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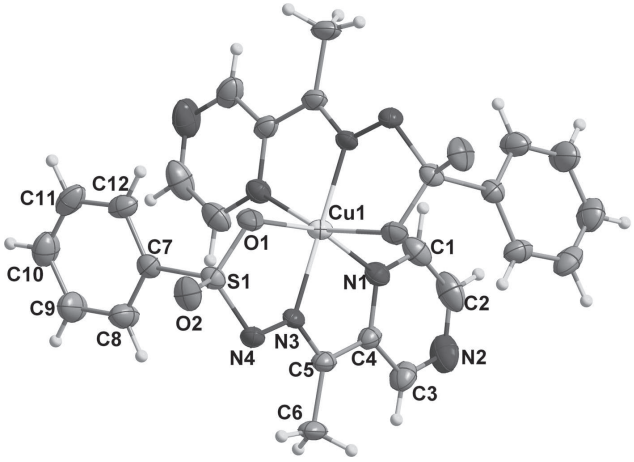
# Crystal Structure of bis(1-(phenylsulfonyl)-2-(1-(pyrazin-2-yl)ethylidene)hydrazin-1-ido-κ$^3$*N*,*N*′,*O*) copper(II), $C_{24}H_{22}N_8O_4S_2Cu$

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## Abstract

$C_{24}H_{22}N_8O_4S_2Cu$, orthorhombic, *Aba*2 (no. 41), $a = 11.9395(18)$ Å, $b = 21.813(3)$ Å, $c = 10.1184(15)$ Å, $V = 2635.2(7)$ Å$^3$, $Z = 4$, $R_{gt}(F) = 0.0395$, $wR_{ref}(F^2) = 0.0912$, $T = 296(2)$ 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

Benzenesulfonyl hydrazide (0.172 g, 1 mmol) and 2-acetopyrazine (0.122 g, 1 mmol) was dissolved in methanol (20 mL). The reaction mixture was refluxed for 1 h and cooled to room temperature. Then copper(II) acetate

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

| | |
|---|---|
| Crystal: | Black block |
| Size: | 0.25 × 0.22 × 0.20 mm |
| Wavelength: | Mo *Kα* radiation (0.71073 Å) |
| $\mu$: | 1.03 mm$^{-1}$ |
| Diffractometer, scan mode: | Bruker APEX-II, $\varphi$ and $\omega$-scans |
| $\theta_{max}$, completeness: | 25°, >99% |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 6422, 2232, 0.050 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\,\sigma(I_{obs})$, 1760 |
| $N(param)_{refined}$: | 177 |
| Programs: | Bruker programs [1], SHELX [2] |

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

| Atom | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.000000 | 0.000000 | 0.88844(12) | 0.0392(3) |
| S1 | −0.10368(13) | −0.10302(7) | 0.72978(17) | 0.0442(4) |
| N1 | −0.0668(5) | 0.0603(3) | 1.0362(5) | 0.0482(14) |
| N2 | −0.1941(8) | 0.1324(3) | 1.2044(8) | 0.089(3) |
| N3 | −0.1611(4) | −0.0201(2) | 0.8778(6) | 0.0395(12) |
| N4 | −0.2023(4) | −0.0604(2) | 0.7845(6) | 0.0447(14) |
| O1 | 0.0036(3) | −0.0704(2) | 0.7304(5) | 0.0532(13) |
| O2 | −0.1389(5) | −0.1284(2) | 0.6063(5) | 0.0658(15) |
| C1 | −0.0191(7) | 0.0981(3) | 1.1174(9) | 0.062(2) |
| H1A | 0.058568 | 0.101068 | 1.119091 | 0.074* |
| C2 | −0.0831(10) | 0.1348(4) | 1.2028(8) | 0.084(3) |
| H2B | −0.046671 | 0.161520 | 1.260007 | 0.101* |
| C3 | −0.2416(8) | 0.0927(3) | 1.1226(9) | 0.067(2) |
| H3A | −0.319137 | 0.088688 | 1.123950 | 0.080* |
| C4 | −0.1809(5) | 0.0568(3) | 1.0352(7) | 0.0453(17) |
| C5 | −0.2314(6) | 0.0126(3) | 0.9445(6) | 0.0455(17) |
| C6 | −0.3554(5) | 0.0051(4) | 0.9295(8) | 0.065(3) |
| H6A | −0.393239 | 0.033407 | 0.986958 | 0.098* |
| H6B | −0.376390 | 0.013237 | 0.839587 | 0.098* |
| H6C | −0.376221 | −0.036027 | 0.952392 | 0.098* |
| C7 | −0.0860(5) | −0.1650(3) | 0.8416(6) | 0.0441(16) |
| C8 | −0.1743(6) | −0.1849(4) | 0.9141(9) | 0.072(2) |
| H8A | −0.243482 | −0.165557 | 0.906875 | 0.086* |
| C9 | −0.1610(7) | −0.2344(4) | 0.9993(10) | 0.089(3) |
| H9A | −0.220939 | −0.247487 | 1.050811 | 0.107* |
| C10 | −0.0612(9) | −0.2637(4) | 1.0078(9) | 0.078(3) |
| H10A | −0.053503 | −0.297776 | 1.062390 | 0.094* |
| C11 | 0.0263(8) | −0.2435(4) | 0.9373(8) | 0.072(2) |
| H11A | 0.094723 | −0.263503 | 0.944778 | 0.087* |
| C12 | 0.0175(6) | −0.1933(3) | 0.8534(7) | 0.059(2) |
| H12A | 0.079245 | −0.179130 | 0.806473 | 0.071* |

monohydrate (0.100 g, 0.5 mmol) was added. After stirring for 1 h, the mixture was filtered and set aside to crystallize for several days, giving black block crystals. The Flack-Parsons parameter is 0.02(2) based on 637 quotients.

## Experimental details

The structure was solved by direct methods and refined with the SHELX crystallographic software package [2]. The hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters.

## Discussion

Schiff bases, including hydrazones [3], semicarbazones [4] and thiosemicarbazones [5] derived from 2-aceto-pyrazine and their metal complexes have been widely investigated due to their excellent biological activities. However, sulfonyl hydrazones has been paid much less attention. As a continuation of our research efforts devoted to Schiff base complexes, the title complex was synthesized and characterized by X-ray diffraction.

In the title complex, the asymmetric unit contains one half of the complex with Ni1 atom lying on the two fold axis. The six-coordinated Cu(II) ion is in a distorted octahedron geometry with the donor sets of four nitrogen and two oxygen atoms from two independent sulfonyl hydrazone ligands. The dihedral angle between the benzene (C7—C12, r.m.s. deviation 0.0091 Å) and pyrazine (C1—C4/N1, N2, r.m.s. deviation 0.0061 Å) ring in each sulfonyl hydrazone is 94.9°. As expected, there exist none classical hydrogen bonds in the crystal. Bond lengths and angles are in the expected ranges.

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