Crystal structure of naphthalen-1-yl-(4-nitro-benzylidene)-amine, $C_{17}H_{12}N_2O_2$

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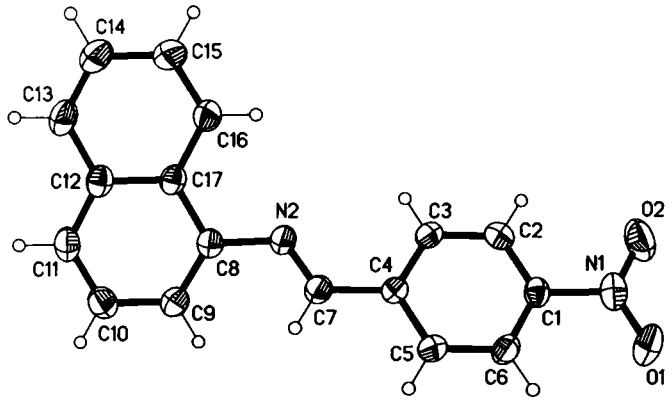

Abstract

$C_{17}H_{12}N_2O_2$, orthorhombic, $P2_12_12_1$ (no. 19), $a = 7.2528(8)$ Å, $b = 12.301(1)$ Å, $c = 15.208(1)$ Å, $V = 1356.8$ Å^3, $Z = 4$, $R_{gt}(F) = 0.046$, $wR_{ref}(F^2) = 0.107$, $T = 273$ K.

Source of material

1-Naphthylamine (0.1 mmol, 14.3 mg) and 4-nitrobenzaldehyde (0.1 mmol, 15.1 mg) were dissolved in methanol (10 ml). The mixture was stirred for 60 min at room temperature to give a clear yellow solution. After allowing the resulting solution to stand in air for 10 d, yellow prismatic crystals were formed at the bottom of the vessel by slow evaporation of the solvent. The crystals were isolated by filtration, washed with methanol and dried in a vacuum desiccator using anhydrous $CaCl_2$ (yield 86 %).
Elemental analysis: found – C, 73.8 %; H, 4.4 %; N, 10.2 %; calc. for $C_{17}H_{12}N_2O_2$ – C, 73.9 %; H, 4.4 %; N, 10.1 %.

Discussion

Schiff base compounds play an important role in the development of coordination chemistry related to catalysis and enzymatic reaction, magnetism and molecular architectures [1,2].
The crystal structure of the title compound is built up by only the $C_{17}H_{12}N_2O_2$ molecules, within which all the bond lengths are in normal ranges [3]. The dihedral angle between the C1 – C6 phenyl ring and the C8 – C17 naphthalene system is 33.8(4)°, and the torsion angles are 178.1(2)° for C2–C3–C4–C7 and –177.7(3)° for C7–C4–C5–C6. As expected, the molecule adopts a *trans* configuration about the C7=N2 bond. The C7=N2 bond length of 1.267(3) Å conforms to the value for a normal C=N double bond. Because of conjugation through the imino double bond C7=N2, the C1 – C6 phenyl ring and the C8 – C17 naphthalene system show a weak distortion. The C7—C4 bond length of 1.469(3) Å is shorter than C–C(=C) of 1.51 Å [4].

Table 1. Data collection and handling.

Crystal:	yellow prism, size 0.14 × 0.32 × 0.34 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.91 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, ω
$2\theta_{max}$:	50.06°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6115, 2385
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1604
$N(param)_{refined}$:	191
Program:	SHELXTL [5]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(2)	4*a*	0.0277	0.3641	0.7409	0.064
H(3)	4*a*	0.0367	0.2416	0.6257	0.059
H(5)	4*a*	0.2154	0.4778	0.4656	0.067
H(6)	4*a*	0.2098	0.5998	0.5814	0.067
H(7)	4*a*	0.1853	0.2953	0.4064	0.061
H(9)	4*a*	0.0339	0.2088	0.3002	0.068
H(10)	4*a*	0.0463	0.0881	0.1820	0.078
H(11)	4*a*	0.1363	–0.0866	0.2035	0.075
H(13)	4*a*	0.2283	–0.2359	0.3041	0.082
H(14)	4*a*	0.2843	–0.2976	0.4418	0.094
H(15)	4*a*	0.2520	–0.1819	0.5626	0.092
H(16)	4*a*	0.1757	–0.0040	0.5423	0.073

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	4*a*	0.1199(3)	0.4921(2)	0.6703(2)	0.046(2)	0.052(2)	0.049(1)	0.008(1)	–0.004(1)	–0.011(1)
C(2)	4*a*	0.0665(3)	0.3861(2)	0.6854(2)	0.052(2)	0.061(2)	0.046(1)	0.001(1)	0.001(1)	0.005(1)
C(3)	4*a*	0.0718(3)	0.3135(2)	0.6167(2)	0.052(2)	0.041(1)	0.054(1)	0.000(1)	–0.001(1)	0.001(1)
C(4)	4*a*	0.1291(4)	0.3471(2)	0.5341(1)	0.044(1)	0.042(1)	0.048(1)	0.000(1)	0.001(1)	–0.001(1)
C(5)	4*a*	0.1790(4)	0.4547(2)	0.5212(2)	0.071(2)	0.044(1)	0.053(1)	–0.002(1)	0.004(1)	0.004(1)

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Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(6)	4*a*	0.1753(4)	0.5278(2)	0.5899(2)	0.067(2)	0.040(1)	0.061(2)	−0.002(1)	0.005(2)	−0.006(1)
C(7)	4*a*	0.1417(4)	0.2705(2)	0.4603(1)	0.053(2)	0.047(2)	0.053(1)	−0.002(1)	0.005(1)	−0.003(1)
C(8)	4*a*	0.1053(3)	0.1027(2)	0.3932(2)	0.044(2)	0.048(1)	0.049(1)	−0.005(1)	0.005(1)	−0.005(1)
C(9)	4*a*	0.0666(4)	0.1366(2)	0.3099(2)	0.061(2)	0.049(2)	0.061(2)	−0.004(1)	−0.001(2)	−0.003(1)
C(10)	4*a*	0.0754(4)	0.0641(2)	0.2383(2)	0.072(2)	0.071(2)	0.054(2)	−0.007(2)	−0.000(2)	−0.003(1)
C(11)	4*a*	0.1262(4)	−0.0402(2)	0.2515(2)	0.069(2)	0.061(2)	0.059(2)	−0.007(2)	0.012(2)	−0.016(1)
C(12)	4*a*	0.1641(4)	−0.0804(2)	0.3361(2)	0.049(2)	0.051(2)	0.060(2)	−0.007(1)	0.006(1)	−0.009(1)
C(13)	4*a*	0.2163(4)	−0.1886(2)	0.3515(2)	0.077(2)	0.050(2)	0.078(2)	−0.007(2)	0.005(2)	−0.017(1)
C(14)	4*a*	0.2495(5)	−0.2256(2)	0.4334(2)	0.098(3)	0.049(2)	0.090(2)	0.001(2)	−0.004(2)	−0.003(2)
C(15)	4*a*	0.2318(5)	−0.1556(2)	0.5061(2)	0.103(3)	0.053(2)	0.073(2)	−0.002(2)	−0.009(2)	0.005(1)
C(16)	4*a*	0.1853(4)	−0.0500(2)	0.4940(2)	0.074(2)	0.051(2)	0.057(2)	−0.006(2)	0.000(2)	−0.006(1)
C(17)	4*a*	0.1513(3)	−0.0088(2)	0.4087(2)	0.044(2)	0.044(1)	0.055(2)	−0.007(1)	0.003(1)	−0.007(1)
N(1)	4*a*	0.1226(3)	0.5685(2)	0.7449(2)	0.060(2)	0.076(2)	0.065(2)	0.004(1)	−0.007(1)	−0.024(1)
N(2)	4*a*	0.0947(3)	0.1718(2)	0.4678(1)	0.053(1)	0.047(1)	0.053(1)	−0.003(1)	0.004(1)	−0.007(1)
O(1)	4*a*	0.1633(4)	0.6631(2)	0.7299(1)	0.116(2)	0.062(1)	0.100(2)	−0.004(1)	−0.001(1)	−0.032(1)
O(2)	4*a*	0.0873(4)	0.5339(2)	0.8180(1)	0.121(2)	0.118(2)	0.055(1)	−0.010(2)	0.006(1)	−0.024(1)

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