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4-Methoxy-2-nitroaniline

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The title molecule, $C_7H_8N_2O_3$, lies on a mirror plane with two of the methyl H atoms related by mirror symmetry. The crystal structure is stabilized by intermolecular N—H···O and C—H···O hydrogen bonds.

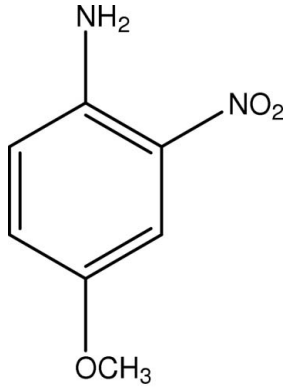
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.001 Å
R factor = 0.033
wR factor = 0.104
Data-to-parameter ratio = 13.6

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

Comment

Nitroaniline-based compounds were reported to have bulk non-linear optical (NLO) properties (Zyss, 1993). We report here the crystal structure of the title compound, (I) (Fig. 1), which crystallizes in the centrosymmetric space group *Pnma*.



(I)

Bond lengths and angles in (I) have normal values (Allen *et al.*, 1987). Except for two symmetry-related H atoms of the methyl group, all atoms lie on a crystallographic mirror plane.

An intramolecular N—H···O hydrogen bond is observed between the amino group and the nearby nitro group. In the

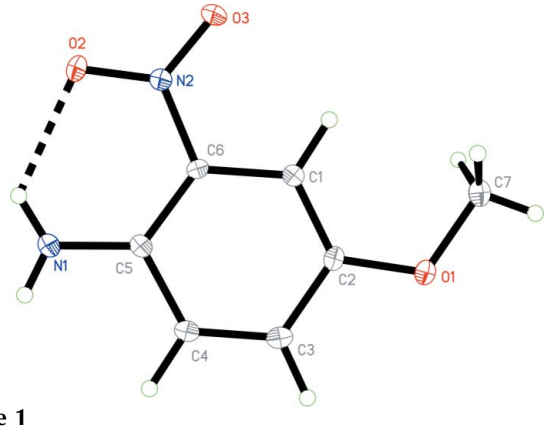


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. A dashed line indicates the intramolecular N—H···O hydrogen bond.

crystal structure, molecules are linked by intermolecular N—H···O and C—H···O hydrogen bonds (Table 1), forming an infinite two-dimensional network in the crystallographic mirror plane (Fig. 2).

Experimental

Commercially available 4-methoxy-2-nitroaniline was further purified by repeated recrystallization from acetone. Single crystals suitable for X-ray analysis were grown by slow evaporation of an acetone solution at room temperature.

Crystal data

$C_7H_8N_2O_3$
M_r = 168.15
Orthorhombic, *Pnma*
a = 16.0264 (4) Å
b = 6.3621 (1) Å
c = 7.1476 (1) Å
V = 728.78 (2) Å^3
Z = 4
D_x = 1.533 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 100.0 (1) K
Block, orange
0.34 × 0.25 × 0.20 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.873, T_{max} = 0.976
13427 measured reflections
1309 independent reflections
1180 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 31.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.104
S = 1.08
1309 reflections
96 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0635P)^2 + 0.1408P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Extinction correction: *SHELXTL*
Extinction coefficient: 0.007 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*1···O2	0.86 (2)	2.06 (2)	2.640 (1)	125 (2)
N1—H1*N*1···O1^{i}	0.86 (2)	2.43 (2)	3.054 (1)	130 (2)
N1—H1*N*2···O3^{ii}	0.81 (2)	2.20 (2)	3.005 (1)	176 (2)
C7—H7*A*···O3^{iii}	0.88 (2)	2.59 (2)	3.461 (1)	169 (1)

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

All H atoms were located in a difference map and refined isotropically. The C—H distances lie in the range 0.88 (2)–1.01 (2) Å.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

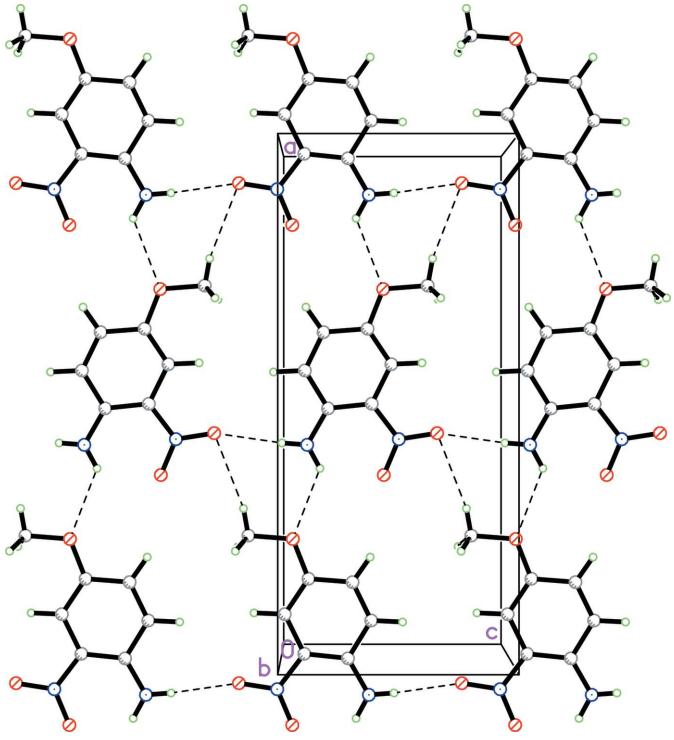


Figure 2
The crystal packing of (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines.

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References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2005). *APEX2* (Version 1.27), *SAINT* (Version 7.12a) and *SADABS* (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Zyss, J. (1993). *Molecular Nonlinear Optics: Materials, Physics, and Devices*. New York: Academic Press.