Tracing the Gas Composition of Titan's Atmosphere with Herschel: Advances and Discoveries

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Morvan D., Banaszkiewicz M., González A.

The Universe explored by Herschel—Noordwijk, 15-18 October 2013
Telescope lens used by Huygens in 1655
Utrecht University Museum
1. Introduction

Titan is covered by a dense atmosphere, which is complex and diverse!

- The origin of Titan’s atmosphere is poorly understood and its chemistry is complicated.

Coustenis et al. (2003)
Nitrogen (N$_2$) | Methane (CH$_4$)

Nitriles e.g.

Hydrogen cyanide (HCN)

Ethane (C$_2$H$_6$)

Benzene (C$_6$H$_6$)

How large and how complex?

More complex molecules
1. Introduction

Sensitive observations of the constituents of the atmosphere are essential to constructing models of the Titans’s atmosphere and its history.

The Universe explored by Herschel– Noordwijk, 15-18 October 2013
1. Introduction

Spectroscopy of Titan has been already performed by:

- Voyager 1 – 2/IRIS
- ISO/SWS
- Cassini/CIRS
- Hanel et al., Science, v 215, 1982
- Cottini et al., 2012
- Coustenis et al. (1998)
- Coustenis et al. (2003)
- Coustenis et al. (2007)
- Nixon et al., 2013

\[ H_2O \]
\[ C_3H_6 \]
Ground-based observations have also improved our knowledge of Titan’s atmospheric composition:

- **IRAM 30-m:**
  - Hidayat et al. 1998
  - Marten et al. 2002

- **SMA:**
  - Gurwell et al. 2004

- **APEX:**
  - Rengele et al. 2011

- **JCMT:**
  - Hidayat et al. 1998
**Herschel Era**

**Instruments onboard Herschel:**

**Heterodyne Instrument for the Far-Infrared (HIFI).**

*PI: F. Helmich, SRON*

Resolutions: 140, 280, 560 kHz, 1.1 MHz

<table>
<thead>
<tr>
<th>SIS Technology</th>
<th>HEB Technology</th>
</tr>
</thead>
<tbody>
<tr>
<td>THz: 0.48, 0.64, 0.80, 0.96, 1.12, 1.27</td>
<td>1.41, 1.91</td>
</tr>
</tbody>
</table>

**HIFI Bands**

- Band 1: 480 – 1150 GHz
- Band 2: 1410-1910 GHz

3 bands in total:

- 55-72 μm
- 72-102 μm
- 102-210 μm

**Photodetector Array Camera and Spectrometer (PACS).**

*PI: A. Poglitsch, MPE*

- 55 – 210 μm

**Spectral and Photometric Imaging Receiver (SPIRE).**

*PI: M. Griffin, Cardiff University*

- Photometer: 250, 350, 500 μm
- Spectrometer: 194- 672 μm
Titan’s Spectroscopy in the Herschel Era

- **Herschel/PACS**: SR = 0.04 cm\(^{-1}\), R = 940-5500
- **Herschel/HIFI**: SR = 4.3 cm\(^{-1}\), R = 1000 - 2500
- **Voyager/IRIS**: SR = 0.5 cm\(^{-1}\), R = 200
- **ISO/SWS**: SR = 0.04 cm\(^{-1}\), R ~ 10\(^{-7}\)
- **ISO/LSW**: SR = 0.04 cm\(^{-1}\), R ~ 10\(^{-7}\)
- **Cassini/CIRS**: SR = 0.04 cm\(^{-1}\), R ~ 10\(^{-7}\)

- **Herschel/SPIRE**: SR = 0.04 cm\(^{-1}\), R = 940-5500

In the framework of the KP “Water and related chemistry in the Solar System” (HssO)

**HssO contributions at this conference**:

- Talks by Hartogh, Lellouch, Rengel
- Posters: Biver, Bockele-Morvan, Calvié, de Val-Borro, Hartogh, Szutowicz

**HssO web site**: [http://www.mps.mpg.de/projects/herschel/HssO/index.htm](http://www.mps.mpg.de/projects/herschel/HssO/index.htm)

• 55 – 671 µm is a rich region with numerous rotational transitions of water and other trace gases
• These line transitions are stronger than those accessible from Earth
• HIFI/PACS/SPIRE higher spectral resolution and sensitivity than previous instruments

Submm range with high sensitivity
Titan’s Observations performed with Herschel

**SPIRE:** Full range spectrum (194 - 671 µm or 15-50 cm$^{-1}$) – July 2010, ~8.9h, SR= 0.04 cm$^{-1}$

**PACS:** Full range spectra (51-220 µm or 50-180 cm$^{-1}$) (twice, 0.63h and 1.1h), R= 1000-5000

Dedicated line scans H$_2$O lines (at 108, 75.4 and 66.4 µm in June 2010, Dec 2010 and July 2011) and CH$_4$. SR= 0.02, 0.04 and 1.11 µm. ~0.3h

**HIFI** spectrally-resolved observation of H$_2$O at 557 GHz (18 cm$^{-1}$ or 538 µm) and at 1097.4 GHz (273 µm) in June 2010, Dec 2010 and June 2011, ~4h each time. SR ~10$^6$

- All Titan observations are disk-averaged and have to be performed near maximum elongation

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Modeling the Titan spectra
Method

\[ \mu_1, \mu_2, \mu_3 \]

\( \mu_i \) = absorption coefficient

T profile
P profile
Vmr profile

Input parameters → Abundance profiles → Radiative Transfer

Comparison with data
Synthetic Spectra

Synthetic spectra
Fitting algorithm: \( \chi^2 \) statistics

New set of parameters

The Universe explored by Herschel–Noordwijk, 15-18 October 2013
The abundance, vertical distribution and origin of H$_2$O in Titan's stratosphere: Observations and photochemical modelling

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\textsuperscript{d} Instituto de Astrofísica de Canarias, La Laguna, Tenerife, 38200, Spain

\textbf{LETTER TO THE EDITOR}

\textbf{Advances and Discoveries}

\textbf{First detection of hydrogen isocyanide (HNC)}

R. Moreno\textsuperscript{1}, E. Lellouch\textsuperscript{1}, L. M. Lara\textsuperscript{2}, R. Courtois\textsuperscript{1}, M. Renger\textsuperscript{3}, N. Biver\textsuperscript{1}, M. R.-R.

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\textsuperscript{3} Max-Planck-Institut für Kernphysik, Universität Heidelberg, 69117 Heidelberg, Germany

\textbf{LETTER TO THE EDITOR}

\textbf{First results of Herschel-SPIRE observations of Titan}\textsuperscript{a}

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\textsuperscript{4} Institute for Astronomy, University of Edinburgh, Royal Observatory, Blackford Hill, Edinburgh, EH9 3HJ, UK

\textbf{LETTER TO THE EDITOR}

\textbf{Herschel/PACS spectroscopy of trace gases of the stratosphere}

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\textbf{LETTER TO THE EDITOR}
1.- Molecular Inventory with Herschel /PACS, SPIRE, and HIFI
Numerous spectral emission features due to:

CH$_4$, CO, HCN, H$_2$O

Rengel et al. 2013, submitted

The Universe explored by Herschel–Noordwijk, 15-18 October 2013
1.- Molecular Inventory with Herschel /PACS, SPIRE, and HIFI

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H$_2$O

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Courtin et al. 2011
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Numerous spectral emission features due to:

- CH₄
- CO
- HCN
- H₂O

Rengel et al. 2013, submitted
Courtin et al. 2012
1. Molecular Inventory with Herschel/PACS, SPIRE, and HIFI

Spectral emission features due to:

- CH$_4$
- CO
- HCN
- H$_2$O

Five dedicated Water vapour line emission with Herschel/PACS and HIFI. Goal: vertical profile of H$_2$O

Moreno et al. 2012

Several H$_2$O far-IR lines detected for the first time in Titan’s atmosphere,
1. Molecular Inventory with Herschel /PACS, SPIRE, and HIFI

Spectral emission features due to:

H₂O

\[ \text{Surprise: Unexpected detection of hydrogen isocyanide (HNC) \rightarrow a specie not previously identified in Titan's atmosphere} \]
2.- Determination of the abundance of the trace constituents:

Step 1: Computation of the synthetic spectra for several abundances
Step 2: Calculation of the best-fit

**CH$_4$:** Origin unknown

Observed and best-fit simulated CH$_4$ lines

Consistent with previous studies:

<table>
<thead>
<tr>
<th>Facility</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>CIRS</td>
<td>1.6±0.5%</td>
<td>Flasar et al. 2005</td>
</tr>
<tr>
<td>GCMS</td>
<td>1.48±0.09%</td>
<td>Niemann et al. 2010</td>
</tr>
<tr>
<td>SPIRE</td>
<td>1.33 ±0.07%</td>
<td>Courtin et al. 2011</td>
</tr>
<tr>
<td>PACS</td>
<td>1.27 ±0.03</td>
<td>Rengel et al. submitted</td>
</tr>
</tbody>
</table>
**CO:** is CO primordial or external? Viable via precipitation of O or O\(^+\) from Enceladus Torus (Hörst et al. 2008; Cassidy & Johnson 2010; Hartogh et al. 2011)

### Observed and best-fit simulated CO lines

For the [60-170] km range altitude

<table>
<thead>
<tr>
<th>Facility</th>
<th>Value [ppm]</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>SPIRE</td>
<td>40±5</td>
<td>Courtin et al. 2011</td>
</tr>
<tr>
<td>CIRS</td>
<td>47±8</td>
<td>De Kok et al 2007</td>
</tr>
<tr>
<td>APEX</td>
<td>30(^{+15}_{-8})</td>
<td>Rengel et al. 2011</td>
</tr>
<tr>
<td>SMA</td>
<td>51±4</td>
<td>Gurwell et al. 2012</td>
</tr>
<tr>
<td>PACS</td>
<td>49±2</td>
<td>Rengel et al. submitted</td>
</tr>
</tbody>
</table>
HCN vertical distribution

- We scaled the distribution from the one by Marten et al 2002, computed the synthetic spectra for several factors, and calculated best-fit distribution of HCN, compared with the profile by CIRS.

Our results confirm the results from Marten et al. 2002.

The CIRS distribution misfits the PACS observations at 1-σ level.

Rengel et al. 2013, submitted
None of the previous water models provides an adequate simultaneous match to the PACS and HIFI observations

→ Photochemical models for water must be revised
3.- Determination of the abundance of the trace constituents: Water vertical distribution

Pressure dependence law as \( q = q_0 (p_0/p)^n \)

- \( q_0 \) is the mixing ratio at the reference pressure level \( p_0 \)

- \( S_a \):
  - \( q_0 = 2.3 \times 10^{-11} \) at \( p_0 = 12.1 \) mbar
  - \( n = 0.49 \)
  - Column density: \( 1.2 (\pm 0.2) \times 10^{14} \) cm\(^{-2}\).
Water Vapour in Titan

PACS – HIFI / Herschel

Moreno et al. 2012

Observed and synthetic spectra

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**H₂O.** Viable via Enceladus plume activity (Hartogh et al. 2011; Moreno et al. 2012).

The Sa distribution is also compatible with the PACS lines from the full scan: computations of the synthetic spectra with Sa (Moreno et al. 2012).

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**Water Vapour in Titan**

PACS / Herschel

Detection for first time

Rengel et al. 2013, submitted
3.- Determination of the abundance of the trace constituents: HNC

First detection of HNC in the Titan’s atmosphere

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HNC distribution: the bulk of HNC is located above 400 km

Models of the HCN line: constant mixing ratio above a given altitude

Origin: reactions

Possible chemical lifetime:

Is HNC restricted to the ionosphere?

Moreno et al. 2011
4.- Isotopic ratios $^{12}\text{C}/^{13}\text{C}$ in CO and HCN

Detection of the isotopes:
- $^{13}\text{CO}(15-14)$ and $(16-15)$
- $^{13}\text{HCN}$ (19-19) and (20-19) but marginal

**Results:**
- $^{12}\text{C}/^{13}\text{C}$ in CO: $122 \pm 62$ vs $87 \pm 6$
- $^{12}\text{C}/^{13}\text{C}$ in HCN: $65 \pm 30$ vs $96 \pm 13$

Consistent with previous works

Detection of the isotopes:
- $^{13}\text{CO}(15-14)$ and $(16-15)$
- $^{13}\text{HCN}$ (19-19) and (20-19)

**Isotopes in Titan**

PACS – SPIRE / Herschel

Observations Best-fit

Courtin et al. 2011

Rengel et al. 2013, submitted
The $^{12}\text{C}/^{13}\text{C}$ isotopic ratio in Titan

Terrestrial value: 89.3

Rengel et al. 2013

The Universe explored by Herschel–Noordwijk, 15-18 October 2013
4. Isotopic ratios $^{14}\text{N}/^{15}\text{N}$ in HCN and $^{16}\text{O}/^{18}\text{O}$ in CO

<table>
<thead>
<tr>
<th>Measurement</th>
<th>$^{14}\text{N}/^{15}\text{N}$</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>IRAM-30m</td>
<td>60-70</td>
<td>Marten et al. 2002</td>
</tr>
<tr>
<td>SMA</td>
<td>$72 \pm 9$ or $94 \pm 13$</td>
<td>Gurwell 2004</td>
</tr>
<tr>
<td>Cassini/CIRS</td>
<td>56 ± 8</td>
<td>Vinatier et al. 2007</td>
</tr>
<tr>
<td>Huygens/GCMS (in N$_2$)</td>
<td>183 ± 5</td>
<td>Niemann et al. 2010</td>
</tr>
<tr>
<td>Herschel/SPIRE</td>
<td>76 ± 6</td>
<td>Courtin et al. 2012</td>
</tr>
</tbody>
</table>

Photolytic fractionation of $^{14}\text{N}^{14}\text{N}$ and $^{14}\text{N}^{15}\text{N}$

<table>
<thead>
<tr>
<th>Measurement</th>
<th>$^{16}\text{O}/^{18}\text{O}$</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>JCMT</td>
<td>$\sim 250$</td>
<td>Owen et al. 1999 (never-published)</td>
</tr>
<tr>
<td>SMA</td>
<td>400 ± 41</td>
<td>Gurwell 2008 (unpublished)</td>
</tr>
<tr>
<td>Herschel/SPIRE</td>
<td>380 ± 60</td>
<td>Courtin et al. 2012</td>
</tr>
</tbody>
</table>

First documented measurement of Titan’s $^{16}\text{O}/^{18}\text{O}$ in CO, value 24% lower than the Terrestrial ratio ($\text{Earth} = 500$) $\Rightarrow$ $^{16}\text{O}/^{18}\text{O}$ depletion in Titan

Precipitation of O$^+$ or O from the Enceladus Torus
Cassini/CIRS

- New Survey between 51 and 671 µm: CH$_4$, CO, HCN, H$_2$O, isotopes
- Determination of abundances
- Unexpected detection of HNC and measurement of $^{16}$O/$^{18}$O ratio

ISO/SWS

PACS

SPIRE

HIFI

Herschel’s Legacy
Herschel’s Legacy

Emerged Implications:

Herschel studies point to

• A denser primitive Titan’s atmosphere: much of the Titan’s atmosphere has been lost over geologic time ($^{14}\text{N}/^{15}\text{N}$)

• $^{18}\text{O}$ enrichment in Titan’s atmosphere: Precipitation of $\text{O}^+$ or $\text{O}$ from the Enceladus plume activity ($^{16}\text{O}/^{18}\text{O}$)

• The content of water vapour in Titan is different as the predictions → Models require a revision

• Above 400 km, Titan’s atmosphere also contains HNC
Future – Synergy with Herschel

- CASSINI/CIRS (extended mission), until 2017. 56 more flybys of Titan.
Future – Synergy with Herschel

- **ALMA:**
  - Titan’s atmospheric chemistry/dynamics

- Search for more complex species
- 3D-mapping and monitoring: seasonal variations
  - Dynamics/photochemistry coupling
  - Direct measurement of mesospheric (500 km) winds
  - Isotopic ratios

SMA 850 micron unresolved observations

Gurwell 2004
Acknowledgments

- HIFI has been designed and built by a consortium of institutes and university departments from across Europe, Canada and the United States under the leadership of SRON Netherlands Institute for Space Research, Groningen, The Netherlands and with major contributions from Germany, France and the US. Consortium members are: Canada: CSA, U.Waterloo; France: CESR, LAB, LERMA, IRAM; Germany: KOSMA, MPIfR, MPS; Ireland, NUI Maynooth; Italy: ASI, IFSI-INAF, Osservatorio Astrofisico di Arcetri-INAF; Netherlands: SRON, TUD; Poland: CAMK, CBK; Spain: Observatorio Astronómico Nacional (IGN), Centro de Astrobiología (CSIC-INTA). Sweden: Chalmers University of Technology - MC2, RSS & GARD; Onsala Space Observatory; Swedish National Space Board, Stockholm University - Stockholm Observatory; Switzerland: ETH Zurich, FHNW; USA: Caltech, JPL, NHSC.

- PACS has been developed by a consortium of institutes led by MPE (Germany) and including UVIE (Austria); KUL, CSL, IMEC (Belgium); CEA, OAMP (France); MPIA (Germany); IFSI, OAP/AOT, OAA/CAISMI, LENS, SISSA (Italy); IAC (Spain). This development has been supported by the funding agencies BMVIT (Austria), ESA-PRODEX (Belgium), CEA/CNES (France), DLR (Germany), ASI (Italy), and CICT/MCT (Spain). Additional funding support for some instrument activities has been provided by ESA.