

Iron Equilibrium Fractionation Factors from *Ab initio*, NRIXS, and Lab Experiments: The Path Forward

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Iron isotope variations have been found in a variety of samples and settings, ranging from hemoproteins to extraterrestrial igneous rocks. The strongest impediment to interpreting iron isotope variations in natural samples is the lack of a robust set of iron equilibrium fractionation factors between phases. Three approaches can be used to estimate equilibrium fractionation factors: *ab initio* calculations [1], NRIXS measurements [1,2], and laboratory experiments [3,4]. Each method has its weaknesses and strengths but evaluating their accuracies can be difficult. Consistency between equilibrium fractionation factors estimated by several independent approaches is a necessary condition to gain confidence in these methods; keeping in mind that natural and synthetic minerals can depart from ideal stoichiometry. Few phases have been studied by the three approaches. Blanchard *et al.* [1] recently estimated the β -factor of goethite using *ab initio* and NRIXS. The β -factor estimated by NRIXS is slightly higher than that predicted by the *ab initio* approach, which itself predicts a higher equilibrium fractionation between goethite and $\text{Fe(II)}_{\text{aq}}$ than is measured [4]. In order to assess the reliability of the equilibrium fractionation factors estimated using the various techniques, we have measured by NRIXS at the APS synchrotron the β -factors for synthetic ferrihydrite, natural goethite, hematite, pyrite, and siderite. *Ab initio* calculations are available for all these phases. We will provide a side-by-side comparison of the NRIXS and *ab initio* approaches with a perspective on what it tells us about laboratory experiments.

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References: [1] Blanchard M. *et al.* (2015) GCA 151, 19-33. [2] Dauphas N. *et al.* (2012) GCA 94, 254-275. [3] Wu L. *et al.* (2011) EST 45, 1847-1852. [4] Frierdich A.J. *et al.* (2014) GCA 139, 383-398.