

VIBRATIONAL SPECTROSCOPY AND A POTENTIAL SURFACE FOR THIOPHOSGENE

BRENT STRICKLER and MARTIN GRUEBELE, *Department of Chemistry and Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, Urbana, IL 61801.*

Vibrationally excited SCCl_2 is a model for nonhydrogenic vibrational energy redistribution (IVR). Spectroscopic characterization of the ground and excited singlet states has been made by fluorescence excitation and high resolution dispersed fluorescence measurements. Using over 500 transitions from several $\tilde{X} \leftarrow \tilde{B}$ dispersed fluorescence spectra, the ground electronic state has been mapped up to 20,200 cm^{-1} with an error $\leq 3 \text{ cm}^{-1}$. The adjustable parameters of an analytical six-dimensional *ab initio* potential surface have been fitted to the fluorescence transitions using a nonlinear least squares algorithm. The fitted potential surface provides an experimental standard for IVR quantum dynamics calculations.