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FOURIER TRANSFORM ¹²CH₃D SPECTRA IN THE REGION 3800 - 8000 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 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.¹ 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 ${}^{12}CH_3D$ 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.*² The theoretical calculations of the involved teams already brought decisive information for the analysis of the main isotopologue³ spectra and will now serve the analysis of ${}^{12}CH_3D$.

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¹ 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: $H_2^{16}O$ intensity measurements around 1200 cm⁻¹ J. Q. S. R. T., **111**, 826-842 (2010).

² M. Rey, A. V. Nikitin and Vl. G. Tyuterev: Accurate first-principles calculations for 12 CH₃D infrared spectra from isotopic and symmetry transformations. *J. C. P.* **141**, 044316 (2014).

³Nikitin, 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 ¹²CH₄ spectra in the 4800 - 5300 cm⁻¹ region. J. Q. S. R. T. **138**,116-123 (2014).