# New analysis of the $^{12}C^{16}O^{+}$ ($B^2\Sigma^+ - X^2\Sigma^+$) system: Spin-orbit and spin-rotation coupling of the $X^2\Sigma^+$ state

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In the present work a new experimental and theoretical analysis of the $B^2\Sigma^+ - X^2\Sigma^+$ system of the molecular ion $^{12}C^{16}O^+$ is performed. New transitions regarding the vibrational levels $v' = 4$ of the $B^2\Sigma^+$ electronic state and the vibrational level $v'' = 7$ of the electronic state $X^2\Sigma^+$ have been recorded. For rationalising the experimental observations, molecular structure calculations were carried out and, from them, a detailed investigation about the fine structure of rotational levels of the $X^2\Sigma^+$ could be performed. For such, the spin-rotational constant, $\gamma$, is characterised through the $\Delta g_\perp$ calculation, the perpendicular component of the electronic g-tensor, in combination with Curl's relation. At equilibrium geometry, the present $\Delta g_\perp$ is computed using the multireference configuration interaction wavefunction to be -2,430 ppm in agreement with the experimental one [-2,344 ppm]. The R-dependence of the g-tensor has been explored in order to estimate the theoretical $\gamma_v$ (**v** = 0-7). In addition, the importance of the lowest $\Pi$ states in this kind of calculation is widely discussed. A comparison between experiment and theory is presented, validating our findings and the methodology employed in our analysis.