GLOBAL FREQUENCY AND INFRARED INTENSITY ANALYSIS OF $^{12}CH_4$ LINES IN THE 900–4800 CM^{-1} REGION

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A new global analysis of methane lines in the 900–4800 cm^{-1} region has been performed thanks to new experimental data for both line positions and intensities. This implies three of the $^{12}CH_4$ polyads, namely the dyad (940–1850 cm^{-1}, 2 vibrational levels, 2 sublevels), the pentad (2150–3350 cm^{-1}, 5 vibrational levels, 9 sublevels) and the octad (3550–4800 cm^{-1}, 8 vibrational levels, 24 sublevels) and some of the associated hot bands. New FTIR spectra of the pentad and octad regions have been recorded with a very high resolution (better than 0.001 cm^{-1} instrumental bandwidth, unapodized) at 78 K using the Bruker IFS 125 HR Zürich prototype (ZP2001) spectrometer[a]. New intensity measurements were performed in the whole region at the Kitt Peak National Observatory. We also used previously recorded high-resolution Raman spectra[b]. The effective Hamiltonian was expanded up to order 6 for the ground state, 6 for the dyad, 5 for the pentad and 5 for the octad. We obtain global root mean square deviations d_{RMS} for line positions $= 1.4 \times 10^{-4}$ cm^{-1} for the dyad, 6.0×10^{-4} cm^{-1} for the pentad and 3.3×10^{-3} cm^{-1} for the octad. This analysis represents a large improvement over the previous one[c] with $d_{\mathrm{RMS}} = 0.041$ cm^{-1} for the octad system.

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