

# Synthesis and X-ray Crystal Structure of the [Ni(HDPE)<sub>2</sub>][NO<sub>3</sub>]<sub>2</sub>·2H<sub>2</sub>O Complex

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Received: April 12, 1991; July 11, 1991

A reação de Ni(NO<sub>3</sub>)<sub>6</sub>H<sub>2</sub>O com 2-((2-piridiletil) imina) - 3 - butanona oxima (HDPE) em solução etanólica (estequiometria 1:2), resulta na formação de cristais vermelhos do complexo [Ni(HDPE)<sub>2</sub>][NO<sub>3</sub>]<sub>2</sub>·2H<sub>2</sub>O (1). A estrutura molecular de (1), foi determinada através de cristalografia de raios-X. O composto é monoclinico, grupo espacial Cc com a=8.502(2)Å, b=18.702(2)Å, c=18.653(2)Å, β=103.22(2)°, Z=4. A estrutura foi refinada a um valor final de R igual a 0.0594 para 2538 reflexões únicas. A estrutura consiste do cátion mononuclear [Ni(HDPE)<sub>2</sub>]<sup>2+</sup>, ânions NO<sub>3</sub><sup>-</sup> e água de cristalização. As moléculas de água estão ligadas através de pontes de hidrogênio a dois grupos hidróxi e dois átomos de oxigênio, um de cada íon NO<sub>3</sub><sup>-</sup>.

The reaction of Ni(NO<sub>3</sub>)<sub>6</sub>H<sub>2</sub>O in ethanolic solution with 2-((2-pyridylethyl)imino)-3-butanone oxime (HDPE) (stoichiometry 1:2), yields red crystals of [Ni(HDPE)<sub>2</sub>][NO<sub>3</sub>]<sub>2</sub>·2H<sub>2</sub>O (1). The crystal structure of (1) has been determined by X-ray crystallography. (1) crystallizes in the monoclinic space group Cc, with a = 8.502(2)Å, b = 18.702(2)Å, c = 18.653(2)Å, β = 103.22(2)°, and Z = 4. The structure was refined to a final R value of 0.0594 for 2538 unique reflections. The structure consists of mononuclear [Ni(HDPE)<sub>2</sub>]<sup>2+</sup> cations and NO<sub>3</sub><sup>-</sup> anions and water of crystallization. The water molecules are linked by hydrogen bonds to two hydroxy and two oxygen atoms, one of each NO<sub>3</sub><sup>-</sup> ion.

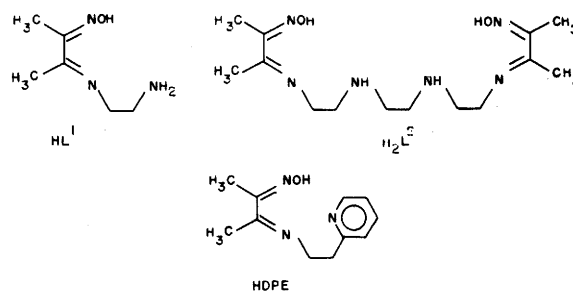
**Key words :** crystal structure, C<sub>22</sub>H<sub>30</sub>N<sub>8</sub>O<sub>8</sub>Ni·2H<sub>2</sub>O

## Introduction

Numerous planar nickel(II) complexes containing ligands such as dioximates,<sup>1</sup> salicylaldoximates<sup>1</sup> and amino-oximates<sup>2</sup> have been synthesized and characterized. These structures are normally stabilized by strong intramolecular NO-H-O hydrogen bonds. However, only few examples of octahedral Ni(II) complexes with undissociated NOH groups have been reported. These include the complexes formed by the tridentate ligand 2-((2-aminoethyl)imino)-3-butanone oxime<sup>3</sup> (HL<sup>1</sup>) and the hexadentate ligand 3,14-dimethyl - 4,7,10,13-tetraaza-3,13-hexadecadiene-2,15-dione dioxime<sup>4</sup> (H<sub>2</sub>L<sup>2</sup>), for which the X-ray crystal structures have been published.

Herein, we report the complete X-ray crystal structure of the nickel(II) complex derived from a closely related tridentate ligand, HDPE. It is interesting to note that replacement of 2-aminoethyl by 2-pyridylethyl in the ligand HL<sup>1</sup>,

enabled us to investigate the effect caused by the formation of six-membered rings in the [Ni(HDPE)<sub>2</sub>]<sup>2+</sup> ion complex.



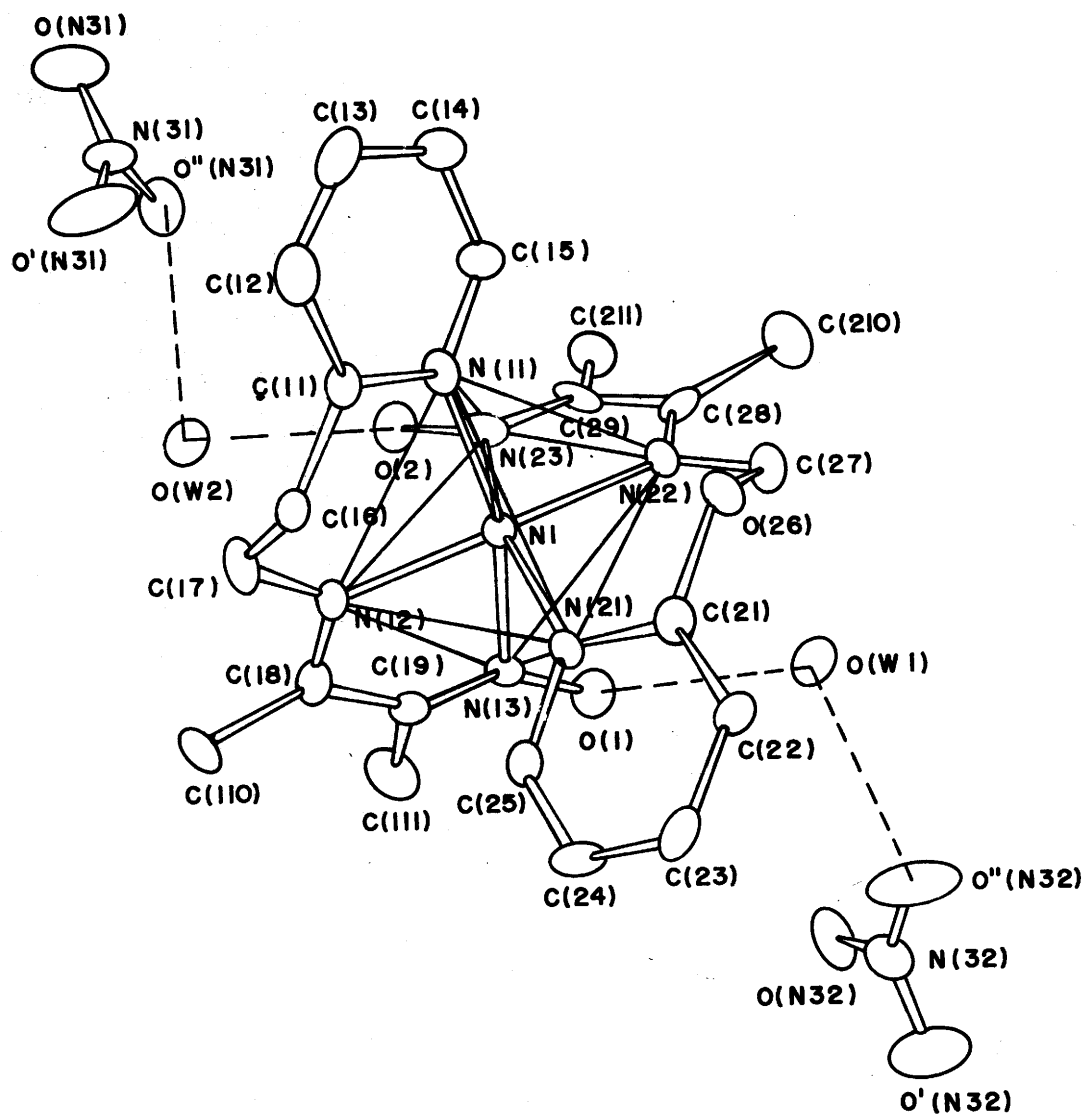


Figure 1. Structure of the  $[Ni(HDPE)_2][NO_3]_2 \cdot 2H_2O$  and atom-labeling scheme, showing the hydrogen bonds (dashed lines).

## Experimental

### Synthesis

The ligand 2 - ((2 - pyridylethyl) imino) - 3 butanone oxime and its nickel(II) complex were prepared according to the method described in the literature.<sup>5</sup> Single crystals suitable for X-ray crystallography were obtained by recrystallization from a methanolic solution of  $[Ni(HDPE)_2][NO_3]_2 \cdot 2H_2O$ . *Anal. Calc.* for  $C_{22}H_{30}N_8O_8Ni \cdot 2H_2O$ : C, 41.99; H, 5.45; N, 17.81. *Found*: C, 42.15; H, 5.36; N, 17.65%.

### X-ray Crystallography

Diffraction measurements were carried out on an Enraf-Nonius CAD-4 diffractometer, using prismatic single crystal with linear dimensions of 0.5x0.13x0.08 mm. Cell dimensions and the orientation matrices were calculated by

least-squares from 25 centred reflections in the range  $10^\circ < \theta < 16.6^\circ$ . All crystal diffraction intensities were measured by the  $\omega$  scan technique using a variable scan speed between 3.85 - 6.67° min<sup>-1</sup>. The intensities of two standard reflections were essentially constant throughout the data collection period. Data were corrected for Lorentz and polarization effects but not for absorption or extinction. A summary of data collection and processing parameters is given in Table 1. The heavy atom was located by Patterson method, with SHELXS-86 system of programs.<sup>6</sup> All other non-hydrogen atoms were determined from successive cycles of difference Fourier synthesis and isotropic least-squares refinement. Hydrogen atoms were located geometrically, all with common isotropic temperature factor of 0.10Å. The water hydrogens were located from dif-

**Table 1.** Crystallographic Data and Summary of Data Collection

Molecular formula	C <sub>22</sub> H <sub>30</sub> N <sub>8</sub> O <sub>8</sub> Ni.2H <sub>2</sub> O
Molecular weight	629.27
Space group	Cc
Cell constants	a=8.502(2)Å b=18.702(2)Å c=18.653(2)Å β=103.22(2)°
Complexes per cell	4
Density	1.448 g.cm <sup>-3</sup>
Radiation used	MoKα (λ=0.71073 Å)
Absorption coefficient	7.36 cm <sup>-1</sup>
Collection range	0° < θ < 25°
h,k,l range	-10 < h < 10, 0 < k < 22, 0 < l < 22
N <sup>o</sup> of unique reflections	2538
N <sup>o</sup> of reflections with I > 2σ(I)	1656
R	0.0594

ference synthesis. The structure was refined anisotropically for all non-hydrogen atoms. The refinement was made by minimization of the function  $\Sigma \omega (|F_o| - K |F_c|)^2$  through block-matrix least-squares, where  $\omega = [\sigma^2(F_o) + 0.001(F_o)^2]^{-1}$ . The final refinement gave R=0.0594, R<sub>w</sub>=0.0544 and all parameters shifts were less than 70% of the corresponding standard deviation. Scattering factors for non-hydrogen atoms from Cromer & Mann<sup>7</sup> with correction for anomalous dispersion from Cromer & Liberman<sup>8</sup>, for hydrogen atoms from Stewart, Davidson & Simpson<sup>9</sup>. Most of the calculations were performed on a Vax 11/780 computer with SHELXS-76 sistem of programs<sup>10</sup>. The final positional parameters and equivalent isotropic temperature factors, calculated as described by Hamilton<sup>11</sup> for all non-hydrogen atoms, are given in Table 2.

### Results and Discussion

Crystals of (1) consist of the mononuclear dication [Ni(HDPE)<sub>2</sub>]<sup>2+</sup>, uncoordinated nitrate anions and water molecules of crystallization. Selected bond distances and angles are summarized in Tables 3 and 4 respectively. The atomic labeling scheme for (1) is shown in Figure 1. The molecule has an approximate two-fold axis which passes through the nickel atom. The nickel(II) ion is bonded to six nitrogen atoms in a distorted octahedral environment in which the two tridentate ligands are in meridional arrangement in such a way, that the two planes defined by the three nitrogen (oxime, imine and pyridyl) are nearly perpendicular to each other. The two halves of the chelate show a close structural similarity. A similar coordination symmetry, has been found in the nickel(II) complexes formed by the tridentate (HL<sup>1</sup>)<sup>3</sup> and the hexadentate (H<sub>2</sub>L<sup>2</sup>)<sup>4</sup> ligands. However, the coordination octahedron in the [Ni(HDPE)<sub>2</sub>]<sup>2+</sup> complex is somewhat less distorted than that in the [Ni(HL<sup>1</sup>)<sub>2</sub>]<sup>2+</sup> and [Ni(H<sub>2</sub>L<sup>2</sup>)<sub>2</sub>]<sup>2+</sup> complexes. The N - Ni - N *cis* angles range from 76.5(3)° to 100.5(3)° in complex (1) whereas in the [Ni(HL<sup>1</sup>)<sub>2</sub>]<sup>2+</sup> and [Ni(H<sub>2</sub>L<sup>2</sup>)<sub>2</sub>]<sup>2+</sup> this variation is more significant, 75.8° to 107.0° and 75.9° to 105.1° respectively. As expected, the largest values are found for those angles that are not included in the chelate rings and the smallest values for angles inside the rings. Interestingly,

**Table 2.** Final Atomic Coordinates and Equivalent Isotropic Temperature Factors for All non-H Atoms (with estimated standard deviations in parentheses)

Atom	x/a	y/b	z/c	Beq Å <sup>2</sup>
Ni	0.0	0.1250(1)	0.0	2.68(3)
N(11)	-0.01529(8)	0.0393(4)	0.0214(4)	2.6(3)
N(12)	0.069(1)	0.1478(4)	0.1101(4)	2.9(3)
N(13)	0.200(1)	0.1996(4)	0.0067(5)	3.2(3)
C(11)	-0.214(1)	0.0419(5)	0.0823(6)	3.0(3)
C(12)	-0.286(1)	-0.0170(7)	0.1032(6)	4.6(4)
C(13)	-0.298(2)	-0.0804(7)	0.0608(7)	5.4(5)
C(14)	-0.235(1)	-0.0830(6)	0.0009(6)	4.5(4)
C(15)	-0.161(1)	-0.0213(5)	-0.0162(5)	3.1(3)
C(16)	-0.192(1)	0.1085(5)	0.1267(6)	4.1(4)
C(17)	-0.021(1)	0.1257(5)	0.1625(5)	4.1(4)
C(18)	0.194(1)	0.1884(5)	0.1309(5)	3.3(3)
C(19)	0.276(1)	0.2094(5)	0.0719(7)	3.6(4)
C(110)	0.255(1)	0.2140(6)	0.2079(6)	5.4(4)
C(111)	0.441(2)	0.2410(7)	0.0899(7)	6.6(5)
O(1)	0.2785(8)	0.2172(4)	-0.0469(4)	5.1(3)
N(21)	-0.170(1)	0.2103(4)	-0.0222(4)	3.1(3)
N(22)	-0.041(1)	0.1018(4)	-0.1096(4)	2.8(3)
N(23)	0.194(1)	0.0519(4)	-0.0066(5)	3.9(3)
C(21)	-0.295(1)	0.2090(6)	-0.0845(5)	3.2(3)
C(22)	-0.394(1)	0.2689(6)	-0.1049(6)	4.3(4)
C(23)	-0.360(1)	0.3300(6)	-0.0609(6)	4.4(4)
C(24)	-0.237(2)	0.3318(6)	-0.0012(6)	4.7(4)
C(25)	-0.144(1)	0.2696(6)	0.0166(5)	3.5(4)
C(26)	-0.321(1)	0.1414(6)	-0.1268(6)	4.3(4)
C(27)	-0.190(2)	0.1247(5)	-0.1646(5)	4.6(4)
C(28)	0.059(1)	0.0615(5)	-0.1315(6)	3.4(3)
C(29)	0.205(1)	0.0388(5)	-0.0723(6)	3.4(4)
C(210)	0.049(1)	0.0347(6)	-0.2066(6)	5.8(5)
C(211)	0.354(1)	0.0071(7)	-0.0902(7)	7.1(5)
O(2)	0.3262(9)	0.0327(4)	0.0480(4)	5.1(3)
N(31)	-0.632(2)	0.1620(5)	-0.3015(6)	5.2(4)
O(N31)	-0.525(1)	0.1385(5)	-0.3279(5)	7.7(4)
O'(N31)	-0.639(1)	0.2231(5)	-0.2865(6)	8.5(4)
O(N31)	-0.724(2)	0.1225(5)	-0.2846(9)	13.6(8)
N(32)	-0.330(2)	-0.0892(6)	-0.2014(6)	5.4(4)
O(N32)	-0.195(1)	-0.1098(5)	-0.1740(5)	8.0(4)
O'(N32)	-0.351(1)	-0.0257(6)	-0.2134(7)	10.1(5)
O(N32)	-0.438(1)	-0.1289(5)	-0.2181(1)	13.4(7)
O(W1)	0.1291(9)	0.2274(4)	-0.1860(4)	5.1(3)
O(W2)	0.3157(9)	0.0237(4)	0.1836(4)	5.4(3)

the N<sub>21</sub>- Ni - N<sub>22</sub> and N<sub>11</sub> - Ni - N<sub>12</sub> bond angles (mean value 90.8(3)°) in (1) are specially noteworthy as they turn out to be significantly greater than the corresponding angles in [Ni(HL<sup>1</sup>)<sub>2</sub>]<sup>2+</sup> (81.5°) and [Ni(H<sub>2</sub>L<sup>2</sup>)<sub>2</sub>]<sup>2+</sup> (82.3°). In fact, this can be interpreted in terms of a better flexibility of the six-membered rings formed by the terminal 2-pyridylethyl groups, which adopt a distorted half-chair configuration with the torsion angles N<sub>21</sub>C<sub>21</sub>C<sub>26</sub>C<sub>27</sub> of -68.9° and N<sub>11</sub>C<sub>11</sub>C<sub>16</sub>C<sub>17</sub> of -65.1°. On the other hand, in the complexes formed by HL<sup>1</sup> and H<sub>2</sub>L<sup>2</sup>, the 2-aminoethyl-imino fragments form the more rigid five-membered rings which adopt the usual gauche conformation.<sup>3,4</sup> In the [Ni(HDPE)<sub>2</sub>]<sup>2+</sup> complex, the five-membered chelate rings including oxime and imine nitrogen donors show slight but significant deviations from planarity, as indicated by the torsional angles of 12.3° and 14.9°. These values may be

**Table 3. Bond Distances(Å) with Estimated Standard Deviations in Parentheses.**

Ni	-	N(11)	2.158(7)
Ni	-	N(12)	2.048(7)
Ni	-	N(13)	2.181(8)
Ni	-	N(21)	2.129(8)
Ni	-	N(22)	2.040(7)
Ni	-	N(23)	2.167(9)
N(11)	-	C(11)	1.35(1)
N(11)	-	C(15)	1.33(1)
N(12)	-	C(17)	1.43(1)
N(12)	-	C(18)	1.29(1)
N(13)	-	C(19)	1.25(1)
N(13)	-	D(1)	1.36(1)
C(11)	-	C(12)	1.36(2)
C(11)	-	C(16)	1.48(1)
C(12)	-	C(13)	1.42(2)
C(13)	-	C(14)	1.35(2)
C(14)	-	C(15)	1.39(1)
C(16)	-	C(17)	1.49(2)
C(18)	-	C(19)	1.48(2)
C(18)	-	C(110)	1.49(1)
C(19)	-	C(111)	1.49(2)
N(21)	-	C(21)	1.38(1)
N(21)	-	C(25)	1.32(1)
N(22)	-	C(27)	1.50(1)
N(22)	-	C(28)	1.27(1)
N(23)	-	C(29)	1.27(1)
N(23)	-	D(2)	1.38(1)
C(21)	-	C(22)	1.40(1)
C(21)	-	C(26)	1.48(1)
C(22)	-	C(23)	1.40(2)
C(23)	-	C(24)	1.34(2)
C(24)	-	C(25)	1.40(2)
C(26)	-	C(27)	1.48(2)
C(28)	-	C(29)	1.52(2)
C(28)	-	C(210)	1.47(2)
C(29)	-	C(211)	1.50(2)
N(31)	-	O(N31)	1.21(2)
N(31)	-	O'(N31)	1.18(1)
N(31)	-	O•(N31)	1.17(2)
N(32)	-	O(N32)	1.21(2)
N(32)	-	O'(32)	1.21(2)
N(32)	-	O•(N32)	1.17(2)

comparable to those found in the  $[\text{Ni}(\text{H}_2\text{L}^2)]^{2+}$  complex (9.0° and 12.1°)<sup>4</sup>.

The Ni - N bond lengths in complex (1) are comparable to those of  $[\text{Ni}(\text{HL}^1)_2]^{2+}$  and  $[\text{Ni}(\text{H}_2\text{L}^2)]^{2+}$ , but longer in (1). For (1), the average Ni - N(imine) and Ni - N(oxime) bond lengths are 2.044(7) and 2.174(8)Å respectively, whereas the corresponding average distances in  $[\text{Ni}(\text{HL}^1)_2]^{2+}$  and  $[\text{Ni}(\text{H}_2\text{L}^2)]^{2+}$  are 2.008(3), 2.135(4)Å and 2.004(3), 2.118(4)Å. The Ni - N(pyridyl) bond lengths, 2.143(7)Å (average) in (1) are close to the Ni - N(amine) bond distances of 2.098(4) and 2.128(6)Å found for  $[\text{Ni}(\text{HL}^1)_2]^{2+}$  and  $[\text{Ni}(\text{H}_2\text{L}^2)]^{2+}$  respectively.

**Table 4. Bond Angles (degree) with Estimated Standard Deviations in Parentheses.**

N(11)	Ni	N(12)	90.9(3)
N(11)	Ni	N(13)	163.6(3)
N(11)	Ni	N(21)	100.5(3)
N(11)	Ni	N(22)	93.2(3)
N(11)	Ni	N(23)	92.3(3)
N(12)	Ni	N(13)	76.6(3)
N(12)	Ni	N(21)	93.7(3)
N(12)	Ni	N(22)	173.4(3)
N(12)	Ni	N(23)	98.1(3)
N(13)	Ni	N(21)	91.0(3)
N(13)	Ni	N(22)	98.4(3)
N(13)	Ni	N(23)	79.2(3)
N(21)	Ni	N(22)	90.7(3)
N(21)	Ni	N(23)	162.4(3)
N(22)	Ni	N(23)	76.5(3)
C(11)	N(11)	C(15)	119.4(8)
C(17)	N(12)	C(18)	119.7(8)
C(19)	N(13)	O(1)	116.5(8)
N(11)	C(11)	C(12)	119.7(9)
N(11)	C(11)	C(16)	118.4(9)
C(12)	C(11)	C(16)	121.8(9)
C(11)	C(12)	C(13)	120.1
C(12)	C(13)	C(14)	120.1
C(13)	C(14)	C(15)	117.1
N(11)	C(15)	C(14)	124.1(9)
C(11)	C(16)	C(17)	114.6(9)
N(12)	C(17)	C(16)	112.0(9)
N(12)	C(18)	C(19)	115.3(9)
N(12)	C(18)	C(110)	124.0(9)
C(19)	C(18)	C(110)	120.7(9)
N(13)	C(19)	C(18)	117.1(9)
N(13)	C(19)	C(111)	112.1
C(18)	C(19)	C(111)	121.1
C(21)	N(21)	C(25)	118.5(8)
C(27)	N(22)	C(28)	118.2(8)
C(29)	N(23)	O(2)	115.7(8)
N(21)	C(21)	C(22)	120.8(9)
N(21)	C(21)	C(26)	117.1(9)
C(22)	C(21)	C(26)	122.1(9)
C(21)	C(22)	C(23)	118.1
C(22)	C(23)	C(24)	122.1
C(23)	C(24)	C(25)	118.1
N(21)	C(25)	C(24)	124.1
C(21)	C(26)	C(27)	113.4(9)
N(22)	C(27)	C(26)	110.1(8)
N(22)	C(28)	C(29)	115.3(9)
N(22)	C(28)	C(210)	128.1
C(29)	C(28)	C(210)	117.1(9)
N(23)	C(29)	C(28)	114.7(9)
N(23)	C(29)	C(211)	123.1
C(28)	C(29)	C(211)	122.5(9)
O(N31)	N(31)	O'(N31)	122.1
O(N31)	N(31)	O.(N31)	119.1
O'(N31)	N(31)	O.(N31)	118.1
O(N32)	N(32)	O'(N32)	118.1
O(N32)	N(32)	O.(N32)	122.1
O'(N32)	N(32)	O.(N32)	120.1

**Table 5.** Distances ( $\text{\AA}$ ) and Angles ( $^\circ$ ) Involved in Hydrogen Bonds.

	O...O	H...O	O-H...O
O(1) --H(O1)...O(W1) <sup>i</sup>	2.62(1)	1.94(7)	125.7(5)
O(2) --H(O2)...O(W2) <sup>i</sup>	2.56(1)	-----	-----
O(W1) <sup>i</sup> --H(OW1)...O <sup>ii</sup> (N32) <sup>iii</sup>	2.78(1)	1.83(1)	152.2(6)
O(W2) <sup>i</sup> --H(OW2)...O <sup>ii</sup> (N31) <sup>ii</sup>	2.83(1)	2.03(1)	153.1(6)

indexes i,ii,iii are referred to the symmetry operations:

i = x ; y ; z, ii = 1 + x ; -y ; 0.5 + z and iii = 0.5 + x ; 0.5 + y ; z

There is unequivocal structural evidence for the presence of the oxime protons in  $[\text{Ni}(\text{HDPE})_2]^{2+}$ . As can be seen the average N-O and N-C(oxime) bond lengths and the average C-N-O bond angle for  $[\text{Ni}(\text{HDPE})_2]^{2+}$  are 1.37(1) $\text{\AA}$ , 1.261 $\text{\AA}$  and 116.1(8) $^\circ$  respectively, whereas the corresponding values in  $[\text{Ni}(\text{HL}^1)_2]^{2+}$  are 1.388(5) $\text{\AA}$ , 1.285(5) $\text{\AA}$  and 113.3(4) $^\circ$ .<sup>3</sup> The values found in the present compound also fall well inside the corresponding ranges of 1.38 $\pm$ 0.03  $\text{\AA}$ , 1.29 $\pm$ 0.02  $\text{\AA}$  and 112 $\pm$ 2 $^\circ$  reported to be characteristic for the uncoordinated oxime group<sup>1,3</sup>.

The water molecules of crystallization are linked by hydrogen bonds to two hydroxy of the oxime groups and two oxygen atoms, one of each  $\text{NO}_3^-$  ion. The distances and angles between atoms involved in hydrogen bond interactions are given in Table 5. It was not possible to determine the distance H...O and the angle O...H...O of the hydrogen bond O(2)·H(O2)·O(W2), due to the impossibility of location of the hydrogen H(O2) linked to the hydroxy group of N(23) in the difference Fourier Synthesis.

The two crystallographically independent nitrate anions in the structure, although with much higher thermal vibration amplitudes than all atoms of the structure, are ordered and do not show any serious distortions from rigorous planarity. The N - O bonds range from 1.17(2) to 1.21(2) $\text{\AA}$  and the O - N - O angles vary between 118.0(1) and 122.0(1) $^\circ$ .

The remaining bond lengths and angles in the ligand molecule can be considered to be within their normally expected values

### Acknowledgements

This work was supported by Grants from CNPq, CAPES, FAPESP and FINEP. We thank Prof. Dr. Ivo Vençato for helpful discussions.

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### Supplementary Material Available:

Listings of observed and calculated structure factors for  $[\text{Ni}(\text{HDPE})_2][\text{NO}_3]_2 \cdot 2\text{H}_2\text{O}$ ; Table of anisotropic thermal parameters; table of atomic coordinates of the H-atoms and isotropic parameters.