First-principles calculations of the methane spectra in the infrared up to 9300 cm^{-1}

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We report global calculations of rovibrational spectra and dipole transition intensities of methane using our recent *ab initio* dipole moment and potential surfaces [1,2]. For the full symmetry account, a recently published variational tensor formalism in normal modes is applied, the convergence of high-J calculations being improved by the use of vibrational eigenfunctions to make a compressed basis set for solving the rovibrational problem [3,4]. For the first time, positions and line intensities at 80 K and 296 K are shown to be in excellent agreement with raw experimental data, even for high energy ranges [5,6], This work is a first step toward the theoretical interpretation of numerous methane bands which remain still unassigned and detailed line-by-line absorption/emission spectra analyses for atmospheric and planetological applications.

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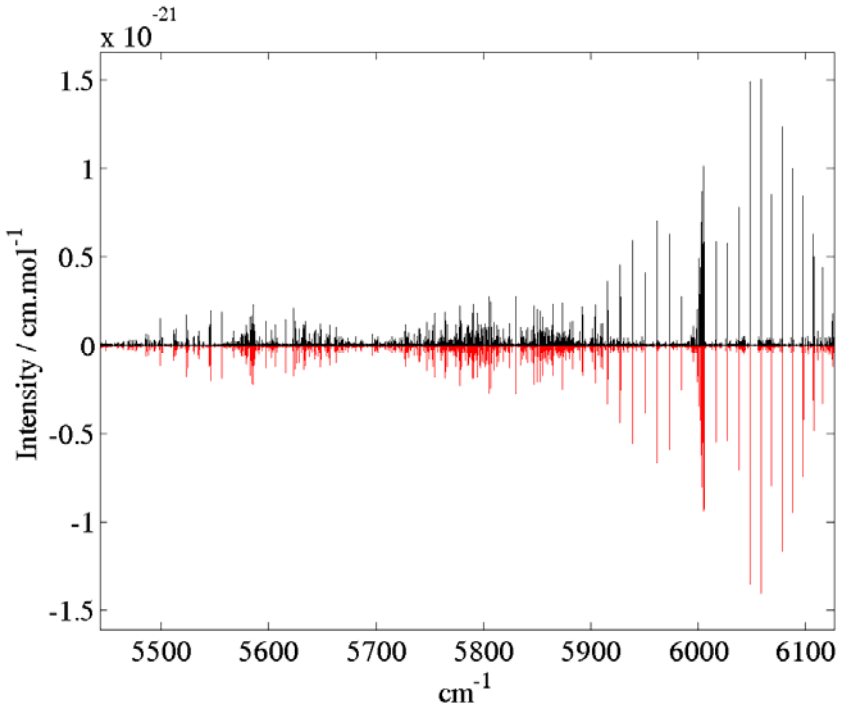

Figure 1 Variational (red) Vs. HITRAN (black)