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The crystal structure of acetato- $\kappa^1 O$ -{(2-(2-(2-aminophenoxy)ethoxy)phenyl)(4-oxo-4-phenylbut-2-en-2-yl)amido- $\kappa^2 N, N', O$ }copper(II), $C_{26}H_{26}CuN_2O_5$

Table 1: Data collection and handling.

Crystal:	Brown block
Size:	0.24 × 0.21 × 0.20 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.96 mm ⁻¹
Diffractometer, scan mode:	Bruker Apex-II, φ and ω
$\theta_{\max}$, completeness:	25.0°, 98 %
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	12593, 4121, 0.025
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3696
$N(\text{param})_{\text{refined}}$:	307
Programs:	Bruker [1], SHELX [2], Olex2 [3]

$\gamma = 100.180(2)^\circ$, $V = 1185.95(11) \text{ \AA}^3$, $Z = 2$, $R_{\text{gt}}(F) = 0.0315$, $wR_{\text{ref}}(F^2) = 0.0869$, $T = 293 \text{ K}$.

CCDC no.: 2047023

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.

Source of material

To the solution of (Z)-3-((2-(2-(2-aminophenoxy)ethoxy)phenyl)amino)-1-phenylbut-2-en-1-one (0.388 g 1 mmol) in chloroform (20 ml) was added the solution of $\text{Cu}(\text{AcO})_2$ (0.182 g, 1 mmol) in chloroform (20 ml) dropwisely. The mixture was stirred for 72 h to get a blue solution and then filtered. The filter residue was washed with methanol 3 times and recrystallized in chloroform to get crystals (0.31 g, yield 60.6%).

Experimental details

The data were scaled and corrected for absorption using SADABS-2016/2 (Bruker, APEX-II CCD). The hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters.

<https://doi.org/10.1515/ncrs-2021-0048>

Received February 2, 2021; accepted February 18, 2021;
published online March 4, 2021

Abstract

$C_{26}H_{26}CuN_2O_5$, triclinic, $P = \bar{1}$ (no. 2), $a = 8.8090(5) \text{ \AA}$, $b = 11.4984(6) \text{ \AA}$, $c = 12.3941(7) \text{ \AA}$, $\alpha = 90.11^\circ$, $\beta = 106.017(2)^\circ$,

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

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
C1	0.3724 (3)	0.27677 (19)	−0.26402 (17)	0.0288 (5)
C2	0.4435 (3)	0.2239 (2)	−0.3336 (2)	0.0408 (6)
H2	0.5469	0.2086	−0.3045	0.049*
C3	0.3623 (3)	0.1934 (3)	−0.4459 (2)	0.0517 (7)
H3	0.4104	0.1567	−0.4910	0.062*
C4	0.2100 (3)	0.2178 (3)	−0.4904 (2)	0.0515 (7)
H4	0.1554	0.1978	−0.5656	0.062*
C5	0.1401 (3)	0.2717 (3)	−0.4232 (2)	0.0520 (7)
H5	0.0380	0.2890	−0.4534	0.062*
C6	0.2192 (3)	0.3008 (2)	−0.3109 (2)	0.0409 (6)
H6	0.1695	0.3367	−0.2663	0.049*
C7	0.4608 (3)	0.30131 (18)	−0.14125 (17)	0.0273 (5)
C8	0.3926 (3)	0.35165 (18)	−0.06931 (17)	0.0278 (5)
H8	0.3030	0.3851	−0.1017	0.033*
C9	0.4477 (3)	0.35678 (17)	0.05037 (17)	0.0261 (5)
C10	0.3326 (3)	0.3918 (2)	0.10953(18)	0.0319 (5)
H10A	0.2404	0.4103	0.0549	0.048*
H10B	0.2990	0.3275	0.1520	0.048*
H10C	0.3852	0.4600	0.1594	0.048*
C11	0.6218 (3)	0.31172 (19)	0.22398 (17)	0.0290 (5)
C12	0.6331 (3)	0.4002 (2)	0.3035 (2)	0.0403 (6)
H12	0.6131	0.4742	0.2803	0.048*
C13	0.6736 (3)	0.3797 (3)	0.4172 (2)	0.0483 (7)
H13	0.6802	0.4396	0.4697	0.058*
C14	0.7041 (3)	0.2706 (3)	0.45208 (19)	0.0469 (7)
H14	0.7285	0.2564	0.5282	0.056*
C15	0.6987 (3)	0.1818 (2)	0.3750 (2)	0.0413 (6)
H15	0.7222	0.1089	0.3993	0.050*
C16	0.6579 (3)	0.2021 (2)	0.26071 (17)	0.0306 (5)
C17	0.7410 (3)	0.0291 (2)	0.2055 (2)	0.0422 (6)
H17A	0.6937	−0.0294	0.2489	0.051*
H17B	0.8500	0.0620	0.2490	0.051*
C18	0.7398 (3)	−0.0256 (2)	0.0951 (2)	0.0398 (6)
H18A	0.7969	−0.0914	0.1069	0.048*
H18B	0.6306	−0.0540	0.0495	0.048*
C19	0.8134 (3)	0.05116 (19)	−0.06852 (18)	0.0309 (5)
C20	0.7568 (3)	−0.0542 (2)	−0.1327 (2)	0.0390 (6)
H20	0.7188	−0.1229	−0.1013	0.047*
C21	0.7576 (3)	−0.0560 (2)	−0.2444 (2)	0.0468 (6)
H21	0.7200	−0.1265	−0.2881	0.056*
C22	0.8129 (3)	0.0447 (2)	−0.2913 (2)	0.0464 (6)
H22	0.8128	0.0422	−0.3663	0.056*
C23	0.8695 (3)	0.1508 (2)	−0.22662 (19)	0.0369 (5)
H23	0.9070	0.2192	−0.2584	0.044*
C24	0.8698 (2)	0.15418 (19)	−0.11510 (18)	0.0286 (5)
C25	0.9836 (2)	0.44472 (19)	0.19143 (17)	0.0279 (5)
C26	1.1113 (3)	0.4787 (3)	0.3018 (2)	0.0497 (7)
H26A	1.1333	0.4086	0.3403	0.075*
H26B	1.2077	0.5207	0.2877	0.075*
H26C	1.0741	0.5284	0.3474	0.075*
N1	0.5848 (2)	0.32681 (15)	0.10547 (14)	0.0266 (4)
N2	0.9184 (2)	0.26092 (15)	−0.04383 (14)	0.0288 (4)
H2A	0.9417	0.3214	−0.0848	0.035*
H2B	1.0080	0.2555	0.0094	0.035*
O1	0.59839 (18)	0.26859 (14)	−0.11157 (12)	0.0343 (4)

Table 2: (continued)

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
O2	0.64757 (19)	0.12037 (13)	0.17772 (12)	0.0341 (4)
O3	0.8192 (2)	0.06715 (13)	0.04194 (12)	0.0362 (4)
O4	0.92797 (18)	0.33458 (13)	0.17032 (12)	0.0314 (3)
O5	0.93758 (19)	0.52259 (14)	0.12852 (13)	0.0366 (4)
Cu1	0.74970 (3)	0.29810 (2)	0.03286 (2)	0.02622 (11)

Comment

Enaminones can be synthesized by condensation reaction of diketone and primary amine [4]. Their group IV metal complexes were not only used as alternatives to metallocene catalysts but also used in the field of optoelectronic technologies for their large nonlinear responses [5, 6]. So, the synthesis and property research of novel enaminone complexes were an important orientation in inorganic chemistry [7, 8]. The molecular structure of the title compound was determined by X-ray single crystal diffraction. There is one complex in the asymmetric unit (see the figure). The bond length of C7–O1, C9–N1 and C1–C2 are 1.289(3), 1.318(3) and 1.392(3) Å respectively, which are in the normal range [9]. Copper was centered in a distorted tetragonal planar coordination geometry. The sum of the bond angles of O1–Cu1–N1, O1–Cu1–N2, O1–Cu1–O4 and O4–Cu1–N1 are 360.13°, which demonstrated that O1, Cu1, N1, O2 and N1 are in the same plane.

Author contribution: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Research funding: National Key R&D program of China (2018YFC1706903), Key projects of Shaanxi Provincial Education Department (20JS033).

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

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