Contribution ID: **80** Type: **POSTER**

57Fe Quadrupole Splitting and Isomer Shift in Various Oxyhemoglobins: Study Using Mössbauer Spectroscopy

Comparison of the heme iron electronic structure in various hemoglobins is very important in order to analyze structure-function relationship of oxygen carriers. It is well known that small stereochemical differences exist in the heme iron in different hemoglobins as well as in non-identical subunits in tetramer. Mössbauer spectroscopy is the most sensitive technique to study iron electronic structure in various species including iron-containing proteins. It was shown earlier that Mössbauer spectroscopy with a high velocity resolution increased possibilities of technique in accuracy of hyperfine parameters evaluation and revealing its small variations [1]. Mössbauer spectra of oxyhemoglobin samples from pig, rabbit, normal human and patients with blood system malignant diseases were measured using spectrometric complex with a high velocity resolution [2] at 90 K in 4096 channels. Then Mössbauer spectra were presented for analysis in 1024 channels by consequent summation of 4 neighboring channels. Mössbauer spectra were fitted in two ways using one quadrupole doublet (model of equivalent iron electronic structure in ⍺–and ⍺–subunits of hemoglobins) and superposition of two quadrupole doublets (model of non-equivalent iron electronic structure in ⍺–and ⍺–subunits of hemoglobins). Small variations of hyperfine parameters obtained within the first model are shown in Fig. 1. Hyperfine parameters obtained using both models were compared with structural and functional properties of hemoglobins.

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Track Classification: Biology, Chemistry, Medicine