

Abstract Submitted
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Radiative charge transfer in ultra-cold collisions of S with Protons¹ P.C. STANCIL, G. SHEN, University of Georgia, J.F. MCCANN, B.M. MCLAUGHLIN, Queens University Belfast — Molecule formation processes involving second-row elements is of prime interest as searches are ongoing in a variety of interstellar and circumstellar media [1]. We have investigated radiative decay processes at ultra-cold temperatures and above for S colliding with H⁺. Previously [1], we have investigated this system for radiative association. We use the MOLPRO quantum chemistry suite of codes to obtain accurate potential energies and transition dipole moments as a function of internuclear distance between low-lying states of the SH⁺ molecular ion complex. A multi-reference configuration-interaction (MRCI) approximation is used to determine all the potential energy curves and transition dipole moments, where the molecular orbitals (MO's) are obtained from state-averaged multiconfiguration-self-consistent-field (MCSCF) calculations. The collision problem is solved using a fully quantum-mechanical approach, an optical potential method, and a semiclassical approximation at higher energies. Rate coefficients are determined for temperatures ranging from micro-Kelvin up to 20,000 K. Further details and a comprehensive set of results will be presented.

[1] P. C. Stancil et al., *Astron. Astrophys. Suppl. Ser.* 143, 107 (2000).

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