

Abstract Submitted
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Ytterbium atom-ion Collisions¹ PENG ZHANG, ALEXANDER DALGARNO, Harvard University, ROBIN COTE, University of Connecticut — Studies of the charge transfer process in collisions of ytterbium atoms (Yb) with ytterbium ions (Yb⁺) at cold and ultracold temperatures are reported. The molecular potential energy curves, $^2\Sigma_g^+$ and $^2\Sigma_u^+$, of Yb₂⁺ are determined at the multi-reference averaged quadratic coupled cluster level of theory with the long range polarization potential described by the accurate dipole polarizability of 142 a.u.. The calculated cross sections are large in the limit of low temperature and show considerable structures that arise from a combination of shape resonances modulated by glory oscillations and Regge oscillations. The thermally averaged charge transfer rate coefficients are in good agreement with the results from a recent experiment and with the Langevin formula at temperatures below 100 K. The scattering lengths for various isotopes computed both from semi-classical theory and from fitting to the effective range expansion are reported and agree well with each other. For higher temperatures, we compare quantal and semiclassical results, and investigate the range of applicability of the Langevin formula.

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