

OBSERVATION AND ANALYSIS OF THE ν_3 and $2\nu_3$ BANDS OF $^{32}\text{S}^{18}\text{O}_3$ AND $^{34}\text{S}^{18}\text{O}_3$

STEVEN W. SHARPE, ROBERT L. SAMS, THOMAS A. BLAKE, *Pacific Northwest National Laboratory, P. O. Box 999, Mail Stop K8-88, 3020 Q Avenue, Richland, WA 99352 (PNNL is operated for the US Department of Energy by the Battelle Memorial Institute under contract DE-AC06-76RLO 1830)*; ARTHUR MAKI, *15012 24th Ave. S. E. Mill Creek, WA 98012*; NICOLAE VULPANOVICI, TONY MASIELLO, JEFFREY BARBER, ENGELENE t.H. CHRYSOSTOM, JOSEPH W. NIBLER, *Department of Chemistry, Oregon State University, 153 Gilbert Hall, Corvallis, OR 97331-4003*; ALFONS WEBER, *National Institute of Standards and Technology, Gaithersburg, MD 20899 and National Science Foundation, 4201 Wilson Boulevard, Arlington, VA 22230*.

We are engaged in a comprehensive investigation of the fundamental and low lying combination and overtone bands of the parent and some isotopic variants of sulfur trioxide. Results and analysis for the Raman^a and infrared^b bands of the parent isotopomer have been published recently. Here, results and analysis of the infrared absorption spectra of the ν_3 and $2\nu_3$ bands of $^{32}\text{S}^{18}\text{O}_3$ and $^{34}\text{S}^{18}\text{O}_3$ recorded separately at a resolution of 0.002 cm^{-1} will be presented. For $^{32}\text{S}^{18}\text{O}_3$, ν_3 is centered at $1348.85320(3)\text{ cm}^{-1}$ with $B' = 0.30879466(7)\text{ cm}^{-1}$, $C' = 0.15436012(6)\text{ cm}^{-1}$ and $C'\zeta = 0.0795934(4)\text{ cm}^{-1}$. The $l = \pm 2$ component of the first overtone of ν_3 is centered at $2692.8899(3)\text{ cm}^{-1}$ with $B' = 0.307815(1)\text{ cm}^{-1}$, $C' = 0.1538331(7)\text{ cm}^{-1}$ and $C'\zeta = 0.078716(2)\text{ cm}^{-1}$. For $^{34}\text{S}^{18}\text{O}_3$, ν_3 is centered at $1330.07810(1)\text{ cm}^{-1}$ with $B' = 0.3088233(3)\text{ cm}^{-1}$ and $C' = 0.15437917(3)\text{ cm}^{-1}$, and $C'\zeta = 0.0770680(3)\text{ cm}^{-1}$. The $l = \pm 2$ component of the first overtone of ν_3 is centered at $2655.45735(4)\text{ cm}^{-1}$ with $B' = 0.3078634(8)\text{ cm}^{-1}$, $C' = 0.15386494(7)\text{ cm}^{-1}$ and $C'\zeta = 0.0762487(3)\text{ cm}^{-1}$. The Hamiltonian for analyzing these bands including splitting and perturbing terms and other fit constants will be presented.

^aE. t.H. Chrysostom, N. Vulpanovici, T. Masiello, J. Barber, J. W. Nibler, A. Weber, A. Maki, T. A. Blake, *J. Mol. Spectrosc.* **210**, 233 (2001).

^bA. Maki, T. A. Blake, R. L. Sams, N. Vulpanovici, J. Barber, E. t.H. Chrysostom, T. Masiello, J. W. Nibler, A. Weber, *J. Mol. Spectrosc.* **210**, 240 (2001).