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Yavuz Köysal*, Hakan Bülbül, Esen Nur Kantar, Emine Coşkun, Songül Şahin and Necmi Dege

Crystal structure of (*E*)-4-nitro-2-((2-phenoxyphenylimino)methyl)phenol, $C_{19}H_{14}N_2O_4$

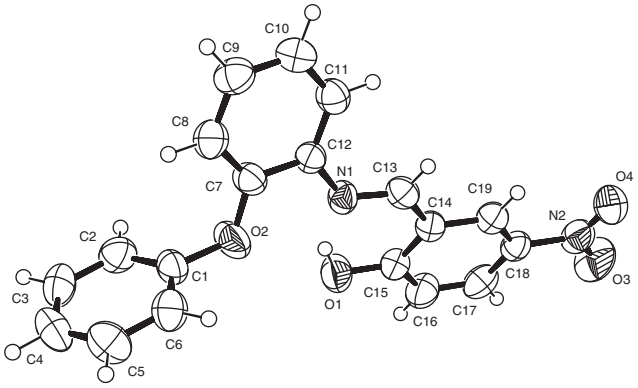

Table 1: Data collection and handling.

Crystal:	Yellow prism
	Size 0.75 × 0.31 × 0.04 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	1.0 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS-II, φ and ω
$2\theta_{max}$, completeness:	53°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	11984, 3354, 0.095
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1390
$N(param)_{refined}$:	230
Programs:	Stoe X-AREA [8], SHELX [9], ORTEP-3 [10], WinGX [11]

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Abstract

$C_{19}H_{14}N_2O_4$, monoclinic, $P2_1/c$ (no. 14), $a = 11.8219(12)$ Å, $b = 6.1210(4)$ Å, $c = 22.356(2)$ Å, $\beta = 94.403(8)°$, $V = 1612.9(3)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0545$, $wR_{ref}(F^2) = 0.0938$, $T = 293(2)$ K.

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

Source of material

The title compound (*E*)-4-nitro-2-((2-phenoxyphenylimino) methyl)phenol was prepared by reflux of a solution containing 2-hydroxy-5-nitrobenzaldehyde (0.157 g, 1.0 mmol) in 20 mL ethanol and a solution containing 2-aminophenylphenylether (2-phenoxyaniline) (0.185 g, 1.0 mmol) in 20 mL ethanol. The reaction mixture was stirred for 1 h under reflux. Crystals of the title compound were obtained from ethanol by slow evaporation (yield 63%, m.p. 433–435 K).

Experimental details

The structure was solved by direct methods and refined by full-matrix least-square techniques. The position of the H1 atom of the OH group was seen in difference Fourier map, and refined isotropically with an O—H bond length of 0.877 Å. All other H atoms were located geometrically and refined using a riding model fixing the aromatic C—H distance at 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic H atoms.

Discussion

Schiff base ligands have been mentioned in the context of many pharmacological activities such as antitumor, antibacterial, antitoxic properties [1]. It is also possible to Schiff bases according to their thermochromic and photochromic characteristics [2, 3].

Our crystallographic investigation shows that the molecule of the title compound, $C_{19}H_{14}N_2O_4$, exists in the phenol-imine tautomeric form in the solid state. Which means that the H atom is located on O1 instead of on N1 (*cf.* the figure). The moleculer structure is not planar. The dihedral angle between the rings C7/C12 and C1/C6 aromatic rings is 87.55(9)°, that shows these rings

***Corresponding author: Yavuz Köysal,** Yesilyurt Demir Celik, Vocational School, Ondokuz Mayıs University, TR-55139, Samsun, Turkey, e-mail: yavuzk@omu.edu.tr
Hakan Bülbül, Esen Nur Kantar and Necmi Dege: Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, TR-55139, Samsun, Turkey
Emine Coşkun and Songül Şahin: Department of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayıs University, TR-55139, Samsun, Turkey

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8047(2)	−0.0491(5)	0.73546(13)	0.0532(8)
C2	0.8420(2)	−0.2497(6)	0.71789(13)	0.0621(9)
H2	0.8287	−0.2952	0.6783	0.075*
C3	0.8991(3)	−0.3819(5)	0.75936(15)	0.0661(9)
H3	0.9238	−0.5189	0.7480	0.079*
C4	0.9201(2)	−0.3144(6)	0.81707(14)	0.0675(10)
H4	0.9605	−0.4038	0.8447	0.081*
C5	0.8818(3)	−0.1150(6)	0.83447(13)	0.0693(10)
H5	0.8951	−0.0702	0.8741	0.083*
C6	0.8238(2)	0.0188(5)	0.79365(13)	0.0618(9)
H6	0.7977	0.1543	0.8054	0.074*
C7	0.6372(2)	0.0844(5)	0.68109(12)	0.0506(8)
C8	0.5681(3)	−0.0624(5)	0.70749(12)	0.0592(8)
H8	0.5991	−0.1650	0.7347	0.071*
C9	0.4523(3)	−0.0558(5)	0.69308(12)	0.0617(9)
H9	0.4053	−0.1556	0.7105	0.074*
C10	0.4060(2)	0.0961(5)	0.65344(13)	0.0597(8)
H10	0.3280	0.1008	0.6444	0.072*
C11	0.4754(2)	0.2421(5)	0.62691(12)	0.0533(8)
H11	0.4439	0.3434	0.5995	0.064*
C12	0.5913(2)	0.2395(5)	0.64058(10)	0.0432(7)
C13	0.6365(2)	0.5610(5)	0.58892(11)	0.0496(8)
H13	0.5640	0.6133	0.5940	0.060*
C14	0.7114(2)	0.6874(5)	0.55480(11)	0.0443(7)
C15	0.8222(2)	0.6147(5)	0.54657(12)	0.0512(7)
C16	0.8903(3)	0.7376(6)	0.51046(14)	0.0660(9)
H16	0.9633	0.6905	0.5044	0.079*
C17	0.8499(3)	0.9259(5)	0.48426(13)	0.0633(9)
H17	0.8955	1.0066	0.4604	0.076*
C18	0.7414(3)	0.9977(5)	0.49297(12)	0.0494(8)
C19	0.6724(2)	0.8813(5)	0.52782(11)	0.0496(7)
H19	0.5998	0.9315	0.5335	0.060*
N1	0.66793(18)	0.3767(4)	0.61257(9)	0.0478(6)
N2	0.6998(3)	1.1973(4)	0.46373(11)	0.0639(8)
O1	0.86261(19)	0.4311(4)	0.57101(10)	0.0669(6)
O2	0.75297(17)	0.0946(4)	0.69292(9)	0.0776(7)
O3	0.7617(2)	1.2950(4)	0.43087(10)	0.0942(8)
O4	0.6041(2)	1.2610(4)	0.47294(10)	0.0769(7)
H1	0.806(3)	0.368(7)	0.5874(17)	0.15(2)*

are almost perpendicular to each other. The C14—C13—N1—C12 torsion angle is −172.9(2)°. The C13 = N1 and the C15—O1 bond distances are 1.288(3) Å and 1.323(3)Å, respectively. The obtained bond distances and angles are in expected normal ranges, and are consistent with our related structures [4–6].

O—H···N and C—H···O hydrogen bonds are observed in crystal packing. In the crystal, there is a weak intermolecular C—H···O hydrogen bond which create centrosymmetric dimers, namely C13—H13···O4 (symmetry code: $-x+1$, $-y+2$, $-z+1$) generates $R_2^2(14)$ ring motifs [7]. There is also a classical intramolecular O—H···N hydrogen-bond [d(N···O) = 2.569(3)Å] which forms an S(6) ring motif [7].

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