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N,*N*′-Bis(3-methoxyphenyl)oxamide

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The molecule of the title compound, $C_{16}H_{16}N_2O_4$, lies on a crystallographically imposed center of symmetry at the midpoint of the C—C bond of the oxamide unit. An intramolecular C—H···O hydrogen bond forms a six-membered ring, and molecules are linked into ribbons along the *a* axis by N—H···O hydrogen bonds.

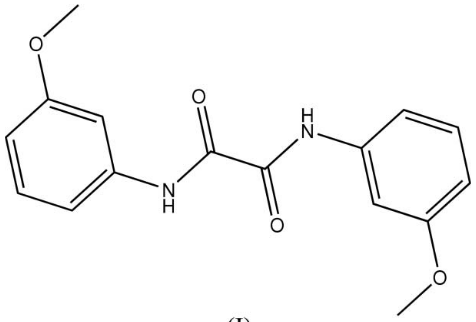
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.098
Data-to-parameter ratio = 13.9

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

Comment

In our ongoing studies of oxalamide derivatives, the title compound, (I), was obtained from the reaction of 3-methoxyaniline and oxalyl chloride. Compound (I) has a crystallographically imposed center of symmetry at the midpoint of the C7—C7^{i} bond [symmetry code: (i): $1 - x, -y, -z$]. All bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987). The dihedral angle between the benzene ring and the N1/C7/O2/N1^{i}/C7^{i}/O2^{i} plane is 31.3 (1)°. An intramolecular C1—H1*B*···O2 hydrogen bond forms a six-membered ring, and molecules are linked into ribbons along the *a* axis (Fig. 2) by N—H···O hydrogen bonds (Table 1). The packing is further stabilized by C—H···π interactions (Table 1; *Cg*1 is the centroid of the C1–C6 benzene ring).



(I)

Experimental

To a solution of 3-methoxyaniline (24.6 g, 0.2 mol) in benzene (70 ml) was added dropwise a solution of oxalyl chloride (6.4 g, 0.05 mol) in benzene (30 ml), and the mixture was stirred at 343 K for 9 h. After cooling to room temperature, water (50 ml) was added to the mixture and the organic phase was washed three times with water to give a solid. Compound (I) was obtained after drying at room temperature for 3 d. Colorless single crystals suitable of (I) for X-ray diffraction study were obtained by slow evaporation of the *N*,*N*-dimethylformamide solution over a period of one day.

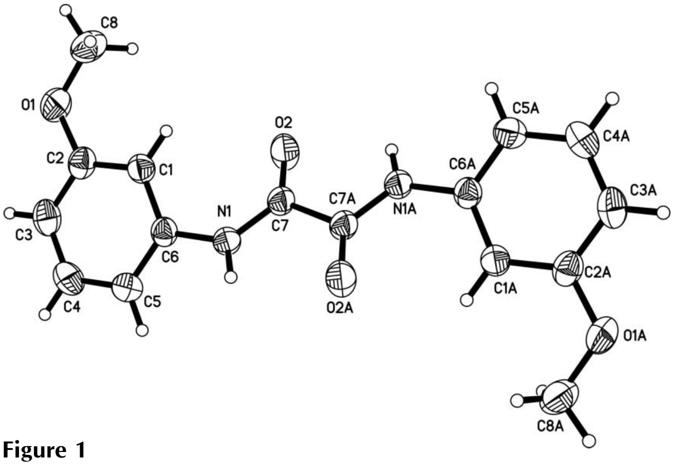


Figure 1

The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The suffix A corresponds to symmetry code $(1 - x, -y, -z)$.

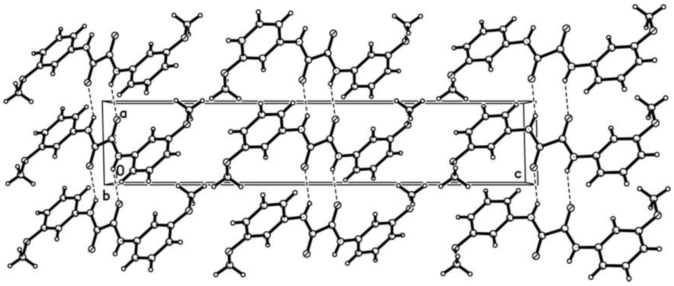


Figure 2

Packing of (I), viewed down the *b* axis, showing the hydrogen-bonded (dashed lines) ribbons.

Crystal data

$C_{16}H_{16}N_2O_4$
$M_r = 300.31$
Monoclinic, $P2_1/c$
$a = 5.0776$ (5) Å
$b = 5.3347$ (6) Å
$c = 26.243$ (3) Å
$\beta = 91.396$ (2)°
$V = 710.65$ (13) Å^3
$Z = 2$
$D_x = 1.403$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 293$ (2) K
Block, colorless
0.39 × 0.22 × 0.10 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.961$, $T_{\max} = 0.990$
3878 measured reflections
1389 independent reflections
1193 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.018$
$\theta_{\max} = 26.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.098$
$S = 1.05$
1389 reflections
100 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2 + 0.1368P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.14$ e Å^{-3}
$\Delta\rho_{\min} = -0.19$ e Å^{-3}

Table 1

Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*B*···*Cg*1$^{\text{ii}}$	0.96	2.74	3.577	146
N1—H1*A*···O2$^{\text{iii}}$	0.86	2.20	2.963 (1)	148
N1—H1*A*···O2$^{\text{i}}$	0.86	2.27	2.681 (1)	109
C1—H1*B*···O2	0.93	2.42	2.918 (2)	113

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

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with N—H = 0.86 Å and C—H distances in the range 0.93–0.96 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C,N})$ and $1.5U_{\text{eq}}$(methyl C).

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*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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