VB/MM – The Validity of the Approximations

Avital Sharir-Ivry, Avital Shurki[†]*

Department of Medicinal Chemistry and Natural Products, The Lise Meitner-Minerva Center for Computational Quantum Chemistry, School of Pharmacy, The Hebrew University of Jerusalem, Jerusalem 91120, Israel

Supporting Information

Table of Content

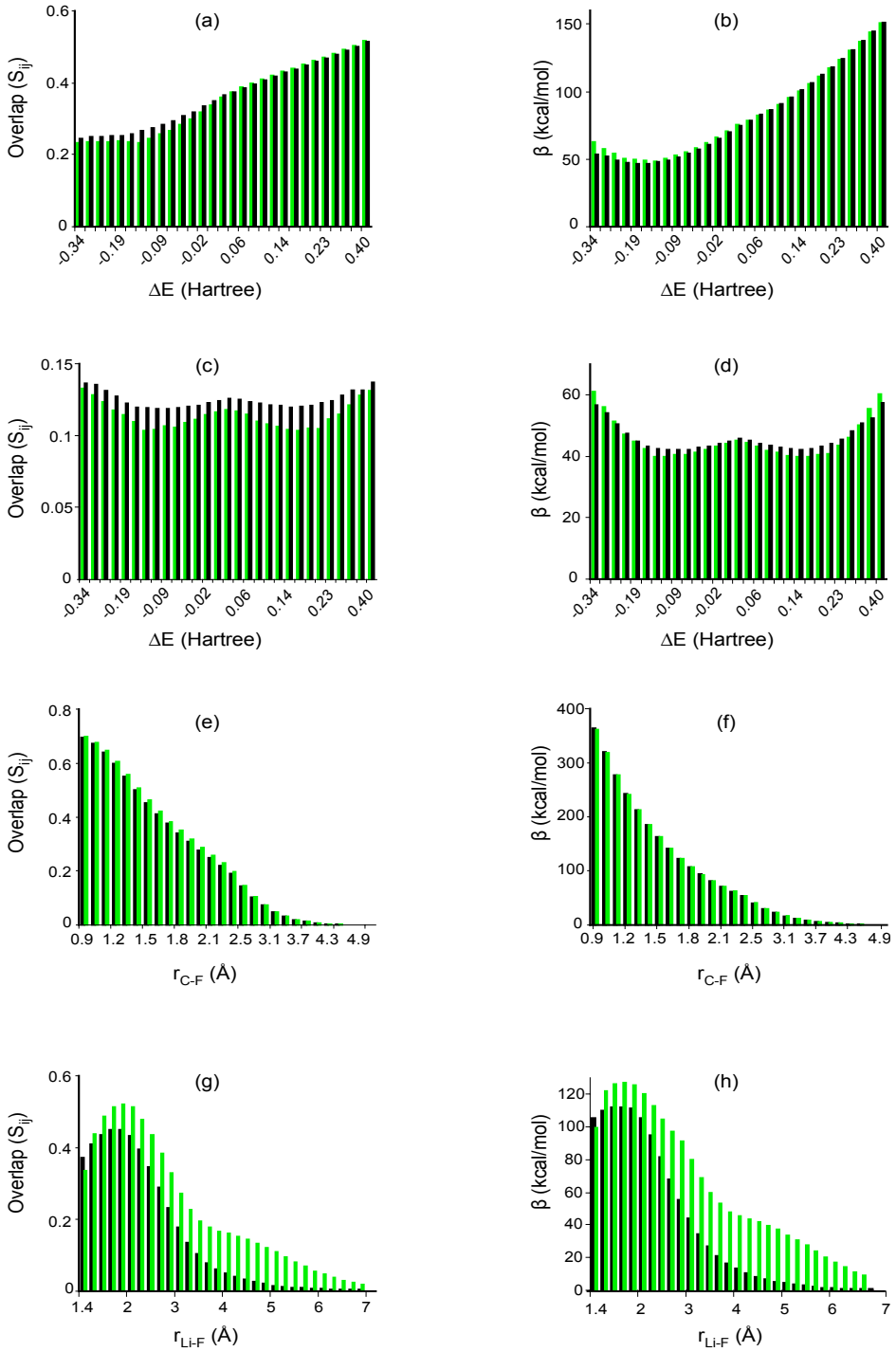

Figure 1S. (a) overlap and (b) reduced resonance integral values between ϕ_{cov}^{P}, **6** and ϕ_{ion}, **7** VB configurations and (c) overlap and (d) reduced resonance integral values between ϕ_{cov}^{R}, **5** and, ϕ_{cov}^{P} **6** VB configurations of various geometries along the S_N2 reaction. (e) overlap and (f) reduced resonance integral values between ϕ_{cov}, **3** and ϕ_{ion}, **4** VB configurations of various geometries along the CH_3F dissociation. (g) overlap and (h) reduced resonance integral values between ϕ_{cov}, **1** and ϕ_{ion}, **2** VB configurations of various geometries along the LiF dissociation. Black bars present the overlap values in the gas phase whereas green bars present the values in solution.

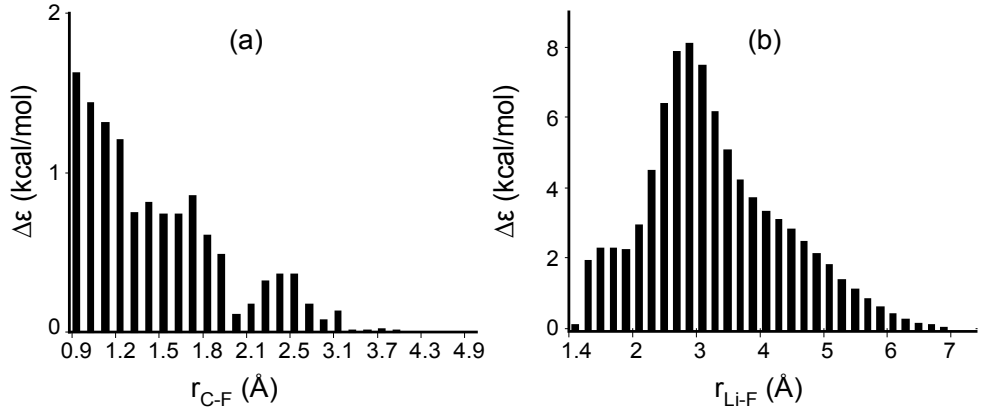

Figure 2S. The absolute energy differences between eigenvalues calculated with and without the approximations for various geometries along (a) CH_3F and (b) LiF dissociation curves.

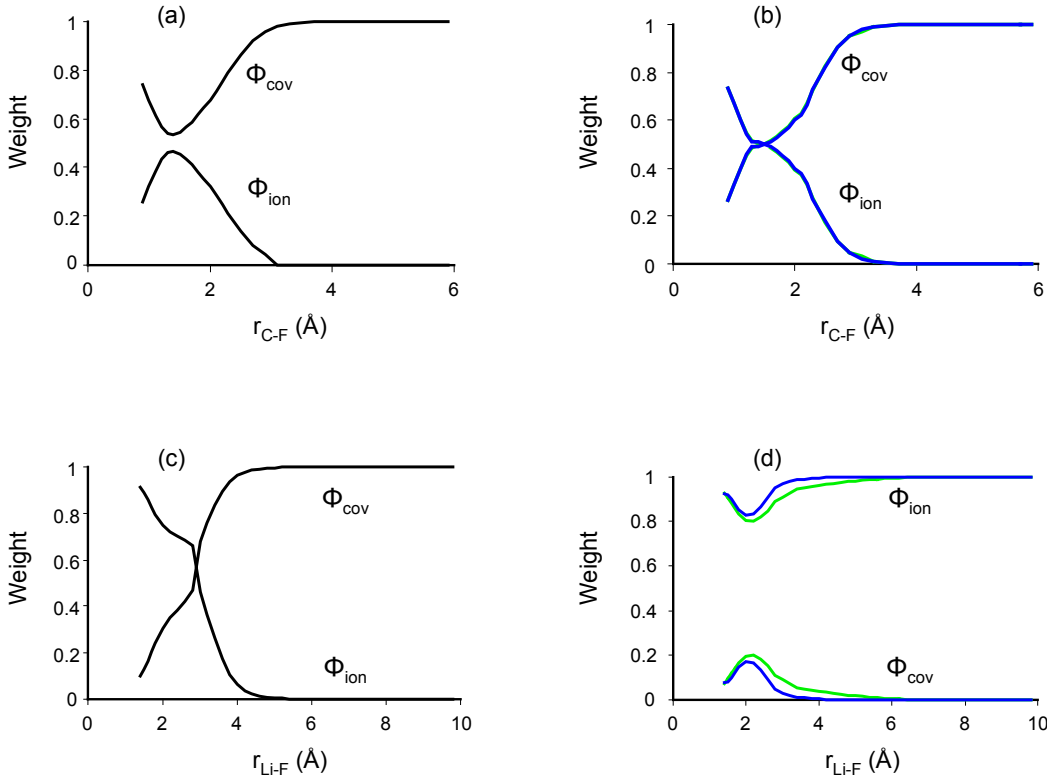

Figure 3S. Weights of the various VB configurations that compose the overall wave function of the gas phase (a) and solution (b) CH_3F dissociation curves, and the gas phase (c) and solution (d) LiF dissociation curves. Solution weights are calculated with the VB/MM (blue) and the DE-VB/MM (green) methods.

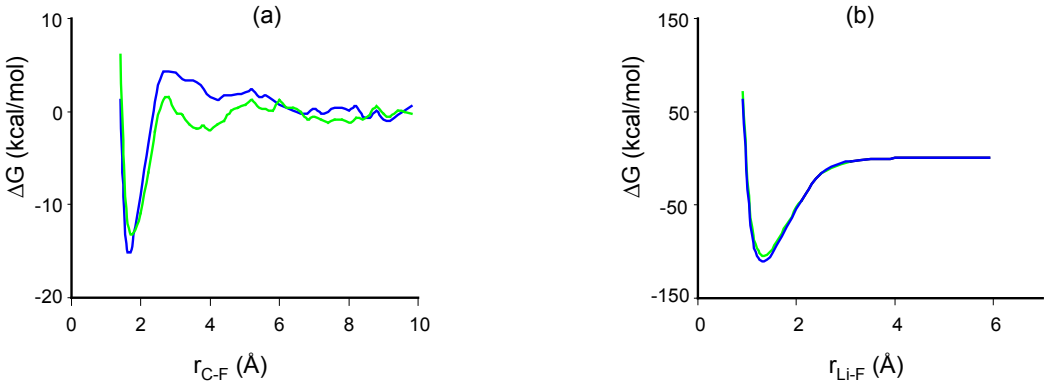

Figure 4S. Dissociation curves of the CH_3F (a) and LiF (b) calculated with VB/MM (blue) and DE-VB/MM (green) methods.