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catena-Poly[[bis(quinolin-8-amine-κ^2N,N')-cadmium(II)]-μ-cyanido-κ^2N:*C*-[dicyanido-nickel(II)]-μ-cyanido-κ^2C:*N*]

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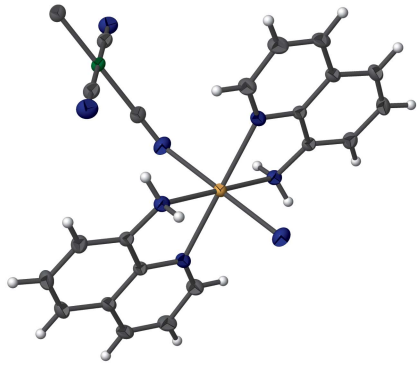
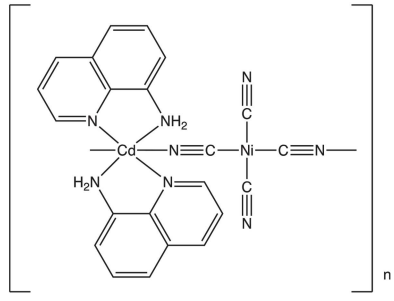
In the title compound, $[CdNi(C_9H_8N_2)_2(CN)_4]_n$, the Cd and Ni atoms both lie on centres of inversion in space group $P2_1/c$. The Cd atom is coordinated by two bidentate quinolin-8-amine ligands and by the N atoms of two cyano ligands, while the square planar Ni atom is coordinated by the C atoms of four cyano ligands. These units form a one-dimensional coordination polymer containing an $(–NC—Ni—CN—Cd–)_n$ backbone, and the coordination polymer chains are linked into a three-dimensional array by a combination of N—H···N and C—H···N hydrogen bonds, augmented by a π–π stacking interaction.

3D view



Chemical scheme



Structure description

Transition-metal coordination compounds in which cyano ligands play the main structure-forming role, so-called cyanocarbanion or cyanometallate complexes, have been the subject of interest for many years, because of their magnetic and luminescent properties (Sieklucka *et al.*, 2011; Benmansour *et al.*, 2007, 2008, 2009, 2012; Setifi *et al.*, 2009; Yuste *et al.*, 2009; Lehchili *et al.*, 2017) including, in particular, their spin-crossover behaviour (Benmansour *et al.*, 2010; Setifi *et al.*, 2013, 2014, Bartual-Murgui *et al.*, 2013). In a continuation of our general study of this area, we now report the crystal and molecular structure of the title compound.

In the structure of the title compound, the Cd and Ni ions both lie on centres of inversion, selected for convenience as those at (0.5, 0.5, 0.5) and (0.5, 0.5, 0), respectively.

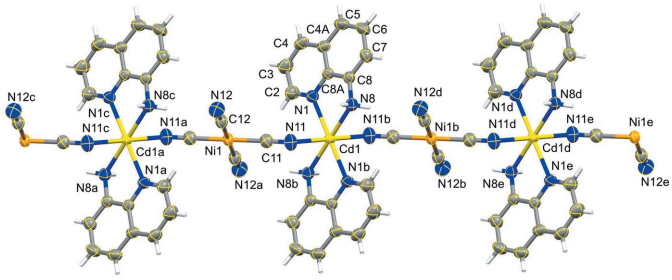


Figure 1
The coordination polymer formed by the title compound. For the sake of clarity many of the C atom labels have been omitted: the atoms marked with a, b, c, d or e are at the symmetry positions $(1-x, 1-y, -z)$, $(1-x, 1-y, 1-z)$, $(x, y, -1+z)$, $(x, y, 1+z)$ and $(1-x, 1-y, 2-z)$, respectively,. Displacement ellipsoids are drawn at the 80% probability level.

The $[Ni(CN)_4]^{2-}$ units adopts the usual square planar configuration, while the Cd centre is coordinated by two bidentate quinolin-8-amine units and by the N atoms of two cyano ligands. The structure thus consists of one-dimensional coordination polymer based on an $(-NC-Ni-CN-Cd-)_n$ backbone and running parallel to [001]. In the reference chain $[Cd\{quinolin\text{-}8\text{-}amine)_2]^{2+}$ units centred at (0.5, 0.5, n + 0.5) alternate with $[Ni(CN)_4]^{2-}$ units centred at (0.5, 0.5, n), where n represents an integer in each case (Fig. 1). There are two types of N—H···N hydrogen bond in the structure (Table 1). Those involving atom H8*A* lie within the coordination polymer chain, but those involving atom H8*B* link the chain along (0.5, 0.5, z) to those along (0.5, 0, z) and (0.5, 1, z), so forming a sheet of hydrogen-bonded chains lying parallel to (100) (Fig. 2). Sheets of this type are linked into a three-dimensional array by two types of direction-specific interactions, a C—H···N hydrogen bond (Table 1) and a π–π stacking interaction. The C—H···N hydrogen bond combines with the inversion symmetry at both metal centres to generate a chain running parallel to the [20$\bar{1}$] direction (Fig. 3), which links the (100) sheets into a three-dimensional structure. In addition, the carbocyclic rings in the quinolin-8-amine ligands at (x, y, z) and ($2-x$, $1-y$, $1-z$), which lie in adjacent (100) sheets, are strictly parallel with an interplanar spacing of 3.4070 (6) Å; the ring-centroid separation is 3.5856 (8) Å, with a ring-centroid offset of *ca* 1.117 (2) Å: the interactions between the two types of ring in these two ligands are similar (Fig. 4).

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

*Cg*1 is the centroid of the C4*A*/C5–C8/C8*A* ring.

D—H···A	D—H	H···A	D···A	D—H···A
N8—H8*A*···N12^{i}	0.880 (18)	2.416 (18)	3.2815 (18)	167.8 (15)
N8—H8*B*···N12^{ii}	0.867 (19)	2.286 (19)	3.1275 (17)	163.9 (17)
C3—H3···*Cg*1^{iii}	0.95	2.78	3.6266 (17)	149
C4—H4···N12^{iv}	0.95	2.58	3.443 (2)	151

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

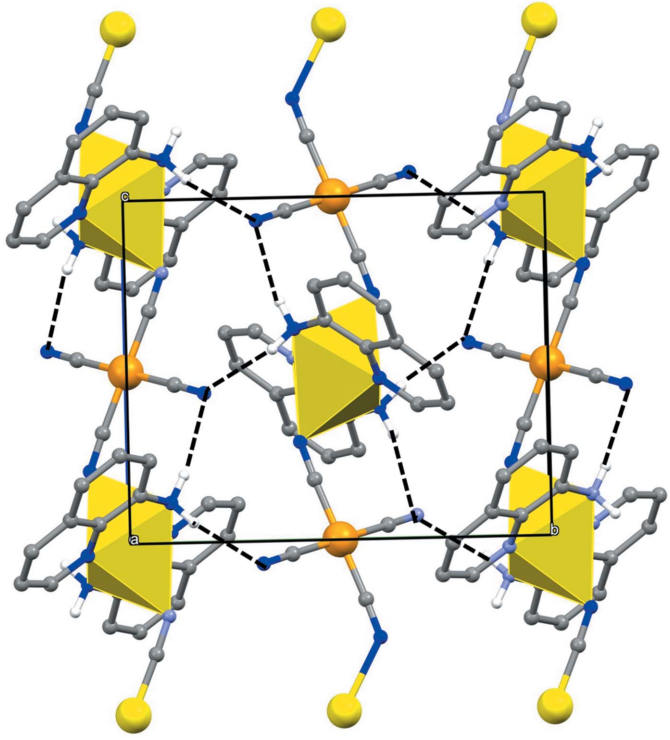


Figure 2
A projection along [100] of part of the crystal structure showing the formation of a hydrogen-bonded sheet of polymer chains, lying parallel to (100). For the sake of clarity, the H atoms bonded to C atoms have been omitted.

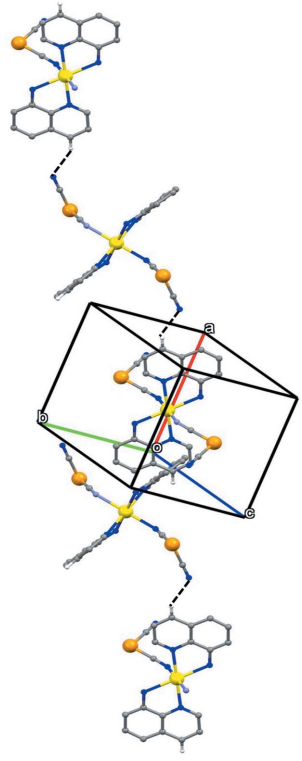


Figure 3
Part of the crystal structure showing the formation of a hydrogen-bonded chain running parallel to the [20$\bar{1}$] direction. For the sake of clarity, the H atoms not involved in the motif shown have been omitted.

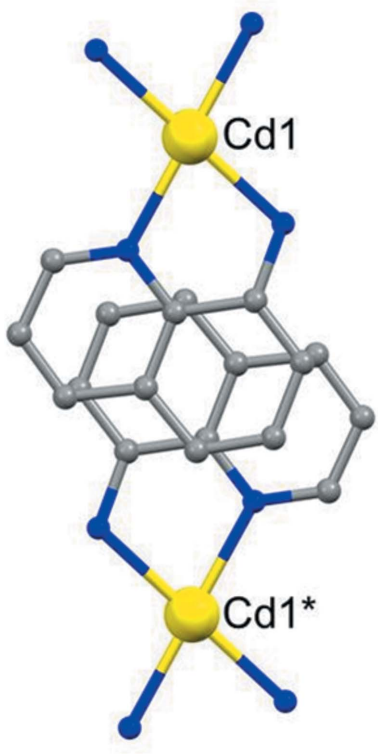


Figure 4
Part of the crystal structure showing the π-stacking of quinolin-8-amine ligands. For the sake of clarity, the unit-cell outline and the H atoms have been omitted: the Cd atom marked with an asterisk (*) is at (1.5, 1/2, 1/2).

The structure of the title compound is very similar to that of the iron(II)–nickel analogue, whose structure has been studied at both 293 K and 120 K, where the iron adopts high-spin and low-spin configurations, respectively (Setifi *et al.*, 2014). This structural similarity of the Cd^{II} and Fe^{II} compounds is somewhat unexpected in view of the different effective radii of these ions (Shannon & Prewitt, 1969, 1970), reflected in the differences between the M—N (M = Cd or Fe) distances in the two compounds, typically around 0.30 Å for each type of bond, itself reflected in the difference between the a repeat vectors, 9.4264 (3) Å for M = Cd but only 9.0035 (5) Å for M = Fe at 120 K.

Synthesis and crystallization

A solution of quinolin-8-amine (0.288 g, 2 mmol) in ethanol (10 ml) was added dropwise with stirring at 323 K to a solution of $Cd[Ni(CN)_4]\cdot H_2O$ (0.293 g, 1 mmol) in water (10 ml). This mixture was stirred for 4 h at 323 K and then filtered. Slow evaporation of the filtrate over a period of one week, at ambient temperature and in the presence of air, gave crystals suitable for single-crystal X-ray diffraction.

Refinement

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$[CdNi(C_9H_8N_2)_2(CN)_4]$
M_r	563.53
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	170
a, b, c (Å)	9.4264 (3), 11.8622 (3), 9.8257 (3)
β (°)	101.088 (2)
V (Å^3)	1078.18 (6)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.89
Crystal size (mm)	0.15 × 0.11 × 0.07
Data collection	
Diffractometer	Rigaku Oxford Diffraction Xcalibur, Eos, Gemini
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.668, 0.885
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22794, 4057, 3319
R_{int}	0.024
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.770
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.022, 0.063, 1.07
No. of reflections	4057
No. of parameters	154
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.55, −0.51

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXS86* (Sheldrick, 2015), *SHELXL2014* (Sheldrick, 2015) and *PLATON* (Spek, 2020).

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Author contributions are as follows. Conceptualization, ZS and MHAD; methodology, ZS and MHAD; investigation, SK and MT; writing (original draft), CG and ZS; writing (review and editing of the manuscript), CG, FS and ZS; visualization, ZS and FS; funding acquisition, ZS and MHAD; resources, FS; supervision, FS.

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References

Bartual-Murgui, C., Akou, A., Shepherd, H. J., Molnár, G., Real, J. A., Salmon, L. & Bousseksou, A. (2013). *Chem. Eur. J.* **19**, 15036–15043.
Benmansour, S., Atmani, C., Setifi, F., Triki, S., Marchivie, M. & Gómez-García, C. J. (2010). *Coord. Chem. Rev.* **254**, 1468–1478.
Benmansour, S., Setifi, F., Gómez-García, C. J., Triki, S., Coronado, E. & Salaün, J. (2008). *J. Mol. Struct.* **890**, 255–262.
Benmansour, S., Setifi, F., Triki, S. & Gómez-García, C. J. (2012). *Inorg. Chem.* **51**, 2359–2365.
Benmansour, S., Setifi, F., Triki, S., Salaün, J.-Y., Vandevelde, F., Sala-Pala, J., Gómez-García, C. J. & Roisnel, T. (2007). *Eur. J. Inorg. Chem.* pp. 186–194.

Benmansour, S., Setifi, F., Triki, S., Thétiot, F., Sala-Pala, J., Gómez-García, C. J. & Colacio, E. (2009). *Polyhedron*, **28**, 1308–1314.
Lehchili, F., Setifi, F., Liu, X., Saneei, A., Kučeráková, M., Setifi, Z., Dušek, M., Poupon, M., Pourayoubi, M. & Reedijk, J. (2017). *Polyhedron*, **131**, 27–33.
Rigaku OD (2015). *CrysAlis PRO*. Agilent Technologies Inc., Santa Clara, CA, USA.
Setifi, F., Benmansour, S., Marchivie, M., Dupouy, G., Triki, S., Sala-Pala, J., Salaün, J.-Y., Gómez-García, C. J., Pillet, S., Lecomte, C. & Ruiz, E. (2009). *Inorg. Chem.* **48**, 1269–1271.
Setifi, F., Charles, C., Houille, S., Thétiot, F., Triki, S., Gómez-García, C. J. & Pillet, S. (2013). *Polyhedron*, **61**, 242–247.
Setifi, F., Milin, E., Charles, C., Thétiot, F., Triki, S. & Gómez-García, C. J. (2014). *Inorg. Chem.* **53**, 97–104.
Shannon, R. D. & Prewitt, C. T. (1969). *Acta Cryst.* B**25**, 925–946.
Shannon, R. D. & Prewitt, C. T. (1970). *Acta Cryst.* B**26**, 1046–1048.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Sieklucka, B., Podgajny, R., Korzeniak, T., Nowicka, B., Pinkowicz, D. & Kozieł, M. (2011). *Eur. J. Inorg. Chem.* pp. 305–326.
Spek, A. L. (2020). *Acta Cryst.* E**76**, 1–11.
Yuste, C., Bentama, A., Marino, N., Armentano, D., Setifi, F., Triki, S., Lloret, F. & Julve, M. (2009). *Polyhedron*, **28**, 1287–1294.

full crystallographic data

IUCrData (2021). **6**, x210568 [https://doi.org/10.1107/S2414314621005680X]

catena-Poly[[bis(quinolin-8-amine-κ^2N,N')cadmium(II)]-μ-cyanido-κ^2N:*C*-[dicyanidonickel(II)]-μ-cyanido-κ^2C:*N*]

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***catena*-Poly[[bis(quinolin-8-amine-κ^2N,N')cadmium(II)]-μ-cyanido-κ^2N:*C*-[dicyanidonickel(II)]-μ-cyanido-κ^2C:*N*]**

Crystal data

$[CdNi(C_9H_8N_2)_2(CN)_4]$
M_r = 563.53
Monoclinic, $P2_1/c$
a = 9.4264 (3) Å
b = 11.8622 (3) Å
c = 9.8257 (3) Å
β = 101.088 (2)°
V = 1078.18 (6) Å^3
Z = 2
$F(000)$ = 560
D_x = 1.736 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4057 reflections
θ = 2.8–33.2°
μ = 1.89 mm^{-1}
T = 170 K
Block, pale yellow
0.15 × 0.11 × 0.07 mm

Data collection

Rigaku Oxford Diffraction Xcalibur, Eos, Gemini diffractometer
Radiation source: fine-focus sealed X-raytube
Graphite monochromator
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.668, T_{max} = 0.885
22794 measured reflections
4057 independent reflections
3319 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 33.2°, θ_{min} = 2.8°
h = −14→12
k = −18→18
l = −12→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.063
S = 1.07
4057 reflections
154 parameters
0 restraints
Primary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0239P)^2 + 0.6589P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.5000	0.5000	0.5000	0.01846 (4)
N1	0.69972 (12)	0.60058 (9)	0.46816 (12)	0.0200 (2)
C2	0.69877 (16)	0.69047 (12)	0.38871 (16)	0.0259 (3)
H2	0.6118	0.7094	0.3266	0.031*
C3	0.82124 (18)	0.75965 (12)	0.39193 (18)	0.0286 (3)
H3	0.8173	0.8224	0.3312	0.034*
C4	0.94535 (17)	0.73487 (12)	0.48371 (16)	0.0246 (3)
H4	1.0286	0.7809	0.4878	0.029*
C4A	0.94994 (14)	0.64063 (11)	0.57272 (13)	0.0200 (2)
C5	1.07330 (15)	0.61251 (13)	0.67437 (15)	0.0252 (3)
H5	1.1583	0.6572	0.6842	0.030*
C6	1.06942 (16)	0.52108 (14)	0.75798 (16)	0.0275 (3)
H6	1.1505	0.5045	0.8288	0.033*
C7	0.94610 (15)	0.45098 (13)	0.74017 (14)	0.0239 (3)
H7	0.9465	0.3868	0.7981	0.029*
C8	0.82593 (14)	0.47349 (11)	0.64121 (13)	0.0181 (2)
C8A	0.82395 (13)	0.57249 (10)	0.55881 (12)	0.0172 (2)
N8	0.70170 (12)	0.40018 (9)	0.61705 (12)	0.0198 (2)
H8A	0.694 (2)	0.3681 (15)	0.6961 (19)	0.024*
H8B	0.713 (2)	0.3478 (16)	0.5586 (19)	0.024*
Ni1	0.5000	0.5000	0.0000	0.01665 (5)
C11	0.50450 (15)	0.44216 (11)	0.17628 (14)	0.0217 (2)
N11	0.50472 (15)	0.41011 (11)	0.28716 (13)	0.0272 (2)
C12	0.62164 (15)	0.38568 (12)	−0.03912 (14)	0.0219 (2)
N12	0.69773 (15)	0.31621 (11)	−0.06549 (14)	0.0292 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.01554 (6)	0.02316 (7)	0.01642 (7)	−0.00368 (4)	0.00242 (4)	0.00056 (4)
N1	0.0186 (5)	0.0198 (5)	0.0214 (5)	−0.0013 (4)	0.0032 (4)	0.0026 (4)
C2	0.0242 (6)	0.0248 (6)	0.0282 (7)	−0.0007 (5)	0.0040 (5)	0.0077 (5)
C3	0.0302 (7)	0.0236 (6)	0.0329 (8)	−0.0038 (5)	0.0088 (6)	0.0078 (5)
C4	0.0241 (7)	0.0227 (6)	0.0287 (7)	−0.0071 (5)	0.0098 (5)	−0.0012 (5)
C4A	0.0184 (5)	0.0209 (5)	0.0214 (5)	−0.0029 (4)	0.0059 (4)	−0.0036 (5)
C5	0.0182 (6)	0.0307 (7)	0.0264 (6)	−0.0041 (5)	0.0032 (5)	−0.0058 (5)
C6	0.0196 (6)	0.0353 (7)	0.0250 (7)	−0.0001 (5)	−0.0023 (5)	−0.0013 (6)
C7	0.0240 (6)	0.0249 (6)	0.0217 (6)	0.0015 (5)	0.0015 (5)	0.0025 (5)
C8	0.0186 (5)	0.0188 (5)	0.0172 (5)	−0.0005 (4)	0.0044 (4)	−0.0011 (4)

C8A	0.0175 (5)	0.0175 (5)	0.0172 (5)	−0.0010 (4)	0.0045 (4)	−0.0012 (4)
N8	0.0223 (5)	0.0171 (5)	0.0202 (5)	−0.0020 (4)	0.0045 (4)	0.0005 (4)
Ni1	0.01888 (11)	0.01653 (10)	0.01467 (10)	0.00374 (8)	0.00356 (8)	−0.00017 (7)
C11	0.0235 (6)	0.0203 (5)	0.0213 (6)	0.0032 (5)	0.0041 (5)	−0.0022 (5)
N11	0.0343 (7)	0.0269 (6)	0.0205 (5)	0.0014 (5)	0.0056 (4)	−0.0007 (5)
C12	0.0244 (6)	0.0217 (6)	0.0196 (5)	0.0029 (5)	0.0040 (4)	0.0016 (5)
N12	0.0300 (6)	0.0264 (6)	0.0326 (6)	0.0073 (5)	0.0094 (5)	0.0018 (5)

Geometric parameters (Å, º)

Cd1—N1	2.3005 (11)	C5—C6	1.365 (2)
Cd1—N1^{i}	2.3005 (11)	C5—H5	0.9500
Cd1—N8	2.3449 (12)	C6—C7	1.412 (2)
Cd1—N8^{i}	2.3449 (12)	C6—H6	0.9500
Cd1—N11^{i}	2.3554 (13)	C7—C8	1.3698 (19)
Cd1—N11	2.3555 (13)	C7—H7	0.9500
N1—C2	1.3205 (17)	C8—C8A	1.4245 (18)
N1—C8A	1.3691 (17)	C8—N8	1.4412 (17)
C2—C3	1.412 (2)	N8—H8A	0.880 (19)
C2—H2	0.9500	N8—H8B	0.868 (19)
C3—C4	1.365 (2)	Ni1—C11	1.8559 (14)
C3—H3	0.9500	Ni1—C11^{ii}	1.8560 (14)
C4—C4A	1.4149 (19)	Ni1—C12	1.8631 (13)
C4—H4	0.9500	Ni1—C12^{ii}	1.8631 (13)
C4A—C5	1.4192 (19)	C11—N11	1.1536 (18)
C4A—C8A	1.4212 (17)	C12—N12	1.1542 (18)
N1—Cd1—N1^{i}	180.0	C6—C5—C4A	119.80 (13)
N1—Cd1—N8	73.80 (4)	C6—C5—H5	120.1
N1^{i}—Cd1—N8	106.20 (4)	C4A—C5—H5	120.1
N1—Cd1—N8^{i}	106.20 (4)	C5—C6—C7	120.64 (14)
N1^{i}—Cd1—N8^{i}	73.80 (4)	C5—C6—H6	119.7
N8—Cd1—N8^{i}	180.0	C7—C6—H6	119.7
N1—Cd1—N11^{i}	92.38 (4)	C8—C7—C6	121.45 (14)
N1^{i}—Cd1—N11^{i}	87.62 (4)	C8—C7—H7	119.3
N8—Cd1—N11^{i}	86.85 (4)	C6—C7—H7	119.3
N8^{i}—Cd1—N11^{i}	93.15 (4)	C7—C8—C8A	118.87 (12)
N1—Cd1—N11	87.62 (4)	C7—C8—N8	122.28 (12)
N1^{i}—Cd1—N11	92.38 (4)	C8A—C8—N8	118.85 (11)
N8—Cd1—N11	93.15 (4)	N1—C8A—C4A	121.24 (11)
N8^{i}—Cd1—N11	86.85 (4)	N1—C8A—C8	119.10 (11)
N11^{i}—Cd1—N11	180.0	C4A—C8A—C8	119.66 (12)
C2—N1—C8A	119.26 (12)	C8—N8—Cd1	109.42 (8)
C2—N1—Cd1	125.91 (9)	C8—N8—H8A	108.3 (12)
C8A—N1—Cd1	113.91 (8)	Cd1—N8—H8A	117.2 (12)
N1—C2—C3	122.93 (14)	C8—N8—H8B	109.8 (12)
N1—C2—H2	118.5	Cd1—N8—H8B	103.4 (12)
C3—C2—H2	118.5	H8A—N8—H8B	108.4 (17)

C4—C3—C2	118.87 (13)	C11—Ni1—C11^{ii}	180.0
C4—C3—H3	120.6	C11—Ni1—C12	91.08 (6)
C2—C3—H3	120.6	C11^{ii}—Ni1—C12	88.92 (6)
C3—C4—C4A	119.94 (13)	C11—Ni1—C12^{ii}	88.92 (6)
C3—C4—H4	120.0	C11^{ii}—Ni1—C12^{ii}	91.08 (6)
C4A—C4—H4	120.0	C12—Ni1—C12^{ii}	180.0
C4—C4A—C5	122.97 (13)	N11—C11—Ni1	177.27 (13)
C4—C4A—C8A	117.66 (12)	C11—N11—Cd1	133.82 (11)
C5—C4A—C8A	119.37 (12)	N12—C12—Ni1	178.59 (13)
C8A—N1—C2—C3	0.4 (2)	Cd1—N1—C8A—C4A	−167.20 (9)
Cd1—N1—C2—C3	168.70 (12)	C2—N1—C8A—C8	−178.04 (12)
N1—C2—C3—C4	−1.9 (2)	Cd1—N1—C8A—C8	12.30 (14)
C2—C3—C4—C4A	0.5 (2)	C4—C4A—C8A—N1	−3.70 (18)
C3—C4—C4A—C5	−177.41 (14)	C5—C4A—C8A—N1	175.86 (12)
C3—C4—C4A—C8A	2.1 (2)	C4—C4A—C8A—C8	176.80 (12)
C4—C4A—C5—C6	179.15 (14)	C5—C4A—C8A—C8	−3.63 (18)
C8A—C4A—C5—C6	−0.4 (2)	C7—C8—C8A—N1	−174.40 (12)
C4A—C5—C6—C7	2.9 (2)	N8—C8—C8A—N1	5.93 (17)
C5—C6—C7—C8	−1.4 (2)	C7—C8—C8A—C4A	5.11 (18)
C6—C7—C8—C8A	−2.6 (2)	N8—C8—C8A—C4A	−174.57 (11)
C6—C7—C8—N8	177.03 (13)	C7—C8—N8—Cd1	160.34 (11)
C2—N1—C8A—C4A	2.46 (19)	C8A—C8—N8—Cd1	−20.00 (13)

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

Hydrogen-bond geometry (Å, º)

*Cg*1 is the centroid of the C4*A*/C5–C8/C8*A* ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N8—H8*A*···N12^{iii}	0.880 (18)	2.416 (18)	3.2815 (18)	167.8 (15)
N8—H8*B*···N12^{iv}	0.867 (19)	2.286 (19)	3.1275 (17)	163.9 (17)
C3—H3···*Cg*1^{v}	0.95	2.78	3.6266 (17)	149
C4—H4···N12^{vi}	0.95	2.58	3.443 (2)	151

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