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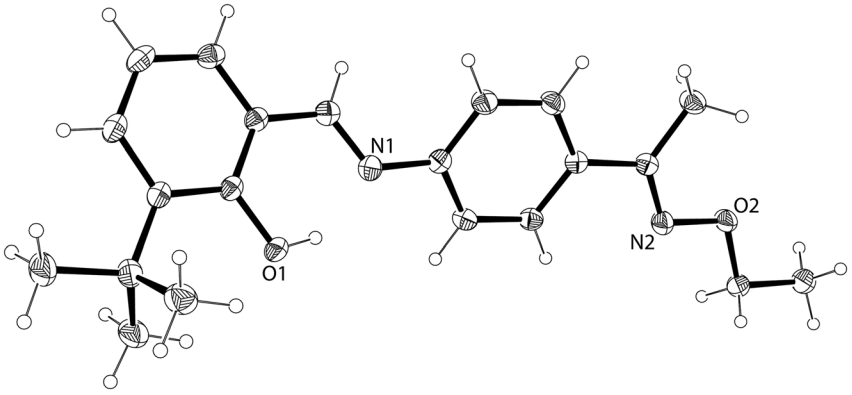
# Synthesis and crystal structure of (*E*)-1-(4-(((*E*)-3-(*tert*-butyl)-2-hydroxybenzylidene)amino)phenyl) ethan-1-one *O*-ethyl oxime, $C_{21}H_{26}N_2O_2$

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**Abstract**

$C_{21}H_{26}N_2O_2$, monoclinic, $P2_1$ (no. 4), $a$ = 7.1425(7) Å, $b$ = 9.2733(8) Å, $c$ = 14.3161(13) Å, $\beta$ = 93.592(4)°, $V$ = 946.36(15) Å$^3$, $Z$ = 2, $R_{gt}(F)$ = 0.0461, $wR_{ref}(F^2)$ = 0.1148, T = 173(2) K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Plate, yellow |
| Size: | 0.27 × 0.25 × 0.06 mm |
| Wavelength: | Mo *K*α radiation (0.71073 Å) |
| $\mu$: | 0.08 mm$^{-1}$ |
| Diffractometer, scan mode: | Bruker D8 venture, $\varphi$ and $\omega$-scans |
| $\theta_{max}$, completeness: | 27.9°, >99% |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 15067, 4486, 0.067 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 3423 |
| $N(param)_{refined}$: | 232 |
| Programs: | Bruker programs [1], SHELX [2], OLEX2 [3] |

## Source of material

The title compound was prepared by a method reported earlier [4, 5]. 3-*tert*–Butyl-2-hydroxy-benzaldehyde (178.23 mg, 1 mmol) dissolved in ethanol solution (5 mL) was added to 1-(4-aminophenyl)ethanone O-ethyl-oxime (178.21 mg, 1 mmol) dissolved in ethanol (5 mL) at 325 K. The mixture was kept stirring for 6 h. The mixture was cooled to room temperature and filtered. The filtrate was recrystallized and several clear yellow crystals were obtained.

## Experimental details

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

## Comment

Schiff base compounds are an important class of ligands in coordination chemistry. Schiff base transition metal complexes are attractive because of their show effective applications in various fields of scientific research. For

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | −0.0353 (3) | 0.5348 (2) | 0.22264 (13) | 0.0391 (5) |
| H1 | 0.025487 | 0.529506 | 0.274695 | 0.059* |
| N1 | 0.0338 (3) | 0.4763 (2) | 0.39732 (15) | 0.0350 (5) |
| C1 | −0.2662 (4) | 0.4364 (3) | 0.31892 (18) | 0.0311 (5) |
| O2 | 0.9063 (3) | 0.4935 (2) | 0.74170 (13) | 0.0410 (5) |
| N2 | 0.7603 (3) | 0.5106 (3) | 0.67280 (16) | 0.0395 (6) |
| C2 | −0.2126 (4) | 0.4882 (3) | 0.23149 (18) | 0.0303 (5) |
| C3 | −0.3403 (4) | 0.4909 (3) | 0.15240 (19) | 0.0316 (6) |
| C4 | −0.5195 (4) | 0.4379 (3) | 0.1643 (2) | 0.0384 (6) |
| H4 | −0.608369 | 0.437851 | 0.112034 | 0.046* |
| C7 | −0.2810 (4) | 0.5464 (3) | 0.05724 (19) | 0.0386 (6) |
| C6 | −0.4486 (4) | 0.3846 (3) | 0.3263 (2) | 0.0378 (6) |
| H6 | −0.485682 | 0.349011 | 0.384577 | 0.045* |
| C5 | −0.5743 (4) | 0.3848 (3) | 0.2497 (2) | 0.0426 (7) |
| H5 | −0.697889 | 0.349021 | 0.254794 | 0.051* |
| C8 | −0.4479 (5) | 0.5504 (4) | −0.0160 (2) | 0.0541 (9) |
| H8A | −0.406212 | 0.588232 | −0.075168 | 0.081* |
| H8B | −0.546358 | 0.612942 | 0.006301 | 0.081* |
| H8C | −0.497521 | 0.452717 | −0.025835 | 0.081* |
| C9 | −0.2055 (5) | 0.7008 (4) | 0.0657 (2) | 0.0531 (8) |
| H9A | −0.179243 | 0.736848 | 0.003538 | 0.080* |
| H9B | −0.089795 | 0.701546 | 0.106281 | 0.080* |
| H9C | −0.299236 | 0.762744 | 0.092765 | 0.080* |
| C10 | −0.1324 (5) | 0.4454 (4) | 0.0212 (2) | 0.0525 (8) |
| H10A | −0.099111 | 0.477382 | −0.040848 | 0.079* |
| H10B | −0.182307 | 0.347051 | 0.016990 | 0.079* |
| H10C | −0.020449 | 0.447125 | 0.064459 | 0.079* |
| C11 | −0.1353 (4) | 0.4311 (3) | 0.40019 (18) | 0.0340 (6) |
| H11 | −0.175716 | 0.393032 | 0.457150 | 0.041* |
| C12 | 0.1696 (4) | 0.4600 (3) | 0.47326 (17) | 0.0320 (6) |
| C13 | 0.1791 (4) | 0.3419 (3) | 0.53270 (19) | 0.0390 (7) |
| H13 | 0.084394 | 0.269874 | 0.527131 | 0.047* |
| C14 | 0.3259 (4) | 0.3281 (3) | 0.60030 (19) | 0.0378 (6) |
| H14 | 0.329210 | 0.247092 | 0.641016 | 0.045* |
| C15 | 0.4686 (4) | 0.4304 (3) | 0.60972 (17) | 0.0303 (5) |
| C16 | 0.4563 (4) | 0.5499 (3) | 0.54949 (17) | 0.0335 (6) |
| H16 | 0.550199 | 0.622488 | 0.554866 | 0.040* |
| C17 | 0.3101 (4) | 0.5634 (3) | 0.48277 (18) | 0.0349 (6) |
| H17 | 0.305259 | 0.644950 | 0.442505 | 0.042* |
| C18 | 0.6306 (4) | 0.4159 (3) | 0.67996 (18) | 0.0319 (6) |
| C19 | 0.6369 (4) | 0.2995 (3) | 0.75214 (19) | 0.0427 (7) |
| H19A | 0.566277 | 0.215654 | 0.727652 | 0.064* |
| H19B | 0.581134 | 0.334833 | 0.808626 | 0.064* |
| H19C | 0.767611 | 0.271685 | 0.767538 | 0.064* |
| C20 | 1.0450 (4) | 0.6024 (3) | 0.7285 (2) | 0.0403 (7) |
| H20A | 0.988715 | 0.699527 | 0.733019 | 0.048* |
| H20B | 1.095478 | 0.592274 | 0.666028 | 0.048* |
| C21 | 1.1987 (4) | 0.5828 (3) | 0.8037 (2) | 0.0452 (7) |
| H21A | 1.250590 | 0.485318 | 0.799812 | 0.068* |
| H21B | 1.147964 | 0.596494 | 0.865150 | 0.068* |
| H21C | 1.297892 | 0.653770 | 0.795363 | 0.068* |

example, these metal complexes are widely applied in ion recognition [6, 7] luminescence materials [8, 9] and supramolecular constructing [10, 11]. Recently, we have also investigated the title compound synthesis, structural characterization, and we predict that this compound can form stable complexes with transition metals [12].

The crystal structure of the title compound is shown in the figure. Compared with reported similar structures, all bond lengths and bond angles are within the normal ranges [4, 5, 13]. In the title compound, there is a strong intramolecular O1—H1···N1 hydrogen bond interaction ($d$(N1···H1) = 1.821 Å, $d$(O1—H1) = 0.840 Å and $d$(O1···N1) = 2.576 Å).

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**Conflict of interest statement:** The authors declare no conflicts of interest regarding this article.

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