



Experiment title:
XANES investigation of local iron environment in synthetic homologues of malarial pigment

Experiment number:
MD-346

Beamline:
ID26

Date of experiment:
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18

Local contact(s):
Marcin Sikora

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Names and affiliations of applicants (* indicates experimentalists):

Monika Walczak^{1*}, Krystyna Lawniczak-Jablonska^{1*}, Anna Wolska^{1*}, Marcin Sikora^{2*}

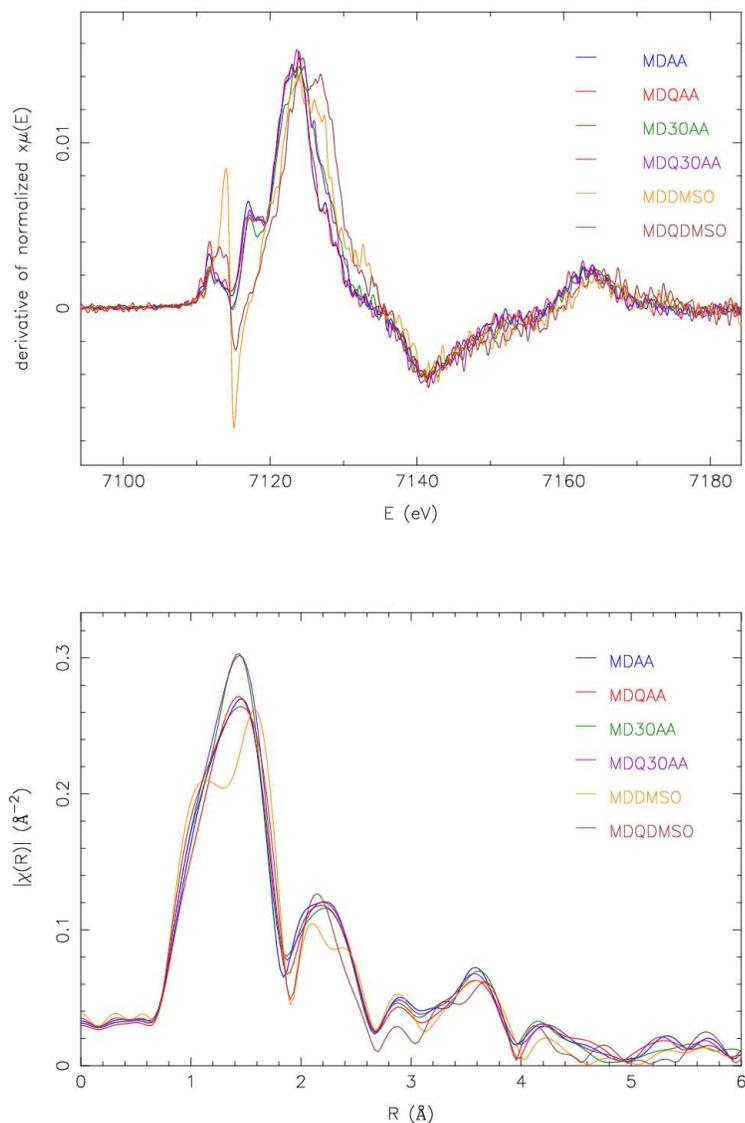
¹Institute of Physics, Polish Academy of Sciences
Al. Lotników 32/46, PL 02-668 Warsaw, Poland

²European Synchrotron Radiation Facility
6 rue Jules Horowitz, Bote Postale 220, 38043 Grenoble, France

Report:

Project was the continuation of performed on station BM26A EXAFS experiment (MD-317) and as well as before concerned newly-synthesized soluble β -hematin-like compound, mesoporphyrin-IX anhydride. The structure of β -hematin is built of chains of dimers. These dimers are formed by the FeIII protoporphyrin-IX molecules through reciprocal iron-carboxylate bonds to one of the propionic side chains of each porphyrin. Mesoporphyrin-IX anhydride (MD) has been studied by extended X-ray absorption fine structure (EXAFS) and X-ray absorption near edge structure (XANES) techniques to determine the ionic state and distribution of atoms around Fe atom in solution with and without presence of antimalarial drug. Spectra were acquired on iron edge using fluorescence detection mode. Because of different chloroquine solubility in pure acetic acid (AA) and acetic acid with water addition solvent, the patterns of spectra shape of MD solved with different water amount were compared. As a second control solvent dimethyl sulfoxide (DMSO) was used. EXAFS spectrum of MD in acetic acid with addition of water with ratio 1:30 (MD30AA) is the same as spectra of that solution after adding chloroquine drug (MDQ30AA). Exactly the same is observed for MD solved in pure acetic acid (MDAA) where change in EXAFS shape of MD after adding antimalarial drug (solution MDQAA) can be omitted. Nevertheless the difference between spectra of MD solved with different ratio of water is obvious and does not depend on the presence of chloroquine.

XANES of MD solvated in acetic acid does not introduce any significant change after drug addition and bigger difference can be observed between spectra of MD solvated with different water ratio (edge shift). Opposite is for DMSO solvent where especially so called peak 1s-3d of quadrupole transition is showing some response for presence of chloroquine. EXAFS spectrum as well indicates changes in pattern for MD solution in DMSO (MDDMSO) after drug addition (MDQDMSO). Firsts atomic neighbors of iron inside protoporphyrin IX ring and also axial oxygen had to be moved.



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