

THEORETICAL INVESTIGATIONS OF THE LIFETIME OF SH ($A^2\Sigma^+$) in Ar \cdots SH and Kr \cdots SH

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The ($A^2\Sigma^+$) state SH molecule provides a prototypical system through which the effect of dimer formation on predissociation dynamics can be investigated. In the gas phase, there is a crossing between this state and the repulsive $a^4\Sigma^-$ state at 1000 cm^{-1} above the vibrational ground state of the diatomic, resulting in the observed lifetime of 1 ns. In recent experiments, Carter and Miller observed that the lifetime is increased by as much as three orders of magnitude when SH is in a dimer with Ar or Kr. Further, the lifetime is found to be sensitive to the intermolecular state of the dimer that is accessed.

In this talk we will present results of our work in modeling these experimental results, using the empirical potential surfaces for the Kr \cdots SH and Ar \cdots SH dimers developed by Korambath and Hayes. We find a simple ballistic model explains many of the experimental trends. Results for approximate quantum calculations of the lifetimes will also be presented.