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Crystal structure of (*E*)-3-((naphthalen-1-ylimino)methyl)-4-nitrophenol, $C_{17}H_{12}N_2O_3$

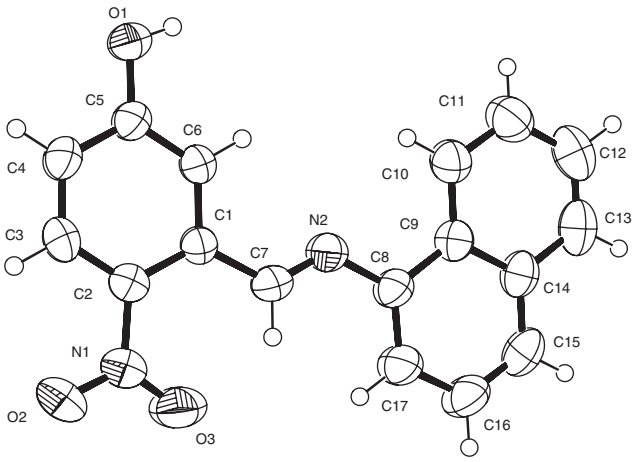

Table 1: Data collection and handling.

Crystal:	Orange plate
Size:	0.60 × 0.27 × 0.03 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	1.0 cm^{-1}
Diffractometer, scan mode:	STOE IPDS 2, ω-scans
$2\theta_{max}$, completeness:	55.2°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	8884, 3177, 0.143
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1601
$N(param)_{refined}$:	199
Programs:	Stoe programs [10], SHELX [11], Platon [12, 13]

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Abstract

$C_{17}H_{12}N_2O_3$, monoclinic, $P2_1/c$ (no. 14), $a = 7.2641(5)$ Å, $b = 12.3968(6)$ Å, $c = 16.1786(13)$ Å, $\beta = 108.200(6)°$, $V = 1384.02(16)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0905$, $wR_{ref}(F^2) = 0.1928$, $T = 293(2)$ K.

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The asymmetric unit of the title crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

(*E*)-3-((naphthalen-1-ylimino)methyl)-4-nitrophenol was prepared by refluxing a mixture of a solution containing 5-hydroxy-2-nitro-benzaldehyde (8.4 mg, 0.05 mmol) in ethanol (20 mL) and a solution containing 1-naphthylamine (7.2 mg, 0.05 mmol) in ethanol (20 mL). The reaction mixture was stirred for 5 h under reflux. Single crystals of the title compound were obtained by slow evaporation of an ethanolic solution (Yield 70%; m.p. 458–459 K).

Experimental details

For least-squares refinement of the crystal structure all H atoms were placed in calculated positions using a suitable riding model, with C—H distances of 0.93 Å and O—H distances of 0.82 Å, $U_{iso}(H) = 1.2U_{eq}(C)$ and $1.5U_{eq}(O)$.

Discussion

Schiff bases are an important class of organic molecules which contain imine and azomethine groups. Schiff bases were first discovered by Hugo Schiff in 1864 [1]. Some Schiff bases show biological activities such as anti-inflammatory, antimicrobial, anticonvulsant, anticancer, analgesic etc. [2–4]. And also, their metal complexes often exhibit antibacterial, antiviral, fungicidal or antitubarculoral activity [5, 6].

In the title compound, $C_{17}H_{12}N_2O_3$, the naphthalen and phenyl ring groups are planar with an r.m.s. deviation of 0.010(4) Å for atom C12 in naphthalen group and −0.005(3) Å for atom C5 in the phenyl group, respectively. However the whole molecule is also nearly planar with the dihedral angle is 5.79(8)° between the related ring systems. The torsion angle around the C1—C7—N2—C8 is −178.8(3)° shows that the molecular structure has E configuration. The C = N bond

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8113(4)	0.3274(2)	0.57499(17)	0.0462(7)
C2	0.8423(4)	0.2748(2)	0.65536(18)	0.0509(7)
C3	0.8641(5)	0.1639(2)	0.6624(2)	0.0587(8)
H3	0.8846	0.1307	0.7161	0.070*
C4	0.8556(5)	0.1028(2)	0.5910(2)	0.0611(8)
H4	0.8695	0.0283	0.5960	0.073*
C5	0.8261(5)	0.1523(2)	0.51121(19)	0.0533(7)
C6	0.8030(4)	0.2627(2)	0.50383(19)	0.0516(7)
H6	0.7812	0.2947	0.4496	0.062*
C7	0.7847(6)	0.4444(2)	0.5587(2)	0.0713(10)
H7	0.7929	0.4883	0.6064	0.086*
C8	0.7328(5)	0.5982(2)	0.4770(2)	0.0560(7)
C9	0.6874(4)	0.6331(2)	0.3892(2)	0.0505(7)
C10	0.6638(5)	0.5607(3)	0.3195(2)	0.0645(9)
H10	0.6797	0.4871	0.3305	0.077*
C11	0.6181(6)	0.5975(3)	0.2363(2)	0.0784(10)
H11	0.6015	0.5489	0.1908	0.094*
C12	0.5959(6)	0.7083(3)	0.2186(3)	0.0858(12)
H12	0.5636	0.7326	0.1615	0.103*
C13	0.6210(5)	0.7801(3)	0.2842(3)	0.0789(11)
H13	0.6085	0.8534	0.2716	0.095*
C14	0.6659(5)	0.7457(2)	0.3714(2)	0.0595(8)
C15	0.6900(5)	0.8186(2)	0.4408(3)	0.0697(9)
H15	0.6761	0.8922	0.4294	0.084*
C16	0.7331(6)	0.7832(2)	0.5236(3)	0.0745(10)
H16	0.7481	0.8325	0.5686	0.089*
C17	0.7554(6)	0.6727(2)	0.5422(2)	0.0715(10)
H17	0.7860	0.6495	0.5995	0.086*
N1	0.8553(4)	0.3349(2)	0.73374(17)	0.0608(7)
N2	0.7547(5)	0.48626(19)	0.49209(18)	0.0784(10)
O1	0.8209(4)	0.08877(15)	0.44248(14)	0.0751(7)
H1	0.8025	0.1262	0.3989	0.113*
O2	0.8685(4)	0.2842(2)	0.80081(15)	0.0903(9)
O3	0.8545(5)	0.4327(2)	0.73294(17)	0.0969(9)

length is 1.154(4) Å, slightly shorther than in related structures [7, 8].

The molecular structure contains O—H···O type intermolecular and C—H···O and C—H···N type intramolecular H bonds. O1—H1···O2 (with symmetry code: x, $-y+1/2, +z-1/2$) creates an infinite chain along the c-axis and generates a C(8) motif [9]. S(6) and S(5) loops are created by the intramolecular H bonds C7—H7···O3 and C10—H10···N2, respectively [9]. There is also π-π stacking which contributes to stabilization between the ring centroids of Cg(1)—Cg(2) [distance between ring centroids is 3.695(2) Å with symmetry code: $1-x$, $1-y$, $1-z$ where Cg(1) belongs to the C1—C6 ring and Cg(2) to C8/C9/C14/C15/C16/C17].

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