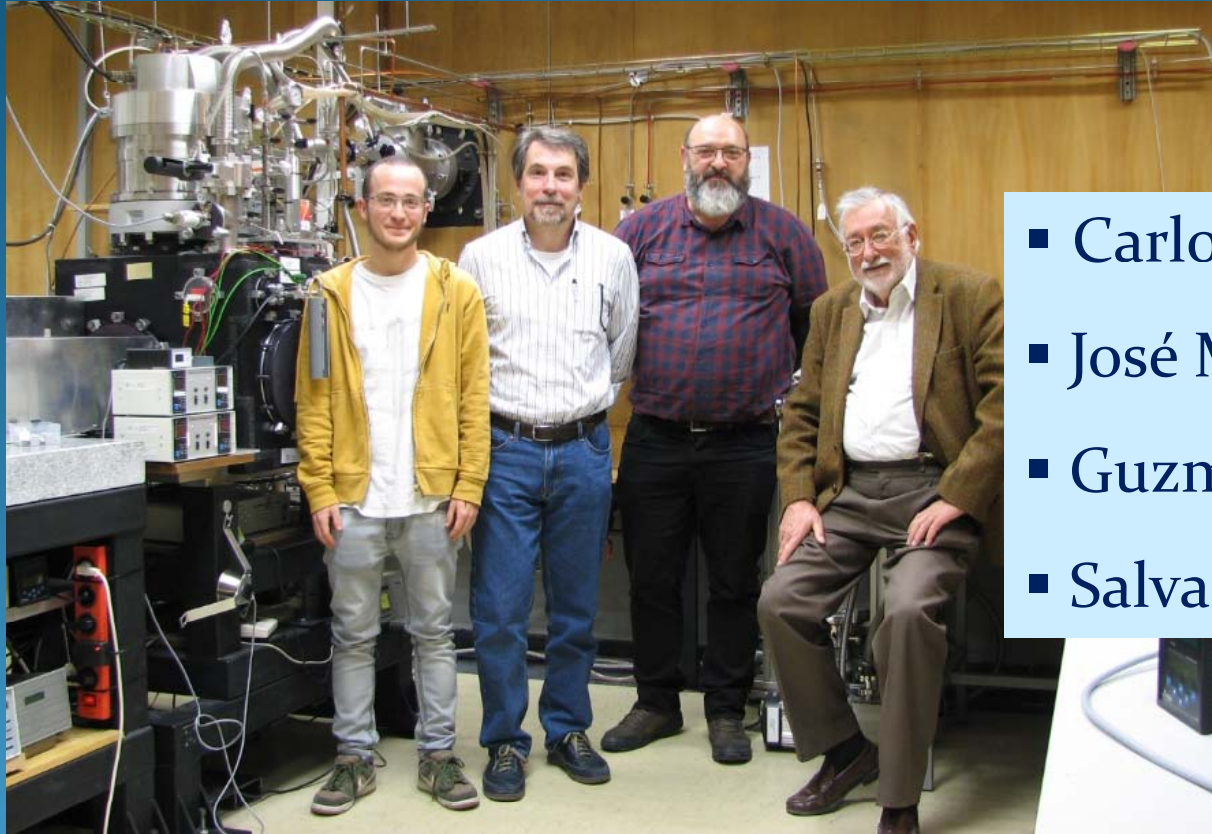


Espectroscopía de microchorros: gases y líquidos fuera del equilibrio

José M^a Fernández

*Laboratorio de Fluidodinámica Molecular
Instituto de Estructura de la Materia, CSIC*

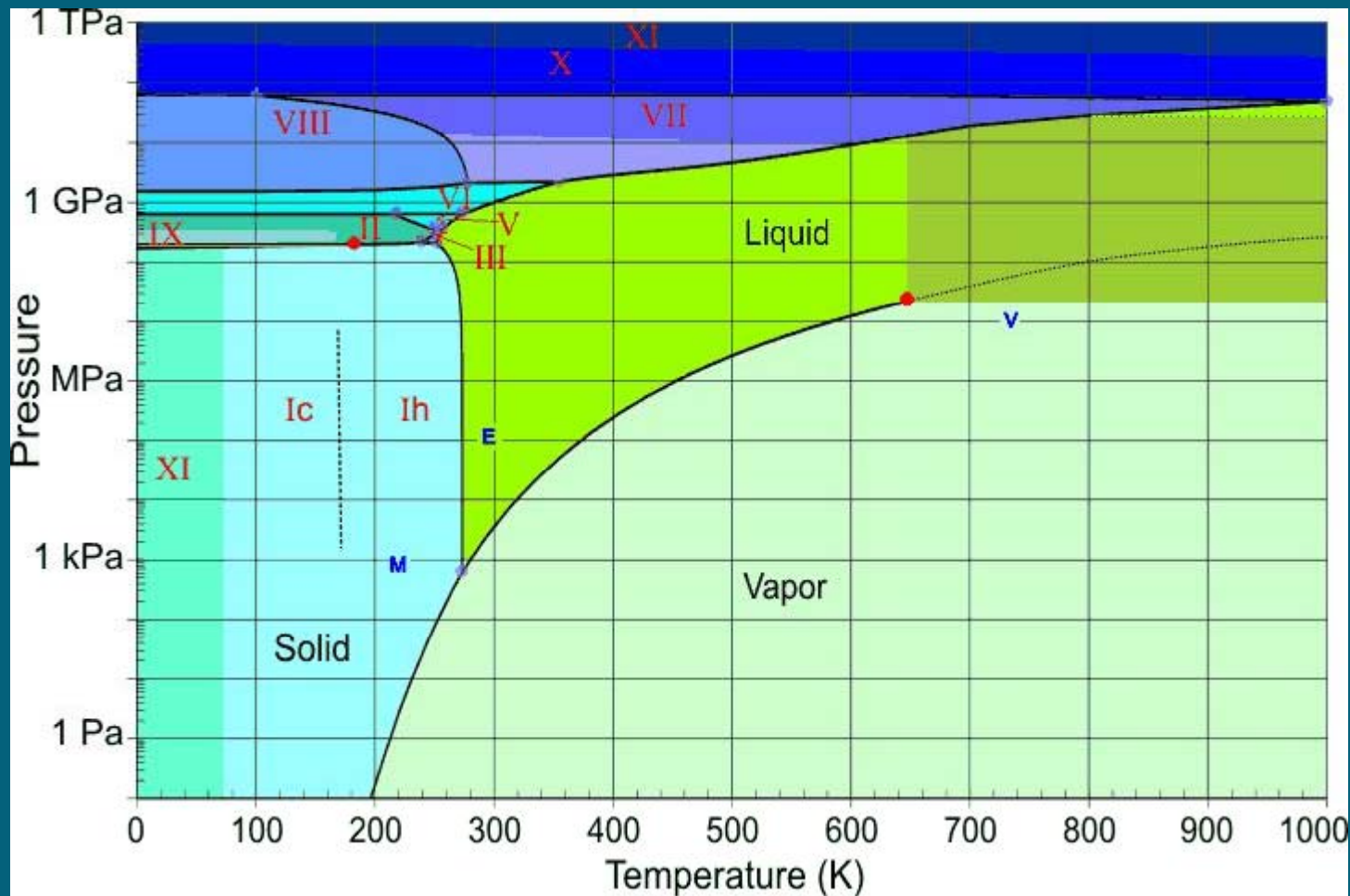
Group of Molecular Fluid Dynamics



- Carlos Álvarez
- José M^a Fernández
- Guzmán Tejeda
- Salvador Montero

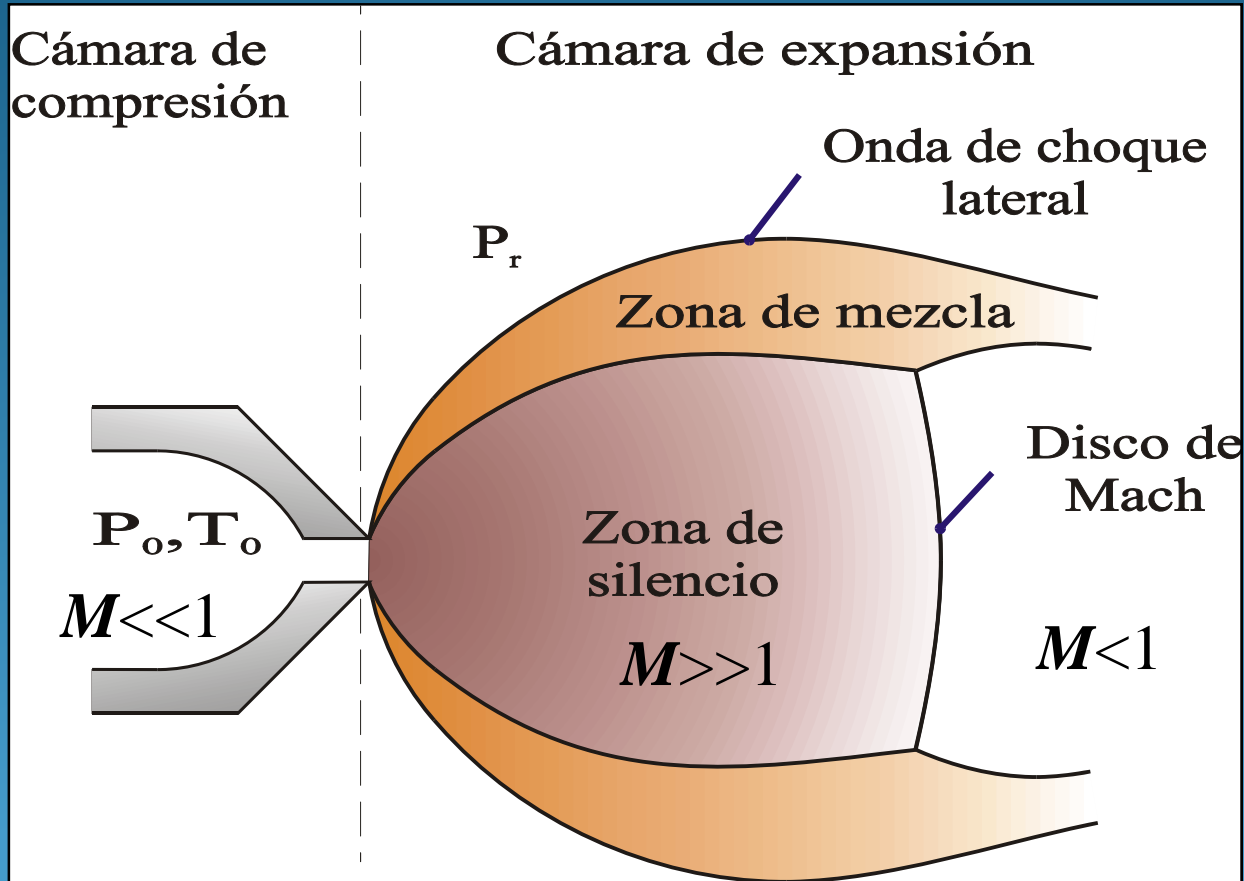
<http://www.iem.csic.es/fismol/fdm/>

Phase diagram (equilibrium)

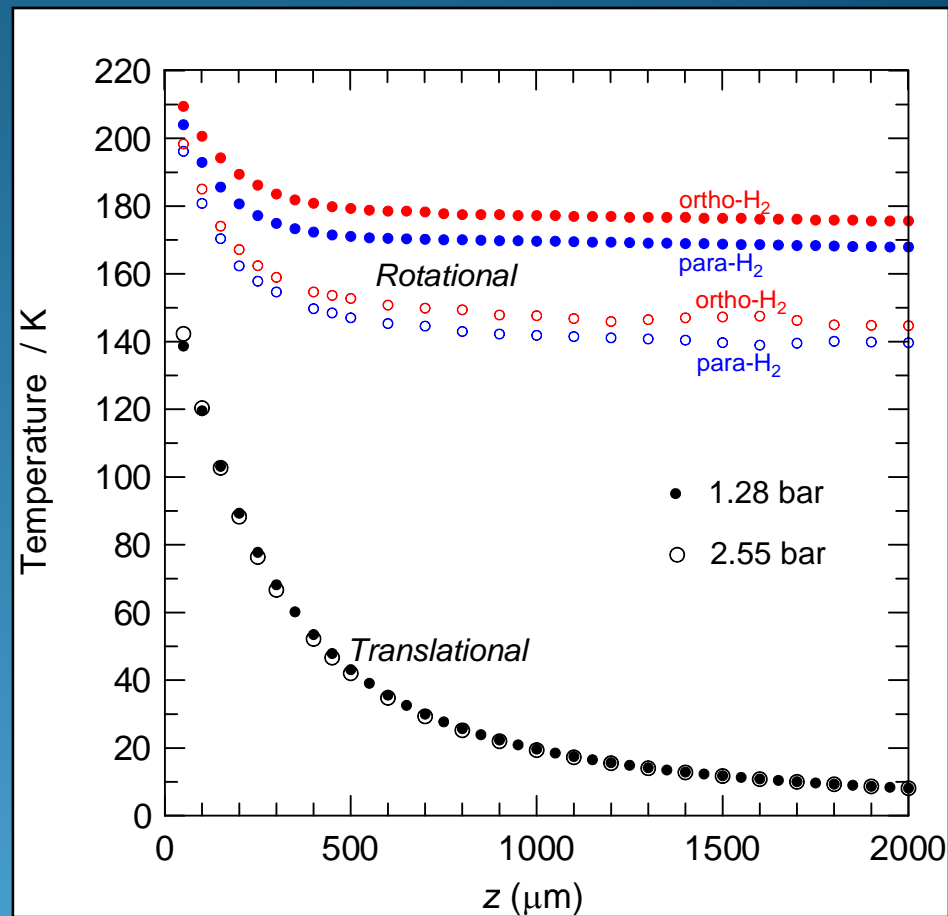
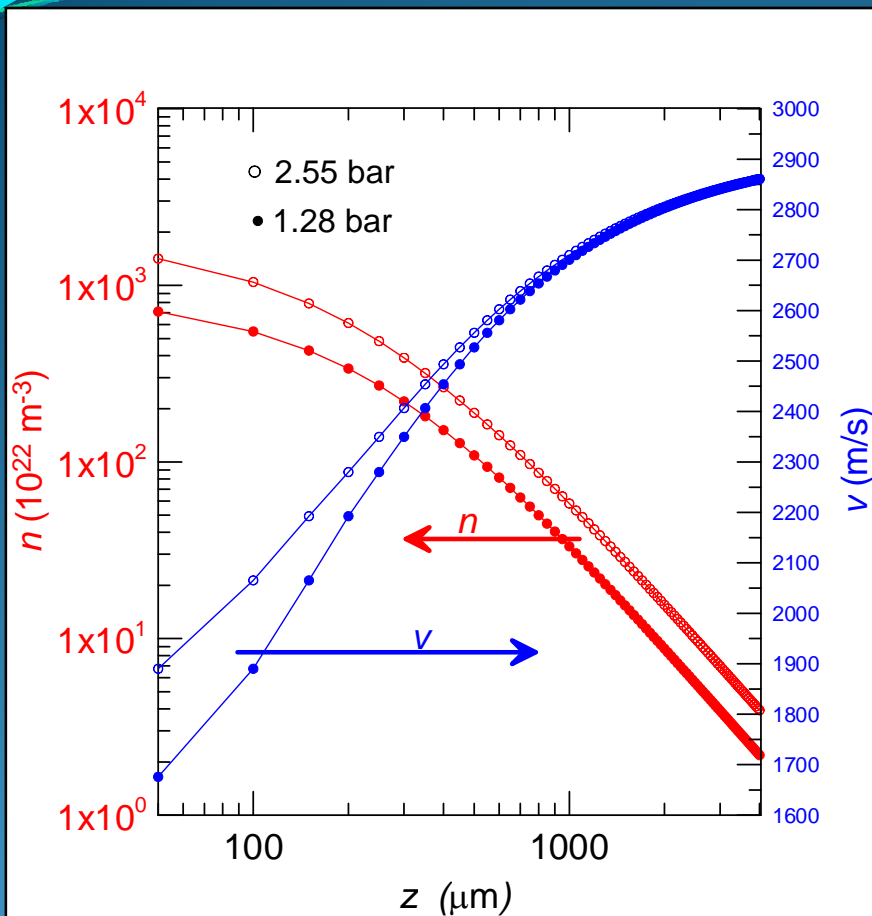


M. Chaplin, Water Structure and Science , <http://www1.lsbu.ac.uk/water/>

Chorros supersónicos de gases. Generalidades



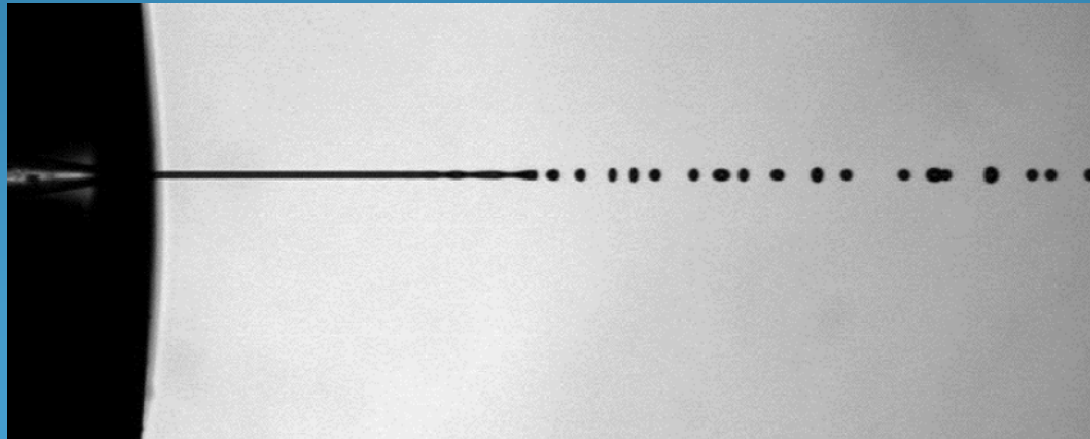
Chorros supersónicos. Zona de silencio



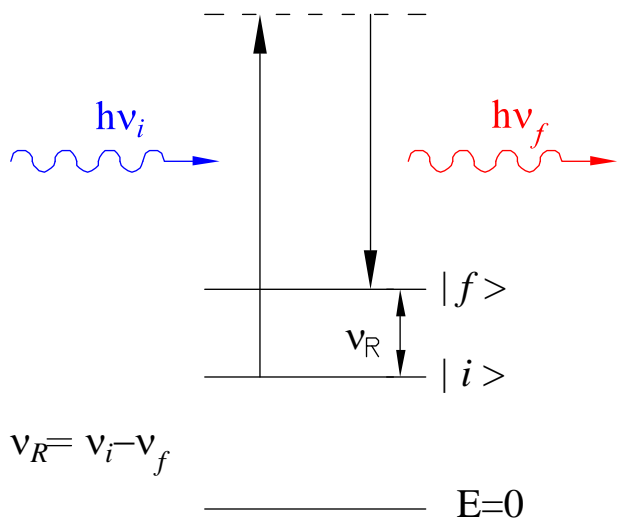
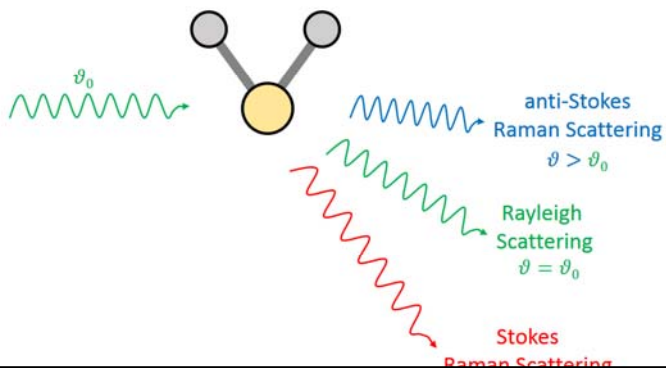
- Se rompe el equilibrio TD: $T_{\text{tras}} \neq T_{\text{rot}} \neq T_{\text{vib}}$
- El chorro supersónico es un sistema dinámico, condicionado por la cinética de colisiones: congelación Trot

Microchorros líquidos subenfriados

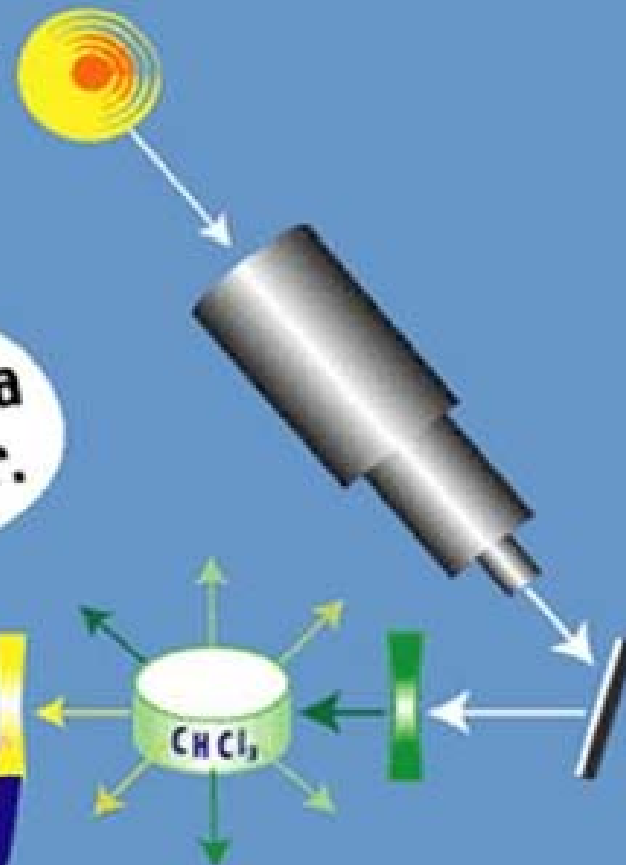
- Tobera < 10 micras
- Líquido presurizado (5-20 bar)
- Se enfrían por evaporación superficial (en vacío)
- Densidad ~ constante
- Fluctuaciones de Rayleigh: rotura en gotas -> líquido



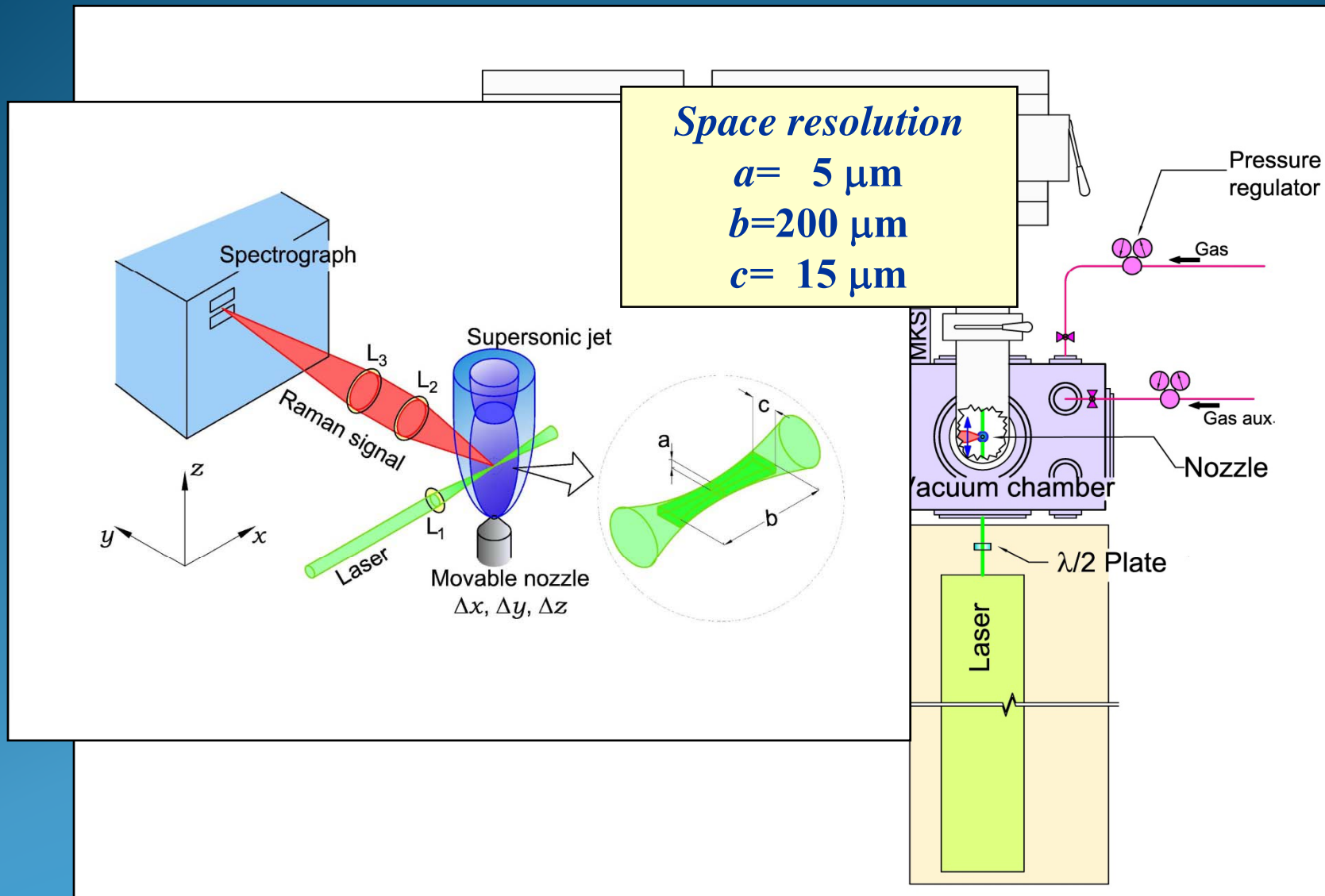
Efecto Raman: Scattering inelástico de luz



Raman, light of a different color.



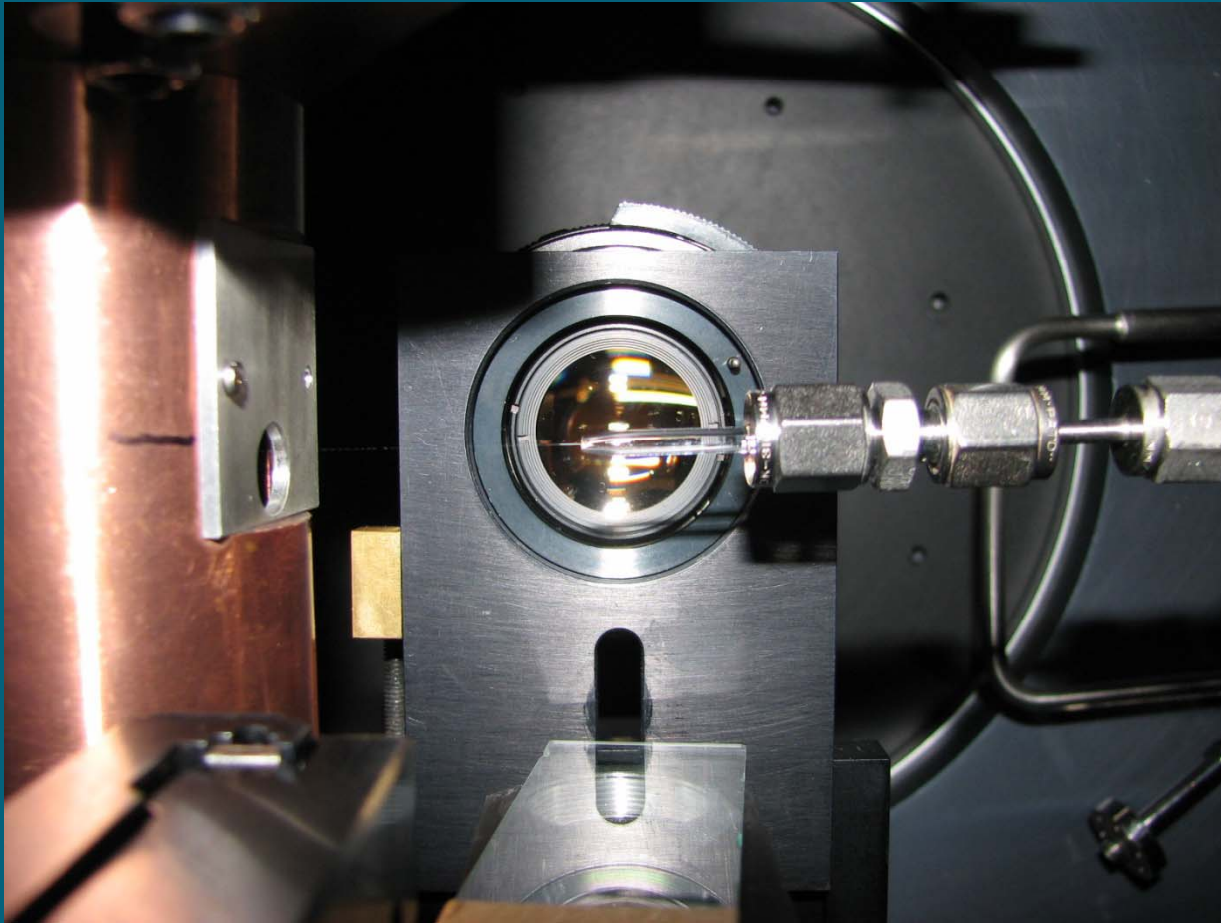
Montaje experimental



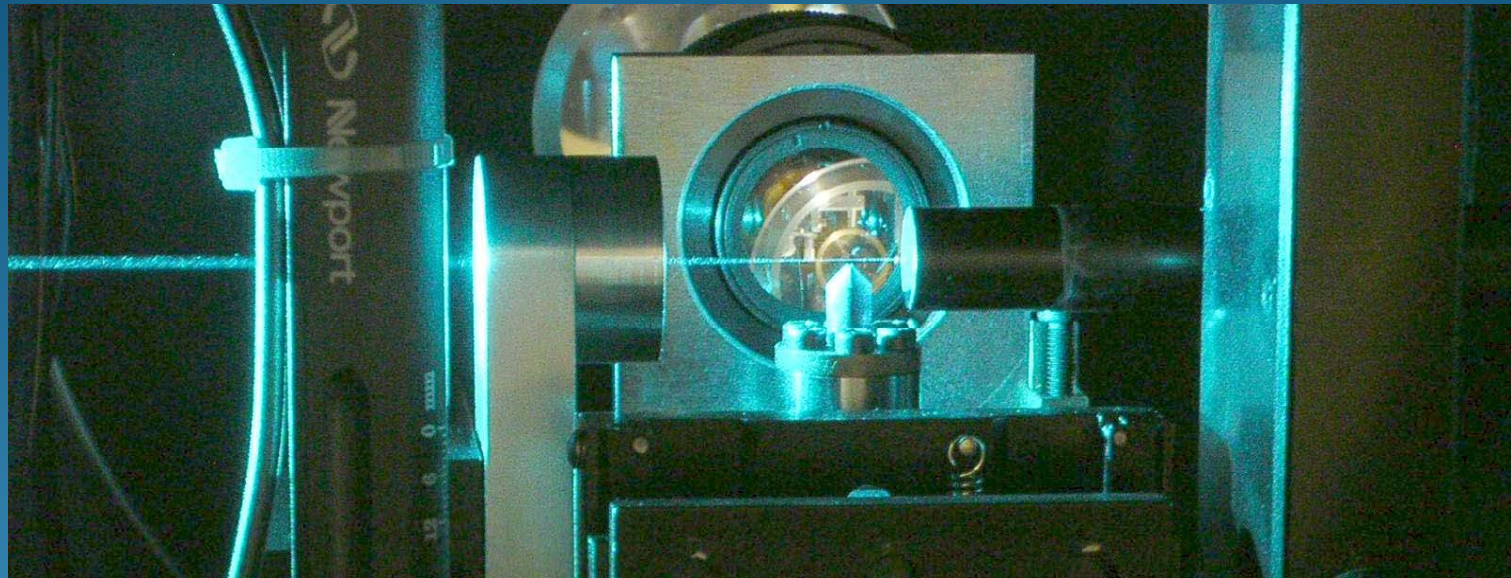
Montaje experimental



Experimental setup (IEM Madrid)



Montaje experimental

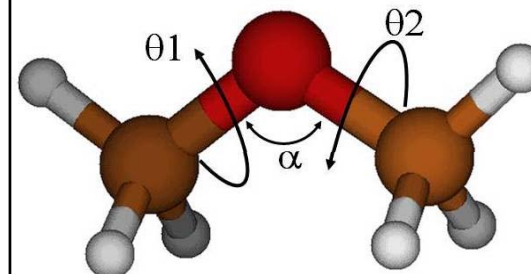
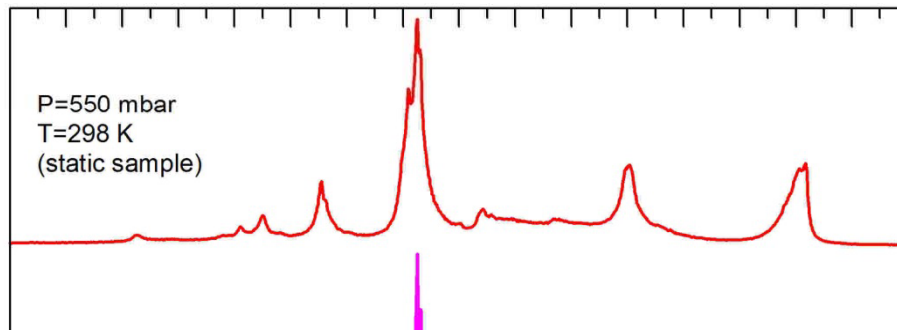


- Movemos la tobera para muestrear el chorro
- Resolución espacial: $1 \mu\text{m}$
- Resolución temporal:
 - Gas: $v \sim 1000 \text{ m/s} \Rightarrow 1 \text{ ns}$
 - Líquido $v \sim 20 \text{ m/s.} \Rightarrow 50 \text{ ns}$

¿Qué podemos estudiar con espectroscopía Raman en chorros de fluidos?

- espectros de moléculas frías
- espectros de moléculas calientes
- mapas de temperaturas en chorros de gases
- mapas de densidades en chorros de gases
- colisiones moleculares inelásticas
- agregación molecular
- solidificación de líquidos subenfriados

Espectroscopía Raman a baja temperatura



Dimetil-eter

THE ASTROPHYSICAL JOURNAL SUPPLEMENT SERIES, 241:13 (9pp), 2019 March

© 2019. The American Astronomical Society. All rights reserved.

<https://doi.org/10.3847/1538-4365/ab041e>

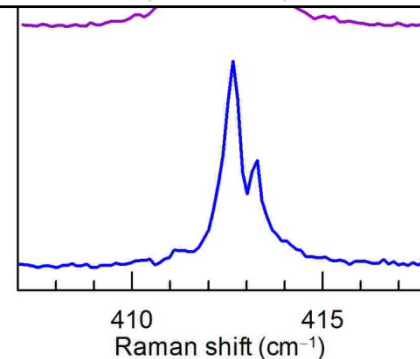
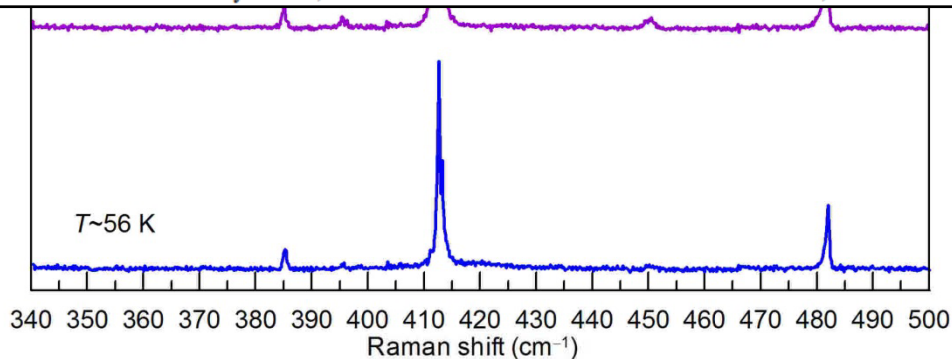


CrossMark

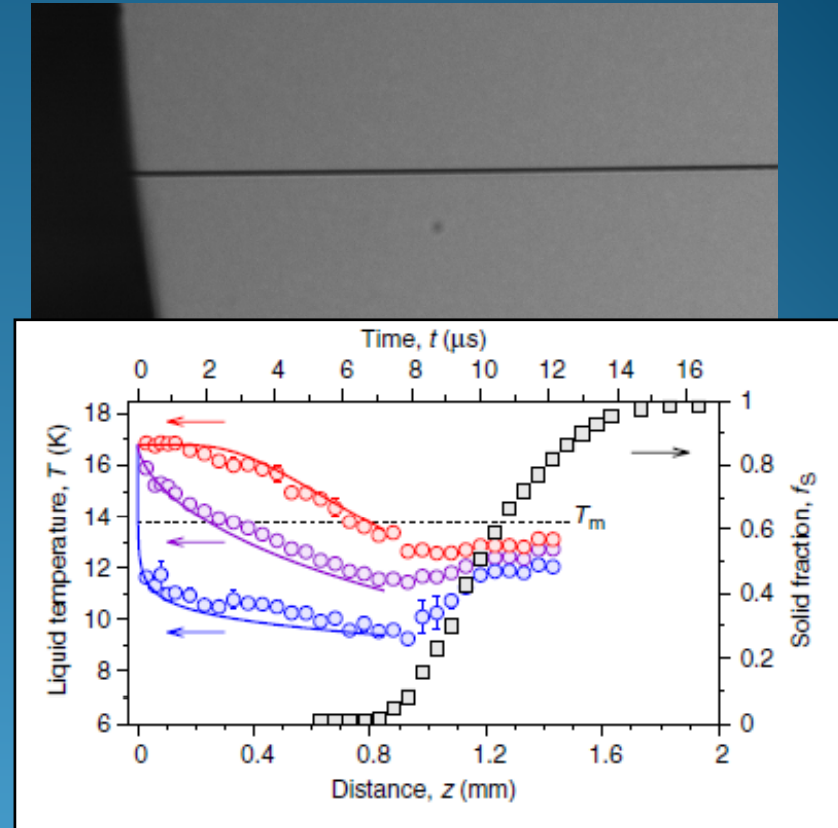
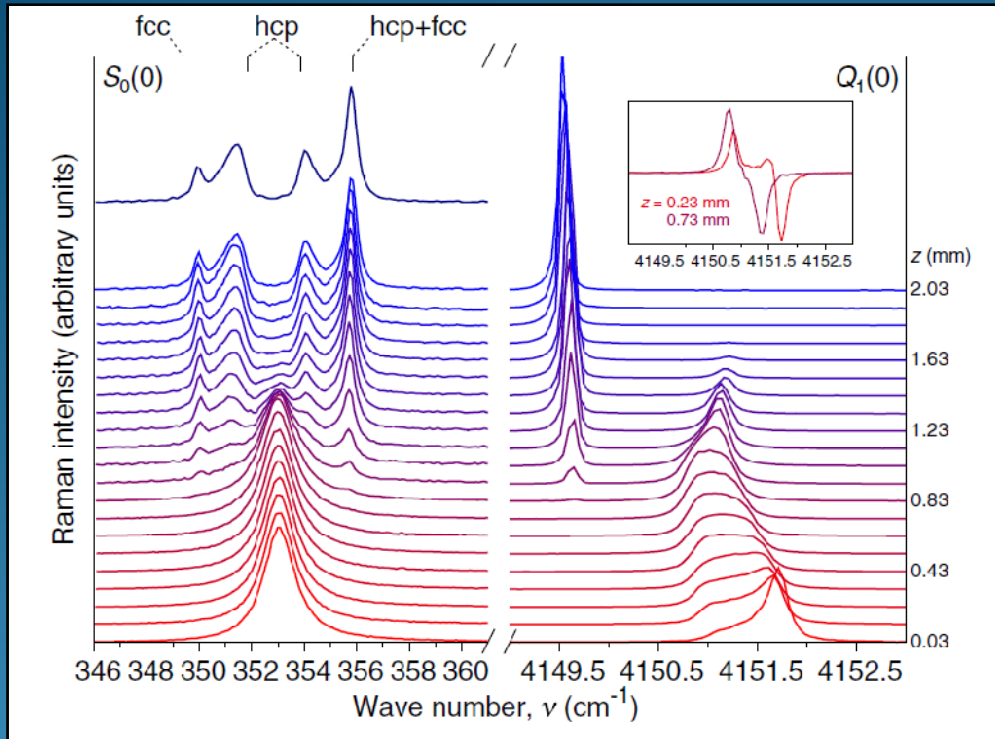
New Spectral Characterization of Dimethyl Ether Isotopologues CH_3OCH_3 and $^{13}\text{CH}_3\text{OCH}_3$ in the THz Region

J. M. Fernández¹ , G. Tejada¹ , M. Carvajal^{2,3} , and M. L. Senent⁴

¹Laboratory of Molecular Fluid Dynamics, Instituto de Estructura de la Materia IEM-CSIC, Unidad Asociada GIFMAN, CSIC-UHU; E-28006 Madrid, Spain



Microchorros de *para*-H₂ y *orto*-D₂ líquidos

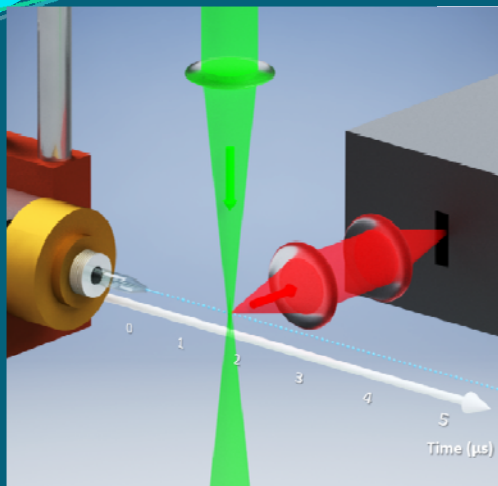


Kühnel, Fernández, Tejada, Kalinin, Montero, Grisenti, Phys. Rev. Lett. **106**, 245301 (2011)

Kühnel, Fernández, Tramonto, Tejada, Moreno, et al., Phys. Rev. B **89**, 180201(R) (2014)

Kühnel, Fernández, Tramonto, Tejada, Moreno, et al., J. Chem. Phys. **143**, 064504 (2015)

Microgotas de agua subenfriada

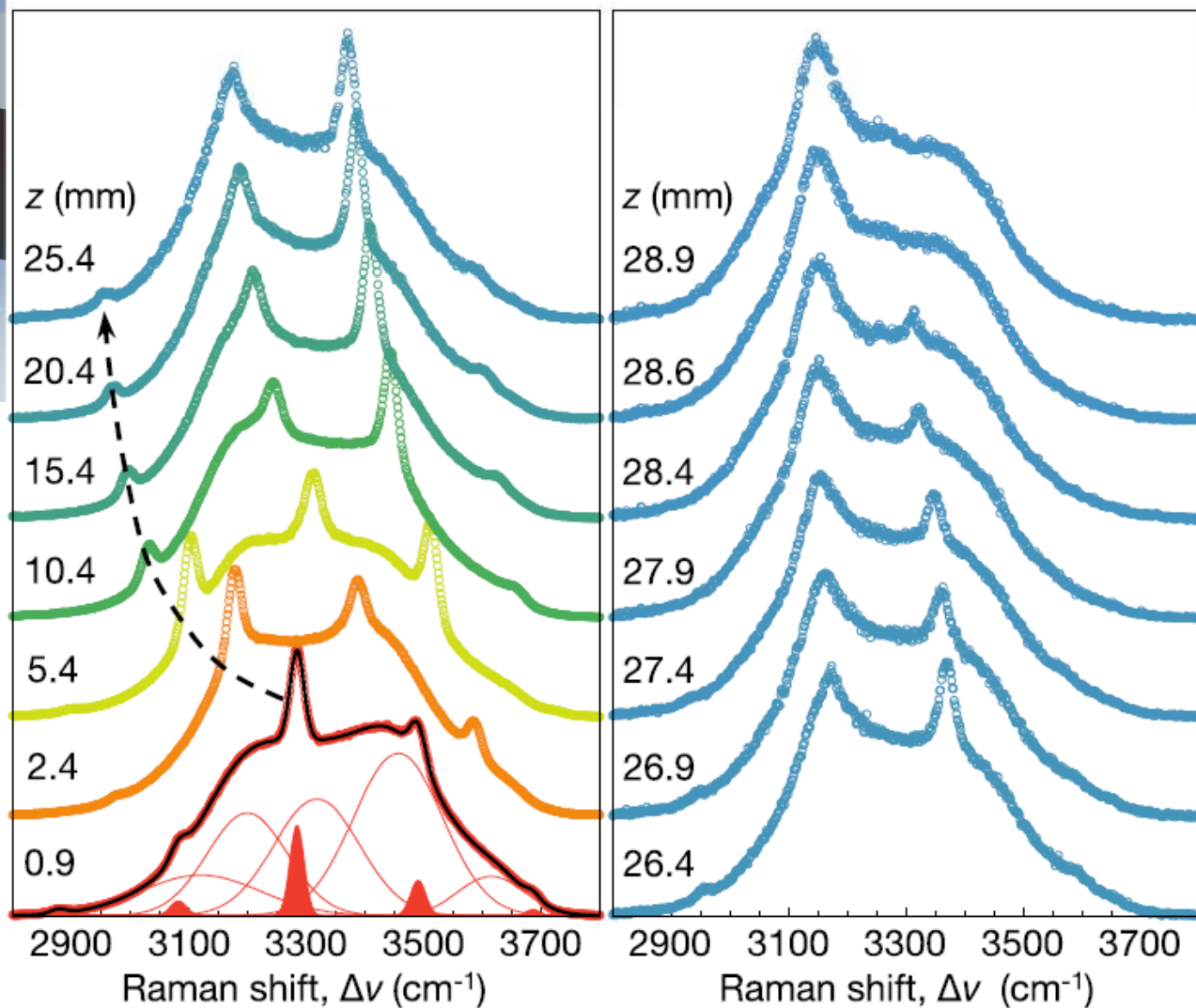


Nozzle

- $d=3.2 \mu\text{m}$
- 966 kHz

Water droplets

- $D=6.4 \mu\text{m}$
- $v=22 \text{ m/s}$



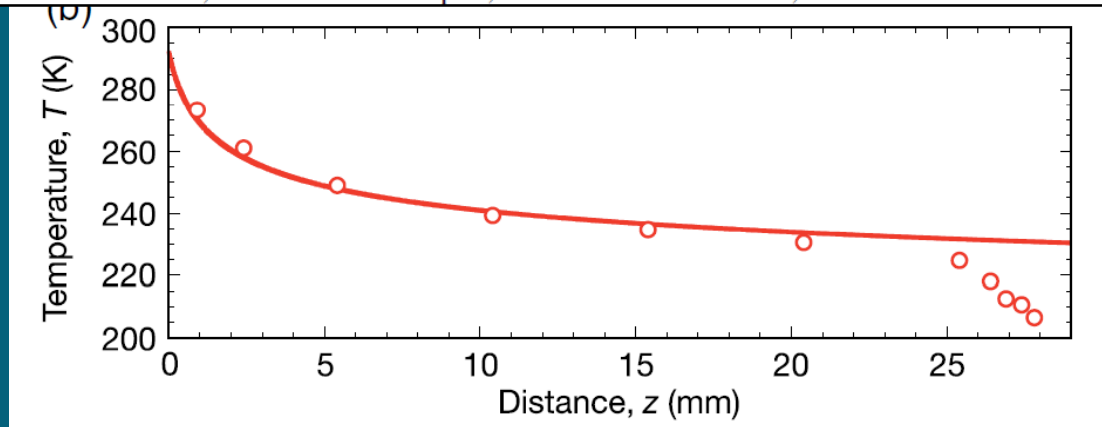
Results. Droplet size and temperature vs distance

PHYSICAL REVIEW LETTERS **120**, 015501 (2018)

Featured in Physics

Shrinking of Rapidly Evaporating Water Microdroplets Reveals their Extreme Supercooling

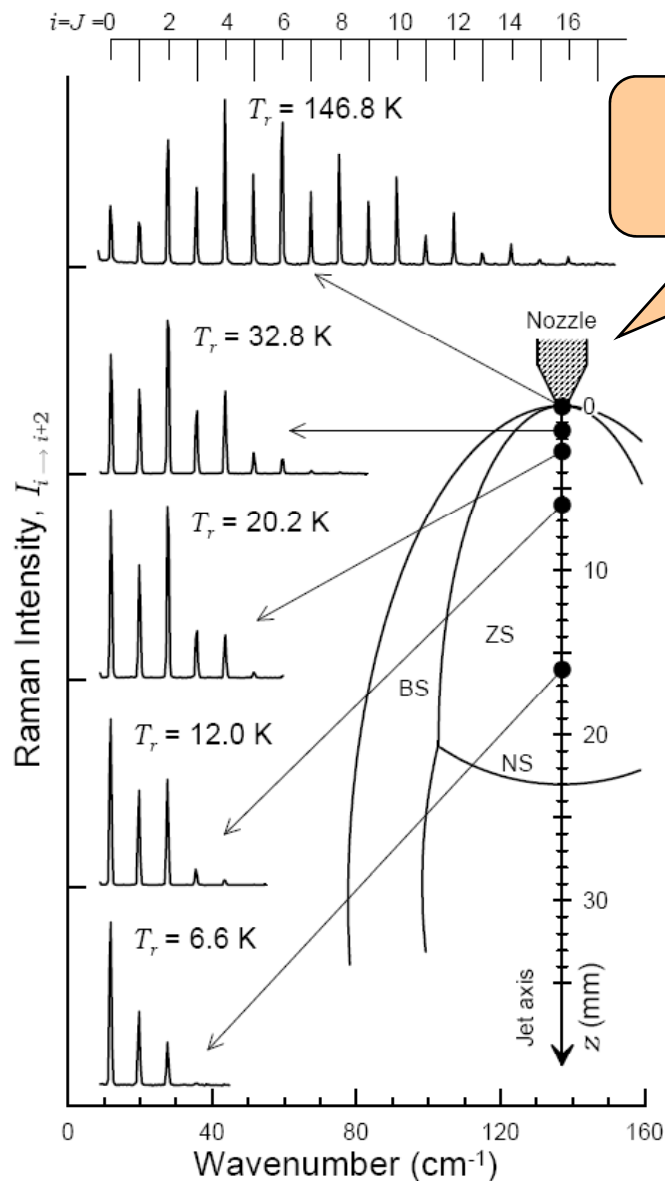
Claudia Goy,¹ Marco A. C. Potenza,² Sebastian Dedera,³ Marilena Tomut,⁴ Emmanuel Guillerm,⁵ Anton Kalinin,^{1,4} Kay-Obbe Voss,⁴ Alexander Schottelius,¹ Nikolaos Petridis,⁴ Alexey Prosvetov,⁴ Guzmán Tejada,⁶ José M. Fernández,⁶ Christina Trautmann,^{4,7} Frédéric Caupin,⁵ Ulrich Glasmacher,³ and Robert E. Grisenti^{1,4,*}



Goy et al. Phys. Rev. Lett. 120, 015501 (2018)

- Size-dependent resonances in the Raman spectra allow to measure the droplet size decrease from evaporative mass losses.
- A fraction of water droplets with initial diameter of 6379 ± 12 nm were found to remain liquid down to 230.6 ± 0.6 K.

Chorros de gases: Relajación rotacional



N_2 , 313 μm nozzle
 $P_0 = 2$ bar, $T_0 = 297$ K

- Seguimiento de la evolución temporal de las poblaciones rotacionales
- Velocidad de relajación rotacional nivel-a-nivel por colisiones inelásticas

Fonfría *et al.*, J. Chem. Phys. **127**, 134305 (2007)

Pérez-Ríos *et al.*, J. Chem. Phys. **134**, 174307 (2011)

Gámez *et al.*, J. Phys. Chem. A **123**, 8496 (2019)

Colisiones inelásticas H₂O:He

THE ASTROPHYSICAL JOURNAL SUPPLEMENT SERIES, 216:3 (8pp), 2015 January

doi:10.1088/0067-0049/216/1/3

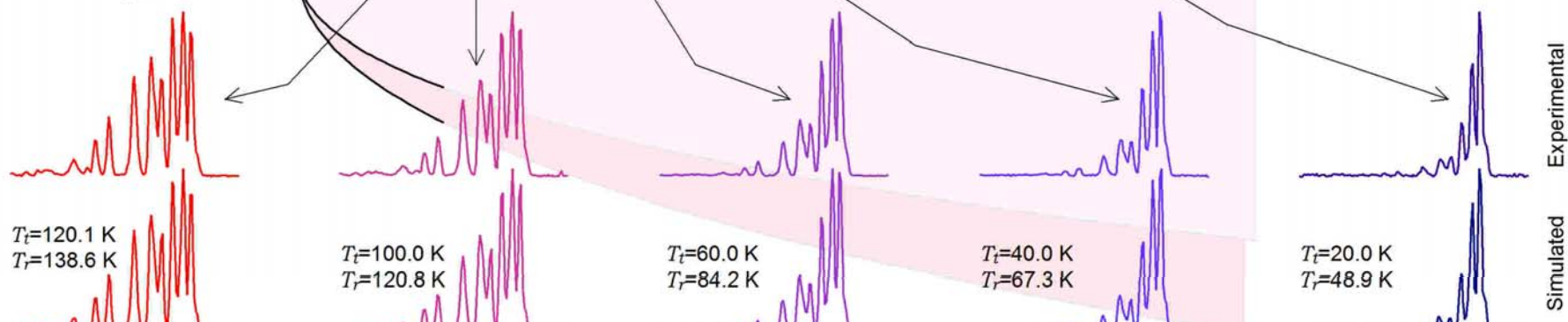
© 2015. The American Astronomical Society. All rights reserved.

LABORATORY STUDY OF RATE COEFFICIENTS FOR H₂O:He INELASTIC COLLISIONS BETWEEN 20 AND 120 K

G. TEJEDA¹, E. CARMONA-NOVILLO², E. MORENO¹, J. M. FERNÁNDEZ¹, M. I. HERNÁNDEZ², AND S. MONTERO¹

¹Laboratory of Molecular Fluid Dynamics, Instituto de Estructura de la Materia, CSIC Serrano 121, E-28006 Madrid, Spain

²Instituto de Física Fundamental, CSIC Serrano 123, E-28006 Madrid, Spain; emsalvador@iem.cfmac.csic.es



THE ASTROPHYSICAL JOURNAL, 808:175 (7pp), 2015 August 1

doi:10.1088/0004-637X/808/2/175

© 2015. The American Astronomical Society. All rights reserved.

BROADENING OF H₂O ROTATIONAL LINES BY COLLISIONS WITH He ATOMS AT LOW TEMPERATURE

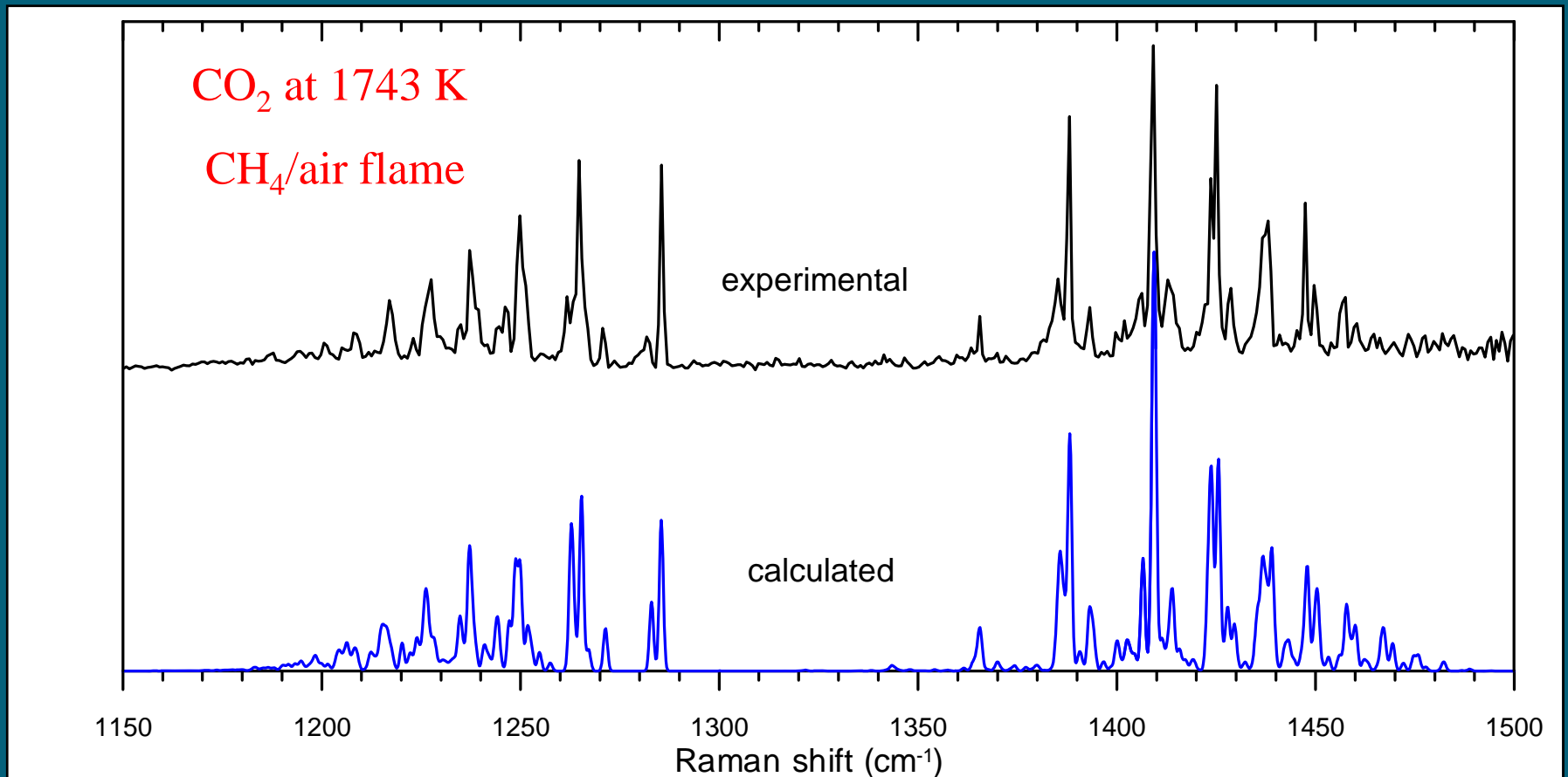
M. I. HERNÁNDEZ¹, J. M. FERNÁNDEZ², G. TEJEDA², E. MORENO², AND S. MONTERO²

¹Instituto de Física Fundamental CSIC, Serrano 123, E-28006 Madrid, Spain

²Laboratory of Molecular Fluid Dynamics, Instituto de Estructura de la Materia CSIC, Serrano 121, E-28006 Madrid, Spain; jm.fernandez@csic.es

Received 2015 April 22; accepted 2015 June 17; published 2015 July 30

Vibrational inelastic collisions in CO₂



Fernández *et al.*, *J. Raman Spectrosc.* **37**, 175 (2006)

Sánchez-Castellanos *et al.*, *Chem. Phys. Lett.* **554**, 208 (2012)

Resumen e ideas a recordar

El FDM-lab ofrece formación en física molecular experimental, con un marcado carácter interdisciplinar:

- Espectroscopía Raman de altas prestaciones
- Láseres de potencia y técnicas ópticas relacionadas
- Dinámica supersónica y subsónica de fluidos
- Alto vacío y criogenia

Posibles temas de trabajo

- colisiones inelásticas V-T, V-V, R-T de moléculas de interés atmosférico (CO₂, N₂, O₂) o astrofísico (+ He, H₂..)
- cartografía de densidad y temperatura de micro-flujos
- cristalización de microchorros/gotas de líquidos subenfriados