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Poly[[μ_3 -dihydrogen [(pyridin-4-yl-methylimino)bis(methylene)]diphosphonato- κ^5 O:O',N,O'':N']copper(II) dihydrate]

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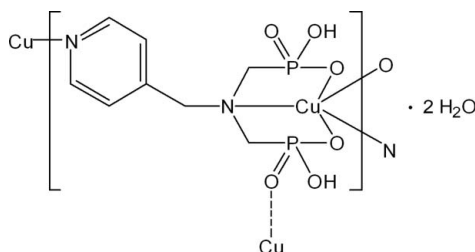
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.046; wR factor = 0.118; data-to-parameter ratio = 16.2.

In the title polymer, $\{[\text{Cu}(\text{C}_8\text{H}_{12}\text{N}_2\text{O}_6\text{P}_2)] \cdot 2\text{H}_2\text{O}\}_n$, the geometry of the five-coordinate Cu^{II} ion can best be described as slightly distorted square-pyramidal formed by one N and two O atoms of an $\text{N}(\text{CH}_2\text{PO}_3\text{H})_2$ group and one N atom from a pyridine ring. The elongated apex of the pyramid is occupied by one O atom from a third diphosphonate ligand. The interconnection of Cu^{2+} ions by the diphosphonate ligands results in the formation of a double-chain array along the b axis, in which the two sub-chains are interlocked by pairs of PO_3 groups. The outside of each sub-chain is decorated by other PO_3 groups. These double chains are further assembled into a three-dimensional supramolecular architecture *via* a large number of $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds between the phosphonate groups and lattice water molecules.

Related literature

For background to metal phosphonate chemistry, see: Maeda (2004); Mao (2007); Shimizu *et al.* (2009). For the synthetic strategy of attaching functional groups to a phosphonic acid ligand, see: Drumel *et al.* (1995); Mao *et al.* (2002); Liang & Shimizu (2007); Du *et al.* (2006, 2010*b*). For a structurally related complex, see: Song & Mao (2005). For the zwitterionic behavior of aminophosphonic acid, see: Yang *et al.* (2008); Du *et al.* (2009, 2010*a*).



Experimental

Crystal data

$[\text{Cu}(\text{C}_8\text{H}_{12}\text{N}_2\text{O}_6\text{P}_2)] \cdot 2\text{H}_2\text{O}$
 $M_r = 393.71$
 Triclinic, $P\bar{1}$
 $a = 8.9250$ (3) Å
 $b = 9.0000$ (3) Å
 $c = 10.5066$ (3) Å
 $\alpha = 75.648$ (2)°
 $\beta = 67.124$ (2)°
 $\gamma = 67.126$ (2)°
 $V = 711.75$ (4) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.80$ mm⁻¹
 $T = 296$ K
 $0.40 \times 0.03 \times 0.02$ mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2008)
 $T_{\text{min}} = 0.605$, $T_{\text{max}} = 0.746$
 7659 measured reflections
 3267 independent reflections
 2309 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.043$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.118$
 $S = 1.03$
 3267 reflections
 202 parameters
 6 restraints
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.50$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.60$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{O1}-\text{H1B} \cdots \text{O1W}$	0.82	1.68	2.494 (4)	169
$\text{O6}-\text{H6C} \cdots \text{O2W}$	0.82	1.75	2.567 (5)	172
$\text{O1W}-\text{H1WA} \cdots \text{O5}^{\text{i}}$	0.83 (2)	1.92 (2)	2.746 (4)	177 (5)
$\text{O1W}-\text{H1WB} \cdots \text{O5}^{\text{ii}}$	0.84 (2)	1.93 (2)	2.747 (4)	167 (5)
$\text{O2W}-\text{H2WA} \cdots \text{O1}^{\text{iii}}$	0.85 (2)	2.09 (3)	2.882 (4)	155 (5)
$\text{O2W}-\text{H2WB} \cdots \text{O3}^{\text{iv}}$	0.85 (2)	1.96 (3)	2.776 (4)	161 (6)

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

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); 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) and DIAMOND (Brandenburg, 2010); 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: FJ2483).

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supporting information

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Poly[[μ_3 -dihydrogen [(pyridin-4-ylmethylimino)bis(methylene)]diphosphonato- κ^5 O:O',N,O'':N'}copper(II)] dihydrate]

Shi-Yong Zhang, Zhong-Gao Zhou and Ke-Jun Wang

S1. Comment

During the past few decades, the syntheses of metal phosphonates with various structures has attracted much attention, owing to their potential applications in areas such as catalysis, ion exchange, intercalation chemistry, and material chemistry (Maeda, 2004; Mao, 2007; Shimizu *et al.*, 2009). The strategy of attaching functional groups such as amine, hydroxyl, carboxylate, sulfonate, and sulfone groups to the phosphonic acid has proven to be an effective method for the isolation of a variety of metal phosphonates with new structures (Drumel *et al.*, 1995; Mao *et al.*, 2002; Liang & Shimizu, 2007; Du *et al.* 2006, 2010*b*). Recently, we are interested in the combination of multiple functional groups to phosphonic acid as a more complex ligand. Herein, we report a copper(II) phosphonate based on an amino-bis(methyl-phosphonic acid) ligand, which contains pyridyl group as an additional functional group. As far as we are aware, only one layered cobalt(II) phosphonate has been reported based on the same ligand (Song & Mao, 2005).

The title compound (I) features a one-dimensional double-chain structure. The formula of it contains one Cu^{2+} ion, one H_2L^{2-} anion and two lattice water molecules. $\text{Cu}(1)$ ion is five-coordinate and its coordination geometry can be described as a slightly distorted square-pyramid (Fig. 1): the square plane is formed by one N and two O atoms of a $\text{N}(\text{CH}_2\text{PO}_3\text{H})_2$ group as well as one N atom of a pyridyl group from two H_2L^{2-} ligand, and the prolonged apex of the pyramid is occupied by one O atom from a third H_2L^{2-} ligand. The H_2L^{2-} ligand in compound (I) acts as a pentadentate chelating and bridging ligand. It chelates one Cu^{2+} ion by its $\text{N}(\text{CH}_2\text{PO}_3\text{H})_2$ group in a tridentate fashion (2O and 1 N), and also bridges with other two Cu^{2+} ions *via* its pyridyl group and a third O atom (Scheme 1). The two phosphonate groups of the H_2L^{2-} ligand both are 1*H*-protonated as the requirement for charge balance and also as indicated by two much longer P—O bonds. It is worthy of note that the strongly basic N atom in the H_2L^{2-} ligand is not protonated but bonded to a Cu^{2+} ion, which is rarely observed for phosphonic acid ligands containing a tertiary amine group (Yang *et al.*, 2008; Du *et al.*, 2009, 2010*a*).

The interconnection of the Cu^{2+} ions by the HL^{2-} anions results in the formation of a one-dimensional double-chain array along the *b*-axis, in which the two sub-chains are inter-locked by pairs of $\text{P}(1)\text{O}_3$ groups and the outside of each sub-chain is decorated by $\text{P}(2)\text{O}_3$ groups. It is worthy of note that such two sub-chains are related by inversion centers, and the shortest $\text{Cd}\cdots\text{Cd}$ distance between them is 5.170 (4) Å while that in each sub-chain is 9.000 (1) Å. These double-chains are further assembled into a three-dimensional supramolecular architecture *via* a large number of hydrogen bonds between the phosphonate groups and lattice water molecules (Fig. 3 and Table 1).

S2. Experimental

4-Pyridyl- $\text{CH}_2\text{N}(\text{CH}_2\text{PO}_3\text{H}_2)_2$ (0.2 mmol) was dissolved in 4 ml H_2O and poured into a test tube, then $\text{CuCl}_2\cdot 2\text{H}_2\text{O}$ (0.15 mmol) dissolved in 8 ml EtOH was carefully layered onto it and left to stand at room temperature. Blue column-shaped crystals of (I) were obtained after about two weeks later. IR data for (I) (KBr, cm^{-1}): 3477(*s*), 3228(*s*), 3141(*m*), 3079(*m*), 2975(*m*), 2913(*m*), 2376(*m*), 1846(*m*), 1624(*s*), 1502(*m*), 1448(*m*), 1433(*m*), 1350(*m*), 1266(*s*), 1221(*m*), 1173(*s*),

1140(*versus*), 1065(*s*), 1051(*s*), 1032(*s*), 945(*s*), 929(*m*), 906(*m*), 866(*m*), 844(*m*), 795(*m*), 742(*m*), 648(*m*), 588(*s*), 524(*m*), 482(*m*), 453(*m*).

S3. Refinement

C-bound H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93 or 0.97 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. H atoms of $-\text{PO}_3\text{H}^-$ groups were also placed in idealized positions and constrained to ride on their parent atoms, with O—H distances of 0.82 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$. Water H atoms were located in a difference map and refined with $U_{\text{iso}}(\text{H})$ values set at $1.5U_{\text{eq}}(\text{O})$. The O—H distances of water were restrained to be 0.85 (1) Å.

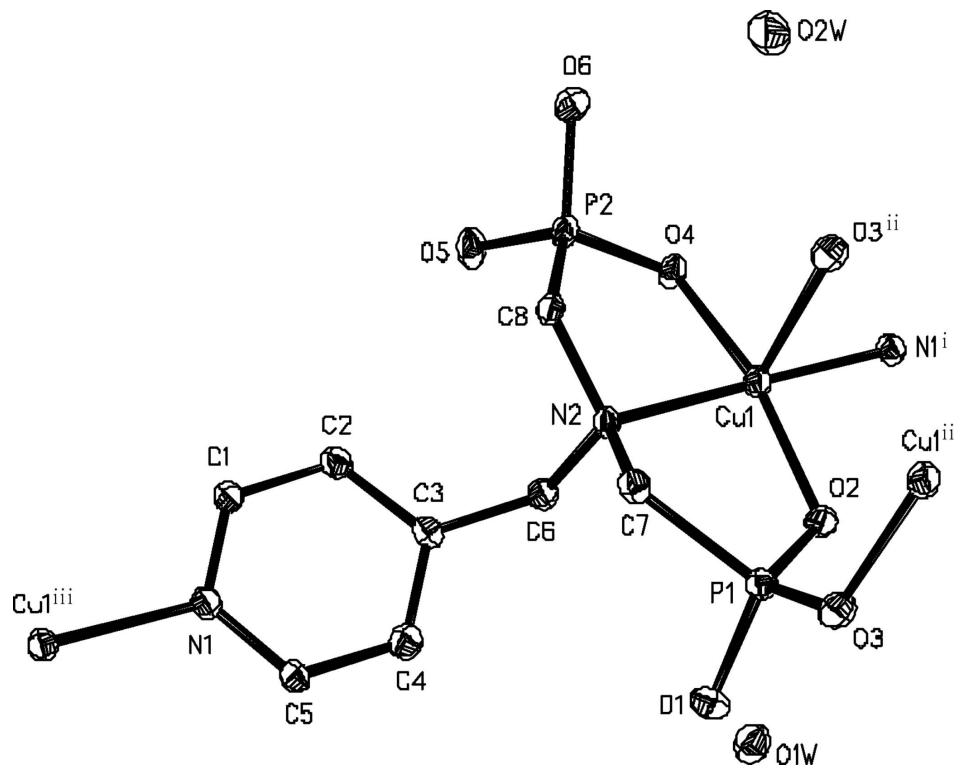
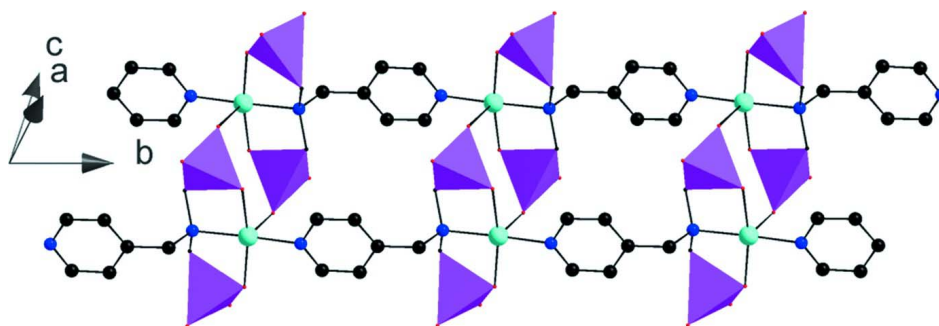
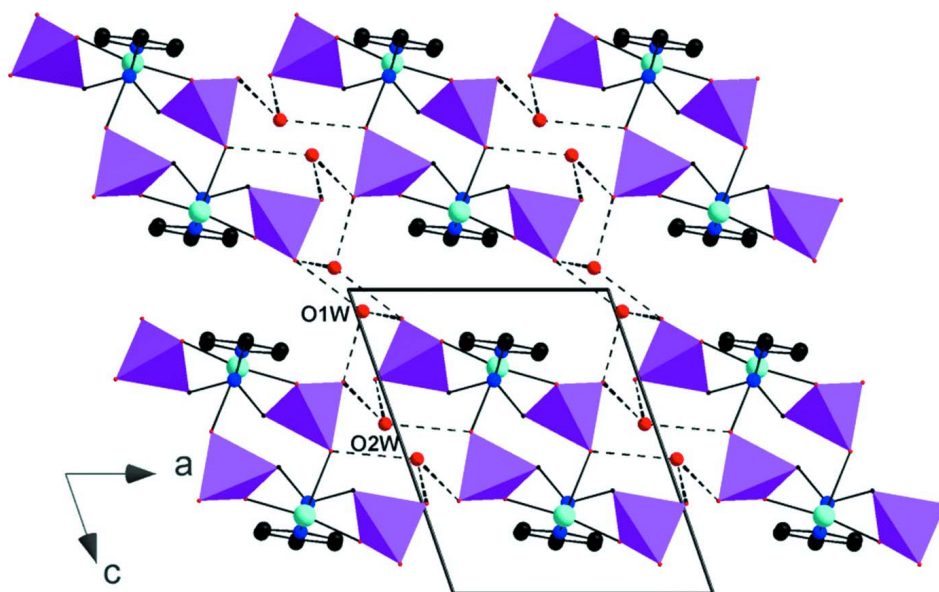


Figure 1

View of the selected unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) $x, y + 1, z$; (ii) $-x + 1, -y + 1, -z + 1$; (iii) $x, y - 1, z$.]

**Figure 2**

View of the double-chain structure of (I) along the *b*-axis. The CPO_3 tetrahedra are shaded in purple. Cu, N and C atoms are drawn as cyan, blue and black circles, respectively.

**Figure 3**

View of the structure of (I) down the *b*-axis. For display details, see the caption for Fig. 2. Hydrogen bonds are represented by dashed lines.

Poly[[μ_3 -dihydrogen [(pyridin-4-ylmethylimino)bis(methylene)]diphosphonato- $\kappa^5\text{O}:O',N,O'':N'$]copper(II)] dihydrate]

Crystal data

$[\text{Cu}(\text{C}_8\text{H}_{12}\text{N}_2\text{O}_6\text{P}_2)] \cdot 2\text{H}_2\text{O}$

$M_r = 393.71$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 8.9250(3)\ \text{\AA}$

$b = 9.0000(3)\ \text{\AA}$

$c = 10.5066(3)\ \text{\AA}$

$\alpha = 75.648(2)^\circ$

$\beta = 67.124(2)^\circ$

$\gamma = 67.126(2)^\circ$

$V = 711.75(4)\ \text{\AA}^3$

$Z = 2$

$F(000) = 402$

$D_x = 1.837\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 1430 reflections

$\theta = 2.1\text{--}27.6^\circ$

$\mu = 1.80\ \text{mm}^{-1}$

$T = 296\ \text{K}$

Needle, blue

$0.40 \times 0.03 \times 0.02\ \text{mm}$

Data collection

Bruker APEXII CCD
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan
(*SADABS*; Bruker, 2008)
 $T_{\min} = 0.605$, $T_{\max} = 0.746$

7659 measured reflections
3267 independent reflections
2309 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.043$
 $\theta_{\text{max}} = 27.6^\circ$, $\theta_{\text{min}} = 2.1^\circ$
 $h = -10 \rightarrow 11$
 $k = -11 \rightarrow 11$
 $l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.118$
 $S = 1.03$
3267 reflections
202 parameters
6 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
 $w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 0.1702P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.50 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.60 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.47006 (6)	0.60143 (5)	0.25556 (5)	0.02485 (17)
P1	0.69833 (14)	0.32696 (12)	0.39341 (11)	0.0237 (2)
P2	0.17163 (14)	0.57368 (13)	0.21239 (12)	0.0265 (3)
N1	0.5076 (4)	-0.1825 (4)	0.2025 (3)	0.0240 (7)
N2	0.4396 (4)	0.3746 (4)	0.2980 (3)	0.0207 (7)
C1	0.3823 (5)	-0.0485 (5)	0.1777 (4)	0.0282 (9)
H1A	0.2869	-0.0590	0.1696	0.034*
C2	0.3912 (5)	0.1042 (5)	0.1641 (4)	0.0293 (10)
H2A	0.3025	0.1945	0.1457	0.035*
C3	0.5301 (5)	0.1261 (4)	0.1773 (4)	0.0233 (9)
C4	0.6596 (6)	-0.0148 (5)	0.1992 (4)	0.0294 (9)
H4A	0.7570	-0.0076	0.2065	0.035*
C5	0.6465 (5)	-0.1652 (5)	0.2102 (4)	0.0273 (9)
H5A	0.7364	-0.2575	0.2233	0.033*
C6	0.5389 (5)	0.2920 (4)	0.1674 (4)	0.0243 (9)

H6A	0.4964	0.3607	0.0933	0.029*
H6B	0.6587	0.2831	0.1412	0.029*
C7	0.5053 (5)	0.2840 (5)	0.4152 (4)	0.0235 (9)
H7A	0.5324	0.1684	0.4164	0.028*
H7B	0.4179	0.3168	0.5029	0.028*
C8	0.2500 (5)	0.4113 (5)	0.3387 (4)	0.0224 (8)
H8A	0.1931	0.4454	0.4312	0.027*
H8B	0.2255	0.3151	0.3391	0.027*
O1	0.8567 (4)	0.1971 (3)	0.3047 (3)	0.0309 (7)
H1B	0.9034	0.2423	0.2302	0.046*
O2	0.6750 (3)	0.4935 (3)	0.3111 (3)	0.0278 (6)
O3	0.7175 (4)	0.3101 (3)	0.5319 (3)	0.0307 (7)
O4	0.2907 (3)	0.6731 (3)	0.1706 (3)	0.0273 (6)
O5	0.1664 (4)	0.5097 (3)	0.0961 (3)	0.0356 (7)
O6	-0.0163 (4)	0.6712 (4)	0.2955 (3)	0.0393 (8)
H6C	-0.0137	0.7334	0.3394	0.059*
O1W	1.0256 (4)	0.3000 (4)	0.0716 (3)	0.0381 (8)
H1WA	1.065 (6)	0.366 (5)	0.078 (5)	0.057*
H1WB	0.964 (6)	0.344 (5)	0.021 (5)	0.057*
O2W	-0.0383 (5)	0.8732 (4)	0.4421 (4)	0.0462 (9)
H2WA	-0.037 (7)	0.965 (4)	0.397 (5)	0.069*
H2WB	0.053 (5)	0.832 (6)	0.464 (6)	0.069*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0279 (3)	0.0187 (3)	0.0339 (3)	-0.0064 (2)	-0.0186 (2)	-0.0011 (2)
P1	0.0258 (6)	0.0185 (5)	0.0290 (6)	-0.0027 (4)	-0.0154 (5)	-0.0030 (4)
P2	0.0283 (6)	0.0233 (5)	0.0369 (6)	-0.0077 (5)	-0.0215 (5)	-0.0020 (5)
N1	0.0277 (18)	0.0195 (17)	0.0268 (19)	-0.0072 (14)	-0.0117 (15)	-0.0025 (14)
N2	0.0248 (17)	0.0177 (16)	0.0235 (17)	-0.0068 (14)	-0.0127 (15)	-0.0014 (13)
C1	0.026 (2)	0.023 (2)	0.042 (3)	-0.0039 (17)	-0.018 (2)	-0.0081 (19)
C2	0.030 (2)	0.022 (2)	0.040 (3)	-0.0025 (18)	-0.020 (2)	-0.0054 (18)
C3	0.028 (2)	0.0192 (19)	0.023 (2)	-0.0061 (17)	-0.0087 (18)	-0.0038 (16)
C4	0.031 (2)	0.028 (2)	0.034 (2)	-0.0097 (19)	-0.015 (2)	-0.0042 (19)
C5	0.028 (2)	0.0169 (19)	0.039 (3)	-0.0065 (17)	-0.017 (2)	-0.0003 (18)
C6	0.028 (2)	0.022 (2)	0.027 (2)	-0.0063 (17)	-0.0142 (18)	-0.0024 (17)
C7	0.031 (2)	0.0188 (19)	0.023 (2)	-0.0078 (17)	-0.0125 (18)	0.0005 (16)
C8	0.023 (2)	0.022 (2)	0.026 (2)	-0.0100 (17)	-0.0100 (18)	-0.0025 (17)
O1	0.0302 (16)	0.0228 (15)	0.0335 (17)	-0.0006 (13)	-0.0123 (14)	-0.0028 (13)
O2	0.0279 (16)	0.0194 (14)	0.0395 (17)	-0.0054 (12)	-0.0194 (14)	0.0008 (13)
O3	0.0312 (17)	0.0335 (16)	0.0321 (17)	-0.0054 (13)	-0.0200 (14)	-0.0043 (13)
O4	0.0315 (16)	0.0234 (14)	0.0367 (17)	-0.0100 (12)	-0.0243 (14)	0.0038 (13)
O5	0.049 (2)	0.0308 (16)	0.0431 (19)	-0.0148 (15)	-0.0302 (16)	-0.0026 (14)
O6	0.0290 (17)	0.0360 (18)	0.061 (2)	-0.0048 (14)	-0.0248 (16)	-0.0111 (16)
O1W	0.041 (2)	0.0387 (19)	0.042 (2)	-0.0163 (16)	-0.0204 (16)	0.0014 (15)
O2W	0.048 (2)	0.0337 (19)	0.061 (2)	-0.0053 (17)	-0.030 (2)	-0.0057 (17)

Geometric parameters (Å, °)

Cu1—O2	1.949 (3)	C2—C3	1.390 (5)
Cu1—O4	1.949 (2)	C2—H2A	0.9300
Cu1—N1 ⁱ	2.008 (3)	C3—C4	1.385 (5)
Cu1—N2	2.080 (3)	C3—C6	1.501 (5)
Cu1—O3 ⁱⁱ	2.315 (3)	C4—C5	1.376 (5)
P1—O3	1.495 (3)	C4—H4A	0.9300
P1—O2	1.514 (3)	C5—H5A	0.9300
P1—O1	1.570 (3)	C6—H6A	0.9700
P1—C7	1.827 (4)	C6—H6B	0.9700
P2—O5	1.497 (3)	C7—H7A	0.9700
P2—O4	1.518 (3)	C7—H7B	0.9700
P2—O6	1.563 (3)	C8—H8A	0.9700
P2—C8	1.831 (4)	C8—H8B	0.9700
N1—C1	1.340 (5)	O1—H1B	0.8200
N1—C5	1.341 (5)	O3—Cu1 ⁱⁱ	2.315 (3)
N1—Cu1 ⁱⁱⁱ	2.008 (3)	O6—H6C	0.8200
N2—C7	1.489 (5)	O1W—H1WA	0.832 (19)
N2—C8	1.492 (5)	O1W—H1WB	0.836 (19)
N2—C6	1.507 (5)	O2W—H2WA	0.846 (19)
C1—C2	1.376 (6)	O2W—H2WB	0.848 (19)
C1—H1A	0.9300		
O2—Cu1—O4	167.12 (11)	C3—C2—H2A	119.4
O2—Cu1—N1 ⁱ	93.65 (12)	C4—C3—C2	115.6 (3)
O4—Cu1—N1 ⁱ	92.92 (12)	C4—C3—C6	122.4 (4)
O2—Cu1—N2	86.48 (11)	C2—C3—C6	121.9 (3)
O4—Cu1—N2	86.29 (11)	C5—C4—C3	121.1 (4)
N1 ⁱ —Cu1—N2	176.50 (13)	C5—C4—H4A	119.4
O2—Cu1—O3 ⁱⁱ	96.97 (11)	C3—C4—H4A	119.4
O4—Cu1—O3 ⁱⁱ	94.37 (11)	N1—C5—C4	121.9 (4)
N1 ⁱ —Cu1—O3 ⁱⁱ	87.53 (12)	N1—C5—H5A	119.0
N2—Cu1—O3 ⁱⁱ	95.93 (11)	C4—C5—H5A	119.0
O3—P1—O2	116.53 (16)	C3—C6—N2	115.5 (3)
O3—P1—O1	108.57 (16)	C3—C6—H6A	108.4
O2—P1—O1	110.13 (17)	N2—C6—H6A	108.4
O3—P1—C7	110.01 (18)	C3—C6—H6B	108.4
O2—P1—C7	103.88 (16)	N2—C6—H6B	108.4
O1—P1—C7	107.31 (17)	H6A—C6—H6B	107.5
O5—P2—O4	115.75 (17)	N2—C7—P1	109.1 (3)
O5—P2—O6	108.56 (17)	N2—C7—H7A	109.9
O4—P2—O6	111.15 (16)	P1—C7—H7A	109.9
O5—P2—C8	112.42 (17)	N2—C7—H7B	109.9
O4—P2—C8	103.00 (16)	P1—C7—H7B	109.9
O6—P2—C8	105.44 (18)	H7A—C7—H7B	108.3
C1—N1—C5	118.3 (3)	N2—C8—P2	108.1 (3)
C1—N1—Cu1 ⁱⁱⁱ	120.0 (3)	N2—C8—H8A	110.1

C5—N1—Cu1 ⁱⁱⁱ	121.1 (3)	P2—C8—H8A	110.1
C7—N2—C8	111.7 (3)	N2—C8—H8B	110.1
C7—N2—C6	112.3 (3)	P2—C8—H8B	110.1
C8—N2—C6	112.8 (3)	H8A—C8—H8B	108.4
C7—N2—Cu1	107.6 (2)	P1—O1—H1B	109.5
C8—N2—Cu1	104.3 (2)	P1—O2—Cu1	119.08 (16)
C6—N2—Cu1	107.7 (2)	P1—O3—Cu1 ⁱⁱ	133.88 (16)
N1—C1—C2	121.7 (4)	P2—O4—Cu1	117.93 (16)
N1—C1—H1A	119.1	P2—O6—H6C	109.5
C2—C1—H1A	119.1	H1WA—O1W—H1WB	109 (4)
C1—C2—C3	121.3 (4)	H2WA—O2W—H2WB	107 (4)
C1—C2—H2A	119.4		

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

Hydrogen-bond geometry (Å, °)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1B \cdots O1W	0.82	1.68	2.494 (4)	169
O6—H6C \cdots O2W	0.82	1.75	2.567 (5)	172
O1W—H1WA \cdots O5 ^{iv}	0.83 (2)	1.92 (2)	2.746 (4)	177 (5)
O1W—H1WB \cdots O5 ^v	0.84 (2)	1.93 (2)	2.747 (4)	167 (5)
O2W—H2WA \cdots O1 ^{vi}	0.85 (2)	2.09 (3)	2.882 (4)	155 (5)
O2W—H2WB \cdots O3 ⁱⁱ	0.85 (2)	1.96 (3)	2.776 (4)	161 (6)

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