GLOBAL ANALYSIS OF THE HIGH TEMPERATURE INFRARED EMISSION SPECTRUM OF 12 CH₄ IN THE DYAD (ν_2/ν_4) REGION

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We report new assignments of vibration-rotation line positions of methane (12 CH₄) in the so-called Dyad (ν_2/ν_4) region (1000 – 1500 cm⁻¹), and the resulting update of the vibration-rotation effective model of methane, previously reported by Nikitin *et al.* [A.V. Nikitin *et al.* PCCP, **15**, (2013), 10071], up to and including the Tetradecad. High resolution (0.01 cm⁻¹) emission spectra of methane have been recorded up to about 1400 K using the high-enthalpy source developed at IPR associated with the Fourier transform spectrometer of the SOLEIL synchrotron facility (AILES beamline). Analysis of these spectra allowed extending rotational assignments in the well-known cold band (Dyad–GS) and related hot bands in the Pentad–Dyad system (3000 cm⁻¹) up to $J_{max} = 30$ and 29, respectively. In addition, 8512 new transitions belonging to the Octad–Pentad (up to J = 28) and Tetradecad–Octad (up to J = 21) hot band systems were successfully identified. As a result, the MeCaSDa database of methane was significantly improved. The line positions assigned in this work, together with the information available in the literature, were fitted using 1096 effective parameters with a dimensionless standard deviation $\sigma = 2.09$. The root mean square deviations d_{RMS} are 3.60×10^{-3} cm⁻¹ for Dyad–GS cold band, 4.47×10^{-3} cm⁻¹ for the Pentad–Dyad, 5.43×10^{-3} cm⁻¹ for the Octad–Pentad and 4.70×10^{-3} cm⁻¹ for the Tetradecad–Octad hot bands. The resulting new line list will contribute to improve opacity and radiative transfer models for hot atmospheres, such as those of hot-Jupiter type exoplanets.