). *Acta Cryst.* E**61**, o4279–o4281.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Stenhouse, J. (1868). *J. Chem. Soc.* pp. 150–151.

Stoe & Cie (2002). *X-AREA* (Version 1.18) and *X-RED32* (Version 1.04). Stoe & Cie, Darmstadt, Germany.

Venkataraman, K. (1970). *The Chemistry of Synthetic Dyes*, ch. VI. New York/London: Academic Press.

Witt, O. N. (1909). *Berichte*, **42**, 2953–2961.

supplementary materials

Acta Cryst. (2007). E**63**, o3662-o3663 [**doi:10.1107/S1600536807036501**]

(*E*)-2-Methyl-4-(phenyldiazenyl)phenol

Ç. Albayrak, I.E. Gümrükçüoglu, M. Odabasoglu and **O. Büyükgüngör**

Comment

Azo compounds were described over 150 years ago (Stenhouse, 1868; Mohlau, 1883; Witt, 1909; Elion, 1923*a*,*b*; Fuch, 1923; Knecht, 1924). They are the oldest and largest class of industrially synthesized organic dyes due to their versatile applications in various fields, such as dyeing textile fibers, biomedical studies, advanced applications in organic synthesis and high technology areas such as lasers, liquid crystalline displays, electro-optical devices and ink-jet printers (Venkataraman, 1970; Egli *et al.*, 1991). There are about 3000 azo dyes currently in use all over the world. The great majority of them are monoazo compounds, which have the common structure unit of the azo chromophore, –N=N–, linking two aromatic systems. The textile industry is the largest consumer of dyestuffs. Although some azo dyes have been reported to be toxic, dozens of additional monoazo dyes are permitted in drugs and cosmetics (Marmion, 1991). The pharmaceutical importance of compounds including an arylazo group has been extensively reported in the literature (Garg & Sharma, 1996; Modest *et al.*, 1957). The oxidation-reduction behaviors of these compounds play an important role in their biological activities (Ravindranath *et al.*, 1983). The structures of some azo derivatives have been the subject of much interest in our laboratory (Odabaşoğlu *et al.*, 2003, 2007; Ersanlı, Albayrak *et al.*, 2004; Ersanlı, Odabaşoğlu *et al.*, 2004; Çakır *et al.*, 2005; Şahin *et al.*, 2005*a*,*b*,*c*,*d*,*e*). In view of the importance of the title compound, (I), we report herein its crystal structure.

In the molecule of the title compound, (I), (Fig. 1) the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987). In the azo group, the N—C and N—N bonds and C—N—N angles are slightly deviate from their normal values (Table 1), due to the disordered N1A and N2A atoms. Aromatic rings adopt a *trans* configuration about the azo functional group, as observed in the structures of other previously reported azo compounds. Except the methyl protons, all atoms are in the same plane and the dihedral angle between the two aromatic rings is 1.38 (7)°.

In the crystal structure, intermolecular O—H···N and C—H···O hydrogen bonds (Table 2) link the molecules (Fig. 2) to form two edge fused $R_2^2(6)$ motifs (Etter, 1990). They are also connected by C—H···π and π···π interactions between (C1–C6) rings at (x, y, z) and $(-x, 1-y, 1-z)$, where the centroid-centroid distance and plane-plane separation are 3.708 (1) Å and 3.418 Å, respectively, (Fig. 3) to form a three-dimensional network.

Experimental

The title compound was prepared according to the literature method (Odabaşoğlu *et al.*, 2003), using aniline and 2-methylphenol as starting materials. The product was crystallized from acetic acid solution to obtain well shaped crystals (yield; 80%, m.p. 408–410 K).

Refinement

When the crystal structure was solved,the atoms N1A and N2A were found to be disordered over two positions. During refinement with anisotropic thermal parameters, the occupancies of disordered N atoms were kept fixed as N1A = 0.63, N1B = 0.37, N2A = 0.63 and N2B = 0.37. H atoms were positioned geometrically with O—H = 0.82 Å (for OH) and C—H

= 0.93 and 0.96 Å for aromatic and methyl H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C,*O*), where x = 1.2 for aromaic H and x = 1.5 for all other H atoms.

Figures

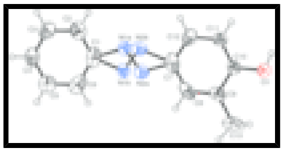


Fig. 1. The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

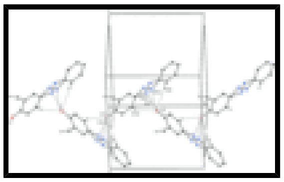


Fig. 2. Part of the crystal structure of (I), showing the formation of $R_2^2(6)$ $R_2^2(6)$ ring motifs. H atoms not involved in intermolecular interactions have been ommited for clarity [symmetry code: (i) $x - 1/2$, $y + 1/2$, $1/2 - z$].

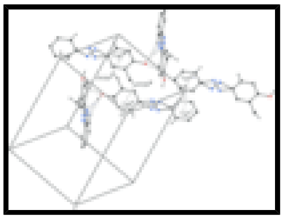


Fig. 3. Part of the crystal structure of (I), showing the formation of C—H···π and π···π interactions·H atoms not involved in intermolecular interactions have been ommited for clarity [symmetry code: (i) $-x$, $1/2 - y$, $-z$; (ii) $-x$, $-y$, z; (iii) $x - 1$, y, $z - 1$; (iv) x, $y - 1$, $z - 1$].

(*E*)-2-Methyl-4-(phenyldiazenyl)phenol

Crystal data

$C_{13}H_{12}N_2O$	F_{000} = 448
M_r = 212.25	D_x = 1.295 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 15802 reflections
a = 9.0537 (6) Å	θ = 1.9–28.0º
b = 10.5716 (9) Å	μ = 0.08 mm^{-1}
c = 12.0287 (7) Å	T = 296 K
β = 108.952 (4)º	Plate, brown
V = 1088.88 (13) Å^3	0.66 × 0.48 × 0.14 mm
Z = 4	

Data collection

Stoe IPDS2 diffractometer	2131 independent reflections
Monochromator: plane graphite	1457 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	R_{int} = 0.049
T = 296 K	θ_{max} = 26.0º
ω scans	θ_{min} = 2.4º
Absorption correction: integration	h = −11→11

(X-RED32; Stoe & Cie, 2002)	
T_{min} = 0.747, T_{max} = 0.949	$k = -13 \rightarrow 13$
15802 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.051$	H-atom parameters constrained
$wR(F^2) = 0.152$	$w = 1/[\sigma^2(F_o^2) + (0.0899P)^2 + 0.0268P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
2131 reflections	$\Delta\rho_{max}$ = 0.17 e Å^{-3}
164 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}	Occ. (<1)
O1	0.73324 (15)	−0.02601 (11)	0.37389 (11)	0.0732 (4)	
H1	0.7186	−0.0445	0.3049	0.110*	
N1A	0.2873 (5)	0.4216 (4)	0.3666 (5)	0.0676 (10)	0.63
N2A	0.3664 (4)	0.3614 (3)	0.4494 (4)	0.0696 (7)	0.63
N1B	0.3083 (6)	0.4176 (4)	0.4572 (5)	0.0504 (11)	0.37
N2B	0.3275 (8)	0.3706 (5)	0.3604 (7)	0.0501 (14)	0.37
C1	0.2013 (2)	0.51896 (18)	0.4215 (3)	0.0841 (7)	
C2	0.0993 (2)	0.5789 (2)	0.3269 (2)	0.0864 (6)	
H2	0.0932	0.5553	0.2511	0.104*	
C3	0.0051 (2)	0.6746 (2)	0.3441 (2)	0.0867 (6)	
H3	−0.0647	0.7148	0.2795	0.104*	
C4	0.0135 (2)	0.71075 (19)	0.4552 (2)	0.0808 (6)	
H4	−0.0501	0.7754	0.4661	0.097*	
C5	0.1155 (3)	0.6516 (2)	0.5498 (2)	0.0852 (6)	
H5	0.1215	0.6762	0.6253	0.102*	

C6	0.2091 (2)	0.5562 (2)	0.5342 (3)	0.0896 (7)
H6	0.2783	0.5162	0.5992	0.108*
C7	0.4448 (3)	0.26581 (18)	0.3974 (3)	0.0822 (7)
C8	0.5429 (3)	0.20592 (19)	0.4970 (2)	0.0795 (6)
H8	0.5426	0.2330	0.5705	0.095*
C9	0.6396 (2)	0.10893 (17)	0.49118 (15)	0.0657 (5)
C10	0.63655 (19)	0.06967 (14)	0.37949 (14)	0.0555 (4)
C11	0.5386 (2)	0.12666 (16)	0.27975 (16)	0.0631 (5)
H11	0.5372	0.0986	0.2061	0.076*
C12	0.4438 (2)	0.22363 (17)	0.2880 (2)	0.0733 (5)
H12	0.3782	0.2616	0.2202	0.088*
C13	0.7481 (3)	0.0461 (2)	0.59793 (18)	0.0968 (8)
H13A	0.8540	0.0581	0.5997	0.145*
H13B	0.7253	−0.0427	0.5955	0.145*
H13C	0.7347	0.0826	0.6671	0.145*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0869 (9)	0.0648 (7)	0.0624 (8)	0.0110 (7)	0.0166 (6)	0.0011 (6)
N1A	0.065 (2)	0.073 (3)	0.063 (3)	−0.0147 (17)	0.0179 (17)	0.005 (2)
N2A	0.0717 (18)	0.074 (2)	0.062 (2)	−0.0149 (15)	0.0205 (17)	0.0044 (16)
N1B	0.055 (2)	0.048 (2)	0.055 (4)	0.0076 (17)	0.027 (2)	−0.002 (2)
N2B	0.060 (3)	0.045 (3)	0.048 (4)	−0.003 (2)	0.021 (2)	0.000 (2)
C1	0.0572 (10)	0.0567 (10)	0.141 (2)	−0.0070 (8)	0.0366 (13)	−0.0023 (12)
C2	0.0700 (12)	0.0943 (15)	0.0991 (17)	−0.0051 (11)	0.0331 (12)	−0.0146 (12)
C3	0.0675 (12)	0.0923 (15)	0.0983 (18)	0.0053 (11)	0.0242 (11)	0.0170 (12)
C4	0.0765 (13)	0.0680 (11)	0.1081 (19)	0.0003 (10)	0.0439 (13)	−0.0014 (11)
C5	0.0815 (13)	0.0839 (13)	0.0917 (16)	−0.0144 (12)	0.0300 (12)	0.0015 (12)
C6	0.0654 (12)	0.0755 (13)	0.118 (2)	−0.0094 (10)	0.0169 (12)	0.0234 (13)
C7	0.0767 (13)	0.0543 (10)	0.136 (2)	−0.0137 (9)	0.0627 (14)	−0.0183 (12)
C8	0.1009 (15)	0.0697 (11)	0.0870 (15)	−0.0335 (11)	0.0571 (13)	−0.0286 (11)
C9	0.0841 (12)	0.0621 (10)	0.0527 (10)	−0.0265 (9)	0.0247 (9)	−0.0069 (8)
C10	0.0651 (9)	0.0490 (8)	0.0531 (10)	−0.0050 (7)	0.0201 (8)	−0.0013 (7)
C11	0.0733 (11)	0.0631 (10)	0.0540 (10)	−0.0020 (8)	0.0220 (8)	0.0033 (7)
C12	0.0668 (11)	0.0610 (10)	0.0928 (15)	0.0018 (8)	0.0268 (10)	0.0148 (9)
C13	0.1265 (19)	0.1026 (16)	0.0507 (12)	−0.0450 (15)	0.0141 (12)	0.0009 (11)

Geometric parameters (Å, °)

C1—C2	1.367 (3)	C7—N2B	1.501 (7)
C1—C6	1.390 (4)	C8—C9	1.365 (3)
C1—N1B	1.418 (6)	C8—H8	0.9300
C1—N1A	1.558 (6)	C9—C10	1.398 (2)
C2—C3	1.381 (3)	C9—C13	1.495 (3)
C2—H2	0.9300	C10—O1	1.3537 (19)
C3—C4	1.368 (3)	C10—C11	1.377 (2)
C3—H3	0.9300	C11—C12	1.362 (3)
C4—C5	1.362 (3)	C11—H11	0.9300

C4—H4	0.9300	C12—H12	0.9300
C5—C6	1.369 (3)	C13—H13A	0.9600
C5—H5	0.9300	C13—H13B	0.9600
C6—H6	0.9300	C13—H13C	0.9600
C7—C12	1.386 (3)	N1A—N2A	1.208 (6)
C7—C8	1.390 (3)	N1B—N2B	1.324 (9)
C7—N2A	1.485 (5)	O1—H1	0.8200

C2—C1—C6	119.1 (2)	C9—C8—H8	118.7
C2—C1—N1B	144.5 (3)	C7—C8—H8	118.7
C6—C1—N1B	96.1 (3)	C8—C9—C10	117.35 (18)
C2—C1—N1A	104.3 (3)	C8—C9—C13	122.9 (2)
C6—C1—N1A	136.5 (3)	C10—C9—C13	119.70 (19)
C1—C2—C3	119.9 (2)	O1—C10—C11	121.83 (16)
C1—C2—H2	120.1	O1—C10—C9	117.30 (16)
C3—C2—H2	120.1	C11—C10—C9	120.87 (17)
C4—C3—C2	120.7 (2)	C12—C11—C10	120.56 (18)
C4—C3—H3	119.7	C12—C11—H11	119.7
C2—C3—H3	119.7	C10—C11—H11	119.7
C5—C4—C3	119.7 (2)	C11—C12—C7	120.1 (2)
C5—C4—H4	120.2	C11—C12—H12	119.9
C3—C4—H4	120.2	C7—C12—H12	119.9
C4—C5—C6	120.4 (2)	C9—C13—H13A	109.5
C4—C5—H5	119.8	C9—C13—H13B	109.5
C6—C5—H5	119.8	H13A—C13—H13B	109.5
C5—C6—C1	120.3 (2)	C9—C13—H13C	109.5
C5—C6—H6	119.9	H13A—C13—H13C	109.5
C1—C6—H6	119.9	H13B—C13—H13C	109.5
C12—C7—C8	118.45 (18)	N2A—N1A—C1	104.3 (6)
C12—C7—N2A	139.7 (3)	N1A—N2A—C7	104.6 (6)
C8—C7—N2A	101.8 (2)	N2B—N1B—C1	106.6 (7)
C12—C7—N2B	99.9 (3)	N1B—N2B—C7	107.2 (7)
C8—C7—N2B	141.7 (3)	C10—O1—H1	109.5
C9—C8—C7	122.63 (19)		

C6—C1—C2—C3	−0.4 (3)	C9—C10—C11—C12	0.7 (3)
N1B—C1—C2—C3	173.1 (3)	C10—C11—C12—C7	−0.1 (3)
N1A—C1—C2—C3	−178.5 (2)	C8—C7—C12—C11	−0.7 (3)
C1—C2—C3—C4	0.4 (3)	N2A—C7—C12—C11	−179.1 (2)
C2—C3—C4—C5	−0.1 (3)	N2B—C7—C12—C11	179.1 (3)
C3—C4—C5—C6	−0.1 (3)	C2—C1—N1A—N2A	−173.9 (3)
C4—C5—C6—C1	0.1 (3)	C6—C1—N1A—N2A	8.5 (4)
C2—C1—C6—C5	0.1 (3)	N1B—C1—N1A—N2A	−1.3 (3)
N1B—C1—C6—C5	−176.1 (2)	C1—N1A—N2A—C7	178.2 (2)
N1A—C1—C6—C5	177.5 (3)	C12—C7—N2A—N1A	−5.9 (4)
C12—C7—C8—C9	1.0 (3)	C8—C7—N2A—N1A	175.6 (2)
N2A—C7—C8—C9	179.94 (18)	N2B—C7—N2A—N1A	−3.0 (5)
N2B—C7—C8—C9	−178.6 (4)	C2—C1—N1B—N2B	9.6 (6)
C7—C8—C9—C10	−0.5 (3)	C6—C1—N1B—N2B	−176.1 (3)
C7—C8—C9—C13	178.53 (17)	N1A—C1—N1B—N2B	−2.9 (4)

C8—C9—C10—O1	179.59 (14)	C1—N1B—N2B—C7	178.2 (3)
C13—C9—C10—O1	0.6 (2)	C12—C7—N2B—N1B	176.7 (4)
C8—C9—C10—C11	−0.4 (2)	C8—C7—N2B—N1B	−3.6 (7)
C13—C9—C10—C11	−179.46 (16)	N2A—C7—N2B—N1B	−1.4 (3)
O1—C10—C11—C12	−179.29 (15)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2B^{i}	0.82	2.10	2.904 (8)	168
O1—H1···N1A^{i}	0.82	2.08	2.891 (6)	172
C2—H2···O1^{ii}	0.93	2.65	3.427 (3)	142
C12—H12···O1^{ii}	0.93	2.57	3.367 (2)	144

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

Fig. 1

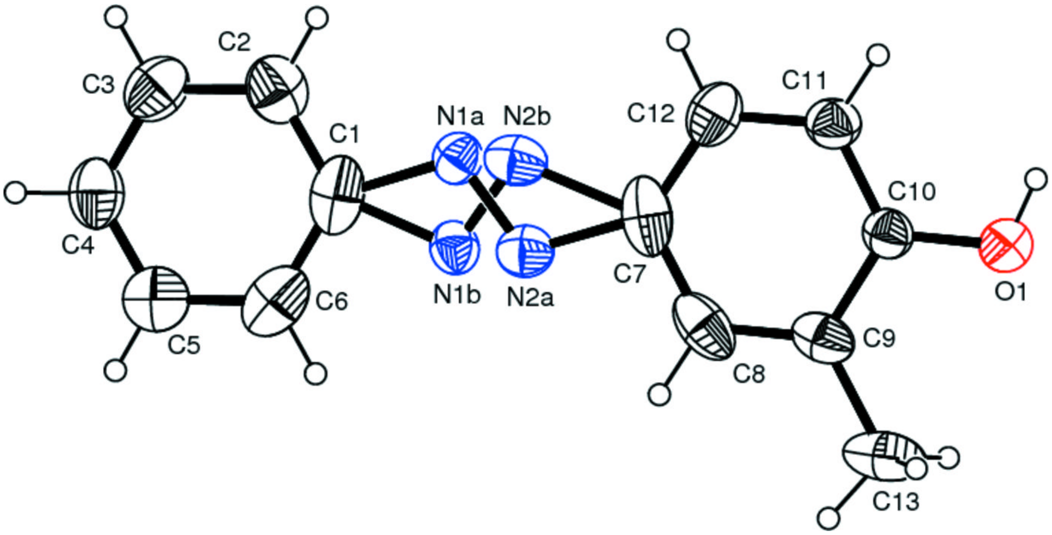


Fig. 2

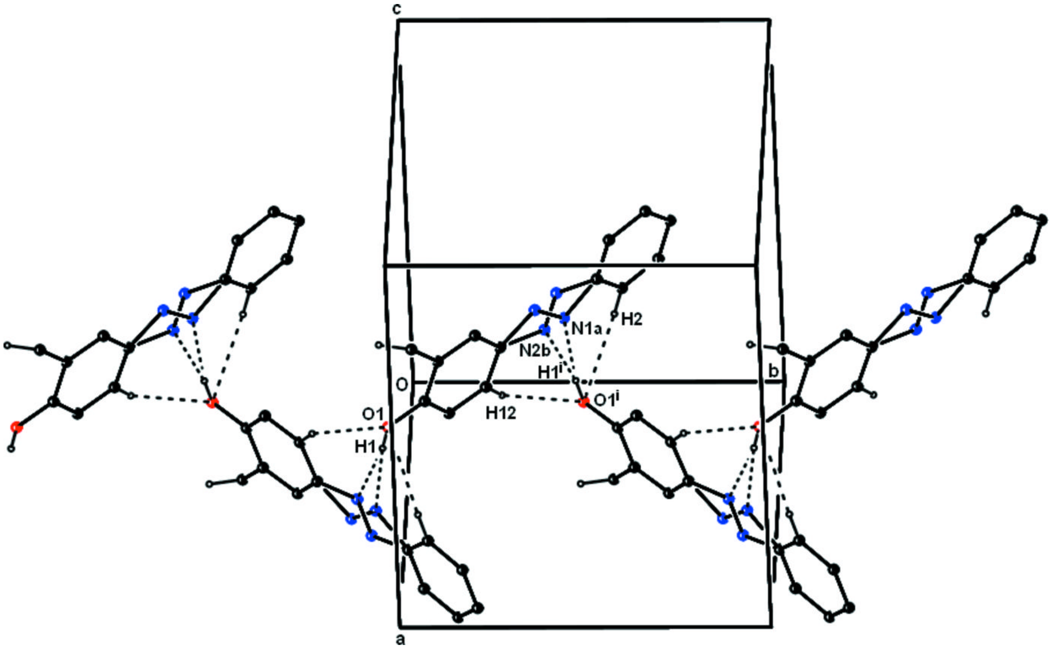


Fig. 3