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Crystal structure of (*E*)-2-(1-((2-aminophenyl)imino)ethyl)-5-fluorophenol, C₁₄H₁₃FN₂O

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Abstract

C₁₄H₁₃FN₂O, orthorhombic, *Pna*2₁ (no. 33), *a* = 7.1841(6) Å, *b* = 23.3361(17) Å, *c* = 7.1672(5) Å, *V* = 1201.57(16) Å³, *Z* = 4, *R*_{gt}(*F*) = 0.0437, *wR*_{ref}(*F*²) = 0.1112, *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

1,2-Diaminobenzene (1 mmol, 0.108 g) and 1-(4-fluoro-2-hydroxyphenyl)ethan-1-one (1 mmol, 0.154 g) were added to ethanol (10 mL). The mixture was refluxed for 2 h. The solution was evaporated slowly at room temperature to obtain colorless prismatic crystals suitable for crystal structure determination.

Experimental details

The H atoms were positioned geometrically with *d*(C–H) = 0.93–0.98 Å and refined as riding with *U*_{iso}(H) = 1.2 *U*_{eq}(carrier) or 1.5 *U*_{eq}(methyl). Solving, refining and finish-

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.32 × 0.24 × 0.21 mm
Wavelength:	Mo Kα radiation (0.71073 Å)
μ:	0.10 mm ^{−1}
Diffraction, scan mode:	Bruker Apex-II, φ and ω
θ _{max} , completeness:	27.5°, >99%
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} , <i>R</i> _{int} :	18144, 2766, 0.033
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ(<i>I</i> _{obs}), 2368
<i>N</i> (<i>param</i>) _{refined} :	166
Programs:	Bruker [1], SHELX [2], Olex2 [3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
C1	−0.6188(4)	−0.17095(11)	−0.3810(4)	0.0518(6)
C2	−0.6659(3)	−0.17561(10)	−0.5641(4)	0.0477(6)
H2	−0.687284	−0.143010	−0.635573	0.057*
C3	−0.6815(3)	−0.22980(10)	−0.6429(3)	0.0396(5)
C4	−0.6500(3)	−0.27925(9)	−0.5331(3)	0.0393(5)
C5	−0.6033(3)	−0.27085(12)	−0.3452(3)	0.0495(6)
H5	−0.582862	−0.302766	−0.270252	0.059*
C6	−0.5864(4)	−0.21708(12)	−0.2673(4)	0.0569(7)
H6	−0.554256	−0.212316	−0.142603	0.068*
C7	−0.6622(3)	−0.33665(9)	−0.6148(3)	0.0400(5)
C8	−0.6417(4)	−0.38792(11)	−0.4923(4)	0.0589(7)
H8A	−0.653706	−0.422074	−0.566010	0.088*
H8B	−0.736710	−0.387390	−0.398180	0.088*
H8C	−0.521432	−0.387298	−0.433940	0.088*
C9	−0.6996(3)	−0.39396(10)	−0.8883(4)	0.0459(5)
C10	−0.5440(3)	−0.41322(9)	−0.9838(3)	0.0417(5)
C11	−0.5582(4)	−0.46375(10)	−1.0856(4)	0.0519(6)
H11	−0.454727	−0.477308	−1.149802	0.062*
C12	−0.7206(4)	−0.49380(11)	−1.0932(5)	0.0647(8)
H12	−0.727117	−0.527180	−1.163832	0.078*
C13	−0.8745(4)	−0.47522(14)	−0.9976(7)	0.0871(12)
H13	−0.984603	−0.496183	−1.000451	0.104*
C14	−0.8635(4)	−0.42496(13)	−0.8972(6)	0.0773(10)
H14	−0.968110	−0.411645	−0.834275	0.093*
F1	−0.6026(3)	−0.11741(8)	−0.3067(3)	0.0790(6)
N1	−0.6902(3)	−0.34021(8)	−0.7933(3)	0.0456(5)
N2	−0.3764(3)	−0.38399(10)	−0.9684(4)	0.0662(7)
H2A	−0.304602	−0.392806	−1.060204	0.079*
H2B	−0.398311	−0.347745	−0.970646	0.079*
O1	−0.7282(3)	−0.23307(7)	−0.8232(2)	0.0533(5)
H1	−0.721416	−0.266470	−0.858027	0.080*

ing of the crystal structure were finished by SHELX [2] and OLEX2 [3].

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Comment

Schiff bases are a class of important synthetic intermediates and they are being used as ligands to form coordination complexes with metal ions. Their complexes can be used for catalysis [4]. Mono-imine compounds are also key intermediates for the syntheses of unsymmetrical tetradentate Schiff base ligands [5]. Herein, we reported the crystal structure of a mono-imine.

The dihedral angle between the two rings (C1–C2–C3–C4–C5–C6 and C9–C10–C11–C12–C13–C14) is 86.39°, which is much larger than that (39.21°) derived from a similar crystal structure determination [6]. It means the two benzene rings are shown in an almost vertical position. The intramolecular O–H···N hydrogen bond stabilises the conformation of the title molecule (*cf.* the figure). The packing of crystal structure is dominated by van der Waals forces.

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