

FIRST HIGH-RESOLUTION SPECTRA AND ROTATIONAL CONSTANTS OF BrNO₂ (NITRYL BROMIDE)

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Nitryl bromide (BrNO₂) 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 BrNO₂. In fact, the only observations of BrNO₂ in the gas phase were possible using flow experiments with gaseous N₂O₅ flowing over NaBr particles.

In this study, a different approach was used: By reaction of highly diluted gaseous ClNO₂ with an aqueous Br⁻ solution, BrNO₂ 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 BrNO₂ 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 ⁷⁹BrNO₂ and ⁸¹BrNO₂ 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 BrNO₂.