Structure of [Cu(tssb)(phen)H₂O]·C₂H₅OH·0.5H₂O (H₂tssb = Schiff Base Derived from Salicylaldehyde and Taurine, phen = 1,10-Phenanthroline)

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A new complex, [Cu(tssb)(phen)H₂O]·C₂H₅OH·0.5H₂O, crystallizes in the triclinic, space group $P\bar{1}$ with cell parameters $a = 10.593(2)$, $b = 11.600(2)$, $c = 21.170(4)$ Å, $\alpha = 103.340(4)^\circ$, $\beta = 96.937(4)^\circ$, $\gamma = 105.056(3)^\circ$, $Z = 4$, $V = 2398.9(7)$ Å³. Its crystal structure was determined and refined to a final $R = 0.0468$ for 10894 independent reflections. The Cu(II) ion forms a distorted octahedral geometry by one nitrogen atom and two oxygen atoms from tssb, two nitrogen atoms from phen and one oxygen atom from water.

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Schiff-base complexes containing sulfur and complexes of amino acid Schiff-bases¹ have recently aroused increasing interest because of their antiviral, anticancer and antibacterial activities. Taurine, an amino acid containing sulfur, is indispensable to human beings, and has important physiological functions. Recently, we have found that the Schiff-base derived from taurine has manifold coordination modes.² Aromatic-ring stacking interaction is an important characteristic of ternary complex, and has important functions in organism, such as stabilizing the double-helical structure³ and the interactions between anticancer drugs and DNA.⁴ Herein we chose H₂tssb, phen and Cu(Ac)₂·4H₂O to synthesize a new compound, [Cu(tssb)(phen)H₂O]·C₂H₅OH·0.5H₂O (see Fig. 1). The crystal structure of the title compound was determined using BRUKER SMART 1000 CCD. The experimental conditions, crystal data and structure refinement results are summarized in Table 1; atomic coordinates and equivalent isotropic displacement parameters are listed in Table 2.

As shown in Fig. 2(a), the crystal contains two crystallographically independent discrete molecules. The Cu(II) ion forms a distorted octahedral geometry by one nitrogen atom and two oxygen atoms from tssb²⁻, two nitrogen atoms from phen and one oxygen atom from terminal water, with O(1) and O(2) at the apical positions. The inter-atomic distances of Cu(1)–O(1), Cu(1)–N(1), Cu(1)–N(2), Cu(1)–O(2), Cu(1)–N(3) and Cu(1)–O(1W) are 2.006(2), 2.101(3), 2.101(2), 2.139(2), 2.042(3) and 2.072(2) Å, respectively. Similar values have been observed in Cu(II) complex of salicylaldehyde Schiff-base.² As expected, all other bond distances and bond angles are within the normal ranges, in good agreement with those of other taurine-containing complexes.^{1–3} The coordination of Cu(2) is similar to that of Cu(1), but the corresponding bond lengths are slightly different (Cu(2)–O(5) 2.2004(2) Å, Cu(2)–N(4) 2.093(3) Å, Cu(2)–O(2W) 2.121(2) Å, Cu(2)–N(5) 2.093(3) Å, Cu(2)–N(6) 2.049(2) Å and Cu(2)–O(6) 2.097(2) Å). The complex is linked by hydrogen bonds and

aromatic-ring stacking forming a three-dimensional structure (see Table 3 and Fig. 2(b)).

Fig. 1 Chemical diagram of the title compound.

Table 1 Crystal and experimental data

CCDC	612502
Formula	C ₂₃ H ₂₆ CuN ₃ O _{6.50} S
Formula weight	544.07
Crystal system	triclinic
Space group	$P\bar{1}$, $Z = 4$
$a = 10.593(2)$ Å	$\alpha = 103.340(4)^\circ$
$b = 11.600(2)$ Å	$\beta = 96.937(4)^\circ$
$c = 21.170(4)$ Å	$\gamma = 105.056(3)^\circ$
$V = 2398.9(7)$ Å ³	$D_c = 1.506$ g cm ⁻³
Linear absorption factor	1.044 mm ⁻¹
$F(0\ 0\ 0) = 1128$	$(\Delta\rho)_{\max} = 0.01$
θ range for data collection	1.01 to 27.5°
No. of reflections used with $I > 2\sigma(I)$	7921
No. of measured reflections	16295 ($R_{\text{int}} = 0.0186$)
$R_1 [I > 2\sigma(I)] = 0.0468$	$wR_2 = 0.1450$
$\Delta\rho_{\max} = 0.940$ e Å ⁻³	$\Delta\rho_{\min} = -0.497$ e Å ⁻³
Crystal dimensions [mm]	0.38 × 0.36 × 0.32
Measurement	BRUKER SMART 1000 CCD
Mo K_α	$\lambda = 0.71073$ Å
Structure determination	direct methods (SHELXS-97) ⁵
Refinement	full matrix least-squares (SHELXL-97) ⁵

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Table 2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for the title compound

Atom	x	y	z	$U(\text{eq})^a$
Cu(1)	815(1)	1477(1)	3304(1)	30(1)
S(1)	-915(1)	3113(1)	2706(1)	36(1)
O(1W)	138(2)	71(2)	2428(1)	40(1)
O(1)	2219(2)	702(2)	3554(1)	35(1)
O(2)	-802(2)	2172(2)	3049(1)	40(1)
O(3)	-1615(3)	3927(3)	3030(1)	57(1)
O(4)	-1463(3)	2564(3)	2004(1)	59(1)
N(1)	1161(3)	2758(3)	4235(1)	35(1)
N(2)	-466(2)	437(2)	3790(1)	34(1)
N(3)	2101(2)	2651(2)	2923(1)	31(1)
C(1)	1978(4)	3888(4)	4449(2)	53(1)
C(2)	2041(5)	4705(4)	5068(2)	70(1)
C(3)	1199(5)	4311(4)	5461(2)	64(1)
C(4)	342(4)	3087(4)	5266(2)	50(1)
C(5)	-494(4)	2553(5)	5667(2)	63(1)
C(6)	-1234(4)	1373(5)	5463(2)	62(1)
C(7)	-1280(3)	591(4)	4825(2)	48(1)
C(8)	-2028(3)	-659(4)	4583(2)	56(1)
C(9)	-1986(4)	-1323(4)	3968(3)	60(1)
C(10)	-1194(3)	-743(3)	3574(2)	45(1)
C(11)	-497(3)	1094(3)	4401(2)	35(1)
C(12)	345(3)	2343(3)	4635(2)	35(1)
C(13)	3505(3)	1237(3)	659(2)	32(1)
C(14)	4372(3)	740(3)	3992(2)	42(1)
C(15)	5738(3)	1207(4)	4081(2)	49(1)
C(16)	6313(3)	2207(4)	3855(2)	49(1)
C(17)	5505(3)	2736(3)	3536(2)	42(1)
C(18)	4102(3)	2279(3)	3432(2)	33(1)
C(19)	3364(3)	2842(3)	3037(2)	33(1)
C(20)	1610(3)	3295(3)	2471(2)	40(1)
C(21)	720(3)	4042(3)	2761(2)	41(1)
Cu(2)	2554(1)	-1829(1)	1863(1)	36(1)
S(2)	4258(1)	-3794(1)	1952(1)	45(1)
O(2W)	-2008(2)	-1705(2)	2802(1)	42(1)
O(5)	2076(2)	-296(2)	1790(1)	37(1)
O(6)	3023(2)	-3440(2)	1951(1)	49(1)
O(7)	4306(4)	-4584(3)	1331(2)	72(1)
O(8)	4486(3)	-4292(3)	2511(2)	60(1)
O(9)	-2206(3)	-34(4)	1595(2)	86(1)
O(10)	3261(3)	-3166(4)	3521(2)	83(1)
N(4)	600(3)	-2902(3)	1411(2)	45(1)
N(5)	2714(3)	-2152(3)	866(1)	40(1)
N(6)	4489(3)	-779(2)	2253(1)	33(1)
C(22)	-411(4)	-3292(4)	1687(2)	62(1)
C(23)	-1704(4)	-3953(5)	1301(3)	83(2)
C(24)	-1896(5)	-4181(5)	630(3)	80(2)
C(25)	-847(4)	-3789(4)	329(2)	62(1)
C(26)	-943(6)	-3993(5)	-377(3)	79(2)
C(27)	97(6)	-3605(5)	-639(2)	78(2)
C(28)	1391(5)	-2954(4)	-238(2)	59(1)
C(29)	2524(6)	-2539(5)	-484(2)	72(1)
C(30)	3728(5)	-1939(5)	-71(2)	66(1)
C(31)	3778(4)	-1764(4)	605(2)	50(1)
C(32)	1525(4)	-2739(3)	449(2)	43(1)
C(33)	406(4)	-3145(3)	742(2)	48(1)
C(34)	2887(3)	615(3)	1644(2)	34(1)
C(35)	2392(4)	1323(4)	1276(2)	46(1)
C(36)	3212(4)	2354(4)	1156(2)	55(1)
C(37)	4568(4)	2726(4)	1380(2)	54(1)
C(38)	5104(4)	2041(3)	1723(2)	44(1)
C(39)	4300(3)	971(3)	1846(2)	34(1)
C(40)	4984(3)	311(3)	2195(2)	35(1)
C(41)	5410(3)	-1300(3)	2589(2)	42(1)
C(42)	5598(4)	-2399(3)	2110(2)	48(1)
C(43)	-2373(8)	-477(9)	903(3)	136(3)
C(44)	-1251(9)	-456(12)	649(2)	197(6)
C(45)	4153(6)	-2748(6)	4136(3)	96(2)
C(46)	4914(5)	-3532(5)	4293(3)	87(2)
O(3W)	7256(5)	-4159(4)	2849(3)	111(2)

a. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Acknowledgments

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Table 3 Hydrogen bond lengths ($\text{\AA}$) and bond angles ($^\circ$) of the title compound

D-H...A	D-H	H-A	D...A	DHA
O(3W)-H(3WA)...O(3) ^a	0.68(7)	2.18(7)	2.857(5)	172(8)
O(3W)-H(3WB)...O(8)	1.16(9)	2.16(9)	2.891(6)	118(6)
O(1W)-H(1WA)...O(5)	0.82	2.12	2.660(3)	123.5
O(1W)-H(1WB)...O(9)	0.83	2.00	2.825(4)	175.8
O(2W)-H(2WA)...O(1)	0.82	2.48	2.815(3)	105.7

a. Symmetry code: $x+1, y-1, z$.

Fig. 2 (a) ORTEP structure of the title compound with atom labeling. The hydrogen atoms are omitted for clarity. (b) Packing diagram of the title compound showing the intermolecular hydrogen bonds and π - π stacking.

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