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The crystal structure of (*E*)-4-(1-(2-aminophenylimino)ethyl)benzene-1,3-diol, $C_{14}H_{14}N_2O_2$

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Abstract

$C_{14}H_{14}N_2O_2$, monoclinic, $P2_1/c$ (no. 14), $a = 8.5030(9)$ Å, $b = 7.6199(8)$ Å, $c = 18.738(2)$ Å, $\beta = 92.852(2)^\circ$, $V = 1212.6(2)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0413$, $wR_{ref}(F^2) = 0.1247$, $T = 296.15$ K.

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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.

Table 1: Data collection and handling.

Crystal:	Colourless needle
Size:	$0.25 \times 0.15 \times 0.09$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.09 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max} , completeness:	28.4° , $>99\%$
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	7366, 2970, 0.020
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 2383
$N(param)_{refined}$:	180
Programs:	Olex2 [1], SHELX [2, 3]

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}
C1	0.79910(13)	0.59584(15)	1.01473(6)	0.0321(3)
C2	0.78761(14)	0.41577(16)	1.02945(7)	0.0376(3)
H2A	0.726955	0.345826	0.998106	0.045*
C3	0.86199(15)	0.33831(16)	1.08811(7)	0.0378(3)
H3	0.850464	0.218784	1.096437	0.045*
C4	0.95506(14)	0.44140(16)	1.13504(6)	0.0330(3)
C5	0.96987(16)	0.61883(16)	1.12255(6)	0.0381(3)
H5	1.031008	0.687104	1.154339	0.046*
C6	0.89486(15)	0.69709(15)	1.06320(6)	0.0343(3)
C7	0.71626(14)	0.67686(17)	0.95268(6)	0.0350(3)
C8	0.61505(18)	0.5646(2)	0.90285(8)	0.0498(4)
H8A	0.561906	0.637629	0.867541	0.075*
H8B	0.538701	0.503428	0.929552	0.075*
H8C	0.679970	0.481192	0.879654	0.075*
C9	0.65313(15)	0.94195(17)	0.88857(7)	0.0393(3)
C10	0.49525(18)	0.9836(2)	0.89420(8)	0.0551(4)
H10	0.440789	0.939143	0.932044	0.066*
C11	0.41809(19)	1.0906(3)	0.84411(9)	0.0629(5)
H11	0.312110	1.117032	0.848096	0.075*
C12	0.4989(2)	1.1578(2)	0.78830(8)	0.0564(4)
H12	0.447421	1.230340	0.754739	0.068*
C13	0.65591(18)	1.11777(18)	0.78209(7)	0.0451(3)
H13	0.709297	1.163115	0.744081	0.054*
C14	0.73539(15)	1.01044(15)	0.83198(6)	0.0350(3)
N1	0.73652(13)	0.84319(14)	0.94306(5)	0.0388(3)
N2	0.89646(13)	0.96567(13)	0.82561(6)	0.0364(2)
H2B	0.9385(19)	1.024(2)	0.7886(9)	0.052(4)*
H2C	0.9538(19)	0.995(2)	0.8664(9)	0.052(4)*
O1	0.91717(13)	0.87011(12)	1.05285(5)	0.0483(3)
H1	0.858(2)	0.894(3)	1.0125(10)	0.093(7)*
O2	1.03401(12)	0.37421(12)	1.19388(4)	0.0433(2)
H2	1.053(2)	0.257(3)	1.1903(11)	0.078(6)*

Source of material

The title compound was prepared as described in literature [4, 5]: A mixture of *o*-phenylenediamine (1.08 g, 10 mmol) and 2,4-dihydroxyacetophenone (1.52 g, 10 mmol) in dry methanol (30 mL) was refluxed for 12 h to give a red solution. The solution was stored at room temperature for 3 days to give crystals suitable for single-crystal X-ray diffraction.

Experimental details

All the hydrogen atoms were positioned geometrically and treated as riding, with C–H = 0.93 Å (aromatic ring) and $U_{\text{iso}}(\text{H}) = 1.2$ times U_{eq} (C, aromatic ring), C–H = 0.96 Å (methyl) and $U_{\text{iso}}(\text{H}) = 1.5$ times U_{eq} (C, methyl).

Comment

Schiff bases can easily form stable complexes with various metal ions and play an important part in inorganic chemistry [6, 7]. Recently, Schiff bases of *o*-phenylenediamine have gained considerable attention due to their remarkable biological activities [8, 9], catalytic activities [10, 11] and fluorescence properties [12, 13]. The current research indicated unsymmetrical Schiff bases of *o*-phenylenediamine ligands could offer much greater diversity of metal-salen species with more flexible and tunable electronic and steric properties, thus their complexes might lead to a possibility for better biological activities and catalytic performances [5, 14]. However, the unsymmetrical Schiff bases of *o*-phenylenediamine ligands are less investigated for the challenge of synthesis. Herein, we reported the crystal structure of a mono-Schiff base compound (*E*)-4-(1-(2-aminophenylimino)ethyl)benzene-1,3-diol.

The title compound was prepared from *o*-phenylenediamine and 2,4-dihydroxyacetophenone, one of the amino groups of *o*-phenylenediamine reacted with the aldehyde group to form a double bond C7=N1, and the N1 atom forms a H-bond to the adjacent phenolic hydroxyl group to form an intramolecular hydrogen bond. Another amino group of *o*-phenylenediamine did not participate in the reaction, and the H atoms which link to N2 atom to form intermolecular hydrogen bonds with two O2 atoms and one O1 atom from three adjacent molecules to form a two-dimensional structure by weak N–H···O interactions.

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