

Bis(tri-2-pyridylamine)nickel(II) bis(perchlorate)

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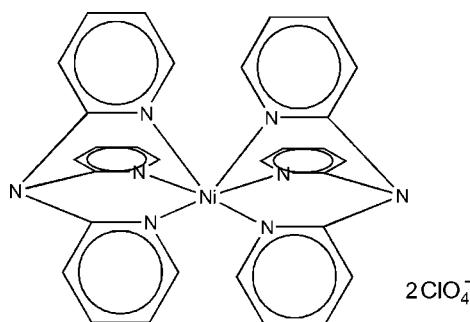
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Key indicators: single-crystal X-ray study; $T = 296\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$; disorder in solvent or counterion; R factor = 0.039; wR factor = 0.096; data-to-parameter ratio = 14.5.

In the title compound, $[\text{Ni}(\text{C}_{15}\text{H}_{12}\text{N}_4)_2](\text{ClO}_4)_2$, the Ni^{II} atom lies on an inversion center and is octahedrally coordinated by the N atoms of two tridentate tri-2-pyridylamine ligands. The two perchlorate anions are disordered over two sites with a refined occupancy ratio of 0.528 (19):0.472 (19).

Related literature

For background to luminescent coordination compounds, see: Liu *et al.* (1997). For related complexes, including the synthesis of 2,2',2''-tpa (tpa is tri-2-pyridylamine), see: Yang *et al.* (1999). For information on the use of 2,2',2''-tpa as a bidentate ligand, see: Wang *et al.* (2009).



Experimental

Crystal data

$[\text{Ni}(\text{C}_{15}\text{H}_{12}\text{N}_4)_2](\text{ClO}_4)_2$	$V = 1617.3 (13)\text{ \AA}^3$
$M_r = 754.18$	$Z = 2$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 8.360 (4)\text{ \AA}$	$\mu = 0.83\text{ mm}^{-1}$
$b = 17.570 (8)\text{ \AA}$	$T = 296\text{ K}$
$c = 11.165 (5)\text{ \AA}$	$0.22 \times 0.15 \times 0.10\text{ mm}$
$\beta = 99.542 (5)^{\circ}$	

Data collection

Bruker SMART CCD area-detector diffractometer	14055 measured reflections
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 1996)	3895 independent reflections
	2611 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.040$
	$T_{\min} = 0.861$, $T_{\max} = 0.920$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$	269 parameters
$wR(F^2) = 0.096$	H-atom parameters constrained
$S = 1.03$	$\Delta\rho_{\max} = 0.25\text{ e \AA}^{-3}$
3895 reflections	$\Delta\rho_{\min} = -0.26\text{ e \AA}^{-3}$

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NK2079).

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Bis(tri-2-pyridylamine)nickel(II) bis(perchlorate)

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Comment

Luminescent organic and coordination compounds have been an active research area for decades because of their various potential applications in materials sciences. It has been demonstrated that 2,2'-dipyridylamine can produce a bright blue luminescence when deprotonated and bound to either an aluminium ion or a boron center (Liu *et al.*, 1997). However, many of the previously reported aluminium or boron compounds based on 2,2'-dipyridylamine are not stable enough for electroluminescent devices. The neutral tripodal ligand 2,2',2"-tripyridylamine and its derivatives with Zn(II), Cd(II) and Hg(II) have been investigated for their optical properties (Yang *et al.*, 1999). However, its complexes with d⁸ metal(II) remain unknown. By using the 2,2',2"-tripyridylamine ligand, we report here the synthesis and crystal structure of the title compound, bis(2,2',2"-tripyridylamine)nickel(II) bis(perchlorate), (I).

The structure of (I) consists of monomeric $[\text{Ni}(2,2',2''\text{-tpa})_2]^{2+}$ cations and associated ClO_4^- anions. The Ni atom lies on an inversion center. As shown in Fig. 1, the Ni center is six-coordinate with an octahedral geometry. In principle, 2,2',2"-tpa can function not only as a tridentate chelating ligand but also as a bidentate chelating ligand where only two pyridyl groups bind to the same central atom (Wang *et al.*, 2009). In the title compound, each 2,2',2"-tpa ligand functions as a tridentate ligand, chelating to the nickel center. The two perchlorate anions are disordered over two sites with a refined occupancy ratio of 0.528 (19) : 0.472 (19).

Experimental

The ligand, 2,2',2"-tpa was synthesized according to the procedure described in the literature (Yang *et al.* (1999)).

A solution of 2,2',2"-tpa (62.11 mg, 0.2 mmol) in acetonitrile (5 ml) was added dropwise to a solution of $\text{Ni}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ (36.58 mg, 0.1 mmol) in acetonitrile (2 ml). The mixture was stirred at room temperature for 5 min and then filtered. Light purple crystals of (I) suitable for X-ray analysis were obtained by slow diffusion of filtrate.

Refinement

The two perchlorate anions are disordered over two sites with a refined occupancy ratio of 0.528 (19) : 0.472 (19). Aromatic H atoms were placed in calculated positions with C—H = 0.93 Å, and refined in riding mode with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

supplementary materials

Figures

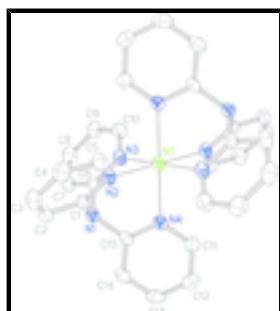


Fig. 1. The structure of (I), shown with 30% probability displacement ellipsoids. The disordered perchlorate anions and H atoms have been omitted for clarity. Unlabeled atoms are related to labeled atoms by inversion symmetry.

Bis(tri-2-pyridylamine)nickel(II) bis(perchlorate)

Crystal data

$[\text{Ni}(\text{C}_{15}\text{H}_{12}\text{N}_4)_2](\text{ClO}_4)_2$

$M_r = 754.18$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 8.360$ (4) Å

$b = 17.570$ (8) Å

$c = 11.165$ (5) Å

$\beta = 99.542$ (5)°

$V = 1617.3$ (13) Å³

$Z = 2$

$F(000) = 772$

$D_x = 1.549$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 7662 reflections

$\theta = 2.2\text{--}27.9$ °

$\mu = 0.83$ mm⁻¹

$T = 296$ K

Block, purple

$0.22 \times 0.15 \times 0.10$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

3895 independent reflections

Radiation source: fine-focus sealed tube graphite

2611 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.040$

Detector resolution: 8.366 pixels mm⁻¹

$\theta_{\text{max}} = 28.4$ °, $\theta_{\text{min}} = 2.3$ °

phi and ω scans

$h = -11 \rightarrow 11$

Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)

$k = -23 \rightarrow 23$

$T_{\text{min}} = 0.861$, $T_{\text{max}} = 0.920$

$l = -14 \rightarrow 14$

14055 measured reflections

Refinement

Refinement on F^2

Primary atom site location: structure-invariant direct methods

Least-squares matrix: full

Secondary atom site location: difference Fourier map

$R[F^2 > 2\sigma(F^2)] = 0.039$

Hydrogen site location: inferred from neighbouring sites

$wR(F^2) = 0.096$

H-atom parameters constrained

$S = 1.03$	$w = 1/[\sigma^2(F_o^2) + (0.0415P)^2 + 0.1545P]$
	where $P = (F_o^2 + 2F_c^2)/3$
3895 reflections	$(\Delta/\sigma)_{\max} = 0.001$
269 parameters	$\Delta\rho_{\max} = 0.25 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\min} = -0.26 \text{ e } \text{\AA}^{-3}$

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.

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 $F^2 > 2\text{sigma}(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Ni1	0.0000	0.0000	0.0000	0.03843 (14)	
N1	0.1260 (2)	-0.05805 (10)	-0.21770 (15)	0.0415 (4)	
N2	0.1529 (2)	-0.09211 (10)	-0.00942 (15)	0.0425 (4)	
N3	-0.1341 (2)	-0.04164 (10)	-0.16286 (16)	0.0425 (5)	
N4	0.1399 (2)	0.05822 (10)	-0.10841 (16)	0.0428 (4)	
C1	0.1923 (3)	-0.10685 (12)	-0.11845 (19)	0.0398 (5)	
C2	0.2910 (3)	-0.16666 (13)	-0.1379 (2)	0.0491 (6)	
H2	0.3180	-0.1751	-0.2143	0.059*	
C3	0.3487 (3)	-0.21360 (14)	-0.0420 (2)	0.0588 (7)	
H3	0.4148	-0.2548	-0.0528	0.071*	
C4	0.3080 (3)	-0.19915 (13)	0.0696 (2)	0.0546 (6)	
H4	0.3456	-0.2305	0.1354	0.066*	
C5	0.2114 (3)	-0.13810 (13)	0.0829 (2)	0.0496 (6)	
H5	0.1852	-0.1281	0.1591	0.060*	
C6	-0.0476 (3)	-0.06409 (12)	-0.24704 (19)	0.0414 (5)	
C7	-0.1176 (3)	-0.09311 (14)	-0.3578 (2)	0.0547 (6)	
H7	-0.0542	-0.1076	-0.4150	0.066*	
C8	-0.2834 (4)	-0.10013 (15)	-0.3818 (2)	0.0647 (7)	
H8	-0.3339	-0.1197	-0.4559	0.078*	
C9	-0.3738 (3)	-0.07818 (14)	-0.2965 (2)	0.0577 (7)	
H9	-0.4861	-0.0832	-0.3110	0.069*	
C10	-0.2954 (3)	-0.04864 (14)	-0.1890 (2)	0.0533 (6)	
H10	-0.3572	-0.0327	-0.1317	0.064*	
C11	0.1900 (3)	0.13045 (13)	-0.0929 (2)	0.0492 (6)	
H11	0.1612	0.1583	-0.0290	0.059*	
C12	0.2822 (3)	0.16462 (14)	-0.1682 (2)	0.0575 (7)	
H12	0.3156	0.2149	-0.1552	0.069*	

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C13	0.3246 (3)	0.12403 (16)	-0.2624 (2)	0.0627 (7)	
H13	0.3886	0.1461	-0.3136	0.075*	
C14	0.2716 (3)	0.05020 (14)	-0.2809 (2)	0.0527 (6)	
H14	0.2970	0.0219	-0.3456	0.063*	
C15	0.1808 (3)	0.01931 (12)	-0.20188 (19)	0.0402 (5)	
Cl1	0.2377 (6)	0.3455 (4)	0.0694 (3)	0.0463 (11)	0.472 (19)
O1	0.1538 (19)	0.3916 (9)	0.1111 (12)	0.128 (5)	0.472 (19)
O2	0.224 (3)	0.2727 (6)	0.1240 (8)	0.153 (7)	0.472 (19)
O3	0.3932 (15)	0.3751 (8)	0.1296 (13)	0.129 (4)	0.472 (19)
O4	0.214 (2)	0.3370 (9)	-0.0534 (9)	0.140 (6)	0.472 (19)
Cl1'	0.2323 (10)	0.3362 (6)	0.0668 (6)	0.095 (2)	0.528 (19)
O1'	0.1418 (16)	0.4114 (7)	0.0767 (15)	0.133 (5)	0.528 (19)
O2'	0.1138 (18)	0.2869 (8)	0.0907 (17)	0.169 (5)	0.528 (19)
O3'	0.3760 (15)	0.3273 (15)	0.1348 (13)	0.205 (9)	0.528 (19)
O4'	0.2693 (18)	0.3279 (7)	-0.0504 (11)	0.109 (4)	0.528 (19)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0488 (3)	0.0391 (2)	0.0291 (2)	0.00336 (19)	0.01177 (17)	-0.00443 (17)
N1	0.0529 (12)	0.0401 (10)	0.0331 (10)	0.0029 (9)	0.0114 (9)	-0.0027 (8)
N2	0.0543 (12)	0.0416 (10)	0.0319 (10)	0.0059 (9)	0.0082 (8)	-0.0038 (8)
N3	0.0476 (12)	0.0456 (11)	0.0343 (10)	0.0033 (9)	0.0069 (9)	-0.0043 (8)
N4	0.0525 (12)	0.0421 (10)	0.0355 (10)	-0.0008 (9)	0.0125 (9)	-0.0026 (8)
C1	0.0457 (13)	0.0387 (12)	0.0355 (11)	0.0002 (10)	0.0079 (10)	-0.0066 (9)
C2	0.0524 (15)	0.0475 (13)	0.0496 (14)	0.0036 (11)	0.0149 (12)	-0.0110 (11)
C3	0.0608 (17)	0.0466 (14)	0.0683 (17)	0.0154 (12)	0.0091 (14)	-0.0037 (13)
C4	0.0587 (16)	0.0474 (14)	0.0553 (15)	0.0077 (12)	0.0022 (13)	0.0065 (12)
C5	0.0603 (16)	0.0517 (14)	0.0369 (13)	0.0048 (12)	0.0080 (11)	0.0005 (11)
C6	0.0542 (15)	0.0386 (12)	0.0321 (11)	0.0019 (10)	0.0092 (10)	-0.0034 (9)
C7	0.0695 (18)	0.0591 (15)	0.0352 (13)	0.0035 (13)	0.0073 (12)	-0.0110 (11)
C8	0.075 (2)	0.0696 (18)	0.0440 (15)	-0.0041 (15)	-0.0063 (14)	-0.0125 (13)
C9	0.0534 (16)	0.0610 (16)	0.0549 (16)	-0.0016 (13)	-0.0021 (13)	-0.0030 (13)
C10	0.0530 (16)	0.0580 (15)	0.0489 (14)	0.0027 (12)	0.0082 (12)	-0.0058 (12)
C11	0.0578 (16)	0.0439 (13)	0.0462 (14)	-0.0016 (11)	0.0095 (12)	-0.0046 (11)
C12	0.0610 (17)	0.0502 (14)	0.0608 (17)	-0.0084 (13)	0.0091 (13)	0.0075 (13)
C13	0.0621 (17)	0.0682 (18)	0.0627 (17)	-0.0046 (14)	0.0242 (14)	0.0156 (14)
C14	0.0595 (16)	0.0600 (16)	0.0426 (14)	0.0065 (13)	0.0199 (12)	0.0062 (11)
C15	0.0434 (13)	0.0465 (13)	0.0317 (11)	0.0049 (10)	0.0095 (10)	0.0010 (9)
Cl1	0.046 (2)	0.072 (2)	0.0231 (16)	0.0105 (14)	0.0106 (12)	-0.0077 (12)
O1	0.158 (8)	0.140 (10)	0.099 (5)	0.080 (7)	0.058 (6)	0.001 (6)
O2	0.31 (2)	0.084 (6)	0.070 (5)	-0.006 (9)	0.037 (8)	0.018 (4)
O3	0.095 (6)	0.186 (10)	0.100 (6)	-0.052 (7)	0.000 (4)	-0.031 (6)
O4	0.195 (12)	0.199 (9)	0.023 (4)	0.091 (8)	0.013 (5)	-0.005 (4)
Cl1'	0.109 (4)	0.101 (3)	0.075 (3)	0.037 (3)	0.014 (3)	-0.020 (2)
O1'	0.107 (5)	0.070 (5)	0.211 (13)	0.027 (4)	-0.004 (6)	-0.036 (6)
O2'	0.169 (9)	0.122 (7)	0.251 (13)	0.007 (7)	0.139 (9)	0.013 (7)
O3'	0.086 (8)	0.36 (3)	0.148 (8)	0.120 (11)	-0.033 (7)	-0.089 (13)

O4'	0.144 (8)	0.120 (6)	0.080 (6)	-0.018 (6)	0.068 (6)	-0.032 (4)
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Geometric parameters (\AA , $^\circ$)

Ni1—N2	2.0755 (19)	C7—C8	1.373 (4)
Ni1—N2 ⁱ	2.0755 (19)	C7—H7	0.9300
Ni1—N4	2.0851 (18)	C8—C9	1.367 (4)
Ni1—N4 ⁱ	2.0851 (18)	C8—H8	0.9300
Ni1—N3 ⁱ	2.1029 (19)	C9—C10	1.370 (3)
Ni1—N3	2.1029 (19)	C9—H9	0.9300
N1—C15	1.436 (3)	C10—H10	0.9300
N1—C1	1.437 (3)	C11—C12	1.370 (3)
N1—C6	1.438 (3)	C11—H11	0.9300
N2—C5	1.337 (3)	C12—C13	1.366 (4)
N2—C1	1.338 (3)	C12—H12	0.9300
N3—C6	1.337 (3)	C13—C14	1.375 (3)
N3—C10	1.337 (3)	C13—H13	0.9300
N4—C15	1.339 (3)	C14—C15	1.368 (3)
N4—C11	1.339 (3)	C14—H14	0.9300
C1—C2	1.375 (3)	C11—O1	1.212 (13)
C2—C3	1.374 (3)	C11—O4	1.361 (11)
C2—H2	0.9300	C11—O2	1.430 (13)
C3—C4	1.369 (3)	C11—O3	1.457 (12)
C3—H3	0.9300	C11'—O3'	1.320 (11)
C4—C5	1.366 (3)	C11'—O2'	1.375 (14)
C4—H4	0.9300	C11'—O4'	1.401 (11)
C5—H5	0.9300	C11'—O1'	1.537 (15)
C6—C7	1.375 (3)		
N2—Ni1—N2 ⁱ	180.0	N3—C6—C7	122.9 (2)
N2—Ni1—N4	86.78 (7)	N3—C6—N1	117.46 (18)
N2 ⁱ —Ni1—N4	93.22 (7)	C7—C6—N1	119.7 (2)
N2—Ni1—N4 ⁱ	93.22 (7)	C8—C7—C6	118.3 (2)
N2 ⁱ —Ni1—N4 ⁱ	86.78 (7)	C8—C7—H7	120.9
N4—Ni1—N4 ⁱ	180.0	C6—C7—H7	120.9
N2—Ni1—N3 ⁱ	94.05 (7)	C9—C8—C7	119.7 (2)
N2 ⁱ —Ni1—N3 ⁱ	85.95 (7)	C9—C8—H8	120.1
N4—Ni1—N3 ⁱ	93.52 (8)	C7—C8—H8	120.1
N4 ⁱ —Ni1—N3 ⁱ	86.48 (8)	C8—C9—C10	118.5 (3)
N2—Ni1—N3	85.95 (7)	C8—C9—H9	120.7
N2 ⁱ —Ni1—N3	94.05 (7)	C10—C9—H9	120.7
N4—Ni1—N3	86.48 (8)	N3—C10—C9	123.0 (2)
N4 ⁱ —Ni1—N3	93.52 (8)	N3—C10—H10	118.5
N3 ⁱ —Ni1—N3	180.0	C9—C10—H10	118.5
C15—N1—C1	113.30 (17)	N4—C11—C12	122.2 (2)
C15—N1—C6	112.77 (17)	N4—C11—H11	118.9
C1—N1—C6	112.15 (17)	C12—C11—H11	118.9

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C5—N2—C1	118.06 (19)	C13—C12—C11	119.2 (2)
C5—N2—Ni1	125.59 (15)	C13—C12—H12	120.4
C1—N2—Ni1	116.34 (14)	C11—C12—H12	120.4
C6—N3—C10	117.54 (19)	C12—C13—C14	119.3 (2)
C6—N3—Ni1	115.96 (15)	C12—C13—H13	120.3
C10—N3—Ni1	126.49 (15)	C14—C13—H13	120.3
C15—N4—C11	118.01 (19)	C15—C14—C13	118.5 (2)
C15—N4—Ni1	116.26 (15)	C15—C14—H14	120.8
C11—N4—Ni1	125.72 (15)	C13—C14—H14	120.8
N2—C1—C2	122.4 (2)	N4—C15—C14	122.8 (2)
N2—C1—N1	117.66 (18)	N4—C15—N1	117.50 (18)
C2—C1—N1	119.90 (19)	C14—C15—N1	119.74 (19)
C3—C2—C1	118.5 (2)	O1—C11—O4	117.6 (10)
C3—C2—H2	120.7	O1—C11—O2	109.8 (9)
C1—C2—H2	120.7	O4—C11—O2	108.8 (9)
C4—C3—C2	119.3 (2)	O1—C11—O3	96.5 (10)
C4—C3—H3	120.3	O4—C11—O3	118.3 (10)
C2—C3—H3	120.3	O2—C11—O3	104.7 (9)
C5—C4—C3	119.0 (2)	O3'—C11'—O2'	115.5 (11)
C5—C4—H4	120.5	O3'—C11'—O4'	101.8 (10)
C3—C4—H4	120.5	O2'—C11'—O4'	113.2 (9)
N2—C5—C4	122.6 (2)	O3'—C11'—O1'	118.1 (12)
N2—C5—H5	118.7	O2'—C11'—O1'	98.6 (8)
C4—C5—H5	118.7	O4'—C11'—O1'	110.1 (9)
N4—Ni1—N2—C5	138.49 (19)	C2—C3—C4—C5	-0.3 (4)
N4 ⁱ —Ni1—N2—C5	-41.51 (19)	C1—N2—C5—C4	-0.4 (3)
N3 ⁱ —Ni1—N2—C5	45.18 (19)	Ni1—N2—C5—C4	178.09 (17)
N3—Ni1—N2—C5	-134.82 (19)	C3—C4—C5—N2	0.9 (4)
N4—Ni1—N2—C1	-42.98 (16)	C10—N3—C6—C7	0.4 (3)
N4 ⁱ —Ni1—N2—C1	137.02 (16)	Ni1—N3—C6—C7	179.54 (18)
N3 ⁱ —Ni1—N2—C1	-136.29 (16)	C10—N3—C6—N1	-178.68 (19)
N3—Ni1—N2—C1	43.71 (16)	Ni1—N3—C6—N1	0.4 (2)
N2—Ni1—N3—C6	-44.10 (16)	C15—N1—C6—N3	-65.0 (2)
N2 ⁱ —Ni1—N3—C6	135.90 (16)	C1—N1—C6—N3	64.4 (2)
N4—Ni1—N3—C6	42.92 (16)	C15—N1—C6—C7	115.9 (2)
N4 ⁱ —Ni1—N3—C6	-137.08 (16)	C1—N1—C6—C7	-114.8 (2)
N2—Ni1—N3—C10	134.9 (2)	N3—C6—C7—C8	-0.9 (4)
N2 ⁱ —Ni1—N3—C10	-45.1 (2)	N1—C6—C7—C8	178.2 (2)
N4—Ni1—N3—C10	-138.1 (2)	C6—C7—C8—C9	0.2 (4)
N4 ⁱ —Ni1—N3—C10	41.9 (2)	C7—C8—C9—C10	0.8 (4)
N2—Ni1—N4—C15	43.27 (16)	C6—N3—C10—C9	0.7 (3)
N2 ⁱ —Ni1—N4—C15	-136.73 (16)	Ni1—N3—C10—C9	-178.30 (18)
N3 ⁱ —Ni1—N4—C15	137.13 (16)	C8—C9—C10—N3	-1.3 (4)
N3—Ni1—N4—C15	-42.87 (16)	C15—N4—C11—C12	-0.8 (3)
N2—Ni1—N4—C11	-137.4 (2)	Ni1—N4—C11—C12	179.82 (18)
N2 ⁱ —Ni1—N4—C11	42.6 (2)	N4—C11—C12—C13	0.1 (4)

N3 ⁱ —Ni1—N4—C11	−43.5 (2)	C11—C12—C13—C14	1.0 (4)
N3—Ni1—N4—C11	136.5 (2)	C12—C13—C14—C15	−1.5 (4)
C5—N2—C1—C2	−0.6 (3)	C11—N4—C15—C14	0.3 (3)
Ni1—N2—C1—C2	−179.22 (17)	Ni1—N4—C15—C14	179.77 (18)
C5—N2—C1—N1	178.7 (2)	C11—N4—C15—N1	−179.87 (19)
Ni1—N2—C1—N1	0.1 (3)	Ni1—N4—C15—N1	−0.4 (3)
C15—N1—C1—N2	64.0 (3)	C13—C14—C15—N4	0.8 (4)
C6—N1—C1—N2	−65.1 (2)	C13—C14—C15—N1	−179.0 (2)
C15—N1—C1—C2	−116.7 (2)	C1—N1—C15—N4	−63.5 (3)
C6—N1—C1—C2	114.2 (2)	C6—N1—C15—N4	65.3 (2)
N2—C1—C2—C3	1.1 (3)	C1—N1—C15—C14	116.3 (2)
N1—C1—C2—C3	−178.2 (2)	C6—N1—C15—C14	−115.0 (2)
C1—C2—C3—C4	−0.6 (4)		

Symmetry codes: (i) $-x, -y, -z$.

supplementary materials

Fig. 1

