

A NEW TREATMENT OF THE $2\nu_3$ (A_1) INFRARED BAND OF METHYL BROMIDE CH_3Br AROUND 1213 cm^{-1}

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The high-resolution Fourier transform infrared spectrum of methyl bromide CH_3Br has been reinvestigated in the $\nu_3 = 2$ vibrational excited state around 1213 cm^{-1} , for both ^{79}Br and ^{81}Br isotopologues.

Thanks to new accurate K-dependent and J-dependent ground state parameters, up to sextic centrifugal distortion constants, 420 new infrared transitions of the $2\nu_3$ band have been assigned for $\text{CH}_3^{79}\text{Br}$ and $\text{CH}_3^{81}\text{Br}$, extending the rotational quantum number values up to $K_{max} = 15$ and $J_{max} = 60$. For each isotopic species, a standard deviation of $2 \times 10^{-4}\text{ cm}^{-1}$ has been obtained for about 700 lines of $2\nu_3$. The new parameter values of the $\nu_3 = 2$ excited state are in good agreement with ones determined previously by infrared spectroscopy, but significantly more accurate.

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