High resolution infrared study of $CH_2{}^{81}BrF$ in the range 920 – 1370 cm^{-1}: rovibrational analysis and resonances of ν_3, ν_4, ν_8, ν_9 fundamentals and $\nu_5+\nu_6$ combination band

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During the past years halogen-containing molecules have attracted a great deal of attention because of their alarming connection with stratospheric ozone depletion and global warming. However, reliable experimental data for many halocarbons are still unavailable, especially for those containing bromine.

High-resolution infrared spectra of CH_2BrF reveal a very dense rotational structure due to the absorptions coming from bromine isotopologues in the natural composition (50.7/49.3 of $^{79/81}Br$). The employment of synthesized isotopically enriched samples are required in order to obtain a less dense structure and to simplify the rovibrational analysis. The IR spectrum of $CH_2{}^{81}BrF$ has been investigated in the range 920 – 1370 cm^{-1} which is of considerable interest being a part of the main atmospheric window. The spectra have been measured at high resolution (0.0030 cm^{-1}) employing a Bruker IFS 120 HR Fourier transform spectrometer. The investigated spectral region is characterized by the absorptions of the ν_9 (936 cm^{-1}), ν_4 (1068 cm^{-1}), ν_8 (1226 cm^{-1}), ν_3 (1314 cm^{-1}) fundamentals and the $\nu_5+\nu_6$ (960 cm^{-1}) combination band.

$CH_2{}^{81}BrF$, a near prolate asymmetric top molecule ($\kappa = -0.986$), belongs to the C_s point group with nine fundamental modes, six of A' ($\nu_1 - \nu_6$) and three of A" ($\nu_7 - \nu_9$) symmetry species. The ν_3 and ν_4 appear as a/b-hybrid bands with predominant *a*-type character whereas ν_8 manifests the typical structure of a *c*-type band. The ν_9 band, in marked contrast with the expected *c*-type structure, appears as a classic *a*-type band, while the $\nu_5+\nu_6$ combination disguises the predicted *a*-/*b*-hybrid appearance because of the high congested spectrum.

Due to the proximity of the band origins of the absorptions investigated to those of close lying overtones and combination bands, several anomalies were found in the observed spectra and different kinds of first order Coriolis resonances were identified. In particular, the established interactions involve the dyads $\nu_3/2\nu_5$, $\nu_8/\nu_6+\nu_9$ and the tetrad $\nu_4/\nu_9/\nu_5+\nu_6/3\nu_6$. In the last system, in spite of the large separation (132 cm^{-1}) between the ν_4 and ν_9 fundamentals, the *a*-type Coriolis resonance seems to be the reason for which ν_9 borrows intensity from the very strong ν_4 and emerges as a pseudo *a*-type band.

The spectral analysis for all the observed bands allowed the line identification up to high J and K_a quantum numbers and the assigned data were fitted using Watson's A-reduction Hamiltonian in the I^r representation and Coriolis operators. Excited state parameters, band origins and coupling terms