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Quantum State Resolved Reactive Scattering Near Conical Intersections: $F(^2P) + HCl \rightarrow HF(v,J) + Cl(^2P)$ and $F(^2P) + H_2O \rightarrow HF(v,J) + OH(^2\Pi)$ via High Resolution IR Spectroscopy on Nascent HF Product ALEXANDER ZOLOT, MICHAEL ZIEMKIEWICZ, MICHAEL DESKEVICH, DAVID NESBITT, JILA, National Institute of Standards and Tehcnology and University of Colorado — State resolved reaction dynamics of the reactions$F(^2P) + HCl \rightarrow HF(v,J) + Cl(^2P)$and $F(^2P) + H_2O \rightarrow HF(v,J) + OH(^2\Pi)$have been studied under rigorous single collision conditions in crossed molecular jets via IR absorbance of the HF product. Supersonic jet collision energies exceed the ground electronic state barrier height predicted by ab initio (DW-MCSCF) calculations, but can not overcome the larger barriers on excited state surfaces. The experimental results reveal highly vibrationally inverted nascent HF populations containing significant population above the average energy available to products for both of the title reactions. Such excited products may be formed by the tail of the collision energy distribution, but may also be favored by the extra ∼1.1 kcal/mol available for reaction with spin-orbit excited fluorine, previously observed in other systems. F+HCl product rotational distributions are found to be particularly non-statistical and are poorly modeled by single surface QCT.

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