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Key indicators

Single-crystal X-ray study
 $T = 294\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.036
 wR factor = 0.098
Data-to-parameter ratio = 15.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

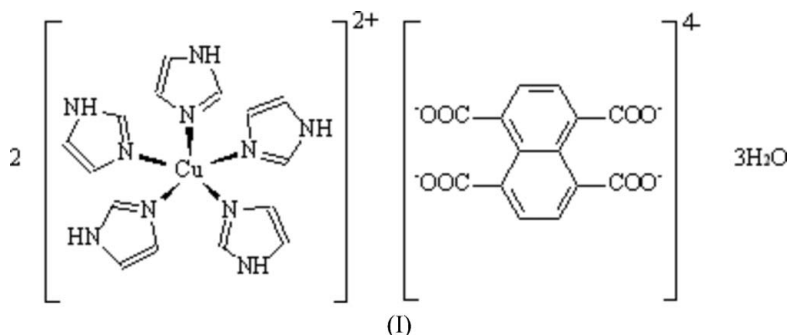
Bis[pentaimidazolecopper(II)] naphthalene-1,4,5,8-tetracarboxylate trihydrate

In the title compound, $[\text{Cu}(\text{C}_3\text{H}_4\text{N}_2)_5]_2(\text{C}_{14}\text{H}_4\text{O}_8) \cdot 3\text{H}_2\text{O}$, the Cu^{II} ion is coordinated by five imidazole ligands in a distorted square-pyramidal geometry. The naphthalenetetracarboxylate anion is located on an inversion center and links with the complex cations *via* $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonding. Hydrogen bonding between solvent water molecules and complex cations stabilizes the crystal structure.

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Comment

Metal complexes with the imidazole ligand have attracted our interest because of their potential applications in areas such as materials and molecular recognition. We present here the title Cu^{II} complex with imidazole, (I).



The crystal structure of (I) consists of Cu^{II} complex cations, naphthalenetetracarboxylate (NTA) anions and solvent water molecules (Fig. 1). The Cu^{II} ion assumes a distorted square pyramidal coordination geometry formed by five imidazole molecules (Table 1). The NTA anion is located on an inversion center and links with the complex cations *via* $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonding (Table 2). Solvent water molecules are also hydrogen bonded with the complex cations, stabilizing the crystal structure.

Experimental

Naphthalene-1,4,5,8-tetracarboxylic acid (6 mmol) was slowly added to an aqueous solution (25 ml) of NaOH (20 mmol) with stirring. An aqueous solution (20 ml) of $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (10 mmol) was mixed with the above solution at room temperature; a large amount of a light-blue precipitate appeared immediately. Solid imidazole (20 mmol) was then added to the mixture with stirring until most of the precipitate had dissolved and the color of the solution had changed to dark blue. The solution was filtered and the filtrate was allowed to stand at room temperature. Single crystals of (I) were obtained by slow evaporation after one week (5.04 g, 43.4%, yield based on Cu).

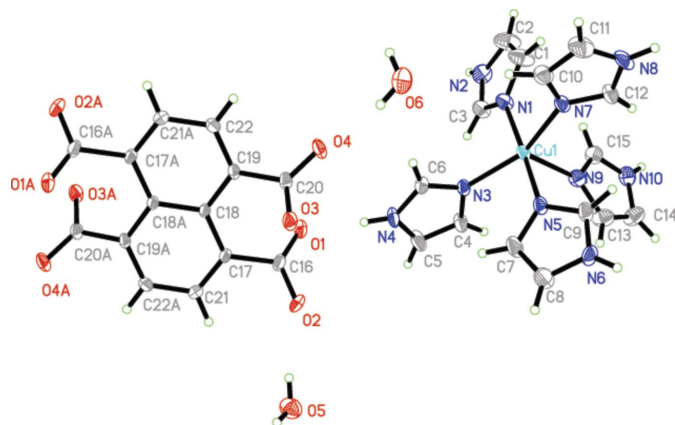


Figure 1
The molecular structure of (I) with 50% probability displacement ellipsoids (arbitrary spheres for H atoms) [symmetry code: (A) $1 - x, 2 - y, 1 - z$].

Crystal data

$[\text{Cu}(\text{C}_3\text{H}_4\text{N}_2)_5]_2(\text{C}_{14}\text{H}_4\text{O}_8) \cdot 3\text{H}_2\text{O}$
 $M_r = 1162.12$
 Monoclinic, $C2/c$
 $a = 19.680(3) \text{ \AA}$
 $b = 17.048(2) \text{ \AA}$
 $c = 16.540(2) \text{ \AA}$
 $\beta = 104.435(2)^\circ$
 $V = 5374.0(12) \text{ \AA}^3$

$Z = 4$
 $D_x = 1.436 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 $\mu = 0.87 \text{ mm}^{-1}$
 $T = 294(2) \text{ K}$
 Block, blue
 $0.24 \times 0.20 \times 0.18 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.819, T_{\max} = 0.860$

14963 measured reflections
 5507 independent reflections
 4006 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$
 $\theta_{\text{max}} = 26.4^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.098$
 $S = 1.04$
 5507 reflections
 348 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.047P)^2 + 2.8814P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.24 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.54 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters ($\text{\AA}, ^\circ$).

Cu1—N1	2.018 (2)	Cu1—N7	2.0068 (19)
Cu1—N3	2.0121 (18)	Cu1—N9	2.202 (2)
Cu1—N5	2.0321 (19)		
N7—Cu1—N3	151.54 (8)	N1—Cu1—N5	176.21 (8)
N7—Cu1—N1	89.86 (8)	N7—Cu1—N9	101.10 (8)
N3—Cu1—N1	90.06 (8)	N3—Cu1—N9	107.32 (8)
N7—Cu1—N5	89.45 (8)	N1—Cu1—N9	92.70 (8)
N3—Cu1—N5	88.77 (7)	N5—Cu1—N9	91.09 (8)

Table 2

Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O5—H5A \cdots O2	0.84	2.13	2.942 (3)	164
O5—H5B \cdots O2 ⁱ	0.87	2.05	2.920 (3)	174
O6—H6A \cdots O4	0.84	2.11	2.903 (3)	158
N2—H2A \cdots O3 ⁱⁱ	0.86	2.02	2.833 (3)	157
N4—H4A \cdots O1	0.86	1.86	2.719 (2)	177
N6—H6C \cdots O3 ⁱⁱⁱ	0.86	1.80	2.640 (2)	165
N8—H8A \cdots O2 ^{iv}	0.86	1.89	2.691 (3)	154
N10—H10A \cdots O4 ^v	0.86	1.88	2.737 (3)	175

Symmetry codes: (i) $-x + 1, y, -z + \frac{3}{2}$; (ii) $x - \frac{1}{2}, -y + \frac{3}{2}, z - \frac{1}{2}$; (iii) $-x + 1, -y + 1, -z + 1$; (iv) $x, -y + 1, z - \frac{1}{2}$; (v) $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$.

Water H atoms were located in a difference Fourier map, and refined as riding in their as-found positions, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. Other H atoms were placed in idealized positions, with $C-H = 0.93 \text{ \AA}$ and $N-H = 0.86 \text{ \AA}$, and refined in riding mode, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$. The crystal structure contains solvent-accessible voids of 39 \AA^3 , but no solvent molecule was found there.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

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