NEW ANALYSIS OF THE ν_3 BAND OF HDCO (MONODEUTERATED FORMALDEHYDE) IN THE 5.8 μm REGION

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Using high-resolution Fourier transform spectra of mono deuterated formaldehyde (HDCO) recorded in the 5.8 μm spectral range at Giessen (Germany), we carried out an extensive analysis of the strong ν_3 fundamental band (carbonyl stretching mode) at 1724.2676 cm^{-1}, starting from results of a previous analysis [a]. For this hybrid band (with both A- and B-type transitions) the analysis was pursued up to high rotational quantum numbers. In this way, it was possible to evidence resonances which perturb the ν_3 lines which are due to the existence of the $2\nu_5$ (at 2059 cm^{-1}) and $\nu_5+\nu_6$ (at 2087 cm^{-1}) dark bands [b]. In addition a local resonance is perturbing the 3^1 levels which is due to a crossing with the 4^1 energy levels. However the 4^1 state is also involved in strong vibration-rotation interactions coupling the $\{5^1,6^1,4^1\}$ system of resonating states of HDCO [c]. Therefore the final energy levels calculation which was performed for the $\{5^1,6^1,4^1,3^1,5^2,5^16^1\}$ resonating states accounts for the observed A- type, B- type C-type Coriolis (and/or) Fermi resonances. In this way it was possible to reproduce the observed line positions, within their experimental uncertainties. Finally using a ν_3 band intensity available in the literature [d] we generated, for the first time, a list of line parameters (positions and intensities) for the 5.8 μm band of HDCO.

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[a] Johns JWC, McKellar ARW., J Mol Spectrosc 1977; 64: 327-339

[b] ν_4, ν_5 and ν_6 correspond to the CHD bending (at 1396 cm^{-1}), the CHD rocking (at 1028 cm^{-1}) and the CHD out of plane (at 1059 cm^{-1}) modes, respectively

[c] A. Perrin, J. M. Flaud, L. Margulès, J. Demaison, H. Mäder and S. Wörmke, J. Mol. Spectrosc. 216, 214 (2002)

[d] Gratien, Nilsson, Doussin, Johnson, Nielsen, Stenstrom and Picquet-Varrault, J. Phys. Chem. 111, 11506 (2007)