EXPERIMENTAL AND *AB-INITIO* STRUCTURE OF $BrNO_2$

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The ν_2 fundamental bands of different isotopomers of $BrNO_2$ ($^{79}Br^{15}N^{16}O_2$, $^{81}Br^{15}N^{16}O_2$, $^{79}Br^{14}N^{18}O_2$, and $^{79}Br^{14}N^{16}O^{18}O$) located around 13 μm, were recorded using high-resolution Fourier-transform infrared spectroscopy. More than 8000 lines of all these isotopomers were reproduced using a Watson-type *A*-reduced Hamiltonian with a root-mean-square deviation of better than 7×10^{-4} cm^{-1}, for the four isotopomers. Rotational and centrifugal distortion constants for the $v_2 = 1$ states as well as for the vibrational ground states of these isotopomers have been determined. For the first time, an analysis of the ground state rotational constants obtained in this study combined with the constants obtained in our previous work on the ν_2 bands of $^{79}Br^{14}N^{16}O_2$ and $^{81}Br^{14}N^{16}O_2$[a], allow us to calculate the r_m-structure of nitryl bromide. A new *ab-initio* structure of nitryl bromide calculated at the CCSD(T)/SDB-aug-cc-pVQZ level of theory is presented and found in fair agreement with the experimental structure.

[a] F. Kwabia Tchana, J. Orphal, I. Kleiner, B. Redlich, R. Mbiake and O. Bouba, *J. Mol. Spectrosc.*, **216**, 2, 292-296 (2002).