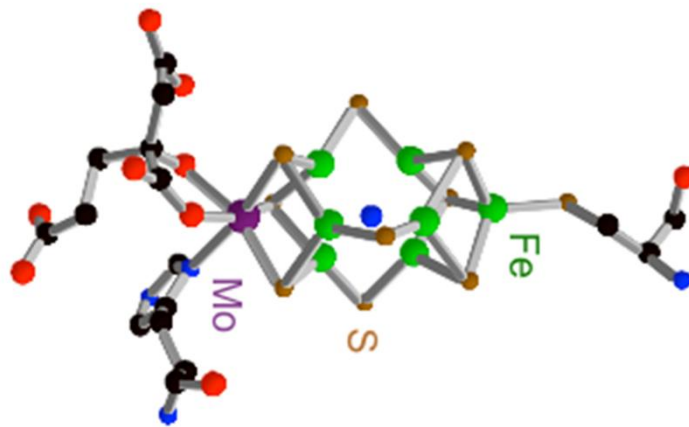
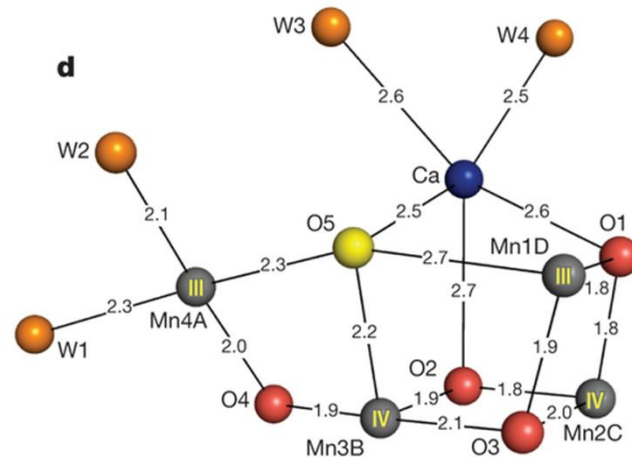
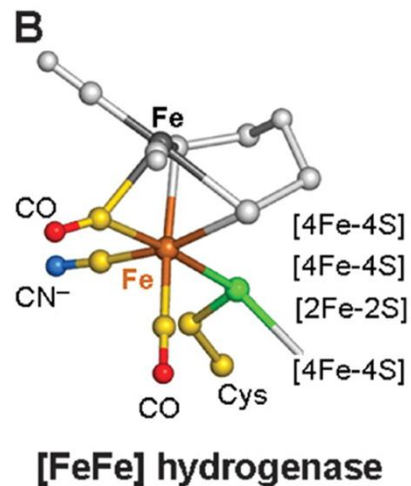
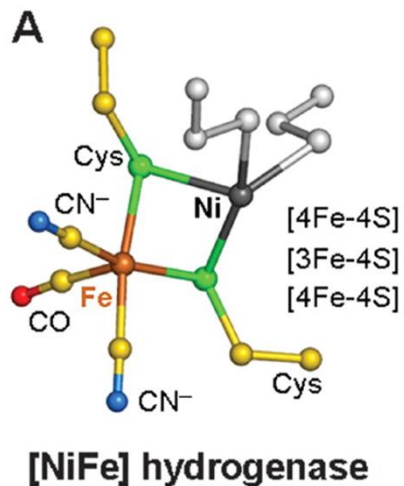
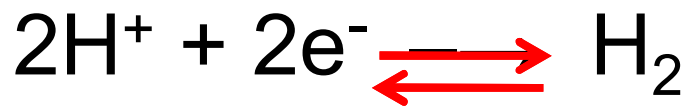


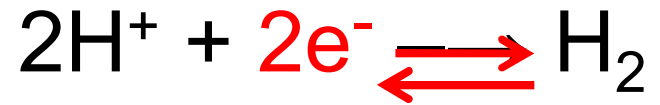
Brainstorming  
metals in biology  
and materials science

# Outline

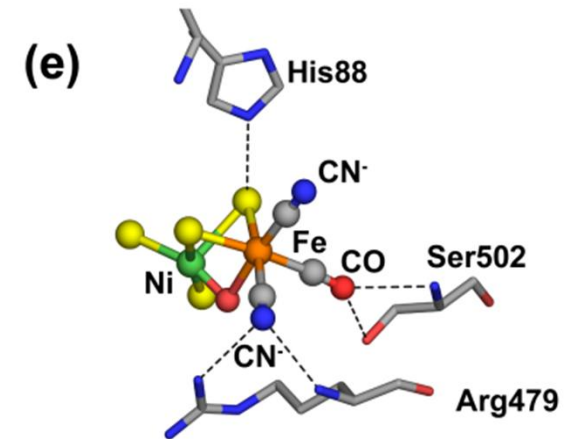
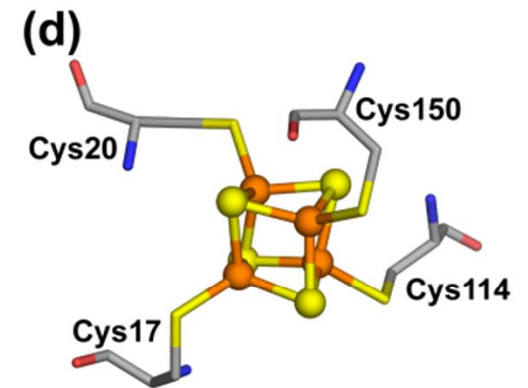
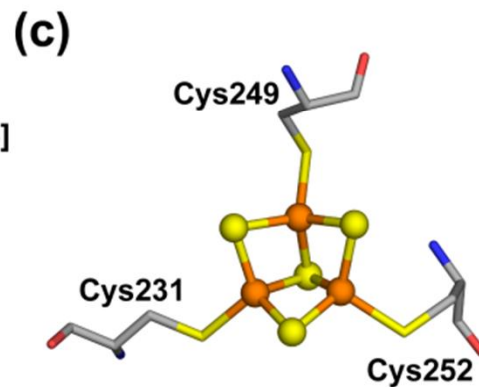
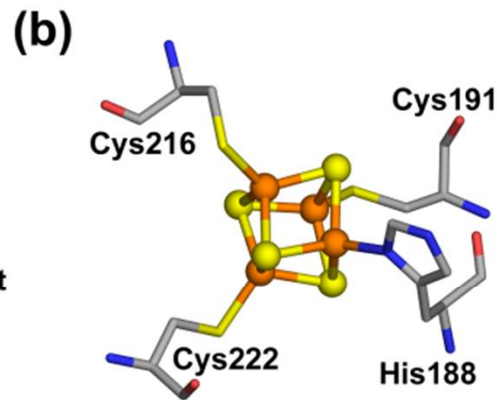
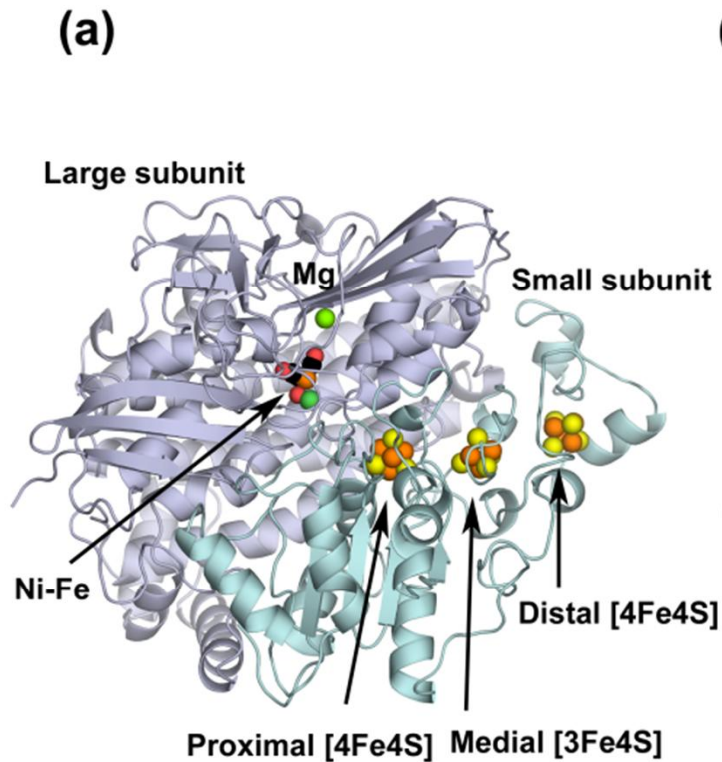
- Time-Resolved
  - Stopped-flow
  - Pump-probe
- Microscopy
- Crystallography
  - Anomalous diffraction
  - Time-dependence of diffraction peaks
- Other nuclei
  - $^{61}\text{Ni}$



# NiFe Hydrogenase



- *Desulfovibrio vulgaris* MF [NiFe] H<sub>2</sub>ase: active site **1 out of 12 Fe**



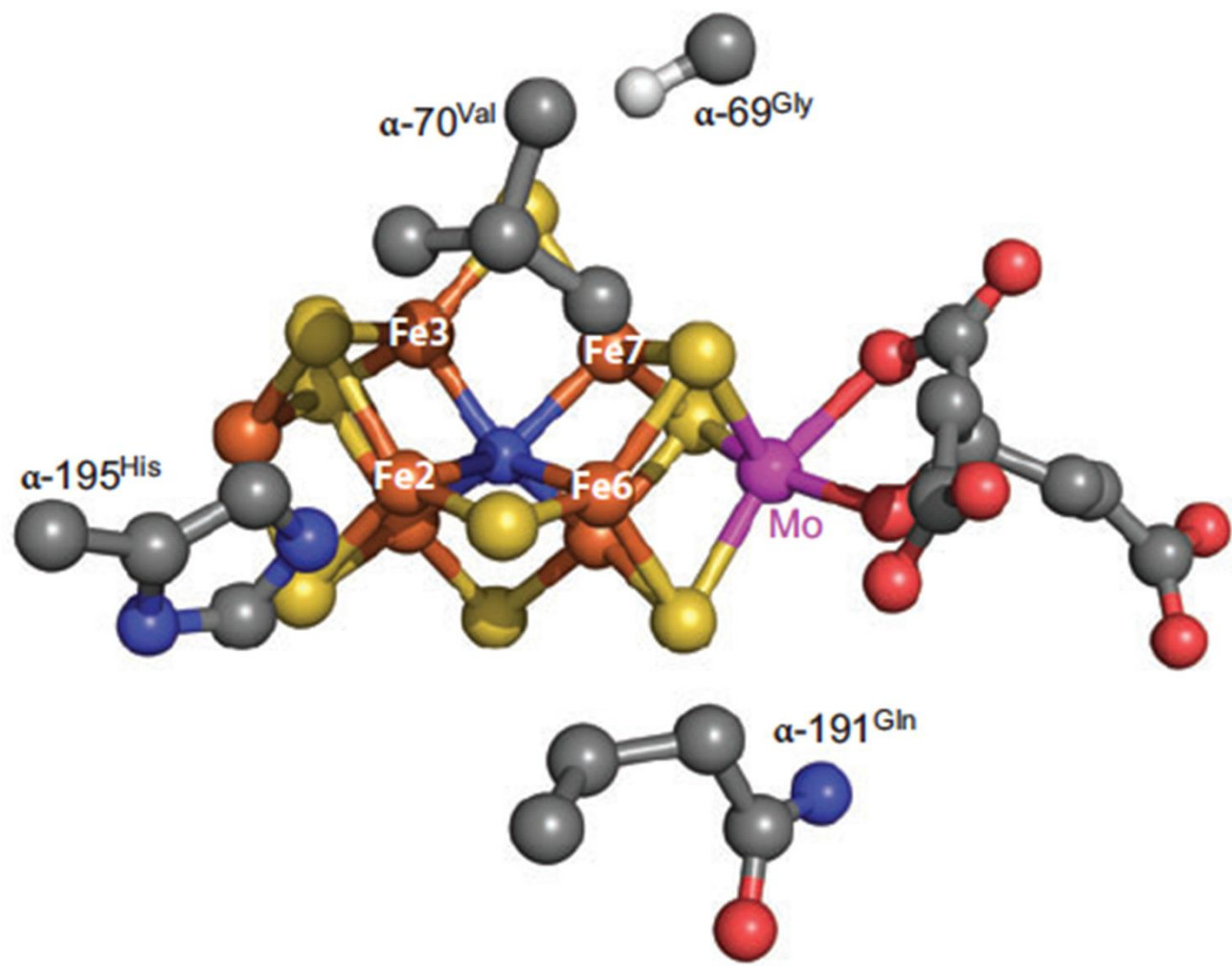
Resting state crystal structures

need spectroscopy for intermediates

anything for metalloenzymes

translates to easier materials science

experiments



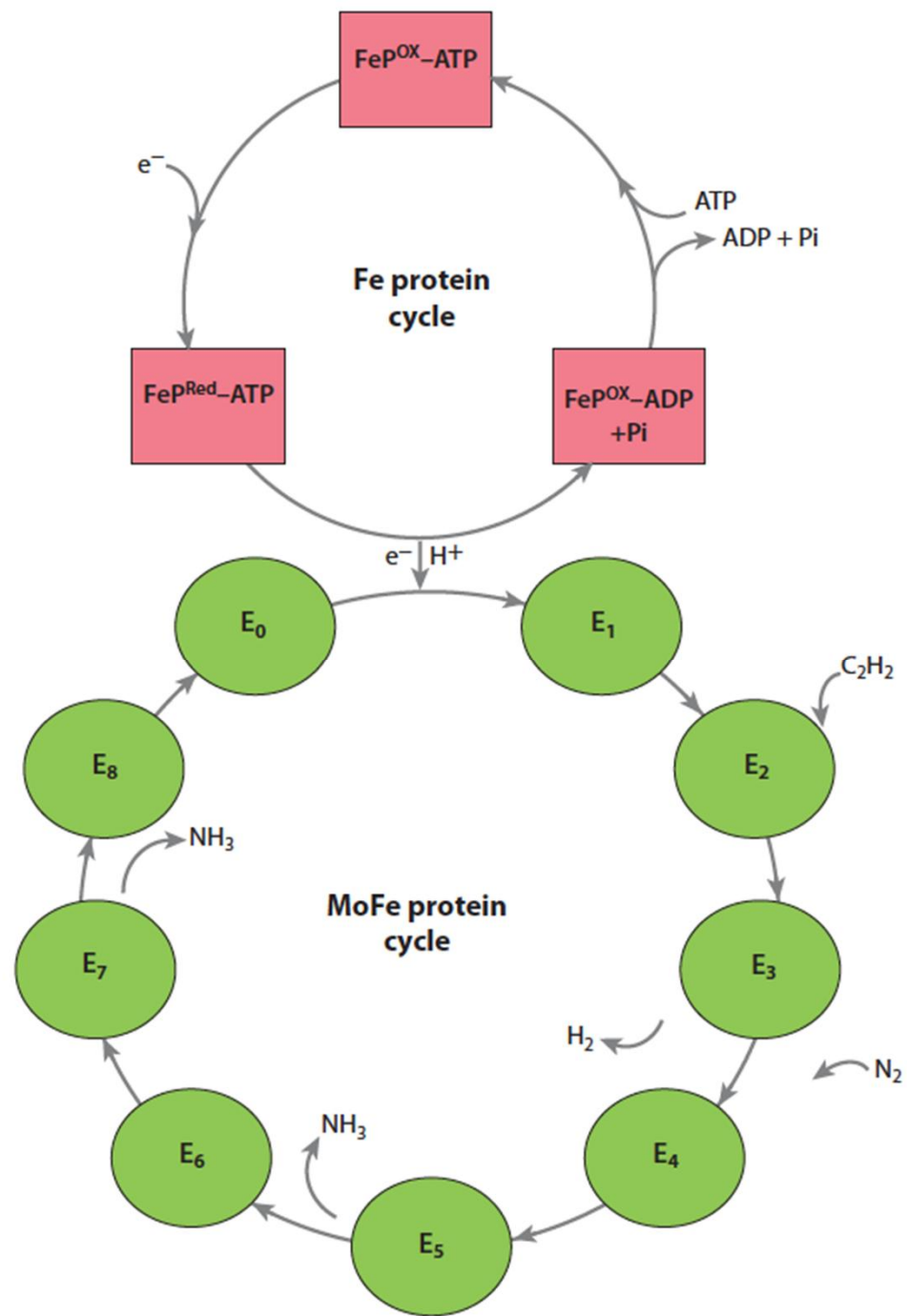
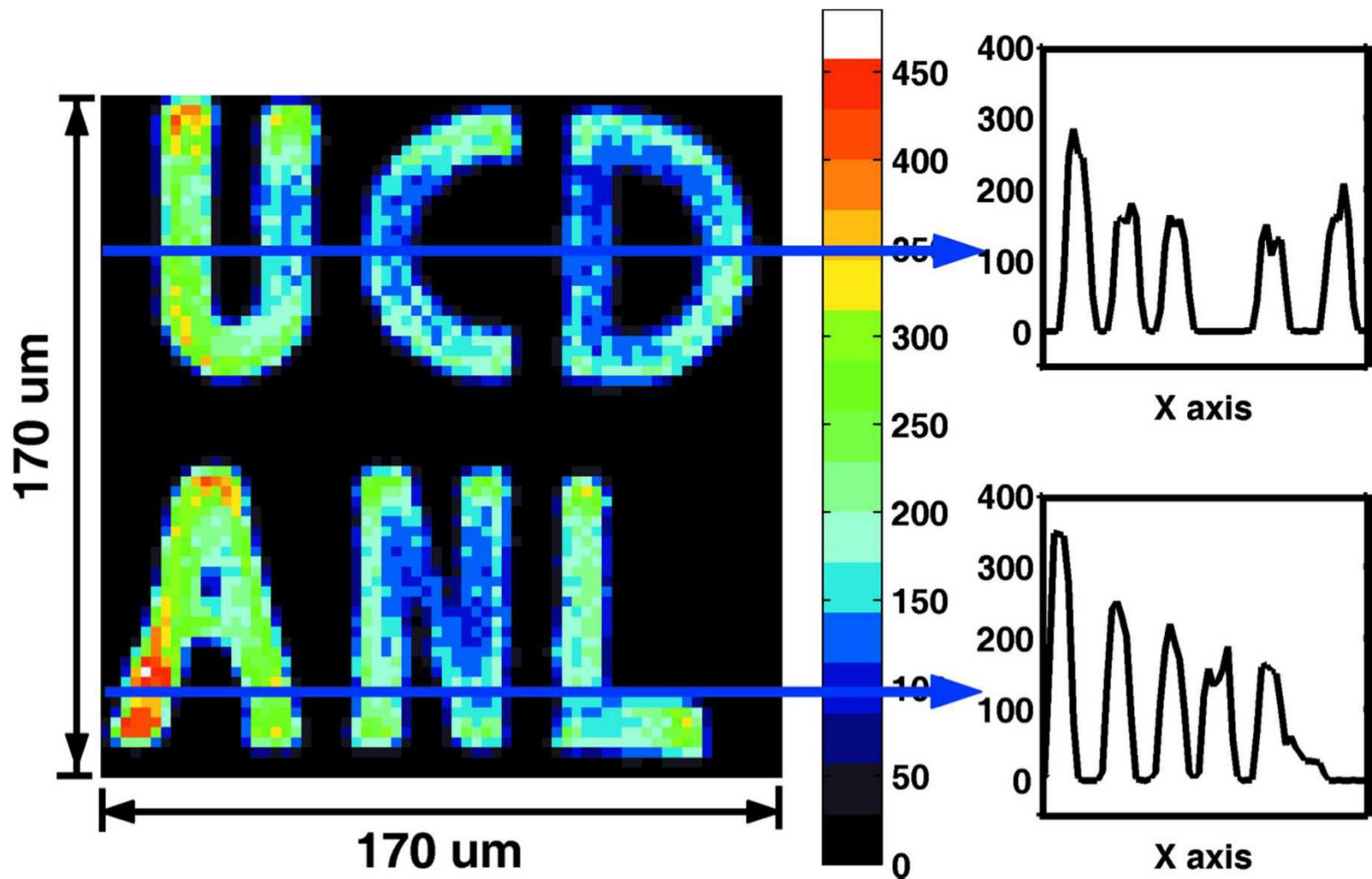


Figure 2

Left: SMS image of the #1 phantom recorded in transmission geometry. Right: intensity distribution along the indicated lines to show the signal-to-noise ratio achieved.





# Vibrational spectroscopy

- Heroic  $\longrightarrow$  routine
- Impossible  $\longrightarrow$  feasible

RIXS of intermediates

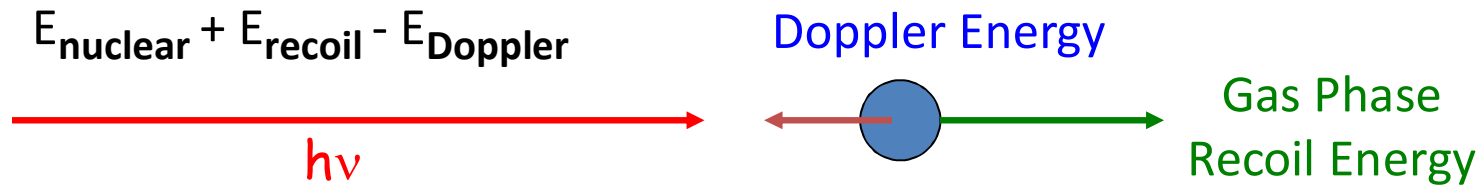
NRVS of intermediates

Hybrid fluorescence / NRVS

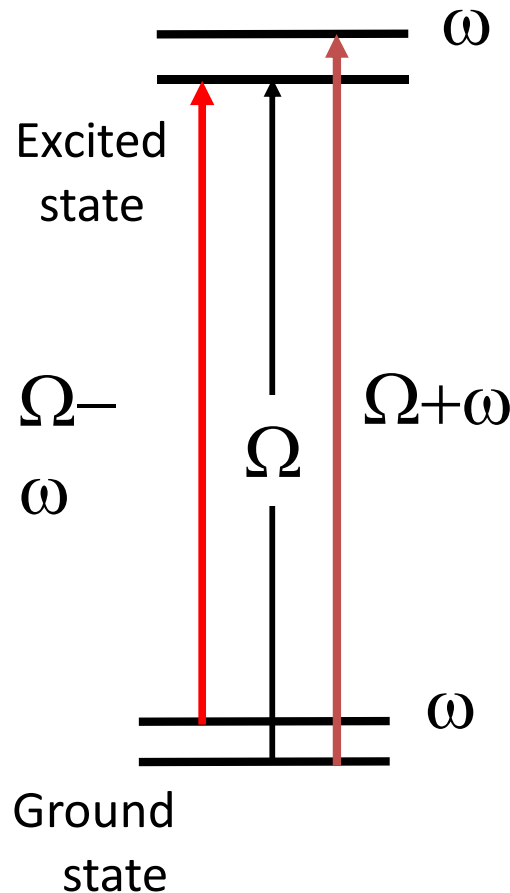
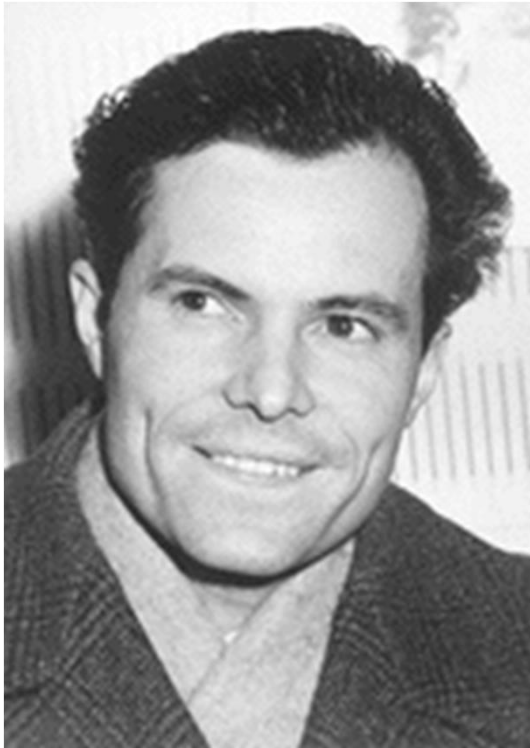
Complicated experiment  $\longrightarrow$  simple interpretation

Magnetic excitations also relevant

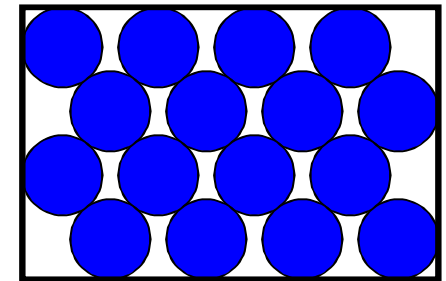
# Nuclear Resonance Vibrational Spectroscopy



- Rudolf Mössbauer
- Nobel Prize - 1961



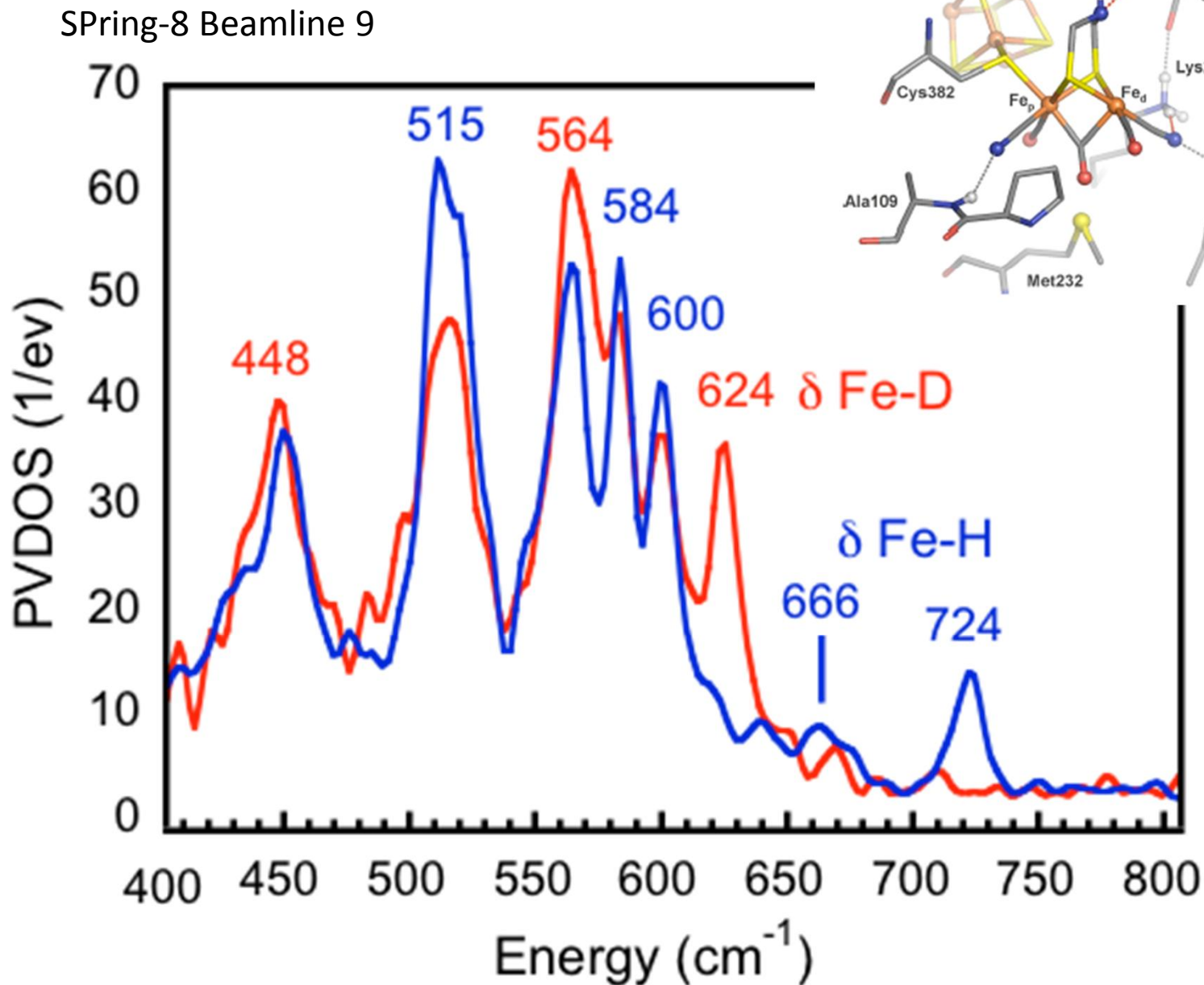
Recoil-Free Absorption

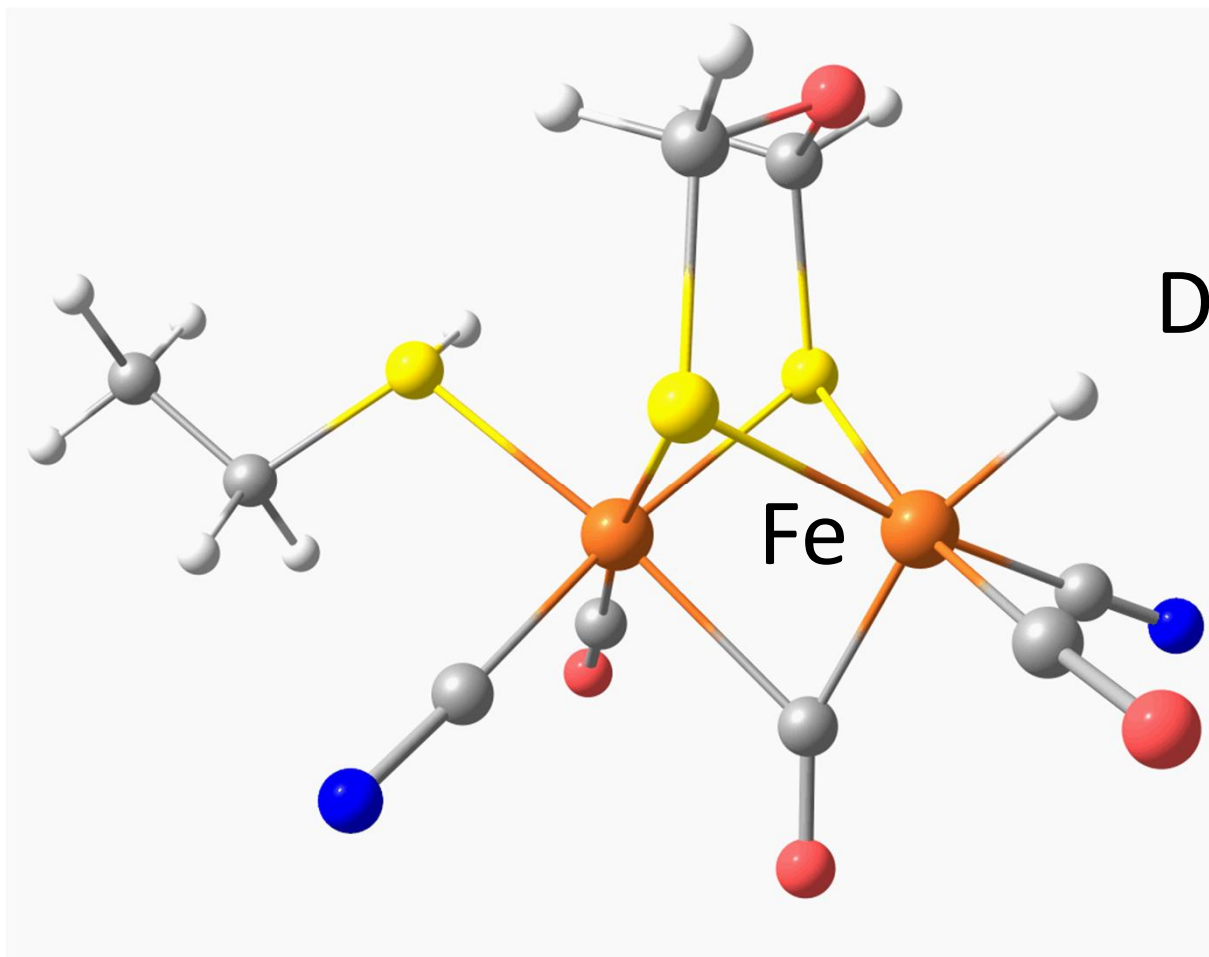


Lattice Recoil Energy  $\sim 0$

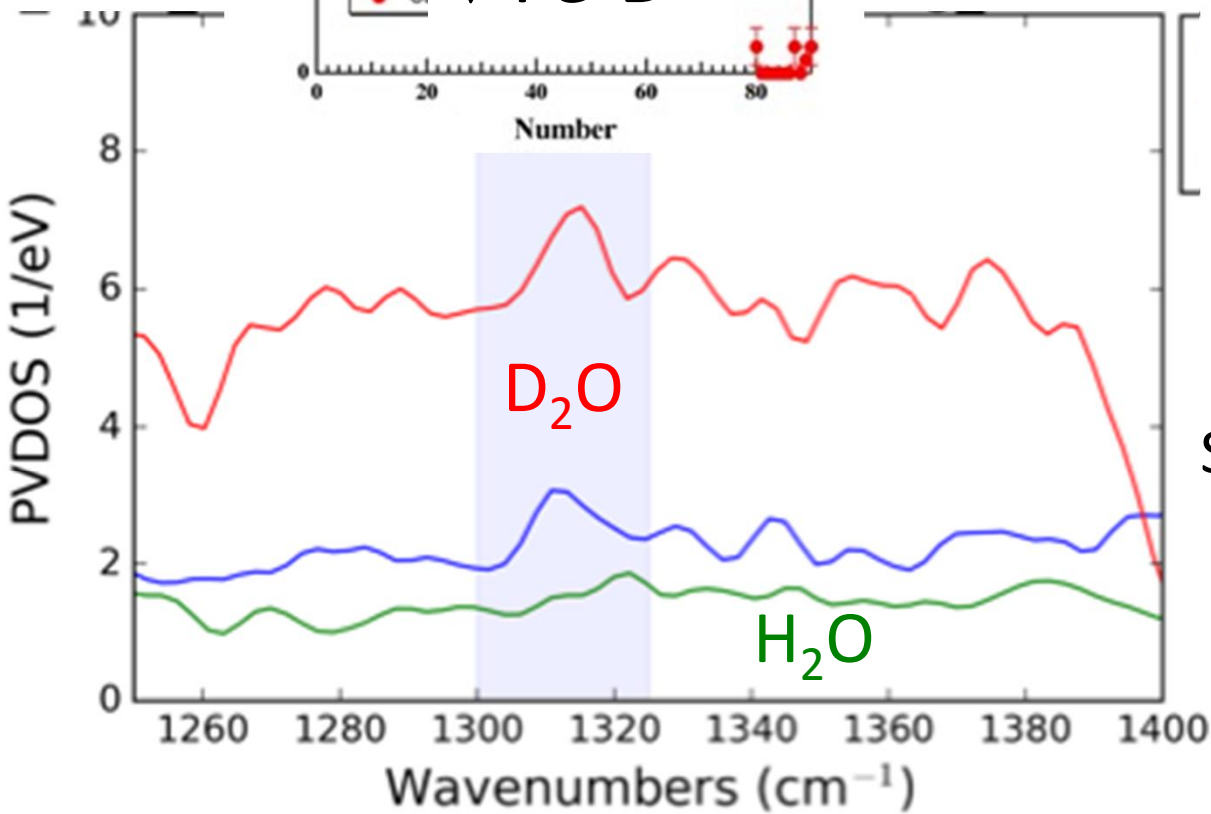
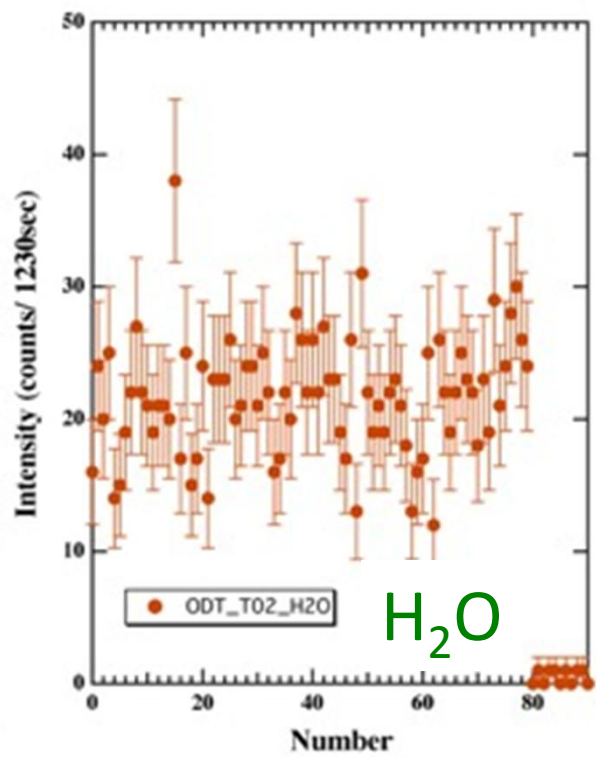
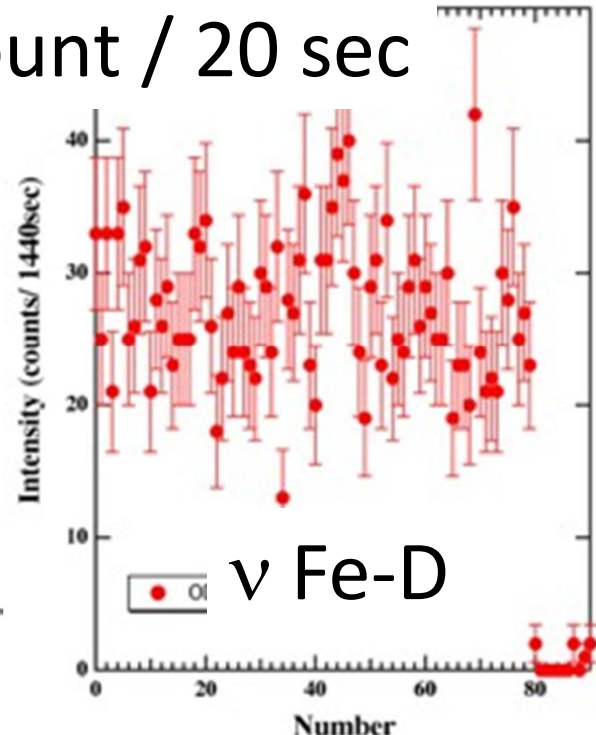
- R. L. Mössbauer  
*Z. Physik* 151, 124 '58

# ODT H<sub>2</sub>ase: H<sub>2</sub>O/H<sub>2</sub> vs. D<sub>2</sub>O/D<sub>2</sub>





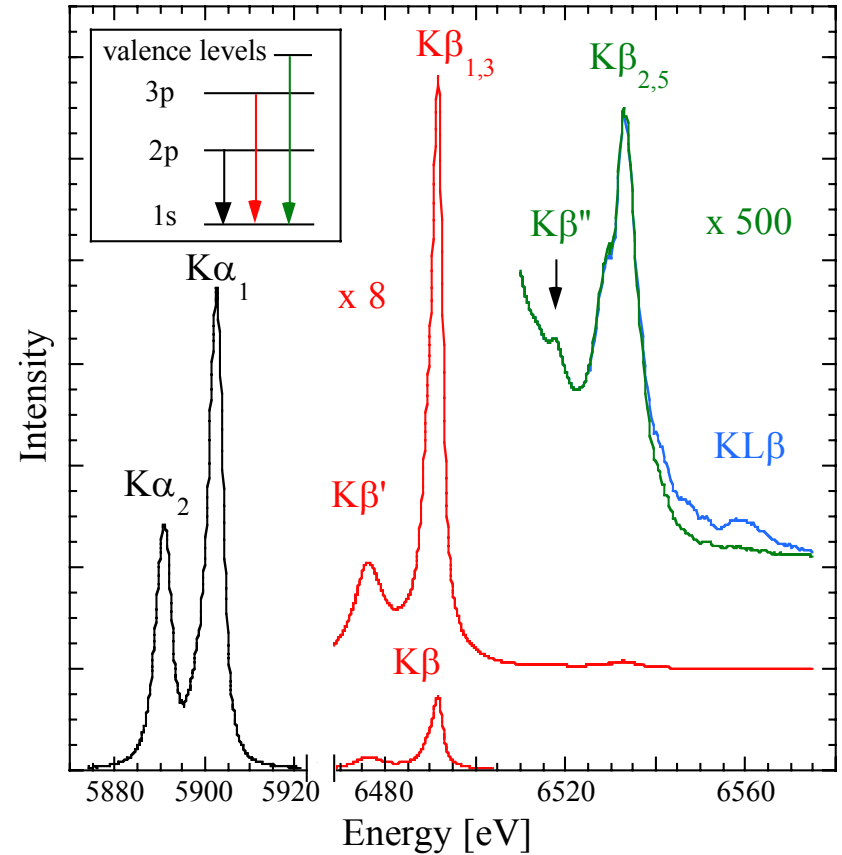
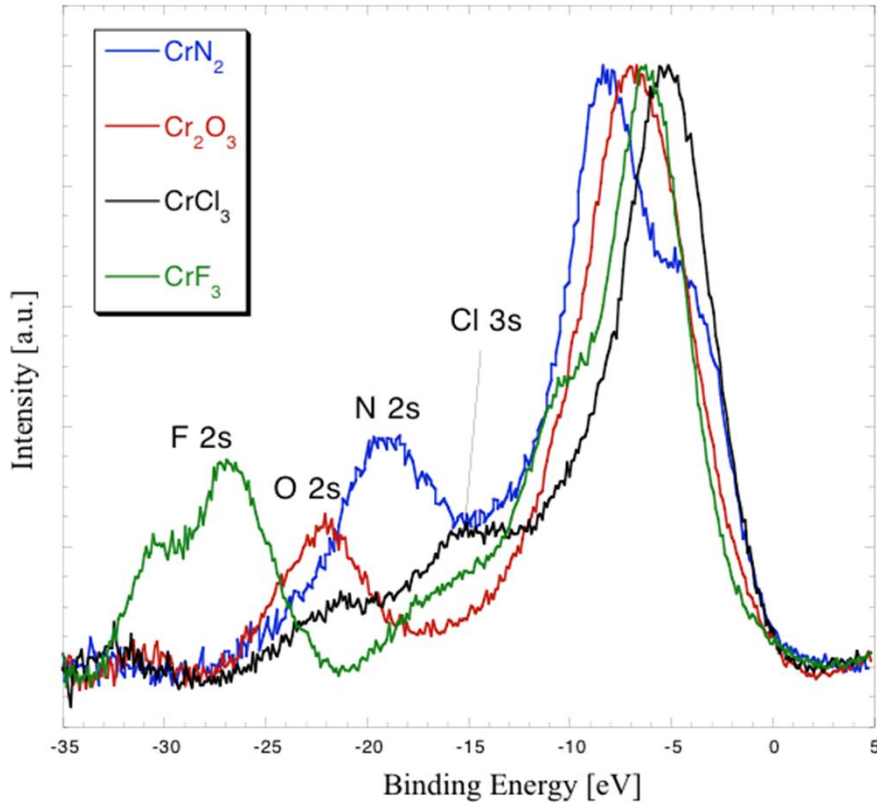
$\sim 1$  count / 20 sec



SPring-8 Beamline XLU-19

# $K\beta''$ -detected NRVS

- heroic



Site- and orientation specific NRVS