

The purpose of this work and the project under which it was created is to develop, compare and validate several theoretical approaches and computation methods used to calculate the cross sections of dissociative recombination. For the most part it is concerned with the indirect dissociative recombination of molecular ions of  $\text{H}_2^+$  in the singlet ungerade channels computed with three distinct approaches. First, the fully numerically solvable two-dimensional approach developed at ÚTF MFF UK as a part of my master's thesis. Second, a vibrational frame transformation method based on the work of Chang and Fano [E. S. Chang and U. Fano, *Phys. Rev. A* **6**, 173 (1972)] and then enhanced into a full energy-dependent form by Gao and Greene [H. Gao and C. H. Greene, *J. Chem. Phys.* **91**, 3988 (1989)], [H. Gao and C. H. Greene, *Phys. Rev. A* **42**, 6946 (1990)], further improved by our own revisions. Third, a two-dimensional R-matrix method based on matching exact 2D solutions from a small interaction region to asymptotic solutions in the non-interacting region. We thoroughly discuss the various advantages and caveats of these methods and, in the later chapters, present our work on employing them for the realistic recombination of  $\text{HeH}^+ + e^-$ . Furthermore, we attempt to extend the presented models to the description of the direct dissociative recombination of  $\text{H}_2^+ + e^-$  in the singlet gerade symmetry.