UNIVERSITÉ DE VERSAILLES ST-QUENTIN-EN-YVELINES

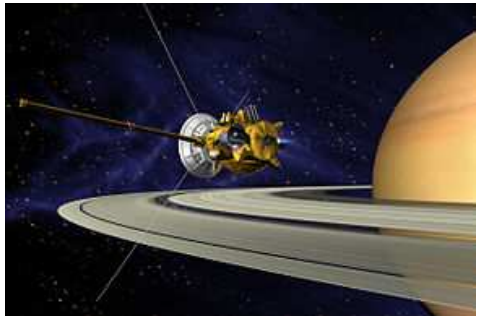
IUF

07 nov 2013 – Journée ESEP

ASTROCHIMIE :
Simuler, Modéliser, Détecter

# Simuler l'atmosphère de Titan en laboratoire

De la complémentarité « Simulation de laboratoire / Mission spatiale »



Artist view of Cassini orbiting Saturn (© NASA)

Nathalie Carrasco

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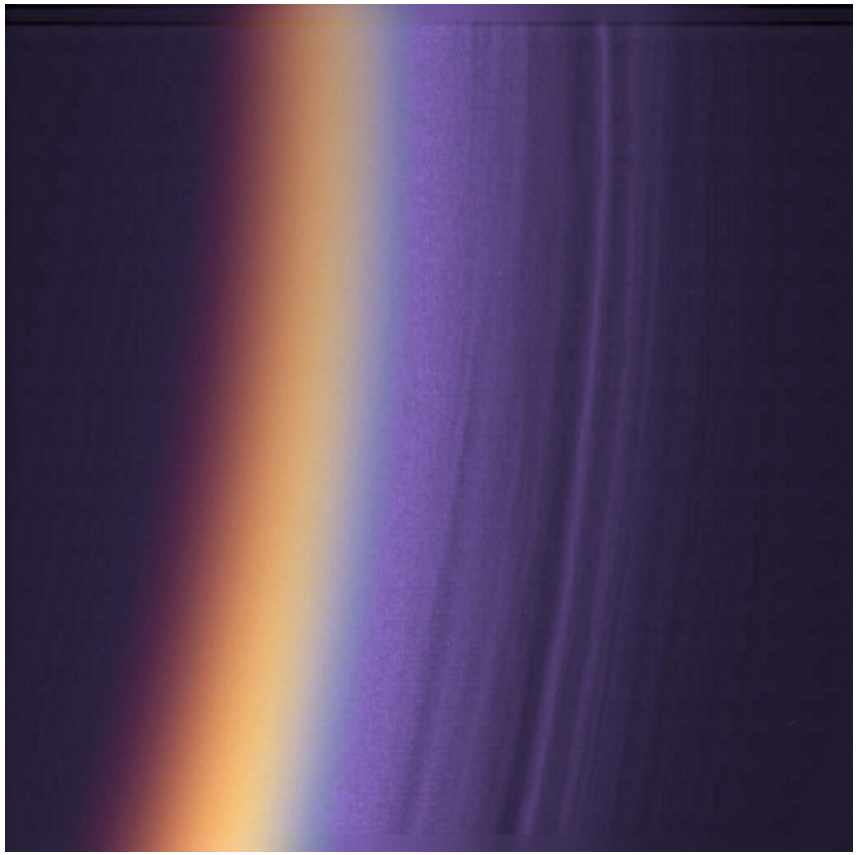
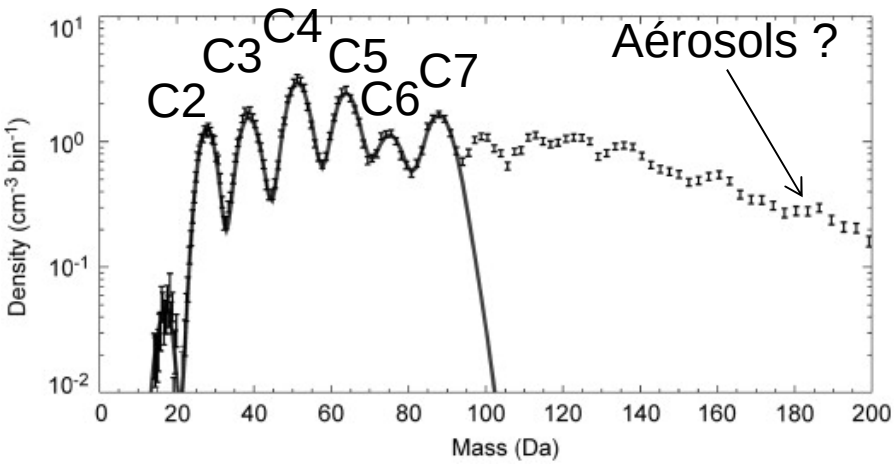
# Haute atmosphère et aérosols



La haute atmosphère de Titan :
une complexité inattendue, qui a pris
tous les modèles chimiques de court




Spectre de masse des ions positifs
in situ: instrument CAPS-IBS-Cassini
( Waite et al. 2007)

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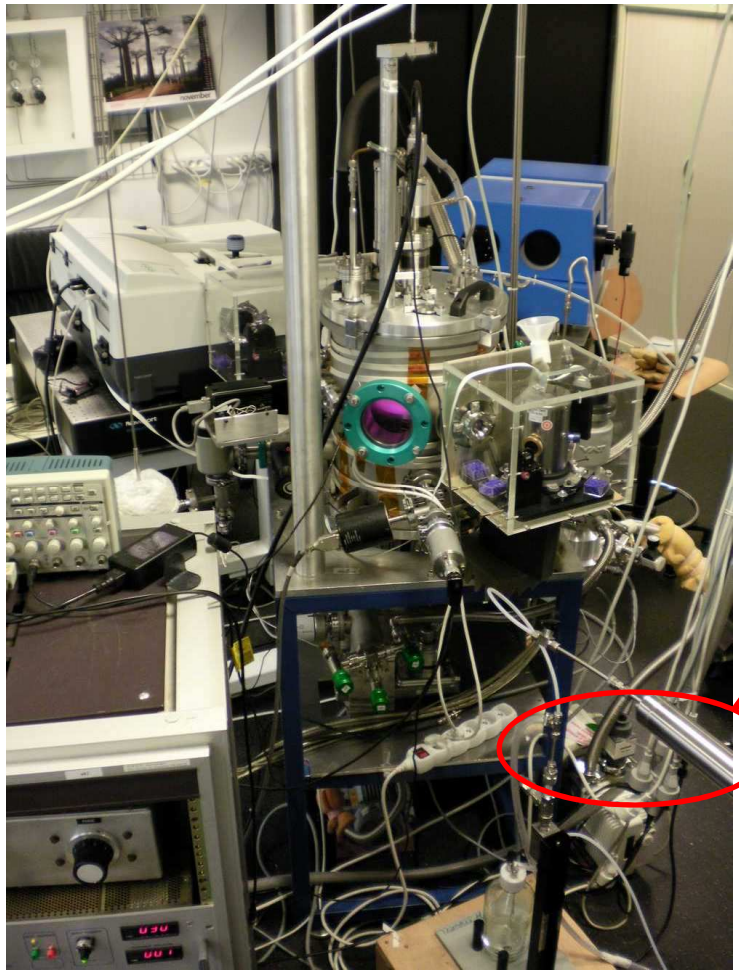
# L‘expérience plasma : PAMPRE



- Décharge plasma RF
  - Plasma « froid »: neutres à température ambiante
  - Plasma « poudreux »: Optimal pour la production d’aérosols
- SMARD: coll. LISA-LATMOS
  - Analyse chimique et granulométrique in-situ

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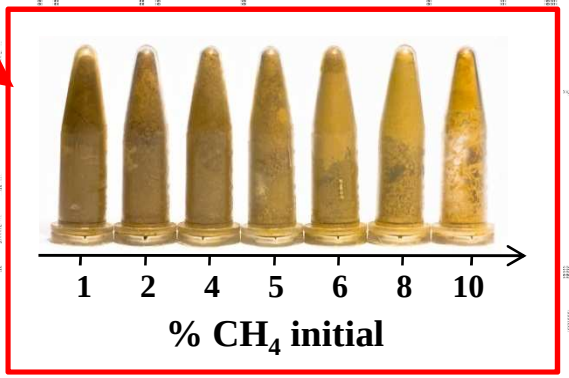
# Collecte des aérosols




**Particules solides (THOLINS) :**

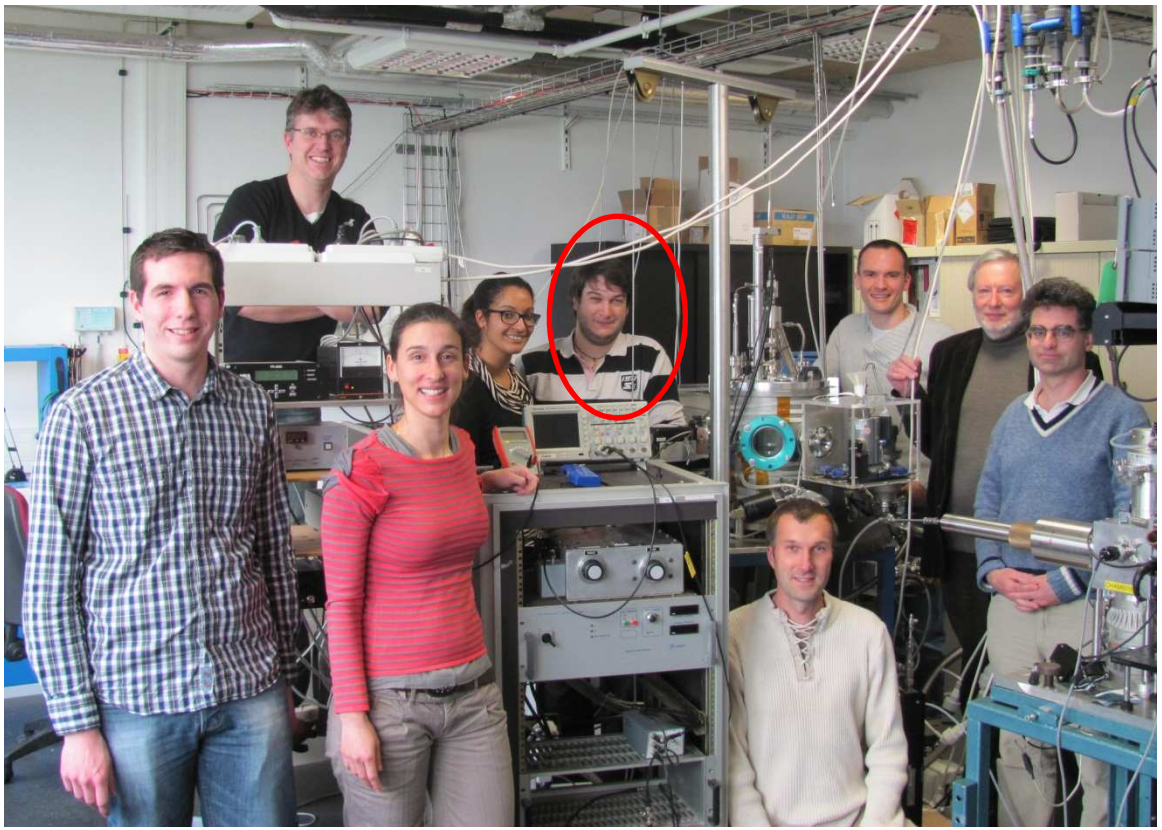
- **production pendant plusieurs heures**
- **déposition dans un cristallisoir**
- **collecte pour analyses *ex situ***

# Analyse des tholins : thèse 2010-2013

Cyril Szopa

Sarah Tigrine

Thomas Gautier



Ludovic Vettier

Guy Cernogora

Jean-Jacques Correia

Benjamin Fleury

Nathalie Carrasco

Pierre Gilbert

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# Propriétés optiques des tholins

- Analysis at SOLEIL Synchrotron facility (France, SMIS Beamline)
- 4000 - 100 $cm^{-1}$ (2.5 - 100 µm)
- Measurements in Absorbance

=> need of offset and/or normalization => Lose information

- Measurement of sample thickness to access the linear absorption coefficient

Beer-Lambert Law:

$$I = I_0 \times \exp(-\sigma \times [n] \times 2d)$$

$$I = I_0 \times \exp(-\varepsilon \times 2d)$$

=> If d is known => ε determination

σ: absorption cross section ($cm^2$)

[n]: absorber density ($cm^{-3}$)

d: pass length (cm)

ε: linear absoprtion coefficient ($cm^{-1}$)

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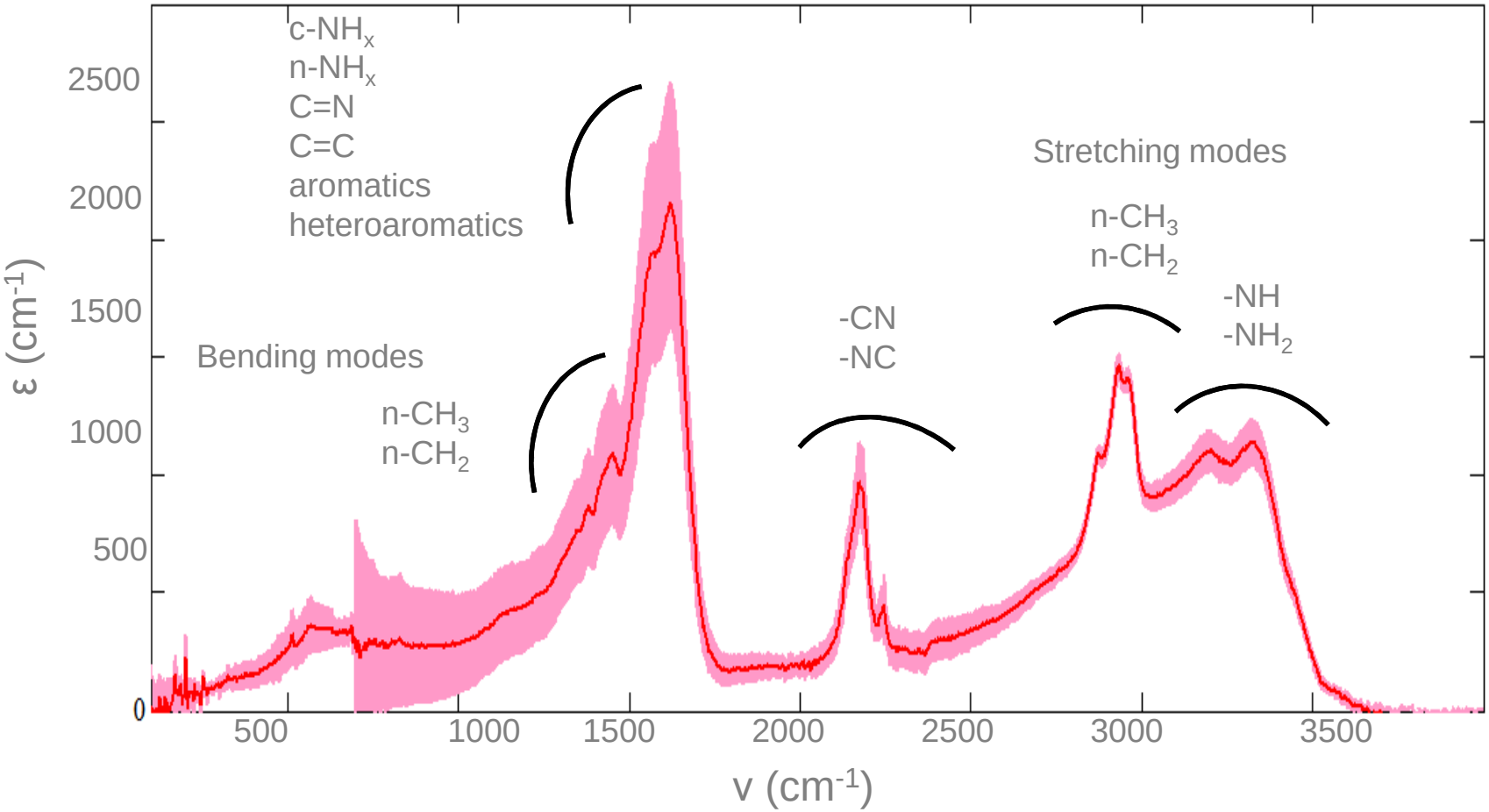
# Spectre infrarouge de tholins du MIR au FIR




Tholins linear absorption coefficient as a function of wavenumber
Pink envelopes provide 2 σ uncertainties

Gautier et al. **(**2012**)** Icarus 221, 320-327.

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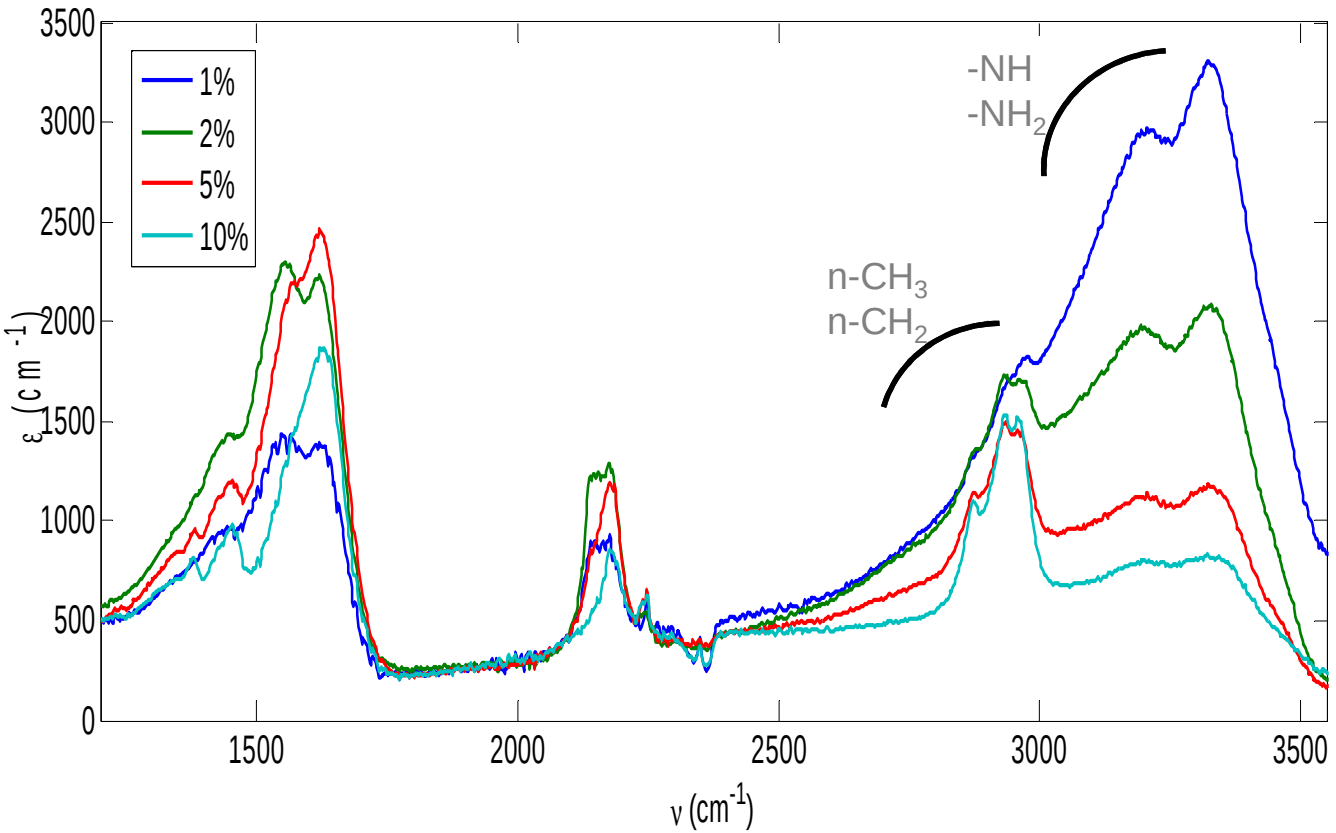
# Influence du méthane sur les bandes amines




Comparison of tholins spectra according to methane percentage in the gas mixture

- Amine decreases when methane increases
- CN and pattern @1600 $cm^{-1}$ maximum for intermediate $\%CH_4$
- Aliphatic structures more visible at high $\%CH_4$
- Might have played a rule during Titan history

Gautier et al. **(**2012**)** Icarus 221, 320-327.

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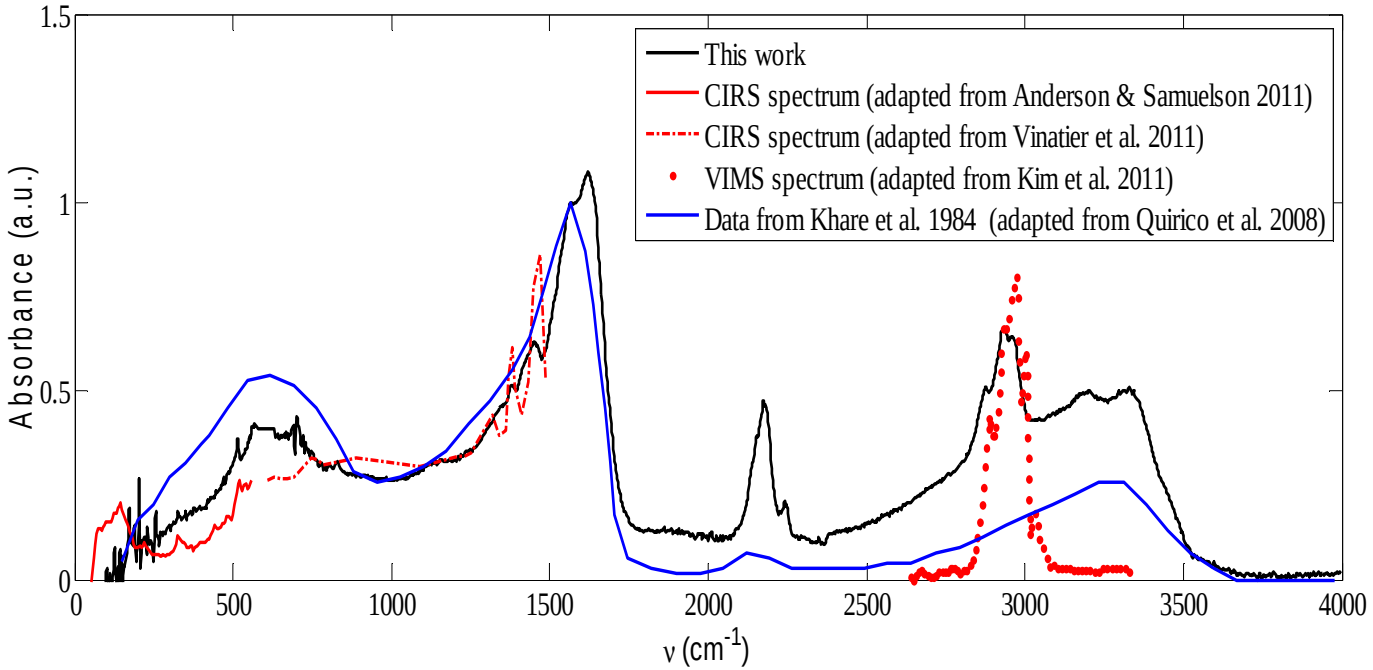
# Comparison aux observations Cassini

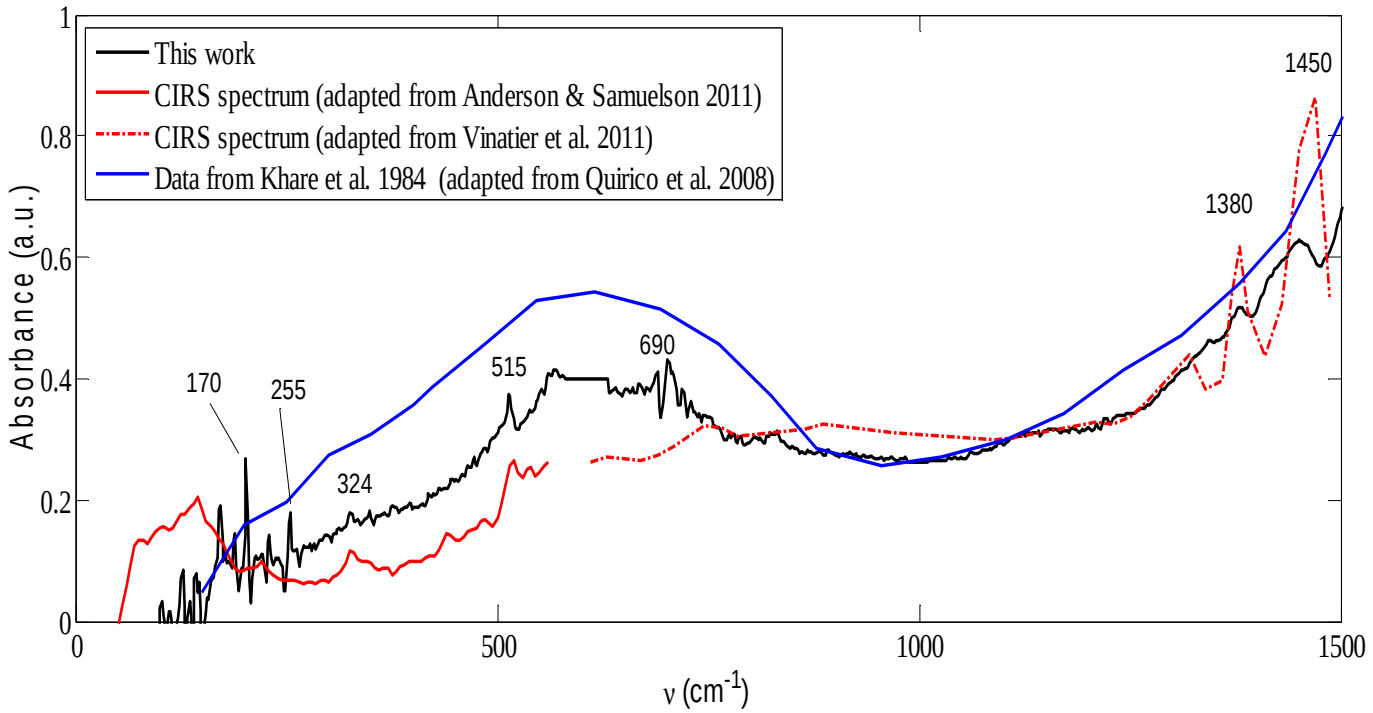



Comparison of PAMPRE tholins (5%) spectra with Cassini

- CIRS (100 – 1500 $cm^{-1}$) (*Vinatier et al. 2011, Anderson et al. 2011*)
- VIMS (2700-3300 $cm^{-1}$) *(Belluci et al. 2009, Rannou et al. 2010)*
- Global agreement in patterns position

Gautier et al. **(**2012**)** Icarus 221, 320-327.

# Comparison aux données CIRS

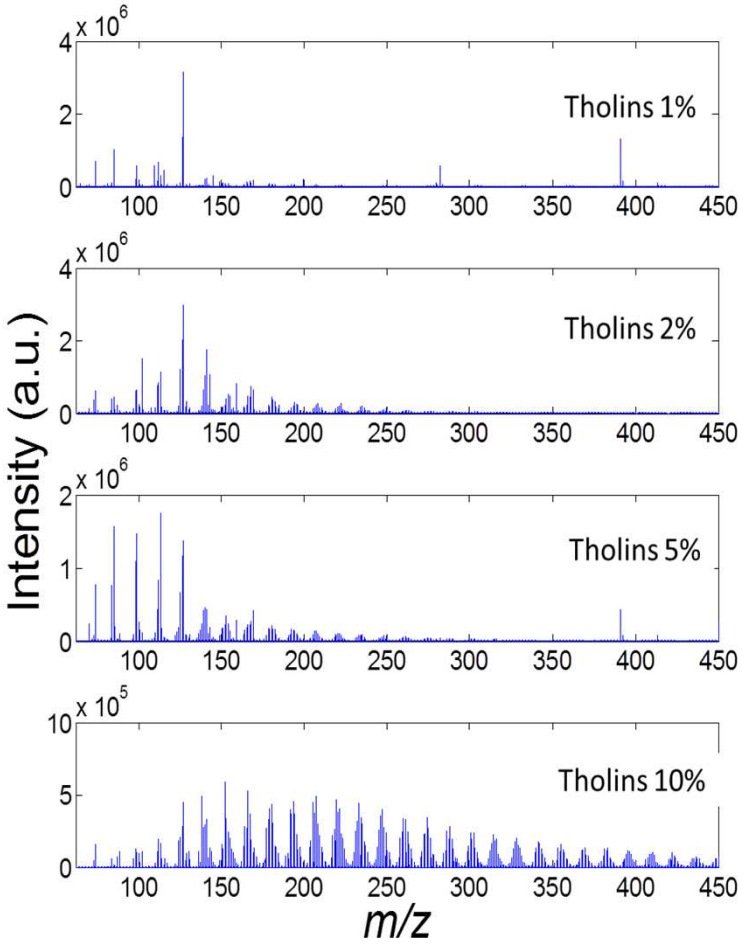



Close up from 0 – 1500 $cm^{-1}$ region

- 1450 – 1380 $cm^{-1}$ bands (aliphatic carbons)
- Confirmed some weak bands suspected in the Far-IR:
  - 515 $cm^{-1}$
  - 324 $cm^{-1}$

Gautier et al. **(**2012**)** Icarus 221, 320-327.

# Analyse chimique des tholins




Tholins orbitrap mass spectra

At 'macro scale':

- 2 structures:
  - *m/z*<150: isolated intense peaks
  - m/z > 150: regularly spaced clusters
- First structure predominant at low %$CH_4$, second at high % $CH_4$
- Co-polymeric shape of the mass spectrum

Gautier et al. (2013) *Nitrogen incorporation in Titan's tholins inferred from statistical approach on high resolution orbitrap mass spectrometry,* to be submitted in Geochimica et Cosmochimica Acta

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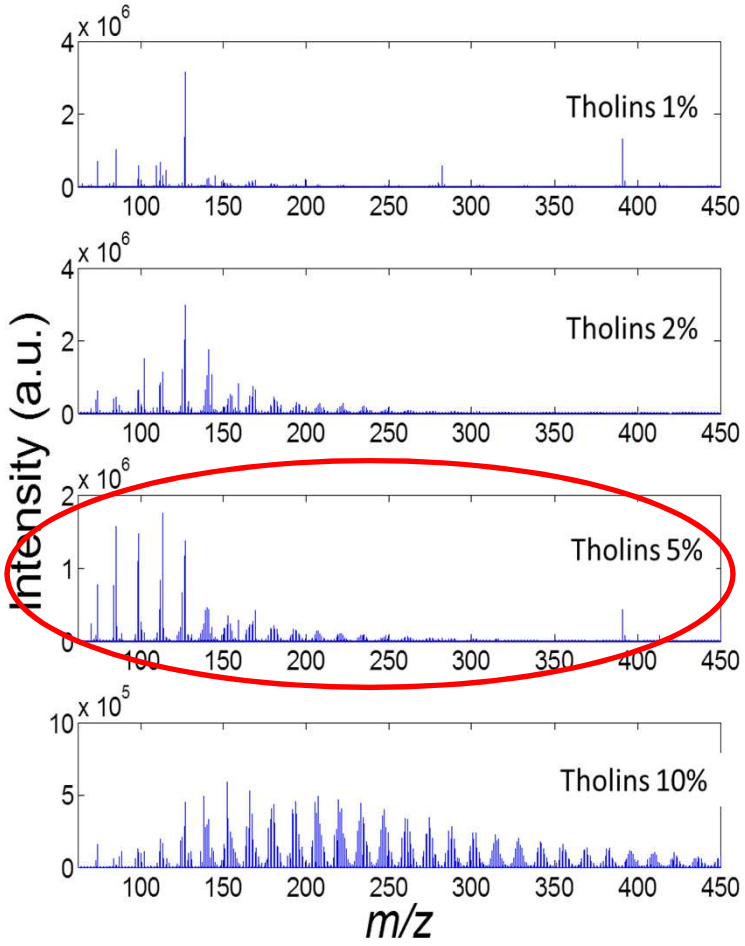
# Analyse chimique des tholins




Close up of Tholins orbitrap mass spectrum around *m/z* 127

At ‘micro scale’:

- All peaks are detected in all samples

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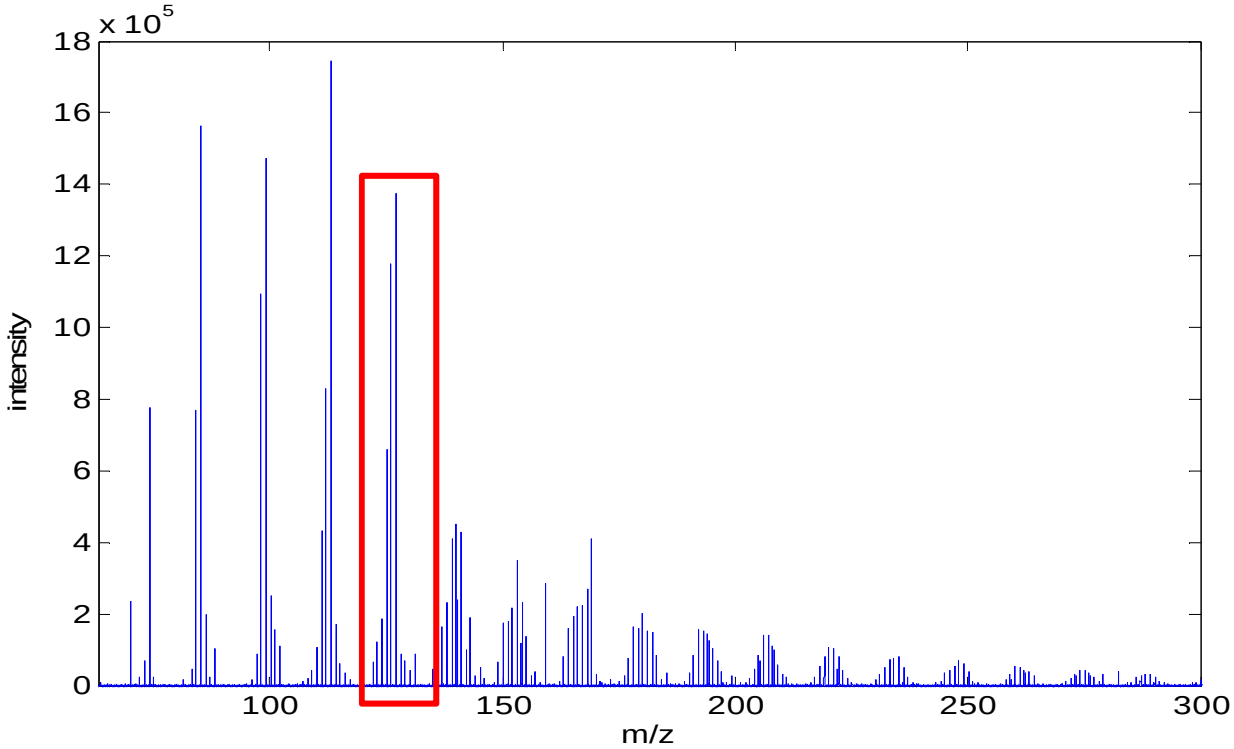
# Analyse chimique des tholins

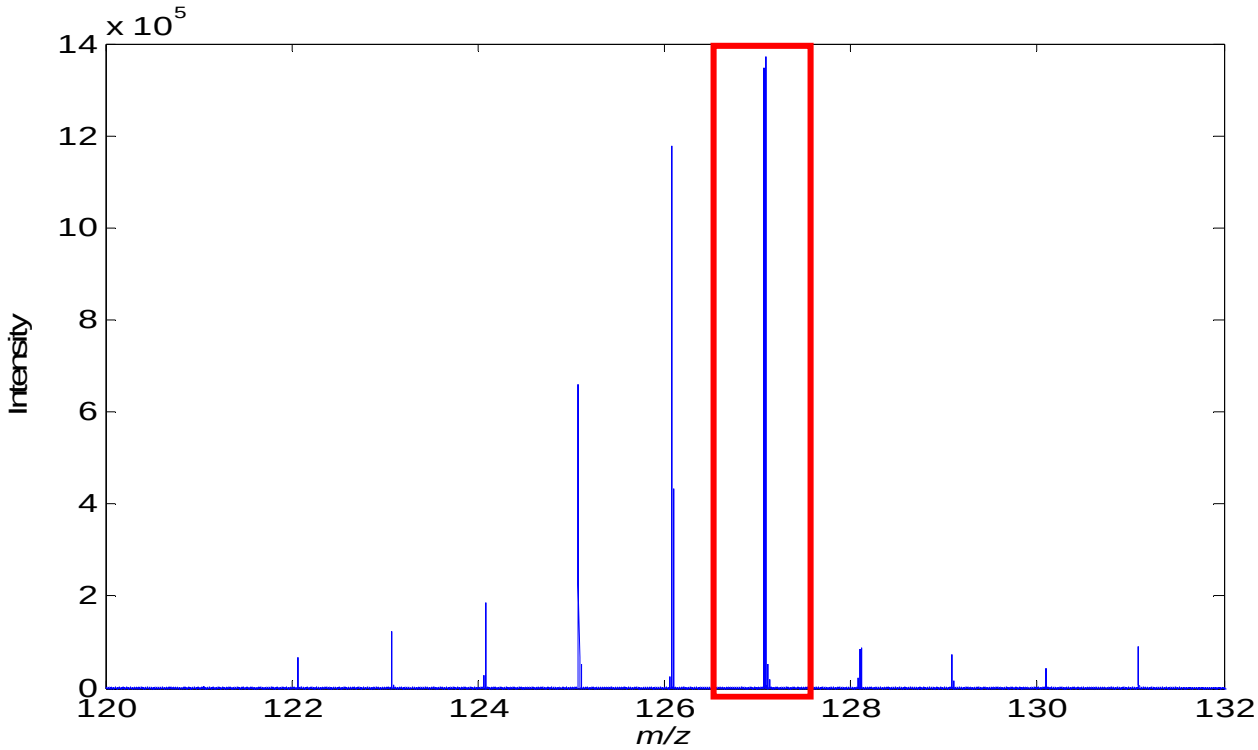



- Access to the formula of the compounds detected
- ~15.000 species detected from *m/z* 60

Haute résolution en masse : Orbitrap

Pernot, Carrasco et al. **(**2010**)** Anal Chem, 82(4), pp 1371–1380
Gautier, Carrasco et al. (2013), en préparation.

# Analyse chimique des tholins

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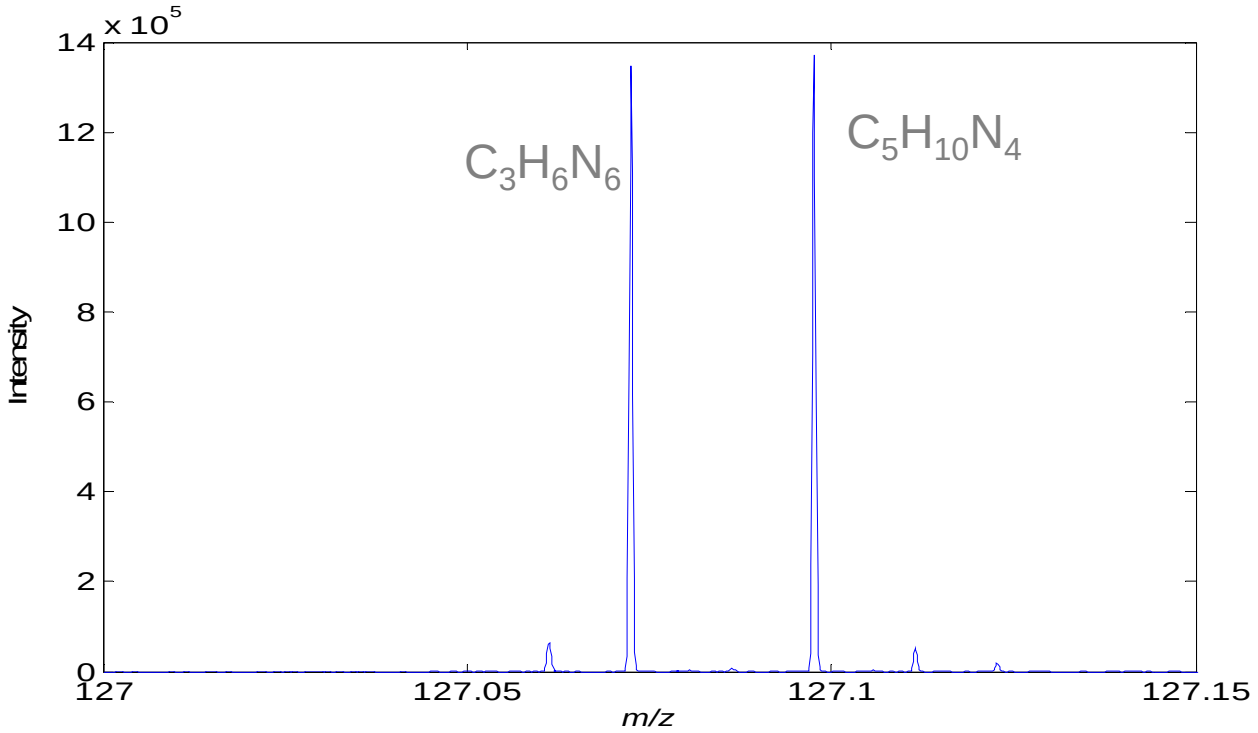


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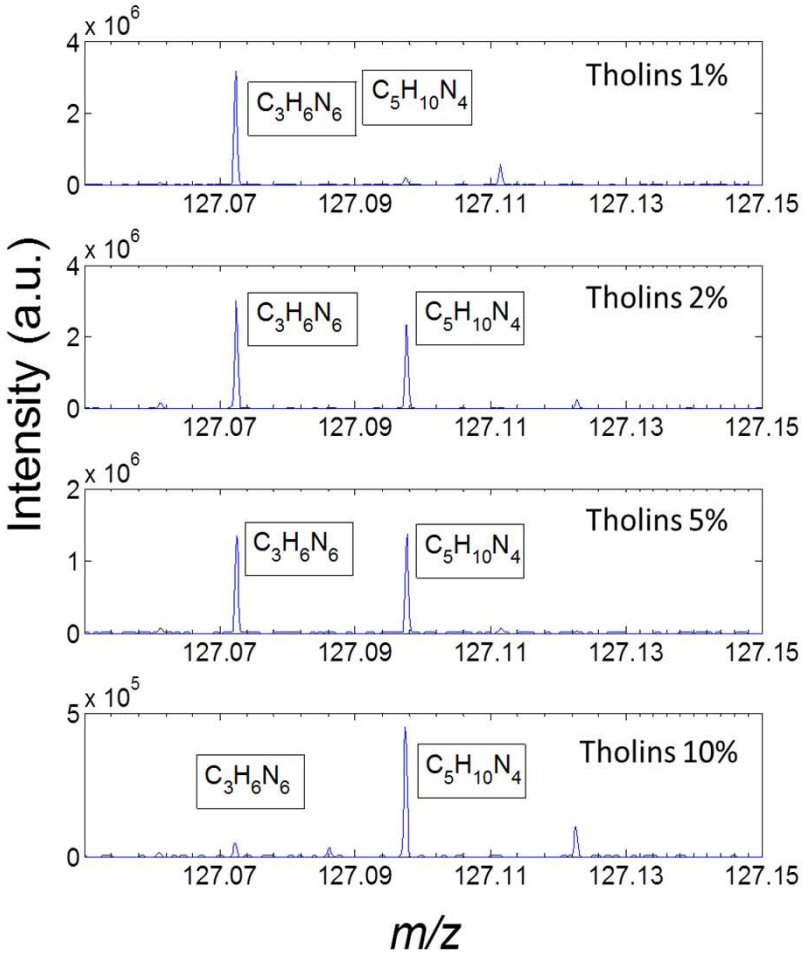


Close up of Tholins orbitrap mass spectrum around *m/z* 127

At 'micro scale':

- All peaks are detected in all samples
- Predominance of highly nitrogeneous molecules at low %$CH_4$ , the opposite at high %$CH_4$
- Progressive transition between the two regimes (high N and high C contents)
- Effect observed in all clusters of the spectrum!

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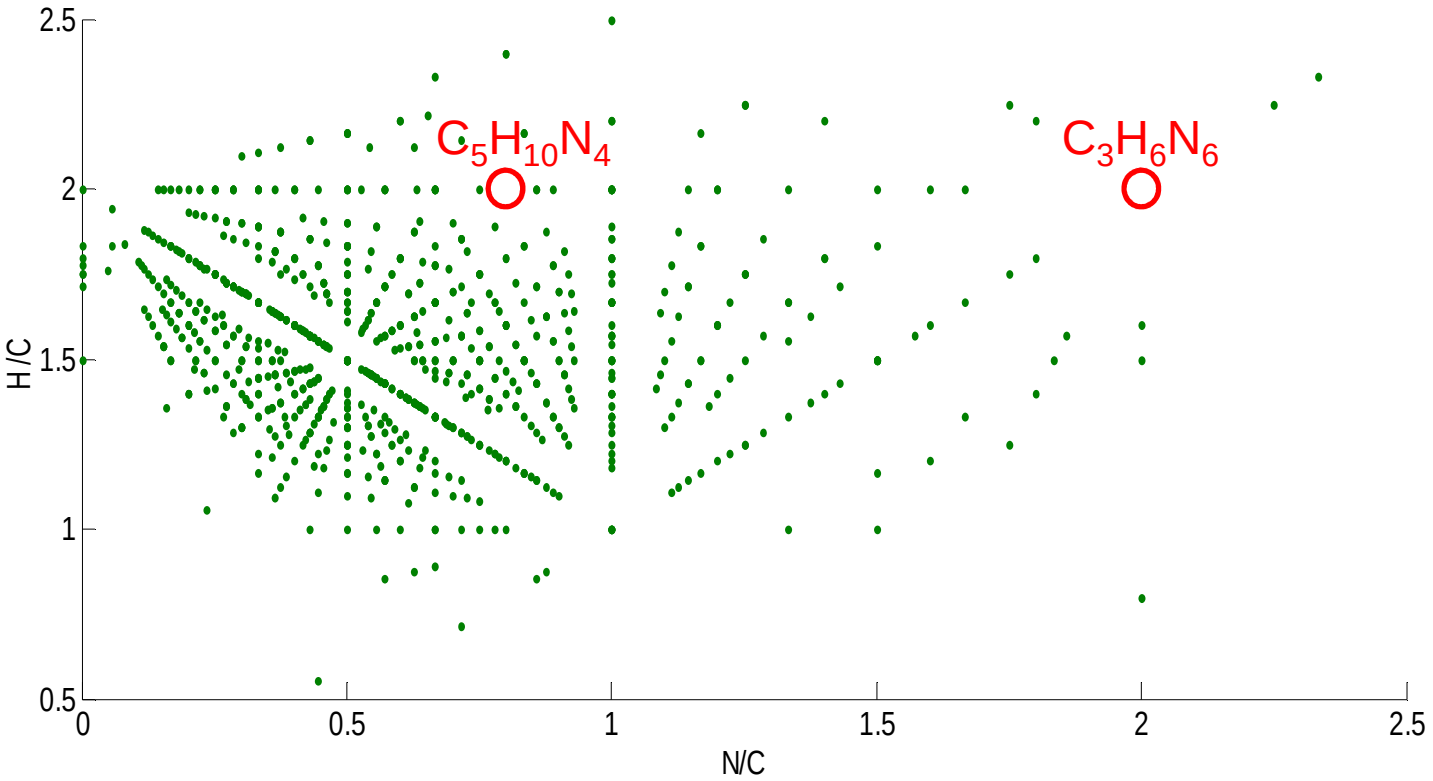
# Diagrammes de Van Krevelen

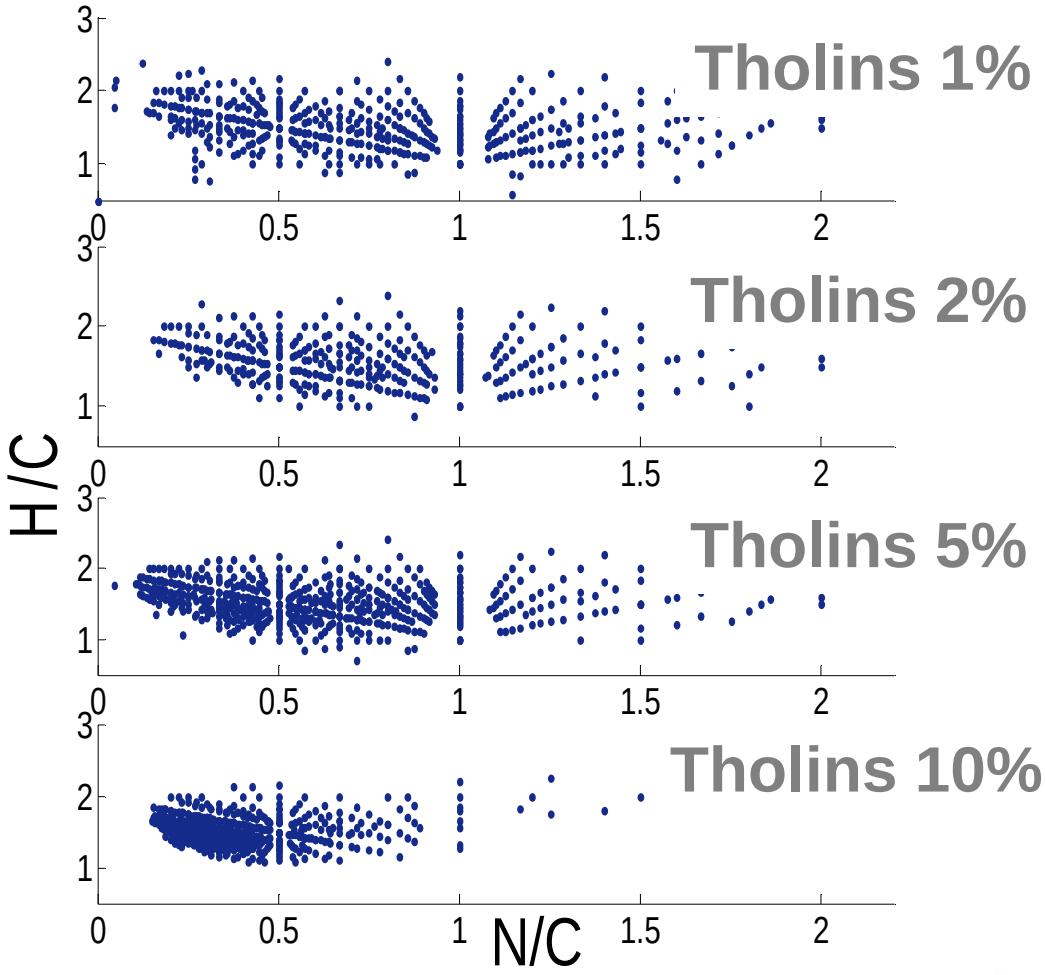
- Each molecule is displaced on the diagram following its H/C and N/C ratio




Gautier et al. (2013) *Nitrogen incorporation in Titan's tholins inferred from statistical approach on high resolution orbitrap mass spectrometry,* to be submitted in Geochimica et Cosmochimica Acta

# Diagrammes de Van Krevelen

- Each molecule is displaced on the diagram following its H/C and N/C ratio
- Depletion of the 'right wing' at high %$CH_4$
- Several polymer families visible

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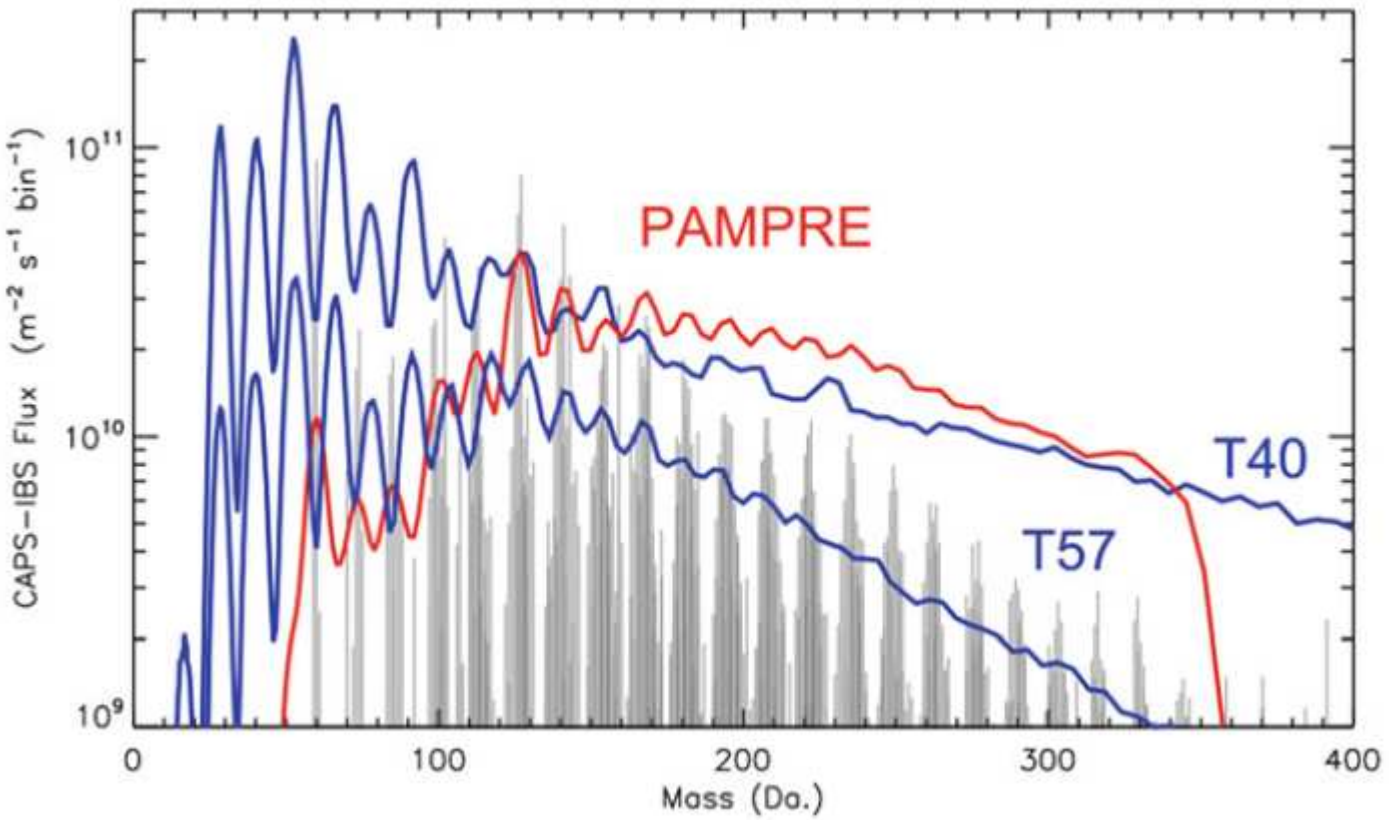
# Comparaison aux données CAPS-IBS




Carrasco et al. **(**2013**)** Chapter 11 in " The Early Evolution of the Atmospheres of Terrestrial Planets ".
Ed. C. Muller, C. A. Nixon, F. Raulin, and J. M. Trigo.,
Springer Astrophysics and Space Science Proceedings, 35:145-154.

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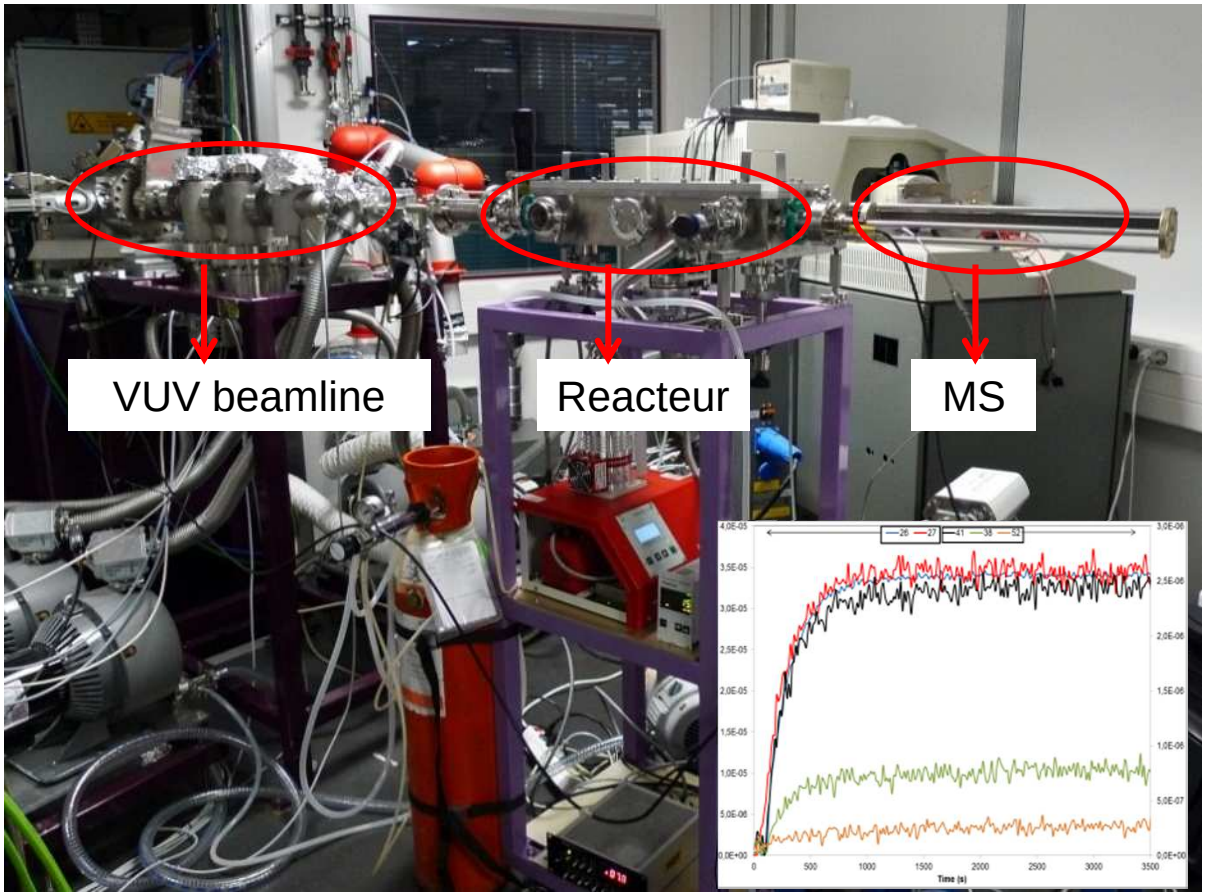
# Nouveau réacteur photochimique: APSIS

- Collaboration LATMOS / LISA / LGPM / LCP / Soleil




- Expérience de photolyse atmosphérique VUV sur synchrotron SOLEIL
- Exobiologie CNES, 2010
- Validité :
  Détection de produits organiques azotés

Peng et al. (2013) JGR Planets, 118 (4), 778-788

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