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Nuclear inelastic scattering for identification of iron ligand modes in dinitrosyl iron complexes and nitrogenase single crystals

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Vibrational iron ligand modes of ⁵⁷Fe labelled complexes can be accessed via synchrotron based nuclear inelastic scattering (NIS). First results of NIS experiments performed in October 2017 at PETRA III, DESY are presented and compared to simulations of the experimental partial density of vibrational states (pDOS). The influence of protonation on the vibrational properties of a dinitrosyl iron complex (DNIC) has been investigated. DNICs are a product of the reaction of the messenger molecule NO with iron sulfur clusters and their reactivity might depend on the protonation state. The density functional theory based simulations confirm the experimentally observed distinct differences between the two protonation states and reproduce the intense features in the pDOS energy region > 500 cm⁻¹ typical for Fe-NO vibrations [1]. Moreover orientation dependent NIS experiments on CO-free and CO-inhibited ⁵⁷Fe enriched nitrogenase single crystals have been performed. Despite the low signal to noise ratio, slight but significant orientation dependent differences are observed for low energy modes < 100 cm⁻¹ as well as in the region of characteristic Fe-CO modes above 460 cm⁻¹ [2].

References
[1] A. L. Speelman et. al., Inorg. Chem., 2016, 55, 5485.
[2] A. D. Scott et. al., J. Am. Chem. Soc., 2014, 136, 15942.

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