Crystal and molecular structure of the tetrahydrate of hexaaquanickel(II) (S*, S*)-ethylenediaminedisuccinato--nickelate(II)

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Crystals of $Ni_2((S^*, S^*)\text{-EDDS}) \cdot 10H_2O$ are monoclinic with lattice parameters $a = 3.065(1)$ nm, $b = 0.9915(5)$ nm, $c = 1.5883(5)$ nm, $\beta = 110.76(2)°$, $V = 4.5132$ nm^3, the space group is $C2/c$, $Z = 8$. The crystal density is $D_0 = 1.748$ Mgm^{-3}, $D_c = 1.72$ Mgm^{-3}, Cu$K\alpha$ ($\lambda = 0.15418$ nm) radiation, $\mu = 2.73$ mm^{-1}, the relative molecular mass is $M_r = 585.84$. The structure was solved by the heavy atom method and refined by the least squares to $R = 0.072$ for 1810 observed diffractions. The structure consists of $[Ni(1)\text{-EDDS}]^{2-}$ complex anions, $[Ni(2)(H_2O)_6]^{2+}$ cations, and crystal water molecules. Both coordination polyhedrons of Ni atom are distorted octahedrons. The coordination polyhedron of Ni(1) atom is formed by two nitrogen atoms of ethylenediamine moiety and by four oxygen atoms of carboxyl groups of EDDS. The complex anion has an (OC-6-13-A) absolute configuration for the (S, S) absolute configuration of the ligand.

Кристаллы $Ni_2((S^*, S^*)\text{-EDDS}) \cdot 10H_2O$ являются моноклинными, $a = 3{,}065(1)$ нм, $b = 0{,}9915(5)$ нм, $c = 1{,}5883(5)$ нм, $\beta = 110{,}76(2)°$, $V = 4{,}5132$ нм^3, пространственная группа симметрии $C2/c$, $Z = 8$. Плотность кристаллов $D_0 = 1{,}748$ мгм$^{-3}$, $D_c = 1{,}72$ мгм$^{-3}$, использованное излучение Cu$K\alpha$ ($\lambda = 0{,}15418$ нм), $\mu = 2{,}73$ мм$^{-1}$, относительная молекулярная масса $M_r = 585{,}84$. Структура была решена методом тяжелого атома и уточнена методом наименьших квадратов до $R = 0{,}072$ для 1810 ненулевых рефлексий. Структура состоит из комплексных анионов $[Ni(1)\text{-EDDS}]^{2-}$, катионов $[Ni(2)(H_2O)_6]^{2+}$ и молекул кристаллической воды. Оба координационных полиэдра атома Ni представляют деформированный октаэдр. Координационный полиэдр атома Ni(1) образован двумя атомами азота от этилендиамина и четырьмя атомами кислорода карбоксильных групп EDDS. Комплексный анион имеет абсолютную конфигурацию (OC-6-13-A) для (S, S) абсолютной конфигурации лиганда.

In order to understand stereochemistry of coordination compounds with multidentate ligands we studied complexes of ethylenediamine-*N*,*N'*-disuccinic acid (further abbreviated as EDDS). This compound was originally synthesized after [1] and by means of Cu(II) complexes it was possible to separate *meso* and *racemic* forms [2]. This amino acid derivative was chosen as a model ligand mainly for the study of a stereospecific coordination.

By X-ray diffraction analysis the structures of (S, S) form of EDDS were determined for Ni(II), Cu(II), and Co(III) metal ions [3—5], of (R, S)-EDDS for Co(III) [6, 7] and of the *racemic* form for Fe(III) [8]. The knowledge obtained so far shows that $[(S, S)\text{-EDDS}]^{4-}$ has an expressive diastereoselectivity on coordination.

The aim of this work is to extend knowledge of the complexes of *racemic* EDDS.

Experimental

Preparation of crystals

Crystals of the title complex were synthesized as follows: (S*,S*)-EDDS · $5H_2O$ (0.03 mol) and fresh $Ni(OH)_2$ xH_2O (0.06 mol) were mixed in H_2O (100 cm^3). Slow evaporation of the formed blue solution gave crystals suitable for X-ray crystallographic study.

For $C_{10}H_{32}N_2Ni_2O_8$ (M_r = 585.84) w_i(calculated): 20.50 % C, 4.78 % N, 5.43 % H, 20.04 % Ni; w_i(found): 21.11 % C, 4.94 % N, 5.10 % H, 20.36 % Ni. The crystal density was measured by the flotation in a bromoform—benzene mixture.

Crystallographic data

For the X-ray diffraction a light blue crystal of needle shape with approximate dimensions $0.1 \times 0.1 \times 0.3$ mm was used. Oscillation and Weissenberg photographs showed that the crystals are monoclinic. A systematic extinction of diffractions of the *hkl* type for $h + k = 2n + 1$ and of the *h0l* type for $h = 2n + 1$ and $l = 2n + 1$ indicated two possible space groups of the symmetry $C2/c$ or Cc. The lattice parameters were refined on Syntex $P2_1$ diffractometer by the least-square method from positional angles of 10 selected reflections using Cu$K\alpha$ radiation. The integral intensities were measured on the same diffractometer using graphite monochromatized Cu$K\alpha$ radiation and Θ—2Θ scan technique in the interval $0 < 2\Theta \leqslant 100°$. The scan rate was determined automatically within 4.88—29.3° min^{-1} in 2Θ. The background was measured at each end of the scan for the half of the reflection scan time. No significant fluctuations were observed in intensities of two standard reflections measured in an interval of 98 measured reflections. Intensities of all reflections were corrected for Lorentz and polarization factors. Empirical absorption correction [9] was made as well. From 2317 measured reflections, 1810 with $I > 1.96\sigma(I)$ were regarded as observed.

The three-dimensional Patterson synthesis calculated from all observed reflections showed positions of both nickel atoms and unambiguously determined the space group as $C2/c$. The positions of other nonhydrogen atoms were determined from successive Fourier syntheses of electron density. The positional and isotropic temperature parameters were refined by the full matrix least squares using relative weights $W=1$ for all observed

Table 1

Final atomic coordinates ($\times 10^4$) with e.s.d.'s in parentheses and equivalent isotropic thermal parameters B_{eq}, defined as

$$B_{eq}=4/3\sum_{i,j} B_{ij}\,\vec{a}_i\,\vec{a}_j$$

Atom	x	y	z	$B_{eq}/(10^{-20}\ m^2)$
Ni(1)	1329(1)	625(2)	2756(1)	3.01
O(1)	955(3)	17(7)	3563(5)	1.75
O(2)	610(3)	952(8)	4436(5)	2.54
O(3)	773(2)	1798(8)	2048(5)	1.90
O(4)	338(3)	3649(8)	1775(5)	2.33
O(5)	1701(3)	1324(8)	1995(5)	2.68
O(6)	2244(3)	495(10)	1489(6)	3.92
O(7)	1101(2)	− 990(8)	1929(5)	2.25
O(8)	1147(3)	−3111(9)	1558(6)	3.79
N(1)	1547(3)	2009(9)	3773(6)	1.89
N(2)	1946(3)	− 361(10)	3406(6)	2.28
C(1)	2246(4)	643(14)	4055(9)	3.23
C(2)	1941(4)	1347(13)	4499(8)	2.51
C(3)	1131(4)	2322(11)	3988(7)	1.48
C(4)	884(4)	991(11)	3989(7)	1.72
C(5)	833(4)	3288(12)	3310(7)	1.75
C(6)	631(4)	2867(11)	2309(7)	1.82
C(7)	2115(4)	− 731(13)	2673(9)	2.75
C(8)	2008(4)	476(14)	2002(8)	2.91
C(9)	1861(4)	−1994(13)	2193(9)	3.05
C(10)	1318(4)	−2036(14)	1869(8)	2.63
Ni(2)	4796(1)	2283(2)	715(1)	3.44
W(1)	4291(3)	3379(8)	− 248(5)	1.94
W(2)	4405(3)	578(8)	166(5)	2.28
W(3)	4403(3)	2524(8)	1542(5)	2.30
W(4)	5318(2)	1322(8)	1720(5)	1.91
W(5)	5163(3)	4020(8)	1202(6)	2.76
W(6)	5165(2)	1946(7)	− 131(5)	1.69
W(7)	1439(3)	4056(12)	1203(7)	6.03
W(8)	1887(4)	4553(10)	3286(8)	5.51
W(9)	3475(5)	1651(20)	1025(12)	13.66
W(10)	2179(7)	2408(21)	271(15)	22.78

reflections to $R = 0.102$. The positions of twelve hydrogen atoms of the EDDS ligand were calculated on the basis of the assumed sp^3 hybridization (bond lengths 0.09 nm, bond angles 109.5°). Calculated positions of H atoms were confronted with difference electron density map (the highest peak was 0.88×10^{30} $(-e)$ m^{-3}. The hydrogen atoms of water molecules were not found.

In final refinement a block-diagonal method was used. The positional coordinates and the anisotropic thermal parameters of the nonhydrogen atoms were refined; the hydrogen atoms were used only for the structure factor calculations with $B = 2.0 \times 10^{-20}$ m^2. Functional $M = \Sigma\, w(|F_o| - |F_c|)^2$ was minimized, and a weighting scheme $w^{-1} = \sigma^2(|F_o|) + (C \cdot |F_o|)^2$ was used. The $\sigma(|F_o|)$ is derived from counting statistics and $C = 0.03$. The value of C was adjusted so that $\langle \Sigma\, w(|F_o| - |F_c|)^2 \rangle$ was constant in different intervals of $|F_o|$. The final $R = \Sigma\, |\Delta F| / \Sigma\, |F_o|$ is 0.072 for the observed reflections and 0.091 for all reflections. A Hamilton weighted residuals $R_w = (\Sigma w |\Delta F|^2 / \Sigma\, w |F_o|^2)^{1/2}$ are 0.104 and 0.110, respectively. There is a disorder in the position of W(10) water molecule. A difference synthesis, calculated without this molecule showed two broad maxima at a distance approximately 0.1 nm, with some unrealistic short interatomic distances. In final refinement the W(10) atom was situated in the mean of both peak positions. The refinement converged to the occupation factor close to unity, but temperature parameters were anomalously high.

Table 2

Coefficients of anisotropic temperature factors ($\times 10^4$). E.s.d.'s are given in parentheses
Temperature factor is of the form $\tau = \exp[-(B_{11}h^2 + \quad + B_{12}hk + \ldots)]$

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Ni(1)	8(0)	80(2)	38(1)	1(1)	15(1)	− 2(2)
O(1)	7(1)	26(8)	28(4)	− 3(5)	19(4)	−12(10)
O(2)	11(1)	37(10)	41(5)	− 4(6)	32(4)	− 4(11)
O(3)	6(1)	50(10)	17(4)	4(5)	4(3)	0(10)
O(4)	8(1)	44(10)	24(4)	14(6)	2(4)	− 3(11)
O(5)	8(1)	66(11)	43(5)	13(6)	26(4)	24(12)
O(6)	12(1)	134(14)	44(5)	3(8)	32(5)	15(14)
O(7)	4(1)	52(10)	37(5)	2(5)	9(4)	−49(11)
O(8)	6(1)	83(12)	67(6)	− 4(6)	12(5)	−57(14)
N(1)	7(1)	36(11)	20(5)	−11(7)	7(4)	3(12)
N(2)	5(1)	73(13)	24(5)	3(7)	7(4)	5(14)
C(1)	4(2)	109(20)	42(8)	11(10)	5(6)	−34(21)
C(2)	5(2)	78(17)	29(7)	2(9)	5(5)	7(18)
C(3)	4(2)	41(14)	22(6)	− 4(8)	14(5)	− 8(15)
C(4)	5(2)	47(14)	22(6)	5(8)	12(5)	15(15)
C(5)	5(2)	51(14)	25(6)	− 1(8)	14(5)	5(15)
C(6)	7(2)	38(14)	26(6)	−14(8)	19(5)	−36(16)
C(7)	6(2)	70(16)	47(8)	10(9)	20(6)	−24(19)
C(8)	8(2)	118(19)	21(6)	−30(10)	13(6)	−12(19)
C(9)	10(2)	55(16)	45(8)	20(10)	22(7)	− 3(18)
C(10)	5(2)	100(18)	25(7)	− 5(9)	7(6)	−34(18)

Table 2 (Continued)

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Ni(2)	11(0)	80(2)	42(1)	3(1)	20(1)	− 1(3)
W(1)	7(1)	39(9)	18(4)	8(5)	5(3)	− 5(10)
W(2)	7(1)	46(10)	26(4)	− 2(6)	5(4)	−14(11)
W(3)	9(1)	64(10)	22(4)	9(6)	17(4)	− 3(11)
W(4)	6(1)	55(10)	16(4)	6(6)	5(3)	−12(10)
W(5)	5(1)	46(10)	48(5)	− 5(5)	4(4)	−27(12)
W(6)	5(1)	42(9)	27(4)	5(5)	17(3)	1(10)
W(7)	12(2)	183(19)	68(7)	− 7(9)	8(6)	− 5(19)
W(8)	17(2)	83(13)	102(8)	−14(8)	49(7)	29(17)
W(9)	23(3)	386(36)	186(16)	−61(17)	25(11)	218(41)
W(10)	65(6)	465(49)	252(24)	−90(27)	−3(19)	505(57)

The refined coordinates of the nonhydrogen atoms are listed in Table 1, the coefficients of anisotropic thermal vibrations are given in Table 2. Values of bond lengths, bond angles, and torsion angles are given in Table 3. Tables of $|F_o|$ and $|F_c|$ can be obtained on request from the authors. Scattering factors for neutral atoms [10] were used. The water molecules in the tables are abbreviated by symbol W.

The calculations were carried out on Nova 1200 with Syntex XTL and on Siemens 4004/150 with NRC program package [11].

Table 3

Interatomic distances, bond angles, and torsion angles for $Ni_2((S^*,S^*)$-EDDS) · $10H_2O$ complex
Standard deviations are given in parentheses

Interatomic distances/nm			
Ni(1)—O(1)	0.209(1)	C(6)—O(3)	0.127(1)
Ni(1)—O(3)	0.204(1)	C(6)—O(4)	0.126(1)
Ni(1)—O(5)	0.205(1)	C(7)—C(8)	0.156(2)
Ni(1)—O(7)	0.203(1)	C(7)—C(9)	0.153(2)
Ni(1)—N(1)	0.204(1)	C(8)—O(5)	0.126(2)
Ni(1)—N(2)	0.205(1)	C(8)—O(6)	0.127(2)
N(1)—C(2)	0.150(1)	C(9)—C(10)	0.156(2)
N(1)—C(3)	0.146(1)	C(10)—O(7)	0.125(2)
N(2)—C(1)	0.149(2)	C(10)—O(8)	0.121(2)
N(2)—C(7)	0.148(2)	Ni(2)—W(1)	0.206(1)
C(1)—C(2)	0.152(2)	Ni(2)—W(2)	0.208(1)
C(3)—C(4)	0.152(2)	Ni(2)—W(3)	0.209(1)
C(3)—C(5)	0.149(2)	Ni(2)—W(4)	0.205(1)
C(4)—O(1)	0.124(1)	Ni(2)—W(5)	0.205(1)
C(4)—O(2)	0.128(1)	Ni(2)—W(6)	0.206(1)
C(5)—C(6)	0.155(2)		

Table 3 (Continued)

Bond angles/°			
N(1)—Ni(1)—N(2)	86.4(4)	O(1)—C(4)—O(2)	124(1)
N(1)—Ni(1)—O(3)	91.6(3)	C(3)—C(4)—O(2)	117(1)
N(1)—Ni(1)—O(7)	169.0(4)	C(3)—C(5)—C(6)	119(1)
N(1)—Ni(1)—O(8)	98.3(4)	O(3)—C(6)—O(4)	123(1)
N(1)—Ni(1)—O(1)	78.8(3)	O(3)—C(6)—C(5)	120(1)
N(2)—Ni(1)—O(7)	89.7(4)	O(4)—C(6)—C(5)	117(1)
N(2)—Ni(1)—O(3)	171.6(4)	N(2)—C(7)—C(8)	107(1)
N(2)—Ni(1)—O(5)	81.5(4)	C(8)—C(7)—C(9)	110(1)
N(2)—Ni(1)—O(1)	99.3(3)	N(2)—C(7)—C(9)	110(1)
O(3)—Ni(1)—O(7)	93.7(3)	O(5)—C(8)—O(6)	125(1)
O(3)—Ni(1)—O(5)	90.7(3)	O(5)—C(8)—C(7)	120(1)
O(3)—Ni(1)—O(1)	88.2(3)	O(6)—C(8)—C(7)	115(1)
O(7)—Ni(1)—O(5)	91.2(3)	C(7)—C(9)—C(10)	119(1)
O(7)—Ni(1)—O(1)	91.7(3)	O(7)—C(10)—O(8)	126(1)
O(5)—Ni(1)—O(1)	176.9(3)	O(7)—C(10)—C(9)	119(1)
Ni(1)—O(1)—C(4)	110.5(7)	O(8)—C(10)—C(9)	114(1)
Ni(1)—O(3)—C(6)	127.7(7)	W(1)—Ni(2)—W(2)	87.0(3)
Ni(1)—O(5)—C(8)	109.7(8)	W(1)—Ni(2)—W(4)	175.8(3)
Ni(1)—O(7)—C(10)	129.0(8)	W(1)—Ni(2)—W(5)	90.2(3)
Ni(1)—N(1)—C(3)	105.0(7)	W(1)—Ni(2)—W(3)	87.5(3)
Ni(1)—N(1)—C(2)	105.3(7)	W(1)—Ni(2)—W(6)	92.5(3)
Ni(1)—N(2)—C(7)	103.8(7)	W(2)—Ni(2)—W(3)	88.9(3)
Ni(1)—N(2)—C(1)	105.1(7)	W(2)—Ni(2)—W(4)	97.1(3)
C(3)—N(1)—C(2)	116(1)	W(2)—Ni(2)—W(5)	177.2(3)
C(1)—N(2)—C(7)	114(1)	W(2)—Ni(2)—W(6)	87.9(3)
C(2)—C(1)—N(2)	107(1)	W(3)—Ni(2)—W(4)	91.6(3)
N(1)—C(2)—C(1)	108(1)	W(3)—Ni(2)—W(5)	91.6(3)
N(1)—C(3)—C(5)	109(1)	W(3)—Ni(2)—W(6)	176.8(3)
C(5)—C(3)—C(4)	112(1)	W(4)—Ni(2)—W(5)	85.7(3)
N(1)—C(3)—C(4)	107(1)	W(4)—Ni(2)—W(6)	88.6(3)
C(3)—C(4)—O(1)	120(1)	W(5)—Ni(2)—W(6)	91.6(3)

Selected torsion angles/°			
Ni(1)—N(1)—C(2)—C(1)	43(1)	C(3)—C(4)—O(1)—Ni(1)	−10(1)
N(1)—C(2)—C(1)—N(2)	−59(1)	C(4)—O(1)—Ni(1)—N(1)	28(1)
C(2)—C(1)—N(2)—Ni(1)	43(1)	O(1)—Ni(1)—N(1)—C(3)	−38(1)
C(1)—N(2)—Ni(1)—N(1)	−16(1)	Ni(1)—N(2)—C(7)—C(8)	39(1)
N(2)—Ni(1)—N(1)—C(2)	−15(1)	N(2)—C(7)—C(8)—O(5)	−20(1)
Ni(1)—N(1)—C(3)—C(5)	−79(1)	C(7)—C(8)—O(5)—Ni(1)	−11(1)
N(1)—C(3)—C(5)—C(6)	61(1)	C(8)—O(5)—Ni(1)—N(2)	28(1)
C(3)—C(5)—C(6)—O(3)	−10(2)	O(5)—Ni(1)—N(2)—C(7)	−37(1)
C(5)—C(6)—O(3)—Ni(1)	−11(2)	C(1)—C(2)—N(1)—C(8)	159(1)
C(6)—O(3)—Ni(1)—N(1)	− 8(1)	C(2)—N(1)—C(3)—C(4)	−73(1)
O(3)—Ni(1)—N(1)—C(3)	50(1)	C(2)—N(1)—C(3)—C(5)	165(1)
Ni(1)—N(2)—C(7)—C(9)	−80(1)	C(4)—C(3)—C(5)—C(6)	−57(1)

Table 3 (Continued)

Selected torsion angles/°			
N(2)— C(7)— C(9)— C(10)	50(1)	C(5)— C(3)— C(4)— O(1)	97(1)
C(7)— C(9)— C(10)— O(7)	7(2)	C(2)—C(1)—N(2)—C(7)	156(1)
C(9)— C(10)— O(7)—Ni(1)	−23(2)	C(1)—N(2)—C(7)—C(8)	−74(1)
C(10)— O(7)—Ni(1)— N(2)	− 6(1)	C(1)—N(2)—C(7)—C(9)	166(1)
O(7)—Ni(1)— N(2)— C(7)	54(1)	C(8)—C(7)—C(9)—C(10)	−68(1)
Ni(1)— N(1)— C(3)— C(4)	43(1)	C(9)—C(7)—C(8)—O(5)	99(1)
N(1)— C(3)— C(4)— O(1)	−23(1)		

Results and discussion

The crystal structure of $Ni_2((S^*, S^*)$-EDDS) $\cdot$ $10H_2O$ consists of complex anions $[Ni(1)(EDDS)]^{2-}$, hydrated cations $[Ni(2)(H_2O)_6]^{2+}$, and crystal water molecules. Complex anions, forming an enantiomeric pair, are related by a centre of symmetry so that there is only one anion in asymmetric unit (Fig. 1). Ni(II) atom of the complex anion is coordinated by two nitrogen atoms of ethylenediamine moiety and by four oxygen atoms of carboxyl groups of the single EDDS. Five chelate

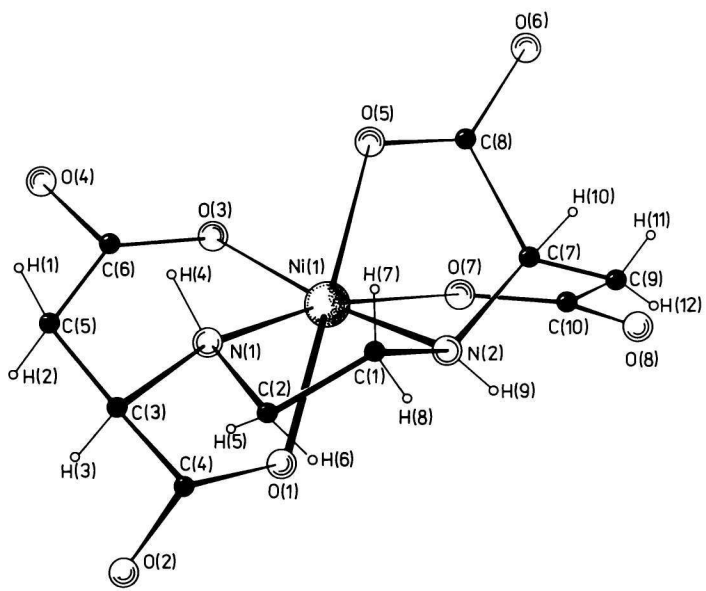

Fig. 1. Perspective representation of $[Ni((S^*,S^*)$-EDDS$)]^{2-}$ complex anion for (OC-6-13-A) absolute configuration and the numbering scheme of the atoms.

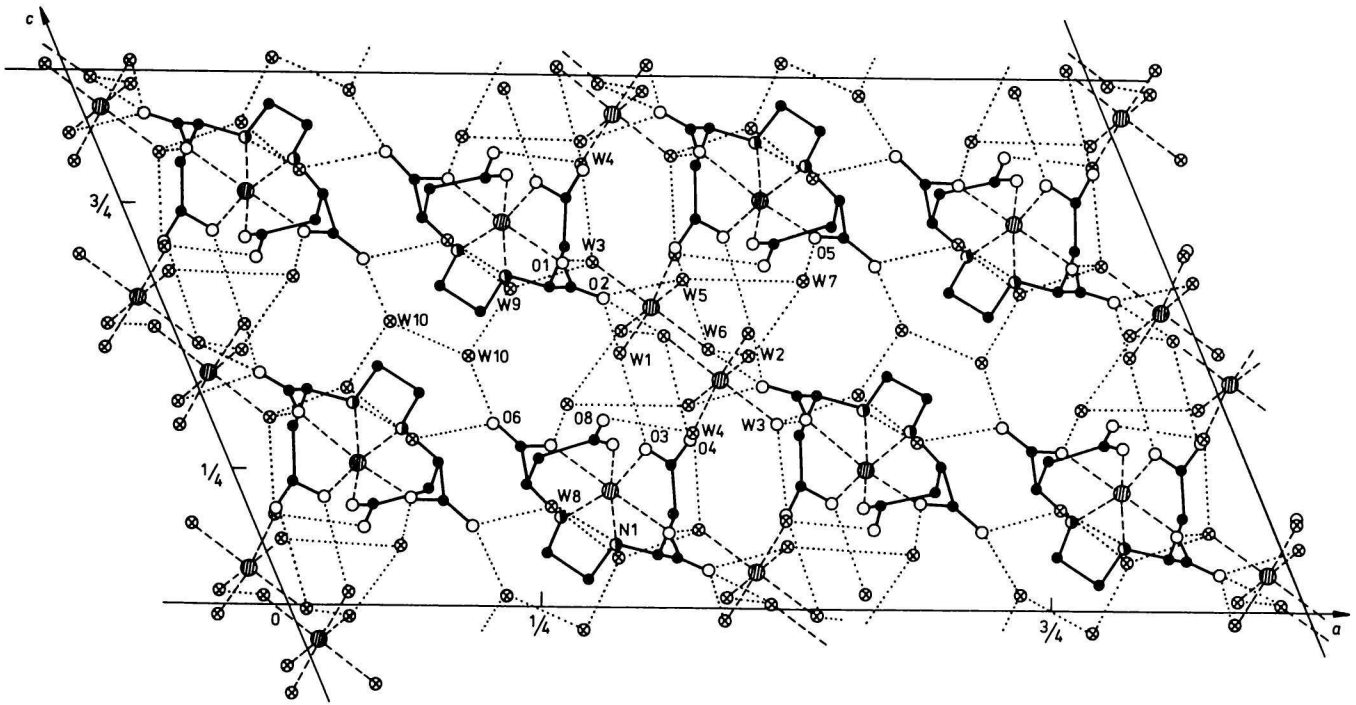

Fig. 2. Projection of unit cell in the direction of *b* axis. Coordination bonds are drawn in dashed lines. The system of hydrogen bonds is dotted.
Atom abbreviation is: ◍ Ni; ◑ N; ○ O; ● C; ⊗ water molecule.

rings are formed. A five-membered ethylenediamine ring (E-ring) and two six-membered β-alanine rings (G-rings) are situated in the equatorial plane. Two five-membered glycine rings (R-rings) are in the axial positions. Ring symbols E, G, and R are according to *Weakliem* and *Hoard* [12]. The values of torsion angles showed that the rings are not planar. E-ring has an almost symmetric *gauche* conformation, G-rings have an asymmetric twisted boat conformation and R-rings have an asymmetric envelope conformation.

The coordination polyhedron of Ni(1) is an octahedron regular from the point of view of bond lengths (0.205 nm) but highly distorted when bond angles are considered. Maximum deviations from the ideal values are $-11°$ from 180° and $+9.3°$ and $-11.2°$ from 90°. The bond lengths in the organic ligand are normal, their mean values are 0.1255 nm for C—O bond (there is no significant difference between coordinated and uncoordinated oxygen atom), 0.1482 nm for N—C bond, and 0.1533 nm for C—C bond.

The coordination polyhedron of Ni(2) is an octahedron, the six donors are water molecules. From the point of view of bond lengths it is also regular (0.206 nm) but the angle distortions are lesser in comparison with Ni(1). The maximum deviation from 180° is $-4°$, and the deviations from 90° are $+7.1°$ and $-4.6°$.

Table 4

Intermolecular hydrogen-bond contacts below 0.3 nm

Atoms		d/nm	Atoms		d/nm
N(1)	W(8^{i})	0.294(2)	W(5)	O(2^{v})	0.293(1)
W(1)	O(2^{v})	0.283(1)	W(5)	W(7^{iii})	0.269(1)
W(1)	O(3^{iv})	0.280(1)	W(6)	O(2^{vii})	0.271(1)
W(2)	W(6^{vi})	0.284(1)	W(6)	O(4^{iv})	0.259(1)
W(2)	W(7^{iv})	0.275(1)	W(7)	O(5^{i})	0.297(1)
W(3)	W(9^{i})	0.280(2)	W(8)	O(6^{v})	0.273(2)
W(3)	O(1^{v})	0.269(1)	W(8)	W(9^{v})	0.276(2)
W(3)	W(4^{ii})	0.285(1)	W(9)	W(10^{iv})	0.249(3)
W(4)	O(4^{iii})	0.265(1)	W(10)	W(10^{iv})	0.242(3)
W(4)	O(8^{iii})	0.270(1)	W(10)	O(6^{i})	0.267(2)

The equivalent positions are:

(i) x, y, z

(ii) $-x, y, \frac{1}{2}-z$

(iii) $x+\frac{1}{2}, y-\frac{1}{2}, z$

(iv) $-\frac{1}{2}-x, \frac{1}{2}-y, -z$

(v) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$

(vi) $-x, -y, -z$

(vii) $x-\frac{1}{2}, -\frac{1}{2}-y, z-\frac{1}{2}$

The absolute configuration of the complex anion, (OC-6-13-A) [13] for (S,S) configuration of the ligand is the same as in all so far studied complexes and this fact further supports conception of the expressive diastereoselectivity of an optical form of EDDS.

The packing of molecules in crystal, on the other hand, is different from the packing found in other structures of (S*,S*)-EDDS. The complex cations and complex anions are alone standing units (Fig. 2) held together only by coulombic forces and hydrogen bonds. In comparison with Ni(II) complex of (S,S)-EDDS and Fe(III) complex of *racemic* EDDS, no oxygen atom of the ligand takes part in the coordination polyhedron of the cation, there is not direct interconnection (*e.g.* coordination bond) among the structure units. In the space between anions and cations, crystal water molecules are situated. The system of hydrogen bonds can be deduced from Table 4.

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