First analysis of the $B^1\Sigma^+(v = 1)$ Rydberg state in the rare $^{12}C^{17}O$ isotopologue on the basis of the 1–v'' progression of the Ångström band system

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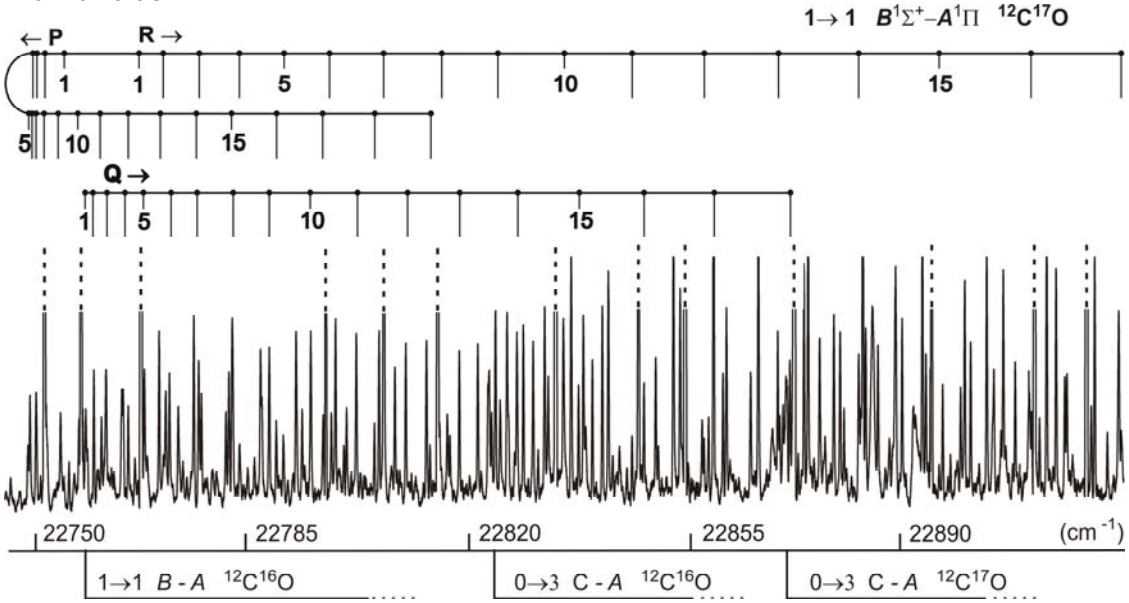
So far unobserved in the rare $^{12}C^{17}O$ isotopologue, the 1 – v'' progression of the Ångström ($B^1\Sigma^+$–$A^1\Pi$) band system was registered under high resolution in the 17 200 – 22 950 cm^{-1} spectral region as an emission spectrum using a high accuracy dispersive optical spectroscopy. The rare $^{12}C^{17}O$ molecules were formed and excited in two steps in a stainless steel hollow-cathode lamp with two anodes. The emission from the discharge was observed with a plane-grating spectrograph and recorded by a photomultiplier tube.

In the studied region, the full rotational structure of the 1–1 and 1–5 bands of the B–A system was observed, in total 111 spectral emission lines up to J''= 21. All those lines were precisely measured with an estimated accuracy of about 0.0030 cm^{-1}, and rotationally analysed. As a result, many molecular constants were determined for the first time for the $B^1\Sigma^+$ (v = 1) state, unobserved so far in the $^{12}C^{17}O$ [1], as well as for the $A^1\Pi$ (v = 5) state. We will also present the results of calculations concerning RKR turning points, FCF factors, relative intensities, and r–centroids for the Ångström band system in the $^{12}C^{17}O$ molecule. We have also determined the value of the $\Delta G_{1/2}$ vibrational quantum, the isotope shifts, as well as the main, isotopically invariant parameters of the $B^1\Sigma^+$ Rydberg state in the CO molecule within the Born-Oppenheimer approximation.

For the $A^1\Pi$, v = 1 and 5 state considerable irregularities of the rotational structure have been observed and analysed in detail. Suspected candidates responsible for these perturbations have been identified. The $B^1\Sigma^+$, v = 1 state has been thoroughly analysed in terms of possible perturbations and it turned out to be completely regular in the $^{12}C^{17}O$ molecule up to the observed maximum J value.



[1] R. Hakalla, W. Szajna, M. Zachwieja, *J. Phys. B: At. Mol. Opt. Phys.*, **2012**, 45, 215102.