

Supplementary Information

Investigation of the high-temperature redox chemistry of $\text{Sr}_2\text{Fe}_{1.5}\text{Mo}_{0.5}\text{O}_{6-\delta}$ via *in situ* neutron diffraction

Daniel E. Bugaris¹, Jason P. Hodges², Ashfia Huq², W. Michael Chance¹, Andreas Heyden³, Fanglin Chen⁴, Hans-Conrad zur Loye¹

¹ *Department of Chemistry and Biochemistry, University of South Carolina, Columbia, SC 29208, USA*

² *Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*

³ *Department of Chemical Engineering, University of South Carolina, Columbia, SC 29208, USA*

⁴ *Department of Mechanical Engineering, University of South Carolina, Columbia, SC 29208, USA*

Figure S1 Powder neutron diffraction profiles for $\text{Sr}_2\text{Fe}_{1.5}\text{Mo}_{0.5}\text{O}_{6-\delta}$ in O_2 in the temperature range 500-850°C.

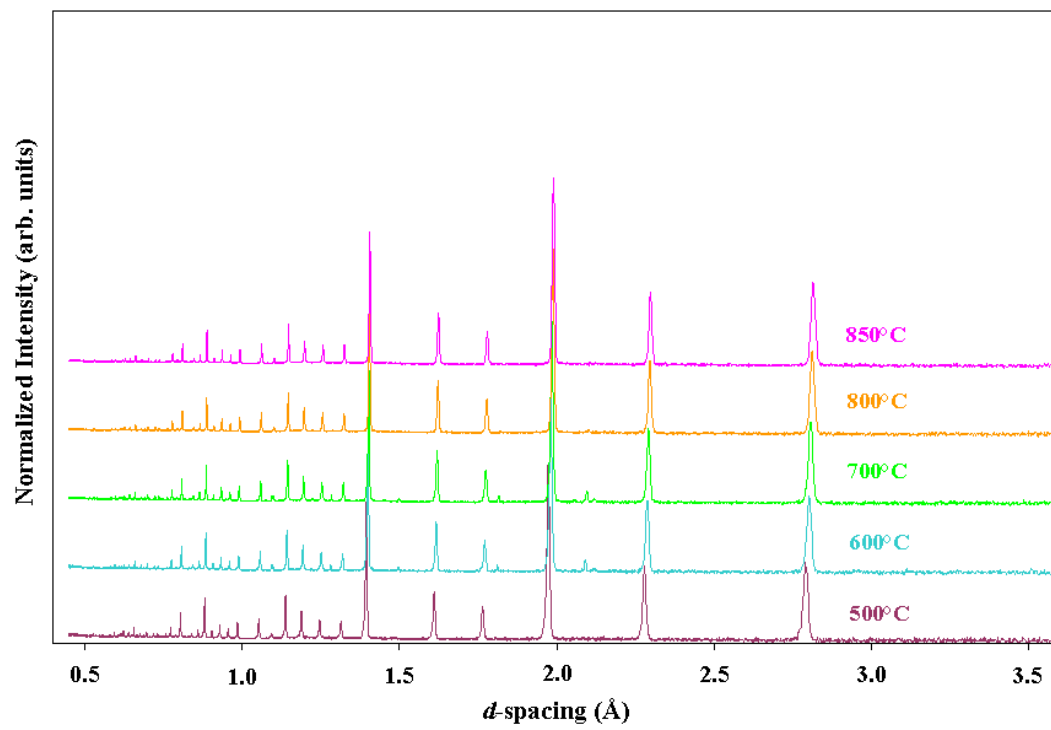


Figure S2 Observed (black crosses), calculated (red line), and difference (blue line) powder neutron diffraction profile for $\text{Sr}_2\text{Fe}_{1.5}\text{Mo}_{0.5}\text{O}_{6-\delta}$ in O_2 at 850°C , refined in the cubic space group $Pm\bar{3}m$. The vertical markers correspond to the allowed Bragg reflections.

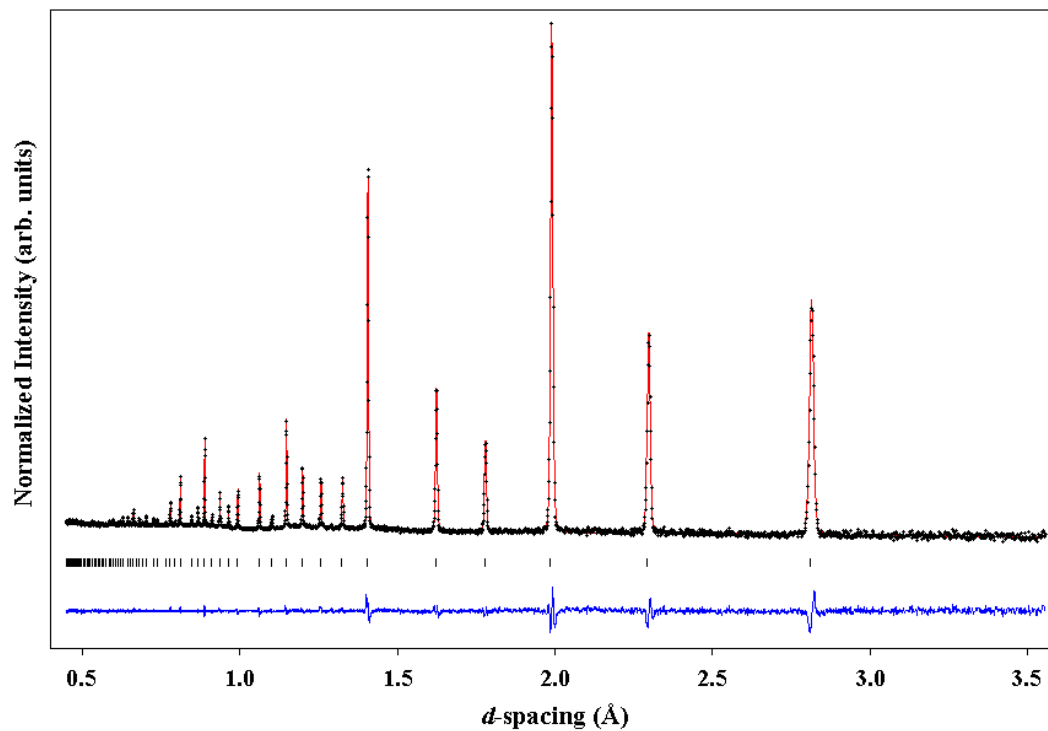


Figure S3 Observed (black crosses), calculated (red line), and difference (blue line) powder neutron diffraction profile for $\text{Sr}_2\text{Fe}_{1.5}\text{Mo}_{0.5}\text{O}_{6.8}$ at 25°C after having been cooled in O_2 , refined in the tetragonal space group $I4/mcm$. The vertical markers correspond to the allowed Bragg reflections.

