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N′-(4-Methoxybenzylidene)-4-nitrobenzohydrazide methanol solvate

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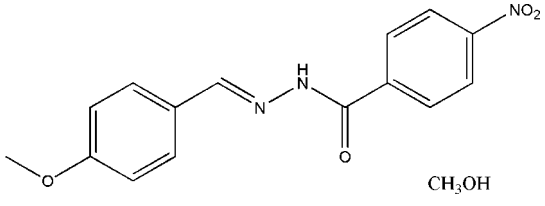
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.058; wR factor = 0.172; data-to-parameter ratio = 15.0.

The title compound, $C_{15}H_{13}N_3O_4\cdot CH_4O$, was synthesized from the reaction of 4-methoxybenzaldehyde with 4-nitrobenzohydrazide in methanol. The benzene rings of the Schiff base molecule are nearly coplanar, making a dihedral angle of 7.0 (3)°. The methanol solvent molecules are linked to the Schiff base molecules by N—H···O, O—H···N and O—H···O hydrogen bonds, forming chains running parallel to the *b* axis.

Related literature

For related structures, see: Brückner *et al.* (2000); Diao (2007); Diao *et al.* (2007, 2008); Harrop *et al.* (2003); Huang *et al.* (2007); Li *et al.* (2007); Ren *et al.* (2002).



Experimental

Crystal data

$C_{15}H_{13}N_3O_4\cdot CH_4O$
M_r = 331.33
Monoclinic, $P2_1/n$
a = 14.719 (3) Å
b = 6.631 (2) Å
c = 18.002 (3) Å
β = 113.17 (3)°
V = 1615.3 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
0.27 × 0.23 × 0.23 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.973, T_{max} = 0.977
9171 measured reflections
3351 independent reflections
1493 reflections with $I > 2\sigma(I)$
R_{int} = 0.065

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.172
S = 0.95
3351 reflections
224 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O5	0.897 (10)	2.049 (13)	2.921 (3)	164 (3)
O5—H5···N3^{i}	0.82	2.56	3.167 (3)	133
O5—H5···O3^{i}	0.82	2.10	2.863 (3)	154

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2199).

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