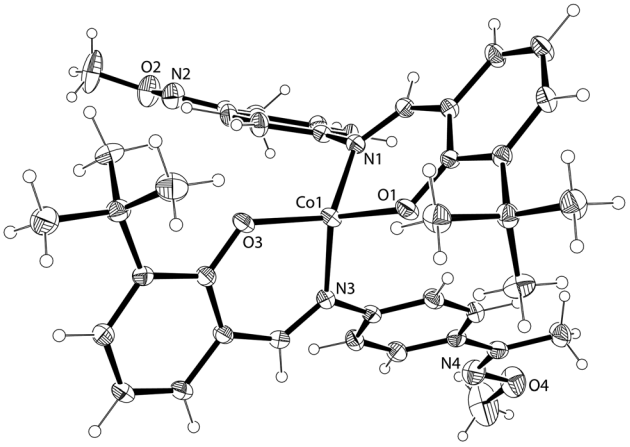
Ji-Xing Zhao*, Da-Qun Chen and Lei-Fang Wu

# Synthesis and crystal structure of bis{2-(*tert*-butyl)-6-((*E*)-((4-((*E*)-1-(methoxyimino) ethyl) phenyl)imino)methyl)phenolato-$\kappa^2N,O$}cobalt(II), $C_{40}H_{46}CoN_4O_4$

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**Abstract**

$C_{40}H_{46}CoN_4O_4$, monoclinic, $P2_1/n$ (no. 14), $a$ = 12.0084(5) Å, $b$ = 28.1263(10) Å, $c$ = 12.0351(5) Å, $\beta$ = 110.800(1)°, $V$ = 3800.0(3) Å$^3$, $Z$ = 4, $R_{gt}(F)$ = 0.0575, $wR_{ref}(F^2)$ = 0.1150, T = 173(2) K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

***Corresponding author: Ji-Xing Zhao**, Analysis and Testing Center, Shihezi University, Xinjiang, 832003, P.R. China,
E-mail: zhaojixing_2016@126.com. https://orcid.org/0000-0002-1322-1860
**Da-Qun Chen and Lei-Fang Wu,** Analysis and Testing Center, Shihezi University, Xinjiang, 832003, P.R. China

## 1 Source of material

The synthesis of the title complex was prepared using a similar method previously reported [4, 5], and its ligand has been synthesized and reported previously [6]. A methanol solution (2 mL) of the cobalt acetate tetrahydrate (49.8 mg, 0.2 mmol) was added dropwise to a dichloromethane solution (2 mL) of organic ligand (named (*E*)-1-(4-(((*E*)-3-(tert-butyl)-2-hydroxybenzylidene)amino)phenyl) ethan-1-one O-methyl oxime) (129.8 mg, 0.4 mmol). The mixture was kept stirring at room temperature for 1 h and then filtered. After the solvent in the filtrate slowly evaporates in a quiet environment for 22 days, several dark red block crystals were obtained.

## 2 Experimental details

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

## 3 Comment

The development of synthetic routes and strategies for Schiff base ligands and their transition metal complexes have potential application value due to their excellent performance in luminescent [7], bioscience [8], magnetic material

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

| | |
|---|---|
| Crystal: | Red block |
| Size: | 0.12 × 0.12 × 0.09 mm |
| Wavelength: | Mo *K*α radiation (0.71073 Å) |
| $\mu$: | 0.50 mm$^{-1}$ |
| Diffractometer, scan mode: | Bruker D8 Venture, $\varphi$ and $\omega$ |
| $\theta_{max}$, completeness: | 25.5°, >99 % |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 42,993, 7074, 0.097 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\sigma(I_{obs})$, 5052 |
| $N(param)_{refined}$: | 452 |
| Programs: | Bruker [1], SHELX [2, 3] |

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

| Atom | x | y | z | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Co1 | 0.71756 (4) | 0.40501 (2) | 0.28207 (4) | 0.03235 (13) |
| O1 | 0.83078 (19) | 0.35536 (8) | 0.33756 (18) | 0.0358 (6) |
| N1 | 0.7832 (2) | 0.44286 (9) | 0.4307 (2) | 0.0308 (6) |
| C1 | 0.9042 (3) | 0.34710 (11) | 0.4457 (3) | 0.0275 (7) |
| N2 | 0.4879 (3) | 0.63024 (11) | 0.4270 (3) | 0.0528 (9) |
| O2 | 0.4472 (2) | 0.67710 (10) | 0.4265 (3) | 0.0676 (9) |
| C2 | 0.9251 (3) | 0.38134 (11) | 0.5389 (3) | 0.0289 (7) |
| O3 | 0.55206 (19) | 0.39183 (8) | 0.21681 (18) | 0.0377 (6) |
| N3 | 0.7231 (2) | 0.43870 (9) | 0.1397 (2) | 0.0313 (6) |
| C3 | 1.0032 (3) | 0.37018 (12) | 0.6548 (3) | 0.0383 (8) |
| H3 | 1.017825 | 0.393122 | 0.716343 | 0.046* |
| C4 | 1.0577 (3) | 0.32711 (12) | 0.6797 (3) | 0.0413 (9) |
| H4 | 1.107797 | 0.319457 | 0.758466 | 0.050* |
| N4 | 1.1099 (3) | 0.58568 (12) | 0.1014 (3) | 0.0560 (9) |
| O4 | 1.2135 (3) | 0.60976 (11) | 0.1102 (3) | 0.0731 (9) |
| C5 | 1.0391 (3) | 0.29410 (12) | 0.5875 (3) | 0.0356 (8) |
| H5 | 1.078786 | 0.264317 | 0.605870 | 0.043* |
| C6 | 0.9664 (3) | 0.30264 (11) | 0.4718 (3) | 0.0293 (7) |
| C7 | 0.8691 (3) | 0.42689 (11) | 0.5238 (3) | 0.0307 (7) |
| H7 | 0.897875 | 0.448058 | 0.589304 | 0.037* |
| C8 | 0.9492 (3) | 0.26562 (11) | 0.3732 (3) | 0.0342 (8) |
| C9 | 1.0265 (3) | 0.22158 (13) | 0.4195 (3) | 0.0489 (10) |
| H9A | 1.013392 | 0.198832 | 0.354364 | 0.073* |
| H9B | 1.005028 | 0.206803 | 0.482830 | 0.073* |
| H9C | 1.110628 | 0.230873 | 0.450853 | 0.073* |
| C10 | 0.8188 (3) | 0.24952 (13) | 0.3252 (3) | 0.0454 (9) |
| H10A | 0.767469 | 0.276809 | 0.290626 | 0.068* |
| H10B | 0.797458 | 0.236259 | 0.390237 | 0.068* |
| H10C | 0.808140 | 0.225184 | 0.263974 | 0.068* |
| C11 | 0.9853 (4) | 0.28704 (13) | 0.2733 (3) | 0.0501 (10) |
| H11A | 0.976014 | 0.263011 | 0.211662 | 0.075* |
| H11B | 1.068630 | 0.297361 | 0.305914 | 0.075* |
| H11C | 0.934267 | 0.314401 | 0.238595 | 0.075* |
| C12 | 0.7410 (3) | 0.48988 (11) | 0.4359 (3) | 0.0305 (7) |
| C16 | 0.5760 (3) | 0.54161 (12) | 0.4146 (3) | 0.0386 (8) |
| H16 | 0.493263 | 0.545545 | 0.399154 | 0.046* |
| C15 | 0.6501 (3) | 0.58150 (11) | 0.4413 (3) | 0.0304 (7) |
| C14 | 0.7704 (3) | 0.57423 (12) | 0.4648 (3) | 0.0367 (8) |
| H14 | 0.822900 | 0.600718 | 0.483033 | 0.044* |
| C13 | 0.8158 (3) | 0.52893 (12) | 0.4624 (3) | 0.0357 (8) |
| H13 | 0.898711 | 0.524793 | 0.478966 | 0.043* |
| C18 | 0.6010 (3) | 0.62976 (12) | 0.4417 (3) | 0.0369 (8) |
| C17 | 0.6199 (3) | 0.49680 (12) | 0.4101 (3) | 0.0383 (8) |
| H17 | 0.567114 | 0.470423 | 0.389131 | 0.046* |
| C19 | 0.6774 (3) | 0.67257 (13) | 0.4573 (4) | 0.0512 (10) |
| H19A | 0.710436 | 0.673802 | 0.393623 | 0.077* |
| H19B | 0.742638 | 0.671023 | 0.534405 | 0.077* |
| H19C | 0.629706 | 0.701152 | 0.454047 | 0.077* |
| C20 | 0.3255 (4) | 0.67373 (18) | 0.4210 (6) | 0.103 (2) |
| H20A | 0.279619 | 0.654222 | 0.352544 | 0.154* |
| H20B | 0.290592 | 0.705623 | 0.412530 | 0.154* |
| H20C | 0.323514 | 0.659041 | 0.494107 | 0.154* |
| C21 | 0.4839 (3) | 0.39238 (11) | 0.1041 (3) | 0.0288 (7) |
| C22 | 0.5216 (3) | 0.41398 (11) | 0.0158 (3) | 0.0299 (7) |
| C23 | 0.4448 (3) | 0.41370 (12) | −0.1047 (3) | 0.0344 (8) |
| H23 | 0.470372 | 0.427992 | −0.163040 | 0.041* |
| C24 | 0.3356 (3) | 0.39346 (12) | −0.1382 (3) | 0.0367 (8) |
| H24 | 0.285062 | 0.393197 | −0.219442 | 0.044* |
| C25 | 0.2981 (3) | 0.37284 (12) | −0.0511 (3) | 0.0347 (8) |
| H25 | 0.220858 | 0.359088 | −0.075420 | 0.042* |
| C26 | 0.3676 (3) | 0.37154 (11) | 0.0680 (3) | 0.0291 (7) |
| C27 | 0.6335 (3) | 0.43681 (12) | 0.0393 (3) | 0.0333 (8) |
| H27 | 0.644141 | 0.452545 | −0.026085 | 0.040* |
| C28 | 0.3215 (3) | 0.34917 (12) | 0.1593 (3) | 0.0373 (8) |
| C29 | 0.1956 (3) | 0.32845 (15) | 0.1007 (4) | 0.0566 (11) |
| H29A | 0.139955 | 0.354019 | 0.061896 | 0.085* |
| H29B | 0.170535 | 0.313458 | 0.161515 | 0.085* |
| H29C | 0.196135 | 0.304665 | 0.041399 | 0.085* |
| C30 | 0.4030 (4) | 0.30833 (14) | 0.2260 (3) | 0.0552 (11) |
| H30A | 0.403147 | 0.283255 | 0.169520 | 0.083* |
| H30B | 0.373494 | 0.295356 | 0.285966 | 0.083* |
| H30C | 0.484171 | 0.320330 | 0.265033 | 0.083* |
| C32 | 0.8250 (3) | 0.46589 (11) | 0.1427 (3) | 0.0311 (7) |
| C31 | 0.3138 (4) | 0.38759 (14) | 0.2471 (3) | 0.0517 (10) |
| H31A | 0.264431 | 0.413992 | 0.203056 | 0.078* |
| H31B | 0.393958 | 0.399291 | 0.292592 | 0.078* |
| H31C | 0.278091 | 0.374001 | 0.301621 | 0.078* |
| C33 | 0.8138 (3) | 0.50891 (12) | 0.0829 (3) | 0.0359 (8) |
| H33 | 0.736902 | 0.520793 | 0.037797 | 0.043* |
| C34 | 0.9134 (3) | 0.53434 (12) | 0.0888 (3) | 0.0365 (8) |
| H34 | 0.904352 | 0.563439 | 0.046427 | 0.044* |
| C35 | 1.0275 (3) | 0.51834 (12) | 0.1556 (3) | 0.0341 (8) |
| C36 | 1.0372 (3) | 0.47548 (12) | 0.2157 (3) | 0.0366 (8) |
| H36 | 1.114049 | 0.463657 | 0.261113 | 0.044* |
| C37 | 0.9377 (3) | 0.44966 (12) | 0.2109 (3) | 0.0368 (8) |
| H37 | 0.946524 | 0.420807 | 0.254215 | 0.044* |
| C38 | 1.1336 (3) | 0.54672 (13) | 0.1625 (3) | 0.0394 (8) |
| C39 | 1.2553 (3) | 0.53074 (15) | 0.2361 (3) | 0.0542 (11) |
| H39A | 1.281157 | 0.505749 | 0.193901 | 0.081* |
| H39B | 1.254751 | 0.518232 | 0.311917 | 0.081* |
| H39C | 1.310451 | 0.557693 | 0.251168 | 0.081* |
| C40 | 1.1772 (5) | 0.65269 (19) | 0.0409 (6) | 0.118 (3) |
| H40A | 1.124380 | 0.644540 | −0.039794 | 0.177* |
| H40B | 1.247710 | 0.669216 | 0.037409 | 0.177* |
| H40C | 1.134834 | 0.673443 | 0.078032 | 0.177* |

[9] and supramolecular structure construction [10, 11] and so on. Schiff base ligands can form stable mononuclear, binuclear, and multinuclear complexes with transition metal ions [12–14].

We report in this article that a new cobalt (II) complex has been prepared. The single crystal structure of the title complex has been characterized by X-ray crystallography (cf. the figure). In the title complex, Co1 is in $N_2O_2$ coordination environment and displays a four-coordinated tetrahedral geometry by two oxygen atoms (O1 and O3) and two nitrogen atoms (N1 and N3) from different ligands. The

Co1–N1 bond length is 1.989(3) Å and the Co1–N3 is 1.980(3) Å. The Co1–O1 bond length is 1.897(2) Å and the Co1–O3 is 1.896(2) Å. The angle of O1–Co1–N1 is 94.11(10)°, O3–Co1–N1 is 119.98(10)°, O1–Co1–N3 is 114.64(11)° and O1–Co1–O3 is 121.10(10)°, respectively. All bond lengths and bond angles are within the normal ranges [14].

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**Competing interests:** The authors declare no conflicts of interest regarding this article.

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