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Charge transfer between O^{6+} and atomic hydrogen Y. WU, P.C. STANCIL, University of Georgia, H.P. LIEBERMANN, R.J. BUENKER, Bergische Universitat Wuppertal, D.R. SCHULTZ, Y. HUI, Oak Ridge National Laboratory —
The charge exchange process has been found to play a dominant role in the production of X-rays and/or EUV photons observed in cometary and planetary atmospheres and from the heliosphere. Charge transfer cross sections, especially state-selective cross sections, are necessary parameters in simulations of X-ray emission. In the present work, charge transfer due to collisions of ground state $O^{6+}(1s^2\ ^1S)$ with atomic hydrogen has been investigated theoretically using the quantum-mechanical molecular-orbital close-coupling method (QMOCC). The multi-reference single- and double-excitation configuration interaction approach (MRDCI) has been applied to compute the adiabatic potential and nonadiabatic couplings, and the atomic basis sets used have been optimized with the method proposed previously to obtain precise potential data. Total and state-selective cross sections are calculated for energies between 10 meV/u and 10 keV/u. The QMOCC results are compared to available experimental and theoretical data as well as to new atomic-orbital close-coupling (AOCC) and classical trajectory Monte Carlo (CTMC) calculations. A recommended set of cross sections, based on the MOCC, AOCC, and CTMC calculations, is deduced which should aid in X-ray modeling studies.

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