

## FOURIER-TRANSFORM MICROWAVE AND MILLIMETERWAVE SPECTROSCOPY OF CH<sub>2</sub>I<sub>2</sub>Br IN ITS GROUND VIBRATIONAL STATE

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Halo-substituted methanes constitute a class of molecules that are important in various fields, from spectroscopy to quantum-chemical calculations. They are also gaining interest due to their potential adverse impact on the atmospheric chemistry.<sup>a</sup>

In the series of the CH<sub>2</sub>LX iodomethanes where  $X = \{F, Cl, Br\}$ , only the rotational spectra of CH<sub>2</sub>IF<sup>b</sup> and CH<sub>2</sub>ICl<sup>c</sup> have been published. We present our investigations on the high-resolution rotational spectroscopy of the two bromine isotopologues of bromiodomethane, CH<sub>2</sub>I<sup>79</sup>Br and CH<sub>2</sub>I<sup>81</sup>Br.

Due to the lack of spectroscopic information available for this compound, high-level quantum-chemical calculations were essential to guide the microwave and millimeterwave spectral assignments of both  $\mu_a$ - and  $\mu_b$ -type transitions. They provided rotational and centrifugal distortion constants (quartic and sextic), as well as the quadrupole-coupling tensor of the iodine ( $I_I = 5/2$ ) and bromine ( $I_{Br} = 3/2$ ) nuclei.

More than 1900 lines have been analyzed, leading to an accurate determination of molecular constants for both isotopologues. The experimental structure ( $r_0$ ) of the title species has been derived from the two sets of rotational constants.

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<sup>b</sup>C. Puzzarini, G. Cazzoli, J. C. López, J. L. Alonso, A. Baldacci, A. Baldan, S. Stopkowicz, L. Cheng and J. Gauss, *J. Chem. Phys.* 62, 174312 (2011).

<sup>c</sup>S. Bailleux, H. Ozeki, S. Sakai, T. Okabayashi, P. Kania and D. Dufлот, *J. Mol. Spectrosc.* 270, 51 (2011).