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(*E*,*E*)-*N*,*N*′-Bis(3,4-methylenedioxybenzylidene)-propane-1,2-diamine

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In the title compound, $C_{19}H_{18}N_2O_4$, the methyl group is disordered. The molecule is centrosymmetric and has a *trans* configuration (*E*,*E*).

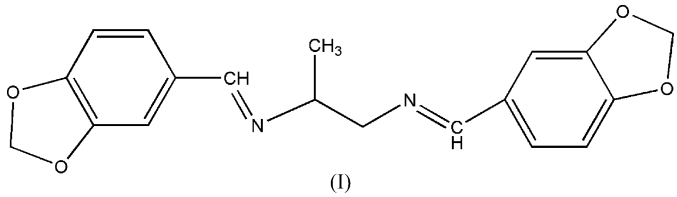
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
Disorder in main residue
R factor = 0.053
wR factor = 0.159
Data-to-parameter ratio = 12.6

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

Comment

Schiff bases are important ligands in the development of Schiff base complexes, because they are potentially capable of forming stable complexes with metal ions (Johnson *et al.*, 1996; Alizadeh *et al.*, 1999). Also, some diamine Schiff bases have shown good anti-inflammatory and analgesic activities (Sondhi *et al.*, 2006). The crystal structures of some diamine Schiff bases have been reported (Xiao & Wang, 2006; Sun *et al.*, 2004). Here we report the crystal structure of a diamine Schiff base, *N*,*N*′-bis(3,4-methylenedioxybenzylidene)-propane-1,2-diamine, (I).



(I)

The molecule of (I) is centrosymmetric. As a result, the methyl group is disordered over two sites, C9 and C9A [symmetry code: (A) $1-x, 1-y, 1-z$], each with 0.5 site occupancy (Fig. 1). The molecule has a *trans* configuration (*E*,*E*), and the geometric parameters are normal.

There are no significant intermolecular interactions in the crystal structure.

Experimental

A mixture containing propane-1,2-diamine (1.48 g, 20 mmol) and 3,4-methylenedioxybenzaldehyde (1.50 g, 10 mmol) was refluxed for about 2 h in ethanol (30 ml); the mixture was then cooled and the product was filtered off, washed with methanol and dried. Yellow crystals of (I) suitable for X-ray structure analysis were obtained by recrystallizing the crude product from ethanol (m.p. 401–402 K).

Crystal data

$C_{19}H_{18}N_2O_4$
M_r = 338.35
Monoclinic, $P2_1/c$
a = 14.325 (3) Å
b = 5.058 (2) Å
c = 12.250 (2) Å
β = 105.968 (2)°
V = 853.3 (4) Å^3
Z = 2
D_x = 1.317 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
Block, yellow
0.56 × 0.50 × 0.41 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.950, T_{max} = 0.963
4114 measured reflections
1490 independent reflections
1011 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.159
S = 1.02
1490 reflections
118 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0871P)^2 + 0.186P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

All H atoms were positioned geometrically and refined as riding on their parent atoms, with C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms, and C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for all other H atoms.

Disorder in the methyl group was identified from a difference Fourier map. The site occupancies were fixed at 0.5 due to the centrosymmetry of the molecule. The disordered C atoms were refined anisotropically with no constraints or restraints.

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*.

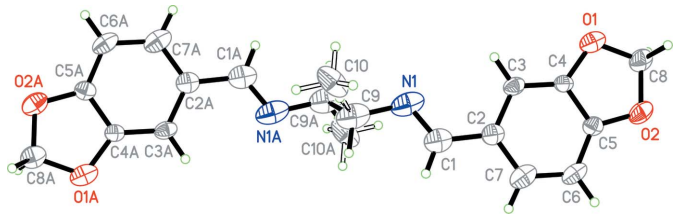


Figure 1
The molecular structure of compound (I), showing the atom-labelling scheme and disordered methyl groups (C10, C10A). Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (A) $-x + 1, -y + 2, -z + 1$].

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