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Diaquabis[(1*R*,2*R*)-(+)–1,2-diphenylethylenediamine-κ^2N,N']nickel(II) dichloride–dichloridobis(1,10-phenanthroline-κ^2N,N')nickel(II) (1/2)

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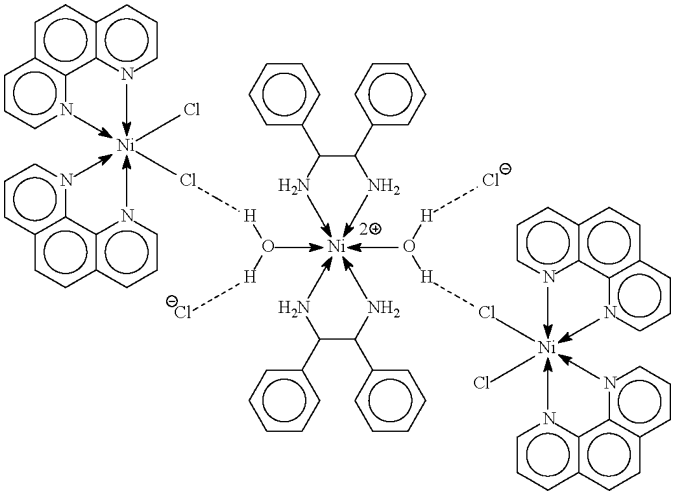
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.013 Å; R factor = 0.056; wR factor = 0.165; data-to-parameter ratio = 17.8.

In the title compound, $[Ni(C_{14}H_{16}N_2)_2(H_2O)_2]Cl_2\cdot 2[NiCl_2(C_{12}H_8N_2)_2]$, the dication, whose Ni atom is chelated by a chiral ligand, lies about a pseudo-inversion site. The dication uses its coordinated water molecules to form hydrogen bonds to the chloride counterion as well as to a coordinated Cl atom of the neutral complex. The three Ni atoms exist in octahedral geometries.

Related literature

For the nickel complexes of *meso*-, *R*,*R*- and *S*,*S*-1,2-diphenylethylenediamine, see: Finney *et al.* (1981); García-Granda & Gómez-Beltrán (1984); García-Granda *et al.* (1990); Murmann & Barnes (2004).



Experimental

Crystal data

$[Ni(C_{14}H_{16}N_2)_2(H_2O)_2]Cl_2\cdot\cdot 2[NiCl_2(C_{12}H_8N_2)_2]$
M_r = 1570.25
Monoclinic, $P2_1$
a = 12.390 (2) Å
b = 13.819 (2) Å
c = 21.261 (3) Å
β = 101.348 (2)°
V = 3569.1 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.06 mm^{-1}
T = 293 (2) K
0.48 × 0.23 × 0.18 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.629, T_{max} = 0.832
22161 measured reflections
14184 independent reflections
7201 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.165
S = 1.02
14184 reflections
796 parameters
590 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}
Absolute structure: Flack (1983), with 5767 Friedel pairs
Flack parameter: −0.07 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H1w1···Cl3	0.82	2.50	3.185 (8)	142
O1w—H1w2···Cl5	0.82	2.41	3.095 (10)	141
O2w—H2w1···Cl1	0.82	2.36	3.182 (8)	180
O2w—H2w2···Cl6	0.82	2.31	3.123 (10)	172

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2291).

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supplementary materials

Acta Cryst. (2007). E**63**, m2123 [**doi:10.1107/S1600536807033296**]

Diaquabis[(1*R*,2*R*)-(+)-1,2-diphenylethylenediamine-κ^2N,N']nickel(II) dichloride-dichloridobis(1,10-phenanthroline-κ^2N,N')nickel(II) (1/2)

Y.-Z. Zhang, Z.-L. Chen and S. W. Ng

Comment

1,2-Diphenylethylenediamine, which can exist in the *meso* and the optically active *R*,*R* and *S*,*S* forms, behaves like ethylenediamine in a number of metal complexes; several nickel(II) complexes have been characterized by crystallography. These have the ligand functioning in the expected chelating mode, as noted in the nitrite/perchlorate, nitrite/chloride (Finney *et al.*, 1981), dichloride (García-Granda & Gómez-Beltrán, 1984; Murmann & Barnes, 2004) and acetate (García-Granda *et al.*, 1990) derivatives. The dichloride complexes are ionic and there is no direct interaction between the four-coordinate cation and the halide.

The attempt to synthesize a similar, mixed-ligand complex, by adding a molar equivalent of 1,10-phenanthroline yielded a cocrystal of dichlorobis(phenanthroline)nickel and diaquabis(diphenylethylenediamine)nickel dichloride (Fig. 1). The trinuclear compound lies on a false inversion site. The nickel atom of the diaquabis(diphenylethylenediamine)nickel cation lies on this site, which also relates the two neutral dichlorobis(phenanthroline)nickel to each other. The cation uses its water molecules to form hydrogen bonds to the free chlorine anion as well as to the chlorine atom of the neutral molecule. The three nickel atoms exist in octahedral geometries.

Experimental

Nickel chloride hexahydrate (0.237 g, 1 mmol), (1*R*,2*R*)-(+)–1,2-diphenylethylenediamine (0.212 g, 1 mmol) and 1,10-phenanthroline (0.198 g, 1 mmol) were placed in a 23-ml, Teflon-lined, Parr bomb along with ethanol (12 ml). The bomb was heated at 413 K for 72 h, and then cooled over 24 h. Green crystals were isolated in 40% yield.

Refinement

The phenyl rings were refined as rigid hexagons of 1.39 Å sides as were the six-membered central ring in the phenanthroline ligands. In the phenanthroline ligands, the N–C distances were restrained to with 0.005 Å of each other, as were the other C–C distances. For the diphenylethylenediamine ligands, the N–C distances were restrained to 1.450±0.005 Å and the aliphatic C–C distances to 1.500±0.005 Å. Additionally, the temperature factors of all carbon, nitrogen and oxygen atoms were restrained to be nearly isotropic. The refinement necessitated somewhat tight restraints.

Carbon-bound H atoms were placed at calculated positions (C–H 0.93 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2 times U_{eq}(C). The water H-atoms were similarly treated (O–H 0.82 Å).

Figures

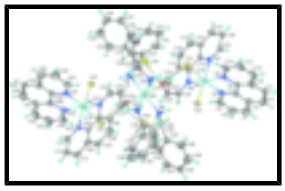


Fig. 1. **Figure 1**. Thermal ellipsoid plot of the cocrystal. Displacement ellipsoids are drawn at the 50% probability level, and H atoms as spheres of arbitrary radii. The dashed lines denote the intermolecular hydrogen bonds.

Diaquabis[(1*R*,2*R*)-(+)–1,2-diphenylethylenediamine- κ^2N,N']nickel(II) dichloride–dichloridobis(1,10-phenanthroline- κ^2N,N')nickel(II) (1/2)

Crystal data

$[Ni(C_{14}H_{16}N_2)_2(H_2O)_2]Cl_2·2[NiCl_2(C_{12}H_8N_2)_2]$	F_{000} = 1620
M_r = 1570.25	D_x = 1.461 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 3615 reflections
a = 12.390 (2) Å	θ = 2.3–24.4º
b = 13.819 (2) Å	μ = 1.06 mm^{-1}
c = 21.261 (3) Å	T = 293 (2) K
β = 101.348 (2)º	Block, green
V = 3569.1 (9) Å^3	0.48 × 0.23 × 0.18 mm
Z = 2	

Data collection

Bruker APEX area-detector diffractometer	14184 independent reflections
Radiation source: fine-focus sealed tube	7201 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.046
T = 293(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −16→14
T_{min} = 0.629, T_{max} = 0.832	k = −15→17
22161 measured reflections	l = −27→27

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.056	$w = 1/[\sigma^2(F_o^2) + (0.0657P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.165	$(\Delta/\sigma)_{max}$ = 0.002

S = 1.02	$\Delta\rho_{max}$ = 0.73 e Å^{-3}
14184 reflections	$\Delta\rho_{min}$ = −0.50 e Å^{-3}
796 parameters	Extinction correction: none
590 restraints	Absolute structure: Flack (1983), 5767 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: −0.07 (3)
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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.29514 (10)	0.5000 (1)	0.49741 (6)	0.0299 (4)
Ni2	0.25490 (14)	0.5183 (2)	0.75226 (8)	0.0338 (2)
Ni3	0.20348 (10)	0.53816 (7)	1.00447 (6)	0.0316 (4)
Cl1	0.2252 (2)	0.6289 (3)	0.55598 (13)	0.0430 (8)
Cl2	0.4373 (2)	0.4691 (3)	0.58756 (13)	0.0421 (9)
Cl3	0.2784 (3)	0.4096 (3)	0.94865 (13)	0.0456 (9)
Cl4	0.0615 (2)	0.5664 (3)	0.91330 (13)	0.0424 (9)
Cl5	0.2419 (3)	0.2174 (3)	0.73513 (16)	0.0572 (11)
Cl6	0.2600 (3)	0.8237 (3)	0.76323 (16)	0.0553 (10)
O1W	0.1792 (6)	0.4053 (7)	0.7986 (3)	0.044 (2)
H1W1	0.1761	0.4221	0.8352	0.065*
H1W2	0.2159	0.3556	0.8000	0.065*
O2W	0.3293 (6)	0.6312 (7)	0.7052 (3)	0.044 (2)
H2W1	0.3028	0.6307	0.6667	0.066*
H2W2	0.3175	0.6838	0.7204	0.066*
N1	0.3601 (6)	0.3954 (7)	0.4420 (4)	0.038 (3)
N2	0.3986 (6)	0.5863 (6)	0.4543 (4)	0.034 (3)
N3	0.1607 (5)	0.5282 (6)	0.4219 (3)	0.030 (2)
N4	0.1767 (5)	0.4016 (7)	0.5181 (3)	0.032 (2)
N5	0.1297 (5)	0.4921 (7)	0.6732 (4)	0.035 (2)
H5A	0.1451	0.5194	0.6397	0.042*
H5B	0.1230	0.4310	0.6661	0.042*
N6	0.1413 (6)	0.6165 (7)	0.7728 (3)	0.035 (2)
H6A	0.1134	0.5957	0.8042	0.042*
H6B	0.1731	0.6710	0.7838	0.042*
N7	0.3814 (6)	0.5373 (7)	0.8346 (4)	0.042 (2)
H7A	0.4106	0.5936	0.8335	0.051*
H7B	0.3539	0.5339	0.8686	0.051*
N8	0.3740 (5)	0.4240 (7)	0.7278 (4)	0.035 (2)
H8A	0.3543	0.3650	0.7320	0.042*

H8B	0.3785	0.4329	0.6884	0.042*
N9	0.1349 (6)	0.6434 (7)	1.0580 (4)	0.038 (3)
N10	0.1035 (7)	0.4532 (7)	1.0484 (4)	0.039 (3)
N11	0.3398 (5)	0.5123 (7)	1.0794 (4)	0.034 (2)
N12	0.3175 (5)	0.6347 (7)	0.9814 (3)	0.033 (2)
C1	0.4366 (5)	0.4348 (6)	0.4119 (3)	0.037 (3)
C2	0.4929 (7)	0.3789 (5)	0.3745 (4)	0.056 (4)
C3	0.5649 (6)	0.4225 (8)	0.3406 (3)	0.076 (5)
H3	0.6025	0.3851	0.3156	0.092*
C4	0.5806 (5)	0.5221 (8)	0.3441 (3)	0.070 (4)
H4	0.6288	0.5513	0.3214	0.084*
C5	0.5244 (7)	0.5780 (5)	0.3814 (4)	0.054 (4)
C6	0.4524 (5)	0.5344 (6)	0.4153 (3)	0.040 (3)
C7	0.4764 (10)	0.2793 (6)	0.3723 (6)	0.072 (5)
H7	0.5165	0.2402	0.3496	0.086*
C8	0.4004 (9)	0.2388 (9)	0.4037 (5)	0.066 (4)
H8	0.3877	0.1725	0.4025	0.079*
C9	0.3432 (10)	0.2998 (7)	0.4373 (5)	0.054 (4)
H9	0.2904	0.2729	0.4576	0.065*
C10	0.5338 (10)	0.6777 (6)	0.3872 (6)	0.070 (4)
H10	0.5800	0.7101	0.3647	0.084*
C11	0.4768 (9)	0.7308 (10)	0.4253 (5)	0.071 (5)
H11	0.4836	0.7978	0.4277	0.086*
C12	0.4090 (9)	0.6821 (7)	0.4600 (5)	0.049 (3)
H12	0.3716	0.7160	0.4869	0.059*
C13	0.0692 (5)	0.4766 (5)	0.4267 (3)	0.031 (3)
C14	−0.0298 (6)	0.4863 (5)	0.3832 (3)	0.034 (3)
C15	−0.1196 (4)	0.4293 (7)	0.3894 (3)	0.055 (4)
H15	−0.1858	0.4358	0.3602	0.066*
C16	−0.1104 (5)	0.3626 (6)	0.4390 (4)	0.048 (3)
H16	−0.1704	0.3244	0.4432	0.057*
C17	−0.0114 (6)	0.3529 (5)	0.4826 (3)	0.041 (3)
C18	0.0784 (4)	0.4099 (6)	0.4764 (3)	0.033 (3)
C19	−0.0362 (8)	0.5558 (7)	0.3345 (4)	0.046 (3)
H19	−0.1014	0.5652	0.3049	0.055*
C20	0.0565 (7)	0.6102 (9)	0.3315 (5)	0.049 (4)
H20	0.0538	0.6570	0.2998	0.059*
C21	0.1533 (8)	0.5951 (8)	0.3758 (4)	0.045 (3)
H21	0.2148	0.6324	0.3732	0.054*
C22	0.0032 (9)	0.2872 (8)	0.5335 (4)	0.061 (4)
H22	−0.0558	0.2487	0.5389	0.073*
C23	0.1023 (7)	0.2777 (9)	0.5760 (5)	0.046 (3)
H23	0.1114	0.2333	0.6095	0.055*
C24	0.1879 (8)	0.3376 (8)	0.5662 (4)	0.040 (3)
H24	0.2555	0.3330	0.5943	0.048*
C25	0.0271 (5)	0.5315 (5)	0.6866 (3)	0.042 (2)
H25	0.0064	0.4906	0.7200	0.051*
C26	0.0539 (5)	0.6301 (5)	0.7160 (3)	0.041 (2)
H26	0.0874	0.6664	0.6852	0.049*

C27	−0.0695 (5)	0.5310 (6)	0.6305 (3)	0.042 (3)
C28	−0.1636 (6)	0.4801 (6)	0.6368 (3)	0.068 (3)
H28	−0.1660	0.4473	0.6747	0.082*
C29	−0.2541 (5)	0.4781 (6)	0.5864 (4)	0.072 (3)
H29	−0.3170	0.4440	0.5906	0.086*
C30	−0.2505 (5)	0.5271 (7)	0.5297 (3)	0.067 (3)
H30	−0.3110	0.5258	0.4960	0.081*
C31	−0.1564 (6)	0.5780 (6)	0.5235 (3)	0.064 (3)
H31	−0.1540	0.6108	0.4856	0.077*
C32	−0.0659 (5)	0.5800 (6)	0.5739 (3)	0.056 (3)
H32	−0.0030	0.6140	0.5697	0.067*
C33	−0.0425 (5)	0.6905 (6)	0.7272 (4)	0.037 (3)
C34	−0.1180 (6)	0.6580 (5)	0.7629 (3)	0.062 (3)
H34	−0.1112	0.5962	0.7806	0.074*
C35	−0.2038 (5)	0.7177 (7)	0.7721 (3)	0.072 (3)
H35	−0.2544	0.6959	0.7959	0.086*
C36	−0.2141 (6)	0.8101 (6)	0.7456 (4)	0.074 (4)
H36	−0.2715	0.8500	0.7518	0.089*
C37	−0.1386 (7)	0.8426 (5)	0.7100 (4)	0.062 (3)
H37	−0.1455	0.9044	0.6923	0.075*
C38	−0.0528 (5)	0.7829 (6)	0.7008 (3)	0.062 (3)
H38	−0.0023	0.8047	0.6769	0.074*
C39	0.4657 (5)	0.4626 (6)	0.8365 (3)	0.040 (2)
H39	0.4373	0.4035	0.8529	0.048*
C40	0.4817 (5)	0.4411 (6)	0.7691 (3)	0.042 (2)
H40	0.5130	0.4990	0.7531	0.050*
C41	0.5703 (5)	0.4891 (6)	0.8827 (3)	0.046 (3)
C42	0.6388 (7)	0.5615 (6)	0.8674 (3)	0.091 (4)
H42	0.6197	0.5946	0.8288	0.109*
C43	0.7357 (6)	0.5843 (6)	0.9100 (4)	0.113 (5)
H43	0.7815	0.6327	0.8998	0.136*
C44	0.7641 (5)	0.5349 (7)	0.9678 (4)	0.079 (4)
H44	0.8290	0.5502	0.9963	0.095*
C45	0.6957 (6)	0.4625 (6)	0.9831 (3)	0.073 (4)
H45	0.7147	0.4294	1.0217	0.087*
C46	0.5988 (6)	0.4396 (5)	0.9405 (3)	0.056 (3)
H46	0.5530	0.3912	0.9507	0.067*
C47	0.5609 (5)	0.3586 (5)	0.7668 (4)	0.041 (3)
C48	0.6560 (6)	0.3785 (5)	0.7438 (4)	0.079 (4)
H48	0.6689	0.4409	0.7305	0.095*
C49	0.7318 (5)	0.3054 (7)	0.7407 (4)	0.098 (5)
H49	0.7955	0.3188	0.7253	0.117*
C50	0.7125 (6)	0.2123 (6)	0.7606 (4)	0.064 (3)
H50	0.7632	0.1634	0.7585	0.077*
C51	0.6174 (7)	0.1923 (5)	0.7836 (3)	0.064 (4)
H51	0.6045	0.1300	0.7969	0.077*
C52	0.5416 (5)	0.2654 (6)	0.7867 (3)	0.055 (3)
H52	0.4779	0.2520	0.8021	0.066*
C53	0.0607 (5)	0.6031 (6)	1.0899 (3)	0.041 (3)

C54	0.0013 (7)	0.6585 (5)	1.1258 (4)	0.056 (4)
C55	−0.0704 (6)	0.6138 (7)	1.1595 (3)	0.066 (4)
H55	−0.1101	0.6508	1.1836	0.079*
C56	−0.0827 (5)	0.5138 (8)	1.1572 (3)	0.076 (4)
H56	−0.1307	0.4839	1.1797	0.091*
C57	−0.0233 (7)	0.4585 (5)	1.1212 (4)	0.054 (4)
C58	0.0484 (5)	0.5031 (6)	1.0876 (3)	0.041 (3)
C59	0.0182 (10)	0.7580 (6)	1.1268 (6)	0.076 (5)
H59	−0.0218	0.7974	1.1493	0.091*
C60	0.0933 (10)	0.7992 (10)	1.0949 (6)	0.077 (5)
H60	0.1048	0.8657	1.0959	0.092*
C61	0.1513 (10)	0.7389 (7)	1.0612 (5)	0.054 (4)
H61	0.2033	0.7658	1.0403	0.065*
C62	−0.0342 (10)	0.3584 (6)	1.1188 (6)	0.070 (4)
H62	−0.0775	0.3266	1.1434	0.083*
C63	0.0209 (9)	0.3075 (9)	1.0789 (5)	0.062 (4)
H63	0.0136	0.2407	1.0753	0.075*
C64	0.0877 (10)	0.3575 (8)	1.0442 (6)	0.056 (4)
H64	0.1230	0.3224	1.0169	0.067*
C65	0.4298 (5)	0.5649 (5)	1.0721 (3)	0.032 (3)
C66	0.5300 (6)	0.5571 (5)	1.1147 (3)	0.044 (3)
C67	0.6183 (4)	0.6146 (7)	1.1068 (3)	0.049 (3)
H67	0.6854	0.6094	1.1354	0.059*
C68	0.6065 (5)	0.6800 (6)	1.0563 (4)	0.059 (4)
H68	0.6656	0.7186	1.0510	0.071*
C69	0.5063 (6)	0.6879 (6)	1.0136 (3)	0.039 (3)
C70	0.4180 (4)	0.6303 (6)	1.0215 (3)	0.031 (3)
C71	0.5383 (9)	0.4863 (7)	1.1623 (5)	0.057 (4)
H71	0.6055	0.4764	1.1899	0.069*
C72	0.4489 (7)	0.4308 (9)	1.1691 (5)	0.053 (4)
H72	0.4548	0.3836	1.2008	0.064*
C73	0.3498 (8)	0.4475 (8)	1.1273 (4)	0.042 (3)
H73	0.2880	0.4126	1.1325	0.050*
C74	0.4920 (8)	0.7537 (8)	0.9627 (4)	0.042 (3)
H74	0.5492	0.7938	0.9565	0.050*
C75	0.3907 (8)	0.7573 (10)	0.9221 (5)	0.056 (4)
H75	0.3798	0.7985	0.8868	0.067*
C76	0.3046 (9)	0.6995 (8)	0.9336 (5)	0.044 (3)
H76	0.2356	0.7061	0.9072	0.053*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0295 (7)	0.0305 (11)	0.0294 (7)	−0.0009 (7)	0.0051 (6)	0.0016 (8)
Ni2	0.0321 (5)	0.0401 (5)	0.0297 (4)	−0.0037 (4)	0.0073 (3)	−0.0004 (4)
Ni3	0.0335 (8)	0.0357 (12)	0.0258 (7)	0.0005 (7)	0.0063 (6)	0.0007 (8)
Cl1	0.0495 (18)	0.039 (2)	0.0415 (17)	0.0118 (15)	0.0121 (14)	−0.0011 (16)
Cl2	0.0401 (17)	0.046 (2)	0.0370 (16)	0.0067 (15)	0.0005 (13)	0.0036 (16)

Cl3	0.057 (2)	0.045 (2)	0.0348 (17)	0.0134 (17)	0.0100 (14)	−0.0015 (16)
Cl4	0.0397 (17)	0.050 (3)	0.0343 (16)	0.0065 (15)	0.0002 (13)	0.0008 (16)
Cl5	0.061 (2)	0.059 (3)	0.0510 (18)	−0.0211 (19)	0.0089 (16)	−0.007 (2)
Cl6	0.070 (2)	0.043 (3)	0.0504 (18)	−0.0181 (19)	0.0063 (17)	−0.0025 (19)
O1W	0.045 (4)	0.053 (5)	0.036 (4)	−0.004 (4)	0.015 (3)	0.008 (4)
O2W	0.054 (4)	0.040 (5)	0.041 (4)	−0.004 (4)	0.015 (4)	0.000 (4)
N1	0.042 (5)	0.042 (6)	0.030 (5)	0.000 (4)	0.006 (4)	−0.005 (4)
N2	0.032 (4)	0.042 (6)	0.029 (4)	−0.010 (4)	0.003 (4)	0.007 (4)
N3	0.038 (4)	0.026 (5)	0.027 (4)	−0.004 (4)	0.005 (3)	0.002 (4)
N4	0.038 (5)	0.030 (5)	0.031 (5)	−0.006 (4)	0.010 (4)	−0.002 (4)
N5	0.028 (4)	0.035 (5)	0.043 (4)	0.003 (3)	0.007 (3)	−0.002 (4)
N6	0.032 (4)	0.043 (5)	0.029 (4)	−0.008 (4)	0.004 (3)	−0.006 (4)
N7	0.040 (4)	0.052 (6)	0.038 (4)	−0.004 (4)	0.012 (3)	−0.006 (4)
N8	0.033 (4)	0.042 (5)	0.033 (4)	0.001 (4)	0.012 (4)	0.004 (4)
N9	0.042 (5)	0.039 (6)	0.033 (5)	0.006 (4)	0.004 (4)	0.002 (4)
N10	0.033 (5)	0.044 (6)	0.037 (5)	−0.001 (4)	0.006 (4)	0.002 (5)
N11	0.038 (4)	0.038 (6)	0.025 (4)	0.005 (5)	0.004 (3)	0.003 (5)
N12	0.038 (5)	0.036 (6)	0.023 (4)	0.002 (4)	0.002 (4)	0.002 (4)
C1	0.027 (5)	0.050 (7)	0.033 (5)	0.008 (5)	0.004 (4)	−0.002 (5)
C2	0.046 (6)	0.079 (8)	0.040 (6)	0.007 (6)	0.004 (5)	−0.005 (6)
C3	0.053 (7)	0.125 (9)	0.052 (7)	0.016 (7)	0.013 (6)	−0.014 (7)
C4	0.042 (6)	0.132 (9)	0.043 (6)	−0.008 (7)	0.022 (5)	0.013 (7)
C5	0.034 (5)	0.085 (8)	0.039 (6)	−0.008 (6)	−0.005 (5)	0.002 (6)
C6	0.031 (5)	0.065 (7)	0.026 (5)	0.001 (5)	0.009 (4)	0.005 (5)
C7	0.072 (7)	0.090 (9)	0.049 (6)	0.028 (6)	0.004 (6)	−0.022 (6)
C8	0.082 (7)	0.053 (7)	0.058 (7)	0.022 (6)	0.005 (6)	−0.013 (6)
C9	0.063 (6)	0.052 (8)	0.045 (6)	0.003 (6)	0.006 (5)	−0.004 (6)
C10	0.056 (7)	0.108 (9)	0.044 (6)	−0.026 (6)	0.004 (5)	0.021 (6)
C11	0.073 (7)	0.062 (8)	0.070 (7)	−0.027 (6)	−0.007 (6)	0.025 (6)
C12	0.048 (6)	0.041 (7)	0.053 (6)	−0.019 (5)	−0.004 (5)	0.005 (5)
C13	0.032 (5)	0.030 (6)	0.030 (5)	−0.003 (4)	0.006 (4)	−0.004 (5)
C14	0.029 (5)	0.036 (6)	0.034 (5)	0.000 (4)	−0.002 (4)	−0.004 (5)
C15	0.042 (6)	0.064 (7)	0.055 (6)	0.002 (6)	0.000 (5)	−0.014 (6)
C16	0.032 (5)	0.047 (7)	0.060 (6)	−0.014 (5)	0.002 (5)	−0.008 (5)
C17	0.042 (6)	0.040 (7)	0.044 (6)	−0.011 (5)	0.013 (5)	−0.002 (5)
C18	0.029 (5)	0.035 (6)	0.034 (5)	−0.007 (5)	0.009 (4)	−0.009 (5)
C19	0.046 (6)	0.056 (7)	0.029 (5)	0.007 (5)	−0.010 (4)	0.002 (5)
C20	0.053 (6)	0.047 (7)	0.044 (6)	0.006 (5)	−0.001 (5)	0.017 (6)
C21	0.053 (6)	0.049 (7)	0.033 (5)	0.005 (5)	0.009 (5)	0.005 (5)
C22	0.058 (6)	0.060 (8)	0.069 (7)	−0.031 (6)	0.025 (6)	−0.017 (6)
C23	0.068 (6)	0.038 (6)	0.036 (5)	−0.010 (5)	0.019 (5)	0.005 (5)
C24	0.045 (5)	0.044 (7)	0.029 (5)	0.010 (5)	0.003 (4)	0.000 (5)
C25	0.036 (4)	0.050 (5)	0.037 (4)	−0.002 (4)	−0.001 (3)	−0.002 (4)
C26	0.034 (4)	0.051 (5)	0.034 (4)	0.003 (4)	−0.002 (4)	0.002 (4)
C27	0.036 (5)	0.059 (6)	0.030 (4)	−0.003 (4)	0.003 (4)	−0.008 (4)
C28	0.056 (6)	0.091 (8)	0.050 (6)	−0.022 (5)	−0.009 (5)	0.008 (5)
C29	0.046 (5)	0.089 (7)	0.072 (6)	−0.029 (5)	−0.012 (5)	0.008 (6)
C30	0.055 (6)	0.085 (7)	0.051 (6)	0.000 (5)	−0.016 (5)	0.002 (5)
C31	0.063 (6)	0.067 (7)	0.057 (6)	0.004 (5)	0.000 (5)	0.008 (5)

C32	0.050 (5)	0.057 (6)	0.053 (6)	−0.009 (5)	−0.005 (5)	−0.007 (5)
C33	0.028 (4)	0.052 (6)	0.030 (4)	0.003 (4)	0.004 (4)	−0.001 (4)
C34	0.059 (6)	0.057 (6)	0.071 (6)	−0.002 (5)	0.016 (5)	0.018 (5)
C35	0.050 (5)	0.094 (8)	0.076 (6)	−0.008 (5)	0.024 (5)	0.015 (6)
C36	0.065 (7)	0.089 (8)	0.069 (7)	0.030 (6)	0.013 (6)	−0.006 (6)
C37	0.063 (6)	0.053 (7)	0.075 (7)	0.006 (5)	0.021 (5)	0.017 (6)
C38	0.057 (6)	0.060 (7)	0.073 (6)	0.015 (5)	0.023 (5)	0.010 (5)
C39	0.039 (4)	0.043 (5)	0.035 (4)	0.003 (4)	−0.001 (4)	−0.002 (4)
C40	0.031 (4)	0.053 (5)	0.039 (5)	0.000 (4)	0.004 (4)	−0.002 (4)
C41	0.041 (5)	0.060 (6)	0.034 (5)	−0.002 (4)	0.004 (4)	−0.003 (5)
C42	0.088 (7)	0.121 (9)	0.057 (6)	−0.057 (6)	−0.004 (5)	0.024 (6)
C43	0.100 (8)	0.141 (10)	0.093 (8)	−0.056 (7)	0.005 (7)	0.014 (7)
C44	0.056 (6)	0.098 (8)	0.070 (7)	−0.006 (6)	−0.020 (5)	−0.013 (6)
C45	0.077 (7)	0.067 (7)	0.065 (6)	0.003 (5)	−0.008 (5)	−0.004 (5)
C46	0.051 (5)	0.067 (6)	0.045 (5)	−0.009 (5)	−0.003 (4)	−0.001 (5)
C47	0.032 (5)	0.056 (6)	0.031 (5)	−0.006 (4)	0.000 (4)	0.000 (4)
C48	0.070 (6)	0.070 (7)	0.108 (8)	0.013 (5)	0.042 (6)	0.033 (6)
C49	0.090 (7)	0.097 (8)	0.120 (8)	0.017 (6)	0.055 (7)	0.032 (7)
C50	0.049 (6)	0.077 (7)	0.069 (6)	0.022 (5)	0.018 (5)	0.018 (6)
C51	0.075 (6)	0.059 (7)	0.060 (6)	0.016 (5)	0.017 (5)	0.010 (6)
C52	0.063 (6)	0.056 (7)	0.055 (5)	0.006 (5)	0.032 (5)	0.003 (5)
C53	0.034 (5)	0.068 (8)	0.021 (5)	0.007 (5)	0.002 (4)	0.000 (5)
C54	0.044 (6)	0.084 (8)	0.040 (6)	0.020 (6)	0.010 (5)	−0.008 (6)
C55	0.038 (6)	0.120 (9)	0.046 (6)	0.014 (6)	0.021 (5)	−0.011 (6)
C56	0.048 (6)	0.133 (9)	0.046 (6)	−0.009 (7)	0.010 (5)	0.004 (7)
C57	0.040 (6)	0.086 (8)	0.038 (6)	−0.013 (6)	0.013 (5)	0.012 (6)
C58	0.031 (5)	0.058 (7)	0.033 (5)	−0.001 (5)	0.001 (4)	0.005 (5)
C59	0.067 (7)	0.097 (9)	0.063 (7)	0.035 (7)	0.010 (6)	−0.021 (7)
C60	0.096 (8)	0.065 (8)	0.070 (7)	0.017 (7)	0.015 (6)	−0.014 (7)
C61	0.070 (7)	0.047 (7)	0.046 (6)	0.007 (6)	0.011 (5)	−0.012 (6)
C62	0.051 (6)	0.093 (8)	0.059 (7)	−0.034 (6)	−0.002 (5)	0.021 (6)
C63	0.063 (7)	0.052 (7)	0.065 (7)	−0.024 (6)	−0.004 (6)	0.012 (6)
C64	0.058 (7)	0.059 (8)	0.048 (6)	−0.009 (6)	0.006 (5)	−0.001 (6)
C65	0.028 (5)	0.034 (6)	0.035 (5)	0.006 (4)	0.007 (4)	−0.008 (5)
C66	0.044 (6)	0.041 (7)	0.046 (6)	0.007 (5)	0.002 (5)	−0.013 (5)
C67	0.027 (5)	0.050 (7)	0.065 (6)	0.004 (5)	−0.003 (5)	−0.007 (6)
C68	0.050 (6)	0.058 (7)	0.074 (7)	−0.011 (6)	0.021 (6)	−0.009 (6)
C69	0.034 (5)	0.044 (7)	0.040 (5)	−0.002 (5)	0.005 (4)	−0.003 (5)
C70	0.035 (5)	0.028 (6)	0.028 (5)	0.005 (5)	0.001 (4)	0.001 (5)
C71	0.050 (6)	0.064 (8)	0.055 (6)	0.016 (6)	0.003 (5)	−0.011 (6)
C72	0.064 (7)	0.051 (7)	0.039 (6)	0.013 (6)	−0.002 (5)	0.013 (6)
C73	0.046 (6)	0.039 (6)	0.039 (5)	0.001 (5)	0.003 (5)	0.005 (5)
C74	0.048 (6)	0.037 (6)	0.042 (5)	−0.012 (5)	0.011 (5)	0.008 (5)
C75	0.078 (7)	0.042 (7)	0.049 (6)	−0.012 (6)	0.011 (6)	0.006 (6)
C76	0.050 (6)	0.039 (7)	0.042 (6)	−0.011 (5)	0.007 (5)	0.003 (5)

Geometric parameters (Å, °)

Ni1—N2	2.090 (9)	C25—H25	0.9800

Ni1—N4	2.109 (8)	C26—C33	1.514 (4)
Ni1—N3	2.109 (7)	C26—H26	0.9800
Ni1—N1	2.120 (10)	C27—C28	1.3900
Ni1—Cl2	2.372 (3)	C27—C32	1.3900
Ni1—Cl1	2.429 (3)	C28—C29	1.3900
Ni2—N6	2.064 (9)	C28—H28	0.9300
Ni2—N5	2.082 (8)	C29—C30	1.3900
Ni2—N8	2.108 (9)	C29—H29	0.9300
Ni2—N7	2.123 (8)	C30—C31	1.3900
Ni2—O1W	2.157 (8)	C30—H30	0.9300
Ni2—O2W	2.156 (8)	C31—C32	1.3900
Ni3—N10	2.059 (10)	C31—H31	0.9300
Ni3—N12	2.071 (9)	C32—H32	0.9300
Ni3—N11	2.112 (7)	C33—C34	1.3900
Ni3—N9	2.125 (10)	C33—C38	1.3900
Ni3—Cl4	2.380 (3)	C34—C35	1.3900
Ni3—Cl3	2.421 (4)	C34—H34	0.9300
O1W—H1W1	0.8200	C35—C36	1.3900
O1W—H1W2	0.8200	C35—H35	0.9300
O2W—H2W1	0.8200	C36—C37	1.3900
O2W—H2W2	0.8200	C36—H36	0.9300
N1—C9	1.338 (5)	C37—C38	1.3900
N1—C1	1.358 (4)	C37—H37	0.9300
N2—C12	1.332 (5)	C38—H38	0.9300
N2—C6	1.365 (4)	C39—C41	1.509 (5)
N3—C21	1.339 (5)	C39—C40	1.515 (5)
N3—C13	1.360 (4)	C39—H39	0.9800
N4—C24	1.340 (5)	C40—C47	1.511 (5)
N4—C18	1.362 (4)	C40—H40	0.9800
N5—C25	1.462 (5)	C41—C42	1.3900
N5—H5A	0.8600	C41—C46	1.3900
N5—H5B	0.8600	C42—C43	1.3900
N6—C26	1.466 (5)	C42—H42	0.9300
N6—H6A	0.8600	C43—C44	1.3900
N6—H6B	0.8600	C43—H43	0.9300
N7—C39	1.464 (5)	C44—C45	1.3900
N7—H7A	0.8600	C44—H44	0.9300
N7—H7B	0.8600	C45—C46	1.3900
N8—C40	1.464 (5)	C45—H45	0.9300
N8—H8A	0.8600	C46—H46	0.9300
N8—H8B	0.8600	C47—C48	1.3900
N9—C61	1.334 (5)	C47—C52	1.3900
N9—C53	1.364 (4)	C48—C49	1.3900
N10—C64	1.337 (5)	C48—H48	0.9300
N10—C58	1.364 (4)	C49—C50	1.3900
N11—C73	1.342 (5)	C49—H49	0.9300
N11—C65	1.365 (4)	C50—C51	1.3900
N12—C76	1.340 (5)	C50—H50	0.9300
N12—C70	1.365 (4)	C51—C52	1.3900

C1—C2	1.3900	C51—H51	0.9300
C1—C6	1.3900	C52—H52	0.9300
C2—C7	1.390 (5)	C53—C54	1.3900
C2—C3	1.3900	C53—C58	1.3900
C3—C4	1.3900	C54—C55	1.3900
C3—H3	0.9300	C54—C59	1.391 (5)
C4—C5	1.3900	C55—C56	1.3900
C4—H4	0.9300	C55—H55	0.9300
C5—C10	1.386 (5)	C56—C57	1.3900
C5—C6	1.3900	C56—H56	0.9300
C7—C8	1.376 (5)	C57—C62	1.389 (5)
C7—H7	0.9300	C57—C58	1.3900
C8—C9	1.386 (5)	C59—C60	1.377 (5)
C8—H8	0.9300	C59—H59	0.9300
C9—H9	0.9300	C60—C61	1.388 (5)
C10—C11	1.384 (5)	C60—H60	0.9300
C10—H10	0.9300	C61—H61	0.9300
C11—C12	1.396 (5)	C62—C63	1.381 (5)
C11—H11	0.9300	C62—H62	0.9300
C12—H12	0.9300	C63—C64	1.395 (5)
C13—C14	1.3900	C63—H63	0.9300
C13—C18	1.3900	C64—H64	0.9300
C14—C15	1.3900	C65—C66	1.3900
C14—C19	1.403 (5)	C65—C70	1.3900
C15—C16	1.3900	C66—C67	1.3900
C15—H15	0.9300	C66—C71	1.395 (5)
C16—C17	1.3900	C67—C68	1.3900
C16—H16	0.9300	C67—H67	0.9300
C17—C18	1.3900	C68—C69	1.3900
C17—C22	1.397 (5)	C68—H68	0.9300
C19—C20	1.384 (5)	C69—C70	1.3900
C19—H19	0.9300	C69—C74	1.398 (5)
C20—C21	1.387 (5)	C71—C72	1.379 (5)
C20—H20	0.9300	C71—H71	0.9300
C21—H21	0.9300	C72—C73	1.387 (5)
C22—C23	1.380 (5)	C72—H72	0.9300
C22—H22	0.9300	C73—H73	0.9300
C23—C24	1.393 (5)	C74—C75	1.377 (5)
C23—H23	0.9300	C74—H74	0.9300
C24—H24	0.9300	C75—C76	1.393 (5)
C25—C26	1.508 (5)	C75—H75	0.9300
C25—C27	1.515 (4)	C76—H76	0.9300
N2—Ni1—N4	166.2 (3)	C23—C24—H24	118.7
N2—Ni1—N3	91.2 (3)	N5—C25—C26	106.7 (6)
N4—Ni1—N3	78.4 (3)	N5—C25—C27	115.3 (6)
N2—Ni1—N1	79.2 (3)	C26—C25—C27	114.0 (6)
N4—Ni1—N1	91.9 (3)	N5—C25—H25	106.8
N3—Ni1—N1	91.9 (4)	C26—C25—H25	106.8
N2—Ni1—Cl2	92.0 (2)	C27—C25—H25	106.8

N4—Ni1—Cl2	98.76 (18)	N6—C26—C25	107.0 (6)
N3—Ni1—Cl2	175.8 (2)	N6—C26—C33	114.8 (6)
N1—Ni1—Cl2	91.4 (3)	C25—C26—C33	116.6 (6)
N2—Ni1—Cl1	96.8 (2)	N6—C26—H26	105.9
N4—Ni1—Cl1	91.9 (3)	C25—C26—H26	105.9
N3—Ni1—Cl1	86.9 (3)	C33—C26—H26	105.9
N1—Ni1—Cl1	175.8 (2)	C28—C27—C32	120.0
Cl2—Ni1—Cl1	90.04 (12)	C28—C27—C25	118.3 (5)
N6—Ni2—N5	81.6 (3)	C32—C27—C25	121.7 (6)
N6—Ni2—N8	176.7 (5)	C27—C28—C29	120.0
N5—Ni2—N8	98.1 (3)	C27—C28—H28	120.0
N6—Ni2—N7	99.7 (3)	C29—C28—H28	120.0
N5—Ni2—N7	177.0 (5)	C30—C29—C28	120.0
N8—Ni2—N7	80.8 (3)	C30—C29—H29	120.0
N6—Ni2—O1W	90.2 (3)	C28—C29—H29	120.0
N5—Ni2—O1W	85.5 (3)	C29—C30—C31	120.0
N8—Ni2—O1W	93.1 (3)	C29—C30—H30	120.0
N7—Ni2—O1W	91.7 (3)	C31—C30—H30	120.0
N6—Ni2—O2W	89.6 (4)	C32—C31—C30	120.0
N5—Ni2—O2W	94.0 (3)	C32—C31—H31	120.0
N8—Ni2—O2W	87.1 (3)	C30—C31—H31	120.0
N7—Ni2—O2W	88.8 (3)	C31—C32—C27	120.0
O1W—Ni2—O2W	179.5 (4)	C31—C32—H32	120.0
N10—Ni3—N12	166.9 (3)	C27—C32—H32	120.0
N10—Ni3—N11	91.4 (3)	C34—C33—C38	120.0
N12—Ni3—N11	78.8 (3)	C34—C33—C26	122.9 (6)
N10—Ni3—N9	78.9 (3)	C38—C33—C26	117.1 (6)
N12—Ni3—N9	92.8 (3)	C35—C34—C33	120.0
N11—Ni3—N9	93.2 (4)	C35—C34—H34	120.0
N10—Ni3—Cl4	92.8 (3)	C33—C34—H34	120.0
N12—Ni3—Cl4	97.50 (18)	C34—C35—C36	120.0
N11—Ni3—Cl4	174.6 (2)	C34—C35—H35	120.0
N9—Ni3—Cl4	90.8 (3)	C36—C35—H35	120.0
N10—Ni3—Cl3	97.3 (2)	C37—C36—C35	120.0
N12—Ni3—Cl3	90.6 (3)	C37—C36—H36	120.0
N11—Ni3—Cl3	85.4 (3)	C35—C36—H36	120.0
N9—Ni3—Cl3	175.9 (2)	C36—C37—C38	120.0
Cl4—Ni3—Cl3	90.83 (11)	C36—C37—H37	120.0
Ni2—O1W—H1W1	109.5	C38—C37—H37	120.0
Ni2—O1W—H1W2	109.5	C37—C38—C33	120.0
H1W1—O1W—H1W2	109.5	C37—C38—H38	120.0
Ni2—O2W—H2W1	109.5	C33—C38—H38	120.0
Ni2—O2W—H2W2	109.5	N7—C39—C41	111.4 (6)
H2W1—O2W—H2W2	109.5	N7—C39—C40	109.7 (6)
C9—N1—C1	118.3 (10)	C41—C39—C40	114.1 (6)
C9—N1—Ni1	130.1 (7)	N7—C39—H39	107.1
C1—N1—Ni1	111.4 (7)	C41—C39—H39	107.1
C12—N2—C6	121.8 (10)	C40—C39—H39	107.1
C12—N2—Ni1	125.7 (7)	N8—C40—C47	112.4 (6)

C6—N2—Ni1	112.4 (7)	N8—C40—C39	109.0 (5)
C21—N3—C13	118.6 (8)	C47—C40—C39	112.6 (6)
C21—N3—Ni1	128.0 (6)	N8—C40—H40	107.5
C13—N3—Ni1	113.1 (5)	C47—C40—H40	107.5
C24—N4—C18	119.8 (8)	C39—C40—H40	107.5
C24—N4—Ni1	127.8 (6)	C42—C41—C46	120.0
C18—N4—Ni1	112.4 (5)	C42—C41—C39	120.5 (6)
C25—N5—Ni2	108.4 (5)	C46—C41—C39	119.5 (6)
C25—N5—H5A	110.0	C43—C42—C41	120.0
Ni2—N5—H5A	110.0	C43—C42—H42	120.0
C25—N5—H5B	110.0	C41—C42—H42	120.0
Ni2—N5—H5B	110.0	C42—C43—C44	120.0
H5A—N5—H5B	108.4	C42—C43—H43	120.0
C26—N6—Ni2	109.5 (5)	C44—C43—H43	120.0
C26—N6—H6A	109.8	C45—C44—C43	120.0
Ni2—N6—H6A	109.8	C45—C44—H44	120.0
C26—N6—H6B	109.8	C43—C44—H44	120.0
Ni2—N6—H6B	109.8	C46—C45—C44	120.0
H6A—N6—H6B	108.2	C46—C45—H45	120.0
C39—N7—Ni2	110.1 (5)	C44—C45—H45	120.0
C39—N7—H7A	109.6	C45—C46—C41	120.0
Ni2—N7—H7A	109.6	C45—C46—H46	120.0
C39—N7—H7B	109.6	C41—C46—H46	120.0
Ni2—N7—H7B	109.6	C48—C47—C52	120.0
H7A—N7—H7B	108.2	C48—C47—C40	117.5 (6)
C40—N8—Ni2	110.6 (5)	C52—C47—C40	122.5 (6)
C40—N8—H8A	109.5	C47—C48—C49	120.0
Ni2—N8—H8A	109.5	C47—C48—H48	120.0
C40—N8—H8B	109.5	C49—C48—H48	120.0
Ni2—N8—H8B	109.5	C50—C49—C48	120.0
H8A—N8—H8B	108.1	C50—C49—H49	120.0
C61—N9—C53	119.3 (10)	C48—C49—H49	120.0
C61—N9—Ni3	129.1 (7)	C49—C50—C51	120.0
C53—N9—Ni3	111.5 (7)	C49—C50—H50	120.0
C64—N10—C58	117.1 (10)	C51—C50—H50	120.0
C64—N10—Ni3	128.9 (7)	C52—C51—C50	120.0
C58—N10—Ni3	114.0 (7)	C52—C51—H51	120.0
C73—N11—C65	119.1 (8)	C50—C51—H51	120.0
C73—N11—Ni3	128.7 (6)	C51—C52—C47	120.0
C65—N11—Ni3	111.9 (5)	C51—C52—H52	120.0
C76—N12—C70	117.5 (8)	C47—C52—H52	120.0
C76—N12—Ni3	128.7 (6)	N9—C53—C54	122.0 (8)
C70—N12—Ni3	113.8 (6)	N9—C53—C58	118.0 (8)
N1—C1—C2	121.4 (8)	C54—C53—C58	120.0
N1—C1—C6	118.4 (8)	C55—C54—C53	120.0
C2—C1—C6	120.0	C55—C54—C59	122.8 (9)
C7—C2—C1	118.9 (9)	C53—C54—C59	117.2 (9)
C7—C2—C3	121.1 (9)	C54—C55—C56	120.0
C1—C2—C3	120.0	C54—C55—H55	120.0

C4—C3—C2	120.0	C56—C55—H55	120.0
C4—C3—H3	120.0	C57—C56—C55	120.0
C2—C3—H3	120.0	C57—C56—H56	120.0
C3—C4—C5	120.0	C55—C56—H56	120.0
C3—C4—H4	120.0	C62—C57—C56	120.7 (9)
C5—C4—H4	120.0	C62—C57—C58	119.3 (9)
C10—C5—C6	115.9 (9)	C56—C57—C58	120.0
C10—C5—C4	124.1 (9)	N10—C58—C57	122.5 (8)
C6—C5—C4	120.0	N10—C58—C53	117.4 (8)
N2—C6—C5	121.8 (8)	C57—C58—C53	120.0
N2—C6—C1	118.2 (8)	C60—C59—C54	121.1 (12)
C5—C6—C1	120.0	C60—C59—H59	119.5
C8—C7—C2	119.7 (11)	C54—C59—H59	119.5
C8—C7—H7	120.2	C59—C60—C61	118.3 (13)
C2—C7—H7	120.2	C59—C60—H60	120.8
C7—C8—C9	118.1 (13)	C61—C60—H60	120.8
C7—C8—H8	121.0	N9—C61—C60	122.1 (13)
C9—C8—H8	121.0	N9—C61—H61	119.0
N1—C9—C8	123.5 (13)	C60—C61—H61	119.0
N1—C9—H9	118.3	C63—C62—C57	118.3 (11)
C8—C9—H9	118.3	C63—C62—H62	120.9
C11—C10—C5	122.4 (11)	C57—C62—H62	120.9
C11—C10—H10	118.8	C62—C63—C64	119.3 (12)
C5—C10—H10	118.8	C62—C63—H63	120.4
C10—C11—C12	118.9 (12)	C64—C63—H63	120.4
C10—C11—H11	120.6	N10—C64—C63	123.3 (12)
C12—C11—H11	120.6	N10—C64—H64	118.3
N2—C12—C11	119.2 (12)	C63—C64—H64	118.3
N2—C12—H12	120.4	N11—C65—C66	121.9 (6)
C11—C12—H12	120.4	N11—C65—C70	118.1 (6)
N3—C13—C14	122.6 (6)	C66—C65—C70	120.0
N3—C13—C18	117.3 (6)	C65—C66—C67	120.0
C14—C13—C18	120.0	C65—C66—C71	117.2 (7)
C13—C14—C15	120.0	C67—C66—C71	122.7 (7)
C13—C14—C19	118.1 (6)	C66—C67—C68	120.0
C15—C14—C19	121.8 (6)	C66—C67—H67	120.0
C16—C15—C14	120.0	C68—C67—H67	120.0
C16—C15—H15	120.0	C69—C68—C67	120.0
C14—C15—H15	120.0	C69—C68—H68	120.0
C15—C16—C17	120.0	C67—C68—H68	120.0
C15—C16—H16	120.0	C68—C69—C70	120.0
C17—C16—H16	120.0	C68—C69—C74	121.1 (7)
C18—C17—C16	120.0	C70—C69—C74	118.9 (7)
C18—C17—C22	117.2 (6)	N12—C70—C69	122.8 (6)
C16—C17—C22	122.8 (6)	N12—C70—C65	117.2 (6)
N4—C18—C17	121.4 (6)	C69—C70—C65	120.0
N4—C18—C13	118.6 (6)	C72—C71—C66	121.3 (10)
C17—C18—C13	120.0	C72—C71—H71	119.3
C20—C19—C14	118.6 (9)	C66—C71—H71	119.3

C20—C19—H19	120.7	C71—C72—C73	117.9 (11)
C14—C19—H19	120.7	C71—C72—H72	121.1
C19—C20—C21	120.1 (10)	C73—C72—H72	121.1
C19—C20—H20	119.9	N11—C73—C72	122.3 (10)
C21—C20—H20	119.9	N11—C73—H73	118.8
N3—C21—C20	121.8 (10)	C72—C73—H73	118.8
N3—C21—H21	119.1	C75—C74—C69	118.1 (9)
C20—C21—H21	119.1	C75—C74—H74	121.0
C23—C22—C17	122.1 (9)	C69—C74—H74	121.0
C23—C22—H22	118.9	C74—C75—C76	120.3 (11)
C17—C22—H22	118.9	C74—C75—H75	119.9
C22—C23—C24	116.8 (10)	C76—C75—H75	119.9
C22—C23—H23	121.6	N12—C76—C75	122.3 (10)
C24—C23—H23	121.6	N12—C76—H76	118.8
N4—C24—C23	122.6 (10)	C75—C76—H76	118.8
N4—C24—H24	118.7		
N2—Ni1—N1—C9	177.9 (11)	C13—C14—C19—C20	1.0 (13)
N4—Ni1—N1—C9	−12.7 (11)	C15—C14—C19—C20	179.8 (8)
N3—Ni1—N1—C9	−91.1 (11)	C14—C19—C20—C21	0.4 (18)
Cl2—Ni1—N1—C9	86.2 (11)	C13—N3—C21—C20	−2.6 (16)
N2—Ni1—N1—C1	3.7 (6)	Ni1—N3—C21—C20	−175.3 (9)
N4—Ni1—N1—C1	173.1 (6)	C19—C20—C21—N3	0.3 (18)
N3—Ni1—N1—C1	94.6 (6)	C18—C17—C22—C23	−0.7 (15)
Cl2—Ni1—N1—C1	−88.1 (6)	C16—C17—C22—C23	179.3 (10)
N4—Ni1—N2—C12	125.7 (13)	C17—C22—C23—C24	0.6 (19)
N3—Ni1—N2—C12	84.5 (10)	C18—N4—C24—C23	0.2 (17)
N1—Ni1—N2—C12	176.1 (10)	Ni1—N4—C24—C23	178.4 (9)
Cl2—Ni1—N2—C12	−92.9 (9)	C22—C23—C24—N4	−0.4 (19)
Cl1—Ni1—N2—C12	−2.6 (10)	Ni2—N5—C25—C26	44.3 (7)
N4—Ni1—N2—C6	−50.8 (16)	Ni2—N5—C25—C27	172.0 (5)
N3—Ni1—N2—C6	−92.1 (6)	Ni2—N6—C26—C25	41.4 (8)
N1—Ni1—N2—C6	−0.4 (6)	Ni2—N6—C26—C33	172.4 (6)
Cl2—Ni1—N2—C6	90.6 (6)	N5—C25—C26—N6	−56.9 (8)
Cl1—Ni1—N2—C6	−179.2 (6)	C27—C25—C26—N6	174.7 (6)
N2—Ni1—N3—C21	−12.3 (9)	N5—C25—C26—C33	173.2 (6)
N4—Ni1—N3—C21	176.9 (10)	C27—C25—C26—C33	44.7 (9)
N1—Ni1—N3—C21	−91.6 (9)	N5—C25—C27—C28	120.6 (7)
Cl1—Ni1—N3—C21	84.4 (9)	C26—C25—C27—C28	−115.4 (6)
N2—Ni1—N3—C13	174.6 (7)	N5—C25—C27—C32	−59.6 (9)
N4—Ni1—N3—C13	3.8 (6)	C26—C25—C27—C32	64.4 (8)
N1—Ni1—N3—C13	95.4 (7)	C32—C27—C28—C29	0.0
Cl1—Ni1—N3—C13	−88.7 (6)	C25—C27—C28—C29	179.8 (7)
N2—Ni1—N4—C24	136.4 (12)	C27—C28—C29—C30	0.0
N3—Ni1—N4—C24	178.7 (10)	C28—C29—C30—C31	0.0
N1—Ni1—N4—C24	87.2 (10)	C29—C30—C31—C32	0.0
Cl2—Ni1—N4—C24	−4.5 (9)	C30—C31—C32—C27	0.0
Cl1—Ni1—N4—C24	−94.8 (9)	C28—C27—C32—C31	0.0
N2—Ni1—N4—C18	−45.3 (17)	C25—C27—C32—C31	−179.8 (7)
N3—Ni1—N4—C18	−3.0 (6)	N6—C26—C33—C34	−70.8 (8)

N1—Ni1—N4—C18	−94.5 (7)	C25—C26—C33—C34	55.4 (8)
Cl2—Ni1—N4—C18	173.8 (6)	N6—C26—C33—C38	108.3 (7)
Cl1—Ni1—N4—C18	83.5 (6)	C25—C26—C33—C38	−125.6 (6)
N6—Ni2—N5—C25	−17.4 (6)	C38—C33—C34—C35	0.0
N8—Ni2—N5—C25	166.0 (6)	C26—C33—C34—C35	179.1 (7)
O1W—Ni2—N5—C25	73.5 (6)	C33—C34—C35—C36	0.0
O2W—Ni2—N5—C25	−106.4 (6)	C34—C35—C36—C37	0.0
N5—Ni2—N6—C26	−13.7 (6)	C35—C36—C37—C38	0.0
N7—Ni2—N6—C26	169.0 (6)	C36—C37—C38—C33	0.0
O1W—Ni2—N6—C26	−99.2 (6)	C34—C33—C38—C37	0.0
O2W—Ni2—N6—C26	80.3 (6)	C26—C33—C38—C37	−179.1 (6)
N6—Ni2—N7—C39	170.6 (6)	Ni2—N7—C39—C41	164.2 (5)
N8—Ni2—N7—C39	−12.7 (6)	Ni2—N7—C39—C40	36.9 (8)
O1W—Ni2—N7—C39	80.1 (6)	Ni2—N8—C40—C47	163.6 (5)
O2W—Ni2—N7—C39	−100.0 (6)	Ni2—N8—C40—C39	38.0 (8)
N5—Ni2—N8—C40	168.5 (6)	N7—C39—C40—N8	−49.8 (9)
N7—Ni2—N8—C40	−14.4 (6)	C41—C39—C40—N8	−175.6 (7)
O1W—Ni2—N8—C40	−105.6 (6)	N7—C39—C40—C47	−175.2 (7)
O2W—Ni2—N8—C40	74.9 (6)	C41—C39—C40—C47	59.0 (9)
N10—Ni3—N9—C61	−179.0 (11)	N7—C39—C41—C42	−73.0 (8)
N12—Ni3—N9—C61	11.2 (11)	C40—C39—C41—C42	51.8 (8)
N11—Ni3—N9—C61	90.2 (11)	N7—C39—C41—C46	107.8 (7)
Cl4—Ni3—N9—C61	−86.3 (10)	C40—C39—C41—C46	−127.3 (6)
N10—Ni3—N9—C53	−2.5 (6)	C46—C41—C42—C43	0.0
N12—Ni3—N9—C53	−172.2 (6)	C39—C41—C42—C43	−179.1 (8)
N11—Ni3—N9—C53	−93.3 (6)	C41—C42—C43—C44	0.0
Cl4—Ni3—N9—C53	90.2 (6)	C42—C43—C44—C45	0.0
N12—Ni3—N10—C64	−127.8 (14)	C43—C44—C45—C46	0.0
N11—Ni3—N10—C64	−86.4 (11)	C44—C45—C46—C41	0.0
N9—Ni3—N10—C64	−179.4 (11)	C42—C41—C46—C45	0.0
Cl4—Ni3—N10—C64	90.3 (10)	C39—C41—C46—C45	179.1 (7)
Cl3—Ni3—N10—C64	−0.9 (11)	N8—C40—C47—C48	117.7 (6)
N12—Ni3—N10—C58	51.0 (17)	C39—C40—C47—C48	−118.8 (6)
N11—Ni3—N10—C58	92.3 (7)	N8—C40—C47—C52	−62.3 (8)
N9—Ni3—N10—C58	−0.7 (6)	C39—C40—C47—C52	61.2 (8)
Cl4—Ni3—N10—C58	−91.0 (6)	C52—C47—C48—C49	0.0
Cl3—Ni3—N10—C58	177.8 (6)	C40—C47—C48—C49	180.0 (6)
N10—Ni3—N11—C73	11.2 (10)	C47—C48—C49—C50	0.0
N12—Ni3—N11—C73	−177.6 (10)	C48—C49—C50—C51	0.0
N9—Ni3—N11—C73	90.2 (10)	C49—C50—C51—C52	0.0
Cl3—Ni3—N11—C73	−86.0 (10)	C50—C51—C52—C47	0.0
N10—Ni3—N11—C65	−175.0 (7)	C48—C47—C52—C51	0.0
N12—Ni3—N11—C65	−3.8 (6)	C40—C47—C52—C51	−180.0 (7)
N9—Ni3—N11—C65	−96.0 (7)	C61—N9—C53—C54	−0.1 (13)
Cl3—Ni3—N11—C65	87.8 (6)	Ni3—N9—C53—C54	−177.0 (3)
N10—Ni3—N12—C76	−134.3 (13)	C61—N9—C53—C58	−177.7 (8)
N11—Ni3—N12—C76	−176.6 (11)	Ni3—N9—C53—C58	5.4 (8)
N9—Ni3—N12—C76	−83.9 (10)	N9—C53—C54—C55	−177.5 (7)
Cl4—Ni3—N12—C76	7.3 (10)	C58—C53—C54—C55	0.0

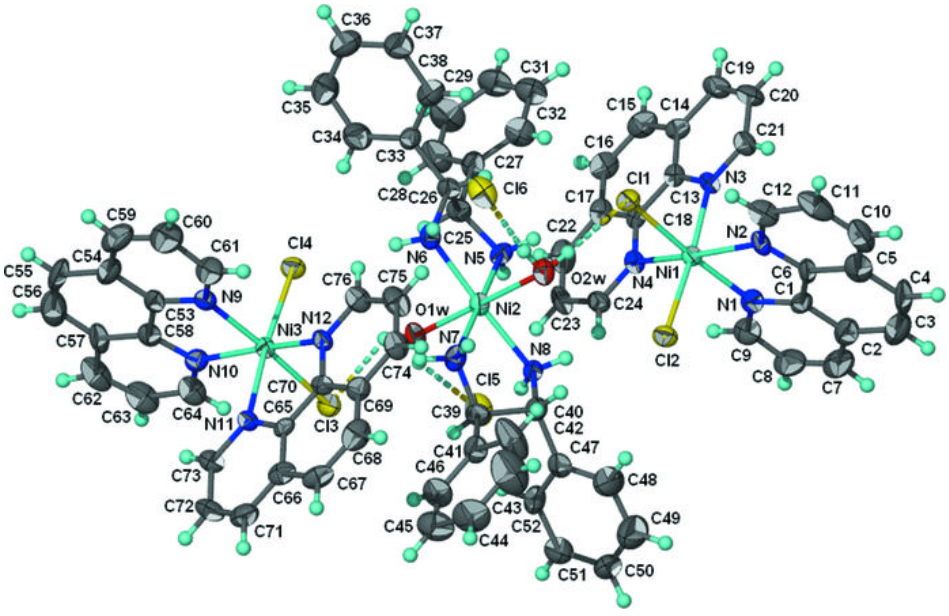
Cl3—Ni3—N12—C76	98.3 (10)	N9—C53—C54—C59	1.8 (9)
N10—Ni3—N12—C70	45.0 (18)	C58—C53—C54—C59	179.3 (9)
N11—Ni3—N12—C70	2.7 (6)	C53—C54—C55—C56	0.0
N9—Ni3—N12—C70	95.4 (7)	C59—C54—C55—C56	−179.3 (10)
Cl4—Ni3—N12—C70	−173.4 (6)	C54—C55—C56—C57	0.0
Cl3—Ni3—N12—C70	−82.4 (6)	C55—C56—C57—C62	179.6 (10)
C9—N1—C1—C2	2.9 (12)	C55—C56—C57—C58	0.0
Ni1—N1—C1—C2	177.9 (4)	C64—N10—C58—C57	−1.3 (12)
C9—N1—C1—C6	178.4 (8)	Ni3—N10—C58—C57	179.8 (3)
Ni1—N1—C1—C6	−6.7 (8)	C64—N10—C58—C53	−177.3 (8)
N1—C1—C2—C7	−5.1 (9)	Ni3—N10—C58—C53	3.8 (8)
C6—C1—C2—C7	179.5 (9)	C62—C57—C58—N10	4.6 (9)
N1—C1—C2—C3	175.4 (7)	C56—C57—C58—N10	−175.8 (7)
C6—C1—C2—C3	0.0	C62—C57—C58—C53	−179.6 (9)
C7—C2—C3—C4	−179.5 (10)	C56—C57—C58—C53	0.0
C1—C2—C3—C4	0.0	N9—C53—C58—N10	−6.3 (9)
C2—C3—C4—C5	0.0	C54—C53—C58—N10	176.0 (7)
C3—C4—C5—C10	−179.2 (10)	N9—C53—C58—C57	177.6 (7)
C3—C4—C5—C6	0.0	C54—C53—C58—C57	0.0
C12—N2—C6—C5	2.6 (12)	C55—C54—C59—C60	177.4 (10)
Ni1—N2—C6—C5	179.3 (3)	C53—C54—C59—C60	−1.9 (16)
C12—N2—C6—C1	−179.7 (8)	C54—C59—C60—C61	0(2)
Ni1—N2—C6—C1	−3.0 (8)	C53—N9—C61—C60	−1.5 (18)
C10—C5—C6—N2	−3.1 (9)	Ni3—N9—C61—C60	174.8 (9)
C4—C5—C6—N2	177.6 (7)	C59—C60—C61—N9	1(2)
C10—C5—C6—C1	179.3 (9)	C56—C57—C62—C63	175.7 (8)
C4—C5—C6—C1	0.0	C58—C57—C62—C63	−4.7 (14)
N1—C1—C6—N2	6.7 (9)	C57—C62—C63—C64	1.9 (18)
C2—C1—C6—N2	−177.7 (7)	C58—N10—C64—C63	−1.7 (18)
N1—C1—C6—C5	−175.5 (7)	Ni3—N10—C64—C63	177.0 (8)
C2—C1—C6—C5	0.0	C62—C63—C64—N10	1.4 (19)
C1—C2—C7—C8	3.8 (15)	C73—N11—C65—C66	−3.5 (12)
C3—C2—C7—C8	−176.7 (9)	Ni3—N11—C65—C66	−178.0 (4)
C2—C7—C8—C9	−0.5 (18)	C73—N11—C65—C70	178.9 (8)
C1—N1—C9—C8	0.6 (18)	Ni3—N11—C65—C70	4.4 (8)
Ni1—N1—C9—C8	−173.3 (8)	N11—C65—C66—C67	−177.6 (8)
C7—C8—C9—N1	−1.8 (19)	C70—C65—C66—C67	0.0
C6—C5—C10—C11	1.2 (15)	N11—C65—C66—C71	5.9 (9)
C4—C5—C10—C11	−179.6 (9)	C70—C65—C66—C71	−176.5 (8)
C5—C10—C11—C12	1.2 (19)	C65—C66—C67—C68	0.0
C6—N2—C12—C11	0.0 (17)	C71—C66—C67—C68	176.3 (8)
Ni1—N2—C12—C11	−176.3 (7)	C66—C67—C68—C69	0.0
C10—C11—C12—N2	−1.8 (18)	C67—C68—C69—C70	0.0
C21—N3—C13—C14	4.2 (12)	C67—C68—C69—C74	179.4 (8)
Ni1—N3—C13—C14	177.9 (4)	C76—N12—C70—C69	−1.8 (12)
C21—N3—C13—C18	−178.0 (8)	Ni3—N12—C70—C69	178.9 (4)
Ni1—N3—C13—C18	−4.2 (8)	C76—N12—C70—C65	178.1 (8)
N3—C13—C14—C15	177.8 (8)	Ni3—N12—C70—C65	−1.2 (8)
C18—C13—C14—C15	0.0	C68—C69—C70—N12	179.9 (8)

N3—C13—C14—C19	−3.4 (9)	C74—C69—C70—N12	0.5 (9)
C18—C13—C14—C19	178.8 (8)	C68—C69—C70—C65	0.0
C13—C14—C15—C16	0.0	C74—C69—C70—C65	−179.4 (8)
C19—C14—C15—C16	−178.7 (8)	N11—C65—C70—N12	−2.2 (9)
C14—C15—C16—C17	0.0	C66—C65—C70—N12	−179.9 (8)
C15—C16—C17—C18	0.0	N11—C65—C70—C69	177.7 (8)
C15—C16—C17—C22	180.0 (9)	C66—C65—C70—C69	0.0
C24—N4—C18—C17	−0.2 (12)	C65—C66—C71—C72	−4.0 (14)
Ni1—N4—C18—C17	−178.7 (4)	C67—C66—C71—C72	179.6 (9)
C24—N4—C18—C13	−179.8 (8)	C66—C71—C72—C73	−0.2 (18)
Ni1—N4—C18—C13	1.8 (8)	C65—N11—C73—C72	−1.1 (16)
C16—C17—C18—N4	−179.6 (8)	Ni3—N11—C73—C72	172.4 (9)
C22—C17—C18—N4	0.4 (9)	C71—C72—C73—N11	2.8 (18)
C16—C17—C18—C13	0.0	C68—C69—C74—C75	179.7 (9)
C22—C17—C18—C13	180.0 (8)	C70—C69—C74—C75	−0.9 (14)
N3—C13—C18—N4	1.7 (9)	C69—C74—C75—C76	2.6 (19)
C14—C13—C18—N4	179.6 (8)	C70—N12—C76—C75	3.5 (18)
N3—C13—C18—C17	−177.9 (8)	Ni3—N12—C76—C75	−177.2 (9)
C14—C13—C18—C17	0.0	C74—C75—C76—N12	−4(2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W1···Cl3	0.82	2.50	3.185 (8)	142
O1W—H1W2···Cl5	0.82	2.41	3.095 (10)	141
O2W—H2W1···Cl1	0.82	2.36	3.182 (8)	180
O2W—H2W2···Cl6	0.82	2.31	3.123 (10)	172

Fig. 1


C36
C37
C38
C29
C31
C35
C32
C34
C33
C27
C28
C26
Cl6
C59
C60
C61
Cl4
C54
C55
C56
N9
C53
C58
C57
N10
C62
C63
C64
N11
Ni3
N12
C76
C75
C25
N6
N5
C22
O2w
N4
Ni1
C24
C23
O1w
Ni2
N7
N8
Cl5
C74
C70
C65
C69
Cl3
C68
C67
C66
C73
C72
C71
C39
C40
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N3
C12
C11
C10
N2
C5
C6
C1
C4
N1
C3
C9
C2
C8
C7
Cl2