metal-organic compounds

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Azido{2-[(tri-2-pyridylmethyl)iminomethyl]phenolato}nickel(II)

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Key indicators: single-crystal X-ray study; T = 295 K; mean σ (C–C) = 0.005 Å; R factor = 0.047; wR factor = 0.097; data-to-parameter ratio = 12.9.

The title compound, $[Ni(C_{23}H_{17}N_4O)(N_3)]$, was obtained by the reaction of the Schiff base ligand 2-[(tri-2-pyridylmethyl)iminomethyl]phenol with sodium azide and nickel(II) perchlorate in methanol solution. The Ni^{II} atom is fourcoordinated by the phenolate O, the imine N and a pyridine N atom of the Schiff base ligand, and by the terminal N atom of an azide ligand, forming a square-planar geometry. The other two pyridyl rings are oriented at an angle of 72.29 (11)° to each other.

Related literature

For related literature, see: Arnold *et al.* (2003); Borisova *et al.* (2007); Bruckner *et al.* (2000); Li & Gao (2007); Li *et al.* (2007); Mondal *et al.* (2001).



Experimental

Crystal data

 $V = 2001.1 (4) Å^{3}$ Z = 4 Mo K\alpha radiation \mu = 1.00 mm^{-1} T = 295 (2) K 0.10 \times 0.08 \times 0.04 mm

Data collection

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Bruker APEX area-detector<br/>diffractometer14754 measured reflections<br/>3723 independent reflections<br/>2616 reflections with I > 2\sigma(I)<br/>R_{int} = 0.081Absorption correction: multi-scan<br/>(SADABS; Bruker, 2002)<br/>T_{min} = 0.906, T_{max} = 0.9662616 reflections with I > 2\sigma(I)<br/>R_{int} = 0.081
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Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$	289 parameters
$wR(F^2) = 0.097$	H-atom parameters constrained
S = 0.94	$\Delta \rho_{\rm max} = 0.48 \ {\rm e} \ {\rm \AA}^{-3}$
3723 reflections	$\Delta \rho_{\rm min} = -0.63 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Ni1-O1	1.815 (2)	Ni1-N2	1.850 (2)
Ni1-N1	1.887 (3)	Ni1-N3	1.898 (3)
O1-Ni1-N2	95.71 (10)	O1-Ni1-N3	87.79 (11)
O1-Ni1-N1 N2-Ni1-N1	178.50 (11) 85.09 (11)	N2-Ni1-N3 N1-Ni1-N3	175.69 (13) 91.46 (12)

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); 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: WN2208).

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Azido{2-[(tri-2-pyridylmethyl)iminomethyl]phenolato}nickel(II)

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Comment

Nickel complexes with Schiff bases have received much attention in recent years due to their pharmacological and catalytic properties (Borisova *et al.*, 2007; Bruckner *et al.*, 2000). 2-(Tri-2-pyridylmethyliminomethyl)phenol is a potential N₄O pentadentate Schiff base ligand and its complexes with copper(II) have been reported (Arnold *et al.*, 2003; Li & Gao, 2007). We report here the crystal structure of the title compound (Fig. 1).

In the mononuclear nickel complex, the environment around the central nickel atom is essentially square-planar, with a maximum deviation of 0.0529 (32) Å for atom N3. Three of the coordination sites are occupied by the phenolate O1, imine N2 and pyridine N1 atoms of the Schiff base ligand and the fourth site by the terminal N atom of an azide ligand. The other two N atoms of the pyridine rings in the Schiff base are distant from the metal. The Ni1—N1 (pyridine) distance is appreciably longer than that for Ni1—N2 (imine), and the Ni—N3 (azide) distance is almost the same as that found in azido {N-[2-(N,N-diethylamino)ethyl]salicylideneiminato}nickel(II) [1.901 (2) Å] (Mondal *et al.*, 2001) and azido {2,4-dibromo-6-[(2-diethylamino)ethyl]phenolato}nickel(II) [1.897 (3) Å] (Li *et al.*, 2007).

Experimental

2-(Tri-2-pyridylmethyliminomethyl)phenol (0.183 g, 0.5 mmol) and Ni(ClO₄)₂·6H₂O (0.183 g, 0.5 mmol) were stirred in methanol (10 ml) for 20 min. To this solution was added a solution of NaN₃ (0.065 g, 1.0 mmol) in water (2 ml). The mixture was stirred for a further 10 min at room temperature, and then filtered. After keeping the filtrate in air for 3 d, brown plate crystals were formed.

Refinement

H atoms were placed at calculated positions and refined in the riding-model approximation, with C—H = 0.93 Å and $U_{iso}(H) = 1.2 \text{Ueq}(C)$.

Figures



Fig. 1. The structure of the title compound, with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity.

Azido{2-[(tri-2-pyridylmethyl)iminomethyl]phenolato}nickel(II)

 $F_{000} = 960$

 $D_{\rm x} = 1.547 \ {\rm Mg \ m^{-3}}$ Mo Kα radiation

Cell parameters from 2703 reflections

 $\lambda = 0.71073 \text{ Å}$

 $\theta = 2.2 - 25.0^{\circ}$

 $\mu = 1.00 \text{ mm}^{-1}$

T = 295 (2) K

Plate, brown

 $0.10 \times 0.08 \times 0.04 \text{ mm}$

Crystal data

[Ni(C₂₃H₁₇N₄O)(N₃)] $M_r = 466.15$ Monoclinic, $P2_1/n$ Hall symbol: -P 2yn *a* = 10.7977 (12) Å *b* = 14.9156 (16) Å *c* = 12.7543 (14) Å $\beta = 103.044 \ (2)^{\circ}$ V = 2001.1 (4) Å³ Z = 4

Data collection

Bruker APEX area-detector diffractometer	3723 independent reflections
Radiation source: fine-focus sealed tube	2616 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\rm int} = 0.081$
T = 295(2) K	$\theta_{max} = 25.5^{\circ}$
ϕ and ω scans	$\theta_{\min} = 2.2^{\circ}$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$h = -13 \rightarrow 12$
$T_{\min} = 0.906, T_{\max} = 0.966$	$k = -18 \rightarrow 17$
14754 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H-atom parameters constrained
$wR(F^2) = 0.097$	$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
<i>S</i> = 0.94	$(\Delta/\sigma)_{\rm max} = 0.001$
3723 reflections	$\Delta \rho_{max} = 0.48 \text{ e} \text{ Å}^{-3}$
289 parameters	$\Delta \rho_{\rm min} = -0.63 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct	Extinction correction: none

methods

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 $F^2 > 2 \operatorname{sigma}(F^2)$ 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 (A^2)

	x	У	Ζ	$U_{\rm iso}*/U_{\rm eq}$
Ni1	0.82925 (4)	0.91145 (3)	0.74918 (3)	0.03162 (15)
N1	1.0057 (2)	0.93353 (17)	0.78930 (19)	0.0319 (6)
N2	0.8733 (2)	0.81489 (16)	0.67416 (19)	0.0292 (6)
N3	0.7952 (3)	1.0088 (2)	0.8344 (3)	0.0571 (9)
N4	0.6969 (3)	1.01342 (19)	0.8625 (2)	0.0430 (8)
N5	0.6054 (3)	1.0224 (2)	0.8930 (2)	0.0580 (9)
N6	1.1723 (3)	0.6869 (2)	0.7657 (2)	0.0490 (8)
N7	1.0587 (3)	0.8768 (2)	0.5391 (2)	0.0439 (7)
01	0.6589 (2)	0.89314 (15)	0.70908 (18)	0.0417 (6)
C1	1.0501 (3)	0.7098 (2)	0.7556 (2)	0.0336 (8)
C2	0.9695 (4)	0.6632 (2)	0.8061 (3)	0.0430 (9)
H2	0.8847	0.6799	0.7963	0.052*
C3	1.0169 (4)	0.5915 (3)	0.8713 (3)	0.0540 (10)
Н3	0.9639	0.5587	0.9051	0.065*
C4	1.1417 (4)	0.5694 (2)	0.8856 (3)	0.0578 (11)
H4	1.1761	0.5222	0.9306	0.069*
C5	1.2157 (4)	0.6183 (3)	0.8320 (3)	0.0586 (11)
Н5	1.3011	0.6030	0.8423	0.070*
C6	1.0479 (3)	0.7177 (2)	0.5191 (3)	0.0387 (8)
H6	1.0390	0.6619	0.5492	0.046*
C7	1.0655 (3)	0.7244 (3)	0.4155 (3)	0.0509 (10)
H7	1.0661	0.6734	0.3737	0.061*
C8	1.0819 (4)	0.8081 (3)	0.3753 (3)	0.0545 (11)
H8	1.0963	0.8146	0.3065	0.065*
С9	1.0765 (4)	0.8817 (3)	0.4388 (3)	0.0556 (11)
H9	1.0858	0.9381	0.4105	0.067*
C10	1.0438 (3)	0.7951 (2)	0.5771 (2)	0.0334 (8)
C11	1.0124 (3)	0.7957 (2)	0.6893 (2)	0.0313 (7)
C12	1.0804 (3)	0.8732 (2)	0.7551 (2)	0.0311 (7)
C13	1.2115 (3)	0.8817 (2)	0.7806 (3)	0.0401 (9)
H13	1.2619	0.8394	0.7564	0.048*
C14	1.2667 (3)	0.9531 (2)	0.8417 (3)	0.0443 (9)
H14	1.3547	0.9596	0.8595	0.053*

C15	1.1901 (3)	1.0148 (2)	0.8761 (3)	0.0451 (9)
H15	1.2254	1.0638	0.9173	0.054*
C16	1.0610 (3)	1.0032 (2)	0.8490 (3)	0.0407 (9)
H16	1.0095	1.0450	0.8728	0.049*
C17	0.7940 (3)	0.7606 (2)	0.6136 (2)	0.0324 (8)
H17	0.8282	0.7152	0.5788	0.039*
C18	0.6602 (3)	0.7650 (2)	0.5961 (2)	0.0299 (7)
C19	0.5858 (3)	0.7001 (2)	0.5293 (2)	0.0349 (8)
H19	0.6258	0.6570	0.4958	0.042*
C20	0.4565 (3)	0.6994 (2)	0.5130 (3)	0.0394 (8)
H20	0.4087	0.6560	0.4694	0.047*
C21	0.3973 (3)	0.7644 (2)	0.5625 (3)	0.0430 (9)
H21	0.3091	0.7643	0.5514	0.052*
C22	0.4660 (3)	0.8284 (2)	0.6270 (3)	0.0398 (9)
H22	0.4240	0.8711	0.6595	0.048*
C23	0.5989 (3)	0.8307 (2)	0.6451 (2)	0.0306 (7)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U ²³
Ni1	0.0290 (2)	0.0333 (2)	0.0331 (2)	0.0004 (2)	0.00817 (17)	-0.0062 (2)
N1	0.0310 (15)	0.0362 (16)	0.0292 (15)	-0.0020 (13)	0.0085 (12)	-0.0003 (12)
N2	0.0279 (15)	0.0329 (15)	0.0278 (14)	0.0004 (12)	0.0084 (12)	-0.0035 (12)
N3	0.0398 (19)	0.058 (2)	0.076 (2)	-0.0026 (17)	0.0191 (18)	-0.0313 (18)
N4	0.044 (2)	0.0416 (18)	0.0398 (18)	0.0105 (16)	0.0026 (16)	-0.0104 (14)
N5	0.050 (2)	0.074 (2)	0.052 (2)	0.0180 (19)	0.0171 (17)	-0.0061 (17)
N6	0.0415 (19)	0.0527 (19)	0.0504 (19)	0.0136 (16)	0.0052 (15)	0.0003 (16)
N7	0.0504 (19)	0.0499 (19)	0.0327 (16)	-0.0009 (15)	0.0122 (14)	0.0014 (14)
01	0.0330 (13)	0.0443 (15)	0.0483 (14)	-0.0006 (11)	0.0105 (11)	-0.0147 (11)
C1	0.036 (2)	0.037 (2)	0.0279 (18)	-0.0005 (16)	0.0066 (15)	-0.0089 (14)
C2	0.049 (2)	0.044 (2)	0.038 (2)	-0.0021 (18)	0.0119 (17)	-0.0045 (17)
C3	0.079 (3)	0.045 (2)	0.036 (2)	-0.005 (2)	0.011 (2)	0.0035 (19)
C4	0.083 (3)	0.035 (2)	0.048 (2)	0.009 (2)	-0.002 (2)	0.0028 (18)
C5	0.054 (3)	0.055 (3)	0.059 (3)	0.015 (2)	-0.004 (2)	-0.009 (2)
C6	0.033 (2)	0.050 (2)	0.036 (2)	-0.0004 (17)	0.0116 (16)	-0.0067 (16)
C7	0.040 (2)	0.074 (3)	0.040 (2)	-0.002 (2)	0.0112 (18)	-0.020 (2)
C8	0.053 (3)	0.082 (3)	0.030 (2)	-0.003 (2)	0.0112 (18)	-0.001 (2)
C9	0.062 (3)	0.067 (3)	0.039 (2)	-0.003 (2)	0.015 (2)	0.012 (2)
C10	0.0247 (18)	0.046 (2)	0.0292 (18)	-0.0002 (16)	0.0064 (14)	-0.0043 (16)
C11	0.0262 (18)	0.0382 (19)	0.0301 (18)	-0.0003 (15)	0.0077 (14)	-0.0028 (15)
C12	0.0300 (18)	0.0384 (19)	0.0258 (17)	-0.0005 (15)	0.0085 (14)	0.0009 (14)
C13	0.0321 (19)	0.050 (2)	0.043 (2)	-0.0024 (17)	0.0181 (16)	-0.0057 (17)
C14	0.030 (2)	0.056 (2)	0.045 (2)	-0.0094 (18)	0.0048 (16)	-0.0035 (19)
C15	0.042 (2)	0.045 (2)	0.047 (2)	-0.0138 (18)	0.0086 (18)	-0.0084 (17)
C16	0.046 (2)	0.037 (2)	0.039 (2)	-0.0041 (17)	0.0096 (17)	-0.0108 (16)
C17	0.0335 (19)	0.0335 (19)	0.0318 (18)	0.0014 (15)	0.0103 (15)	-0.0045 (15)
C18	0.0290 (18)	0.0352 (19)	0.0244 (16)	0.0012 (15)	0.0037 (14)	0.0044 (14)
C19	0.035 (2)	0.041 (2)	0.0277 (18)	-0.0020 (16)	0.0051 (15)	-0.0006 (15)

$\begin{array}{ccccccc} C22 & 0.031 (2) & 0.051 (2) & 0.040 (2) & 0.0043 (17) & 0.0106 (16) & -0.0003 (17) \\ C23 & 0.0303 (19) & 0.0327 (19) & 0.0294 (17) & -0.0007 (15) & 0.0082 (14) & -0.0030 (15) \\ \hline \\ $	C20 C21	0.037 (2) 0.0291 (19)	0.045 (2) 0.057 (2)	0.0331 (19) 0.040 (2)	-0.0087 (17) -0.0065 (18)	0.0019 (16) 0.0025 (16)	0.0004 (16) 0.0038 (18)
Geometric parameters ($\hat{4}, \hat{2}$) Nil—Ol 1.815 (2) C7—C8 1.376 (5) Nil—N1 1.887 (3) C7—17 0.9300 Nil—N2 1.850 (2) C8—C9 1.373 (5) Nil—N3 1.898 (3) C8—H18 0.9300 NI—C12 1.345 (4) C9—H9 0.9300 NI—C16 1.345 (4) C10—C11 1.543 (4) N2—C17 1.298 (4) C12—C13 1.385 (4) N2—C11 1.498 (4) C13—C14 1.374 (6) N4—N5 1.148 (4) C14—C15 1.374 (5) N4—N5 1.148 (4) C15—C16 1.370 (4) N7—C10 1.335 (4) C15—C16 1.370 (4) N7—C9 1.339 (3) C16—H116 0.9300 C1—C2 1.332 (4) C17—C18 1.413 (4) C1—C1 1.540 (4) C17—C18 1.414 (4) C3—C1 1.380 (5) C18—C19 1.414 (4) C3—C2 1.330 (5) C19—C10 1.356 (4) C1—C11 1.540 (4) C17—C18 1.341 (4) C3—C13 1.380 (5) </td <td>C22 C23</td> <td>0.031 (2) 0.0303 (19)</td> <td>0.051 (2) 0.0327 (19)</td> <td>0.040 (2) 0.0294 (17)</td> <td>0.0043 (17) -0.0007 (15)</td> <td>0.0106 (16) 0.0082 (14)</td> <td>-0.0003 (17) 0.0030 (15)</td>	C22 C23	0.031 (2) 0.0303 (19)	0.051 (2) 0.0327 (19)	0.040 (2) 0.0294 (17)	0.0043 (17) -0.0007 (15)	0.0106 (16) 0.0082 (14)	-0.0003 (17) 0.0030 (15)
Nil-O11.815 (2)C7-C81.376 (5)Nil-N11.887 (3)C7-H70.9300Nil-N21.850 (2)C8-C91.373 (5)Nil-N31.888 (3)C8-H80.9300NI-C121.345 (4)C10-C111.543 (4)N2-C171.228 (4)C11-C121.517 (4)N2-C171.298 (4)C12-C131.385 (4)N3-N41.197 (4)C13-C141.374 (4)N4-N51.148 (4)C13-C140.9300N6-C11.340 (4)C14-C151.374 (5)N6-C51.343 (5)C14-H140.9300N7-C101.335 (4)C15-C161.370 (4)N7-C91.339 (4)C15-H150.9300O1-C231.390 (3)C16-H160.9300C1-C21.322 (4)C17-C181.413 (4)C1-C111.540 (4)C17-H170.9300C2-C31.380 (5)C19-C201.364 (4)C3-C41.350 (5)C19-C201.364 (4)C3-C41.350 (5)C19-C201.364 (4)C3-C41.350 (5)C19-C211.330 (5)C4-C51.371 (5)C20-C211.366 (4)C6-C71.381 (4)C22-C231.401 (4)C6-H50.9300C21-H220.9300C4-H50.9300C21-H220.9300C4-H50.9300C21-H220.9300C5-H50.9300C12-C11-C111122 (3)N1-N1N7.69 (13)N2-C11-C12113 (4)C6-H60.9300C21-H22 <td>Geometric para</td> <td>meters (Å, °)</td> <td></td> <td></td> <td></td> <td></td> <td></td>	Geometric para	meters (Å, °)					
n.t. of, i.t. of, $C7-H7$ 09300 Nil-N2 1.850 (2) C8-C9 1.373 (5) Nil-N2 1.850 (2) C8-H8 09300 Nil-C12 1.345 (4) C9-H9 09300 Ni-C16 1.345 (4) C10-C11 1.543 (4) N2-C17 1.298 (4) C11-C12 1.517 (4) N2-C11 1.488 (4) C13-C14 1.535 (4) N4-N5 1.148 (4) C13-C14 0.9300 N6-C1 1.340 (4) C14-C15 1.374 (5) N6-C5 1.335 (4) C15-C16 1.370 (4) N7-C9 1.339 (4) C15-H15 0.9300 N1-C22 1.382 (4) C17-C18 1.413 (4) C1-C11 1.540 (4) C17-H17 0.9300 C1-C2 1.382 (4) C17-H17 0.9300 C1-C2 1.380 (5) C18-C23 1.407 (4) C2-H2 0.9300 C18-C19 1.344 (4) C3-H3 0.9300 C21-C20 1.364 (4) C3-H3 0.9300 C21-C22 1.366 (4) C4	Ni1-01		1 815 (2)	C7—C8	3	13	76 (5)
Nil-N2 1850 (2) C8-C9 1.373 (5) Nil-N3 1.589 (3) C8-H8 0.9300 NI-C12 1.345 (4) C10-C11 1.543 (4) N2-C17 1.298 (4) C11-C12 1.517 (4) N2-C11 1.498 (4) C12-C13 1.385 (4) N3-N4 1.197 (4) C13-C14 1.374 (4) N4-N5 1.148 (4) C13-H13 0.9300 N6-C1 1.345 (4) C14-C15 1.374 (5) N6-C5 1.343 (5) C14-H114 0.9300 N7-C10 1.355 (4) C15-C16 1.370 (4) N7-C9 1.339 (4) C15-H15 0.9300 C1-C2 1.382 (4) C17-C18 1.413 (4) C1-C1 1.540 (4) C17-H17 0.9300 C2-C3 1.380 (5) C18-C23 1.407 (4) C2-H2 0.9300 C16-H16 0.9300 C2-H3 0.9300 C19-H19 0.9300 C4-C4 1.360 (5) C19-C20 1.366 (4) C3-C4 1.380 (6) C20-C21 1.390 (5) C4-H4	Ni1—N1		1.813 (2)	С7—Н2	7	0.9	300
Nill-N3 1.898 (3) C8-H8 0.9300 Nil-C12 1.345 (4) C9-H9 0.9300 Nil-C16 1.345 (4) C10-C11 1.543 (4) N2-C17 1.298 (4) C12-C13 1.385 (4) N2-C11 1.498 (4) C13-C14 1.374 (4) N4-N5 1.148 (4) C13-C14 1.374 (4) N4-N5 1.148 (4) C13-C14 1.370 (4) N7-C9 1.335 (4) C15-C16 1.370 (4) N7-C9 1.339 (4) C15-C16 0.9300 C1-C2 1.382 (4) C17-C18 1.413 (4) C1-C11 1.540 (4) C17-H17 0.9300 C1-C2 1.380 (5) C18-C13 1.444 (4) C2-C3 1.380 (5) C18-C19 1.414 (4) C3-C4 1.360 (5) C19-C20 1.364 (4) C3-C4 1.360 (5) C19-C20 1.366 (4) C3-H2 0.9300 C2-C23 1.401 (4) C3-C4 1.377 (4) C21-H21 0.9300	Ni1—N2		1.850 (2)	C8—C9)	1.3	73 (5)
N1-C12 1345 (4) C9-H9 0.9300 N1-C16 1.345 (4) C10-C11 1.543 (4) N2-C17 1.298 (4) C12-C13 1.385 (4) N3-N4 1.197 (4) C13-C14 1.374 (4) N4-N5 1.148 (4) C13-L14 0.9300 N6-C1 1.340 (4) C14-L15 1.374 (5) N6-C5 1.343 (5) C14-H14 0.9300 N7-C10 1.335 (4) C15-C16 1.370 (4) N7-C9 1.339 (3) C16-H16 0.9300 C1-C21 1.382 (4) C17-C18 1.413 (4) C1-C11 1.540 (4) C17-H17 0.9300 C2-C3 1.380 (5) C18-C13 1.407 (4) C2-H2 0.9300 C18-C19 1.414 (4) C3-H3 0.9300 C19-C21 1.390 (5) C4-C5 1.373 (5) C20-C21 1.390 (5) C4-H4 0.9300 C21-H21 0.9300 C4-C5 1.371 (4) C22-C23 1.401 (4)	Ni1—N3		1.898 (3)	C8—H8	3	0.9	300
N1-C16 1.345 (4) C10-C11 1.543 (4) N2-C17 1.298 (4) C11-C12 1.517 (4) N2-C11 1.498 (4) C12-C13 1.385 (4) N3-N4 1.197 (4) C13-C14 1.374 (4) N4-N5 1.148 (4) C13-H13 0.9300 N6-C1 1.340 (4) C14-C15 1.374 (5) N6-C2 1.343 (5) C14-H14 0.9300 N7-C10 1.355 (4) C15-C16 1.370 (4) N7-C9 1.339 (4) C15-H15 0.9300 C1-C2 1.382 (4) C17-C18 1.413 (4) C1-C11 1.540 (4) C17-H17 0.9300 C2-C3 1.380 (5) C18-C19 1.414 (4) C3-C4 1.360 (5) C19-C20 1.364 (4) C3-H3 0.9300 C19-C12 0.9300 C4-C5 1.377 (5) C20-C21 1.390 (5) C4-H4 0.9300 C21-C22 0.9300 C4-C4 1.361 (4) C22-L122 0.9300 <tr< td=""><td>N1—C12</td><td></td><td>1.345 (4)</td><td>С9—Н9</td><td>)</td><td>0.9</td><td>300</td></tr<>	N1—C12		1.345 (4)	С9—Н9)	0.9	300
N2-C17 1298 (4) C1I-C12 1.517 (4) N2-C11 1.498 (4) C12-C13 1.385 (4) N3-N4 1.197 (4) C13-C14 1.374 (4) N4-N5 1.148 (4) C13-C14 1.374 (5) N6-C1 1.340 (4) C14-C15 1.374 (5) N6-C5 1.343 (5) C14-H14 0.9300 N7-C9 1.339 (4) C15-C16 1.370 (4) N7-C9 1.339 (4) C15-H15 0.9300 C1-C2 1.382 (4) C17-C18 1.413 (4) C1-C11 1.540 (4) C17-H17 0.9300 C2-C3 1.380 (5) C18-C19 1.414 (4) C2-C4 1.360 (5) C19-C20 1.364 (4) C3-H3 0.9300 C19-H19 0.9300 C4-C5 1.373 (5) C20-C21 1.390 (5) C4-H4 0.9300 C20-H20 0.9300 C4-H4 0.9300 C21-C22 1.366 (4) C6-C7 1.381 (4) C22-C23 1.401 (4)	N1-C16		1.345 (4)	C10—C	211	1.5	43 (4)
N2-C11 1.498 (4) C12-C13 1.385 (4) N3-N4 1.197 (4) C13-C14 1.374 (4) N4-N5 1.148 (4) C13-H13 0.9300 N6-C1 1.340 (4) C14-C15 1.374 (5) N6-C5 1.343 (5) C14-H14 0.9300 N7-C10 1.335 (4) C15-C16 1.370 (4) N7-C9 1.339 (3) C16-H16 0.9300 C1-C2 1.382 (4) C17-C18 1.413 (4) C1-C2 1.380 (5) C18-C19 1.414 (4) C2-C3 1.380 (5) C18-C19 1.414 (4) C3-C4 1.360 (5) C19-C20 1.364 (4) C3-C4 1.360 (5) C19-C20 1.366 (4) C4-C5 1.373 (5) C2O-C21 1.390 (5) C4-C4 1.381 (4) C21-H21 0.9300 C5-H5 0.9300 C21-H22 0.9300 C6-C7 1.381 (4) C22-C23 1.401 (4) C6-C7 1.381 (4) C22-C12 0.9300 <	N2—C17		1.298 (4)	C11—C	212	1.5	17 (4)
N3-N41.197 (4)C13-C141.374 (4)N4-N51.148 (4)C13-H130.9300N6-C11.340 (4)C14-C151.374 (5)N6-C51.334 (5)C14-H140.9300N7-C101.335 (4)C15-C161.370 (4)N7-C91.339 (4)C15-H150.9300C1-C21.382 (4)C17-C181.413 (4)C1-C111.540 (4)C17-H170.9300C2-C31.380 (5)C18-C231.407 (4)C2-C31.380 (5)C19-C201.364 (4)C3-C41.360 (5)C19-C201.364 (4)C3-C41.360 (5)C19-C201.364 (4)C3-C41.373 (5)C20-C211.390 (5)C4-C51.373 (5)C20-C211.390 (5)C4-C40.9300C21-H200.9300C5-H50.9300C21-H210.9300C6-C71.381 (4)C22-C231.401 (4)C6-H60.9300C22-H220.9300C1-Ni1-N1178 (50 (11)C4-C10-C11113 (6)C1-Ni1-N391.46 (12)N2-C11-C12105.8 (2)O1-Ni1-N391.46 (12)N2-C11-C10107.1 (2)N2-Ni1-N391.46 (12)N2-C11-C10107.8 (2)C12-NI-N11116.0 (2)C1-C11-C10117.3 (3)N2-NI-N391.46 (12)N2-C11-C11111.3 (2)N2-NI-N391.46 (12)N2-C11-C11113.3 (3)C1-NI-N391.46 (12)N2-C11-C11113.3 (3)C12-NI-N391.46 (12)N2-C11-C1	N2-C11		1.498 (4)	C12—C	213	1.3	85 (4)
N4—N51.148 (4)C13—H130.9300N6—C11.340 (4)C14—C151.374 (5)N6—C51.343 (5)C14—H140.9300N7—C101.335 (4)C15—C161.370 (4)N7—C91.339 (4)C15—H150.9300C1—C231.309 (3)C16—H160.9300C1—C21.82 (4)C17—C181.413 (4)C1—C111.540 (4)C17—H170.9300C2—C31.380 (5)C18—C231.407 (4)C2—C31.380 (5)C19—C191.414 (4)C3—C41.360 (5)C19—C191.414 (4)C3—C41.360 (5)C19—C191.390 (5)C4—C51.373 (5)C20—C211.390 (5)C4—C51.373 (5)C20—C211.390 (5)C4—H40.9300C21—C221.366 (4)C6—C101.377 (4)C21—H210.9300C5—H50.9300C22—H220.9300C6—C71.381 (4)C22—C231.401 (4)C6—C60.9300C22—H220.9300C1—N1178.50 (11)N2—C11—C1113.6 (3)O1—N1—N1178.50 (11)N2—C11—C1107.1 (2)N2—N1=N391.46 (12)N2—C11—C1107.1 (2)N2—N1=N391.46 (12)N2—C11—C10109.7 (3)C12—N1—N1125.4 (2)N1—C12—C13121.3 (3)C12—N1—N1125.4 (2)N1—C12—C11116.0 (3)C17—N2=N11116.0 (2)C1—C12116.0 (3)C17=N2=N11116.70 (19)C14—C13—C12116.0 (3	N3—N4		1.197 (4)	C13—C	214	1.3	74 (4)
N6-C1 1.340 (4)C14-C15 1.374 (5)N6-C5 1.343 (5)C14-H14 0.9300 N7-C10 1.335 (4)C15-C16 1.370 (4)N7-C9 1.339 (4)C15-H15 0.9300 C1-C23 1.309 (3)C16-H16 0.9300 C1-C2 1.382 (4)C17-C18 1.413 (4)C2-C3 1.380 (5)C18-C23 1.407 (4)C2-H2 0.9300 C18-C19 1.414 (4)C3-C4 1.360 (5)C19-C20 1.364 (4)C3-C4 1.360 (5)C19-C20 1.364 (4)C3-H3 0.9300 C19-H19 0.9300 C4-C5 1.373 (5)C20-C21 1.390 (5)C4-H4 0.9300 C20-H20 0.9300 C5-H5 0.9300 C21-C22 1.366 (4)C6-C10 1.377 (4)C21-H21 0.9300 C6-C7 1.381 (4)C22-C23 1.401 (4)C6-H6 0.9300 C22-H22 0.9300 C1-N1-N1 178.50 (11)C6-C10-C11 122.9 (3)N2-Ni1-N1 87.79 (11)N2-C11-C1 113.6 (3)O1-Ni1-N2 9.711 (10)N7-C10-C11 122.9 (3)N2-Ni1-N3 175.69 (13)C12-C11-C10 177.8 (2)C12-N1-N1 18.6 (3) $C12-C11-C10$ 114.7 (3)C12-N1-N3 175.69 (13) $C12-C11-C10$ 114.7 (3)C12-N1-N1 125.6 (2) $C1-C1-C11$ 122.8 (3)C11-N2-N11 125.6 (2) $C13-C12-C11$ 126.6 (3)C11-N2-N11 <td>N4—N5</td> <td></td> <td>1.148 (4)</td> <td>C13—H</td> <td>113</td> <td>0.9</td> <td>300</td>	N4—N5		1.148 (4)	C13—H	113	0.9	300
N6-C5 1.343 (5) C14-H14 0.9300 N7-C10 1.335 (4) C15-C16 1.370 (4) N7-C9 1.339 (4) C15-H15 0.9300 O1-C23 1.309 (3) C16-H16 0.9300 C1-C2 1.382 (4) C17-C18 1.413 (4) C1-C11 1.540 (4) C17-C18 1.413 (4) C2-C3 1.380 (5) C18-C23 1.407 (4) C2-C4 1.360 (5) C19-C20 1.364 (4) C3-C4 1.360 (5) C19-C20 1.364 (4) C3-H2 0.9300 C19-H19 0.9300 C4-C5 1.373 (5) C20-C21 1.366 (4) C5-H5 0.9300 C1-H21 0.9300 C5-H5 0.9300 C21-H21 0.9300 C6-C7 1.381 (4) C22-C23 1.401 (4) C6-C7 1.381 (4) C22-C23 1.401 (4) C6-H6 0.9300 C22-H22 0.9300 O1-Ni1-N2 95.71 (10) N7-C10-C11 113.6 (3) O1-Ni1-N3 87.79 (11) N2-C11-C1 107.1 (2)	N6—C1		1.340 (4)	C14—C	215	1.3	74 (5)
N7C101.335 (4)C15C161.370 (4)N7C91.339 (4)C15H150.9300O1C231.309 (3)C16H160.9300C1C11.382 (4)C17C181.413 (4)C1C111.540 (4)C17H170.9300C2C31.380 (5)C18C231.407 (4)C2H20.9300C18C191.414 (4)C3C41.360 (5)C19C201.364 (4)C3H30.9300C19H190.9300C4C51.373 (5)C20C211.390 (5)C4H40.9300C20H200.9300C5H50.9300C21C221.366 (4)C6-C101.377 (4)C21H210.9300C6-C71.381 (4)C22C231.401 (4)C6-C160.9300C22H220.9300O1Ni1-N295.71 (10)N7C10C11113.6 (3)O1-Ni1-N387.79 (11)N2C11C1113.6 (3)O1-Ni1-N391.46 (12)N2C11C1107.1 (2)N2Ni1-N391.46 (12)N2C11C1107.8 (2)C12N1-N391.46 (12)N2C11C1107.8 (2)C12N1-N391.46 (12)N2C11C1107.8 (2)C12N1-N391.46 (12)N2C11C1107.8 (2)C12N1-N391.46 (12)N2C11C1107.8 (2)C12N1-N391.46 (12)N2C11C1107.8 (2)C12N1-N391.46 (12)N2C11C1107.8 (2)C12N1-N1116.0 (2)C1C11C110	N6—C5		1.343 (5)	C14—H	I14	0.9	300
N7C91.339 (4)C15H150.9300O1C231.309 (3)C16H160.9300C1C21.382 (4)C17C181.413 (4)C1C111.540 (4)C17H170.9300C2C31.380 (5)C18C231.407 (4)C2H20.9300C18C191.414 (4)C3C41.360 (5)C19C201.364 (4)C3H30.9300C19H190.9300C4C51.373 (5)C20C211.390 (5)C4H40.9300C21C221.366 (4)C5H50.9300C21C221.366 (4)C6C101.377 (4)C21H210.9300C5H50.9300C22H220.9300C6C71.381 (4)C22C231.401 (4)C6H60.9300C22H220.9300O1Ni1-N1178.50 (11)C6-C10-C11113.6 (3)O1-Ni1-N1178.50 (11)N2-C11-C12105.8 (2)O1-Ni1-N387.79 (11)N2-C11-C1107.1 (2)N2-Ni1-N3175.69 (13)C12-C11-C1107.8 (2)C12-N1-C16118.6 (3)C12-C11-C10107.8 (2)C12-N1-N1116.0 (2)C1-C11-C10114.7 (3)C15-N1-N1125.4 (2)N1-C12-C13121.3 (3)C12-N1-N1125.6 (2)C13-C12-C11122.8 (3)C12-N1-N1125.6 (2)C13-C12-C11122.8 (3)C12-N2-N11116.70 (19)C14-C13-H13120.2N4-N3-N11121.0 (2)C14-C13-H13120.2	N7—C10		1.335 (4)	C15—C	216	1.3	70 (4)
01C23 $1.309(3)$ $C16H16$ 0.9300 $C1C2$ $1.382(4)$ $C17C18$ $1.413(4)$ $C1C11$ $1.540(4)$ $C17H17$ 0.9300 $C2C3$ $1.380(5)$ $C18C23$ $1.407(4)$ $C2H2$ 0.9300 $C18C19$ $1.414(4)$ $C3C4$ $1.360(5)$ $C19C20$ $1.364(4)$ $C3H3$ 0.9300 $C19H19$ 0.9300 $C4C5$ $1.373(5)$ $C20C21$ $1.390(5)$ $C4H4$ 0.9300 $C21C22$ $1.366(4)$ $C6C10$ $1.377(4)$ $C21H21$ 0.9300 $C6C7$ $1.381(4)$ $C22C23$ $1.401(4)$ $C6H6$ 0.9300 $C22H22$ 0.9300 $O1Ni-N2$ $9.5.71(10)$ $N7C10C11$ $113.6(3)$ $O1Ni-N1$ $178.50(11)$ $C6C1C11$ $113.6(3)$ $O1N1-N1$ $178.50(11)$ $N2C11C12$ $105.8(2)$ $O1N1-N3$ $9.77(1)$ $N2C11C12$ $105.8(2)$ $N2N1-N1$ $N5.09(13)$ $C12C11C10$ $107.8(2)$ $C12N1C16$ $118.6(3)$ $C12C11C10$ $107.8(2)$ $C12N1C16$ $118.6(3)$ $C12C11C10$ $107.8(2)$ $C1N1N11$ $125.6(2)$ $C13C12C11$ $122.8(3)$ $C1N2N11$ $125.6(2)$ $C13C12C11$ $122.8(3)$ $C1N2N11$ $125.6(2)$ $C13C12C11$ $125.8(3)$ $C1N2N11$ $125.6(2)$ $C13C12C11$ $125.8(3)$ $C1N2N11$ $105.9(4)$	N7—C9		1.339 (4)	C15—H	115	0.9	300
C1-C2 $1.382 (4)$ C17-C18 $1.413 (4)$ C1-C11 $1.540 (4)$ C17-H17 0.9300 C2-C3 $1.380 (5)$ C18-C23 $1.407 (4)$ C2-H2 0.9300 C18-C19 $1.414 (4)$ C3-C4 $1.360 (5)$ C19-C20 $1.364 (4)$ C3-H3 0.9300 C19-H19 0.9300 C4-C5 $1.373 (5)$ C20-C21 $1.390 (5)$ C4-H4 0.9300 C20-H20 0.9300 C5-H5 0.9300 C21-C22 $1.366 (4)$ C6-C10 $1.377 (4)$ C21-H21 0.9300 C6-C7 $1.381 (4)$ C22-C23 $1.401 (4)$ C6-H6 0.9300 C22-H22 0.9300 C1-NiI-N2 $9.571 (10)$ N7-C10-C11 $113.6 (3)$ O1-NiI-N1 $178.50 (11)$ C6-C10-C11 $122.9 (3)$ N2-Ni1-N1 $85.09 (11)$ N2-C11-C1 $107.1 (2)$ N1-Ni-N3 $91.46 (12)$ N2-C11-C1 $107.1 (2)$ N1-Ni1-N3 $91.46 (12)$ N2-C11-C10 $107.8 (2)$ C12-NI-Ni1 $116.0 (2)$ C1-C11-C10 $107.8 (2)$ C12-NI-Ni1 $125.4 (2)$ N1-C12-C13 $121.3 (3)$ C12-NI-Ni1 $125.4 (2)$ N1-C12-C11 $122.8 (3)$ C14-N2-Ni1 $125.6 (2)$ $C13-C12-C11$ $122.8 (3)$ C14-N2-Ni1 $121.0 (2)$ $C14-C13-H13$ 120.2 N5-N4-N3 $175.9 (4)$ $C12-C13-H13$ 120.2 N5-N4-N3 $175.9 (4)$ $C12-C13-H13$ 120.2	O1—C23		1.309 (3)	C16—H	116	0.9	300
C1C111.540 (4)C17H170.9300C2C31.380 (5)C18C231.407 (4)C2H20.9300C18C191.414 (4)C3C41.360 (5)C19C201.364 (4)C3H30.9300C19H190.9300C4C51.373 (5)C20C211.390 (5)C4H40.9300C20H200.9300C5H50.9300C21C221.366 (4)C6C101.377 (4)C21H210.9300C6C71.381 (4)C22C231.401 (4)C6H60.9300C22H220.9300O1Ni1-N295.71 (10)N7C10C11113.6 (3)O1Ni1-N1178.50 (11)C6C10C11122.9 (3)N2Ni1-N185.09 (11)N2C11C12105.8 (2)O1-Ni1-N3175.69 (13)C12C11C11107.1 (2)N1-Ni1-N391.46 (12)N2C11C10107.8 (2)C12-N1-C16118.6 (3)C12C11C10107.7 (3)C12-N1-N1116.0 (2)C1C11C10107.7 (3)C12-N1-N11116.0 (2)C1C11C10114.7 (3)C12-N1-N11116.0 (2)C1C11C10114.7 (3)C12-N1-N11116.0 (2)C1C11C10114.7 (3)C12-N1-N11116.0 (2)C1C11C10114.7 (3)C12-N1-N11116.0 (19)C14C13C11128.8 (3)C12-N1-N11125.6 (2)C13C12C11128.8 (3)C11-N2-N11125.6 (2)C13C12C11129.6 (3)N4-N3-N11<	C1—C2		1.382 (4)	C17—C	218	1.4	13 (4)
C2C31.380 (5)C18C231.407 (4)C2-H20.9300C18C191.414 (4)C3C41.360 (5)C19C201.364 (4)C3-H30.9300C19H190.9300C4C51.373 (5)C20C211.390 (5)C4H40.9300C20H200.9300C5H50.9300C21C221.366 (4)C6-C101.377 (4)C21H210.9300C6-C71.381 (4)C22C231.401 (4)C6-H60.9300C22H220.9300O1Ni1-N295.71 (10)N7C10C11113.6 (3)O1Ni1-N1178.50 (11)C6-C10-C11122.9 (3)N2Ni1-N185.09 (11)N2C11C12105.8 (2)O1-Ni1-N387.79 (11)N2C11C11111.3 (2)N2-Ni1-N3175.69 (13)C12C11C10107.1 (2)N1-Ni1-N391.46 (12)N2C11C10107.8 (2)C12-N1-Ni1116.0 (2)C1C11C10107.7 (3)C12-N1-Ni1125.4 (2)N1C12C13121.3 (3)C17-N2-C11117.7 (3)N1C12C11116.0 (3)C17-N2-Ni1125.6 (2)C13C12C11122.8 (3)C11-N2-Ni1125.6 (2)C13C12C11122.8 (3)C11-N2-Ni1125.6 (2)C13C12C11122.8 (3)C11-N2-Ni1125.6 (2)C13C12C11122.8 (3)C1-N4-N3-Ni1121.0 (2)C14C13H13120.2N5-N4-N3175.9 (4)C12C13H13120.2N5-N4-N3	C1—C11		1.540 (4)	C17—H	117	0.9	300
C2-H20.9300C18-C191.414 (4)C3-C41.360 (5)C19-C201.364 (4)C3-H30.9300C19-H190.9300C4-C51.373 (5)C20-C211.390 (5)C4-H40.9300C20-H200.9300C5-H50.9300C21-C221.366 (4)C6-C101.377 (4)C21-H210.9300C6-C71.381 (4)C22-C231.401 (4)C6-H60.9300C22-H220.9300O1-Ni1-N295.71 (10)N7-C10-C11113.6 (3)O1-Ni1-N1178.50 (11)C6-C10-C11122.9 (3)N2-Ni1-N185.09 (11)N2-C11-C12105.8 (2)O1-Ni1-N387.79 (11)N2-C11-C1111.3 (2)N2-Ni1-N391.46 (12)N2-C11-C1107.1 (2)N1-Ni1-N391.46 (12)N2-C11-C10109.7 (3)C12-N1-C16118.6 (3)C12-C11-C10109.7 (3)C12-N1-Ni115.6 (2)C1-C11-C10114.7 (3)C14-N1-Ni1125.4 (2)N1-C12-C11116.0 (3)C17-N2-Ni1116.0 (19)C14-C13-C12119.6 (3)C11-N2-Ni1126.6 (2)C13-C12-C11122.8 (3)C11-N2-Ni1126.9 (2)C14-C13-H13120.2N5-N4-N3175.9 (4)C12-C13-H13120.2C1-N6-C5116.8 (3)C13-C14-C15119.0 (3)	C2—C3		1.380 (5)	C18—C	223	1.4	07 (4)
C3-C41.360 (5)C19-C201.364 (4)C3-H30.9300C19-H190.9300C4-C51.373 (5)C20-C211.390 (5)C4-H40.9300C20-H200.9300C5-H50.9300C21-C221.366 (4)C6-C101.377 (4)C21-H210.9300C6-C71.381 (4)C22-C231.401 (4)C6-H60.9300C22-H220.9300O1-Ni1-N295.71 (10)N7-C10-C11113.6 (3)O1-Ni1-N1178.50 (11)C6-C10-C11122.9 (3)N2-Ni1-N185.09 (11)N2-C11-C12105.8 (2)O1-Ni1-N387.99 (11)N2-C11-C1111.3 (2)N2-Ni1-N3175.69 (13)C12-C11-C1107.1 (2)N1-Ni1-N391.46 (12)N2-C11-C10109.7 (3)C12-N1-C16118.6 (3)C12-C11-C10109.7 (3)C12-N1-Ni1115.0 (2)C1-C11-C10114.7 (3)C12-N1-Ni1125.4 (2)N1-C12-C11116.0 (3)C17-N2-Ni1125.6 (2)C13-C12-C11122.8 (3)C11-N2-Ni1116.70 (19)C14-C13-C12119.6 (3)C11-N2-Ni1120.2C14-C13-H13120.2N5-N4-N3175.9 (4)C12-C13-H13120.2C1-N6-C5116.8 (3)C13-C14-C15119.0 (3)	С2—Н2		0.9300	C18—C	219	1.4	14 (4)
C3—H3 0.9300 C19—H19 0.9300 C4—C5 1.373 (5) C20—C21 1.390 (5) C4—H4 0.9300 C20—H20 0.9300 C5—H5 0.9300 C21—C22 1.366 (4) C6—C10 1.377 (4) C21—H21 0.9300 C6—C7 1.381 (4) C22—C23 1.401 (4) C6—H6 0.9300 C22—H22 0.9300 O1—Ni1—N2 95.71 (10) N7—C10—C11 113.6 (3) O1—Ni1—N1 178.50 (11) C6—C10—C11 122.9 (3) N2—Ni1—N1 85.09 (11) N2—C11—C12 105.8 (2) O1—Ni1—N3 87.79 (11) N2—C11—C1 111.3 (2) N2—Ni1—N3 175.69 (13) C12—C11—C1 107.1 (2) N1—Ni1—N3 91.46 (12) N2—C11—C10 107.8 (2) C12—N1—C16 118.6 (3) C12—C11—C10 109.7 (3) C12—N1—Ni1 116.0 (2) C1—C11—C10 114.7 (3) C14—N1—Ni1 125.4 (2) N1—C12—C13 121.3 (3) C17—N2—C11 117.7 (3) N1—C12—C11 16.0 (3) C17—N2—C11 117.7 (3)<	C3—C4		1.360 (5)	C19—C	220	1.3	64 (4)
C4—C51.373 (5)C20—C211.390 (5)C4—H40.9300C20—H200.9300C5—H50.9300C21—C221.366 (4)C6—C101.377 (4)C21—H210.9300C6—C71.381 (4)C22—C231.401 (4)C6—H60.9300C22—H220.9300O1—Ni1—N295.71 (10)N7—C10—C11113.6 (3)O1—Ni1—N1178.50 (11)C6—C10—C11122.9 (3)N2—Ni1—N185.09 (11)N2—C11—C12105.8 (2)O1—Ni1—N387.79 (11)N2—C11—C1111.3 (2)N2—Ni1—N3175.69 (13)C12—C11—C1107.1 (2)N1—Ni1—N391.46 (12)N2—C11—C10109.7 (3)C12—N1—C16118.6 (3)C12—C11—C10109.7 (3)C12—N1—Ni1116.0 (2)C1—C11—C10114.7 (3)C14—N1—Ni1125.4 (2)N1—C12—C11116.0 (3)C17—N2—Ni1125.6 (2)C13—C12—C11122.8 (3)C11—N2—Ni1125.6 (2)C13—C12—C11122.8 (3)C11—N2—Ni1121.0 (2)C14—C13—H13120.2N5—N4—N3175.9 (4)C12—C13—H13120.2N5—N4—N3175.9 (4)C12—C13—H13120.2C1—N6—C5116.8 (3)C13—C14—C15119.0 (3)	С3—Н3		0.9300	C19—H	119	0.9	300
C4—H40.9300C20—H200.9300C5—H50.9300C21—C221.366 (4)C6—C101.377 (4)C21—H210.9300C6—C71.381 (4)C22—C231.401 (4)C6—H60.9300C22—H220.9300O1—Ni1—N295.71 (10)N7—C10—C11113.6 (3)O1—Ni1—N1178.50 (11)C6—C10—C11122.9 (3)N2—Ni1—N185.09 (11)N2—C11—C12105.8 (2)O1—Ni1—N387.79 (11)N2—C11—C1111.3 (2)N2—Ni1—N3175.69 (13)C12—C11—C1107.1 (2)N1—Ni1—N391.46 (12)N2—C11—C10107.8 (2)C12—N1—C16118.6 (3)C12—C11—C10114.7 (3)C16—N1—Ni1125.4 (2)N1—C12—C13121.3 (3)C17—N2—C11117.7 (3)N1—C12—C11116.0 (3)C17—N2—Ni1125.6 (2)C13—C12—C11122.8 (3)C11—N2—Ni1116.70 (19)C14—C13—C12119.6 (3)N4—N3—Ni1121.0 (2)C14—C13—H13120.2N5—N4—N3175.9 (4)C12—C13—H13120.2C1—N6—C5116.8 (3)C13—C14—C15119.0 (3)	C4—C5		1.373 (5)	C20—C	21	1.3	90 (5)
C5-H5 0.9300 C21-C22 1.366 (4)C6-C10 1.377 (4)C21-H21 0.9300 C6-C7 1.381 (4)C22-C23 1.401 (4)C6-H6 0.9300 C22-H22 0.9300 O1-Ni1-N2 95.71 (10)N7-C10-C11 113.6 (3)O1-Ni1-N1 178.50 (11)C6-C10-C11 122.9 (3)N2-Ni1-N1 85.09 (11)N2-C11-C12 105.8 (2)O1-Ni1-N3 87.79 (11)N2-C11-C1 111.3 (2)N2-Ni1-N3 175.69 (13)C12-C11-C1 107.1 (2)N1-Ni1-N3 91.46 (12)N2-C11-C10 107.8 (2)C12-N1-C16 118.6 (3)C12-C11-C10 109.7 (3)C12-N1-Ni1 116.0 (2)C1-C11-C10 114.7 (3)C16-N1-Ni1 125.4 (2)N1-C12-C13 121.3 (3)C17-N2-Ni1 115.6 (2) $C13-C12-C11$ 122.8 (3)C11-N2-Ni1 116.70 (19) $C14-C13-C12$ 119.6 (3)N4-N3-Ni1 121.0 (2) $C14-C13-H13$ 120.2 N5-N4-N3 175.9 (4) $C12-C13-H13$ 120.2 C1-N6-C5 116.8 (3) $C13-C14-C15$ 119.0 (3)	C4—H4		0.9300	C20—H	120	0.9	300
C6—C101.377 (4)C21—H210.9300C6—C71.381 (4)C22—C231.401 (4)C6—H60.9300C22—H220.9300O1—Ni1—N295.71 (10)N7—C10—C11113.6 (3)O1—Ni1—N1178.50 (11)C6—C10—C11122.9 (3)N2—Ni1—N185.09 (11)N2—C11—C12105.8 (2)O1—Ni1—N387.79 (11)N2—C11—C1111.3 (2)N2—Ni1—N3175.69 (13)C12—C11—C1107.1 (2)N1—Ni1—N391.46 (12)N2—C11—C10107.8 (2)C12—N1—C16118.6 (3)C12—C11—C10109.7 (3)C12—N1—Ni116.0 (2)C1—C11—C10114.7 (3)C16—N1—Ni1125.4 (2)N1—C12—C13121.3 (3)C17—N2—C11117.7 (3)N1—C12—C11116.0 (3)C17—N2—Ni1125.6 (2)C13—C12—C11122.8 (3)C11—N2—Ni1125.6 (2)C14—C13—C12119.6 (3)N4—N3—Ni1121.0 (2)C14—C13—H13120.2N5—N4—N3175.9 (4)C12—C13—H13120.2C1—N6—C5116.8 (3)C13—C14—C15119.0 (3)	С5—Н5		0.9300	C21—C	222	1.3	66 (4)
C6—C7 $1.381 (4)$ C22—C23 $1.401 (4)$ C6—H6 0.9300 C22—H22 0.9300 O1—Ni1—N2 $95.71 (10)$ $N7$ —C10—C11 $113.6 (3)$ O1—Ni1—N1 $178.50 (11)$ C6—C10—C11 $122.9 (3)$ N2—Ni1—N1 $85.09 (11)$ N2—C11—C12 $105.8 (2)$ O1—Ni1—N3 $87.79 (11)$ N2—C11—C1 $111.3 (2)$ N2—Ni1—N3 $175.69 (13)$ C12—C11—C1 $107.1 (2)$ N1—Ni1—N3 $91.46 (12)$ N2—C11—C10 $109.7 (3)$ C12—N1—C16 $118.6 (3)$ C12—C11—C10 $109.7 (3)$ C14—N1—Ni1 $125.4 (2)$ N1—C12—C13 $121.3 (3)$ C17—N2—C11 $117.7 (3)$ N1—C12—C11 $116.0 (3)$ C17—N2—Ni1 $125.6 (2)$ C13—C12—C11 $122.8 (3)$ C11—N2—Ni1 120.2 C14—C13—C12 $119.6 (3)$ N4—N3—Ni1 $121.0 (2)$ C14—C13—H13 120.2 N5—N4—N3 $175.9 (4)$ C12—C13—H13 120.2 C1—N6—C5 $116.8 (3)$ C13—C14—C15 $119.0 (3)$	C6—C10		1.377 (4)	C21—H	121	0.9	300
C6—H60.9300C22—H220.9300O1—Ni1—N295.71 (10)N7—C10—C11113.6 (3)O1—Ni1—N1178.50 (11)C6—C10—C11122.9 (3)N2—Ni1—N185.09 (11)N2—C11—C12105.8 (2)O1—Ni1—N387.79 (11)N2—C11—C1111.3 (2)N2—Ni1—N3175.69 (13)C12—C11—C1107.1 (2)N1—Ni1—N391.46 (12)N2—C11—C10107.8 (2)C12—N1—C16118.6 (3)C12—C11—C10109.7 (3)C12—N1—Ni1116.0 (2)C1—C11—C10114.7 (3)C16—N1—Ni1125.4 (2)N1—C12—C13121.3 (3)C17—N2—C11117.7 (3)N1—C12—C11116.0 (3)C17—N2—Ni1125.6 (2)C13—C12—C11122.8 (3)C11—N2—Ni1116.70 (19)C14—C13—H13120.2N4—N3—Ni1121.0 (2)C14—C13—H13120.2N5—N4—N3175.9 (4)C12—C13—H13120.2C1—N6—C5116.8 (3)C13—C14—C15119.0 (3)	С6—С7		1.381 (4)	C22—C	223	1.4	01 (4)
O1Ni1N295.71 (10)N7C10C11113.6 (3)O1Ni1N1178.50 (11)C6C10C11122.9 (3)N2Ni1N185.09 (11)N2C11C12105.8 (2)O1Ni1N387.79 (11)N2C11C1111.3 (2)N2Ni1N3175.69 (13)C12C11C1107.1 (2)N1Ni1N391.46 (12)N2C11C10107.8 (2)C12N1C16118.6 (3)C12C11C10109.7 (3)C12N1Ni1116.0 (2)C1C11C10114.7 (3)C16N1Ni1125.4 (2)N1C12C13121.3 (3)C17N2C11117.7 (3)N1C12C11116.0 (3)C11N2Ni1125.6 (2)C13C12C11122.8 (3)C11N2Ni1116.70 (19)C14C13C12119.6 (3)N4N3Ni1121.0 (2)C14C13H13120.2N5N4N3175.9 (4)C12C13H13120.2C1N6C5116.8 (3)C13C14C15119.0 (3)	С6—Н6		0.9300	С22—Н	122	0.9	300
O1Ni1N1 178.50 (11) C6C10C11 122.9 (3) N2Ni1N1 85.09 (11) N2C11C12 105.8 (2) O1Ni1N3 87.79 (11) N2C11C1 111.3 (2) N2Ni1N3 175.69 (13) C12C11C1 107.1 (2) N1Ni1N3 91.46 (12) N2C11C10 107.8 (2) C12N1C16 118.6 (3) C12C11C10 109.7 (3) C12N1Ni1 116.0 (2) C1C11C10 114.7 (3) C16N1Ni1 125.4 (2) N1C12C13 121.3 (3) C17N2C11 117.7 (3) N1C12C11 116.0 (3) C17N2Ni1 125.6 (2) C13C12C11 122.8 (3) C11N2Ni1 116.70 (19) C14C13C12 119.6 (3) N4N3Ni1 121.0 (2) C14C13H13 120.2 N5N4N3 175.9 (4) C12C13H13 120.2 C1N6C5 116.8 (3) C13C14C15 119.0 (3)	O1—Ni1—N2		95.71 (10)	N7—C1	10—C11	113	3.6 (3)
N2-Ni1-N1 85.09 (1) N2-C11-C12 105.8 (2) O1-Ni1-N3 87.79 (1) N2-C11-C1 111.3 (2) N2-Ni1-N3 175.69 (13) C12-C11-C1 107.1 (2) N1-Ni1-N3 91.46 (12) N2-C11-C10 107.8 (2) C12-N1-C16 118.6 (3) C12-C11-C10 109.7 (3) C12-N1-Ni1 116.0 (2) C1-C11-C10 114.7 (3) C16-N1-Ni1 125.4 (2) N1-C12-C13 121.3 (3) C17-N2-C11 117.7 (3) N1-C12-C11 116.0 (3) C17-N2-Ni1 125.6 (2) C13-C12-C11 122.8 (3) C11-N2-Ni1 116.70 (19) C14-C13-C12 119.6 (3) N4-N3-Ni1 121.0 (2) C14-C13-H13 120.2 N5-N4-N3 175.9 (4) C12-C13-H13 120.2 C1-N6-C5 116.8 (3) C13-C14-C15 119.0 (3)	O1—Ni1—N1		178.50 (11)	C6—C1	0—C11	122	2.9 (3)
O1—Ni1—N387.79 (11)N2—C11—C1111.3 (2)N2—Ni1—N3175.69 (13)C12—C11—C1107.1 (2)N1—Ni1—N391.46 (12)N2—C11—C10107.8 (2)C12—N1—C16118.6 (3)C12—C11—C10109.7 (3)C12—N1—Ni1116.0 (2)C1—C11—C10114.7 (3)C16—N1—Ni1125.4 (2)N1—C12—C13121.3 (3)C17—N2—C11117.7 (3)N1—C12—C11116.0 (3)C17—N2—Ni1125.6 (2)C13—C12—C11122.8 (3)C11—N2—Ni1116.70 (19)C14—C13—C12119.6 (3)N4—N3—Ni1121.0 (2)C14—C13—H13120.2N5—N4—N3175.9 (4)C12—C13—H13120.2C1—N6—C5116.8 (3)C13—C14—C15119.0 (3)	N2—Ni1—N1		85.09 (11)	N2—C	11—C12	105	5.8 (2)
N2-Ni1-N3175.69 (13)C12-C11-C1107.1 (2)N1-Ni1-N391.46 (12)N2-C11-C10107.8 (2)C12-N1-C16118.6 (3)C12-C11-C10109.7 (3)C12-N1-Ni1116.0 (2)C1-C11-C10114.7 (3)C16-N1-Ni1125.4 (2)N1-C12-C13121.3 (3)C17-N2-C11117.7 (3)N1-C12-C11116.0 (3)C17-N2-Ni1125.6 (2)C13-C12-C11122.8 (3)C11-N2-Ni1116.70 (19)C14-C13-C12119.6 (3)N4-N3-Ni1121.0 (2)C14-C13-H13120.2N5-N4-N3175.9 (4)C12-C13-H13120.2C1-N6-C5116.8 (3)C13-C14-C15119.0 (3)	O1—Ni1—N3		87.79 (11)	N2—C1	11—C1	111	.3 (2)
N1—Ni1—N391.46 (12)N2—C11—C10107.8 (2)C12—N1—C16118.6 (3)C12—C11—C10109.7 (3)C12—N1—Ni1116.0 (2)C1—C11—C10114.7 (3)C16—N1—Ni1125.4 (2)N1—C12—C13121.3 (3)C17—N2—C11117.7 (3)N1—C12—C11116.0 (3)C17—N2—Ni1125.6 (2)C13—C12—C11122.8 (3)C11—N2—Ni1116.70 (19)C14—C13—C12119.6 (3)N4—N3—Ni1121.0 (2)C14—C13—H13120.2N5—N4—N3175.9 (4)C12—C13—H13120.2C1—N6—C5116.8 (3)C13—C14—C15119.0 (3)	N2—Ni1—N3		175.69 (13)	C12—C	C11—C1	107	7.1 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N1—Ni1—N3		91.46 (12)	N2—C	11—C10	107	7.8 (2)
C12—N1—Ni1116.0 (2)C1—C11—C10114.7 (3)C16—N1—Ni1125.4 (2)N1—C12—C13121.3 (3)C17—N2—C11117.7 (3)N1—C12—C11116.0 (3)C17—N2—Ni1125.6 (2)C13—C12—C11122.8 (3)C11—N2—Ni1116.70 (19)C14—C13—C12119.6 (3)N4—N3—Ni1121.0 (2)C14—C13—H13120.2N5—N4—N3175.9 (4)C12—C13—H13120.2C1—N6—C5116.8 (3)C13—C14—C15119.0 (3)	C12—N1—C16		118.6 (3)	C12—C	C11—C10	109	9.7 (3)
C16N1Ni1125.4 (2)N1C12C13121.3 (3)C17N2C11117.7 (3)N1C12C11116.0 (3)C17N2Ni1125.6 (2)C13C12C11122.8 (3)C11N2Ni1116.70 (19)C14C13C12119.6 (3)N4N3Ni1121.0 (2)C14C13H13120.2N5N4N3175.9 (4)C12C13H13120.2C1N6C5116.8 (3)C13C14C15119.0 (3)	C12—N1—Ni1		116.0 (2)	C1—C1	1—C10	114	4.7 (3)
C17—N2—C11117.7 (3)N1—C12—C11116.0 (3)C17—N2—Ni1125.6 (2)C13—C12—C11122.8 (3)C11—N2—Ni1116.70 (19)C14—C13—C12119.6 (3)N4—N3—Ni1121.0 (2)C14—C13—H13120.2N5—N4—N3175.9 (4)C12—C13—H13120.2C1—N6—C5116.8 (3)C13—C14—C15119.0 (3)	C16—N1—Ni1		125.4 (2)	N1—C1	12—C13	121	1.3 (3)
C17—N2—Ni1125.6 (2)C13—C12—C11122.8 (3)C11—N2—Ni1116.70 (19)C14—C13—C12119.6 (3)N4—N3—Ni1121.0 (2)C14—C13—H13120.2N5—N4—N3175.9 (4)C12—C13—H13120.2C1—N6—C5116.8 (3)C13—C14—C15119.0 (3)	C17—N2—C11		117.7 (3)	N1—C1	12—C11	116	5.0 (3)
C11—N2—Ni1116.70 (19)C14—C13—C12119.6 (3)N4—N3—Ni1121.0 (2)C14—C13—H13120.2N5—N4—N3175.9 (4)C12—C13—H13120.2C1—N6—C5116.8 (3)C13—C14—C15119.0 (3)	C17—N2—Ni1		125.6 (2)	C13—C	C12—C11	122	2.8 (3)
N4—N3—Ni1121.0 (2)C14—C13—H13120.2N5—N4—N3175.9 (4)C12—C13—H13120.2C1—N6—C5116.8 (3)C13—C14—C15119.0 (3)	C11—N2—Ni1		116.70 (19)	C14—C	C13—C12	119	9.6 (3)
N5—N4—N3175.9 (4)C12—C13—H13120.2C1—N6—C5116.8 (3)C13—C14—C15119.0 (3)	N4—N3—Ni1		121.0 (2)	C14—C	С13—Н13	120).2
C1—N6—C5 116.8 (3) C13—C14—C15 119.0 (3)	N5—N4—N3		175.9 (4)	C12—C	С13—Н13	120).2
	C1—N6—C5		116.8 (3)	C13—C	C14—C15	119	9.0 (3)

C10—N7—C9	116.9 (3)	C13—C14—H14	120.5
C23—O1—Ni1	127.6 (2)	C15—C14—H14	120.5
N6—C1—C2	122.5 (3)	C16—C15—C14	119.1 (3)
N6—C1—C11	113.4 (3)	C16—C15—H15	120.5
C2—C1—C11	123.9 (3)	C14—C15—H15	120.5
C3—C2—C1	118.9 (4)	N1—C16—C15	122.5 (3)
С3—С2—Н2	120.5	N1—C16—H16	118.8
C1—C2—H2	120.5	C15—C16—H16	118.8
C4—C3—C2	119.4 (4)	N2—C17—C18	125.3 (3)
С4—С3—Н3	120.3	N2—C17—H17	117.3
С2—С3—Н3	120.3	С18—С17—Н17	117.3
C3—C4—C5	118.3 (4)	C23—C18—C17	122.0 (3)
C3—C4—H4	120.8	C23—C18—C19	119.0 (3)
С5—С4—Н4	120.8	C17—C18—C19	119.0 (3)
N6—C5—C4	124.0 (4)	C20-C19-C18	121.3 (3)
N6—C5—H5	118.0	С20—С19—Н19	119.3
С4—С5—Н5	118.0	С18—С19—Н19	119.3
C10—C6—C7	118.8 (3)	C19—C20—C21	119.1 (3)
С10—С6—Н6	120.6	С19—С20—Н20	120.5
С7—С6—Н6	120.6	C21—C20—H20	120.5
C8—C7—C6	118.6 (3)	C22—C21—C20	121.2 (3)
С8—С7—Н7	120.7	C22—C21—H21	119.4
С6—С7—Н7	120.7	C20-C21-H21	119.4
C9—C8—C7	118.7 (3)	C21—C22—C23	120.9 (3)
С9—С8—Н8	120.7	C21—C22—H22	119.6
С7—С8—Н8	120.7	C23—C22—H22	119.6
N7—C9—C8	123.7 (4)	O1—C23—C22	117.7 (3)
N7—C9—H9	118.2	O1—C23—C18	123.8 (3)
С8—С9—Н9	118.2	C22—C23—C18	118.5 (3)
N7—C10—C6	123.3 (3)		
N2—Ni1—N1—C12	-3.4 (2)	N7-C10-C11-N2	80.5 (3)
N3—Ni1—N1—C12	174.0 (2)	C6-C10-C11-N2	-95.5 (3)
N2—Ni1—N1—C16	177.2 (3)	N7-C10-C11-C12	-34.3 (4)
N3—Ni1—N1—C16	-5.4 (3)	C6-C10-C11-C12	149.7 (3)
O1—Ni1—N2—C17	1.9 (3)	N7—C10—C11—C1	-154.9 (3)
N1—Ni1—N2—C17	-176.8 (3)	C6—C10—C11—C1	29.1 (4)
O1—Ni1—N2—C11	-175.1 (2)	C16—N1—C12—C13	0.2 (4)
N1—Ni1—N2—C11	6.2 (2)	Ni1—N1—C12—C13	-179.2 (2)
O1—Ni1—N3—N4	21.3 (3)	C16—N1—C12—C11	179.3 (3)
N1—Ni1—N3—N4	-160.0 (3)	Ni1—N1—C12—C11	-0.1 (3)
N2—Ni1—O1—C23	-1.5 (3)	N2-C11-C12-N1	4.5 (3)
N3—Ni1—O1—C23	-179.0 (3)	C1—C11—C12—N1	-114.3 (3)
C5—N6—C1—C2	-3.0 (5)	C10-C11-C12-N1	120.6 (3)
C5—N6—C1—C11	173.1 (3)	N2-C11-C12-C13	-176.4 (3)
N6-C1-C2-C3	1.4 (5)	C1—C11—C12—C13	64.8 (4)
C11—C1—C2—C3	-174.3 (3)	C10-C11-C12-C13	-60.3 (4)
C1—C2—C3—C4	1.0 (5)	N1—C12—C13—C14	-0.1 (5)
C2—C3—C4—C5	-1.6 (5)	C11—C12—C13—C14	-179.2 (3)
C1—N6—C5—C4	2.5 (5)	C12-C13-C14-C15	-0.1 (5)

C3—C4—C5—N6	-0.2 (6)	C13—C14—C15—C16	0.3 (5)
С10—С6—С7—С8	1.9 (5)	C12—N1—C16—C15	0.0 (5)
С6—С7—С8—С9	-1.8 (6)	Ni1—N1—C16—C15	179.4 (2)
C10—N7—C9—C8	-0.9 (5)	C14—C15—C16—N1	-0.3 (5)
C7—C8—C9—N7	1.4 (6)	C11—N2—C17—C18	175.7 (3)
C9—N7—C10—C6	1.0 (5)	Ni1—N2—C17—C18	-1.3 (4)
C9—N7—C10—C11	-175.0 (3)	N2-C17-C18-C23	-0.3 (5)
C7-C6-C10-N7	-1.5 (5)	N2-C17-C18-C19	-178.9 (3)
C7-C6-C10-C11	174.1 (3)	C23-C18-C19-C20	-1.0 (4)
C17—N2—C11—C12	175.5 (2)	C17-C18-C19-C20	177.6 (3)
Ni1—N2—C11—C12	-7.3 (3)	C18-C19-C20-C21	0.6 (5)
C17—N2—C11—C1	-68.4 (3)	C19—C20—C21—C22	-0.2 (5)
Ni1—N2—C11—C1	108.8 (2)	C20—C21—C22—C23	0.3 (5)
C17—N2—C11—C10	58.2 (3)	Ni1-01-C23-C22	178.8 (2)
Ni1—N2—C11—C10	-124.6 (2)	Ni1-01-C23-C18	0.5 (4)
N6-C1-C11-N2	176.2 (2)	C21—C22—C23—O1	-179.0 (3)
C2-C1-C11-N2	-7.8 (4)	C21—C22—C23—C18	-0.7 (5)
N6-C1-C11-C12	-68.6 (3)	C17—C18—C23—O1	0.7 (5)
C2-C1-C11-C12	107.5 (3)	C19—C18—C23—O1	179.3 (3)
N6-C1-C11-C10	53.4 (3)	C17—C18—C23—C22	-177.5 (3)
C2-C1-C11-C10	-130.5 (3)	C19—C18—C23—C22	1.0 (4)

Fig. 1

