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N,*N*′-Bis(3,4,5-trimethoxybenzylidene)hydrazine

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In the title compound, $C_{20}H_{24}N_2O_6$, the molecule possesses a crystallographically imposed centre of symmetry at the mid-point of the N—N bond. The central C═N—N═C linkage is therefore planar.

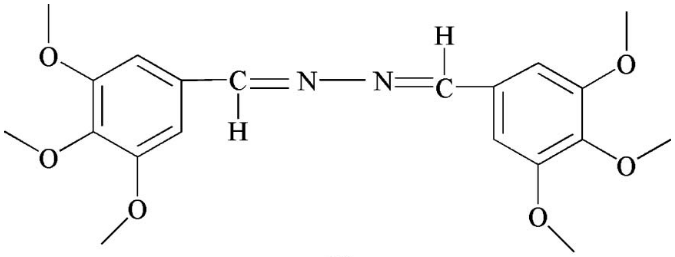
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.139
Data-to-parameter ratio = 15.4

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

Comment

To date, a large number of azine compounds containing both a diimine linkage and N—N bonding have been synthesized because they are used in coordination chemistry (Xu *et al.*, 1997; Armstrong *et al.*, 1998; Kesslen *et al.*, 1999; Kundu *et al.*, 2005; Zheng *et al.*, 2005). In this context, an X-ray crystal structure determination of the title compound, (I), was carried out.



(I)

In the molecule of (I), there is an inversion centre at the mid-point of the N1—N1^{i} bond [symmetry code: (i) $-x + 1$, $-y + 2$, $-z + 1$] and the C═N—N═C linkage is planar (Fig. 1). The N—N bond length, 1.419 (3) Å, is slightly greater than that observed in related azine compounds (Liu *et al.*, 2004; Sengül *et al.*, 2004; Xu *et al.*, 2005). The C═N—N angle, 112.2 (2)°, is similar to that observed in *N*,*N*′-bis(3-hydroxy-4-methoxybenzylidene)hydrazine (Duan *et al.*, 2005), but

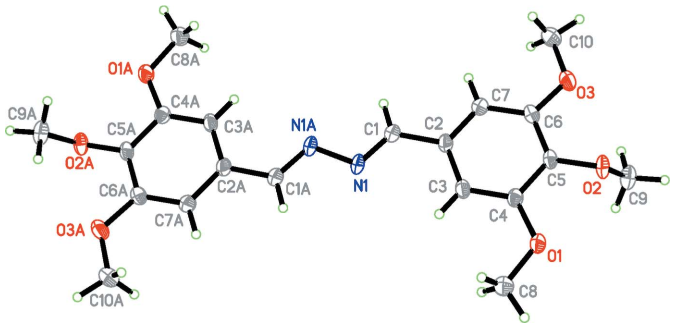


Figure 1
View of the molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level for non-H atoms. [Symmetry code: (A) $1 - x$, $2 - y$, $1 - z$.]

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significantly smaller than the ideal value of 120° expected for an sp^2 N atom, as a consequence of the repulsion between the N lone pairs and the adjacent C═N bond. The O atoms of the methoxy groups attached to the benzene ring do not deviate substantially from the plane of the ring; a maximum deviation of 0.0699 (2) Å is observed for atom O2.

Experimental

The title compound was synthesized by the reaction of 3,4,5-trimethoxybenzaldehyde with hydrazine hydrate in refluxing ethanol (Liu *et al.*, 2004). Single crystals suitable for X-ray analysis were obtained by slow evaporation at 298 K of a tetrahydrofuran solution.

Crystal data

$C_{20}H_{24}N_2O_6$
$M_r = 388.41$
Monoclinic, $C2/c$
$a = 29.879$ (10) Å
$b = 4.9185$ (18) Å
$c = 14.040$ (5) Å
$\beta = 103.754$ (6)°
$V = 2004.2$ (12) Å^3
$Z = 4$
$D_x = 1.287$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 294$ (2) K
Block, light yellow
0.22 × 0.18 × 0.14 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.979$, $T_{\max} = 0.987$
5201 measured reflections
2004 independent reflections
1280 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.033$
$\theta_{\max} = 26.2°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.139$
$S = 1.01$
2004 reflections
130 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0802P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.16$ e Å^{-3}
$\Delta\rho_{\min} = -0.22$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C4	1.365 (2)	O3—C6	1.370 (2)
O2—C5	1.375 (2)	N1—N1$^{\rm i}$	1.419 (3)
C1—N1—N1$^{\rm i}$	112.2 (2)		
N1$^{\rm i}$—N1—C1—C2	−179.4 (2)		

Symmetry code: (i) $-x + 1, -y + 2, -z + 1$.

All H atoms were positioned geometrically and refined using a riding model. Constrained distances: 0.93 Å for Csp^2—H and 0.96 Å for Csp^3—H. $U_{\rm iso}$(H) values were fixed at $1.2U_{\rm eq}$(aromatic C) and $1.5U_{\rm eq}$(methyl C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 1997); software used to prepare material for publication: *SHELXTL*.

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