CARS AND INFRARED STUDIES OF $^{32}S^{16}O_3$: HOW CAN SUCH A SIMPLE MOLECULE GIVE SUCH A COMPLEX SPECTRUM?

JEFFREY BARBER, ENGELENE t.H. CHRYSOSTOM, TONY MASIELLO, JOSEPH W. NIBLER, *Department of Chemistry, Oregon State University, Corvallis, OR 97331*; ARTHUR MAKI, *15012 24th Ave. S. E. Mill Creek, WA 98012*; ALFONS WEBER, *National Science Foundation, Arlington, VA 22230 and National Institute of Standards and Technology, Gaithersburg, MD 20899*; THOMAS A. BLAKE, ROBERT L. SAMS, *Pacific Northwest National Laboratory, Richland, WA 99352*.

Sulfur trioxide is an important participant in reactions in the upper atmosphere and also in a number of industrial processes. It is a D_{3h} planar oblate top whose spectroscopy is surprisingly incomplete, in part due to its extreme corrosive properties. We report here a comprehensive investigation of all four fundamental bands of $^{32}S^{16}O_3$. High resolution (0.001 cm^{-1}) coherent anti-Stokes Raman scattering (CARS) has been used at Oregon State University to examine the Q-branch structure of the IR-inactive ν_1 symmetric stretching mode of $^{32}S^{16}O_3$. This spectrum reveals two intense Q-branch regions, with complex vibrational-rotational structure. The modeling of this has been challenging and involves a subtle combination of Fermi-resonances, indirect Coriolis interactions, and l-resonances with nearby hidden states; $2\nu_4$ (l= 0, $\pm$ 2), $\nu_2 + \nu_4$ ($l = \pm$ 1), $2\nu_2$ (l =0). The analysis of the perturbed ν_1 spectrum, achieved by locating these states via high-resolution infrared hot-band studies performed at Pacific Northwest National Laboratory, will be presented in this talk.