

## EXPERIMENTAL AND *AB-INITIO* STRUCTURE OF BrNO<sub>2</sub>

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The  $\nu_2$  fundamental bands of different isotopomers of BrNO<sub>2</sub> (<sup>79</sup>Br<sup>15</sup>N<sup>16</sup>O<sub>2</sub>, <sup>81</sup>Br<sup>15</sup>N<sup>16</sup>O<sub>2</sub>, <sup>79</sup>Br<sup>14</sup>N<sup>18</sup>O<sub>2</sub>, and <sup>79</sup>Br<sup>14</sup>N<sup>16</sup>O<sup>18</sup>O) located around 13  $\mu\text{m}$ , 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  $7 \times 10^{-4} \text{ cm}^{-1}$ , for the four isotopomers. Rotational and centrifugal distortion constants for the  $\nu_2 = 1$  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  $\nu_2$  bands of <sup>79</sup>Br<sup>14</sup>N<sup>16</sup>O<sub>2</sub> and <sup>81</sup>Br<sup>14</sup>N<sup>16</sup>O<sub>2</sub><sup>a</sup>, 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.

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<sup>a</sup>F. Kwabia Tchana, J. Orphal, I. Kleiner, B. Redlich, R. Mbiaké and O. Bouba, *J. Mol. Spectrosc.*, **216**, 2, 292-296 (2002).