

Lithium Isotope Effect Accompanying Electrochemical Insertion of Lithium into Liquid Gallium

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Z. Naturforsch. **65a**, 461 – 467 (2010); received September 7, 2009

Lithium was electrochemically inserted from a 1 : 2 (v/v) mixed solution of ethylene carbonate (EC) and methylethyl carbonate (MEC) containing 1 M LiClO₄ into liquid gallium to observe lithium isotope effects accompanying the insertion. It was observed that the lighter isotope ⁶Li was preferentially fractionated into liquid gallium with the single-stage lithium isotope separation factors *S*, ranging from 1.005 to 1.031 at 50 °C and 1.003 to 1.024 at 25 °C. The lithium isotope effects estimated by molecular orbital calculations at the B3LYP/6-311G(d) level of theory agreed qualitatively with those of the experiments, but the quantitative agreement of the two was not satisfactory.

Key words: Lithium Isotope Effects; Electrochemical Insertion; Gallium; Molecular Orbital Calculation; Reduced Partition Function Ratio.