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[*N*,*N*′-Bis(pyrrol-2-ylmethylene)cyclohexane-1,2-diaminato-κ^4N]nickel(II)

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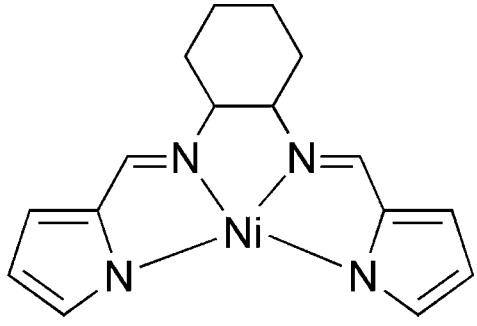
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.010 Å; disorder in main residue; R factor = 0.061; wR factor = 0.136; data-to-parameter ratio = 14.6.

The tetradentate Schiff base ligand derived from the condensation of pyrrole-2-carbaldehyde and cyclohexane-1,2-diamine forms a square-planar four-coordinate Ni complex, [Ni($C_{16}H_{18}N_4$)]. The compound crystallizes with two crystallographically independent molecules in the asymmetric unit.

Related literature

For related literature, see: Bacchi *et al.* (2003); Baleizao & Garcia (2006); Bella *et al.* (2004); Carey *et al.* (2004); Downing & Urbach (1971); Maruyama *et al.* (1990); Rigamonti *et al.* (2006); Tedim *et al.* (2006); Weber (1967).



Experimental

Crystal data

[Ni($C_{16}H_{18}N_4$)]
M_r = 325.05
Monoclinic, $P2_1/c$
a = 21.379 (3) Å
b = 8.6247 (10) Å
c = 17.475 (2) Å
β = 111.697 (2)°
V = 2993.9 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.29 mm^{-1}
T = 294 (2) K
0.26 × 0.22 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.730, T_{max} = 0.800
16412 measured reflections
6100 independent reflections
4081 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.136
S = 1.15
6100 reflections
418 parameters
12 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—N2	1.850 (4)	Ni2—N6	1.844 (5)
Ni1—N3	1.855 (4)	Ni2—N7	1.851 (4)
Ni1—N1	1.887 (4)	Ni2—N8	1.883 (4)
Ni1—N4	1.889 (4)	Ni2—N5	1.888 (5)
N2—Ni1—N3	84.00 (19)	N6—Ni2—N7	84.9 (2)
N2—Ni1—N1	84.78 (19)	N7—Ni2—N8	84.12 (19)
N3—Ni1—N4	84.49 (19)	N6—Ni2—N5	84.3 (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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2334).

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supplementary materials

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[*N*,*N*'-Bis(pyrrol-2-ylmethylene)cyclohexane-1,2-diaminato-κ^4N]nickel(II)

J.-M. Chen, W.-J. Ruan, F. Gao, Y.-H. Zhang and Z.-A. Zhu

Comment

salen ligands (salen = *N*,*N*'-bis(salicyldene)ethylenediamine) and their complexes have received continuous and intensive attention because of their capabilities to serve as catalysts of organic reactions (Baleizao & Garcia, 2006), models of catalytic centers of metalloenzymes (Maruyama *et al.*, 1990; Carey *et al.*, 2004) and nonlinear optical materials (Rigamonti *et al.*, 2006; Tedim *et al.*, 2006). On the contrary, little is known about the ligand behaviour of the analogous compounds derived from pyrrole 2-carboxaldehyde and about the properties of their complexes (Weber, 1967; Downing & Urbach, 1971; Bacchi *et al.*, 2003, Bella *et al.*, 2004). In the present work, we have prepared the title compound (I) and determined its crystal structure.

The complex crystallizes with two crystallographically independent, but quite similar molecules in the asymmetric unit. In both molecules, the ligand is bideprotonated and the Ni(II) ion is tetracoordinated in a square planar environment, with the pyrrole and imine nitrogen atoms as donors. The coordination induces the formation of three five-membered chelate rings, and the N—Ni—N angles are less than 90°. The Ni—N (pyrrole) distances are significantly longer than the Ni—N (imine) distances.

Experimental

The title complex was synthesized by dissolving *N*,*N*'-bis(pyrrol-2- ylmethylene)cyclohexylenediamine (1 mmol, 268 mg) in ethanol (15 ml), with the addition of nickel(II) acetate (1 mmol, 212 mg) dissolved in distilled water (5 ml). The mixture was stirred at room temperature for 2 h and the resulting red–brown precipitate was filtered, dried and chromatographed on silica gel eluted with $CHCl_3$. Crystals suitable for X-ray diffraction analysis were obtained by recrystallization from a $CHCl_3$ solution. Elemental composition, calculated: C 59.12, H 5.58, N 17.24%; found: C 59.14, H 5.45, N 17.35%. M^+ = 324 g mol^{-1}. ^{1}H NMR (300 MHz, $CDCl_3$, 298 K, TMS): 7.23 (s, 2H, H imine), 6.80 (s, 2H, H pyrrole α), 6.59 (t, J = 3.6 Hz, 2H, H pyrrole γ), 6.13 (t, J = 3.0 Hz, 2H, *H*

pyrrole β), 3.34 (t, J = 3.5 Hz, 2H, CH), 2.24–1.31 (m, 8H, CH_2).

Refinement

The two cyclohexane-1,2-diamine groups are disordered, with site-occupation factors of 0.495 (15) for atoms C6 and C11, 0.505 (15) for atoms C6' and C11', and 0.50 (3) for atoms C22, C27, C22' and C27'. H atoms were positioned geometrically and allowed to ride on their parent C atoms, with C—H ranging from 0.93 to 0.98 Å and U_{iso}(H) = 1.2Ueq(C).

Figures

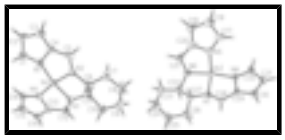


Fig. 1. A view of the title complex, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented by circles of arbitrary size, and only one set of disordered C atoms are represented.

[*N*,*N*'-Bis(pyrrol-2-ylmethylene)cyclohexane-1,2-diaminato-κ^4N]nickel(II)

Crystal data

$[Ni(C_{16}H_{18}N_4)]$	F_{000} = 1360
M_r = 325.05	D_x = 1.442 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 21.379 (3) Å	Cell parameters from 4354 reflections
b = 8.6247 (10) Å	θ = 2.5–25.5º
c = 17.475 (2) Å	μ = 1.29 mm^{-1}
β = 111.697 (2)º	T = 294 (2) K
V = 2993.9 (6) Å^3	Block, red
Z = 8	0.26 × 0.22 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer	6100 independent reflections
Radiation source: fine-focus sealed tube	4081 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.040
T = 294(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 1.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −26→25
T_{min} = 0.730, T_{max} = 0.800	k = −10→7
16412 measured reflections	l = −20→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.061	H-atom parameters constrained
$wR(F^2)$ = 0.136	$w = 1/[\sigma^2(F_o^2) + 10.3102P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.15	$(\Delta/\sigma)_{max}$ = 0.001
6100 reflections	$\Delta\rho_{max}$ = 0.39 e Å^{-3}
418 parameters	$\Delta\rho_{min}$ = −0.41 e Å^{-3}

12 restraints

Primary atom site location: structure-invariant direct methods

Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.00459 (17)

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)
Ni1	1.03966 (3)	0.31724 (8)	0.46424 (4)	0.0414 (2)	
Ni2	0.46464 (3)	0.30951 (8)	0.42360 (4)	0.0433 (2)	
N1	1.0592 (2)	0.4251 (5)	0.3818 (3)	0.0465 (11)	
N2	0.9512 (2)	0.3281 (5)	0.3915 (3)	0.0474 (11)	
N3	1.0027 (2)	0.2221 (5)	0.5330 (3)	0.0469 (11)	
N4	1.1217 (2)	0.3006 (5)	0.5555 (3)	0.0459 (11)	
N5	0.4469 (3)	0.4146 (5)	0.3230 (3)	0.0508 (12)	
N6	0.5536 (2)	0.3479 (5)	0.4403 (3)	0.0515 (12)	
N7	0.4986 (2)	0.2207 (5)	0.5273 (3)	0.0449 (11)	
N8	0.3804 (2)	0.2682 (5)	0.4305 (3)	0.0437 (11)	
C1	1.1105 (3)	0.4849 (7)	0.3641 (4)	0.0562 (15)	
H1	1.1558	0.4715	0.3962	0.067*	
C2	1.0866 (4)	0.5684 (8)	0.2921 (4)	0.0667 (18)	
H2	1.1124	0.6202	0.2675	0.080*	
C3	1.0173 (4)	0.5614 (7)	0.2631 (4)	0.0613 (17)	
H3	0.9876	0.6084	0.2157	0.074*	
C4	1.0007 (3)	0.4706 (6)	0.3183 (3)	0.0482 (14)	
C5	0.9415 (3)	0.4129 (7)	0.3273 (3)	0.0542 (15)	
H5	0.8986	0.4350	0.2895	0.065*	
C6	0.9065 (4)	0.2229 (14)	0.4133 (6)	0.047 (4)	0.495 (15)
H6A	0.9163	0.1172	0.4006	0.056*	0.495 (15)
C11	0.9294 (4)	0.2363 (14)	0.5065 (7)	0.047 (4)	0.495 (15)
H11A	0.9185	0.3402	0.5205	0.057*	0.495 (15)
C6'	0.9007 (4)	0.2944 (15)	0.4278 (6)	0.050 (4)	0.505 (15)
H6B	0.8968	0.3850	0.4596	0.060*	0.505 (15)
C11'	0.9339 (4)	0.1640 (15)	0.4875 (6)	0.050 (4)	0.505 (15)
H11B	0.9373	0.0735	0.4553	0.060*	0.505 (15)
C22	0.6002 (8)	0.249 (3)	0.5056 (13)	0.057 (5)	0.50 (3)
H22A	0.5986	0.1425	0.4848	0.068*	0.50 (3)

C27	0.5722 (7)	0.251 (3)	0.5742 (11)	0.046 (4)	0.50 (3)
H27A	0.5767	0.3567	0.5959	0.056*	0.50 (3)
C22'	0.6023 (7)	0.322 (3)	0.5298 (11)	0.050 (5)	0.50 (3)
H22B	0.5981	0.4097	0.5631	0.060*	0.50 (3)
C27'	0.5723 (7)	0.183 (3)	0.5538 (12)	0.046 (4)	0.50 (3)
H27B	0.5773	0.0947	0.5214	0.055*	0.50 (3)
C7	0.8311 (3)	0.2486 (8)	0.3704 (4)	0.0646 (18)	
H7A	0.8220	0.3590	0.3691	0.078*	0.495 (15)
H7B	0.8174	0.2133	0.3138	0.078*	0.495 (15)
H7C	0.8074	0.3414	0.3436	0.078*	0.505 (15)
H7D	0.8353	0.1818	0.3278	0.078*	0.505 (15)
C8	0.7908 (4)	0.1694 (14)	0.4093 (5)	0.129 (4)	
H8A	0.7676	0.0857	0.3728	0.155*	
H8B	0.7565	0.2421	0.4104	0.155*	
C9	0.8204 (4)	0.1035 (12)	0.4915 (6)	0.113 (3)	
H9A	0.8095	−0.0061	0.4868	0.136*	
H9B	0.7973	0.1494	0.5244	0.136*	
C10	0.8935 (3)	0.1169 (7)	0.5396 (4)	0.0586 (16)	
H10A	0.9143	0.0165	0.5406	0.070*	0.495 (15)
H10B	0.9001	0.1440	0.5959	0.070*	0.495 (15)
H10C	0.9102	0.0181	0.5656	0.070*	0.505 (15)
H10D	0.9007	0.1930	0.5829	0.070*	0.505 (15)
C12	1.0435 (3)	0.2008 (6)	0.6084 (3)	0.0508 (14)	
H12	1.0295	0.1614	0.6490	0.061*	
C13	1.1108 (3)	0.2424 (6)	0.6237 (3)	0.0479 (14)	
C14	1.1706 (3)	0.2436 (7)	0.6910 (4)	0.0601 (16)	
H14	1.1770	0.2104	0.7439	0.072*	
C15	1.2192 (3)	0.3041 (8)	0.6645 (4)	0.0642 (17)	
H15	1.2644	0.3198	0.6963	0.077*	
C16	1.1871 (3)	0.3367 (6)	0.5807 (4)	0.0514 (14)	
H16	1.2082	0.3776	0.5472	0.062*	
C17	0.3959 (4)	0.4642 (7)	0.2550 (4)	0.0617 (17)	
H17	0.3508	0.4398	0.2417	0.074*	
C18	0.4210 (4)	0.5572 (8)	0.2080 (4)	0.072 (2)	
H18	0.3959	0.6039	0.1580	0.086*	
C19	0.4893 (4)	0.5680 (7)	0.2480 (4)	0.071 (2)	
H19	0.5191	0.6250	0.2317	0.085*	
C20	0.5050 (4)	0.4761 (7)	0.3185 (4)	0.0573 (16)	
C21	0.5638 (3)	0.4361 (7)	0.3859 (4)	0.0609 (17)	
H21	0.6064	0.4702	0.3909	0.073*	
C23	0.6741 (3)	0.3039 (9)	0.5423 (4)	0.0725 (19)	
H23A	0.6960	0.2780	0.5042	0.087*	0.50 (3)
H23B	0.6747	0.4158	0.5477	0.087*	0.50 (3)
H23C	0.6779	0.2379	0.4992	0.087*	0.50 (3)
H23D	0.6929	0.4044	0.5380	0.087*	0.50 (3)
C24	0.7123 (4)	0.2366 (13)	0.6217 (6)	0.127 (4)	
H24A	0.7394	0.3196	0.6553	0.153*	
H24B	0.7434	0.1636	0.6128	0.153*	
C25	0.6814 (4)	0.1572 (11)	0.6722 (5)	0.103 (3)	

H25A	0.6971	0.2081	0.7255	0.124*	
H25B	0.6993	0.0525	0.6812	0.124*	
C26	0.6071 (3)	0.1450 (7)	0.6440 (4)	0.0592 (16)	
H26A	0.5932	0.1695	0.6896	0.071*	0.50 (3)
H26B	0.5937	0.0391	0.6273	0.071*	0.50 (3)
H26C	0.5911	0.2148	0.6764	0.071*	0.50 (3)
H26D	0.5951	0.0402	0.6535	0.071*	0.50 (3)
C28	0.4559 (3)	0.1853 (6)	0.5596 (3)	0.0461 (13)	
H28	0.4685	0.1472	0.6129	0.055*	
C29	0.3878 (3)	0.2089 (6)	0.5076 (3)	0.0439 (13)	
C30	0.3251 (3)	0.1884 (7)	0.5121 (4)	0.0581 (15)	
H30	0.3162	0.1509	0.5570	0.070*	
C31	0.2781 (3)	0.2348 (7)	0.4368 (4)	0.0603 (16)	
H31	0.2315	0.2333	0.4212	0.072*	
C32	0.3138 (3)	0.2840 (7)	0.3890 (4)	0.0544 (15)	
H32	0.2943	0.3225	0.3357	0.065*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0458 (4)	0.0390 (4)	0.0391 (4)	0.0018 (3)	0.0154 (3)	−0.0003 (3)
Ni2	0.0506 (4)	0.0389 (4)	0.0453 (4)	−0.0012 (3)	0.0233 (3)	−0.0032 (3)
N1	0.053 (3)	0.047 (3)	0.040 (2)	0.003 (2)	0.018 (2)	0.002 (2)
N2	0.047 (3)	0.051 (3)	0.040 (2)	0.000 (2)	0.011 (2)	−0.003 (2)
N3	0.045 (3)	0.051 (3)	0.046 (3)	0.006 (2)	0.019 (2)	0.006 (2)
N4	0.046 (3)	0.043 (3)	0.047 (3)	0.004 (2)	0.016 (2)	0.001 (2)
N5	0.071 (3)	0.041 (3)	0.049 (3)	0.000 (2)	0.033 (3)	−0.006 (2)
N6	0.060 (3)	0.052 (3)	0.054 (3)	−0.001 (2)	0.035 (3)	−0.004 (2)
N7	0.041 (2)	0.043 (3)	0.050 (3)	−0.002 (2)	0.016 (2)	−0.001 (2)
N8	0.046 (3)	0.040 (3)	0.047 (3)	−0.002 (2)	0.019 (2)	−0.002 (2)
C1	0.062 (4)	0.054 (4)	0.057 (4)	0.003 (3)	0.028 (3)	0.002 (3)
C2	0.095 (5)	0.060 (4)	0.059 (4)	−0.008 (4)	0.045 (4)	0.004 (3)
C3	0.086 (5)	0.055 (4)	0.043 (3)	0.004 (4)	0.024 (3)	0.005 (3)
C4	0.063 (4)	0.039 (3)	0.043 (3)	0.004 (3)	0.020 (3)	−0.002 (3)
C5	0.059 (4)	0.048 (3)	0.045 (3)	0.010 (3)	0.006 (3)	−0.003 (3)
C6	0.049 (8)	0.037 (8)	0.052 (8)	0.000 (6)	0.016 (6)	−0.007 (6)
C11	0.044 (7)	0.046 (8)	0.061 (9)	0.010 (6)	0.031 (6)	0.000 (7)
C6'	0.056 (8)	0.054 (9)	0.047 (8)	−0.004 (7)	0.027 (6)	−0.006 (7)
C11'	0.051 (8)	0.050 (9)	0.060 (9)	0.006 (6)	0.033 (7)	0.007 (7)
C22	0.061 (9)	0.055 (10)	0.064 (10)	−0.019 (8)	0.035 (8)	−0.023 (8)
C27	0.044 (7)	0.047 (10)	0.053 (9)	−0.002 (7)	0.023 (6)	−0.021 (7)
C22'	0.040 (7)	0.062 (12)	0.045 (8)	−0.010 (7)	0.013 (6)	−0.017 (8)
C27'	0.049 (7)	0.036 (10)	0.053 (9)	0.006 (7)	0.019 (6)	−0.011 (7)
C7	0.044 (3)	0.071 (4)	0.074 (4)	0.002 (3)	0.017 (3)	−0.005 (3)
C8	0.057 (5)	0.217 (12)	0.108 (7)	−0.036 (7)	0.025 (5)	0.017 (8)
C9	0.072 (6)	0.139 (9)	0.142 (8)	−0.019 (5)	0.055 (6)	0.032 (7)
C10	0.062 (4)	0.054 (4)	0.068 (4)	−0.006 (3)	0.034 (3)	−0.008 (3)
C12	0.063 (4)	0.043 (3)	0.050 (3)	0.010 (3)	0.026 (3)	0.002 (3)

C13	0.059 (4)	0.043 (3)	0.042 (3)	0.009 (3)	0.019 (3)	0.003 (2)
C14	0.063 (4)	0.064 (4)	0.044 (3)	0.003 (3)	0.008 (3)	0.006 (3)
C15	0.054 (4)	0.060 (4)	0.062 (4)	0.005 (3)	0.003 (3)	0.002 (3)
C16	0.048 (3)	0.046 (3)	0.059 (4)	0.003 (3)	0.018 (3)	−0.002 (3)
C17	0.090 (5)	0.048 (4)	0.051 (4)	0.006 (3)	0.030 (4)	−0.003 (3)
C18	0.114 (6)	0.056 (4)	0.051 (4)	0.004 (4)	0.036 (4)	0.002 (3)
C19	0.117 (6)	0.044 (4)	0.078 (5)	0.001 (4)	0.067 (5)	0.001 (3)
C20	0.088 (5)	0.043 (3)	0.056 (4)	0.003 (3)	0.044 (4)	−0.004 (3)
C21	0.071 (4)	0.051 (4)	0.082 (5)	−0.013 (3)	0.053 (4)	−0.014 (3)
C23	0.049 (4)	0.081 (5)	0.091 (5)	−0.009 (4)	0.030 (4)	−0.020 (4)
C24	0.053 (5)	0.170 (10)	0.138 (9)	−0.011 (6)	0.011 (5)	0.045 (8)
C25	0.061 (5)	0.136 (8)	0.092 (6)	0.015 (5)	0.004 (4)	0.012 (6)
C26	0.060 (4)	0.052 (4)	0.058 (4)	0.005 (3)	0.012 (3)	−0.010 (3)
C28	0.049 (3)	0.040 (3)	0.049 (3)	−0.002 (3)	0.017 (3)	0.009 (3)
C29	0.047 (3)	0.041 (3)	0.046 (3)	0.000 (2)	0.020 (3)	−0.002 (2)
C30	0.056 (4)	0.059 (4)	0.068 (4)	−0.005 (3)	0.033 (3)	−0.006 (3)
C31	0.044 (3)	0.062 (4)	0.075 (4)	−0.001 (3)	0.022 (3)	−0.003 (3)
C32	0.046 (3)	0.051 (4)	0.057 (4)	0.000 (3)	0.010 (3)	−0.006 (3)

Geometric parameters (Å, °)

Ni1—N2	1.850 (4)	C27'—H27B	0.9800
Ni1—N3	1.855 (4)	C7—C8	1.452 (10)
Ni1—N1	1.887 (4)	C7—H7A	0.9700
Ni1—N4	1.889 (4)	C7—H7B	0.9700
Ni2—N6	1.844 (5)	C7—H7C	0.9700
Ni2—N7	1.851 (4)	C7—H7D	0.9700
Ni2—N8	1.883 (4)	C8—C9	1.454 (8)
Ni2—N5	1.888 (5)	C8—H8A	0.9700
N1—C1	1.347 (7)	C8—H8B	0.9700
N1—C4	1.387 (7)	C9—C10	1.481 (9)
N2—C5	1.290 (7)	C9—H9A	0.9700
N2—C6	1.466 (8)	C9—H9B	0.9700
N2—C6'	1.470 (8)	C10—H10A	0.9700
N3—C12	1.297 (7)	C10—H10B	0.9700
N3—C11	1.466 (8)	C10—H10C	0.9700
N3—C11'	1.477 (9)	C10—H10D	0.9700
N4—C16	1.340 (7)	C12—C13	1.410 (8)
N4—C13	1.390 (7)	C12—H12	0.9300
N5—C17	1.351 (7)	C13—C14	1.379 (8)
N5—C20	1.378 (7)	C14—C15	1.388 (9)
N6—C21	1.297 (7)	C14—H14	0.9300
N6—C22	1.480 (18)	C15—C16	1.396 (8)
N6—C22'	1.543 (16)	C15—H15	0.9300
N7—C28	1.274 (6)	C16—H16	0.9300
N7—C27	1.503 (15)	C17—C18	1.391 (9)
N7—C27'	1.504 (15)	C17—H17	0.9300
N8—C32	1.345 (7)	C18—C19	1.368 (10)
N8—C29	1.394 (6)	C18—H18	0.9300

C1—C2	1.374 (8)	C19—C20	1.397 (9)
C1—H1	0.9300	C19—H19	0.9300
C2—C3	1.378 (9)	C20—C21	1.412 (9)
C2—H2	0.9300	C21—H21	0.9300
C3—C4	1.387 (8)	C23—C24	1.446 (10)
C3—H3	0.9300	C23—H23A	0.9700
C4—C5	1.423 (8)	C23—H23B	0.9700
C5—H5	0.9300	C23—H23C	0.9700
C6—C7	1.521 (9)	C23—H23D	0.9700
C6—C11	1.523 (9)	C24—C25	1.454 (8)
C6—H6A	0.9800	C24—H24A	0.9700
C11—C10	1.520 (9)	C24—H24B	0.9700
C11—H11A	0.9800	C25—C26	1.484 (9)
C6'—C7	1.507 (9)	C25—H25A	0.9700
C6'—C11'	1.520 (9)	C25—H25B	0.9700
C6'—H6B	0.9800	C26—H26A	0.9700
C11'—C10	1.523 (8)	C26—H26B	0.9700
C11'—H11B	0.9800	C26—H26C	0.9700
C22—C27	1.53 (3)	C26—H26D	0.9700
C22—C23	1.545 (17)	C28—C29	1.417 (7)
C22—H22A	0.9800	C28—H28	0.9300
C27—C26	1.485 (18)	C29—C30	1.383 (7)
C27—H27A	0.9800	C30—C31	1.388 (8)
C22'—C23	1.477 (15)	C30—H30	0.9300
C22'—C27'	1.49 (3)	C31—C32	1.389 (8)
C22'—H22B	0.9800	C31—H31	0.9300
C27'—C26	1.511 (18)	C32—H32	0.9300
N2—Ni1—N3	84.00 (19)	C7—C8—C9	122.0 (7)
N2—Ni1—N1	84.78 (19)	C7—C8—H8A	106.8
N3—Ni1—N1	168.47 (19)	C9—C8—H8A	106.8
N2—Ni1—N4	167.79 (19)	C7—C8—H8B	106.8
N3—Ni1—N4	84.49 (19)	C9—C8—H8B	106.8
N1—Ni1—N4	106.5 (2)	H8A—C8—H8B	106.7
N6—Ni2—N7	84.9 (2)	C8—C9—C10	120.8 (6)
N6—Ni2—N8	168.2 (2)	C8—C9—H9A	107.1
N7—Ni2—N8	84.12 (19)	C10—C9—H9A	107.1
N6—Ni2—N5	84.3 (2)	C8—C9—H9B	107.1
N7—Ni2—N5	169.0 (2)	C10—C9—H9B	107.1
N8—Ni2—N5	106.4 (2)	H9A—C9—H9B	106.8
C1—N1—C4	106.2 (5)	C9—C10—C11	114.4 (6)
C1—N1—Ni1	142.4 (4)	C9—C10—C11'	113.2 (6)
C4—N1—Ni1	111.2 (4)	C11—C10—C11'	27.7 (5)
C5—N2—C6	131.7 (6)	C9—C10—H10A	108.7
C5—N2—C6'	125.4 (6)	C11—C10—H10A	108.7
C6—N2—C6'	27.4 (5)	C11'—C10—H10A	83.8
C5—N2—Ni1	114.9 (4)	C9—C10—H10B	108.7
C6—N2—Ni1	112.9 (4)	C11—C10—H10B	108.7
C6'—N2—Ni1	114.9 (4)	C11'—C10—H10B	129.9
C12—N3—C11	124.8 (6)	H10A—C10—H10B	107.6

C12—N3—C11'	131.3 (6)	C9—C10—H10C	108.9
C11—N3—C11'	28.7 (5)	C11—C10—H10C	128.6
C12—N3—Ni1	115.7 (4)	C11'—C10—H10C	108.9
C11—N3—Ni1	114.8 (4)	H10A—C10—H10C	28.4
C11'—N3—Ni1	112.3 (4)	H10B—C10—H10C	81.1
C16—N4—C13	106.7 (5)	C9—C10—H10D	108.9
C16—N4—Ni1	142.2 (4)	C11—C10—H10D	83.3
C13—N4—Ni1	110.8 (4)	C11'—C10—H10D	109.0
C17—N5—C20	106.2 (5)	H10A—C10—H10D	130.6
C17—N5—Ni2	142.1 (5)	H10B—C10—H10D	28.8
C20—N5—Ni2	111.3 (4)	H10C—C10—H10D	107.7
C21—N6—C22	131.0 (8)	N3—C12—C13	114.4 (5)
C21—N6—C22'	126.6 (8)	N3—C12—H12	122.8
C22—N6—C22'	28.7 (6)	C13—C12—H12	122.8
C21—N6—Ni2	115.7 (4)	C14—C13—N4	109.4 (5)
C22—N6—Ni2	112.3 (6)	C14—C13—C12	136.3 (6)
C22'—N6—Ni2	113.8 (6)	N4—C13—C12	114.3 (5)
C28—N7—C27	125.3 (8)	C13—C14—C15	106.9 (5)
C28—N7—C27'	130.8 (8)	C13—C14—H14	126.5
C27—N7—C27'	26.2 (5)	C15—C14—H14	126.5
C28—N7—Ni2	116.5 (4)	C14—C15—C16	106.7 (5)
C27—N7—Ni2	114.5 (7)	C14—C15—H15	126.7
C27'—N7—Ni2	112.1 (7)	C16—C15—H15	126.7
C32—N8—C29	106.1 (5)	N4—C16—C15	110.3 (6)
C32—N8—Ni2	142.5 (4)	N4—C16—H16	124.9
C29—N8—Ni2	111.2 (3)	C15—C16—H16	124.9
N1—C1—C2	110.6 (6)	N5—C17—C18	109.9 (6)
N1—C1—H1	124.7	N5—C17—H17	125.1
C2—C1—H1	124.7	C18—C17—H17	125.1
C1—C2—C3	107.4 (6)	C19—C18—C17	107.9 (6)
C1—C2—H2	126.3	C19—C18—H18	126.0
C3—C2—H2	126.3	C17—C18—H18	126.0
C2—C3—C4	106.6 (6)	C18—C19—C20	106.0 (6)
C2—C3—H3	126.7	C18—C19—H19	127.0
C4—C3—H3	126.7	C20—C19—H19	127.0
N1—C4—C3	109.2 (5)	N5—C20—C19	109.9 (6)
N1—C4—C5	112.9 (5)	N5—C20—C21	113.7 (5)
C3—C4—C5	137.9 (6)	C19—C20—C21	136.4 (7)
N2—C5—C4	115.5 (5)	N6—C21—C20	114.5 (6)
N2—C5—H5	122.2	N6—C21—H21	122.7
C4—C5—H5	122.2	C20—C21—H21	122.7
N2—C6—C7	117.1 (7)	C24—C23—C22'	111.7 (8)
N2—C6—C11	104.3 (7)	C24—C23—C22	113.7 (9)
C7—C6—C11	112.4 (8)	C22'—C23—C22	28.7 (6)
N2—C6—H6A	107.5	C24—C23—H23A	108.8
C7—C6—H6A	107.5	C22'—C23—H23A	131.4
C11—C6—H6A	107.5	C22—C23—H23A	108.8
N3—C11—C10	117.0 (7)	C24—C23—H23B	108.8
N3—C11—C6	102.5 (7)	C22'—C23—H23B	83.5

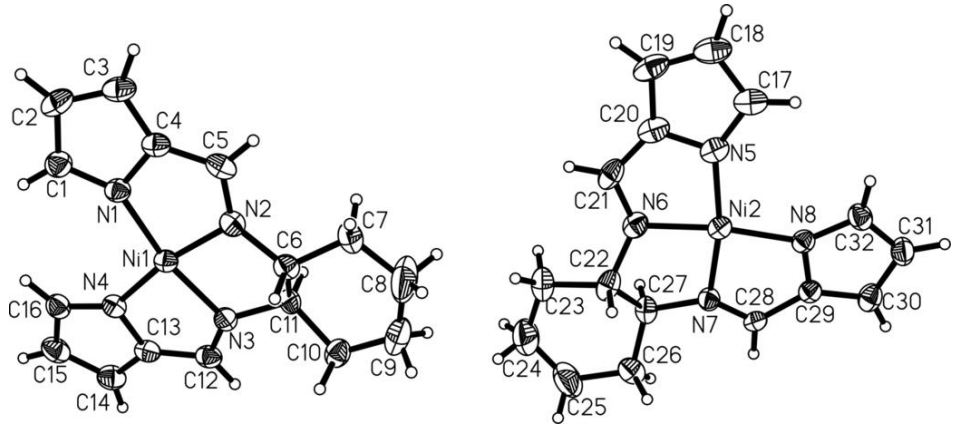
C10—C11—C6	110.3 (8)	C22—C23—H23B	108.8
N3—C11—H11A	108.9	H23A—C23—H23B	107.7
C10—C11—H11A	108.9	C24—C23—H23C	109.3
C6—C11—H11A	108.9	C22'—C23—H23C	109.1
N2—C6'—C7	117.8 (7)	C22—C23—H23C	82.1
N2—C6'—C11'	102.2 (7)	H23A—C23—H23C	30.0
C7—C6'—C11'	111.0 (8)	H23B—C23—H23C	131.1
N2—C6'—H6B	108.5	C24—C23—H23D	109.3
C7—C6'—H6B	108.5	C22'—C23—H23D	109.4
C11'—C6'—H6B	108.5	C22—C23—H23D	129.2
N3—C11'—C6'	103.8 (7)	H23A—C23—H23D	80.4
N3—C11'—C10	116.1 (7)	H23B—C23—H23D	29.2
C6'—C11'—C10	112.5 (8)	H23C—C23—H23D	107.9
N3—C11'—H11B	108.0	C23—C24—C25	123.4 (7)
C6'—C11'—H11B	108.0	C23—C24—H24A	106.5
C10—C11'—H11B	108.0	C25—C24—H24A	106.5
N6—C22—C27	104.5 (15)	C23—C24—H24B	106.5
N6—C22—C23	115.8 (12)	C25—C24—H24B	106.5
C27—C22—C23	108.0 (17)	H24A—C24—H24B	106.5
N6—C22—H22A	109.4	C24—C25—C26	120.2 (7)
C27—C22—H22A	109.4	C24—C25—H25A	107.3
C23—C22—H22A	109.4	C26—C25—H25A	107.3
C26—C27—N7	116.6 (13)	C24—C25—H25B	107.3
C26—C27—C22	114.5 (17)	C26—C25—H25B	107.3
N7—C27—C22	101.9 (14)	H25A—C25—H25B	106.9
C26—C27—H27A	107.8	C25—C26—C27	112.3 (8)
N7—C27—H27A	107.8	C25—C26—C27'	112.6 (8)
C22—C27—H27A	107.8	C27—C26—C27'	26.3 (5)
C23—C22'—C27'	114.1 (17)	C25—C26—H26A	109.1
C23—C22'—N6	116.1 (12)	C27—C26—H26A	109.1
C27'—C22'—N6	101.8 (15)	C27'—C26—H26A	128.9
C23—C22'—H22B	108.2	C25—C26—H26B	109.1
C27'—C22'—H22B	108.2	C27—C26—H26B	109.1
N6—C22'—H22B	108.2	C27'—C26—H26B	85.1
C22'—C27'—N7	104.7 (14)	H26A—C26—H26B	107.9
C22'—C27'—C26	111.9 (17)	C25—C26—H26C	109.1
N7—C27'—C26	115.0 (12)	C27—C26—H26C	85.4
C22'—C27'—H27B	108.3	C27'—C26—H26C	109.3
N7—C27'—H27B	108.3	H26A—C26—H26C	26.6
C26—C27'—H27B	108.3	H26B—C26—H26C	129.2
C8—C7—C6'	114.9 (6)	C25—C26—H26D	109.1
C8—C7—C6	113.9 (7)	C27—C26—H26D	128.9
C6'—C7—C6	26.5 (5)	C27'—C26—H26D	108.9
C8—C7—H7A	108.8	H26A—C26—H26D	83.3
C6'—C7—H7A	84.2	H26B—C26—H26D	26.7
C6—C7—H7A	108.8	H26C—C26—H26D	107.8
C8—C7—H7B	108.8	N7—C28—C29	114.6 (5)
C6'—C7—H7B	127.8	N7—C28—H28	122.7
C6—C7—H7B	108.8	C29—C28—H28	122.7

H7A—C7—H7B	107.7	C30—C29—N8	109.6 (5)
C8—C7—H7C	108.5	C30—C29—C28	137.1 (5)
C6'—C7—H7C	108.5	N8—C29—C28	113.3 (5)
C6—C7—H7C	128.9	C29—C30—C31	106.6 (5)
H7A—C7—H7C	27.7	C29—C30—H30	126.7
H7B—C7—H7C	82.1	C31—C30—H30	126.7
C8—C7—H7D	108.5	C30—C31—C32	107.0 (5)
C6'—C7—H7D	108.6	C30—C31—H31	126.5
C6—C7—H7D	84.9	C32—C31—H31	126.5
H7A—C7—H7D	129.8	N8—C32—C31	110.6 (5)
H7B—C7—H7D	27.3	N8—C32—H32	124.7
H7C—C7—H7D	107.5	C31—C32—H32	124.7
N2—Ni1—N1—C1	−179.6 (7)	C28—N7—C27—C26	42 (2)
N3—Ni1—N1—C1	167.3 (8)	C27'—N7—C27—C26	−70 (3)
N4—Ni1—N1—C1	5.2 (7)	Ni2—N7—C27—C26	−161.0 (11)
N2—Ni1—N1—C4	7.0 (4)	C28—N7—C27—C22	167.2 (13)
N3—Ni1—N1—C4	−6.1 (12)	C27'—N7—C27—C22	55 (2)
N4—Ni1—N1—C4	−168.2 (3)	Ni2—N7—C27—C22	−36 (2)
N3—Ni1—N2—C5	169.7 (4)	N6—C22—C27—C26	174.1 (9)
N1—Ni1—N2—C5	−7.7 (4)	C23—C22—C27—C26	−62 (3)
N4—Ni1—N2—C5	150.1 (8)	N6—C22—C27—N7	47 (2)
N3—Ni1—N2—C6	−17.1 (6)	C23—C22—C27—N7	171.2 (10)
N1—Ni1—N2—C6	165.5 (6)	C21—N6—C22'—C23	−41 (2)
N4—Ni1—N2—C6	−36.7 (12)	C22—N6—C22'—C23	69 (2)
N3—Ni1—N2—C6'	12.8 (7)	Ni2—N6—C22'—C23	162.1 (12)
N1—Ni1—N2—C6'	−164.6 (7)	C21—N6—C22'—C27'	−165.9 (12)
N4—Ni1—N2—C6'	−6.8 (13)	C22—N6—C22'—C27'	−56 (2)
N2—Ni1—N3—C12	−170.2 (4)	Ni2—N6—C22'—C27'	38 (2)
N1—Ni1—N3—C12	−157.0 (9)	C23—C22'—C27'—N7	−173.9 (9)
N4—Ni1—N3—C12	5.7 (4)	N6—C22'—C27'—N7	−48 (2)
N2—Ni1—N3—C11	−13.1 (6)	C23—C22'—C27'—C26	61 (3)
N1—Ni1—N3—C11	0.1 (13)	N6—C22'—C27'—C26	−173.3 (9)
N4—Ni1—N3—C11	162.8 (6)	C28—N7—C27'—C22'	−145.7 (13)
N2—Ni1—N3—C11'	18.2 (6)	C27—N7—C27'—C22'	−57 (3)
N1—Ni1—N3—C11'	31.3 (13)	Ni2—N7—C27'—C22'	44 (2)
N4—Ni1—N3—C11'	−165.9 (6)	C28—N7—C27'—C26	−22 (2)
N2—Ni1—N4—C16	−157.8 (8)	C27—N7—C27'—C26	66 (3)
N3—Ni1—N4—C16	−177.4 (6)	Ni2—N7—C27'—C26	166.7 (11)
N1—Ni1—N4—C16	−1.0 (7)	N2—C6'—C7—C8	160.8 (9)
N2—Ni1—N4—C13	14.6 (11)	C11'—C6'—C7—C8	43.5 (12)
N3—Ni1—N4—C13	−5.0 (4)	N2—C6'—C7—C6	66.9 (12)
N1—Ni1—N4—C13	171.5 (4)	C11'—C6'—C7—C6	−50.4 (12)
N6—Ni2—N5—C17	−177.9 (7)	N2—C6—C7—C8	−164.8 (9)
N7—Ni2—N5—C17	−166.6 (9)	C11—C6—C7—C8	−44.0 (12)
N8—Ni2—N5—C17	−3.0 (7)	N2—C6—C7—C6'	−66.4 (12)
N6—Ni2—N5—C20	−6.2 (4)	C11—C6—C7—C6'	54.3 (12)
N7—Ni2—N5—C20	5.1 (12)	C6'—C7—C8—C9	−15.5 (15)
N8—Ni2—N5—C20	168.7 (4)	C6—C7—C8—C9	13.7 (15)
N7—Ni2—N6—C21	−171.0 (4)	C7—C8—C9—C10	0.9 (17)

N8—Ni2—N6—C21	−148.9 (9)	C8—C9—C10—C11	15.0 (14)
N5—Ni2—N6—C21	6.8 (4)	C8—C9—C10—C11'	−15.3 (14)
N7—Ni2—N6—C22	19.3 (11)	N3—C11—C10—C9	−160.8 (8)
N8—Ni2—N6—C22	41.4 (16)	C6—C11—C10—C9	−44.3 (11)
N5—Ni2—N6—C22	−162.9 (11)	N3—C11—C10—C11'	−66.9 (11)
N7—Ni2—N6—C22'	−11.9 (11)	C6—C11—C10—C11'	49.7 (11)
N8—Ni2—N6—C22'	10.2 (16)	N3—C11'—C10—C9	163.4 (8)
N5—Ni2—N6—C22'	165.9 (11)	C6'—C11'—C10—C9	44.0 (12)
N6—Ni2—N7—C28	170.0 (4)	N3—C11'—C10—C11	64.8 (12)
N8—Ni2—N7—C28	−5.5 (4)	C6'—C11'—C10—C11	−54.5 (12)
N5—Ni2—N7—C28	158.7 (9)	C11—N3—C12—C13	−159.5 (7)
N6—Ni2—N7—C27	10.8 (11)	C11'—N3—C12—C13	164.7 (8)
N8—Ni2—N7—C27	−164.8 (11)	Ni1—N3—C12—C13	−5.0 (6)
N5—Ni2—N7—C27	−0.5 (16)	C16—N4—C13—C14	0.1 (6)
N6—Ni2—N7—C27'	−17.7 (10)	Ni1—N4—C13—C14	−175.1 (4)
N8—Ni2—N7—C27'	166.7 (10)	C16—N4—C13—C12	178.9 (5)
N5—Ni2—N7—C27'	−29.0 (15)	Ni1—N4—C13—C12	3.7 (6)
N6—Ni2—N8—C32	156.7 (9)	N3—C12—C13—C14	179.0 (6)
N7—Ni2—N8—C32	178.9 (6)	N3—C12—C13—N4	0.7 (7)
N5—Ni2—N8—C32	2.0 (7)	N4—C13—C14—C15	0.3 (7)
N6—Ni2—N8—C29	−17.4 (12)	C12—C13—C14—C15	−178.1 (6)
N7—Ni2—N8—C29	4.8 (4)	C13—C14—C15—C16	−0.5 (7)
N5—Ni2—N8—C29	−172.1 (3)	C13—N4—C16—C15	−0.4 (6)
C4—N1—C1—C2	0.7 (7)	Ni1—N4—C16—C15	172.2 (5)
Ni1—N1—C1—C2	−172.9 (5)	C14—C15—C16—N4	0.6 (7)
N1—C1—C2—C3	0.1 (7)	C20—N5—C17—C18	−0.4 (6)
C1—C2—C3—C4	−0.9 (7)	Ni2—N5—C17—C18	171.5 (5)
C1—N1—C4—C3	−1.3 (6)	N5—C17—C18—C19	−0.9 (7)
Ni1—N1—C4—C3	174.5 (4)	C17—C18—C19—C20	1.9 (7)
C1—N1—C4—C5	178.8 (5)	C17—N5—C20—C19	1.6 (6)
Ni1—N1—C4—C5	−5.4 (6)	Ni2—N5—C20—C19	−173.1 (4)
C2—C3—C4—N1	1.4 (7)	C17—N5—C20—C21	179.6 (5)
C2—C3—C4—C5	−178.7 (7)	Ni2—N5—C20—C21	4.9 (6)
C6—N2—C5—C4	−165.1 (8)	C18—C19—C20—N5	−2.2 (7)
C6'—N2—C5—C4	160.6 (7)	C18—C19—C20—C21	−179.5 (7)
Ni1—N2—C5—C4	6.5 (6)	C22—N6—C21—C20	161.6 (14)
N1—C4—C5—N2	−0.5 (7)	C22'—N6—C21—C20	−161.8 (13)
C3—C4—C5—N2	179.6 (7)	Ni2—N6—C21—C20	−5.7 (7)
C5—N2—C6—C7	−22.2 (14)	N5—C20—C21—N6	0.4 (7)
C6'—N2—C6—C7	65.9 (12)	C19—C20—C21—N6	177.6 (7)
Ni1—N2—C6—C7	166.1 (6)	C27'—C22'—C23—C24	−46 (3)
C5—N2—C6—C11	−147.1 (8)	N6—C22'—C23—C24	−163.4 (13)
C6'—N2—C6—C11	−59.0 (12)	C27'—C22'—C23—C22	55 (3)
Ni1—N2—C6—C11	41.2 (9)	N6—C22'—C23—C22	−63 (2)
C12—N3—C11—C10	−47.1 (12)	N6—C22—C23—C24	160.6 (13)
C11'—N3—C11—C10	66.8 (12)	C27—C22—C23—C24	44 (2)
Ni1—N3—C11—C10	158.2 (6)	N6—C22—C23—C22'	68 (2)
C12—N3—C11—C6	−167.9 (7)	C27—C22—C23—C22'	−48 (2)
C11'—N3—C11—C6	−54.0 (11)	C22'—C23—C24—C25	16.1 (18)

Ni1—N3—C11—C6	37.4 (9)	C22—C23—C24—C25	−15.0 (17)
N2—C6—C11—N3	−47.1 (10)	C23—C24—C25—C26	−1.5 (16)
C7—C6—C11—N3	−175.0 (7)	C24—C25—C26—C27	−13.7 (15)
N2—C6—C11—C10	−172.5 (7)	C24—C25—C26—C27'	14.8 (15)
C7—C6—C11—C10	59.7 (12)	N7—C27—C26—C25	165.2 (11)
C5—N2—C6'—C7	45.8 (13)	C22—C27—C26—C25	46 (2)
C6—N2—C6'—C7	−67.9 (13)	N7—C27—C26—C27'	69 (2)
Ni1—N2—C6'—C7	−160.1 (7)	C22—C27—C26—C27'	−50 (2)
C5—N2—C6'—C11'	167.7 (7)	C22'—C27'—C26—C25	−43 (2)
C6—N2—C6'—C11'	54.0 (12)	N7—C27'—C26—C25	−162.2 (11)
Ni1—N2—C6'—C11'	−38.1 (10)	C22'—C27'—C26—C27	52 (3)
C12—N3—C11'—C6'	147.2 (8)	N7—C27'—C26—C27	−67 (2)
C11—N3—C11'—C6'	58.5 (12)	C27—N7—C28—C29	161.5 (12)
Ni1—N3—C11'—C6'	−42.8 (10)	C27'—N7—C28—C29	−165.7 (13)
C12—N3—C11'—C10	23.2 (14)	Ni2—N7—C28—C29	4.8 (6)
C11—N3—C11'—C10	−65.5 (12)	C32—N8—C29—C30	0.3 (6)
Ni1—N3—C11'—C10	−166.8 (7)	Ni2—N8—C29—C30	176.5 (4)
N2—C6'—C11'—N3	48.5 (10)	C32—N8—C29—C28	−179.9 (5)
C7—C6'—C11'—N3	174.9 (7)	Ni2—N8—C29—C28	−3.6 (6)
N2—C6'—C11'—C10	174.8 (7)	N7—C28—C29—C30	179.2 (6)
C7—C6'—C11'—C10	−58.8 (12)	N7—C28—C29—N8	−0.6 (7)
C21—N6—C22—C27	148.9 (11)	N8—C29—C30—C31	0.3 (7)
C22'—N6—C22—C27	56 (2)	C28—C29—C30—C31	−179.5 (6)
Ni2—N6—C22—C27	−43 (2)	C29—C30—C31—C32	−0.7 (7)
C21—N6—C22—C23	30 (2)	C29—N8—C32—C31	−0.7 (6)
C22'—N6—C22—C23	−63 (2)	Ni2—N8—C32—C31	−175.0 (5)
Ni2—N6—C22—C23	−162.1 (11)	C30—C31—C32—N8	0.9 (7)

Fig. 1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