Isotopic effects in the theoretical methane intensities : $^{13}CH_4$, $^{12}CH_3D$ and $^{12}CD_4$

Michaël Rey[a], A. V. Nikitin[b], and Vl. G. Tyuterev[a]

[a] GSMA, UMR CNRS 7331, Université de Reims Champagne Ardenne, Moulin de la Housse, BP 1039-51687 REIMS Cedex 2, France : michael.rey@univ-reims.fr
[b] Laboratory of Theoretical Spectroscopy, Institute of Atmospheric Optics, SB RAS, 634055 TOMSK, Russia

We focus on the calculations of dipole transition intensities and rovibrational spectra for $^{13}CH_4$, $^{12}CH_3D$ and $^{12}CD_4$. Global variational calculations were performed using our recent potential energy and dipole moment surfaces [1,2] initially derived for $^{12}CH_4$, combined with the tensor formalism proposed in previous works [3,4,5]. Isotopic substitutions and symmetry breakdown were studied from theoretical considerations. Isotopic vibrational band center shifts due to the H->D and 12->13 substitutions were calculated and compared with experimental values. These shifts were found to be quite irregular, but their variational predictions were very accurate [6,7], of the order of 0.01 cm^{-1} , and could thus be used for a precise calculation of line positions. Rovibrational line intensities computed from the *ab initio* dipole moment surfaces agree very well with those available in the HITRAN 2012 database [8]. Our preliminary results suggest that numerous bands of methane isotopologues which remain still unassigned could be identified and modeled using the proposed approach.

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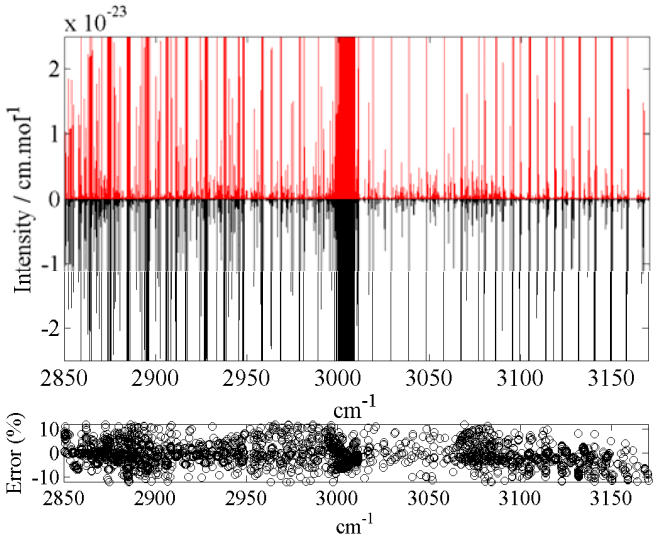

Figure 1 Variational (black) Vs. HITRAN (red) for $^{13}CH_4$