NEAR-DISSOCIATION THEORY ANALYSIS FOR THE DISSOCIATION ENERGY AND VIBRATIONAL EXTRAPOLATION FOR Ba^+-Ar

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Panov *et al.*[a] recently reported dispersed emission and both low and high resolution $B\,^2\Pi - X\,^2\Sigma^+$ excitation spectra for the Ba^+-Ar complex. Their analysis of those data involved merging a high quality electronic structure calculation with an RKR potential for the well. However, while reasonable dissociation energies were obtained, their approach does not readily provide any estimate of the uncertainties. The present paper shows that equivalent (or better) results, which also include realistic estimates of the extrapolation uncertainties, can be obtained by simply applying near-dissociation expansion (NDE) fits directly to the experimental data.

[a] S.I. Panov, J.M. Williamson and T.A. Miller, *J. Chem. Phys.* **102**, 7359 (1995)