Mass-independent Hg isotope fractionations caused by nuclear volume effects

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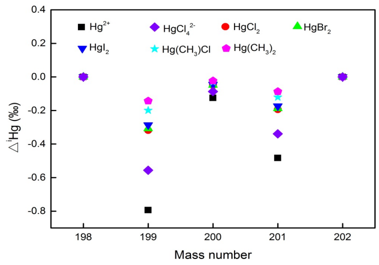
W. H. King (1984) and Y. Fujii *et al* (1989) first noticed an anomalous isotope effect and called it as the nuclear volume effect (NVE). The NVE is an isotope fractionation driving force caused by differences in nuclear charge density, nuclear size and nuclear shape of isotopes, especially for heavy elements. Bigeleisen (1996) first calculated the NVE for U isotopes. Later, tremendous efforts have been made on checking the NVEs of isotope systems including Mo, Zn, Cr, Ni, Te, etc., by Dr. Toshiyuki Fujii and his co-workers. By using quantum chemistry calculation methods, Schauble (2007) also showed that NVE could affect isotope fractionations of some heavy elements (e.g., Hg, Tl) to astonishing degrees [1] and he extended such calculation to solids (Schauble, 2013).

Hg isotope system is a very unique one. It shows not only odd number mass-independent fractionations but also even number mass-independent fractionations [2,3]. The mechansim of the Δ^{200}Hg mass-independent fractionation is still not clear. Here we provide a NVE investigation on mass-independent Hg isotope fractionation using full-electron relativistic quantum mechanics calculation. Dirac 13.1 software package is used for this study. We find that the NVE can cause mass-independent Hg isotope fractionations for both odd and even number cases. However, the degree of the $\Delta^{200/198}$Hg mass-independent fractionation is quite small. The figure at below shows the results (relative to elememtal Hg). Our results can only explain part of Δ^{200}Hg data but not those large MIF Hg data found recently (e.g., [3]). Our data generally agree with the experiments of Ghosh *et al* (2008, 2013) [4].



[1] Schauble (2007) *GCA*, **71**, 2170-2189. [2] Gratz *et al* (2010) *EST*, **44**, 7764-7770. [3] Chen *et al* (20123) *GCA*, **90**, 33-46. [4] Ghosh *et al* (2013) *Chem. Geol.*, **336**, 5-12.