

## ABSORPTION OF THE MONONUCLEAR Fe(III) COORDINATION COMPOUNDS

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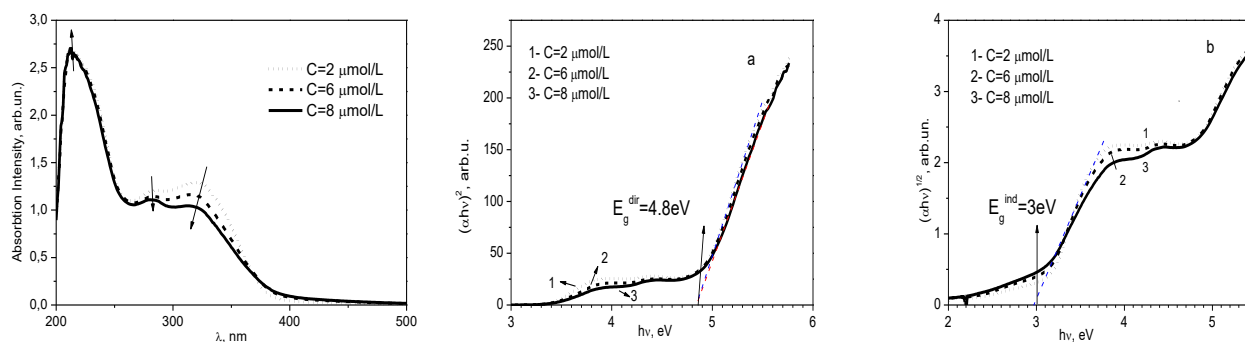
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This paper presents the study of wide-gap semiconductors in the form of two new Fe(III) mononuclear coordination compounds ( $[\text{Fe}(\text{H}_2\text{L})(\text{H}_2\text{O})_2] \cdot \text{X}_2 \cdot 2.5\text{H}_2\text{O}$ , where  $\text{X}=\text{NO}_3^-$ ,  $\text{ClO}_4^-$ ) based on the 2,6-diacetylpyridine bis(picolinoylhydrazone) ( $\text{H}_2\text{L}$ ).

Optical absorption spectra were measured using **UV-Vis Spectrophotometer (PerkinElmer Lambda 25)** at 300 K in the wavelength range 200-500 nm measured. The UV-vis spectral titration of  $\text{H}_2\text{L}$  with  $\text{Fe}^{3+}$  were carried out by gradually increasing the amount of  $\text{Fe}^{3+}$  (10-100  $\mu\text{L}$ ) in the ethanol media of ligand. The spectra of three concentrations of  $\text{Fe}^{3+}$  (Fig.1) represent a series of curves characterized by the position of the absorption maxima at the same wavelength and differing only in their intensities. Upon successive addition of  $\text{Fe}^{3+}$  the absorbance bands gradually decreases in intensity, accompanied by the appearance of shoulder peaks in the region of 250-400 nm.

To estimate the band gap  $E_g$ , Tauc coordinates were used [1]:  $(\alpha \cdot h\nu)^{1/n} = h\nu - E_g$ , where  $\alpha$  is the absorption coefficient,  $E_g$  is the band gap,  $n$  is a constant depending on the type of electronic transition in the material.

An analysis of the optical absorption spectra under the assumption of direct allowed transitions ( $n=1/2$ ) is presented in the inset to figure 2a. Approximation of the intrinsic absorption edge constructed in coordinates  $(\alpha h\nu)^2$  from  $(h\nu)$  gives the value of the direct band gap ( $E_g^{\text{dir}}$ ). Approximation of the intrinsic absorption edge plotted in coordinates  $(\alpha h\nu)^{1/2}$  from  $(h\nu)$ , which corresponds to allowed indirect transitions, shows the value of the indirect band gap ( $E_g^{\text{indir}}$ ) (Fig. 2b).



**Figure 1.** Absorption spectra at various concentration  $s(C)$

**Figure 2.** The edge of the optical absorption band in the Tauc coordinates of the sample for three concentrations

Approximations of the curves of the intrinsic absorption edge taken for different concentrations converge at one point and give the exact value of the width of the direct ( $E_g^{\text{dir}} = 4.8 \text{ eV}$ ) and indirect ( $E_g^{\text{indir}} = 3.0 \text{ eV}$ ) band gap.

These values agree well with those theoretically calculated from the band structure.

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[1] Tauc J. Optical Properties and Electronic Structure of Amorphous Germanium /J.Tauc, R.Grigorovici, A.Vancu. *Physica status solidi*. 1966. Vol. 2, I. 15. P. 627–637.