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3-Methoxybenzamide oxime

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.055
wR factor = 0.150
Data-to-parameter ratio = 14.6

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

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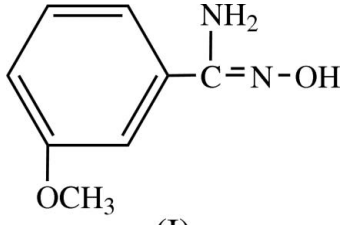
The asymmetric unit of the title compound, $C_8H_{10}N_2O_2$, contains two molecules which are linked by O—H···N hydrogen-bonding interactions, leading to the formation of a dimer of topology $R_2^2(8)$ according to graph-set theory.

Comment

As shown in Fig. 1, the two molecules in the asymmetric unit of the title compound, (I), form a dimer of topology $R_2^2(8)$ according to graph-set theory (Etter, 1990), through O—H···N hydrogen bonds (Table 1). There are also N—H···O hydrogen bonds linking the dimers and forming a two-dimensional network (Fig. 2). The two benzene rings in the dimer make a dihedral angle of 54.83 (9)°.



(I)

Experimental

3-Methoxybenzonitrile (20 mmol) was dissolved in ethanol (8 ml), hydroxylamine hydrochloride (20 mmol) was dissolved in ethanol (6 ml) and potassium carbonate (10 mmol) was dissolved in water (10 ml); these three separate solutions were mixed. The resulting mixture was refluxed for 24 h. After cooling and filtering, crude

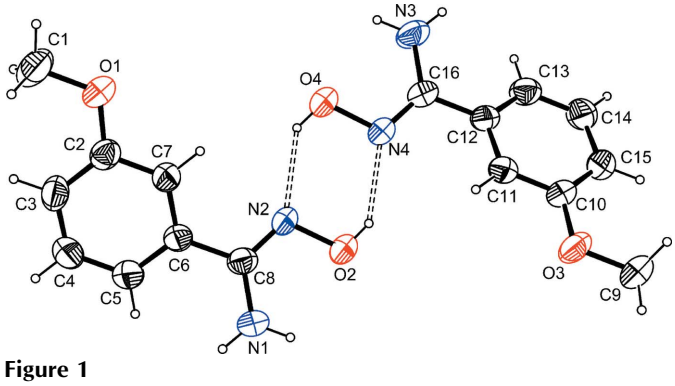


Figure 1
A view of the dimer structure of compound (I), with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii. Hydrogen bonds are shown as dashed lines.

compound (I) was obtained. Pure compound (I) was obtained by crystallization from a solution in a mixture of ethanol (6 ml) and water (2 ml). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_8H_{10}N_2O_2$
M_r = 166.18
Monoclinic, $P2_1/c$
a = 6.8630 (14) Å
b = 18.910 (4) Å
c = 12.893 (3) Å
β = 101.77 (3)°
V = 1638.1 (6) Å^3
Z = 8
D_x = 1.348 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
Block, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.971, T_{max} = 0.990
3491 measured reflections
3219 independent reflections
1994 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.150
S = 1.02
3219 reflections
221 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0677P)^2 + 0.2578P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N4	0.82	2.05	2.751 (3)	143
O4—H4A···N2	0.82	2.09	2.777 (3)	141
N1—H1B···O1^{i}	0.86	2.65	3.449 (3)	155
N1—H1A···O4^{i}	0.86	2.30	3.098 (3)	154
N3—H3A···O2^{ii}	0.86	2.37	3.166 (3)	155

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

All H atoms were treated as riding on their parent atoms, with C—H = 0.93 ($C_{aromatic}$) or 0.96 Å (CH_3), N—H = 0.86 Å and O—H = 0.82 Å, with $U_{iso}(H) = 1.2U_{eq}(C_{aromatic}, NH_2, OH)$ or $1.5U_{eq}(C_{methyl})$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

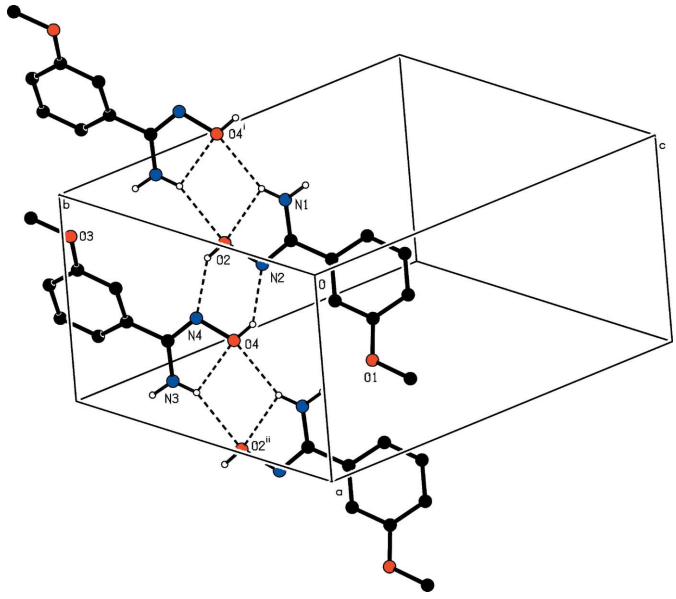


Figure 2
A partial packing view, showing the O—H···N and N—H···O hydrogen bonds as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry codes: (i) $x-1, y, z$; (ii) $1+x, y, z$.]

References

Burnett, M. N. & Johnson, C. K. (1996). *ORTEPIII*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Etter, M. C. (1990). *Acc. Chem. Res.* **23**, 120–126.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.