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Diaquabis(ethylenediamine-κ^2N,N')-copper(II) bis(sulfamerazinate)

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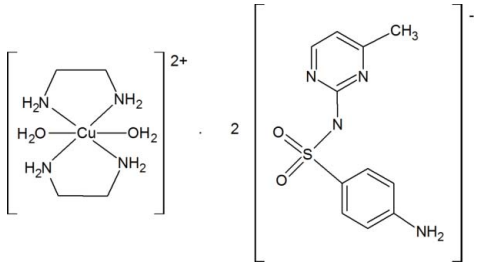
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.097; data-to-parameter ratio = 18.7.

The asymmetric unit of the title compound, $[Cu(C_2H_8N_2)_2(H_2O)_2](C_{11}H_{11}N_4O_2S)_2$, contains one sulfamerazinate anion in a general position and one half-cation that is located on a center of inversion. The Cu^{II} cation shows a strong Jahn–Teller distortion. It is coordinated by four N atoms of two ethylenediamine ligands in the basal plane and two O atoms at much longer distances in the axial positions in a bipyramidal coordination. In the crystal, the building blocks are connected by N—H···N, O—H···N, N—H···O and O—H···O hydrogen bonding into a two-dimensional network parallel to (001).

Related literature

For the antibacterial activity of sulfonamides, see: Anand (1980); Kratz *et al.* (2000); Grave *et al.* (2010). For uses of sulfamerazine, see: Murphy *et al.* (1943); Clark *et al.* (1943); Earle (1944); Forbes *et al.* (1946). The crystal structure of sulfamerazine was reported by Acharya *et al.* (1982). For a related compound in which sulfathiazole acts as a deprotonated counter-ion, see: Anacona *et al.* (2002).



Experimental

Crystal data

$[Cu(C_2H_8N_2)_2(H_2O)_2](C_{11}H_{11}N_4O_2S)_2$
M_r = 746.41
Triclinic, $P\overline{1}$
a = 7.5429 (4) Å
b = 8.1800 (5) Å
c = 14.8434 (8) Å
α = 75.299 (5)°
β = 82.800 (5)°
γ = 78.873 (5)°
V = 866.40 (9) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.81 mm^{-1}
T = 293 K
0.41 × 0.36 × 0.17 mm

Data collection

Oxford Diffraction Gemini diffractometer
Absorption correction: analytical (de Meulenaer & Tompa, 1965)
T_{min} = 0.723, T_{max} = 0.869
4738 measured reflections
4020 independent reflections
3361 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.097
S = 1.05
4020 reflections
215 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1NA···O2^{i}	0.97	2.09	3.022 (3)	162
O1W—H1W···O1	0.85	2.07	2.816 (2)	145
N1—H1NB···O1	0.97	2.41	3.219 (2)	140
O1W—H2W···N11^{ii}	0.95	1.92	2.858 (2)	171
N2—H2NA···O2^{ii}	0.97	2.33	3.189 (3)	147
N2—H2NA···N11^{ii}	0.97	2.47	3.319 (3)	145
N2—H2NB···O2^{iii}	0.97	2.42	3.277 (3)	147
N14—H14A···N12^{iv}	0.93	2.09	3.003 (3)	166
N14—H14B···O1^{v}	0.95	2.21	2.993 (3)	140
N14—H14B···N13^{v}	0.95	2.44	3.215 (3)	139

Symmetry codes: (i) $-x+2, -y, -z$; (ii) $x-1, y, z$; (iii) $-x+1, -y, -z$; (iv) $x-1, y+1, z$; (v) $x, y+1, z$.

Data collection: *GEMINI* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: NC2325).

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