Abstract Submitted
for the DAMOP08 Meeting of
The American Physical Society

Electric field control of chemical reactions TIMUR TSCHERBUL, ROMAN KREMS, Department of Chemistry, University of British Columbia — We develop the formalism for rigorous quantum scattering calculations of probabilities for chemical reactions in the presence of an external electric field. The approach is based on the Fock-Delves hyperspherical coordinates and adiabatic partitioning of the total Hamiltonian. The adiabatic channel wave functions are expanded in basis sets of hyperangular functions corresponding to different reaction arrangements and the effects of external fields are included in each chemical arrangement separately. We show that the chemical reaction of vibrationally excited LiF molecules with H atoms at temperatures below 1 K can be significantly modified by external electric fields. In particular, we demonstrate that (i) electric fields may enhance the s-wave reaction cross section by several orders of magnitude, (ii) reactive scattering resonances at low collision energies may be shifted and suppressed by electric fields of $\sim$ 100 kV/cm; (iii) the chemical reaction becomes more probable than inelastic energy transfer at high electric fields.

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Date submitted: 31 Jan 2008 Electronic form version 1.4