ESRF	**Experiment title: Unravelling dimetal-carboxylate catalysis in enzymes by means of nuclear inelastic scattering**	**Experiment number**: LS-2422
Beamline: ID-18	**Date of experiment**: from: 10/12/2015 to: 13/12/2015	**Date of report**: 01/03/2016
Shifts: 9	**Local contact(s)**: Aleksandr Chumakov, Rudolf Rüffer	*Received at ESRF:*

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Report:

Within experiment LS-2422 we have obtained NIS data sets for the following ribonucleotide reductase [1-5] R2 samples: (i) the ribonucleotide reductase R2 subunit from *escherichia coli* in its oxidised state, (ii) the R2 subunit from *saccharopolyspora erythraea* in its oxidised state, reconstituted with manganese and ^{57}Fe and (iii) the R2 subunit from *saccharopolyspora erythraea* in its oxidised state, reconstituted with ^{57}Fe. The partial density of vibrational states (pDOS) derived from the obtained data sets are shown in Figure 1. From the data we clearly see a different mode distribution between the R2a class protein and the two R2c class proteins, resulting in a increased intensity in the energy range from 400-500 cm^{-1} for the R2a protein, and an increased intensity in the range from 200-300 cm^{-1} for the R2c protein. The most eye-catching difference between the manganese-iron and the iron-only reconstituted R2c sample is the 5-band structure from 180-290 cm^{-1} and the intense band at 355 cm^{-1} for the purely with ^{57}Fe reconstitued sample.

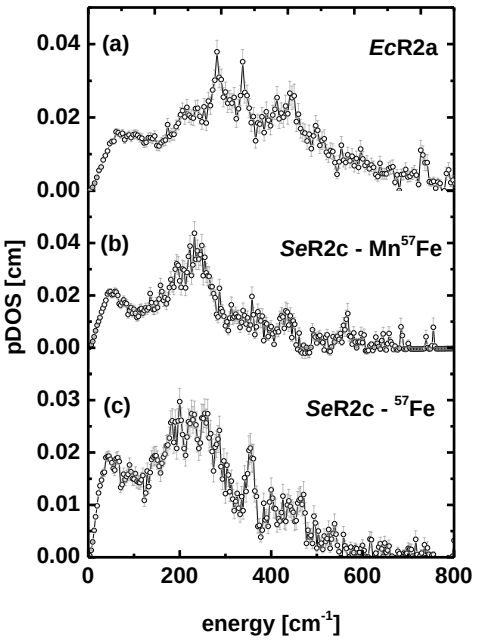

Figure 1: NIS data of (a) the R2a from *escherichia coli*, reconstituted with ^{57}Fe; (b) R2c from *saccharopolyspora erythraea*, reconstituted with Mn and ^{57}Fe and (c) R2c from *saccharopolyspora erythraea*, reconstituted with ^{57}Fe. The data have been measured at ID-18 of ESRF during LS-2422 with an energy resolution of 0.74 meV (~ 6 cm^{-1}) and a temperature setting of 20 K.

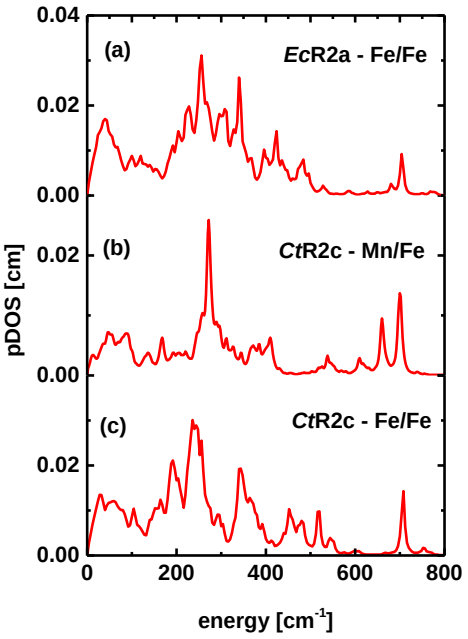

Figure 2: DFT derived simulated pDOS of (a) *Ec*R2a with a diiron center (1MXR) (b) *Ct*R2c (1SYY) as a model for *Se*R2c with a Mn/Fe center and (c) *Ct*R2c (1SYY) as a model for *Se*R2c with a Fe/Fe center. Geometry optimization and normal mode analysis was done using GAUSSIAN 09, Rev.D. The crystallographic structure of *Ct*R2c was used as the structure of *Se*R2c is not yet available.

The experimental data shown in Fig. 1 are currently being analysed by theoretical quantum chemical calculations which are coupled to molecular mechanics calculations in order to perform a full normal mode analysis of the iron containing proteins (QM/MM calculations) [6,7]. With this approach we will be able to test structures of the metal sites in these proteins which are very susceptible to radiation damage. First results are presented in Figure 2.

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