Ab initio Molecular Orbital Calculations of Reduced Partition Function Ratios of Polyboric Acids and Polyborate Anions

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Molecular orbital calculations at the HF/6-31G(d) level were carried out for polyboric acids and polyborate anions up to a pentamer to estimate their ^{11}B-to-^{10}B isotopic reduced partition function ratios (RPFRs) and examine the additivity of logarithms of RPFRs. Approximate RPFR-values calculated by the use of the additivity agreed with exact RPFR-values within a margin of 1% error. This error was equivalent to a 5% error on ln(RPFR). The equilibrium constants of mono boron isotope exhange reactions between three-coordinate boron and four-coordinate boron ranged from 1.0203 to 1.0360 at 25 °C, indicating the importance of exact evaluation of RPFRs of polymers.

Key words: Ab initio Molecular Orbital Calculations; Polyborates; Reduced Partition Function Ratios; Boron Isotope Exchange; Isotope Fractionation.