High-resolution VUV and Vis Fourier-transform spectroscopy and extended deperturbation analysis of the ^{13}C^{18}O A$^1\Pi(v = 2)$ level

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Abstract

Spectral measurements were performed within the VUV (66,450–68,450 cm^{-1}) and Vis (19,100–25,000 cm^{-1}) ranges, achieving measurement accuracies of approximately 0.04 cm^{-1} for the VUV-FT spectroscopy (SOLEIL synchrotron) and 0.007 cm^{-1} for the Vis-FT spectroscopy (University of Rzeszów). A total of 787 radiative transitions were analysed, covering various electronic states.

A comprehensive deperturbation analysis of the A$^1\Pi(v = 2)$ level was performed using 1008 spectral lines and the `PGOPHER` program [1]. As a result, 38 floated parameters were obtained. Moreover, 429 ro-vibronic term values of the states under consideration were obtained. The interference between two indirect perturbation paths for the e-symmetry component between the A$^1\Pi(v = 2)$, a$^3\Pi(v = 13)$ and e$^3\Sigma^-(v = 4)$ levels was discovered. Moreover, two other indirect couplings of a$^3\Pi(v = 13)$ with A$^1\Pi(v = 2)$ were observed, namely via the d$^3\Delta(v = 7)$ and I$^1\Sigma^-(v = 3)$ intermediary levels.

The results are part of the studies on the electronic state of A$^1\Pi$ and its interactions in various isotopologues of carbon monoxide, which were undertaken by our research group [2,3]. The work aims to provide valuable information on the energetic structures of the CO molecule and the dynamics of unimolecular perturbations.

References

1. C. Western, *J. Quant. Spectrosc. Radiat. Transf.*, **186**, 221–242 (2017).
2. R. Hakalla et al., *RSC Advances*, **6**, 31588–31606 (2016).
3. S. Ryzner et al., *Spectrochim. Acta A*, **279**, 121367 (2022).