

ISOMORPHISM IN THE THIOSACCHARINATES OF Mg, Co(II), Ni(II) AND Zn(II): COMPARISON WITH THE ANALOGOUS METAL SACCHARINATES

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The thiosaccharinates of magnesium, cobalt(II), nickel(II) and zinc(II) were synthesized and studied by infrared spectroscopy and powder X-ray diffraction and their structural properties were compared with the corresponding characteristics of the analogous metal saccharinates.

The very close similarity of the infrared spectra of the studied thiosaccharinates of magnesium, cobalt(II), nickel(II) and zinc(II) indicates isomorphism between them. Additional evidence is obtained from the study of their powder diffraction patterns which are also similar and confirm the isomorphism.

Contrary to the case of the corresponding saccharinates which are hydrates (the magnesium salt crystallizes as a heptahydrate, structurally different from the hexahydrates of the saccharinates of cobalt(II), nickel(II) and zinc(II) which form an isomorphous series), the studied metal(II) thiosaccharinates are anhydrous.

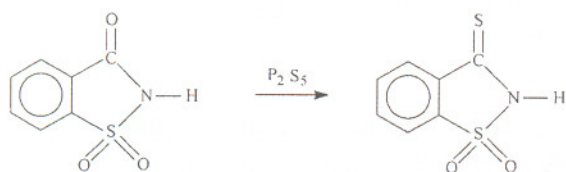
Only a single pair of strong bands was found in the infrared region where the SO₂ stretching vibrations are expected to appear, this being indicative for the existence of only one type of SO₂ groups in the structure.

Since various factors determine the frequency of the SO₂ stretchings, it is difficult to use the positions of the $\nu_{as}(\text{SO}_2)$ and $\nu_s(\text{SO}_2)$ bands as a tool for making conclusions about the type of metal-to-ligand bonding in the studied metal thiosaccharinates.

Key words: thiosaccharinates; magnesium; cobalt(II); nickel(II); zinc(II); isomorphism; analogous metal saccharinates

INTRODUCTION

1,2-benzisothiazol-3(2H)-one 1,1-dioxide, commonly known as saccharin, is cyclic imide which forms several types of metal saccharinates showing thereby different coordination patterns. Treated with P₂S₅ saccharin transforms into its thioanalogue thiosaccharin (1,2-benzisothiazol-3(2H)-thione 1,1-dioxide) (see Scheme 1). Thiosaccharin also forms metal thiosaccharinates, but less is known about its coordination ability.



Scheme 1

We have prepared and studied the structural characteristics (crystal structures and infrared spectra) of a series of metal saccharinates (including those of Mg, Co(II), Ni(II) and Zn(II)) [1–3], as well as thiosaccharinates of Na, K, Cd, Pb(II), Ca, Sr, Ba, Mn(II), Cu(II) and Hg(II) and thiosaccharin itself [4–12]. The structural characteristics of various metal saccharinates have also been studied by other authors [13–17] while, with the exception of the crystal structures of thiosaccharin [12] and its compounds with Na [4] and K [5] published by us, there are no structural examples of metal complexes with thiosaccharin.

In the course of the investigation of various metal thiosaccharinates we have prepared and studied the infrared spectra as well as the X-ray diagrams of the thiosaccharinates of Mg, Co(II), Ni(II) and Zn(II).

EXPERIMENTAL

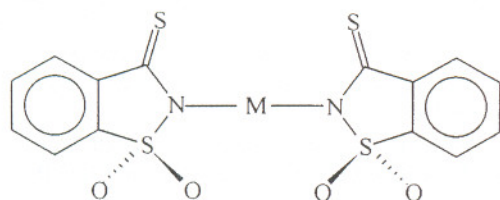
The studied compounds were synthesized for the first time by addition of an alcoholic solution of thiosaccharin to an aqueous solution of $Mg(NO_3) \cdot 6H_2O$, $Co(NO_3) \cdot 6H_2O$, $NiSO_4 \cdot 6H_2O$ and $ZnSO_4 \cdot 7H_2O$, respectively. The mixture was refluxed up to 373 K for 15 min. After cooling to room temperature, corresponding polycrystalline yellow substances (needle-shaped tiny little crystals) were obtained.

The infrared spectra were recorded on a Perkin Elmer 580 spectrophotometer and System 2000 FT IR interferometer using KBr discs. The band fitting was performed with the program GRAMS/32 [18].

The X-ray powder diagrams were obtained on a JEOL diffractometer using $CuK\alpha$ radiation ($\lambda = 154.178$ pm).

RESULTS AND DISCUSSION

The results of the elemental analysis for the studied metal thiosaccharinates are given in Table 1. They confirm the predicted formula $M(\text{thiosac})_2$ (see Scheme 2).



M = Mg, Co, Ni, Zn

Scheme 2

The infrared spectra of the title compounds are shown in Fig. 1. The very close similarity of the infrared spectra of the studied thiosaccharinates of Mg, Co(II), Ni(II) and Zn(II) indicates isomorphism between them.

Since the similarity between the infrared spectra can not a priori be taken as a proof that the studied compounds have the same crystal structure [9, 19], additional evidence about the isomorphism between the thiosaccharinates of Mg, Co(II), Ni(II) and Zn(II) was obtained from the study of their powder diffraction patterns. As can be seen from Fig. 2, the diffraction diagrams of the studied compounds are also very similar to each other, classifying the title compounds as members of the isomorphous series.

Unfortunately, our efforts to prepare the appropriate monocrystals for crystal structure determination of the title compounds were unsuccessful. In order to obtain some structural informations, the infrared spectra of the title compounds and the *ab initio* results for the thiosaccharin and deprotonated thiosaccharin [20] as well as the results of the normal coordinate analysis for compounds of similar type [21–23] were used.

Table 1

Elemental analysis for the studied thiosaccharinates of Mg, Co(II), Ni(II) and Zn(II)

Molecular formula	M_r	Elemental analysis (in mass %)					
		C		H		N	
		Cal.	Exp.	Cal.	Exp.	Cal.	Exp.
$C_{14}H_8N_2O_4S_4Mg$	420.65	39.97	37.57	1.92	2.13	6.66	6.22
$C_{14}H_8N_2O_4S_4Co$	455.27	36.93	38.85	1.77	1.96	6.15	5.96
$C_{14}H_8N_2O_4S_4Ni$	455.05	36.95	37.56	1.78	2.01	6.15	6.09
$C_{14}H_8N_2O_4S_4Zn$	461.71	36.42	36.74	1.75	1.94	6.06	5.99

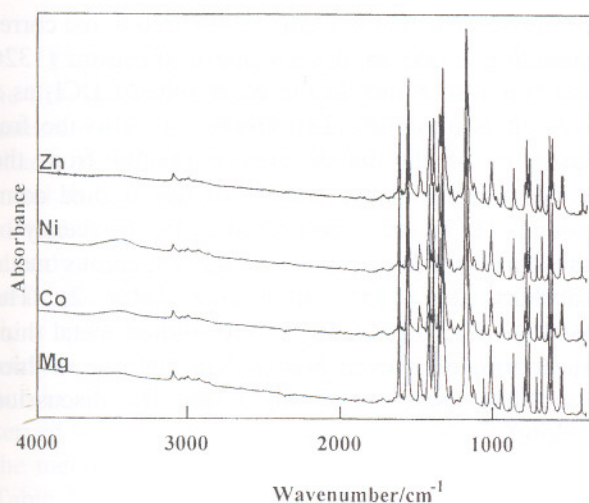


Fig. 1. The FTIR spectra of the thiosaccharinates of Mg, Co(II), Ni(II) and Zn(II)

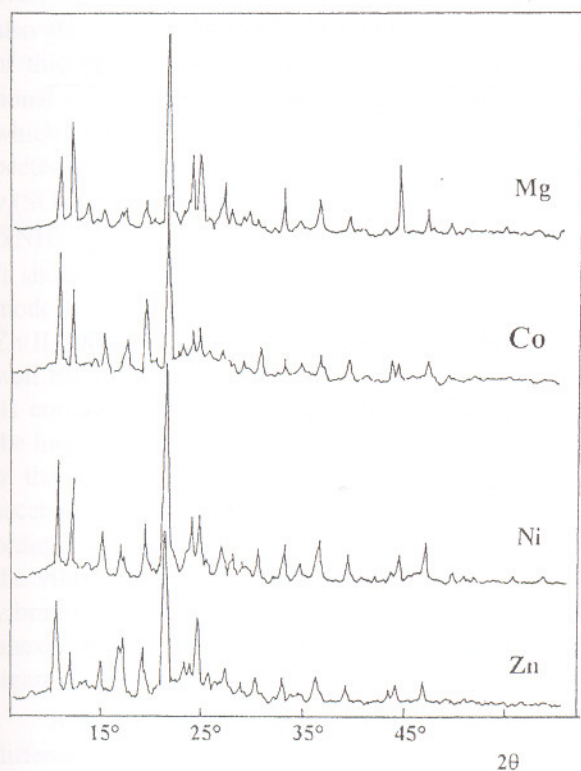


Fig. 2. The powder diffraction patterns of the thiosaccharinates of Mg, Co(II), Ni(II) and Zn(II)

Our main interest was focused on the frequencies of the bands due to the stretchings of the SO_2 groups. Although it is well known that the assignment of the bands originating from the SO_2 stretching vibrations in the saccharin and metal saccharinates [e.g. 24] as well as in thiosaccharin itself and

metal thiosaccharinates [6, 8, 11, 12] is accompanied by some difficulties concerning the presence of additional bands in the same spectral region [20–23], the strongest bands appearing in the spectra of the studied title compounds at 1330 cm^{-1} and 1176 cm^{-1} are assumed as antisymmetric [$\nu_{\text{as}}(\text{SO}_2)$] and symmetric [$\nu_{\text{s}}(\text{SO}_2)$] SO_2 stretching vibrations, respectively, Fig. 3. Generally, the antisymmetric sulphonyl stretching mode and the symmetric one in sulphones are considered to be good (characteristic) group vibrations manifested by the most prominent bands in the infrared spectrum. According to the *ab initio* calculations for the saccharin and thiosaccharin, that is applicable for the $\nu_{\text{as}}(\text{SO}_2)$ mode and partly in the case of the $\nu_{\text{s}}(\text{SO}_2)$ mode [e.g. 20, 25].

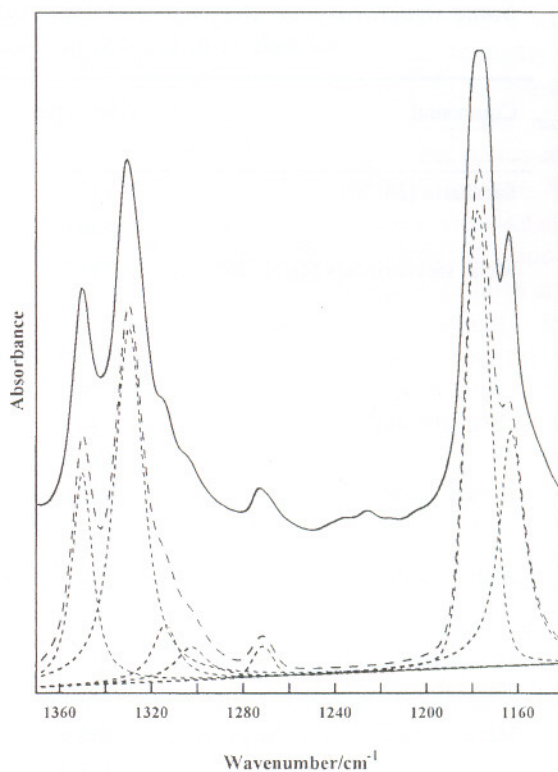


Fig. 3. The results of the curve-fitting procedure in the $\nu(\text{SO}_2)$ region in the FTIR spectrum of zinc(II) thiosaccharinate, the representative of the isomorphous series: original spectrum (full line); reconstructed spectrum (dashed line); the component bands (dotted lines)

Both, IR spectral analysis [24] as well as the *ab initio* force field treatment [25] have shown that the frequencies of the antisymmetric and symmetric SO_2 stretchings in metal saccharinates are lower than in saccharin itself. This lowering varies on going from one compound to another and is caused by various factors. Similarly, the *ab initio* treat-

ment for thiosaccharin and its deprotonated analogue [20] has shown that the frequencies of the $\nu(\text{SO}_2)$ modes decrease on going from thiosaccharin to metal thiosaccharinates. It is worth mentioning that the frequency of the $\nu_{\text{as}}(\text{SO}_2)$ mode in the spectra of the title compounds (1330 cm^{-1}) is, as expected, lower than the corresponding mode in thiosaccharin itself (1377 cm^{-1}) at the same time being considerably higher compared to the frequency of the respective mode in the corresponding metal saccharinates (1288 cm^{-1} in Co, Ni and Zn compounds and 1265 cm^{-1} in the Mg compound). The higher $\nu_{\text{as}}(\text{SO}_2)$ mode in the spectrum

of thiosaccharin (1377 cm^{-1}) compared to the corresponding mode in the saccharin spectrum (1326 cm^{-1}) is also found in the cases when CDCl_3 as a solvent is used [20, 25]. Higher are also the frequencies of the bands arising mainly from the $\nu_{\text{s}}(\text{SO}_2)$ mode in the spectra of the studied compounds (1176 cm^{-1}) compared to the frequency of the corresponding modes of the analogous metal saccharinates (1155 cm^{-1}) (see Table 2). The $\nu_{\text{s}}(\text{SO}_2)$ mode frequency in the studied metal thiosaccharinates is even higher than that one in thiosaccharin itself (1155 cm^{-1}) (see the discussion below).

Table 2

Some structural and spectroscopic data concerning the SO_2 groups in some metal saccharinates as well as in thiosaccharin and its compounds with various metals

Compound	R(S-O)/pm	$\angle(\text{O-S-O})^\circ$	Frequency data/ cm^{-1}				
			ν_{as}	ν_{s}	Δ	Δ'	Δ''
Saccharin [26, 27]	142.9	117.7	1335	1180	155		
	140.9						
Metal saccharinates Mg [1, 26]	144.5	114.4	1265	1155	110	70	25
	144.9						
	142.2						
	144.5						
Co(II) [13, 26]	144.7	116.5	1288	1155	133	47	25
	143.8						
Ni(II) [13, 26]	144.8	116.9	1288	1155	133	47	25
	143.8						
Zn(II) [14, 26]	144.6	116.7	1288	1155	133	47	25
	143.4						
Thiosaccharin [12]	143.1	117.5	1377	1155	222		
	142.5						
Metal thiosaccharinates Na [4, 6]	145.8	113.5	1270	1160	110	107	-5
	143.9						
K [5, 6]	144.3	113.7	1270	1160	110	107	-5
	144.2						
Hg(II) [11]			1309	1153	156	78	2
Mg			1330	1176	154	47	-21
Co(II)			1330	1176	154	47	-21
Ni(II)			1330	1176	154	47	-21
Zn(II)			1330	1176	154	47	-21

$\Delta = \nu_{\text{as}} - \nu_{\text{s}}$; $\Delta' = \nu_{\text{as}}(\text{sac}) - \nu_{\text{as}}(\text{M-sac})$ or $\Delta' = \nu_{\text{as}}(\text{thiosac}) - \nu_{\text{as}}(\text{M-thiosac})$;

$\Delta'' = \nu_{\text{s}}(\text{sac}) - \nu_{\text{s}}(\text{M-sac})$ or $\Delta'' = \nu_{\text{s}}(\text{thiosac}) - \nu_{\text{s}}(\text{M-thiosac})$;

sac, M-sac, thiosac and M-thiosac denotes saccharin, metal saccharinate, thiosaccharin and metal thiosaccharinate, respectively.

The lowering of the frequency of the symmetric SO_2 mode in the spectra of the metal saccharinates compared to the corresponding mode in saccharin as well as its lowering in the spectra of the metal thiosaccharinates compared to the spectrum of thiosaccharin itself is also expected, as it was already stated, according to the *ab initio* force field treatment [20, 25, respectively]. These expectations agree well with the results of the IR spectral analysis of metal saccharinates and saccharin itself but do not correspond with the experimentally observed frequencies for the symmetric SO_2 modes in the metal thiosaccharinates and thiosaccharin (see Table 2). As seen from Table 2, namely, except for the case of the Hg(II) compound, the frequency of the $\nu_s(\text{SO}_2)$ mode in the spectra of metal thiosaccharinates is higher than that one in the spectrum of thiosaccharin. It should be born in mind, however, that the *ab initio* force field treatment [20] also shows that the $\nu_s(\text{SO}_2)$ mode in the spectrum of thiosaccharin is mixed with at least two additional modes, one of them being the $\delta(\text{NH})$ mode which in the spectra of metal thiosaccharinates expectedly disappears. This is not the case with the $\nu_s(\text{SO}_2)$ mode in the spectrum of saccharin, where $\delta(\text{NH})$ mode is not a component of $\nu_s(\text{SO}_2)$ mode. It should be one of the reasons why the $\nu_s(\text{SO}_2)$ mode in the thiosaccharinates of Mg Co(II), Ni(II), Zn(II), Na and K does not follow the same already well established spectral pattern for saccharin and its compounds and instead to the lower, shifts to the higher frequencies. The presence of C=S group in the thiosaccharinates, instead of C=O group in saccharinates, with highly delocalized normal coordinates involved in more pronounced mixing of the vibrations in the region of the symmetric SO_2 vibrations could be additional explanation for the unexpected spectral behavior of thiosaccharinato ligand of the studied compounds.

It is interesting to mention that the frequency difference between the antisymmetric and symmetric SO_2 stretching vibrations in the spectra of the studied metal thiosaccharinates [$\Delta = \nu_{\text{as}}(\text{SO}_2) - \nu_s(\text{SO}_2) = 154 \text{ cm}^{-1}$] is larger compared to the corresponding value in the spectra of saccharinates of Co(II), Ni(II), Z(II) ($\Delta = 133 \text{ cm}^{-1}$) [26] and Mg ($\Delta = 110 \text{ cm}^{-1}$) [24, 26] (see Table 2). It could be related to the possible existence of larger O-S-O angle in the thiosaccharinate ligand of the studied metal thiosaccharinates compared to the values of the O-S-O angles in the saccharinate ligands of the analogous metal saccharinates, [24]. A slightly

more pronounced frequency difference between the antisymmetric and symmetric SO_2 stretching vibrations in deprotonated thiosaccharin (136 cm^{-1}) [20] compared to deprotonated saccharin (126 cm^{-1}) [25] is also found in the spectra recorded in DMSO- d_6 as well.

The appearance of the single pair of strong bands (see Fig. 2) in the region where the $\nu_{\text{as}}(\text{SO}_2)$ and $\nu_s(\text{SO}_2)$ modes are expected [6, 28–31] indicates the existence of only one type of SO_2 groups in the structure of the studied compounds [24]. The band shape analysis of the spectral region where the stretching SO_2 vibrations are expected, namely, has shown that the bands with smaller intensity appear as a result of other type of vibrations expected according to the *ab initio* force field treatment for thiosaccharin and its nitranion [20] while the *rest* of the bands with rather weak intensity are probably due to the combinations or overtones. Unfortunately, similarly to the case of the metal saccharinates [24], the positions of the bands arising from the antisymmetric and symmetric SO_2 stretching vibrations can not be used to make conclusions about the type of metal-to-ligand bonding in the studied metal thiosaccharinates (whose crystal structures are not determined). Namely, it is well known that various factors determine the frequencies of the SO_2 stretches [24] (e.g. the participation of the electron-donor atoms from the thiosaccharin ligand in the hydrogen bonding and/or in coordination sphere around the metal atom as well as the value of the O-S-O angle in the SO_2 group).

In order to obtain more precise structural information about the title compound, the spectroscopic characteristics of the thiosaccharinates of Mg, Co(II), Ni(II) and Zn(II) are compared with the ones of the analogous metal saccharinates with known crystal structures.

The comparison has shown that, contrary to the corresponding saccharinates of Mg, Co(II), Ni(II) and Zn(II) which are hydrates, the studied thiosaccharinates of Mg, Co(II), Ni(II) and Zn(II) are anhydrous. Otherwise, the saccharinates of Co(II), Ni(II) and Zn(II) are isomorphous hexahydrates [2], while the Mg saccharinate is heptahydrate [1] and expectedly does not belong to the isomorphous series of the saccharinates of bivalent Mn, Fe, Co, Ni, Cu, Zn and Cd [26]. The structural differences between the above mentioned isomorphous metal saccharinates, on the one hand, and the saccharinate of magnesium, on the other hand, are very clearly seen by the appearance of their

infrared spectra shown in Fig. 4. Namely, the infrared spectrum of Mg saccharinate heptahydrate in the region between 4000 and 400 cm^{-1} differs from the spectra of the isomorphous hexahydrated saccharinates of Mn(II), Fe(II), Co(II), Ni(II), Cu(II), Zn(II) and Cd(II). The differences are especially pronounced in the region of the stretching H_2O , CO and SO_2 vibrations as well as in the region of the H_2O librational modes.

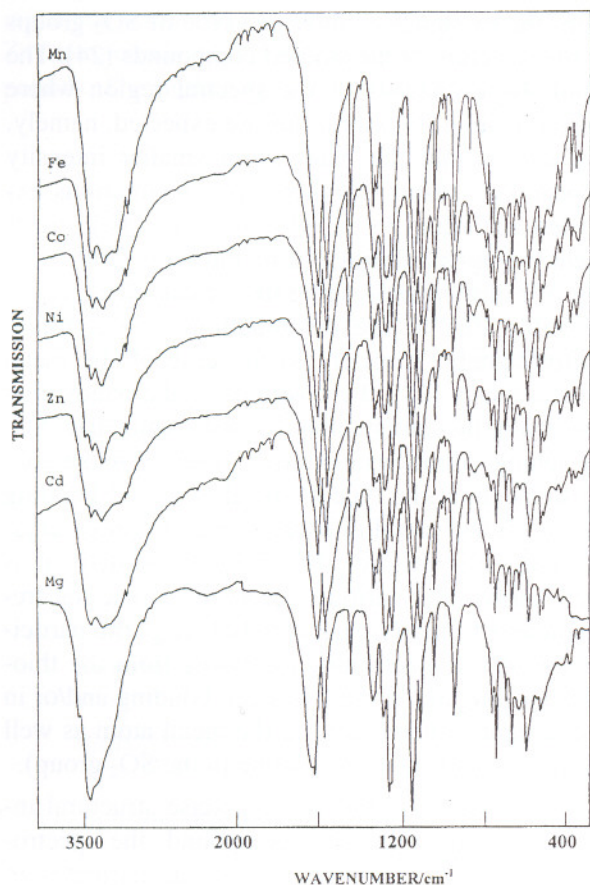


Fig. 4. The infrared spectra of the isomorphous hexahydrated saccharinates of Mn(II), Fe(II), Co(II), Ni(II), Cu(II), Zn(II) and Cd(II) compared to the spectrum of the Mg saccharinate heptahydrate in the region between 4000 and 400 cm^{-1}

Additional evidence about the previously determined [1, 2] structural dissimilarities between the saccharinates of Co(II) (as a represent of the isomorphous series) and Mg is obtained by the ap-

CONCLUSION

This work has confirmed the expected changes of the ligation properties of thiosaccharin compared to saccharin appeared due to the substitution of the oxygen atom in saccharin by sulfur

pearance of their infrared spectra in the region of the stretching OD vibrations of the isotopically isolated HOD molecules (where the D content does not exceed 3%), Fig. 5. Namely, the number of the bands originating from the stretching O-D vibrations in the spectrum of the Mg saccharinate heptahydrate is considerably larger (at least eight) compared to the number of the bands originating from the corresponding $\nu(\text{OD})$ modes in the spectrum of Co(II) saccharinate hexahydrate where only three types of crystallographically different water molecules exist (being manifested by the appearance of five bands in the spectrum). It corresponds (at least qualitatively) with the existence of seven crystallographically different water molecules (14 OH groups) in the structure of the heptahydrate of Mg saccharinate [1], manifested by presence of 14 hydrogen bonds with different $\text{O}_w \cdots \text{A}$ ($\text{A} = \text{proton acceptor}$) distances (some of them being very close to each other). On the other hand, in the structure of M(II) saccharinate hexahydrate ($\text{M} = \text{Mn, Fe, Co, Ni, Zn, Cd}$) [2, 13–15] only five different $\text{O}_w \cdots \text{A}$ distances appear in the structure.

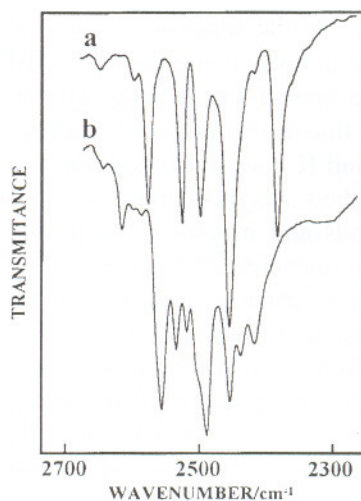


Fig. 5. The infrared spectra of Co(II) saccharinate hexahydrate (a) and Mg saccharinate heptahydrate (b) in the region of the stretching OD vibrations of the isotopically isolated HOD molecules

atom in thiosaccharin. The study of the title compounds has shown that, contrary to the saccharinate of the magnesium, which does not belong to the isomorphous series of the saccharinates of Co(II),

Ni(II) and Zn(II), the magnesium thiosaccharinate is a member of the group of isomorphous thiosaccharinates of Co(II), Ni(II) and Zn(II). It has been also shown that the thiosaccharinate compounds are anhydrous. Obviously, in all examined com-

pounds the ligand has the role of the decisive factor for the molecular structure of the compound.

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Резиме

ИЗОМОРФИЗАМ КАЈ ТИОСАХАРИНАТИТЕ НА Mg, Co(II), Ni(II) И Zn(II): СПОРЕДБА СО АНАЛОГНИТЕ МЕТАЛНИ САХАРИНАТИ

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Клучни зборови: тиосахаринати; магнезиум; кобалт(II); никел(II), цинк(II); изоморфизам; аналогни метални сахаринати

Синтетизирани се и испитувани тиосахаринатите на магнезиум, кобалт(II), никел(II) и цинк(II) со мето-

дите на инфрацрвена спектроскопија и рендгенска дифракција на спрашени обрасци. Нивните структурни

карактеристики се споредени со оние кај аналогните метални сахаринати.

Големата сличност на инфрацрвените спектри на изучуваните тиосахаринати на магнезиум, кобалт(II), никел(II) и цинк(II) укажуваат дека овие соединенија се изоморфни. Тоа го потврдуваат нивните рендгенограми на спрашени обрасци.

За разлика од соодветните сахаринати кои се хидрати (магнезиумовото соединение кристализира како хептахидрат и е структурно различно од хексахидратните сахаринати на кобалт, никел и цинк, кои се изоморфни), изучуваните метални тиосахаринати се безводни.

Постоењето на само еден пар ленти со силен интензитет во подрачјето на инфрацрвениот спектар каде што се очекуваат валентните SO_2 -вибрации укажува на постоење на само еден тип SO_2 -групи во нивните структури.

Со оглед на тоа што различни фактори влијаат врз фреквенцијата на SO_2 -валентните вибрации, положбите на лентите $\nu_{\text{as}}(\text{SO}_2)$ и $\nu_s(\text{SO}_2)$ тешко е да се употребат за донесување заклучоци за типот на врската метал-лиганд кај изучуваните метални тиосахаринати.