Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(1-Ammonioethylidenediphosphonato-κ^2O,O)-(2,2′-bipyridyl-κ^2N,N')chloridocopper(II)

Ming Li and Ju-Tang Sun*

College of Chemistry and Molecular Sciences, Wuhan University, Wuhan 430072, People's Republic of China

Correspondence e-mail: hlik@163.com

Received 19 March 2007
Accepted 26 March 2007

In the title complex, $[Cu(C_2H_8NO_6P_2)Cl(C_{10}H_8N_2)]$, the Cu^{II} atom has a slightly distorted square-pyramidal geometry. O—H···O, N—H···O and O—H···Cl interactions form a two-dimensional layer structure. Adjacent layers are linked to form a three-dimensional structure through π–π interactions.

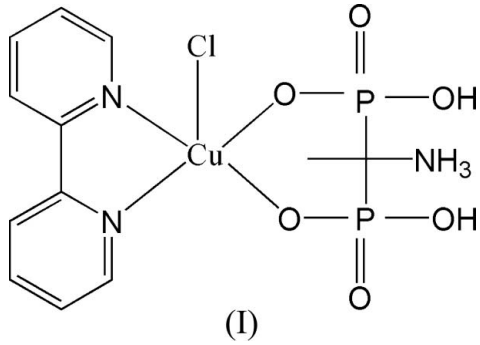
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.029
wR factor = 0.083
Data-to-parameter ratio = 17.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Metal organophosphonates have been widely investigated in the past two decades due to their potential applications as catalysts, sensors, sorbents, and magnetic and luminescent materials (Clearfield, 1996; Finn *et al.*, 2003). Among the diverse organophosphonic acids, phosphonic acids and diphosphonic acids containing functional groups, such as crown ether, –COOH, –OH, –NR_2 or mixed groups, are excellent precursors for the preparation of hybrid materials (Clearfield, 2002, and references therein; Yin *et al.*, 2003). 1-Aminoethylidenediphosphonic acid ($AEDPH_4$) contains an –NH_2 group, which exists as a zwitterion by transfer of one H atom to the amino group. Deprotonation of this group will result in predictable hydrogen-bonded aggregates from stronger P—O—H···O—P to weaker C—H···X hydrogen bonds. However, little attention has been paid to the structural study of metal–AEDP compounds (Yin *et al.*, 2005; Ding *et al.*, 2006; Li *et al.*, 2006). We present here the title new AEDP-containing complex, (I).



(I)

The Cu^{II} ion of (I) is coordinated by two phosphonate O atoms from the 1-aminoethylidenediphosphonate ligand, two N atoms from the 2,2′-bipyridyl ligand and one Cl^- ion in a distorted square-pyramidal geometry (Fig. 1).

Molecules of (I) are connected by a pair of strong O—H···O hydrogen bonds [O2—H2···O3^{i}; symmetry code: (i) $-x, 1-y, 1-z$] to form a dimer. These dimers are then linked to form a layer structure parallel to the *bc* plane *via* O—H···Cl and N—H···O interactions, as shown in Fig. 2. Details of the hydrogen bonds are given in Table 1. The shortest

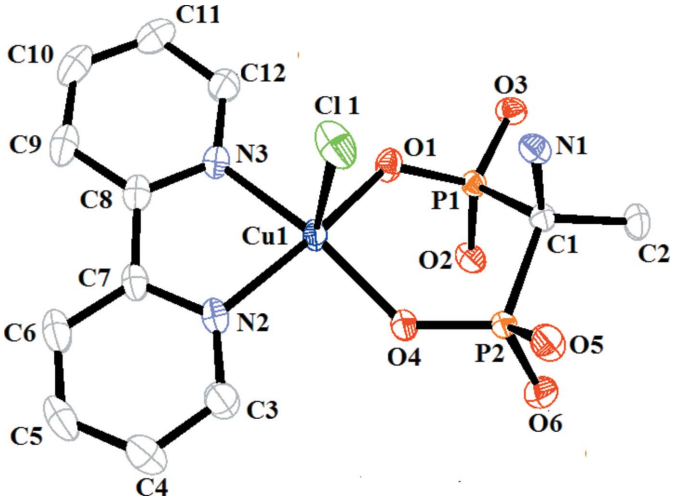


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. All H atoms have been omitted for clarity.

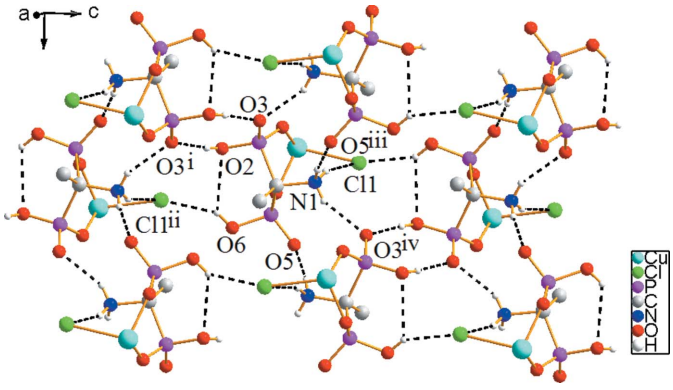


Figure 2
The two-dimensional layer structure in (I), formed *via* various hydrogen bonds, including O—H···O, N—H···O and O—H···Cl. The 2,2′-bipyridyl ligands have been omitted for clarity. [Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$.]

plane-to-plane (3.311 Å) and centroid-to-centroid (3.544 Å) distances between 2,2′-bipyridyl ligands in two neighbouring layers (symmetry relationship: $1-x, 1-y, 1-z$) suggest a π–π stacking interaction between them. These weak π–π interactions, together with the C—H···O and C—H···Cl hydrogen bonds, link adjacent layers to form a three-dimensional structure.

Experimental

$CuCl_2{\cdot}2H_2O$ (0.0426 g, 0.25 mmol), 2,2′-bipyridyl (0.0390 g, 0.25 mmol), $AEDPH_4$ (0.1025 g, 0.5 mmol) and H_2O (1.0 ml) were mixed and sealed in a Teflon-lined autoclave and heated at 353 K. Blue crystals of (I) suitable for single-crystal analysis were obtained after 6 d (0.0489 g, yield 42.5% based on 2,2′-bipyridyl).

Crystal data

$[Cu(C_2H_8NO_6P_2)Cl(C_{10}H_8N_2)]$
$M_r = 459.21$
Monoclinic, $P2_1/c$
$a = 13.1203\ (12)$ Å
$b = 8.6490\ (8)$ Å
$c = 15.1501\ (14)$ Å
$\beta = 108.3670\ (10)^\circ$
$V = 1631.6\ (3)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 1.74$ mm^{-1}
$T = 293\ (2)$ K
0.37 × 0.30 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.566$, $T_{max} = 0.701$
10176 measured reflections
3913 independent reflections
3464 reflections with $I > 2/s(I)$
$R_{int} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.083$
$S = 1.04$
3913 reflections
230 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.79$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O3^{i}	0.89	2.04	2.845 (2)	151
N1—H1B···Cl1	0.89	2.33	3.1899 (16)	161
N1—H1C···O5^{ii}	0.89	1.88	2.762 (2)	174
O2—H2···O3^{iii}	0.82	1.73	2.5316 (18)	167
O6—H6A···Cl1^{iv}	0.82	2.44	3.1357 (15)	143
O6—H6A···O2	0.82	2.55	3.120 (2)	128

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

All H atoms were positioned geometrically and treated as riding, with C—H = 0.93 Å (aromatic) or 0.96 Å (methyl), N—H = 0.89 Å and O—H = 0.82 Å, and with $U_{iso}(H) = 1.2U_{eq}$(C,N,O), or $1.5U_{eq}$(C) for methyl H.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Bruker, 2000).

This work was financially supported by the National Natural Science Foundation of China (grant No. 20471044).

References

Brandenburg, K. (1999). *DIAMOND*. Release 2.1c. Crystal Impact GbR, Bonn, Germany.
Bruker (1997). *SMART* (Version 5.611), *SAINT* (Version 6.0) and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2000). *SADABS* (Version 2.03) and *SHELXTL* (Version 6.12). Bruker AXS Inc., Madison, Wisconsin, USA.
Clearfield, A. (1996). *Curr. Opin. Solid State Mater. Sci.* **1**, 268–278.
Clearfield, A. (2002). *Recent Opin. Solid Mater. Sci.* **6**, 495–506.
Ding, D.-G., Yin, M.-C., Lu, H.-J., Fan, Y.-T., Hou, H.-W. & Wang, Y.-T. (2006). *J. Solid State Chem.* **179**, 747–752.
Finn, R. C., Zubieta, J. & Haushalter, R. C. (2003). *Prog. Inorg. Chem.* **51**, 421–601.

Li, M., Chen, S.-P., Xiang, J.-F., He, H.-J., Yuan, L.-J. & Sun, J.-T. (2006). *Cryst. Growth Des.* **6**, 1250–1252.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Yin, P., Gao, S., Zheng, L.-M., Wang, Z.-M. & Xin, X.-Q. (2003). *Chem. Commun.* pp. 1076–1077.
Yin, P., Wang, X.-C., Gao, S. & Zheng, L.-M. (2005). *J. Solid State Chem.* **178**, 1049–1053.