NEW ANALYSIS OF THE $\nu_3$ BAND OF HDCO (MONODEUTERATED FORMALDEHYDE) IN THE 5.8 $\mu$m REGION

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Using high-resolution Fourier transform spectra of mono deuterated formaldehyde (HDCO) recorded in the 5.8 $\mu$m spectral range at Giessen (Germany), we carried out an extensive analysis of the strong $\nu_3$ 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 $\nu_3$ 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 $\{5^1, 6^1, 4^1, 3^1, 5^2, 5^1 6^1\}$ 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 $\nu_5$ 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 $\mu$m band of HDCO.

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aJohns JWC, McKellar ARW., J Mol Spectrosc 1977; 64: 327-339
b$\nu_4$, $\nu_5$ and $\nu_6$ 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