

**FOURIER TRANSFORM  $^{12}\text{CH}_3\text{D}$  SPECTRA IN THE REGION 3800 – 8000  $\text{cm}^{-1}$ . DIRECT COMPARISON TO AB INITIO CALCULATION.**

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The spectra of  $^{12}\text{CH}_3\text{D}$  isotopologue has been recorded in the all region 3800 - 8000  $\text{cm}^{-1}$  using the Step-by-Step Fourier Transform spectrometer of G.S.M.A. at Reims university. The region was studied using four optical filters with maximum optical path differences of 0.7 and 1 meter. The Fourier Transform Spectrometer was fitted with a tungsten light source. The light power was limited at the entrance of the spectrometer using a 5 mm-diameter iris. The detection was performed using a pair of InSb detectors.<sup>1</sup> The  $^{12}\text{CH}_3\text{D}$  gaz has been purchased at EURISO-TOP with an isotopic purity of 98 %. It was used to fill our 2 meter base long White-type cell built in the frame of a previous french ANR support for methane studies. Two absorption paths of 8 and 40 meters were used with the same amount of gaz corresponding to a pressure of 1.7 torr.

The spectra obtained show an important number of structures belonging to several polyads of  $^{12}\text{CH}_3\text{D}$  and the determination of lines parameters will be made further. This poster presents the first comparison to the *ab initio* calculations of Rey et al.<sup>2</sup> The theoretical calculations of the involved teams already brought decisive information for the analysis of the main isotopologue<sup>3</sup> spectra and will now serve the analysis of  $^{12}\text{CH}_3\text{D}$ .

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<sup>1</sup> J. J. Plateaux, A. Barbe and A. Delahaigue: Reims high resolution Fourier transform spectrometer. Data reduction for ozone. *Spec. Acta A*, **51**, 1153-1169 (1995), L. Régalia, C. Oudot, X. Thomas, P. Von der Heyden, D. Decatoire: FTS improvements and connection with a long White cell. Application:  $\text{H}_2^{16}\text{O}$  intensity measurements around 1200  $\text{cm}^{-1}$  *J. Q. S. R. T.*, **111**, 826-842 (2010).

<sup>2</sup> M. Rey, A. V. Nikitin and V. G. Tyuterev: Accurate first-principles calculations for  $^{12}\text{CH}_3\text{D}$  infrared spectra from isotopic and symmetry transformations. *J. C. P.* **141**, 044316 (2014).

<sup>3</sup> Nikitin, A.V. , Thomas, X., Régalia, L., Daumont, L., Rey, M., Tashkun, S.A. , Tyuterev, V. and Brown, L.R. , Measurements and modeling of long-path  $^{12}\text{CH}_4$  spectra in the 4800 – 5300  $\text{cm}^{-1}$  region. *J. Q. S. R. T.* **138**,116-123 (2014).