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Dimethylammonium diaqua(pyridine-2,4-dicarboxylato-κ^2N,O^2)cuprate(II)

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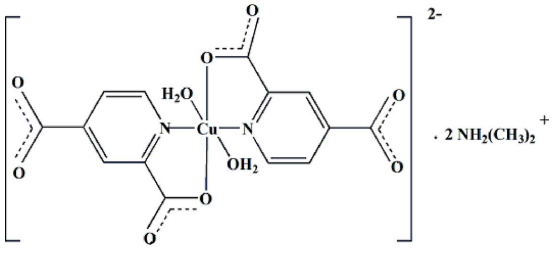
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.029; wR factor = 0.079; data-to-parameter ratio = 13.6.

The asymmetric unit of the title compound, $(C_2H_8N)_2[Cu(C_7H_3NO_4)_2(H_2O)_2]$, contains one-half of a mononuclear $[Cu(C_7H_3NO_4)_2(H_2O)_2]^{2-}$ anion, one dimethylammonium cation and one aqua ligand. The Cu^{II} atom, lying on an inversion center, is coordinated by two symmetry-related N atoms and two O atoms from one pyridine-2,4-dicarboxylate ligand and two symmetry-related aqua ligands and exhibits a distorted octahedral *trans*-$[CuN_2O_4]$ coordination geometry. Multiple crystallographically independent O—H···O and N—H···O hydrogen bonds form a three-dimensional network in the crystal structure.

Related literature

For the structural diversity and potential applications of coordination polymers constructed from metal ions and bridging ligands, see: Eddaoudi *et al.* (2001); Kitagawa *et al.* (2004). For general background to metal complexes of pyridine-2,4-dicarboxylates, see: Mahata & Natarajan (2005); Bai *et al.* (2008); Chen & Beatty (2008). For similar structures, see: Zou *et al.* (2008); Noro *et al.* (2005). For comparative bond lengths and angles, see: Chutia *et al.* (2009); Klein *et al.* (1982).



Experimental

Crystal data

$(C_2H_8N)_2[Cu(C_7H_3NO_4)_2(H_2O)_2]$
M_r = 521.98
Monoclinic, $P2_1/n$
a = 7.9854 (7) Å
b = 9.4648 (8) Å
c = 14.9380 (12) Å
β = 103.540 (1)°
V = 1097.64 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.06 mm^{-1}
T = 293 K
0.31 × 0.16 × 0.16 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.732, T_{max} = 0.849
5508 measured reflections
2160 independent reflections
1992 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.079
S = 1.06
2160 reflections
159 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O1	1.9733 (11)	Cu1—O1*W*	2.4162 (15)
Cu1—N1	1.9810 (14)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1*W*—H1*WA*···O4^{i}	0.83 (2)	1.85 (2)	2.680 (2)	174
O1*W*—H1Wb···O3^{ii}	0.81 (2)	2.00 (2)	2.809 (2)	172
N2—H2*A*···O3	0.90	1.92	2.783 (2)	161
N2—H2*B*···O2^{iii}	0.90	1.94	2.778 (2)	154

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2257).

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supporting information

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Dimethylammonium diaqua(pyridine-2,4-dicarboxylato-κ^2N,O^2)cuprate(II)

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S1. Comment

Coordination polymers constructed from metal ions and bridging ligands have been of great interest due to their structural diversity and many potential applications (Eddaoudi *et al.*, 2001; Kitagawa *et al.*, 2004). Pyridinedicarboxylates(pydc) have been extensively studied as excellent bridging ligands in the area of metal-organic frameworks (Mahata *et al.*, 2005; Bai *et al.* 2008; Chen *et al.* 2008). Herein we report the crystal structure of the title compound $[Cu(2,4\text{-pydc})_2(H_2O)_2][NH_2(CH_3)_2]_2$, (2,4-pydc= pyridine-2,4-dicarboxylate) .The Cu^{II} atom, lying on an inversion center, is coordinated by two symmetry-related N atoms and two O atoms from one pyridine-2,4-dicarboxylate ligand and two symmetry-related aqua ligands and exhibits a distorted octahedral trans-[CuN_2O_4] coordination geometry (Table 1 and Fig. 1). The bond lengths and angles are all in normal ranges (Chutia *et al.*, 2009; Klein *et al.*, 1982). Multiple crystallographically independent hydrogen bonds form a three-dimensional network in the crystal structure, Table 2.

S2. Experimental

A solution of $Cu(NO_3)_2.3H_2O$ (0.024 g, 0.1 mmol) in H_2O (3 ml) was added to a suspending solution of 2,4-pydc (0.017 g, 0.1 mmol) in H_2O and DMF(1:1, 7 ml). The mixture was stirred for 30 minutes and sealed in a 15 ml Teflon-lined stainless steel autoclave and heated at 423 K for 3 d under autogenous pressure. When cooled to room temperature, green block crystals of the title compound were obtained (yield 0.045 g, 86% based on Cu).

S3. Refinement

H atoms of the pyridine ring were positioned geometrically and refined as riding atoms, with C—H = 0.93-0.96 Å and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5 U_{eq}(C) for CH_3 group. H atoms of water molecule were located in a difference Fourier map and refined as riding, with U_{iso}(H) = 1.2U_{eq}(O).

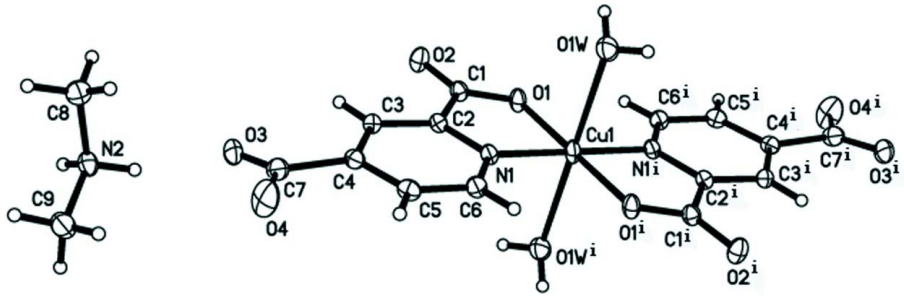

Figure 1

Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) -*x*, 1 - *y*, 2 - *z*.]

Dimethylammonium diaqua(pyridine-2,4-dicarboxylato-κ^2N,O^2)cuprate(II)

Crystal data

$(C_2H_8N)_2[Cu(C_7H_3NO_4)_2(H_2O)_2]$
$M_r = 521.98$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.9854$ (7) Å
$b = 9.4648$ (8) Å
$c = 14.9380$ (12) Å
$\beta = 103.540$ (1)°
$V = 1097.64$ (16) Å^3
$Z = 2$
$F(000) = 542$
$D_x = 1.579$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3343 reflections
$\theta = 2.6$–$26.0°$
$\mu = 1.06$ mm^{-1}
$T = 293$ K
Block, green
0.31 × 0.16 × 0.16 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.732$, $T_{max} = 0.849$
5508 measured reflections
2160 independent reflections
1992 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.6°$
$h = -9 \rightarrow 9$
$k = -7 \rightarrow 11$
$l = -12 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.079$
$S = 1.06$
2160 reflections
159 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2 + 0.427P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.0000	0.5000	1.0000	0.02668 (12)
N1	0.15726 (18)	0.55054 (15)	0.92027 (9)	0.0235 (3)
N2	0.7815 (2)	0.47684 (16)	0.59707 (11)	0.0302 (3)
H2A	0.6957	0.4670	0.6264	0.036*
H2B	0.8078	0.3904	0.5793	0.036*
O1	0.15272 (15)	0.33417 (12)	1.02961 (8)	0.0291 (3)
O2	0.38987 (16)	0.24074 (13)	0.99920 (9)	0.0337 (3)
O3	0.57116 (18)	0.46822 (17)	0.72146 (10)	0.0393 (3)
O4	0.4794 (2)	0.68865 (19)	0.68723 (12)	0.0618 (5)
O1W	0.18306 (19)	0.62993 (16)	1.12457 (10)	0.0400 (3)
H1WA	0.126 (3)	0.687 (2)	1.1473 (16)	0.048*
H1WB	0.250 (2)	0.594 (2)	1.1680 (12)	0.048*

C1	0.2761 (2)	0.33162 (18)	0.98819 (11)	0.0253 (3)
C2	0.2792 (2)	0.45160 (18)	0.92182 (11)	0.0223 (3)
C3	0.3928 (2)	0.45788 (18)	0.86496 (11)	0.0234 (3)
H3	0.4755	0.3880	0.8674	0.028*
C4	0.3812 (2)	0.57093 (18)	0.80377 (11)	0.0249 (3)
C5	0.2608 (2)	0.67552 (18)	0.80637 (11)	0.0277 (4)
H5	0.2545	0.7549	0.7690	0.033*
C6	0.1501 (2)	0.66179 (18)	0.86455 (11)	0.0269 (4)
H6	0.0686	0.7319	0.8649	0.032*
C7	0.4887 (2)	0.5772 (2)	0.73205 (12)	0.0337 (4)
C8	0.9339 (3)	0.5361 (3)	0.66186 (15)	0.0414 (5)
H8A	1.0242	0.5513	0.6303	0.062*
H8B	0.9728	0.4712	0.7118	0.062*
H8C	0.9037	0.6244	0.6856	0.062*
C9	0.7204 (3)	0.5659 (2)	0.51421 (13)	0.0409 (5)
H9A	0.6653	0.6490	0.5306	0.061*
H9B	0.6396	0.5134	0.4686	0.061*
H9C	0.8166	0.5931	0.4898	0.061*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.03408 (19)	0.02407 (18)	0.02744 (19)	0.00826 (11)	0.01843 (13)	0.00608 (11)
N1	0.0288 (7)	0.0230 (7)	0.0207 (6)	0.0025 (6)	0.0095 (5)	0.0003 (6)
N2	0.0352 (8)	0.0289 (8)	0.0295 (8)	−0.0024 (6)	0.0136 (7)	−0.0061 (6)
O1	0.0363 (7)	0.0269 (6)	0.0297 (6)	0.0071 (5)	0.0190 (5)	0.0078 (5)
O2	0.0357 (7)	0.0289 (7)	0.0411 (7)	0.0097 (5)	0.0183 (6)	0.0119 (6)
O3	0.0368 (7)	0.0531 (8)	0.0329 (7)	0.0035 (6)	0.0183 (6)	0.0039 (6)
O4	0.0617 (10)	0.0642 (11)	0.0720 (11)	0.0089 (8)	0.0411 (9)	0.0378 (9)
O1W	0.0444 (8)	0.0413 (8)	0.0345 (7)	0.0109 (6)	0.0095 (6)	−0.0020 (6)
C1	0.0304 (8)	0.0230 (8)	0.0242 (8)	0.0016 (7)	0.0097 (7)	0.0016 (6)
C2	0.0258 (8)	0.0208 (8)	0.0209 (7)	−0.0009 (6)	0.0070 (6)	−0.0010 (6)
C3	0.0236 (8)	0.0235 (8)	0.0240 (8)	0.0001 (6)	0.0074 (6)	−0.0001 (7)
C4	0.0245 (8)	0.0276 (9)	0.0228 (8)	−0.0058 (6)	0.0062 (6)	0.0009 (7)
C5	0.0333 (9)	0.0245 (9)	0.0250 (8)	−0.0027 (7)	0.0063 (7)	0.0059 (7)
C6	0.0320 (8)	0.0231 (8)	0.0260 (8)	0.0043 (7)	0.0079 (7)	0.0026 (7)
C7	0.0277 (9)	0.0459 (12)	0.0287 (9)	−0.0047 (8)	0.0090 (7)	0.0085 (8)
C8	0.0349 (10)	0.0507 (12)	0.0376 (11)	−0.0059 (9)	0.0066 (8)	−0.0036 (10)
C9	0.0472 (11)	0.0445 (12)	0.0319 (10)	0.0041 (9)	0.0110 (8)	0.0005 (9)

Geometric parameters (Å, º)

Cu1—O1	1.9733 (11)	O1W—H1WB	0.815 (10)
Cu1—O1^{i}	1.9733 (11)	C1—C2	1.512 (2)
Cu1—N1^{i}	1.9810 (14)	C2—C3	1.381 (2)
Cu1—N1	1.9810 (14)	C3—C4	1.396 (2)
Cu1—O1W^{i}	2.4162 (15)	C3—H3	0.9300
Cu1—O1W	2.4162 (15)	C4—C5	1.387 (2)

N1—C6	1.335 (2)	C4—C7	1.523 (2)
N1—C2	1.347 (2)	C5—C6	1.383 (2)
N2—C8	1.477 (3)	C5—H5	0.9300
N2—C9	1.483 (3)	C6—H6	0.9300
N2—H2A	0.9000	C8—H8A	0.9600
N2—H2B	0.9000	C8—H8B	0.9600
O1—C1	1.281 (2)	C8—H8C	0.9600
O2—C1	1.234 (2)	C9—H9A	0.9600
O3—C7	1.253 (2)	C9—H9B	0.9600
O4—C7	1.242 (2)	C9—H9C	0.9600
O1W—H1WA	0.832 (10)		

O1—Cu1—O1^{i}	179.998 (1)	N1—C2—C3	122.38 (15)
O1—Cu1—N1^{i}	96.81 (5)	N1—C2—C1	114.25 (14)
O1^{i}—Cu1—N1^{i}	83.18 (5)	C3—C2—C1	123.33 (15)
O1—Cu1—N1	83.19 (5)	C2—C3—C4	118.89 (16)
O1^{i}—Cu1—N1	96.81 (5)	C2—C3—H3	120.6
N1^{i}—Cu1—N1	180.00 (5)	C4—C3—H3	120.6
O1—Cu1—O1W^{i}	89.92 (5)	C5—C4—C3	117.97 (15)
O1^{i}—Cu1—O1W^{i}	90.08 (5)	C5—C4—C7	120.04 (15)
N1^{i}—Cu1—O1W^{i}	89.18 (5)	C3—C4—C7	121.90 (16)
N1—Cu1—O1W^{i}	90.82 (5)	C6—C5—C4	119.98 (15)
O1—Cu1—O1W	90.08 (5)	C6—C5—H5	120.0
O1^{i}—Cu1—O1W	89.91 (5)	C4—C5—H5	120.0
N1^{i}—Cu1—O1W	90.82 (5)	N1—C6—C5	121.69 (15)
N1—Cu1—O1W	89.18 (5)	N1—C6—H6	119.2
O1W^{i}—Cu1—O1W	180.00 (5)	C5—C6—H6	119.2
C6—N1—C2	118.96 (14)	O4—C7—O3	126.71 (18)
C6—N1—Cu1	128.65 (12)	O4—C7—C4	116.09 (18)
C2—N1—Cu1	112.29 (11)	O3—C7—C4	117.13 (16)
C8—N2—C9	113.01 (16)	N2—C8—H8A	109.5
C8—N2—H2A	109.0	N2—C8—H8B	109.5
C9—N2—H2A	109.0	H8A—C8—H8B	109.5
C8—N2—H2B	109.0	N2—C8—H8C	109.5
C9—N2—H2B	109.0	H8A—C8—H8C	109.5
H2A—N2—H2B	107.8	H8B—C8—H8C	109.5
C1—O1—Cu1	114.32 (10)	N2—C9—H9A	109.5
Cu1—O1W—H1WA	110.7 (17)	N2—C9—H9B	109.5
Cu1—O1W—H1WB	124.4 (18)	H9A—C9—H9B	109.5
H1WA—O1W—H1WB	106 (2)	N2—C9—H9C	109.5
O2—C1—O1	125.07 (15)	H9A—C9—H9C	109.5
O2—C1—C2	119.13 (14)	H9B—C9—H9C	109.5
O1—C1—C2	115.80 (14)		

Symmetry code: (i) $-x$, $-y+1$, $-z+2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O4^{ii}	0.83 (2)	1.85 (2)	2.680 (2)	174
O1*W*—H1Wb···O3^{iii}	0.81 (2)	2.00 (2)	2.809 (2)	172
N2—H2*A*···O3	0.90	1.92	2.783 (2)	161
N2—H2*B*···O2^{iv}	0.90	1.94	2.778 (2)	154

Symmetry codes: (ii) *x*−1/2, −*y*+3/2, *z*+1/2; (iii) −*x*+1, −*y*+1, −*z*+2; (iv) *x*+1/2, −*y*+1/2, *z*−1/2.