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Diaquabis[3-(2-pyridyl)-1*H*-pyrazole-κ^2N^2,N^3]cadmium(II) dinitrate

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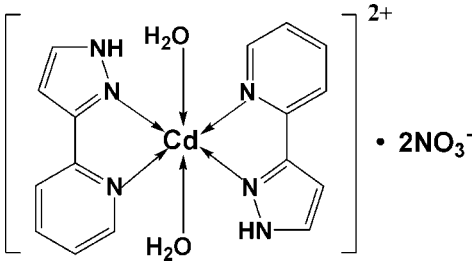
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.024; wR factor = 0.057; data-to-parameter ratio = 15.7.

In the title centrosymmetric compound, $[Cd(C_8H_7N_3)_2(H_2O)_2](NO_3)_2$, the Cd^{II} atom lies on a center of symmetry and is six-coordinated by four N donors from two distinct chelating 3-(2-pyridyl)-1*H*-pyrazole ligands and two O atoms from two water molecules, in a distorted octahedral geometry. The Cd^{II} mononuclear units and nitrate ions are linked through intermolecular O—H···O, N—H···O and C—H···O hydrogen-bonding interactions, forming a three-dimensional framework.

Related literature

For related literature, see: Bell *et al.* (2003); Hu *et al.* (2006); Liu *et al.* (2006, 2007); Paul *et al.* (2004); Steel (2005); Ward *et al.* (2001); Zou *et al.* (2004, 2005, 2006). For hydrogen-bond details, see: Desiraju & Steiner (1999).



Experimental

Crystal data

$[Cd(C_8H_7N_3)_2(H_2O)_2](NO_3)_2$
M_r = 562.78
Monoclinic, $P2_1/n$
a = 8.1283 (16) Å
b = 10.461 (2) Å
c = 12.309 (3) Å
β = 94.04 (3)°
V = 1044.0 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.11 mm^{-1}
T = 293 (2) K
0.22 × 0.18 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.795, T_{max} = 0.845
6639 measured reflections
2377 independent reflections
1810 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.057
S = 0.93
2377 reflections
151 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N3	2.2900 (17)	Cd1—N2	2.3539 (18)
Cd1—O1*W*	2.3133 (18)		
N3—Cd1—N3^{i}	180	O1*W*—Cd1—N2	93.57 (7)
N3—Cd1—O1*W*^{i}	91.87 (6)	N3—Cd1—N2^{i}	107.13 (6)
N3—Cd1—O1*W*	88.13 (6)	O1*W*—Cd1—N2^{i}	86.43 (7)
O1*W*^{i}—Cd1—O1*W*	180	N2—Cd1—N2^{i}	180
N3—Cd1—N2	72.87 (6)		

Symmetry code: (i) $-x+1, -y+2, -z+1$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O2^{ii}	0.85	2.34	3.096 (3)	148
O1*W*—H1*WA*···O3^{ii}	0.85	2.28	3.036 (3)	149
O1*W*—H1*WB*···O2^{iii}	0.85	2.12	2.944 (3)	164
N1—H1*B*···O1^{iv}	0.86	2.10	2.956 (3)	171
N1—H1*B*···O3^{iv}	0.86	2.60	3.170 (3)	125
O1*W*—H1*WB*···O1^{iii}	0.85	2.50	3.138 (2)	133
C1—H1*A*···O3^{v}	0.93	2.53	3.319 (3)	143
C8—H8*A*···O1^{vi}	0.93	2.39	3.253 (3)	153

Symmetry codes: (ii) $-x, -y+2, -z+1$; (iii) $x+\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (iv) $x+\frac{3}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (v) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (vi) $-x-\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2499).

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supplementary materials

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Diaquabis[3-(2-pyridyl)-1*H*-pyrazole- κ^2N^2,N^3]cadmium(II) dinitrate

C.-S. Liu

Comment

In recent years, much attention has been focused on the synthetic approach and the structural control of metal-organic coordination architectures with ligands based on pyrazolyl-pyridine chelating units (Steel, 2005; Ward *et al.*, 2001). Many novel functional complexes with 3-(2-pyridyl)-1*H*-pyrazole (*L*) and/or 3-(2-pyridyl)pyrazole ligands have been reported (Bell *et al.*, 2003; Paul *et al.*, 2004; Singh *et al.,* 2003; Ward *et al.*, 2001). Recently, we have used 3-(2-pyridyl)-1*H*-pyrazole and its derivatives to obtain complexes with various structures, including discrete multinuclear molecules, one- and two-dimensional coordination polymers, which exhibit luminescent and magnetic properties (Hu *et al.*, 2006; Liu *et al.*, 2006, 2007; Zou *et al.*, 2004,2005,2006). Now we report here the crystal structure of a cadmium(II) complex of *L* ligand, $[Cd(L)_2(H_2O)_2]^{2+}\cdot 2NO_3^{2-}$, the title compound.

In the title centrosymmetric complex, the Cd^{II} center is six-coordinated by four N donors from two *L* ligands and two O atoms from two water molecules (Table 1). The *L* ligand chelates to the Cd^{II} atom, which lies on an inversion center, in a nearly isobidentate manner [Cd1—N2 = 2.3539 (18) Å and Cd1—N3 = 2.2900 (17) Å]. The two other coordination sites are occupied by two water molecules. The coordination geometry around the Cd^{II} center can be described as a distorted octahedron (Fig. 1). The distortion from the ideal octahedral geometry is evident from the bond angles given in Table 1.

The Cd^{II} mononuclear units are linked to nitrate anions through intermolecular O–H···O, N–H···O and C–H···O (Desiraju & Steiner, 1999) hydrogen-bonding interactions (Table 2) involving the coordinated water molecules and free nitrate anions, forming a three-dimensional framework (Fig. 2).

Experimental

3-(2-Pyridyl)-1*H*-pyrazole) (0.1 mmol) and $Cd(NO_3)_2$ (0.1 mmol) were added to methanol (15 ml) containing water (5 ml). In few minutes, a white solid appeared which then was filtered. The resulting solution was kept at room temperature. Colourless single crystals of the title compound suitable for X-ray analysis were obtained by slow evaporation of the solvent after several days (yield: 30%). Analysis calculated for ($C_{16}H_{18}CdN_8O_8$): C 34.15, H 3.22, N 19.91%; found: C 34.26, H 3.14, N 18.77%.

Refinement

H atoms of the water molecule were located in a difference map and were allowed to ride on the parent atom, with U_{iso} = $1.2U_{eq}$(O). The remaining H atoms were included in calculated positions and treated in the subsequent refinement as riding atoms, with C—H = 0.93 Å, N—H = 0.86 Å and i>U_{iso}(H) = $1.2U_{eq}$(C,N).

Figures

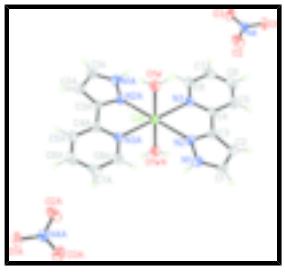

Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. Atoms labelled with the suffix A are generated by the symmetry operation (1 − *x*, 2 − *y*, 1 − *z*).

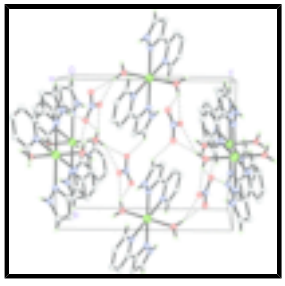

Fig. 2. Part of the crystal packing in the title compound. Hydrogen bonds are shown as dashed lines. For clarity only H atoms involved in the interactions are shown.

Diaquabis[3-(2-pyridyl)-1*H*-pyrazole- κ^2N^2,N^3]cadmium(II) dinitrate

Crystal data

$[Cd(C_8H_7N_3)_2(H_2O)_2](NO_3)_2$	F_{000} = 564
M_r = 562.78	D_x = 1.790 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 666 reflections
a = 8.1283 (16) Å	θ = 2.3–22.5º
b = 10.461 (2) Å	μ = 1.11 mm^{-1}
c = 12.309 (3) Å	*T* = 293 (2) K
β = 94.04 (3)º	Block, colourless
V = 1044.0 (4) Å^3	0.22 × 0.18 × 0.16 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	2377 independent reflections
Radiation source: fine-focus sealed tube	1810 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.032
T = 293(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 2.6º
Absorption correction: multi-scan (SADABS; Bruker, 1998)	*h* = −10→10
T_{min} = 0.795, T_{max} = 0.845	*k* = −14→13
6639 measured reflections	*l* = −15→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.025$	H-atom parameters constrained
$wR(F^2) = 0.057$	$w = 1/[\sigma^2(F_o^2) + (0.0278P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.93$	$(\Delta/\sigma)_{max} = 0.001$
2377 reflections	$\Delta\rho_{max} = 0.43$ e Å^{-3}
151 parameters	$\Delta\rho_{min} = -0.25$ 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}
Cd1	0.5000	1.0000	0.5000	0.03912 (8)
C1	0.7329 (3)	0.6068 (2)	0.5375 (2)	0.0564 (6)
H1A	0.8148	0.5450	0.5353	0.068*
C2	0.5940 (3)	0.5968 (2)	0.5903 (2)	0.0559 (6)
H2A	0.5605	0.5283	0.6315	0.067*
C3	0.5102 (3)	0.7142 (2)	0.56918 (17)	0.0423 (5)
C4	0.3529 (3)	0.7578 (2)	0.60517 (17)	0.0419 (5)
C5	0.2468 (3)	0.6775 (2)	0.6560 (2)	0.0593 (7)
H5A	0.2746	0.5923	0.6686	0.071*
C6	0.1009 (3)	0.7249 (3)	0.6875 (2)	0.0669 (8)
H6A	0.0294	0.6719	0.7224	0.080*
C7	0.0596 (3)	0.8489 (3)	0.6681 (2)	0.0610 (7)
H7A	−0.0398	0.8816	0.6890	0.073*
C8	0.1675 (3)	0.9247 (2)	0.6172 (2)	0.0536 (6)
H8A	0.1393	1.0095	0.6030	0.064*
N1	0.7326 (2)	0.72088 (19)	0.48873 (18)	0.0529 (5)
H1B	0.8102	0.7479	0.4506	0.064*
N2	0.5972 (2)	0.78798 (17)	0.50643 (15)	0.0444 (4)

N3	0.3126 (2)	0.88119 (17)	0.58709 (14)	0.0416 (4)
N4	−0.4146 (2)	0.79729 (19)	0.84554 (14)	0.0449 (4)
O1	−0.4736 (2)	0.69650 (17)	0.87871 (16)	0.0685 (5)
O2	−0.2770 (2)	0.7968 (2)	0.81080 (17)	0.0818 (6)
O3	−0.4952 (3)	0.89658 (17)	0.84575 (19)	0.0767 (6)
O1W	0.3392 (2)	0.96843 (16)	0.33963 (14)	0.0583 (5)
H1WA	0.3421	1.0117	0.2814	0.070*
H1WB	0.2902	0.8984	0.3236	0.070*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03983 (12)	0.03118 (11)	0.04703 (13)	−0.00183 (10)	0.00790 (8)	0.00727 (10)
C1	0.0514 (14)	0.0395 (13)	0.0765 (18)	0.0158 (11)	−0.0076 (13)	−0.0038 (12)
C2	0.0613 (15)	0.0411 (12)	0.0636 (16)	0.0000 (12)	−0.0068 (12)	0.0072 (12)
C3	0.0481 (12)	0.0337 (10)	0.0436 (12)	−0.0016 (10)	−0.0064 (9)	0.0007 (9)
C4	0.0517 (12)	0.0379 (11)	0.0353 (11)	−0.0125 (10)	−0.0017 (9)	0.0024 (9)
C5	0.0677 (17)	0.0509 (14)	0.0596 (15)	−0.0166 (13)	0.0075 (13)	0.0097 (12)
C6	0.0603 (16)	0.075 (2)	0.0674 (17)	−0.0231 (15)	0.0199 (14)	0.0018 (15)
C7	0.0428 (13)	0.0773 (19)	0.0655 (16)	−0.0073 (13)	0.0222 (12)	−0.0123 (15)
C8	0.0530 (13)	0.0493 (14)	0.0594 (15)	−0.0037 (12)	0.0100 (12)	−0.0038 (12)
N1	0.0448 (10)	0.0454 (11)	0.0690 (13)	0.0079 (9)	0.0072 (9)	−0.0014 (10)
N2	0.0426 (10)	0.0353 (9)	0.0553 (11)	0.0040 (8)	0.0036 (8)	0.0031 (9)
N3	0.0402 (9)	0.0412 (10)	0.0440 (10)	−0.0051 (8)	0.0069 (8)	0.0009 (8)
N4	0.0498 (11)	0.0432 (10)	0.0414 (10)	−0.0084 (9)	0.0017 (8)	−0.0012 (8)
O1	0.0753 (12)	0.0446 (10)	0.0860 (13)	−0.0143 (9)	0.0072 (10)	0.0178 (10)
O2	0.0574 (11)	0.1002 (16)	0.0920 (15)	−0.0163 (11)	0.0359 (10)	−0.0100 (13)
O3	0.0805 (13)	0.0438 (10)	0.1049 (16)	0.0108 (10)	−0.0012 (11)	−0.0007 (11)
O1W	0.0690 (11)	0.0541 (10)	0.0504 (9)	−0.0187 (8)	−0.0056 (8)	0.0104 (8)

Geometric parameters (Å, °)

Cd1—N3	2.2900 (17)	C5—C6	1.367 (4)
Cd1—N3^{i}	2.2900 (17)	C5—H5A	0.93
Cd1—O1W^{i}	2.3133 (18)	C6—C7	1.357 (4)
Cd1—O1W	2.3133 (18)	C6—H6A	0.93
Cd1—N2	2.3539 (18)	C7—C8	1.366 (3)
Cd1—N2^{i}	2.3539 (18)	C7—H7A	0.93
C1—N1	1.336 (3)	C8—N3	1.341 (3)
C1—C2	1.346 (4)	C8—H8A	0.93
C1—H1A	0.93	N1—N2	1.337 (2)
C2—C3	1.420 (3)	N1—H1B	0.86
C2—H2A	0.93	N4—O2	1.226 (2)
C3—N2	1.330 (3)	N4—O3	1.228 (2)
C3—C4	1.456 (3)	N4—O1	1.239 (2)
C4—N3	1.346 (3)	O1W—H1WA	0.85
C4—C5	1.384 (3)	O1W—H1WB	0.85
N3—Cd1—N3^{i}	180	C6—C5—C4	119.3 (3)

N3—Cd1—O1W^{i}	91.87 (6)	C6—C5—H5A	120.4
N3^{i}—Cd1—O1W^{i}	88.13 (6)	C4—C5—H5A	120.4
N3—Cd1—O1W	88.13 (6)	C7—C6—C5	120.4 (2)
N3^{i}—Cd1—O1W	91.87 (6)	C7—C6—H6A	119.8
O1W^{i}—Cd1—O1W	180	C5—C6—H6A	119.8
N3—Cd1—N2	72.87 (6)	C6—C7—C8	118.4 (2)
N3^{i}—Cd1—N2	107.13 (6)	C6—C7—H7A	120.8
O1W^{i}—Cd1—N2	86.43 (7)	C8—C7—H7A	120.8
O1W—Cd1—N2	93.57 (7)	N3—C8—C7	122.4 (2)
N3—Cd1—N2^{i}	107.13 (6)	N3—C8—H8A	118.8
N3^{i}—Cd1—N2^{i}	72.87 (6)	C7—C8—H8A	118.8
O1W^{i}—Cd1—N2^{i}	93.57 (7)	C1—N1—N2	111.8 (2)
O1W—Cd1—N2^{i}	86.43 (7)	C1—N1—H1B	124.1
N2—Cd1—N2^{i}	180	N2—N1—H1B	124.1
N1—C1—C2	108.2 (2)	C3—N2—N1	105.52 (17)
N1—C1—H1A	125.9	C3—N2—Cd1	112.07 (13)
C2—C1—H1A	125.9	N1—N2—Cd1	140.14 (14)
C1—C2—C3	104.6 (2)	C8—N3—C4	119.2 (2)
C1—C2—H2A	127.7	C8—N3—Cd1	124.93 (16)
C3—C2—H2A	127.7	C4—N3—Cd1	115.83 (14)
N2—C3—C2	109.9 (2)	O2—N4—O3	120.3 (2)
N2—C3—C4	120.58 (18)	O2—N4—O1	119.7 (2)
C2—C3—C4	129.5 (2)	O3—N4—O1	120.0 (2)
N3—C4—C5	120.3 (2)	Cd1—O1W—H1WA	126.6
N3—C4—C3	117.32 (18)	Cd1—O1W—H1WB	123.3
C5—C4—C3	122.4 (2)	H1WA—O1W—H1WB	107.7
N1—C1—C2—C3	0.1 (3)	O1W^{i}—Cd1—N2—C3	83.94 (15)
C1—C2—C3—N2	0.3 (3)	O1W—Cd1—N2—C3	−96.06 (15)
C1—C2—C3—C4	179.9 (2)	N3—Cd1—N2—N1	−168.5 (2)
N2—C3—C4—N3	−10.1 (3)	N3^{i}—Cd1—N2—N1	11.5 (2)
C2—C3—C4—N3	170.3 (2)	O1W^{i}—Cd1—N2—N1	−75.4 (2)
N2—C3—C4—C5	169.8 (2)	O1W—Cd1—N2—N1	104.6 (2)
C2—C3—C4—C5	−9.8 (4)	C7—C8—N3—C4	1.5 (4)
N3—C4—C5—C6	0.1 (4)	C7—C8—N3—Cd1	179.34 (19)
C3—C4—C5—C6	−179.9 (2)	C5—C4—N3—C8	−1.1 (3)
C4—C5—C6—C7	0.7 (4)	C3—C4—N3—C8	178.82 (19)
C5—C6—C7—C8	−0.3 (4)	C5—C4—N3—Cd1	−179.15 (17)
C6—C7—C8—N3	−0.8 (4)	C3—C4—N3—Cd1	0.8 (2)
C2—C1—N1—N2	−0.4 (3)	O1W^{i}—Cd1—N3—C8	100.70 (18)
C2—C3—N2—N1	−0.5 (2)	O1W—Cd1—N3—C8	−79.30 (18)
C4—C3—N2—N1	179.83 (19)	N2—Cd1—N3—C8	−173.62 (19)
C2—C3—N2—Cd1	−166.96 (15)	N2^{i}—Cd1—N3—C8	6.38 (19)
C4—C3—N2—Cd1	13.4 (2)	O1W^{i}—Cd1—N3—C4	−81.39 (16)
C1—N1—N2—C3	0.6 (3)	O1W—Cd1—N3—C4	98.61 (16)
C1—N1—N2—Cd1	160.79 (18)	N2—Cd1—N3—C4	4.29 (14)

N3—Cd1—N2—C3	−9.12 (14)	N2^{i}—Cd1—N3—C4	−175.71 (14)
N3^{i}—Cd1—N2—C3	170.88 (14)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WA···O2^{ii}	0.85	2.34	3.096 (3)	148
O1W—H1WA···O3^{ii}	0.85	2.28	3.036 (3)	149
O1W—H1WB···O2^{iii}	0.85	2.12	2.944 (3)	164
N1—H1B···O1^{iv}	0.86	2.10	2.956 (3)	171
N1—H1B···O3^{iv}	0.86	2.60	3.170 (3)	125
O1W—H1WB···O1^{iii}	0.85	2.50	3.138 (2)	133
C1—H1A···O3^{v}	0.93	2.53	3.319 (3)	143
C8—H8A···O1^{vi}	0.93	2.39	3.253 (3)	153

Symmetry codes: (ii) −*x*, −*y*+2, −*z*+1; (iii) *x*+1/2, −*y*+3/2, *z*−1/2; (iv) *x*+3/2, −*y*+3/2, *z*−1/2; (v) −*x*+1/2, *y*−1/2, −*z*+3/2; (vi) −*x*−1/2, *y*+1/2, −*z*+3/2.

Fig. 1

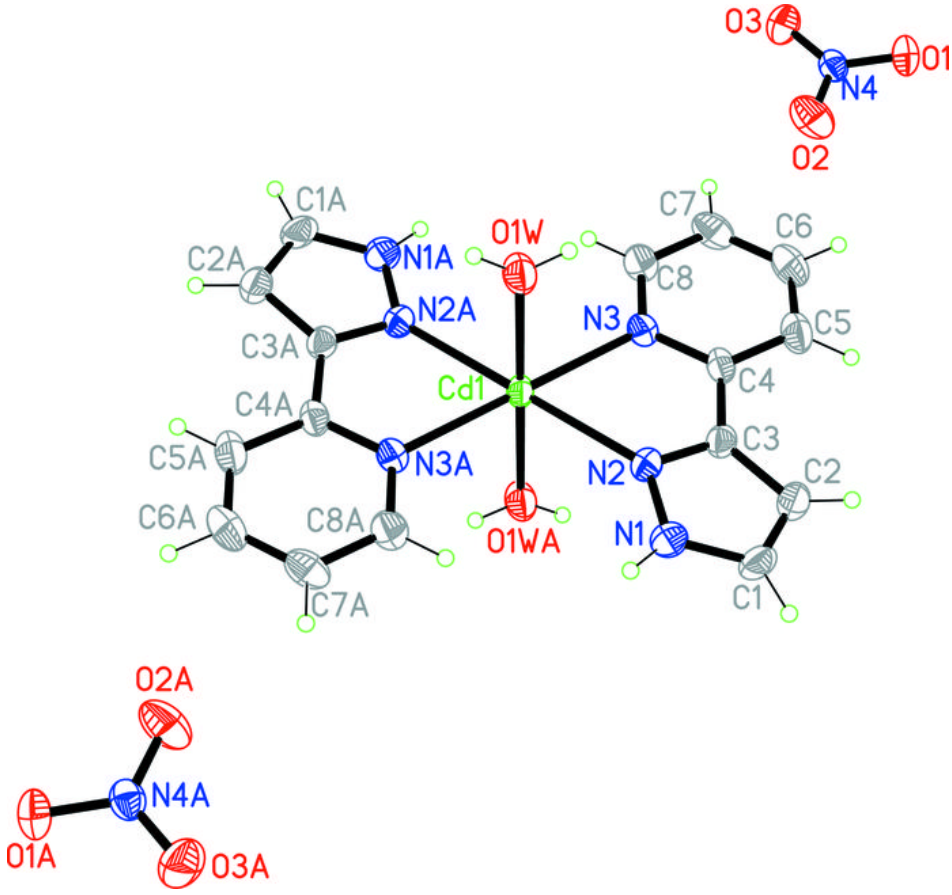
O3
O1
N4
O2
C1A
C2A
N1A
O1W
C7
C6
C8
N2A
N3
C5
C3A
Cd1
C4
C4A
C3
C5A
N3A
N2
C2
C6A
C8A
O1WA
N1
C7A
C1
O2A
N4A
O1A
O3A

Fig. 2