High Resolution Infrared Spectroscopy of $CH_2D^{79}Br$: Analysis of the ν_4 and ν_8 Interacting Fundamental Bands

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The high resolution (0.0030 cm^{-1}) infrared spectrum of monodeutero methyl bromide, $CH_2D^{79}Br$, previously studied in the range 550 – 1080 cm^{-1} [1, 2] has now been recorded between 1125 and 1360 cm^{-1} employing the Bruker IFS 120 HR Fourier transform spectrometer located at the MAX-lab (Lund University, Sweden). This spectral region is characterized by the absorption associated with the ν_4 (1225 cm^{-1}) and ν_8 (1252 cm^{-1}) bands.

CH_2DBr, a near prolate asymmetric top molecule (κ = –0.998), belongs to the C_s symmetry group with nine normal vibrations, six of A' (ν_1 – ν_6) and three of A" (ν_7 – ν_9) symmetry species. The ν_4 fundamental appears as an *a*-/*b*-hybrid band with predominant *a*-type character whereas ν_8 manifests the typical structure of a *c*-type band.

These close lying levels undergo to mutual interactions through both *a*- and *b*-Coriolis coupling mainly affecting the low K_a sublevels. Owing to these interactions, some transitions of ν_8 with selection rules $\Delta K_a = 0$ and $\Delta K_c = 0, \pm 2$ have been identified in the spectrum. The rovibrational structure of the two fundamentals is further complicated by two additional resonances: *b*-type Coriolis interaction between ν_8 and the $2\nu_6$ overtone and anharmonic resonance between ν_4 and $\nu_5+\nu_6$ combination.

Preliminary results, obtained by fitting transitions up to J'=70 and K_a'=10 for both fundamentals, will be presented.

[1] A. Baldacci, P. Stoppa, S. Giorgianni, R. Wugt Larsen, *Mol. Phys.* **2010**, *108*, 733.
[2] A. Baldacci, R. Visinoni, R. Wugt Larsen, *Chem. Phys. Lett.* **2010**, *499*, 40.