Abstract Submitted
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**Bond coordinates as an alternative: Low energy reactive collisions of He2+ with He; comparison of TD and TI quantum calculations** MANUEL LARA, JILA, University of Colorado, ENRICO BODO, Dept. of Chemistry and INFM, University of Rome "La Sapienza", Italy , FRANCO A. GIANTURCO[1], Dept. of Chemistry, University of Rome "La Sapienza", Italy — "Reactive" and "inelastic" processes in the ionic $He_3^+$ system[1] have been separated and analyzed through the simulation of the $^3He + ^4He_2$ collision. The combined use of TD and TI techniques allowed the study for both high and very low kinetic energies; the agreement between the corresponding results in the medium energy range is very good. Influence of the internal excitation of the reagents and implications on the dynamics of evaporation in He clusters will be discussed[2,3]. Emphasis will be made on the TD wavepacket propagation methodology used for the calculation of state-to-state transition probabilies, based bond coordinates: This method[4] was suggested recently by one of the authors, and is applied for the first time to a process with three open channels. Bond coordinates can have several advantages over the use of standard Jacobi ones [1] E. Scifoni, E. Bodo and F. A. Gianturco, Eur. Phys. J. D, 30, 363 (2004) [2] E. Bodo, F. A. Gianturco, A. Dalgarno, J. Phys. B 35 (2002) 2391. [3] E. Bodo and F. A. Gianturco, Eur. Phys. J. D, 31 (2004) 423 [4] M. Lara, A. Aguado, O. Roncero,and M. Paniagua. J. Chem. Phys., 113, 1781 (2000)

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