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Effect of solvent on isotopic properties of complexes SiF_4 and BF_3 in the processes of isotope separation of silicon and boron by chemical exchange rectification

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Abstract

Ab initio quantum-chemical calculation of isotope reduced partition function ratios (β-factors) and separation factors of isotopes of silicon and boron in the systems fluoride of the element – its complex with organic solvent have been carried out. These systems are used for separation of isotopes of boron and silicone by the method of chemical exchange rectification (chemical isotope exchange method with thermal phase reversal).

It has been shown that the common ab initio calculations of vibrational frequencies of the fluoride of boron or silicon and their complex with solvent can not predict experimental values of isotope separation factor. And for the correct description it is necessary to take into account the polarizing effect of solvent on the complex. This effect has been used to study the Polarized Continuum Model (PCM). In all cases for the systems previously studied we found out that our theoretical results corresponded well with experimental results. This opens a possibility for directed search for isotope separation systems by the method of chemical exchange rectification.