

Crustal contamination in the British and Irish Palaeogene Igneous Province: Mechanisms, timing and implications for the formation of granitic magmas

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Old and lithologically variable terranes, such as those in the northern British Isles, preserve distinct and diverse crustal isotopic end-members. Similarly, individual crustal lithologies comprise various isotopic sinks, representative of various sources. Hence, while a partial melt/restite of these crustal lithologies may not be fully representative of the original protolith, it can be identified individually, further constraining crustal contamination. Therefore a magma's course may be traced isotopically, providing a picture of a granite's ascent and storage at both a local and crustal scale. Samples from the Drumadoon Igneous Complex, Isle of Arran, Scotland, and the Carlingford Igneous Centre, NE Ireland, were analysed for major and trace elements and Sr and Nd isotopes, aiming to reveal both magma chamber-scale processes and larger-scale crustal pathways. The Arran data point towards major involvement of the Grampian terrane, despite the Drumadoon Igneous Complex being within the Midland Valley. Therefore, while the magmas originated at depth on the northern side of the Highland Boundary Fault (HBF), they have crossed this boundary during their evolution and ascent, most likely during shallow-level emplacement. The HBF has a sub-vertical orientation, therefore the magma is unlikely to have taken a direct vertical traverse through the crust, but rather experienced significant lateral transport. At Carlingford, all samples trend markedly towards local Silurian crust, reflecting the involvement of a single crustal end-member. Nevertheless, our data imply contamination was not straightforward. We see a time sequence of variably overprinted processes, from initial contamination by crustal partial melts, to bulk contamination, and final assimilation of the remaining restite during transport and emplacement. At both centres, granitic magmas appear to result from high levels of contamination during differentiation, producing a characteristic bimodal "Bunsen-Daly Gap". Significantly, the intermediate compositions that bridge this gap at Drumadoon and Carlingford are not the products of fractional crystallisation, but rather appear to be the result of both mixing of end-member compositions and variable amounts of crustal contamination during storage, transport and emplacement.

Silicon isotopic fractionation: Assessments from first-principles methods

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Equilibrium isotopic fractionation between solids is a thermodynamic property, which is determined by the vibrational properties of the system. In this work, we employ an *ab initio* method (Density Functional Perturbation Theory) to obtain the complete phonon dispersion, which in turn, is used to calculate the free energy of a material of a given isotopic composition. Finally, the equilibrium isotopic fractionation is determined from the difference in free energy of materials of different isotopic compositions. We use PBE functionals, combined with the use of pseudo-potentials and planewave basis sets. This methodology has proved to be successful in reproducing the physical and chemical properties of complex systems. Within this framework, we have recently developed a methodology to predict equilibrium fractionation factors as a function of temperature [1].

Silicon is a major component of Earth crust. Measurements of various isotopic compositions in Nature show that, in general, the silicon composition follows the oxygen composition, and shows a positive correlation with silicon content [2]. Further observations, as well as theoretical arguments, predicted that silicon isotopic fractionation properties could be related to the degree of polymerization of silica units in silicates[3].

In this study, we have focused on the study of the systematic trends in Si fractionation, and on its relationship with oxygen fractionation or silicate polymerization. Our work consists in a comparative study of materials presenting several degrees of silicate polymerization: nesosilicates (forsterite), inosilicates (clinoenstatite), phyllosilicates (kaolinite and lizardite), and tectosilicates (quartz). Oxygen isotopic fractionation has been computed and compared to existing experimental data with which they agree well given the calculation uncertainty. Silicon isotopic fractionation has also been computed and compared to their oxygen counterparts. Silicon fractionation between quartz and other materials is systematically positive and range from 0.2 to 0.8 permil at 1000°C. Beyond that, they roughly follow the trends of oxygen fractionation. Nevertheless, a clear correlation between silicate polymerization and silicon fractionation has not been observed.

References

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