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(*E*)-*N*′-[4-(Dimethylamino)benzylidene]-4-methylbenzohydrazide methanol monosolvate

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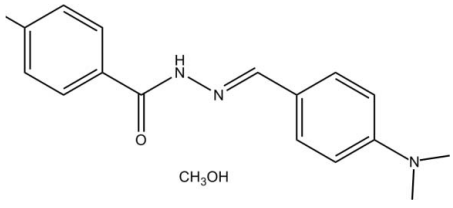
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.060; wR factor = 0.169; data-to-parameter ratio = 16.7.

In the title compound, $C_{17}H_{19}N_3O\cdot CH_3OH$, the hydrazone molecule exists in a *trans* geometry with respect to the methylidene unit and the dihedral angle between the two substituted benzene rings is 42.6 (2)°. In the crystal, the components are linked through N—H···O and O—H···O hydrogen bonds, forming [100] chains of alternating hydrazone and methanol molecules.

Related literature

For the hydrazone compounds reported by one of the authors recently and background refereences, see: Liu (2010*a*,*b*).



Experimental

Crystal data

$C_{17}H_{19}N_3O\cdot CH_4O$
M_r = 313.39
Triclinic, $P\overline{1}$
a = 6.3874 (18) Å
b = 11.724 (3) Å
c = 11.975 (3) Å
α = 78.830 (3)°
β = 77.138 (3)°
γ = 84.807 (3)°
V = 856.7 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 K
0.20 × 0.18 × 0.13 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.984, T_{max} = 0.990
5975 measured reflections
3613 independent reflections
1755 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.169
S = 1.00
3613 reflections
216 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 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
N2—H2*B*···O2^{i}	0.90 (1)	2.02 (1)	2.905 (3)	168 (2)
O2—H2···O1	0.82	1.92	2.720 (3)	166

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: HB6324).

References

Bruker (1998). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Liu, H. (2010*a*). *Acta Cryst.* E**66**, o1582.
Liu, H. (2010*b*). *Acta Cryst.* E**66**, o2026.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2011). E**67**, o2139 [doi:10.1107/S1600536811029394]

(*E*)-*N*′-[4-(Dimethylamino)benzylidene]-4-methylbenzohydrazide methanol monosolvate

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S1. Comment

Recently, the author has reported two new hydrazone compounds (Liu, 2010*a*,*b*). As a further study on these compounds, in the present work, the title new hydrazone compound, (I), which crystallised as a methanol solvate, is reported.

In the title compound (Fig. 1), the methanol molecule is linked to the hydrazone molecule through O—H···O and O—H···N hydrogen bonds (Table 1). The hydrazone molecule exists in a *trans* geometry with respect to the methylidene unit. The dihedral angle between the two substituted benzene rings is 42.6 (2)°. In the crystal structure, the hydrazone and the methanol molecules are linked through N—H···O and O—H···O, hydrogen bonds (Table 1), to form chains along the *a* axis (Fig. 2).

S2. Experimental

4-Dimethylaminobenzaldehyde (1.0 mmol, 153 mg) and 4-methylbenzohydrazide (1.0 mmol, 150 mg) were mixed in 50 mL methanol. The mixture was stirred at ambient temperature for 2 h and filtered. Colorless blocks of the title compound were formed by slow evaporation of the filtrate for a week.

S3. Refinement

The amino hydrogen atom was located in an electronic density map and refined isotropically, with the N—H distance restrained to 0.90 (1)Å. Other hydrogen atoms were placed in calculated positions, with C—H = 0.93–0.96 Å, O—H = 0.82 Å, and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(O and methyl C).

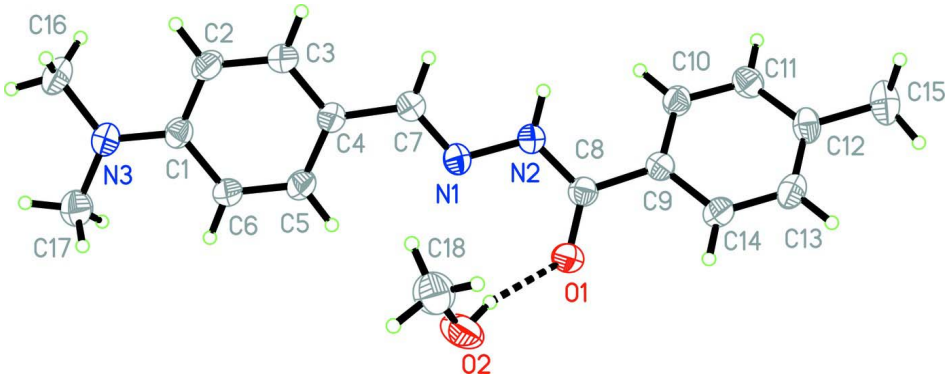

Figure 1

Molecular structure of the title compound with 30% probability displacement ellipsoids. Hydrogen bonds are shown as dashed lines.

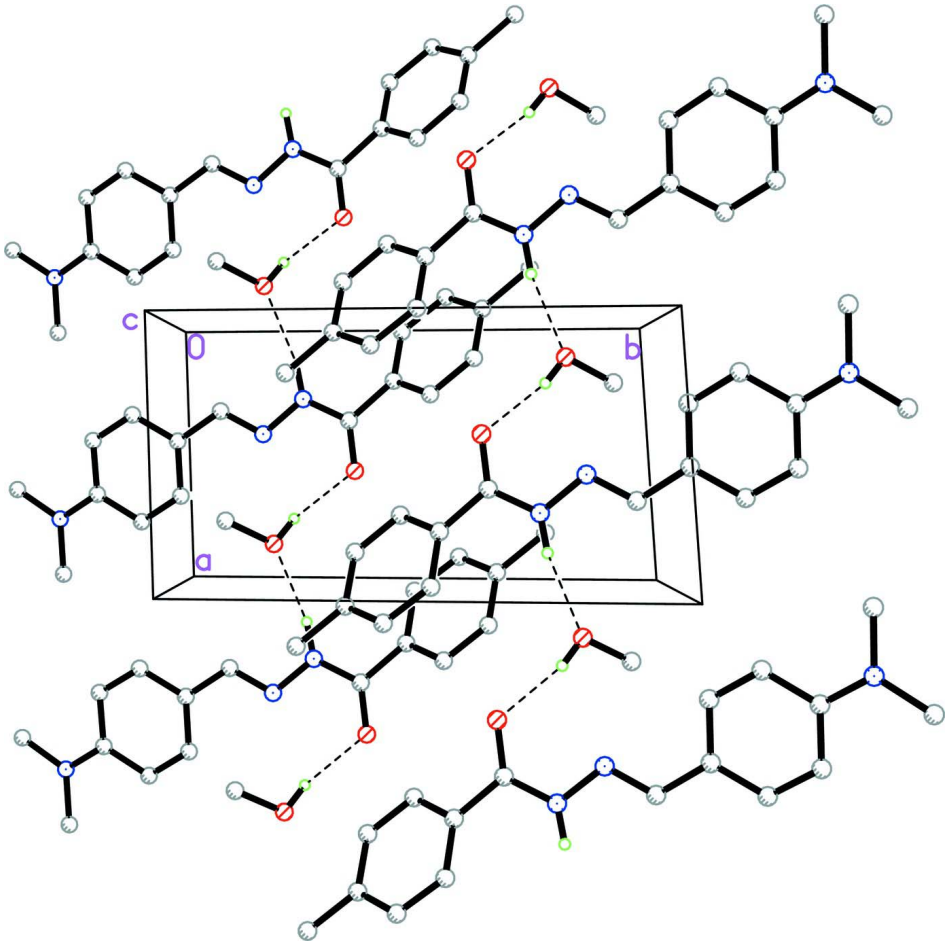

Figure 2

Packing structure of the title compound, viewed along the *c* axis. Hydrogen bonds are shown as dashed lines. Hydrogen atoms not involved in hydrogen bonding have been omitted.

(*E*)-*N*′-[4-(Dimethylamino)benzylidene]-4-methylbenzohydrazide methanol monosolvate

Crystal data

$C_{17}H_{19}N_3O\cdot CH_4O$
$M_r = 313.39$
Triclinic, $P\overline{1}$
$a = 6.3874\ (18)$ Å
$b = 11.724\ (3)$ Å
$c = 11.975\ (3)$ Å
$\alpha = 78.830\ (3)°$
$\beta = 77.138\ (3)°$
$\gamma = 84.807\ (3)°$
$V = 856.7\ (4)$ Å^3
$Z = 2$
$F(000) = 336$
$D_x = 1.215$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 744 reflections
$\theta = 2.6–24.9°$
$\mu = 0.08$ mm^{-1}
$T = 298$ K
Block, colorless
0.20 × 0.18 × 0.13 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.984$, $T_{max} = 0.990$

5975 measured reflections
3613 independent reflections
1755 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.7°$
$h = -8 \rightarrow 8$
$k = -14 \rightarrow 13$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.169$
$S = 1.00$
3613 reflections
216 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0667P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.4251 (3)	0.17760 (17)	0.23171 (17)	0.0519 (6)
N2	0.2884 (3)	0.26788 (18)	0.27010 (18)	0.0518 (5)
N3	0.7692 (4)	−0.29356 (18)	0.03356 (18)	0.0603 (6)
O1	0.5681 (3)	0.37103 (15)	0.27273 (17)	0.0699 (6)
O2	0.8472 (3)	0.19729 (18)	0.3439 (2)	0.0945 (7)
H2	0.7518	0.2406	0.3205	0.142*
C1	0.6665 (4)	−0.2025 (2)	0.0848 (2)	0.0493 (6)
C2	0.4491 (4)	−0.2032 (2)	0.1361 (2)	0.0584 (7)
H2A	0.3721	−0.2677	0.1391	0.070*
C3	0.3463 (4)	−0.1095 (2)	0.1824 (2)	0.0595 (7)
H3	0.2001	−0.1121	0.2154	0.071*
C4	0.4524 (4)	−0.0118 (2)	0.1816 (2)	0.0498 (6)
C5	0.6711 (4)	−0.0127 (2)	0.1337 (2)	0.0563 (7)
H5	0.7481	0.0511	0.1331	0.068*
C6	0.7761 (4)	−0.1051 (2)	0.0874 (2)	0.0557 (7)
H6	0.9233	−0.1033	0.0571	0.067*
C7	0.3337 (4)	0.0872 (2)	0.2259 (2)	0.0547 (7)
H7	0.1853	0.0847	0.2511	0.066*
C8	0.3731 (4)	0.3636 (2)	0.2844 (2)	0.0494 (6)
C9	0.2198 (4)	0.4615 (2)	0.31429 (19)	0.0450 (6)

C10	0.0261 (4)	0.4838 (2)	0.2788 (2)	0.0518 (7)
H10	−0.0156	0.4341	0.2368	0.062*
C11	−0.1058 (4)	0.5789 (2)	0.3052 (2)	0.0566 (7)
H11	−0.2332	0.5937	0.2783	0.068*
C12	−0.0529 (5)	0.6528 (2)	0.3707 (2)	0.0541 (7)
C13	0.1388 (5)	0.6292 (2)	0.4075 (2)	0.0601 (7)
H13	0.1772	0.6769	0.4525	0.072*
C14	0.2749 (4)	0.5360 (2)	0.3787 (2)	0.0534 (7)
H14	0.4051	0.5231	0.4029	0.064*
C15	−0.2024 (5)	0.7539 (2)	0.4031 (2)	0.0797 (9)
H15A	−0.1317	0.8013	0.4390	0.119*
H15B	−0.3298	0.7250	0.4567	0.119*
H15C	−0.2408	0.7996	0.3343	0.119*
C16	0.6496 (5)	−0.3900 (2)	0.0267 (2)	0.0713 (8)
H16A	0.6002	−0.4333	0.1035	0.107*
H16B	0.7407	−0.4398	−0.0206	0.107*
H16C	0.5283	−0.3608	−0.0073	0.107*
C17	0.9965 (5)	−0.2948 (2)	−0.0162 (3)	0.0775 (9)
H17A	1.0262	−0.2307	−0.0798	0.116*
H17B	1.0406	−0.3666	−0.0439	0.116*
H17C	1.0740	−0.2879	0.0421	0.116*
C18	0.7566 (5)	0.1029 (3)	0.4231 (3)	0.0921 (11)
H18A	0.8683	0.0469	0.4421	0.138*
H18B	0.6613	0.0677	0.3895	0.138*
H18C	0.6774	0.1288	0.4925	0.138*
H2B	0.1469 (18)	0.257 (2)	0.292 (2)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0519 (13)	0.0437 (12)	0.0603 (14)	0.0045 (11)	−0.0138 (10)	−0.0106 (10)
N2	0.0470 (13)	0.0442 (12)	0.0652 (14)	0.0003 (11)	−0.0110 (11)	−0.0142 (10)
N3	0.0649 (16)	0.0474 (13)	0.0717 (15)	−0.0017 (12)	−0.0149 (12)	−0.0181 (11)
O1	0.0476 (12)	0.0561 (12)	0.1090 (16)	−0.0009 (9)	−0.0189 (10)	−0.0201 (10)
O2	0.0519 (13)	0.0742 (15)	0.147 (2)	0.0031 (11)	−0.0245 (13)	0.0062 (14)
C1	0.0572 (17)	0.0415 (14)	0.0500 (15)	−0.0037 (13)	−0.0151 (12)	−0.0048 (12)
C2	0.0613 (18)	0.0485 (16)	0.0673 (18)	−0.0154 (14)	−0.0106 (14)	−0.0129 (13)
C3	0.0467 (16)	0.0586 (17)	0.0754 (19)	−0.0063 (13)	−0.0093 (13)	−0.0198 (15)
C4	0.0513 (16)	0.0435 (15)	0.0556 (16)	−0.0021 (12)	−0.0122 (12)	−0.0100 (12)
C5	0.0564 (18)	0.0445 (15)	0.0668 (18)	−0.0111 (13)	−0.0067 (14)	−0.0102 (13)
C6	0.0454 (15)	0.0507 (16)	0.0707 (18)	−0.0079 (13)	−0.0059 (13)	−0.0148 (14)
C7	0.0490 (16)	0.0510 (16)	0.0647 (18)	−0.0015 (13)	−0.0106 (13)	−0.0137 (13)
C8	0.0491 (16)	0.0465 (15)	0.0519 (15)	−0.0034 (13)	−0.0116 (12)	−0.0057 (12)
C9	0.0453 (15)	0.0428 (14)	0.0447 (14)	−0.0027 (12)	−0.0084 (11)	−0.0037 (11)
C10	0.0550 (17)	0.0513 (16)	0.0525 (15)	−0.0004 (13)	−0.0147 (13)	−0.0142 (12)
C11	0.0539 (17)	0.0612 (17)	0.0537 (16)	0.0036 (14)	−0.0137 (13)	−0.0080 (13)
C12	0.0670 (19)	0.0428 (15)	0.0464 (15)	0.0046 (13)	−0.0049 (13)	−0.0044 (12)
C13	0.076 (2)	0.0510 (16)	0.0545 (17)	−0.0121 (15)	−0.0065 (14)	−0.0174 (13)

C14	0.0561 (16)	0.0490 (16)	0.0579 (16)	−0.0079 (13)	−0.0166 (13)	−0.0088 (13)
C15	0.101 (3)	0.0611 (19)	0.0695 (19)	0.0140 (17)	−0.0032 (17)	−0.0179 (15)
C16	0.091 (2)	0.0502 (17)	0.076 (2)	−0.0128 (16)	−0.0134 (16)	−0.0202 (14)
C17	0.073 (2)	0.073 (2)	0.088 (2)	−0.0007 (17)	−0.0077 (17)	−0.0311 (17)
C18	0.090 (3)	0.074 (2)	0.112 (3)	0.004 (2)	−0.035 (2)	−0.005 (2)

Geometric parameters (Å, º)

N1—C7	1.275 (3)	C9—C10	1.383 (3)
N1—N2	1.392 (3)	C9—C14	1.386 (3)
N2—C8	1.344 (3)	C10—C11	1.378 (3)
N2—H2B	0.897 (10)	C10—H10	0.9300
N3—C1	1.376 (3)	C11—C12	1.384 (3)
N3—C17	1.441 (3)	C11—H11	0.9300
N3—C16	1.445 (3)	C12—C13	1.379 (4)
O1—C8	1.232 (3)	C12—C15	1.508 (3)
O2—C18	1.387 (3)	C13—C14	1.382 (3)
O2—H2	0.8200	C13—H13	0.9300
C1—C2	1.388 (3)	C14—H14	0.9300
C1—C6	1.402 (3)	C15—H15A	0.9600
C2—C3	1.374 (3)	C15—H15B	0.9600
C2—H2A	0.9300	C15—H15C	0.9600
C3—C4	1.381 (3)	C16—H16A	0.9600
C3—H3	0.9300	C16—H16B	0.9600
C4—C5	1.387 (3)	C16—H16C	0.9600
C4—C7	1.450 (3)	C17—H17A	0.9600
C5—C6	1.366 (3)	C17—H17B	0.9600
C5—H5	0.9300	C17—H17C	0.9600
C6—H6	0.9300	C18—H18A	0.9600
C7—H7	0.9300	C18—H18B	0.9600
C8—C9	1.485 (3)	C18—H18C	0.9600
C7—N1—N2	115.7 (2)	C9—C10—H10	119.7
C8—N2—N1	119.3 (2)	C10—C11—C12	121.4 (3)
C8—N2—H2B	121.7 (17)	C10—C11—H11	119.3
N1—N2—H2B	118.6 (17)	C12—C11—H11	119.3
C1—N3—C17	121.3 (2)	C13—C12—C11	117.7 (2)
C1—N3—C16	120.4 (2)	C13—C12—C15	121.2 (3)
C17—N3—C16	118.3 (2)	C11—C12—C15	121.1 (3)
C18—O2—H2	109.5	C12—C13—C14	121.3 (2)
N3—C1—C2	121.3 (2)	C12—C13—H13	119.4
N3—C1—C6	121.7 (2)	C14—C13—H13	119.4
C2—C1—C6	117.0 (2)	C13—C14—C9	120.7 (3)
C3—C2—C1	120.8 (2)	C13—C14—H14	119.6
C3—C2—H2A	119.6	C9—C14—H14	119.6
C1—C2—H2A	119.6	C12—C15—H15A	109.5
C2—C3—C4	122.3 (2)	C12—C15—H15B	109.5
C2—C3—H3	118.9	H15A—C15—H15B	109.5

C4—C3—H3	118.9	C12—C15—H15C	109.5
C3—C4—C5	116.9 (2)	H15A—C15—H15C	109.5
C3—C4—C7	120.0 (2)	H15B—C15—H15C	109.5
C5—C4—C7	123.0 (2)	N3—C16—H16A	109.5
C6—C5—C4	121.6 (2)	N3—C16—H16B	109.5
C6—C5—H5	119.2	H16A—C16—H16B	109.5
C4—C5—H5	119.2	N3—C16—H16C	109.5
C5—C6—C1	121.3 (2)	H16A—C16—H16C	109.5
C5—C6—H6	119.3	H16B—C16—H16C	109.5
C1—C6—H6	119.3	N3—C17—H17A	109.5
N1—C7—C4	122.5 (2)	N3—C17—H17B	109.5
N1—C7—H7	118.7	H17A—C17—H17B	109.5
C4—C7—H7	118.7	N3—C17—H17C	109.5
O1—C8—N2	122.2 (2)	H17A—C17—H17C	109.5
O1—C8—C9	121.1 (2)	H17B—C17—H17C	109.5
N2—C8—C9	116.8 (2)	O2—C18—H18A	109.5
C10—C9—C14	118.1 (2)	O2—C18—H18B	109.5
C10—C9—C8	123.2 (2)	H18A—C18—H18B	109.5
C14—C9—C8	118.6 (2)	O2—C18—H18C	109.5
C11—C10—C9	120.7 (2)	H18A—C18—H18C	109.5
C11—C10—H10	119.7	H18B—C18—H18C	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*B*···O2^{i}	0.90 (1)	2.02 (1)	2.905 (3)	168 (2)
O2—H2···O1	0.82	1.92	2.720 (3)	166

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