Crystal structure of (2,2′-((naphthalen-1-ylmethyl)azanediyl)diacetato-κ³N,O,O′)-
(1,10-phenanthroline-κ²N,N′)-copper(II) trihydrate, CuC₂₇H₂₇N₃O₇

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Abstract
CuC₂₇H₂₇N₃O₇, orthorhombic, Pca₂₁ (no. 29), a = 22.9142(18) Å, b = 7.3271(6) Å, c = 14.7386(11) Å, V = 2474.5(3) Å³, Z = 4, Rgt(F) = 0.0443, wRref(F²) = 0.0990, T = 294(2) K.

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The asymmetric unit of the title crystal structure is shown in the figure. Table 1 contains crystallographic data and

Table 1: Data collection and handling.

<table>
<thead>
<tr>
<th>Crystal:</th>
<th>Blue block</th>
</tr>
</thead>
<tbody>
<tr>
<td>Size:</td>
<td>0.12 × 0.10 × 0.10 mm</td>
</tr>
<tr>
<td>Wavelength:</td>
<td>Mo Kα radiation (0.71073 Å)</td>
</tr>
<tr>
<td>λ:</td>
<td>0.94 mm⁻¹</td>
</tr>
<tr>
<td>Diffractometer, scan mode:</td>
<td>φ and ω</td>
</tr>
<tr>
<td>θmax, completeness:</td>
<td>28.3°, &gt;99%</td>
</tr>
<tr>
<td>N(hkl)measured, N(hkl)unique, Rint:</td>
<td>16,736, 5352, 0.044</td>
</tr>
<tr>
<td>Criterion for Iobs, N(hkl)gt:</td>
<td>Iobs &gt; 2 σ(Iobs), 4224</td>
</tr>
<tr>
<td>N(param)refined:</td>
<td>352</td>
</tr>
<tr>
<td>Programs:</td>
<td>Bruker [1], SHELX [2–4], Diamond [5], Olex2 [6], PLATON [7]</td>
</tr>
</tbody>
</table>

Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

All the reagents and solvents were used as obtained without further purification. N-(1-naphthylmethyl)iminodiacetic acid...
**Experimental details**

H atoms were synthesized as riding, with C–H distances of 0.93 Å (aromatic) and 0.97 Å (methylene); $U_{iso}(H) = 1.2U_{eq}$ (aromatic and methylene C). H atoms bonded to water O atoms were initially found in difference maps, and refined with constraint of $O$–$H = 0.82$ Å and $U_{iso}(H)$ values were set equal to 1.5 times of their parent atoms.

**Comment**

$2,2'$-(1-naphthylmethyl)iminodiacetic acid (H$_2$NamIDA) is a frequently used organic starting material in the synthesis of metal-organic compounds as supra-molecular building blocks or as biological probe [9–12]. As the continuation of our earlier work aiming to design new useful DNA cleaving agents [13, 14], we have synthesized new mixed ligated copper(II) complexes formed by NamIDA and 1,10-phenanthroline.

The title compound was crystallized in the orthorhombic space Pca2$_1$ group. In its asymmetric unit, there is a neutral metal coordination ion and three free water molecules. The central copper (II) is five-coordinated by a [NO$_3$] donor set from each one NamIDA diaionic ligands and one phenanthroline molecule. The coordination...
configuration around Cu(II) center can be best described as a distorted square pyramidal polyhedron with a $\tau$ parameter of 0.13 [15]. The square plane is constituted by each two carboxylate oxygen and two phenanthroline nitrogen atoms, and the aliphatic amine N1 atom resides at the axial position. The Cu–O (1.990(3) Å and 1.949(3) Å) bond distances are slightly shorter than the Cu–N bond lengths (2.017(3) Å and 2.008(4) Å). The axial Cu1–N1 bond (2.323(3) Å) are apparently longer than the four basal Cu–O and Cu–N bond which is similar to some analogs [9, 11].

In the crystal, the coordination ions are linked into a two-dimensional network parallel to the (100) plane by six O–H⋯O hydrogen bonds. Due to the two aromatic naphthyl and phenanthroline rings existing in the molecular structure, there are also strong π⋯π stacking interactions, which further consolidated the crystal packing. For instance, the centroid-to-centroid distance between the six-numbered C16–C19/C27/N2 and C10–C15 rings is only 3.525(2) Å with a dihedral angle of 3.3(1)$^\circ$. There is also another π⋯π stacking interaction between the C19–C22/C26/C27 and C10–C15 rings with the centroid-to-centroid distance and dihedral angle of 3.653(3) Å and 2.4(1)$^\circ$, respectively [7].

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

**References**