OBSERVATION OF ROOM TEMPERATURE, ROTATIONALLY-RESOLVED INFRARED SPECTRA OF VAPOR PHASE SULFURIC ACID

THOMAS A. BLAKE, ROBERT L. SAMS, , *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).*

While recording high-resolution, mid-infrared spectra of weak overtone and combination bands of sulfur trioxide using a Bruker IFS 120HR Fourier transform spectrometer and White cell, we observed eight rotationally resolved bands that have a rotational line spacing for a molecule with a B value of approximately 0.162 cm^{-1}(B'' = 0.3485 $\mathrm{cm}^{-1}$for $^{32}\mathrm{S}^{16}\mathrm{O}_3$). We believe these bands belong to $\mathrm{H}_2{}^{32}\mathrm{S}^{16}\mathrm{O}_4$, which was created by the reaction of sulfur trioxide with water in the volume and surfaces of the White cell. Nominal pathlengths were twenty or forty meters and the sample pressure of sulfur trioxide was varied between 0.1 and 10 Torr. The observed band centers and our tentative assignment of these bands are as follows: 3600.9 $\mathrm{cm}^{-1}\nu_1(a)$, O - H symmetric stretch; 1247.5 $\mathrm{cm}^{-1}\nu_2(a)$, O - S - O symmetric stretch; 1099.1 $\mathrm{cm}^{-1}\nu_3(a)$, S - $(\mathrm{OH})_2$ symmetric bend; 828.3 $\mathrm{cm}^{-1}\nu_4(a)$, S(- $\mathrm{OH})_2$ symmetric stretch; 3602.9 $\mathrm{cm}^{-1}\nu_9(b)$, O - H antisymmetric stretch; 1486.9 $\mathrm{cm}^{-1}\nu_{10}(b)$, O - S - O antisymmetric stretch; 1149.7 $\mathrm{cm}^{-1}\nu_{11}(b)$, S - $(\mathrm{OH})_2$ symmetric bend; 897.3 $\mathrm{cm}^{-1}\nu_{12}(b)$, S(- $\mathrm{OH})_2$ symmetric stretch. The room temperature vapor pressure of sulfuric acid is very small and consequently its room temperature, vapor phase spectrum has not, to our knowledge, been reported in the past.