NEW ANALYSIS OF THE CORIOLIS-INTERACTING ν_2 AND ν_5 BANDS OF $CH_3{}^{79}Br$ AND $CH_3{}^{81}Br$

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Methyl bromide (CH_3Br) has been identified as one of the major sources of atmospheric bromine. Atmospheric methyl bromide originates from both natural (algae, phytoplankton) and anthropogenic sources (agricultural fumigant): the tropospheric mixing ratio of CH_3Br is 9-11 pptV in the Northern hemisphere and about 8 pptv in the Southern hemisphere, with an increase of about 0.15 pptV per year[a]. However, until present, no attempts have been made to determine atmospheric concentrations of CH_3Br using infrared spectroscopy. Although the line positions in this region have been studied previously at medium spectral resolution[b], little is known about the line intensities. The purpose of the present work is to complete and extend the previous studies of the 1200-1600 cm^{-1} spectral range and to provide a prediction of line positions and intensities accurate enough to determine optimal spectral windows for future atmospheric detection of CH_3Br. The ν_2 (A_1) and ν_5 (E) fundamental bands of $CH_3{}^{79}Br$ and $CH_3{}^{81}Br$ have been recorded at LPPM with a high-resolution Fourier-transform infrared spectrometer (unapodized resolution of 0.004 cm^{-1}). For both isotopomers, we assigned 3037 lines for the parallel bands, 4530 for the perpendicular bands, and in addition 80 perturbation-allowed transitions, with $J \leq 68$ and $K \leq 11$. By taking into account the xy-Coriolis interaction between the two bands, it has been possible to generate an accurate prediction of the whole spectrum, with a standard deviation of better than 7×10^{-4} cm^{-1}. The ground state axial rotational constants A_0 were redetermined from allowed and perturbation-allowed infrared transitions observed in the ν_2 and ν_5 bands around the local crossing. The A_0 values obtained for both isotopomers are more accurate but fully compatible with those obtained previously.

[a]World Meteorological Organization (WMO),"Scientific Assessment of Ozone Depletion: 1998", Report 44, WMO Global Ozone Research And Monitoring Project, Chapter 2, Geneva, Switzerland, 1999.

[b]R. Anttila, C. Betrencourt-Stirnemann, and J. Dupre, *J. Mol. Spectrosc.*, **100**, 54, (1983).