Supporting Information:

## A C<sub>2</sub>-Symmetric Nickel Diamine Complex as an Asymmetric Catalyst for Enecarbamate Additions to Butane-2,3-dione

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Experimental Section:

General:

All reactions were carried out under an argon atmosphere in dried glassware. Reaction solvents were distilled prior to use by standard procedures. Preparative thin layer chromatography was carried out using Wakogel B-F5. Butane-2,3-dione 1 was freshly distilled from anhydrous magnesium sulfate under reduced pressure at room temperature prior to use.<sup>1</sup> Enecarbamates 2ac were prepared according to the method reported by Kagan *et al.*<sup>2</sup> Diamine ligand 5 was prepared according top a reported procedure.<sup>3</sup> Metal triflate compounds that were not commercially available from the usual suppliers (Ni(OTf)<sub>2</sub> & Co(OTf)<sub>2</sub>) were prepared in accordance with literature methods.<sup>4a-c</sup> High-performance liquid chromatography was conducted using the following apparatus: SHIMADZU LC-10AT (liquid chromatograph), SHIMADZU SPD-10A (UV detector) and SHIMADZU C-R6A Chromatopac (CHIRACEL AD-H column, ipropylalcohol:hexanes 1:19 as eluent, 0.5 mL flow rate, unless otherwise stated). Proton and  $^{13}$ C NMR spectra were recorded in CDCl<sub>3</sub> on JEOL JNM-LA300, JNM-LA400, JNM-DE400 or JNM-DE600, tetramethyl silane ( $\delta = 0$ ) or residual solvent peak (CHCl<sub>3</sub> = 7.26 in CDCl<sub>3</sub>) served as standards for <sup>1</sup>H NMR, CDCl<sub>3</sub> ( $\delta$  = 77.0) for <sup>13</sup>C NMR. Mass spectra were recorded on a BRUKER DIALATONICS<sup>®</sup> BIOTOF<sup>®</sup> II machine. Melting points of crystalline materials are uncorrected and were determined on YAZAWA BY-1 apparatus. IR spectra were measured on a JASCO FT/IR-610. X-Ray diffraction analysis was carried out on a Rigaku RAXIS-RAPID diffractometer (see later).

General Procedure for Catalysed Reactions:

Metal triflates were weighed in a dry-box into dried two necked flasks fitted with 3-way taps. Diamine ligand corresponding to 1.0 molar equivalent was added under a flow of argon, the flask was sealed and evacuated-back-filled with argon (3 cycles). Dry solvents were added *via* syringe to give the stated concentration with respect to metal triflate. The solutions were stirred at the specified temperature and enecarbamates (**2a-c**) (corresponding to the given catalyst loading) were added rapidly under a flow a of argon, followed by freshly distilled diketone **1a-b**. Reactions were stirred at that temperature for the stated time. Reactions were quenched at the

<sup>1</sup>Perrin, D.D.; Armarego, W.L.F. Purification of Laboratory Chemicals, 3rd ed.; Pergamon Press: Oxford, England, 1998.

<sup>2</sup>Suen, Y.H.; Horeau, A.; Kagan, H.B. Bull. Soc. Chim. Fr. 1965, 5, 1454.

<sup>&</sup>lt;sup>3</sup> Kobayashi, S.; Matsubara, R.; Nakamura, Y.; Kitagawa, H.; Sugira, M. J. Am. Chem. Soc. 2003, 125, 2507.

<sup>&</sup>lt;sup>4</sup> (a) Boumizane, K.; Herzog-Cance, M.H.; Jones, D.J.; Pascal, J.L.; Potier, J.; Roziere, J. *Polyhedron* **1991**, *10*, 2757.(b) Jansky, M.T.; Yoke, J.T. *J. Inorg. Nucl. Chem.* **1979**, *41*, 1707. (c) Dixon, N.E.; Lawrance, G.A.; Lay, P.A.; Sargeson, A.M.; Taubes, H. *Inorg. Synth.* **1986**, *24*, 243.

given temperature by addition of 3 N HCl<sub>aqu</sub> solution, and then stirred at room temperature (exposed to air) for ~1 min, transferred to a separating funnel and extracted with EtOAc (3 times). The organic fractions were combined dried over magnesium sulfate and solvent removed *in vacuo*. These residues were loaded onto preparative TLC plates with DCM and purified by eluting with benzene/acetone 7/1 (rf ~ 0.36).

Analytical Data:



Compound **4a**:<sup>5</sup>

<sup>1</sup>H NMR ( $\delta$ ; 600 MHz; CDCl<sub>3</sub>) 1.31 (3H, s, CH<sub>3</sub>-C-OH), 2.31 (3H, s, CH<sub>3</sub>-C=O), 3.17 (1H, d, J = 17.9, CHH), 3.73 (1H, d, J = 17.2, CHH), 4.30-4.48 (1H, br s, OH), 7.41 (2H, t, J = 7.6, Ph 3- and 5-H), 7.53 (1H, t, J = 7.6, Ph 4-H), 7.87 (2H, d, J = 8.2, Ph 2- and 6-H). <sup>13</sup>C NMR ( $\delta$ ; 150 MHz; CDCl<sub>3</sub>) 24.3 (H<sub>3</sub>C-C=O), 25.2 (H<sub>3</sub>C-C-OH), 47.1 (CH<sub>2</sub>), 78.2 (C-OH), 128.3 (Ph 2- and 6-CH), 128.7 (Ph 3- and 5-CH), 133.9 (Ph 4-CH), 136.1 (Ph 1-C), 200.6 (O=C-Ph), 213.4 (O=C-Me). (Found: [M+H]<sup>+</sup>, *m/z*, (ESI) 207.1029. C<sub>12</sub>H<sub>15</sub>O<sub>3</sub> requires 207.1021) IR (neat) 1675 (C=O), 1711 (C=O) and 3461 (br O-H). HPLC analysis of ee under stated conditions major enantiomer 26.9 min, minor enantiomer 28.1 min.



Compound **4b**:<sup>5</sup>

<sup>1</sup>H NMR ( $\delta$ ; 600 MHz; CDCl<sub>3</sub>) 1.29 (3H, s, CH<sub>3</sub>-C-OH), 2.31 (3H, s, CH<sub>3</sub>-C=O), 3.10 (1H, d, *J* = 17.9, CHH), 3.69 (1H, d, *J* = 17.2, CHH), 3.81 (3H, *s*, O-CH<sub>3</sub>), 4.41-4.62 (1H, br s, OH), 6.86 (2H, d, *J* = 8.9, Ar 2- and 6-H), 7.85 (2H, d, *J* = 8.9, Ar 3- and 5-H). <sup>13</sup>C NMR ( $\delta$ ; 150 MHz; CDCl<sub>3</sub>) 24.4 (H<sub>3</sub>C-C=O), 25.1 (H<sub>3</sub>C-C-OH), 46.7 (CH<sub>2</sub>), 55.5 (O-CH<sub>3</sub>), 78.3 (C-OH), 113.8 (Ar 3- and 5-CH), 129.2 (Ar 1-C), 130.7 (Ar 2- and 6-CH), 164.1 (Ar 4-C-OMe), 199.01 (O=C-Ph), 213.7 (O=C-Me). M.p. 123-124 C. Anal. calcd. for C<sub>13</sub>H<sub>17</sub>O<sub>4</sub>: C, 66.09; H, 6.83. Found: C, 65.99; H, 6.70. (Found: [M+H]<sup>+</sup>, *m/z*, (ESI) 237.1134. C<sub>13</sub>H<sub>17</sub>O<sub>4</sub> requires 237.1127). IR (neat) 1171 (C-O), 1668 (C=O), 1715 (C=O) and 3503 (O-H) cm<sup>-1</sup>. HPLC analysis of ee under stated conditions major enantiomer 53.1 min, minor enantiomer 57.0 min.



Compound **4c**:

<sup>1</sup>H NMR ( $\delta$ ; 600 MHz; CDCl<sub>3</sub>) 1.31 (3H, s, CH<sub>3</sub>-C-OH), 2.30 (3H, s, CH<sub>3</sub>-C=O), 3.14 (1H, d, J = 18.0, CHH), 3.69 (1H, d, J = 18.0, CHH), 4.21-4.49 (1H, br s, OH), 7.38 (2H, d, J = 8.9, Ar 3- and 5-H), 7.81 (2H, d, J = 8.2, Ar 2- and 6-H). <sup>13</sup>C NMR ( $\delta$ ; 150 MHz; CDCl<sub>3</sub>) 23.9 (H<sub>3</sub>C-C=O),

<sup>&</sup>lt;sup>5</sup> Arime, T.; Takahashi, H.; Kobayashi, S.; Yamaguchi, S.; Mori, N. Synth. Commun. 1995, 25, 389.

24.8 (H<sub>3</sub>C-C-OH), 46.7 (CH<sub>2</sub>), 77.9 (C-OH), 128.7 (Ar 3- and 5-CH), 129.4 (Ar 2- and 6-CH), 134.1 (Ar 1-C), 140.1 (Ar 4-C-Cl), 199.01 (O=C-Ph), 212.8 (O=C-Me). (Found:  $[M+H]^+$ , *m/z*, (ESI) 241.0635. C<sub>12</sub>H<sub>14</sub>ClO<sub>3</sub> requires 241.0631). IR (neat) 1683 (C=O), 1714 (C=O) and 3462 (br O-H) cm<sup>-1</sup>. HPLC analysis of ee under stated conditions major enantiomer 33.1 min, minor enantiomer 36.8 min.

Compounds 4d and 4e isolated as a mixture:



<sup>1</sup>H NMR spectral data reported together, 1H of compound **4e** is given as 1H integration whereas 1H for **4d** is given as 7H (i.e ratio is 7:1), also se attached spectrum. <sup>1</sup>H NMR ( $\delta$ ; 600 MHz; CDCl<sub>3</sub>) 0.86 (3H, t, J = 7.6, **4e** CH<sub>2</sub>CH<sub>3</sub>), 1.02 (21H, t, J = 6.9, **4d**, CH<sub>2</sub>CH<sub>3</sub>), 1.30 (21H, s, **4d** CH<sub>3</sub>-C-OH), 1.69-1.78 (2H, m, **4e** CH<sub>2</sub>CH<sub>3</sub>), 2.28 (3H, s, **4e** H<sub>3</sub>C-C=O), 2.68-2.81 (14H, m, **4d** CH<sub>2</sub>CH<sub>3</sub>), 3.14 (7H, d, J = 17.9, **4d** CHH), 3.26 (1H, d, J = 17.2, **4e** CHH), 3.59 (1H, d, J = 17.2, **4e** CHH), 3.77 (7H, d, J = 17.8, **4d** CHH), 4.26-4.48 (7.3H, br with br side peak, **4d** + **4e** OH), 7.27-7.33 (2H, br m, **4e** Ph 2- & 5-H), 7.40 (14H, t, J = 8.3, **4d** Ph 3- & 5-H), 7.53 (8H, app t, J = 7.6, , **4d** + **4e** Ph 4-H), 7.87 (16H, app d, J = 7.9, , **4d** + **4e** Ph 2- & 6-H). Copy of <sup>13</sup>C spectrum of mixture also included (see later), assignments not given (i.e. mostly major product observed some peaks for minor can be seen but are inconclusive). (Found: [M+H]<sup>+</sup>, *m/z*, (ESI) 221.1176. C<sub>13</sub>H<sub>17</sub>O<sub>3</sub> requires 221.1178). IR (neat) 1672 (C=O), 1709 (C=O) and 3462 (br O-H) cm<sup>-1</sup>. HPLC analysis of ee (eluent = 9:1 hexane:*i*-propyl alcochol, *flow rate* = 0.2 mL/min) **4d** major enantiomer 47.6 min, **4d** minor enantiomer 53.6 min and **4e** major enantiomer 51.4 min, **4e** minor enantiomer 57.2 min.



Compound 7:

Racemic diamine 5 (0.1107 g, 0.282 mmol) was combined with nickel(II) bromide (0.0670 g, 0.307 mmol) under an argon atmosphere. Acetonitrile (20 mL) was added and the mixture heated at reflux for 0.5 hours then stirred at room temperature for 8 hours, resulting in a light blue solution. Solvent was removed *in vacuo* and the brown solid was triturated with hexane, the pink/brown residue was taken up in CH<sub>2</sub>Cl<sub>2</sub> and filtered to remove a small amount of insoluble material. Solvent was removed *in vacuo* once more and the brown/pink solid obtained was dried *in vacuo* at 85 C for a further 6 hours. Dissolution in CH<sub>2</sub>Cl<sub>2</sub> gave a bright pink/red solution which readily provided deep purple crystals by slow addition of hexane. X-Ray crystal structure analysis failed to give data of sufficient quality for publication but a tetrahedral coordination environment about nickel was tentatively assigned. Upon drying, the purple crystals of 7, were isolated in 61 % yield (0.1050 g, not including XRD sample). Proton NMR spectroscopy could not provide evidence of structure in a variety of solvents, see attached spectrum recorded in CDCl<sub>3</sub> by way of an example. M.p 249-251 C, IR (neat) 3409 (br N-H), 1635, 1456 and 669 cm<sup>-1</sup>. Anal. calcd. for  $C_{28}H_{28}Br_2N_2Ni$ : C, 55.04; H, 4.62; N, 4.58. Found: C, 54.67; H, 4.70; N,

4.54. (*m/z*; FAB) 531 (M<sup>+</sup> - Br, 88 %), 451 (M<sup>+</sup> - 2Br, 100 %). (Found:  $[M-2Br+H]^+$ , *m/z*, (ESI) 451.486. C<sub>28</sub>H<sub>29</sub>N<sub>2</sub>Ni requires 451.1684).



Compound 8:

Silver triflate (0.0430 g, 0.167 mmol) was stirred in CH<sub>2</sub>Cl<sub>2</sub> (10 mL), at room temperature, protected from light. To the resulting mixture purple crystals of compound 7 (0.0453g, 0.074 mmol) were added. Although dry CH<sub>2</sub>Cl<sub>2</sub> was used no precautions concerning exclusion of air or moisture were taken after addition of the solid materials. After 10 hours a grey precipitate (consistent with the formation of silver bromide) was removed by filtration and the light blue/green solution was concentrated in vacuo. Dissolution in (wet) acetone, filtration through celite, solvent removal in vacuo, dissolution in CH<sub>2</sub>Cl<sub>2</sub> and subsequent diffusion of diethyl ether gave a light blue precipitate corresponding to 94 % yield of 8 (0.0497 g, 0.069 mmol). The isolated blue powder was split into a number of portion and recrystallisations were attempted. Crystals suitable for XRD conformation of structure 8 were obtained by dissolving 8 in CH<sub>2</sub>Cl<sub>2</sub>  $/Et_2O$  (10/1) and layering this solution with hexane. No precautions concerning exclusion of light, atmospheric oxygen or water were taken during crystal preparation and the resultant blue crystals were stored in ambient conditions with no apparent decomposition. As with compound 7 no useful NMR data could be obtained the <sup>1</sup>H spectrum recorded in acetone- $d_6$  is included for comparison. M.p 157-159 C, IR (neat) 3397 (br OH<sub>2</sub>+ NH), 1650, 1455, 1250, 1168 (CF<sub>3</sub>) and 1029 (SO) cm<sup>-1</sup>. (Found:  $[M+H]^+$ , m/z, (ESI) 785.5168. C<sub>30</sub>H<sub>33</sub>F<sub>6</sub>N<sub>2</sub>NiO<sub>8</sub>S<sub>2</sub> requires 785.0936. Found  $[M-OH_2+H]^+$ , m/z, (ESI) 766.8783.  $C_{30}H_{31}F_6N_2NiO_7S_2$  requires 767.0830. Found  $[M^+ OTf+H]^+$ , m/z, (ESI) 639.4411.  $C_{29}H_{33}F_3N_2NiO_5S$  requires 639.1416. Found  $[M^+-2OTf+H]^+$ , m/z, (ESI) 487.4356. C<sub>28</sub>H<sub>33</sub>N<sub>2</sub>NiO<sub>2</sub> requires 487.1895. Found  $[M^+-2(H_2O+OTf)+H]^+$ , m/z, (ESI) 451.4564. C<sub>28</sub>H<sub>29</sub>N<sub>2</sub>Ni requires 451.1684).

## Kinetic Data:

Determination of Observed Rate Constant ( $k_{obs.}$ ) for Reaction of **1a** with **2a**: Calculated conversions are tabulated and represented graphically.  $k_{obs}$  Corresponds to the slope of the second plot.



bold type-face, benzyl carbamate serves as internal standard



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Non-Linear Effect Experiments:

Tabulated here is the data pertaining to Figure 1 in the main text and the associated discussion. The data point for 100% ee ligand is taken from Table 1, entry 1 in the main text. A plot showing approximate correlation between yield of **4a** and ee of **5** is also given.

Low ee 5 was prepared by combination of 0.007M stock solutions of R 5 and racemic 5, other experimental conditions match those of Table 1, entry 1 in the main text.

L	igand 5 ee/%l	Product 4a ee/%	%Yield <b>4a</b> /%
	100	76	67
	77	76	69
	50	79	52
	35	78	57
	10	58	32







Compound 4b:





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### Crystal Data for Compound 8:



#### Data Collection

A blue block crystal of  $C_{30}H_{32}O_8N_2S_2NiF_6$  having approximate dimensions of 0.10 x 0.10 x 0.10 mm was mounted on a glass fiber. All measurements were made on a Rigaku RAXIS RAPID imaging plate area detector with graphite monochromated Mo-K $\alpha$  radiation. Indexing was performed from 3 oscillations that were exposed for 90 seconds. The crystal-to-detector distance was 127.40 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive monoclinic cell with dimensions:

a = 11.503(8) Å

 $\begin{array}{ll} b = & 15.70(2) \ \text{\AA} & \beta = & 92.82(3)^0 \\ c = & 18.53(1) \ \text{\AA} & \\ V = & 3342(4) \ \text{\AA}^3 \end{array}$ 

For Z = 4 and F.W. = 785.40, the calculated density is 1.56 g/cm<sup>3</sup>. The systematic absences of:

h01: 
$$h \pm 2n$$

 $0k0: k \pm 2n$ 

uniquely determine the space group to be:

#### P2<sub>1</sub>/a (#14)

The data were collected at a temperature of  $-173 \pm 1^{\circ}$ C to a maximum 20 value of 54.9°. A total of 55 oscillation images were collected. A sweep of data was done using  $\omega$  scans from 130.0 to 190.0° in 3.0° step, at  $\chi$ =45.0° and  $\phi$  = 0.0°. The exposure rate was 120.0 [sec./°]. A second sweep was performed using  $\omega$  scans from 0.0 to 160.0° in 4.0° step, at  $\chi$ =45.0° and  $\phi$  = 180.0°. The exposure rate was 120.0 [sec./°]. The crystal-to-detector distance was 127.40 mm. Readout was performed in the 0.100 mm pixel mode.

#### Data Reduction

Of the 29278 reflections that were collected, 7603 were unique ( $R_{int} = 0.030$ ); equivalent reflections were merged.

The linear absorption coefficient,  $\mu$ , for Mo-K $\alpha$  radiation is 7.9 cm<sup>-1</sup>. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.83 to 1.00. The data were corrected for Lorentz and polarization effects.

#### Structure Solution and Refinement

The structure was solved by direct methods<sup>1</sup> and expanded using Fourier techniques<sup>2</sup>. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement<sup>3</sup> on  $F^2$  was based on 4965 observed reflections and 492 variable parameters and converged (largest parameter shift was 0.01 times its esd) with unweighted and weighted agreement factors of:

R1 = 
$$\Sigma$$
 ||Fo| - |Fc|| /  $\Sigma$  |Fo| = 0.024  
wR2 = [ $\Sigma$  ( w (Fo<sup>2</sup> - Fc<sup>2</sup>)<sup>2</sup>)/ $\Sigma$  w(Fo<sup>2</sup>)<sup>2</sup>]<sup>1/2</sup> = 0.030

The standard deviation of an observation of unit weight<sup>4</sup> was 1.02. A Robust-resistant weighting scheme was used<sup>5</sup>. Plots of  $\Sigma$  w (|Fo| - |Fc|)<sup>2</sup> versus |Fo|, reflection order in data collection, sin  $\theta/\lambda$  and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.31 and -0.34 e<sup>-</sup>/Å<sup>3</sup>, respectively.

Neutral atom scattering factors were taken from Cromer and Waber<sup>6</sup>. Anomalous dispersion effects were included in Fcalc<sup>7</sup>; the values for  $\Delta f$  and  $\Delta f''$  were those of Creagh and McAuley<sup>8</sup>. The values for the mass attenuation coefficients are those of Creagh and Hubbell<sup>9</sup>. All calculations were performed using the CrystalStructure<sup>10,11</sup> crystallographic software package.

(1) SIR2002: Burla, M.C., Camalli, M., Carrozzini, B., Cascarano, G.L., Giacovazzo, C., Polidori, G., Spagna., R. (2003).

(2) <u>DIRDIF99</u>: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least Squares function minimized:

 $\Sigma w (F_0^2 - F_c^2)^2$  where w = Least Squares weights.

(4) Standard deviation of an observation of unit weight:

 $[\Sigma w (F_0^2 - F_c^2)^2 / (N_0 - N_V)]^{1/2}$ 

where:  $N_0 =$  number of observations

 $N_V$  = number of variables

(5) Carruthers, J.R. and Watkin, D.J. (1979), Acta Cryst, A35, 698-699

(6) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 À (1974).

(7) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).
 (8) Creagh, D. C. & McAuley, W.J.; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(9) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(10) CrystalStructure 3.6.0: Crystal Structure Analysis Package, Rigaku and Rigaku/MSC (2000-2004). 9009 New Trails Dr. The Woodlands TX 77381 USA.

(11) CRYSTALS Issue 10: Watkin, D.J., Prout, C.K. Carruthers, J.R. & Betteridge, P.W. Chemical Crystallography Laboratory, Oxford, UK. (1996)

EXPERIMENTA	L DETAILS
A. Crystal	Data
Empirical Formula	$C_{30}H_{32}O_8N_2S_2NiF_6$
Formula Weight	785.40
Crystal Color, Habit	blue, block
Crystal Dimensions	0.10 X 0.10 X 0.10 mm
Crystal System	monoclinic
Lattice Type	Primitive
Indexing Images	3 oscillations @ 90.0 seconds
Detector Position	127.40 mm
Pixel Size	0.100 mm
Lattice Parameters	a = 11.303(8) A h = 15.70(2) Å
	D = 15.70(2) A a = 18.52(1) Å
	C = 18.55(1) A
	$\beta = 92.82(3)^{\circ}$
	$V = 3342(4) Å^3$
Space Group	P2 <sub>1</sub> /a (#14)
Z value	4
D <sub>calc</sub>	$1.561 \text{ g/cm}^3$
Foo	1616.00
	1
$\mu$ (MoK $\alpha$ )	7.91 cm <sup>-1</sup>
B. Intensity Me	asurements
Diffractometer	Rigaku RAXIS-RAPID
Kadiation	$MOK\alpha (\lambda = 0./10/5 A)$
Detactor Apartura	220 mm v 256 mm
Data Images	200 mm x 200 mm
$\frac{1}{1}$	120.0 100.00
$ω$ oscillation Range ( $\chi$ =45.0, $φ$ =0.0)	130.0 - 190.0
Exposure Rate	
(1) associated as $(1) = 45.0$ $(1) = 180.0$	120.0 sec./
$\omega$ oscillation Kange ( $\chi$ =45.0, $\varphi$ =180.0)	$120.0 \text{ sec.}^{10}$ $0.0 - 160.0^{0}$
Exposure Rate $(\chi=45.0, \phi=180.0)$	120.0 sec./ <sup>0</sup> 0.0 - 160.0 <sup>0</sup> 120.0 sec./ <sup>0</sup>
Exposure Rate Detector Position	120.0 sec./ <sup>0</sup> 0.0 - 160.0 <sup>0</sup> 120.0 sec./ <sup>0</sup> 127.40 mm
Exposure Rate Detector Position Pixel Size	120.0 sec./ <sup>0</sup> 0.0 - 160.0 <sup>0</sup> 120.0 sec./ <sup>0</sup> 127.40 mm 0.100 mm
Exposure Rate Detector Position Pixel Size $2\theta_{max}$	120.0 sec./ <sup>0</sup> 0.0 - 160.0 <sup>0</sup> 120.0 sec./ <sup>0</sup> 127.40 mm 0.100 mm 54.9 <sup>0</sup>
Exposure Rate Detector Position Pixel Size $2\theta_{max}$ No. of Reflections Measured	120.0 sec./ <sup>0</sup> 0.0 - 160.0 <sup>0</sup> 120.0 sec./ <sup>0</sup> 127.40 mm 0.100 mm 54.9 <sup>0</sup> Total: 29278
Exposure Rate Detector Position Pixel Size $2\theta_{max}$ No. of Reflections Measured	120.0 sec./ <sup>0</sup> 0.0 - 160.0 <sup>0</sup> 120.0 sec./ <sup>0</sup> 127.40 mm 0.100 mm 54.9 <sup>0</sup> Total: 29278 Unique: 7603 (R <sub>int</sub> = 0.030)
Exposure Rate Detector Position Pixel Size $2\theta_{max}$ No. of Reflections Measured Corrections	120.0 sec. <sup>70</sup> $0.0 - 160.0^{\circ}$ 120.0 sec. <sup>70</sup> 127.40 mm 0.100 mm $54.9^{\circ}$ Total: 29278 Unique: 7603 (R <sub>int</sub> = 0.030) Lorentz-polarization
Exposure Rate Detector Position Pixel Size $2\theta_{max}$ No. of Reflections Measured Corrections	120.0 sec. <sup>10</sup> $0.0 - 160.0^{\circ}$ 120.0 sec. <sup>10</sup> 127.40 mm 0.100 mm $54.9^{\circ}$ Total: 29278 Unique: 7603 (R <sub>int</sub> = 0.030) Lorentz-polarization Absorption
Exposure Rate Detector Position Pixel Size $2\theta_{max}$ No. of Reflections Measured Corrections	120.0 sec. <sup>70</sup> $0.0 - 160.0^{\circ}$ 120.0 sec. <sup>70</sup> 127.40 mm 0.100 mm 54.9° Total: 29278 Unique: 7603 (R <sub>int</sub> = 0.030) Lorentz-polarization Absorption (trans. factors: 0.8297 - 1.0000)
Exposure Rate Detector Position Pixel Size $2\theta_{max}$ No. of Reflections Measured Corrections C. Structure Solution	120.0 sec. <sup>70</sup> 0.0 - 160.0 <sup>0</sup> 120.0 sec. <sup>70</sup> 127.40 mm 0.100 mm 54.9 <sup>0</sup> Total: 29278 Unique: 7603 (R <sub>int</sub> = 0.030) Lorentz-polarization Absorption (trans. factors: 0.8297 - 1.0000) and Refinement
Exposure Rate Detector Position Pixel Size $2\theta_{max}$ No. of Reflections Measured Corrections C. Structure Solution	120.0 sec. <sup>70</sup> $0.0 - 160.0^{0}$ 120.0 sec. <sup>70</sup> 127.40 mm 0.100 mm 54.9 <sup>0</sup> Total: 29278 Unique: 7603 (R <sub>int</sub> = 0.030) Lorentz-polarization Absorption (trans. factors: 0.8297 - 1.0000) and Refinement Direct Methods
a) oscination Range (χ=45.0, φ=180.0)         Exposure Rate         Detector Position         Pixel Size         2θmax         No. of Reflections Measured         Corrections         C. Structure Solution         Refinement	120.0 sec. <sup>70</sup> $0.0 - 160.0^{0}$ 120.0 sec. <sup>70</sup> 127.40 mm 0.100 mm 54.9 <sup>0</sup> Total: 29278 Unique: 7603 (R <sub>int</sub> = 0.030) Lorentz-polarization Absorption (trans. factors: 0.8297 - 1.0000) and Refinement Direct Methods Full-matrix least-squares on F <sup>2</sup>
w oscination Range (χ=45.0, φ=180.0)         Exposure Rate         Detector Position         Pixel Size         2θmax         No. of Reflections Measured         Corrections         C. Structure Solution         Refinement         Function Minimized	120.0 sec. <sup>70</sup> 0.0 - 160.0 <sup>0</sup> 120.0 sec. <sup>70</sup> 127.40 mm 0.100 mm 54.9 <sup>0</sup> Total: 29278 Unique: 7603 (R <sub>int</sub> = 0.030) Lorentz-polarization Absorption (trans. factors: 0.8297 - 1.0000) and Refinement Direct Methods Full-matrix least-squares on F <sup>2</sup> $\Sigma$ w (Fo <sup>2</sup> - Fc <sup>2</sup> ) <sup>2</sup>
w oscination Kange (χ=45.0, φ=180.0)         Exposure Rate         Detector Position         Pixel Size         2θmax         No. of Reflections Measured         Corrections         C. Structure Solution         Structure Solution         Refinement         Function Minimized         Least Squares Weights	120.0 sec. <sup>70</sup> 0.0 - 160.0 <sup>0</sup> 120.0 sec. <sup>70</sup> 127.40 mm 0.100 mm 54.9 <sup>0</sup> Total: 29278 Unique: 7603 (R <sub>int</sub> = 0.030) Lorentz-polarization Absorption (trans. factors: 0.8297 - 1.0000) and Refinement Direct Methods Full-matrix least-squares on F <sup>2</sup> $\Sigma$ w (Fo <sup>2</sup> - Fc <sup>2</sup> ) <sup>2</sup> Chebychev polynomial with 3 parameters
a) oscination Range (χ=45.0, φ=180.0)         Exposure Rate         Detector Position         Pixel Size         2θmax         No. of Reflections Measured         Corrections         C. Structure Solution         Refinement         Function Minimized         Least Squares Weights	120.0 sec. <sup>10</sup> 0.0 - 160.0 <sup>0</sup> 120.0 sec. <sup>10</sup> 127.40 mm 0.100 mm 54.9 <sup>0</sup> Total: 29278 Unique: 7603 (R <sub>int</sub> = 0.030) Lorentz-polarization Absorption (trans. factors: 0.8297 - 1.0000) and Refinement Direct Methods Full-matrix least-squares on F <sup>2</sup> $\Sigma$ w (Fo <sup>2</sup> - Fc <sup>2</sup> ) <sup>2</sup> Chebychev polynomial with 3 parameters 6419.4300,8908.6800,3224.1100,
Exposure Rate Detector Position Pixel Size $2\theta_{max}$ No. of Reflections Measured Corrections C. Structure Solution Refinement Function Minimized Least Squares Weights $2\theta_{max}$ cutoff	120.0 sec. <sup>70</sup> 0.0 - 160.0 <sup>0</sup> 120.0 sec. <sup>70</sup> 127.40 mm 0.100 mm 54.9 <sup>0</sup> Total: 29278 Unique: 7603 (R <sub>int</sub> = 0.030) Lorentz-polarization Absorption (trans. factors: 0.8297 - 1.0000) and Refinement Direct Methods Full-matrix least-squares on F <sup>2</sup> $\Sigma$ w (Fo <sup>2</sup> - Fc <sup>2</sup> ) <sup>2</sup> Chebychev polynomial with 3 parameters 6419.4300,8908.6800,3224.1100, 0.0 <sup>0</sup>

No. Observations	(I>2.00o(I))		4965	
No. Variables			492	
Reflection/Parame	eter Ratio		10.09	
Residuals: $RI (I \ge 1)$	$2.00\sigma(1)$		0.024	
Goodness of Fit I	/2.000(1)) ndicator		1.022	
Max Shift/Error in	n Final Cycle		0.010	
Maximum peak ir	Final Diff. Map		$0.31 e^{-}/Å^{3}$	
Minimum peak in	Final Diff. Map		$-0.34 e^{-/Å^3}$	
Table 1. Atomic c	coordinates and $B_{iso}/B_{eq}$			
atom	X	у	Z	B <sub>eq</sub>
Ni(1)	0.06505(2)	0.11118(1)	0.80246(1)	0.818(4)
S(1)	-0.20562(3)	0.08024(2)	0.77150(2)	0.968(7)
S(2)	0.33925(3)	0.14390(3)	0.86285(2)	1.012(7)
F(1)	-0.40922(8)	0.05515(7)	0.70709(6)	2.44(2)
F(2) F(2)	-0.30/1/(8) 0.2648(1)	0.15062(6) 0.01788(7)	0.65578(5)	1./3(2)
F(3) F(4)	-0.2048(1) 0.39/35(0)	0.01/88(7) 0.03194(7)	0.04428(3) 0.96318(6)	2.40(2) 2.87(3)
F(5)	0.53880(8)	0.03194(7) 0.07594(7)	0.90318(0)	2.53(2)
F(6)	0.4154(1)	-0.01262(7)	0.85459(6)	3.03(3)
O(1)	-0.09678(9)	0.11238(8)	0.74405(5)	1.30(2)
O(2)	-0.2610(1)	0.13947(8)	0.81783(6)	1.62(2)
O(3)	-0.1997(1)	-0.00667(7)	0.79510(6)	1.56(2)
O(4)	0.22119(9)	0.11111(7)	0.86665(5)	1.23(2)
O(5)	0.37492(9)	0.15447(7)	0.78966(6)	1.44(2)
O(6)	0.36785(9)	0.21204(7)	0.911/3(6)	1.50(2)
O(7)	0.0709(1) 0.0170(1)	0.24015(7) 0.12066(7)	0.78806(6) 0.80887(6)	1.31(2) 1.21(2)
N(1)	-0.0170(1) 0.1458(1)	0.13000(7) 0.08805(8)	0.89887(0)	1.21(2) 0.91(3)
N(2)	0.0657(1)	-0.02076(8)	0.81399(7)	0.91(3)
C(1)	-0.3017(1)	0.0761(1)	0.68967(9)	1.47(3)
C(2)	0.4275(1)	0.0550(1)	0.89817(9)	1.78(4)
C(3)	0.0919(1)	-0.0562(1)	0.88829(8)	1.16(3)
C(4)	0.0072(1)	-0.1231(1)	0.91178(7)	1.13(3)
C(5)	-0.1018(1)	-0.0993(1)	0.93355(8)	1.54(3)
C(6)	-0.1792(1) 0.1460(2)	-0.1599(1)	0.95836(9)	2.09(4)
C(7)	-0.1409(2) -0.0389(1)	-0.2449(1) -0.2691(1)	0.90148(9)	2.32(4) 1.90(4)
C(9)	0.0376(1)	-0.2091(1)	0.91378(8)	1 40(3)
C(10)	0.1459(1)	-0.05547(9)	0.75992(8)	0.93(3)
C(11)	0.1303(1)	-0.1500(1)	0.74726(8)	1.28(3)
C(12)	0.0258(1)	-0.1823(1)	0.71728(9)	1.51(3)
C(13)	0.0110(2)	-0.2695(1)	0.7076(1)	2.17(4)
C(14)	0.0996(2)	-0.3247(1)	0.7297(1)	2.43(4)
C(15)	0.2038(2)	-0.2938(1)	0.7595(1)	2.23(4)
C(10) C(17)	0.2190(1) 0.1303(1)	-0.2064(1) 0.0037(1)	0.76795(9)	1.00(4)
C(17) C(18)	0.1303(1) 0.2101(1)	-0.0037(1)	0.63259(8)	1.02(3)
C(19)	0.3301(1)	-0.0257(1)	0.64107(8)	1.35(3)
C(20)	0.4018(1)	-0.0515(1)	0.58718(9)	1.64(3)
C(21)	0.3534(1)	-0.0888(1)	0.52466(9)	1.86(4)
C(22)	0.2350(2)	-0.1011(1)	0.51651(9)	2.07(4)
C(23)	0.1634(1)	-0.0745(1)	0.57028(9)	1.66(3)
C(24)	0.1099(1) 0.1092(1)	0.1451(1) 0.1577(1)	0.64486(8)	1.22(3)
C(25)	0.1983(1) 0.3103(1)	0.1377(1) 0.1862(1)	0.38/81(8) 0.60604(8)	1.14(3) 1.24(3)
C(20) C(27)	0.3103(1) 0.3898(1)	0.1802(1) 0.2000(1)	0.55315(9)	1.54(5)
C(28)	0.3570(2)	0.1872(1)	0.48096(9)	1.97(4)
C(29)	0.2456(2)	0.1600(1)	0.46194(9)	2.21(4)
C(30)	0.1670(1)	0.1447(1)	0.51501(9)	1.83(4)
$B_{eq} = 8/3 \pi^2 (U_{11})(a)$	$(a^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2$	+ $2U_{12}(aa*bb*)\cos\gamma + 2U_1$	$_3(aa^*cc^*)cos \beta + 2U_{23}(bb^*cc^*)$	*)cos α)
Table 2. Atomic c	coordinates and B iso involv	ving hydrogens/Bea		
atom	X	у	Z	B <sub>eq</sub>
H(1)	-0.1239	-0.0410	0.9315	1.866
H(2)	-0.2535	-0.1429	0.9734	2.520
H(3)	-0.1989	-0.2861	0.9792	2.756
H(4)	-0.01/4	-0.3275	0.9407	2.296

$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H(5)	0 1113	-0.2263		0 8980	1 672	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H(6)	0.0905	-0.0104		0.9217	1.389	
$\begin{array}{ c c c c } \hline 10000(1) & 0.038(1) & 0.8945(9) & 1.044 \\ \hline 1101 & 0.02534 & 0.1442 & 0.7325 & 1.386 \\ \hline 1101 & 0.0592 & 0.2913 & 0.6556 & 2.620 \\ \hline 11021 & 0.0893 & 0.3843 & 0.7245 & 2.977 \\ \hline 11051 & 0.0523 & 0.0114 & 0.715 & 1.241 \\ \hline 1101 & 0.0523 & 0.0114 & 0.6715 & 1.241 \\ \hline 1101 & 0.0818 & 0.0853 & 0.5648 & 1.998 \\ \hline 1101 & 0.0222 & 0.1272 & 0.4739 & 2.483 \\ \hline 1101 & 0.3627 & 0.0011 & 0.6843 & 1.593 \\ \hline 1101 & 0.3627 & 0.011 & 0.6843 & 1.593 \\ \hline 1101 & 0.3252 & 0.0114 & 0.5256 & 1.779 \\ \hline 1101 & 0.3252 & 0.0114 & 0.6233 & 1.454 \\ \hline 1109 & 0.4836 & 0.0434 & 0.5926 & 1.799 \\ \hline 1101 & 0.3257 & 0.0101 & 0.6843 & 1.593 \\ \hline 1122 & 0.0924 & 0.1994 & 0.6641 & 1.474 \\ \hline 1123 & 0.0327 & 0.0100 & 0.6643 & 1.593 \\ \hline 1123 & 0.0924 & 0.1994 & 0.6441 & 1.474 \\ \hline 1123 & 0.0922 & 0.1501 & 0.4125 & 2.685 \\ \hline 1123 & 0.0924 & 0.1994 & 0.6442 & 2.400 \\ \hline 1123 & 0.0924 & 0.1974 & 0.4446 & 2.410 \\ \hline 1123 & 0.062(2) & 0.1001 & 0.798(1) & 2.6(5) \\ \hline 1126 & 0.4108 & 0.1974 & 0.4446 & 2.410 \\ \hline 1126 & 0.062(2) & 0.1001 & 0.798(1) & 2.6(5) \\ \hline 1126 & 0.062(2) & 0.1001 & 0.798(1) & 2.6(5) \\ \hline 1130 & 0.022(2) & 0.1001 & 0.798(1) & 2.6(5) \\ \hline 1130 & 0.022(2) & 0.1001 & 0.798(1) & 2.0(5) \\ \hline 1130 & 0.022(2) & 0.1001 & 0.798(1) & 2.0(5) \\ \hline 1130 & 0.022(2) & 0.1001 & 0.0798(1) & 2.0(5) \\ \hline 1130 & 0.022(2) & 0.1001 & 0.0292(1) & 0.00019(7) & 0.00009(7) \\ \hline 1130 & 0.0002(7) & 0.00035(9) & 0.00035(9) & 0.00019(7) & 0.00009(7) \\ \hline 1130 & 0.0102(7) & 0.0246(1) & 0.022(1) & 0.00017(1) & 0.00007(1) \\ \hline 1130 & 0.0102(7) & 0.0144(2) & 0.0002(7) & -0.0003(1) & -0.0007(7) & 0.00009(7) \\ \hline 1130 & 0.0102(7) & 0.0144(2) & 0.0122(7) & 0.00019(7) & 0.00009(7) \\ \hline 1130 & 0.0102(7) & 0.0144(7) & 0.000019(7) & 0.00009(7) \\ \hline 1140 & 0.0177(6) & 0.0137(6) & 0.0007(6) & 0.0007(7) & 0.00009(7) \\ \hline 1140 & 0.0177(6) & 0.0138(6) & 0.0007(6) & 0.0007(7) & -0.0084(7) & 0.0007(7) \\ \hline 1140 & 0.0134(7) & 0.0124(7) & 0.0004(7) & 0.0007(7) & 0.0008(7) \\ \hline 1140 & 0.0134(7) & 0.0138(6) & 0.0007(6) & 0.0007(6) & 0.0007(6) \\ \hline 1141(7) & 0.0107(7) & 0.0138(6) & 0.0007(6) &$	H(7)	0.1676	-0.0805		0.8895	1.363	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H(8)	-0.000(1)	-0.038(1)		0.8045(9)	1.0(4)	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H(9)	0.2233	-0.0460		0.7785	1.086	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H(10)	-0.0354	-0.1442		0.7032	1.821	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H(11)	-0.0592	-0.2913		0.6856	2.620	
$\begin{split} &   1(3) & 0.241 & -0.3320 & 0.774 & 2.726 \\   1(5) & 0.0533 & -0.0114 & 0.6715 & 1.241 \\   1(5) & 0.0533 & -0.0114 & 0.6715 & 1.241 \\   1(7) & 0.2022 & -0.1272 & 0.4739 & 2.483 \\   1(7) & 0.2022 & -0.1272 & 0.4739 & 2.483 \\   1(9) & 0.4857 & -0.0631 & 0.3926 & 1.993 \\   1(7) & 0.2027 & -0.0001 & 0.3926 & 1.994 \\   1(2) & 0.2377 & -0.0001 & 0.1949 & 0.6641 & 1.474 \\   1(2) & 0.2327 & 0.1949 & 0.6555 & 1.614 \\   1(2) & 0.2327 & 0.1949 & 0.6555 & 1.614 \\   1(2) & 0.2327 & 0.1949 & 0.6555 & 1.614 \\   1(2) & 0.0724 & 0.1974 & 0.4446 & 2.410 \\   1(2) & 0.0724 & 0.1974 & 0.4446 & 2.410 \\   1(2) & 0.0972 & 0.1510 & 0.4125 & 2.685 \\   1(2) & 0.0907 & 0.1255 & 0.5015 & 2.159 \\   1(2) & 0.002(2) & 0.286(1) & 0.798(1) & 2.6(5) \\   1(3) & 0.012(2) & 0.286(1) & 0.798(1) & 2.6(5) \\   1(3) & 0.012(2) & 0.198(1) & 0.991(1) & 3.0(5) \\   1(3) & 0.002(2) & 0.198(1) & 0.991(1) & 3.0(5) \\   1(3) & 0.002(2) & 0.198(1) & 0.0101(7) & 0.0000(9) \\   1(1) & 0.0088(9) & 0.0033(9) & 0.01297(9) & 0.0010(9) & 0.0010(51) & 0.0000(1) \\   1(1) & 0.0098(9) & 0.0033(9) & 0.01297(9) & 0.0010(9) & 0.0010(51) & 0.0000(61) \\   1(1) & 0.0098(9) & 0.0033(9) & 0.01297(9) & 0.0010(9) & 0.0010(51) & 0.0000(5) \\   1(1) & 0.0098(9) & 0.0033(9) & 0.01297(9) & 0.0010(9) & 0.0010(51) & 0.0000(5) \\   1(1) & 0.0098(9) & 0.0038(9) & 0.01292(9) & 0.0010(9) & 0.0010(51) & 0.0000(5) \\   1(1) & 0.0098(5) & 0.0038(6) & 0.0075(5) & 0.0000(5) & 0.0027(5) \\   1(1) & 0.0198(5) & 0.0142(2) & -0.002(1) & -0.0015(1) & 0.0026(1) \\   1(1) & 0.0198(5) & 0.0138(6) & 0.0075(5) & 0.0000(5) & 0.0007(5) \\   1(1) & 0.0198(6) & 0.0127(2) & 0.0142(2) & -0.002(1) & -0.0015(1) & 0.0027(5) \\   1(1) & 0.0198(6) & 0.0127(5) & 0.0006(5) & -0.0005(5) \\   1(1) & 0.0198(6) & 0.0127(5) & 0.0006(5) & -0.0005(5) \\   1(1) & 0.0198(6) & 0.0127(5) & 0.0006(5) & -0.0005(5) \\   1(1) & 0.0198(6) & 0.0127(5) & 0.0006(5) & -0.0005(5) \\   1(1) & 0.0198(6) & 0.0127(6) & 0.0005(5) & -0.0005(5) \\   1(1) & 0.0112(5) & 0.0138(6) & 0.0007(5) & -0.0005(5) \\   1(1) & 0.0138(6) & 0.0007(5) & -0.0003(5) & 0.0007$	H(12)	0.0893	-0.3845		0.7245	2.977	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H(13)	0.2641	-0.3320		0.7748	2.726	
H(16)       0.0523       -0.0114       0.6715       1.241         H(17)       0.2022       -0.1272       0.4739       2.483         H(19)       0.4836       -0.0434       0.5926       1.979         H(20)       0.3627       -0.0011       0.6843       1.593         H(21)       0.222(2)       0.100(1)       0.7199(9)       1.9(4)         H(23)       0.0416       0.1214       0.6220       1.458         H(23)       0.0416       0.1214       0.6253       1.614         H(23)       0.4663       0.2191       0.5666       2.100       -         H(23)       0.4663       0.2191       0.5666       2.100       -         H(23)       0.4663       0.2191       0.5666       2.100       -         H(30)       0.1232(2)       0.288(1)       0.798(1)       3.65       -         H(30)       0.1232(2)       0.288(1)       0.798(1)       3.65       -         H(31)       0.026(2)       0.139(1)       0.932(1)       3.065       -         H(31)       0.028(2)       0.139(1)       0.932(1)       3.065       -         H(31)       0.0084(9)       0.0122(2)       0.00019(7)	H(14)	0.2913	-0.1851		0.7874	2.000	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H(15)	0.0523	-0.0114		0.6715	1.241	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H(16)	0.0818	-0.0833		0.5648	1.998	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H(17)	0.2022	-0.1272		0.4739	2.483	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H(18)	0.4021	-0.1064		0.4874	2.304	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H(19)	0.4836	-0.0434		0.5926	1.979	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	H(20)	0.3627	-0.0011		0.6843	1.593	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H(21)	0.223(2)	0.100(1)		0.7190(9)	1.9(4)	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H(22)	0.0924	0.1994		0.6641	1.4/4	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H(23) H(24)	0.0410	0.1214		0.6220	1.438	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	П(24) Ц(25)	0.5527	0.1949		0.0333	2 100	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	H(26)	0.4003	0.2191		0.3003	2.100	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	H(27)	0.4108	0.1974		0.44440	2.410	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	H(28)	0.2232	0.1310		0.4125	2.085	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H(20)	0.0907 0.012(2)	0.1255		0.3013	2.139	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H(29)	0.012(2) 0.123(2)	0.208(1) 0.268(1)		0.788(1) 0.700(1)	2.0(5)	
$\begin{array}{c ccccc} 1 & 0.020(2) & 0.10(1) & 0.020(1) & 2.6(5) \\ \hline Peg=8/3 \pi^2(U_{11}(aer)^2 + U_{22}(ber)^2 + U_{12}(aer^{bbr}) + 2U_{12}(aer^{bbr}) + 2U_{23}(be^{br}) + 2$	H(31)	0.123(2) 0.028(2)	0.208(1)		0.799(1) 0.932(1)	3.0(3) 3.0(5)	
$\begin{array}{c} \mbox{H} (J_2) = 0.002(2) = 0.003(2) $	H(32)	-0.028(2)	0.139(1) 0.169(1)		0.932(1) 0.899(1)	2.0(5)	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	n(32)	-0.002(2)	0.109(1)		0.099(1)	2.0(3)	
$ Table 3. Anisotropic Displacement Parameters \\ atom U_1 U_2 U_3 U_3 U_12 U_1 U_1 U_2 U_3 U_23 \\ Ni(1) 0.00985(9) 0.00835(9) 0.01292(9) 0.00019(9) 0.00109(7) 0.00009(9) \\ S(1) 0.0110(2) 0.0114(2) 0.0127(2) -0.018(1) -0.0015(1) 0.0010(1) \\ S(2) 0.0114(2) 0.0127(2) 0.0142(2) -0.0018(1) -0.0017(1) 0.0026(1) \\ F(1) 0.0179(5) 0.0348(7) 0.0389(6) -0.0106(5) -0.0102(5) 0.0078(5) \\ F(2) 0.0227(5) 0.0160(5) 0.0248(5) 0.0017(4) -0.0066(4) 0.0045(4) \\ F(3) 0.0469(7) 0.0226(6) 0.0228(5) 0.0077(5) -0.0084(5) -0.0109(5) \\ F(4) 0.0271(6) 0.0432(7) 0.0386(6) 0.0075(5) -0.0029(4) 0.0112(5) \\ F(6) 0.0360(6) 0.0197(6) 0.0482(8) 0.0093(5) -0.0079(5) -0.0029(5) \\ O(1) 0.0133(5) 0.0173(6) 0.0187(5) -0.0002(5) -0.0074(4) 0.0025(5) \\ O(2) 0.0193(6) 0.0234(7) 0.0188(6) 0.0056(5) 0.0013(4) -0.0018(5) \\ O(3) 0.0185(6) 0.0150(6) 0.0252(6) -0.0028(5) -0.001(4) 0.0022(5) \\ O(2) 0.0193(6) 0.0234(7) 0.0188(6) 0.0056(5) 0.0013(4) -0.0018(5) \\ O(3) 0.0185(6) 0.0150(6) 0.0252(6) -0.0028(5) -0.0012(4) 0.0028(5) \\ O(3) 0.0185(6) 0.0173(5) 0.0173(5) -0.0011(5) -0.0012(4) 0.0028(5) \\ O(7) 0.0119(6) 0.0126(6) 0.0173(5) -0.0014(5) 0.00006(5) 0.0008(5) \\ O(7) 0.0119(6) 0.0128(6) 0.0250(7) 0.0004(6) 0.0017(5) -0.0008(5) \\ O(7) 0.0119(6) 0.0128(6) 0.0250(7) 0.0004(6) 0.0017(5) -0.0003(5) 0.0001(5) \\ C(1) 0.0113(7) 0.0116(7) 0.0129(6) -0.0025(5) 0.0006(5) 0.0009(5) \\ O(7) 0.0119(6) 0.0128(6) 0.0250(7) 0.0004(6) 0.0017(5) -0.0003(5) 0.0001(5) \\ C(1) 0.0113(9) 0.0161(9) 0.0121(7) 0.0005(6) -0.0003(5) 0.0001(5) \\ C(2) 0.0156(8) 0.023(1) 0.0128(7) -0.0004(6) 0.0017(6) \\ C(3) 0.0177(8) 0.0148(8) 0.0124(7) -0.0003(5) -0.0003(6) 0.0017(6) \\ C(4) 0.0118(8) 0.0184(9) 0.021(7) -0.0005(6) 0.0005(7) \\ C(10) 0.0117(7) 0.0058(8) -0.0158(9) -0.0188(9) -0.0056(8) 0.0005(7) \\ C(10) 0.0117(7) 0.0058(8) -$	$B_{eq} = 8/3 \pi^{2}(U)$	$U_{11}(aa^*)^2 + U_{22}(bb^*)^2$	$+ U_{33}(cc^*)^2 + 2U_{12}(aa^*b)$	(1300) $(1300)$ $(1300)$	$(aa^*cc^*)cos \beta + 2U_{23}(bb^*)$	$cc^*)cos \alpha$	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Table 3. Anis	otropic Displacemen	t Parameters				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	atom	U <sub>11</sub>	$U_{22}$	$U_{33}$	$0_{12}$	U <sub>13</sub>	$U_{23}$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Ni(1)	0.00985(9)	0.00835(9)	0.01292(9)	0.00019(9)	0.00109(7)	0.00009(9)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	S(1)	0.0110(2)	0.0114(2)	0.0142(2)	-0.0002(1)	-0.0015(1)	0.0010(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	S(2)	0.0114(2)	0.0127(2)	0.0142(2)	-0.0018(1)	-0.0017(1)	0.0026(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	F(1)	0.0179(5)	0.0348(7)	0.0389(6)	-0.0106(5)	-0.0102(5)	0.0078(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	F(2)	0.0287(5)	0.0160(5)	0.0204(5)	0.0014(4)	-0.0066(4)	0.0045(4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	F(3)	0.0469(7)	0.0226(6)	0.0228(5)	0.0077(5)	-0.0084(5)	-0.0100(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	F(4)	0.0271(6)	0.0432(7)	0.0386(6)	0.0075(5)	0.0000(5)	0.0279(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	F(5)	0.0123(5)	0.0411(7)	0.0422(6)	0.0031(5)	-0.0029(4)	0.0112(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	F(6)	0.0360(6)	0.0197(6)	0.0584(8)	0.0093(5)	-0.00/9(5)	-0.0029(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O(1)	0.0133(5)	0.01/3(6)	0.0187(5)	-0.0002(5)	-0.000/(4)	0.0025(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O(2)	0.0195(6)	0.0234(7)	0.0188(6)	0.0050(5)	0.0013(4)	-0.0018(5)
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	O(3)	0.0185(6)	0.0150(6)	0.0252(6)	-0.0028(5)	-0.0040(5)	0.0062(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O(4)	0.0124(5) 0.0158(6)	0.0109(0) 0.0226(7)	0.0173(5)	-0.0011(5)	-0.0012(4)	0.0028(5) 0.0017(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O(3)	0.0138(0) 0.0211(6)	0.0230(7) 0.0176(6)	0.0130(3)	-0.0041(3)	0.0000(4) 0.0005(5)	0.0017(3) 0.0008(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O(0)	0.0211(0) 0.0110(6)	0.0170(0) 0.0128(6)	0.0180(0)	-0.0003(3)	-0.0003(3)	0.0008(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O(7)	0.0119(0) 0.0141(6)	0.0128(0) 0.0170(7)	0.0230(7)	0.0004(0)	0.0017(5)	-0.0012(5)
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	N(1)	0.0141(0) 0.0111(7)	0.0170(7)	0.0130(0)	0.0039(3)	0.0007(5)	-0.0008(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N(1)	0.0111(7) 0.0085(6)	0.0107(7) 0.0116(7)	0.0129(0)	-0.0002(5)	-0.0000(3)	0.0019(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\Gamma(2)$	0.0083(0) 0.0183(9)	0.0110(7) 0.0161(9)	0.0144(7) 0.0210(8)	-0.0003(3)	-0.0003(3)	-0.0016(7)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(2)	0.0105(9)	0.0101(9) 0.023(1)	0.0210(0)	0.0020(7)	-0.0043(7)	0.0070(8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(3)	0.0170(0)	0.023(1) 0.0140(8)	0.0205(7)	0.0021(7)	-0.0004(6)	0.0007(6)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(4)	0.0177(0)	0.0184(9)	0.0121(7)	-0.0029(6)	-0.0008(6)	0.0007(6)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(5)	0.0212(8)	0.025(1)	0.0125(7)	0.0045(7)	-0.0004(6)	0.0025(7)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(6)	0.0170(9)	0.046(1)	0.0122(8)	-0.0031(8)	0.0006(7)	0.0059(8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(7)	0.031(1)	0.039(1)	0.0180(9)	-0.0188(9)	-0.0056(8)	0.0096(8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(8)	0.034(1)	0.0158(9)	0.0217(9)	-0.0066(8)	-0.0045(8)	0.0053(7)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(9)	0.0200(9)	0.0163(9)	0.0168(8)	0.0005(7)	0.0006(6)	0.0005(7)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(10)	0.0117(7)	0.0095(8)	0.0139(7)	0.0006(6)	0.0010(6)	0.0001(6)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(11)	0.0222(9)	0.0124(8)	0.0146(8)	-0.0009(7)	0.0067(6)	0.0014(7)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(12)	0.0213(9)	0.0156(9)	0.0208(8)	-0.0013(7)	0.0060(7)	-0.0022(7)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(13)	0.033(1)	0.023(1)	0.028(1)	-0.0122(8)	0.0125(8)	-0.0082(8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(14)	0.050(1)	0.0102(9)	0.034(1)	-0.0017(9)	0.0221(9)	-0.0040(8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(15)	0.040(1)	0.0148(9)	0.032(1)	0.0099(8)	0.0157(9)	0.0032(8)
C(17)         0.0133(8)         0.0084(8)         0.0170(7)         -0.0010(6)         -0.0013(6)         -0.0018(6)           C(18)         0.0178(8)         0.0089(8)         0.0141(7)         0.0000(6)         0.0021(6)         0.0023(6)           C(19)         0.0204(8)         0.0158(9)         0.0150(8)         0.0012(7)         0.0002(6)         -0.0010(6)	C(16)	0.0238(9)	0.0178(9)	0.0220(9)	0.0047(7)	0.0064(7)	0.0023(7)
C(18)0.0178(8)0.0089(8)0.0141(7)0.0000(6)0.0021(6)0.0023(6)C(19)0.0204(8)0.0158(9)0.0150(8)0.0012(7)0.0002(6)-0.0010(6)	C(17)	0.0133(8)	0.0084(8)	0.0170(7)	-0.0010(6)	-0.0013(6)	-0.0018(6)
C(19) 0.0204(8) 0.0158(9) 0.0150(8) 0.0012(7) 0.0002(6) -0.0010(6)	C(18)	0.0178(8)	0.0089(8)	0.0141(7)	0.0000(6)	0.0021(6)	0.0023(6)
	C(19)	0.0204(8)	0.0158(9)	0.0150(8)	0.0012(7)	0.0002(6)	-0.0010(6)

C(20)	0.0184(8)	0.0	(203(9))	0.0240(9)	0.0048	8(7)	0.0038(7)	0.0013(7)
	0.0101(0)	0.0		0.0217(0)	0.0010	·(()	0.0050(7)	0.0015(7)
C(21)	0.030(1)	0.0	)21(1)	0.0217(9)	0.0038	5(7)	0.0122(7)	-0.0014(7)
C(22)	0.039(1)	0.0	0.23(1)	0.0165(8)	-0.0071	(8)	0.0051(7)	-0.0067(8)
0(22)	0.000(1)	0.0	20(1)	0.0105(0)	0.0071	(0)	0.0001(7)	0.0007(0)
C(23)	0.0217(9)	0.0	)205(9)	0.0211(8)	-0.00/0	)(7)	0.0021(7)	-0.0030(7)
C(24)	0.0164(8)	0.0	(109(7))	0.0187(8)	0.0017	7(6)	-0.0006(6)	0.0024(7)
0(25)	0.0201(0)	0.0	0004(0)	0.0151(0)	0.001/		0.0010(()	0.0019(())
C(25)	0.0201(8)	0.0	JU84(8)	0.0151(8)	0.0016	<b>(</b> 0)	0.0019(6)	0.0018(6)
C(26)	0.0225(9)	0.0	)120(8)	0.0166(8)	0.0007	(7)	0.0022(6)	0.0009(6)
COT	0.0242(0)	0.0	157(0)	0.0271(0)	0.000	1(7)	0.0059(7)	0.0002(7)
C(27)	0.0245(9)	0.0	1137(9)	0.02/1(9)	-0.000	I(7)	0.0038(7)	0.0002(7)
C(28)	0.034(1)	0.0	D20(1)	0.0229(9)	0.0020	)(8)	0.0153(8)	0.0019(7)
cipó	0.045(1)	0.0	$\eta_{2}\epsilon(1)$	0.0130(8)	0.000	3(0)	0.0032(7)	0.0007(7)
C(29)	0.043(1)	0.0	)20(1)	0.0150(8)	-0.000	5(9)	0.0032(7)	-0.0007(7)
C(30)	0.0247(9)	0.0	)241(9)	0.0205(9)	-0.0029	9(8)	-0.0018(7)	0.0006(7)
			2		. 2 . 2	.2		
The general	temperature fac	tor expressio	n: exp(-2π <sup>2</sup> (a* <sup>2</sup> l	J11h <sup>2</sup> + b* <sup>2</sup> U2	$2k^2 + c^{*2}U_{33}$	$l^2 + 2a^*b^*U_1$	2hk + 2a*c*U13	$hl + 2b*c*U_{23}kl))$
		1	1 \ \	11 2			2 15	23 //
Table 4. Bo	nd lengths (Å)							
atom	atom	di	stanco		atom		atom	dictorio
atom	atom	ui	stance		atom		atom	uistance
Ni(1)	O(1)	2.1	107(1)		Ni(1)		O(4)	2.105(1)
Ni(1)	O(7)	2 (	344(1)		Ni(1)		O(8)	2.084(1)
	0(7)	2.0					0(0)	2.004(1)
N1(1)	N(1)	2.0	J/5(1)		N1(1)		N(2)	2.083(1)
S(1)	0(1)	14	464(1)		S(1)		O(2)	1.436(1)
		1.	42.4(1)				C(1)	1.022(2)
5(1)	O(3)	1.4	+34(1)		5(1)		$\mathcal{C}(1)$	1.855(2)
S(2)	O(4)	1.4	457(1)		S(2)		O(5)	1.445(1)
SO	0(6)	1	120(1)		S(D)		$C(\mathbf{n})$	1.927(2)
5(2)	0(0)	1.4	+50(1)		3(2)		C(2)	1.82/(2)
F(1)	C(1)	1.3	335(2)		F(2)		C(1)	1.327(2)
Fa	റസ്	1 /	326(2)		EA		cò	1 321(2)
1(5)		1	520(2)		r(4)		$\mathcal{L}(2)$	1.331(2)
F(5)	C(2)	1.3	321(2)		F(6)		C(2)	1.337(2)
N(1)	C(17)	1./	181(2)		N(1)		C(24)	1 405(2)
IN(1)	C(17)	1	+0+(2)		1(1)		C(24)	1.495(2)
N(2)	C(3)	1.5	502(2)		N(2)		C(10)	1.498(2)
CÓ	CÌÁ	1.4	512(2)		CÌÁ		C(5)	1 387(2)
0(5)	C(+)	1	512(2)		C(4)		0(5)	1.567(2)
C(4)	C(9)	1	391(2)		C(5)		C(6)	1.397(3)
C(6)	C(7)	13	386(3)		C(7)		C(8)	1 380(3)
	C(7)	1	000(0)					1.511(2)
C(8)	C(9)	1.:	392(2)		C(10)		$C(\Pi)$	1.511(2)
C(10)	C(17)	1.5	540(2)		C(11)		C(12)	1.395(2)
C(11)	0(10)	1 /	101(2)		C(12)		C(12)	1 201(2)
$C(\Pi)$	C(10)	1	<b>591</b> (2)		C(12)		C(13)	1.391(3)
C(13)	C(14)	1.3	385(3)		C(14)		C(15)	1.382(3)
C(15)	C(16)	1 3	201(2)		C(17)		C(18)	1 517(2)
C(13)	C(10)	1	591(2)		C(17)		C(18)	1.31/(2)
C(18)	C(19)	1.3	391(2)		C(18)		C(23)	1.390(2)
CÌLIÓ	còm	1.3	286(2)		còm		cèn	1 300(2)
C(1))	C(20)	1	560(2)		C(20)		C(21)	1.570(2)
C(21)	C(22)	1	376(3)		C(22)		C(23)	1.388(2)
C(24)	C(25)	14	516(2)		C(25)		C(26)	1.389(2)
	C(25)	1	2)				C(20)	1.309(2)
C(25)	C(30)	1	594(2)		C(26)		C(27)	1.390(2)
C(27)	C(28)	13	386(2)		C(28)		C(29)	1 380(3)
	C(20)	1.	200(2)		0(20)		0(2))	1.500(5)
C(29)	C(30)	1	589(5)					
Table 5 Bo	nd lengths invol	ving hydroge	ns (Å)					
10010 5. 00	nu tengens mvoi	ving nyeroge	113 (11)					1. (
atom	atom	dis	stance		atom		atom	distance
O(7)	H(29)	0.8	31(2)		O(7)		H(30)	0.77(2)
0 m	Han	0.9			ဂဏ်		น่าวา	0.80(2)
0(8)	11(51)	0.0	30(2)		0(8)		11(52)	0.80(2)
N(1)	H(21)	0.9	<del>)</del> 3(2)		N(2)		H(8)	0.81(2)
C(3)	HG	0.0	9502		cà		H(7)	0.9500
	11(0)	0.5	201				11(7)	0.0500
U(5)	H(1)	0.9	J01		C(6)		H(2)	0.9499
C(7)	H(3)	0.0	9500		C(8)		H(4)	0.9501
C	Ц(5)	0.0	0500		C(10)		цю́	0.9500
C(3)	п(5)	0.9	/500		C(10)		11(7)	0.2500
C(12)	H(10)	0.9	9500		C(13)		H(11)	0.9500
C(14)	H(12)	0.0	9500		cùs		H(13)	0.9500
	11(12)	0.5	2500				11(15)	0.9500
C(16)	H(14)	0.9	9500		C(17)		H(15)	0.9500
C(19)	H(20)	0.0	9500		C(20)		H(19)	0.9500
C(21)	II(10)	0.	501		C(20)		II(17)	0.0500
U(21)	H(18)	0.9	7501		C(22)		r1(17)	0.9500
C(23)	H(16)	0.0	9500		C(24)		H(22)	0.9500
còń	HON	0.0	0500		COO		нàń	0.9501
C(24)	<u>п(23)</u>	0.9	500		C(20)		11(24)	0.9501
C(27)	H(25)	0.9	¥500		C(28)		H(26)	0.9500
C(29)	HOT	0.0	9500		ല്ദത്		H(28)	0.9501
	11(27)	0.5			C(50)		n(20)	0.9501
H(8)	N(2)	0.8	31(2)		H(11)		C(13)	0.9500
Table 6. Bo	nd angles ( <sup>0</sup> )							
atom	atom	atom	angle		atom	atom	atom	angle
NE(1)	0(1)	0(1)	104 50/00			NI:(1)	0(1)	17( 40(4)
INI(1)	O(1)	S(1)	124.58(6)		U(4)	N1(1)	O(1)	1/6.48(4)
O(7)	Ni(1)	O(1)	87.59(5)		O(8)	Ni(1)	O(1)	90.72(4)
N(1)	NG(1)	0(1)	Q0 04(A)		N(2)	NG(1)	O(1)	02 44(5)
19(1)	181(1)	O(1)	89.06(4)		1N(Z)	INI(1)	O(1)	93.44(3)
Ni(1)	O(4)	S(2)	138.06(6)		O(7)	Ni(1)	O(4)	92.39(5)
$O(\hat{8})$	Ni(1)	O(4)	85 75(4)		NÌÌÌ	NiĉIŚ	$\hat{\mathbf{O}}(4)$	94 46(4)
N(0)	11(1) ht(1)		05.75(4)					
N(2)	N1(1)	O(4)	86.74(5)		U(8)	N1(1)	<b>O</b> (7)	89.17(5)
N(1)	Ni(1)	O(7)	92.46(5)		N(2)	Ni(1)	O(7)	177 31(5)

N(1)	Ni(1)	O(8)	178 35(5)	N(2)	Ni(1)	O(8)	93 30(5)
N(2)	Ni(1)	N(1)	85.08(5)	Ni(1)	N(1)	C(17)	107.37(9)
Ni(1)	N(1)	C(24)	115 58(9)	Ni(1)	N(2)	C(3)	11754(9)
Ni(1)	N(2)	C(10)	107.00(9)	O(3)	S(1)	O(1)	113 91(7)
$\Omega(2)$	S(1)	O(1)	113 36(7)	C(1)	S(1)	O(1)	10248(7)
O(2)	S(1)	O(1)	116.76(7)	C(1)	S(1)	O(1)	102.40(7) 104.48(7)
C(1)	S(1)	O(2)	102.60(7)	S(1)	S(1)	O(2) E(1)	104.40(7) 100.7(1)
$\mathcal{C}(1)$	S(1) = C(1)	U(3)	111.0(1)	S(1)	C(1)	$\Gamma(1)$ $\Gamma(2)$	109.7(1) 110.5(1)
S(1)	C(1)	$\Gamma(2)$	111.9(1)	S(1)	C(1)	$\Gamma(3)$	110.5(1)
0(5)	S(2)	O(4)	113.21(6)	0(6)	S(2)	0(4)	114.82(6)
C(2)	S(2)	0(4)	102.43(7)	0(6)	S(2)	0(5)	116.18(7)
C(2)	S(2)	0(5)	104.20(7)	C(2)	S(2)	O(6)	103.79(7)
S(2)	C(2)	F(4)	110.7(1)	S(2)	C(2)	F(5)	110.9(1)
S(2)	C(2)	F(6)	110.5(1)	F(1)	C(1)	F(2)	108.0(1)
F(1)	C(1)	F(3)	108.2(1)	F(2)	C(1)	F(3)	108.5(1)
F(4)	C(2)	F(5)	108.6(1)	F(4)	C(2)	F(6)	107.7(1)
F(5)	C(2)	F(6)	108.3(1)	N(1)	C(17)	C(10)	108.9(1)
C(24)	N(1)	C(17)	113.1(1)	N(1)	C(17)	C(18)	113.5(1)
N(1)	C(24)	C(25)	116.3(1)	C(10)	N(2)	C(3)	112.1(1)
N(2)	C(3)	C(4)	114.7(1)	N(2)	C(10)	C(17)	108.9(1)
N(2)	C(10)	C(11)	112.9(1)	C(3)	C(4)	C(5)	120.0(1)
C(3)	C(4)	C(9)	121.0(1)	C(9)	C(4)	C(5)	118.9(1)
C(4)	C(5)	C(6)	120.8(2)	C(4)	C(9)	C(8)	120.3(2)
C(5)	C(6)	C(7)	119.7(2)	CíÓ	C(7)	C(8)	119.8(2)
C(7)	C(8)	C(9)	120 5(2)	C(17)	C(10)	C(11)	112.3(1)
C(10)	C(11)	C(12)	120.8(1)	C(10)	C(11)	C(16)	120.1(1)
C(10)	C(17)	C(12)	111 4(1)	C(16)	C(11)	C(12)	120.1(1) 110.0(2)
C(10)	C(17)	C(13)	120 5(2)	C(10)	C(11)	C(12)	119.0(2) 120.7(2)
C(12)	C(12)	C(13)	119 6(2)	C(13)	C(14)	C(15)	120.7(2) 120.6(2)
C(12)	C(15)	C(14)	119.0(2)	C(13)	C(14)	C(13)	120.0(2) 121.0(1)
C(14)	C(13)	C(10)	120.0(1)	C(17)	C(18)	C(19)	121.0(1)
C(17)	C(18)	C(23)	120.0(1)	C(23)	C(18)	C(19)	118.9(1)
C(18)	C(19)	C(20)	120.6(1)	C(18)	C(23)	C(22)	120.7(2)
C(19)	C(20)	C(21)	119.7(1)	C(20)	C(21)	C(22)	120.3(2)
C(21)	C(22)	C(23)	119.9(2)	C(24)	C(25)	C(26)	121.3(1)
C(24)	C(25)	C(30)	120.3(1)	C(30)	C(25)	C(26)	118.4(1)
C(25)	C(26)	C(27)	120 9(1)	C(25)	C(30)	C(29)	120 9(2)
· · ·	· /	0(=/)	120.9(1)	C(23)	C(30)	$\mathcal{C}(2^{j})$	120.9(2)
C(26)	C(27)	C(28)	120.0(2)	C(23) C(27)	C(28)	C(29)	119.7(2)
C(26) C(28)	C(27) C(29)	C(28) C(30)	120.0(2) 120.1(2)	C(23) C(27)	C(28)	C(29)	119.7(2)
C(26) C(28) Table 7. Bond	C(27) C(29)	$\begin{array}{c} C(28) \\ C(30) \end{array}$	120.0(1) 120.0(2) 120.1(2)	C(27)	C(28)	C(29)	119.7(2)
C(26) C(28) Table 7. Bond	C(27) C(29) I angles involvin	C(28) C(30) ng hydrogens ( <sup>0</sup> ) atom	120.0(2) 120.1(2) angle	atom	atom	atom	angle
C(26) C(28) Table 7. Bond atom	C(27) C(29) d angles involvin atom Q(7)	C(28) C(30) atom H(29)	angle 120.1(2)	atom Ni(1)	atom Q(7)	atom H(30)	angle 124(1)
C(26) C(28) Table 7. Bond atom Ni(1) Ni(1)	C(27) C(29) I angles involvir atom O(7) O(8)	C(28) C(30) ng hydrogens ( <sup>0</sup> ) atom H(29) H(31)	angle 120(1) 120.1(2)	atom Ni(1)	atom O(7) O(8)	atom H(30) H(32)	angle 124(1) 115(1)
C(26) C(28) Table 7. Bond atom Ni(1) Ni(1) Ni(1)	$\begin{array}{c} C(27) \\ C(29) \\ 1 \text{ angles involvin} \\ of (7) \\ O(8) \\ N(1) \end{array}$	C(28) C(30) ng hydrogens ( <sup>0</sup> ) atom H(29) H(31) H(21)	angle 120(1) 120.1(2) angle 120(1) 112(1) 102(1)	atom Ni(1) Ni(1) Ni(1)	atom O(7) O(8) N(2)	atom H(30) H(32) H(8)	angle 124(1) 115(1)
C(26) C(28) Table 7. Bond atom Ni(1) Ni(1) Ni(1) Ni(1)	C(27) C(29) d angles involvin atom O(7) O(8) N(1) O(7)	C(28) C(30) ng hydrogens ( <sup>0</sup> ) atom H(29) H(31) H(21) H(20)	angle 120(1) 120.1(2) angle 120(1) 112(1) 102(1) 109(2)	atom Ni(1) Ni(1) Ni(1) Ni(1)	atom O(7) O(8) N(2) O(8)	atom H(30) H(32) H(8) H(31)	angle 124(1) 115(1) 107(1) 105(2)
C(26) C(28) Table 7. Bond atom Ni(1) Ni(1) Ni(1) H(30) N(1)	$\begin{array}{c} C(27) \\ C(29) \\ \hline angles involvin \\ atom \\ O(7) \\ O(8) \\ N(1) \\ O(7) \\ O(7) \\ C(17) \end{array}$	C(28) C(30) atom H(29) H(31) H(21) H(29) H(15)	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4	atom Ni(1) Ni(1) Ni(1) H(32) H(21)	atom O(7) O(8) N(2) O(8) N(1)	atom H(30) H(32) H(8) H(31) C(17)	angle 124(1) 115(1) 107(1) 105(2) 110(1)
C(26) C(28) Table 7. Bond atom Ni(1) Ni(1) Ni(1) H(30) N(1) H(21)	C(27) C(29) d angles involvir atom O(7) O(8) N(1) O(7) C(17) N(1)	C(28) C(30) ng hydrogens ( <sup>0</sup> ) atom H(29) H(31) H(21) H(29) H(15) C(24)	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 107(1)	atom Ni(1) Ni(1) Ni(1) H(32) H(21) N(1)	atom O(7) O(8) N(2) O(8) N(1) C(24)	atom H(30) H(32) H(8) H(31) C(17) H(22)	angle 124(1) 115(1) 107(1) 105(2) 110(1) 107 8
C(26) C(28) Table 7. Bond atom Ni(1) Ni(1) Ni(1) H(30) N(1) H(21) N(1)	C(27) C(29) I angles involvir atom O(7) O(8) N(1) O(7) C(17) N(1) C(17) N(1)	C(28) C(30) ng hydrogens ( <sup>0</sup> ) atom H(29) H(31) H(21) H(29) H(15) C(24) H(23)	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 107(1) 107.4	atom Ni(1) Ni(1) Ni(1) H(32) H(21) N(1) N(2)	atom O(7) O(8) N(2) O(8) N(1) C(24) C(24)	atom H(30) H(32) H(8) H(31) C(17) H(22) H(6)	angle 124(1) 115(1) 107(1) 105(2) 110(1) 107.8 107.9
C(26) C(28) Table 7. Bond atom Ni(1) Ni(1) Ni(1) H(30) N(1) H(21) N(1) N(2)	C(27) C(29) I angles involvir atom O(7) O(8) N(1) O(7) C(17) N(1) C(24) C(24)	C(28) C(30) atom H(29) H(31) H(21) H(29) H(15) C(24) H(23) U(2)	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 107(1) 107.4 107(2) 107.4	atom Ni(1) Ni(1) Ni(1) H(32) H(21) N(1) N(2) W(2)	atom O(7) O(8) N(2) O(8) N(1) C(24) C(3) N(2)	atom H(30) H(32) H(8) H(31) C(17) H(22) H(6) C(2)	angle 124(1) 115(1) 107(1) 105(2) 110(1) 107.8 107.9 102(1)
C(26) C(28) Table 7. Bond atom Ni(1) Ni(1) Ni(1) H(30) N(1) H(21) N(1) N(2) V(2)	C(27) C(29) I angles involvir atom O(7) O(8) N(1) O(7) C(17) N(1) C(24) C(3) N(2)	C(28) C(30) atom H(29) H(31) H(21) H(21) H(29) H(15) C(24) H(23) H(7) C(20)	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 107(1) 107.4 107.4 108.2 109(1)	atom Ni(1) Ni(1) Ni(1) H(32) H(21) N(1) N(2) H(8) N(2)	atom O(7) O(8) N(2) O(8) N(1) C(24) C(3) N(2) C(10)	atom H(30) H(32) H(8) H(31) C(17) H(22) H(6) C(3)	angle 124(1) 115(1) 107(1) 105(2) 110(1) 107.8 107.9 102(1) 107.2
C(26) C(28) Table 7. Bond atom Ni(1) Ni(1) Ni(1) H(30) N(1) H(21) N(1) N(2) H(8) U(2)	C(27) C(29) d angles involvin atom O(7) O(8) N(1) O(7) C(17) N(1) C(24) C(3) N(2) C(2)	C(28) C(30) atom H(29) H(31) H(21) H(21) H(29) H(15) C(24) H(23) H(7) C(10) C(24)	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 107(1) 107.4 108.2 109(1) 107.0	atom Ni(1) Ni(1) Ni(1) H(32) H(21) N(1) N(2) H(8) N(2) H(8) N(2)	atom O(7) O(8) N(2) O(8) N(1) C(24) C(3) N(2) C(10) C(20)	atom H(30) H(32) H(8) H(31) C(17) H(22) H(6) C(3) H(9) C(4)	angle 124(1) 115(1) 107(1) 105(2) 110(1) 107.8 107.9 102(1) 107.3 109.5
C(26) C(28) Table 7. Bond atom Ni(1) Ni(1) Ni(1) H(30) N(1) H(21) N(1) N(2) H(8) H(6) U(2)	$\begin{array}{c} C(27) \\ C(29) \\ \hline angles involvin \\ atom \\ O(7) \\ O(8) \\ N(1) \\ O(7) \\ C(17) \\ N(1) \\ C(24) \\ C(3) \\ N(2) \\ C(3) \\ N(2) \\ C(3) \\ O(7) \\ C(3) \\ O(7) \\$	C(28) C(30) atom H(29) H(31) H(21) H(21) H(29) H(15) C(24) H(23) H(7) C(10) C(4) U(0)	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 107(1) 107.4 108.2 109(1) 107.9 109.4	atom Ni(1) Ni(1) Ni(1) H(32) H(21) N(1) N(2) H(8) N(2) H(7) (2) H(7) (2)	atom O(7) O(8) N(2) O(8) N(1) C(24) C(3) N(2) C(10) C(3) C(10) C(3)	atom H(30) H(32) H(8) H(31) C(17) H(22) H(6) C(3) H(9) C(4) U(1)	angle 124(1) 115(1) 107(1) 105(2) 110(1) 107.8 107.9 102(1) 107.3 108.5
C(26) C(28) Table 7. Bonc atom Ni(1) Ni(1) Ni(1) H(30) N(1) H(21) N(1) N(2) H(8) H(6) H(7)	$\begin{array}{c} C(27) \\ C(29) \\ \hline \\ angles involvin \\ atom \\ O(7) \\ O(8) \\ N(1) \\ O(7) \\ C(17) \\ N(1) \\ C(24) \\ C(3) \\ N(2) \\ C(3) \\ C(3)$	C(28) C(30) atom H(29) H(31) H(21) H(21) H(29) H(15) C(24) H(7) C(10) C(4) H(6) U(2)	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 102(1) 109(2) 107.4 107(1) 107.4 108.2 109(1) 107.9 109.4	atom Ni(1) Ni(1) Ni(1) H(32) H(21) N(1) N(2) H(8) N(2) H(7) C(4)	atom O(7) O(8) N(2) O(8) N(1) C(24) C(3) N(2) C(10) C(3) C(5) O(5)	$\begin{array}{c} \text{atom} \\ \text{H(30)} \\ \text{H(32)} \\ \text{H(8)} \\ \text{H(31)} \\ \text{C(17)} \\ \text{H(22)} \\ \text{H(6)} \\ \text{C(3)} \\ \text{H(9)} \\ \text{C(4)} \\ \text{H(1)} \\ \end{array}$	angle 124(1) 115(1) 107(1) 105(2) 110(1) 107.8 107.9 102(1) 107.3 108.5 119.5
C(26) C(28) Table 7. Bond atom Ni(1) Ni(1) Ni(1) H(30) N(1) H(21) N(1) N(2) H(8) H(6) H(7) C(4) S(2)	C(27) C(29) d angles involvin atom O(7) O(8) N(1) O(7) C(17) N(1) C(24) C(3) N(2) C(3) C(3) C(3) C(9) O(2) O(2) O(3) C(3)	C(28) C(30) mg hydrogens ( <sup>0</sup> ) atom H(29) H(31) H(21) H(29) H(15) C(24) H(23) H(7) C(10) C(10) C(10) C(4) H(6) H(5) U(2)	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 109(2) 107.4 107(1) 107.4 108.2 109(1) 107.9 109.4 119.8 120.2	atom Ni(1) Ni(1) Ni(1) H(32) H(21) N(1) N(2) H(8) N(2) H(7) C(4) H(7) C(4) H(1)	atom O(7) O(8) N(2) O(8) N(1) C(24) C(3) N(2) C(10) C(3) C(5) C(5) C(5)	atom H(30) H(32) H(8) H(31) C(17) H(22) H(6) C(3) H(9) C(4) H(1) C(6) C(2)	angle 124(1) 119.7(2) angle 124(1) 115(1) 107(1) 105(2) 110(1) 107.8 107.9 102(1) 107.3 108.5 119.5 119.7
C(26) C(28) Table 7. Bond atom Ni(1) Ni(1) Ni(1) H(30) N(1) H(21) N(1) H(21) N(1) N(2) H(8) H(6) H(6) H(7) C(4) C(5)	$\begin{array}{c} C(27) \\ C(29) \\ \hline \\ A angles involvin \\ atom \\ O(7) \\ O(8) \\ N(1) \\ O(7) \\ C(17) \\ N(1) \\ C(24) \\ C(3) \\ C(3) \\ C(3) \\ C(3) \\ C(3) \\ C(9) \\ C(6) \\ C(6) \\ C(7) \\ C($	C(28) C(30) mg hydrogens ( <sup>0</sup> ) atom H(29) H(31) H(21) H(29) H(15) C(24) H(23) H(7) C(10) C(4) H(6) H(5) H(2)	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 107(1) 107.4 108.2 109(1) 107.9 109.4 119.8 120.2	atom Ni(1) Ni(1) Ni(1) H(32) H(21) N(1) N(2) H(8) N(2) H(7) C(4) H(1) H(2)	atom O(7) O(8) N(2) O(8) N(1) C(24) C(3) N(2) C(10) C(3) C(5) C(5) C(5) C(6)	$\begin{array}{c} \text{atom} \\ \text{H(30)} \\ \text{H(32)} \\ \text{H(8)} \\ \text{H(31)} \\ \text{C(17)} \\ \text{H(22)} \\ \text{H(6)} \\ \text{C(3)} \\ \text{H(9)} \\ \text{C(4)} \\ \text{H(1)} \\ \text{C(6)} \\ \text{C(7)} \\ \end{array}$	angle 124(1) 119.7(2) 119.7(2) 119.7(2) 115(1) 107(1) 105(2) 110(1) 107.8 107.9 102(1) 107.3 108.5 119.5 119.7 120.1
C(26) C(28) Table 7. Bond atom Ni(1) Ni(1) Ni(1) H(30) N(1) H(21) N(1) H(21) N(1) N(2) H(8) H(6) H(7) C(4) C(5) C(6)	$\begin{array}{c} C(27) \\ C(29) \\ \hline \\ angles involvin \\ atom \\ O(7) \\ O(8) \\ N(1) \\ O(7) \\ C(17) \\ N(1) \\ C(24) \\ C(3) \\ C(3) \\ C(3) \\ C(3) \\ C(3) \\ C(9) \\ C(6) \\ C(7) \\ \hline \end{array}$	C(28) C(30) atom H(29) H(31) H(21) H(21) H(29) H(15) C(24) H(23) H(7) C(10) C(4) H(6) H(6) H(5) H(2) H(3)	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 107(1) 107.4 109(1) 107.4 109(1) 107.9 109.4 119.8 120.2 119.8	atom Ni(1) Ni(1) Ni(1) H(32) H(21) N(1) N(2) H(7) C(4) H(1) H(2) C(7)	atom O(7) O(8) N(2) O(8) N(1) C(24) C(3) N(2) C(10) C(3) C(5) C(5) C(5) C(6) C(8)	$\begin{array}{c} \text{atom} \\ \text{H}(30) \\ \text{H}(32) \\ \text{H}(8) \\ \text{H}(31) \\ \text{C}(17) \\ \text{H}(22) \\ \text{H}(6) \\ \text{C}(3) \\ \text{H}(9) \\ \text{C}(4) \\ \text{H}(1) \\ \text{C}(6) \\ \text{C}(7) \\ \text{H}(4) \end{array}$	angle 124(1) 119.7(2) 119.7(2) 119.7(2) 107.1(1) 105(2) 110(1) 107.8 107.9 102(1) 107.3 108.5 119.5 119.7 120.1 119.7
C(26) C(28) Table 7. Bond atom Ni(1) Ni(1) Ni(1) H(30) N(1) H(21) N(1) N(2) H(8) H(6) H(7) C(4) C(5) C(6) H(3)	$\begin{array}{c} C(27) \\ C(29) \\ \hline \\ angles involvin \\ atom \\ O(7) \\ O(8) \\ N(1) \\ O(7) \\ C(17) \\ N(1) \\ C(24) \\ C(3) \\ N(2) \\ C(3) \\ C(3) \\ C(3) \\ C(3) \\ C(3) \\ C(3) \\ C(6) \\ C(7) \\ C(7) \\ C(7) \end{array}$	C(28) C(30) atom H(29) H(31) H(21) H(21) H(29) H(15) C(24) H(23) H(7) C(10) C(4) H(6) H(5) H(2) H(3) C(8)	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 107(1) 107.4 109(1) 107.9 109.4 119.8 120.2 119.8 120.2 119.8 120.4	atom Ni(1) Ni(1) Ni(1) H(32) H(21) N(1) N(2) H(7) C(4) H(1) H(2) C(7) C(8)	atom O(7) O(8) N(2) O(8) N(1) C(24) C(3) N(2) C(10) C(3) C(5) C(5) C(5) C(6) C(8) C(9)	$\begin{array}{c} \text{atom} \\ \text{H(30)} \\ \text{H(32)} \\ \text{H(8)} \\ \text{H(31)} \\ \text{C(17)} \\ \text{H(22)} \\ \text{H(6)} \\ \text{C(3)} \\ \text{H(9)} \\ \text{C(4)} \\ \text{H(1)} \\ \text{C(6)} \\ \text{C(7)} \\ \text{H(4)} \\ \text{H(5)} \end{array}$	angle 124(1) 119.7(2) 119.7(2) 119.7(2) 107(1) 105(2) 110(1) 107.8 107.9 102(1) 107.3 108.5 119.5 119.7 120.1 119.7 119.9
C(26) C(28) Table 7. Bonc atom Ni(1) Ni(1) Ni(1) H(30) N(1) H(21) N(1) N(1) N(2) H(8) H(6) H(7) C(4) C(5) C(6) H(3) H(4)	$\begin{array}{c} C(27) \\ C(29) \\ \hline \\ angles involvin \\ atom \\ O(7) \\ O(8) \\ N(1) \\ O(7) \\ C(17) \\ N(1) \\ C(24) \\ C(3) \\ N(2) \\ C(3) \\ N(2) \\ C(3) \\ C(3) \\ C(3) \\ C(3) \\ C(3) \\ C(3) \\ C(7) \\ C(7) \\ C(7) \\ C(7) \\ C(8) \\ \end{array}$	C(28) C(30) ng hydrogens ( <sup>0</sup> ) atom H(29) H(31) H(21) H(21) H(29) H(15) C(24) H(23) H(7) C(10) C(4) H(6) H(5) H(2) H(3) C(8) C(9)	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 102(1) 109(2) 107.4 107(1) 107.4 107(1) 107.4 108.2 109(1) 107.9 109.4 119.8 120.2 119.8 120.4 119.7	$\begin{array}{c} \text{atom} \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{H}(32) \\ \text{H}(21) \\ \text{H}(21) \\ \text{N}(1) \\ \text{N}(2) \\ \text{H}(8) \\ \text{N}(2) \\ \text{H}(7) \\ \text{C}(4) \\ \text{H}(7) \\ \text{C}(4) \\ \text{H}(1) \\ \text{H}(2) \\ \text{C}(7) \\ \text{C}(7) \\ \text{C}(8) \\ \text{H}(9) \end{array}$	$\begin{array}{c} c(38)\\ C(28)\\ \end{array}$ atom O(7) O(8) N(2) O(8) N(1) C(24) C(3) N(2) C(10) C(3) C(5) C(5) C(5) C(5) C(5) C(6) C(8) C(9) C(10)\\ \end{array}	$\begin{array}{c} c(29) \\ c(3) \\ c(17) \\ c(17) \\ c(17) \\ c(17) \\ c(17) \\ c(17) \\ c(11) \\ $	angle 124(1) 119.7(2) 119.7(2) 110.7(1) 107(1) 107(1) 107.8 107.9 102(1) 107.3 108.5 119.5 119.7 120.1 119.7 119.9 108.2
C(26) C(28) Table 7. Bonc atom Ni(1) Ni(1) Ni(1) H(30) N(1) H(21) N(1) N(1) N(2) H(8) H(6) H(7) C(4) C(4) C(5) C(6) H(3) H(4) H(9)	$\begin{array}{c} C(27) \\ C(29) \\ \hline \\ A angles involvin \\ atom \\ O(7) \\ O(8) \\ N(1) \\ O(7) \\ C(17) \\ N(1) \\ C(24) \\ C(3) \\ C(7) \\ C(7) \\ C(7) \\ C(7) \\ C(7) \\ C(8) \\ C(10) \\ \end{array}$	C(28) C(30) ng hydrogens ( <sup>0</sup> ) atom H(29) H(31) H(21) H(29) H(15) C(24) H(23) H(7) C(10) C(4) H(6) H(5) H(2) H(3) C(8) C(9) C(17)	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 107(1) 107.4 109(1) 107.9 109.4 119.8 120.2 119.8 120.2 119.8 120.4 119.7 107.0	$\begin{array}{c} \text{atom} \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{H}(32) \\ \text{H}(21) \\ \text{H}(21) \\ \text{N}(1) \\ \text{H}(2) \\ \text{H}(8) \\ \text{N}(2) \\ \text{H}(7) \\ \text{C}(4) \\ \text{H}(1) \\ \text{H}(2) \\ \text{C}(7) \\ \text{C}(8) \\ \text{H}(9) \\ \text{C}(10) \end{array}$	$\begin{array}{c} \text{atom} \\ \text{O}(7) \\ \text{O}(8) \\ \text{N}(2) \\ \text{O}(8) \\ \text{N}(1) \\ \text{C}(24) \\ \text{C}(3) \\ \text{N}(2) \\ \text{C}(10) \\ \text{C}(3) \\ \text{C}(5) \\ \text{C}(5) \\ \text{C}(5) \\ \text{C}(6) \\ \text{C}(8) \\ \text{C}(9) \\ \text{C}(10) \\ \text{C}(17) \end{array}$	$\begin{array}{c} \text{atom} \\ \text{H(30)} \\ \text{H(32)} \\ \text{H(8)} \\ \text{H(31)} \\ \text{C(17)} \\ \text{H(22)} \\ \text{H(6)} \\ \text{C(23)} \\ \text{H(9)} \\ \text{C(4)} \\ \text{H(1)} \\ \text{C(6)} \\ \text{C(7)} \\ \text{H(4)} \\ \text{H(5)} \\ \text{C(11)} \\ \text{H(15)} \end{array}$	angle 124(1) 119.7(2) angle 124(1) 115(1) 107(1) 105(2) 110(1) 107.8 107.9 102(1) 107.3 108.5 119.7 120.1 119.7 120.1 119.7 119.9 108.2 107.5
C(26) C(28) Table 7. Bond atom Ni(1) Ni(1) H(30) N(1) H(21) N(1) N(2) H(8) H(6) H(7) C(4) C(5) C(6) H(3) H(4) H(4) H(9) C(11)	$\begin{array}{c} C(27) \\ C(29) \\ \hline \\ C(29) \\ \hline \\ angles involvin \\ atom \\ O(7) \\ O(8) \\ N(1) \\ O(7) \\ C(17) \\ N(1) \\ C(24) \\ C(24) \\ C(3) \\ N(2) \\ C(3) \\ C(7) \\ C(7) \\ C(7) \\ C(7) \\ C(7) \\ C(7) \\ C(8) \\ C(10) \\ C(12) \\ \end{array}$	C(28) C(30) ng hydrogens ( <sup>0</sup> ) atom H(29) H(31) H(21) H(29) H(15) C(24) H(7) C(10) C(4) H(6) H(5) H(2) H(3) C(8) C(9) C(17) H(10)	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 109(2) 107.4 107(1) 107.4 108.2 109(1) 107.9 109.4 119.8 120.2 119.8 120.2 119.8 120.4 119.7 107.0 119.5	$\begin{array}{c} \text{atom} \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{H}(32) \\ \text{H}(21) \\ \text{H}(21) \\ \text{N}(1) \\ \text{H}(2) \\ \text{H}(8) \\ \text{N}(2) \\ \text{H}(7) \\ \text{C}(4) \\ \text{H}(1) \\ \text{H}(2) \\ \text{C}(7) \\ \text{C}(4) \\ \text{H}(9) \\ \text{C}(70) \\ \text{C}(10) \\ \text{C}(11) \end{array}$	$\begin{array}{c} \text{atom} \\ \text{O}(7) \\ \text{O}(8) \\ \text{N}(2) \\ \text{O}(8) \\ \text{N}(1) \\ \text{C}(24) \\ \text{C}(3) \\ \text{N}(2) \\ \text{C}(10) \\ \text{C}(3) \\ \text{C}(5) \\ \text{C}(5) \\ \text{C}(5) \\ \text{C}(5) \\ \text{C}(6) \\ \text{C}(8) \\ \text{C}(9) \\ \text{C}(10) \\ \text{C}(17) \\ \text{C}(16) \end{array}$	$\begin{array}{c} \text{atom} \\ \text{H(30)} \\ \text{H(32)} \\ \text{H(8)} \\ \text{H(31)} \\ \text{C(17)} \\ \text{H(22)} \\ \text{H(6)} \\ \text{C(3)} \\ \text{H(9)} \\ \text{C(4)} \\ \text{H(1)} \\ \text{C(6)} \\ \text{C(7)} \\ \text{H(4)} \\ \text{H(5)} \\ \text{C(11)} \\ \text{H(15)} \\ \text{H(14)} \end{array}$	angle 124(1) 119.7(2) angle 124(1) 115(1) 107(1) 105(2) 110(1) 107.8 107.9 102(1) 107.3 108.5 119.5 119.7 120.1 119.7 120.1 119.7 119.9 108.2 107.5 119.8
C(26) C(28) Table 7. Bond atom Ni(1) Ni(1) H(30) N(1) H(21) N(1) H(21) N(1) H(21) N(2) H(8) H(6) H(7) C(4) C(5) C(6) H(4) H(4) H(9) C(11) H(10)	C(27) C(29) A angles involvir atom O(7) O(8) N(1) O(7) C(17) N(1) C(24) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(2) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(2) C(3)	C(28) C(30) ng hydrogens ( <sup>0</sup> ) atom H(29) H(31) H(21) H(29) H(15) C(24) H(23) H(7) C(10) C(24) H(6) H(5) H(2) H(3) C(8) C(9) C(17) H(10) C(13)	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 107(1) 107.4 108.2 109(1) 107.9 109.4 119.8 120.2 119.8 120.4 119.7 107.0 119.5 120.0	$\begin{array}{c} \text{atom} \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{H}(32) \\ \text{H}(21) \\ \text{H}(21) \\ \text{N}(2) \\ \text{H}(2) \\ \text{H}(3) \\ \text{N}(2) \\ \text{H}(3) \\ \text{N}(2) \\ \text{H}(7) \\ \text{C}(4) \\ \text{H}(1) \\ \text{H}(2) \\ \text{C}(7) \\ \text{C}(4) \\ \text{H}(1) \\ \text{H}(2) \\ \text{C}(7) \\ \text{C}(8) \\ \text{H}(9) \\ \text{C}(10) \\ \text{C}(11) \\ \text{C}(12) \end{array}$	$\begin{array}{c} \text{atom} \\ \text{O}(7) \\ \text{O}(8) \\ \text{N}(2) \\ \text{O}(8) \\ \text{N}(1) \\ \text{C}(24) \\ \text{C}(3) \\ \text{N}(2) \\ \text{C}(10) \\ \text{C}(3) \\ \text{C}(5) \\ \text{C}(5) \\ \text{C}(5) \\ \text{C}(5) \\ \text{C}(6) \\ \text{C}(8) \\ \text{C}(9) \\ \text{C}(10) \\ \text{C}(17) \\ \text{C}(16) \\ \text{C}(13) \end{array}$	$\begin{array}{c} \text{atom} \\ \text{H(30)} \\ \text{H(32)} \\ \text{H(8)} \\ \text{H(31)} \\ \text{C(17)} \\ \text{H(22)} \\ \text{H(6)} \\ \text{C(3)} \\ \text{H(9)} \\ \text{C(4)} \\ \text{H(1)} \\ \text{C(6)} \\ \text{C(7)} \\ \text{H(4)} \\ \text{H(1)} \\ \text{C(5)} \\ \text{C(11)} \\ \text{H(15)} \\ \text{H(14)} \\ \text{H(11)} \end{array}$	angle 124(1) 119.7(2) 119.7(2) 110.7(1) 105(2) 110(1) 107.8 107.9 102(1) 107.3 108.5 119.5 119.7 120.1 119.7 120.1 119.7 119.9 108.2 107.5 119.8 120.5
C(26) C(28) Table 7. Bond atom Ni(1) Ni(1) H(30) N(1) H(21) N(1) H(21) N(1) H(21) N(2) H(8) H(6) H(7) C(4) C(5) C(6) H(3) H(4) H(9) C(11) H(10) H(11)	C(27) C(29) A angles involvir atom O(7) O(8) N(1) O(7) C(17) N(1) C(24) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(2) C(3) C(3) C(3) C(3) C(2) C(3) C(3) C(3) C(3) C(2) C(3) C(3) C(2) C(3) C(3) C(2) C(3) C(3) C(3) C(2) C(3) C(3) C(3) C(3) C(2) C(3)	C(28) C(30) ng hydrogens (°) atom H(29) H(31) H(21) H(29) H(15) C(24) H(23) H(7) C(10) C(24) H(6) H(5) H(2) H(3) C(8) C(9) C(17) H(10) C(13) C(14)	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 107(1) 107.4 109(1) 107.9 109.4 119.8 120.2 119.8 120.4 119.7 107.0 119.5 120.0 119.9	$\begin{array}{c} \text{atom} \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{H}(32) \\ \text{H}(21) \\ \text{N}(1) \\ \text{H}(32) \\ \text{H}(21) \\ \text{N}(2) \\ \text{H}(3) \\ \text{N}(2) \\ \text{H}(3) \\ \text{N}(2) \\ \text{H}(7) \\ \text{C}(4) \\ \text{H}(1) \\ \text{H}(2) \\ \text{C}(7) \\ \text{C}(4) \\ \text{H}(1) \\ \text{H}(2) \\ \text{C}(7) \\ \text{C}(8) \\ \text{H}(9) \\ \text{C}(10) \\ \text{C}(11) \\ \text{C}(12) \\ \text{C}(13) \end{array}$	$\begin{array}{c} \text{atom} \\ \text{O}(7) \\ \text{O}(8) \\ \text{N}(2) \\ \text{O}(8) \\ \text{N}(1) \\ \text{C}(24) \\ \text{C}(3) \\ \text{N}(2) \\ \text{C}(10) \\ \text{C}(3) \\ \text{C}(5) \\ \text{C}(5) \\ \text{C}(5) \\ \text{C}(6) \\ \text{C}(8) \\ \text{C}(9) \\ \text{C}(10) \\ \text{C}(17) \\ \text{C}(16) \\ \text{C}(13) \\ \text{C}(14) \end{array}$	$\begin{array}{c} \text{atom} \\ \text{H(30)} \\ \text{H(32)} \\ \text{H(31)} \\ \text{C(17)} \\ \text{H(22)} \\ \text{H(6)} \\ \text{C(17)} \\ \text{H(22)} \\ \text{H(6)} \\ \text{C(3)} \\ \text{H(9)} \\ \text{C(4)} \\ \text{H(1)} \\ \text{C(6)} \\ \text{C(7)} \\ \text{H(4)} \\ \text{H(5)} \\ \text{C(11)} \\ \text{H(15)} \\ \text{H(14)} \\ \text{H(11)} \\ \text{H(11)} \\ \text{H(12)} \end{array}$	angle 124(1) 119.7(2) 119.7(2) 119.7(2) 110(1) 105(2) 110(1) 107.8 107.9 102(1) 107.3 108.5 119.5 119.7 120.1 119.7 119.9 108.2 107.5 119.8 120.5 120.1
C(26) C(28) Table 7. Bond atom Ni(1) Ni(1) Ni(1) H(30) N(1) H(21) N(1) H(21) N(1) N(2) H(8) H(6) H(7) C(4) C(5) C(6) H(3) H(4) H(9) C(11) H(10) H(11) C(14)	$\begin{array}{c} C(27) \\ C(29) \\ \hline \\ angles involvin \\ atom \\ O(7) \\ O(8) \\ N(1) \\ O(7) \\ C(17) \\ N(1) \\ C(24) \\ C(3) \\ N(2) \\ C(3) \\ C(1) \\ C(12) \\ C(12) \\ C(12) \\ C(13) \\ C(15) \end{array}$	$\begin{array}{c} C(28) \\ C(28) \\ C(30) \\ \\ atom \\ H(29) \\ H(31) \\ H(21) \\ H(21) \\ H(29) \\ H(15) \\ C(24) \\ H(15) \\ C(24) \\ H(23) \\ H(7) \\ C(10) \\ C(4) \\ H(6) \\ H(5) \\ H(2) \\ H(3) \\ C(8) \\ C(9) \\ C(17) \\ H(10) \\ C(13) \\ C(14) \\ H(13) \\ \end{array}$	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 107(1) 107.4 109(2) 107.4 109(1) 107.9 109.4 119.8 120.2 119.8 120.2 119.8 120.4 119.7 107.0 119.5 120.0 119.9 120.3	$\begin{array}{c} \text{atom} \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{H}(32) \\ \text{H}(21) \\ \text{N}(1) \\ \text{N}(2) \\ \text{H}(21) \\ \text{N}(2) \\ \text{H}(7) \\ \text{C}(4) \\ \text{H}(1) \\ \text{H}(2) \\ \text{C}(7) \\ \text{C}(4) \\ \text{H}(1) \\ \text{H}(2) \\ \text{C}(7) \\ \text{C}(8) \\ \text{H}(9) \\ \text{C}(10) \\ \text{C}(11) \\ \text{C}(12) \\ \text{C}(13) \\ \text{H}(12) \end{array}$	$\begin{array}{c} \text{atom} \\ \text{O}(7) \\ \text{O}(8) \\ \text{N}(2) \\ \text{O}(8) \\ \text{N}(1) \\ \text{C}(24) \\ \text{C}(3) \\ \text{C}(10) \\ \text{C}(3) \\ \text{C}(5) \\ \text{C}(5) \\ \text{C}(5) \\ \text{C}(6) \\ \text{C}(8) \\ \text{C}(9) \\ \text{C}(10) \\ \text{C}(17) \\ \text{C}(16) \\ \text{C}(13) \\ \text{C}(14) \\ \text{C}(14) \end{array}$	$\begin{array}{c} \text{atom} \\ \text{H(30)} \\ \text{H(32)} \\ \text{H(8)} \\ \text{H(31)} \\ \text{C(17)} \\ \text{H(22)} \\ \text{H(6)} \\ \text{C(3)} \\ \text{H(9)} \\ \text{C(4)} \\ \text{H(1)} \\ \text{C(6)} \\ \text{C(7)} \\ \text{H(4)} \\ \text{H(5)} \\ \text{C(11)} \\ \text{H(15)} \\ \text{H(14)} \\ \text{H(15)} \\ \text{H(11)} \\ \text{H(11)} \\ \text{H(11)} \\ \text{H(12)} \\ \text{C(15)} \end{array}$	angle 124(1) 119.7(2) 119.7(2) 119.7(2) 107.1 105(2) 110(1) 107.8 107.9 102(1) 107.3 108.5 119.5 119.7 120.1 119.7 120.1 119.7 119.9 108.2 107.5 119.8 120.5 120.1 119.3
C(26) C(28) Table 7. Bonc atom Ni(1) Ni(1) Ni(1) H(30) N(1) H(21) N(1) N(2) H(8) H(6) H(7) C(4) C(5) C(6) H(3) H(4) H(9) C(11) H(10) H(11) C(14) C(15)	C(27) C(29) A angles involvin atom O(7) O(8) N(1) O(7) C(17) N(1) C(24) C(3) N(2) C(3) C(2) C(3) C(2) C(3) C(10) C(12) C(12) C(12) C(13) C(15) C(16)	$\begin{array}{c} C(28) \\ C(28) \\ C(30) \\ \end{array}$ ng hydrogens ( $^{0}$ ) atom H(29) H(31) H(21) H(21) H(29) H(15) C(24) H(23) H(7) C(10) C(4) H(5) H(2) H(3) C(8) C(9) C(17) H(10) C(13) C(14) H(13) H(14) \\ \end{array}	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 107(1) 107.4 107(1) 107.4 109(1) 107.9 109.4 119.8 120.2 119.8 120.4 119.7 107.0 119.5 120.0 119.5	atom Ni(1) Ni(1) Ni(1) H(32) H(21) N(1) N(2) H(7) C(4) H(7) C(4) H(7) C(4) H(7) C(4) H(7) C(4) H(1) H(2) C(7) C(10) C(11) C(12) C(13) H(12) H(13)	$\begin{array}{c} c(38)\\ c(28)\\ c(28)\\ c(28)\\ c(3)\\ c(28)\\ c(3)\\ c(5)\\ c(5)\\ c(5)\\ c(6)\\ c(8)\\ c(7)\\ c(10)\\ c(17)\\ c(16)\\ c(13)\\ c(14)\\ c(14)\\ c(15)\\ c(15)\\ c(15)\\ c(16)\\ c(15)\\ c(16)\\ c(17)\\ c(16)\\ c(15)\\ c(16)\\ c(15)\\ c(16)\\ c(17)\\ c(16)\\ c(15)\\ c(16)\\ c(17)\\ c(16)\\ c(15)\\ c(16)\\ c(15)\\ c(16)\\ c(16)\\ c(15)\\ c(16)\\ c(16)\\ c(16)\\ c(15)\\ c(16)\\ c(16)$	$\begin{array}{c} c(29) \\ c(3) \\ c(17) \\ c(17) \\ c(17) \\ c(17) \\ c(11) \\ c(16) \\ c(17) \\ c(16) \\ $	angle 124(1) 115(1) 107(1) 105(2) 110(1) 107.8 102(1) 107.3 108.5 119.5 119.7 120.1 119.7 119.9 108.2 107.5 119.8 120.1 119.3 120.2
C(26) C(28) Table 7. Bonc atom Ni(1) Ni(1) Ni(1) H(30) N(1) H(21) N(1) N(2) H(8) H(6) H(7) C(4) C(4) C(4) C(5) C(6) H(3) H(4) H(9) C(11) H(10) H(11) C(14) C(15) H(15)	C(27) C(29) A angles involvir atom O(7) O(8) N(1) O(7) C(17) N(1) C(24) C(24) C(24) C(24) C(3) N(2) C(3) C(3) C(3) C(3) C(3) C(3) C(7) C(7) C(7) C(7) C(7) C(7) C(7) C(10) C(12) C(12) C(12) C(13) C(15) C(17)	$\begin{array}{c} C(28) \\ C(28) \\ C(30) \\ \hline \\ \  \  \  \  \  \  \  \  \  \  \  \  \$	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 107(1) 107.4 109(1) 107.9 109.4 119.8 120.2 119.8 120.2 119.8 120.4 119.7 107.0 119.5 120.0 119.5 107.8	$\begin{array}{c} \text{atom} \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{H}(32) \\ \text{H}(21) \\ \text{H}(21) \\ \text{H}(21) \\ \text{N}(2) \\ \text{H}(32) \\ \text{H}(7) \\ \text{C}(4) \\ \text{H}(7) \\ \text{C}(7) \\ \text{C}(7) \\ \text{C}(8) \\ \text{H}(9) \\ \text{C}(10) \\ \text{C}(11) \\ \text{C}(12) \\ \text{C}(13) \\ \text{H}(12) \\ \text{H}(13) \\ \text{C}(18) \end{array}$	$\begin{array}{c} c(38) \\ c(28) \\ c(28) \\ c(28) \\ c(3) \\ c(5) \\ c(3) \\ c(5) \\ c(5) \\ c(6) \\ c(6) \\ c(7) \\ c(10) \\ c(17) \\ c(16) \\ c(17) \\ c(16) \\ c(13) \\ c(14) \\ c(15) \\ c(19) \\$	$\begin{array}{c} c(29) \\ c(30) \\ c(17) \\ c(17) \\ c(17) \\ c(17) \\ c(17) \\ c(22) \\ c(17) \\ c(22) \\ c(23) \\ c(23) \\ c(23) \\ c(23) \\ c(14) \\ c(16) \\ c(7) \\ c(16) \\ c(7) \\ c(16) \\ c$	angle 124(1) 119.7(2) 119.7(2) 119.7(2) 110.7(1) 107.1) 107.1) 105(2) 110.7(1) 107.8 107.9 102.(1) 107.3 108.5 119.7 120.1 119.7 119.9 108.2 107.5 119.8 120.5 120.1 119.3
C(26) C(28) Table 7. Bonc atom Ni(1) Ni(1) Ni(1) H(30) N(1) H(21) N(1) N(2) H(8) H(6) H(7) C(4) C(5) C(6) H(3) H(4) H(4) H(4) H(9) C(11) H(10) H(11) C(14) C(15) H(15) C(18)	C(27) C(29) A angles involvir atom O(7) O(8) N(1) O(7) C(17) N(1) C(24) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(2) C(3) C(10) C(12) C(13) C(15) C(16) C(17) C(23)	$\begin{array}{c} C(28) \\ C(28) \\ C(30) \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ $	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 109(2) 107.4 109(1) 107.9 109.4 119.8 120.2 119.8 120.2 119.8 120.4 119.7 107.0 119.5 120.0 119.9 120.3 119.5 107.8 119.4	$\begin{array}{c} \text{atom} \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{H}(32) \\ \text{H}(21) \\ \text{H}(21) \\ \text{N}(1) \\ \text{N}(2) \\ \text{H}(3) \\ \text{H}(3) \\ \text{H}(2) \\ \text{H}(3) \\ \text{C}(4) \\ \text{H}(1) \\ \text{H}(2) \\ \text{C}(7) \\ \text{C}(4) \\ \text{H}(1) \\ \text{H}(2) \\ \text{C}(7) \\ \text{C}(8) \\ \text{H}(9) \\ \text{C}(10) \\ \text{C}(11) \\ \text{C}(12) \\ \text{C}(13) \\ \text{H}(12) \\ \text{H}(13) \\ \text{C}(18) \\ \text{H}(20) \end{array}$	$\begin{array}{c} \text{atom} \\ \text{O}(7) \\ \text{O}(8) \\ \text{N}(2) \\ \text{O}(8) \\ \text{N}(1) \\ \text{C}(24) \\ \text{C}(3) \\ \text{N}(2) \\ \text{C}(10) \\ \text{C}(3) \\ \text{C}(5) \\ \text{C}(5) \\ \text{C}(5) \\ \text{C}(5) \\ \text{C}(5) \\ \text{C}(6) \\ \text{C}(7) \\ \text{C}(10) \\ \text{C}(17) \\ \text{C}(16) \\ \text{C}(17) \\ \text{C}(16) \\ \text{C}(13) \\ \text{C}(14) \\ \text{C}(14) \\ \text{C}(15) \\ \text{C}(19) \\ \text{C}(19) \\ \end{array}$	$\begin{array}{c} \text{atom} \\ \text{H(30)} \\ \text{H(32)} \\ \text{H(8)} \\ \text{H(31)} \\ \text{C(17)} \\ \text{H(22)} \\ \text{H(6)} \\ \text{C(3)} \\ \text{H(9)} \\ \text{C(4)} \\ \text{H(1)} \\ \text{C(6)} \\ \text{C(7)} \\ \text{H(4)} \\ \text{H(1)} \\ \text{C(6)} \\ \text{C(11)} \\ \text{H(5)} \\ \text{C(11)} \\ \text{H(15)} \\ \text{H(14)} \\ \text{H(11)} \\ \text{H(12)} \\ \text{C(15)} \\ \text{C(16)} \\ \text{H(20)} \\ \text{C(20)} \end{array}$	angle 124(1) 119.7(2) 119.7(2) 119.7(2) 119.7(2) 107(1) 105(2) 110(1) 107.8 107.9 102(1) 107.3 108.5 119.5 119.7 120.1 119.7 119.9 108.2 107.5 119.8 120.5 120.1 119.3 120.2
C(26) C(28) Table 7. Bond atom Ni(1) Ni(1) Ni(1) H(30) N(1) H(21) N(1) H(21) N(1) N(2) H(8) H(6) H(7) C(4) C(5) C(4) C(5) C(6) H(3) H(4) H(4) H(9) C(11) H(10) H(11) C(14) C(15) H(15) C(18) C(19)	C(27) C(29) A angles involvir atom O(7) O(8) N(1) O(7) C(17) N(1) C(24) C(3) N(2) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(2) C(3) C(1) C(12) C(12) C(12) C(13) C(15) C(17) C(23) C(20)	$\begin{array}{c} C(28) \\ C(28) \\ C(30) \\ \end{array}$ ng hydrogens ( $^{0}$ ) atom H(29) H(31) H(21) H(29) H(15) C(24) H(23) H(7) C(10) C(4) H(6) H(5) H(2) H(3) C(4) H(6) H(5) H(2) H(3) C(8) C(9) C(17) H(10) C(13) C(14) H(13) H(14) C(18) H(16) H(19)	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 107(1) 107.4 109(1) 107.9 109.4 119.8 120.2 119.8 120.4 119.7 107.0 119.5 120.0 119.9 120.3 119.5 107.8 119.4 120.4 119.4 120.4	$\begin{array}{c} \text{atom} \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{H}(32) \\ \text{H}(21) \\ \text{H}(21) \\ \text{N}(1) \\ \text{H}(2) \\ \text{H}(32) \\ \text{H}(2) \\ \text{H}(3) \\ \text{N}(2) \\ \text{H}(3) \\ \text{H}(4) \\ \text{H}(1) \\ \text{H}(2) \\ \text{C}(4) \\ \text{H}(1) \\ \text{H}(2) \\ \text{C}(4) \\ \text{H}(1) \\ \text{H}(2) \\ \text{C}(7) \\ \text{C}(4) \\ \text{H}(1) \\ \text{H}(2) \\ \text{C}(7) \\ \text{C}(4) \\ \text{H}(1) \\ \text{H}(2) \\ \text{C}(10) \\ \text{C}(11) \\ \text{C}(12) \\ \text{C}(13) \\ \text{H}(12) \\ \text{H}(13) \\ \text{C}(18) \\ \text{H}(20) \\ \text{H}(19) \end{array}$	$\begin{array}{c} \text{atom} \\ \text{O}(7) \\ \text{O}(8) \\ \text{N}(2) \\ \text{O}(8) \\ \text{N}(1) \\ \text{C}(24) \\ \text{C}(3) \\ \text{N}(2) \\ \text{C}(10) \\ \text{C}(3) \\ \text{C}(5) \\ \text{C}(5) \\ \text{C}(5) \\ \text{C}(5) \\ \text{C}(5) \\ \text{C}(6) \\ \text{C}(8) \\ \text{C}(9) \\ \text{C}(10) \\ \text{C}(17) \\ \text{C}(16) \\ \text{C}(13) \\ \text{C}(14) \\ \text{C}(14) \\ \text{C}(14) \\ \text{C}(15) \\ \text{C}(19) \\ \text{C}(20) \end{array}$	atom H(30) H(32) H(8) H(31) C(17) H(22) H(6) C(3) H(9) C(4) H(1) C(6) C(7) H(4) H(1) C(6) C(7) H(4) H(15) H(14) H(15) H(14) H(11) H(12) C(15) C(16) H(20) C(20) C(20) C(21)	angle 119.7(2) angle 124(1) 115(1) 107(1) 105(2) 110(1) 107.8 107.9 102(1) 107.3 108.5 119.5 119.7 120.1 119.7 108.2 107.5 119.8 120.5 120.1 119.3 120.2 119.9
$\begin{array}{c} C(26) \\ C(28) \\ \hline \\ Table 7. Bond \\ atom \\ Ni(1) \\ Ni(1) \\ Ni(1) \\ H(30) \\ N(1) \\ H(21) \\ N(1) \\ H(21) \\ N(1) \\ H(21) \\ N(1) \\ H(21) \\ N(2) \\ H(8) \\ H(6) \\ H(7) \\ C(4) \\ C(5) \\ C(6) \\ H(3) \\ H(4) \\ H(9) \\ C(11) \\ H(10) \\ H(11) \\ C(11) \\ H(10) \\ H(11) \\ C(14) \\ C(15) \\ H(15) \\ C(18) \\ C(19) \\ C(20) \end{array}$	$\begin{array}{c} C(27) \\ C(29) \\ \hline \\ \hline \\ angles involvin \\ atom \\ O(7) \\ O(8) \\ N(1) \\ O(7) \\ C(17) \\ N(1) \\ C(24) \\ C(3) \\ N(2) \\ C(3) \\ C(1) \\ C(12) \\ C(12) \\ C(12) \\ C(12) \\ C(12) \\ C(12) \\ C(13) \\ C(15) \\ C(16) \\ C(17) \\ C(23) \\ C(20) \\ C(21) \\ \end{array}$	$\begin{array}{c} C(28) \\ C(30) \\ \hline \\ atom \\ H(29) \\ H(31) \\ H(21) \\ H(21) \\ H(29) \\ H(15) \\ C(24) \\ H(23) \\ H(7) \\ C(10) \\ C(24) \\ H(6) \\ H(5) \\ H(2) \\ H(3) \\ C(4) \\ H(6) \\ H(5) \\ H(2) \\ H(3) \\ C(8) \\ C(9) \\ C(17) \\ H(10) \\ C(13) \\ C(14) \\ H(13) \\ H(14) \\ C(18) \\ H(16) \\ H(19) \\ H(18) \\ \end{array}$	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 109(2) 107.4 109(1) 107.9 109.4 119.8 120.2 119.8 120.2 119.8 120.4 119.7 107.0 119.5 120.0 119.5 120.0 119.5 107.8 119.4 120.4 120.1 120.2 120.1 120.2 120.1 120.2 120.1 120.2 120.2 120.1 120.2 120.	$\begin{array}{c} \text{atom} \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{Ni}(1) \\ \text{H}(32) \\ \text{H}(21) \\ \text{H}(21) \\ \text{N}(2) \\ \text{H}(21) \\ \text{N}(2) \\ \text{H}(32) \\ \text{H}(2) \\ \text{H}(3) \\ \text{N}(2) \\ \text{H}(7) \\ \text{C}(4) \\ \text{H}(1) \\ \text{H}(2) \\ \text{C}(7) \\ \text{C}(4) \\ \text{H}(1) \\ \text{H}(2) \\ \text{C}(7) \\ \text{C}(8) \\ \text{H}(9) \\ \text{C}(10) \\ \text{C}(11) \\ \text{C}(12) \\ \text{C}(13) \\ \text{H}(12) \\ \text{H}(12) \\ \text{H}(13) \\ \text{C}(18) \\ \text{H}(20) \\ \text{H}(19) \\ \text{C}(21) \end{array}$	atom O(7) O(8) N(2) O(8) N(1) C(24) C(3) C(10) C(3) C(5) C(5) C(6) C(3) C(5) C(6) C(10) C(17) C(16) C(13) C(14) C(14) C(15) C(19) C(22) C(22)	atom H(30) H(32) H(8) H(31) C(17) H(22) H(6) C(3) H(9) C(4) H(1) C(6) C(7) H(4) H(1) C(6) C(7) H(4) H(15) H(14) H(15) H(14) H(11) H(12) C(15) C(16) H(20) C(20) C(21) H(17)	angle 119.7(2) angle 124(1) 115(1) 107(1) 105(2) 110(1) 107.8 107.9 102(1) 107.3 108.5 119.5 119.7 120.1 119.7 120.1 119.8 120.5 120.1 119.3 120.2 119.3 120.2 119.9 120.1
C(26) C(28) Table 7. Bond atom Ni(1) Ni(1) Ni(1) H(30) N(1) H(21) N(1) N(2) H(8) H(6) H(7) C(4) C(5) C(6) H(3) H(4) H(9) C(11) H(10) H(11) C(14) C(15) H(15) C(18) C(19) C(20) H(18)	C(27) C(29) 1 angles involvin atom O(7) O(8) N(1) O(7) C(17) C(17) N(1) C(24) C(3) N(2) C(3) C(2) C(12) C(12) C(12) C(12) C(12) C(12) C(12) C(13) C(12) C(12) C(12) C(13) C(12) C(12) C(13) C(12) C(12) C(13) C(12) C(13) C(12) C(12) C(13) C(12) C(13) C(21)	$\begin{array}{c} C(28) \\ C(28) \\ C(30) \\ \end{array}$ ng hydrogens ( $^{0}$ ) atom H(29) H(31) H(21) H(21) H(29) H(15) C(24) H(23) H(7) C(10) C(4) H(6) H(2) H(3) C(8) C(9) C(17) H(10) C(13) C(14) H(13) H(14) C(18) H(16) H(19) H(18) C(22) H(18) H(18) C(22) H(	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 107(1) 107.4 108.2 109(1) 107.9 109.4 119.8 120.2 119.8 120.2 119.8 120.4 119.7 107.0 119.5 120.0 119.9 120.3 119.5 107.8 119.4 120.4 120.1 119.7	atom Ni(1) Ni(1) Ni(1) H(32) H(21) N(1) N(2) H(32) H(21) N(2) H(7) C(4) H(7) C(4) H(7) C(4) H(7) C(4) H(7) C(4) H(1) H(2) C(7) C(8) H(9) C(10) C(11) C(12) C(13) H(12) H(13) C(18) H(20) H(19) C(21) C(22) C(22)	atom O(7) O(8) N(2) O(8) N(1) C(24) C(3) N(2) C(10) C(3) C(5) C(5) C(6) C(7) C(10) C(17) C(16) C(17) C(16) C(13) C(14) C(14) C(14) C(19) C(19) C(19) C(22) C(23)	atom H(30) H(32) H(8) H(31) C(17) H(22) H(6) C(3) H(9) C(4) H(1) C(6) C(7) H(4) H(1) C(6) C(7) H(4) H(15) H(14) H(15) H(14) H(11) H(12) C(15) C(16) H(20) C(20) C(21) H(17) H(16)	angle 119.7(2) angle 124(1) 115(1) 107(1) 105(2) 110(1) 107.8 102(1) 107.3 108.5 119.5 119.7 120.1 119.7 119.9 108.2 107.5 119.8 120.2 119.3 120.2 119.9 120.1 119.9 120.1 119.9
C(26) C(28) Table 7. Bonc atom Ni(1) Ni(1) Ni(1) H(30) N(1) H(21) N(1) N(2) H(8) H(6) H(7) C(4) C(5) C(6) H(3) H(4) H(9) C(11) H(10) H(11) C(14) C(15) H(15) C(18) C(19) C(20) H(18) H(17) H(18) H(17) H(18) H(17) H(18) H(17) H(18) H(18) H(17) H(18) H(18) H(18) H(18) H(18) H(18) H(18) H(18) H(18) H(18) H(18) H(18) H(18) H(17) H(18) H(17) H(18) H(17) H(18) H(18) H(17) H(18) H(17) H(18) H(17) H(18) H(17) H(18) H(17) H(18) H(17) H(18) H(17) H(18) H(17) H(18) H(17) H(18) H(18) H(17) H(18) H(18) H(18) H(18) H(18) H(18) H(18) H(18) H(18) H(19) H(18) H(19) H(18) H(19) H(19) H(19) H(18) H(19) H(	C(27) C(29) I angles involvir atom O(7) O(8) N(1) O(7) C(17) N(1) C(24) C(3) N(2) C(3) C(2) C(12) C(12) C(12) C(12) C(12) C(12) C(13) C(15) C(16) C(17) C(23) C(20) C(21) C(21) C(21) C(21) C(22) C(21) C(22) C(21) C(22) C(21) C(22) C(21) C(22) C(21) C(22) C(21) C(22) C(21) C(22) C(21) C(22) C(22) C(21) C(22)	$\begin{array}{c} C(28) \\ C(28) \\ C(30) \\ \hline \\ \  \  \  \  \  \  \  \  \  \  \  \  \$	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 107(1) 107.4 109(1) 107.9 109.4 119.8 120.2 119.8 120.4 119.7 107.0 119.5 120.0 119.5 107.8 119.4 120.4 120.3 119.5 107.8 119.4 120.4 120.1 119.7 120.0 119.5 107.8 119.4 120.0 119.4 120.0 119.5 107.8 119.4 120.0 119.4 120.0 119.4 120.0 119.5 107.8 119.4 120.4 120.1 119.7 120.0 119.5 120.0 120.	atom Ni(1) Ni(1) Ni(1) H(32) H(21) N(1) H(2) H(7) C(4) H(7) C(4) H(7) C(4) H(7) C(4) H(1) H(2) C(7) C(7) C(7) C(7) C(8) H(9) C(10) C(11) C(12) C(13) H(12) H(13) C(18) H(20) H(19) C(21) C(22) H(22)	atom O(7) O(8) N(2) O(8) N(1) C(24) C(3) C(10) C(3) C(5) C(5) C(5) C(5) C(5) C(6) C(8) C(9) C(10) C(17) C(16) C(17) C(16) C(13) C(14) C(14) C(15) C(19) C(20) C(22) C(24) C(24) C(24) C(23) C(24) C(23) C(24) C(23) C(24) C(23) C(24) C(23) C(24) C(23) C(24) C(23) C(23) C(23) C(24) C(23) C(24) C(23) C(24) C(23) C(24) C(25) C(25) C(10) C(17) C(16) C(19) C(19) C(20) C(22) C(23) C(24) C(24) C(24) C(24) C(25) C(25) C(25) C(25) C(25) C(24) C(25) C	atom H(30) H(32) H(8) H(31) C(17) H(22) H(6) C(3) H(9) C(4) H(1) C(6) C(7) H(4) H(1) C(6) C(7) H(4) H(5) C(11) H(15) H(14) H(15) H(14) H(11) C(15) C(16) H(20) C(20) C(21) H(17) H(16) C(25)	angle 119.7(2) angle 124(1) 115(1) 107(1) 105(2) 110(1) 107.8 102(1) 107.3 108.5 119.5 119.7 120.1 119.7 119.9 108.2 107.5 119.8 120.5 120.1 119.3 120.2 119.3 120.2 119.9 120.2 119.9 120.1 119.9 107.8
C(26) C(28) Table 7. Bonc atom Ni(1) Ni(1) Ni(1) H(30) N(1) H(21) N(1) H(21) N(1) N(2) H(8) H(6) H(7) C(4) C(4) C(5) C(6) H(3) H(4) H(9) C(11) H(10) H(10) H(11) C(14) C(15) H(15) C(18) C(19) C(20) H(18) H(17) H(23) H(17) H(23) H(17) H(17) H(18) H(17) H(18) H(17) H(18) H(17	C(27) C(29) A angles involvir atom O(7) O(8) N(1) O(7) C(17) N(1) C(24) C(24) C(3) N(2) C(3) C(3) C(3) C(3) C(3) C(3) C(7) C(7) C(7) C(7) C(7) C(7) C(12) C(12) C(12) C(12) C(12) C(13) C(15) C(16) C(17) C(23) C(20) C(21) C(21) C(22) C(22) C(24) C(21) C(23) C(20) C(21) C(21) C(22) C(23) C(23) C(23) C(24) C(25) C(24) C(25	$\begin{array}{c} C(28) \\ C(28) \\ C(30) \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ $	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 107(1) 107.4 109(1) 107.9 109.4 119.8 120.2 119.8 120.2 119.8 120.4 119.7 107.0 119.5 120.0 119.5 107.8 119.4 120.4 120.1 119.7 120.0 119.5 107.8 119.4 120.4 120.1 119.7 120.0 119.7 120.0 119.5 107.8 119.4 120.4 120.3 119.5 107.8 119.4 120.4 120.3 119.5 107.8 119.4 120.4 120.4 120.5 107.8 119.4 120.4 120.4 120.5 107.8 119.4 120.4 120.4 120.5 107.8 119.7 120.0 119.5 107.8 119.4 120.4 120.4 120.5 107.8 119.4 120.4 120.4 120.5 107.8 119.4 120.4 120.4 120.5 107.8 119.5 107.8 119.7 107.8 119.7 107.8 119.7 107.8 119.4 120.4 120.4 120.5 107.8 119.7 120.0 119.5 107.8 119.4 120.4 120.4 120.5 107.8 119.5 107.8 119.7 107.8 119.7 107.8 119.7 107.8 119.4 120.4 120.4 120.4 120.5 107.8 119.5 107.8 119.7 107.8 119.7 107.8 119.7 107.8 119.7 107.8 119.7 107.8 119.7 107.0 119.5 107.8 119.7 107.0 119.5 107.8 119.7 107.0 119.5 107.8 119.7 107.0 119.7 107.8 119.7 107.0 119.7 107.8 119.7 107.0 119.7 107.8 119.7 120.0 120.	atom Ni(1) Ni(1) Ni(1) H(32) H(21) N(1) N(2) H(7) C(4) H(7) C(4) H(7) C(4) H(7) C(4) H(1) H(2) C(7) C(8) H(9) C(10) C(11) C(12) C(13) H(12) H(12) H(13) C(18) H(20) H(19) C(21) C(22) H(23)	atom O(7) O(8) N(2) O(8) N(1) C(24) C(3) C(10) C(3) C(5) C(5) C(5) C(5) C(6) C(7) C(10) C(17) C(16) C(17) C(16) C(13) C(14) C(14) C(14) C(15) C(19) C(20) C(22) C(23) C(24) C(24) C(24) C(24) C(24) C(24) C(24) C(24) C(24) C(24) C(24) C(24) C(24) C(24) C(24) C(24) C(24) C(24) C(24) C(25) C(25) C(26) C(27) C(20) C(22) C(22) C(24) C(24) C(24) C(24) C(24) C(24) C(24) C(25) C(26) C(27)	atom H(30) H(32) H(8) H(31) C(17) H(22) H(6) C(17) H(22) H(6) C(23) H(9) C(4) H(1) C(6) C(7) H(4) H(1) C(6) C(7) H(4) H(5) C(11) H(15) H(14) H(11) H(15) H(14) H(11) H(12) C(15) C(16) H(20) C(21) H(17) H(16) C(25) H(22)	angle 124(1) 119.7(2) 119.7(2) 119.7(2) 119.7(2) 107(1) 105(2) 110(1) 107.8 107.9 102(1) 107.3 108.5 119.7 120.1 119.7 120.1 119.7 120.1 119.9 108.2 107.5 119.8 120.2 119.3 120.2 119.3 120.2 119.9 120.1 119.5 120.1 119.5 120.2 119.5 120.2 119.3 120.2 119.9 120.2 119.3 120.2 119.9 120.2 119.9 120.2 119.3 120.2 119.9 120.2 119.9 120.2 119.3 120.2 119.9 120.1 119.9 120.2 119.3 120.2 119.9 120.1 119.9 120.2 119.3 120.2 119.9 120.1 119.9 120.2 119.3 120.2 119.9 120.1 119.9 120.2 119.9 120.2 119.9 120.2 119.9 120.2 119.9 120.2 119.9 120.2 119.9 120.2
$\begin{array}{c} C(26) \\ C(28) \\ \hline \\ Table 7. Bonc \\ atom \\ Ni(1) \\ Ni(1) \\ Ni(1) \\ H(30) \\ N(1) \\ H(21) \\ N(1) \\ H(21) \\ N(1) \\ N(2) \\ H(8) \\ H(6) \\ H(7) \\ C(2) \\ H(8) \\ H(6) \\ H(7) \\ C(4) \\ C(5) \\ C(6) \\ H(3) \\ H(4) \\ H(9) \\ C(11) \\ H(10) \\ H(11) \\ C(14) \\ C(15) \\ H(15) \\ C(18) \\ C(19) \\ C(20) \\ H(18) \\ H(17) \\ H(23) \\ C(25) \\ \end{array}$	C(27) C(29) A angles involvir atom O(7) O(8) N(1) O(7) C(17) N(1) C(24) C(3) N(2) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(2) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(3) C(12) C(12) C(12) C(12) C(12) C(12) C(12) C(12) C(12) C(12) C(13) C(15) C(16) C(17) C(23) C(20) C(21) C(21) C(22) C(22) C(24)	$\begin{array}{c} C(28) \\ C(28) \\ C(30) \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ $	angle 120.0(2) 120.1(2) angle 120(1) 112(1) 102(1) 109(2) 107.4 109(2) 107.4 109(1) 107.9 109.4 119.8 120.2 119.8 120.2 119.8 120.2 119.8 120.4 119.7 107.0 119.5 120.0 119.4 120.4 120.1 119.7 120.0 108.0 109.1 109.1 109.1 109.2 109.2 109.2 109.4 119.5 120.0 119.4 120.4 120.1 119.7 120.0 108.0 109.1 109.2 109.2 109.4 119.5 120.0 119.4 120.4 120.1 119.7 120.0 108.0 109.1 109.1 109.2 109.2 109.4 119.5 120.0 119.4 120.2 119.7 120.0 109.4 119.7 120.0 109.4 119.7 120.0 109.4 119.7 120.0 109.4 119.7 120.0 109.4 119.7 120.0 119.7 120.0 109.4 119.7 120.0 119.7 120.0 119.7 120.0 119.7 120.0 120.0 120.0 120.0 120.1 120.1 120.2 120.4 120.4 120.4 120.0 120.	atom Ni(1) Ni(1) Ni(1) Ni(1) H(32) H(21) H(21) N(1) H(2) H(3) H(2) H(3) H(2) H(3) H(2) H(3) H(7) C(4) H(7) C(4) H(7) C(4) H(7) C(4) H(7) C(4) H(7) C(4) H(7) C(4) H(7) C(4) H(7) C(4) H(7) C(4) H(2) C(7) C(8) H(9) C(10) C(11) C(12) C(13) H(12) H(13) C(18) H(20) H(19) C(21) C(22) H(22) H(22) H(23) C	atom O(7) O(8) N(2) O(8) N(1) C(24) C(3) C(5) C(5) C(5) C(5) C(5) C(6) C(7) C(10) C(17) C(16) C(17) C(16) C(17) C(16) C(17) C(16) C(17) C(16) C(17) C(16) C(17) C(16) C(17) C(16) C(17) C(16) C(17) C(16) C(17) C(16) C(17) C(16) C(17) C(16) C(17) C(16) C(17) C(16) C(17) C(16) C(19) C(20) C(22) C(23) C(24) C(24) C(24) C(23) C(24) C(25) C(20) C(20) C(22) C(23) C(24) C(24) C(24) C(24) C(24) C(25) C(25) C(27)	atom H(30) H(32) H(8) H(31) C(17) H(22) H(6) C(3) H(9) C(4) H(1) C(6) C(7) H(4) H(1) C(6) C(7) H(4) H(5) C(11) H(15) H(14) H(15) H(14) H(11) H(15) C(16) H(12) C(16) H(20) C(21) H(17) H(16) C(25) H(22) H(22) H(22)	angle 124(1) 119.7(2) 119.7(2) 119.7(2) 119.7(2) 107(1) 105(2) 110(1) 107.8 107.9 102(1) 107.3 108.5 119.5 119.7 120.1 119.7 120.1 119.8 120.5 120.1 119.3 120.2 119.3 120.2 119.9 120.1 119.9 120.1 119.9 120.1 119.9 120.1 119.9

H(24) H(25) C(28)	C(26) C(27) C(29)	C(27) C(28) H(27)		120.0 119.8 119.8	C(26) C(27) H(26)	C(27) C(28) C(28)	H(2) H(2) C(2)	5) 6) 9)	120.2 120.3 120.0
C(29)	C(30)	H(28)		119.6	H(27)	C(29)	C(3)	0)	120.1
atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
O(7)	Ni(1)	O(1)	S(1)	-122.73(8)	O(8)	Ni(1)	O(1)	S(1)	-33.59(8)
N(1)	Ni(1)	O(1)	<b>S</b> (1)	144.77(8)	N(2)	Ni(1)	O(1)	S(1)	59.75(8)
O(7)	Ni(1)	O(4)	S(2)	-50.6(1)	O(8)	Ni(1)	O(4)	S(2)	-139.6(1)
N(1)	Ni(1)	O(4)	S(2)	42.1(1)	N(2)	Ni(1)	O(4)	S(2)	126.9(1)
O(1) O(4)	Ni(1) Ni(1)	N(1) N(1)	C(17)	-78.55(9) 101.33(9)	O(1)	Ni(1) Ni(1)	N(1) N(1)	C(24) C(24)	48.70(9)
O(7)	Ni(1)	N(1)	C(17)	-166.07(8)	O(7)	Ni(1)	N(1)	C(24) C(24)	-38.8(1)
N(2)	Ni(1)	N(1)	C(17)	15.01(8)	N(2)	Ni(1)	N(1)	C(24)	142.2(1)
O(1)	Ni(1)	N(2)	C(3)	-130.8(1)	O(1)	Ni(1)	N(2)	C(10)	102.11(9)
O(4)	Ni(1)	N(2)	C(3)	45.6(1)	O(4)	Ni(1)	N(2)	C(10)	-81.42(9)
O(8) N(1)	Ni(1)	N(2)	C(3)	-39.9(1)	O(8)	Ni(1)	N(2)	C(10)	-166.9'/(8)
O(2)	S(1)	O(1)	$N_{i}(1)$	80 90(8)	O(3)	S(1)	O(1)	$N_i(1)$	-55 81(9)
C(1)	S(1)	O(1)	Ni(1)	-167.11(6)	O(1)	S(1) = S(1)	C(1)	F(1)	-174.3(1)
O(1)	S(1)	C(1)	F(2)	-54.4(1)	O(1)	S(1)	C(1)	F(3)	66.6(1)
O(2)	S(1)	C(1)	F(1)	-55.8(1)	O(2)	S(1)	C(1)	F(2)	64.0(1)
O(2)	S(1)	C(1)	F(3)	-175.0(1)	O(3)	S(1)	C(1)	F(1)	67.0(1)
O(3)	S(1) = S(2)	C(1)	F(2)	-173.2(1)	O(3)	S(1)	C(1)	F(3)	-52.2(1)
C(2)	S(2) = S(2)	O(4)	Ni(1) Ni(1)	-20.3(1) -138 12(9)	O(0)	S(2) = S(2)	C(2)	F(4)	-54 9(1)
O(4)	S(2) = S(2)	C(2)	F(5)	-175.5(1)	O(4)	S(2) = S(2)	C(2)	F(6)	64.3(1)
O(5)	S(2)	C(2)	F(4)	-173.1(1)	O(5)	S(2)	C(2)	F(5)	66.3(1)
O(5)	S(2)	C(2)	F(6)	-53.9(1)	O(6)	S(2)	C(2)	F(4)	64.8(1)
O(6)	S(2)	C(2)	F(5)	-55.7(1)	O(6)	S(2)	C(2)	F(6)	-175.9(1)
$N_1(1)$	N(1)	C(17)	C(10)	-40.1(1)	$N_1(1)$	N(1)	C(17)	C(18)	-164.9(1)
C(24) Ni(1)	N(1) N(1)	C(17) C(24)	C(10) C(25)	-108.8(1) 153.9(1)	C(24) C(17)	N(1) N(1)	C(17) C(24)	C(18) C(25)	-81.8(2)
Ni(1)	N(2)	C(24) C(3)	C(23) C(4)	131.0(1)	C(10)	N(2)	C(24) C(3)	C(23) C(4)	-104.4(1)
Ni(1)	N(2)	C(10)	C(11)	-164.0(1)	Ni(1)	N(2)	C(10)	C(17)	-38.6(1)
C(3)	N(2)	C(10)	C(11)	65.8(2)	C(3)	N(2)	C(10)	C(17)	-168.8(1)
N(2)	C(3)	C(4)	C(5)	-76.3(2)	N(2)	C(3)	C(4)	C(9)	105.4(2)
C(3)	C(4)	C(5)	C(6)	-177.2(1)	C(9)	C(4)	C(5)	C(6)	1.1(2)
C(3)	C(4) C(5)	C(9)	C(8)	1/6.3(1)	C(5)	C(4)	C(9)	C(8)	-2.1(2)
C(4) C(6)	C(3) C(7)	C(0) C(8)	C(9)	-0.4(2)	C(3)	C(0) C(8)	C(7)	C(3) C(4)	1.7(2)
N(2)	C(10)	C(11)	C(12)	63.9(2)	N(2)	C(10)	C(11)	C(16)	-113.7(2)
C(17)	C(10)	C(11)	C(12)	-59.6(2)	C(17)	C(10)	C(11)	C(16)	122.7(2)
N(2)	C(10)	C(17)	N(1)	53.7(2)	N(2)	C(10)	C(17)	C(18)	179.7(1)
C(11)	C(10)	C(17)	N(1)	179.4(1)	C(11)	C(10)	C(17)	C(18)	-54.6(2)
C(10)	C(11)	C(12)	C(13)	-178.2(2)	C(16)	C(11)	C(12)	C(13)	-0.6(2)
C(10) C(11)	C(11) C(12)	C(10) C(13)	C(15) C(14)	1//.1(2) 1.7(3)	C(12)	C(11) C(13)	C(16) C(14)	C(15) C(15)	-0.5(2) 1 7(3)
C(11) C(13)	C(12) C(14)	C(15)	C(14) C(16)	0.6(3)	C(12) C(14)	C(15)	C(14) C(16)	C(13) C(11)	0.6(3)
N(1)	C(17)	C(18)	C(19)	55.4(2)	N(1)	C(17)	C(18)	C(23)	-123.8(2)
C(10)	C(17)	C(18)	C(19)	-68.0(2)	C(10)	C(17)	C(18)	C(23)	112.8(2)
C(17)	C(18)	C(19)	C(20)	-177.0(1)	C(23)	C(18)	C(19)	C(20)	2.2(2)
C(17)	C(18)	C(23)	C(22)	177.6(2)	C(19)	C(18)	C(23)	C(22)	-1.6(2)
C(18)	C(19)	C(20)	C(21)	-1.1(2) 1 4(2)	C(19)	C(20)	C(21)	C(22)	-0.7(3)
N(1)	C(21) C(24)	C(22) C(25)	C(25)	1.4(3) -54 9(2)	N(1)	C(22) C(24)	C(25)	C(18) C(30)	-0.2(3) 128 1(2)
C(24)	C(24) C(25)	C(26)	C(20) C(27)	-178.0(1)	C(30)	C(24) C(25)	C(26)	C(27)	-1.0(2)
C(24)	C(25)	C(30)	C(29)	176.9(2)	C(26)	C(25)	C(30)	C(29)	-0.3(3)
C(25)	C(26)	C(27)	C(28)	1.4(3)	C(26)	C(27)	C(28)	C(29)	-0.5(3)
C(27)	C(28)	C(29)	C(30)	-0.7(3)	C(28)	C(29)	C(30)	C(25)	1.1(3)
The sign is	positive if w	hen looking	from atom 2	to atom 3 a clock-wise	motion of ator	n 1 would su	perimpose it	on atom 4.	
Table 9. Di	istances beyc	nd the asym	metric unit c	out to 3.60 Å	- 4		- 4		1:
atom Ni(1)	s(1)		3 1755(A)		atom Ni(1)		S(2)		3 3343(4)
Ni(1)	O(3)		3,560(1)		Ni(1)		C(3)		3.080(2)
Ni(1)	C(10)		2.899(1)		Ni(1)		C(17)		2.889(2)
Ni(1)	C(24)		3.037(2)		S(1)		F(1)		2.606(1)
S(1)	F(2)		2.634(1)		S(1)		F(3)		2.611(1)
S(1)	O(8)		3.224(1)		S(1)		N(2)		3.554(1)

S(2)	F(4)	2 614(1)	S(2)	F(5)	2 609(1)
S(2)	$\Gamma(4)$	2.616(1)	S(2)	$O(7)^{1}$	2.000(1)
5(2)	F(0)	2.010(1)	5(2)	$O(7)^{2}$	3.303(1)
F(1)	F(2)	2.154(1)	F(1)	F(3)	2.156(2)
F(1)	O(2)	2.920(2)	F(1)	O(3)	3.004(1)
F(1)	$O(5)^{2}$	3.363(1)	F(1)	$O(7)^{3)}$	3.559(2)
F(1)	$C(19)^{2}$	3 426(2)	F(1)	$C(20)^{2}$	3 463(2)
$\Gamma(1)$	E(1)	2.154(1)	F(1)	O(1)	2.916(1)
F(2)	F(5)	2.134(1)	F(2)	O(1)	2.910(1)
F(2)	0(2)	3.028(1)	F(2)	O(7) <sup>3</sup>	3.355(2)
F(2)	$C(21)^{4}$	3.496(2)	F(2)	$C(22)^{4}$	3.427(2)
F(2)	$C(24)^{3}$	3.351(2)	F(2)	$C(25)^{3}$	3.264(2)
F(2)	$C(26)^{3)}$	3 060(2)	F(3)	O(1)	3,000(1)
$\Gamma(2)$	0(2)	3.000(2)	F(2)	$C(21)^{4}$	3.000(1)
F(3)	0(3)	2.883(1)	F(3)	C(21) <sup>4</sup>	3.430(2)
F(3)	C(22)*	3.286(2)	F(3)	C(29)*	3.430(2)
F(4)	F(5)	2.154(1)	F(4)	F(6)	2.155(2)
F(4)	O(4)	2.891(1)	F(4)	Q	2.995(2)
F(5)	5(1) F(6)	2.051(1) 2.156(2)	F(5)	$O(2)^{(5)}$	3.030(2)
$\Gamma(5)$	1(0)	2.130(2)	F(5)	0(2)	3.030(2)
F(5)	0(5)	3.023(1)	F(5)	O(6)	2.913(1)
F(6)	O(4)	2.977(2)	F(6)	O(5)	2.914(2)
F(6)	C(10)	3,550(2)	O(1)	O(2)	2.423(2)
oùí	ດໄພ	2 429(2)	O(1)	O(7)	2 873(2)
O(1)	O(8)	2.022(1)	O(1)	N(1)	2.073(2)
0(1)	0(8)	2.962(1)	0(1)	N(I)	2.955(2)
O(1)	N(2)	3.050(2)	0(1)	C(1)	2.581(2)
O(1)	C(17)	3.380(2)	O(1)	C(24)	3.118(2)
O(2)	$F(5)^{2}$	3.030(2)	O(2)	O(3)	2.443(2)
0(2)	$O(6)^{3)}$	3 226(2)	O(2)	$O(7)^{3)}$	2.741(2)
O(2)	O(0)	3.120(2)	O(2)	O(1)	2.741(2)
O(2)	0(8)	3.120(2)	0(2)	C(1)	2.595(2)
O(3)	O(8)	3.516(2)	O(3)	N(2)	3.063(2)
O(3)	C(1)	2.580(2)	O(3)	C(5)	3.111(2)
0(3)	$C(15)^{6}$	3.379(2)	O(4)	O(5)	2.424(1)
O(4)	0(6)	2 432(1)	O(4)	O(7)	2.995(2)
O(4)	O(0)	2.752(1)		$\mathbf{N}(1)$	2.993(2)
0(4)	0(8)	2.850(2)	0(4)	N(1)	3.069(2)
O(4)	N(2)	2.875(2)	O(4)	C(2)	2.571(2)
O(4)	C(3)	3.055(2)	O(4)	C(10)	3.366(2)
O(5)	$F(1)^{5}$	3 363(1)	0(5)	0(6)	2.441(2)
O(5)	$O(7)^{1)}$	2 798(2)	O(5)	N(1)	3 163(2)
O(5)	O(7)	2.502(2)	0(5)		3.103(2)
0(5)	C(2)	2.595(2)	0(5)	C(26)	3.482(2)
O(6)	$O(2)^{1}$	3.226(2)	O(6)	$O(7)^{1}$	3.434(2)
O(6)	$O(8)^{1}$	2.818(2)	O(6)	C(2)	2.575(2)
O(7)	$S(2)^{3}$	3.563(1)	O(7)	$F(1)^{(1)}$	3.559(2)
O(7)	$E(2)^{1}$	3 355(2)	O(7)	$O(2)^{(1)}$	2.741(2)
O(7)	$\Gamma(2)$	3.555(2)	0(7)	O(2)	2.741(2)
O(7)	0(5)*	2.798(2)	O(7)	0(6)	3.434(2)
O(7)	O(8)	2.898(2)	O(7)	N(1)	2.975(2)
O(7)	C(24)	3.096(2)	O(8)	$O(6)^{3)}$	2.818(2)
O(8)	N(2)	3 030(2)	O(8)	C(3)	3 200(2)
N(1)	N(2)	2811(2)	N(1)	C(10)	2.200(2)
N(1)	$\Gamma(2)$	2.511(2)	N(1)	C(10)	2.400(2)
N(1)	C(18)	2.510(2)	N(1)	C(19)	3.069(2)
N(1)	C(25)	2.557(2)	N(1)	C(26)	3.127(2)
N(2)	C(4)	2.538(2)	N(2)	C(5)	3.249(2)
N(2)	C(9)	3.508(2)	N(2)	C(11)	2.507(2)
N(2)	$\dot{C(12)}$	3 126(2)	N(2)	CÌLŃ	3 533(2)
N(2)	C(17)	$2 \sqrt{72}(2)$	C(3)	C(5)	2.555(2)
N(2)	C(17)	2.472(2)	C(3)		2.311(2)
C(3)	C(9)	2.527(2)	C(3)	C(10)	2.488(2)
C(3)	C(11)	3.050(2)	C(4)	C(6)	2.420(2)
C(4)	C(7)	2.794(2)	C(4)	C(8)	2.413(2)
$\vec{C}(4)$	C(10)	3 469(2)	C(4)	C(11)	3 449(2)
C(4)	C(7)	2.40(2)	$C(\tau)$	C(11)	2.77(2)
C(5)	C(7)	2.406(3)	C(5)	C(8)	2.763(2)
C(5)	C(9)	2.393(2)	C(6)	C(8)	2.392(3)
C(6)	C(9)	2.775(2)	C(7)	C(9)	2.407(3)
C(9)	C(11)	3.440(2)	C(9)	C(16)	3.494(2)
cũm	cùź	2 528(2)	cùm	CUD	2 517(2)
C(10)	C(12)	2.526(2)	C(10)	C(10)	2.517(2) 2.165(2)
C(10)	C(18)	2.320(2)	C(10)	C(19)	5.105(2)
C(10)	C(23)	3.542(2)	C(11)	C(13)	2.418(3)
C(11)	C(14)	2.783(3)	C(11)	C(15)	2.418(2)
C(11)	C(17)	2.534(2)	C(11)	C(18)	2.962(2)
càń	C(23)	3 525(2)	cùź	C(14)	2400(3)
C(12)	C(15)	2.323(2)	C(12)	C(14)	2.700(3)
C(12)	C(15)	2.111(5)	C(12)	C(10)	2.401(2)
C(12)	C(17)	5.104(2)	C(12)	C(18)	3.548(2)
C(13)	C(15)	2.404(3)	C(13)	C(16)	2.775(3)
C(14)	C(16)	2.397(3)	C(15)	$O(3)^{7}$	3.379(2)
cùń	C(19)	2 532(2)	CUT	C(23)	2 519(2)
-(17)	~(1))	(-)	~(1))	-()	2.217(2)

C(17) C(18) C(18) C(19) C(19) C(20) C(20) C(21) C(22) C(22) C(22) C(24) C(24) C(25) C(25) C(26) C(26) C(27) C(28)	$\begin{array}{c} C(24) \\ C(20) \\ C(22) \\ C(25) \\ F(1)^{5)} \\ C(22) \\ C(25) \\ F(1)^{5)} \\ C(23) \\ F(3)^{4)} \\ F(2)^{4)} \\ C(28)^{8)} \\ F(2)^{1)} \\ C(30) \\ C(27) \\ C(29) \\ C(28) \\ C(30) $	2.485(2) 2.412(2) 2.414(2) 3.148(2) 3.426(2) 2.770(2) 3.379(2) 3.463(2) 2.768(2) 3.430(2) 3.430(2) 3.427(2) 3.489(3) 3.351(2) 2.525(2) 2.417(2) 2.421(2) 2.405(2) 2.390(2) 2.764(2) 2.399(3)	C(17) C(18) C(18) C(19) C(19) C(20) C(21) C(21) C(21) C(22) C(23) C(24) C(25) C(25) C(26) C(26) C(26) C(27) C(28) C(29)	$\begin{array}{c} C(25) \\ C(21) \\ C(24) \\ C(30) \\ C(21) \\ C(23) \\ C(26) \\ C(22) \\ F(2)^4 \\ C(23) \\ F(3)^4 \\ C(30) \\ C(26) \\ F(2)^{1)} \\ C(28) \\ F(2)^{1)} \\ C(28) \\ F(2)^{1)} \\ C(29) \\ C(29) \\ C(29) \\ C(29) \\ F(3)^{4)} \end{array}$	3.276(2) 2.782(2) 3.074(2) 3.591(2) 2.401(2) 2.395(2) 3.395(2) 2.399(2) 3.496(2) 2.392(2) 3.286(2) 3.286(2) 3.286(2) 3.264(2) 2.796(2) 3.060(2) 2.767(2) 2.393(2) 3.489(3) 3.430(2)
Symmetry Opera (1) X+1/2,-Y+1, (3) X+1/2-1,-Y+1, (5) X+1,Y,Z (7) X+1/2,-Y+1, (9) -X+1/2,Y+1, (9) -X+1/2,D, D,	ators: /2,Z +1/2,Z /2-1,Z /2,-Z+1	(2) X-1,Y,Z (4) -X,-Y,-Z+1 (6) X+1/2-1,-Y+1/2-1,Z (8) -X+1/2,Y+1/2-1	I,-Z+1		
atom	atom	distance	atom	atom	distance
Ni(1)	H(6)	2 9232	Ni(1)	H(7)	3 5863
Ni(1)	H(8)	2.45(2)	Ni(1)	H(9)	3.1115
Ni(1)	H(15)	3.0949	Ni(1)	H(21)	2.45(2)
Ni(1)	H(22)	2.9433	Ni(1)	H(23)	3.3452
Ni(1)	H(29)	2.55(2)	Ni(1)	H(30)	2.56(2)
Ni(1)	H(31)	2.50(2)	Ni(1)	H(32)	2.53(2)
S(1)	H(8)	3.04(2)	S(1)	$H(30)^{1}$	3.15(2)
S(1)	H(32)	3.14(2)	S(2)	H(9)	3.5929
S(2)	H(21)	3.00(2)	$\tilde{S}(2)$	$H(29)^{2}$	2.84(2)
S(2)	H(30)	3.33(2)	S(2)	$H(32)^{2}$	3.20(2)
F(1)	$H(12)^{3}$	2 6998	F(1)	$H(19)^{4}$	2.8555
F(1)	$H(20)^{4}$	2,7809	F(1)	$H(29)^{1}$	3 29(2)
F(1)	$H(30)^{1}$	3 27(2)	F(2)	$H(17)^{5}$	2,7669
F(2)	$H(18)^{5}$	2 9033	F(2)	$H(22)^{1}$	2.6319
F(2)	$H(24)^{1}$	2.9105	F(2)	$H(25)^{4)}$	3 2047
F(2)	$H(29)^{1}$	3.52(2)	F(2)	$H(30)^{1}$	3.09(2)
F(3)	$H(12)^{3}$	3.1079	F(3)	$H(17)^{5}$	2.9013
F(3)	$H(18)^{5}$	3.1625	F(3)	$H(19)^{4}$	3.1540
F(3)	$H(27)^{5}$	2.9009	F(4)	$H(4)^{6}$	3.3984
F(4)	H(7)	3.3810	F(5)	$H(29)^{2}$	3.26(2)
F(5)	$H(30)^{2}$	3.29(2)	F(6)	$H(4)^{6}$	3.0539
F(6)	H(7)	3.1399	F(6)	H(9)	2.6150
F(6)	$H(12)^{6}$	3.5920	F(6)	H(14)	3.2784
F(6)	H(20)	3.1877	O(1)	H(8)	2.81(2)
O(1)	H(15)	2.9581	O(1)	H(22)	3.0180
O(1)	H(23)	2.8326	O(1)	$H(24)^{1}$	3.5174
O(1)	H(29)	2.85(2)	O(1)	H(32)	3.01(2)
O(2)	$H(29)^{1}$	3.01(2)	O(2)	$H(30)^{1}$	1.99(2)
O(2)	H(32)	2.72(2)	O(3)	H(1)	2.6863
O(3)	H(8)	2.34(2)	O(3)	H(10)	3.3835
O(3)	$H(12)^{3)}$	3.1960	O(3)	$H(13)^{3)}$	2.5922
O(4)	H(6)	2.6627	O(4)	H(7)	3.1040
O(4)	H(9)	2.9594	O(4)	H(21)	2.74(2)
O(4)	H(30)	2.96(2)	O(4)	H(31)	2.62(2)
O(4)	H(32)	3.46(2)	O(5)	H(20)	3.1253
O(5)	H(21)	2.29(2)	O(5)	H(24)	2.5878
O(5)	$H(29)^{2}$	1.99(2)	O(5)	H(30)	3.41(2)
O(5)	$H(30)^{2}$	3.10(2)	O(5)	$H(32)^{2}$	3.48(2)
O(6)	$H(29)^{2}$	2.92(2)	O(6)	H(30)	3.53(2)
O(6)	$H(31)^{2}$	2.99(2)	O(6)	$H(32)^{2}$	2.05(2)
O(7)	H(21)	3.13(2)	O(7)	H(22)	2.4080

O(7)	H(23)	3 5998	O(7)	H(31)	3.17(2)
O(7)	H(23)	2.84(2)	O(2)	II(31)	2.0256
O(7)	п(52)	2.84(2)	0(8)	H(1)	5.0550
O(8)	H(6)	2.5615	O(8)	H(8)	3.18(2)
O(8)	H(29)	3.02(2)	O(8)	H(30)	3.31(2)
N(1)	H(8)	3.21(2)	N(1)	H(9)	2.6232
N(1)	H(15)	1 9871	N(1)	H(20)	2 9082
N(1)	L(22)	2 0012	N(1)	H(22)	1 0064
N(1)	П(22)	2.0015	N(I)	H(23)	1.9904
N(1)	H(24)	2.9221	N(1)	H(29)	3.59(2)
N(1)	H(30)	3.33(2)	N(2)	H(1)	3.1715
N(2)	H(6)	2.0087	N(2)	H(7)	2.0125
N(2)	H(0)	1 9985	N(2)	H(10)	3 0136
N(2)	$\Pi(J)$ $\Pi(15)$	2 (41)	N(2)	11(10)	2.0100
N(2)	H(15)	2.0410	N(2)	H(21)	3.21(2)
N(2)	H(31)	3.37(2)	C(1)	$H(12)^{3}$	3.3356
C(1)	$H(17)^{5}$	3.3887	C(1)	$H(18)^{5}$	3.4572
C(1)	$H(19)^{4}$	3.5239	$\mathbf{C}(1)$	$H(30)^{1}$	3.32(2)
C(2)	H(0)	3 5266	C(3)	H(1)	2 6554
C(2)	11(5)	3.5200	C(3)		1.0((2))
C(3)	H(5)	2.6851	C(3)	H(8)	1.86(2)
C(3)	H(9)	2.5982	C(3)	H(31)	3.27(2)
C(4)	H(1)	2.0302	C(4)	H(2)	3.2751
C(4)	H(4)	3 2683	C(4)	HÓ	2.0379
C(4)	Ц(б)	2.0179	C(4)	H(3)	2.0379
C(4)	H(0)	2.0176		H(7)	2.0249
C(4)	H(8)	2.40(2)	C(5)	H(2)	2.0461
C(5)	H(3)	3.2645	C(5)	H(5)	3.2520
C(5)	H(6)	2.6340	C(5)	H(7)	3.2564
C(5)	H(8)	2.88(2)	C(5)	$H(13)^{3}$	3 /271
C(3)	$\Pi(0)$	2.00(2)		$\Pi(13)$	2.0220
C(6)	H(1)	2.0421	C(6)	H(3)	2.0330
C(6)	H(4)	3.2495	C(6)	$H(5)^{3}$	3.1604
C(6)	$H(13)^{3}$	3.4328	C(7)	H(1)	3.2625
C(7)	H(2)	2.0359	C(7)	H(4)	2.0264
C(7)	H(5)	3 2600	C(7)	$H(5)^{3}$	3 0010
C(7)	II(3) $II(14)^{3}$	2.4497	C(n)	11(3)	2.2510
C(7)	H(14)*	3.448/	C(8)	H(2)	3.2510
C(8)	$H(2)^{0}$	3.5881	C(8)	H(3)	2.0331
C(8)	H(5)	2.0391	C(8)	$H(14)^{3}$	3.4258
CÒ	HÌÌ	3 2506	CÒ	$H(2)^{6}$	3 4850
C(0)	H(1)	3 2657	C(0)	H(2) <sup>6</sup>	3 2004
C(3)	11(3)	3.2037	C(9)	11(3)	2.1700
C(9)	H(4)	2.0375	C(9)	H(6)	3.1/80
C(9)	H(7)	2.5630	C(9)	H(8)	3.38(2)
C(10)	H(6)	3.1750	C(10)	H(7)	2.4334
CÌIÓ	H(8)	1 93(2)	C(10)	H(10)	2.6786
C(10)	H(0) H(14)	26676	C(10)	H(15)	2.0700
C(10)	П(14)	2.0070	C(10)	H(13)	2.0570
C(10)	H(20)	3.0418	C(10)	H(21)	2.72(2)
C(11)	H(5)	3.0561	C(11)	H(7)	2.8651
C(11)	H(8)	2.58(2)	C(11)	H(9)	2.0206
càń	H(10)	2 0375	càń	H(11)	3 2769
C(11)	II(10) II(12)	2.0375	C(11)	$\Pi(14)$	2 0279
	П(15)	3.2/43		H(14)	2.0576
$C(\Pi)$	H(15)	2.7185	C(11)	H(16)	3.5556
C(12)	H(5)	3.5110	C(12)	H(8)	2.81(2)
C(12)	H(9)	3.2820	C(12)	H(11)	2.0437
C(12)	H(12)	3.2592	C(12)	$H(13)^{3}$	3.2500
C(12)	H(14)	3 2600	C(12)	H(15)	2 8357
C(12)	$\Pi(14)$	3.2142	C(12)	11(10)	2.0337
C(12)	H(10)	5.5142	C(13)	H(10)	2.0397
C(13)	H(12)	2.0348	C(13)	H(13)	3.2613
C(13)	$H(13)^{3}$	3.5355	C(13)	$H(14)^{3}$	3.0728
C(13)	$H(26)^{7}$	3.0472	C(14)	H(5)	3.4763
C(14)	H(10)	3 2570	C(14)	H(11)	2 0327
C(14)	H(10)	2.0220			2.0527
C(14)	H(13)	2.0339	C(14)	H(14)	3.2522
C(14)	H(19) <sup>3)</sup>	3.4912	C(14)	H(26) <sup>7)</sup>	3.2441
C(14)	$H(27)^{7}$	3.4306	C(15)	H(5)	3.0173
$\dot{C(15)}$	H(10) <sup>6)</sup>	3.3693	C(15)	H(11)	3.2585
C(15)	H(11) <sup>6)</sup>	3 3862	C(15)	H(12)	2 0242
C(15)	II(11)	2.0251	C(15)	11(12) $11(27)^{7}$	2.0242
C(15)	H(14)	2.0351	C(15)	H(27)''	3.4463
C(16)	H(5)	2.7805	C(16)	H(7)	3.0761
C(16)	H(9)	2.5260	C(16)	H(10)	3.2577
cùố	H(11) <sup>6</sup>	3 0366	CÌLÔ	H(12)	3 2520
C(16)	H(12)	2 0/13	C(17)	H(8)	2 72(2)
	11(13)	2.0413		11(0)	2.12(2)
C(17)	H(9)	2.0318	C(17)	H(10)	2.9340
C(17)	H(16)	2.6615	C(17)	H(20)	2.6800
C(17)	H(21)	2.01(2)	C(17)	H(22)	3.2491
C(17)	H(23)	2 5175	C(18)	H(9)	2 70/0
C(17)	II(20)	2.5175	C(10)	II(J)	2.7047
U(18)	п(10)	3.3708	C(18)	п(15)	2.0215

C(18)	H(16)	2 0327	C(18)	H(17)	3 2604
C(18)	$\Pi(10)$	2.0527	C(10)	11(17)	2.0220
C(18)	H(19)	3.2699	C(18)	H(20)	2.0320
C(18)	H(21)	2.66(2)	C(18)	H(23)	3.1354
C(19)	H(9)	2.8988	C(19)	$H(11)^{6}$	3.2329
C(19)	$H(12)^{6}$	3.5798	C(19)	H(15)	3.2802
C(19)	HÌLA	3 2520	C(19)	H(18)	3 2591
C(10)	H(10)	2.0294	C(10)	11(10)	2.2371
C(19)	H(19)	2.0384	C(19)	H(21)	2.76(2)
C(19)	H(24)	3.4749	C(20)	H(11) <sup>69</sup>	3.0879
C(20)	$H(12)^{6}$	3.4051	C(20)	H(17)	3.2571
C(20)	H(18)	2.0390	C(20)	H(20)	2.0366
C(20)	$H(26)^{8)}$	3 2206	C(21)	H(16)	3 2487
C(20)	$\Pi(20)$ $\Pi(17)$	2.02(0	C(21)	11(10)	2.0277
C(21)	H(1/)	2.0269	C(21)	H(19)	2.03//
C(21)	H(19) <sup>%</sup>	3.5987	C(21)	H(20)	3.2603
C(21)	$H(25)^{8}$	3.4154	C(21)	$H(26)^{8}$	3.2311
C(22)	H(16)	2.0356	C(22)	H(18)	2.0226
$\dot{c}\dot{c}\dot{z}\dot{z}\dot{z}$	H(19)	3 2540	C(23)	H(15)	2 5231
C(22)	H(17)	2.0267	C(23)	LI(19)	2.0201
C(23)	$\Pi(17)$	2.0507	C(23)	H(18)	3.2491
C(23)	H(20)	3.2509	C(23)	H(23)	3.5309
C(23)	H(28)	3.4755	C(23)	H(28) <sup>3)</sup>	3.2516
C(24)	H(15)	2.5972	C(24)	H(21)	1.98(2)
C(24)	H(24)	2.6782	C(24)	$H(25)^{1}$	3 0271
C(24)	H(28)	2 6710	C(24)	H(20)	3.51(2)
C(24)	H(20)	2.0/19	C(24)	$\Pi(23)$ $\Pi(15)$	2.51(2)
C(24)	H(30)	3.45(2)	C(25)	H(15)	3.3393
C(25)	H(20)	3.5575	C(25)	H(21)	2.60(2)
C(25)	H(22)	2.0207	C(25)	H(23)	2.0224
C(25)	H(24)	2 0281	C(25)	H(25)	3 2728
C(25)	$H(25)^{1}$	3 30/19	C(25)	H(27)	3 2763
C(25)	H(29)	2.0274	C(25)	11(27)	2 2042
C(25)	H(28)	2.0374	C(26)	H(17)	3.2843
C(26)	H(20)	3.3204	C(26)	H(21)	2.72(2)
C(26)	H(22)	2.7841	C(26)	H(23)	3.2809
C(26)	H(25)	2.0403	C(26)	H(26)	3.2638
C(26)	H(28)	3 2490	C(27)	$H(17)^{9}$	2 9/60
C(20)	11(20)	2.0204	C(27)	H(17)	2.1170
C(27)	H(18)	2.9394	C(27)	H(22)	3.41/8
C(27)	$H(23)^{2}$	3.5102	C(27)	H(24)	2.0389
C(27)	H(26)	2.0375	C(27)	H(27)	3.2505
C(28)	$H(17)^{9}$	3.1161	C(28)	$H(18)^{8}$	3.0783
C(28)	$H(19)^{(8)}$	3 2512	C(28)	H(24)	3 2620
C(28)	H(25)	2 0330	C(28)	H(27)	2 0276
C(20)	H(29)	2.0550	C(20)	11(27)	2.0270
C(28)	H(28)	3.2532	C(29)	$H(1/)^{2}$	3.58/0
C(29)	H(25)	3.2497	C(29)	H(26)	2.0295
C(29)	H(28)	2.0330	C(30)	$H(16)^{5}$	3.3002
C(30)	H(22)	3.0564	C(30)	H(23)	2.5346
CÌGM	H(24)	3 2470	CÌ3Ú	$H(25)^{(1)}$	3 3207
C(30)	ц(26)	2 2560	C(30)	H(27)	2 0 2 9 4
C(30)	H(20)	3.2309	C(30)	$\Pi(27)$	2.0364
H(2)	C(8) <sup>5</sup>	3.5881	H(2)	C(9) <sup>37</sup>	3.4850
H(3)	$C(9)^{3}$	3.2094	H(4)	$F(4)^{3}$	3.3984
H(4)	$F(6)^{3}$	3.0539	H(5)	$C(6)^{6}$	3.1604
H(5)	$C(7)^{6}$	3 0010	H(8)	Ni(1)	2.45(2)
H(8)	S(1)	3.04(2)	H(8)	0(1)	281(2)
11(0)	O(2)	3.04(2)	11(0)	O(1)	2.01(2) 2.19(2)
H(8)	O(3)	2.34(2)	H(8)		5.10(2)
H(8)	N(1)	3.21(2)	H(8)	C(3)	1.86(2)
H(8)	C(4)	2.40(2)	H(8)	C(5)	2.88(2)
H(8)	C(9)	3.38(2)	H(8)	C(10)	1.93(2)
H(8)	cừn	2 58(2)	H(8)	$\dot{C(12)}$	2 81(2)
L(0)	C(17)	2.30(2)	H(10)	$C(12)^{3}$	2 2602
H(8)	C(17)	2.72(2)	H(10)		3.3093
H(11)	$C(\Pi)$	3.2769	H(11)	C(12)	2.0437
H(11)	C(14)	2.0327	H(11)	C(15)	3.2585
H(11)	$C(15)^{3}$	3.3862	H(11)	$C(16)^{3}$	3.0366
H(11)	$C(19)^{3}$	3.2329	H(11)	$C(20)^{3}$	3.0879
HÀIŃ	F(1) <sup>6)</sup>	2 6998	HÌIÍ	F(3) <sup>6)</sup>	3 1070
U(12)	$E(6)^{3}$	2 5020	U(12)	$O(2)^{(0)}$	2 1040
п(12) H(12)	F(0)	3.3720	П(12) Н(12)	C(3)	5.1900
H(12)	C(1)"	5.5556	H(12)	C(19)"	3.5798
H(12)	$C(20)^{3}$	3.4051	H(13)	O(3) <sup>6)</sup>	2.5922
H(13)	$C(5)^{6)}$	3.4271	H(13)	$C(6)^{6}$	3.4328
HÌISÍ	$C(12)^{6}$	3 2500	H(13)	$C(13)^{6}$	3 5355
H(14)	$C(7)^{6}$	3 // 87	H(14)	$C(8)^{(6)}$	3 1750
11(14)	C(1)	2.0720	11(14)	C(0)	2.4230
H(14)	C(13)"	5.0/28	н(16)	C(30)"	5.3002
H(17)	$F(2)^{3}$	2.7669	H(17)	$F(3)^{3}$	2.9013
H(17)	$C(1)^{5}$	3.3887	H(17)	$C(26)^{7}$	3.2843
H(17)	$C(27)^{7}$	2.9460	H(17)	$C(28)^{7}$	3.1161
· · · · ·			and the second		

H(17)	$C(29)^{7}$	3.5870	H(18)	$F(2)^{5}$	2.9033
H(18)	$F(3)^{5}$	3.1625	H(18)	$C(1)^{5}$	3.4572
H(18)	$C(27)^{8)}$	2.9394	H(18)	$C(28)^{8)}$	3.0783
H(19)	$F(1)^{10}$	2.8555	H(19)	$F(3)^{10}$	3.1540
H(19)	$C(1)^{10}$	3.5239	H(19)	$C(14)^{6}$	3.4912
H(19)	$C(21)^{8)}$	3.5987	H(19)	$C(28)^{(8)}$	3.2512
H(20)	$F(1)^{10}$	2.7809	H(22)	$F(2)^{2}$	2.6319
H(22)	$C(27)^{1}$	3.4178	H(23)	$C(27)^{1}$	3.5102
H(24)	$F(2)^{2}$	2.9106	H(24)	$O(1)^{2}$	3.5174
H(25)	$F(2)^{10}$	3.2047	H(25)	$C(21)^{8)}$	3.4154
H(25)	$C(24)^{2}$	3.0271	H(25)	$C(25)^{2)}$	3.3049
H(25)	$C(30)^{2}$	3.3207	H(26)	$C(13)^{9)}$	3.0472
H(26)	$C(14)^{9}$	3.2441	H(26)	$C(20)^{8)}$	3.2206
H(26)	$C(21)^{8)}$	3.2311	H(27)	$F(3)^{5}$	2.9009
H(27)	$C(14)^{9)}$	3.4306	H(27)	$C(15)^{9)}$	3.4463
H(28)	$C(23)^{5}$	3.2516	H(29)	$S(2)^{(1)}$	2.84(2)
H(29)	$F(1)^{2}$	3.29(2)	H(29)	$F(2)^{2}$	3.52(2)
H(29)	$F(5)^{1}$	3.26(2)	H(29)	$O(2)^{2)}$	3.01(2)
H(29)	$O(5)^{1)}$	1.99(2)	H(29)	$O(6)^{1)}$	2.92(2)
H(30)	$S(1)^{2}$	3.15(2)	H(30)	$F(1)^{2}$	3.27(2)
H(30)	$F(2)^{2}$	3.09(2)	H(30)	$F(5)^{1}$	3.29(2)
H(30)	$O(2)^{2)}$	1.99(2)	H(30)	$O(5)^{1)}$	3.10(2)
H(30)	$C(1)^{2)}$	3.32(2)	H(31)	$O(6)^{1)}$	2.99(2)
H(32)	$S(2)^{1)}$	3.20(2)	H(32)	$O(5)^{1)}$	3.48(2)
H(32)	$O(6)^{1)}$	2.05(2)			
Symmetry	Operators:				
(1) X+1/2-	1,-Y+1/2,Z		(2) $X+1/2, -Y+1/2, Z$		
(3) X+1/2-	1,-Y+1/2-1,Z		(4) X-1,Y,Z		
(5) -X,-Y,-	Z+1	(6) X+1/2,-Y+	1/2-1,Z		
(7) -X+1/2	,Y+1/2-1,-Z+1		(8) -X+1,-Y,-Z+1		
(9) -X+1/2	,Y+1/2,-Z+1		(10) X+1,Y,Z		