

• 非传统稳定同位素地球化学：分馏理论、分析方法和地质应用 •

## Extreme Lithium Isotopic Fractionation Between Quartz and Garnet in Leucogranites from the Southeastern Margin of North China Craton

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We report Li concentrations and isotopic compositions for minerals and bulk rocks of garnet-bearing leucogranites from the southeastern margin of the North China craton. The five leucogranite samples have low Li concentrations (1.8–4.3 ppm) and considerably variable but slightly higher  $\delta^7\text{Li}$  values (+4.0 to +13.1‰) compared to an average of 2.2‰ for granites worldwide. Quartz has relatively low Li concentrations (~1 ppm) but is strongly enriched in  $^7\text{Li}$ , with  $\delta^7\text{Li}$  values ranging from +27.0‰ to +38.5‰. By contrast, garnet has unusually high Li concentrations (27.7–50.4 ppm) and depleted but relatively homogeneous isotopic compositions, with  $\delta^7\text{Li}$  values ranging from -1.0‰ to +0.3‰. Plagioclase has 3.1–4.2 ppm Li and  $\delta^7\text{Li}$  values of +1.8‰ to +8.9‰,

whereas those for K-feldspar are 0.9–2.8 ppm and +3.4 to +11.4‰, respectively. Biotite has very high Li concentrations (241 ppm) and  $\delta^7\text{Li}$  values of +7.3‰ falling within the range of plagioclase. These observations indicate that significant Li isotopic fractionation between minerals could occur during magmatic and/or metamorphic processes. The extreme inter-mineral isotopic fractionations, with  $\delta^7\text{Li}_{\text{quartz-garnet}}$  (=  $\delta^7\text{Li}_{\text{quartz}} - \delta^7\text{Li}_{\text{garnet}}$ ) up to 33.7‰, could be explained by equilibrium isotope fractionation related to the variation of coordination number and the bond strength of Li to its neighboring atoms in different minerals. This finding helps to understand the behavior of the lithium isotopes during subduction and crustal recycling processes.

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## 核体积效应对重元素稳定同位素分馏的影响

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早在1947年Bigeleisen–Mayer就建立了化学交换反应中平衡态的同位素分馏理论。这个理论认为, 在温度一定的情况下, 化学交换反应中的同位素富集系数与质量差  $\Delta m$  成正比, 并且与产物中的两个同位素的质量  $m'$  和成反比, 即Bigeleisen–Mayer公式。然而, 这个理论并不是对元素周期表中的每一个元素适用。1989年Fujii发现 $^{235}\text{U}$ 在U(IV)和U(VI)的交换反应中的异常同位素效应, 该异常效应违背了Bigeleisen–Mayer理论, 且被称为“核体积效应”。核体积效应是一种由核电荷密度和核大小和形状的不同引起的同位素效应。1996年Bigeleisen对1947年建立的同位素分馏理论进行修正, 在质量变化项的基础上加入了核体积变化项。对于交换反应:  $A'Y + AX = A'X + AY$ , 核体积效应的表达式为:  $\ln K_a = (kT^{-1}) \{ [E^0(AX) - E^0(A'X)] - [E^0(AY) - E^0(A'Y)] \}$ 。其中 $E^0$ 是基态的电子能, 且核体积效应项与

$1/T$ 成正比。因此当温度恒定时, 核体积效应项只与电子能之差有关。

此后Fujii等人通过实验研究了核体积效应对不同重元素同位素分馏的影响, 例如Ti、Zn、Zr、Fe、Gd、Nd、Cr、Sr、Mo、Ru、Te、Cd和Sn等元素。2006年Schauble从理论计算上也研究了核体积效应对Hg、Tl和其他重元素稳定同位素分馏的影响。他们研究得出的结论一致。对于轻元素而言, 交换反应中影响同位素分馏的主要因素是质量效应, 核体积效应可以忽略不计, 但是对于重元素而言, 核体积效应则是影响交换反应中同位素分馏的主要因素, 且随着重元素原子序数的增大, 核体积效应对其同位素的分馏更为重要。因此, 在计算重元素的同位素分馏系数时, 务必要考虑核体积效应的影响。我们使用量子化学计算方法, 示范了如何进行Hg、Tl等同位素体系的平衡分馏系数的计算。