FIRST HIGH-RESOLUTION SPECTRA AND ROTATIONAL CONSTANTS OF $BrNO_2$ (NITRYL BROMIDE)

J. ORPHAL, *Institute of Environmental Physics, University of Bremen, P. O. Box 330440, 28334 Bremen, Germany*; B. REDLICH, H. GROTHE, and H. WILLNER, *Institute of Physical Chemistry, University of Hannover, Callinstr. 9, 30167 Hannover, Germany*; A. FRENZEL and C. ZETZSCH, *Fraunhofer-Institute of Toxicology and Aerosol Research, Fuchsstr. 1, 30625 Hannover, Germany*.

Nitryl bromide ($BrNO_2$) formed by heterogeneous reactions on polar stratospheric clouds and on sea-salt particles in the marine troposphere. However, no rotationally resolved spectra have been reported up to now, and nothing is known about rotational constants, structure, and force field of $BrNO_2$. In fact, the only observations of $BrNO_2$ in the gas phase were possible using flow experiments with gaseous N_2O_5 flowing over NaBr particles.

In this study, a different approach was used: By reaction of highly diluted gaseous $ClNO_2$ with an aqueous Br^- solution, $BrNO_2$ was formed and trapped at low temperature. The crude product was purified by trap-to-trap condensations and fractional sublimation in vacuo.

High-resolution infrared spectra of the ν_4 band of $BrNO_2$ around 1660 cm^{-1} were measured with resolutions of up to 0.002 cm^{-1}, using the Bruker IFS-120HR FTS at University of Hannover. For the first time, rotational constants for the $^{79}BrNO_2$ and $^{81}BrNO_2$ isotopomers were determined for the ν_4 and ground vibrational states. The constants were used for determination of a first substitution structure and, together with infrared band centers, the harmonic force field of $BrNO_2$.