IUCrData

ISSN 2414-3146

Bis(acetato-κO)bis{2-[4-(pyridin-2-yl)phenyl]-1*H*-imidazo[4,5-*f*][1,10]phenanthroline-$\kappa^2 N,N'$}-cadmium(II)

Lei-Qun Guo and Yin-Hua Jiang*

School of Chemistry and Chemical Engineering, Jiangsu University, 212013 Zhenjiang, Jiangsu, People's Republic of China. *Correspondence e-mail: guoleiqun0606@163.com

Received 31 December 2015
Accepted 13 January 2016

Edited by V. V. Chernyshev, Moscow State University, Russia

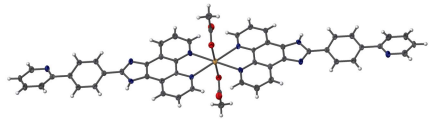
Keywords: crystal structure; Cd^{II} complex; hydrogen bonds.

CCDC reference: 885941

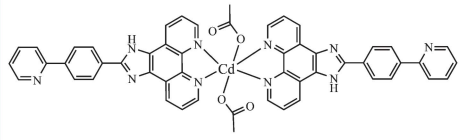
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $[Cd(CH_3COO)(C_{24}H_{15}N_5)]$, comprises one-half of the centrosymmetric molecule. The Cd^{II} ion, situated on a centre of inversion, is coordinated by two O atoms from two acetate ligands and four N atoms from two 2-[4-(pyridin-2-yl)phenyl]-1*H*-imidazo[4,5-*f*][1,10]-phenanthroline (*L*) ligands in a distorted octahedral geometry. In the *L* ligand, the terminal phenyl and pyridine rings are turned away from the mean plane of the imidazo[4,5-*f*][1,10]phenanthroline fragment in opposite directions, at 11.1 (1) and 10.5 (1)°, respectively. In the crystal, N—H···O hydrogen bonds link molecules related by translation along the *a* axis into linear chains, and weak C—H···N interactions link these chains into layers parallel to the (011) plane.

3D view



Chemical scheme



Structure description

In recent years, the design and synthesis of novel metal-organic coordination polymers based on 1,10-phenanthroline-derivates ligands have attracted much attention (Wang *et al.*, 2011; Xu *et al.*, 2011; Kong *et al.*, 2015). We report herein the crystal structure of the title molecular complex (I) (Fig. 1). In (I), the Cd^{II} ion, situated on a centre of inversion, is six-coordinated by two O atoms from two acetato ligands and four N atoms from two 2-(4-pyridine-2-yl-phenyl)-1*H*-imidazo[4,5-*f*] [1,10]phenanthroline ligands in a distorted octahedral geometry. Such a centrosymmetric coordination of the transition metal atom (Cd) is similar to those observed in the related structures with CCDC refcodes PUPTOK (Wang *et al.*, 2010), WEJLUT (Che, 2006) and WEJNUV (Che *et al.*, 2006). However, all three of the aforementioned compounds are polymeric, while (I) is a 0D molecular complex. In the crystal, the adjacent molecules are linked *via* N—H···O hydrogen bonds

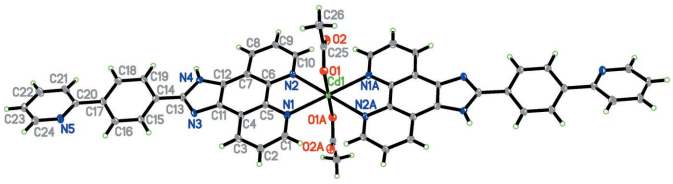


Figure 1
The molecular structure of (I), showing the atomic numbering and 50% probability displacement ellipsoids. [Symmetry code: (A) $-x$, $-y+1$, $-z+1$.]

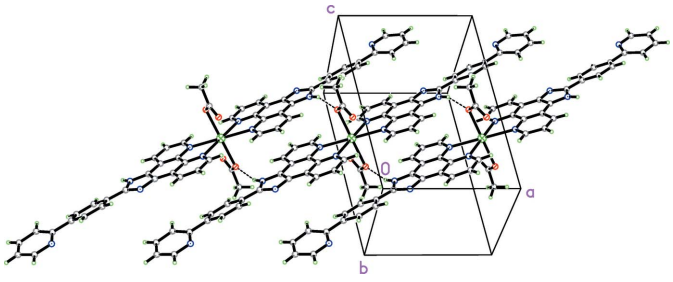


Figure 2
A portion of the crystal packing showing the formation of a hydrogen-bonded (dashed lines) linear chain of molecules.

(Table 1) into linear chains along the axis *a* (Fig. 2), and weak C—H···N interactions (Table 1) link these chains into layers parallel to the (011) plane.

Synthesis and crystallization

A mixture of $Cd(CH_3COO)_2{\cdot}4H_2O$ (0.25 mmol), 2-(4-pyridine-2-yl-phenyl)-1*H*-imidazo[4,5-*f*][1,10]phenanthroline (0.5 mmol) and H_2O (10 ml) was stirred at room temperature for 15 min. When the pH value had been adjusted to about 7.08 with NaOH, the mixture was transferred into a 25 ml Teflon-lined stainless-steel reactor, heated to 453 K for nine days, and then slowly cooled to room temperature at a rate of 5 K h^{-1}. Pale-yellow block crystals of the title complex were isolated, washed with distilled water, and dried in air (yield: 46% based on Cd^{II}).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

This work was supported financially by Jiangsu University.

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···O1^{i}	0.86	1.93	2.724 (4)	153
C9—H9···N5^{ii}	0.93	2.61	3.523 (5)	168

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Cd(C_2H_3O_2)(C_{24}H_{15}N_5)]$
M_r	977.31
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	9.2984 (12), 9.3261 (14), 12.5747 (16)
α, β, γ (°)	107.160 (2), 103.719 (3), 96.550 (2)
V (Å^3)	992.1 (2)
Z	1
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.62
Crystal size (mm)	0.25 × 0.20 × 0.18
Data collection	
Diffractometer	Bruker *SMART APEX* CCD diffractometer
Absorption correction	Multi-scan (*SADABS*; Bruker, 2005)
T_{min}, T_{max}	0.861, 0.897
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6876, 3448, 3170
R_{int}	0.041
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.596
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.122, 1.07
No. of reflections	3448
No. of parameters	293
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.19, −0.95

Computer programs: *APEX2* (Bruker, 2005), *SAINT* (Bruker, 2005), *SHELXTL* (Sheldrick, 2008).

References

Bruker (2005). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Che, G.-B. (2006). *Acta Cryst.* E**62**, m1244–m1246.
Che, G.-B., Lin, X.-F. & Liu, C.-B. (2006). *Acta Cryst.* E**62**, m1456–m1458.
Kong, Z. G., Guo, S. N., Zhou, X. L., Zhao, Z. Y. & Lv, J. Q. (2015). *Chin. J. Struct. Chem.* **34**, 606–610.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wang, X.-L., Chen, Y.-Q., Liu, G.-C., Zhang, J.-X., Lin, H.-Y. & Chen, B.-K. (2010). *Inorg. Chim. Acta*, **363**, 773–778.
Wang, X.-Y., Ma, S. & He, Y. (2011). *Acta Cryst.* E**67**, m325.
Xu, H.-B., Ma, S. & He, Y. (2011). *Acta Cryst.* E**67**, m326.

full crystallographic data

IUCrData (2016). **1**, x160063 [doi:10.1107/S2414314616000638]

Bis(acetato-κO)bis{2-[4-(pyridin-2-yl)phenyl]-1*H*-imidazo[4,5-*f*][1,10]phenanthroline-$\kappa^2 N,N'$}cadmium(II)

Lei-Qun Guo and Yin-Hua Jiang

Bis(acetato-κO)bis{2-[4-(pyridin-2-yl)phenyl]-1*H*-imidazo[4,5-*f*][1,10]phenanthroline-$\kappa^2 N,N'$}cadmium(II)

Crystal data

$[Cd(C_2H_3O_2)(C_{24}H_{15}N_5)]$
M_r = 977.31
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 9.2984 (12) Å
b = 9.3261 (14) Å
c = 12.5747 (16) Å
α = 107.160 (2)°
β = 103.719 (3)°
γ = 96.550 (2)°
V = 992.1 (2) Å^3
Z = 1
$F(000)$ = 498
D_x = 1.636 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1729 reflections
θ = 2.1–23.6°
μ = 0.62 mm^{-1}
T = 293 K
Block, pale-yellow
0.25 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.861, T_{max} = 0.897
6876 measured reflections
3448 independent reflections
3170 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 25.1°, θ_{min} = 3.3°
h = −11→10
k = −11→8
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.122
S = 1.07
3448 reflections
293 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0696P)^2 + 0.0238P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.95 e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.1738 (4)	0.7815 (5)	0.7460 (3)	0.0222 (9)
H1	0.0793	0.8077	0.7310	0.027*
C2	0.2863 (4)	0.8767 (5)	0.8459 (4)	0.0260 (9)
H2	0.2669	0.9633	0.8957	0.031*
C3	0.4248 (4)	0.8383 (5)	0.8677 (3)	0.0242 (9)
H3	0.5022	0.8992	0.9330	0.029*
C4	0.4507 (2)	0.7022 (2)	0.78865 (19)	0.0209 (9)
C5	0.33294 (19)	0.6156 (3)	0.6911 (2)	0.0193 (8)
C6	0.3560 (2)	0.4885 (3)	0.61043 (17)	0.0183 (8)
C7	0.4969 (2)	0.4479 (2)	0.62734 (19)	0.0203 (9)
C12	0.61462 (19)	0.5344 (3)	0.7249 (2)	0.0199 (8)
C11	0.5915 (2)	0.6616 (3)	0.80555 (17)	0.0195 (8)
C8	0.5160 (4)	0.3161 (5)	0.5384 (4)	0.0224 (9)
H8	0.6090	0.2866	0.5457	0.027*
C9	0.3958 (4)	0.2363 (5)	0.4440 (3)	0.0232 (9)
H9	0.4052	0.1507	0.3871	0.028*
C10	0.2590 (4)	0.2859 (4)	0.4350 (4)	0.0225 (9)
H10	0.1779	0.2311	0.3705	0.027*
C13	0.8247 (4)	0.6499 (5)	0.8649 (3)	0.0217 (9)
C14	0.9828 (4)	0.6839 (4)	0.9361 (3)	0.0210 (9)
C15	1.0378 (4)	0.8222 (5)	1.0267 (3)	0.0224 (9)
H15	0.9748	0.8921	1.0399	0.027*
C16	1.1848 (4)	0.8580 (5)	1.0977 (4)	0.0234 (9)
H16	1.2201	0.9521	1.1569	0.028*
C17	1.2810 (4)	0.7524 (5)	1.0806 (3)	0.0207 (9)
C18	1.2244 (4)	0.6149 (5)	0.9902 (4)	0.0266 (10)
H18	1.2866	0.5440	0.9779	0.032*
C19	1.0785 (4)	0.5791 (5)	0.9177 (4)	0.0249 (9)
H19	1.0442	0.4862	0.8572	0.030*
C20	1.4371 (4)	0.7911 (4)	1.1599 (4)	0.0222 (9)
C21	1.5513 (5)	0.7191 (5)	1.1270 (4)	0.0323 (10)
H21	1.5321	0.6469	1.0537	0.039*
C22	1.6934 (5)	0.7574 (5)	1.2057 (4)	0.0393 (12)
H22	1.7704	0.7095	1.1861	0.047*
C23	1.7198 (4)	0.8663 (5)	1.3124 (4)	0.0303 (10)

H23	1.8144	0.8940	1.3666	0.036*
C24	1.6021 (4)	0.9332 (5)	1.3369 (4)	0.0288 (10)
H24	1.6203	1.0082	1.4089	0.035*
C25	−0.0756 (4)	0.2401 (5)	0.5775 (4)	0.0230 (9)
C26	−0.1180 (5)	0.1365 (5)	0.6414 (4)	0.0304 (10)
H26A	−0.1043	0.0352	0.6042	0.046*
H26B	−0.2219	0.1332	0.6405	0.046*
H26C	−0.0550	0.1747	0.7202	0.046*
Cd1	0.0000	0.5000	0.5000	0.02133 (17)
N1	0.1936 (3)	0.6574 (4)	0.6721 (3)	0.0208 (7)
N2	0.2376 (3)	0.4062 (4)	0.5128 (3)	0.0207 (7)
N3	0.7245 (3)	0.7336 (4)	0.8941 (3)	0.0218 (7)
N4	0.7646 (3)	0.5293 (4)	0.7644 (3)	0.0210 (7)
H4	0.8114	0.4627	0.7319	0.025*
N5	1.4633 (4)	0.8975 (4)	1.2639 (3)	0.0262 (8)
O1	−0.0839 (3)	0.3810 (3)	0.6190 (3)	0.0278 (7)
O2	−0.0346 (3)	0.1899 (3)	0.4899 (3)	0.0305 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.015 (2)	0.028 (2)	0.023 (2)	0.0088 (16)	0.0054 (16)	0.0053 (18)
C2	0.025 (2)	0.029 (2)	0.022 (2)	0.0069 (17)	0.0051 (17)	0.0061 (19)
C3	0.021 (2)	0.026 (2)	0.018 (2)	−0.0006 (16)	0.0019 (17)	0.0011 (18)
C4	0.016 (2)	0.025 (2)	0.019 (2)	0.0031 (15)	0.0034 (16)	0.0049 (17)
C5	0.0136 (19)	0.025 (2)	0.021 (2)	0.0060 (15)	0.0039 (16)	0.0096 (18)
C6	0.0120 (19)	0.020 (2)	0.018 (2)	−0.0010 (14)	0.0001 (15)	0.0047 (17)
C7	0.020 (2)	0.021 (2)	0.020 (2)	0.0023 (16)	0.0056 (16)	0.0085 (18)
C12	0.016 (2)	0.022 (2)	0.020 (2)	0.0040 (15)	0.0038 (16)	0.0065 (17)
C11	0.016 (2)	0.019 (2)	0.017 (2)	0.0006 (15)	0.0010 (15)	0.0012 (17)
C8	0.016 (2)	0.023 (2)	0.029 (2)	0.0046 (16)	0.0053 (17)	0.0109 (19)
C9	0.021 (2)	0.019 (2)	0.023 (2)	0.0013 (16)	0.0035 (17)	0.0012 (17)
C10	0.016 (2)	0.021 (2)	0.024 (2)	0.0012 (16)	0.0010 (16)	0.0025 (18)
C13	0.014 (2)	0.027 (2)	0.022 (2)	0.0029 (16)	0.0019 (16)	0.0086 (18)
C14	0.019 (2)	0.021 (2)	0.022 (2)	0.0025 (16)	0.0027 (16)	0.0081 (18)
C15	0.020 (2)	0.022 (2)	0.022 (2)	0.0074 (16)	0.0045 (17)	0.0016 (17)
C16	0.022 (2)	0.020 (2)	0.023 (2)	0.0036 (16)	0.0030 (17)	0.0027 (18)
C17	0.017 (2)	0.024 (2)	0.020 (2)	0.0014 (16)	0.0021 (16)	0.0084 (18)
C18	0.018 (2)	0.023 (2)	0.032 (2)	0.0061 (16)	0.0033 (18)	0.0018 (19)
C19	0.019 (2)	0.021 (2)	0.027 (2)	0.0014 (16)	0.0006 (18)	0.0020 (18)
C20	0.021 (2)	0.019 (2)	0.023 (2)	0.0017 (16)	0.0021 (17)	0.0060 (18)
C21	0.026 (2)	0.025 (2)	0.031 (3)	0.0032 (18)	0.0037 (19)	−0.006 (2)
C22	0.016 (2)	0.032 (3)	0.051 (3)	0.0074 (18)	−0.001 (2)	−0.004 (2)
C23	0.014 (2)	0.031 (3)	0.037 (3)	0.0028 (17)	−0.0054 (18)	0.009 (2)
C24	0.024 (2)	0.030 (2)	0.026 (2)	0.0042 (18)	0.0007 (18)	0.0058 (19)
C25	0.0131 (19)	0.026 (2)	0.029 (2)	0.0038 (16)	0.0024 (17)	0.0102 (19)
C26	0.029 (2)	0.030 (2)	0.031 (2)	0.0016 (18)	0.0084 (19)	0.011 (2)
Cd1	0.0144 (2)	0.0254 (3)	0.0198 (3)	0.00243 (16)	0.00164 (17)	0.00412 (19)

N1	0.0151 (17)	0.0254 (19)	0.0229 (18)	0.0072 (13)	0.0055 (14)	0.0082 (15)
N2	0.0160 (17)	0.0210 (18)	0.0192 (17)	0.0005 (13)	−0.0011 (13)	0.0041 (15)
N3	0.0157 (17)	0.0229 (19)	0.0191 (18)	0.0019 (13)	−0.0008 (14)	0.0012 (15)
N4	0.0181 (17)	0.0178 (17)	0.0254 (18)	0.0095 (13)	0.0060 (14)	0.0028 (15)
N5	0.0176 (18)	0.029 (2)	0.0263 (19)	0.0043 (14)	0.0012 (15)	0.0050 (16)
O1	0.0246 (15)	0.0257 (17)	0.0307 (16)	0.0052 (12)	0.0072 (12)	0.0067 (13)
O2	0.0278 (16)	0.0359 (18)	0.0264 (17)	0.0070 (13)	0.0086 (13)	0.0077 (14)

Geometric parameters (Å, º)

C1—N1	1.316 (5)	C16—C17	1.408 (5)
C1—C2	1.402 (5)	C16—H16	0.9300
C1—H1	0.9300	C17—C18	1.384 (6)
C2—C3	1.363 (5)	C17—C20	1.488 (5)
C2—H2	0.9300	C18—C19	1.383 (5)
C3—C4	1.448 (4)	C18—H18	0.9300
C3—H3	0.9300	C19—H19	0.9300
C4—C5	1.3900	C20—N5	1.334 (5)
C4—C11	1.3900	C20—C21	1.398 (6)
C5—N1	1.382 (3)	C21—C22	1.384 (6)
C5—C6	1.3900	C21—H21	0.9300
C6—N2	1.385 (3)	C22—C23	1.370 (6)
C6—C7	1.3900	C22—H22	0.9300
C7—C12	1.3900	C23—C24	1.372 (6)
C7—C8	1.459 (4)	C23—H23	0.9300
C12—N4	1.376 (3)	C24—N5	1.334 (5)
C12—C11	1.3900	C24—H24	0.9300
C11—N3	1.391 (3)	C25—O2	1.230 (5)
C8—C9	1.367 (5)	C25—O1	1.282 (5)
C8—H8	0.9300	C25—C26	1.503 (6)
C9—C10	1.394 (5)	C26—H26A	0.9600
C9—H9	0.9300	C26—H26B	0.9600
C10—N2	1.323 (5)	C26—H26C	0.9600
C10—H10	0.9300	Cd1—O1^{i}	2.326 (3)
C13—N3	1.331 (5)	Cd1—O1	2.326 (3)
C13—N4	1.363 (5)	Cd1—N1	2.399 (3)
C13—C14	1.472 (5)	Cd1—N1^{i}	2.399 (3)
C14—C15	1.389 (5)	Cd1—N2	2.455 (3)
C14—C19	1.401 (6)	Cd1—N2^{i}	2.455 (3)
C15—C16	1.385 (5)	N4—H4	0.8600
C15—H15	0.9300		
N1—C1—C2	124.1 (3)	C18—C19—C14	119.5 (4)
N1—C1—H1	118.0	C18—C19—H19	120.2
C2—C1—H1	118.0	C14—C19—H19	120.2
C3—C2—C1	117.9 (4)	N5—C20—C21	121.5 (4)
C3—C2—H2	121.0	N5—C20—C17	117.0 (4)
C1—C2—H2	121.0	C21—C20—C17	121.5 (4)

C2—C3—C4	119.5 (3)	C22—C21—C20	118.8 (4)
C2—C3—H3	120.2	C22—C21—H21	120.6
C4—C3—H3	120.2	C20—C21—H21	120.6
C5—C4—C11	120.0	C23—C22—C21	119.6 (4)
C5—C4—C3	118.5 (2)	C23—C22—H22	120.2
C11—C4—C3	121.4 (2)	C21—C22—H22	120.2
N1—C5—C6	119.6 (2)	C22—C23—C24	117.8 (4)
N1—C5—C4	120.4 (2)	C22—C23—H23	121.1
C6—C5—C4	120.0	C24—C23—H23	121.1
N2—C6—C5	118.8 (2)	N5—C24—C23	124.2 (4)
N2—C6—C7	121.2 (2)	N5—C24—H24	117.9
C5—C6—C7	120.0	C23—C24—H24	117.9
C12—C7—C6	120.0	O2—C25—O1	122.6 (4)
C12—C7—C8	122.3 (2)	O2—C25—C26	120.6 (4)
C6—C7—C8	117.7 (2)	O1—C25—C26	116.8 (4)
N4—C12—C7	134.5 (2)	C25—C26—H26A	109.5
N4—C12—C11	105.5 (2)	C25—C26—H26B	109.5
C7—C12—C11	120.0	H26A—C26—H26B	109.5
C12—C11—C4	120.0	C25—C26—H26C	109.5
C12—C11—N3	110.5 (2)	H26A—C26—H26C	109.5
C4—C11—N3	129.4 (2)	H26B—C26—H26C	109.5
C9—C8—C7	119.4 (3)	O1^{i}—Cd1—O1	180.000 (1)
C9—C8—H8	120.3	O1^{i}—Cd1—N1	93.95 (10)
C7—C8—H8	120.3	O1—Cd1—N1	86.05 (10)
C8—C9—C10	118.6 (4)	O1^{i}—Cd1—N1^{i}	86.05 (10)
C8—C9—H9	120.7	O1—Cd1—N1^{i}	93.95 (10)
C10—C9—H9	120.7	N1—Cd1—N1^{i}	180.0
N2—C10—C9	123.9 (3)	O1^{i}—Cd1—N2	83.71 (10)
N2—C10—H10	118.1	O1—Cd1—N2	96.29 (10)
C9—C10—H10	118.1	N1—Cd1—N2	68.72 (10)
N3—C13—N4	113.0 (3)	N1^{i}—Cd1—N2	111.28 (10)
N3—C13—C14	122.9 (4)	O1^{i}—Cd1—N2^{i}	96.29 (10)
N4—C13—C14	124.2 (4)	O1—Cd1—N2^{i}	83.71 (10)
C15—C14—C19	118.9 (4)	N1—Cd1—N2^{i}	111.28 (10)
C15—C14—C13	119.0 (4)	N1^{i}—Cd1—N2^{i}	68.72 (10)
C19—C14—C13	122.1 (4)	N2—Cd1—N2^{i}	180.000 (1)
C16—C15—C14	121.2 (4)	C1—N1—C5	119.5 (3)
C16—C15—H15	119.4	C1—N1—Cd1	123.2 (2)
C14—C15—H15	119.4	C5—N1—Cd1	117.3 (2)
C15—C16—C17	120.2 (4)	C10—N2—C6	119.2 (3)
C15—C16—H16	119.9	C10—N2—Cd1	125.2 (2)
C17—C16—H16	119.9	C6—N2—Cd1	115.6 (2)
C18—C17—C16	117.9 (3)	C13—N3—C11	104.0 (3)
C18—C17—C20	122.7 (4)	C13—N4—C12	107.0 (3)
C16—C17—C20	119.5 (4)	C13—N4—H4	126.5
C19—C18—C17	122.3 (4)	C12—N4—H4	126.5
C19—C18—H18	118.8	C24—N5—C20	118.1 (4)
C17—C18—H18	118.8	C25—O1—Cd1	105.5 (2)

N1—C1—C2—C3	0.0 (6)	C17—C20—C21—C22	−178.5 (4)
C1—C2—C3—C4	−0.3 (6)	C20—C21—C22—C23	−1.3 (7)
C2—C3—C4—C5	1.1 (5)	C21—C22—C23—C24	0.1 (7)
C2—C3—C4—C11	177.9 (3)	C22—C23—C24—N5	0.9 (7)
C11—C4—C5—N1	−178.4 (3)	C2—C1—N1—C5	−0.5 (6)
C3—C4—C5—N1	−1.5 (3)	C2—C1—N1—Cd1	−178.7 (3)
C11—C4—C5—C6	0.0	C6—C5—N1—C1	−177.1 (3)
C3—C4—C5—C6	176.9 (3)	C4—C5—N1—C1	1.2 (4)
N1—C5—C6—N2	−0.3 (3)	C6—C5—N1—Cd1	1.2 (3)
C4—C5—C6—N2	−178.7 (3)	C4—C5—N1—Cd1	179.58 (13)
N1—C5—C6—C7	178.4 (3)	O1^{i}—Cd1—N1—C1	95.5 (3)
C4—C5—C6—C7	0.0	O1—Cd1—N1—C1	−84.5 (3)
N2—C6—C7—C12	178.6 (3)	N2—Cd1—N1—C1	177.2 (3)
C5—C6—C7—C12	0.0	N2^{i}—Cd1—N1—C1	−2.8 (3)
N2—C6—C7—C8	0.3 (3)	O1^{i}—Cd1—N1—C5	−82.8 (2)
C5—C6—C7—C8	−178.3 (3)	O1—Cd1—N1—C5	97.2 (2)
C6—C7—C12—N4	−177.2 (3)	N2—Cd1—N1—C5	−1.1 (2)
C8—C7—C12—N4	1.1 (4)	N2^{i}—Cd1—N1—C5	178.9 (2)
C6—C7—C12—C11	0.0	C9—C10—N2—C6	−0.9 (6)
C8—C7—C12—C11	178.2 (3)	C9—C10—N2—Cd1	179.3 (3)
N4—C12—C11—C4	177.9 (2)	C5—C6—N2—C10	179.4 (3)
C7—C12—C11—C4	0.0	C7—C6—N2—C10	0.8 (4)
N4—C12—C11—N3	−0.4 (3)	C5—C6—N2—Cd1	−0.8 (3)
C7—C12—C11—N3	−178.3 (2)	C7—C6—N2—Cd1	−179.40 (13)
C5—C4—C11—C12	0.0	O1^{i}—Cd1—N2—C10	−82.5 (3)
C3—C4—C11—C12	−176.8 (3)	O1—Cd1—N2—C10	97.5 (3)
C5—C4—C11—N3	177.9 (3)	N1—Cd1—N2—C10	−179.2 (3)
C3—C4—C11—N3	1.2 (3)	N1^{i}—Cd1—N2—C10	0.8 (3)
C12—C7—C8—C9	−179.6 (3)	O1^{i}—Cd1—N2—C6	97.7 (2)
C6—C7—C8—C9	−1.3 (4)	O1—Cd1—N2—C6	−82.3 (2)
C7—C8—C9—C10	1.2 (6)	N1—Cd1—N2—C6	1.0 (2)
C8—C9—C10—N2	−0.2 (6)	N1^{i}—Cd1—N2—C6	−179.0 (2)
N3—C13—C14—C15	−11.1 (6)	N4—C13—N3—C11	−0.3 (4)
N4—C13—C14—C15	170.1 (4)	C14—C13—N3—C11	−179.2 (3)
N3—C13—C14—C19	166.8 (4)	C12—C11—N3—C13	0.5 (3)
N4—C13—C14—C19	−11.9 (6)	C4—C11—N3—C13	−177.6 (2)
C19—C14—C15—C16	0.5 (6)	N3—C13—N4—C12	0.1 (4)
C13—C14—C15—C16	178.5 (4)	C14—C13—N4—C12	178.9 (3)
C14—C15—C16—C17	−1.3 (6)	C7—C12—N4—C13	177.6 (2)
C15—C16—C17—C18	1.1 (6)	C11—C12—N4—C13	0.2 (3)
C15—C16—C17—C20	−178.3 (4)	C23—C24—N5—C20	−0.7 (6)
C16—C17—C18—C19	0.0 (6)	C21—C20—N5—C24	−0.6 (6)
C20—C17—C18—C19	179.3 (4)	C17—C20—N5—C24	179.4 (3)
C17—C18—C19—C14	−0.7 (6)	O2—C25—O1—Cd1	−2.0 (4)
C15—C14—C19—C18	0.5 (6)	C26—C25—O1—Cd1	177.7 (3)
C13—C14—C19—C18	−177.4 (4)	O1^{i}—Cd1—O1—C25	114 (100)
C18—C17—C20—N5	−157.8 (4)	N1—Cd1—O1—C25	−119.9 (2)

C16—C17—C20—N5	21.5 (6)	N1^{i}—Cd1—O1—C25	60.1 (2)
C18—C17—C20—C21	22.2 (6)	N2—Cd1—O1—C25	−51.8 (2)
C16—C17—C20—C21	−158.5 (4)	N2^{i}—Cd1—O1—C25	128.2 (2)
N5—C20—C21—C22	1.5 (7)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···O1^{ii}	0.86	1.93	2.724 (4)	153
C9—H9···N5^{iii}	0.93	2.61	3.523 (5)	168

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