First analysis of the Herzberg ($C^1\Sigma^+ \rightarrow A^1\Pi$) band system in the lesser-abundant $^{13}C^{17}O$ isotopologue

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It has been presented high-resolution emission spectra measurements of the so far non-analysed in the $^{13}C^{17}O$ isotopologue, the Herzberg band system. The $C \rightarrow A(0,1),(0,2)$, and $(0,3)$ bands have been recorded in the 22 950 – 26 050 cm^{-1} region using high-accuracy dispersive optical spectroscopy [1–3]. The $^{13}C^{17}O$ molecules were formed and excited in a stainless steel hollow-cathode lamp with two anodes. All 224 rovibrational spectra lines, up to $J = 30$, were precisely measured with an estimated accuracy of about 0.0030 cm^{-1}, and rotationally analysed.

We are going to present the values of molecular parameters determined for the first time in $^{13}C^{17}O$: the merged rotational constants of the $C^1\Sigma^+(v = 0)$ Rydberg state and the individual rotational constants of the $A^1\Pi(v = 3)$ state, the rotational and vibrational equilibrium constants for the $C^1\Sigma^+$ state, the band origins of the $C \rightarrow A$ system, the isotope shifts, and the $\Delta G^C_{1/2}$ vibrational quantum as well as the RKR turning points, Franck - Condon factors, relative intensities, and r-centroids for the Herzberg band system as well as the main, isotopically invariant parameters of the $C^1\Sigma^+$ state in the CO molecule within the Born-Oppenheimer approximation.

The combined analysis of now obtained Herzberg bands and earlier analyzed Ångström ($B^1\Sigma^+ \rightarrow A^1\Pi$) system [4, 5] yielded a precise relative characteristic of the $C^1\Sigma^+(v = 0)$ and $B^1\Sigma^+(v = 0, 1)$ Rydberg states in the $^{13}C^{17}O$ molecule, among others: ν^{CB}_{00}, ν^{CB}_{01} vibrational quanta.

For the $A^1\Pi(v = 3)$ state of $^{13}C^{17}O$, considerable irregularities of the rotational structure have been observed and analysed in detail. Simultaneously, the $C^1\Sigma^+(v = 0)$ state was observed to be quite regular up to the observed $J_{\max}$ level.

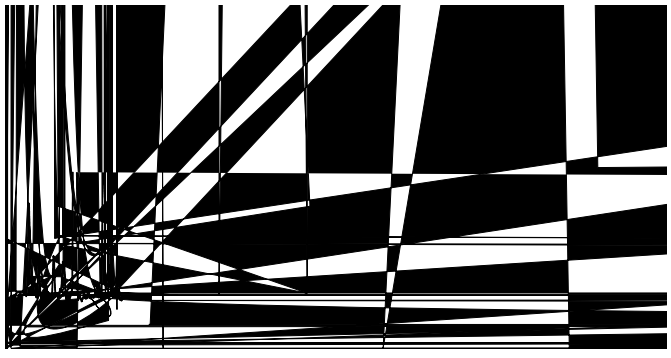

Figure 1: *The emission spectrum of carbon monoxide showing the first observation and rotational interpretation of the $C \rightarrow A(0,3)$ transition in the ^{13}C ^{17}O isotopologue, on an expanded scale. Peaks of the atomic Th calibration lines are marked with broken lines.*

References

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