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Crystal structure of 1-{4-[(2-hydroxy-5-nitrobenzylidene)amino]phenyl}ethanone O-methyl oxime, \( \text{C}_{16}\text{H}_{15}\text{N}_{3}\text{O}_{4} \)

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Abstract
\( \text{C}_{16}\text{H}_{15}\text{N}_{3}\text{O}_{4} \), monoclinic, \( P_{2}/c \) (no. 14), \( a = 6.4730(5) \, \text{Å}, b = 8.1564(6) \, \text{Å}, c = 27.511(2) \, \text{Å}, \beta = 90.113(2)° \), \( V = 1652.47(19) \, \text{Å}^3 \), \( Z = 4 \), \( R_{gt}(F) = 0.0623 \), \( wR_{ref}(F^2) = 0.1360 \), \( T = 153(2) \, \text{K} \).

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The 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
The title compound was prepared by modification of the reported method [4, 5]. 2-Hydroxy-5-nitrobenzaldehyde (167.2 mg, 1 mmol) dissolved in ethanol solution (4 mL) was added to 1-(4-aminophenyl)ethanone O-methyl oxime (164.2 mg, 1 mmol) dissolved in ethanol solution (4 mL). The solution had been stirred at 328 K. Sever hours later, the mixture was filtered at room temperature. The filtrate was allowed to stand for 16 days at room temperature by slow evaporation. Several block yellow crystals were obtained (yield 75.2%, m.p. 375–383 K). Anal. calcd. for \( \text{C}_{16}\text{H}_{15}\text{N}_{3}\text{O}_{4} \): C, 61.34%; H, 4.83%; N, 13.41%; Found: C, 61.52%; H, 4.95%; N, 13.37%.

Experimental details
Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment
Oxime-type compounds are also considered a very important class of organic molecules [4–7]. Various properties of oxime-type compounds along with their applications in some fields of chemistry increased interest. For example, some oxime from complexes [8–11], which are used as analytical reagents for the detection and determination of some metal ions. Other compounds represent nonlinear optical materials.

Table 1: Data collection and handling.

<table>
<thead>
<tr>
<th>Crystal:</th>
<th>Yellow block</th>
</tr>
</thead>
<tbody>
<tr>
<td>Size:</td>
<td>0.22 × 0.19 × 0.18 mm</td>
</tr>
<tr>
<td>Wavelength:</td>
<td>Mo Kα radiation (0.71073 Å)</td>
</tr>
<tr>
<td>𝜇:</td>
<td>0.11 mm⁻¹</td>
</tr>
<tr>
<td>Diffractometer, scan mode:</td>
<td>Bruker APEX2, ω</td>
</tr>
<tr>
<td>𝜃max, completeness:</td>
<td>26.0°, 97%</td>
</tr>
<tr>
<td>( N(hkl) \text{measured} ), ( N(hkl) \text{unique} ), ( R_{int} ):</td>
<td>10517, 2761, 0.051</td>
</tr>
<tr>
<td>Criterion for ( I_{obs} ), ( N(hkl) \text{gt} ):</td>
<td>( I_{obs} &gt; 2 \sigma(I_{obs}), 1994 )</td>
</tr>
<tr>
<td>( n(\text{param}) \text{refined} ):</td>
<td>211</td>
</tr>
<tr>
<td>Programs:</td>
<td>Bruker [1], Olex2 [2], SHELX [3]</td>
</tr>
</tbody>
</table>

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and many of them show supramolecular architectures [12–16].

The current work reports the synthesis of title compound. The title structure is built up by the C_{16}H_{13}N_{4}O_{4} molecules. All bond lengths are in normal ranges [4–6]. There is a strong intramolecular O1···H1···N2 hydrogen bond interaction (d(N2···H1) = 1.799 Å, d(O1···H1) = 0.84 Å and d(O1···N2) = 2.553 Å) in the title structure (cf. the figure).

References


8. Li, Q. L.; Li, P. P.; Ma, J. X.; Zhao, J. X.; Zhao, L.: Crystal structure of bis(2-(((E)-(E)-1-((methoxyimino)ethyl)phenyl)imino)methyl)phenolato-κ²N,N,Ozinc(II), C_{16}H_{14}N_{2}O_{5}Zn. Z. Kristallogr. NCS 233 (2018) 637–639.


