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## Key indicators

Single-crystal X-ray study

T = 150 K

Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$ 

R factor = 0.039

wR factor = 0.105

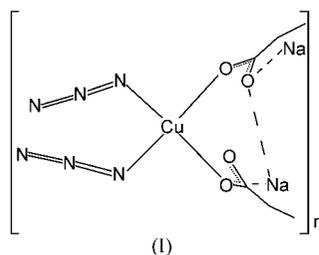
Data-to-parameter ratio = 15.0

For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Poly[di- $\mu_4$ -acetato-di- $\mu_2$ -azido-copper(II)-  
disodium(I)] at 150 K

In the structure of the title compound,  $[\text{CuNa}_2(\text{C}_2\text{H}_3\text{O}_2)_2(\text{N}_3)_2]_n$ , the copper(II) cation is coordinated by two N atoms of two symmetry-related azide anions and two O atoms of two symmetry-related carboxylate anions within a distorted tetragonal plane. The sodium cation is surrounded by four O atoms of four symmetry-equivalent carboxylate anions and two N atoms of two azide anions within an irregular polyhedron. The copper(II) cations are located on a twofold axis, whereas all other atoms are located in general positions. The copper(II) and sodium cations are connected *via* the carboxylate anions into sheets parallel to (010). These sheets are linked by the azide anions *via*  $\mu$ -N,N coordination into a three-dimensional coordination network.

## Comment

Recently, we investigated the synthesis, structures and properties of new coordination polymers based on transition metal cations, N-donor ligands and cyanide, thiocyanate or azide anions (Näther & Greve, 2003). During our investigations, we obtained crystals of the title compound, (I), by accident.



In the structure of (I), the copper(II) cation is located on a twofold axis, whereas all other atoms are located in general positions. Each copper(II) cation is fourfold coordinated by two N atoms of two symmetry-equivalent azide anions and two symmetry-equivalent carboxylate O atoms within a distorted tetragonal plane. The Cu–N [1.947 (3) Å] and Cu–O [1.988 (2) Å] bond lengths are in the range of those found in other structures retrieved from the Cambridge Structural Database (CSD; Version 5.25 of 2004; Allen, 2002). The copper cation is connected to the *syn* lone pair of that O atom which exhibits the shorter C–O bond length. The C–O...Cu angle of 111.23 (18)° shows that the copper cation is approximately oriented in the direction of the O-atom lone pair. There are no additional long Cu–O or Cu–N contacts perpendicular to the N<sub>2</sub>O<sub>2</sub> plane, which are very often found in copper(II) cations due to Jahn–Teller distortion. The sodium cation is surrounded by four O atoms of four symmetry-equivalent carboxylate anions and two N atoms of two azide anions within an irregular polyhedron. The Na–N

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and Na—O bond lengths are in the usual range found in other structures retrieved from the CSD. The copper(II) and the sodium cations are connected *via* the carboxylate anions into sheets parallel to (010). These sheets are linked by the azide anions *via*  $\mu$ -*N,N* coordination into a three-dimensional structure.

## Experimental

The title compound was prepared by reaction of copper(II) acetate (90.95 mg, 0.5 mmol), sodium azide (65.16 mg, 1 mmol) and 2-methylpyrazine (0.05 ml, 0.5 mmol) in acetonitrile (4 ml). After 6 d, blue crystals formed, which were filtered off and washed with ethanol and diethyl ether. The product consisted of a blue crystalline powder and some larger single crystals suitable for structure analysis. The homogeneity of the sample was confirmed by X-ray powder diffraction.

### Crystal data

[CuNa<sub>2</sub>(C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>)<sub>2</sub>(N<sub>3</sub>)<sub>2</sub>]  
*M<sub>r</sub>* = 311.67  
 Monoclinic, *P*2<sub>1</sub>/*n*  
*a* = 6.6691 (4) Å  
*b* = 7.8721 (7) Å  
*c* = 9.7547 (6) Å  
 $\beta$  = 94.404 (7)°  
*V* = 510.61 (6) Å<sup>3</sup>  
*Z* = 2

*D<sub>x</sub>* = 2.027 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 4743 reflections  
 $\theta$  = 2.5–28°  
 $\mu$  = 2.24 mm<sup>-1</sup>  
*T* = 150 (2) K  
 Block, blue  
 0.08 × 0.05 × 0.05 mm

### Data collection

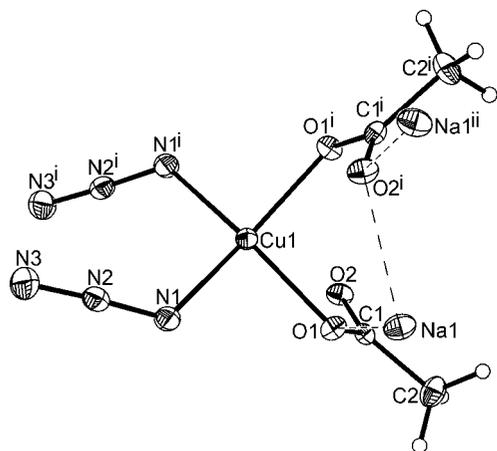
Stoe Imaging Plate Diffraction  
 System diffractometer  
 $\varphi$  scans  
 4743 measured reflections  
 1200 independent reflections  
 1077 reflections with *I* > 2σ(*I*)

*R*<sub>int</sub> = 0.046  
 $\theta_{\max}$  = 28.1°  
*h* = -8 → 8  
*k* = -10 → 10  
*l* = -12 → 12

### Refinement

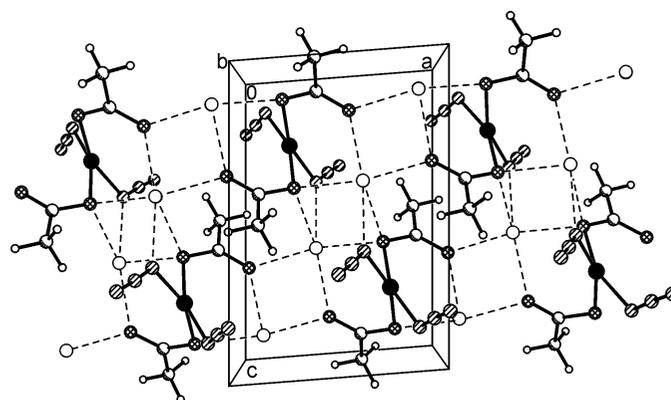
Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.039  
*wR* (*F*<sup>2</sup>) = 0.105  
*S* = 1.09  
 1200 reflections  
 80 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0567P)^2 + 1.0984P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.54 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.71 \text{ e \AA}^{-3}$   
 Extinction correction: *SHELXL97*  
 Extinction coefficient: 0.066 (7)



**Figure 1**

The crystal structure of the title compound, showing the copper coordination, the atom labelling and displacement ellipsoids at the 50% probability level. The Na coordination is shown as dashed lines. [Symmetry codes: (i)  $-x + \frac{3}{2}, y, -z + \frac{3}{2}$ ; (ii)  $-x + \frac{1}{2}, y, z - \frac{3}{2}$ ]



**Figure 2**

The crystal structure of the title compound viewed along the *b* axis. The Na coordination is shown as dashed lines.

**Table 1**

Selected geometric parameters (Å, °).

Cu1—N1 <sup>i</sup>	1.947 (3)	N1—Na1 <sup>ii</sup>	2.441 (3)
Cu1—N1	1.947 (3)	N3—Na1 <sup>iv</sup>	2.539 (3)
Cu1—O1	1.988 (2)	Na1—O2 <sup>i</sup>	2.369 (3)
Cu1—O1 <sup>i</sup>	1.988 (2)	Na1—O2 <sup>v</sup>	2.378 (2)
O1—Na1	2.382 (2)	Na1—N1 <sup>ii</sup>	2.441 (3)
O1—Na1 <sup>ii</sup>	2.669 (3)	Na1—N3 <sup>vi</sup>	2.539 (3)
O2—Na1 <sup>i</sup>	2.369 (3)	Na1—O1 <sup>ii</sup>	2.669 (3)
O2—Na1 <sup>iii</sup>	2.378 (2)		
N1 <sup>i</sup> —Cu1—N1	97.86 (16)	O2 <sup>i</sup> —Na1—O2 <sup>v</sup>	82.67 (9)
N1 <sup>i</sup> —Cu1—O1	158.59 (10)	O2 <sup>i</sup> —Na1—O1	81.04 (8)
N1—Cu1—O1	88.33 (10)	O2 <sup>v</sup> —Na1—O1	147.54 (9)
N1 <sup>i</sup> —Cu1—O1 <sup>i</sup>	88.33 (10)	O2 <sup>i</sup> —Na1—N1 <sup>ii</sup>	163.92 (10)
N1—Cu1—O1 <sup>i</sup>	158.59 (10)	O2 <sup>v</sup> —Na1—N1 <sup>ii</sup>	109.15 (10)
O1—Cu1—O1 <sup>i</sup>	93.32 (13)	O1—Na1—N1 <sup>ii</sup>	93.15 (10)
C1—O1—Cu1	111.23 (18)	O2 <sup>i</sup> —Na1—N3 <sup>vi</sup>	82.70 (10)
C1—O1—Na1	132.08 (18)	O2 <sup>v</sup> —Na1—N3 <sup>vi</sup>	113.03 (10)
Cu1—O1—Na1	104.47 (9)	O1—Na1—N3 <sup>vi</sup>	92.50 (10)
C1—O1—Na1 <sup>ii</sup>	113.56 (18)	N1 <sup>ii</sup> —Na1—N3 <sup>vi</sup>	82.58 (10)
Cu1—O1—Na1 <sup>ii</sup>	97.71 (9)	O2 <sup>i</sup> —Na1—O1 <sup>ii</sup>	129.60 (9)
C1—O2—Na1 <sup>i</sup>	124.02 (19)	O2 <sup>v</sup> —Na1—O1 <sup>ii</sup>	80.56 (8)
C1—O2—Na1 <sup>iii</sup>	128.2 (2)	O1—Na1—O1 <sup>ii</sup>	88.53 (8)
N2—N1—Cu1	124.0 (2)	N1 <sup>ii</sup> —Na1—O1 <sup>ii</sup>	64.72 (8)
N2—N1—Na1 <sup>ii</sup>	129.1 (2)	N3 <sup>vi</sup> —Na1—O1 <sup>ii</sup>	147.29 (10)
N2—N3—Na1 <sup>iv</sup>	150.3 (3)		

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

The positions of the methyl H atoms were idealized, then refined as rigid groups allowed to rotate but not tip, with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ .

Data collection: *IPDS* (Stoe & Cie, 1998); cell refinement: *IPDS*; data reduction: *IPDS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *CIFTAB* in *SHELXL97*.

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