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## Key indicators

Single-crystal X-ray study  
 $T = 298$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å  
 $R$  factor = 0.071  
 $wR$  factor = 0.172  
Data-to-parameter ratio = 12.0For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

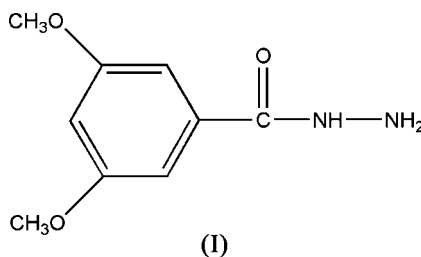
## 3,5-Dimethoxybenzohydrazide

The title compound,  $\text{C}_9\text{H}_{12}\text{N}_2\text{O}_3$ , was synthesized by the reaction of ethyl 3,5-dimethoxybenzoate with hydrazine. X-ray analysis reveals that the asymmetric unit contains two independent molecules.  $\text{N}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds link the molecules into layers. Molecules in adjacent layers are linked *via*  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds.

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## Comment

*N*-Benzoylhydrazine is a compound of considerable biological and chemical importance (Mead *et al.*, 1958). Among the important features of *N*-benzoylhydrazine derivatives are the donor ability of the N and O centres and the potential to explore both the steric and electronic effects on the ligand framework (Bahgat, 2004). We report here the crystal structure of the title compound, (I).

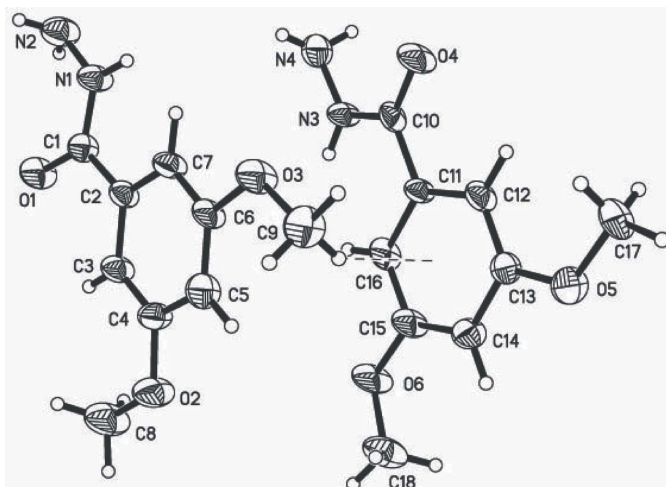


The asymmetric unit of (I) consists of two independent molecules (Fig. 1), *A* (O1–O3/N1/N2/C1–C9) and *B* (O4–O6/N3/N4/C10–C18), which have similar geometries. A  $\text{C}-\text{H}\cdots\pi$  interaction involving the C11–C16 benzene ring (centroid  $C_g$ ) is observed between the two independent molecules (Table 1). Each molecule is nearly planar: the dihedral angle between the aromatic ring and the  $\text{N}-\text{N}-\text{C}=\text{O}$  group is  $9.7(4)^\circ$  for molecule *A* and  $7.2(4)^\circ$  for molecule *B*. In molecule *A*, the largest deviation from the least-squares plane through all the atoms is  $0.220(4)$  Å for atom O1; in molecule *B*, it is  $0.232(4)$  Å for atom O4.

The crystal packing shows that the molecules of (I) are linked *via*  $\text{N}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds to form layers. The molecules of adjacent layers are linked *via*  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds (Table 1).

## Experimental

Compound (I) was synthesized by the reaction of ethyl 3,5-dimethoxybenzoate (2 mmol) with hydrazine (2 mmol). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.



**Figure 1**

The structure of the asymmetric unit of (I), showing 50% probability displacement ellipsoids. The dashed line represents the C—H... $\pi$  interaction between the two independent molecules.

#### Crystal data

$C_9H_{12}N_2O_3$	$V = 933.9 (5) \text{ \AA}^3$
$M_r = 196.21$	$Z = 4$
Triclinic, $P\bar{1}$	$D_x = 1.395 \text{ Mg m}^{-3}$
$a = 8.705 (3) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 10.082 (3) \text{ \AA}$	$\mu = 0.11 \text{ mm}^{-1}$
$c = 10.981 (3) \text{ \AA}$	$T = 298 (2) \text{ K}$
$\alpha = 104.222 (2)^\circ$	Block, colourless
$\beta = 90.735 (3)^\circ$	$0.49 \times 0.17 \times 0.15 \text{ mm}$
$\gamma = 90.916 (3)^\circ$	

#### Data collection

Bruker SMART CCD area-detector diffractometer	4831 measured reflections
$\varphi$ and $\omega$ scans	3217 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1120 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.950$ , $T_{\max} = 0.984$	$R_{\text{int}} = 0.074$
	$\theta_{\text{max}} = 25.0^\circ$

#### Refinement

Refinement on $F^2$	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.071$	$w = 1/[\sigma^2(F_o^2) + (0.0427P)^2]$
$wR(F^2) = 0.172$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.95$	$(\Delta/\sigma)_{\text{max}} = 0.002$
3217 reflections	$\Delta\rho_{\text{max}} = 0.27 \text{ e \AA}^{-3}$
269 parameters	$\Delta\rho_{\text{min}} = -0.26 \text{ e \AA}^{-3}$

**Table 1**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$C_g$  is the centroid of the C11–C16 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 $\cdots$ O4 <sup>i</sup>	0.86	2.10	2.925 (5)	162
N2—H2B $\cdots$ O1 <sup>iii</sup>	0.85 (4)	2.36 (4)	3.199 (6)	170 (6)
N3—H3 $\cdots$ O1 <sup>iii</sup>	0.86	2.11	2.947 (6)	164
N4—H4A $\cdots$ O4 <sup>i</sup>	0.85 (4)	2.25 (4)	3.098 (6)	174 (4)
C7—H7 $\cdots$ O4 <sup>i</sup>	0.93	2.37	3.284 (6)	167
C16—H16 $\cdots$ O1 <sup>iii</sup>	0.93	2.33	3.239 (7)	165
C9—H9B $\cdots$ C <sub>g</sub>	0.96	2.61	3.462 (6)	148

Symmetry codes: (i)  $-x + 1, -y + 2, -z + 1$ ; (ii)  $-x, -y + 1, -z + 1$ ; (iii)  $-x + 1, -y + 1, -z + 1$ .

H atoms of the  $-\text{NH}_2$  groups were located in a difference map and refined isotropically with a fixed  $U_{\text{iso}}$  value of  $0.08 \text{ \AA}^2$ ; the N—H distances were restrained to be equal to within  $\pm 0.03 \text{ \AA}$ . The remaining H atoms were placed in idealized positions (N—H =  $0.86 \text{ \AA}$  and C—H =  $0.93\text{--}0.96 \text{ \AA}$ ) and allowed to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2$  or  $1.5$  (methyl) times  $U_{\text{eq}}(\text{C,N})$ .

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1999); 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, 1999); software used to prepare material for publication: SHELXTL.

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