Crystal structure of 2-nitro-*N'*-(2-methoxynaphthylidene)-benzohydrazide, C₁₉H₁₅N₃O₄

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Abstract

C₁₉H₁₅N₃O₄, monoclinic, *P*12₁/*c*1 (no. 14), *a* = 10.909(4) Å, *b* = 11.084(4) Å, *c* = 14.888(6) Å, β = 105.360(6)°, *V* = 1735.9 Å³, *Z* = 4, *R*_g(*F*) = 0.050, *wR*_{ref}(*F*²) = 0.131, *T* = 298 K.

Source of material

2-Methoxy-1-naphthylaldehyde and 2-nitrobenzohydrazide of analytical reagent (AR) grade were purchased from Aldrich and were used as obtained. 2-Methoxy-1-naphthylaldehyde (186.2 mg, 1.0 mmol) and 2-nitrobenzohydrazide (181.2 mg, 1.0 mmol) were dissolved in a methanol solution (50 ml). The mixture was stirred for 30 min at room temperature. The resulting solution was left in air for a few days, yielding colorless block-shaped crystals.

Experimental details

H1 atom was located in a difference map and refined with N—H distance restrained to 0.90(1) Å. The remaining H atoms were positioned geometrically [*d*(C—H) = 0.93–0.96 Å] and refined using a riding model, with *U*_{iso}(H) = 1.2 *U*_{eq}(C) and 1.5 *U*_{eq}(C19). A rotating group model was applied for the methyl group.

Discussion

Schiff bases are a kind of versatile compounds, which possess excellent biological properties [1–3]. Recently, a large number of

Schiff bases derived from the reaction of aldehydes with benzohydrazides have been reported [4–6].

In the title crystal structure, all the bond lengths are comparable with those observed in other similar compounds [4–8]. The dihedral angle between the C1–C6 benzene ring and the C9–C18 naphthyl ring is 73.6(2)°. The dihedral angle between the O3/N3/O4 plane and the C1–C6 benzene ring is 17.0(2)°. The C19 atom deviates from the least-squares plane of C9–C18 by 0.245(2) Å. The torsion angles of C1–C7–N1–N2 and C7–N1–N2–C8 are 3.6(2)° and 0.7(2)°, respectively. In the crystal structure, molecules are linked through intermolecular N—H...O hydrogen bonds to form dimers.

Table 1. Data collection and handling.

Crystal:	colorless block, size 0.30 × 0.32 × 0.32 mm
Wavelength:	Mo <i>K</i> _α radiation (0.71073 Å)
μ :	0.96 cm ^{−1}
Diffractometer, scan mode:	Bruker SMART 1000 CCD, ω
$2\theta_{\max}$:	54°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	14186, 3765
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ (<i>I</i> _{obs}), 2288
<i>N</i> (<i>param</i>) _{refined} :	239
Programs:	SHELXS-97 [9], SHELXL-97 [10], SHELXTL [11],

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(3)	4e	0.8244	−0.0288	1.0956	0.073
H(4)	4e	0.8042	−0.0013	1.2442	0.090
H(5)	4e	0.8494	0.1821	1.3152	0.093
H(6)	4e	0.9151	0.3403	1.2396	0.076
H(8)	4e	0.6950	0.5032	0.8977	0.051
H(11)	4e	0.2951	0.4904	0.7085	0.080
H(12)	4e	0.1764	0.3923	0.7895	0.082
H(14)	4e	0.1561	0.2816	0.9267	0.082
H(15)	4e	0.2448	0.1995	1.0679	0.088
H(16)	4e	0.4627	0.2079	1.1309	0.079
H(17)	4e	0.5903	0.3004	1.0535	0.063
H(19A)	4e	0.4396	0.5419	0.6277	0.159
H(19B)	4e	0.5530	0.6330	0.6577	0.159
H(19C)	4e	0.4309	0.6506	0.6930	0.159
H(1)	4e	0.881(2)	0.482(1)	0.979(1)	0.080

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
O(1)	4e	1.0600(1)	0.3963(1)	1.09887(9)	0.0403(8)	0.0575(8)	0.0655(9)	−0.0125(6)	0.0072(6)	0.0050(7)
O(2)	4e	0.5415(1)	0.5200(1)	0.7565(1)	0.068(1)	0.086(1)	0.0599(9)	−0.0027(8)	0.0128(8)	0.0255(8)
O(3)	4e	0.9588(1)	0.1885(1)	0.9551(1)	0.087(1)	0.069(1)	0.067(1)	−0.0142(8)	0.0419(9)	−0.0047(8)
O(4)	4e	0.8473(2)	0.0301(2)	0.9448(1)	0.139(2)	0.085(1)	0.061(1)	−0.051(1)	0.017(1)	−0.0240(9)
N(1)	4e	0.8610(1)	0.4171(1)	1.0093(1)	0.0348(9)	0.0436(9)	0.059(1)	−0.0075(7)	0.0087(7)	0.0082(8)
N(2)	4e	0.7378(1)	0.3742(1)	0.9834(1)	0.0345(8)	0.0417(8)	0.0543(9)	−0.0047(7)	0.0099(7)	0.0040(7)
N(3)	4e	0.8963(2)	0.1188(2)	0.9867(1)	0.058(1)	0.049(1)	0.047(1)	−0.0072(8)	0.0084(8)	−0.0015(8)
C(1)	4e	0.9084(2)	0.2528(2)	1.1201(1)	0.034(1)	0.047(1)	0.043(1)	−0.0019(8)	0.0092(8)	0.0028(9)
C(2)	4e	0.8816(2)	0.1406(2)	1.0800(1)	0.043(1)	0.048(1)	0.038(1)	−0.0048(8)	0.0067(8)	0.0032(9)
C(3)	4e	0.8425(2)	0.0457(2)	1.1249(2)	0.072(2)	0.051(1)	0.058(1)	−0.013(1)	0.012(1)	0.008(1)
C(4)	4e	0.8306(2)	0.0622(2)	1.2130(2)	0.092(2)	0.075(2)	0.062(2)	−0.020(1)	0.027(1)	0.019(1)
C(5)	4e	0.8575(2)	0.1713(2)	1.2551(2)	0.097(2)	0.093(2)	0.051(1)	−0.016(2)	0.034(1)	0.004(1)
C(6)	4e	0.8965(2)	0.2663(2)	1.2096(1)	0.075(2)	0.067(1)	0.053(1)	−0.009(1)	0.025(1)	−0.009(1)
C(7)	4e	0.9501(2)	0.3599(2)	1.0739(1)	0.041(1)	0.041(1)	0.046(1)	−0.0058(9)	0.0146(9)	−0.0051(9)
C(8)	4e	0.6618(2)	0.4374(2)	0.9222(1)	0.043(1)	0.036(1)	0.050(1)	−0.0050(8)	0.0152(9)	−0.0010(9)
C(9)	4e	0.5265(2)	0.4142(1)	0.8877(1)	0.038(1)	0.035(1)	0.048(1)	−0.0016(8)	0.0094(8)	−0.0042(8)
C(10)	4e	0.4653(2)	0.4644(2)	0.8028(1)	0.051(1)	0.049(1)	0.055(1)	−0.0014(9)	0.011(1)	0.003(1)
C(11)	4e	0.3340(2)	0.4560(2)	0.7660(2)	0.053(1)	0.075(2)	0.061(1)	0.006(1)	−0.003(1)	0.007(1)
C(12)	4e	0.2639(2)	0.3974(2)	0.8145(2)	0.040(1)	0.074(2)	0.084(2)	−0.003(1)	0.002(1)	−0.009(1)
C(13)	4e	0.3185(2)	0.3441(2)	0.9012(2)	0.042(1)	0.044(1)	0.073(1)	−0.0060(9)	0.018(1)	−0.011(1)
C(14)	4e	0.2436(2)	0.2861(2)	0.9517(2)	0.048(1)	0.058(1)	0.102(2)	−0.013(1)	0.027(1)	−0.011(1)
C(15)	4e	0.2959(2)	0.2371(2)	1.0352(2)	0.072(2)	0.057(1)	0.107(2)	−0.019(1)	0.051(2)	−0.004(1)
C(16)	4e	0.4268(2)	0.2426(2)	1.0730(2)	0.074(2)	0.059(1)	0.074(2)	−0.010(1)	0.034(1)	0.007(1)
C(17)	4e	0.5031(2)	0.2979(2)	1.0267(1)	0.050(1)	0.049(1)	0.061(1)	−0.0056(9)	0.020(1)	0.001(1)
C(18)	4e	0.4522(2)	0.3515(2)	0.9388(1)	0.041(1)	0.0317(9)	0.055(1)	−0.0045(8)	0.0135(9)	−0.0085(8)
C(19)	4e	0.4868(3)	0.5922(2)	0.6773(2)	0.111(2)	0.105(2)	0.095(2)	−0.000(2)	0.013(2)	0.057(2)

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