

CALCULATION OF CO (7–0) OVERTONE LINE INTENSITIES AND ALL CO BANDS ANALYSIS

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Accurate studies of high overtone transitions of CO molecule provide a challenge to both experiment and theory as the lines are very weak: below 2×10^{-29} cm molecule⁻¹ at 296 K. The details of the experimental measurements of the lines of 0-7 band are given in the separate, purely experimental talk/poster (and published in the Ref. ¹) of the same team of authors (in reverse order). In particular, intensities of 14 lines in the sixth overtone (7–0) band of carbon monoxide (¹²C¹⁶O) are measured in the visible range between 14300 and 14500 cm^{-1} using a frequency-stabilized cavity ring-down spectrometer. In this poster we concentrate on the theoretical part of the paper mentioned above. Agreement between theory and experiment within the experimental uncertainty of a few percent for the 14 lines of 0-7 band of CO is obtained. However, this agreement is only achieved after issues with stability of the Davidson correction to the MRCI (multi-reference configuration interaction) calculations are resolved.

The problem of the theoretical calculations from the first principles of the line intensities of CO molecule for all the bands, known with high accuracy, that is 0-0, 0-1, 0-2, 0-3, 0-4, 0-6, 0-7 bands is considered. The calculations are presented, which reproduce all the above mentioned experimentally known line intensities close to experimental accuracy

¹A. Balashov, K. Bielska, G. Li, A. Kyuberis, S. Wojtewicz, J. Domyslawska, R. Ciurylo, N.F. Zobov, D. Lisak, J. Tennyson, O. L. Polyansky, *J. Chem. Phys.*, accepted, (2023)