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catena-Poly[[(benzoato-κ^2O,O')chloridocadmium(II)]-μ-2,2′-diphenyl-1,1′-(butane-1,4-diyl)diimidazole-$\kappa^2N^3:N^{3'}$]

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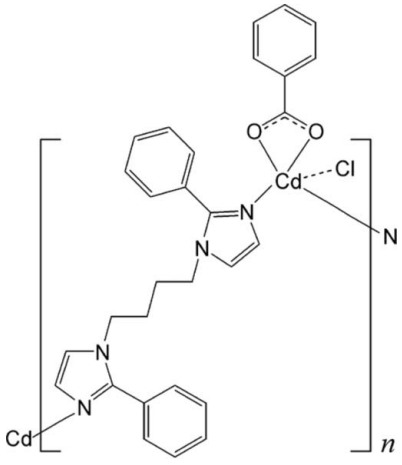
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.009 Å; H-atom completeness 63%; disorder in main residue; R factor = 0.052; wR factor = 0.161; data-to-parameter ratio = 20.0.

The title Cd^{II} coordination polymer, $[Cd(C_7H_5O_2)Cl(C_{22}H_{22}N_4)]_n$, was obtained by reaction of $CdCl_2\cdot2.5H_2O$, benzoic acid (HL) and 2,2′-diphenyl-1,1′-(butane-1,4-diyl)diimidazole (bbip). Each Cd^{II} cation is five-coordinated by a ClO_2N_2 donor set in a distorted trigonal–bipyramidal geometry. In the bbip ligand, three C atoms and one N atom are disordered equally over two positions; another two C atoms are disordered over two positions, the site-occupancy ratio being 0.6:0.4. The bbip ligand acts as a bridging bidentate ligand, linking Cd^{II} centres into a one-dimensional zigzag chain; adjacent chains are further connected through face-to-face π–π interactions between the imidazole rings [with an average face-to-face distance of 3.560 (8) Å], resulting in the formation of a two-dimensional supramolecular layer.

Related literature

The bond distances and angles in the title compound are normal (Ma *et al.*, 2000).



Experimental

Crystal data

$[Cd(C_7H_5O_2)Cl(C_{22}H_{22}N_4)]$
M_r = 611.40
Monoclinic, $P2_1/c$
a = 20.0290 (16) Å
b = 9.0893 (7) Å
c = 15.5393 (13) Å
β = 98.197 (2)°
V = 2800.0 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.91 mm^{-1}
T = 293 (2) K
0.32 × 0.25 × 0.22 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.74, T_{max} = 0.79
16824 measured reflections
6748 independent reflections
4217 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.161
S = 1.00
6748 reflections
338 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.85 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.258 (3)	Cd1—O1	2.430 (4)
Cd1—N4^{i}	2.259 (3)	Cd1—Cl	2.4361 (13)
Cd1—O2	2.336 (3)		
N1—Cd1—N4^{i}	94.39 (13)	O2—Cd1—O1	54.47 (13)
N1—Cd1—O2	128.78 (14)	N1—Cd1—Cl	111.06 (10)
N4^{i}—Cd1—O2	91.65 (12)	N4^{i}—Cd1—Cl	113.59 (10)
N1—Cd1—O1	93.84 (13)	O2—Cd1—Cl	112.63 (11)
N4^{i}—Cd1—O1	140.93 (13)	O1—Cd1—Cl	98.70 (11)

Symmetry code: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PR2014).

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supplementary materials

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catena-Poly[[(benzoato-κ^2O,O')chloridocadmium(II)]-μ-2,2'-diphenyl-1,1'-(butane-1,4-diyl)diimidazole-$\kappa^2N^3:N^{3'}$]

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Comment

As part of an investigation of the transition metal application there is a need to prepare further examples of these compounds. In this paper, the structure of the title compound, (I), is described.

As shown in Fig. 1, the Cd^{II} ions is coordinated by one Cl^- anion, two oxygen atoms from the chelating carboxylate of *L* anion and two nitrogen atoms of two bbip ligands. Each Cd^{II} cation has a distorted trigonal bipyramidal coordination sphere. As illustrated in Fig. 2, each bbip molecule in (I) coordinates to two Cd^{II} cations through its two aromatic N atoms, thus acing as a bridging bidentate ligand. The Cd^{II} cations are bridged by bbip ligand to form a zigzag chain along the *c* axis, with the separation between the Cd^{II} atoms bridged by bbip ligand of 14.509 (1) Å. A fascinating structural feature of (I) is that there exist face-to-face π-π interactions between the imidazolyl ring and phenyl ring of adjacent bbip ligands (with the centroid-to-centriod and average face-to-face distances of 3.644 (7)–3.752 (2) Å and 3.647 (8)–3.760 (2) Å, respectively. Fig. 2). Along the *b* axis, parallel 1-D chains further stack to form 2-D supermolecular structure (Fig. 3) *via* face-to-face π-π interactions between imidazolyl rings, with the centroid-to-centriod distance of 3.607 (2) Å and average face-to-face distance of 3.560 (8) Å.

Experimental

The ligand bbip was synthesized according to the literature (Ma *et al.*, 2000) but an imidazole was replaced by 2-phenylimidazole. A mixture of $CdCl_2{\cdot}2.5H_2O$ (0.091 g, 0.4 mmol), HL (0.049 g, 0.4 mmol), bbip (0.137 g, 0.40 mmol), and water (8 ml) was sealed in a Teflon reactor (15 ml) and heated at 160 °C for 3 days. After the mixture had been cooled to room temperature at 10 °C.h^{-1}, colorless crystals of (I) were obtained. Yield: 73%.

Refinement

Disorderd bbip ligand was refined using isotropic C and N atoms split over two sites, with a total occupancy of 1. Some of the carbon H atoms attached to disordered part could not be positioned reliably and were not included in the refinement. Other aromatic H-atoms were refined using a riding model with d(C—H) = 0.93 Å, U_{iso}=1.2U_{eq} (C).

Figures

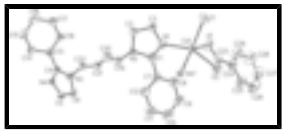

Fig. 1. A view of the local coordination of the Cd^{II} cation in (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms have been omitted for clarity.

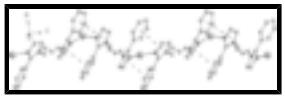

Fig. 2. View of the face-to-face π-π interactions in bbip ligands. L^- and Cl^- anions have been omitted for clarity.

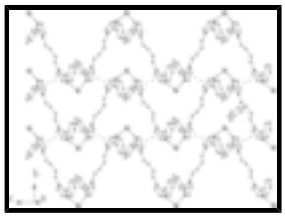

Fig. 3. The packing diagram of part of the crystal structure of (I), showing the face-to-face π-π interactions. L^- and Cl^- anions have been omitted for clarity.

catena-Poly[[(benzoato-κ^2*O*,*O*')chloridocadmium(II)]-μ-2,2'-diphenyl-1,1'-\ (butane-1,4-diyl)diimidazole-κ^2*N*^{3}:*N*$^{3'}$]

Crystal data

$[Cd(C_7H_5O_2)Cl(C_{22}H_{22}N_4)]$	F_{000} = 1240
M_r = 611.40	D_x = 1.450 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4217 reflections
a = 20.0290 (16) Å	θ = 2.1–28.3º
b = 9.0893 (7) Å	μ = 0.91 mm^{-1}
c = 15.5393 (13) Å	T = 293 (2) K
β = 98.197 (2)º	Block, colorless
V = 2800.0 (4) Å^3	0.32 × 0.25 × 0.22 mm
Z = 4	

Data collection

Bruker APEX CCD area-detector diffractometer	6748 independent reflections
Radiation source: fine-focus sealed tube	4217 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.035
T = 293(2) K	θ_{max} = 28.3º
ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −22→26
T_{min} = 0.74, T_{max} = 0.79	k = −11→12
16824 measured reflections	l = −19→20

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.052	H-atom parameters constrained
$wR(F^2)$ = 0.161	$w = 1/[\sigma^2(F_o^2) + (0.0894P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.001$
6748 reflections	$\Delta\rho_{max} = 0.85$ e Å^{-3}
338 parameters	$\Delta\rho_{min} = -0.54$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cd1	0.222863 (16)	1.42407 (3)	0.871874 (19)	0.05373 (15)	
C1	0.2233 (3)	1.1196 (6)	0.7681 (3)	0.0660 (13)	
C2	0.1379 (6)	1.1311 (14)	0.6578 (7)	0.061 (3)	0.50
C2'	0.1237 (6)	1.0990 (12)	0.6842 (8)	0.053 (3)*	0.50
C3	0.1337 (2)	1.2422 (6)	0.7139 (3)	0.0653 (12)	
C4	0.1836 (2)	0.3373 (5)	0.4985 (3)	0.0509 (10)	
C5	0.2792 (2)	0.2428 (5)	0.5504 (3)	0.0597 (11)	
H5	0.3165	0.1806	0.5583	0.072*	
C6	0.2715 (2)	0.3616 (6)	0.5988 (3)	0.0619 (12)	
H6	0.3015	0.3952	0.6459	0.074*	
C7	0.2856 (3)	1.0733 (6)	0.8239 (4)	0.0708 (14)	
C8	0.3412 (3)	1.1618 (7)	0.8307 (4)	0.0845 (16)	
H8	0.3412	1.2462	0.7969	0.101*	
C9	0.3981 (3)	1.1239 (9)	0.8890 (5)	0.104 (2)	
H9	0.4361	1.1839	0.8947	0.125*	
C10	0.3982 (3)	1.0008 (9)	0.9369 (5)	0.101 (2)	
H10	0.4368	0.9760	0.9748	0.121*	
C11	0.3434 (3)	0.9120 (7)	0.9313 (5)	0.094 (2)	
H11	0.3443	0.8278	0.9655	0.113*	
C12	0.2868 (3)	0.9470 (6)	0.8750 (4)	0.0795 (16)	
H12	0.2490	0.8866	0.8708	0.095*	
C13	0.1176 (2)	0.3626 (5)	0.4443 (3)	0.0573 (11)	
C14	0.0745 (2)	0.2432 (6)	0.4254 (3)	0.0688 (13)	
H14	0.0858	0.1515	0.4498	0.083*	
C15	0.0152 (3)	0.2619 (8)	0.3703 (4)	0.0871 (17)	
H15	−0.0130	0.1815	0.3562	0.104*	

C16	−0.0034 (3)	0.3980 (9)	0.3355 (5)	0.098 (2)	
H16	−0.0443	0.4102	0.2995	0.117*	
C17	0.0394 (3)	0.5151 (8)	0.3547 (4)	0.0872 (17)	
H17	0.0274	0.6070	0.3311	0.105*	
C18	0.0988 (2)	0.4988 (6)	0.4072 (3)	0.0654 (12)	
H18	0.1274	0.5792	0.4188	0.078*	
C19'	0.2226 (6)	0.9355 (13)	0.6431 (8)	0.064 (3)*	0.40
C19	0.1970 (4)	0.8646 (10)	0.6951 (5)	0.0617 (19)*	0.60
C20	0.1926 (4)	0.8506 (11)	0.5946 (6)	0.058 (2)*	0.50
C20'	0.1816 (6)	0.8000 (14)	0.6443 (8)	0.081 (3)*	0.50
C21	0.2224 (4)	0.7045 (11)	0.5700 (6)	0.064 (2)*	0.60
C21'	0.2161 (6)	0.6732 (14)	0.6005 (8)	0.053 (3)*	0.40
C22	0.1782 (6)	0.5320 (15)	0.6152 (8)	0.067 (3)*	0.50
C22'	0.1852 (5)	0.5691 (12)	0.5948 (7)	0.050 (2)*	0.50
C23	0.3401 (3)	1.5518 (5)	0.8487 (4)	0.0688 (13)	
C24	0.4080 (3)	1.6253 (7)	0.8387 (4)	0.0763 (14)	
C25	0.4608 (3)	1.6183 (9)	0.9056 (5)	0.105 (2)	
H25	0.4565	1.5642	0.9553	0.126*	
C26	0.5195 (4)	1.6906 (12)	0.8992 (6)	0.137 (3)	
H26	0.5549	1.6859	0.9448	0.164*	
C27	0.5269 (4)	1.7698 (14)	0.8265 (8)	0.155 (4)	
H27	0.5670	1.8192	0.8226	0.186*	
C28	0.4739 (4)	1.7760 (14)	0.7586 (6)	0.162 (4)	
H28	0.4784	1.8288	0.7085	0.195*	
C29	0.4158 (4)	1.7046 (9)	0.7657 (4)	0.114 (2)	
H29	0.3803	1.7094	0.7202	0.137*	
N1	0.19153 (17)	1.2451 (4)	0.7736 (2)	0.0558 (9)	
N2	0.1798 (4)	1.0148 (7)	0.7192 (4)	0.0441 (16)	0.50
N2'	0.1943 (5)	1.0566 (10)	0.6890 (6)	0.059 (2)*	0.50
N3	0.21146 (18)	0.4242 (4)	0.5661 (2)	0.0585 (10)	
N4	0.22479 (16)	0.2261 (4)	0.4880 (2)	0.0517 (8)	
O1	0.29828 (19)	1.5411 (5)	0.7832 (3)	0.0891 (12)	
O2	0.33107 (18)	1.5115 (4)	0.9222 (3)	0.0798 (10)	
Cl	0.13732 (7)	1.61591 (14)	0.86482 (10)	0.0804 (4)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0710 (3)	0.0409 (2)	0.0458 (2)	−0.00401 (14)	−0.00363 (15)	−0.00112 (12)
C1	0.072 (3)	0.062 (3)	0.059 (3)	0.005 (2)	−0.005 (2)	−0.025 (2)
C2	0.063 (7)	0.073 (7)	0.050 (6)	−0.005 (5)	0.016 (5)	−0.013 (5)
C3	0.066 (3)	0.064 (3)	0.062 (3)	0.001 (2)	−0.004 (2)	−0.009 (2)
C4	0.055 (2)	0.050 (2)	0.046 (2)	0.0013 (19)	−0.0006 (18)	−0.0086 (18)
C5	0.058 (3)	0.067 (3)	0.050 (2)	0.012 (2)	−0.0049 (19)	−0.003 (2)
C6	0.057 (3)	0.071 (3)	0.054 (2)	0.001 (2)	−0.006 (2)	−0.008 (2)
C7	0.060 (3)	0.067 (3)	0.083 (4)	0.007 (2)	0.000 (3)	−0.029 (3)
C8	0.068 (3)	0.081 (4)	0.101 (4)	0.004 (3)	−0.002 (3)	−0.008 (3)
C9	0.065 (4)	0.105 (5)	0.134 (6)	−0.004 (3)	−0.020 (4)	−0.017 (5)

C10	0.075 (4)	0.110 (6)	0.108 (5)	0.021 (4)	−0.020 (3)	−0.015 (4)
C11	0.087 (4)	0.083 (4)	0.108 (5)	0.026 (3)	−0.005 (4)	−0.011 (3)
C12	0.070 (3)	0.070 (4)	0.094 (4)	0.013 (3)	−0.001 (3)	−0.020 (3)
C13	0.049 (2)	0.057 (3)	0.063 (3)	0.001 (2)	0.002 (2)	−0.014 (2)
C14	0.054 (3)	0.070 (3)	0.081 (3)	−0.005 (2)	0.004 (2)	−0.008 (3)
C15	0.058 (3)	0.100 (5)	0.099 (4)	−0.012 (3)	−0.004 (3)	−0.022 (4)
C16	0.061 (3)	0.120 (6)	0.103 (5)	0.014 (4)	−0.018 (3)	−0.020 (4)
C17	0.066 (3)	0.087 (4)	0.101 (4)	0.018 (3)	−0.013 (3)	−0.005 (4)
C18	0.056 (3)	0.059 (3)	0.078 (3)	0.006 (2)	−0.003 (2)	−0.006 (3)
C23	0.076 (3)	0.054 (3)	0.072 (3)	−0.001 (2)	−0.005 (3)	−0.008 (2)
C24	0.059 (3)	0.086 (4)	0.085 (4)	−0.006 (3)	0.010 (3)	−0.015 (3)
C25	0.064 (4)	0.128 (6)	0.117 (6)	−0.001 (4)	−0.007 (3)	−0.013 (4)
C26	0.065 (4)	0.196 (10)	0.146 (8)	−0.028 (5)	0.008 (4)	−0.032 (7)
C27	0.089 (6)	0.205 (11)	0.180 (10)	−0.037 (6)	0.050 (6)	−0.038 (9)
C28	0.116 (7)	0.241 (13)	0.142 (8)	−0.049 (8)	0.057 (6)	0.001 (8)
C29	0.102 (5)	0.155 (7)	0.087 (5)	−0.038 (5)	0.024 (4)	0.003 (4)
N1	0.065 (2)	0.046 (2)	0.054 (2)	0.0006 (17)	0.0000 (17)	−0.0097 (16)
N2	0.063 (4)	0.033 (3)	0.033 (3)	−0.009 (3)	−0.002 (3)	−0.003 (3)
N3	0.055 (2)	0.063 (2)	0.055 (2)	0.0071 (17)	−0.0039 (17)	−0.0193 (17)
N4	0.0530 (19)	0.051 (2)	0.0474 (19)	0.0031 (16)	−0.0040 (15)	−0.0065 (15)
O1	0.083 (3)	0.107 (3)	0.073 (2)	−0.023 (2)	−0.004 (2)	−0.018 (2)
O2	0.079 (2)	0.078 (3)	0.078 (3)	−0.019 (2)	−0.0043 (19)	0.012 (2)
Cl	0.0931 (9)	0.0445 (6)	0.0991 (10)	0.0147 (6)	−0.0011 (8)	0.0033 (6)

Geometric parameters (Å, °)

Cd1—N1	2.258 (3)	C15—H15	0.9300
Cd1—N4^{i}	2.259 (3)	C16—C17	1.372 (9)
Cd1—O2	2.336 (3)	C16—H16	0.9300
Cd1—O1	2.430 (4)	C17—C18	1.351 (7)
Cd1—Cl	2.4361 (13)	C17—H17	0.9300
C1—N1	1.315 (6)	C18—H18	0.9300
C1—N2'	1.403 (10)	C19'—C20	1.182 (14)
C1—N2	1.434 (8)	C19'—C19	1.205 (14)
C1—C7	1.475 (7)	C19'—N2'	1.470 (15)
C2—C2'	0.608 (12)	C19'—C20'	1.482 (18)
C2—C3	1.344 (11)	C19'—N2	1.716 (15)
C2—N2'	1.347 (14)	C19—C20'	0.997 (12)
C2—N2	1.583 (14)	C19—N2	1.469 (11)
C2'—N2	1.404 (13)	C19—C20	1.557 (12)
C2'—C3	1.386 (12)	C19—N2'	1.748 (13)
C2'—N2'	1.459 (15)	C20—C20'	0.951 (13)
C3—N1	1.378 (5)	C20—C21	1.526 (13)
C4—N4	1.330 (5)	C20—C21'	1.679 (16)
C4—N3	1.368 (5)	C20'—C21'	1.551 (17)
C4—C13	1.482 (6)	C21—C21'	0.581 (13)
C5—C6	1.337 (7)	C21—C22'	1.517 (15)
C5—N4	1.361 (5)	C21'—C22'	1.128 (15)
C5—H5	0.9300	C21'—C22	1.526 (18)

C6—N3	1.360 (5)	C22—N3	1.460 (13)
C6—H6	0.9300	C22'—N3	1.509 (11)
C7—C8	1.366 (8)	C23—O1	1.227 (6)
C7—C12	1.394 (8)	C23—O2	1.236 (6)
C8—C9	1.394 (8)	C24—C29	1.371 (9)
C8—H8	0.9300	C24—C25	1.376 (8)
C9—C10	1.343 (10)	C25—C26	1.362 (10)
C9—H9	0.9300	C25—H25	0.9300
C10—C11	1.356 (10)	C26—C27	1.366 (13)
C10—H10	0.9300	C26—H26	0.9300
C11—C12	1.368 (8)	C27—C28	1.386 (11)
C11—H11	0.9300	C27—H27	0.9300
C12—H12	0.9300	C28—C29	1.351 (10)
C13—C14	1.391 (6)	C28—H28	0.9300
C13—C18	1.394 (7)	C29—H29	0.9300
C14—C15	1.372 (7)	N2—N2'	0.699 (9)
C14—H14	0.9300	N4—Cd1^{ii}	2.259 (3)
C15—C16	1.380 (9)		
N1—Cd1—N4^{i}	94.39 (13)	C19'—C20—C21'	118.6 (10)
N1—Cd1—O2	128.78 (14)	C19—C20—C21'	92.8 (7)
N4^{i}—Cd1—O2	91.65 (12)	C20—C20'—C19	106.1 (15)
N1—Cd1—O1	93.84 (13)	C20—C20'—C19'	52.8 (10)
N4^{i}—Cd1—O1	140.93 (13)	C19—C20'—C19'	53.9 (9)
O2—Cd1—O1	54.47 (13)	C20—C20'—C21'	80.4 (11)
N1—Cd1—Cl	111.06 (10)	C19—C20'—C21'	132.7 (12)
N4^{i}—Cd1—Cl	113.59 (10)	C19'—C20'—C21'	109.2 (10)
O2—Cd1—Cl	112.63 (11)	C20—C20'—C21	61.1 (10)
O1—Cd1—Cl	98.70 (11)	C19—C20'—C21	134.3 (11)
N1—C1—N2'	105.5 (5)	C19'—C20'—C21	95.3 (9)
N1—C1—N2	110.3 (5)	C21'—C21—C20	94.9 (19)
N1—C1—C7	125.9 (4)	C22'—C21—C20	114.8 (8)
N2'—C1—C7	127.4 (5)	C21'—C21—C20'	61.9 (18)
N2—C1—C7	121.4 (5)	C22'—C21—C20'	86.7 (7)
C2'—C2—C3	81.0 (17)	C20—C21—C22	113.0 (7)
C2'—C2—N2'	88 (2)	C20'—C21—C22	83.4 (7)
C3—C2—N2'	105.7 (8)	C21—C21'—C22'	122 (2)
C2'—C2—N2	62.0 (18)	C21—C21'—C22	135 (2)
C3—C2—N2	100.8 (7)	C21—C21'—C20'	99 (2)
C2—C2'—N2	96 (2)	C22'—C21'—C20'	112.5 (11)
C2—C2'—C3	73.3 (17)	C22—C21'—C20'	107.3 (10)
N2—C2'—C3	108.3 (8)	C21—C21'—C20	64.9 (17)
C2—C2'—N2'	67.4 (18)	C22'—C21'—C20	130.8 (11)
C3—C2'—N2'	97.9 (8)	C22—C21'—C20	132.4 (10)
C2—C3—N1	109.0 (6)	N3—C22—C21'	102.3 (9)
N1—C3—C2'	108.1 (6)	N3—C22—C21	95.0 (7)
N4—C4—N3	109.9 (3)	C21'—C22'—N3	123.0 (10)
N4—C4—C13	124.6 (4)	N3—C22'—C21	115.4 (8)
N3—C4—C13	125.5 (4)	O1—C23—O2	124.8 (5)

C6—C5—N4	110.2 (4)	O1—C23—C24	117.2 (5)
C6—C5—H5	124.9	O2—C23—C24	118.0 (5)
N4—C5—H5	124.9	O1—C23—Cd1	64.6 (3)
C5—C6—N3	107.2 (4)	O2—C23—Cd1	60.2 (3)
C5—C6—H6	126.4	C24—C23—Cd1	178.2 (4)
N3—C6—H6	126.4	C29—C24—C25	118.9 (6)
C8—C7—C12	119.6 (5)	C29—C24—C23	121.2 (5)
C8—C7—C1	119.3 (5)	C25—C24—C23	119.8 (6)
C12—C7—C1	120.9 (5)	C26—C25—C24	120.1 (8)
C7—C8—C9	119.1 (6)	C26—C25—H25	120.0
C7—C8—H8	120.4	C24—C25—H25	120.0
C9—C8—H8	120.4	C25—C26—C27	120.8 (8)
C10—C9—C8	120.2 (6)	C25—C26—H26	119.6
C10—C9—H9	119.9	C27—C26—H26	119.6
C8—C9—H9	119.9	C26—C27—C28	119.3 (8)
C9—C10—C11	121.5 (6)	C26—C27—H27	120.3
C9—C10—H10	119.2	C28—C27—H27	120.3
C11—C10—H10	119.2	C29—C28—C27	119.5 (9)
C10—C11—C12	119.5 (7)	C29—C28—H28	120.2
C10—C11—H11	120.2	C27—C28—H28	120.2
C12—C11—H11	120.2	C28—C29—C24	121.4 (7)
C11—C12—C7	120.1 (6)	C28—C29—H29	119.3
C11—C12—H12	120.0	C24—C29—H29	119.3
C7—C12—H12	120.0	C1—N1—C3	107.9 (4)
C14—C13—C18	118.9 (4)	C1—N1—Cd1	125.3 (3)
C14—C13—C4	118.4 (4)	C3—N1—Cd1	126.5 (3)
C18—C13—C4	122.6 (4)	N2'—N2—C2'	80.3 (12)
C15—C14—C13	119.3 (5)	N2'—N2—C1	73.3 (10)
C15—C14—H14	120.3	C2'—N2—C1	103.6 (7)
C13—C14—H14	120.3	N2'—N2—C19	101.5 (12)
C14—C15—C16	121.1 (5)	C2'—N2—C19	127.7 (7)
C14—C15—H15	119.4	C1—N2—C19	127.2 (6)
C16—C15—H15	119.4	N2'—N2—C2	57.8 (11)
C17—C16—C15	119.0 (5)	C1—N2—C2	96.0 (6)
C17—C16—H16	120.5	C19—N2—C2	126.2 (6)
C15—C16—H16	120.5	N2'—N2—C19'	57.9 (11)
C18—C17—C16	121.0 (6)	C2'—N2—C19'	114.4 (8)
C18—C17—H17	119.5	C1—N2—C19'	108.5 (7)
C16—C17—H17	119.5	C2—N2—C19'	98.0 (7)
C17—C18—C13	120.6 (5)	N2—N2'—C2	96.2 (13)
C17—C18—H18	119.7	N2—N2'—C1	78.2 (11)
C13—C18—H18	119.7	C2—N2'—C1	109.3 (8)
C20—C19'—C19	81.5 (10)	N2—N2'—C19'	98.3 (13)
C20—C19'—N2'	127.0 (11)	C2—N2'—C19'	124.3 (10)
C19—C19'—N2'	81.0 (9)	C1—N2'—C19'	126.2 (9)
N2'—C19'—C20'	111.3 (10)	N2—N2'—C2'	71.6 (11)
C20—C19'—N2	117.0 (10)	C1—N2'—C2'	102.4 (7)
C19—C19'—N2	57.2 (7)	C19'—N2'—C2'	127.7 (9)
C20'—C19'—N2	90.4 (8)	N2—N2'—C19	55.4 (10)

C20'—C19—C19'	84.1 (12)	C2—N2'—C19	122.6 (8)
C20'—C19—N2	133.7 (11)	C1—N2'—C19	110.7 (7)
C19'—C19—N2	79.2 (8)	C2'—N2'—C19	106.8 (7)
C19'—C19—C20	48.6 (7)	C6—N3—C4	106.7 (4)
N2—C19—C20	110.5 (7)	C6—N3—C22	122.1 (6)
C20'—C19—N2'	122.8 (11)	C4—N3—C22	128.4 (6)
C19'—C19—N2'	56.1 (7)	C6—N3—C22'	125.6 (5)
C20—C19—N2'	91.8 (6)	C4—N3—C22'	127.5 (5)
C20'—C20—C19'	87.4 (13)	C4—N4—C5	106.0 (3)
C20'—C20—C21	85.8 (11)	C4—N4—Cd1^{ii}	128.1 (3)
C19'—C20—C21	123.1 (10)	C5—N4—Cd1^{ii}	123.9 (3)
C19'—C20—C19	49.9 (8)	C23—O1—Cd1	88.3 (4)
C21—C20—C19	110.7 (7)	C23—O2—Cd1	92.4 (3)
C20'—C20—C21'	65.6 (11)		
C3—C2—C2'—N2	−107.4 (8)	C26—C27—C28—C29	0.6 (17)
N2'—C2—C2'—N2	−1.2 (10)	C27—C28—C29—C24	−0.4 (16)
N2'—C2—C2'—C3	106.3 (7)	C25—C24—C29—C28	−0.2 (12)
N2—C2—C2'—C3	107.4 (8)	C23—C24—C29—C28	176.3 (8)
C3—C2—C2'—N2'	−106.3 (7)	N2'—C1—N1—C3	15.6 (7)
N2—C2—C2'—N2'	1.2 (10)	N2—C1—N1—C3	−13.9 (6)
C2'—C2—C3—N1	92.2 (18)	C7—C1—N1—C3	−176.3 (5)
N2'—C2—C3—N1	6.9 (11)	N2'—C1—N1—Cd1	−169.0 (5)
N2—C2—C3—N1	33.2 (9)	N2—C1—N1—Cd1	161.5 (4)
N2'—C2—C3—C2'	−85 (2)	C7—C1—N1—Cd1	−0.9 (8)
N2—C2—C3—C2'	−59.1 (17)	C2—C3—N1—C1	−14.6 (8)
N2—C2'—C3—C2	90 (2)	C2'—C3—N1—C1	12.5 (7)
N2'—C2'—C3—C2	63.5 (17)	C2—C3—N1—Cd1	170.1 (7)
C2—C2'—C3—N1	−96.6 (18)	C2'—C3—N1—Cd1	−162.9 (6)
N2—C2'—C3—N1	−6.1 (10)	N4^{i}—Cd1—N1—C1	−54.7 (4)
N2'—C2'—C3—N1	−33.1 (9)	O2—Cd1—N1—C1	40.9 (5)
N4—C5—C6—N3	−1.0 (6)	O1—Cd1—N1—C1	87.0 (4)
N1—C1—C7—C8	−55.0 (8)	Cl—Cd1—N1—C1	−172.1 (4)
N2'—C1—C7—C8	110.4 (8)	C23—Cd1—N1—C1	66.8 (4)
N2—C1—C7—C8	144.4 (6)	N4^{i}—Cd1—N1—C3	119.8 (4)
N1—C1—C7—C12	119.7 (6)	O2—Cd1—N1—C3	−144.5 (4)
N2'—C1—C7—C12	−74.8 (9)	O1—Cd1—N1—C3	−98.4 (4)
N2—C1—C7—C12	−40.9 (8)	Cl—Cd1—N1—C3	2.4 (4)
C12—C7—C8—C9	−0.1 (9)	C23—Cd1—N1—C3	−118.7 (4)
C1—C7—C8—C9	174.7 (5)	C2—C2'—N2—N2'	2(2)
C7—C8—C9—C10	0.8 (10)	C3—C2'—N2—N2'	−72.0 (13)
C8—C9—C10—C11	−1.1 (12)	C2—C2'—N2—C1	72.3 (19)
C9—C10—C11—C12	0.7 (11)	C3—C2'—N2—C1	−1.9 (10)
C10—C11—C12—C7	0.0 (9)	N2'—C2'—N2—C1	70.1 (10)
C8—C7—C12—C11	−0.2 (9)	C2—C2'—N2—C19	−95 (2)
C1—C7—C12—C11	−174.9 (5)	C3—C2'—N2—C19	−169.0 (8)
N4—C4—C13—C14	45.0 (7)	N2'—C2'—N2—C19	−97.0 (14)
N3—C4—C13—C14	−135.3 (5)	C3—C2'—N2—C2	−74.2 (18)
N4—C4—C13—C18	−131.0 (5)	N2'—C2'—N2—C2	−2(2)

N3—C4—C13—C18	48.8 (7)	C2—C2'—N2—C19'	−46 (2)
C18—C13—C14—C15	0.6 (7)	C3—C2'—N2—C19'	−119.9 (9)
C4—C13—C14—C15	−175.5 (4)	N2'—C2'—N2—C19'	−47.9 (11)
C13—C14—C15—C16	−1.9 (9)	N1—C1—N2—N2'	85.1 (12)
C14—C15—C16—C17	1.8 (10)	C7—C1—N2—N2'	−111.6 (12)
C15—C16—C17—C18	−0.4 (10)	N1—C1—N2—C2'	9.8 (8)
C16—C17—C18—C13	−0.9 (9)	N2'—C1—N2—C2'	−75.3 (11)
C14—C13—C18—C17	0.8 (7)	C7—C1—N2—C2'	173.2 (7)
C4—C13—C18—C17	176.7 (5)	N1—C1—N2—C19	177.0 (7)
C20—C19'—C19—C20'	6.7 (11)	N2'—C1—N2—C19	91.9 (14)
N2'—C19'—C19—C20'	136.5 (10)	C7—C1—N2—C19	−19.7 (11)
N2—C19'—C19—C20'	136.7 (10)	N1—C1—N2—C2	31.3 (7)
C20—C19'—C19—N2	−130.0 (8)	N2'—C1—N2—C2	−53.8 (10)
N2'—C19'—C19—N2	−0.2 (6)	C7—C1—N2—C2	−165.3 (6)
C20'—C19'—C19—N2	−136.7 (10)	N1—C1—N2—C19'	131.8 (6)
N2'—C19'—C19—C20	129.8 (10)	N2'—C1—N2—C19'	46.7 (11)
C20'—C19'—C19—C20	−6.7 (11)	C7—C1—N2—C19'	−64.8 (8)
N2—C19'—C19—C20	130.0 (8)	C20'—C19—N2—N2'	−70.5 (19)
C20—C19'—C19—N2'	−129.8 (10)	C19'—C19—N2—N2'	0.3 (14)
C20'—C19'—C19—N2'	−136.5 (10)	C20—C19—N2—N2'	−37.5 (13)
N2—C19'—C19—N2'	0.2 (6)	C20'—C19—N2—C2'	16 (2)
C19—C19'—C20—C20'	−7.0 (11)	C19'—C19—N2—C2'	86.8 (12)
N2'—C19'—C20—C20'	−78.8 (16)	C20—C19—N2—C2'	49.0 (12)
N2—C19'—C20—C20'	−53.3 (13)	N2'—C19—N2—C2'	86.5 (14)
C19—C19'—C20—C21	−90.2 (12)	C20'—C19—N2—C1	−148.2 (14)
N2'—C19'—C20—C21	−162.0 (11)	C19'—C19—N2—C1	−77.3 (10)
C20'—C19'—C20—C21	−83.2 (13)	C20—C19—N2—C1	−115.2 (8)
N2—C19'—C20—C21	−136.5 (10)	N2'—C19—N2—C1	−77.7 (13)
N2'—C19'—C20—C19	−71.8 (13)	C20'—C19—N2—C2	−12.2 (19)
C20'—C19'—C20—C19	7.0 (11)	C19'—C19—N2—C2	58.7 (11)
N2—C19'—C20—C19	−46.3 (8)	C20—C19—N2—C2	20.8 (12)
C19—C19'—C20—C21'	−67.3 (12)	N2'—C19—N2—C2	58.3 (12)
N2'—C19'—C20—C21'	−139.1 (12)	C20'—C19—N2—C19'	−70.8 (16)
C20'—C19'—C20—C21'	−60.3 (11)	C20—C19—N2—C19'	−37.9 (8)
N2—C19'—C20—C21'	−113.6 (11)	N2'—C19—N2—C19'	−0.3 (14)
C19'—C19—C20—C20'	168.6 (18)	C2'—C2—N2—N2'	−177 (2)
N2—C19—C20—C20'	−137.9 (15)	C3—C2—N2—N2'	−103.7 (14)
N2'—C19—C20—C20'	−151.7 (15)	C3—C2—N2—C2'	73.6 (18)
C20'—C19—C20—C19'	−168.6 (18)	N2'—C2—N2—C2'	177 (2)
N2—C19—C20—C19'	53.5 (10)	C2'—C2—N2—C1	−111.4 (19)
N2'—C19—C20—C19'	39.6 (9)	C3—C2—N2—C1	−37.8 (9)
C20'—C19—C20—C21	−52.3 (14)	N2'—C2—N2—C1	66.0 (11)
C19'—C19—C20—C21	116.4 (12)	C2'—C2—N2—C19	102.4 (19)
N2—C19—C20—C21	169.8 (7)	C3—C2—N2—C19	176.0 (7)
N2'—C19—C20—C21	156.0 (7)	N2'—C2—N2—C19	−80.2 (14)
C20'—C19—C20—C21'	−42.8 (14)	C2'—C2—N2—C19'	138.9 (19)
C19'—C19—C20—C21'	125.8 (11)	C3—C2—N2—C19'	−147.5 (8)
N2—C19—C20—C21'	179.3 (7)	N2'—C2—N2—C19'	−43.8 (12)
N2'—C19—C20—C21'	165.5 (7)	C20—C19'—N2—N2'	−121.4 (17)

C19'—C20—C20'—C19	8.7 (14)	C19—C19'—N2—N2'	−179.6 (16)
C21—C20—C20'—C19	132.1 (11)	C20'—C19'—N2—N2'	−152.3 (15)
C21'—C20—C20'—C19	131.9 (13)	C20—C19'—N2—C2'	−61.6 (14)
C21—C20—C20'—C19'	123.4 (10)	C19—C19'—N2—C2'	−119.9 (10)
C19—C20—C20'—C19'	−8.7 (14)	N2'—C19'—N2—C2'	59.7 (13)
C21'—C20—C20'—C19'	123.2 (9)	C20'—C19'—N2—C2'	−92.5 (10)
C19'—C20—C20'—C21'	−123.2 (9)	C20—C19'—N2—C1	−176.8 (10)
C21—C20—C20'—C21'	0.3 (8)	C19—C19'—N2—C1	125.0 (8)
C19—C20—C20'—C21'	−131.9 (13)	N2'—C19'—N2—C1	−55.4 (12)
C19'—C20—C20'—C21	−123.4 (10)	C20'—C19'—N2—C1	152.3 (8)
C19—C20—C20'—C21	−132.1 (11)	C20—C19'—N2—C19	58.2 (10)
C21'—C20—C20'—C21	−0.3 (8)	N2'—C19'—N2—C19	179.6 (16)
C19'—C19—C20'—C20	−8.6 (14)	C20'—C19'—N2—C19	27.3 (7)
N2—C19—C20'—C20	60.3 (19)	C20—C19'—N2—C2	−77.7 (12)
N2'—C19—C20'—C20	34.3 (18)	C19—C19'—N2—C2	−135.9 (9)
N2—C19—C20'—C19'	68.9 (14)	N2'—C19'—N2—C2	43.7 (12)
C20—C19—C20'—C19'	8.6 (14)	C20'—C19'—N2—C2	−108.6 (9)
N2'—C19—C20'—C19'	42.8 (10)	C2'—N2—N2'—C2	−1.0 (9)
C19'—C19—C20'—C21'	83.2 (18)	C1—N2—N2'—C2	−108.5 (8)
N2—C19—C20'—C21'	152.1 (13)	C19—N2—N2'—C2	125.8 (8)
C20—C19—C20'—C21'	92 (2)	C19'—N2—N2'—C2	126.1 (11)
N2'—C19—C20'—C21'	126.0 (15)	C2'—N2—N2'—C1	107.5 (6)
C19'—C19—C20'—C21	56.6 (17)	C19—N2—N2'—C1	−125.7 (6)
N2—C19—C20'—C21	125.5 (14)	C2—N2—N2'—C1	108.5 (8)
C20—C19—C20'—C21	65.2 (16)	C19'—N2—N2'—C1	−125.4 (9)
N2'—C19—C20'—C21	99.4 (16)	C2'—N2—N2'—C19'	−127.1 (9)
C19—C19'—C20'—C20	169.7 (17)	C1—N2—N2'—C19'	125.4 (9)
N2'—C19'—C20'—C20	122.8 (14)	C19—N2—N2'—C19'	−0.3 (11)
N2—C19'—C20'—C20	134.4 (12)	C2—N2—N2'—C19'	−126.1 (11)
C20—C19'—C20'—C19	−169.7 (17)	C1—N2—N2'—C2'	−107.5 (6)
N2'—C19'—C20'—C19	−46.8 (11)	C19—N2—N2'—C2'	126.8 (8)
N2—C19'—C20'—C19	−35.2 (8)	C2—N2—N2'—C2'	1.0 (9)
C20—C19'—C20'—C21'	60.9 (12)	C19'—N2—N2'—C2'	127.1 (9)
C19—C19'—C20'—C21'	−129.4 (14)	C2'—N2—N2'—C19	−126.8 (8)
N2'—C19'—C20'—C21'	−176.3 (10)	C1—N2—N2'—C19	125.7 (6)
N2—C19'—C20'—C21'	−164.6 (9)	C2—N2—N2'—C19	−125.8 (8)
C20—C19'—C20'—C21	47.2 (10)	C19'—N2—N2'—C19	0.3 (11)
C19—C19'—C20'—C21	−143.1 (12)	C2'—C2—N2'—N2	2(2)
N2'—C19'—C20'—C21	170.0 (9)	C3—C2—N2'—N2	82.4 (14)
N2—C19'—C20'—C21	−178.4 (7)	C2'—C2—N2'—C1	−77.3 (19)
C20'—C20—C21—C21'	−1(2)	C3—C2—N2'—C1	2.8 (12)
C19'—C20—C21—C21'	83 (2)	N2—C2—N2'—C1	−79.6 (12)
C19—C20—C21—C21'	28 (2)	C2'—C2—N2'—C19'	106.8 (19)
C20'—C20—C21—C22'	34.6 (12)	C3—C2—N2'—C19'	−173.1 (10)
C19'—C20—C21—C22'	118.6 (12)	N2—C2—N2'—C19'	104.5 (16)
C19—C20—C21—C22'	63.8 (10)	C3—C2—N2'—C2'	80.1 (18)
C21'—C20—C21—C22'	35.3 (15)	N2—C2—N2'—C2'	−2(2)
C19'—C20—C21—C20'	84.1 (14)	C2'—C2—N2'—C19	55 (2)
C19—C20—C21—C20'	29.2 (8)	C3—C2—N2'—C19	135.0 (9)

C21'—C20—C21—C20'	1(2)	N2—C2—N2'—C19	52.5 (10)
C20'—C20—C21—C22	28.2 (12)	N1—C1—N2'—N2	−104.2 (11)
C19'—C20—C21—C22	112.3 (12)	C7—C1—N2'—N2	88.0 (13)
C19—C20—C21—C22	57.4 (9)	N1—C1—N2'—C2	−11.7 (10)
C21'—C20—C21—C22	28.9 (16)	N2—C1—N2'—C2	92.4 (13)
C20—C20'—C21—C21'	179 (2)	C7—C1—N2'—C2	−179.5 (8)
C19—C20'—C21—C21'	95 (3)	N1—C1—N2'—C19'	164.1 (9)
C19'—C20'—C21—C21'	137 (2)	N2—C1—N2'—C19'	−91.7 (15)
C20—C20'—C21—C22'	−148.9 (11)	C7—C1—N2'—C19'	−3.7 (14)
C19—C20'—C21—C22'	126.5 (18)	N1—C1—N2'—C2'	−36.3 (9)
C19'—C20'—C21—C22'	169.2 (9)	N2—C1—N2'—C2'	67.9 (11)
C21'—C20'—C21—C22'	31.9 (17)	C7—C1—N2'—C2'	155.9 (7)
C19—C20'—C21—C20	−84.5 (19)	N1—C1—N2'—C19	−149.8 (5)
C19'—C20'—C21—C20	−41.9 (9)	N2—C1—N2'—C19	−45.7 (10)
C21'—C20'—C21—C20	−179 (2)	C7—C1—N2'—C19	42.4 (10)
C20—C20'—C21—C22	−154.0 (11)	C20—C19'—N2'—N2	72.4 (18)
C19—C20'—C21—C22	121.4 (18)	C19—C19'—N2'—N2	0.3 (13)
C19'—C20'—C21—C22	164.1 (9)	C20'—C19'—N2'—N2	30.0 (16)
C21'—C20'—C21—C22	26.8 (18)	C20—C19'—N2'—C2	−31 (2)
C20—C21—C21'—C22'	124.0 (17)	C19—C19'—N2'—C2	−103.0 (13)
C20'—C21—C21'—C22'	124 (2)	C20'—C19'—N2'—C2	−73.4 (15)
C22—C21—C21'—C22'	−1.7 (12)	N2—C19'—N2'—C2	−103.4 (16)
C22'—C21—C21'—C22	1.7 (12)	C20—C19'—N2'—C1	153.8 (12)
C20—C21—C21'—C22	126 (2)	C19—C19'—N2'—C1	81.8 (11)
C20'—C21—C21'—C22	125 (3)	C20'—C19'—N2'—C1	111.4 (12)
C22'—C21—C21'—C20'	−124 (2)	N2—C19'—N2'—C1	81.4 (14)
C20—C21—C21'—C20'	0.4 (13)	C20—C19'—N2'—C2'	−1(2)
C22—C21—C21'—C20'	−125 (3)	C19—C19'—N2'—C2'	−72.8 (13)
C22'—C21—C21'—C20	−124.0 (17)	C20'—C19'—N2'—C2'	−43.1 (16)
C20'—C21—C21'—C20	−0.4 (13)	N2—C19'—N2'—C2'	−73.1 (13)
C22—C21—C21'—C20	−126 (2)	C20—C19'—N2'—C19	72.0 (13)
C20—C20'—C21'—C21	−1(2)	C20'—C19'—N2'—C19	29.6 (7)
C19—C20'—C21'—C21	−104 (3)	N2—C19'—N2'—C19	−0.3 (13)
C19'—C20'—C21'—C21	−46 (2)	C2—C2'—N2'—N2	−178 (2)
C20—C20'—C21'—C22'	−130.6 (14)	C3—C2'—N2'—N2	114.3 (12)
C19—C20'—C21'—C22'	126.2 (18)	N2—C2'—N2'—C2	178 (2)
C19'—C20'—C21'—C22'	−175.6 (12)	C3—C2'—N2'—C2	−68.2 (17)
C21—C20'—C21'—C22'	−130 (3)	C2—C2'—N2'—C1	109.6 (18)
C20—C20'—C21'—C22	−143.3 (12)	N2—C2'—N2'—C1	−72.9 (10)
C19—C20'—C21'—C22	113.6 (18)	C3—C2'—N2'—C1	41.4 (9)
C19'—C20'—C21'—C22	171.8 (10)	C2—C2'—N2'—C19'	−91 (2)
C21—C20'—C21'—C22	−143 (2)	N2—C2'—N2'—C19'	86.3 (14)
C19—C20'—C21'—C20	−103 (2)	C3—C2'—N2'—C19'	−159.4 (10)
C19'—C20'—C21'—C20	−44.9 (9)	C2—C2'—N2'—C19	−134.0 (18)
C21—C20'—C21'—C20	1(2)	N2—C2'—N2'—C19	43.5 (9)
C20'—C20—C21'—C21	179 (2)	C3—C2'—N2'—C19	157.8 (7)
C19'—C20—C21'—C21	−109 (2)	C20'—C19—N2'—N2	125.9 (16)
C19—C20—C21'—C21	−153.5 (19)	C19'—C19—N2'—N2	−179.6 (16)
C20'—C20—C21'—C22'	67.9 (17)	C20—C19—N2'—N2	145.2 (13)

C19'—C20—C21'—C22'	140.1 (15)	C20'—C19—N2'—C2	52.6 (16)
C21—C20—C21'—C22'	−111 (3)	C19'—C19—N2'—C2	107.1 (13)
C19—C20—C21'—C22'	95.2 (15)	N2—C19—N2'—C2	−73.4 (13)
C20'—C20—C21'—C22	50.6 (15)	C20—C19—N2'—C2	71.8 (10)
C19'—C20—C21'—C22	122.8 (14)	C20'—C19—N2'—C1	−175.9 (11)
C21—C20—C21'—C22	−129 (3)	C19'—C19—N2'—C1	−121.4 (11)
C19—C20—C21'—C22	77.9 (13)	N2—C19—N2'—C1	58.2 (11)
C19'—C20—C21'—C20'	72.3 (14)	C20—C19—N2'—C1	−156.6 (7)
C21—C20—C21'—C20'	−179 (2)	C20'—C19—N2'—C19'	−54.5 (13)
C19—C20—C21'—C20'	27.3 (9)	N2—C19—N2'—C19'	179.6 (16)
C21—C21'—C22—N3	54 (3)	C20—C19—N2'—C19'	−35.2 (8)
C22'—C21'—C22—N3	60 (4)	C20'—C19—N2'—C2'	73.4 (14)
C20'—C21'—C22—N3	175.9 (9)	C19'—C19—N2'—C2'	127.9 (11)
C20—C21'—C22—N3	149.0 (11)	N2—C19—N2'—C2'	−52.5 (11)
C22'—C21'—C22—C21	6(5)	C20—C19—N2'—C2'	92.7 (8)
C20'—C21'—C22—C21	122 (3)	C5—C6—N3—C4	1.2 (5)
C20—C21'—C22—C21	95 (3)	C5—C6—N3—C22	163.7 (7)
C21'—C21—C22—N3	−128 (3)	C5—C6—N3—C22'	−173.6 (7)
C22'—C21—C22—N3	62 (6)	N4—C4—N3—C6	−1.0 (5)
C20—C21—C22—N3	170.6 (7)	C13—C4—N3—C6	179.2 (4)
C20'—C21—C22—N3	−174.4 (7)	N4—C4—N3—C22	−162.0 (8)
C22'—C21—C22—C21'	−170 (7)	C13—C4—N3—C22	18.2 (10)
C20—C21—C22—C21'	−62 (3)	N4—C4—N3—C22'	173.7 (7)
C20'—C21—C22—C21'	−46 (3)	C13—C4—N3—C22'	−6.1 (9)
C21—C21'—C22'—N3	72 (3)	C21'—C22—N3—C6	80.4 (10)
C22—C21'—C22'—N3	−103 (4)	C21—C22—N3—C6	90.1 (7)
C20'—C21'—C22'—N3	−171.3 (9)	C21'—C22—N3—C4	−121.2 (8)
C20—C21'—C22'—N3	154.7 (10)	C21—C22—N3—C4	−111.5 (7)
C22—C21'—C22'—C21	−175 (4)	C21'—C22—N3—C22'	−26.4 (18)
C20'—C21'—C22'—C21	117 (3)	C21—C22—N3—C22'	−16.7 (19)
C20—C21'—C22'—C21	83 (3)	C21'—C22'—N3—C6	49.6 (15)
C20—C21—C22'—C21'	−65 (2)	C21—C22'—N3—C6	69.6 (10)
C20'—C21—C22'—C21'	−47 (2)	C21'—C22'—N3—C4	−124.0 (12)
C22—C21—C22'—C21'	9(6)	C21—C22'—N3—C4	−104.0 (8)
C21'—C21—C22'—N3	−118 (3)	C21'—C22'—N3—C22	136 (3)
C20—C21—C22'—N3	176.5 (7)	C21—C22'—N3—C22	156 (3)
C20'—C21—C22'—N3	−165.5 (8)	N3—C4—N4—C5	0.4 (5)
C22—C21—C22'—N3	−109 (6)	C13—C4—N4—C5	−179.9 (4)
N1—Cd1—C23—O1	49.2 (3)	N3—C4—N4—Cd1^{ii}	−163.9 (3)
N4^{i}—Cd1—C23—O1	156.9 (3)	C13—C4—N4—Cd1^{ii}	15.9 (6)
O2—Cd1—C23—O1	−178.5 (5)	C6—C5—N4—C4	0.4 (5)
Cl—Cd1—C23—O1	−73.7 (3)	C6—C5—N4—Cd1^{ii}	165.5 (3)
N1—Cd1—C23—O2	−132.3 (3)	O2—C23—O1—Cd1	−1.6 (6)
N4^{i}—Cd1—C23—O2	−24.6 (4)	C24—C23—O1—Cd1	−179.6 (4)
O1—Cd1—C23—O2	178.5 (5)	N1—Cd1—O1—C23	−135.5 (3)
Cl—Cd1—C23—O2	104.8 (3)	N4^{i}—Cd1—O1—C23	−33.7 (4)
O1—C23—C24—C29	14.5 (9)	O2—Cd1—O1—C23	0.8 (3)
O2—C23—C24—C29	−163.7 (6)	Cl—Cd1—O1—C23	112.5 (3)

O1—C23—C24—C25	−169.0 (6)	O1—C23—O2—Cd1	1.6 (6)
O2—C23—C24—C25	12.8 (8)	C24—C23—O2—Cd1	179.7 (4)
C29—C24—C25—C26	0.6 (11)	N1—Cd1—O2—C23	61.2 (4)
C23—C24—C25—C26	−176.0 (7)	$N4^{i}$—Cd1—O2—C23	158.2 (3)
C24—C25—C26—C27	−0.4 (14)	O1—Cd1—O2—C23	−0.8 (3)
C25—C26—C27—C28	−0.2 (17)	Cl—Cd1—O2—C23	−85.3 (3)

Symmetry codes: (i) *x*, −*y*+3/2, *z*+1/2; (ii) *x*, −*y*+3/2, *z*−1/2.

Fig. 1

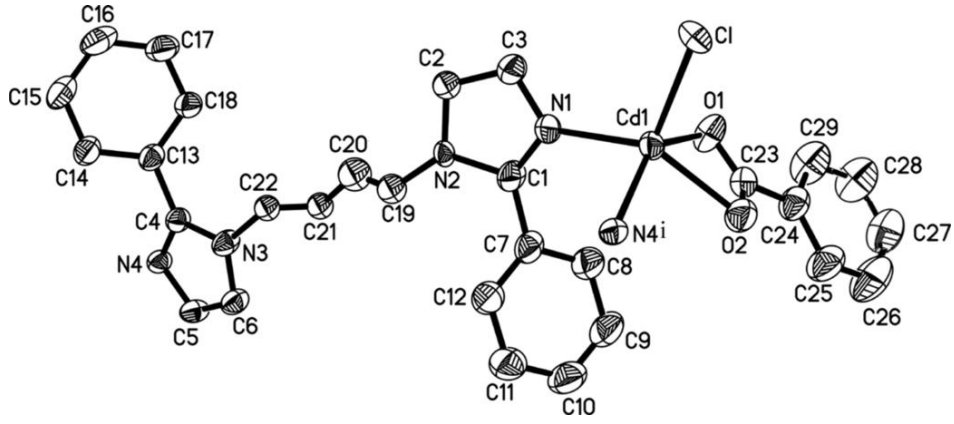
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Fig. 2

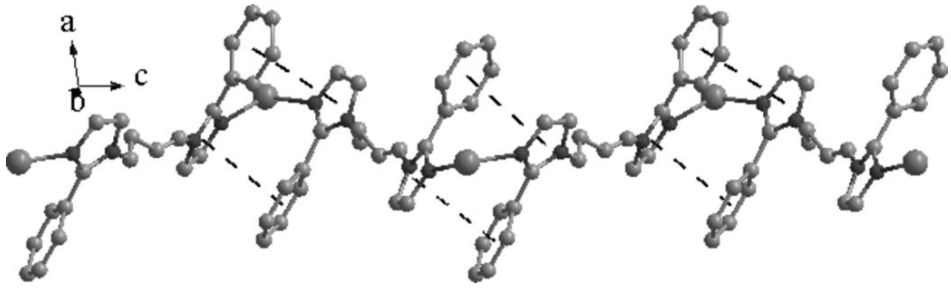

Fig. 3