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Bis(2-aminopyridinium) diaquabis(malonato-κ^2O,O')cuprate(II)

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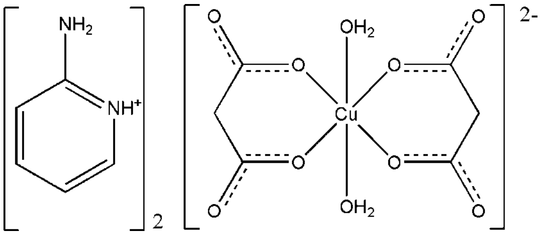
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.027; wR factor = 0.075; data-to-parameter ratio = 11.1.

The Cu^{II} ion in the title compound, $(C_5H_7N_2)_2[Cu(C_3H_2O_4)_2(H_2O)_2]$, is located on an inversion centre and coordinated by four O atoms from two bidentate malonate (mal) ligands in the equatorial plane and two O atoms from two coordinated water molecules in the axial positions, forming an elongated octahedral geometry. Each $[Cu(mal)_2(H_2O)_2]^{2-}$ anion bridges two 2-aminopyridinium cations *via* N—H···O hydrogen bonds and symmetry-related anions *via* O—H···O hydrogen bonds, to form an infinite one-dimensional chain. Additional O—H···O and C—H···O hydrogen bonds generate two-dimensional sheets that are joined into a three-dimensional network *via* N—H···O, C—H···O and interlayer π–π interactions between aminopyridinium cations (symmetry code: $1 - x, 1 - y, 2 - z$).

Related literature

For related literature, see: Chattopadhyay *et al.* (1993); Lenstra & Kataeva (2001); Rodríguez-Martin *et al.* (2002); Ruiz-Pérez *et al.* (2000); Bernstein *et al.* (1995).



Experimental

Crystal data

$(C_5H_7N_2)_2[Cu(C_3H_2O_4)_2(H_2O)_2]$
M_r = 493.92
Triclinic, $P\bar{1}$
a = 7.0433 (13) Å
b = 7.9116 (15) Å
c = 9.5767 (18) Å
α = 96.096 (2)°
β = 107.865 (2)°
γ = 103.743 (2)°
V = 484.03 (16) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.19 mm^{-1}
T = 298 (2) K
0.50 × 0.40 × 0.30 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
T_{min} = 0.587, T_{max} = 0.716
1987 measured reflections
1659 independent reflections
1616 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.075
S = 1.14
1659 reflections
150 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O3	1.9293 (14)	Cu1—O5	2.665 (2)
Cu1—O1	1.9336 (14)		
O3—Cu1—O1	92.20 (6)	O1—Cu1—O5	95.04 (7)
O3—Cu1—O5	84.65 (6)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.86	1.91	2.756 (2)	168
N2—H2C···O2	0.86	2.14	2.930 (3)	152
N2—H2D···O4^{i}	0.86	2.35	3.172 (3)	161
O5—H5A···O2^{ii}	0.83 (4)	1.99 (4)	2.807 (3)	171 (3)
O5—H5B···O4^{iii}	0.76 (3)	2.31 (3)	3.043 (3)	161 (3)
C5—H5···O3^{i}	0.93	2.45	3.209 (3)	139
C6—H6···O4^{iv}	0.93	2.59	3.514 (3)	172
C7—H7···O2^{v}	0.93	2.49	3.278 (3)	142

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

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SK3114).

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supplementary materials

Acta Cryst. (2007). E**63**, m1331-m1332 [**doi:10.1107/S1600536807015851**]

Bis(2-aminopyridinium) diaquabis(malonato-*κ*^{2}*O*,*O*')cuprate(II)

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Comment

The title complex, (I), $(C_5H_5N_2H)_2[Cu(mal)_2(H_2O)_2]$ (Fig. 1), was synthesized from purely aqueous media by mixing the reactants in stoichiometric

ratio and adjusting the pH of the mixture with dilute NaOH. Selected geometric data are listed in Table 1.

The asymmetric unit of (I) consists of one diaquabis(malonato)cuprate(II) anion

and two protonated 2-aminopyridine cations. The coordination around Cu in the mononuclear unit is elongated octahedral, forming a CuO_6 chromophore. Four carboxylate O atoms from two bidentate malonate anions build the equatorial plane, with Cu—O bonds nearly identical [1.929 (15) and 1.933 (15) Å for Cu1—O3 and Cu1—O1, respectively], whereas two water molecules occupy the axial sites [2.665 (2) Å for Cu1—O5]. The values of the Cu—O(malonate) bonds and bond angles around Cu1 agree well with those previously reported for other malonate-containing Cu^{II} complexes. The axial Cu1—O5 bond is somewhat longer than that in the similar unit reported by other authors, *e.g.* $[Cu(H_2O)_4][Cu(mal)_2(H_2O)_2]$ (Chattopadhyay *et al.*, 1993), $\{[Cu(H_2O)_4]_2[Cu(mal)_2(H_2O)_2]\}$ (Reference?), $[Cu(mal)_2(H_2O)_2]\{[Cu(H_2O)_4][Cu(mal)_2(H_2O)_2]\}$ (Ruiz-Pérez *et al.* 2000) and $[M^{II}(H_2O)_6][Cu^{II}(mal)_2(H_2O)_2]$ (Rodríguez-Martin *et al.* 2002).

Compound (I) is in form of a dianion. A comparison of the geometry of the current anion with that of the related neutral complex $[Cu(Hmal)_2(H_2O)_2]$ (Lenstra & Kataeva, 2001) indicates shorter Cu—O bonds in the equatorial plane and longer axial bonds in (I), consistent with a Jahn–Teller effect. The

malonate ligands show a twist–boat conformation, with the methylene C atom out

of the chelate ring plane.

The supramolecular interactions in (I) are listed in Table 2. The monomeric anionic units link to one another *via* strong complementary O5—H5A···O2 hydrogen bonds generating an $R_2^2(12)$ (Bernstein *et al.*, 1995) hydrogen-bonded supramolecular synthon, to give an infinite one-dimensional tape along the *a* axis (Fig. 2). Each monomeric unit also binds two 2-aminopyridine ligands *via* N2—H2C···O2 and N1—H1···O1 hydrogen bonds through the formation of an $R_2^2(8)$ hydrogen-bonding synthon (Fig. 2). Each such layer links adjacent layers along the *b* axis *via* O5—H5B···O4 hydrogen bonds, generating an $R_2^2(12)$ cyclic motif (Fig. 3). The aminopyridine unit from one layer also participates in hydrogen bonding *via* a C7—H7···O2 hydrogen bond with the adjacent layer to give a two-dimensional sheet. It is interesting to note that one H atom (H5A) of the coordinated water molecule helps the monomeric unit to grow one-dimensionally and the other H atom (H5B) helps the one-dimensional chains to grow two-dimensionally. These two-dimensional sheets propagate along the *c* axis direction through interlayer N2—H2D···O4 and C5—H5···O3 hydrogen bonds. Interlayer π–π (Fig. 4) stacking between aminopyridine moieties also provides additional stabilization of the ultimate three-dimensional structure (Fig. 5).

Experimental

Copper(II) acetate monohydrate (0.199 g, 1 mmol) was dissolved in water (20 ml) and allowed to react with malonic acid (0.208 g, 2 mmol) in water (10 ml) to give a clear blue solution. A warm aqueous solution (10 ml) of 2-aminopyridine (0.188 g, 2 mmol) was added dropwise to the above blue solution with continuous

stirring. The pH of this solution was adjusted to 5.20 by dropwise addition of dilute NaOH. This solution was heated at 323 K for 1 h with continuous stirring

and then filtered and kept for crystallization. Flat blue single crystals of (I) suitable for X-ray analysis were separated after several weeks from the mother liquor by slow evaporation at room temperature. The crystals were filtered off, washed with cold water and dried on filter paper (yield 0.24 g, 48%). Analysis, calculated for $C_{16}H_{22}N_4O_{10}Cu$: C 38.91, H 4.49, N 11.34%; found: C 38.22, H 3.89, N 10.91%.

Refinement

H atoms attached to C and N atoms were placed in geometrically idealized positions, with Csp^2—H = 0.93, Csp^3—H = 0.97 and Nsp^2—H = 0.86 Å, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C,*N*). H atoms attached to O (water) were located in a difference Fourier map and refined freely.

Figures

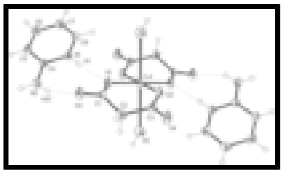

Fig. 1. The structure of (I), with displacement ellipsoids drawn at the 30% probability level. Dotted lines indicate hydrogen bonds. Unlabelled atoms are generated by the inversion operation (1 − *x*, 1 − *y*, 1 − *z*).

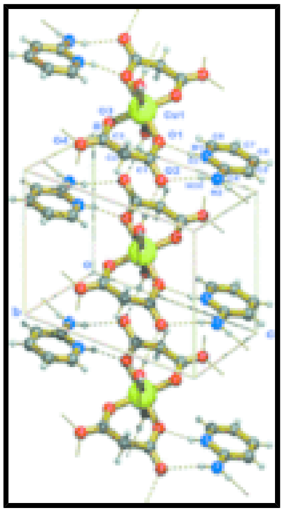

Fig. 2. The one-dimensional assembly of monomeric units along the *a* axis with 2-aminopyridinium. Dashed lines indicate hydrogen bonds.

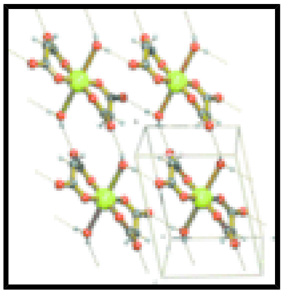

Fig. 3. The two-dimensional assembly of monomeric units. Aminopyridinium ligands have been omitted for clarity. Dashed lines indicate hydrogen bonds.

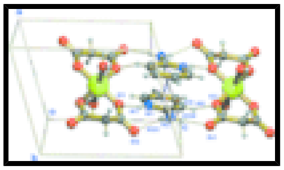

Fig. 4. The π–π stacking (blue dotted line) between aminopyridine units. N2—H2D···O4 and C5—H5···O3 hydrogen bonds (dashed lines) help to grow the structure along *c* axis.

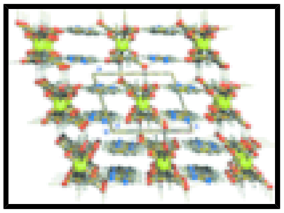

Fig. 5. The packing of complex (I), resulting in the three-dimensional assembly. Dotted lines indicate hydrogen bonds.

Bis(2-aminopyridinium) diaquabis(malonato-κ^2*O,O'*)cuprate(II)

Crystal data

$(C_5H_7N_2)_2[Cu(C_3H_2O_4)_2(H_2O_1)_2]$

M_r = 493.92

Triclinic, $P\bar{1}$

Hall symbol: -P 1

a = 7.0433 (13) Å

b = 7.9116 (15) Å

c = 9.5767 (18) Å

α = 96.096 (2)º

β = 107.865 (2)º

γ = 103.743 (2)º

V = 484.03 (16) Å^3

Z = 1

F_{000} = 255

D_x = 1.694 Mg m^{-3}

Mo *K*α radiation
λ = 0.71073 Å

Cell parameters from 1903 reflections

θ = 3.2–26.9º

μ = 1.19 mm^{-1}

T = 298 (2) K

Block, blue

0.50 × 0.40 × 0.30 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 298(2) K

ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 2000)

1659 independent reflections

1616 reflections with $I > 2\sigma(I)$

R_{int} = 0.013

θ_{max} = 25.0º

θ_{min} = 2.3º

$h = -8 \rightarrow 8$

$T_{\min} = 0.587$, $T_{\max} = 0.716$	$k = -7 \rightarrow 9$
1987 measured reflections	$l = -11 \rightarrow 10$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.028$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.075$	$w = 1/[\sigma^2(F_o^2) + (0.0298P)^2 + 0.2343P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.14$	$(\Delta/\sigma)_{\max} = 0.001$
1659 reflections	$\Delta\rho_{\max} = 0.21$ e Å^{-3}
150 parameters	$\Delta\rho_{\min} = -0.27$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	$U_{\rm iso}$*/$U_{\rm eq}$
Cu1	0.5000	0.5000	0.5000	0.03666 (15)
O1	0.3286 (2)	0.5451 (2)	0.61517 (16)	0.0376 (3)
O2	0.1202 (3)	0.6770 (2)	0.68071 (18)	0.0439 (4)
O3	0.3648 (2)	0.6104 (2)	0.34319 (15)	0.0369 (3)
O4	0.2336 (3)	0.8215 (2)	0.26013 (18)	0.0486 (4)
O5	0.7799 (3)	0.8175 (3)	0.6047 (2)	0.0528 (5)
C1	0.2326 (3)	0.6633 (3)	0.6054 (2)	0.0303 (4)
C2	0.2668 (4)	0.7969 (3)	0.5094 (2)	0.0390 (5)
H2A	0.3917	0.8911	0.5679	0.047*
H2B	0.1517	0.8487	0.4899	0.047*
C3	0.2884 (3)	0.7385 (3)	0.3595 (2)	0.0325 (4)
C4	0.2435 (3)	0.4109 (3)	0.9537 (2)	0.0338 (4)
C5	0.2439 (3)	0.3007 (3)	1.0592 (2)	0.0403 (5)
H5	0.2326	0.3410	1.1503	0.048*
C6	0.2608 (4)	0.1344 (3)	1.0272 (3)	0.0494 (6)

H6	0.2603	0.0608	1.0967	0.059*
C7	0.2791 (4)	0.0732 (3)	0.8911 (3)	0.0497 (6)
H7	0.2896	−0.0408	0.8690	0.060*
C8	0.2810 (4)	0.1815 (3)	0.7930 (3)	0.0439 (5)
H8	0.2933	0.1425	0.7019	0.053*
N1	0.2655 (3)	0.3464 (2)	0.82503 (19)	0.0355 (4)
H1	0.2697	0.4138	0.7606	0.043*
N2	0.2258 (3)	0.5744 (2)	0.9738 (2)	0.0424 (4)
H2C	0.2285	0.6366	0.9057	0.051*
H2D	0.2117	0.6180	1.0550	0.051*
H5A	0.889 (6)	0.788 (5)	0.630 (4)	0.076 (11)*
H5B	0.803 (5)	0.908 (4)	0.651 (3)	0.056 (10)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0490 (2)	0.0496 (3)	0.0299 (2)	0.03156 (18)	0.02295 (17)	0.01711 (16)
O1	0.0514 (9)	0.0448 (8)	0.0358 (8)	0.0291 (7)	0.0264 (7)	0.0181 (6)
O2	0.0540 (9)	0.0571 (10)	0.0429 (9)	0.0338 (8)	0.0308 (8)	0.0194 (7)
O3	0.0502 (9)	0.0432 (8)	0.0275 (7)	0.0250 (7)	0.0175 (6)	0.0102 (6)
O4	0.0646 (11)	0.0630 (11)	0.0404 (9)	0.0396 (9)	0.0268 (8)	0.0283 (8)
O5	0.0483 (11)	0.0505 (12)	0.0596 (12)	0.0219 (9)	0.0138 (9)	0.0073 (10)
C1	0.0349 (10)	0.0336 (10)	0.0250 (9)	0.0146 (9)	0.0108 (8)	0.0036 (8)
C2	0.0555 (13)	0.0354 (11)	0.0379 (11)	0.0233 (10)	0.0233 (10)	0.0116 (9)
C3	0.0341 (10)	0.0373 (11)	0.0308 (10)	0.0143 (9)	0.0133 (8)	0.0107 (8)
C4	0.0303 (10)	0.0374 (11)	0.0307 (10)	0.0056 (9)	0.0100 (8)	0.0057 (8)
C5	0.0471 (12)	0.0443 (13)	0.0305 (11)	0.0103 (10)	0.0156 (9)	0.0103 (9)
C6	0.0576 (15)	0.0451 (14)	0.0442 (13)	0.0100 (11)	0.0160 (11)	0.0183 (11)
C7	0.0602 (15)	0.0338 (12)	0.0541 (15)	0.0132 (11)	0.0196 (12)	0.0057 (10)
C8	0.0500 (13)	0.0419 (12)	0.0383 (12)	0.0106 (10)	0.0176 (10)	−0.0001 (10)
N1	0.0394 (9)	0.0397 (10)	0.0288 (9)	0.0101 (8)	0.0137 (7)	0.0093 (7)
N2	0.0559 (12)	0.0402 (10)	0.0381 (10)	0.0170 (9)	0.0229 (9)	0.0095 (8)

Geometric parameters (Å, °)

Cu1—O3^{i}	1.9293 (14)	C4—N2	1.328 (3)
Cu1—O3	1.9293 (14)	C4—N1	1.350 (3)
Cu1—O1	1.9336 (14)	C4—C5	1.403 (3)
Cu1—O1^{i}	1.9336 (14)	C5—C6	1.360 (3)
Cu1—O5	2.665 (2)	C5—H5	0.9300
O1—C1	1.273 (2)	C6—C7	1.396 (4)
O2—C1	1.238 (2)	C6—H6	0.9300
O3—C3	1.272 (2)	C7—C8	1.338 (3)
O4—C3	1.230 (3)	C7—H7	0.9300
O5—H5A	0.83 (4)	C8—N1	1.347 (3)
O5—H5B	0.76 (3)	C8—H8	0.9300
C1—C2	1.498 (3)	N1—H1	0.8600
C2—C3	1.524 (3)	N2—H2C	0.8600

C2—H2A	0.9700	N2—H2D	0.8600
C2—H2B	0.9700		
O3^{i}—Cu1—O3	180.0	O4—C3—C2	117.50 (18)
O3^{i}—Cu1—O1	87.80 (6)	O3—C3—C2	119.42 (17)
O3—Cu1—O1	92.20 (6)	N2—C4—N1	118.51 (19)
O3^{i}—Cu1—O1^{i}	92.20 (6)	N2—C4—C5	124.0 (2)
O3—Cu1—O1^{i}	87.80 (6)	N1—C4—C5	117.5 (2)
O1—Cu1—O1^{i}	180.0	C6—C5—C4	119.5 (2)
O3—Cu1—O5	84.65 (6)	C6—C5—H5	120.3
O3^{i}—Cu1—O5	95.35 (6)	C4—C5—H5	120.3
O1^{i}—Cu1—O5	84.96 (7)	C5—C6—C7	120.6 (2)
O1—Cu1—O5	95.04 (7)	C5—C6—H6	119.7
C1—O1—Cu1	126.40 (13)	C7—C6—H6	119.7
C3—O3—Cu1	126.18 (13)	C8—C7—C6	118.8 (2)
H5A—O5—H5B	107 (3)	C8—C7—H7	120.6
O2—C1—O1	121.31 (18)	C6—C7—H7	120.6
O2—C1—C2	118.82 (18)	C7—C8—N1	120.5 (2)
O1—C1—C2	119.74 (17)	C7—C8—H8	119.7
C1—C2—C3	119.44 (18)	N1—C8—H8	119.7
C1—C2—H2A	107.5	C8—N1—C4	123.03 (19)
C3—C2—H2A	107.5	C8—N1—H1	118.5
C1—C2—H2B	107.5	C4—N1—H1	118.5
C3—C2—H2B	107.5	C4—N2—H2C	120.0
H2A—C2—H2B	107.0	C4—N2—H2D	120.0
O4—C3—O3	123.06 (18)	H2C—N2—H2D	120.0
O3^{i}—Cu1—O1—C1	157.70 (18)	C1—C2—C3—O4	151.5 (2)
O3—Cu1—O1—C1	−22.30 (18)	C1—C2—C3—O3	−29.9 (3)
O1—Cu1—O3—C3	31.54 (17)	N2—C4—C5—C6	179.4 (2)
O1^{i}—Cu1—O3—C3	−148.46 (17)	N1—C4—C5—C6	−1.6 (3)
Cu1—O1—C1—O2	177.25 (15)	C4—C5—C6—C7	0.4 (4)
Cu1—O1—C1—C2	−7.0 (3)	C5—C6—C7—C8	0.5 (4)
O2—C1—C2—C3	−145.0 (2)	C6—C7—C8—N1	−0.1 (4)
O1—C1—C2—C3	39.2 (3)	C7—C8—N1—C4	−1.2 (3)
Cu1—O3—C3—O4	168.22 (16)	N2—C4—N1—C8	−178.8 (2)
Cu1—O3—C3—C2	−10.4 (3)	C5—C4—N1—C8	2.0 (3)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.86	1.91	2.756 (2)	168
N2—H2C···O2	0.86	2.14	2.930 (3)	152
N2—H2D···O4^{ii}	0.86	2.35	3.172 (3)	161
O5—H5A···O2^{iii}	0.83 (4)	1.99 (4)	2.807 (3)	171 (3)
O5—H5B···O4^{iv}	0.76 (3)	2.31 (3)	3.043 (3)	161 (3)
C5—H5···O3^{ii}	0.93	2.45	3.209 (3)	139

C6—H6···O4^{v}	0.93	2.59	3.514 (3)	172
C7—H7···O2^{vi}	0.93	2.49	3.278 (3)	142

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

Fig. 1

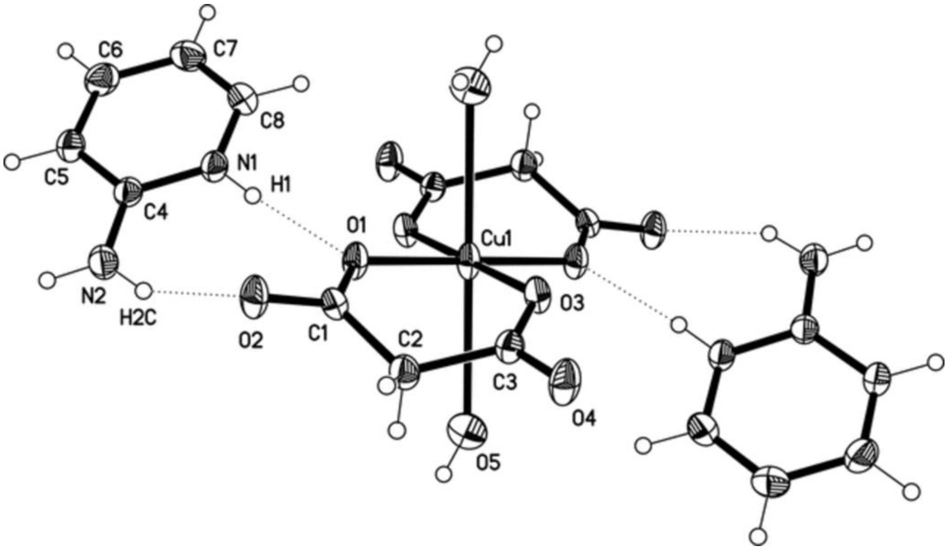

Fig. 2

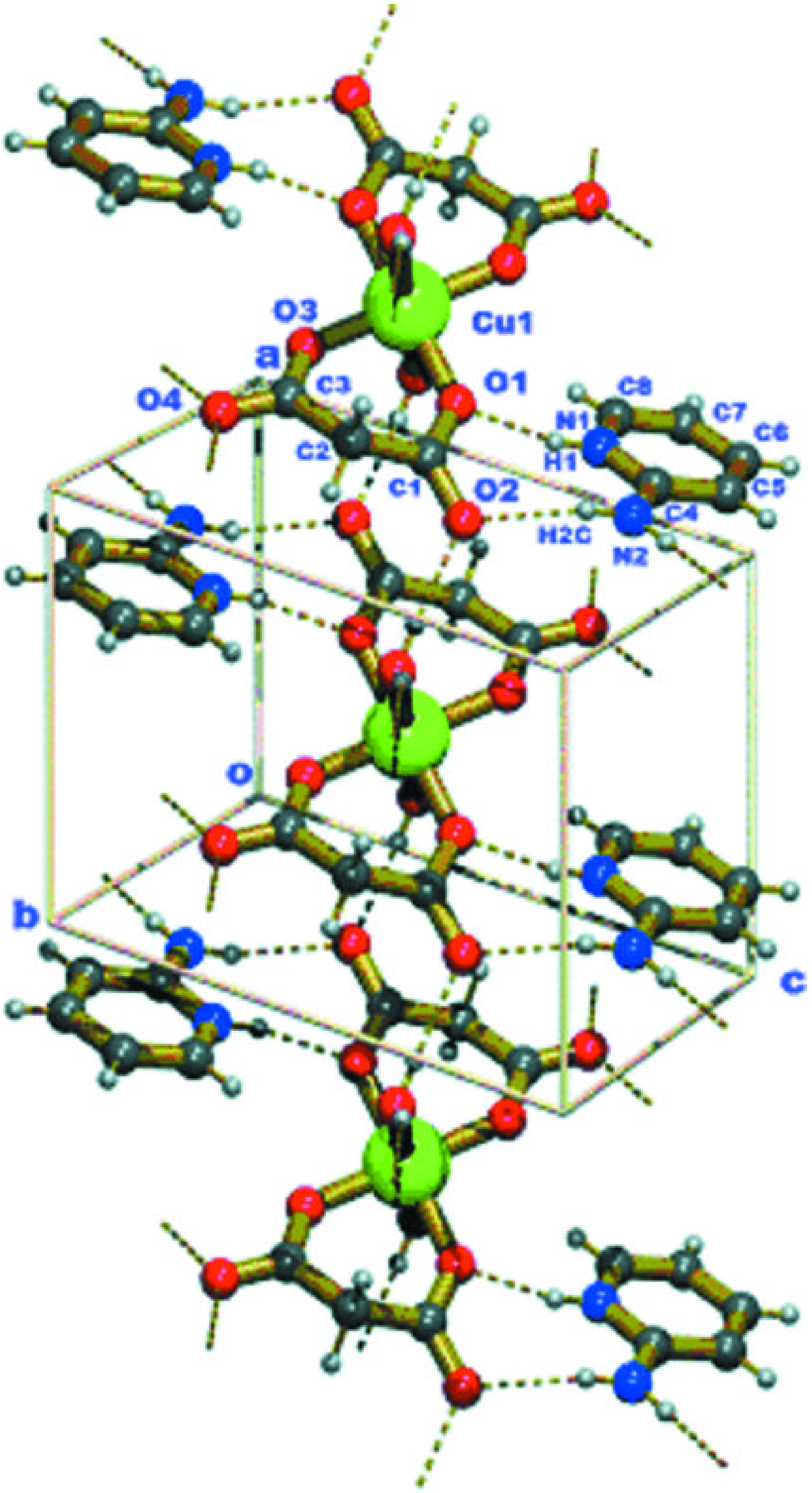

Fig. 3

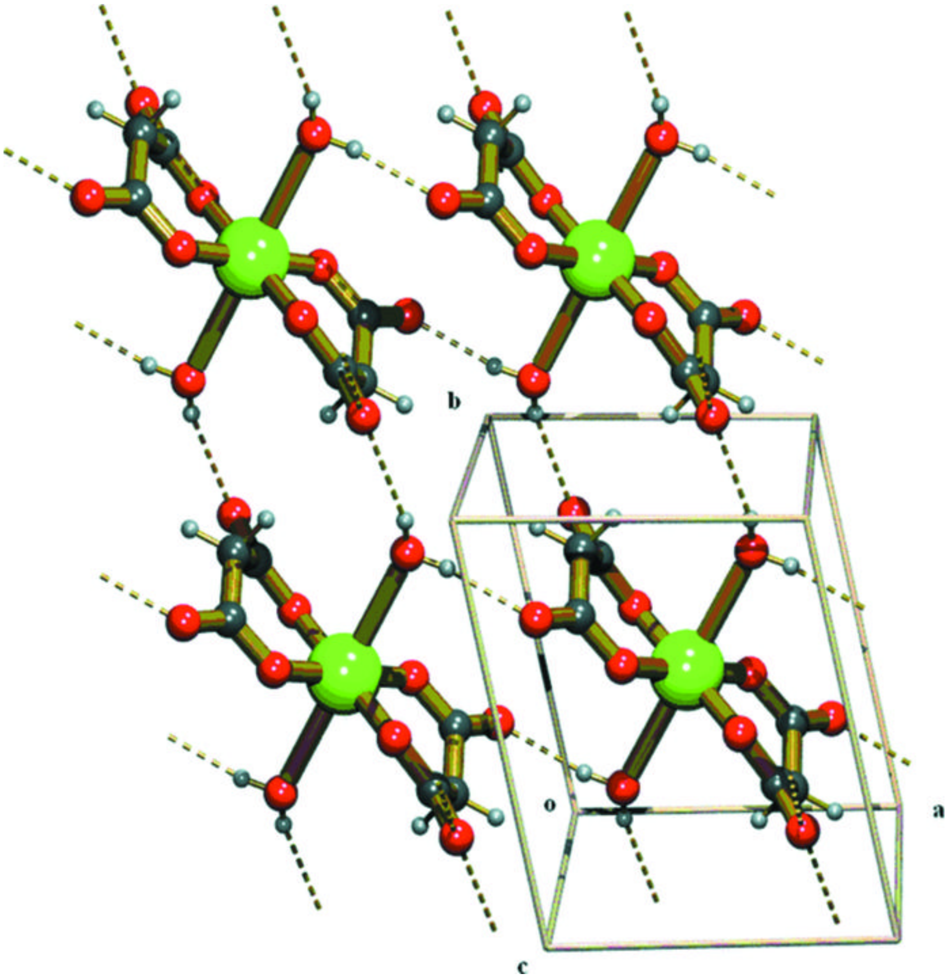

Fig. 4

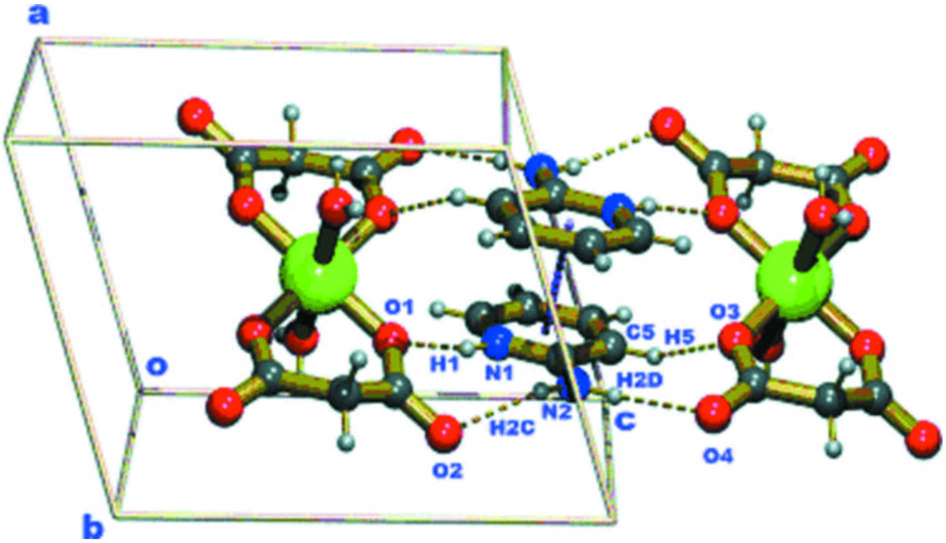

Fig. 5