THEORETICAL INVESTIGATIONS OF THE LIFETIME OF SH AND SD ($^2\Sigma^+$) IN M···SH/D (M=Ne,Ar,Kr) COMPLEXES

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The lifetimes of SH and SD in the $^2\Sigma^+$ electronic state are investigated as a function of the intermolecular vibrational states of Ne···SH, Ar···SH and Kr···SH. Model potentials are developed for these systems and the lifetimes, calculated from these potentials, agree well with those reported by Miller and co-workers.[a] The calculated lifetimes are analyzed using an empirical ballistic model that assumes that the rare gas atom blocks electronic predissociation for certain geometrically defined geometries. The results of the ballistic model are found to be in good agreement with the more demanding adiabatic calculations of the dynamics and with the experimental lifetimes.

[a] B. Applegate, M.-C. Yang and T. A. Miller, J. Chem. Phys. (submitted)