

**COMPARISON OF THE IR SPECTRA OF COMPLEX COMPOUNDS WITH
MIXED LIGANDS WITH THE RESULTS OF QUANTUM CHEMICAL
VIBRATION ANALYSIS**

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Abstract

In this article, the structure of complex compounds of Co(II), Ni(II), Cu(II) succinates with ethanolamines with mixed ligands is studied by comparing the vibration frequencies of the quantum-chemical analysis with the vibration frequencies of the practically obtained IR-spectra.

Keywords: metal succinate, monoethanolamine, diethanolamine, triethanolamine, IR spectrum.

This method of analysis is based on the change of vibration frequencies as a result of the impact of infrared rays on the substance. Infrared radiation is also called "thermal" radiation, because all solid and liquid objects heated to a certain temperature emit energy in the infrared spectrum. Usually, wave frequency is used to study IR-spectra. Depending on the changes in the specific absorption spectra of atomic groups, the positions of the maxima observed in the infrared spectra provide information about the structure of an individual compound or the components of complex substances.

IR-spectra of free molecules of ligands are as follows are represented by peaks (cm⁻¹) [1-4]:

Monoethanolamine: 3360- $\nu(\text{OH})$, 3290- $\nu_{\text{as}}(\text{NH}_2)$, 3200- $\nu_{\text{s}}(\text{NH}_2)$, 1660- $\delta(\text{NH}_2)$, 1290- $\nu(\text{C-N})$, 1070- $\nu(\text{C-O})$.

Diethanolamine: 3400- $\nu(\text{OH})$, 3310- $\nu_{\text{as}}(\text{NH})$, 3200- $\nu_{\text{s}}(\text{NH})$, 1694- $\delta(\text{NH})$, 1278- $\nu(\text{C-N})$, 1022- $\nu(\text{C-O})$.

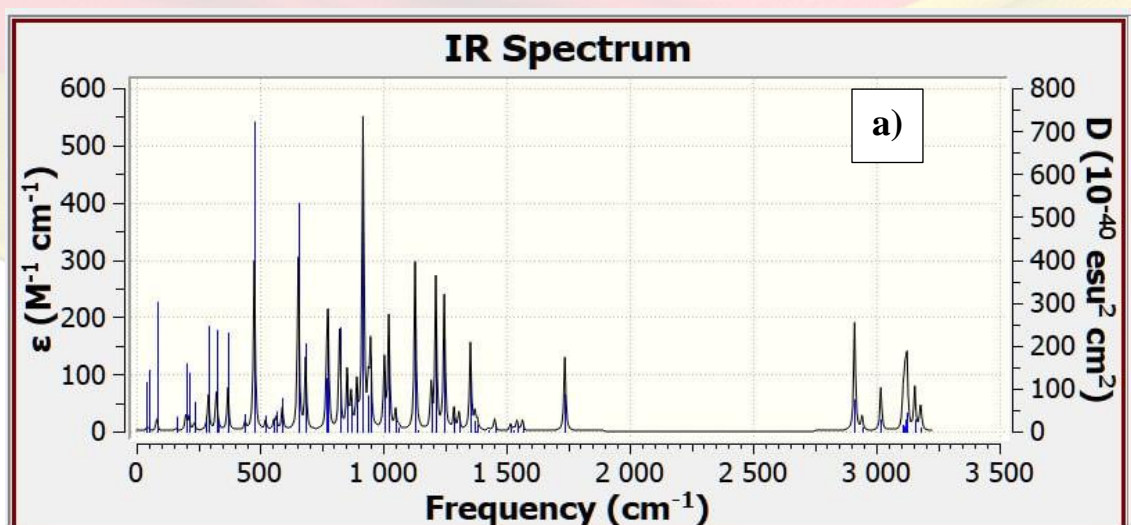
Triethanolamine: 3600 – $\nu(\text{OH})$, 1607- $\nu(\text{C-N})$, 1050- $\nu(\text{C-O})$, 1066- $\nu(\text{CN})$.

Succinic acid: 905 – $\nu(\text{OH})$, 1420- $\nu(\text{C-O})$, 1720- $\nu(\text{C=O})$.

It is possible to make a sufficient conclusion about the formation of coordination bonds in complex compounds using the quantum-chemical method of IR-spectroscopy and comparing with the spectra obtained in practice. If the vibrational frequencies generated by quantum-chemical calculations match or closely match the experimentally obtained frequencies, then the predicted analysis will be confirmed.

In the mixed-ligand metallocomplex compounds of cobalt(II), nickel(II) and copper(II) succinates obtained with MEA in a 1:1 ratio, changes in the valence vibrations of C-O bonds were observed, in which the valence vibrations of C-O, NH bonds were 24-51 cm^{-1} increased to And the vibrational frequencies of the C=O bond decreased by 5-88 cm^{-1} , respectively. From this, it can be shown that the nitrogen atom of the amino group and the oxygen of the carbonyl group of succinic acid participate in the formation of complexes with cobalt, nickel and copper succinate in the ratio of MEA 1:1 (Fig.1).

In the IR-spectra of compounds obtained with 1:2 and 1:3 ratio of MEA, it was noted that the absorption frequency of valence vibrations of C-O and NH bonds increased by 4-24 cm^{-1} , and no change was observed in the vibration frequencies of C=O bond. It follows that the coordination bond in complexes with metals is formed through the nitrogen of the amino group and the oxygen of the hydroxyl group in MEA.



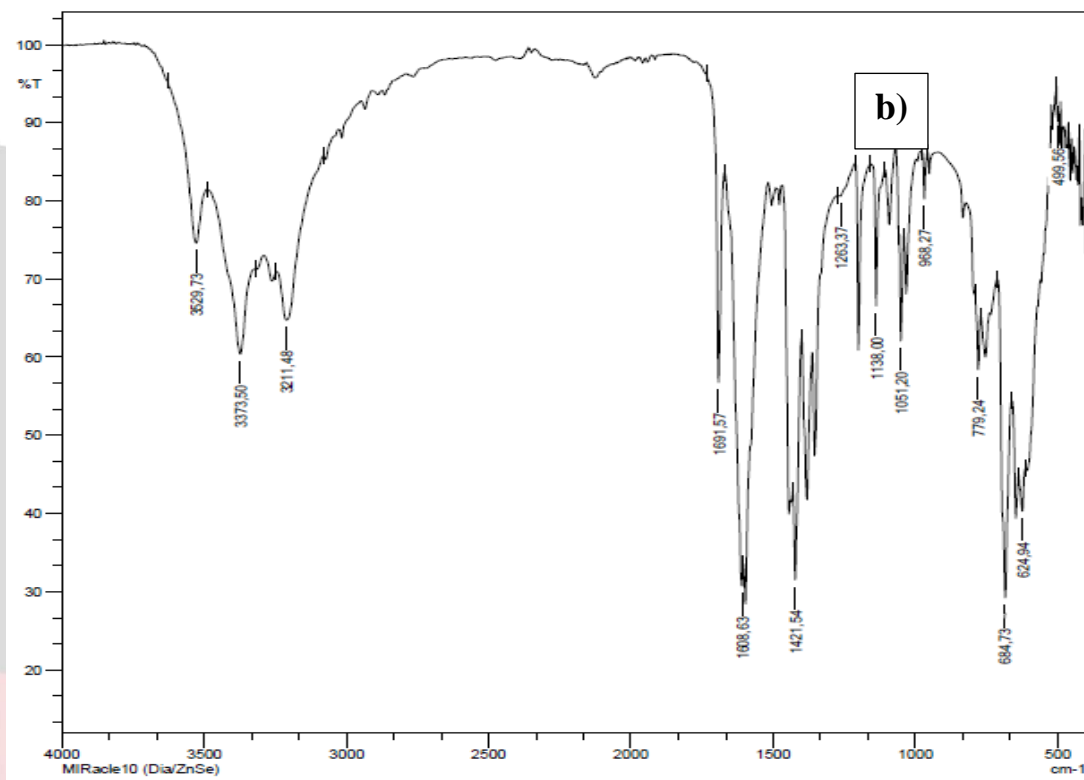
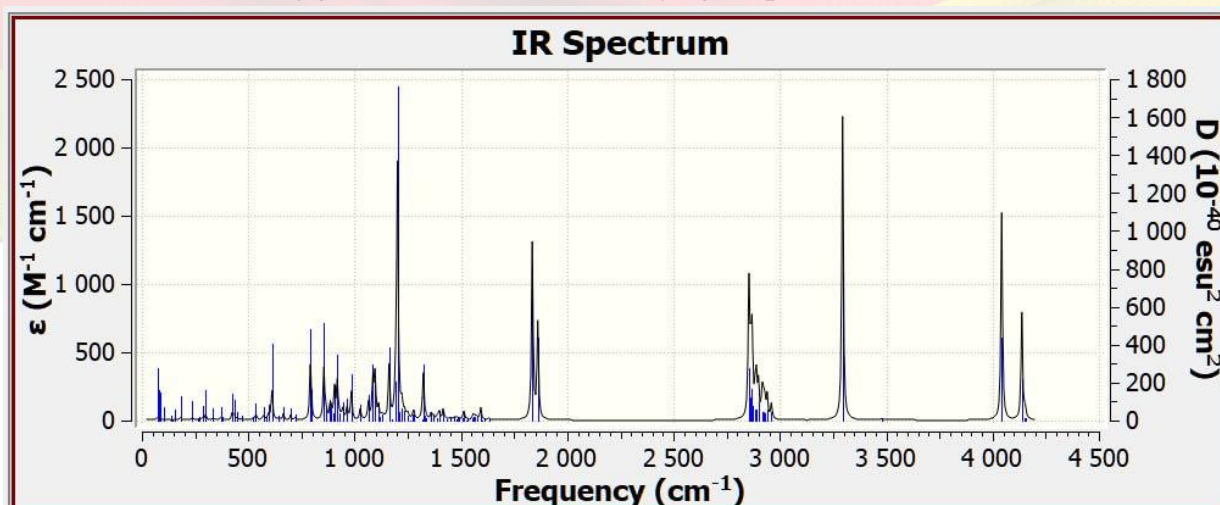


Figure 1. Quantum-chemical (a) and practical (b) IR-spectra of the complex compound [Cu(Suc)(MEA)]

In the complexes of DEA with cobalt(II), nickel(II) and copper(II) succinates in a ratio of 1:1, it was noted that the absorption frequencies of the valence vibrations of the oxygen atom in the hydroxyl group decreased by 13-18 cm^{-1} , and no change was observed in the NH bond. In addition, a change in the vibrational frequencies of the C=O bond in succinate was also observed. This indicates that the metal ions are coordinated through the oxygen of the hydroxyl group in DEA and the oxygen atom of the carbonyl group in succinate.



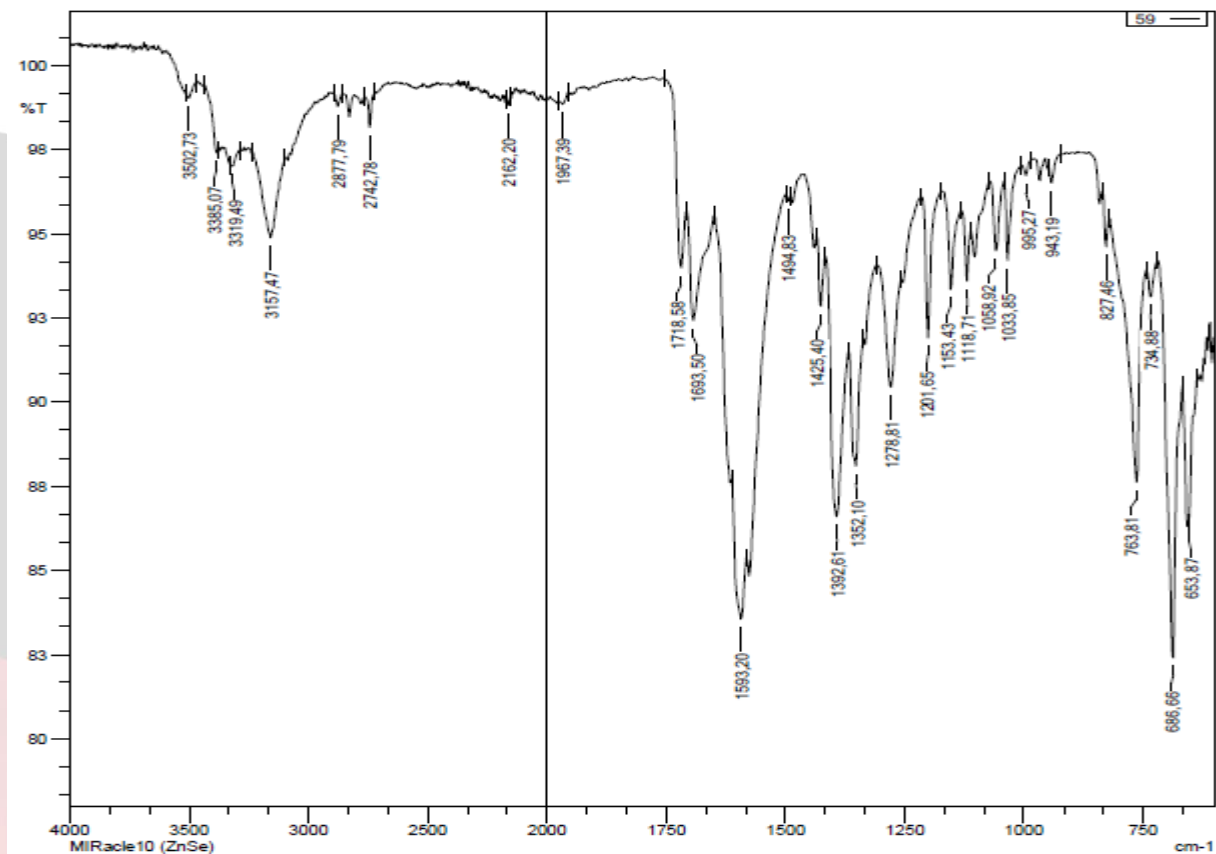
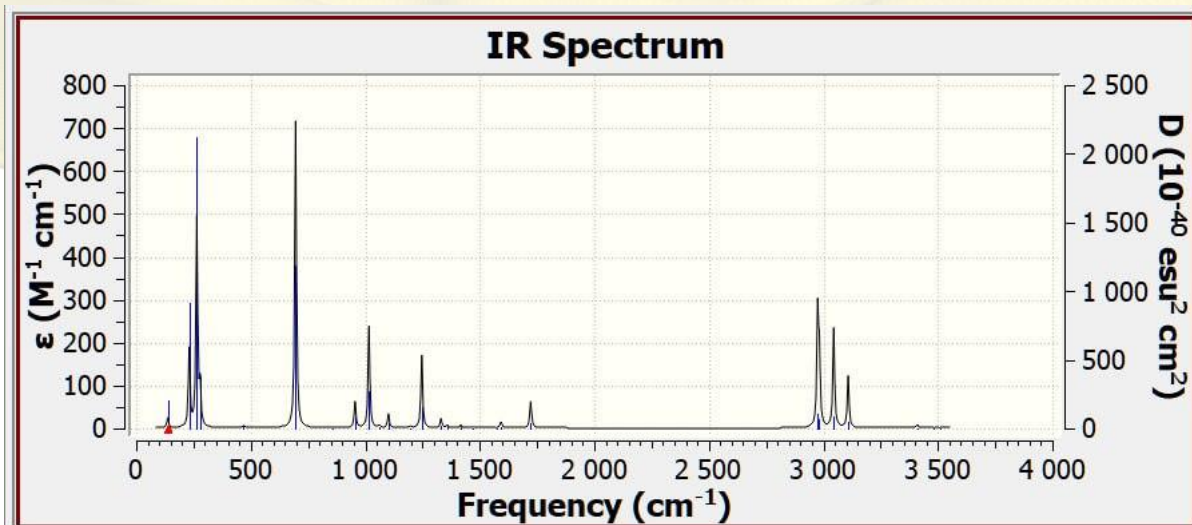


Figure 2. Quantum-chemical (a) and practical (b) IR-spectra of the complex compound [Ni(Suc)(DEA)₂]

In mixed ligand metallocomplexes of cobalt(II), nickel(II), copper(II) succinate obtained with DEA in a ratio of 1:2, changes in the valence vibrations of C-O and NH bonds were observed, while the valence vibrations of the C-O bond increased by 85 cm⁻¹. And the vibrational frequencies of the NH bond decreased by 71 cm⁻¹. From this, it can be shown that the formation of DEA complexes with cobalt(II), nickel(II), copper(II) ions in a ratio of 1:2 involves nitrogen and hydroxyl oxygen atoms of the amino group (Fig. 2).



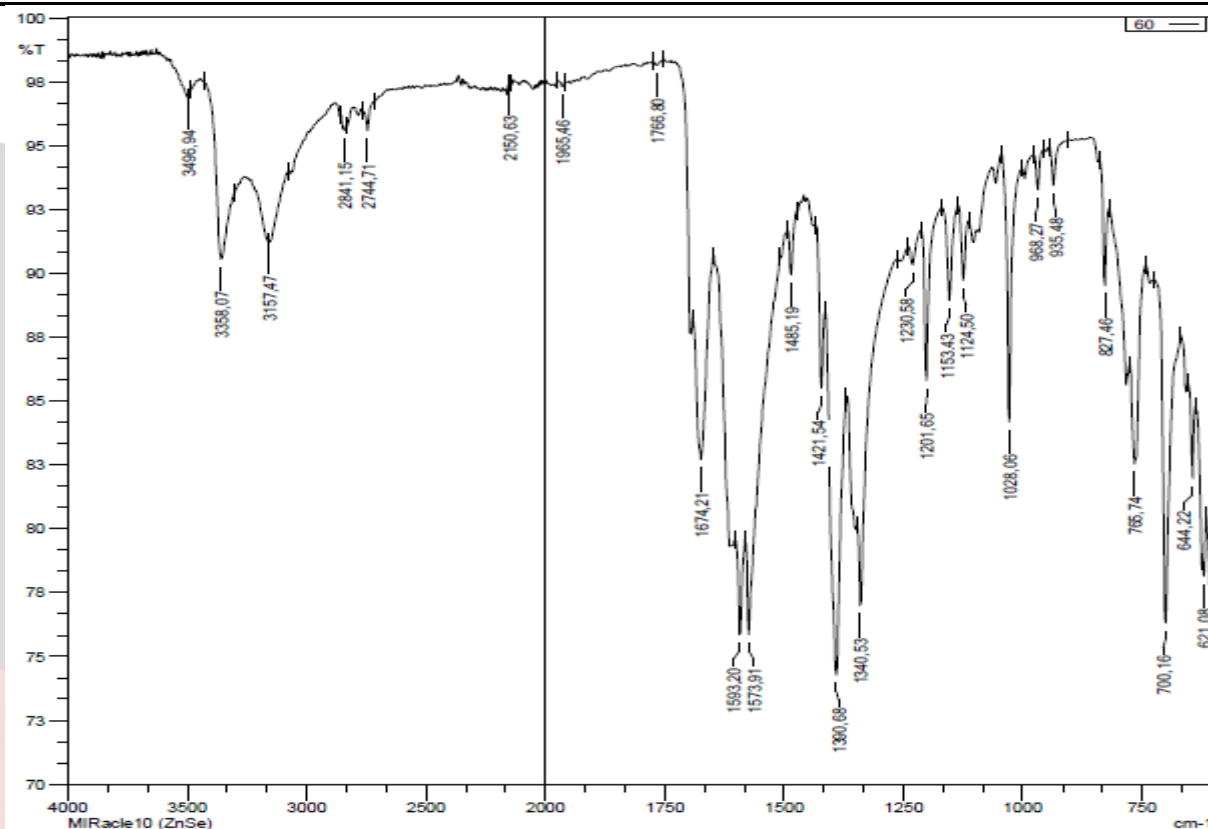


Figure 3. Quantum-chemical (a) and practical (b) infrared spectra of the complex compound [Co(Suc)(TEA)₂]

In the mixed ligand complex compounds of cobalt(II), nickel(II), copper(II) obtained with DEA in a ratio of 1:3, the decrease in the absorption frequencies of the valence vibrations of the oxygen atom of the hydroxyl group in DEA by 9-17 cm⁻¹ indicates its coordination with metal ions. No change was observed in the vibrational frequencies of the NH bond in DEA. In complexes of TEA with cobalt(II), nickel(II), copper(II) succinate in 1:1, 1:2 and 1:3 ratios, the absorption frequencies of the valence vibrations of the nitrogen atom contained in TEA decrease by 9-17 cm⁻¹. A change in C-O bond valence vibrations is observed, in which C-O bond valence vibrations increase by 12-85 cm⁻¹. This shows that nitrogen atom and hydroxyl groups of TEA are coordinated with metal ions through oxygen atoms (Fig. 3).

Table 1 Quantum-chemically calculated and IR-spectrum main vibrational frequencies of synthesized complex compounds

	[Cu(Suc)(MEA)]		[Co(Suc)(TEA) ₂]		[Ni(Suc)(DEA) ₂]	
	theoretical	practical	theoretical	Practical	theoretical	Practical
v(O-H)	3330	3373	3361	3358	3310	3319
v(C-O)	1053	1051	1002	1028	1035	1034
δ(NH ₂)	1662	1608	-	-	-	-
δ(N-H)	-	-	-	-	1694	1693.5
v(C-N)	-	-	1338	1352	-	-
v(C=O)	1750	1692	1793	1767	1739	1714
v(M-O)	701	683	681	700	684	686

By comparing the practically obtained IR-spectra of complex compounds with mixed ligands synthesized in different proportions with the results of the theoretical calculation analysis of quantum-chemical vibrations, it can be concluded that the values of the vibration frequencies of the theoretical vibration frequencies and IR-spectra are close to each other. This means that it is the coordination bonds formed in the spheres and indicates that octahedral complex compounds are formed.

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