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(*E*)-4-Methoxy-*N*-(3,4-methylenedioxybenzylidene)aniline

Shu-Ping Yang,[a]* Li-Jun Han,[b] Da-Qi Wang[c] and Zhi-Qun Yu[a]

[a]Department of Chemical Engineering, Huaihai Institute of Technology, Lianyungang 222005, People's Republic of China, [b]Department of Mathematics and Science, Huaihai Institute of Technology, Lianyungang 222005, People's Republic of China, and [c]College of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of China
Correspondence e-mail: yangshuping@hhit.edu.cn

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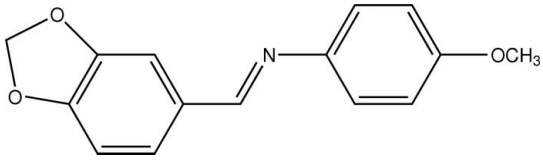
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.015 Å; R factor = 0.103; wR factor = 0.303; data-to-parameter ratio = 6.8.

The title compound, $C_{15}H_{13}NO_3$, crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit. The *A* molecules are linked by two C—H···O hydrogen bonds into a sheet of $R_4^4(33)$ rings, and the *B* molecules are linked into a *C*(13) chain by C—H···O hydrogen bonds. The molecules are also connected by three C—H···π interactions, resulting in a three-dimensional structure.

Related literature

For related literature, see: Allen *et al.* (1987); Bernstein *et al.* (1995); Yang *et al.* (2007*a*,*b*).



Experimental

Crystal data

$C_{15}H_{13}NO_3$
M_r = 255.26
Monoclinic, $P2_1$
a = 14.497 (2) Å
b = 6.119 (1) Å
c = 14.732 (2) Å
β = 102.819 (2)°
V = 1274.3 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
0.57 × 0.18 × 0.11 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.949, T_{max} = 0.990
6121 measured reflections
2363 independent reflections
1115 reflections with $I > 2\sigma(I)$
R_{int} = 0.099

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.103
$wR(F^2)$ = 0.303
S = 0.95
2363 reflections
345 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

*Cg*2*A* and *Cg*2*B* are the centroids of the rings C9*A*–C17*A* and C9*B*–C17*B*, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C8*A*—H8*A*···O3*A*^{i}	0.97	2.58	3.28 (2)	129
C8*B*—H8*C*···O3*B*^{i}	0.97	2.57	3.36 (2)	139
C15*A*—H15*B*···O2*A*^{ii}	0.96	2.60	3.32 (2)	132
C13*A*—H13*A*···*Cg*2*B*	0.93	3.05	3.69 (4)	127
C10*A*—H10*A*···*Cg*2*A*^{iii}	0.93	2.70	3.45 (4)	138
C13*B*—H13*B*···*Cg*2*A*^{iv}	0.93	3.09	3.70 (4)	124

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2399).

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supplementary materials

Acta Cryst. (2007). E**63**, o4098 [**doi:10.1107/S1600536807045503**]

(*E*)-4-Methoxy-*N*-(3,4-methylenedioxybenzylidene)aniline

S.-P. Yang, L.-J. Han, D.-Q. Wang and Z.-Q. Yu

Comment

We have reported recently the crystal structures of some Schiff bases compounds (Yang *et al.*, 2007*a*,*b*). As part of our study of Schiff bases compounds, we report here the crystal structure of the title compound (I).

The compound (I) crystallizes in monoclinic space group $P2_1/c$, with two independent molecules in the asymmetric unit. In the asymmetric unit, the molecules *A* and *B* are likned by one C—H···π intercation [C13A···*Cg*2B = 3.69 (4) Å, H13A···*Cg*2B = 3.05 Å, C13A—H13A···*Cg*2B = 127°; where *Cg*2B is the centroid of the ring C9B–C17B] (Table 1 and Fig. 1). The molecules *A* and *B* have an E configuration, the dihedral angle between the two benzene rings are 46.3 (3)° for molecule *A* and 43.5 (2)° for molecule *B*, respectively. The geometric parameters in (I) are normal (Allen *et al.*, 1987).

In the crystal structure of (I), atom C8A in the molecule *A* at (*x*, *y*, *z*) acts as hydrogen-bond donor, *via* H8A, to atom O3A in the molecule *A* at (*x*, *y*, −1 + *z*), forming a simple *C*(13) chain (Bernstein *et al.*, 1995). Similarly, atom C15A at (*x*, *y*, *z*) acts as hydrogen-bond donor, *via* H15B, to O2A at (*x*, −1 + *y*, 1 + *z*), producing a *C*(14) chain. The combination of the two chains generates a $R_4^4(33)$ ring (Table 1 and Fig. 2).

In (I), atom C8B in the molecule *B* at (*x*, *y*, *z*) acts as hydrogen-bond donor, *via* H8C, to atom O3B in the molecule *B* at (*x*, *y*, −1 + *z*), forming a simple *C*(13) chain running parallel to the [001] direction (Table 1 and Fig.3).

The molecules are also connected by three C—H···π interactions, resulting in a three-dimensional structure (see Table 1).

Experimental

The mixture containing piperonaldehyde (1.5 g, 10 mmol) and 4-methoxyaniline (1.23 g, 10 mmol) was refluxed for about 4 h in ethanol (30 ml), then the reaction mixture was cooled and the products were filtered off, washed with ethanol and dried. Colourless crystals of (I) suitatble for X-ray structure analysis were obtained by recrystallizing the crude product from ethanol [m.p.383–385 K].

Refinement

H atoms were placed in calculated positions with C—H = 0.93–0.97 Å, and refined in riding mode with U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

Figures

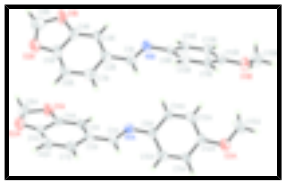


Fig. 1. A view of the two independent molecules of (I) in the asymmetric unit, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

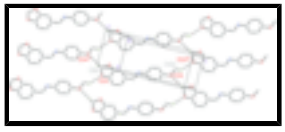


Fig. 2. A view of part of the crystal structure of molecule *A*, showing $R_4^4(33)$ rings. For clarity, H atoms bonded to C atoms have been omitted. Dashed lines indicate hydrogen bonds [Symmetry codes: (*) *x*, *y*,-1 + *z*; (#) *x*, −1 + *y*, 1 + *z*].

Fig. 3. A view of part of the crystal structure of molecule *B*, showing the formation of a *C*(13) chain along [001]. For clarity, H atoms bonded to C atoms have been omitted. Dashed lines indicate hydrogen bonds [Symmetry codes: (*) *x*, *y*, −1 + *z*; (#) *x*, *y*, 1 + *z*].

(*E*)-4-Methoxy-*N*-(3,4-methylenedioxybenzylidene)aniline

Crystal data

$C_{15}H_{13}NO_3$	F_{000} = 536
M_r = 255.26	D_x = 1.331 Mg m^{-3}
Monoclinic, $P2_1$	Melting point: 383 K
Hall symbol: P 2yb	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 14.497 (2) Å	Cell parameters from 741 reflections
b = 6.1192 (14) Å	θ = 2.3–21.0º
c = 14.732 (2) Å	μ = 0.09 mm^{-1}
β = 102.819 (2)º	*T* = 298 (2) K
V = 1274.3 (4) Å^3	Needle, colourless
Z = 4	0.57 × 0.18 × 0.11 mm

Data collection

Bruker SMART CCD area-detector diffractometer	2363 independent reflections
Radiation source: fine-focus sealed tube	1115 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.099
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −17→17
T_{min} = 0.949, T_{max} = 0.990	*k* = −7→7
6121 measured reflections	*l* = −17→12

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites

Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.103$	$w = 1/[\sigma^2(F_o^2) + (0.1804P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.303$	$(\Delta/\sigma)_{max} = 0.026$
$S = 0.95$	$\Delta\rho_{max} = 0.33$ e Å^{-3}
2363 reflections	$\Delta\rho_{min} = -0.29$ e Å^{-3}
345 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), with 1668 Freidel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: −10 (10)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2$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}
N1A	0.6221 (5)	0.9203 (17)	0.3790 (6)	0.056 (2)
O1A	0.5892 (6)	0.9143 (17)	0.0183 (5)	0.089 (3)
O2A	0.6377 (6)	1.2521 (18)	−0.0237 (6)	0.089 (3)
O3A	0.6112 (5)	0.7729 (15)	0.7511 (5)	0.074 (2)
C1A	0.6309 (7)	1.118 (2)	0.3467 (7)	0.061 (3)
H1A	0.6380	1.2347	0.3881	0.073*
C2A	0.6299 (7)	1.162 (2)	0.2514 (8)	0.061 (3)
C3A	0.6029 (7)	0.995 (2)	0.1830 (6)	0.055 (3)
H3A	0.5837	0.8580	0.1989	0.066*
C4A	0.6063 (7)	1.044 (2)	0.0925 (7)	0.060 (3)
C5A	0.6351 (8)	1.250 (2)	0.0672 (8)	0.063 (3)
C6A	0.6617 (8)	1.416 (2)	0.1340 (8)	0.074 (3)
H6A	0.6821	1.5520	0.1180	0.089*
C7A	0.6564 (7)	1.369 (2)	0.2239 (8)	0.065 (3)
H7A	0.6709	1.4784	0.2685	0.078*
C8A	0.6020 (12)	1.046 (3)	−0.0599 (8)	0.106 (5)
H8A	0.6462	0.9762	−0.0913	0.127*
H8B	0.5421	1.0648	−0.1042	0.127*
C9A	0.6204 (6)	0.8953 (18)	0.4729 (6)	0.048 (2)
C14A	0.6592 (7)	0.6977 (18)	0.5177 (7)	0.055 (3)

H14A	0.6855	0.5962	0.4838	0.066*
C13A	0.6591 (6)	0.6538 (19)	0.6074 (7)	0.054 (3)
H13A	0.6873	0.5264	0.6349	0.065*
C12A	0.6169 (7)	0.798 (2)	0.6591 (6)	0.056 (3)
C11A	0.5796 (7)	0.9931 (18)	0.6168 (7)	0.053 (3)
H11A	0.5537	1.0945	0.6511	0.064*
C10A	0.5803 (6)	1.037 (2)	0.5270 (7)	0.058 (3)
H10A	0.5531	1.1664	0.5006	0.070*
C15A	0.6397 (11)	0.565 (2)	0.7928 (8)	0.107 (5)
H15A	0.5998	0.4524	0.7595	0.161*
H15B	0.6341	0.5659	0.8565	0.161*
H15C	0.7042	0.5366	0.7903	0.161*
N1B	0.8902 (5)	0.4200 (18)	0.4322 (5)	0.058 (2)
O1B	0.9310 (6)	0.4245 (16)	0.0858 (5)	0.087 (3)
O2B	0.8841 (6)	0.7662 (16)	0.0242 (5)	0.083 (3)
O3B	0.8685 (5)	0.2769 (16)	0.8033 (5)	0.073 (2)
C1B	0.8780 (6)	0.617 (2)	0.3959 (7)	0.059 (3)
H1B	0.8673	0.7332	0.4329	0.070*
C2B	0.8809 (7)	0.658 (2)	0.2997 (8)	0.058 (3)
C3B	0.9081 (7)	0.501 (2)	0.2429 (6)	0.054 (3)
H3B	0.9264	0.3628	0.2669	0.065*
C4B	0.9082 (7)	0.545 (2)	0.1546 (7)	0.060 (3)
C5B	0.8787 (7)	0.760 (2)	0.1160 (7)	0.061 (3)
C6B	0.8521 (7)	0.914 (2)	0.1707 (8)	0.068 (3)
H6B	0.8331	1.0519	0.1467	0.082*
C7B	0.8534 (7)	0.866 (2)	0.2635 (8)	0.062 (3)
H7B	0.8359	0.9717	0.3016	0.074*
C8B	0.9174 (12)	0.556 (3)	0.0050 (10)	0.114 (5)
H8C	0.8717	0.4874	−0.0450	0.137*
H8D	0.9766	0.5708	−0.0148	0.137*
C9B	0.8867 (6)	0.3895 (17)	0.5252 (6)	0.044 (2)
C10B	0.9184 (6)	0.539 (2)	0.5986 (6)	0.056 (3)
H10B	0.9446	0.6712	0.5860	0.068*
C11B	0.9114 (7)	0.493 (2)	0.6877 (6)	0.055 (3)
H11B	0.9336	0.5949	0.7343	0.066*
C12B	0.8717 (6)	0.298 (2)	0.7113 (7)	0.052 (3)
C13B	0.8436 (7)	0.150 (2)	0.6423 (7)	0.064 (3)
H13B	0.8205	0.0154	0.6561	0.077*
C14B	0.8489 (7)	0.1971 (19)	0.5499 (7)	0.058 (3)
H14B	0.8260	0.0946	0.5038	0.069*
C15B	0.8285 (10)	0.076 (2)	0.8290 (8)	0.094 (4)
H15D	0.7652	0.0589	0.7926	0.141*
H15E	0.8273	0.0800	0.8939	0.141*
H15F	0.8665	−0.0456	0.8176	0.141*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

N1A	0.065 (5)	0.049 (6)	0.058 (6)	0.006 (5)	0.021 (4)	−0.002 (5)
O1A	0.142 (7)	0.066 (6)	0.057 (5)	0.008 (6)	0.021 (5)	0.001 (5)
O2A	0.129 (7)	0.076 (7)	0.068 (6)	0.000 (6)	0.038 (5)	0.021 (6)
O3A	0.098 (5)	0.062 (6)	0.056 (5)	0.003 (5)	0.005 (4)	0.011 (5)
C1A	0.062 (6)	0.064 (9)	0.052 (7)	−0.005 (6)	−0.001 (5)	0.014 (6)
C2A	0.069 (6)	0.052 (7)	0.065 (7)	0.006 (6)	0.019 (5)	0.011 (7)
C3A	0.084 (7)	0.030 (6)	0.047 (6)	−0.003 (5)	0.004 (5)	0.003 (5)
C4A	0.066 (7)	0.065 (9)	0.052 (7)	0.013 (7)	0.017 (5)	−0.008 (7)
C5A	0.083 (7)	0.047 (8)	0.062 (7)	0.008 (6)	0.021 (6)	0.019 (7)
C6A	0.077 (7)	0.054 (8)	0.091 (9)	−0.009 (6)	0.016 (7)	0.017 (8)
C7A	0.077 (7)	0.051 (8)	0.063 (7)	−0.002 (6)	0.010 (6)	0.005 (6)
C8A	0.148 (12)	0.114 (15)	0.060 (8)	−0.017 (12)	0.033 (8)	0.008 (10)
C9A	0.064 (6)	0.038 (7)	0.038 (6)	−0.015 (5)	0.006 (5)	0.003 (5)
C14A	0.080 (7)	0.040 (7)	0.053 (7)	0.000 (6)	0.030 (5)	0.005 (5)
C13A	0.039 (5)	0.046 (7)	0.068 (7)	−0.007 (5)	−0.009 (5)	0.008 (6)
C12A	0.067 (6)	0.058 (8)	0.044 (6)	−0.004 (6)	0.015 (5)	−0.002 (6)
C11A	0.082 (7)	0.024 (6)	0.049 (6)	−0.003 (5)	0.003 (5)	0.003 (5)
C10A	0.057 (6)	0.040 (7)	0.068 (7)	−0.001 (5)	−0.004 (5)	−0.002 (6)
C15A	0.165 (13)	0.065 (11)	0.090 (9)	0.006 (10)	0.024 (9)	0.034 (9)
N1B	0.070 (5)	0.056 (7)	0.043 (5)	−0.004 (5)	0.003 (4)	−0.007 (5)
O1B	0.153 (8)	0.065 (6)	0.048 (4)	0.011 (6)	0.031 (5)	0.009 (5)
O2B	0.120 (6)	0.066 (7)	0.064 (5)	0.007 (6)	0.021 (4)	0.011 (5)
O3B	0.092 (5)	0.081 (7)	0.044 (4)	−0.014 (5)	0.010 (3)	0.005 (5)
C1B	0.055 (6)	0.068 (9)	0.048 (6)	−0.007 (6)	0.003 (5)	−0.008 (6)
C2B	0.063 (6)	0.041 (7)	0.069 (7)	−0.003 (5)	0.009 (5)	−0.002 (6)
C3B	0.083 (7)	0.044 (7)	0.033 (5)	−0.003 (6)	0.011 (5)	0.007 (5)
C4B	0.079 (7)	0.057 (9)	0.050 (7)	−0.015 (6)	0.025 (5)	−0.002 (7)
C5B	0.072 (7)	0.064 (9)	0.041 (6)	−0.021 (7)	0.002 (5)	0.002 (7)
C6B	0.081 (7)	0.052 (8)	0.071 (8)	0.005 (6)	0.012 (6)	0.007 (7)
C7B	0.062 (6)	0.054 (8)	0.069 (8)	−0.008 (6)	0.011 (5)	−0.007 (6)
C8B	0.171 (14)	0.084 (13)	0.097 (10)	0.024 (12)	0.049 (10)	−0.014 (10)
C9B	0.049 (5)	0.034 (6)	0.041 (5)	−0.002 (5)	−0.006 (4)	−0.005 (5)
C10B	0.044 (5)	0.051 (7)	0.072 (7)	−0.009 (5)	0.010 (5)	−0.015 (6)
C11B	0.072 (6)	0.052 (8)	0.036 (5)	−0.012 (6)	0.000 (5)	0.001 (5)
C12B	0.045 (5)	0.055 (7)	0.051 (6)	0.001 (5)	0.005 (4)	−0.006 (6)
C13B	0.089 (7)	0.047 (7)	0.056 (7)	0.000 (6)	0.012 (6)	−0.003 (6)
C14B	0.078 (7)	0.043 (7)	0.048 (6)	−0.005 (6)	0.006 (5)	−0.014 (5)
C15B	0.137 (11)	0.067 (10)	0.082 (8)	−0.010 (9)	0.035 (8)	0.009 (8)

Geometric parameters (Å, °)

N1A—C1A	1.315 (15)	N1B—C1B	1.315 (15)
N1A—C9A	1.397 (11)	N1B—C9B	1.396 (11)
O1A—C4A	1.330 (13)	O1B—C4B	1.352 (13)
O1A—C8A	1.452 (15)	O1B—C8B	1.414 (16)
O2A—C5A	1.348 (13)	O2B—C5B	1.373 (12)
O2A—C8A	1.42 (2)	O2B—C8B	1.423 (18)
O3A—C12A	1.385 (11)	O3B—C12B	1.373 (11)
O3A—C15A	1.434 (15)	O3B—C15B	1.447 (16)

C1A—C2A	1.426 (13)	C1B—C2B	1.448 (14)
C1A—H1A	0.9300	C1B—H1B	0.9300
C2A—C7A	1.411 (17)	C2B—C3B	1.388 (15)
C2A—C3A	1.426 (16)	C2B—C7B	1.402 (17)
C3A—C4A	1.379 (13)	C3B—C4B	1.329 (12)
C3A—H3A	0.9300	C3B—H3B	0.9300
C4A—C5A	1.403 (17)	C4B—C5B	1.462 (18)
C5A—C6A	1.406 (17)	C5B—C6B	1.351 (17)
C6A—C7A	1.375 (14)	C6B—C7B	1.396 (14)
C6A—H6A	0.9300	C6B—H6B	0.9300
C7A—H7A	0.9300	C7B—H7B	0.9300
C8A—H8A	0.9700	C8B—H8C	0.9700
C8A—H8B	0.9700	C8B—H8D	0.9700
C9A—C10A	1.390 (14)	C9B—C14B	1.381 (15)
C9A—C14A	1.431 (14)	C9B—C10B	1.412 (13)
C14A—C13A	1.349 (12)	C10B—C11B	1.369 (12)
C14A—H14A	0.9300	C10B—H10B	0.9300
C13A—C12A	1.394 (14)	C11B—C12B	1.404 (15)
C13A—H13A	0.9300	C11B—H11B	0.9300
C12A—C11A	1.397 (16)	C12B—C13B	1.352 (13)
C11A—C10A	1.353 (13)	C13B—C14B	1.410 (13)
C11A—H11A	0.9300	C13B—H13B	0.9300
C10A—H10A	0.9300	C14B—H14B	0.9300
C15A—H15A	0.9600	C15B—H15D	0.9600
C15A—H15B	0.9600	C15B—H15E	0.9600
C15A—H15C	0.9600	C15B—H15F	0.9600
C1A—N1A—C9A	118.9 (10)	C1B—N1B—C9B	119.4 (10)
C4A—O1A—C8A	106.6 (11)	C4B—O1B—C8B	108.0 (10)
C5A—O2A—C8A	106.1 (10)	C5B—O2B—C8B	105.5 (10)
C12A—O3A—C15A	116.4 (10)	C12B—O3B—C15B	116.1 (9)
N1A—C1A—C2A	123.2 (12)	N1B—C1B—C2B	121.7 (11)
N1A—C1A—H1A	118.4	N1B—C1B—H1B	119.2
C2A—C1A—H1A	118.4	C2B—C1B—H1B	119.2
C7A—C2A—C3A	119.3 (10)	C3B—C2B—C7B	119.6 (10)
C7A—C2A—C1A	120.6 (12)	C3B—C2B—C1B	123.0 (11)
C3A—C2A—C1A	120.2 (12)	C7B—C2B—C1B	117.4 (11)
C4A—C3A—C2A	117.6 (11)	C4B—C3B—C2B	120.7 (12)
C4A—C3A—H3A	121.2	C4B—C3B—H3B	119.6
C2A—C3A—H3A	121.2	C2B—C3B—H3B	119.6
O1A—C4A—C3A	128.6 (12)	C3B—C4B—O1B	132.5 (12)
O1A—C4A—C5A	109.4 (10)	C3B—C4B—C5B	120.1 (11)
C3A—C4A—C5A	122.0 (11)	O1B—C4B—C5B	107.4 (9)
O2A—C5A—C6A	128.6 (12)	C6B—C5B—O2B	131.0 (12)
O2A—C5A—C4A	110.3 (11)	C6B—C5B—C4B	119.7 (9)
C6A—C5A—C4A	121.0 (10)	O2B—C5B—C4B	109.4 (11)
C7A—C6A—C5A	117.1 (12)	C5B—C6B—C7B	119.4 (12)
C7A—C6A—H6A	121.4	C5B—C6B—H6B	120.3
C5A—C6A—H6A	121.4	C7B—C6B—H6B	120.3
C6A—C7A—C2A	122.9 (12)	C6B—C7B—C2B	120.5 (11)

C6A—C7A—H7A	118.5	C6B—C7B—H7B	119.7
C2A—C7A—H7A	118.5	C2B—C7B—H7B	119.7
O2A—C8A—O1A	107.2 (10)	O1B—C8B—O2B	109.7 (10)
O2A—C8A—H8A	110.3	O1B—C8B—H8C	109.7
O1A—C8A—H8A	110.3	O2B—C8B—H8C	109.7
O2A—C8A—H8B	110.3	O1B—C8B—H8D	109.7
O1A—C8A—H8B	110.3	O2B—C8B—H8D	109.7
H8A—C8A—H8B	108.5	H8C—C8B—H8D	108.2
C10A—C9A—N1A	126.9 (10)	C14B—C9B—N1B	118.4 (9)
C10A—C9A—C14A	115.8 (8)	C14B—C9B—C10B	115.6 (9)
N1A—C9A—C14A	117.2 (10)	N1B—C9B—C10B	126.0 (10)
C13A—C14A—C9A	122.3 (10)	C11B—C10B—C9B	121.4 (10)
C13A—C14A—H14A	118.8	C11B—C10B—H10B	119.3
C9A—C14A—H14A	118.9	C9B—C10B—H10B	119.3
C14A—C13A—C12A	120.3 (10)	C10B—C11B—C12B	122.2 (10)
C14A—C13A—H13A	119.9	C10B—C11B—H11B	118.9
C12A—C13A—H13A	119.8	C12B—C11B—H11B	118.9
O3A—C12A—C13A	126.3 (11)	C13B—C12B—O3B	127.6 (11)
O3A—C12A—C11A	115.5 (10)	C13B—C12B—C11B	117.0 (9)
C13A—C12A—C11A	118.2 (9)	O3B—C12B—C11B	115.3 (9)
C10A—C11A—C12A	121.3 (10)	C12B—C13B—C14B	121.2 (11)
C10A—C11A—H11A	119.4	C12B—C13B—H13B	119.4
C12A—C11A—H11A	119.4	C14B—C13B—H13B	119.4
C11A—C10A—C9A	122.1 (10)	C9B—C14B—C13B	122.5 (10)
C11A—C10A—H10A	119.0	C9B—C14B—H14B	118.8
C9A—C10A—H10A	118.9	C13B—C14B—H14B	118.8
O3A—C15A—H15A	109.5	O3B—C15B—H15D	109.5
O3A—C15A—H15B	109.5	O3B—C15B—H15E	109.5
H15A—C15A—H15B	109.5	H15D—C15B—H15E	109.5
O3A—C15A—H15C	109.5	O3B—C15B—H15F	109.5
H15A—C15A—H15C	109.5	H15D—C15B—H15F	109.5
H15B—C15A—H15C	109.5	H15E—C15B—H15F	109.5
C9A—N1A—C1A—C2A	−177.6 (8)	C9B—N1B—C1B—C2B	−180.0 (7)
N1A—C1A—C2A—C7A	−168.5 (10)	N1B—C1B—C2B—C3B	−8.3 (15)
N1A—C1A—C2A—C3A	10.9 (15)	N1B—C1B—C2B—C7B	170.7 (10)
C7A—C2A—C3A—C4A	1.5 (15)	C7B—C2B—C3B—C4B	−0.1 (15)
C1A—C2A—C3A—C4A	−177.9 (9)	C1B—C2B—C3B—C4B	178.9 (9)
C8A—O1A—C4A—C3A	179.6 (11)	C2B—C3B—C4B—O1B	179.8 (10)
C8A—O1A—C4A—C5A	−3.6 (13)	C2B—C3B—C4B—C5B	−0.5 (15)
C2A—C3A—C4A—O1A	176.4 (10)	C8B—O1B—C4B—C3B	179.8 (13)
C2A—C3A—C4A—C5A	0.0 (15)	C8B—O1B—C4B—C5B	0.1 (13)
C8A—O2A—C5A—C6A	−179.2 (13)	C8B—O2B—C5B—C6B	179.6 (13)
C8A—O2A—C5A—C4A	4.8 (14)	C8B—O2B—C5B—C4B	−0.4 (13)
O1A—C4A—C5A—O2A	−0.8 (13)	C3B—C4B—C5B—C6B	0.4 (15)
C3A—C4A—C5A—O2A	176.3 (9)	O1B—C4B—C5B—C6B	−179.8 (9)
O1A—C4A—C5A—C6A	−177.1 (10)	C3B—C4B—C5B—O2B	−179.6 (9)
C3A—C4A—C5A—C6A	−0.1 (17)	O1B—C4B—C5B—O2B	0.2 (11)
O2A—C5A—C6A—C7A	−176.9 (10)	O2B—C5B—C6B—C7B	−179.8 (10)
C4A—C5A—C6A—C7A	−1.3 (17)	C4B—C5B—C6B—C7B	0.2 (15)

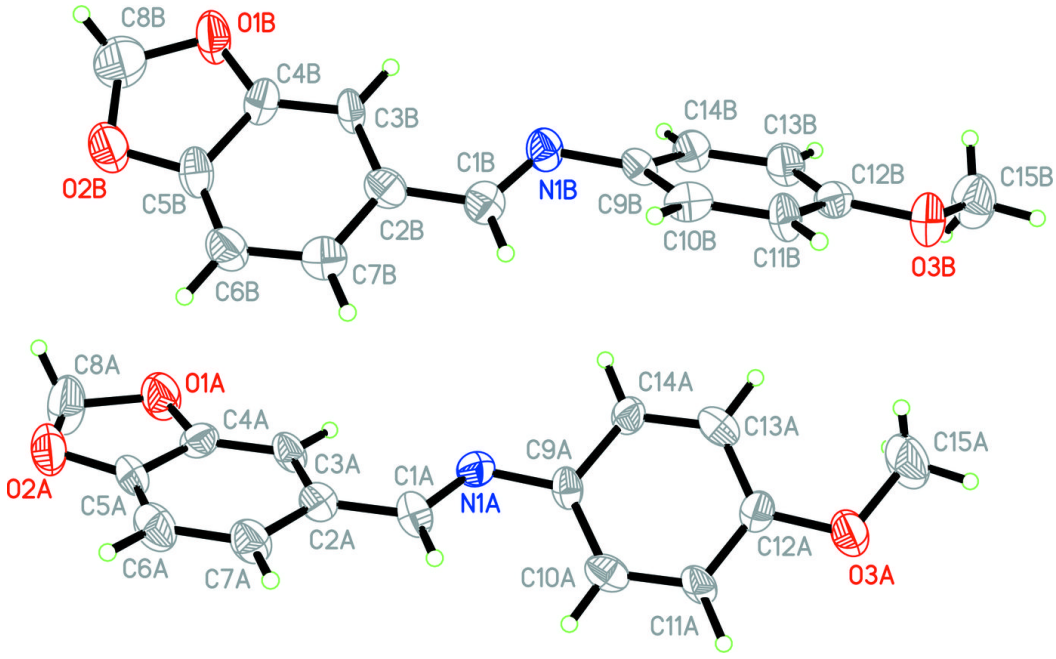
C5A—C6A—C7A—C2A	2.9 (16)	C5B—C6B—C7B—C2B	−0.8 (15)
C3A—C2A—C7A—C6A	−3.1 (16)	C3B—C2B—C7B—C6B	0.7 (15)
C1A—C2A—C7A—C6A	176.3 (9)	C1B—C2B—C7B—C6B	−178.3 (8)
C5A—O2A—C8A—O1A	−6.8 (15)	C4B—O1B—C8B—O2B	−0.4 (16)
C4A—O1A—C8A—O2A	6.4 (15)	C5B—O2B—C8B—O1B	0.5 (15)
C1A—N1A—C9A—C10A	35.4 (14)	C1B—N1B—C9B—C14B	145.3 (10)
C1A—N1A—C9A—C14A	−148.3 (9)	C1B—N1B—C9B—C10B	−34.5 (14)
C10A—C9A—C14A—C13A	−1.5 (13)	C14B—C9B—C10B—C11B	0.0 (14)
N1A—C9A—C14A—C13A	−178.3 (9)	N1B—C9B—C10B—C11B	179.8 (9)
C9A—C14A—C13A—C12A	2.6 (13)	C9B—C10B—C11B—C12B	−0.7 (15)
C15A—O3A—C12A—C13A	−9.1 (15)	C15B—O3B—C12B—C13B	−1.5 (15)
C15A—O3A—C12A—C11A	173.5 (11)	C15B—O3B—C12B—C11B	−179.5 (10)
C14A—C13A—C12A—O3A	179.5 (9)	C10B—C11B—C12B—C13B	2.6 (14)
C14A—C13A—C12A—C11A	−3.2 (13)	C10B—C11B—C12B—O3B	−179.2 (9)
O3A—C12A—C11A—C10A	−179.6 (9)	O3B—C12B—C13B—C14B	178.3 (9)
C13A—C12A—C11A—C10A	2.8 (15)	C11B—C12B—C13B—C14B	−3.8 (14)
C12A—C11A—C10A—C9A	−1.9 (15)	N1B—C9B—C14B—C13B	179.0 (9)
N1A—C9A—C10A—C11A	177.6 (9)	C10B—C9B—C14B—C13B	−1.2 (14)
C14A—C9A—C10A—C11A	1.2 (13)	C12B—C13B—C14B—C9B	3.2 (15)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8A—H8A···O3A^{i}	0.97	2.58	3.28 (2)	129
C8B—H8C···O3B^{i}	0.97	2.57	3.36 (2)	139
C15A—H15B···O2A^{ii}	0.96	2.60	3.32 (2)	132
C13A—H13A···Cg2B	0.93	3.05	3.69 (4)	127
C10A—H10A···Cg2A^{iii}	0.93	2.70	3.45 (4)	138
C13B—H13B···Cg2A^{iv}	0.93	3.09	3.70 (4)	124

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

Fig. 1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C1A
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Fig. 2

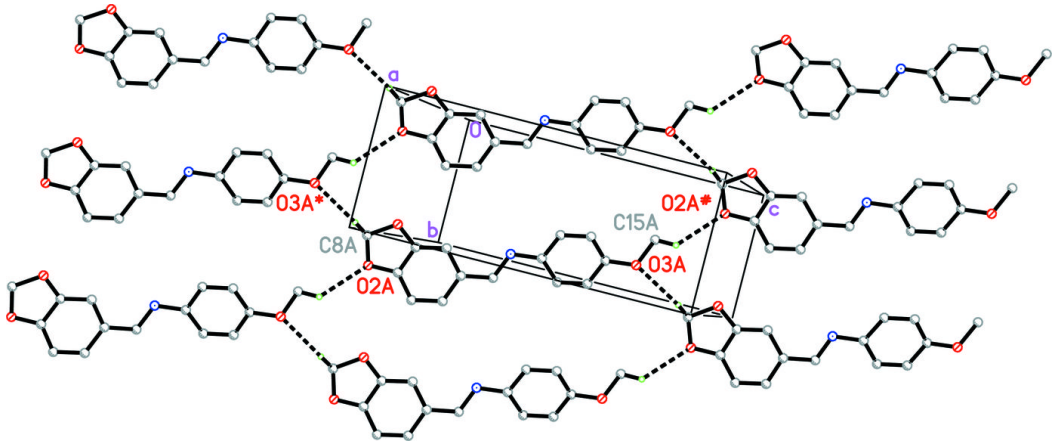

Fig. 3