Theoretical study of reduced partitioning function ratios of Zn-bearing minerals and metals

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The isotopic fractionation of Zn between metallic- and silicate phases has been used to trace the partitioning of Zn into the Earth's core and to study the Zn isotopic composition of the bulk silicate Earth [1, 2]. In order to understand the behaviour of Zn during natural processes, such as partial melting and fractional crystallisation, theoretical approaches to quantifying its isotopic composition in common high temperature phases are paramount. Here we theoretically calculate the reduced partition function ratios (lnβ) for ^{66}Zn/^{64}Zn for zinc metal, Zn-bearing olivine, sphalerite, and gahnite (Zn-spinel). Calculations with three different programs: SIESTA, Quantum Espresso (QE), and VASP have been performed to assess any bias between them. Furthermore, lnβ was calculated by both the full-frequency calculation (Full) and the force constant approximation (FCA). Results obtained using SIESTA yield the best consistency between FCA and Full calculations. On the other hand, agreement between the FCA and Full methods was non-systematic using QE and VASP. Our results for sphalerite and gahnite using SIESTA and QE show heavy Zn enrichment in gahnite, consistentent with previous work [3]. We provide the first results for olivine, and find that it is enriched in the lighter isotopes (~0.15 per mil) compared to gahnite (Zn-spinel), in agreement with natural olivine-spinel pairs in peridotites [2]. This difference supports the observation that mantle minerals are isotopically fractionated relative to one another and that partial melting should produce Zn isotopic fractionation [4]. Finally, Zn metal is slightly enriched in the lighter isotopes (~0.1 per mil at 1000 K) compared to olivine, suggesting that the Earth's core may be isotopically fractionated compared to the mantle.

[1] Mahan, Siebert, Pringle & Moynier (2016) *GCA* **196**, 252-270. [2] Wang, Liu, Liu, Huang, Xiao, Chu, Zhao & Tang (2017) *GCA* **198** 151-167. [3] Ducher, Blanchard & Balan (2016) *Chemical Geology* **443**, 87-96. [4] Doucet, Mattielli, Ionov, Debouge & Golovin (2016) *EPSL*, **451**, 232-240.