

## EXERCISE 5.1.

The seminar topics this year are: IR, Raman, XPS, SEM, AFM, HRTEM, ED, EELS. Please look at a little bit of these techniques already now to be able to answer to the following question:

Which of these techniques could give similar information of the sample as the XANES technique? Please discuss this with a few sentences.

Also, please read the attached research paper, and explain the usefulness of the systematic approach in interpreting the XANES data.

M. Karppinen, H. Yamauchi, Y. Yasukawa, J. Lindén, T.S. Chan, R.S. Liu, & J.M. Chen, Valence state of iron in the  $\text{Sr}_2\text{Fe}(\text{Mo,W,Ta})\text{O}_{6.0}$  double-perovskite system: an Fe *K*-edge and  $L_{2,3}$ -edge XANES study, *Chemistry of Materials* **15**, 4118-4121 (2003).

## EXERCISE 5.2.

Please read one of the two research articles and explain why EXAFS is uniquely suitable to address the research question.

You can earn an extra point, if you read/answer both papers.

Vega-Castillo et al,

On the local order of amorphous  $\text{La}_2\text{Mo}_2\text{O}_{6.7}$ ,

*Dalton Transactions* **46**, 7273 (2017).

Walshe et al.,

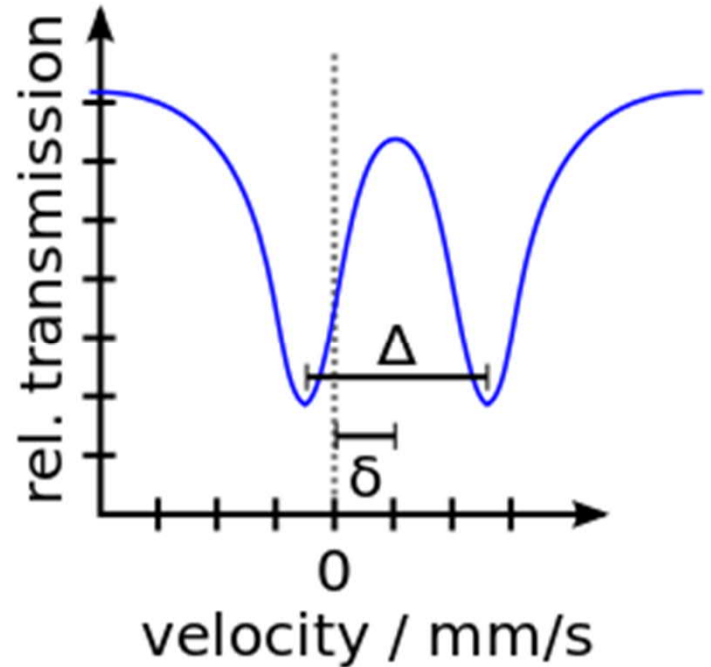
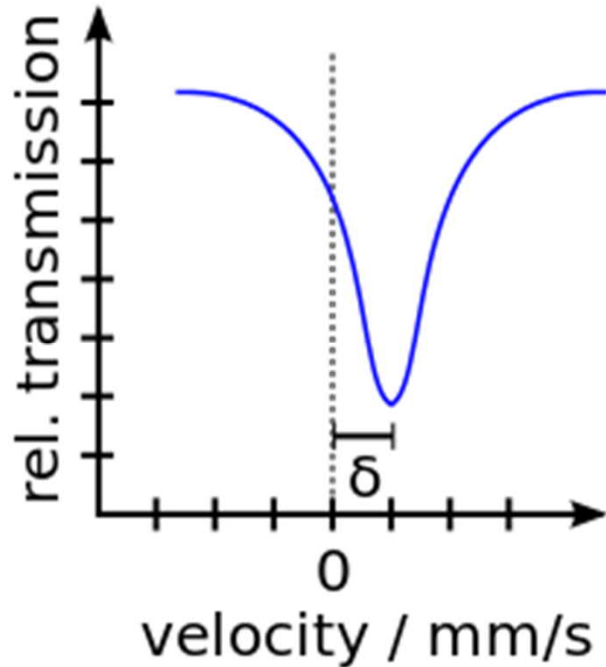
An EXAFS and HR-XANES study of the uranyl peroxides  $[\text{UO}_2(\eta^2\text{-O}_2)(\text{H}_2\text{O})_2] \cdot n\text{H}_2\text{O}$  ( $n = 0, 2$ ) and uranyl (oxy)hydroxide  $[(\text{UO}_2)_4\text{O}(\text{OH})_6] \cdot 6\text{H}_2\text{O}$ ,

*Dalton Transactions* **43**, 4400 (2014).

### EXERCISE 5.3.

Below are two  $^{57}\text{Fe}$  Mössbauer spectra. What can you tell of the two samples, individually and in comparison to each other.

Also, explain why the energy axis in the spectra is given in the units of mm/s.



## EXERCISE 5.4.

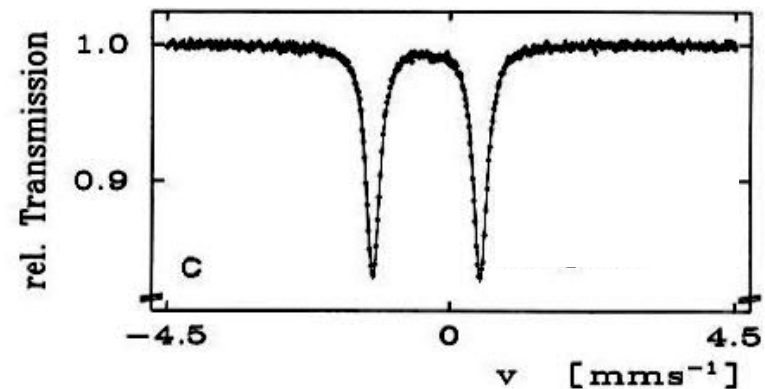
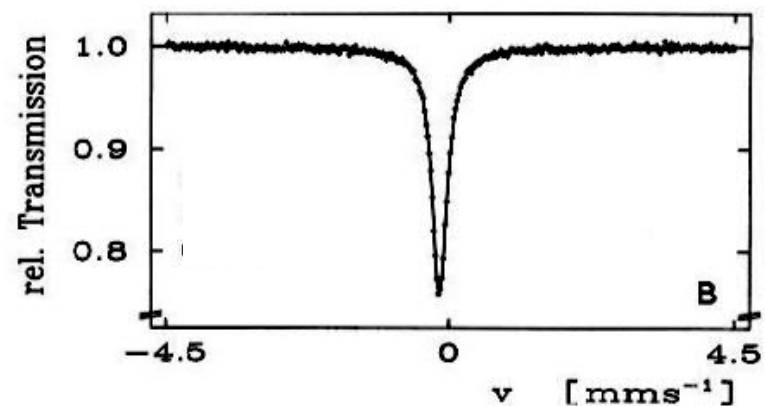
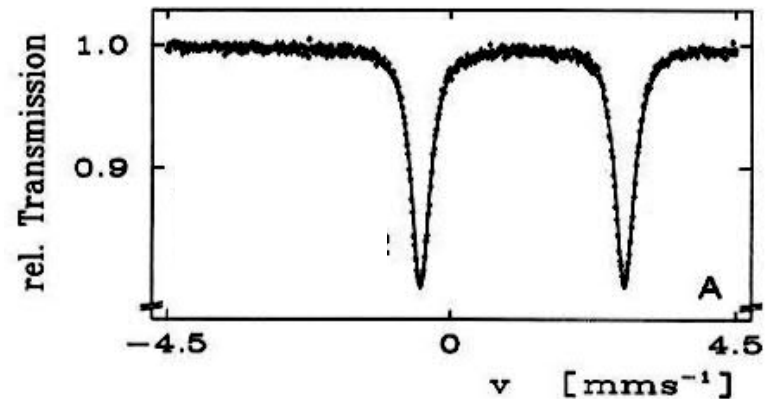
Here are Mössbauer spectra (A, B, & C) for three Fe(II) compounds:

$\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$  (high-spin  $S=2$ )

$\text{K}_4[\text{Fe}(\text{CN})_6]$  (cubic; low-spin  $S=0$ )

$\text{Na}_2[\text{Fe}(\text{CN})_5\text{NO}]$  (tetragonal; low-spin  $S=0$ )

Please assign each spectrum to the correct compound, and explain WHY!



## EXERCISE 5.5.

Assign the four Mössbauer spectra to the four compounds, and explain WHY!

- $\alpha\text{-Fe}_2\text{O}_3$  (antiferromagnetic)
- $\text{KFe(III)[Fe(II)(CN)}_6]$
- $\text{FeSO}_4$
- $\text{NdFeO}_3$  (perovskite)



mm/s

