

Systematic XAS study on the reduction and uptake of Tc by magnetite and mackinawite

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Supplementary Information

Table S1. Description of the experimental conditions for the synthesis of the Fe minerals studied in this work.

Fe minerals	Recipe	[Fe] _{tot}	Particle size	Reference
Magnetite (Fe ₃ O ₄)	60 mL of 6 M NH ₄ OH + 50 mL of Fe(II)/Fe(III) solution with [Fe(II)]=0.4 M and [Fe(III)]=0.8 M	0.5 M	~10 nm	Jolivet et al. (1992) ¹
Mackinawite (FeS)	100 mL of 0.6 M Fe(II) solution ((NH ₄) ₂ Fe(SO ₄) ₂ · 6H ₂ O) + 100 mL of 0.6 M Na ₂ S	0.3 M	2 to 10 nm	Rickard et al. (2006) ²

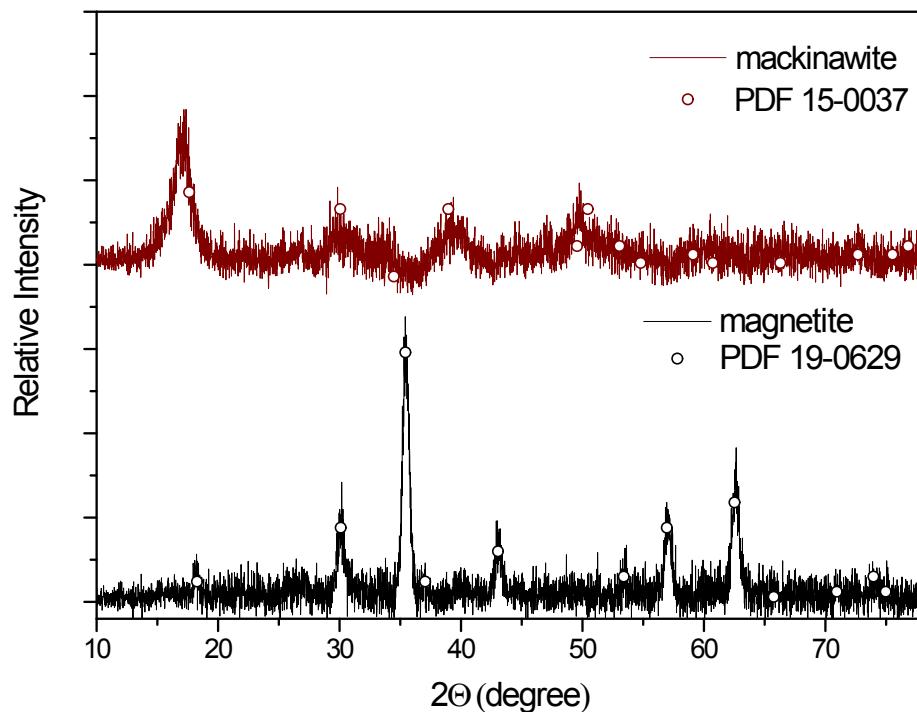


Figure S1. XRD patterns of magnetite and mackinawite phases synthesized in the present work. Small circles indicate peak positions and relative intensities reported for the corresponding reference materials (JCPDS PDF files 19-0629³ and 15-0037⁴).

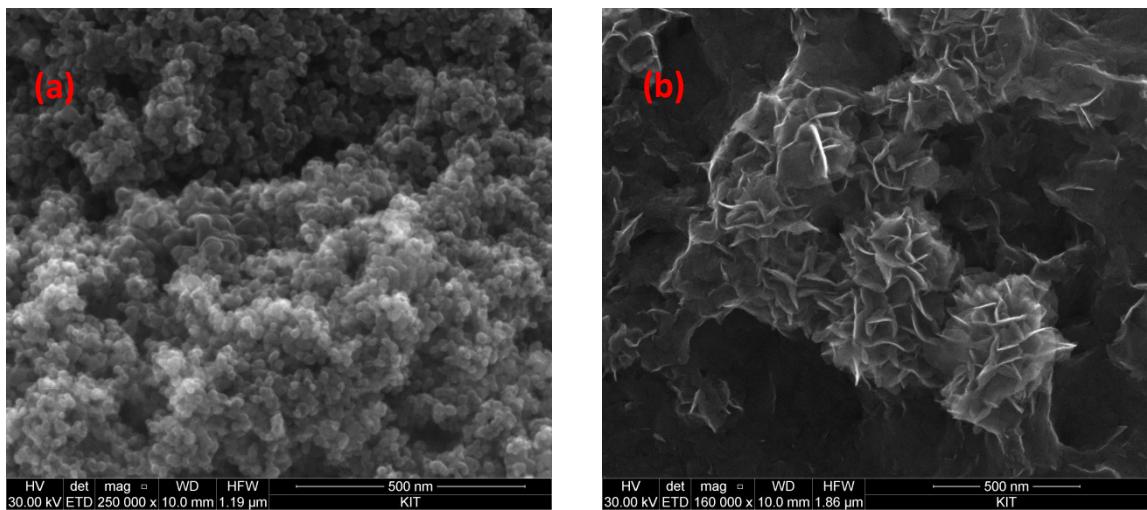


Figure S2. SEM pictures of magnetite (a) and mackinawite (b) solid phases equilibrated with a Tc-containing solution for 6 weeks.

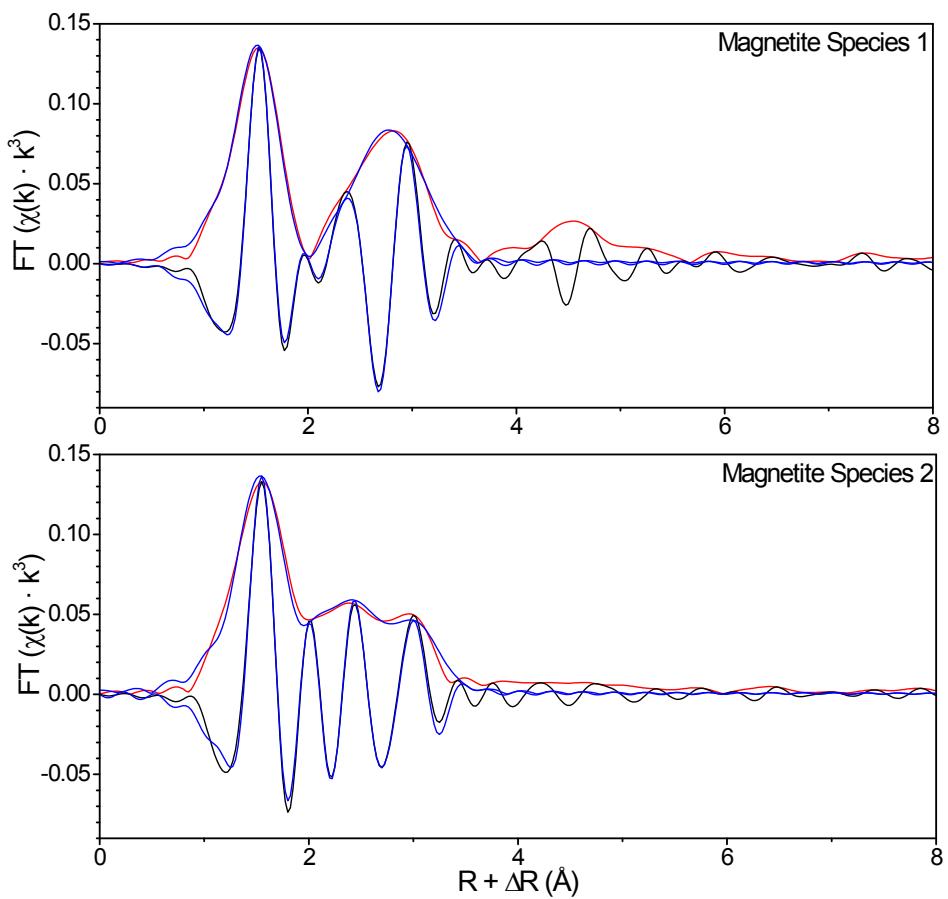


Figure S3. Tc-K edge EXAFS fits of the two ITFA-derived Tc species in the magnetite system. Shown is the experimental Fourier Transform magnitude (red) and imaginary part (black) as well as their respective fits (blue).

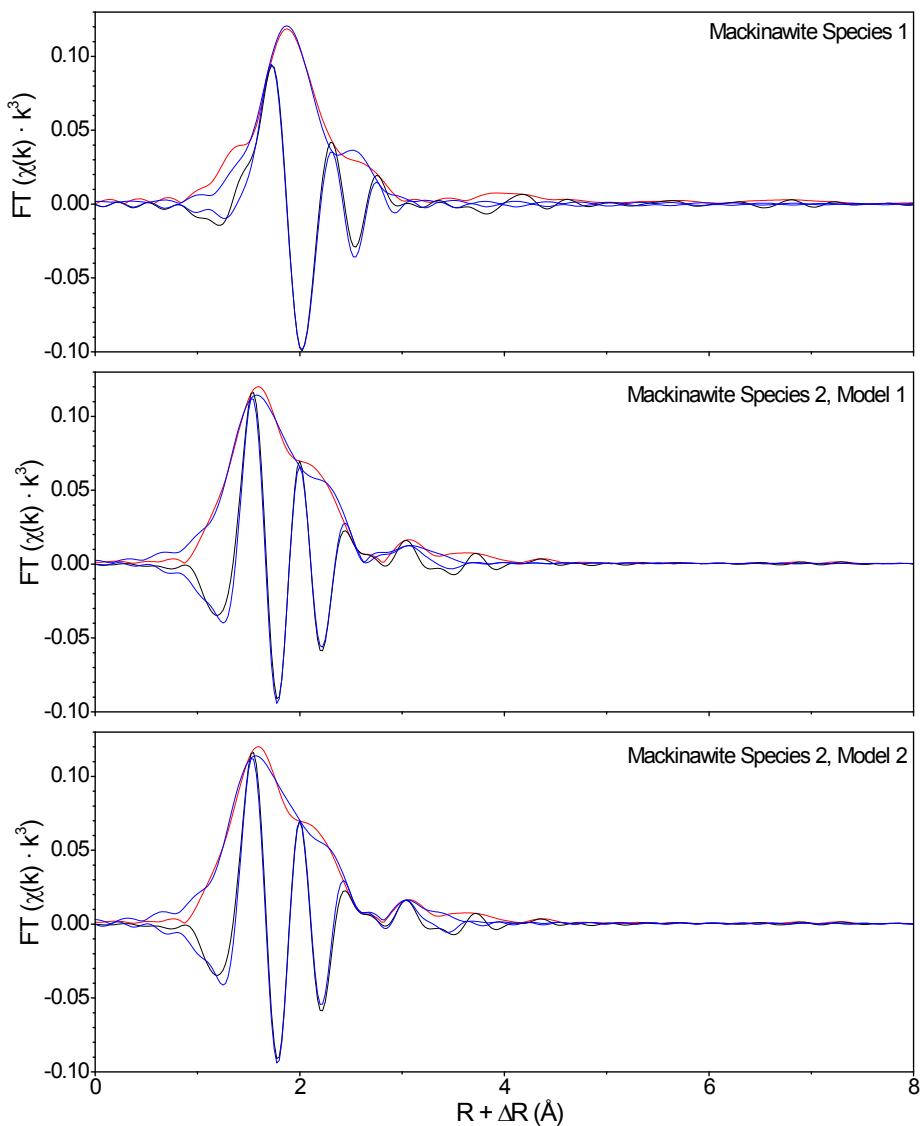


Figure S4. Tc-K edge EXAFS fits of the two ITFA-derived Tc species in the mackinawite system. Shown is the experimental Fourier Transform magnitude (red) and imaginary part (black) as well as their respective fits (blue).

References

1. J. P. Jolivet, P. Belleville, E. Tronc and J. Livage, *Influence of Fe(II) on the Formation of the Spinel Iron-Oxide in Alkaline-Medium*. Clays and Clay Minerals, 1992. **40**(5): p. 531-539.
2. D. Rickard, *Characteristics of mackinawite, tetragonal FeS*. Geochimica Et Cosmochimica Acta, 2006. **70**(18): p. A533-A533.
3. H. E. Swanson, H. F. McMurdie, M. C. Morris and E. H. Evans, *Standart X-ray diffraction powder patterns*. U.S. Department of Commerce, 1967.
4. T. E. Howard, C. Milton, C. E. C. T., I. Adler, C. Mead, B. Ingram and R. Berner, *Valleriite and the new iron sulfide, mackinawite*. Mineralogy and Petrology, 1964. **475-D**: p. D64-D69.