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# Poly[[tris(1,10-phenanthroline)tris($\mu_3$-succinato)tricadmium(II)] tetrahydrate]

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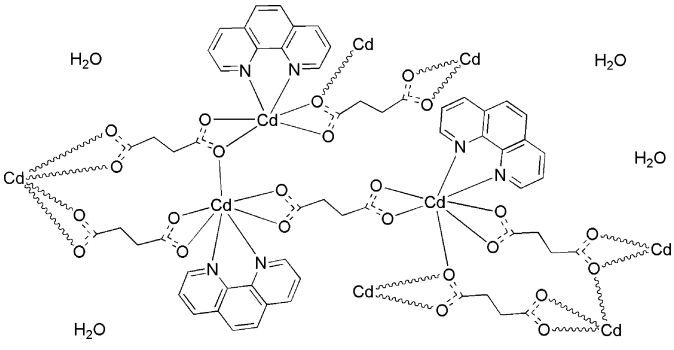
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.035; $wR$ factor = 0.073; data-to-parameter ratio = 16.1.

The title complex, $\{[Cd_3(C_4H_4O_4)_3(C_{12}H_8N_2)_3]\cdot 4H_2O\}_n$, has been isolated from the hydrothermal reaction of cadmium acetate with 1,10-phenanthroline (phen) and succinic acid. The structure features two-dimensional networks formed by succinate ligands bridging Cd atoms in two different coordination modes. A twofold rotation axis passes through one Cd atom. In one coordination mode, the Cd atoms are in a distorted octahedral $CdO_4N_2$ arrangement and the coordination atoms come from one phen ligand and two succinate ligands. In the other coordination mode, the Cd atoms are in the decahedral $CdO_5N_2$ geometries and the coordination atoms come from one phen ligand and three succinate ligands.

## Related literature

For related literature, see: Zheng & Lin (2001).




## Experimental

### Crystal data

$[Cd_3(C_4H_4O_4)_3(C_{12}H_8N_2)_3]\cdot 4H_2O$
$M_r$ = 1298.09
Monoclinic, $C2/c$
$a$ = 11.1875 (6) Å
$b$ = 21.4051 (15) Å
$c$ = 20.2455 (12) Å
$\beta$ = 100.847 (1)°
$V$ = 4761.6 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.41 mm$^{-1}$
$T$ = 298 (2) K
0.32 × 0.20 × 0.20 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.662, $T_{max}$ = 0.766
16149 measured reflections
5526 independent reflections
4640 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.073

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.073
$S$ = 0.97
5526 reflections
343 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.74 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.79 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O7—H7$A$···O8$^{i}$ | 0.791 (18) | 2.174 (19) | 2.962 (4) | 174 (5) |
| O7—H7$B$···O5 | 0.804 (18) | 2.048 (19) | 2.847 (3) | 172 (4) |
| O8—H8$A$···O4$^{ii}$ | 0.823 (18) | 2.04 (2) | 2.857 (3) | 169 (4) |
| O8—H8$B$···O6 | 0.806 (19) | 2.015 (19) | 2.818 (3) | 174 (4) |

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

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: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXTL* (Bruker, 1997).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2314).

## References

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# supplementary materials

*Acta Cryst.* (2007). E**63**, m2889 [ **doi:10.1107/S1600536807051665** ]

# Poly[[tris(1,10-phenanthroline)tris($\mu_3$-succinato)tricadmium(II)] tetrahydrate]

**X.-Y. Wang, X.-T. Deng, C.-G. Wang and M. Wang**

## Comment

Succinic acid is a flexible bridging spacer to constitute coordination polymers. The simultaneous coordination of hydroxide and succinate groups to transition metal atoms tends to form coordination polymers with three-dimensional open framework [Zheng *et al.* (2001)] . Introduction of a second competing ligand such as phen has been found to lower the dimensionality of the structure since its chelation to the metal ion leaves fewer sites for succinate coordination. In structure (I), the Cd atoms are in the distorted octahedral $CdO_4N_2$ and decahedral $CdO_5N_2$ geometries. (Fig. 1) The succinato ligands have two coordination modes (Fig. 2). In the first mode, the carboxylate group bidentately bridges two Cd atoms. In the other mode, one chelating O atom bonds to the second Cd atom. The Cd atoms are interlinked by the succinate ligands to generate two-dimensional networks, in which existing stacking interactions between phen rings and hydrogen bonds.

## Experimental

A mixture of $Cd(CH_3COO)_2{\cdot}2H_2O$ (0.266 g, 1 mmol), succinic acid (0.465 g, 4 mmol), 1,10-phenanthroline hydrate (0.396 g, 2 mmol) and $H_2O$ (10 ml) was heated in a 23 ml stainless steel reactor with a Teflon liner at 453 K for 72 h. Colorless block-shape crystals of the title complex were obtained.

## Refinement

H atoms bonded to O atoms were located in difference maps and then included in the refinement with bond-length restraints of O–H = 0.82 (2) Å, with $U_{iso}$(H)= 1.5$U_{eq}$ All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C–H distances of 0.93 and 0.97 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$.

## Figures

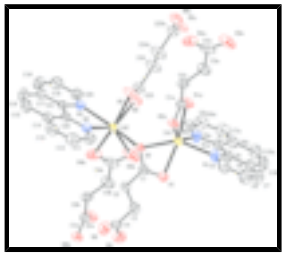

Fig. 1. The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level. The H atoms and water molecules have been omitted for clarity. [symmety codes:(*a*) −*x*,*y*, 1/2 − *z*;(*b*) 1 − *x*,*y*, 1/2 − *z*; (*d*) −*x*,-*y*,1 − *z*]

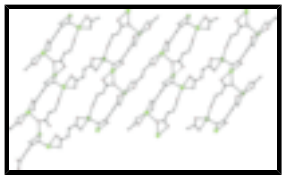

Fig. 2. The molecular structure of (I), showing two-dimensional networks omitting water molecules and phen ligands.

## Poly[[[(1,10-phenanthroline)cadmium(II)]-μ-succnicate-κ$^4$*O*,*O*,*O*'O'] hydrate]

### *Crystal data*

| | |
|---|---|
| $[Cd_3(C_4H_4O_4)_3(C_{12}H_8N_2)_3]\cdot 4H_2O$ | $F_{000}$ = 2584 |
| $M_r$ = 1298.09 | $D_x$ = 1.811 Mg m$^{-3}$ |
| Monoclinic, *C*2/*c* | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: -C 2yc | Cell parameters from 6336 reflections |
| *a* = 11.1875 (6) Å | θ = 2.5–28.2º |
| *b* = 21.4051 (15) Å | μ = 1.41 mm$^{-1}$ |
| *c* = 20.2455 (12) Å | *T* = 298 (2) K |
| β = 100.8470 (10)º | Block, colorless |
| *V* = 4761.6 (5) Å$^3$ | 0.32 × 0.20 × 0.20 mm |
| *Z* = 4 | |

### *Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 5526 independent reflections |
| Radiation source: fine-focus sealed tube | 4640 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.073 |
| *T* = 298(2) K | $\theta_{max}$ = 27.8º |
| φ and ω scans | $\theta_{min}$ = 1.9º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | *h* = −14→14 |
| $T_{min}$ = 0.662, $T_{max}$ = 0.766 | *k* = −22→27 |
| 16149 measured reflections | *l* = −18→26 |

### *Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.035 | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2)$ = 0.073 | $w = 1/[\sigma^2(F_o^2) + (0.0314P)^2]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| *S* = 0.97 | $(\Delta/\sigma)_{max}$ = 0.002 |
| 5526 reflections | $\Delta\rho_{max}$ = 0.74 e Å$^{-3}$ |
| 343 parameters | $\Delta\rho_{min}$ = −0.78 e Å$^{-3}$ |
| 4 restraints | Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.00223 (7) |

*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 | 0.5000 | 0.450298 (13) | 0.2500 | 0.03689 (9) |
| Cd2 | 0.785266 (16) | 0.558555 (9) | 0.372822 (9) | 0.02702 (8) |
| N1 | 0.4185 (2) | 0.36355 (11) | 0.18944 (13) | 0.0408 (6) |
| N2 | 0.73872 (19) | 0.66078 (10) | 0.33202 (11) | 0.0320 (5) |
| N3 | 0.86461 (19) | 0.63215 (11) | 0.45773 (11) | 0.0324 (5) |
| O1 | 0.63997 (18) | 0.46118 (10) | 0.18172 (10) | 0.0470 (5) |
| O2 | 0.66807 (15) | 0.51931 (9) | 0.27212 (9) | 0.0328 (4) |
| O3 | 1.0882 (2) | 0.46530 (13) | 0.15096 (13) | 0.0661 (7) |
| O4 | 1.01226 (19) | 0.56006 (11) | 0.14051 (11) | 0.0531 (6) |
| O5 | 0.59517 (19) | 0.55649 (11) | 0.41393 (12) | 0.0566 (7) |
| O6 | 0.74168 (19) | 0.49423 (10) | 0.45879 (11) | 0.0498 (5) |
| C1 | 0.7021 (2) | 0.50054 (12) | 0.21886 (13) | 0.0296 (6) |
| C2 | 0.8143 (2) | 0.52649 (13) | 0.19883 (13) | 0.0321 (6) |
| H2A | 0.8672 | 0.5432 | 0.2384 | 0.038* |
| H2B | 0.7914 | 0.5607 | 0.1676 | 0.038* |
| C3 | 0.8840 (2) | 0.47844 (15) | 0.16635 (17) | 0.0467 (8) |
| H3A | 0.9004 | 0.4426 | 0.1960 | 0.056* |
| H3B | 0.8332 | 0.4644 | 0.1248 | 0.056* |
| C4 | 1.0029 (3) | 0.50216 (17) | 0.15113 (14) | 0.0446 (8) |
| C5 | 0.3448 (3) | 0.36281 (16) | 0.13045 (17) | 0.0515 (8) |
| H5 | 0.3145 | 0.4007 | 0.1121 | 0.062* |
| C6 | 0.3099 (3) | 0.30888 (18) | 0.09421 (18) | 0.0598 (9) |
| H6 | 0.2596 | 0.3108 | 0.0521 | 0.072* |
| C7 | 0.3511 (3) | 0.25281 (17) | 0.12167 (18) | 0.0571 (9) |
| H7 | 0.3290 | 0.2160 | 0.0982 | 0.069* |
| C8 | 0.4264 (3) | 0.25086 (14) | 0.18520 (16) | 0.0423 (7) |
| C9 | 0.4599 (2) | 0.30787 (13) | 0.21748 (14) | 0.0362 (6) |
| C10 | 0.4661 (3) | 0.19347 (15) | 0.21870 (16) | 0.0549 (9) |
| H10 | 0.4449 | 0.1557 | 0.1970 | 0.066* |
| C11 | 0.6760 (3) | 0.67523 (14) | 0.27157 (14) | 0.0408 (7) |
| H11 | 0.6429 | 0.6430 | 0.2431 | 0.049* |
| C12 | 0.6576 (3) | 0.73636 (16) | 0.24886 (15) | 0.0491 (8) |
| H12 | 0.6125 | 0.7445 | 0.2063 | 0.059* |

| | | | | |
|---|---|---|---|---|
| C13 | 0.7060 (3) | 0.78405 (14) | 0.28923 (16) | 0.0468 (8) |
| H13 | 0.6956 | 0.8251 | 0.2741 | 0.056* |
| C14 | 0.7718 (2) | 0.77134 (13) | 0.35386 (14) | 0.0367 (6) |
| C15 | 0.8255 (3) | 0.81935 (14) | 0.39966 (17) | 0.0464 (7) |
| H15 | 0.8172 | 0.8610 | 0.3864 | 0.056* |
| C16 | 0.8867 (3) | 0.80530 (15) | 0.46072 (16) | 0.0491 (8) |
| H16 | 0.9198 | 0.8373 | 0.4895 | 0.059* |
| C17 | 0.9027 (2) | 0.74159 (14) | 0.48317 (14) | 0.0388 (7) |
| C18 | 0.9684 (3) | 0.72468 (15) | 0.54706 (15) | 0.0475 (8) |
| H18 | 1.0030 | 0.7552 | 0.5774 | 0.057* |
| C19 | 0.9806 (3) | 0.66304 (16) | 0.56400 (15) | 0.0483 (8) |
| H19 | 1.0238 | 0.6511 | 0.6059 | 0.058* |
| C20 | 0.9279 (3) | 0.61835 (14) | 0.51804 (14) | 0.0402 (7) |
| H20 | 0.9375 | 0.5765 | 0.5302 | 0.048* |
| C21 | 0.8526 (2) | 0.69322 (13) | 0.43960 (12) | 0.0308 (6) |
| C22 | 0.7853 (2) | 0.70819 (13) | 0.37350 (13) | 0.0310 (6) |
| C23 | 0.6369 (3) | 0.51558 (15) | 0.45537 (15) | 0.0413 (7) |
| C24 | 0.5619 (3) | 0.48871 (19) | 0.50365 (18) | 0.0600 (10) |
| H24A | 0.5593 | 0.4437 | 0.4983 | 0.072* |
| H24B | 0.6037 | 0.4975 | 0.5492 | 0.072* |
| O7 | 0.3967 (2) | 0.64187 (12) | 0.38792 (14) | 0.0622 (7) |
| H7A | 0.345 (3) | 0.630 (2) | 0.407 (2) | 0.093* |
| H7B | 0.449 (3) | 0.6154 (16) | 0.393 (2) | 0.093* |
| O8 | 0.8093 (2) | 0.39279 (12) | 0.54661 (12) | 0.0548 (6) |
| H8A | 0.870 (2) | 0.4015 (19) | 0.5751 (16) | 0.082* |
| H8B | 0.795 (4) | 0.4228 (14) | 0.5223 (18) | 0.082* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cd1 | 0.02758 (14) | 0.02503 (16) | 0.0631 (2) | 0.000 | 0.02148 (13) | 0.000 |
| Cd2 | 0.02656 (11) | 0.02609 (12) | 0.03117 (12) | −0.00091 (7) | 0.01250 (8) | −0.00017 (8) |
| N1 | 0.0353 (12) | 0.0292 (13) | 0.0587 (16) | −0.0019 (10) | 0.0106 (11) | 0.0041 (11) |
| N2 | 0.0343 (11) | 0.0322 (13) | 0.0310 (12) | 0.0016 (10) | 0.0103 (9) | 0.0010 (10) |
| N3 | 0.0362 (12) | 0.0311 (13) | 0.0324 (12) | 0.0007 (9) | 0.0128 (10) | 0.0015 (10) |
| O1 | 0.0385 (11) | 0.0575 (14) | 0.0496 (13) | −0.0221 (10) | 0.0201 (10) | −0.0225 (11) |
| O2 | 0.0295 (9) | 0.0364 (11) | 0.0350 (10) | −0.0037 (8) | 0.0127 (8) | −0.0059 (8) |
| O3 | 0.0409 (12) | 0.0809 (19) | 0.0837 (18) | −0.0104 (12) | 0.0299 (12) | −0.0349 (15) |
| O4 | 0.0417 (12) | 0.0665 (17) | 0.0543 (14) | −0.0193 (11) | 0.0172 (10) | 0.0069 (12) |
| O5 | 0.0424 (12) | 0.0763 (18) | 0.0572 (14) | 0.0027 (11) | 0.0247 (11) | 0.0284 (12) |
| O6 | 0.0500 (12) | 0.0432 (13) | 0.0642 (14) | 0.0047 (10) | 0.0316 (11) | 0.0120 (11) |
| C1 | 0.0264 (12) | 0.0305 (15) | 0.0335 (14) | 0.0007 (10) | 0.0101 (11) | 0.0031 (11) |
| C2 | 0.0320 (13) | 0.0345 (15) | 0.0319 (14) | −0.0093 (11) | 0.0116 (11) | −0.0011 (11) |
| C3 | 0.0364 (15) | 0.0452 (19) | 0.064 (2) | −0.0122 (13) | 0.0230 (15) | −0.0141 (16) |
| C4 | 0.0331 (15) | 0.072 (2) | 0.0319 (16) | −0.0175 (15) | 0.0157 (12) | −0.0220 (15) |
| C5 | 0.0461 (18) | 0.046 (2) | 0.060 (2) | −0.0029 (15) | 0.0047 (16) | 0.0103 (16) |
| C6 | 0.055 (2) | 0.065 (3) | 0.056 (2) | −0.0097 (18) | 0.0013 (17) | 0.0028 (18) |
| C7 | 0.055 (2) | 0.050 (2) | 0.067 (2) | −0.0192 (17) | 0.0125 (17) | −0.0137 (18) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C8 | 0.0390 (15) | 0.0310 (16) | 0.061 (2) | −0.0066 (12) | 0.0186 (15) | −0.0038 (14) |
| C9 | 0.0298 (13) | 0.0275 (15) | 0.0547 (18) | −0.0018 (11) | 0.0167 (12) | −0.0005 (12) |
| C10 | 0.061 (2) | 0.0271 (16) | 0.080 (3) | −0.0087 (14) | 0.0217 (18) | −0.0086 (15) |
| C11 | 0.0446 (16) | 0.0415 (18) | 0.0365 (16) | 0.0027 (13) | 0.0082 (13) | −0.0006 (13) |
| C12 | 0.0499 (18) | 0.058 (2) | 0.0382 (17) | 0.0103 (16) | 0.0056 (14) | 0.0115 (15) |
| C13 | 0.0520 (18) | 0.0348 (17) | 0.057 (2) | 0.0097 (14) | 0.0190 (16) | 0.0129 (15) |
| C14 | 0.0374 (14) | 0.0297 (15) | 0.0468 (17) | 0.0027 (12) | 0.0172 (13) | 0.0032 (12) |
| C15 | 0.0513 (18) | 0.0258 (16) | 0.063 (2) | −0.0011 (13) | 0.0137 (16) | −0.0008 (14) |
| C16 | 0.0548 (18) | 0.0301 (17) | 0.061 (2) | −0.0092 (14) | 0.0079 (16) | −0.0080 (15) |
| C17 | 0.0391 (15) | 0.0344 (16) | 0.0444 (17) | −0.0051 (12) | 0.0118 (13) | −0.0064 (13) |
| C18 | 0.0512 (18) | 0.048 (2) | 0.0405 (18) | −0.0096 (15) | 0.0005 (14) | −0.0127 (15) |
| C19 | 0.0488 (18) | 0.058 (2) | 0.0365 (17) | −0.0036 (16) | 0.0026 (14) | 0.0002 (15) |
| C20 | 0.0440 (16) | 0.0386 (17) | 0.0385 (16) | 0.0026 (13) | 0.0090 (13) | 0.0035 (13) |
| C21 | 0.0305 (13) | 0.0308 (15) | 0.0341 (15) | −0.0005 (11) | 0.0138 (11) | −0.0013 (11) |
| C22 | 0.0293 (13) | 0.0297 (15) | 0.0367 (15) | −0.0010 (11) | 0.0129 (11) | −0.0001 (12) |
| C23 | 0.0432 (16) | 0.0452 (18) | 0.0407 (17) | −0.0085 (14) | 0.0210 (13) | 0.0028 (14) |
| C24 | 0.0496 (19) | 0.076 (3) | 0.062 (2) | 0.0037 (18) | 0.0282 (17) | 0.0248 (19) |
| O7 | 0.0657 (17) | 0.0497 (16) | 0.0671 (17) | −0.0044 (13) | 0.0022 (13) | 0.0110 (13) |
| O8 | 0.0580 (14) | 0.0522 (15) | 0.0531 (16) | 0.0038 (12) | 0.0081 (11) | 0.0067 (11) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Cd1—O1$^{i}$ | 2.2873 (19) | C6—C7 | 1.366 (5) |
| Cd1—O1 | 2.2873 (19) | C6—H6 | 0.9300 |
| Cd1—N1 | 2.315 (2) | C7—C8 | 1.399 (4) |
| Cd1—N1$^{i}$ | 2.315 (2) | C7—H7 | 0.9300 |
| Cd1—O2 | 2.3667 (17) | C8—C9 | 1.402 (4) |
| Cd1—O2$^{i}$ | 2.3667 (17) | C8—C10 | 1.433 (4) |
| Cd1—C1$^{i}$ | 2.683 (2) | C9—C9$^{i}$ | 1.447 (5) |
| Cd2—O4$^{ii}$ | 2.331 (2) | C10—C10$^{i}$ | 1.349 (6) |
| Cd2—O6 | 2.341 (2) | C10—H10 | 0.9300 |
| Cd2—O2 | 2.3613 (17) | C11—C12 | 1.389 (4) |
| Cd2—N2 | 2.362 (2) | C11—H11 | 0.9300 |
| Cd2—N3 | 2.377 (2) | C12—C13 | 1.355 (4) |
| Cd2—O5 | 2.426 (2) | C12—H12 | 0.9300 |
| Cd2—O3$^{ii}$ | 2.545 (3) | C13—C14 | 1.402 (4) |
| N1—C5 | 1.318 (4) | C13—H13 | 0.9300 |
| N1—C9 | 1.363 (3) | C14—C22 | 1.409 (4) |
| N2—C11 | 1.328 (3) | C14—C15 | 1.438 (4) |
| N2—C22 | 1.357 (3) | C15—C16 | 1.330 (4) |
| N3—C20 | 1.324 (3) | C15—H15 | 0.9300 |
| N3—C21 | 1.357 (4) | C16—C17 | 1.438 (4) |
| O1—C1 | 1.249 (3) | C16—H16 | 0.9300 |
| O2—C1 | 1.274 (3) | C17—C21 | 1.407 (4) |
| O3—C4 | 1.239 (4) | C17—C18 | 1.409 (4) |
| O3—Cd2$^{ii}$ | 2.545 (3) | C18—C19 | 1.364 (4) |
| O4—C4 | 1.265 (4) | C18—H18 | 0.9300 |

| | | | |
|---|---|---|---|
| O4—Cd2$^{ii}$ | 2.331 (2) | C19—C20 | 1.386 (4) |
| O5—C23 | 1.241 (4) | C19—H19 | 0.9300 |
| O6—C23 | 1.248 (3) | C20—H20 | 0.9300 |
| C1—C2 | 1.497 (3) | C21—C22 | 1.443 (3) |
| C2—C3 | 1.514 (4) | C23—C24 | 1.516 (4) |
| C2—H2A | 0.9700 | C24—C24$^{iii}$ | 1.448 (6) |
| C2—H2B | 0.9700 | C24—H24A | 0.9700 |
| C3—C4 | 1.509 (4) | C24—H24B | 0.9700 |
| C3—H3A | 0.9700 | O7—H7A | 0.791 (18) |
| C3—H3B | 0.9700 | O7—H7B | 0.804 (18) |
| C5—C6 | 1.384 (5) | O8—H8A | 0.823 (18) |
| C5—H5 | 0.9300 | O8—H8B | 0.806 (19) |
| O1$^{i}$—Cd1—O1 | 168.31 (11) | C4—C3—H3B | 108.8 |
| O1$^{i}$—Cd1—N1 | 98.96 (9) | C2—C3—H3B | 108.8 |
| O1—Cd1—N1 | 90.44 (8) | H3A—C3—H3B | 107.7 |
| O1$^{i}$—Cd1—N1$^{i}$ | 90.44 (8) | O3—C4—O4 | 122.3 (3) |
| O1—Cd1—N1$^{i}$ | 98.96 (9) | O3—C4—C3 | 119.7 (3) |
| N1—Cd1—N1$^{i}$ | 73.37 (12) | O4—C4—C3 | 117.9 (3) |
| O1$^{i}$—Cd1—O2 | 115.59 (7) | N1—C5—C6 | 123.8 (3) |
| O1—Cd1—O2 | 56.00 (6) | N1—C5—H5 | 118.1 |
| N1—Cd1—O2 | 145.11 (7) | C6—C5—H5 | 118.1 |
| N1$^{i}$—Cd1—O2 | 100.42 (7) | C7—C6—C5 | 118.5 (3) |
| O1$^{i}$—Cd1—O2$^{i}$ | 56.00 (6) | C7—C6—H6 | 120.7 |
| O1—Cd1—O2$^{i}$ | 115.59 (7) | C5—C6—H6 | 120.7 |
| N1—Cd1—O2$^{i}$ | 100.42 (7) | C6—C7—C8 | 119.9 (3) |
| N1$^{i}$—Cd1—O2$^{i}$ | 145.11 (7) | C6—C7—H7 | 120.0 |
| O2—Cd1—O2$^{i}$ | 102.76 (9) | C8—C7—H7 | 120.0 |
| O1$^{i}$—Cd1—C1$^{i}$ | 27.67 (7) | C7—C8—C9 | 117.7 (3) |
| O1—Cd1—C1$^{i}$ | 143.51 (8) | C7—C8—C10 | 122.7 (3) |
| N1—Cd1—C1$^{i}$ | 100.42 (8) | C9—C8—C10 | 119.6 (3) |
| N1$^{i}$—Cd1—C1$^{i}$ | 117.52 (8) | N1—C9—C8 | 121.8 (3) |
| O2—Cd1—C1$^{i}$ | 112.32 (7) | N1—C9—C9$^{i}$ | 118.86 (16) |
| O2$^{i}$—Cd1—C1$^{i}$ | 28.34 (7) | C8—C9—C9$^{i}$ | 119.32 (18) |
| O4$^{ii}$—Cd2—O6 | 115.91 (8) | C10$^{i}$—C10—C8 | 120.94 (18) |
| O4$^{ii}$—Cd2—O2 | 107.38 (7) | C10$^{i}$—C10—H10 | 119.5 |
| O6—Cd2—O2 | 105.85 (7) | C8—C10—H10 | 119.5 |
| O4$^{ii}$—Cd2—N2 | 95.84 (8) | N2—C11—C12 | 123.0 (3) |
| O6—Cd2—N2 | 137.87 (7) | N2—C11—H11 | 118.5 |
| O2—Cd2—N2 | 88.71 (7) | C12—C11—H11 | 118.5 |
| O4$^{ii}$—Cd2—N3 | 80.55 (7) | C13—C12—C11 | 119.5 (3) |
| O6—Cd2—N3 | 87.36 (8) | C13—C12—H12 | 120.3 |
| O2—Cd2—N3 | 158.64 (7) | C11—C12—H12 | 120.3 |
| N2—Cd2—N3 | 70.53 (7) | C12—C13—C14 | 119.8 (3) |
| O4$^{ii}$—Cd2—O5 | 166.83 (8) | C12—C13—H13 | 120.1 |

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|---|---|---|---|
| O6—Cd2—O5 | 54.24 (7) | C14—C13—H13 | 120.1 |
| O2—Cd2—O5 | 84.81 (7) | C13—C14—C22 | 117.3 (3) |
| N2—Cd2—O5 | 89.26 (7) | C13—C14—C15 | 123.1 (3) |
| N3—Cd2—O5 | 89.78 (8) | C22—C14—C15 | 119.6 (3) |
| O4$^{ii}$—Cd2—O3$^{ii}$ | 53.26 (7) | C16—C15—C14 | 121.2 (3) |
| O6—Cd2—O3$^{ii}$ | 83.13 (7) | C16—C15—H15 | 119.4 |
| O2—Cd2—O3$^{ii}$ | 78.21 (8) | C14—C15—H15 | 119.4 |
| N2—Cd2—O3$^{ii}$ | 138.96 (7) | C15—C16—C17 | 121.3 (3) |
| N3—Cd2—O3$^{ii}$ | 120.76 (8) | C15—C16—H16 | 119.3 |
| O5—Cd2—O3$^{ii}$ | 127.25 (8) | C17—C16—H16 | 119.3 |
| C5—N1—C9 | 118.2 (3) | C21—C17—C18 | 117.6 (3) |
| C5—N1—Cd1 | 127.3 (2) | C21—C17—C16 | 119.2 (3) |
| C9—N1—Cd1 | 114.31 (19) | C18—C17—C16 | 123.1 (3) |
| C11—N2—C22 | 118.1 (2) | C19—C18—C17 | 119.3 (3) |
| C11—N2—Cd2 | 125.57 (19) | C19—C18—H18 | 120.3 |
| C22—N2—Cd2 | 116.27 (17) | C17—C18—H18 | 120.3 |
| C20—N3—C21 | 118.2 (2) | C18—C19—C20 | 119.3 (3) |
| C20—N3—Cd2 | 125.52 (19) | C18—C19—H19 | 120.4 |
| C21—N3—Cd2 | 115.99 (17) | C20—C19—H19 | 120.4 |
| C1—O1—Cd1 | 94.09 (16) | N3—C20—C19 | 123.4 (3) |
| C1—O2—Cd2 | 129.59 (15) | N3—C20—H20 | 118.3 |
| C1—O2—Cd1 | 89.78 (15) | C19—C20—H20 | 118.3 |
| Cd2—O2—Cd1 | 132.66 (8) | N3—C21—C17 | 122.1 (2) |
| C4—O3—Cd2$^{ii}$ | 87.5 (2) | N3—C21—C22 | 118.2 (2) |
| C4—O4—Cd2$^{ii}$ | 96.86 (18) | C17—C21—C22 | 119.7 (3) |
| C23—O5—Cd2 | 90.14 (17) | N2—C22—C14 | 122.3 (2) |
| C23—O6—Cd2 | 93.92 (18) | N2—C22—C21 | 118.7 (2) |
| O1—C1—O2 | 120.1 (2) | C14—C22—C21 | 119.0 (2) |
| O1—C1—C2 | 119.1 (2) | O5—C23—O6 | 121.7 (3) |
| O2—C1—C2 | 120.8 (2) | O5—C23—C24 | 121.3 (3) |
| C1—C2—C3 | 113.1 (2) | O6—C23—C24 | 117.0 (3) |
| C1—C2—H2A | 109.0 | C24$^{iii}$—C24—C23 | 116.3 (4) |
| C3—C2—H2A | 109.0 | C24$^{iii}$—C24—H24A | 108.2 |
| C1—C2—H2B | 109.0 | C23—C24—H24A | 108.2 |
| C3—C2—H2B | 109.0 | C24$^{iii}$—C24—H24B | 108.2 |
| H2A—C2—H2B | 107.8 | C23—C24—H24B | 108.2 |
| C4—C3—C2 | 114.0 (3) | H24A—C24—H24B | 107.4 |
| C4—C3—H3A | 108.8 | H7A—O7—H7B | 107 (4) |
| C2—C3—H3A | 108.8 | H8A—O8—H8B | 107 (4) |
| O1$^{i}$—Cd1—N1—C5 | 95.2 (3) | O5—Cd2—O6—C23 | −0.51 (18) |
| O1—Cd1—N1—C5 | −77.8 (3) | O3$^{ii}$—Cd2—O6—C23 | −147.46 (19) |
| N1$^{i}$—Cd1—N1—C5 | −177.0 (3) | Cd1—O1—C1—O2 | −2.2 (3) |
| O2—Cd1—N1—C5 | −92.7 (3) | Cd1—O1—C1—C2 | 179.6 (2) |
| O2$^{i}$—Cd1—N1—C5 | 38.4 (3) | Cd2—O2—C1—O1 | 153.3 (2) |
| C1$^{i}$—Cd1—N1—C5 | 67.2 (3) | Cd1—O2—C1—O1 | 2.1 (3) |

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|---|---|---|---|
| O1$^{i}$—Cd1—N1—C9 | −89.39 (19) | Cd2—O2—C1—C2 | −28.5 (3) |
| O1—Cd1—N1—C9 | 97.6 (2) | Cd1—O2—C1—C2 | −179.7 (2) |
| N1$^{i}$—Cd1—N1—C9 | −1.62 (14) | O1—C1—C2—C3 | −37.5 (4) |
| O2—Cd1—N1—C9 | 82.7 (2) | O2—C1—C2—C3 | 144.2 (3) |
| O2$^{i}$—Cd1—N1—C9 | −146.26 (19) | C1—C2—C3—C4 | −175.1 (2) |
| C1$^{i}$—Cd1—N1—C9 | −117.43 (19) | Cd2$^{ii}$—O3—C4—O4 | 0.8 (3) |
| O4$^{ii}$—Cd2—N2—C11 | 103.4 (2) | Cd2$^{ii}$—O3—C4—C3 | −177.5 (2) |
| O6—Cd2—N2—C11 | −116.4 (2) | Cd2$^{ii}$—O4—C4—O3 | −0.8 (3) |
| O2—Cd2—N2—C11 | −4.0 (2) | Cd2$^{ii}$—O4—C4—C3 | 177.4 (2) |
| N3—Cd2—N2—C11 | −178.8 (2) | C2—C3—C4—O3 | 150.8 (3) |
| O5—Cd2—N2—C11 | −88.8 (2) | C2—C3—C4—O4 | −27.5 (4) |
| O3$^{ii}$—Cd2—N2—C11 | 66.3 (3) | C9—N1—C5—C6 | −2.2 (5) |
| O4$^{ii}$—Cd2—N2—C22 | −73.61 (18) | Cd1—N1—C5—C6 | 173.0 (3) |
| O6—Cd2—N2—C22 | 66.6 (2) | N1—C5—C6—C7 | 2.0 (5) |
| O2—Cd2—N2—C22 | 179.05 (18) | C5—C6—C7—C8 | 0.2 (5) |
| N3—Cd2—N2—C22 | 4.20 (17) | C6—C7—C8—C9 | −1.9 (5) |
| O5—Cd2—N2—C22 | 94.23 (18) | C6—C7—C8—C10 | 175.8 (3) |
| O3$^{ii}$—Cd2—N2—C22 | −110.64 (19) | C5—N1—C9—C8 | 0.3 (4) |
| O4$^{ii}$—Cd2—N3—C20 | −78.7 (2) | Cd1—N1—C9—C8 | −175.6 (2) |
| O6—Cd2—N3—C20 | 38.1 (2) | C5—N1—C9—C9$^{i}$ | −179.5 (3) |
| O2—Cd2—N3—C20 | 167.36 (19) | Cd1—N1—C9—C9$^{i}$ | 4.7 (4) |
| N2—Cd2—N3—C20 | −178.4 (2) | C7—C8—C9—N1 | 1.7 (4) |
| O5—Cd2—N3—C20 | 92.3 (2) | C10—C8—C9—N1 | −176.0 (3) |
| O3$^{ii}$—Cd2—N3—C20 | −42.3 (2) | C7—C8—C9—C9$^{i}$ | −178.5 (3) |
| O4$^{ii}$—Cd2—N3—C21 | 94.91 (18) | C10—C8—C9—C9$^{i}$ | 3.7 (5) |
| O6—Cd2—N3—C21 | −148.27 (18) | C7—C8—C10—C10$^{i}$ | −176.7 (4) |
| O2—Cd2—N3—C21 | −19.0 (3) | C9—C8—C10—C10$^{i}$ | 0.9 (6) |
| N2—Cd2—N3—C21 | −4.78 (17) | C22—N2—C11—C12 | 0.9 (4) |
| O5—Cd2—N3—C21 | −94.07 (18) | Cd2—N2—C11—C12 | −176.0 (2) |
| O3$^{ii}$—Cd2—N3—C21 | 131.33 (17) | N2—C11—C12—C13 | 0.6 (5) |
| O1$^{i}$—Cd1—O1—C1 | 47.76 (16) | C11—C12—C13—C14 | −1.3 (5) |
| N1—Cd1—O1—C1 | −168.60 (18) | C12—C13—C14—C22 | 0.6 (4) |
| N1$^{i}$—Cd1—O1—C1 | −95.37 (18) | C12—C13—C14—C15 | −179.8 (3) |
| O2—Cd1—O1—C1 | 1.21 (15) | C13—C14—C15—C16 | 179.7 (3) |
| O2$^{i}$—Cd1—O1—C1 | 89.62 (17) | C22—C14—C15—C16 | −0.8 (5) |
| C1$^{i}$—Cd1—O1—C1 | 83.1 (2) | C14—C15—C16—C17 | 0.6 (5) |
| O4$^{ii}$—Cd2—O2—C1 | 1.1 (2) | C15—C16—C17—C21 | 0.0 (5) |
| O6—Cd2—O2—C1 | −123.3 (2) | C15—C16—C17—C18 | 179.1 (3) |
| N2—Cd2—O2—C1 | 96.8 (2) | C21—C17—C18—C19 | 0.0 (4) |
| N3—Cd2—O2—C1 | 110.3 (3) | C16—C17—C18—C19 | −179.1 (3) |
| O5—Cd2—O2—C1 | −173.8 (2) | C17—C18—C19—C20 | −0.2 (5) |
| O3$^{ii}$—Cd2—O2—C1 | −44.0 (2) | C21—N3—C20—C19 | 1.2 (4) |
| O4$^{ii}$—Cd2—O2—Cd1 | 140.17 (11) | Cd2—N3—C20—C19 | 174.7 (2) |
| O6—Cd2—O2—Cd1 | 15.78 (12) | C18—C19—C20—N3 | −0.4 (5) |

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|---|---|---|---|
| N2—Cd2—O2—Cd1 | −124.11 (11) | C20—N3—C21—C17 | −1.4 (4) |
| N3—Cd2—O2—Cd1 | −110.69 (18) | Cd2—N3—C21—C17 | −175.53 (19) |
| O5—Cd2—O2—Cd1 | −34.73 (11) | C20—N3—C21—C22 | 179.1 (2) |
| O3$^{ii}$—Cd2—O2—Cd1 | 95.05 (12) | Cd2—N3—C21—C22 | 5.0 (3) |
| O1$^{i}$—Cd1—O2—C1 | −171.79 (14) | C18—C17—C21—N3 | 0.9 (4) |
| O1—Cd1—O2—C1 | −1.18 (15) | C16—C17—C21—N3 | 180.0 (3) |
| N1—Cd1—O2—C1 | 16.8 (2) | C18—C17—C21—C22 | −179.6 (2) |
| N1$^{i}$—Cd1—O2—C1 | 92.65 (15) | C16—C17—C21—C22 | −0.5 (4) |
| O2$^{i}$—Cd1—O2—C1 | −113.61 (15) | C11—N2—C22—C14 | −1.6 (4) |
| C1$^{i}$—Cd1—O2—C1 | −141.66 (14) | Cd2—N2—C22—C14 | 175.58 (19) |
| O1$^{i}$—Cd1—O2—Cd2 | 38.54 (13) | C11—N2—C22—C21 | 179.4 (2) |
| O1—Cd1—O2—Cd2 | −150.85 (14) | Cd2—N2—C22—C21 | −3.4 (3) |
| N1—Cd1—O2—Cd2 | −132.82 (13) | C13—C14—C22—N2 | 0.9 (4) |
| N1$^{i}$—Cd1—O2—Cd2 | −57.02 (12) | C15—C14—C22—N2 | −178.7 (2) |
| O2$^{i}$—Cd1—O2—Cd2 | 96.72 (11) | C13—C14—C22—C21 | 179.8 (2) |
| C1$^{i}$—Cd1—O2—Cd2 | 68.67 (12) | C15—C14—C22—C21 | 0.2 (4) |
| O4$^{ii}$—Cd2—O5—C23 | −43.9 (5) | N3—C21—C22—N2 | −1.1 (3) |
| O6—Cd2—O5—C23 | 0.51 (18) | C17—C21—C22—N2 | 179.4 (2) |
| O2—Cd2—O5—C23 | 114.3 (2) | N3—C21—C22—C14 | 179.9 (2) |
| N2—Cd2—O5—C23 | −156.9 (2) | C17—C21—C22—C14 | 0.4 (4) |
| N3—Cd2—O5—C23 | −86.4 (2) | Cd2—O5—C23—O6 | −0.9 (3) |
| O3$^{ii}$—Cd2—O5—C23 | 43.4 (2) | Cd2—O5—C23—C24 | 179.8 (3) |
| O4$^{ii}$—Cd2—O6—C23 | 169.29 (18) | Cd2—O6—C23—O5 | 0.9 (3) |
| O2—Cd2—O6—C23 | −71.82 (19) | Cd2—O6—C23—C24 | −179.8 (3) |
| N2—Cd2—O6—C23 | 34.4 (2) | O5—C23—C24—C24$^{iii}$ | 2.8 (6) |
| N3—Cd2—O6—C23 | 91.13 (19) | O6—C23—C24—C24$^{iii}$ | −176.5 (4) |

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

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O7—H7A···O8$^{iii}$ | 0.791 (18) | 2.174 (19) | 2.962 (4) | 174 (5) |
| O7—H7B···O5 | 0.804 (18) | 2.048 (19) | 2.847 (3) | 172 (4) |
| O8—H8A···O4$^{iv}$ | 0.823 (18) | 2.04 (2) | 2.857 (3) | 169 (4) |
| O8—H8B···O6 | 0.806 (19) | 2.015 (19) | 2.818 (3) | 174 (4) |

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

**Fig. 1**

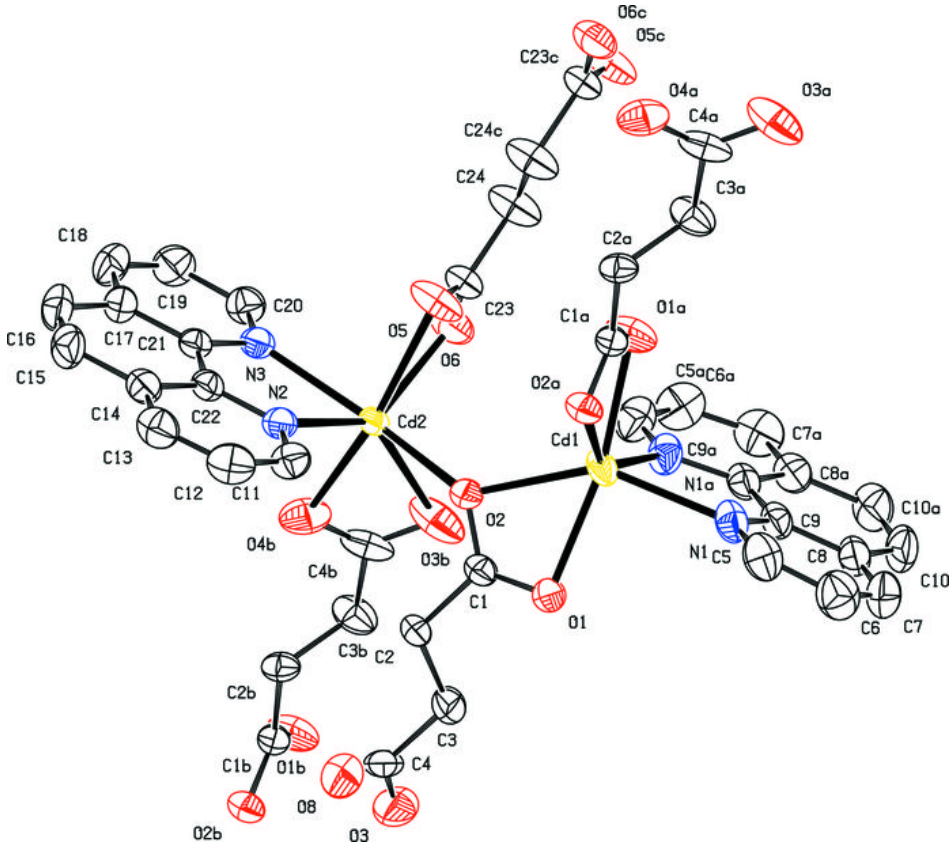
O6c
O5c
C23c
O4a
O3a
C4a
C24c
C24
C3a
C18
C2a
C19
C20
C23
C1a
O1a
O5
C16
C17
C21
O6
N3
C15
N2
O2a
C5a
C6a
C14
C22
Cd2
Cd1
C7a
C9a
C13
C8a
N1a
C12
C11
O2
C10a
C9
O4b
O3b
N1
C5
C8
C4b
C1
C10
O1
C6
C7
C3b
C2
C2b
C3
C1b
O1b
C4
O8
O2b
O3

**Fig. 2**