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Quantum dynamics of Li+HF→LiF+H reaction at low temperatures[1] N. BALAKRISHNAN, JISHA HAZRA, Department of Chemistry, University of Nevada Las Vegas, Las Vegas, NV 89154 — We report a quantum dynamics study of the Li+HF→LiF+H reaction at low temperatures of interest to cooling and trapping experiments. Contributions from non-zero partial waves are analyzed and results show narrow resonances in the energy dependence of the cross section that survive partial wave summation. Results obtained using two ab initio electronic potential energy surfaces for the LiHF system show strong sensitivity to the choice of the potential. In particular, small differences in the barrier heights of the two potential surfaces are found to dramatically influence the reaction cross sections at low energies. Comparison with recent measurements of the reaction cross section shows similar energy dependence in the threshold regime and an overall good agreement with experimental data compared to previous theoretical results.

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