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Towards a full quantum mechanical treatment of atom-triatom inelastic collisions[1] H. DA SILVA JR, N. BALAKRISHNAN, University of Nevada, Las Vegas — Despite computational methodologies designed to model atomic and molecular inelastic collisions being widely available nowadays, these are yet restricted to small systems such as atom–diatom and diatom–diatom within the time-independent quantum mechanical approach. Moreover, recent advances in AMO physics brought to attention physical conditions (i.e. ultracold collisions, light–assisted excited colliding partners, high atomic densities etc.) and heavy atomic/molecular species (often also charged) that are nearly numerically intractable. In particular, after steady advances in the early 90's, the atom–triatom case is yet lacking a full quantum mechanical approach. In this work we propose a time–independent formalism, based on a set of arrangement–fixed Jacobi coordinates, to model collisions and scattering of an atom by a triatomic target, accounting for all degrees of freedom. Numerical results are presented for the case study H_2O + H.

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