Molecular Orbital Estimation of Reduced Partition Function Ratios of Lithium Interacting with Aromatic Hydrocarbons with Condensed Benzene Rings

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Molecular orbital calculations at the B3LYP/6-311G(d) level were carried out to elucidate the lithium isotope effects accompanying chemical insertion of lithium from 1-methoxybutane solution containing lithium and naphthalene to graphite. The lithium atom between the graphene layers of graphite was modeled as lithium atoms in 1:1 complexes of lithium and simple aromatic hydrocarbons with condensed benzene rings. The ^{7}Li-to-^{6}Li isotopic reduced partition function ratio (RPFR) was found to be a decreasing function of the number of benzene rings adjacent to the benzene ring above which the lithium atom was located, and was "saturated" at 1.04570 at 25 °C. The most plausible lithium species in the 1-methoxybutane solution was a lithium atom interacting with a naphthalene molecule and solvated by a 1-methoxybutane molecule in the contact ion pair manner. Its RPFR value was 1.07126 at 25 °C. The two RPFR values gave a single-stage separation factor of 1.024 for the lithium isotopes, which agreed well with the experimental value of 1.023.

Key words: Lithium Isotopes; Graphite; Reduced Partition Function Ratio; Molecular Orbital Calculations.