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Bis{5-methoxy-2-[(2-morpholinoethyl)iminomethyl- κN]phenolato- κO^{1} }nickel(II)

Nooraziah Mohd Lair, Hapipah Mohd Ali and Seik Weng Ng*

Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia Correspondence e-mail: seikweng@um.edu.my

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Key indicators: single-crystal X-ray study; T = 100 K; mean σ (C–C) = 0.002 Å; R factor = 0.026; wR factor = 0.079; data-to-parameter ratio = 16.7.

The asymmetric unit of the crystal structure of the title compound, $[Ni(C_{14}H_{19}N_2O_3)_2]$, contains two independent Ni^{II} complex molecules, with the metal atoms each located on a center of inversion. Each metal atom is chelated by two Schiff base anions in a distorted square-planar coordination environment.

Related literature

The Schiff base exists in the zwitterionic form; see: Mohd Lair et al. (2009).



10299 measured reflections 5978 independent reflections

 $R_{\rm int} = 0.014$

5388 reflections with $I > 2\sigma(I)$

Experimental

Crystal data

[Ni(C ₁₄ H ₁₉ N ₂ O ₃) ₂]	$\gamma = 61.926 \ (1)^{\circ}$
$M_r = 585.33$	V = 1349.45 (3) Å ³
Triclinic, $P\overline{1}$	Z = 2
a = 10.3358 (1) Å	Mo $K\alpha$ radiation
b = 10.4502 (1) Å	$\mu = 0.77 \text{ mm}^{-1}$
c = 14.8764 (2) Å	$T = 100 { m K}$
$\alpha = 72.482 \ (1)^{\circ}$	$0.45 \times 0.35 \times 0.25 \text{ mm}$
$\beta = 78.847 (1)^{\circ}$	

Data collection Bruker SMART APEX

DIUKEI SMARI AFEA
diffractometer
Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)
$T_{\min} = 0.724, \ T_{\max} = 0.831$

Refinement

N

N

$R[F^2 > 2\sigma(F^2)] = 0.026$	357 parameters
$wR(F^2) = 0.079$	H-atom parameters constrained
S = 1.02	$\Delta \rho_{\rm max} = 0.24 \text{ e } \text{\AA}^{-3}$
5978 reflections	$\Delta \rho_{\rm min} = -0.45 \text{ e } \text{\AA}^{-3}$

Table 1

Selected bond lengths (Å).

li1-01	1.9001 (9)	Ni2-O4	1.8873 (9)
Ni1-N1	2.0077 (10)	Ni2-N3	2.0105 (10)

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: X-SEED (Barbour, 2001); software used to prepare material for publication: publCIF (Westrip, 2009).

We thank the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2537).

References

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Acta Cryst. (2009). E65, m733 [doi:10.1107/S1600536809020790]

Bis{5-methoxy-2-[(2-morpholinoethyl)iminomethyl-*KN*]phenolato-*KO*¹}nickel(II)

N. Mohd Lair, H. Mohd Ali and S. W. Ng

Experimental

The Schiff base was synthesized as described (Mohd Lair *et al.*, 2009). The Schiff base (0.25 g, 2 mmol) and nickel(II) acetate (0.29 g, 1 mmol) were heated in ethanol (50 ml) for 5 hours. Large crystals appeared after a day.

Refinement

Hydrogen atoms were placed at calculated positions (C–H 0.95–0.98 Å) and were treated as riding on their parent carbon atoms, with U(H) set to 1.2–1.5 times $U_{eq}(C)$.

Figures



Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of the two independent molecules of $Ni(C_{14}H_{19}N_2O_3)_2$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

Bis{5-methoxy-2-[(2-morpholinoethyl)iminomethyl- κN]phenolato- κO^{1} }nickel(II)

Crystal data	
[Ni(C ₁₄ H ₁₉ N ₂ O ₃) ₂]	Z = 2
$M_r = 585.33$	$F_{000} = 620$
Triclinic, <i>P</i> T	$D_{\rm x} = 1.441 {\rm Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
a = 10.3358 (1) Å	Cell parameters from 7081 reflections
b = 10.4502 (1) Å	$\theta = 2.4 - 28.3^{\circ}$
c = 14.8764 (2) Å	$\mu = 0.77 \text{ mm}^{-1}$
$\alpha = 72.482 \ (1)^{\circ}$	T = 100 K
$\beta = 78.847 \ (1)^{\circ}$	Block, brown
$\gamma = 61.926 \ (1)^{\circ}$	$0.45\times0.35\times0.25~mm$
$V = 1349.45 (3) Å^3$	

Data collection

Bruker SMART APEX diffractometer

5978 independent reflections

Radiation source: fine-focus sealed tube	5388 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\rm int} = 0.014$
T = 100 K	$\theta_{\text{max}} = 27.5^{\circ}$
ω scans	$\theta_{\min} = 1.4^{\circ}$
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	$h = -13 \rightarrow 13$
$T_{\min} = 0.724, T_{\max} = 0.831$	$k = -13 \rightarrow 13$
10299 measured reflections	$l = -19 \rightarrow 18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.026$	H-atom parameters constrained
$wR(F^2) = 0.079$	$w = 1/[\sigma^2(F_0^2) + (0.0486P)^2 + 0.3802P]$ where $P = (F_0^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{\rm max} = 0.001$
5978 reflections	$\Delta \rho_{max} = 0.24 \text{ e} \text{ Å}^{-3}$
357 parameters	$\Delta \rho_{\rm min} = -0.45 \text{ e} \text{ Å}^{-3}$
Primary atom site location: structure-invariant direct	

Primary atom site location: structure-invariant direct methods Extinction correction: none

	x	У	Z	$U_{\rm iso}*/U_{\rm eq}$
Ni1	0.5000	0.5000	0.5000	0.01251 (7)
Ni2	0.0000	0.5000	0.5000	0.01139 (7)
01	0.64797 (11)	0.38684 (10)	0.41957 (7)	0.0219 (2)
O2	0.85765 (11)	0.09562 (10)	0.19085 (7)	0.0217 (2)
O3	0.11665 (11)	0.31275 (11)	0.96822 (7)	0.0226 (2)
O4	0.07976 (11)	0.42908 (10)	0.38957 (6)	0.0201 (2)
O5	0.33314 (11)	0.09974 (10)	0.18575 (7)	0.0204 (2)
O6	-0.43863 (13)	0.32859 (12)	0.95338 (8)	0.0333 (3)
N1	0.40989 (12)	0.35698 (11)	0.53370 (7)	0.0165 (2)
N2	0.25322 (12)	0.28136 (11)	0.78382 (8)	0.0171 (2)
N3	0.00294 (12)	0.30250 (11)	0.57283 (7)	0.0160 (2)
N4	-0.25854 (12)	0.37022 (11)	0.78592 (8)	0.0171 (2)
C1	0.65173 (14)	0.28594 (14)	0.38318 (9)	0.0169 (2)
C2	0.75883 (14)	0.24097 (13)	0.30890 (9)	0.0177 (3)
H2	0.8281	0.2812	0.2890	0.021*
C3	0.76314 (14)	0.13913 (14)	0.26538 (9)	0.0175 (3)
C4	0.66694 (15)	0.07116 (14)	0.29655 (9)	0.0199 (3)
H4	0.6729	-0.0013	0.2677	0.024*
C5	0.56494 (14)	0.11209 (13)	0.36923 (9)	0.0182 (3)
H5	0.5003	0.0664	0.3907	0.022*
C6	0.55269 (14)	0.22006 (13)	0.41341 (9)	0.0163 (2)
C7	0.94834 (15)	0.17079 (15)	0.15000 (10)	0.0242 (3)

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

H7A	1.0063	0.1341	0.0949	0.036*
H7B	1.0146	0.1511	0.1967	0.036*
H7C	0.8862	0.2786	0.1304	0.036*
C8	0.44220 (14)	0.25732 (13)	0.48793 (9)	0.0168 (2)
H8	0.3858	0.2025	0.5060	0.020*
C9	0.29494 (14)	0.36405 (14)	0.61125 (9)	0.0175 (2)
H9A	0.2377	0.3156	0.6020	0.021*
H9B	0.2268	0.4698	0.6103	0.021*
C10	0.36353 (14)	0.28583 (14)	0.70611 (9)	0.0179 (3)
H10A	0.4373	0.1824	0.7049	0.022*
H10B	0.4148	0.3389	0.7171	0.022*
C11	0.32412 (15)	0.17738 (14)	0.87014 (9)	0.0202 (3)
H11A	0.3874	0.2113	0.8890	0.024*
H11B	0.3868	0.0767	0.8586	0.024*
C12	0.20802 (15)	0.17037 (14)	0.94837 (9)	0.0219 (3)
H12A	0.1467	0.1342	0.9296	0.026*
H12B	0.2564	0.0981	1.0062	0.026*
C13	0.04749 (15)	0.41852 (15)	0.88474 (10)	0.0220 (3)
H13A	-0.0127	0.5181	0.8984	0.026*
H13B	-0.0188	0.3884	0.8658	0.026*
C14	0.15997 (15)	0.42874 (14)	0.80402 (9)	0.0195 (3)
H14A	0.1089	0.5005	0.7469	0.023*
H14B	0.2219	0.4659	0.8210	0.023*
C15	0.13013 (14)	0.29600 (13)	0.37536 (9)	0.0156 (2)
C16	0.20321 (14)	0.27219 (13)	0.28691 (9)	0.0162 (2)
H16	0.2144	0.3520	0.2402	0.019*
C17	0.25856 (14)	0.13342 (14)	0.26797 (9)	0.0163 (2)
C18	0.24168 (14)	0.01325 (14)	0.33586 (9)	0.0183 (3)
H18	0.2780	-0.0812	0.3220	0.022*
C19	0.17215 (14)	0.03538 (13)	0.42195 (9)	0.0175 (2)
H19	0.1615	-0.0455	0.4678	0.021*
C20	0.11576 (13)	0.17479 (13)	0.44478 (9)	0.0157 (2)
C21	0.37176 (15)	0.21061 (15)	0.11990 (9)	0.0214 (3)
H21A	0.4315	0.1707	0.0662	0.032*
H21B	0.4280	0.2368	0.1512	0.032*
H21C	0.2821	0.3000	0.0974	0.032*
C22	0.05326 (13)	0.18669 (13)	0.53806 (9)	0.0158 (2)
H22	0.0479	0.0999	0.5794	0.019*
C23	-0.04492 (14)	0.27936 (13)	0.67398 (9)	0.0175 (2)
H23A	0.0000	0.3175	0.7062	0.021*
H23B	-0.0106	0.1710	0.7028	0.021*
C24	-0.21159 (14)	0.35923 (14)	0.68823 (9)	0.0183 (3)
H24A	-0.2481	0.4609	0.6459	0.022*
H24B	-0.2553	0.3042	0.6709	0.022*
C25	-0.22424 (19)	0.22319 (15)	0.85116 (10)	0.0287 (3)
H25A	-0.1165	0.1614	0.8506	0.034*
H25B	-0.2685	0.1715	0.8307	0.034*
C26	-0.2839 (2)	0.24170 (16)	0.94997 (10)	0.0335 (4)
H26A	-0.2591	0.1421	0.9939	0.040*

-0.2373	0.2910	0.9708	0.040*
-0.47234 (17)	0.47365 (16)	0.89310 (10)	0.0264 (3)
-0.4271	0.5223	0.9159	0.032*
-0.5801	0.5354	0.8956	0.032*
-0.41669 (15)	0.46615 (16)	0.79223 (10)	0.0224 (3)
-0.4690	0.4266	0.7673	0.027*
-0.4378	0.5681	0.7529	0.027*
	-0.2373 -0.47234 (17) -0.4271 -0.5801 -0.41669 (15) -0.4690 -0.4378	-0.2373 0.2910 -0.47234 (17) 0.47365 (16) -0.4271 0.5223 -0.5801 0.5354 -0.41669 (15) 0.46615 (16) -0.4690 0.4266 -0.4378 0.5681	-0.23730.29100.9708-0.47234 (17)0.47365 (16)0.89310 (10)-0.42710.52230.9159-0.58010.53540.8956-0.41669 (15)0.46615 (16)0.79223 (10)-0.46900.42660.7673-0.43780.56810.7529

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.01396 (11)	0.01469 (11)	0.01148 (12)	-0.00886 (9)	0.00226 (8)	-0.00429 (8)
Ni2	0.01437 (11)	0.00926 (11)	0.01011 (12)	-0.00527 (8)	0.00115 (8)	-0.00286 (8)
01	0.0239 (5)	0.0239 (5)	0.0250 (5)	-0.0154 (4)	0.0058 (4)	-0.0119 (4)
02	0.0252 (5)	0.0203 (5)	0.0203 (5)	-0.0112 (4)	0.0053 (4)	-0.0080 (4)
03	0.0262 (5)	0.0214 (5)	0.0158 (5)	-0.0079 (4)	0.0025 (4)	-0.0051 (4)
O4	0.0277 (5)	0.0132 (4)	0.0181 (5)	-0.0089 (4)	0.0029 (4)	-0.0051 (3)
05	0.0245 (5)	0.0185 (4)	0.0187 (5)	-0.0098 (4)	0.0050 (4)	-0.0083 (4)
O6	0.0490 (7)	0.0321 (6)	0.0244 (6)	-0.0273 (5)	0.0166 (5)	-0.0102 (4)
N1	0.0167 (5)	0.0199 (5)	0.0139 (5)	-0.0098 (4)	0.0014 (4)	-0.0036 (4)
N2	0.0182 (5)	0.0162 (5)	0.0156 (5)	-0.0077 (4)	0.0016 (4)	-0.0039 (4)
N3	0.0180 (5)	0.0156 (5)	0.0141 (5)	-0.0078 (4)	-0.0004 (4)	-0.0030 (4)
N4	0.0209 (5)	0.0157 (5)	0.0137 (5)	-0.0085 (4)	0.0010 (4)	-0.0027 (4)
C1	0.0187 (6)	0.0156 (5)	0.0156 (6)	-0.0078 (5)	-0.0017 (5)	-0.0021 (4)
C2	0.0181 (6)	0.0158 (6)	0.0185 (6)	-0.0084 (5)	0.0004 (5)	-0.0027 (5)
C3	0.0188 (6)	0.0147 (6)	0.0146 (6)	-0.0052 (5)	-0.0012 (5)	-0.0013 (5)
C4	0.0239 (6)	0.0185 (6)	0.0196 (6)	-0.0102 (5)	-0.0026 (5)	-0.0052 (5)
C5	0.0201 (6)	0.0176 (6)	0.0182 (6)	-0.0104 (5)	-0.0029 (5)	-0.0017 (5)
C6	0.0181 (6)	0.0157 (5)	0.0144 (6)	-0.0079 (5)	-0.0025 (5)	-0.0011 (4)
C7	0.0235 (7)	0.0238 (7)	0.0240 (7)	-0.0115 (6)	0.0067 (6)	-0.0073 (5)
C8	0.0179 (6)	0.0176 (6)	0.0158 (6)	-0.0097 (5)	-0.0027 (5)	-0.0008 (4)
C9	0.0166 (6)	0.0217 (6)	0.0168 (6)	-0.0117 (5)	0.0018 (5)	-0.0046 (5)
C10	0.0169 (6)	0.0211 (6)	0.0171 (6)	-0.0102 (5)	0.0017 (5)	-0.0049 (5)
C11	0.0211 (6)	0.0183 (6)	0.0177 (6)	-0.0068 (5)	0.0010 (5)	-0.0040 (5)
C12	0.0266 (7)	0.0192 (6)	0.0170 (6)	-0.0101 (5)	0.0016 (5)	-0.0024 (5)
C13	0.0214 (6)	0.0215 (6)	0.0184 (7)	-0.0068 (5)	0.0015 (5)	-0.0044 (5)
C14	0.0213 (6)	0.0168 (6)	0.0185 (6)	-0.0081 (5)	0.0014 (5)	-0.0040 (5)
C15	0.0152 (6)	0.0143 (5)	0.0175 (6)	-0.0062 (5)	-0.0023 (5)	-0.0041 (4)
C16	0.0178 (6)	0.0148 (5)	0.0149 (6)	-0.0068 (5)	-0.0010 (5)	-0.0028 (4)
C17	0.0148 (6)	0.0187 (6)	0.0160 (6)	-0.0068 (5)	-0.0008 (5)	-0.0062 (5)
C18	0.0197 (6)	0.0149 (5)	0.0215 (7)	-0.0074 (5)	0.0001 (5)	-0.0072 (5)
C19	0.0188 (6)	0.0147 (5)	0.0201 (6)	-0.0088 (5)	-0.0015 (5)	-0.0029 (5)
C20	0.0158 (6)	0.0153 (5)	0.0170 (6)	-0.0075 (5)	-0.0020 (5)	-0.0036 (5)
C21	0.0230 (7)	0.0207 (6)	0.0177 (6)	-0.0090 (5)	0.0027 (5)	-0.0041 (5)
C22	0.0161 (6)	0.0148 (5)	0.0169 (6)	-0.0081 (5)	-0.0012 (5)	-0.0022 (4)
C23	0.0219 (6)	0.0156 (5)	0.0136 (6)	-0.0085 (5)	0.0006 (5)	-0.0021 (4)
C24	0.0206 (6)	0.0206 (6)	0.0158 (6)	-0.0116 (5)	0.0000 (5)	-0.0035 (5)
C25	0.0451 (9)	0.0177 (6)	0.0179 (7)	-0.0133 (6)	0.0060 (6)	-0.0025 (5)

$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C26	0.0531 (10)	0.0207 (7)	0.0174 (7)	-0.0136 (7)	0.0068 (7)	-0.0021 (5)
C28 0.0266 (6) 0.0297 (7) 0.0189 (7) -0.0126 (6) 0.0119 (5) -0.0082 (5) Geometric parameters (Å, ?) Nil-Ot ¹ 1.9001 (9) C9-H9B 0.9900 Nil-Ni ¹ 2.0077 (10) C10-H10A 0.9900 Nil-Ni ¹ 2.0077 (10) C10-H10A 0.9900 Ni2-O4 ^a 1.8873 (9) C11-C12 1.5136 (18) Ni2-O4 1.8873 (9) C11-H11A 0.9900 Ni2-N3 ^a 2.0105 (10) C12-H12A 0.9900 O1-C1 1.3052 (15) C12-H12A 0.9900 O2-C3 1.3627 (16) C13-U13A 0.9900 O3-C12 1.4312 (16) C14-H11A 0.9900 O4-C15 1.3048 (15) C14-H11A 0.9900 O5-C17	C27	0.0274 (7)	0.0302 (7)	0.0207 (7)	-0.0135 (6)	0.0075 (6)	-0.0090 (6)
Geometric parameters ($4, 6'$) Nil—Ol ¹ 19001 (9) C9—H9R 0.9900 Nil—Ol 20077 (10) C10—H10A 0.9900 Nil—N1 2.0077 (10) C10—H10B 0.9900 Ni2—O4 ⁱⁱ 1.8873 (9) C11—C12 1.5136 (18) Ni2—O4 ⁱⁱ 1.8873 (9) C11—H11A 0.9900 Ni2—N3 2.0105 (10) C12—H12A 0.9900 OL=C1 1.36527 (16) C12—H12A 0.9900 OL=C1 1.36527 (16) C13—H13A 0.9900 O2—C3 1.3627 (16) C13—H13B 0.9900 O3—C12 1.4312 (16) C14—H14A 0.9900 O3—C13 1.4312 (16) C14—H14A 0.9900 O4—C15 1.3048 (15) C15—C20 1.4225 (16) O5—C21 1.4360 (15) C15—C16 1.4140 (18) O5—C21 1.4360 (15) C18—C17 1.3329 (17) O4—C15 1.2928 (17) C16—C17 1.3329 (17) O4—C24 1.4450 (16) C19—H19 0.9500 N2—C10 1.4550 (16) C19—C22 1.4347 (18)	C28	0.0206 (6)	0.0297 (7)	0.0189 (7)	-0.0126 (6)	0.0019 (5)	-0.0082 (5)
$\begin{split} \mathbf{N}_{1} = 01^{1} & 1.9001 (9) & C9 = H9A & 0.9900 \\ \mathbf{N}_{1} = -\mathbf{N}_{1}^{1} & 2.0077 (10) & C10 = H10A & 0.9900 \\ \mathbf{N}_{1} = -\mathbf{N}_{1}^{1} & 2.0077 (10) & C10 = H10B & 0.9900 \\ \mathbf{N}_{1} = -\mathbf{N}_{1}^{1} & 2.0077 (10) & C10 = H10B & 0.9900 \\ \mathbf{N}_{2} = -\mathbf{N}_{3}^{2} & 2.0077 (10) & C11 = H11A & 0.9900 \\ \mathbf{N}_{2} = -\mathbf{N}_{3}^{2} & 2.0105 (10) & C11 = H11A & 0.9900 \\ \mathbf{N}_{2} = -\mathbf{N}_{3}^{2} & 2.0105 (10) & C12 = H12A & 0.9900 \\ \mathbf{O}_{2} = -C3 & 1.3627 (16) & C13 = H13A & 0.9900 \\ \mathbf{O}_{2} = -C7 & 1.4319 (16) & C13 = H13A & 0.9900 \\ \mathbf{O}_{3} = -C13 & 1.3627 (16) & C13 = H13A & 0.9900 \\ \mathbf{O}_{3} = -C13 & 1.3627 (16) & C13 = H13B & 0.9900 \\ \mathbf{O}_{4} = -C15 & 1.3048 (15) & C14 = H14A & 0.9900 \\ \mathbf{O}_{4} = -C15 & 1.3048 (15) & C15 = C16 & 1.4140 (18) \\ \mathbf{O}_{5} = -C17 & 1.3613 (16) & C15 = C16 & 1.4140 (18) \\ \mathbf{O}_{5} = -C17 & 1.3613 (16) & C15 = C16 & 1.4140 (18) \\ \mathbf{O}_{5} = -C17 & 1.3613 (16) & C15 = C16 & 1.4140 (18) \\ \mathbf{O}_{5} = -C17 & 1.3613 (16) & C15 = C16 & 1.4149 (17) \\ \mathbf{N}_{1} = C9 & 1.4786 (15) & C15 = C20 & 1.4225 (16) \\ \mathbf{O}_{6} = -C26 & 1.419 (2) & C16 = C17 & 1.3829 (17) \\ \mathbf{O}_{6} = -C27 & 1.4244 (17) & C16 = H16 & 0.9500 \\ \mathbf{N}_{1} = -C8 & 1.2928 (17) & C17 = C18 & 1.4149 (17) \\ \mathbf{N}_{2} = -C10 & 1.4650 (16) & C19 = -C20 & 1.4141 (17) \\ \mathbf{N}_{2} = -C10 & 1.4650 (16) & C19 = -C20 & 1.4141 (17) \\ \mathbf{N}_{2} = -C10 & 1.4650 (16) & C19 = -C22 & 1.4281 (18) \\ \mathbf{N}_{3} = -C23 & 1.3830 (18) & C23 = -H23A & 0.9900 \\ \mathbf{C}_{4} = -C3 & 1.3830 (18) & C23 = -H23A & 0.9900 \\ \mathbf{C}_{4} = -C3 & 1.3830 (18) & C23 = -H23A & 0.9900 \\ \mathbf{C}_{4} = -C3 & 1.3830 (18) & C23 = H23A & 0.9900 \\ \mathbf{C}_{4} = -C4 & 1.4129 (18) & C24 = H24B & 0.9900 \\ \mathbf{C}_{5} = -H44 & 0.9500 & C26 = H26A & 0.9900 \\ \mathbf{C}_{5} = -H5 & 0.9500 & C26 = H25A & 0.9900 \\ \mathbf{C}_{5} = -H75 & 0.9500 & C26 = H25A & 0.9900 \\ \mathbf{C}_{5} = -H77 & 0.9800 & C27 = H27A & 0.9900 \\ \mathbf{C}_{5} = -H77 & 0.9800 & C27 = H27A & 0.9900 \\ \mathbf{C}_{5} = -H77 & 0.9800 & C27 = H27A & 0.9900 \\ \mathbf{C}_{5} = -H77 & 0.9800 & C27 = H27A & 0.9900 \\ \mathbf{C}_{5} = -H77 & 0.9800 & C27 = H27A & $	Geometric pa	rameters (Å, °)					
Init of 1 Nit - O1 1.9001 (9) C9 - H9B 0.9900 Nit - N1 2.0077 (10) C10 - H10A 0.9900 Nit - N1 2.0077 (10) C10 - H10B 0.9900 Ni2 - O4 ⁴ 1.8873 (9) C11 - C12 1.5136 (18) Ni2 - N3 2.0105 (10) C11 - H11B 0.9900 Ol - C1 1.3622 (15) C12 - H12A 0.9900 O2 - C3 1.3627 (16) C13 - C14 1.5180 (18) O2 - C7 1.4319 (16) C13 - H13B 0.9900 O3 - C12 1.4327 (16) C14 - H14A 0.9900 O3 - C12 1.3633 (16) C15 - C16 1.4420 (18) O5 - C17 1.3613 (16) C15 - C16 1.4420 (18) O5 - C27 1.4224 (17) C16 - C17 1.3829 (17) O6 - C26 1.419 (2) C16 - C17 1.3829 (17) O6 - C27 1.4244 (17) C16 - H16 0.9500 N1 - C9 1.4786 (15) C18 - C19 1.3697 (18) N2 - C11 1.4653 (16) C19 - H19 0.95	Ni1_01 ⁱ		1 9001 (9)	C9—	Н9А	0.9	900
NII-DY D300 (9) CI-DID 0.9300 NII-NI 2.0077 (10) C10-H10B 0.9900 NI2-O4 ⁴ 1.8873 (9) C11-C12 1.5136 (18) NI2-O4 ⁴ 1.8873 (9) C11-H11A 0.9900 NI2-N3 ⁴ 2.0105 (10) C12-H12A 0.9900 NI2-N3 ⁴ 2.0105 (10) C12-H12B 0.9900 O2-C3 1.3627 (16) C13-C14 1.5180 (18) O2-C7 1.4319 (16) C13-H13A 0.9900 O3-C12 1.4237 (16) C13-H13A 0.9900 O3-C13 1.4319 (16) C15-C16 1.4140 (18) O5-C21 1.3048 (15) C14-H14B 0.9900 O5-C17 1.3613 (16) C15-C20 1.4225 (17) O6-C26 1.419 (2) C16-C17 1.3829 (17) O6-C27 1.4244 (17) C16-H116 0.9500 N1-C8 1.2928 (17) C17-C18 1.4149 (17) N1-C8 1.2928 (17) C14-H14B 0.9500 N2-C11 1.4633 (16)	Ni1_01		1 9001 (9)	C9	HOR	0.0	900
NII—NI 2.507 (10) C10—II.0A 0.5900 NII—NI 2.007 (10) C10—II.0B 0.9900 NI2—O4 ⁱⁱ 1.8873 (9) C11—C12 1.5136 (18) NI2—N3 ⁱⁱ 2.0105 (10) C11—H11A 0.9900 NI2—N3 2.0105 (10) C12—H12A 0.9900 O1—C1 1.3052 (15) C12—H12A 0.9900 O2—C3 1.3627 (16) C13—H13A 0.9900 O3—C12 1.4237 (16) C13—H13A 0.9900 O3—C13 1.4312 (16) C14—H14A 0.9900 O4—C15 1.3048 (15) C14—H14A 0.9900 O5—C17 1.3613 (16) C15—C20 1.4225 (16) O6—C24 1.419 (2) C16—C17 1.3829 (17) O1—C15 1.3048 (15) C18—C19 1.3697 (18) N2—C10 1.4630 (16) C19—C20 1.4140 (18) O5—C21 1.4786 (15) C18—C19 1.3697 (18) N2—C10 1.4650 (16) C19—C20 1.4141 (17) N2—C11 1.4630 (16) <td></td> <td></td> <td>2,0077(10)</td> <td>C10</td> <td>H10A</td> <td>0.5</td> <td>9900</td>			2,0077(10)	C10	H10A	0.5	9900
NIN1 2.007 (10) C10f10B 0.9900 Ni2-O4 ^µ I.8873 (9) C11C12 I.5136 (18) Ni2-O4 I.8873 (9) C11H11A 0.9900 Ni2-N3 ^µ 2.0105 (10) C12H12A 0.9900 OlC1 1.3052 (15) C12H12B 0.9900 O2-C3 1.3627 (16) C13C14 1.5180 (18) O2-C7 I.4319 (16) C13H13A 0.9900 O3-C12 I.4237 (16) C13H13A 0.9900 O3-C13 I.4312 (16) C14H14B 0.9900 O4-C15 1.3048 (15) C14H14B 0.9900 O5-C21 1.4350 (15) C15-C20 1.4252 (16) O6-C26 I.419 (2) C16-C17 I.3829 (17) O6-C26 I.419 (2) C16-C17 I.3829 (17) O6-C26 I.419 (2) C18-C19 I.3697 (18) N2-C11 I.4633 (16) C18-H18 0.9500 N2-C21 I.4786 (15) C18-C19 I.3697 (18) N2-C21 I.4780 (16) <td>NII—NI</td> <td></td> <td>2.0077 (10)</td> <td>C10-</td> <td>-HIOA</td> <td>0.9</td> <td>900</td>	NII—NI		2.0077 (10)	C10-	-HIOA	0.9	900
N204* 1.8873 (9) C11C12 1.515 (18) Ni203 ⁱⁱ 2.0105 (10) C11H11A 0.9900 Ni2N3 2.0105 (10) C12H12A 0.9900 OlC1 1.3052 (15) C12H12A 0.9900 O2C3 1.3627 (16) C13H13A 0.9900 O3C12 1.4237 (16) C13H13B 0.9900 O3C12 1.4237 (16) C14H14A 0.9900 O4C15 1.3484 (15) C14H14B 0.9900 O4C15 1.3484 (15) C14H14B 0.9900 O5C17 1.3613 (16) C15C16 1.4140 (18) O5C21 1.4360 (15) C15C20 1.4225 (16) O6-C22 1.424 (17) C16H16 0.9500 N1C8 1.2928 (17) C17C18 1.4149 (17) N2C11 1.4633 (16) C18C19 1.3697 (18) N2C14 1.4700 (16) C19C20 1.4411 (17) N2C14 1.4700 (16) C19H21A 0.9800 N4C24 1.4651 (17) C21H21A 0.9800 N4C25 <td< td=""><td></td><td></td><td>2.0077 (10)</td><td>C10-</td><td>-HIUB</td><td>0.9</td><td>900</td></td<>			2.0077 (10)	C10-	-HIUB	0.9	900
N2-O4 1.88/3 (9) C11-H11A 0.9900 Ni2-N3 ⁱⁱ 2.0105 (10) C11-H11B 0.9900 Ol-C1 1.3052 (15) C12-H12A 0.9900 O2-C3 1.3627 (16) C13-C14 1.5180 (18) O2-C7 1.4319 (16) C13-H13A 0.9900 O3-C12 1.4237 (16) C13-H13A 0.9900 O3-C13 1.4312 (16) C14-H14B 0.9900 O5-C17 1.3613 (16) C15-C16 1.4140 (18) O5-C21 1.4360 (15) C15-C20 1.4225 (16) O6-C25 1.419 (2) C16-C17 1.3829 (17) O6-C27 1.4244 (17) C16-H16 0.9500 N1-C8 1.2928 (17) C17-C18 1.4149 (17) N1-C9 1.4786 (15) C18-C19 1.3697 (18) N2-C11 1.4633 (16) C19-H19 0.9500 N2-C14 1.4700 (16) C19-H19 0.9500 N3-C22 1.2974 (16) C20-C22 1.4281 (18) N3-C22 1.2974 (16) <	N12—O4"		1.8873 (9)	C11-	-012	1.3	0136 (18)
N2-AS ¹⁰ 2.0105 (10)C11-H11B0.9900Ni2-N32.0105 (10)C12-H12A0.9900O2-C31.3052 (15)C12-H12B0.9900O2-C31.3627 (16)C13-C141.5180 (18)O2-C71.4319 (16)C13-H13A0.9900O3-C131.4312 (16)C14-H14A0.9900O3-C131.4312 (16)C14-H14B0.9900O4-C151.3048 (15)C14-H14B0.9900O5-C171.3613 (16)C15-C161.4140 (18)O5-C211.4264 (17)C16-C171.3829 (17)O6-C261.419 (2)C16-C171.3829 (17)O6-C271.4244 (17)C16-H160.9500NI-C81.2928 (17)C17-C181.4149 (17)N1-C91.4760 (15)C18-C191.3697 (18)N2-C111.4633 (16)C19-H190.9500N2-C101.4650 (16)C19-H190.9500N2-C111.4631 (17)C21-H21A0.9800N4-C241.4614 (17)C21-H21A0.9800N4-C241.4614 (17)C21-H21A0.9800N4-C251.4667 (16)C23-H23A0.9900C2-C31.3680 (18)C23-H23B0.9900C2-C41.4129 (18)C24-H24A0.9900C2-C51.3698 (19)C25-C261.512 (2)C4-H40.9500C2-H25A0.9900C3-C41.4129 (18)C24-H24B0.9900C3-C41.4126 (17)C25-H25A0.9900C3-C41.4129 (18)C24-H24B <td>N12—O4</td> <td></td> <td>1.8873 (9)</td> <td>C11–</td> <td>-H11A</td> <td>0.9</td> <td>900</td>	N12—O4		1.8873 (9)	C11–	-H11A	0.9	900
N2-M32.0105 (10)C12-H12A0.9900O1-C11.3052 (15)C12-H12B0.9900O2-C31.3627 (16)C13-C141.5180 (18)O2-C71.4319 (16)C13-H13A0.9900O3-C121.4227 (16)C14-H14A0.9900O3-C131.4312 (16)C14-H14A0.9900O4-C151.3048 (15)C14-H14B0.9900O5-C171.3613 (16)C15-C161.4140 (18)O5-C211.4360 (15)C15-C161.4225 (16)O6-C261.419 (2)C16-C171.3829 (17)O6-C271.4244 (17)C16-H160.9500N1-C81.2928 (17)C17-C181.4141 (17)N1-C91.4786 (15)C18-C191.3667 (18)N2-C101.4650 (16)C19-C201.4141 (17)N2-C141.4700 (16)C19-H190.9500N3-C231.4740 (16)C20-C221.4281 (18)N3-C231.4740 (16)C21-H21A0.9800N4-C241.4614 (17)C21-H21A0.9800N4-C251.4667 (16)C22-H220.9500C1-C21.4223 (17)C23-H23A0.9900C2-C31.3830 (18)C23-H23B0.9900C2-C41.4149 (18)C24-H24A0.9900C2-C51.3698 (19)C24-H24A0.9900C3-C41.4149 (17)C24-H24B0.9900C3-C41.4149 (17)C24-H24B0.9900C3-C41.4149 (18)C24-H24B0.9900C3-C41.3698 (19)C24-H	Ni2—N3 ¹¹		2.0105 (10)	C11–	-H11B	0.9	9900
Ol-Cl $1.3627 (16)$ $Cl2-Hl2B$ 0.9900 $O2-C3$ $1.3627 (16)$ $Cl3-Cl4$ $1.5180 (18)$ $O2-C7$ $1.4319 (16)$ $Cl3-Hl3A$ 0.9900 $O3-Cl2$ $1.4237 (16)$ $Cl3-Hl3A$ 0.9900 $O3-Cl3$ $1.4312 (16)$ $Cl4-Hl4A$ 0.9900 $O4-Cl5$ $1.3048 (15)$ $Cl4-Hl4B$ 0.9900 $O5-Cl7$ $1.3613 (16)$ $Cl5-Cl6$ $1.4140 (18)$ $O5-C21$ $1.4360 (15)$ $Cl5-Cl6$ $1.4225 (16)$ $O6-C26$ $1.419 (2)$ $Cl6-Cl7$ $1.3829 (17)$ $O6-C27$ $1.4224 (17)$ $Cl6-Hl6$ 0.9500 $NI-C8$ $1.2928 (17)$ $Cl7-Cl8$ $1.4149 (17)$ $NI-C9$ $1.4786 (15)$ $Cl8-Cl9$ $1.3697 (18)$ $N2-Cl1$ $1.4633 (16)$ $Cl8-Hl8$ 0.9500 $N2-Cl1$ $1.4650 (16)$ $Cl9-C22$ $1.4211 (17)$ $N2-Cl4$ $1.4700 (16)$ $Cl-H21A$ 0.9800 $N4-C24$ $1.461 (17)$ $C2l-H21B$ 0.9800 $N4-C24$ $1.4667 (16)$ $C22-H22$ 0.9500 $N4-C24$ $1.463 (16)$ $C21-H21B$ 0.9900 $Cl-C2$ $1.4420 (18)$ $C23-C24$ $1.5235 (18)$ $Cl-C3$ $1.3830 (18)$ $C23-H23A$ 0.9900 $Cl-C4$ $1.4129 (18)$ $C24-H24B$ 0.9900 $Cl-C5$ $1.3698 (19)$ $C25-C26$ $1.512 (2)$ $Cl-C4$ $1.4146 (17)$ $C25-H25A$ 0.9900 $Cl-C5-H12A$ 0.9900 $C2-H25A$ 0.9900 <td< td=""><td>Ni2—N3</td><td></td><td>2.0105 (10)</td><td>C12–</td><td>-H12A</td><td>0.9</td><td>900</td></td<>	Ni2—N3		2.0105 (10)	C12–	-H12A	0.9	900
02-C3 $1.3627 (16)$ $C13-C14$ $1.5180 (18)$ $02-C7$ $1.4319 (16)$ $C13-H13A$ 0.9900 $03-C12$ $1.4327 (16)$ $C13-H13B$ 0.9900 $03-C13$ $1.4312 (16)$ $C14-H14A$ 0.9900 $04-C15$ $1.3048 (15)$ $C14-H14B$ 0.9900 $05-C17$ $1.3613 (16)$ $C15-C16$ $1.4140 (18)$ $05-C21$ $1.4360 (15)$ $C15-C20$ $1.4225 (16)$ $06-C26$ $1.419 (2)$ $C16-C17$ $1.3829 (17)$ $06-C27$ $1.4244 (17)$ $C16-H16$ 0.9500 $NI-C8$ $1.2928 (17)$ $C17-C18$ $1.4149 (17)$ $NI-C9$ $1.4786 (15)$ $C18-H18$ 0.9500 $N2-C11$ $1.4633 (16)$ $C19-C20$ $1.4141 (17)$ $N2-C11$ $1.4630 (16)$ $C19-H19$ 0.9500 $N3-C22$ $1.2974 (16)$ $C20-C22$ $1.4281 (18)$ $N3-C23$ $1.4740 (16)$ $C21-H21A$ 0.9800 $N4-C24$ $1.667 (16)$ $C22-H22$ 0.9800 $N4-C24$ $1.464 (17)$ $C21-H21B$ 0.9800 $N4-C25$ $1.4667 (16)$ $C22-H22$ 0.9500 $C1-C6$ $1.4223 (17)$ $C23-H23A$ 0.9900 $C2-G2$ $1.3830 (18)$ $C23-H23A$ 0.9900 $C2-G4$ $1.4129 (18)$ $C24-H24B$ 0.9900 $C2-G4$ $1.4129 (18)$ $C25-H25A$ 0.9900 $C-C4$ $1.4129 (18)$ $C25-H25A$ 0.9900 $C-C5$ $1.5080 (19)$ $C25-H25A$ 0.9900 $C-C6$	O1—C1		1.3052 (15)	C12–	-H12B	0.9	900
02-C7 $1.4319 (16)$ $C13-H13A$ 0.9900 $03-C12$ $1.4327 (16)$ $C13-H13B$ 0.9900 $03-C13$ $1.4312 (16)$ $C14-H14B$ 0.9900 $05-C17$ $1.3613 (16)$ $C15-C16$ $1.4140 (18)$ $05-C21$ $1.4360 (15)$ $C15-C16$ $1.4225 (16)$ $06-C26$ $1.419 (2)$ $C16-C17$ $1.3829 (17)$ $06-C27$ $1.4244 (17)$ $C16-H16$ 0.9500 $N1-C8$ $1.2928 (17)$ $C17-C18$ $1.4149 (17)$ $N1-C9$ $1.4786 (15)$ $C18-C19$ $1.3697 (18)$ $N2-C11$ $1.4653 (16)$ $C19-C20$ $1.4141 (17)$ $N2-C10$ $1.4650 (16)$ $C19-C20$ $1.4141 (17)$ $N2-C14$ $1.4700 (16)$ $C19-H19$ 0.9500 $N3-C22$ $1.2974 (16)$ $C20-C22$ $1.4281 (18)$ $N3-C23$ $1.4740 (16)$ $C21-H21A$ 0.9800 $N4-C24$ $1.461 (17)$ $C21-H21B$ 0.9800 $N4-C25$ $1.4667 (16)$ $C22-H22$ 0.9500 $C1-C2$ $1.4201 (18)$ $C23-C24$ $1.523 (18)$ $C1-C2$ $1.4201 (18)$ $C23-H23A$ 0.9900 $C2-C3$ $1.3698 (19)$ $C25-C26$ $1.512 (2)$ $C2-H44$ 0.9500 $C24-H24B$ 0.9900 $C3-C4$ $1.4210 (18)$ $C26-H25A$ 0.9900 $C3-C4$ $1.4146 (17)$ $C25-H25A$ 0.9900 $C3-C6$ $1.4129 (18)$ $C26-H26B$ 0.9900 $C5-C6$ $1.4146 (17)$ $C25-H25A$ 0.9900 <	O2—C3		1.3627 (16)	C13–	C14	1.5	5180 (18)
03-C12 $1.4237 (16)$ $C13-H13B$ 0.9900 $03-C13$ $1.4312 (16)$ $C14-H14A$ 0.9900 $04-C15$ $1.3048 (15)$ $C14-H14B$ 0.9900 $05-C17$ $1.3613 (16)$ $C15-C16$ $1.4140 (18)$ $05-C21$ $1.4360 (15)$ $C15-C20$ $1.4225 (16)$ $06-C26$ $1.419 (2)$ $C16-C17$ $1.3829 (17)$ $06-C27$ $1.4244 (17)$ $C16-H16$ 0.9500 $N1-C8$ $1.2928 (17)$ $C17-C18$ $1.4149 (17)$ $N1-C9$ $1.4786 (15)$ $C18-C19$ $1.3697 (18)$ $N2-C11$ $1.4633 (16)$ $C19-C20$ $1.4141 (17)$ $N2-C10$ $1.4650 (16)$ $C19-C20$ $1.4141 (17)$ $N2-C14$ $1.4700 (16)$ $C20-C22$ $1.4281 (18)$ $N3-C22$ $1.2974 (16)$ $C20-C22$ $1.4281 (18)$ $N3-C23$ $1.4740 (16)$ $C21-H21A$ 0.9800 $N4-C24$ $1.4614 (17)$ $C21-H21B$ 0.9800 $N4-C25$ $1.4667 (16)$ $C22-H22$ 0.9500 $C1-C2$ $1.4231 (17)$ $C23-H23B$ 0.9900 $C2-C3$ $1.3830 (18)$ $C23-H23B$ 0.9900 $C2-C4$ $1.4129 (18)$ $C24-H24B$ 0.9900 $C2-H2$ 0.9500 $C24-H24B$ 0.9900 $C2-H2$ 0.9500 $C25-H25A$ 0.9900 $C3-C4$ $1.4129 (18)$ $C24-H24B$ 0.9900 $C3-C4$ $1.4129 (18)$ $C24-H24B$ 0.9900 $C3-C4$ $1.4129 (18)$ $C25-H25A$ 0.9900	O2—C7		1.4319 (16)	C13–	-H13A	0.9	900
03-C13 $1.4312 (16)$ $C14-H14A$ 0.9900 $04-C15$ $1.3048 (15)$ $C14-H14B$ 0.9900 $05-C17$ $1.3613 (16)$ $C15-C16$ $1.4140 (18)$ $05-C21$ $1.4360 (15)$ $C15-C20$ $1.4225 (16)$ $06-C26$ $1.419 (2)$ $C16-C17$ $1.3829 (17)$ $06-C27$ $1.4244 (17)$ $C16-H16$ 0.9500 $N1-C8$ $1.2928 (17)$ $C17-C18$ $1.4149 (17)$ $N1-C9$ $1.4786 (15)$ $C18-C19$ $1.3697 (18)$ $N2-C11$ $1.4633 (16)$ $C18-H18$ 0.9500 $N2-C10$ $1.4650 (16)$ $C19-C20$ $1.4141 (17)$ $N2-C14$ $1.4700 (16)$ $C19-H19$ 0.9500 $N3-C22$ $1.2974 (16)$ $C20-C22$ $1.4281 (18)$ $N3-C23$ $1.4740 (16)$ $C21-H21A$ 0.9800 $N4-C24$ $1.4614 (17)$ $C21-H21B$ 0.9800 $N4-C25$ $1.4667 (16)$ $C22-H22$ 0.9500 $C1-C2$ $1.4221 (17)$ $C23-H23A$ 0.9900 $C2-C3$ $1.3830 (18)$ $C23-H23A$ 0.9900 $C2-C4$ $1.4129 (18)$ $C24-H24A$ 0.9900 $C2-C5$ $1.3698 (19)$ $C25-C26$ $1.512 (2)$ $C4-C5$ $1.3698 (19)$ $C25-H25A$ 0.9900 $C2-H2A$ 0.9500 $C2-H26A$ 0.9900 $C3-C4$ $1.4270 (18)$ $C26-H26B$ 0.9900 $C5-H35$ 0.9900 $C2-H27A$ 0.9900 $C5-H35$ 0.9900 $C2-H27A$ 0.9900 $C5-H35$ <t< td=""><td>O3—C12</td><td></td><td>1.4237 (16)</td><td>C13–</td><td>-H13B</td><td>0.9</td><td>900</td></t<>	O3—C12		1.4237 (16)	C13–	-H13B	0.9	900
04-C15 $1.3048 (15)$ $C14-H14B$ 0.9900 $05-C17$ $1.313 (16)$ $C15-C16$ $1.4140 (18)$ $05-C21$ $1.4360 (15)$ $C15-C20$ $1.4225 (16)$ $06-C26$ $1.419 (2)$ $C16-C17$ $1.3229 (17)$ $06-C27$ $1.4244 (17)$ $C16-H16$ 0.9500 $N1-C8$ $1.2928 (17)$ $C17-C18$ $1.4149 (17)$ $N1-C9$ $1.4786 (15)$ $C18-C19$ $1.3697 (18)$ $N2-C11$ $1.4633 (16)$ $C19-C20$ $1.4141 (17)$ $N2-C10$ $1.4650 (16)$ $C19-H19$ 0.9500 $N2-C14$ $1.4700 (16)$ $C21-H21A$ 0.9800 $N-C22$ $1.2974 (16)$ $C20-C22$ $1.4281 (18)$ $N3-C23$ $1.4740 (16)$ $C21-H21A$ 0.9800 $N4-C24$ $1.4614 (17)$ $C21-H21B$ 0.9800 $N4-C25$ $1.4667 (16)$ $C22-H22$ 0.9500 $C1-C2$ $1.4221 (17)$ $C23-H23A$ 0.9900 $C2-C3$ $1.3830 (18)$ $C23-H23A$ 0.9900 $C2-C3$ $1.3698 (19)$ $C25-C26$ $1.512 (2)$ $C4-C5$ $1.3698 (19)$ $C25-H25A$ 0.9900 $C3-C4$ $1.4127 (18)$ $C26-H26A$ 0.9900 $C5-C6$ $1.4146 (17)$ $C25-H25A$ 0.9900 C	O3—C13		1.4312 (16)	C14–	-H14A	0.9	900
05-C17 $1.3613 (16)$ $C15-C16$ $1.4140 (18)$ $05-C21$ $1.4360 (15)$ $C15-C20$ $1.4225 (16)$ $06-C26$ $1.419 (2)$ $C16-C17$ $1.3829 (17)$ $06-C27$ $1.4244 (17)$ $C16-H16$ 0.9500 $N1-C8$ $1.2928 (17)$ $C17-C18$ $1.4149 (17)$ $N1-C9$ $1.4786 (15)$ $C18-C19$ $1.3697 (18)$ $N2-C11$ $1.4633 (16)$ $C18-H18$ 0.9500 $N2-C10$ $1.4650 (16)$ $C19-C20$ $1.4141 (17)$ $N2-C14$ $1.4700 (16)$ $C19-H19$ 0.9500 $N3-C22$ $1.2974 (16)$ $C20-C22$ $1.4281 (18)$ $N3-C23$ $1.4740 (16)$ $C21-H21A$ 0.9800 $N4-C24$ $1.4631 (17)$ $C21-H21B$ 0.9800 $N4-C25$ $1.4667 (16)$ $C22-H22$ 0.9500 $C1-C2$ $1.4221 (18)$ $C23-C24$ $1.5235 (18)$ $C1-C2$ $1.4231 (17)$ $C23-H23A$ 0.9900 $C2-C3$ $1.3830 (18)$ $C23-H23A$ 0.9900 $C2-C4$ $1.4129 (18)$ $C24-H24A$ 0.9900 $C2-H2$ 0.9500 $C2-H25A$ 0.9900 $C4-C5$ $1.3698 (19)$ $C25-C26$ $1.512 (2)$ $C4-H4$ 0.9500 $C25-H25A$ 0.9900 $C5-H5$ 0.9500 $C2-H25B$ 0.9900 $C5-H5$ 0.9500 $C25-H25A$ 0.9900 $C5-H5$ 0.9500 $C2-H25B$ 0.9900 $C5-H5$ 0.9500 $C2-H25B$ 0.9900 $C5-H5$ 0.9500 <td< td=""><td>O4—C15</td><td></td><td>1.3048 (15)</td><td>C14–</td><td>-H14B</td><td>0.9</td><td>900</td></td<>	O4—C15		1.3048 (15)	C14–	-H14B	0.9	900
05-C21 $1.4360 (15)$ $C15-C20$ $1.4225 (16)$ $06-C26$ $1.419 (2)$ $C16-C17$ $1.3829 (17)$ $06-C27$ $1.4244 (17)$ $C16-H16$ 0.9500 $N1-C8$ $1.2928 (17)$ $C17-C18$ $1.4149 (17)$ $N1-C9$ $1.4786 (15)$ $C18-C19$ $1.3697 (18)$ $N2-C11$ $1.4633 (16)$ $C19-C20$ $1.4141 (17)$ $N2-C10$ $1.4650 (16)$ $C19-C20$ $1.4141 (17)$ $N2-C14$ $1.4700 (16)$ $C19-H19$ 0.9500 $N3-C22$ $1.2974 (16)$ $C20-C22$ $1.4281 (18)$ $N3-C23$ $1.4740 (16)$ $C21-H21A$ 0.9800 $N4-C24$ $1.4614 (17)$ $C21-H21B$ 0.9800 $N4-C25$ $1.4667 (16)$ $C22-H22$ 0.9500 $C1-C2$ $1.4221 (18)$ $C23-C24$ $1.5235 (18)$ $C1-C4$ $1.4221 (17)$ $C23-H23A$ 0.9900 $C2-C3$ $1.3830 (18)$ $C23-H23A$ 0.9900 $C2-C4$ $1.4129 (18)$ $C24-H24B$ 0.9900 $C2-C5$ $1.3698 (19)$ $C25-C26$ $1.512 (2)$ $C4-H4$ 0.9500 $C2-H25A$ 0.9900 $C3-C4$ $1.4126 (17)$ $C25-H25A$ 0.9900 $C5-C6$ $1.4146 (17)$ $C25-H25B$ 0.9900 $C5-C6$ $1.4127 (18)$ $C26-H26B$ 0.9900 $C5-C6$ $1.4127 (18)$ $C26-H26B$ 0.9900 $C5-H5$ 0.9500 $C27-H27A$ 0.9900 $C5-H5$ 0.9800 $C27-H27A$ 0.9900 $C5-H5$ <t< td=""><td>O5—C17</td><td></td><td>1.3613 (16)</td><td>C15–</td><td>C16</td><td>1.4</td><td>140 (18)</td></t<>	O5—C17		1.3613 (16)	C15–	C16	1.4	140 (18)
06-C26 $1.419 (2)$ $C16-C17$ $1.3829 (17)$ $06-C27$ $1.4244 (17)$ $C16-H16$ 0.9500 $N1-C8$ $1.2928 (17)$ $C17-C18$ $1.4149 (17)$ $N1-C9$ $1.4786 (15)$ $C18-C19$ $1.3697 (18)$ $N2-C11$ $1.4633 (16)$ $C18-H18$ 0.9500 $N2-C10$ $1.4650 (16)$ $C19-C20$ $1.4141 (17)$ $N2-C14$ $1.4700 (16)$ $C21-H21A$ 0.9800 $N3-C22$ $1.2974 (16)$ $C20-C22$ $1.4281 (18)$ $N3-C23$ $1.4740 (16)$ $C21-H21A$ 0.9800 $N4-C24$ $1.4614 (17)$ $C21-H21B$ 0.9800 $N4-C25$ $1.4667 (16)$ $C22-H22$ 0.9500 $C1-C2$ $1.4201 (18)$ $C23-C24$ $1.5235 (18)$ $C1-C6$ $1.4223 (17)$ $C23-H23A$ 0.9900 $C2-C3$ $1.3830 (18)$ $C23-H24A$ 0.9900 $C2-H2$ 0.9500 $C24-H24A$ 0.9900 $C3-C4$ $1.4129 (18)$ $C24-H24B$ 0.9900 $C4-C5$ $1.3698 (19)$ $C25-C26$ $1.512 (2)$ $C4-H44$ 0.9500 $C25-H25A$ 0.9900 $C5-H5$ 0.9500 $C26-H26B$ 0.9900 $C5-H5$ 0.9500 $C26-H26B$ 0.9900 $C5-H5$ 0.9800 $C27-H27A$ 0.9900 $C7-H7A$ 0.9800 $C27-H27B$ 0.9900 $C7-H7A$ 0.9800 $C27-H27B$ 0.9900 $C5-H5$ 0.9900 $C7-H27B$ 0.9900 $C7-H7C$ 0.9800 $C27-H27B$ <	O5—C21		1.4360 (15)	C15–	C20	1.4	225 (16)
06-C27 $1.4244 (17)$ $C16-H16$ 0.9500 $N1-C8$ $1.2928 (17)$ $C17-C18$ $1.4149 (17)$ $N1-C9$ $1.4786 (15)$ $C18-C19$ $1.3697 (18)$ $N2-C11$ $1.4633 (16)$ $C18-H18$ 0.9500 $N2-C10$ $1.4650 (16)$ $C19-C20$ $1.4141 (17)$ $N2-C14$ $1.4700 (16)$ $C20-C22$ $1.4281 (18)$ $N3-C22$ $1.2974 (16)$ $C20-C22$ $1.4281 (18)$ $N3-C23$ $1.4740 (16)$ $C21-H21A$ 0.9800 $N4-C24$ $1.4614 (17)$ $C21-H21B$ 0.9800 $N4-C25$ $1.4667 (16)$ $C22-H22$ 0.9500 $C1-C2$ $1.4201 (18)$ $C23-C24$ $1.5235 (18)$ $C1-C6$ $1.4223 (17)$ $C23-H23A$ 0.9900 $C2-C3$ $1.3830 (18)$ $C23-H24A$ 0.9900 $C2-H2$ 0.9500 $C24-H24A$ 0.9900 $C3-C4$ $1.4129 (18)$ $C24-H24B$ 0.9900 $C4-C5$ $1.3698 (19)$ $C25-C26$ $1.512 (2)$ $C4-H44$ 0.9500 $C25-H25A$ 0.9900 $C5-C6$ $1.4146 (17)$ $C25-H25B$ 0.9900 $C5-C6$ $1.41270 (18)$ $C26-H26A$ 0.9900 $C5-C6$ $1.41270 (18)$ $C26-H26B$ 0.9900 $C5-C6$ $1.41270 (18)$ $C26-H26B$ 0.9900 $C7-H7A$ 0.9800 $C27-H27A$ 0.9900 $C7-H7A$ 0.9800 $C27-H27B$ 0.9900 $C7-H7A$ 0.9800 $C27-H27B$ 0.9900 $C7-H7B$ 0.9800	O6—C26		1.419 (2)	C16–	C17	1.3	8829 (17)
N1-C81.2928 (17)C17-C181.4149 (17)N1-C91.4786 (15)C18-C191.3697 (18)N2-C111.4633 (16)C18-H180.9500N2-C101.4650 (16)C19-C201.4141 (17)N2-C141.4700 (16)C19-H190.9500N3-C221.2974 (16)C20-C221.4281 (18)N3-C231.4740 (16)C21-H21A0.9800N4-C241.4614 (17)C21-H21B0.9800N4-C251.4667 (16)C22-H220.9500C1-C21.4201 (18)C23-C241.5235 (18)C1-C61.4223 (17)C23-H23A0.9900C2-C31.3830 (18)C23-H23B0.9900C2-C41.4129 (18)C24-H24A0.9900C3-C41.4129 (18)C24-H24B0.9900C4-C51.3698 (19)C25-C261.512 (2)C4-H40.9500C25-H25A0.9900C5-C61.4146 (17)C25-H25A0.9900C5-H50.9500C26-H26A0.9900C5-H50.9500C26-H26A0.9900C5-H50.9500C26-H26A0.9900C5-H50.9800C27-C281.5109 (19)C7-H7A0.9800C27-H27B0.9900C7-H7B0.9800C27-H27B0.9900C7-H7C0.9800C27-H27B0.9900C8-H80.9500C28-H28A0.9900	O6—C27		1.4244 (17)	C16–	-H16	0.9	9500
N1-C9 $1.4786 (15)$ $C18-C19$ $1.3697 (18)$ N2-C11 $1.4633 (16)$ $C18-H18$ 0.9500 N2-C10 $1.4650 (16)$ $C19-C20$ $1.4141 (17)$ N2-C14 $1.4700 (16)$ $C19-H19$ 0.9500 N3-C22 $1.2974 (16)$ $C20-C22$ $1.4281 (18)$ N3-C23 $1.4740 (16)$ $C21-H21A$ 0.9800 N4-C24 $1.4614 (17)$ $C21-H21B$ 0.9800 N4-C28 $1.4637 (16)$ $C22-H22$ 0.9500 N4-C25 $1.4667 (16)$ $C22-H22$ 0.9500 C1-C2 $1.4201 (18)$ $C23-C24$ $1.5235 (18)$ C1-C6 $1.4223 (17)$ $C23-H23B$ 0.9900 C2-C3 $1.3830 (18)$ $C23-H23B$ 0.9900 C2-H2 0.9500 $C24-H24B$ 0.9900 C3-C4 $1.4129 (18)$ $C25-C26$ $1.512 (2)$ C4-C5 $1.3698 (19)$ $C25-H25A$ 0.9900 C5-C6 $1.4146 (17)$ $C25-H25B$ 0.9900 C5-H5 0.9500 $C26-H26A$ 0.9900 C5-H5 0.9500 $C26-H26A$ 0.9900 C5-H5 0.9800 $C27-C28$ $1.5109 (19)$ C7-H7A 0.9800 $C27-H27A$ 0.9900 C7-H7B 0.9800 $C27-H27B$ 0.9900 C7-H7C 0.9800 $C27-H27B$ 0.9900 C8-H8 0.9500 $C28-H28A$ 0.9900	N1—C8		1.2928 (17)	C17–	C18	1.4	149 (17)
N2C11 $1.4633(16)$ $C18H18$ 0.9500 N2C10 $1.4650(16)$ $C19C20$ $1.4141(17)$ N2C14 $1.4700(16)$ $C19H19$ 0.9500 N3C22 $1.2974(16)$ $C20C22$ $1.4281(18)$ N3C23 $1.4740(16)$ $C21H21A$ 0.9800 N4C24 $1.4614(17)$ $C21H21B$ 0.9800 N4C25 $1.4667(16)$ $C22H22$ 0.9500 C1C2 $1.4201(18)$ $C23C24$ $1.5235(18)$ C1C6 $1.4223(17)$ $C23H23A$ 0.9900 C2C3 $1.3830(18)$ $C23H23B$ 0.9900 C2C4 $1.4129(18)$ $C24H24A$ 0.9900 C3C4 $1.4129(18)$ $C24H24B$ 0.9900 C4C5 $1.3698(19)$ $C25C26$ $1.512(2)$ C4H4 0.9500 $C25H25A$ 0.9900 C5C6 $1.4146(17)$ $C25H25B$ 0.9900 C5C76 $1.4146(17)$ $C25H26B$ 0.9900 C5C6 $1.4146(17)$ $C25H26B$ 0.9900 C5C76 $1.4270(18)$ $C26-H26B$ 0.9900 C6C8 $1.4270(18)$ $C26-H26B$ 0.9900 C7H7A 0.9800 $C27-H27A$ 0.9900 C7H7B 0.9800 $C27-H27B$ 0.9900 C7H7A 0.9800 $C27-H27B$ 0.9900 C7H7A 0.9800 $C27-H27B$ 0.9900	N1-C9		1.4786 (15)	C18–	C19	1.3	697 (18)
N2C10 $1.4650 (16)$ $C19C20$ $1.4141 (17)$ N2C14 $1.4700 (16)$ $C19H19$ 0.9500 N3C22 $1.2974 (16)$ $C20C22$ $1.4281 (18)$ N3C23 $1.4740 (16)$ $C21H21A$ 0.9800 N4C24 $1.4614 (17)$ $C21H21B$ 0.9800 N4C25 $1.4667 (16)$ $C22H22$ 0.9500 C1C2 $1.4201 (18)$ $C23C24$ $1.5235 (18)$ C1C6 $1.4223 (17)$ $C23-H23A$ 0.9900 C2C3 $1.3830 (18)$ $C23-H23B$ 0.9900 C2H2 0.9500 $C24-H24A$ 0.9900 C3C4 $1.4129 (18)$ $C24-H24A$ 0.9900 C3C4 $1.4129 (18)$ $C25-H25A$ 0.9900 C4C5 $1.3698 (19)$ $C25-H25A$ 0.9900 C5C6 $1.4146 (17)$ $C25-H25B$ 0.9900 C5C76 $1.4146 (17)$ $C25-H25B$ 0.9900 C5C78 $1.4470 (18)$ $C26-H26B$ 0.9900 C5H7A 0.9800 $C27-C28$ $1.5109 (19)$ C7H7A 0.9800 $C27-H27A$ 0.9900 C7H7B 0.9800 $C27-H27A$ 0.9900 C7H7B 0.9800 $C27-H27B$ 0.9900 C8H8 0.9500 $C28-H28A$ 0.9900	N2-C11		1.4633 (16)	C18–	-H18	0.9	9500
N2C14 1.4700 (16) C19H19 0.9500 N3C22 1.2974 (16) C20C22 1.4281 (18) N3C23 1.4740 (16) C21H21A 0.9800 N4C24 1.4614 (17) C21H21B 0.9800 N4C28 1.4667 (16) C22H22 0.9500 C1C2 1.4201 (18) C23C24 1.5235 (18) C1C6 1.4223 (17) C23H23A 0.9900 C2C3 1.3830 (18) C23H23B 0.9900 C2H2 0.9500 C24H24A 0.9900 C3C4 1.4129 (18) C24H24B 0.9900 C3C4 1.4129 (18) C24H24B 0.9900 C4C5 1.3698 (19) C25C26 1.512 (2) C4H4 0.9500 C25H25A 0.9900 C5C6 1.4146 (17) C25H25B 0.9900 C5H5 0.9500 C26-H26A 0.9900 C5H5 0.9500 C26-H26B 0.9900 C5H5 0.9800 C27C28 1.5109 (19) C7H7A 0.9800 C27C28 1	N2-C10		1.4650 (16)	C19–	-C20	1.4	141 (17)
N3-C22 $1.2974(16)$ $C20-C22$ $1.4281(18)$ N3-C23 $1.4740(16)$ $C21-H21A$ 0.9800 N4-C24 $1.4614(17)$ $C21-H21B$ 0.9800 N4-C28 $1.4631(17)$ $C21-H21C$ 0.9800 N4-C25 $1.4667(16)$ $C22-H22$ 0.9500 C1-C2 $1.4201(18)$ $C23-C24$ $1.5235(18)$ C1-C6 $1.4223(17)$ $C23-H23A$ 0.9900 C2-C3 $1.3830(18)$ $C23-H23B$ 0.9900 C2-H2 0.9500 $C24-H24A$ 0.9900 C3-C4 $1.4129(18)$ $C24-H24B$ 0.9900 C3-C4 $1.4129(18)$ $C25-C26$ $1.512(2)$ C4-H4 0.9500 $C25-H25A$ 0.9900 C5-C6 $1.4146(17)$ $C25-H25B$ 0.9900 C5-H5 0.9500 $C26-H26A$ 0.9900 C5-H5 0.9500 $C26-H26B$ 0.9900 C7-H7A 0.9800 $C27-C28$ $1.5109(19)$ C7-H7A 0.9800 $C27-H27A$ 0.9900 C7-H7B 0.9800 $C27-H27B$ 0.9900 C8-H8 0.9500 $C28-H28A$ 0.9900	N2-C14		1.4700 (16)	C19–	-H19	0.9	9500
N3—C231.4740 (16)C21—H21A0.9800N4—C241.4614 (17)C21—H21B0.9800N4—C281.4631 (17)C21—H21C0.9800N4—C251.4667 (16)C22—H220.9500C1—C21.4201 (18)C23—C241.5235 (18)C1—C61.4223 (17)C23—H23A0.9900C2—C31.3830 (18)C23—H23B0.9900C2—H20.9500C24—H24A0.9900C3—C41.4129 (18)C24—H24B0.9900C4—C51.3698 (19)C25—C261.512 (2)C4—H40.9500C25—H25A0.9900C5—C61.4146 (17)C25—H25B0.9900C5—H50.9500C26—H26A0.9900C5—H50.9500C26—H26B0.9900C6—C81.4270 (18)C26—H26B0.9900C7—H7A0.9800C27—C281.5109 (19)C7—H7B0.9800C27—H27A0.9900C7—H7R0.9800C27—H27B0.9900C8—H80.9500C28—H28A0.9900	N3—C22		1.2974 (16)	C20–	C22	1.4	281 (18)
N4—C241.4614 (17)C21—H21B0.9800N4—C281.4631 (17)C21—H21C0.9800N4—C251.4667 (16)C22—H220.9500C1—C21.4201 (18)C23—C241.5235 (18)C1—C61.4223 (17)C23—H23A0.9900C2—C31.3830 (18)C23—H23B0.9900C2—H20.9500C24—H24A0.9900C3—C41.4129 (18)C24—H24B0.9900C4—C51.3698 (19)C25—C261.512 (2)C4—H40.9500C25—H25A0.9900C5—C61.4146 (17)C25—H25B0.9900C5—H50.9500C26—H26A0.9900C5—H50.9500C26—H26B0.9900C6—C81.4270 (18)C26—H26B0.9900C7—H7A0.9800C27—C281.5109 (19)C7—H7B0.9800C27—H27A0.9900C7—H7B0.9800C27—H27A0.9900C8—H80.9500C28—H28A0.9900	N3—C23		1.4740 (16)	C21–	-H21A	0.9	9800
N4—C281.4631 (17)C21—H21C0.9800N4—C251.4667 (16)C22—H220.9500C1—C21.4201 (18)C23—C241.5235 (18)C1—C61.4223 (17)C23—H23A0.9900C2—C31.3830 (18)C23—H23B0.9900C2—H20.9500C24—H24A0.9900C3—C41.4129 (18)C24—H24B0.9900C4—C51.3698 (19)C25—C261.512 (2)C4—H40.9500C25—H25A0.9900C5—C61.4146 (17)C25—H25B0.9900C5—H50.9500C26—H26B0.9900C6—C81.4270 (18)C26—H26B0.9900C7—H7A0.9800C27—C281.5109 (19)C7—H7B0.9800C27—H27A0.9900C7—H7C0.9800C27—H27B0.9900C8—H80.9500C28—H28A0.9900	N4—C24		1.4614 (17)	C21-	-H21B	0.9	9800
N4—C251.4667 (16)C22—H220.9500C1—C21.4201 (18)C23—C241.5235 (18)C1—C61.4223 (17)C23—H23A0.9900C2—C31.3830 (18)C23—H23B0.9900C2—H20.9500C24—H24A0.9900C3—C41.4129 (18)C24—H24B0.9900C4—C51.3698 (19)C25—C261.512 (2)C4—H40.9500C25—H25A0.9900C5—C61.4146 (17)C25—H25B0.9900C5—H50.9500C26—H26A0.9900C6—C81.4270 (18)C26—H26B0.9900C7—H7A0.9800C27—C281.5109 (19)C7—H7B0.9800C27—H27A0.9900C7—H7C0.9800C27—H27B0.9900C8—H80.9500C28—H28A0.9900	N4—C28		1.4631 (17)	C21-	-H21C	0.9	9800
C1C21.4201 (18)C23C241.5235 (18)C1C61.4223 (17)C23H23A0.9900C2C31.3830 (18)C23H23B0.9900C2H20.9500C24H24A0.9900C3C41.4129 (18)C24H24B0.9900C4C51.3698 (19)C25C261.512 (2)C4H40.9500C25H25A0.9900C5C61.4146 (17)C25H25B0.9900C5H50.9500C26H26A0.9900C5H50.9500C26H26B0.9900C6C81.4270 (18)C26H26B0.9900C7H7A0.9800C27C281.5109 (19)C7H7B0.9800C27H27A0.9900C7H7C0.9800C27H27A0.9900C8H80.9500C28H28A0.9900	N4—C25		1.4667 (16)	C22–	-H22	0.9	9500
C1C61.4223 (17)C23H23A0.9900C2C31.3830 (18)C23H23B0.9900C2H20.9500C24H24A0.9900C3C41.4129 (18)C24H24B0.9900C4C51.3698 (19)C25C261.512 (2)C4H40.9500C25H25A0.9900C5C61.4146 (17)C25H25B0.9900C5H50.9500C26H26A0.9900C6C81.4270 (18)C26H26B0.9900C7H7A0.9800C27C281.5109 (19)C7H7B0.9800C27H27A0.9900C7H7C0.9800C27H27B0.9900C8H80.9500C28H28A0.9900	C1—C2		1.4201 (18)	C23–	C24	1.5	5235 (18)
C2—C31.3830 (18)C23—H23B0.9900C2—H20.9500C24—H24A0.9900C3—C41.4129 (18)C24—H24B0.9900C4—C51.3698 (19)C25—C261.512 (2)C4—H40.9500C25—H25A0.9900C5—C61.4146 (17)C25—H25B0.9900C5—H50.9500C26—H26A0.9900C6—C81.4270 (18)C26—H26B0.9900C7—H7A0.9800C27—C281.5109 (19)C7—H7B0.9800C27—H27A0.9900C7—H7C0.9800C27—H27B0.9900C8—H80.9500C28—H28A0.9900	C1—C6		1.4223 (17)	C23–	-H23A	0.9	900
C2—H20.9500C24—H24A0.9900C3—C41.4129 (18)C24—H24B0.9900C4—C51.3698 (19)C25—C261.512 (2)C4—H40.9500C25—H25A0.9900C5—C61.4146 (17)C25—H25B0.9900C5—H50.9500C26—H26A0.9900C6—C81.4270 (18)C26—H26B0.9900C7—H7A0.9800C27—C281.5109 (19)C7—H7B0.9800C27—H27A0.9900C7—H7C0.9800C27—H27B0.9900C8—H80.9500C28—H28A0.9900	C2—C3		1.3830 (18)	C23–	-H23B	0.9	900
C3—C41.4129 (18)C24—H24B0.9900C4—C51.3698 (19)C25—C261.512 (2)C4—H40.9500C25—H25A0.9900C5—C61.4146 (17)C25—H25B0.9900C5—H50.9500C26—H26A0.9900C6—C81.4270 (18)C26—H26B0.9900C7—H7A0.9800C27—C281.5109 (19)C7—H7B0.9800C27—H27A0.9900C7—H7C0.9800C27—H27B0.9900C8—H80.9500C28—H28A0.9900	С2—Н2		0.9500	C24–	-H24A	0.9	900
C4—C51.3698 (19)C25—C261.512 (2)C4—H40.9500C25—H25A0.9900C5—C61.4146 (17)C25—H25B0.9900C5—H50.9500C26—H26A0.9900C6—C81.4270 (18)C26—H26B0.9900C7—H7A0.9800C27—C281.5109 (19)C7—H7B0.9800C27—H27A0.9900C7—H7C0.9800C27—H27B0.9900C8—H80.9500C28—H28A0.9900	C3—C4		1.4129 (18)	C24–	-H24B	0.9	900
C4—H40.9500C25—H25A0.9900C5—C61.4146 (17)C25—H25B0.9900C5—H50.9500C26—H26A0.9900C6—C81.4270 (18)C26—H26B0.9900C7—H7A0.9800C27—C281.5109 (19)C7—H7B0.9800C27—H27A0.9900C7—H7C0.9800C27—H27B0.9900C8—H80.9500C28—H28A0.9900	C4—C5		1.3698 (19)	C25–	C26	1.5	512 (2)
C5—C61.4146 (17)C25—H25B0.9900C5—H50.9500C26—H26A0.9900C6—C81.4270 (18)C26—H26B0.9900C7—H7A0.9800C27—C281.5109 (19)C7—H7B0.9800C27—H27A0.9900C7—H7C0.9800C27—H27B0.9900C8—H80.9500C28—H28A0.9900	C4—H4		0.9500	C25–	-H25A	0.9	900
C5—H50.9500C26—H26A0.9900C6—C81.4270 (18)C26—H26B0.9900C7—H7A0.9800C27—C281.5109 (19)C7—H7B0.9800C27—H27A0.9900C7—H7C0.9800C27—H27B0.9900C8—H80.9500C28—H28A0.9900	C5—C6		1.4146 (17)	C25-	–H25B	0.9	9900
C6—C81.4270 (18)C26—H26B0.9900C7—H7A0.9800C27—C281.5109 (19)C7—H7B0.9800C27—H27A0.9900C7—H7C0.9800C27—H27B0.9900C8—H80.9500C28—H28A0.9900	С5—Н5		0.9500	C26–	-H26A	0.9	9900
C7—H7A0.9800C27—C281.5109 (19)C7—H7B0.9800C27—H27A0.9900C7—H7C0.9800C27—H27B0.9900C8—H80.9500C28—H28A0.9900	С6—С8		1.4270 (18)	C26–	–H26B	0.9	9900
C7—H7B0.9800C27—H27A0.9900C7—H7C0.9800C27—H27B0.9900C8—H80.9500C28—H28A0.9900	С7—Н7А		0.9800	C27–	C28	1.5	5109 (19)
C7—H7C0.9800C27—H27B0.9900C8—H80.9500C28—H28A0.9900	С7—Н7В		0.9800	C27–	–H27A	0.9	9900
C8—H8 0.9500 C28—H28A 0.9900	С7—Н7С		0.9800	C27–	–H27B	0.9	900
	С8—Н8		0.9500	C28–	-H28A	0.9	9900

C9—C10	1.5197 (18)	C28—H28B	0.9900
O1 ⁱ —Ni1—O1	180.00 (5)	O3—C12—H12B	109.3
O1 ⁱ —Ni1—N1 ⁱ	91.36 (4)	C11—C12—H12B	109.3
O1—Ni1—N1 ⁱ	88.64 (4)	H12A—C12—H12B	108.0
O1 ⁱ —Ni1—N1	88.64 (4)	O3—C13—C14	111.45 (11)
01—Ni1—N1	91.36 (4)	O3—C13—H13A	109.3
N1 ⁱ —Ni1—N1	180.000 (1)	C14—C13—H13A	109.3
04 ⁱⁱ —Ni2—O4	180.000 (1)	O3—C13—H13B	109.3
O4 ⁱⁱ —Ni2—N3 ⁱⁱ	91.43 (4)	C14—C13—H13B	109.3
O4—Ni2—N3 ⁱⁱ	88.57 (4)	H13A—C13—H13B	108.0
O4 ⁱⁱ —Ni2—N3	88.57 (4)	N2—C14—C13	110.41 (10)
04—Ni2—N3	91.43 (4)	N2—C14—H14A	109.6
N3 ⁱⁱ —Ni2—N3	180.00 (8)	C13—C14—H14A	109.6
C1 - O1 - Ni1	129 48 (8)	N2-C14-H14B	109.6
$C_3 = 0_2 = C_7$	117.40 (10)	C13—C14—H14B	109.6
C12—O3—C13	109.77 (10)	H14A—C14—H14B	108.1
C15—O4—Ni2	131.19 (8)	O4—C15—C16	117.97 (11)
C17—O5—C21	117.05 (10)	O4—C15—C20	123.00 (12)
C26—O6—C27	108.78 (11)	C16—C15—C20	119.02 (11)
C8—N1—C9	115.10 (10)	C17—C16—C15	120.42 (11)
C8—N1—Ni1	123.43 (9)	C17—C16—H16	119.8
C9—N1—Ni1	121.41 (8)	C15—C16—H16	119.8
C11—N2—C10	110.51 (10)	O5—C17—C16	124.33 (11)
C11—N2—C14	108.13 (10)	O5—C17—C18	114.78 (11)
C10—N2—C14	112.35 (10)	C16—C17—C18	120.89 (12)
C22—N3—C23	115.73 (10)	C19—C18—C17	118.91 (11)
C22—N3—Ni2	124.12 (9)	C19—C18—H18	120.5
C23—N3—Ni2	120.03 (8)	C17—C18—H18	120.5
C24—N4—C28	109.14 (10)	C18—C19—C20	122.07 (11)
C24—N4—C25	111.97 (10)	C18—C19—H19	119.0
C28—N4—C25	109.90 (11)	C20—C19—H19	119.0
01—C1—C2	118.41 (11)	C19—C20—C15	118.67 (12)
O1—C1—C6	123.26 (12)	C19—C20—C22	118.84 (11)
C2—C1—C6	118.33 (12)	C15—C20—C22	122.41 (11)
C3—C2—C1	120.54 (12)	O5—C21—H21A	109.5
С3—С2—Н2	119.7	O5—C21—H21B	109.5
C1—C2—H2	119.7	H21A—C21—H21B	109.5
O2—C3—C2	124.17 (11)	O5—C21—H21C	109.5
02—C3—C4	114.60 (12)	H21A—C21—H21C	109.5
C2—C3—C4	121.22 (12)	H21B—C21—H21C	109.5
C5—C4—C3	118.52 (12)	N3-C22-C20	127.44 (11)
C5—C4—H4	120.7	N3-C22-H22	116.3
$C_3 = C_4 = H_4$	120.7	C20—C22—H22	110.5
C4 = C5 = U5	122.20 (12)	N3	111.20 (10)
$C_4 = C_5 = H_5$	110.9	$1N_{3} = 0.23 = 1123 \text{ A}$	109.4
	110.9	$U_{24} - U_{23} - \Pi_{23} A$	109.4
U3-U0-U1	119.11 (12)	NJ	109.4

C5—C6—C8	118.53 (11)	С24—С23—Н23В	109.4
C1—C6—C8	122.35 (12)	H23A—C23—H23B	108.0
O2—C7—H7A	109.5	N4—C24—C23	111.74 (11)
O2—C7—H7B	109.5	N4—C24—H24A	109.3
H7A—C7—H7B	109.5	C23—C24—H24A	109.3
O2—C7—H7C	109.5	N4—C24—H24B	109.3
H7A—C7—H7C	109.5	C23—C24—H24B	109.3
Н7В—С7—Н7С	109.5	H24A—C24—H24B	107.9
N1—C8—C6	127.62 (11)	N4—C25—C26	109.78 (11)
N1—C8—H8	116.2	N4—C25—H25A	109.7
С6—С8—Н8	116.2	C26—C25—H25A	109.7
N1—C9—C10	110.54 (10)	N4—C25—H25B	109.7
N1—C9—H9A	109.5	С26—С25—Н25В	109.7
С10—С9—Н9А	109.5	H25A—C25—H25B	108.2
N1—C9—H9B	109.5	O6—C26—C25	111.08 (14)
С10—С9—Н9В	109.5	O6—C26—H26A	109.4
Н9А—С9—Н9В	108.1	C25—C26—H26A	109.4
N2—C10—C9	111.81 (10)	O6—C26—H26B	109.4
N2	109.3	С25—С26—Н26В	109.4
C9—C10—H10A	109.3	H26A—C26—H26B	108.0
N2—C10—H10B	109.3	O6—C27—C28	111.46 (12)
C9—C10—H10B	109.3	O6—C27—H27A	109.3
H10A—C10—H10B	107.9	С28—С27—Н27А	109.3
N2—C11—C12	109.55 (11)	O6—C27—H27B	109.3
N2—C11—H11A	109.8	С28—С27—Н27В	109.3
C12—C11—H11A	109.8	H27A—C27—H27B	108.0
N2—C11—H11B	109.8	N4—C28—C27	111.16 (12)
C12—C11—H11B	109.8	N4—C28—H28A	109.4
H11A—C11—H11B	108.2	C27—C28—H28A	109.4
O3—C12—C11	111.61 (10)	N4—C28—H28B	109.4
O3—C12—H12A	109.3	C27—C28—H28B	109.4
C11—C12—H12A	109.3	H28A—C28—H28B	108.0
N1 ⁱ —Ni1—O1—C1	-162.51 (11)	C13—O3—C12—C11	58.29 (14)
N1—Ni1—O1—C1	17.49 (11)	N2-C11-C12-O3	-60.30 (15)
N3 ⁱⁱ —Ni2—O4—C15	173.30 (12)	C12—O3—C13—C14	-56.79 (14)
N3—Ni2—O4—C15	-6.70 (12)	C11—N2—C14—C13	-57.87 (14)
O1 ⁱ —Ni1—N1—C8	166.44 (11)	C10—N2—C14—C13	179.90 (11)
O1—Ni1—N1—C8	-13.56 (11)	O3—C13—C14—N2	57.68 (15)
O1 ⁱ —Ni1—N1—C9	-10.58 (9)	Ni2—O4—C15—C16	-170.87 (9)
01—Ni1—N1—C9	169.42 (9)	Ni2—O4—C15—C20	8.59 (19)
O4 ⁱⁱ —Ni2—N3—C22	-177.97 (11)	O4—C15—C16—C17	-179.89 (11)
O4—Ni2—N3—C22	2.03 (11)	C20-C15-C16-C17	0.63 (18)
O4 ⁱⁱ —Ni2—N3—C23	-2.22 (9)	C21—O5—C17—C16	8.00 (18)
O4—Ni2—N3—C23	177.78 (9)	C21—O5—C17—C18	-171.33 (11)
Ni1—O1—C1—C2	166.26 (9)	C15—C16—C17—O5	-178.45 (12)
Ni1—O1—C1—C6	-12.93 (19)	C15-C16-C17-C18	0.85 (19)
O1—C1—C2—C3	-177.25 (12)	O5—C17—C18—C19	177.94 (12)

C6—C1—C2—C3	1.99 (18)	C16-C17-C18-C19	-1.43 (19)		
C7—O2—C3—C2	-6.01 (18)	C17—C18—C19—C20	0.51 (19)		
C7—O2—C3—C4	174.14 (11)	C18—C19—C20—C15	0.94 (19)		
C1—C2—C3—O2	176.76 (11)	C18—C19—C20—C22	-175.93 (12)		
C1—C2—C3—C4	-3.39 (19)	O4-C15-C20-C19	179.04 (12)		
O2—C3—C4—C5	-177.91 (11)	C16-C15-C20-C19	-1.50 (18)		
C2—C3—C4—C5	2.23 (19)	O4—C15—C20—C22	-4.20 (19)		
C3—C4—C5—C6	0.3 (2)	C16-C15-C20-C22	175.25 (12)		
C4—C5—C6—C1	-1.59 (19)	C23—N3—C22—C20	-175.40 (12)		
C4—C5—C6—C8	179.30 (12)	Ni2—N3—C22—C20	0.52 (19)		
O1—C1—C6—C5	179.65 (12)	C19—C20—C22—N3	176.48 (12)		
C2—C1—C6—C5	0.45 (18)	C15-C20-C22-N3	-0.3 (2)		
O1—C1—C6—C8	-1.3 (2)	C22—N3—C23—C24	-108.75 (12)		
C2—C1—C6—C8	179.52 (11)	Ni2—N3—C23—C24	75.15 (12)		
C9—N1—C8—C6	-176.67 (12)	C28—N4—C24—C23	171.84 (10)		
Ni1—N1—C8—C6	6.13 (19)	C25—N4—C24—C23	-66.25 (14)		
C5-C6-C8-N1	-176.71 (12)	N3-C23-C24-N4	-165.34 (10)		
C1—C6—C8—N1	4.2 (2)	C24—N4—C25—C26	-176.26 (12)		
C8—N1—C9—C10	101.55 (13)	C28—N4—C25—C26	-54.79 (17)		
Ni1—N1—C9—C10	-81.20 (11)	C27—O6—C26—C25	-61.61 (15)		
C11—N2—C10—C9	167.06 (10)	N4-C25-C26-O6	60.01 (17)		
C14—N2—C10—C9	-72.06 (13)	C26—O6—C27—C28	59.59 (16)		
N1-C9-C10-N2	-175.82 (10)	C24—N4—C28—C27	176.61 (11)		
C10-N2-C11-C12	-177.93 (10)	C25—N4—C28—C27	53.46 (15)		
C14—N2—C11—C12	58.71 (13)	O6—C27—C28—N4	-56.47 (16)		
Symmetry codes: (i) $-x+1$, $-y+1$, $-z+1$; (ii) $-x$, $-y+1$, $-z+1$.					



