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Hexaaquacadmium(II) bis{[*N*-(2-oxidobenzylidene)glycyl-L-leucinato]-cuprate(II)} dihydrate

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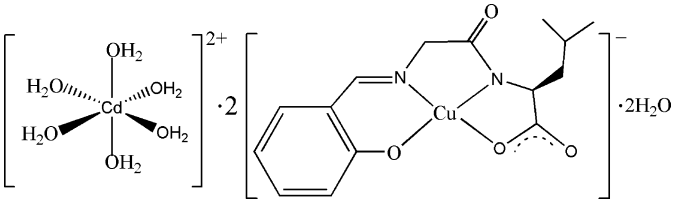
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.024; wR factor = 0.054; data-to-parameter ratio = 14.0.

The title compound, $[Cd(H_2O)_6][Cu(C_{15}H_{17}N_2O_4)]_2\cdot 2H_2O$, has a chiral structure. Copper has a square-planar coordination with two N and two O atoms of the quadridentate chiral Schiff base ligand. The Cd^{2+} ion is coordinated by six aqua ligands with a slightly distorted octahedral configuration. Ions are linked by O—H···O hydrogen bonds, and the $[Cd(H_2O)_6]^{2+}$ cations and $[CuL]^-$ anions (L = Schiff base derived from glycyl-L-leucine and salicylaldehyde) occupy a stacking structure within well separated columns along the a axis. The two crystallographically independent copper–Schiff base anions each have a chiral carbon centre with an S configuration. They are related by a non-crystallographic twofold rotation axis parallel to the [010] direction.

Related literature

For related literature, see: Liu *et al.* (2004).



Experimental

Crystal data

$[Cd(H_2O)_6][Cu(C_{15}H_{17}N_2O_4)]_2\cdot 2H_2O$
M_r = 962.22
Monoclinic, $P2_1$
a = 7.0569 (6) Å
b = 17.4745 (14) Å
c = 15.9430 (13) Å
β = 100.680 (1)°
V = 1932.0 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.71 mm^{-1}
T = 296 (2) K
0.30 × 0.28 × 0.23 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.602, T_{max} = 0.678
15044 measured reflections
6936 independent reflections
6430 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.054
S = 1.01
6936 reflections
494 parameters
361 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Absolute structure: Flack (1983), 3005 Friedel pairs
Flack parameter: 0.008 (9)

Table 1
Selected geometric parameters (Å, °).

Cd1—O10	2.228 (2)	Cu1—N2	1.903 (2)
Cd1—O13	2.268 (3)	Cu1—N1	1.927 (3)
Cd1—O12	2.280 (2)	Cu1—O2	1.954 (2)
Cd1—O9	2.281 (2)	Cu2—O5	1.878 (2)
Cd1—O11	2.285 (2)	Cu2—N4	1.895 (3)
Cd1—O14	2.373 (2)	Cu2—N3	1.915 (3)
Cu1—O1	1.886 (2)	Cu2—O6	1.945 (2)
O1—Cu1—N2	179.61 (11)	O5—Cu2—N4	174.48 (11)
O1—Cu1—N1	95.61 (11)	O5—Cu2—N3	96.40 (11)
N2—Cu1—N1	84.62 (11)	N4—Cu2—N3	84.99 (11)
O1—Cu1—O2	95.93 (10)	O5—Cu2—O6	95.53 (10)
N2—Cu1—O2	83.87 (11)	N4—Cu2—O6	83.99 (10)
N1—Cu1—O2	167.28 (11)	N3—Cu2—O6	165.06 (12)

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

D—H···A	D—H	H···A	D···A	D—H···A
O16—H16B···O8^{i}	0.85	1.94	2.783 (4)	171
O16—H16A···O4^{ii}	0.85	2.11	2.937 (4)	165
O15—H15B···O5	0.878 (18)	1.91 (2)	2.769 (3)	164 (4)
O15—H15A···O14^{iii}	0.861 (19)	1.980 (19)	2.828 (4)	168 (4)
O14—H14D···O4^{iv}	0.865 (18)	1.86 (2)	2.714 (4)	171 (3)
O14—H14E···O3	0.838 (17)	2.073 (18)	2.911 (3)	177 (3)
O12—H12B···O8^{v}	0.85	2.12	2.853 (3)	144
O10—H10A···O6^{vi}	0.85	1.93	2.685 (3)	147
O10—H10B···O2	0.85	2.52	3.261 (3)	147
O9—H9A···O15	0.85	1.81	2.652 (4)	167
O9—H9B···O2	0.84	1.99	2.812 (3)	166

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); 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: SI2059).

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supporting information

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Hexaaquacadmium(II) bis{[*N*-(2-oxidobenzylidene)glycyl-L-leucinato]cuprate(II)} dihydrate

Guolin Zhang, Lihua Ye, Yanyan Zhang and Wenlong Liu

S1. Comment

We are making a systematic investigation of chiral complexes of Schiff base derived from chiral dipeptides to which little attention has been given, and recently reported a chiral Cu(II)—Sr(II)—Na(I) complex of a Schiff base ligand resulting from the condensation of glycyl-*L*-tyrosine with *N*-5-bromosalicylaldehyde (Liu *et al.*, 2004). Herein, we report the synthesis and structure of a Cu(II)—Cd(II) chiral Schiff base complex derived from glycyl-*L*-leucine and salicylaldehyde.

The asymmetric unit consists of two $[CuL]^-$ anions ($[Cu1L]^-$ and $[Cu2L]^-$)(*L* is a Schiff base derived from glycyl-*L*-leucine and salicylaldehyde), one cation $[Cd^{II}$, O9, O10, O11, O12, O13 and O14$]^{2+}$, and two uncoordinated water molecules (O15 and O16) (Fig. 1). $[CuL]^-$ has an approximate square-planar structure. The two crystallographically independent copper-Schiff base anions each have a chiral carbon centre (C10 and C25) with S-configuration. They are related by a non-crystallographic twofold rotation axis parallel to the [0 1 0] direction (Fig. 2). The deprotonated Schiff base ligand is a triple negatively charged quadridentate ONNO chelant, coordinating to the Cu^{II} ion *via* one phenolic oxygen, one deprotonated amide nitrogen atom, one imino nitrogen atom and one carboxylate oxygen. The Cu—O and Cu—N bond distances are in the range of 1.878 (2)–1.954 (2) Å and 1.895 (3)–1.927 (3) Å, respectively (Table 1). The best-fit least-squares plane through the four basal and Cu atoms shows these atoms to be nearly coplanar. The Cd^{II} is coordinated by six aqua ligands with a slightly distorted octahedral geometry. The six Cd—O bonds in the structure are in the range of 2.228 (2)–2.373 (2) Å.

The anions and cations linked by O—H···O hydrogen bonds (Table 2) form well separated columns along the *a*-axis in the stacking structure of (Fig. 3). The intermolecular and intramolecular hydrogen bonds in the title compound play an important role in the stabilization of the whole structure.

S2. Experimental

Glycyl-*L*-leucine (5 mmol), salicylaldehyde (5 mmol) and LiOH (10 mmol) were dissolved in MeOH/H_2O (30 ml, v:v = 1:1) and refluxed for 30 min. Then $Cu(ClO_4)_2.6H_2O$ (5 mmol) was added to the solution and the resulting solution was adjusted to the pH 9–11 by using 5 mol.L^{-1} NaOH solution. After stirring at room temperature (25 °C) for 1 hr, $CdCl_2.6H_2O$ (2.5 mmol) was added. A violet precipitate was obtained immediately. After stirring for 30 min and then filtered, the precipitate was recrystallized in water. The violet crystals suitable for X-ray diffraction were obtained after 1 week.

S3. Refinement

The water H atoms were located in a difference Fourier map and refined in riding mode, with a distance restraint of O—H = 0.85 Å and U_{iso}(H) = 1.5U_{eq}(O). All other H atoms were positioned geometrically and constrained as riding atoms, with C—H distances of 0.93–0.98 Å and U_{iso}(H) set to 1.2 or 1.5$_{eq}$(C) of the parent atom. The refinement of the structure

was performed using 361 least-squares restraints by applying SIMU and *DFIX* instructions of *SHELXTL*.

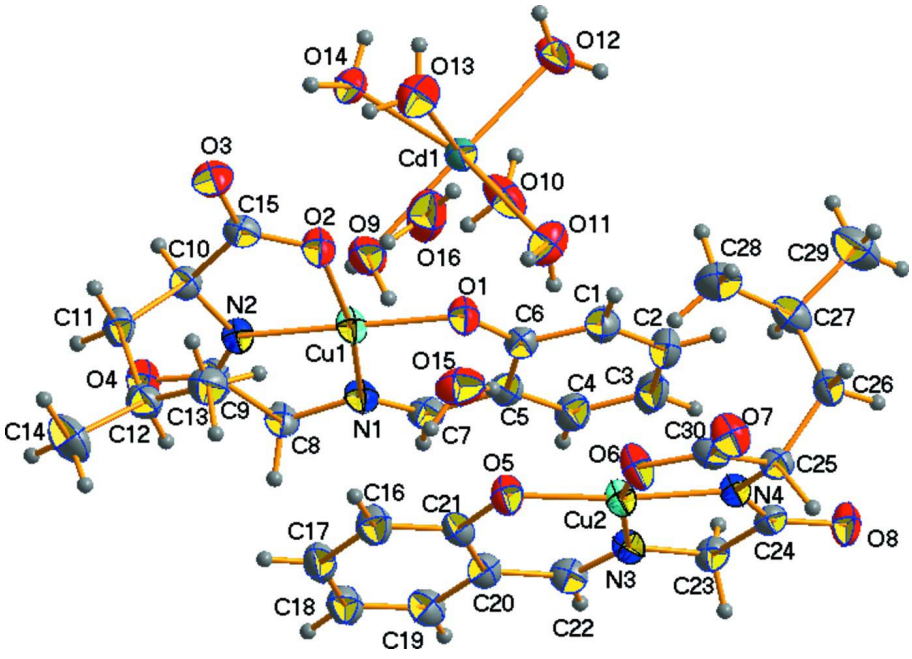

Figure 1

The molecular structure of the title compound, with atom labels and 50% probability displacement ellipsoids.

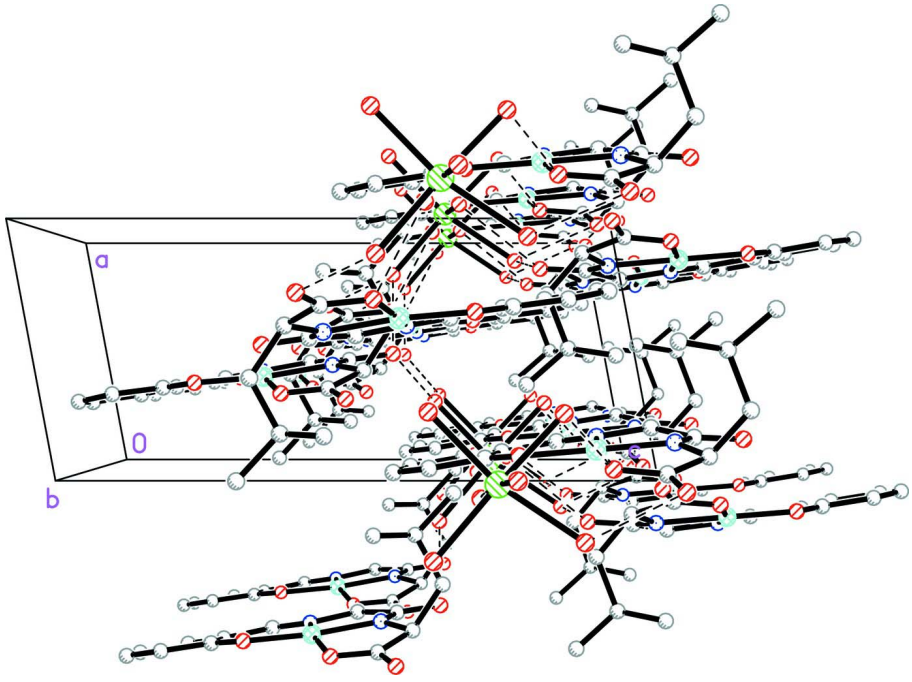

Figure 2

View of the title structure in *ac* projection showing the non-crystallographic twofold rotation symmetry between the $[CuL]^-$ anions.

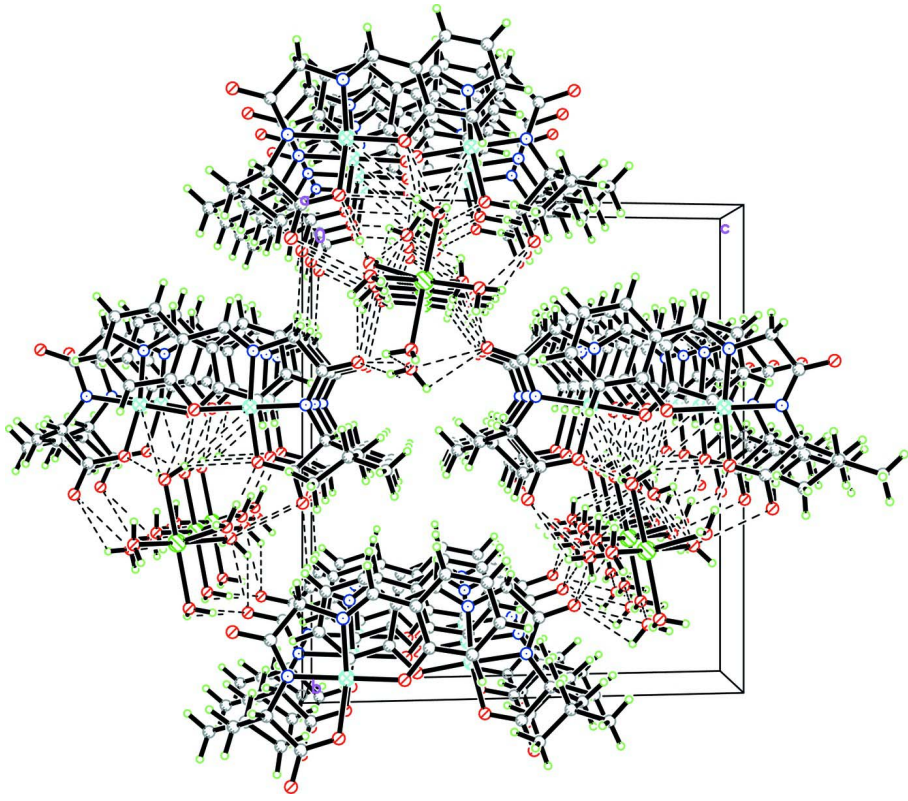

Figure 3

The packing of the title compound, viewed down the *a* axis, showing a separated columns stacking structure connected by O—H···O hydrogen bonds, indicated by dashed lines.

Hexaaquacadmium(II) bis{[*N*-(2-oxidobenzylidene)glycyl-*L*-leucinato]cuprate(II)} dihydrate

Crystal data

$[Cd(H_2O)_6][Cu(C_{15}H_{17}N_2O_4)]_2\cdot 2H_2O$
$M_r = 962.22$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 7.0569\ (6)$ Å
$b = 17.4745\ (14)$ Å
$c = 15.9430\ (13)$ Å
$\beta = 100.680\ (1)°$
$V = 1932.0\ (3)$ Å^3
$Z = 2$
$F(000) = 984$
$D_x = 1.654$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7167 reflections
$\theta = 2.3–26.6°$
$\mu = 1.71$ mm^{-1}
$T = 296$ K
Block, violet
0.30 × 0.28 × 0.23 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min} = 0.602$, $T_{max} = 0.678$
15044 measured reflections
6936 independent reflections
6430 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.3°$
$h = -8\rightarrow 8$
$k = -19\rightarrow 21$
$l = -19\rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.054$
$S = 1.01$
6936 reflections
494 parameters
361 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
$w = 1/[\sigma^2(F_o^2) + (0.0201P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}
Absolute structure: Flack (1983), 3005 Friedel pairs
Absolute structure parameter: 0.008 (9)

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_{iso}*/U_{eq}
Cd1	0.05438 (3)	0.678849 (13)	0.730726 (13)	0.03116 (6)
Cu1	0.14923 (5)	0.41364 (2)	0.89059 (2)	0.03101 (9)
Cu2	0.60569 (6)	0.40862 (2)	0.62847 (2)	0.03172 (10)
C1	0.0796 (5)	0.3718 (2)	0.6304 (2)	0.0395 (8)
H1	0.0698	0.4219	0.6102	0.047*
C2	0.0601 (5)	0.3127 (2)	0.5729 (2)	0.0424 (9)
H2	0.0361	0.3235	0.5148	0.051*
C3	0.0753 (5)	0.2376 (2)	0.5997 (2)	0.0448 (9)
H3	0.0632	0.1978	0.5603	0.054*
C4	0.1088 (5)	0.2223 (2)	0.6863 (2)	0.0394 (8)
H4	0.1167	0.1717	0.7047	0.047*
C5	0.1315 (5)	0.2817 (2)	0.7474 (2)	0.0342 (7)
C6	0.1140 (4)	0.3592 (2)	0.7193 (2)	0.0318 (7)
C7	0.1665 (4)	0.25880 (19)	0.8363 (2)	0.0336 (7)
H7	0.1742	0.2067	0.8483	0.040*
C8	0.2178 (5)	0.27673 (18)	0.9874 (2)	0.0326 (7)
H8A	0.3478	0.2569	1.0036	0.039*
H8B	0.1283	0.2355	0.9921	0.039*
C9	0.1871 (4)	0.34199 (18)	1.0471 (2)	0.0290 (7)
C10	0.1302 (5)	0.47934 (18)	1.0534 (2)	0.0309 (7)
H10	0.0151	0.4695	1.0780	0.037*
C11	0.2893 (5)	0.5061 (2)	1.1262 (2)	0.0360 (8)
H11A	0.2568	0.5572	1.1426	0.043*

H11B	0.2880	0.4729	1.1748	0.043*
C12	0.4951 (5)	0.5080 (2)	1.1086 (2)	0.0398 (8)
H12	0.5295	0.4556	1.0954	0.048*
C13	0.5223 (5)	0.5579 (2)	1.0346 (2)	0.0514 (10)
H13A	0.6571	0.5612	1.0325	0.077*
H13B	0.4730	0.6082	1.0418	0.077*
H13C	0.4542	0.5360	0.9824	0.077*
C14	0.6328 (6)	0.5326 (3)	1.1889 (3)	0.0626 (11)
H14A	0.5961	0.5821	1.2063	0.094*
H14B	0.7617	0.5348	1.1776	0.094*
H14C	0.6278	0.4962	1.2336	0.094*
C15	0.0748 (4)	0.54010 (18)	0.9829 (2)	0.0315 (7)
C16	0.6727 (5)	0.3991 (2)	0.8915 (2)	0.0422 (8)
H16	0.6679	0.4511	0.9035	0.051*
C17	0.7038 (5)	0.3480 (2)	0.9577 (2)	0.0431 (8)
H17	0.7222	0.3661	1.0135	0.052*
C18	0.7085 (5)	0.2701 (2)	0.9435 (2)	0.0432 (9)
H18	0.7309	0.2356	0.9888	0.052*
C19	0.6789 (5)	0.2451 (2)	0.8600 (2)	0.0394 (8)
H19	0.6805	0.1928	0.8495	0.047*
C20	0.6466 (5)	0.29517 (19)	0.7907 (2)	0.0324 (7)
C21	0.6478 (4)	0.37532 (19)	0.8058 (2)	0.0325 (7)
C22	0.6117 (5)	0.26192 (19)	0.7058 (2)	0.0337 (7)
H22	0.6095	0.2088	0.7019	0.040*
C23	0.5484 (5)	0.26228 (18)	0.5525 (2)	0.0333 (7)
H23A	0.4279	0.2342	0.5451	0.040*
H23B	0.6512	0.2262	0.5493	0.040*
C24	0.5385 (4)	0.32158 (19)	0.4817 (2)	0.0296 (7)
C25	0.5794 (5)	0.45912 (18)	0.4560 (2)	0.0308 (7)
H25	0.6829	0.4480	0.4244	0.037*
C26	0.3991 (5)	0.4801 (2)	0.3906 (2)	0.0364 (8)
H26A	0.4222	0.5293	0.3662	0.044*
H26B	0.3856	0.4428	0.3448	0.044*
C27	0.2086 (5)	0.4847 (2)	0.4204 (2)	0.0429 (8)
H27	0.1841	0.4347	0.4442	0.052*
C28	0.2036 (6)	0.5437 (3)	0.4880 (3)	0.0611 (11)
H28A	0.2386	0.5926	0.4681	0.092*
H28B	0.2930	0.5299	0.5387	0.092*
H28C	0.0758	0.5465	0.5005	0.092*
C29	0.0475 (6)	0.5000 (3)	0.3436 (3)	0.0704 (13)
H29A	0.0448	0.4595	0.3027	0.106*
H29B	0.0710	0.5478	0.3177	0.106*
H29C	−0.0741	0.5022	0.3622	0.106*
C30	0.6475 (4)	0.52643 (19)	0.5175 (2)	0.0342 (8)
N1	0.1872 (4)	0.30447 (16)	0.89864 (17)	0.0316 (7)
N2	0.1733 (3)	0.40911 (15)	1.01137 (15)	0.0289 (5)
N3	0.5838 (4)	0.29972 (16)	0.63589 (16)	0.0311 (6)
N4	0.5587 (4)	0.39243 (14)	0.50891 (16)	0.0287 (6)

O1	0.1267 (3)	0.41864 (13)	0.77098 (13)	0.0369 (5)
O2	0.0898 (3)	0.52136 (12)	0.90607 (14)	0.0374 (6)
O3	0.0209 (4)	0.60371 (13)	1.00130 (16)	0.0443 (6)
O4	0.1794 (3)	0.32572 (13)	1.12385 (15)	0.0391 (6)
O5	0.6277 (3)	0.42809 (12)	0.74572 (13)	0.0382 (6)
O6	0.6665 (4)	0.51242 (13)	0.59822 (15)	0.0405 (6)
O7	0.6854 (3)	0.58814 (13)	0.48932 (15)	0.0427 (6)
O8	0.5149 (3)	0.29840 (13)	0.40516 (14)	0.0399 (6)
O9	0.2842 (4)	0.64352 (15)	0.84431 (15)	0.0493 (7)
H9A	0.3804	0.6232	0.8274	0.074*
H9B	0.2295	0.6115	0.8707	0.074*
O10	−0.0061 (4)	0.55560 (14)	0.70150 (17)	0.0501 (7)
H10B	0.0342	0.5289	0.7458	0.075*
H10A	−0.1269	0.5493	0.6860	0.075*
O11	0.2908 (3)	0.67554 (17)	0.65034 (14)	0.0486 (6)
H11D	0.3784	0.7078	0.6694	0.073*
H11C	0.3389	0.6308	0.6530	0.073*
O12	−0.1939 (3)	0.69629 (14)	0.61856 (15)	0.0494 (7)
H12A	−0.1492	0.6987	0.5726	0.074*
H12B	−0.2501	0.7381	0.6260	0.074*
O13	0.0777 (4)	0.80624 (15)	0.75778 (18)	0.0505 (7)
H13E	−0.0350	0.8253	0.7486	0.076*
H13D	0.1301	0.8135	0.8096	0.076*
O14	−0.1360 (3)	0.67596 (16)	0.83875 (14)	0.0382 (5)
H14D	−0.147 (5)	0.7248 (10)	0.845 (2)	0.057*
H14E	−0.092 (5)	0.6565 (17)	0.8865 (15)	0.057*
O15	0.5499 (4)	0.58134 (15)	0.7677 (2)	0.0545 (7)
H15A	0.656 (4)	0.605 (2)	0.788 (3)	0.082*
H15B	0.590 (6)	0.5359 (14)	0.755 (3)	0.082*
O16	0.4485 (4)	0.84117 (19)	0.75926 (18)	0.0655 (9)
H16A	0.5562	0.8284	0.7892	0.098*
H16B	0.4512	0.8324	0.7072	0.098*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03613 (11)	0.02655 (12)	0.03007 (12)	−0.00048 (11)	0.00428 (8)	−0.00025 (12)
Cu1	0.0439 (2)	0.0219 (2)	0.02635 (19)	−0.00039 (18)	0.00396 (16)	0.00266 (17)
Cu2	0.0432 (2)	0.0210 (2)	0.0280 (2)	−0.00213 (18)	−0.00093 (16)	−0.00087 (18)
C1	0.0453 (18)	0.0391 (19)	0.0342 (18)	0.0029 (15)	0.0074 (15)	−0.0012 (15)
C2	0.049 (2)	0.049 (2)	0.0300 (18)	0.0006 (17)	0.0085 (15)	−0.0053 (17)
C3	0.0473 (19)	0.049 (2)	0.0378 (19)	−0.0040 (17)	0.0073 (15)	−0.0172 (17)
C4	0.0461 (18)	0.0306 (18)	0.0408 (19)	−0.0014 (14)	0.0061 (15)	−0.0062 (15)
C5	0.0352 (16)	0.0338 (18)	0.0332 (17)	0.0010 (14)	0.0051 (13)	−0.0029 (14)
C6	0.0308 (15)	0.0348 (18)	0.0302 (16)	0.0016 (13)	0.0062 (12)	−0.0012 (14)
C7	0.0373 (17)	0.0234 (16)	0.0398 (18)	0.0017 (13)	0.0062 (14)	−0.0008 (15)
C8	0.0425 (18)	0.0225 (16)	0.0324 (17)	0.0029 (14)	0.0064 (14)	0.0056 (14)
C9	0.0311 (16)	0.0281 (17)	0.0275 (17)	−0.0029 (13)	0.0048 (13)	0.0025 (14)

C10	0.0349 (17)	0.0264 (16)	0.0326 (17)	0.0002 (13)	0.0096 (13)	0.0034 (14)
C11	0.0474 (18)	0.0290 (17)	0.0310 (17)	−0.0012 (15)	0.0058 (14)	−0.0031 (14)
C12	0.0408 (18)	0.0351 (18)	0.0406 (19)	0.0030 (15)	0.0004 (15)	−0.0030 (16)
C13	0.044 (2)	0.059 (2)	0.050 (2)	0.0036 (18)	0.0076 (17)	0.004 (2)
C14	0.056 (2)	0.072 (3)	0.052 (2)	−0.009 (2)	−0.0109 (19)	−0.001 (2)
C15	0.0314 (16)	0.0235 (17)	0.0387 (19)	−0.0016 (13)	0.0041 (14)	0.0008 (14)
C16	0.0477 (18)	0.040 (2)	0.0380 (18)	−0.0031 (16)	0.0052 (15)	−0.0022 (16)
C17	0.0427 (18)	0.057 (2)	0.0298 (18)	−0.0022 (17)	0.0056 (14)	0.0035 (17)
C18	0.0435 (19)	0.050 (2)	0.0364 (19)	0.0010 (16)	0.0079 (15)	0.0096 (17)
C19	0.0427 (17)	0.0344 (18)	0.0408 (19)	−0.0006 (15)	0.0071 (15)	0.0078 (15)
C20	0.0350 (16)	0.0305 (17)	0.0326 (17)	−0.0022 (13)	0.0084 (13)	0.0032 (14)
C21	0.0337 (16)	0.0334 (17)	0.0290 (16)	−0.0010 (13)	0.0021 (13)	0.0035 (14)
C22	0.0382 (17)	0.0226 (16)	0.0401 (18)	−0.0017 (13)	0.0069 (14)	0.0021 (15)
C23	0.0397 (18)	0.0231 (17)	0.0370 (18)	−0.0006 (13)	0.0068 (14)	−0.0036 (14)
C24	0.0264 (15)	0.0302 (18)	0.0329 (18)	0.0012 (13)	0.0075 (13)	−0.0012 (14)
C25	0.0345 (16)	0.0251 (17)	0.0330 (17)	0.0014 (13)	0.0068 (13)	0.0026 (13)
C26	0.0477 (19)	0.0312 (18)	0.0279 (17)	0.0023 (15)	0.0012 (15)	−0.0001 (14)
C27	0.0410 (18)	0.042 (2)	0.043 (2)	−0.0024 (15)	−0.0002 (15)	0.0082 (16)
C28	0.045 (2)	0.076 (3)	0.064 (3)	0.008 (2)	0.0113 (19)	−0.004 (2)
C29	0.048 (2)	0.088 (3)	0.066 (3)	0.002 (2)	−0.011 (2)	0.010 (2)
C30	0.0315 (16)	0.0297 (19)	0.0390 (19)	−0.0002 (14)	0.0008 (14)	0.0022 (16)
N1	0.0400 (16)	0.0246 (16)	0.0300 (15)	0.0014 (12)	0.0056 (12)	0.0042 (12)
N2	0.0369 (13)	0.0211 (13)	0.0282 (13)	−0.0035 (12)	0.0044 (10)	−0.0011 (12)
N3	0.0328 (15)	0.0254 (15)	0.0328 (16)	−0.0031 (11)	−0.0001 (12)	−0.0029 (13)
N4	0.0359 (14)	0.0202 (15)	0.0281 (14)	−0.0004 (10)	0.0008 (11)	−0.0006 (11)
O1	0.0566 (14)	0.0249 (12)	0.0282 (11)	0.0040 (11)	0.0050 (10)	0.0016 (11)
O2	0.0579 (15)	0.0232 (13)	0.0306 (13)	0.0031 (11)	0.0067 (11)	0.0029 (10)
O3	0.0563 (15)	0.0272 (13)	0.0488 (15)	0.0093 (11)	0.0080 (12)	−0.0019 (12)
O4	0.0543 (15)	0.0300 (13)	0.0340 (13)	−0.0021 (11)	0.0103 (11)	0.0053 (11)
O5	0.0575 (14)	0.0234 (14)	0.0317 (12)	0.0012 (10)	0.0033 (10)	−0.0032 (10)
O6	0.0622 (16)	0.0239 (13)	0.0301 (13)	−0.0106 (11)	−0.0057 (11)	0.0014 (10)
O7	0.0563 (15)	0.0261 (13)	0.0438 (15)	−0.0090 (11)	0.0041 (12)	0.0071 (11)
O8	0.0583 (16)	0.0330 (14)	0.0283 (13)	−0.0032 (12)	0.0081 (11)	−0.0082 (10)
O9	0.0445 (14)	0.0643 (17)	0.0391 (14)	0.0055 (12)	0.0078 (11)	0.0095 (13)
O10	0.0642 (16)	0.0272 (14)	0.0483 (15)	−0.0054 (12)	−0.0170 (13)	0.0046 (12)
O11	0.0589 (14)	0.0389 (14)	0.0533 (14)	−0.0068 (16)	0.0241 (11)	−0.0025 (15)
O12	0.0587 (15)	0.0384 (16)	0.0438 (14)	0.0141 (12)	−0.0096 (11)	−0.0047 (12)
O13	0.0626 (18)	0.0347 (16)	0.0559 (17)	−0.0028 (13)	0.0150 (14)	−0.0038 (14)
O14	0.0487 (12)	0.0294 (12)	0.0372 (12)	0.0039 (14)	0.0101 (10)	−0.0007 (14)
O15	0.0487 (16)	0.0359 (16)	0.081 (2)	0.0024 (13)	0.0162 (14)	−0.0107 (15)
O16	0.0576 (17)	0.090 (2)	0.0504 (17)	−0.0138 (16)	0.0138 (13)	−0.0207 (16)

Geometric parameters (Å, º)

Cd1—O10	2.228 (2)	C16—C21	1.407 (4)
Cd1—O13	2.268 (3)	C16—H16	0.9300
Cd1—O12	2.280 (2)	C17—C18	1.381 (5)
Cd1—O9	2.281 (2)	C17—H17	0.9300

Cd1—O11	2.285 (2)	C18—C19	1.380 (5)
Cd1—O14	2.373 (2)	C18—H18	0.9300
Cu1—O1	1.886 (2)	C19—C20	1.394 (5)
Cu1—N2	1.903 (2)	C19—H19	0.9300
Cu1—N1	1.927 (3)	C20—C21	1.421 (5)
Cu1—O2	1.954 (2)	C20—C22	1.452 (5)
Cu2—O5	1.878 (2)	C21—O5	1.318 (4)
Cu2—N4	1.895 (3)	C22—N3	1.279 (4)
Cu2—N3	1.915 (3)	C22—H22	0.9300
Cu2—O6	1.945 (2)	C23—N3	1.461 (4)
C1—C2	1.371 (5)	C23—C24	1.524 (4)
C1—C6	1.410 (4)	C23—H23A	0.9700
C1—H1	0.9300	C23—H23B	0.9700
C2—C3	1.379 (5)	C24—O8	1.267 (4)
C2—H2	0.9300	C24—N4	1.311 (4)
C3—C4	1.382 (5)	C25—N4	1.462 (4)
C3—H3	0.9300	C25—C26	1.533 (4)
C4—C5	1.413 (5)	C25—C30	1.549 (5)
C4—H4	0.9300	C25—H25	0.9800
C5—C6	1.424 (5)	C26—C27	1.509 (5)
C5—C7	1.450 (4)	C26—H26A	0.9700
C6—O1	1.319 (4)	C26—H26B	0.9700
C7—N1	1.261 (4)	C27—C28	1.497 (5)
C7—H7	0.9300	C27—C29	1.532 (5)
C8—N1	1.473 (4)	C27—H27	0.9800
C8—C9	1.526 (4)	C28—H28A	0.9600
C8—H8A	0.9700	C28—H28B	0.9600
C8—H8B	0.9700	C28—H28C	0.9600
C9—O4	1.267 (4)	C29—H29A	0.9600
C9—N2	1.300 (4)	C29—H29B	0.9600
C10—N2	1.457 (4)	C29—H29C	0.9600
C10—C11	1.530 (4)	C30—O7	1.217 (4)
C10—C15	1.543 (4)	C30—O6	1.292 (4)
C10—H10	0.9800	O9—H9A	0.8535
C11—C12	1.530 (5)	O9—H9B	0.8358
C11—H11A	0.9700	O10—H10B	0.8500
C11—H11B	0.9700	O10—H10A	0.8501
C12—C13	1.507 (5)	O11—H11D	0.8500
C12—C14	1.518 (5)	O11—H11C	0.8499
C12—H12	0.9800	O12—H12A	0.8500
C13—H13A	0.9600	O12—H12B	0.8499
C13—H13B	0.9600	O13—H13E	0.8500
C13—H13C	0.9600	O13—H13D	0.8500
C14—H14A	0.9600	O14—H14D	0.865 (18)
C14—H14B	0.9600	O14—H14E	0.838 (17)
C14—H14C	0.9600	O15—H15A	0.861 (19)
C15—O3	1.228 (4)	O15—H15B	0.878 (18)
C15—O2	1.291 (4)	O16—H16A	0.8493

C16—C17	1.370 (5)	O16—H16B	0.8483
O10—Cd1—O13	173.25 (11)	C18—C17—H17	119.2
O10—Cd1—O12	82.86 (9)	C19—C18—C17	117.7 (3)
O13—Cd1—O12	92.07 (10)	C19—C18—H18	121.1
O10—Cd1—O9	89.13 (9)	C17—C18—H18	121.1
O13—Cd1—O9	95.67 (10)	C18—C19—C20	122.6 (3)
O12—Cd1—O9	171.42 (9)	C18—C19—H19	118.7
O10—Cd1—O11	89.41 (10)	C20—C19—H19	118.7
O13—Cd1—O11	95.55 (10)	C19—C20—C21	119.3 (3)
O12—Cd1—O11	95.64 (9)	C19—C20—C22	117.5 (3)
O9—Cd1—O11	87.30 (9)	C21—C20—C22	123.2 (3)
O10—Cd1—O14	91.09 (10)	O5—C21—C16	118.4 (3)
O13—Cd1—O14	85.05 (10)	O5—C21—C20	124.8 (3)
O12—Cd1—O14	96.66 (9)	C16—C21—C20	116.8 (3)
O9—Cd1—O14	80.38 (8)	N3—C22—C20	125.3 (3)
O11—Cd1—O14	167.66 (8)	N3—C22—H22	117.3
O1—Cu1—N2	179.61 (11)	C20—C22—H22	117.3
O1—Cu1—N1	95.61 (11)	N3—C23—C24	110.2 (3)
N2—Cu1—N1	84.62 (11)	N3—C23—H23A	109.6
O1—Cu1—O2	95.93 (10)	C24—C23—H23A	109.6
N2—Cu1—O2	83.87 (11)	N3—C23—H23B	109.6
N1—Cu1—O2	167.28 (11)	C24—C23—H23B	109.6
O5—Cu2—N4	174.48 (11)	H23A—C23—H23B	108.1
O5—Cu2—N3	96.40 (11)	O8—C24—N4	127.4 (3)
N4—Cu2—N3	84.99 (11)	O8—C24—C23	118.4 (3)
O5—Cu2—O6	95.53 (10)	N4—C24—C23	114.2 (3)
N4—Cu2—O6	83.99 (10)	N4—C25—C26	115.1 (3)
N3—Cu2—O6	165.06 (12)	N4—C25—C30	107.0 (3)
C2—C1—C6	122.1 (3)	C26—C25—C30	111.7 (3)
C2—C1—H1	119.0	N4—C25—H25	107.6
C6—C1—H1	119.0	C26—C25—H25	107.6
C1—C2—C3	121.2 (3)	C30—C25—H25	107.6
C1—C2—H2	119.4	C27—C26—C25	118.3 (3)
C3—C2—H2	119.4	C27—C26—H26A	107.7
C2—C3—C4	118.8 (3)	C25—C26—H26A	107.7
C2—C3—H3	120.6	C27—C26—H26B	107.7
C4—C3—H3	120.6	C25—C26—H26B	107.7
C3—C4—C5	121.5 (3)	H26A—C26—H26B	107.1
C3—C4—H4	119.2	C28—C27—C26	113.9 (3)
C5—C4—H4	119.2	C28—C27—C29	110.0 (3)
C4—C5—C6	119.3 (3)	C26—C27—C29	109.2 (3)
C4—C5—C7	116.6 (3)	C28—C27—H27	107.8
C6—C5—C7	124.0 (3)	C26—C27—H27	107.8
O1—C6—C1	118.9 (3)	C29—C27—H27	107.8
O1—C6—C5	124.1 (3)	C27—C28—H28A	109.5
C1—C6—C5	117.0 (3)	C27—C28—H28B	109.5
N1—C7—C5	124.7 (3)	H28A—C28—H28B	109.5

N1—C7—H7	117.7	C27—C28—H28C	109.5
C5—C7—H7	117.7	H28A—C28—H28C	109.5
N1—C8—C9	109.9 (3)	H28B—C28—H28C	109.5
N1—C8—H8A	109.7	C27—C29—H29A	109.5
C9—C8—H8A	109.7	C27—C29—H29B	109.5
N1—C8—H8B	109.7	H29A—C29—H29B	109.5
C9—C8—H8B	109.7	C27—C29—H29C	109.5
H8A—C8—H8B	108.2	H29A—C29—H29C	109.5
O4—C9—N2	127.8 (3)	H29B—C29—H29C	109.5
O4—C9—C8	118.1 (3)	O7—C30—O6	123.1 (3)
N2—C9—C8	114.1 (3)	O7—C30—C25	120.2 (3)
N2—C10—C11	114.8 (3)	O6—C30—C25	116.7 (3)
N2—C10—C15	106.9 (3)	C7—N1—C8	121.5 (3)
C11—C10—C15	113.2 (3)	C7—N1—Cu1	125.4 (2)
N2—C10—H10	107.2	C8—N1—Cu1	112.5 (2)
C11—C10—H10	107.2	C9—N2—C10	124.3 (3)
C15—C10—H10	107.2	C9—N2—Cu1	117.8 (2)
C12—C11—C10	117.2 (3)	C10—N2—Cu1	116.3 (2)
C12—C11—H11A	108.0	C22—N3—C23	122.3 (3)
C10—C11—H11A	108.0	C22—N3—Cu2	124.5 (2)
C12—C11—H11B	108.0	C23—N3—Cu2	113.0 (2)
C10—C11—H11B	108.0	C24—N4—C25	125.3 (3)
H11A—C11—H11B	107.3	C24—N4—Cu2	117.5 (2)
C13—C12—C14	110.0 (3)	C25—N4—Cu2	116.36 (19)
C13—C12—C11	114.8 (3)	C6—O1—Cu1	125.4 (2)
C14—C12—C11	109.5 (3)	C15—O2—Cu1	114.9 (2)
C13—C12—H12	107.4	C21—O5—Cu2	125.1 (2)
C14—C12—H12	107.4	C30—O6—Cu2	115.9 (2)
C11—C12—H12	107.4	Cd1—O9—H9A	110.6
C12—C13—H13A	109.5	Cd1—O9—H9B	104.7
C12—C13—H13B	109.5	H9A—O9—H9B	110.5
H13A—C13—H13B	109.5	Cd1—O10—H10B	109.6
C12—C13—H13C	109.5	Cd1—O10—H10A	109.3
H13A—C13—H13C	109.5	H10B—O10—H10A	109.5
H13B—C13—H13C	109.5	Cd1—O11—H11D	109.9
C12—C14—H14A	109.5	Cd1—O11—H11C	108.8
C12—C14—H14B	109.5	H11D—O11—H11C	109.5
H14A—C14—H14B	109.5	Cd1—O12—H12A	109.2
C12—C14—H14C	109.5	Cd1—O12—H12B	108.4
H14A—C14—H14C	109.5	H12A—O12—H12B	109.5
H14B—C14—H14C	109.5	Cd1—O13—H13E	108.7
O3—C15—O2	122.7 (3)	Cd1—O13—H13D	109.6
O3—C15—C10	119.8 (3)	H13E—O13—H13D	109.5
O2—C15—C10	117.6 (3)	Cd1—O14—H14D	98 (3)
C17—C16—C21	121.9 (3)	Cd1—O14—H14E	120 (3)
C17—C16—H16	119.1	H14D—O14—H14E	109 (3)
C21—C16—H16	119.1	H15A—O15—H15B	103 (3)
C16—C17—C18	121.5 (3)	H16A—O16—H16B	108.8

C16—C17—H17	119.2

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O16—H16*B*···O8^{i}	0.85	1.94	2.783 (4)	171
O16—H16*A*···O4^{ii}	0.85	2.11	2.937 (4)	165
O15—H15*B*···O5	0.88 (2)	1.91 (2)	2.769 (3)	164 (4)
O15—H15*A*···O14^{iii}	0.86 (2)	1.98 (2)	2.828 (4)	168 (4)
O14—H14*D*···O4^{iv}	0.87 (2)	1.86 (2)	2.714 (4)	171 (3)
O14—H14*E*···O3	0.84 (2)	2.07 (2)	2.911 (3)	177 (3)
O13—H13*E*···O4^{iv}	0.85	2.44	2.870 (4)	112
O12—H12*B*···O8^{v}	0.85	2.12	2.853 (3)	144
O12—H12*A*···O7^{vi}	0.85	2.51	2.809 (3)	102
O11—H11*C*···O15	0.85	2.30	2.879 (4)	125
O11—H11*D*···O8^{i}	0.85	2.20	2.779 (4)	126
O10—H10*A*···O6^{vi}	0.85	1.93	2.685 (3)	147
O10—H10*B*···O2	0.85	2.52	3.261 (3)	147
O10—H10*B*···O1	0.85	2.05	2.729 (3)	136
O9—H9*A*···O15	0.85	1.81	2.652 (4)	167
O9—H9*B*···O2	0.84	1.99	2.812 (3)	166

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