

Abstract Submitted
for the DAMOP08 Meeting of
The American Physical Society

Quantum dynamics of F + HCl and F + DCl reactions at ultralow energies¹ BALAKRISHNAN NADUVALATH, GOULVEN QUÉMÉNER, University of Nevada Las Vegas — Quantum scattering calculations of $F + HCl \rightarrow HF + Cl$ and $F + DCl \rightarrow DF + Cl$ reactions have been carried out at cold and ultracold temperatures. The effect of rotational and vibrational excitations of the HCl molecule on the reactivity is investigated. The reactivity of the F + DCl system is found to be significantly lower than that of the F + HCl reaction indicating the importance of quantum tunneling at low energies. For both reactions, Feshbach resonances occur at low energies due to decay of quasibound states of the FHCl and FDCl complexes supported by the van der Waals interaction potential. We also explored the validity of the coupled-states approximation for cold collisions and we found that it is generally valid for the background scattering but it fails to reproduce the resonances or to correctly describe the Wigner threshold behavior of cross sections when the diatom is initially in an excited rotational level.

¹This work is supported by NSF grant No. PHY-0555565.

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Date submitted: 31 Jan 2008

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