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Di-μ-chlorido-bis(chlorido{2-[(2*S*)-pyrrolidin-2-yl]-1*H*-benzimidazole}-cadmium(II))

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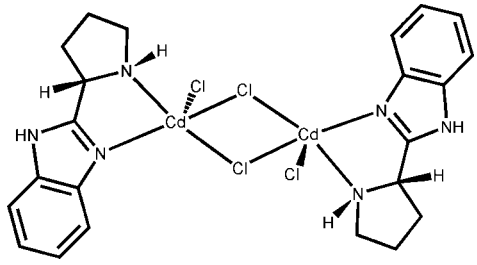
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.027; wR factor = 0.061; data-to-parameter ratio = 19.0.

The title binuclear compound, $[Cd_2Cl_4(C_{11}H_{12}N_3)_2]$, was synthesized by the hydrothermal reaction of $CdCl_2$ and the homochiral ligand 2-[(2*S*)-pyrrolidin-2-yl]-1*H*-benzimidazole. Each of the two crystallographically independent Cd atoms has a slightly distorted trigonal–bipyramidal geometry and is coordinated by two N atoms from the organic ligand, and by one terminal and two bridging Cl^- anions. The crystal structure involves intermolecular N—H···Cl hydrogen bonds. One C atom of a pyrrolidine ring is disordered over two positions; the site occupany factors are *ca* 0.8 and 0.2.

Related literature

For the physical properties of non-centrosymmetric solid materials, see: Zyss (1993); Agullo-Lopez *et al.* (1994); Newnham *et al.* (1975); Qu *et al.* (2004). For synthesis of the organic ligand, see: Aminabhavi *et al.* (1986).



Experimental

Crystal data

$[Cd_2Cl_4(C_{11}H_{12}N_3)_2]$
M_r = 741.09
Monoclinic, $P2_1$
a = 9.365 (6) Å
b = 8.103 (5) Å
c = 17.691 (12) Å
β = 99.673 (12)°
V = 1323.4 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.03 mm^{-1}
T = 293 (2) K
0.4 × 0.3 × 0.3 mm

Data collection

Rigaku Mercury2 CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.701, T_{max} = 1.000
(expected range = 0.381–0.543)
13823 measured reflections
6010 independent reflections
5622 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.061
S = 1.04
6010 reflections
317 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}
Absolute structure: Flack (1983), with 2870 Friedel pairs
Flack parameter: −0.03 (2)

Table 1
Selected bond lengths (Å).

Cd1—N2	2.266 (3)	Cd1—Cl1	2.6026 (18)
Cd1—N1	2.394 (3)	Cd1—Cd2	3.8485 (16)
Cd1—Cl3	2.5063 (14)	Cl1—Cl2	3.472 (2)
Cd1—Cl2	2.5605 (16)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···Cl3^{i}	0.86	2.35	3.191 (3)	168
N6—H6A···Cl4^{ii}	0.86	2.43	3.267 (4)	164

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1999); software used to prepare material for publication: *SHELXTL/PC*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2093).

References

Agullo-Lopez, F., Cabrera, J. M. & Agullo-Rueda, F. (1994). *Electrooptics: Phenomena, Materials and Applications*. New York: Academic Press.
Aminabhavi, T. M., Biradar, N. S. & Patil, S. B. (1986). *Inorg. Chim. Acta*, **125**, 125–128.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Newnham, R. E. (1975). *Structure–Property Relations*. New York: Springer.
Qu, Z.-R., Zhao, H., Wang, Y.-P., Wang, X.-S., Ye, Q., Li, Y.-H., Xiong, R.-G., Abrahams, B. H., Liu, Z.-G., Xue, Z.-L. & You, X.-Z. (2004). *Chem. Eur. J.* **10**, 54–60.
Rigaku (2005). *CrystalClear*. Version 1.4.0. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1999). *SHELXTL/PC*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Zyss, J. (1993). *Molecular Nonlinear Optics: Materials, Physics and Devices*. New York: Academic Press.

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supplementary materials

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Di-μ-chlorido-bis(chlorido{2-[(2*S*)-pyrrolidin-2-yl]-1*H*-benzimidazole}cadmium(II))

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Comment

Phenomena such as triboluminescence, second harmonic generation (SHG), piezoelectricity, pyroelectricity and ferroelectricity are only found in noncentrosymmetric bulk materials (Zyss, 1993; Agullo-Lopez *et al.,* 1994; Newnham *et al.*, 1975). There has been very strong interest in employing crystal-engineering strategies to generate materials with desirable properties. Such approaches have succeeded in producing chiral or noncentrosymmetric coordination polymers and organic compounds (Qu *et al.*, 2004). We have focused on the synthesis of noncentrosymmetric coordination compounds by the hydrothermal reaction of the chiral ligand and inoganic salt. Here we report the crystal structure of the title compound prepared from $CdCl_2$ and benzimidazole-derived chiral ligand.

As shown in Fig. 1, the Cd ions are chelated by the chiral organic ligand and thus the compound has to form chiral crystals. Each of the two crystallographically independent pentacoordinated Cd atoms has a slightly distorted trigonal-bipyramidal geometry and is coordinated by two N atoms from the organic ligand, and by one terminal and two bridging Cl^- anions. The two Cd centers are bridged by two chlorine atoms to give a dicadmium framework with a Cd—Cd separation of 3.8485 (16) Å and a Cl—Cl distance of 3.472 (2) Å.

Experimental

The homochiral ligand, (*S*)-2-[pyrrolidin-2-yl]-1*H*-benzimidazole, was synthesized by the reaction of (*S*)-pyrrolidine-2-carboxylic acid and benzene-1,2-diamine according to the procedure described in the literature (Aminabhavi *et al.*, 1986). A mixture of *S*-2-(pyrrolidin-2-yl)-1*H*-benzimidazole (18.7 mg, 0.1 mmol) and $CdCl_2$ (18.3 mg, 0.1 mmol) and water (1 ml) sealed in a glass tube were kept at 70 °C. Crystals suitable for X-ray analysis were obtained after 3 days.

Refinement

All H atoms were included in calculated positions with C—H = 0.93–0.97 Å and N—H=0.86 Å and with U_{iso}(H) = 1.2U_{eq}(C,*N*). One of the pyrrolidine rings is disordered with the C10 atom occupying two positions, C10 nad C10', with the occupancy factors of 0.81 (2) and 0.19 (2), respectively.

Figures

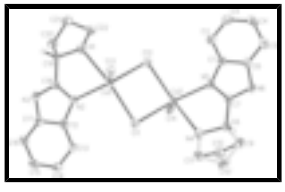


Fig. 1. A view of the title compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level and all hydrogen atoms, except H8a and H19*a*, were omitted for clarity.

Di-μ-chlorido-bis(chlorido{2-[(2*S*)-pyrrolidin-2-yl]-1*H*- benzimidazole}cadmium(II))

Crystal data

$[Cd_2Cl_4(C_{11}H_{12}N_3)_2]$	F_{000} = 728
M_r = 741.09	D_x = 1.860 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 11574 reflections
a = 9.365 (6) Å	θ = 3.3–27.4º
b = 8.103 (5) Å	μ = 2.03 mm^{-1}
c = 17.691 (12) Å	T = 293 (2) K
β = 99.673 (12)º	Prism, colourless
V = 1323.4 (15) Å^3	0.4 × 0.3 × 0.3 mm
Z = 2	

Data collection

Rigaku Mercury2 CCD diffractometer	6010 independent reflections
Radiation source: fine-focus sealed tube	5622 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.036
Detector resolution: 13.66 pixels mm^{-1}	θ_{max} = 27.5º
T = 293(2) K	θ_{min} = 3.4º
ω scans	h = −12→12
Absorption correction: multi-scan (CrystalClear; Rigaku, 2005)	k = −10→10
T_{min} = 0.701, T_{max} = 1.000	l = −22→22
13823 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.027	$w = 1/[\sigma^2(F_o^2) + (0.0194P)^2 + 0.0229P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.061	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.04	$\Delta\rho_{max}$ = 0.57 e Å^{-3}
6010 reflections	$\Delta\rho_{min}$ = −0.30 e Å^{-3}
317 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983)
Primary atom site location: structure-invariant direct methods	Flack parameter: −0.03 (2)
Secondary atom site location: difference Fourier map	

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	0.89212 (3)	0.09969 (3)	0.681550 (14)	0.03784 (7)	
Cd2	0.70149 (3)	−0.19423 (3)	0.803532 (14)	0.03883 (7)	
Cl1	0.94116 (11)	−0.02794 (13)	0.81846 (6)	0.0536 (3)	
Cl2	0.64668 (9)	−0.04558 (12)	0.67049 (5)	0.0442 (2)	
Cl3	1.03862 (11)	−0.05990 (11)	0.60033 (5)	0.0499 (2)	
Cl4	0.55426 (12)	−0.04372 (12)	0.88338 (6)	0.0538 (2)	
N1	0.8156 (3)	0.2880 (3)	0.57844 (15)	0.0387 (6)	
H1A	0.8586	0.2380	0.5428	0.046*	
N2	0.9917 (3)	0.3464 (3)	0.72100 (14)	0.0341 (6)	
N3	1.0317 (3)	0.6107 (4)	0.69852 (15)	0.0389 (6)	
H3A	1.0233	0.7052	0.6761	0.047*	
N4	0.8371 (3)	−0.4053 (4)	0.88192 (15)	0.0398 (6)	
H4C	0.9229	−0.4063	0.8655	0.048*	
N5	0.5980 (3)	−0.4390 (3)	0.76447 (15)	0.0359 (7)	
N6	0.5622 (3)	−0.7033 (4)	0.78519 (16)	0.0403 (7)	
H6A	0.5742	−0.7996	0.8057	0.048*	
C1	0.4788 (4)	−0.4917 (4)	0.71093 (19)	0.0372 (8)	
C2	0.3925 (4)	−0.4088 (6)	0.6516 (2)	0.0499 (9)	
H2A	0.4059	−0.2969	0.6434	0.060*	
C3	0.2868 (4)	−0.4999 (6)	0.6066 (2)	0.0522 (10)	
H3B	0.2275	−0.4476	0.5662	0.063*	
C4	0.2664 (4)	−0.6681 (6)	0.6188 (2)	0.0504 (10)	
H4A	0.1945	−0.7250	0.5864	0.061*	
C5	0.3504 (4)	−0.7521 (5)	0.6781 (2)	0.0478 (9)	
H5A	0.3363	−0.8634	0.6874	0.057*	
C6	0.4568 (4)	−0.6603 (4)	0.7237 (2)	0.0389 (8)	
C7	0.6417 (4)	−0.5683 (4)	0.80687 (18)	0.0344 (8)	
C8	0.7681 (4)	−0.5709 (4)	0.87137 (19)	0.0400 (8)	
H8A	0.8393	−0.6513	0.8594	0.048*	
C9	0.7265 (5)	−0.6156 (6)	0.9492 (2)	0.0632 (12)	0.83 (2)
H9A	0.6288	−0.6592	0.9427	0.076*	0.83 (2)
H9B	0.7927	−0.6971	0.9757	0.076*	0.83 (2)
C9'	0.7265 (5)	−0.6156 (6)	0.9492 (2)	0.0632 (12)	0.17 (2)

H9'A	0.6271	−0.5849	0.9512	0.076*	0.17 (2)
H9'B	0.7386	−0.7328	0.9596	0.076*	0.17 (2)
C10	0.7372 (11)	−0.4563 (12)	0.9930 (3)	0.067 (3)	0.83 (2)
H10A	0.6478	−0.3939	0.9814	0.080*	0.83 (2)
H10B	0.7588	−0.4761	1.0479	0.080*	0.83 (2)
C10'	0.827 (6)	−0.520 (3)	1.0028 (14)	0.060 (11)	0.17 (2)
H10C	0.9152	−0.5819	1.0188	0.072*	0.17 (2)
H10D	0.7845	−0.4950	1.0479	0.072*	0.17 (2)
C11	0.8590 (5)	−0.3676 (6)	0.9658 (2)	0.0608 (12)	0.83 (2)
H11A	0.8537	−0.2498	0.9747	0.073*	0.83 (2)
H11B	0.9520	−0.4084	0.9915	0.073*	0.83 (2)
C11'	0.8590 (5)	−0.3676 (6)	0.9658 (2)	0.0608 (12)	0.17 (2)
H11C	0.9581	−0.3336	0.9840	0.073*	0.17 (2)
H11D	0.7944	−0.2801	0.9762	0.073*	0.17 (2)
C12	1.0924 (3)	0.4106 (4)	0.78235 (18)	0.0330 (7)	
C13	1.1658 (4)	0.3332 (5)	0.8477 (2)	0.0488 (10)	
H13A	1.1499	0.2229	0.8582	0.059*	
C14	1.2641 (5)	0.4293 (6)	0.8966 (2)	0.0565 (11)	
H14A	1.3155	0.3809	0.9405	0.068*	
C15	1.2880 (4)	0.5930 (6)	0.8813 (2)	0.0527 (10)	
H15A	1.3553	0.6520	0.9156	0.063*	
C16	1.2163 (4)	0.6723 (5)	0.8167 (2)	0.0479 (10)	
H16A	1.2320	0.7827	0.8064	0.057*	
C17	1.1176 (4)	0.5762 (4)	0.76791 (18)	0.0360 (7)	
C18	0.9634 (4)	0.4698 (4)	0.67212 (18)	0.0321 (7)	
C19	0.8754 (4)	0.4578 (4)	0.59312 (18)	0.0341 (7)	
H19A	0.9402	0.4804	0.5563	0.041*	
C20	0.7473 (4)	0.5766 (5)	0.5758 (2)	0.0531 (10)	
H20A	0.7757	0.6793	0.5543	0.064*	
H20B	0.7066	0.6006	0.6216	0.064*	
C21	0.6403 (4)	0.4832 (5)	0.5179 (2)	0.0514 (10)	
H21A	0.5422	0.5239	0.5156	0.062*	
H21B	0.6664	0.4889	0.4672	0.062*	
C22	0.6568 (4)	0.3081 (6)	0.5497 (2)	0.0472 (8)	
H22A	0.6021	0.2945	0.5913	0.057*	
H22B	0.6231	0.2278	0.5101	0.057*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.04699 (14)	0.02405 (12)	0.04211 (14)	−0.00259 (11)	0.00645 (10)	0.00146 (10)
Cd2	0.05097 (15)	0.02408 (12)	0.04213 (14)	−0.00421 (11)	0.00980 (11)	−0.00005 (10)
Cl1	0.0559 (6)	0.0497 (6)	0.0501 (5)	−0.0185 (5)	−0.0057 (4)	0.0168 (5)
Cl2	0.0464 (5)	0.0394 (5)	0.0442 (5)	−0.0079 (4)	−0.0002 (4)	0.0072 (4)
Cl3	0.0707 (6)	0.0331 (4)	0.0523 (5)	0.0026 (4)	0.0285 (5)	0.0066 (4)
Cl4	0.0748 (6)	0.0339 (5)	0.0594 (6)	0.0037 (5)	0.0305 (5)	0.0009 (4)
N1	0.0454 (16)	0.0296 (14)	0.0396 (15)	0.0028 (13)	0.0031 (12)	−0.0069 (13)
N2	0.0406 (15)	0.0281 (15)	0.0321 (14)	−0.0051 (12)	0.0015 (12)	0.0026 (11)

N3	0.0501 (16)	0.0257 (14)	0.0388 (15)	−0.0055 (15)	0.0017 (12)	0.0033 (14)
N4	0.0415 (15)	0.0361 (14)	0.0431 (15)	−0.0023 (15)	0.0108 (12)	0.0015 (14)
N5	0.0498 (17)	0.0247 (15)	0.0336 (15)	−0.0022 (12)	0.0082 (12)	−0.0002 (11)
N6	0.0535 (17)	0.0223 (13)	0.0452 (16)	−0.0026 (15)	0.0084 (13)	0.0002 (14)
C1	0.0413 (19)	0.0369 (18)	0.0348 (18)	−0.0063 (16)	0.0101 (14)	−0.0011 (15)
C2	0.052 (2)	0.047 (2)	0.050 (2)	−0.007 (2)	0.0064 (17)	0.012 (2)
C3	0.045 (2)	0.068 (3)	0.042 (2)	−0.002 (2)	0.0037 (17)	0.007 (2)
C4	0.040 (2)	0.068 (3)	0.045 (2)	−0.016 (2)	0.0108 (16)	−0.014 (2)
C5	0.052 (2)	0.037 (2)	0.058 (2)	−0.0125 (18)	0.0189 (18)	−0.0133 (18)
C6	0.0426 (19)	0.034 (2)	0.0428 (19)	−0.0035 (15)	0.0161 (15)	−0.0043 (15)
C7	0.045 (2)	0.0286 (17)	0.0333 (17)	−0.0022 (15)	0.0158 (15)	0.0020 (14)
C8	0.051 (2)	0.0294 (17)	0.0381 (18)	−0.0009 (16)	0.0027 (15)	−0.0003 (14)
C9	0.086 (3)	0.058 (3)	0.043 (2)	−0.027 (2)	0.003 (2)	0.012 (2)
C9'	0.086 (3)	0.058 (3)	0.043 (2)	−0.027 (2)	0.003 (2)	0.012 (2)
C10	0.089 (5)	0.076 (6)	0.038 (3)	−0.021 (4)	0.019 (3)	−0.006 (3)
C10'	0.11 (3)	0.041 (15)	0.029 (12)	0.020 (16)	−0.002 (14)	0.000 (10)
C11	0.079 (3)	0.054 (3)	0.045 (2)	−0.019 (2)	−0.002 (2)	−0.0026 (19)
C11'	0.079 (3)	0.054 (3)	0.045 (2)	−0.019 (2)	−0.002 (2)	−0.0026 (19)
C12	0.0392 (17)	0.0326 (18)	0.0283 (16)	−0.0026 (14)	0.0085 (13)	0.0002 (13)
C13	0.055 (2)	0.048 (2)	0.0392 (19)	−0.0135 (18)	−0.0050 (16)	0.0118 (17)
C14	0.063 (3)	0.065 (3)	0.037 (2)	−0.015 (2)	−0.0062 (18)	0.0075 (19)
C15	0.052 (2)	0.068 (3)	0.0374 (19)	−0.017 (2)	0.0045 (16)	−0.012 (2)
C16	0.051 (2)	0.039 (2)	0.053 (2)	−0.0126 (17)	0.0070 (18)	−0.0086 (18)
C17	0.0454 (18)	0.0308 (18)	0.0328 (17)	−0.0022 (16)	0.0097 (14)	−0.0050 (14)
C18	0.0384 (18)	0.0268 (16)	0.0319 (16)	−0.0034 (14)	0.0088 (14)	0.0010 (14)
C19	0.0390 (17)	0.0338 (17)	0.0305 (17)	−0.0015 (14)	0.0086 (13)	0.0017 (14)
C20	0.063 (2)	0.034 (2)	0.059 (2)	0.0101 (19)	0.0006 (19)	0.0048 (18)
C21	0.044 (2)	0.056 (3)	0.051 (2)	0.0107 (19)	−0.0026 (16)	0.0069 (19)
C22	0.0424 (19)	0.048 (2)	0.048 (2)	−0.003 (2)	−0.0006 (15)	0.000 (2)

Geometric parameters (Å, °)

Cd1—N2	2.266 (3)	C5—C6	1.388 (5)
Cd1—N1	2.394 (3)	C5—H5A	0.9300
Cd1—Cl3	2.5063 (14)	C7—C8	1.500 (5)
Cd1—Cl2	2.5605 (16)	C8—C9	1.536 (5)
Cd1—Cl1	2.6026 (18)	C8—H8A	0.9800
Cd1—Cd2	3.8485 (16)	C9—C10	1.500 (9)
Cd2—N5	2.264 (3)	C9—H9A	0.9700
Cd2—N4	2.422 (3)	C9—H9B	0.9700
Cd2—Cl4	2.4574 (14)	C10—C11	1.495 (7)
Cd2—Cl1	2.5931 (16)	C10—H10A	0.9700
Cd2—Cl2	2.6169 (17)	C10—H10B	0.9700
Cl1—Cl2	3.472 (2)	C10'—H10C	0.9700
N1—C19	1.492 (4)	C10'—H10D	0.9700
N1—C22	1.497 (4)	C11—H11A	0.9700
N1—H1A	0.9002	C11—H11B	0.9700
N2—C18	1.319 (4)	C12—C13	1.391 (5)
N2—C12	1.412 (4)	C12—C17	1.393 (5)

N3—C18	1.353 (4)	C13—C14	1.391 (6)
N3—C17	1.379 (4)	C13—H13A	0.9300
N3—H3A	0.8600	C14—C15	1.379 (7)
N4—C8	1.488 (5)	C14—H14A	0.9299
N4—C11	1.495 (5)	C15—C16	1.382 (6)
N4—H4C	0.9001	C15—H15A	0.9300
N5—C7	1.313 (4)	C16—C17	1.392 (5)
N5—C1	1.404 (4)	C16—H16A	0.9300
N6—C7	1.343 (4)	C18—C19	1.502 (4)
N6—C6	1.384 (4)	C19—C20	1.529 (5)
N6—H6A	0.8600	C19—H19A	0.9800
C1—C2	1.386 (5)	C20—C21	1.511 (5)
C1—C6	1.406 (5)	C20—H20A	0.9700
C2—C3	1.376 (6)	C20—H20B	0.9701
C2—H2A	0.9300	C21—C22	1.525 (6)
C3—C4	1.398 (6)	C21—H21A	0.9700
C3—H3B	0.9300	C21—H21B	0.9699
C4—C5	1.380 (6)	C22—H22A	0.9700
C4—H4A	0.9300	C22—H22B	0.9701
N2—Cd1—N1	74.18 (10)	N6—C6—C1	105.5 (3)
N2—Cd1—Cl3	113.28 (8)	C5—C6—C1	122.5 (4)
N1—Cd1—Cl3	90.84 (8)	N5—C7—N6	112.5 (3)
N2—Cd1—Cl2	138.31 (7)	N5—C7—C8	125.2 (3)
N1—Cd1—Cl2	94.86 (8)	N6—C7—C8	122.3 (3)
Cl3—Cd1—Cl2	106.85 (5)	N4—C8—C7	110.7 (3)
N2—Cd1—Cl1	93.71 (8)	N4—C8—C9	105.7 (3)
N1—Cd1—Cl1	161.07 (7)	C7—C8—C9	113.5 (3)
Cl3—Cd1—Cl1	107.49 (5)	N4—C8—H8A	109.3
Cl2—Cd1—Cl1	84.50 (3)	C7—C8—H8A	108.9
N2—Cd1—Cd2	125.37 (7)	C9—C8—H8A	108.7
N1—Cd1—Cd2	135.57 (7)	C10—C9—C8	104.8 (4)
Cl3—Cd1—Cd2	110.63 (5)	C10—C9—H9A	110.8
Cl2—Cd1—Cd2	42.55 (3)	C8—C9—H9A	110.8
Cl1—Cd1—Cd2	42.11 (3)	C10—C9—H9B	110.8
N5—Cd2—N4	73.29 (11)	C8—C9—H9B	110.8
N5—Cd2—Cl4	110.95 (8)	H9A—C9—H9B	108.9
N4—Cd2—Cl4	108.18 (8)	C11—C10—C9	103.6 (5)
N5—Cd2—Cl1	143.62 (8)	C11—C10—H10A	111.0
N4—Cd2—Cl1	86.97 (8)	C9—C10—H10A	111.0
Cl4—Cd2—Cl1	104.08 (5)	C11—C10—H10B	111.0
N5—Cd2—Cl2	96.87 (8)	C9—C10—H10B	111.0
N4—Cd2—Cl2	147.63 (7)	H10A—C10—H10B	109.0
Cl4—Cd2—Cl2	104.14 (5)	H10C—C10'—H10D	108.3
Cl1—Cd2—Cl2	83.57 (4)	N4—C11—C10	103.7 (4)
N5—Cd2—Cd1	125.88 (7)	N4—C11—H11A	111.0
N4—Cd2—Cd1	120.66 (8)	C10—C11—H11A	111.0
Cl4—Cd2—Cd1	111.91 (5)	N4—C11—H11B	111.0
Cl1—Cd2—Cd1	42.30 (3)	C10—C11—H11B	111.0
Cl2—Cd2—Cd1	41.42 (3)	H11A—C11—H11B	109.0

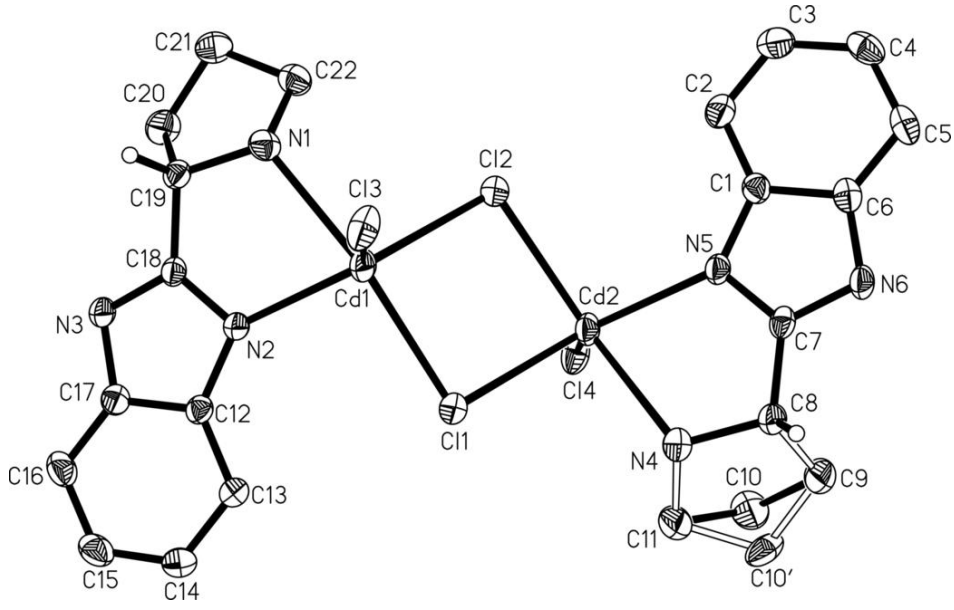
Cd2—Cl1—Cd1	95.59 (4)	C13—C12—C17	120.7 (3)
Cd2—Cl1—Cl2	48.51 (3)	C13—C12—N2	130.2 (3)
Cd1—Cl1—Cl2	47.23 (3)	C17—C12—N2	109.0 (3)
Cd1—Cl2—Cd2	96.03 (3)	C12—C13—C14	116.6 (4)
Cd1—Cl2—Cl1	48.26 (4)	C12—C13—H13A	121.8
Cd2—Cl2—Cl1	47.92 (3)	C14—C13—H13A	121.6
C19—N1—C22	106.4 (3)	C15—C14—C13	121.9 (4)
C19—N1—Cd1	113.56 (19)	C15—C14—H14A	119.4
C22—N1—Cd1	118.7 (2)	C13—C14—H14A	118.7
C19—N1—H1A	109.8	C14—C15—C16	122.5 (4)
C22—N1—H1A	110.3	C14—C15—H15A	118.8
Cd1—N1—H1A	97.7	C16—C15—H15A	118.8
C18—N2—C12	105.0 (3)	C15—C16—C17	115.6 (4)
C18—N2—Cd1	116.1 (2)	C15—C16—H16A	122.6
C12—N2—Cd1	138.5 (2)	C17—C16—H16A	121.8
C18—N3—C17	107.9 (3)	N3—C17—C16	131.8 (4)
C18—N3—H3A	126.2	N3—C17—C12	105.5 (3)
C17—N3—H3A	125.9	C16—C17—C12	122.7 (3)
C8—N4—C11	107.0 (3)	N2—C18—N3	112.5 (3)
C8—N4—Cd2	112.98 (19)	N2—C18—C19	125.4 (3)
C11—N4—Cd2	113.3 (3)	N3—C18—C19	122.0 (3)
C8—N4—H4C	110.1	N1—C19—C18	110.7 (3)
C11—N4—H4C	110.0	N1—C19—C20	106.7 (3)
Cd2—N4—H4C	103.5	C18—C19—C20	115.8 (3)
C7—N5—C1	106.2 (3)	N1—C19—H19A	108.2
C7—N5—Cd2	116.6 (2)	C18—C19—H19A	107.6
C1—N5—Cd2	136.3 (2)	C20—C19—H19A	107.6
C7—N6—C6	107.9 (3)	C21—C20—C19	103.2 (3)
C7—N6—H6A	126.2	C21—C20—H20A	111.0
C6—N6—H6A	125.9	C19—C20—H20A	111.1
C2—C1—N5	131.3 (3)	C21—C20—H20B	110.9
C2—C1—C6	120.7 (4)	C19—C20—H20B	111.4
N5—C1—C6	107.9 (3)	H20A—C20—H20B	109.1
C3—C2—C1	116.7 (4)	C20—C21—C22	101.6 (3)
C3—C2—H2A	122.3	C20—C21—H21A	111.9
C1—C2—H2A	121.0	C22—C21—H21A	111.6
C2—C3—C4	122.5 (4)	C20—C21—H21B	111.2
C2—C3—H3B	118.6	C22—C21—H21B	111.1
C4—C3—H3B	118.9	H21A—C21—H21B	109.2
C5—C4—C3	121.5 (4)	N1—C22—C21	105.0 (3)
C5—C4—H4A	119.1	N1—C22—H22A	110.6
C3—C4—H4A	119.4	C21—C22—H22A	110.6
C4—C5—C6	116.1 (4)	N1—C22—H22B	110.9
C4—C5—H5A	122.2	C21—C22—H22B	110.9
C6—C5—H5A	121.8	H22A—C22—H22B	108.9
N6—C6—C5	132.0 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3A···Cl3^{i}	0.86	2.35	3.191 (3)	168
N6—H6A···Cl4^{ii}	0.86	2.43	3.267 (4)	164

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

Fig. 1


C21
C22
C20
N1
C19
C18
N3
N2
C17
C12
C16
C13
C15
C14
Cl3
Cd1
Cl2
Cl1
Cd2
Cl4
C3
C4
C2
C5
C1
C6
N5
N6
C7
C8
N4
C10
C9
C11
C10′