STRUCURE AND INTERACTIONS OF ULTRACOLD Yb IONS AND Rb ATOMS

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Abstract. In order to study ultracold charge-transfer processes in hybrid atom-ion traps, we have mapped out the potential energy curves and molecular parameters for several low lying states of the $RbYb^+$ system. We employ both a multi-reference configuration interaction (MRCI) and a full configuration interaction (FCI) approach. Turning points, crossing points, potential minima and spectroscopic molecular constants are obtained for the lowest five molecular states. Long-range parameters, including the dispersion coefficients are estimated from our *ab initio* data. The separated-atom ionization potentials and atomic polarizability of the ytterbium atom (α_d=128.4 atomic units) are in good agreement with experiment and previous calculations. We will present dynamical calculations for (adiabatic) scattering lengths for the two lowest (Yb,Rb^+) channels that were carried out in our work. We find that the pseudo potential approximation is rather limited in validity, and only applies to nK temperatures. The adiabatic scattering lengths for both the triplet and singlet channels, are large and negative in the FCI approximation.

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Keywords: Ultracold, potential curves, scattering lengths, molecular constants

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