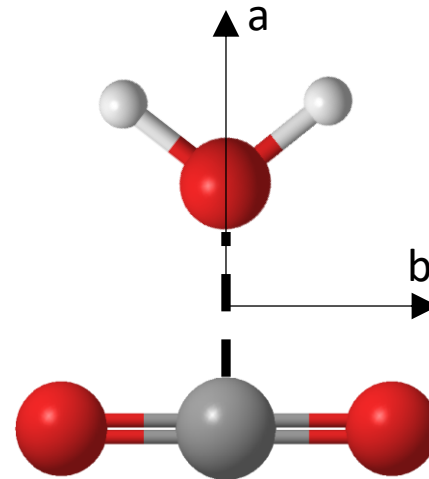
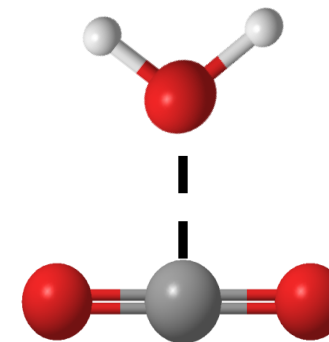


Spectres à haute résolution de D_2O-CO_2 autour des triples excitations vibrationnelle de D_2O

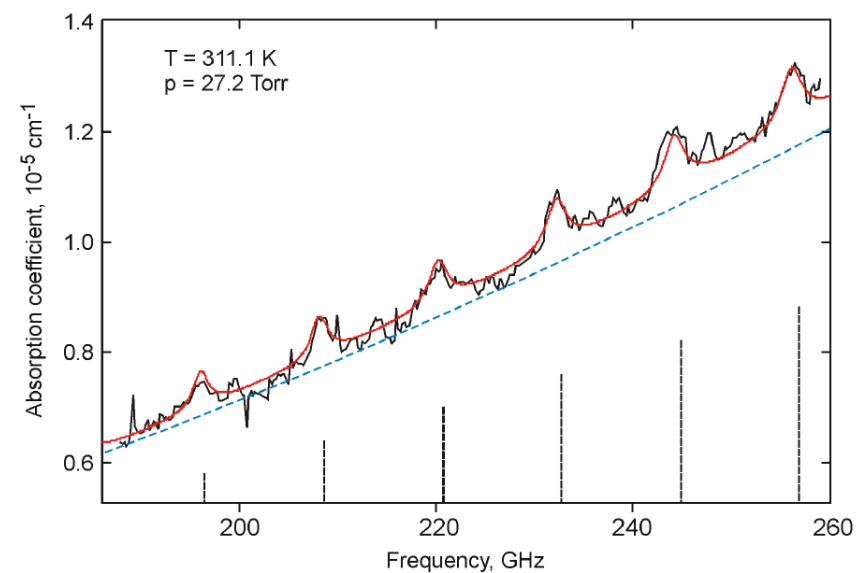


Motivations

- Le CO_2 et l'eau sont les principaux gaz à effet de serre
- Première étape de la nucléation
- Formation de l'acide carbonique
- Bon modèle pour les collisions



Dimère de l'eau observé à température ambiante en laboratoire

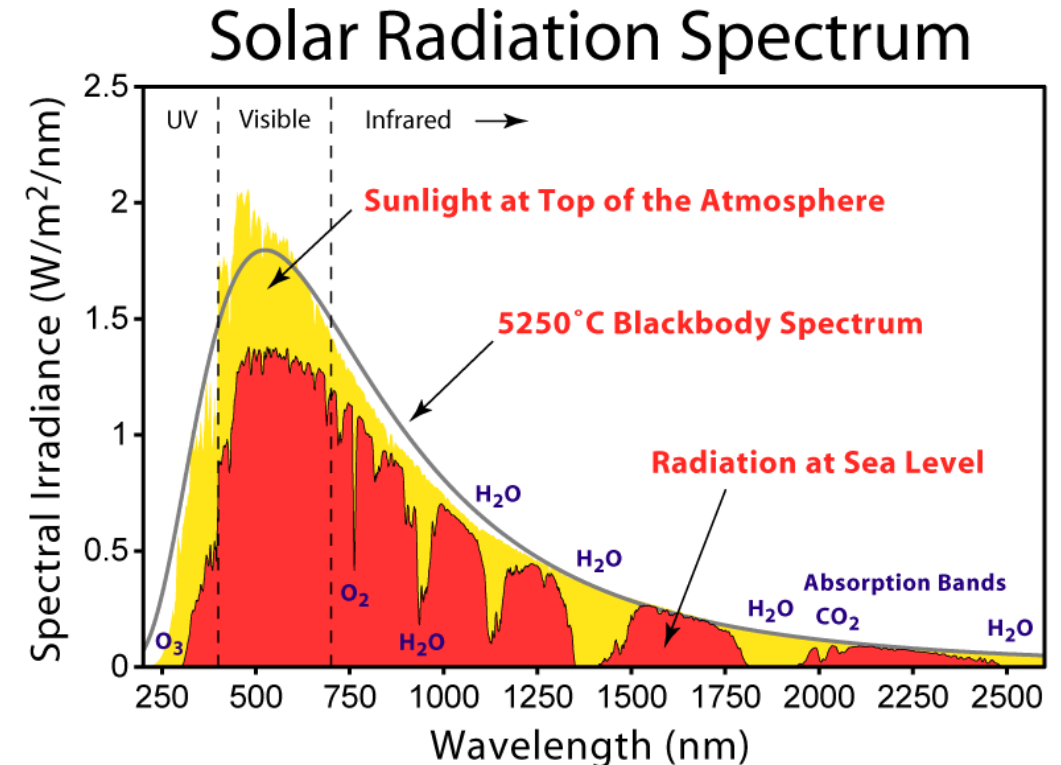


M.Y. Tretyakov, E. Serov, M. Koshelev, V. Parshin, A. Krupnov, Water dimer rotationally resolved millimeter-wave spectrum observation at room temperature, *Physical review letters* 110 (2013) 093001

E. Serov, M. Koshelev, T. Odintsova, V. Parshin, M.Y. Tretyakov, Rotationally resolved water dimer spectra in atmospheric air and pure water vapour in the 188–258 GHz range, *Physical Chemistry Chemical Physics* 16 (2014) 26221-26233

Intérêts de l'étude des excitations vibrationnelles multiples

- Maximum de la lumière solaire est situé dans le visible
- Pas encore étudié
- Plus d'énergie insérée dans le complexe pourrait mener à une réactivité accrue
- Système dynamique intéressant

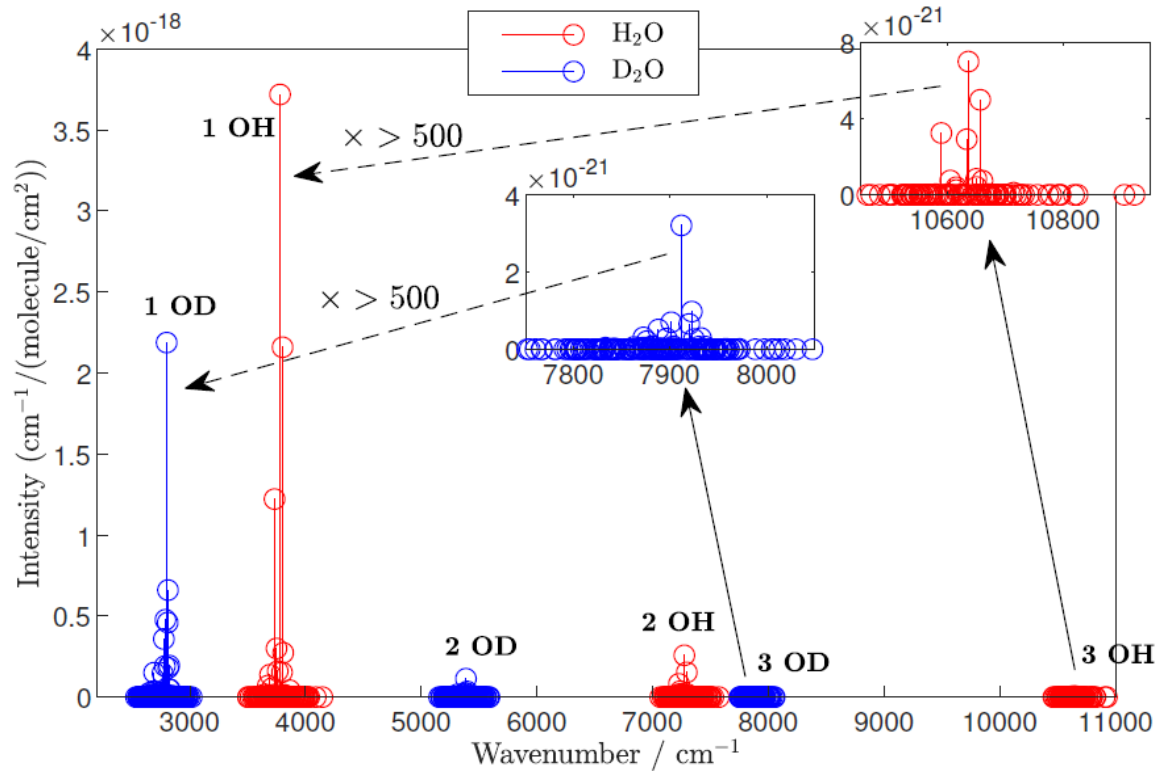


Adapted from: S. Gorjian and H. Ebadi, "Chapter 1 - introduction," in *Photovoltaic Solar Energy Conversion*, edited by S. Gorjian and A. Shukla (Academic Press, 2020) pp. 1–26.

Challenges

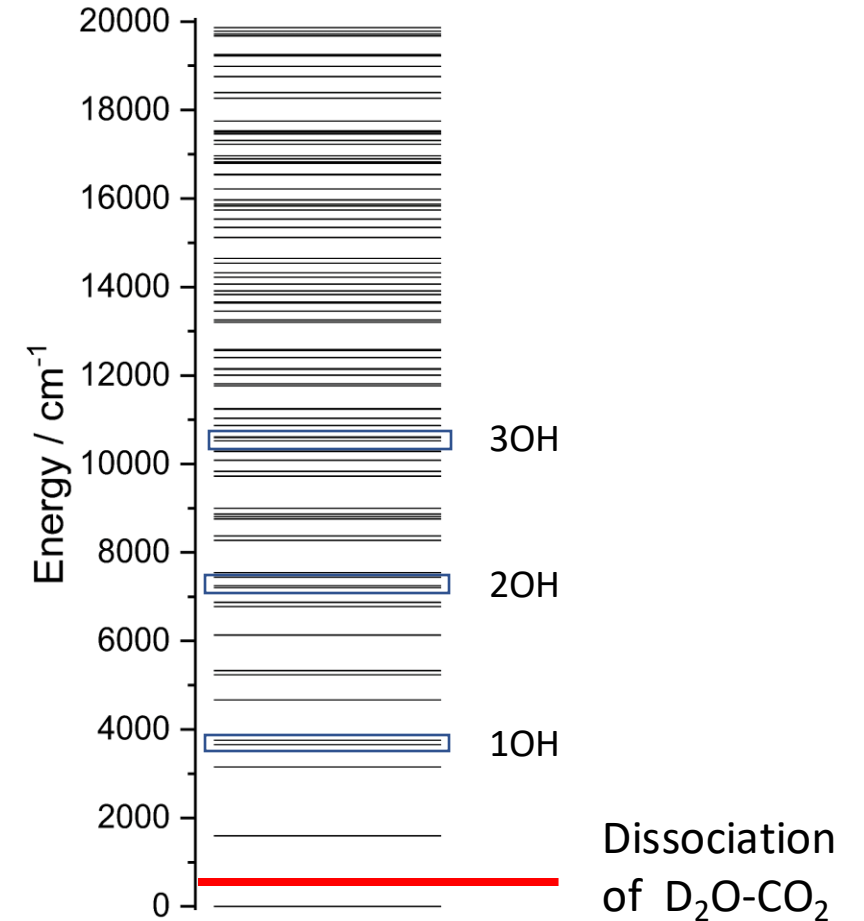
Observation

Diminution de la section efficace d'absorption



Compréhension

Augmentation de la densité d'états vibrationnelle



Dispositif expérimental : FANTASIO

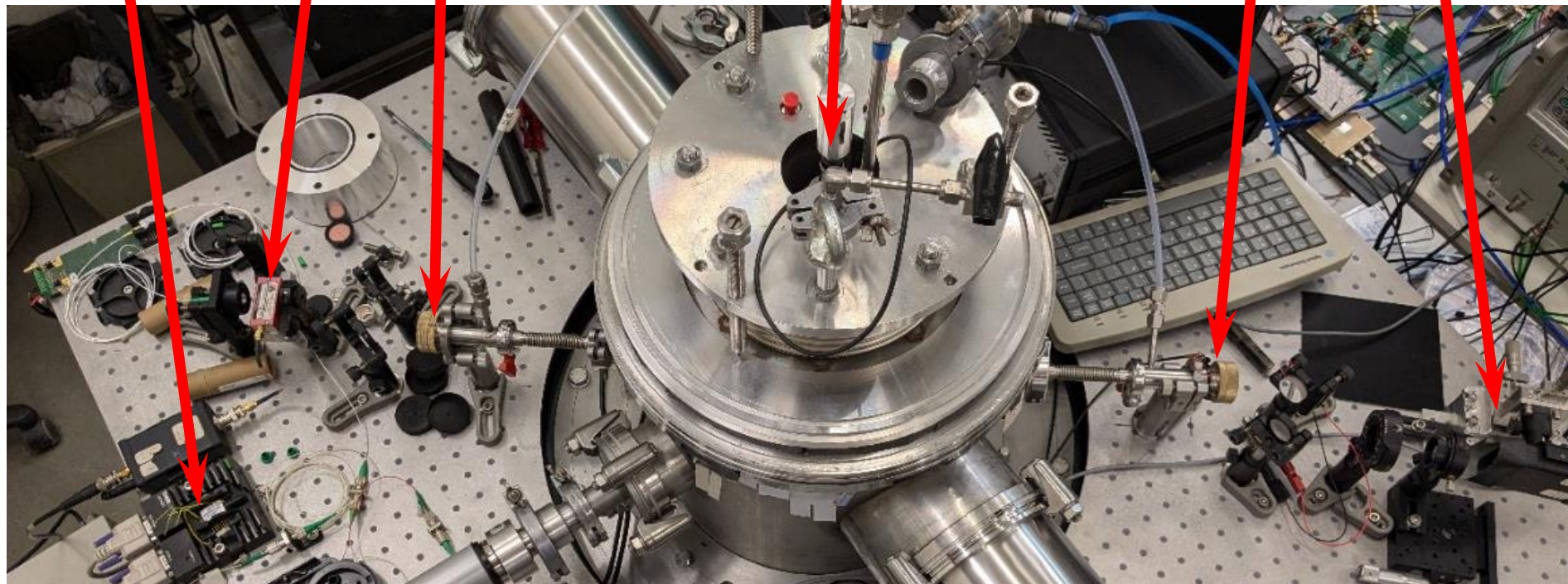
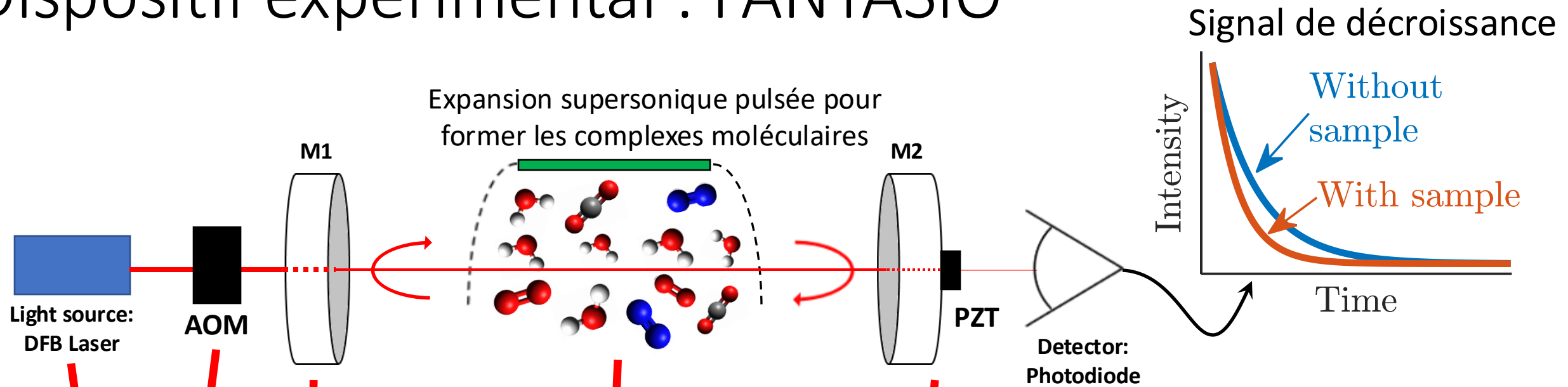
- Source de complexes de Van der Waals:
Expansion supersonique
- Spectromètre infrarouge proche:
CW-CRDS^a



FANTASIO set-up^b
Fourier trANsform, Tunable diode and
quadropole mAss spectrometers interfaced
to a Supersonic expansiOn



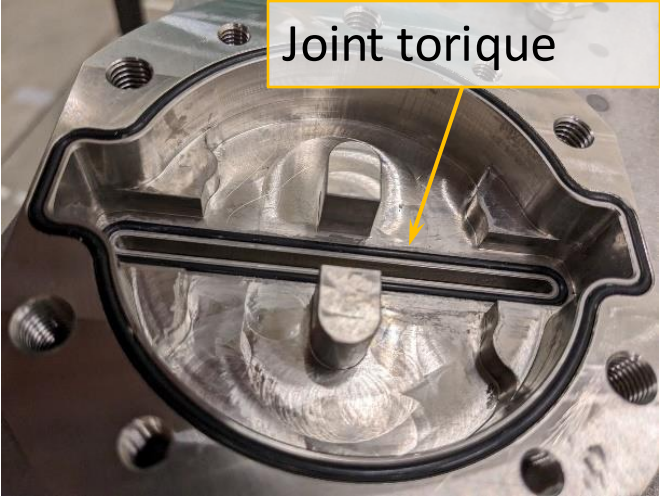
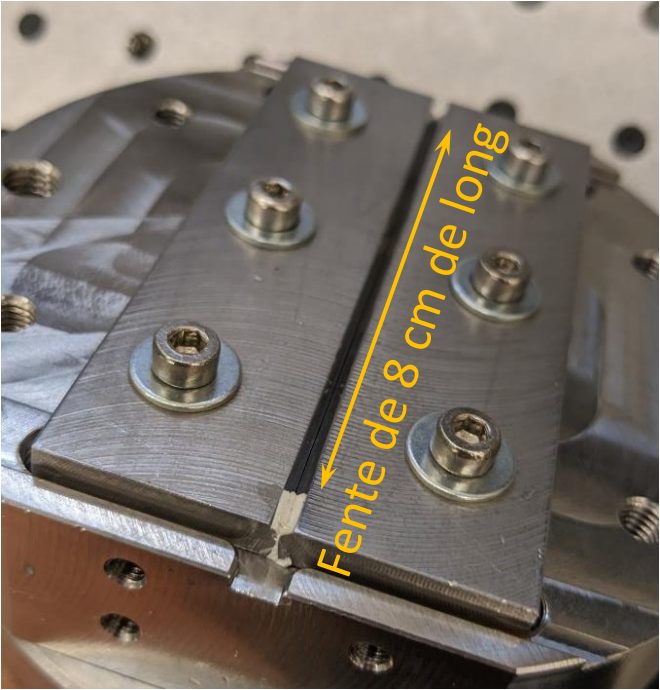
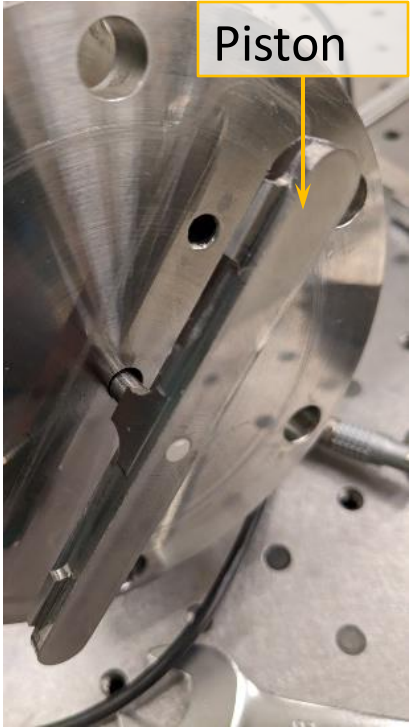
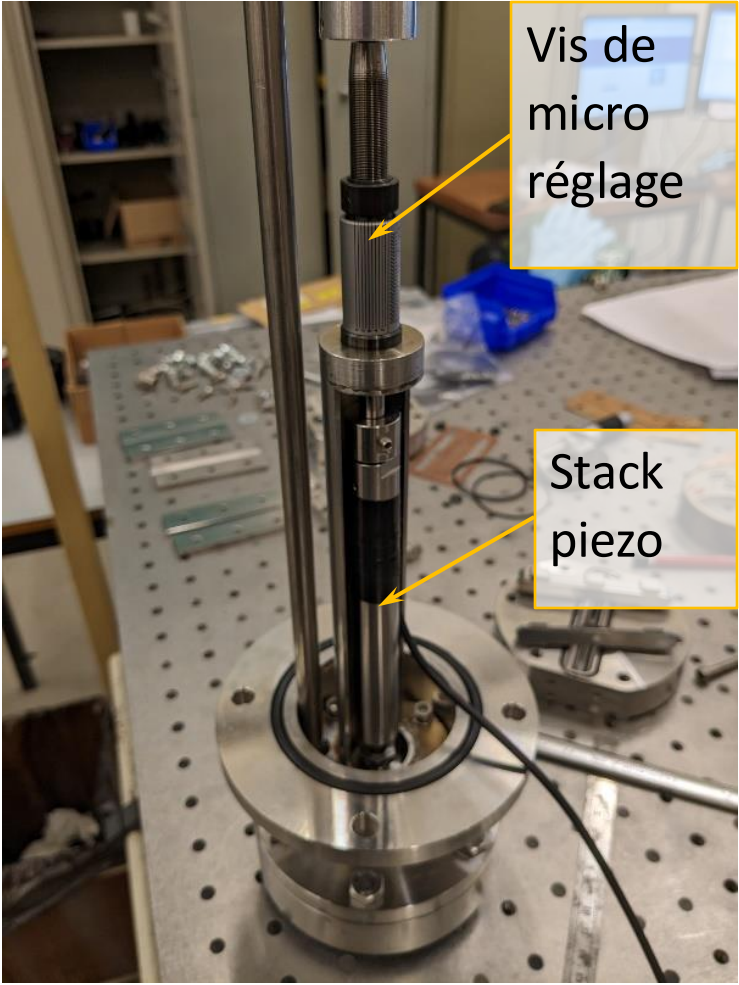
Dispositif expérimental : FANTASIO



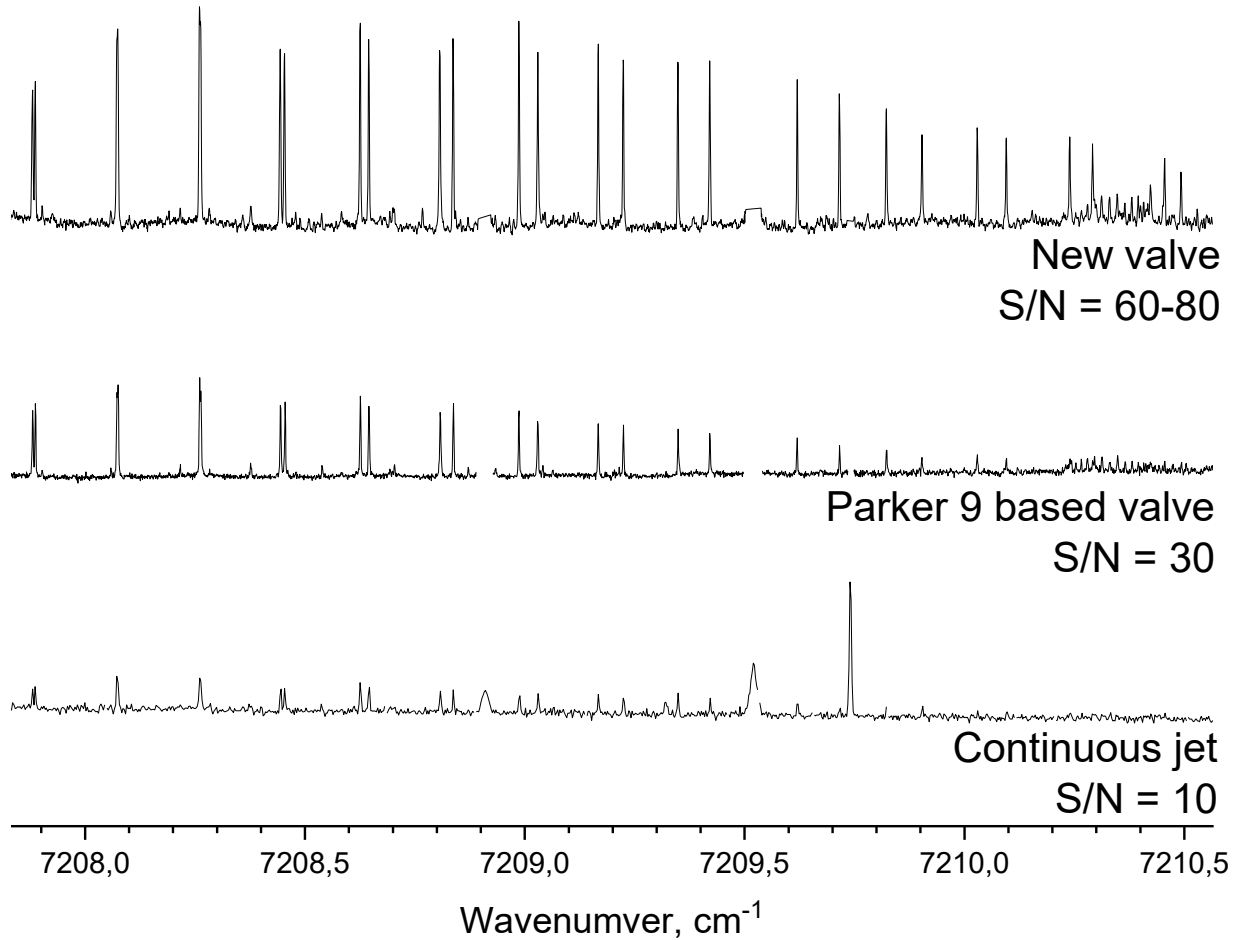
$L \approx 75 \text{ cm}$
 $l \approx 8 \text{ cm}$
 $R \approx 99.9995 \%$
 $\tau_0 \approx 100 \mu\text{s}$

La lumière parcourt environ **30 km** à l'intérieur de la cavité (environ 3 km à l'intérieur du jet).

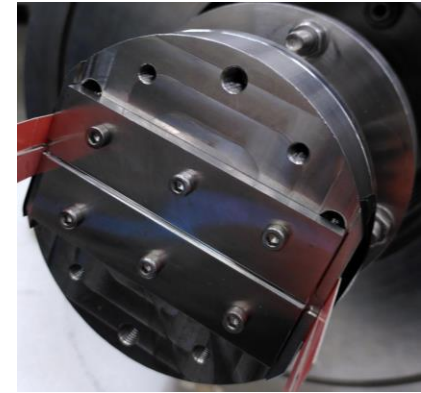
Nouvelle fente pulsée



Amélioration du spectre de Ar-H₂O



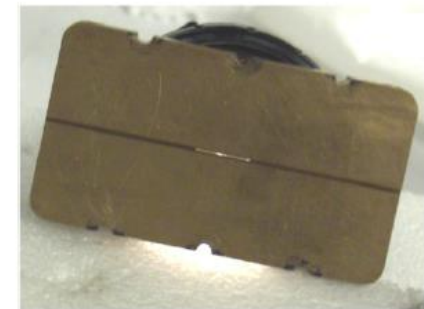
$\Pi(1_{01}), (200) \leftarrow \Sigma(1_{01}), (000)$



$l = 8 \text{ cm}, D = 50 \mu\text{m}$

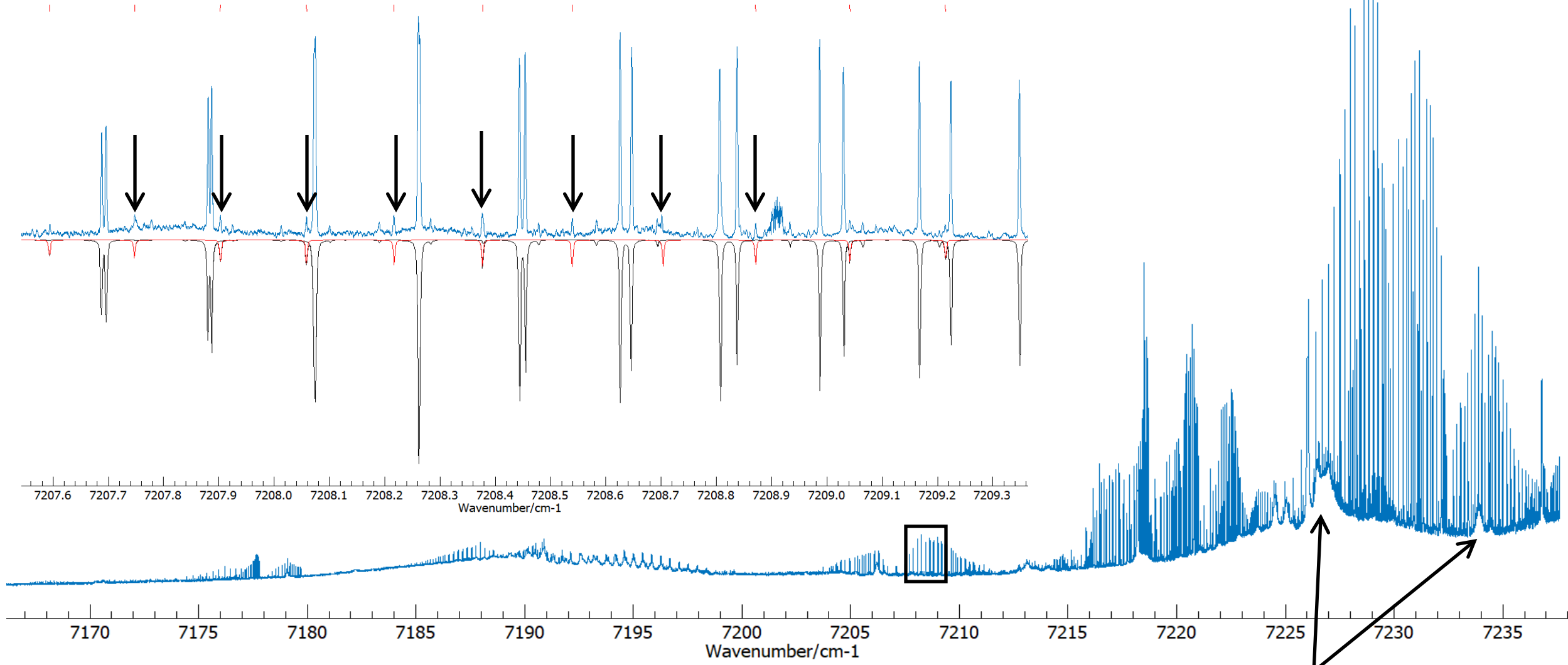


$l = 2.5 \text{ cm}, D = 50 \mu\text{m}$



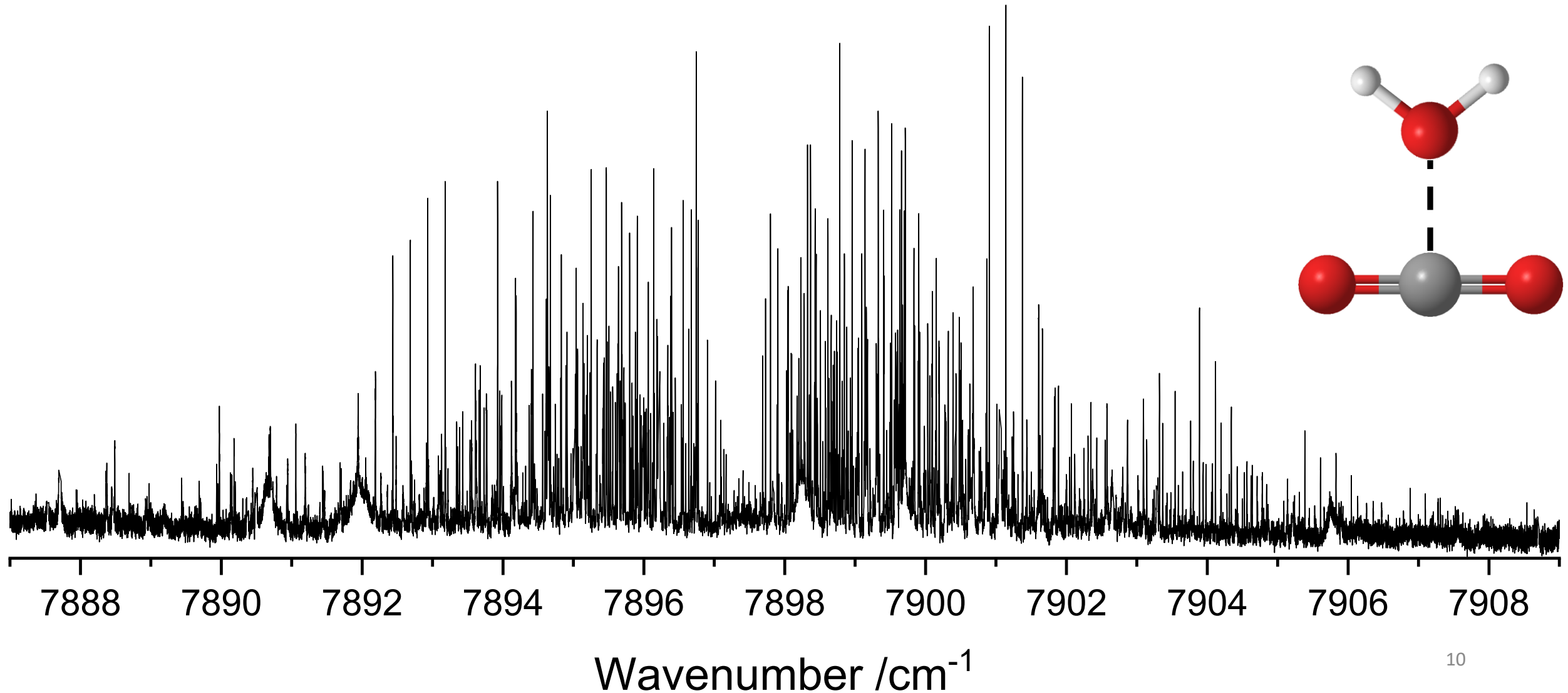
$l = 1 \text{ cm}, D = 12 \mu\text{m}$

Ar-H₂¹⁸O dans la gamme 20H (0,2 % d'abondance naturelle)

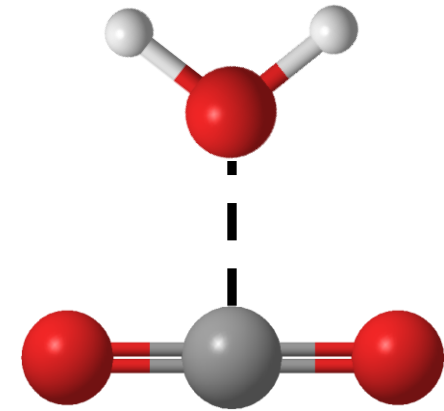
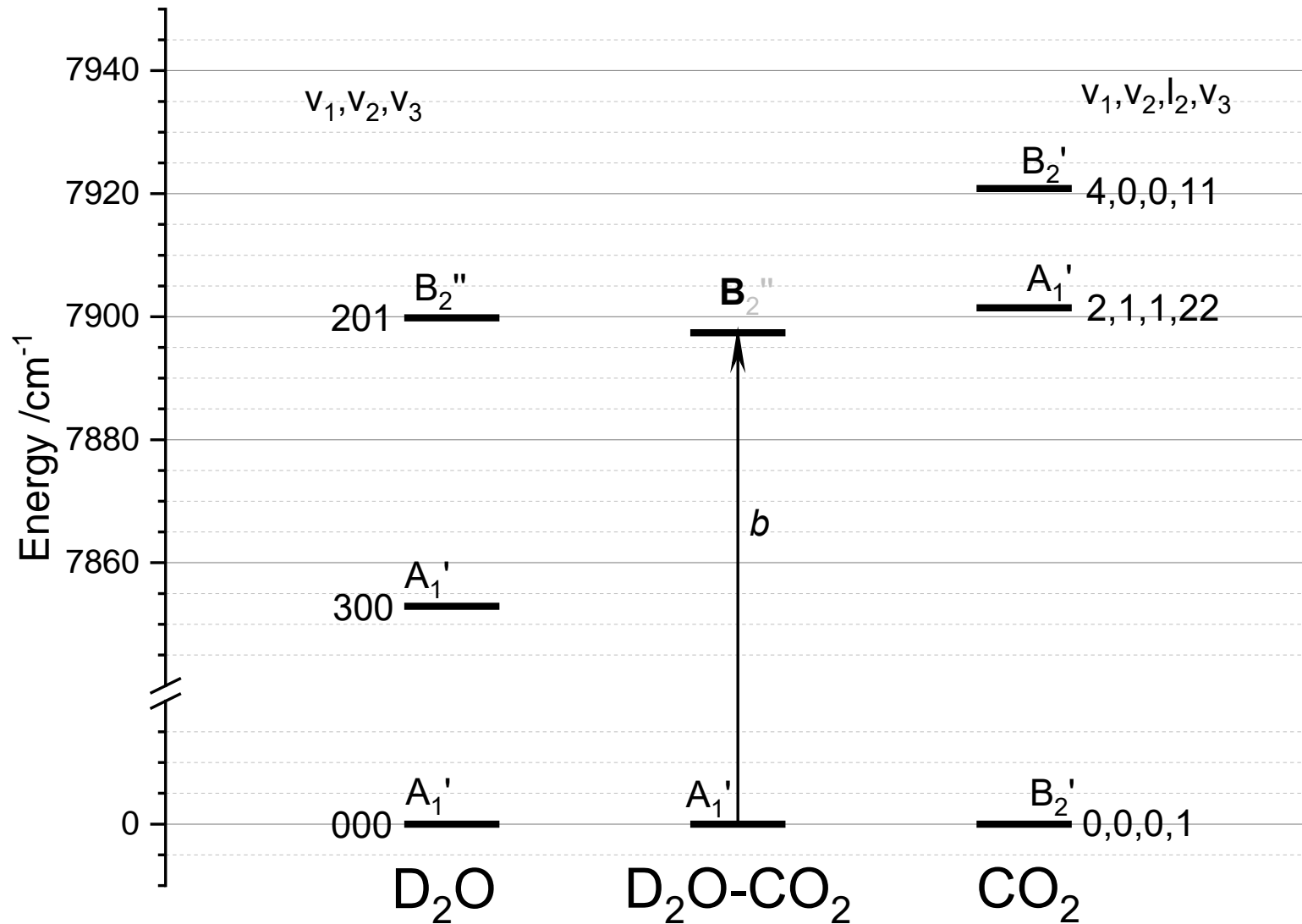


Dimère d'eau

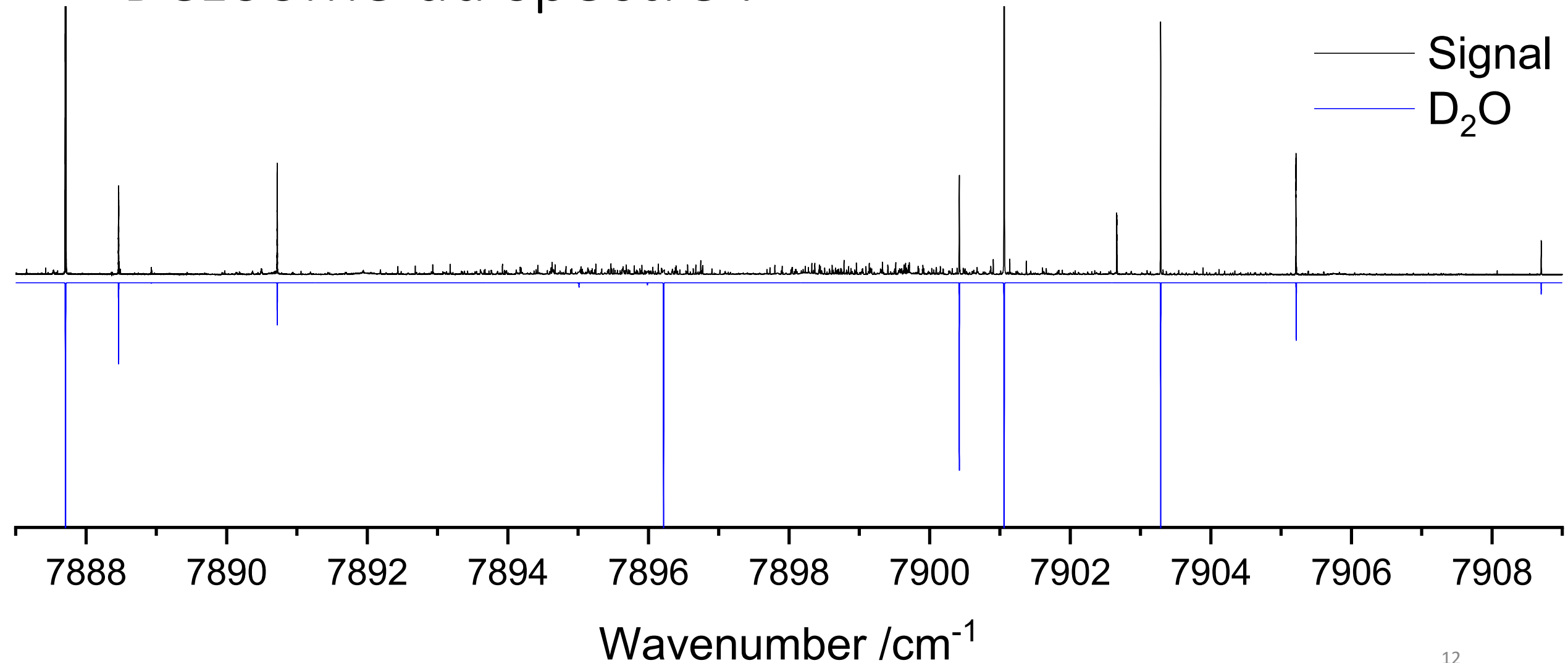
Le spectre de D_2O-CO_2 aux alentours de la triple élongation
OD de D_2O $(\nu_1', \nu_2', \nu_3') \leftarrow (\nu_1'', \nu_2'', \nu_3'') = (2, 0, 1) \leftarrow (0, 0, 0)$:



Attribution vibrationnelle

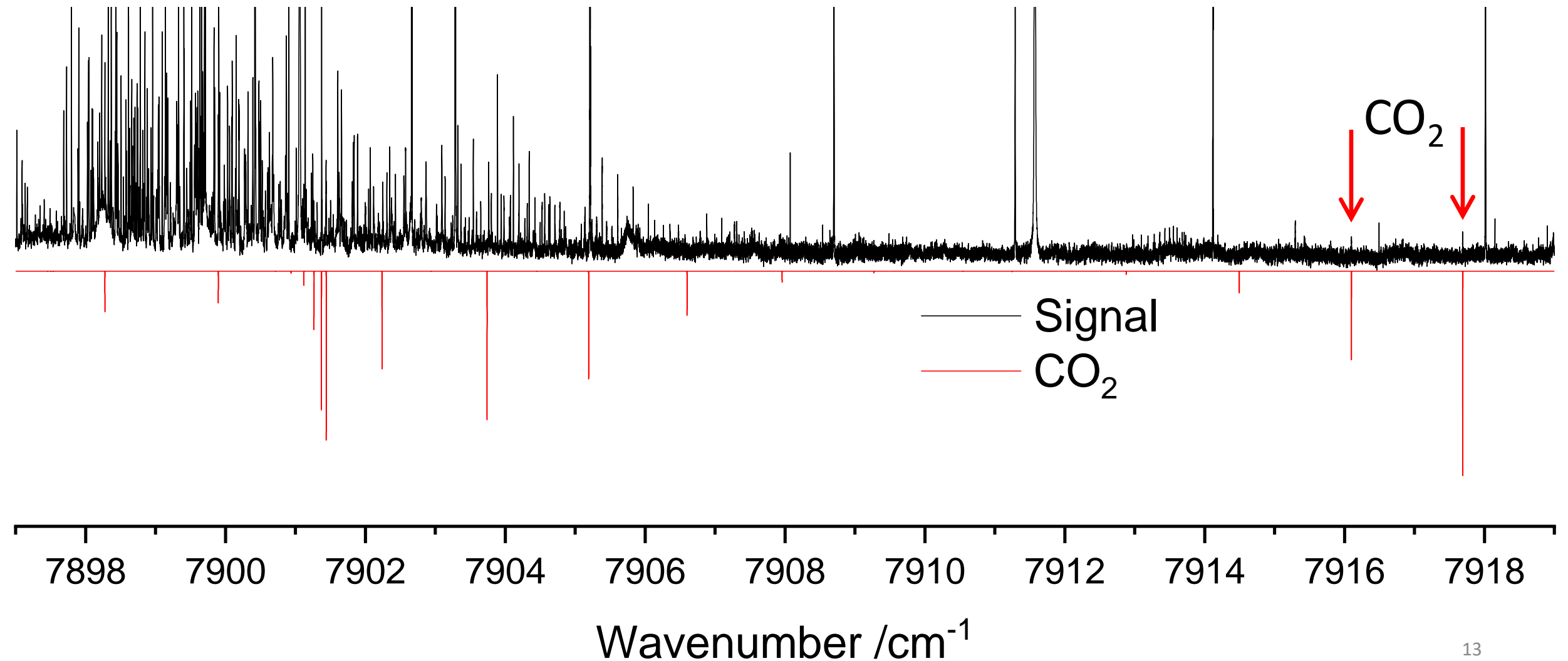


Attribution vibrationnelle : D₂O ?
Dézooome du spectre :



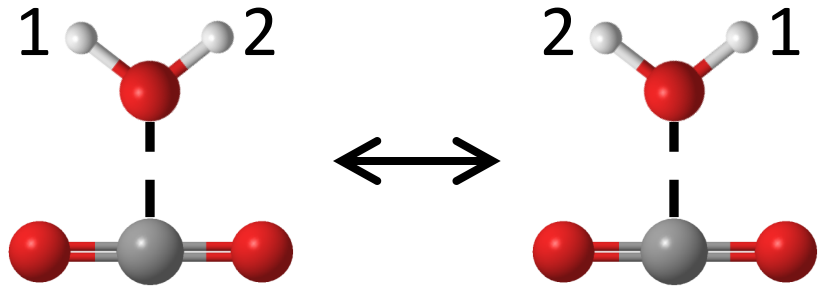
Attribution vibrationnelle : CO₂?

Zoom du spectre :



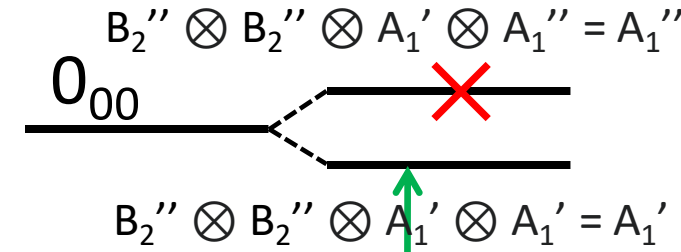
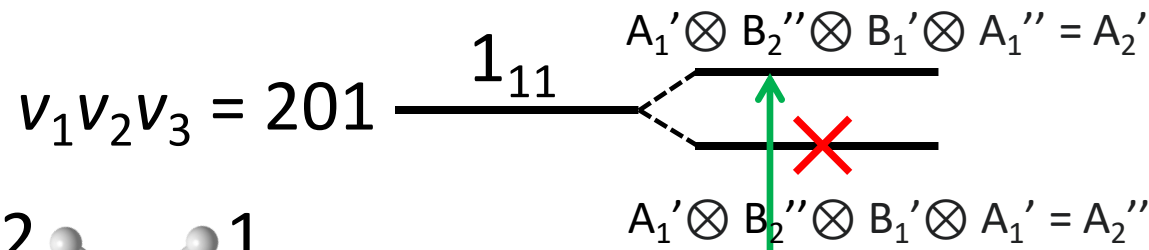
Attribution rotationnelle:

Le modèle

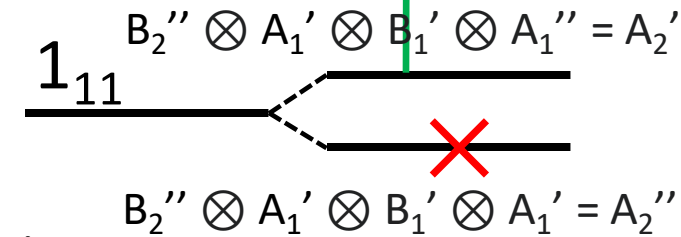
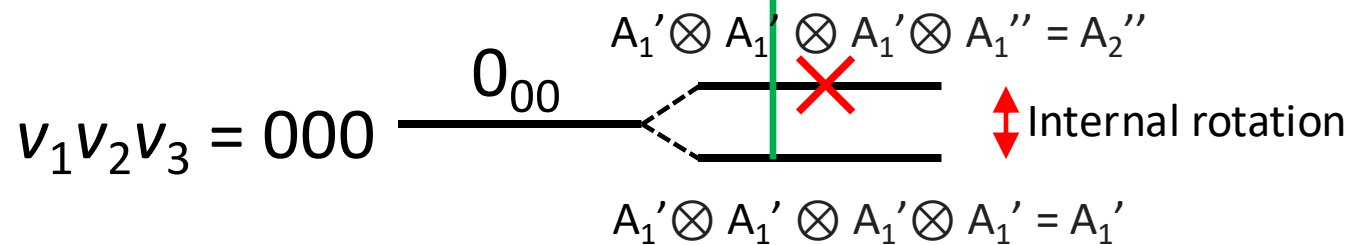


Ortho

Para

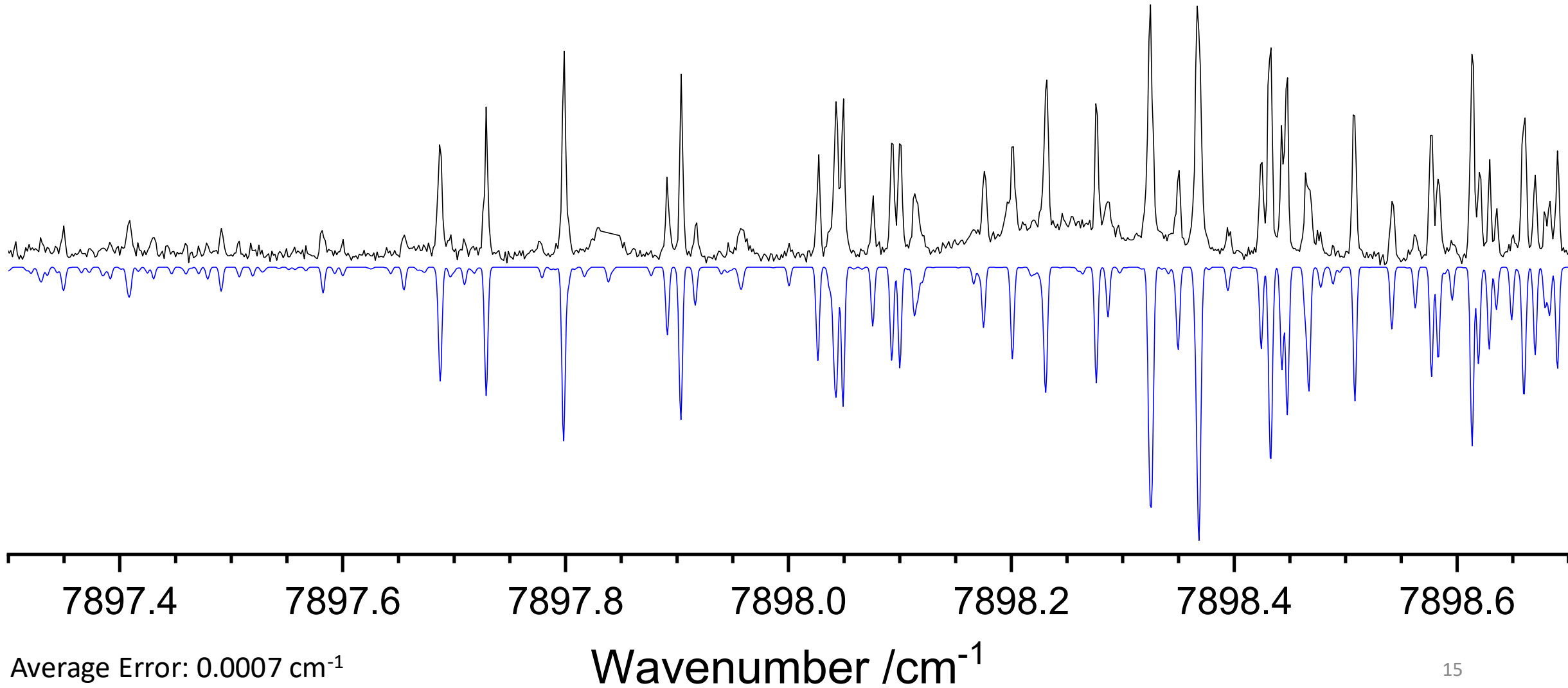


$$\Gamma = \Gamma_{ns} \otimes \Gamma_v \otimes \Gamma_r \otimes \Gamma_{ir} \otimes \Gamma_e \otimes \Gamma_{es}$$

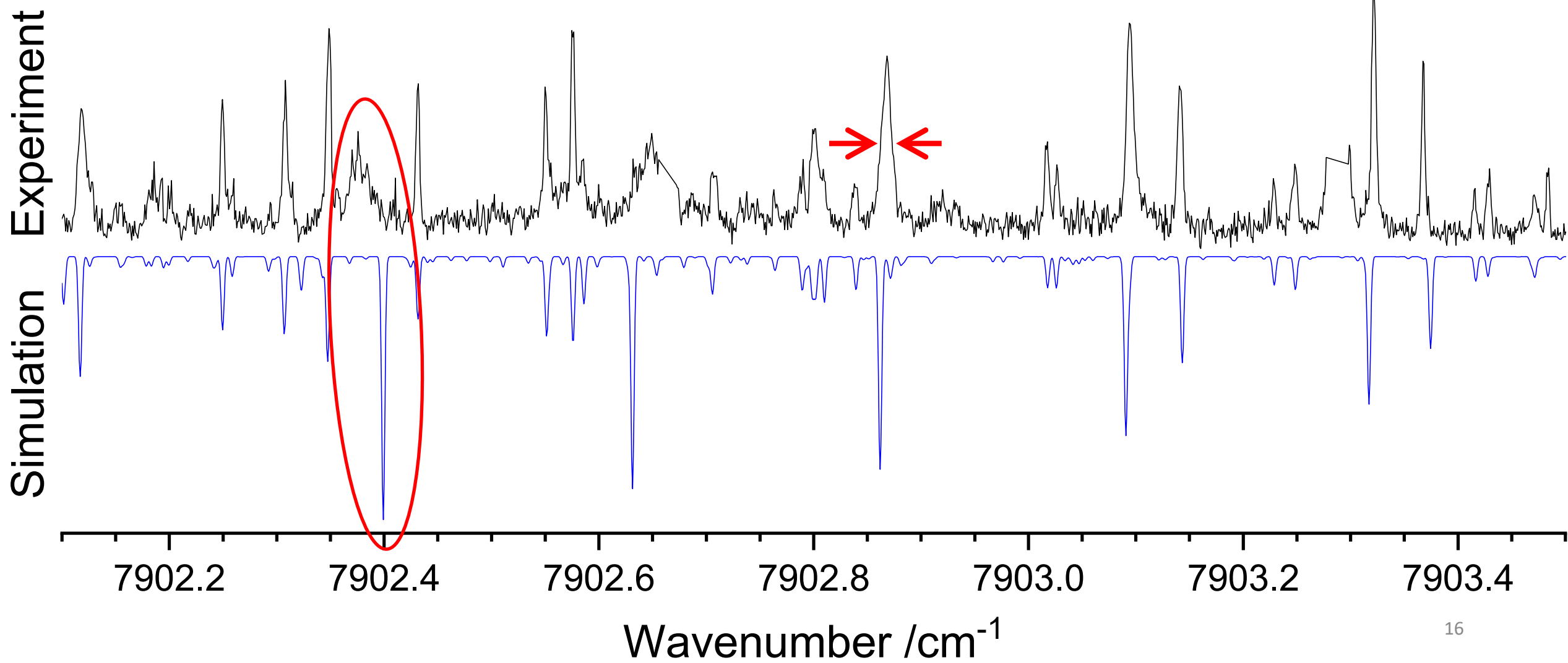


Qualité du modèle

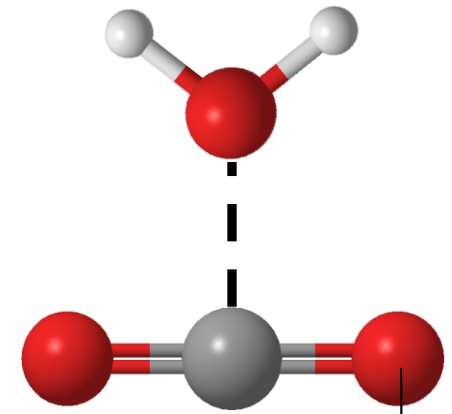
Experiment
Simulation



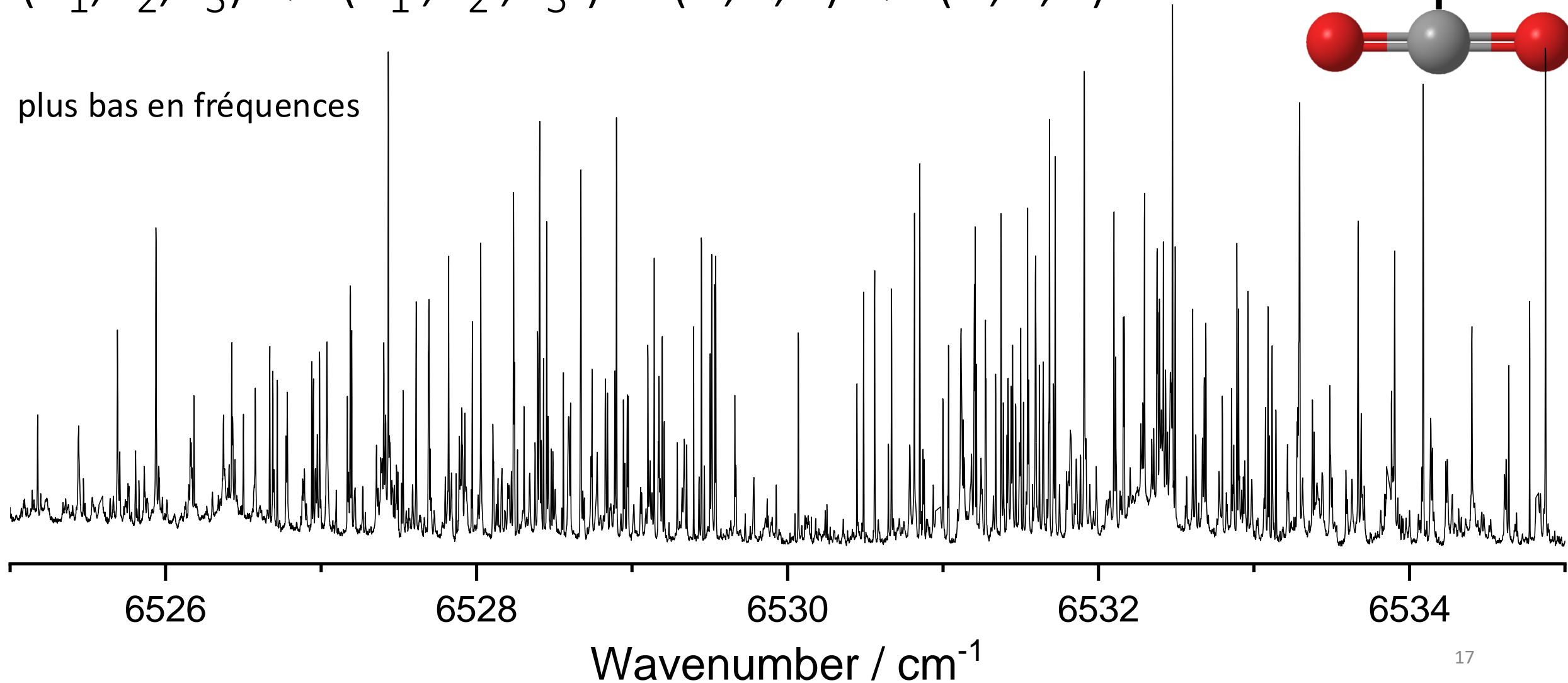
Observation de perturbations locales



Spectre de D₂O-CO₂ aux alentours
de la triple excitation vibrationnelle de D₂O
 $(v_1, v_2, v_3) \leftarrow (v_1', v_2', v_3') = (1, 1, 1) \leftarrow (0, 0, 0)$:

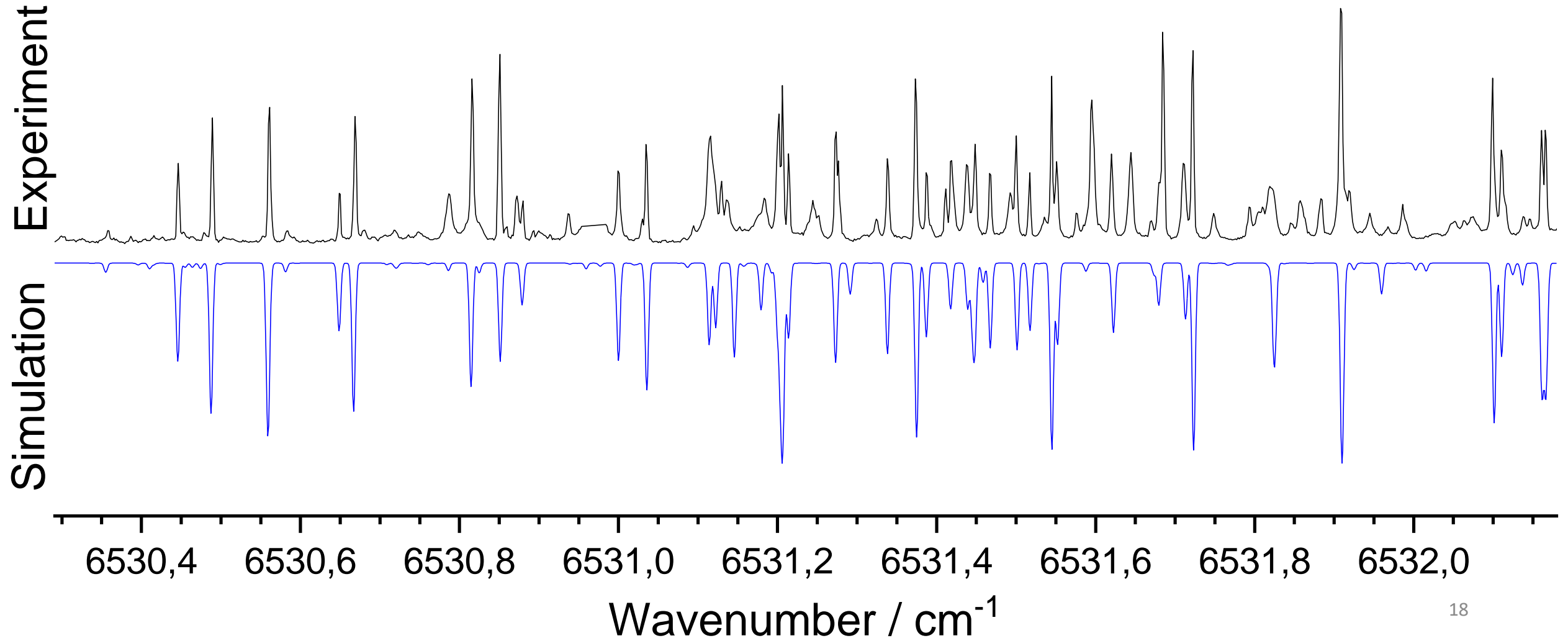


plus bas en fréquences



Qualité du modèle

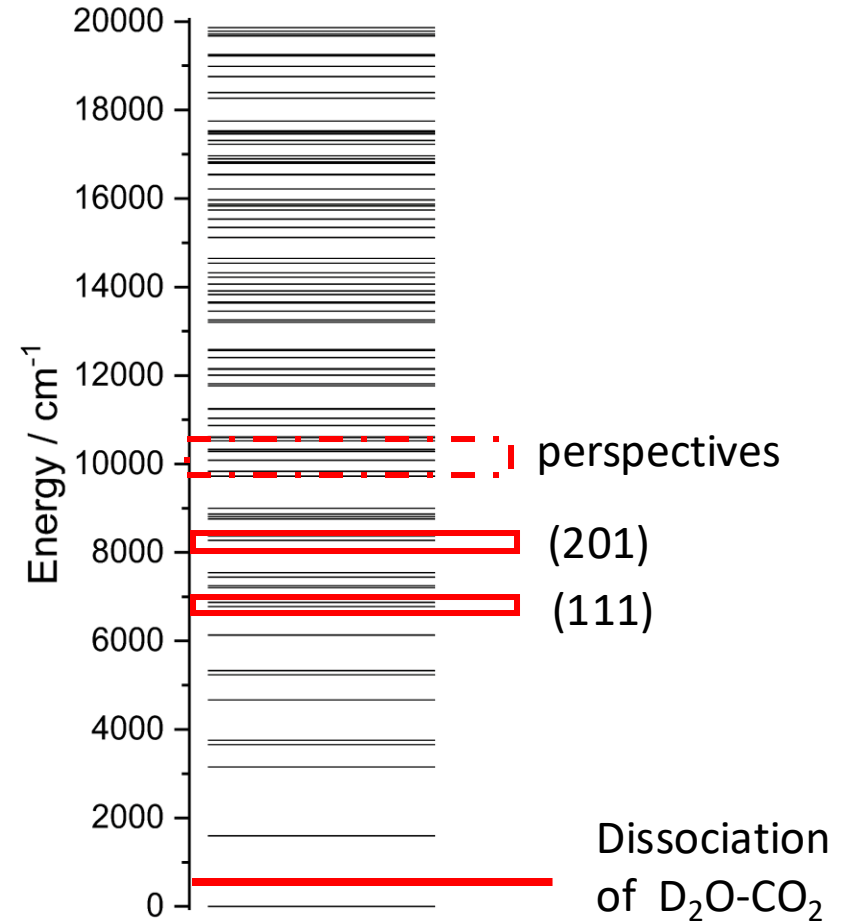
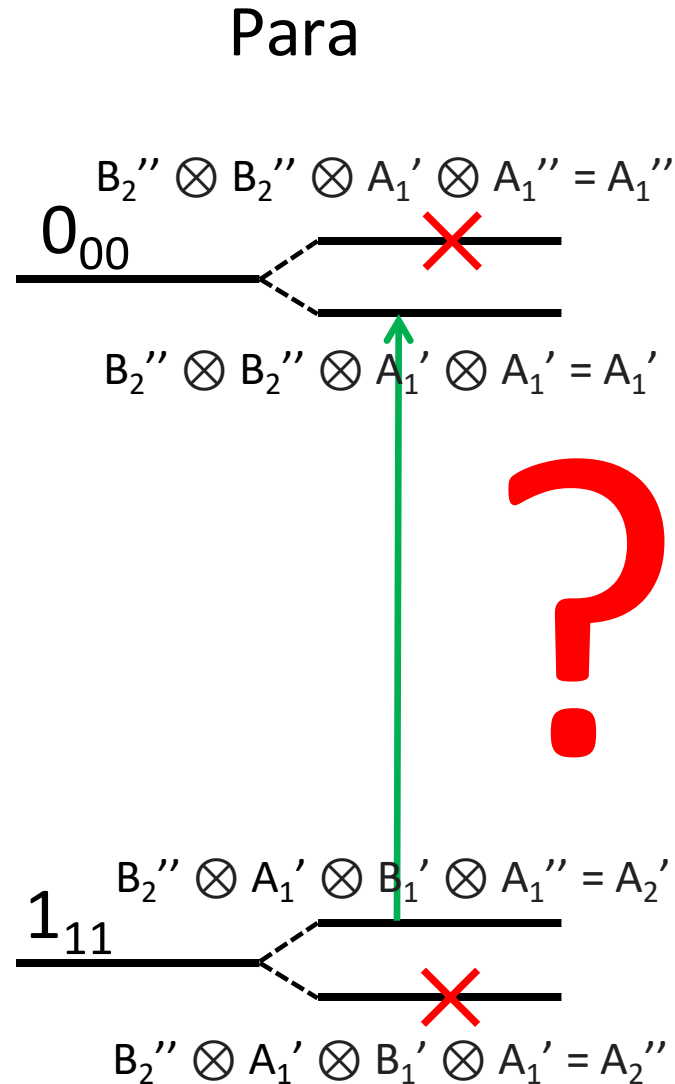
Observation uniquement de la composante Ortho.
Absence de la composante Para.



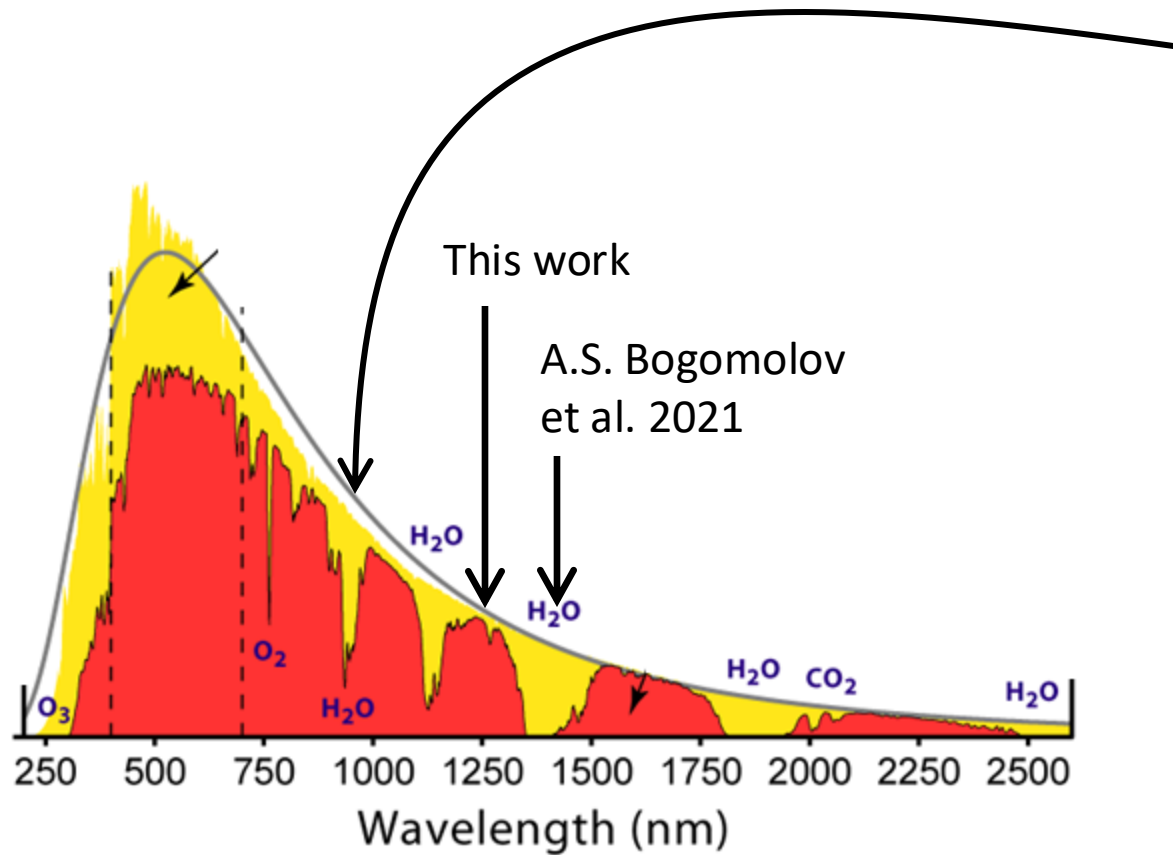
Dynamique de Photodissociation dépendante du spin nucléaire?

Anomalie déjà observée dans ce travail

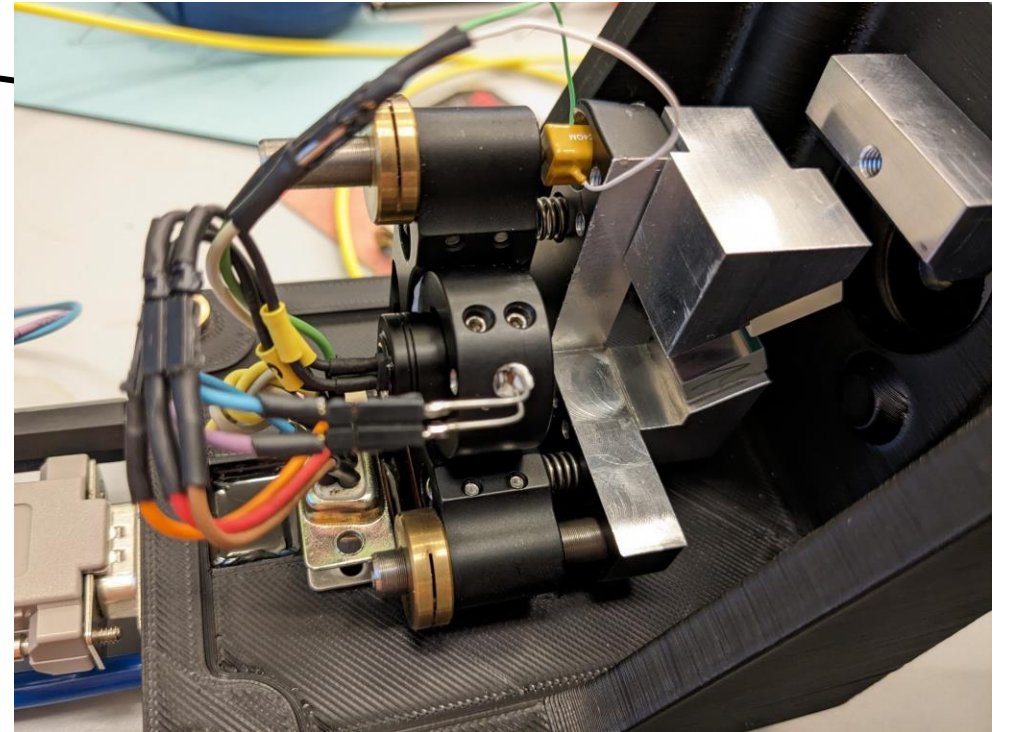
Bardlay, A.; McKellar, A.; Moazzen-Ahmadi, N. New Infrared Spectra of Acetylene-Water Dimers: First Determination of the A Rotational Constant and Another K-Dependent Anomaly. *The Journal of Physical Chemistry A* **2024**, *128* (36), 7628-7633.



Perspectives



Nouvelles sources laser ECDL



Perspectives

- Accuracy

- On a reçu le peigne de fréquence

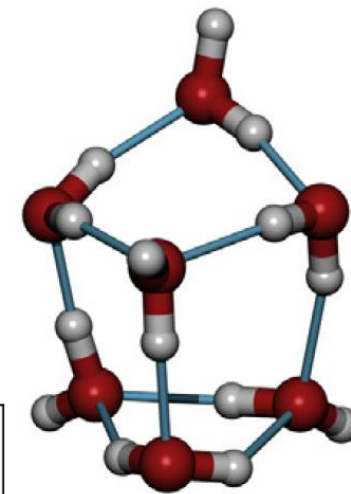
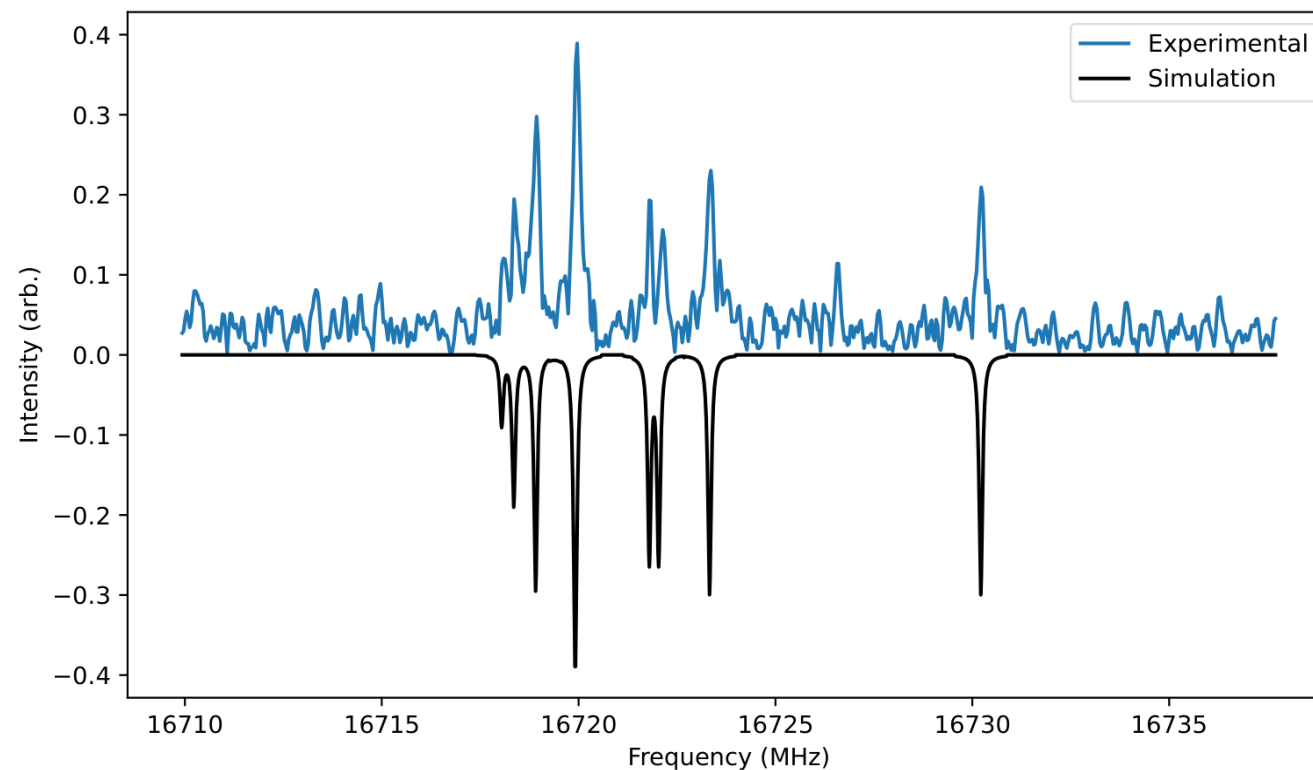
En collaboration

avec Alexis Libert et Arthémise Altman

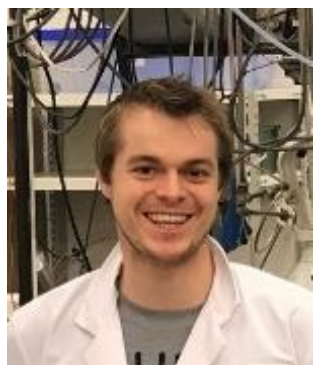
- Complexes plus grands et spectroscopie micro-ondes

En collaboration avec Simon Collignon

Water heptamer PR1 structure



Merci pour votre attention !



Robin Glorieux



Simon Collignon



Clément Lauzin



Ricardo De Abreu



Alexis Libert



E. Arthémise ALTMAN



Michel Herman



Nasser Moazzen-Ahmadi