# High-temperature hypersonic Laval nozzle for non-LTE cavity ringdown spectroscopy **@**

Cite as: J. Chem. Phys. **152**, 134201 (2020); https://doi.org/10.1063/5.0003886 Submitted: 05 February 2020 . Accepted: 09 March 2020 . Published Online: 01 April 2020

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COLLECTIONS

This paper was selected as Featured

#### DUDÁS Eszter - 25/06/2020 nISMS







## Astronomical observations

EXOPLANET (HOT JUPITER)

1000 - 3000K CH<sub>4</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>

> Theoretical molecular model

Experimental data

Atmospheric modelling

## e-PYTHEAS project

## SMAUG Spectroscopy of Molecules Accelerated in Uniform Gas flows



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**Objective:** record high temperature spectral data

- \* Small hydrocarbons (CH<sub>4</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>)
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- \* overcrowded for polyatomic molecules
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### Challenges: HT spectra

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## Our approach:

- \* Decoupling internal degrees of freedom
- \*  $T_{rot} \ll T_{vib}$

#### **Non-LTE spectroscopy**



**Decoupling internal degrees of freedom of molecules** 

- high vibrational levels thermally populated
- high-J rotational levels thermally de-populated

simplified rotational structure

- → few molecular collisions
- $\rightarrow$  low energy transfer V-T & V-R
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- $\rightarrow$  low energy transfer V-T & V-R
- → decoupled internal degrees of freedom

Adiabatic expansion:  
$$c_P T_0 = c_P T + \frac{1}{2} u^2$$

$$Mach = \frac{speed \ of \ gas}{speed \ of \ sound} = \frac{u}{\sqrt{\gamma rT}} \propto \sqrt{\frac{E_{kinetic}}{E_{thermal}}}$$

Accelerate the gas  $\rightarrow$  Laval nozzle



- $\rightarrow$  low energy transfer V-T & V-R
- $\rightarrow$  decoupled internal degrees of freedom

Adiabatic expansion:  $c_P T_0 = c_P T + \frac{1}{2} u^2$ 



Accelerate the gas  $\rightarrow$  Laval nozzle









Temperature /K







Temperature /K



**Pressure /Torr** 

2

3

4

5

6

d



100 b 500K 80 1000K 0.4 1500K 60 2000K 0.3 40 0.2 20 0.1 0 0 2 3 4 5 6 7 15 10 1 Radial distance from axis /mm









Temperature /K



Temperature /K



**Pressure /Torr** 









5 0 5

10 15



## Preliminary study on carbon monoxide



## Preliminary study on carbon monoxide





#### Preliminary study on carbon monoxide





**CO non-LTE conditions:** T<sub>rot</sub> = 12.6 (1) K T<sub>vib</sub> = 1345 (56) K

#### **Application to non-LTE spectroscopy of methane**



6120 - 6140 cm<sup>-1</sup>

6193 - 6219 cm<sup>-1</sup>

#### LTE vs non-LTE spectra



#### LTE vs non-LTE spectra CH<sub>4</sub>



Evolution of the Int. abs. cross-sections of RO-s in diff. polyads

#### LTE vs non-LTE spectra CH<sub>4</sub>



Evolution of the Int. abs. cross-sections of RO-s in diff. polyads

#### **Temperature extraction - T**<sub>rot</sub>



 $T_{rot} = 30 (3) K$ 





$$\bar{\sigma}_{ij}(T_{rot}, T_{vib}^{I}, T_{vib}^{II}) = \bar{\sigma}_{ij}(T_0) \frac{Q_0(T_0)}{Q_{rot}(T_{rot}) \times Q_{vib}(T_{vib}^{II}) \times Q_{vib}(T_{vib}^{II})} \times exp\left[\frac{E_i}{kT_0} - \frac{1}{k} \left(\frac{E_i^{pol}}{T_{vib}^{I}} + \frac{E_i^{vib}}{T_{vib}^{II}} + \frac{E_i^{rot}}{T_{vib}}\right)\right]$$



$$\bar{\sigma}_{ij}(T_{rot}, T_{vib}^{I}, T_{vib}^{II}) = \overline{\sigma}_{ij}(T_0) \frac{Q_0(T_0)}{Q_{rot}(T_{rot}) \times Q_{vib}(T_{vib}^{I}) \times Q_{vib}(T_{vib}^{II})} \times exp\left[ \underbrace{E_i}_{kT_0} - \frac{1}{k} \underbrace{E_i^{vib}}_{T_{vib}} + \underbrace{E_i^{vib}}_{T_{vib}} + \underbrace{E_i^{rot}}_{T_{vib}} \right]$$

## TheoReTS database



#### **Temperature extraction – T<sup>I</sup>**<sub>vib</sub> & T<sup>II</sup><sub>vib</sub>



#### **Conclusions and perspectives**

Performance of the SMAUG setup has been characterized

- Line identification using TheoReTS
- Insertion of new hot bands into TheoReTS

Limitations of the current experimental system:

➤ (T<sub>0</sub>)<sub>max</sub> ~ 2000K

 $\succ$  graphite heating element  $\rightarrow$  limited variety of molecules can be

studied



### **The PLATYPUS Project**







#### In collaboration with Christine Charles, Dimitrios Tsifakis, Rod Boswell,

Space Plasma, Power and Propulsion Laboratory (SP3), Australian National University

#### Acknowledgments

- > ANR (e-PYTHEAS project) is acknowledged for the PhD grant
- Colleagues at the Molecular Physics Department
- Technical staff of IPR

- Christine Charles, Dimitrios Tsifakis, Rod Boswell
  Space Plasma, Power and Propulsion Laboratory (SP3)
- Dr. Vinayak N. Kulkarni Indian Institute of Technology Guwahati
- Professor Robert Gamache
  University of Massachusetts Lowell