



Internally consistent database for oxygen isotope fractionation in minerals: theory and applications

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Stable isotopes are important tools for a wide range of applications in Earth sciences as the oxygen isotopic signature of minerals records the physical and chemical conditions of equilibration. Oxygen isotope fractionation between minerals has often been used for thermometry, but also to investigate samples that experienced fluid-rock interactions. The petrological interpretation of oxygen isotope trends requires the knowledge of equilibrium fractionation between two phases and its evolution with temperature. A few well-documented compilations of fractionation factors are available in the literature, but they are either restricted to small chemical systems or based on different methods making the data not consistent with each other.

In this study, we report the first internally consistent database for oxygen fractionation that includes fractionation factors for most major and accessory phases and a pure H₂O fluid phase. This database has been derived simultaneously using a least square regression technique based on a large dataset of experimental, theoretical and natural data from the literature. All the constraints for a given phase contributed to the refinement of its fractionation properties making the final database internally consistent.

This database can be applied in a general thermodynamic framework to model the evolution of $\delta^{18}\text{O}$ in minerals through their metamorphic history. At fixed P and T and for a given bulk rock composition, it is possible to predict the mineral assemblage, mineral mode and compositions using Gibbs free energy minimization. If the bulk rock $\delta^{18}\text{O}$ is known, the $\delta^{18}\text{O}$ values of each phase at any given P-T can be predicted and compared with data from mineral and mineral zone analyses. If the $\delta^{18}\text{O}$ of one phase is known, it is possible to recalculate the $\delta^{18}\text{O}$ of the other phases in equilibrium and the bulk $\delta^{18}\text{O}$. These results enhance our ability to investigate samples that experienced complex thermal histories and/or fluid-rock interactions. They also provide a strong theoretical basis for evaluating to what extent a rock has evolved either as an open system with respect to oxygen isotopes or as a closed system fully or partially re-equilibrated.