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N,*N*′-Bis(3,5-dimethoxyphenyl)oxamide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.069
wR factor = 0.152
Data-to-parameter ratio = 14.1

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

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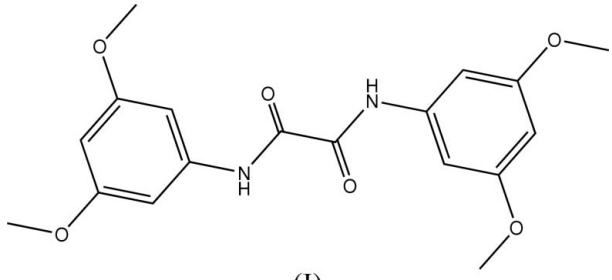
The molecule of the title compound, $C_{18}H_{20}N_2O_6$, lies on a crystallographically imposed center of symmetry at the mid-point of the C—C bond of the oxamide unit. The crystal structure is stabilized by π–π interactions.

Comment

N,*N*′-Diphenyloxamide and its derivatives have been widely applied in a number of materials as anti-oxidants, ultraviolet absorbents and metal ion passivators (Feng *et al.*, 1997). We report here the synthesis and crystal structure of *N*,*N*′-bis(3,5-dimethoxyphenyl)oxamide, (I).



(I)

Compound (I) has a crystallographically imposed center of symmetry at the mid-point of the C9—C9^{i} bond [symmetry code: (i) $2-x, 1-y, -z$]. The bond lengths and angles are within normal ranges (Allen *et al.*, 1987). However, the C9—C9^{i} bond length [1.527 (7) Å] is longer than the typical Csp^2—Csp^2 single bond distance (1.460 Å). The molecule of (I) is almost planar. Weak N—H···O and C—H···O interactions (Table 1) are observed in the molecular structure. The crystal structure is stabilized by π–π interactions between the benzene rings at (x, y, z) and ($1-x$, $1-y$, $1-z$), with a centroid–centroid distance of 3.670 (2) Å.

Experimental

To a solution of 3,5-dimethoxyaniline (15.3 g, 0.1 mol) in CH_2Cl_2 (30 ml) was added dropwise a solution of oxalyl chloride (3.2 g, 0.025 mol) in CH_2Cl_2 (10 ml), and the mixture was stirred at 353 K for 2 h. After cooling to room temperature, the solvent was removed *in vacuo*, and the residue was subjected to column chromatography (petroleum ether/EtOAc 3:1) to give (I) as a yellow solid (5.6 g, 62%). Single crystals of (I) suitable for an X-ray diffraction study were obtained by slow evaporation of a $CHCl_3$ solution at room temperature over a period of 3 d.

Crystal data

$C_{18}H_{20}N_2O_6$
M_r = 360.36
Monoclinic, $P2_1/c$
a = 6.7851 (7) Å
b = 15.6234 (15) Å
c = 8.0308 (8) Å
β = 92.59 (3)°
V = 850.45 (15) Å^3
Z = 2
D_x = 1.407 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 (2) K
Block, yellow
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.979, T_{max} = 0.989
1805 measured reflections
1672 independent reflections
747 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.152
S = 0.98
1672 reflections
119 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0455P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.023 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	2.22	2.665 (4)	112
C2—H2···O1	0.93	2.33	2.935 (5)	123

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

H atoms were placed in idealized positions and refined as riding, with C—H = 0.93 or 0.96 Å, N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(C,N), or 1.5U_{eq}(C) for methyl H.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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, 2001); software used to prepare material for publication: *SHELXL97*.

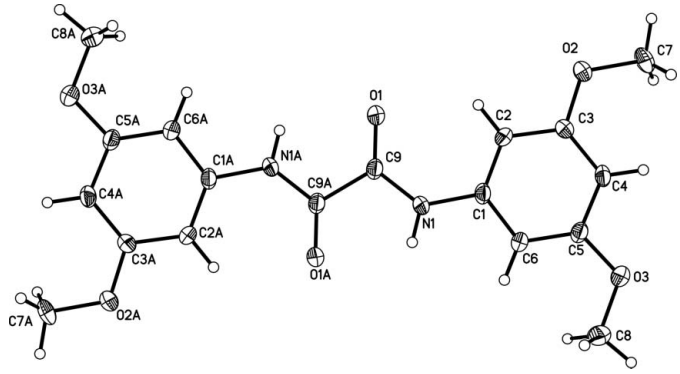


Figure 1
The molecular structure of (I), showing the labeling scheme. Displacement ellipsoids are drawn at the 30% probability level. The suffix A corresponds to symmetry code $(2-x, 1-y, -z)$.

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