

# Poly[propane-1,3-diammonium [cuprate(II)-bis( $\mu_2$ -pyridine-2,3-dicarboxylato)] trihydrate]

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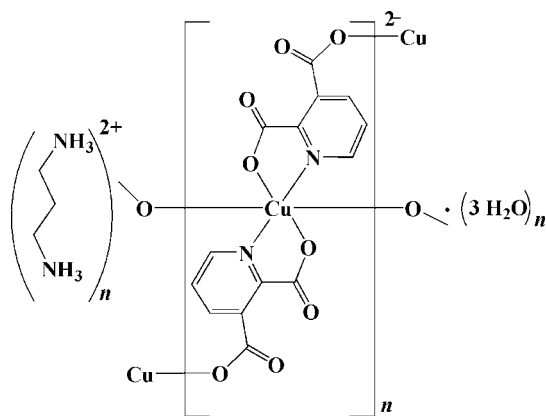
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Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å; disorder in main residue;  $R$  factor = 0.063;  $wR$  factor = 0.176; data-to-parameter ratio = 12.4.

The title polymeric compound  $\{(\text{C}_3\text{H}_{12}\text{N}_2)[\text{Cu}(\text{C}_7\text{H}_3\text{NO}_4)_2] \cdot 3\text{H}_2\text{O}\}_n$  or  $\{(\text{pnH}_2)[\text{Cu}(\text{py-2,3-dc})_2] \cdot 3\text{H}_2\text{O}\}_n$  (pn is propane-1,3-diamine and py-2,3-dc is pyridine-2,3-dicarboxylic acid), was synthesized by reaction of copper(II) chloride dihydrate with a proton-transfer compound, propane-1,3-diammonium pyridine-2,3-dicarboxylate or  $(\text{pnH}_2)(\text{py-2,3-dc})$ , in aqueous solution. The anion is a six-coordinate complex (site symmetry  $\bar{1}$ ), with a distorted octahedral geometry around  $\text{Cu}^{\text{II}}$ , consisting of two bidentate pyridine-2,3-dicarboxylate groups and two O atoms of bridging ligands from  $(\text{py-2,3-dc})^{2-}$  fragments, which are located in *trans* positions. The  $(\text{pnH}_2)^{2+}$  cation is disordered over two sites by the center of inversion. Intermolecular hydrogen bonds,  $\pi-\pi$  [centroid-centroid distances of 3.539 (3) Å] and  $\text{C}-\text{O} \cdots \pi$  stacking interactions [ $\text{O} \cdots \text{Cg} = 3.240$  (5) Å; Cg is the center of the pyridine ring], connect the various components into a supramolecular structure.

## Related literature

For related literature, see: Aghabozorg, Attar Gharamaleki, Ghadermazi *et al.* (2007); Aghabozorg, Attar Gharamaleki, Ghasemikhah *et al.* (2007); Aghabozorg, Daneshvar *et al.* (2007).



## Experimental

### Crystal data

$(\text{C}_3\text{H}_{12}\text{N}_2)[\text{Cu}(\text{C}_7\text{H}_3\text{NO}_4)_2] \cdot 3\text{H}_2\text{O}$   
 $M_r = 523.94$   
Triclinic,  $P\bar{1}$   
 $a = 6.6857$  (12) Å  
 $b = 7.8251$  (18) Å  
 $c = 9.9188$  (9) Å  
 $\alpha = 82.6561$  (10)°  
 $\beta = 84.0079$  (13)°

$\gamma = 71.9520$  (17)°  
 $V = 488.20$  (15) Å<sup>3</sup>  
 $Z = 1$   
Mo  $K\alpha$  radiation  
 $\mu = 1.19$  mm<sup>-1</sup>  
 $T = 100$  (2) K  
0.21 × 0.16 × 0.15 mm

### Data collection

Bruker SMART APEXII CCD diffractometer  
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)  
 $T_{\text{min}} = 0.775$ ,  $T_{\text{max}} = 0.836$

10997 measured reflections  
2348 independent reflections  
2310 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.026$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.063$   
 $wR(F^2) = 0.176$   
 $S = 1.01$   
2348 reflections

189 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.69$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.93$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Cu1—O1	1.960 (4)	Cu1—O4 <sup>i</sup>	2.549 (4)
Cu1—N1	1.970 (4)		
O1 <sup>ii</sup> —Cu1—N1 <sup>ii</sup>	83.39 (16)	O4 <sup>i</sup> —Cu1—O4 <sup>iii</sup>	180
O1—Cu1—N1 <sup>ii</sup>	96.61 (16)		

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

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
N2—H2A $\cdots$ O3	0.91	1.96	2.854 (1)	167
N2—H2B $\cdots$ O2 <sup>iv</sup>	0.91	2.01	2.830 (1)	150
N3—H3B $\cdots$ N2 <sup>v</sup>	0.91	1.56	2.283 (1)	134
N3—H3B $\cdots$ O2W <sup>vi</sup>	0.91	1.95	2.852 (13)	174
N3—H3C $\cdots$ O3 <sup>iv</sup>	0.91	2.42	3.041 (10)	126
N3—H3C $\cdots$ O4 <sup>iv</sup>	0.91	2.08	2.991 (1)	174
N3—H3D $\cdots$ O1WA <sup>vii</sup>	0.91	2.03	2.934 (1)	170
N3—H3D $\cdots$ O1WB <sup>viii</sup>	0.91	2.51	3.407 (15)	170
O1WA—H3W $\cdots$ O1 <sup>viii</sup>	0.89	2.11	2.764 (1)	130

# metal-organic compounds

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1WA-H4W\cdots O3^i$	0.97	1.74	2.696 (1)	168
$O2W-H1W\cdots O1WA$	0.87	2.00	2.779 (15)	148
$O2W-H1W\cdots O1WB$	0.87	1.59	2.350 (1)	145
$O2W-H2W\cdots O3^{ix}$	0.85	1.92	2.768 (1)	179
$C5-H5\cdots O1WA^x$	0.95	2.60	3.534 (13)	169
$C8-H8A\cdots O2$	0.99	2.37	2.891 (11)	112
$C8-H8B\cdots O4^i$	0.99	2.49	3.396 (11)	153

Symmetry codes: (i)  $x-1, y, z$ ; (iv)  $-x+1, -y+2, -z+1$ ; (v)  $-x, -y+2, -z+1$ ; (vi)  $x-1, y+1, z$ ; (vii)  $x, y+1, z$ ; (viii)  $x, y-1, z$ ; (ix)  $-x+1, -y+1, -z+1$ ; (x)  $-x, -y+1, -z+2$ .

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2184).

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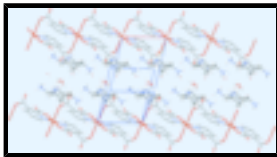


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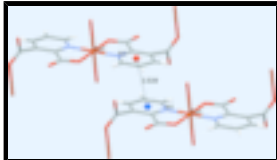
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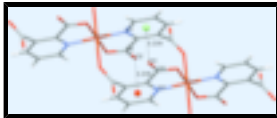
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