A global analysis of bending states up to $v_4 + v_5 = 3$ of acetylenes isotopologues $^{12}C^{13}CD_2$, $^{12}C_2HD$ and $^{13}C_2HD$

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In recent years, much effort has been devoted to the study of the infrared spectra of the rare isotopologues of acetylene. In particular, the ro-vibrational transitions involving the low-lying bending states have been thoroughly investigated. Important improvements have been achieved for what concerns non-centrosymmetric isotopologues containing Deuterium and ^{13}C, i.e. $^{12}C^{13}CD_2$, $^{12}C_2HD$ and $^{13}C_2HD$.

In the case of $^{12}C^{13}CD_2$, it is the first time that a high resolution study of the bending states up to $v_4 + v_5 = 3$ has been performed. Twenty seven bands have been observed in the range 450 - 1700 cm^{-1} and 3210 rotation vibration transitions have been analysed, allowing the characterization of the ground state and of 13 vibrationally excited bending states.

An analogous global analysis has been performed for $^{12}C_2HD$ and $^{13}C_2HD$ but, in addition, pure rotational microwave transitions, recorded in the range 100 – 700 GHz for the ground state and for excited states up to $v_4 + v_5 = 3$, have been included in the data set. 5317 infrared data and 168 microwave transitions have been fitted simultaneously for $^{12}C_2HD$, whereas 4894 infrared and 143 microwave data for $^{13}C_2HD$.

For each isotopologue, a very accurate set of vibrational and rotational spectroscopic parameters has been obtained. They include also l–type interaction and Darling–Dennison anharmonic parameters. Some of them have been determined with an extremely high precision.