

## **A fast open data reduction workflow for the electron microprobe flank method to determine $\text{Fe}^{3+}/\Sigma\text{Fe}$ contents in minerals**

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### **ABSTRACT**

Knowing the  $\text{Fe}^{3+}/\Sigma\text{Fe}$  ratio in minerals is important to understand the formation and evolution of minerals and their host rocks. Variable  $\text{Fe}^{3+}/\Sigma\text{Fe}$  in, e.g., garnet is accompanied by a change of their characteristic  $\text{Fe}L\alpha$  and  $\text{Fe}L\beta$  X-ray emission lines, which can be quantified with electron microprobe measurements using the flank method. Previously, the required data reduction process to determine the  $\text{Fe}^{3+}/\Sigma\text{Fe}$  was complex. Here, we present a new data reduction tool taking garnet data as an example. This new Flank Reduction app is a freely available, graphical user interface (GUI)-driven, web-based application to reduce flank method data quickly and easily. The entire data reduction process is achieved in minutes compared to hours or days, as it was before. Flank Reduction provides comprehensive insights into, e.g., the flank method standards employed, data obtained, and errors through a wide array of controls and visualization tools. Documentation with comprehensive information on the flank method, data reduction, as well as training material such as video tutorials or sample data sets, are available on a dedicated webpage. Flank Reduction emphasizes the high value of Findable, Accessible, Interoperable, Reproducible (FAIR) and open research software and demonstrates how current developments in coding and app implementation can facilitate the development of powerful and expandable research software.

**Keywords:** Oxidation state, ferrous/ferric iron, flank method, garnet, electron microprobe, data reduction, Python