P-02

X-RAY ABSORPTION FOR CHARACTERIZING LOCAL ENVIRONMENT IN MALARIA PIGMENT

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Malaria is still one of the most devastating infectious diseases in the world. Moreover, *Plasmodium* parasite which causes malaria illness has recently become widely resistant to commonly used antimalarial therapies. Therefore, new antimalarial drugs are desperately needed. However, precise mechanism of action of currently drugs as well as haem detoxification by *plasmodium* is still not well understood.

The *plasmodium* parasite has a complicated life cycle, with several developmental stages. One of *Plasmodium* parasite's intraerythrocytic phases uses hemoglobin (oxygen carrying enzyme) as a nutrient source. During hemoglobin's degradation process the haem is released and subsequently the parasite converts it into microcrystalline material, called hemozoin, by its polymerization. Mechanism of haem polymerization and its inhibition is unclear. The crystallographicaly and spectroscopicaly similar to malaria pigment is synthetic β-hematin, which could be used as substitute of hemozoin in antimalarial drug research.

The bonding of Fe-ion in hemozoin and β-hematin has been the subject of our investigation. Using x-ray absorption spectroscopy we tried to determine local environment of Fe-ion in the malaria pigment and β-hematin, in relation with previous diffraction and spectroscopic results. The measurements of Fe K-edge of x-ray absorption were performed at the HASYLAB beamline A1 in the fluorescence mode using a five-elements Si detector. The samples were cooled down to LN temperature. The Si monochromator was operated in two crystalline mode.

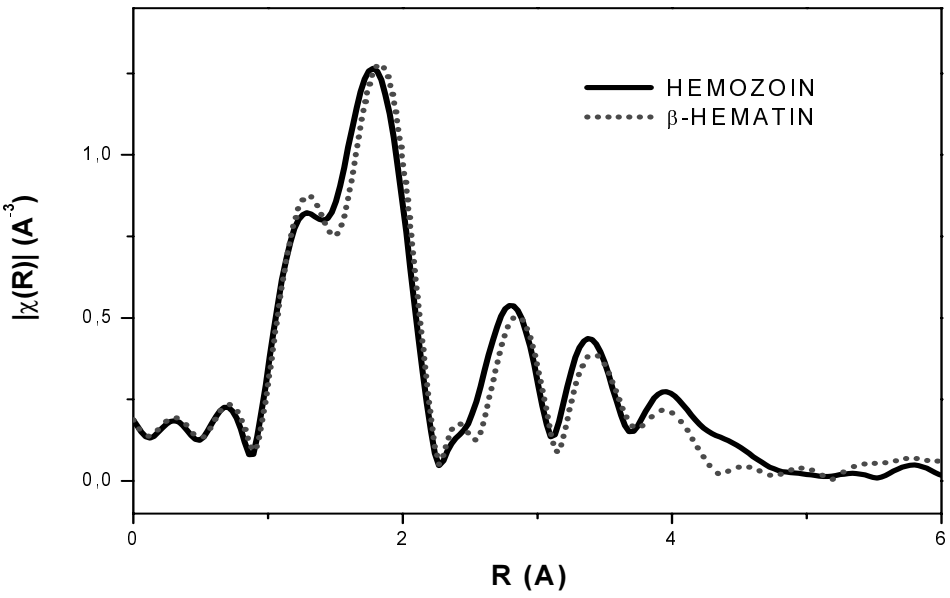

Figure 1. Radial distribution of atoms around the Fe in hemozoin and β-hematin.

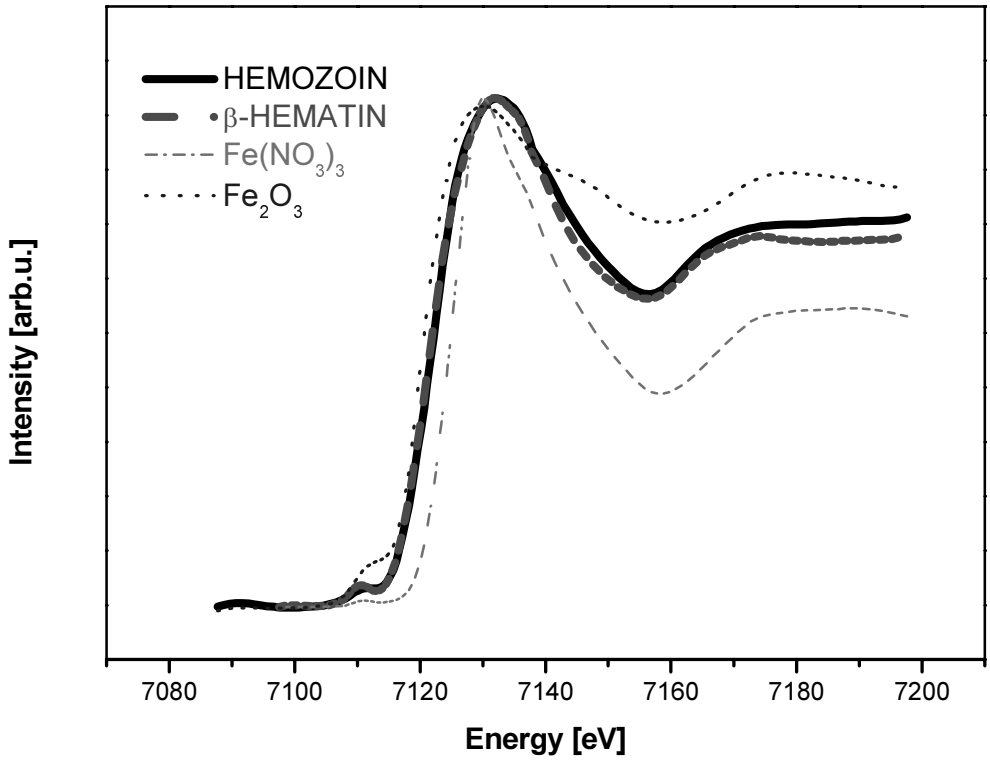

Figure 2. XANES spectra of hemozoin, β-hematin and reference spectra of Fe_2O_3 and $Fe(NO_3)_3$.

The radial distribution of atoms around Fe obtained from EXAFS (extended x-ray absorption fine structure) averaged from three spectra and taken in *k*-range up to 10 $Å^{-1}$ are presented in Fig. 1. One can see that radial distributions of atoms around Fe in malaria pigment and β-hematin differ only in details, therefore both materials have very similar atomic surrounding, nevertheless some difference with atomic distance can be responsible for small shift in the position of peaks.

The information about the nature of chemical bonding one can get from the XANES (x-ray absorption near edge structure). In the Fig. 2 the XANES spectra of hemozoin, β-hematin and reference spectra of Fe_2O_3 and $Fe(NO_3)_3$ are presented. Judging from the shift of the Fe-edge the ionic state of Fe in hemozoin and β-hematin are identical and very similar to that in Fe_2O_3. This evidence that the ionic state of iron in the both investigated materials is Fe^{+3}.

The model of atomic distribution constructed using the FeFF8 will be presented and discussed with reference to diffraction data.

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