AB INITIO VARIATIONAL PREDICTIONS FOR HIGH-RESOLUTION LASER SPECTROSCOPY: ASSIGNMENT OF 107 NEW SUB-BANDS OF METHANE IN THE ICOSAD RANGE 6280-7800 CM^{-1}

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A detailed study of methane spectra in the highly congested icosad range 6280-7800 cm^{-1} has been performed using variational global calculations[1] derived from accurate *ab initio* potential energy and dipole moment surfaces[2,3]. For the very first time, the experimental WKLMC line lists[4] −recorded at 80 and 296 K using very sensitive laser techniques (DAS, CRDS) and considered as the most significant advance in methane spectroscopy in the near infrared− have been partly assigned from first principles predictions[5]. Among the 20 bands and the 134 sub-levels contain in the icosad system, 19 and 107, respectively, have been identified for line intensities I$\geq$10^{-27} cm/molecule. Finally a total of 12900 transitions and 7300 energy levels was assigned, which represent about 20% of the experimental list at 80 K. This gives approximately 98, 85, 62 and 50% of assigned lines for measured intensities $\geq$10^{-23}, $\geq$10^{-24}, $\geq$10^{-25} and $\geq$10^{-26} cm/molecule, respectively. This work clearly demonstrates the validity of our recent global calculations. It could be used in various applications, as the generation of accurate high-temperature line lists. Simultaneously, the modeling of the methane spectra at 80K in the 6539-6800 cm^{-1} region is currently in progress[6] and should allow to validate the global assignments. This work is supported by French-Russian LIA SAMI and Tomsk State University Mendeleev grant program.

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