



2017 ESO Calibration Workshop:

The second generation VLT
instruments and friends



Molecular Line Parameters & VAMDC

an atmospheric/laboratory physicist point of view

C. Janssen

LERMA, Paris, France

LERMA - Laboratoire d'Etudes du Rayonnement et de la Matière en Astrophysique on the campus JUSSIEU



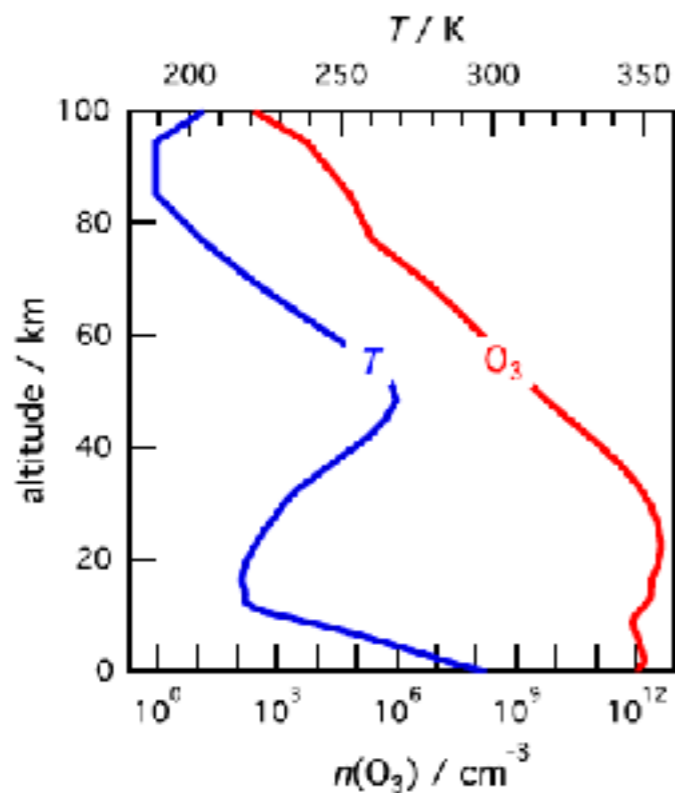
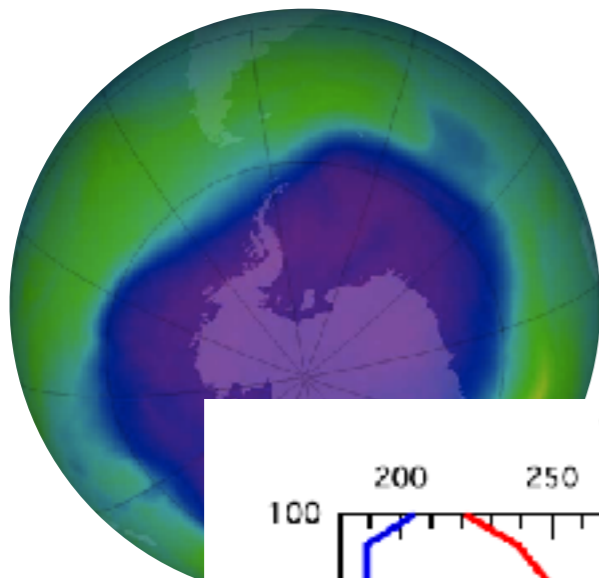
The SMILE group

*Spectroscopie Moléculaire et Instrumentation Laser
pour l'Environnement*

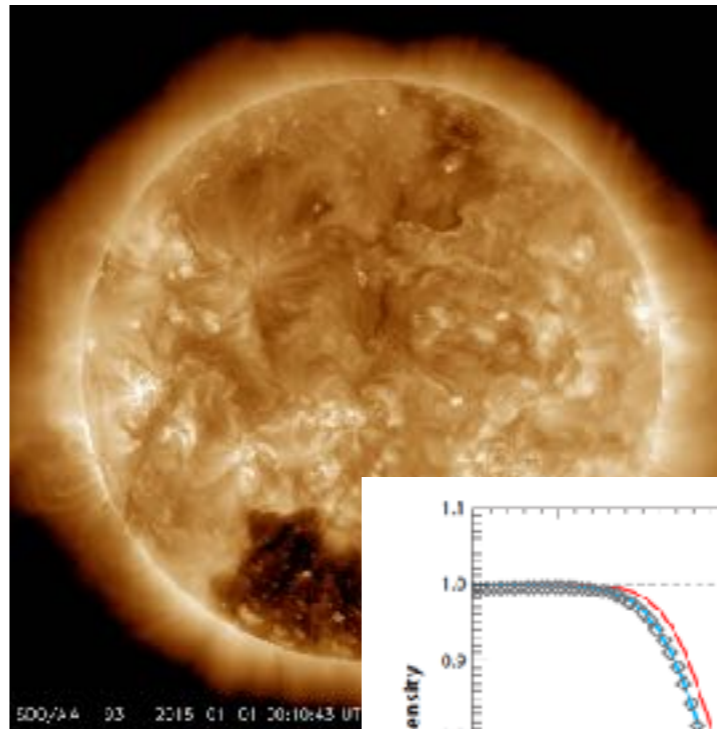
- ▶ (High Resolution) Molecular Spectroscopy
- ▶ Remote Sensing
- ▶ Chemical Kinetics & Atmospheric Chemistry

Phys. Conditions

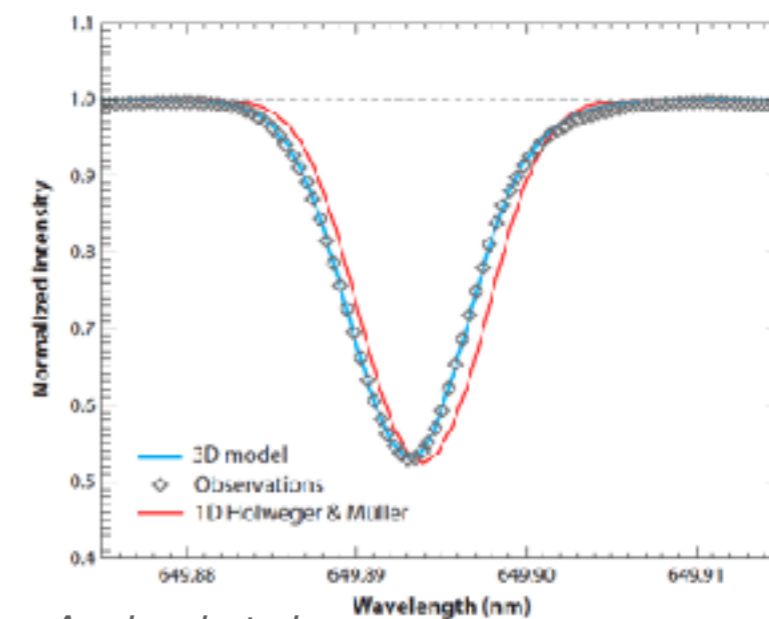
$T \sim 200 - 300 \text{ K}$



credits NASA



$T \sim 6000 \text{ K}$

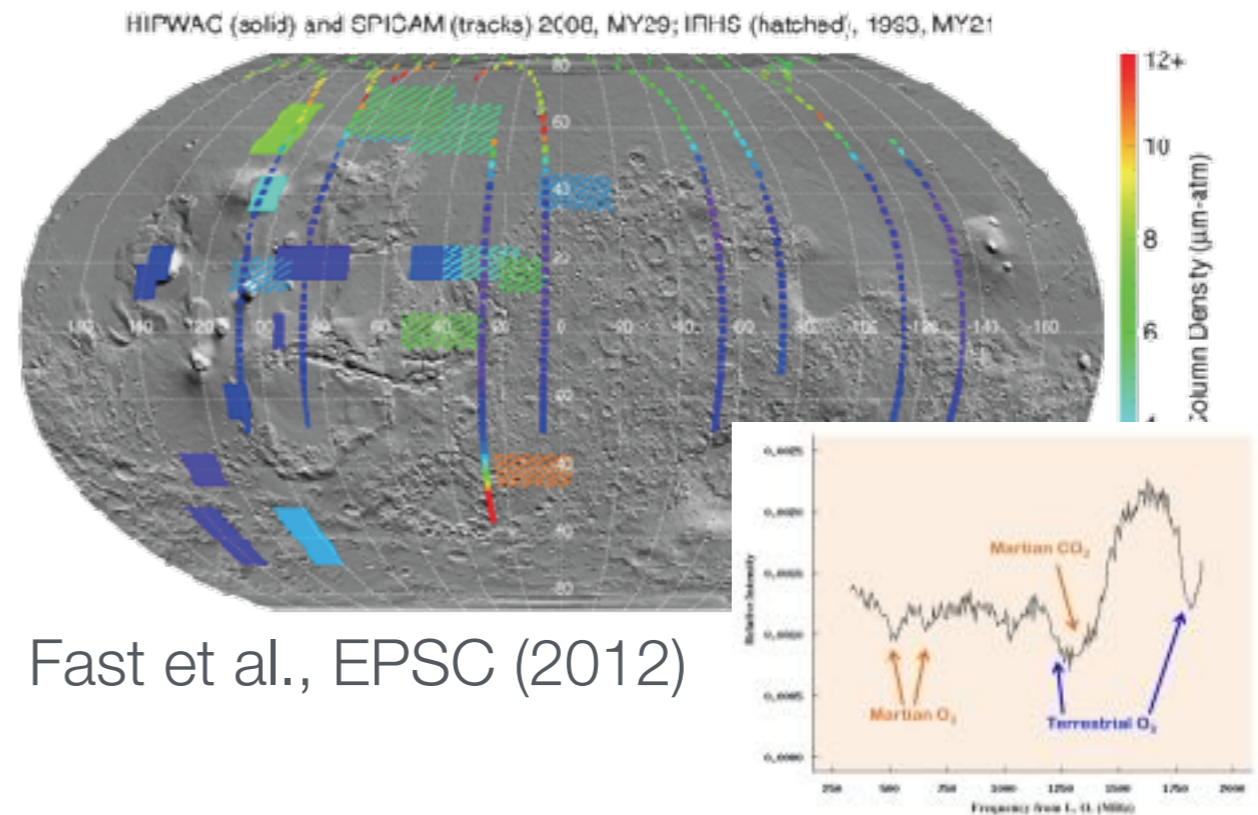


Asplund et al.
Ann Rev Astron Astrophys **47**, 481 (2009)

Ozone in the solar system

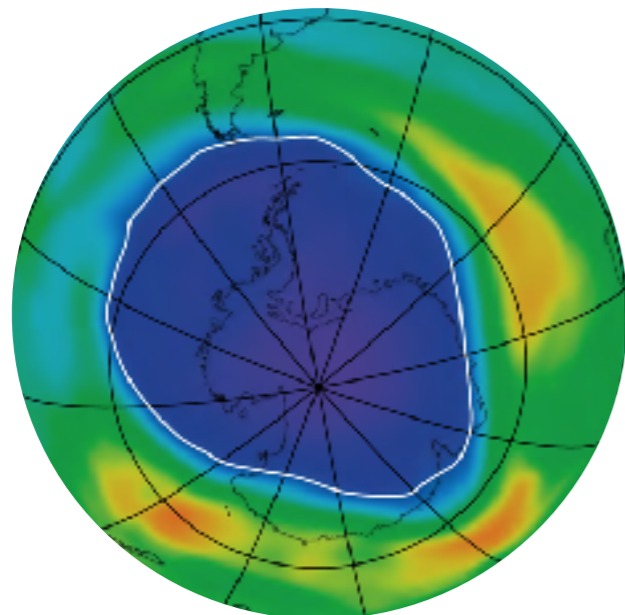


Pollution

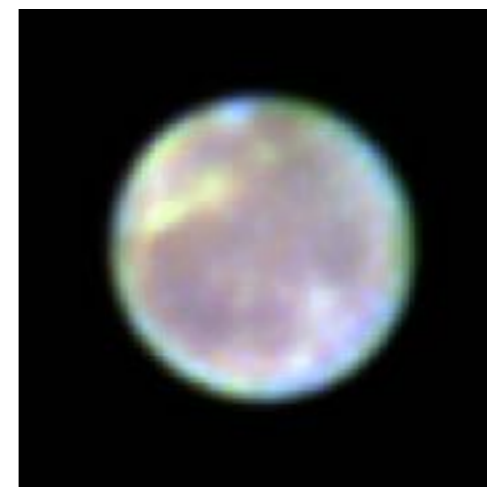


Fast et al., EPSC (2012)

Ozone hole



From *Scientific Assessment of Ozone Depletion* (2014)

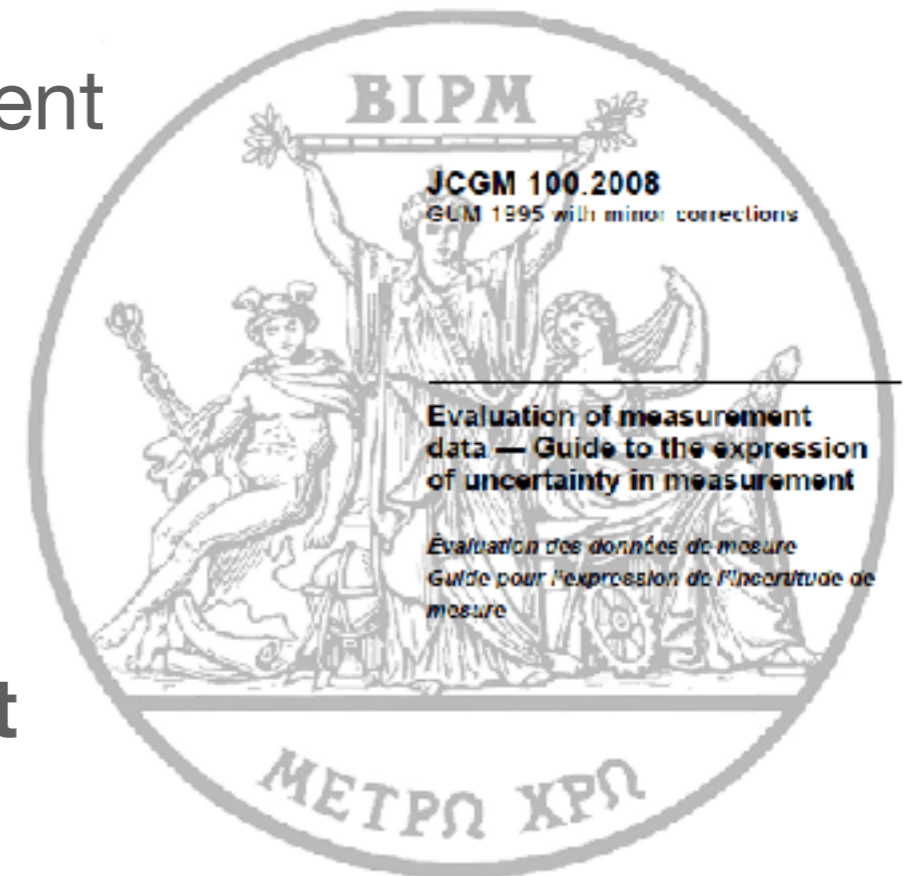


Planetary bodies

Noll et al., *Science* **273** (1996)

Metrology

- ▶ "Science of measurement"
- ▶ GUM - Guide to the Expression of Uncertainty in Measurement
 - ▶ Uncertainty is integral part of measurement
 - ▶ Need common rules
 - ▶ **Assure traceability**
 - ▶ (link to primary standards)
 - ▶ **Provide (complete) uncertainty budget**

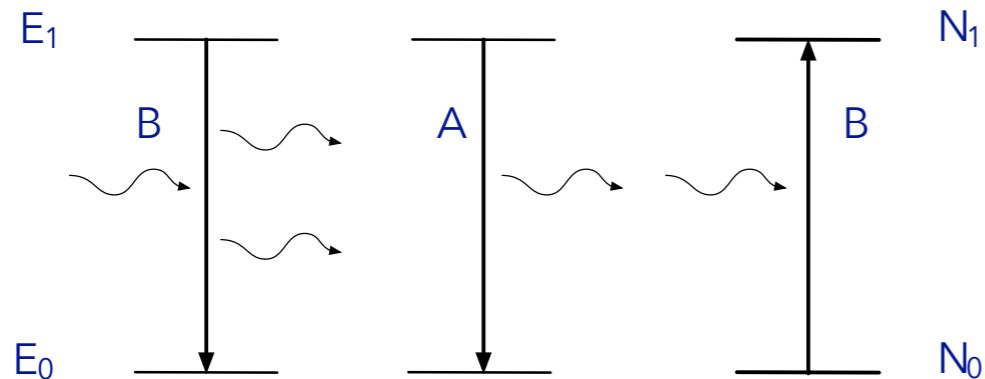


Outline

- ▶ Introduction :
 - ▶ A phenomenological primer on molecular line parameters
 - ▶ Problems associated with spectroscopic data of ozone
- ▶ Multispectral Measurements (FTS & TDL): UV, 5 and 10 μm , incl. pressure shifting using QCLs
- ▶ The VAMDC infrastructure as resource of molecular data
(presentation of work by M.L. Dubernet, C.M. Zwölf, N. Moreau, and Y.A. Ba)

Molecular Line Parameters

- ▶ weak field / linear absorption



- ▶ use semi-empirical formulae for line-shape & parameters

$$\Gamma_L/p = \gamma(T) = \gamma_0(T_{ref}) \left(\frac{T}{T_{ref}} \right)^n$$

$$\Delta_L/p = \delta(T) = \delta_0(T_{ref}) + \delta'(T - T_{ref})$$

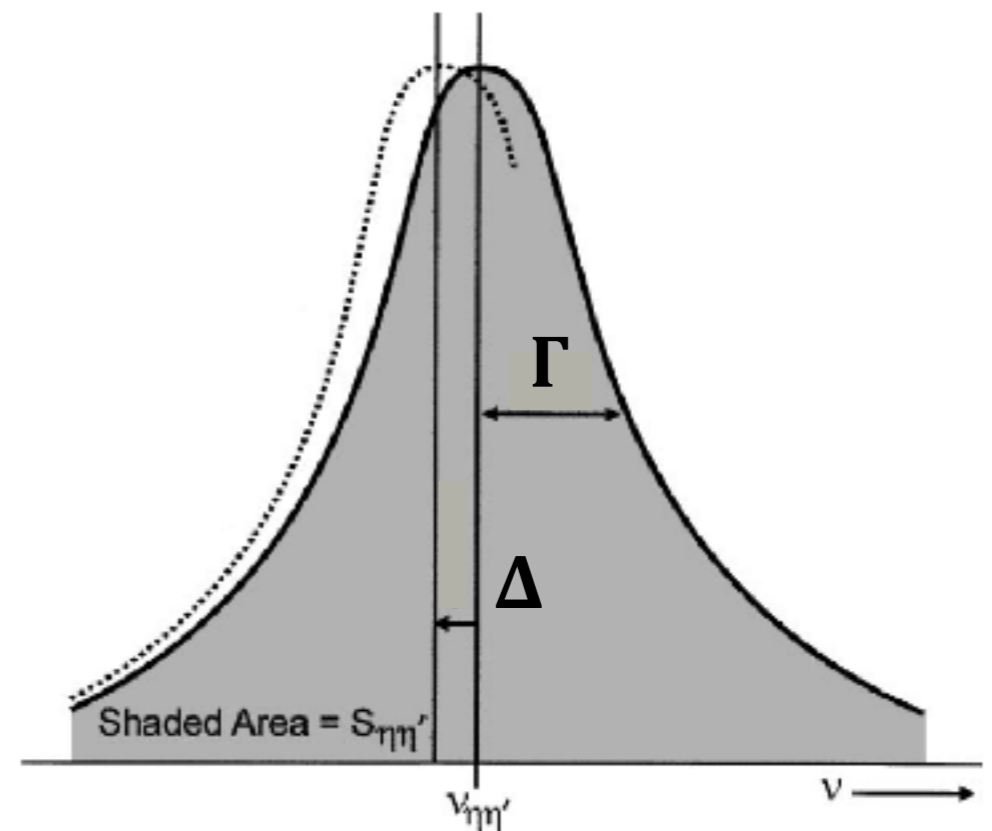
- ▶ resolved ro-vibrational transitions

$$S_{\eta\eta'} = \frac{h\nu_{\eta\eta'}}{c} \frac{n_{\eta}}{N} \left(1 - \frac{g_{\eta}n_{\eta'}}{g_{\eta'}n_{\eta}} \right) B_{\eta\eta'}$$

- ▶ cross section of ind. transition

$$S = \int \sigma(\nu) d\nu$$

$$\sigma(\nu) = S \times f(\nu)$$

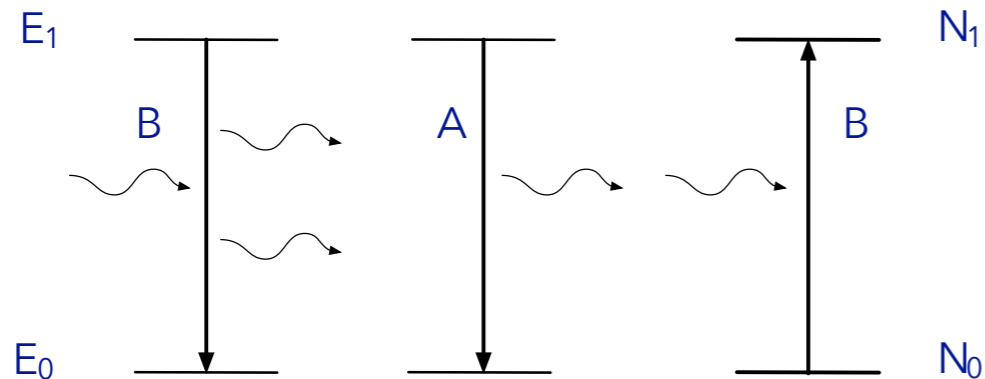


adapted from Rothman et al.,
J Quant Spectrosc. Radial. Trans. **60**, 1998

Molecular Line Parameters

▶ weak field / linear absorption

▶ most commonly used: Voigt



$$\nu = \int \mathcal{G}(\Gamma_D, \nu) \mathcal{L}(\Gamma_L, \nu' - \nu) d\nu'$$

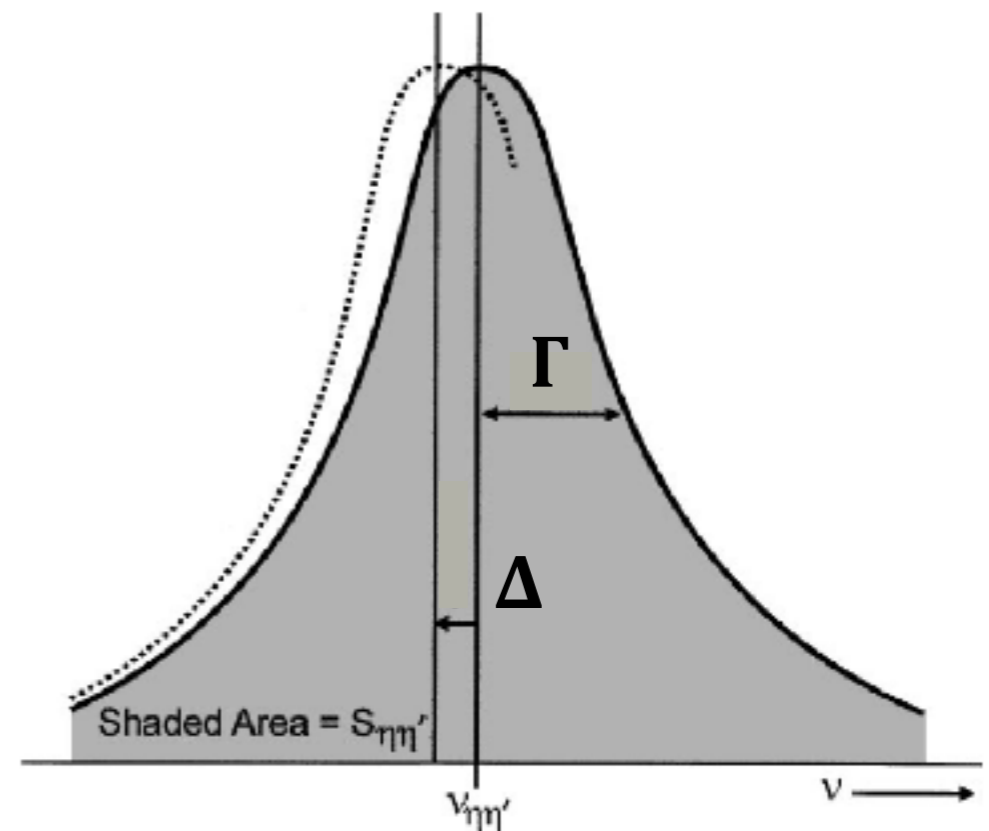
▶ resolved ro-vibrational transitions

$$S_{\eta\eta'} = \frac{h\nu_{\eta\eta'}}{c} \frac{n_{\eta}}{N} \left(1 - \frac{g_{\eta}n_{\eta'}}{g_{\eta'}n_{\eta}} \right) B_{\eta\eta'}$$

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adapted from Rothman et al.,
J Quant Spectrosc. Radial. Trans. **60**, 1998

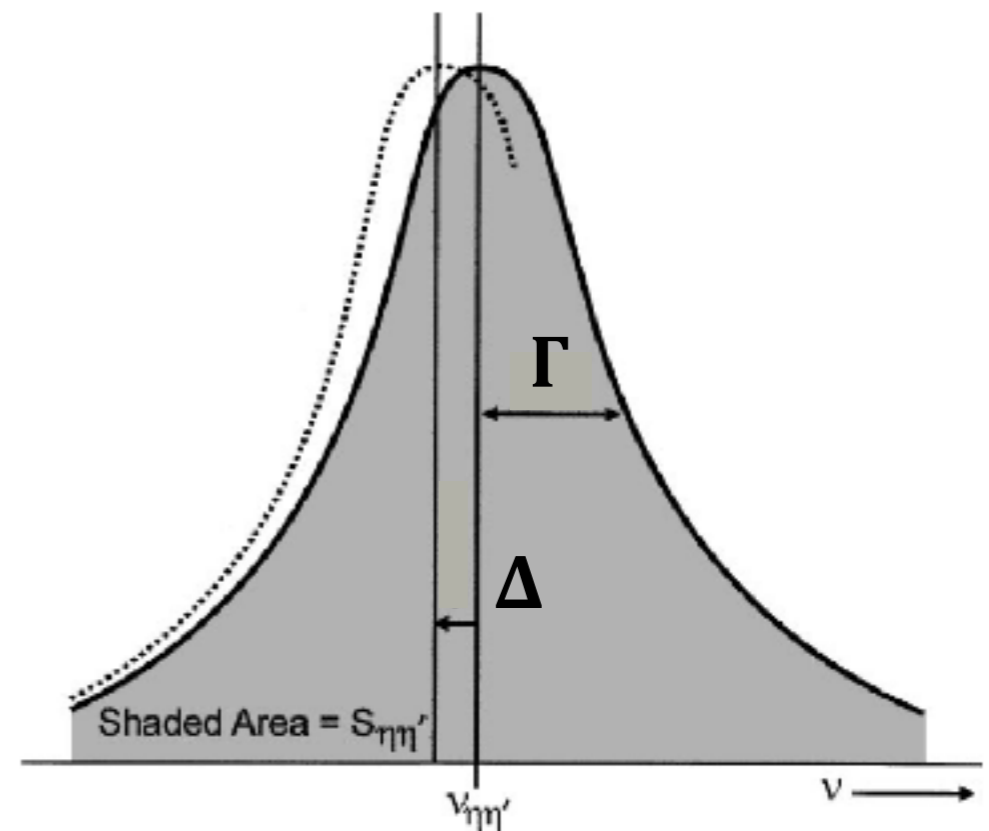
Molecular Line Parameters

- ▶ weak field / linear absorption
- ▶ most commonly used: Voigt

High resolution spectroscopy reveals limits of Voigt profile
Preparation for more general line shape model
(Dicke effect, velocity and phase changing collisions,):

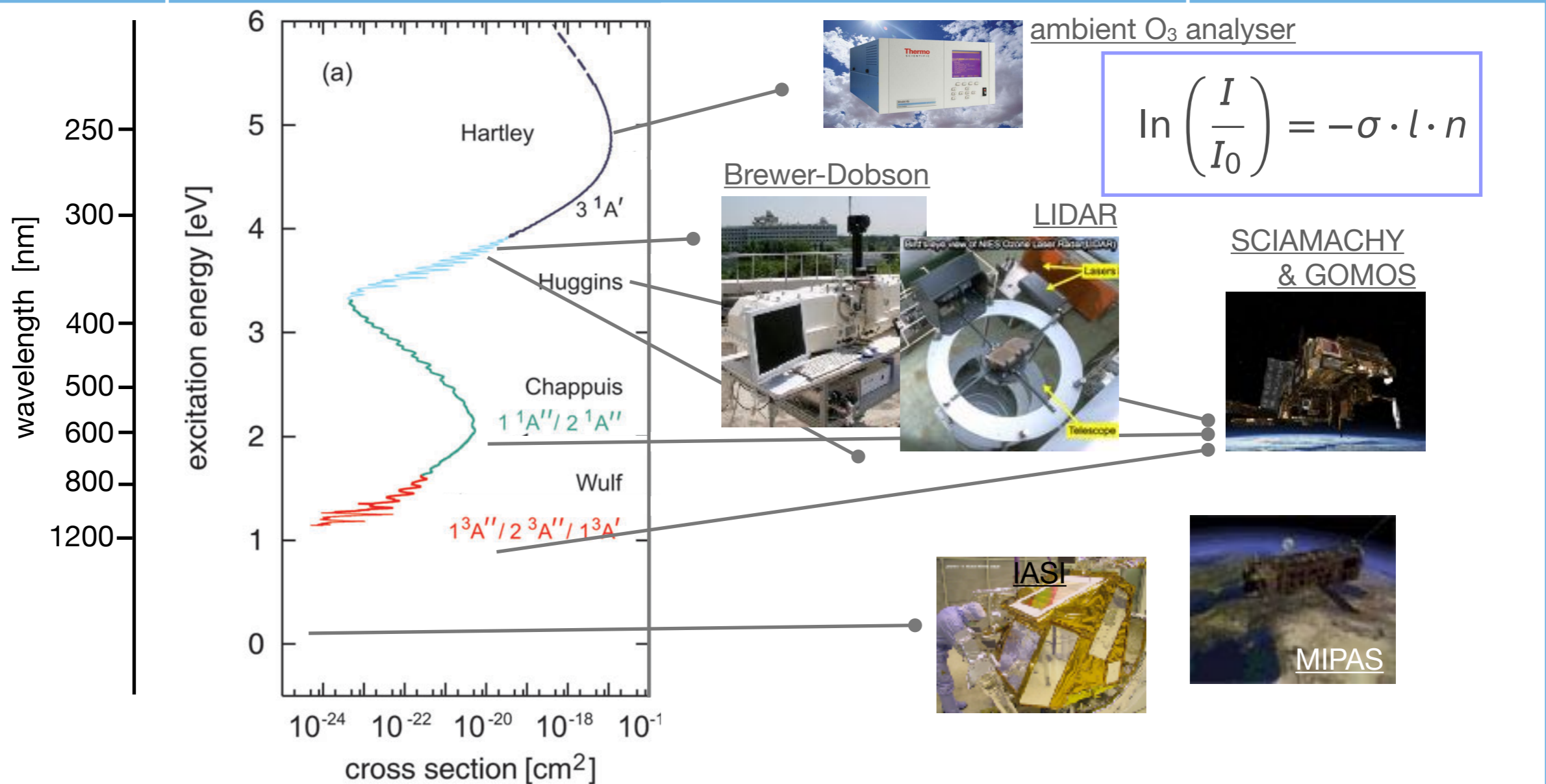
$$HTP(\Gamma_D, \Gamma_0, \Delta_0, \Gamma_2, \Delta_2, \nu_{VC}, \eta; \Delta\nu)$$

eg Wcisło et al., *J Quant Spectrosc. Radial. Trans.* **177**, 75 (2016)



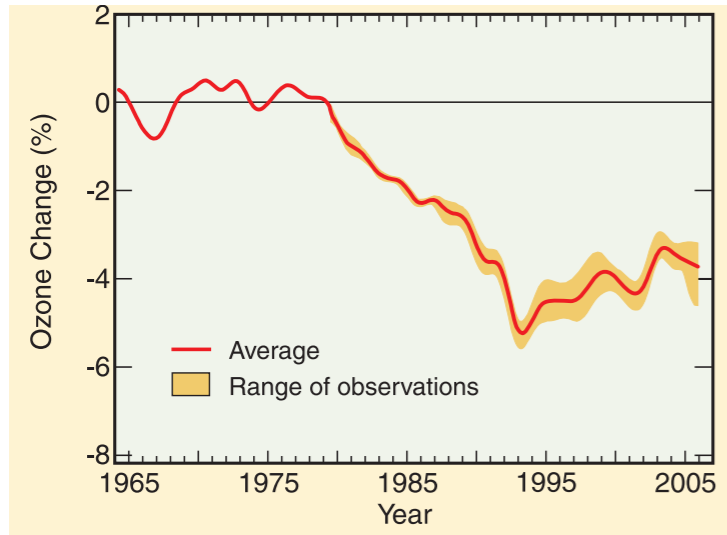
adapted from Rothman et al.,
J Quant Spectrosc. Radial. Trans. **60**, 1998

Ozone Spectroscopy & Measurement



Ozone Spectroscopic Data Quality

- ▶ target uncertainty : $< 1\%$



Scientific Assessment of Ozone Depletion 2010, WMO

Atmos. Meas. Tech. Discuss., 7, 2071–2106, 2014
 www.atmos-meas-tech-discuss.net/7/2071/2014/
 doi:10.5194/amt-7-2071-2014
 © Author(s) 2014. CC Attribution 3.0 License.



This discussion paper is/has been under review for the journal Atmospheric Measurement Techniques (AMT). Please refer to the corresponding final paper in AMT if available.

Quality assessment of ozone total column amounts as monitored by ground-based solar absorption spectrometry in the near infrared ($> 3000\text{ cm}^{-1}$)

O. E. García¹, M. Schneider^{1,2}, F. Hase², T. Blumenstock², E. Sepúlveda^{1,3}, and Y. González¹

Rel. retrieval bias using recommended data

	UV	VIS	3 μm	5 μm	10 μm	14 μm
UV					-4%	
VIS				0 ?		
3 μm					7%	
5 μm		0 ?			?	
10 μm	4%		-7%	?		?
14 μm					?	

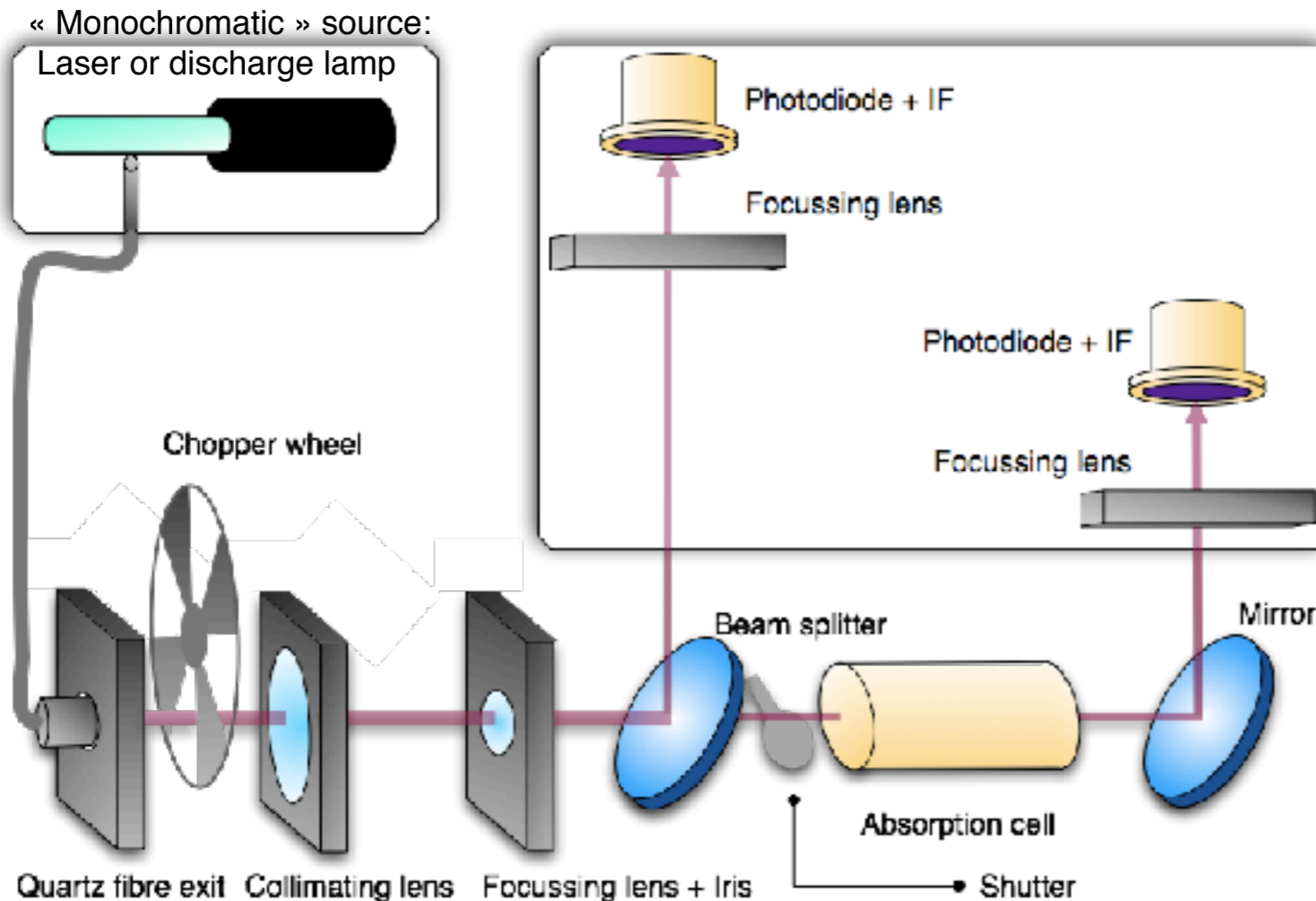
- ▶ Inconsistencies in atmospheric & laboratory data (+ data bases)

- ▶ Lab: IR (10 μm / 1000 cm^{-1}) - UV (300 nm):
 - ▶ 5.5 % (Picquet-Varrault et al., 2005) &
 - ▶ 4.0 (± 0.1)% (Gratien et al., 2010)
- ▶ Column-O₃: FTIR (962 - 1044 cm^{-1}) - Brewer (303.2 - 320.1 nm) @ Izaña:
 - ▶ 4.2 ± 0.7 % (e.g. Viatte et al., *Atmos. Meas. Tech.* 4, 2011)

3. How do other ranges compare ?

Reference values at selected wavelengths with metrological quality

Cross section @ 253/325 nm

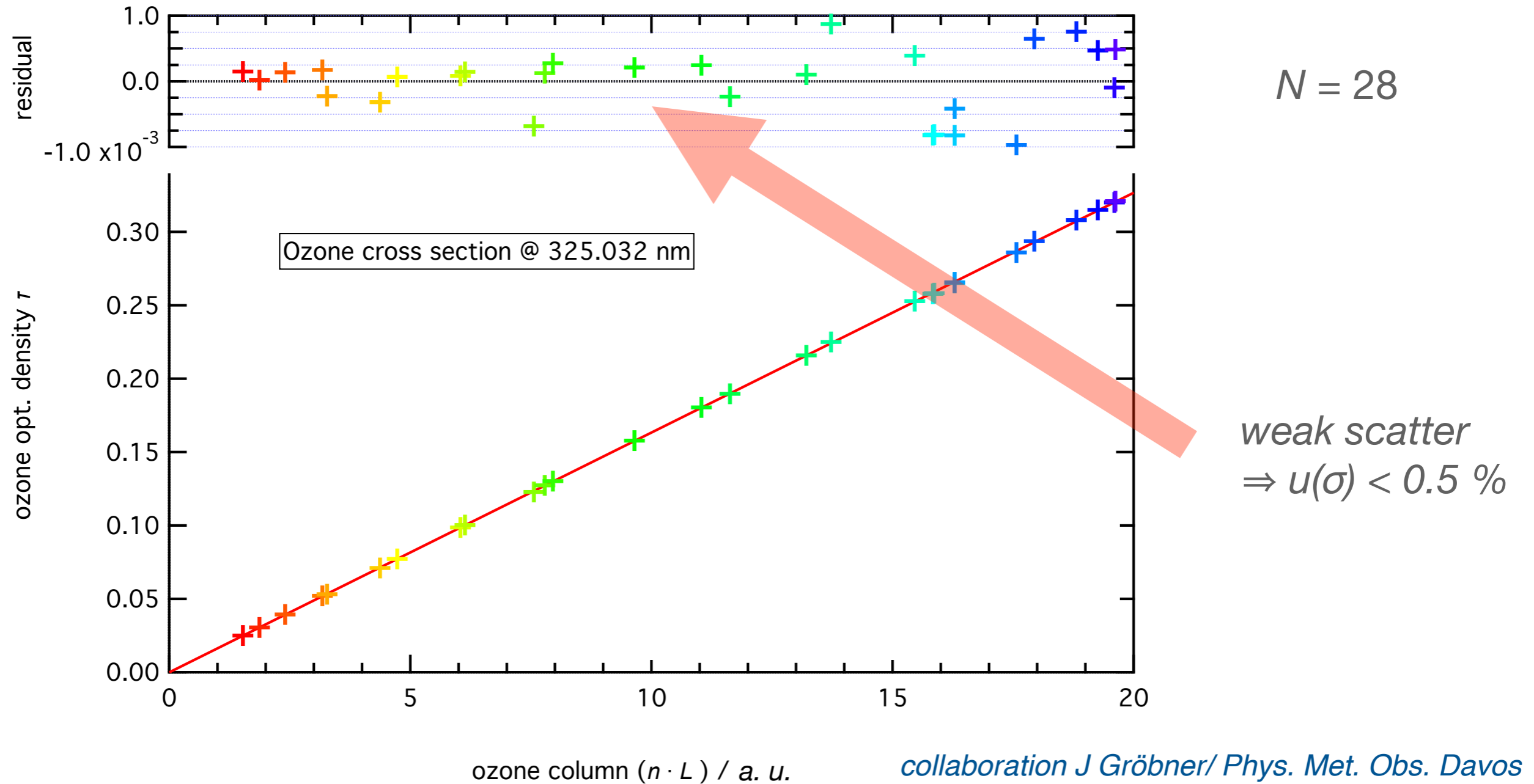


”Resolving power” $\sim 3 \cdot 10^6$

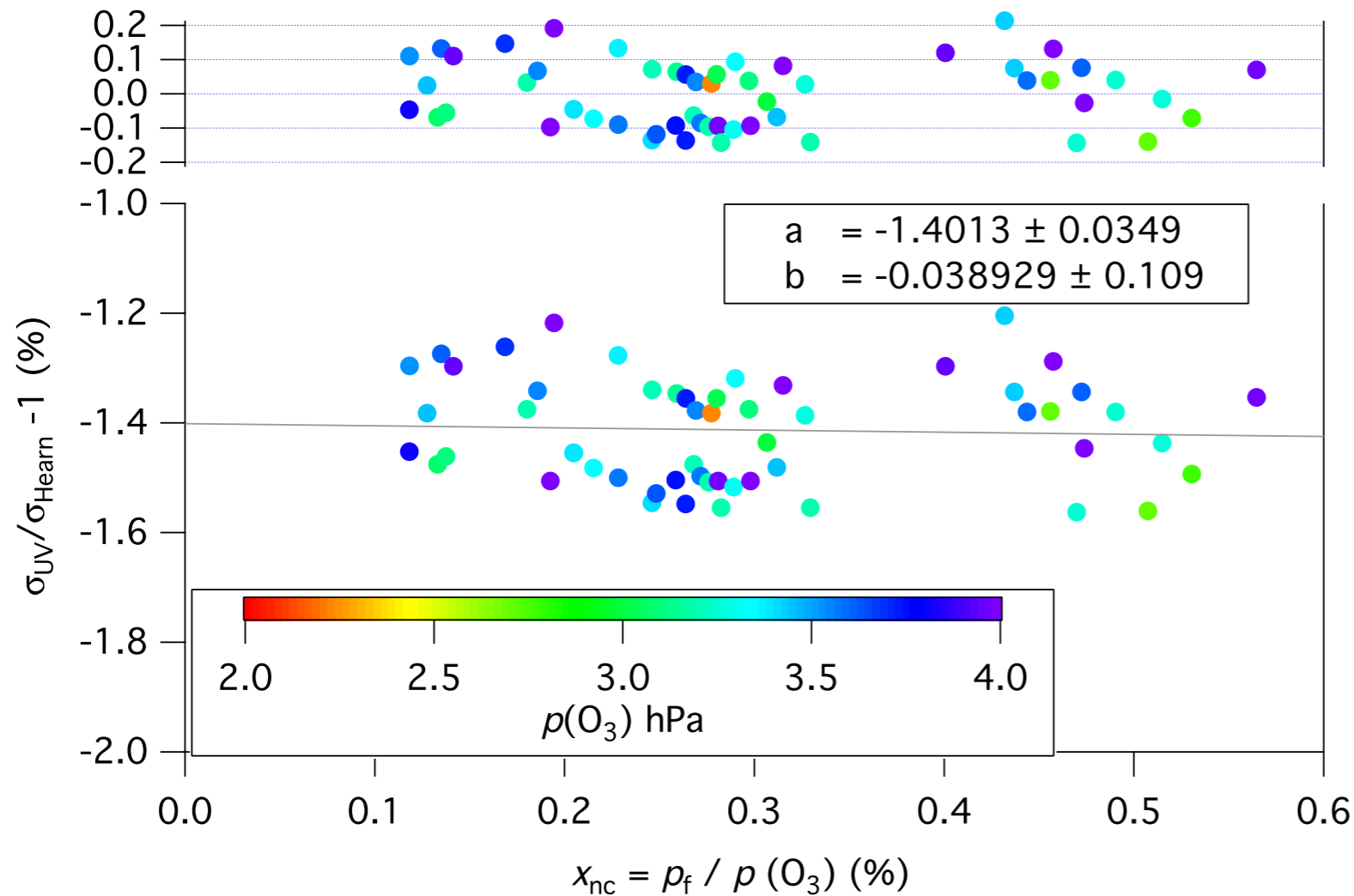
$$\ln \left(\frac{I_0}{I} \right) = \sigma \cdot L \cdot n \quad \Rightarrow \quad \sigma = \underbrace{\frac{k_B T}{(1 - x_c - x_{nc}) p}}_{n^{-1}} \cdot L^{-1} \cdot \ln (I_0 / I)$$

UV measurements @ 325 nm

Preliminary results



UV measurements @ 253 nm



$N = 55$

$$\sigma_{LERMA} = (1.131 \pm 0.7\%) \cdot 10^{-17} \text{ cm}^2$$

$$\sigma_{Hearn/BIPM} = (1.148 \pm 2.1\%) \cdot 10^{-17} \text{ cm}^2$$

$$\sigma_{Viallon/BIPM} = (1.127 \pm 0.9\%) \cdot 10^{-17} \text{ cm}^2$$

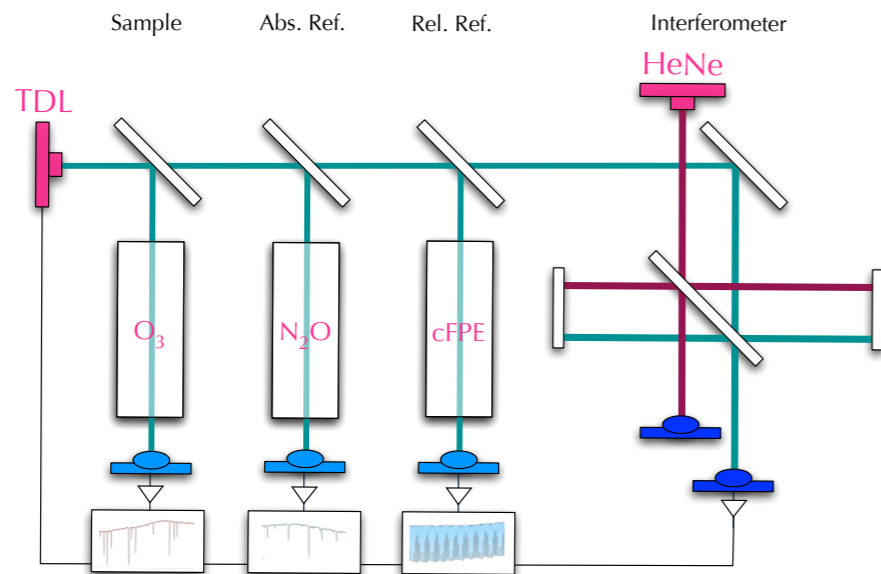
(officially recommended)

Viallon et al., *AMT*, **8**, 2015

**High resolution study of
individual molecular line
transitions
(almost metrological
quality)**

IR studies at LERMA

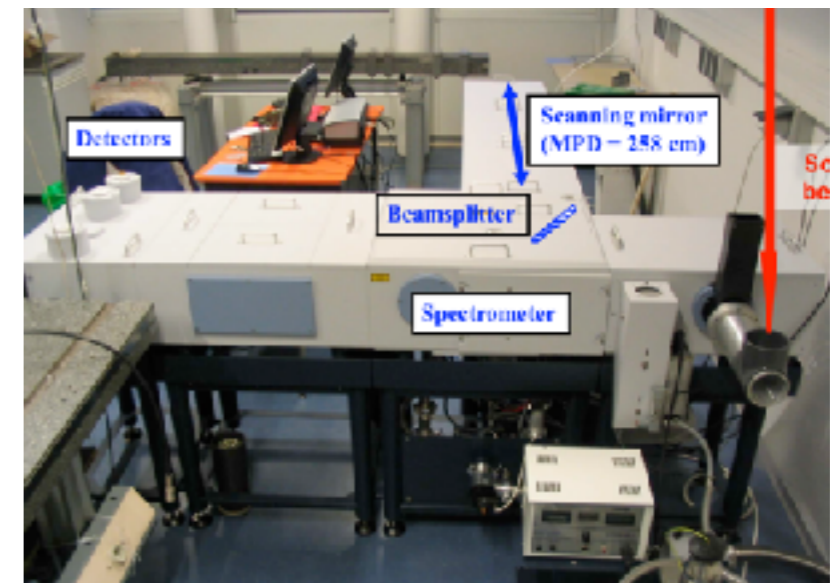
Lab: Interferometrically controlled tunable TDL (R ~ 10⁸)



- high spectral resolution ($< 5 \times 10^{-8}$)
- interferometer based stabilization
- **1 out of 2 systems** explicitly mentioned for spectroscopy on future satellite missions (Harrison et al., JQSRT **112**, 2011)

Guinet et al. JQSRT **110**, 2010

Atmosphere: FTS-Paris (R ~ 10⁶)

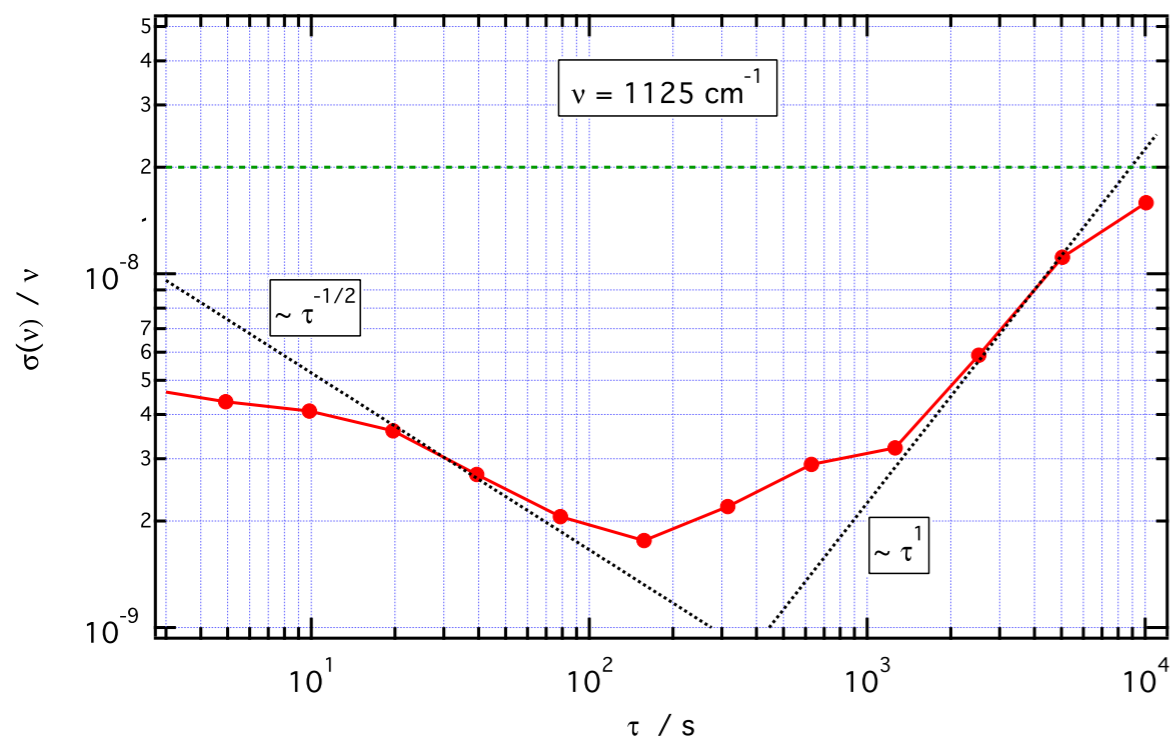
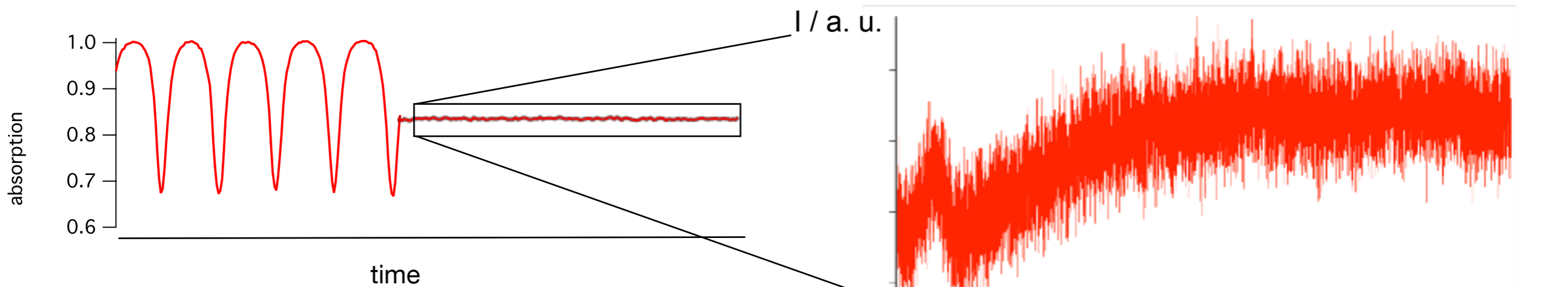


- ground based FTS, part of the air quality research station of UPMC at Paris
- Bruker HR125, resolution: **0.0024 cm⁻¹**
- MCT and InSb detectors: access to **950-1400 cm⁻¹** and **1950-3200 cm⁻¹**

Té et al. RSI **81**, 2010

Frequency stabilization

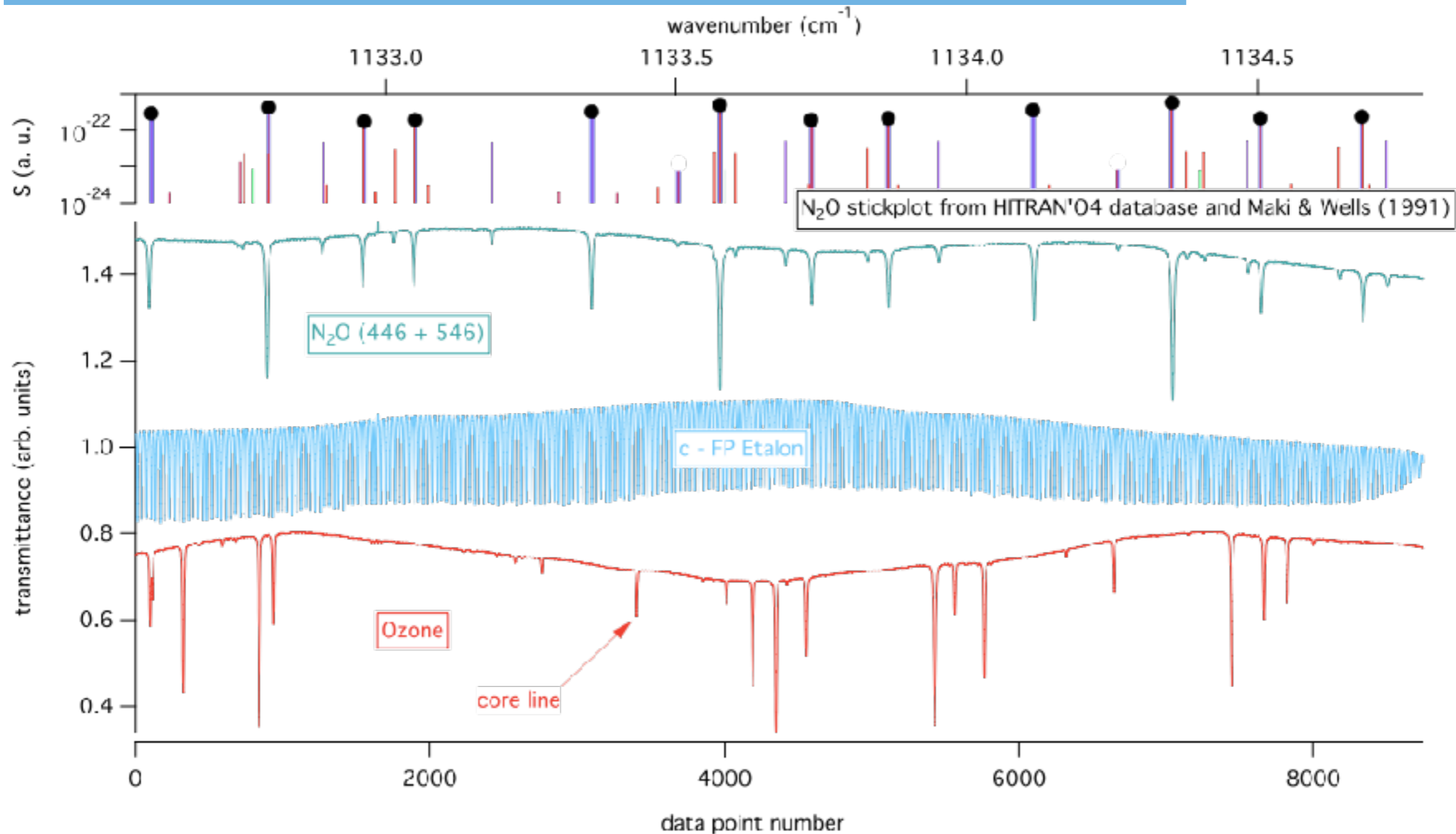
$$D = k_d \lambda_d = k_{\text{HeNe}} \lambda_{\text{HeNe}}$$



$$\begin{aligned} \Delta\nu/\nu &= 5 \cdot 10^{-9} \text{ (1/2 h)} \\ \Delta\nu/\nu &= 1 \cdot 10^{-8} \text{ (1h)} \\ \Delta\nu/\nu &= 2 \cdot 10^{-8} \text{ (3h)} \end{aligned}$$

compare to:
- 10^{-6} FTIR

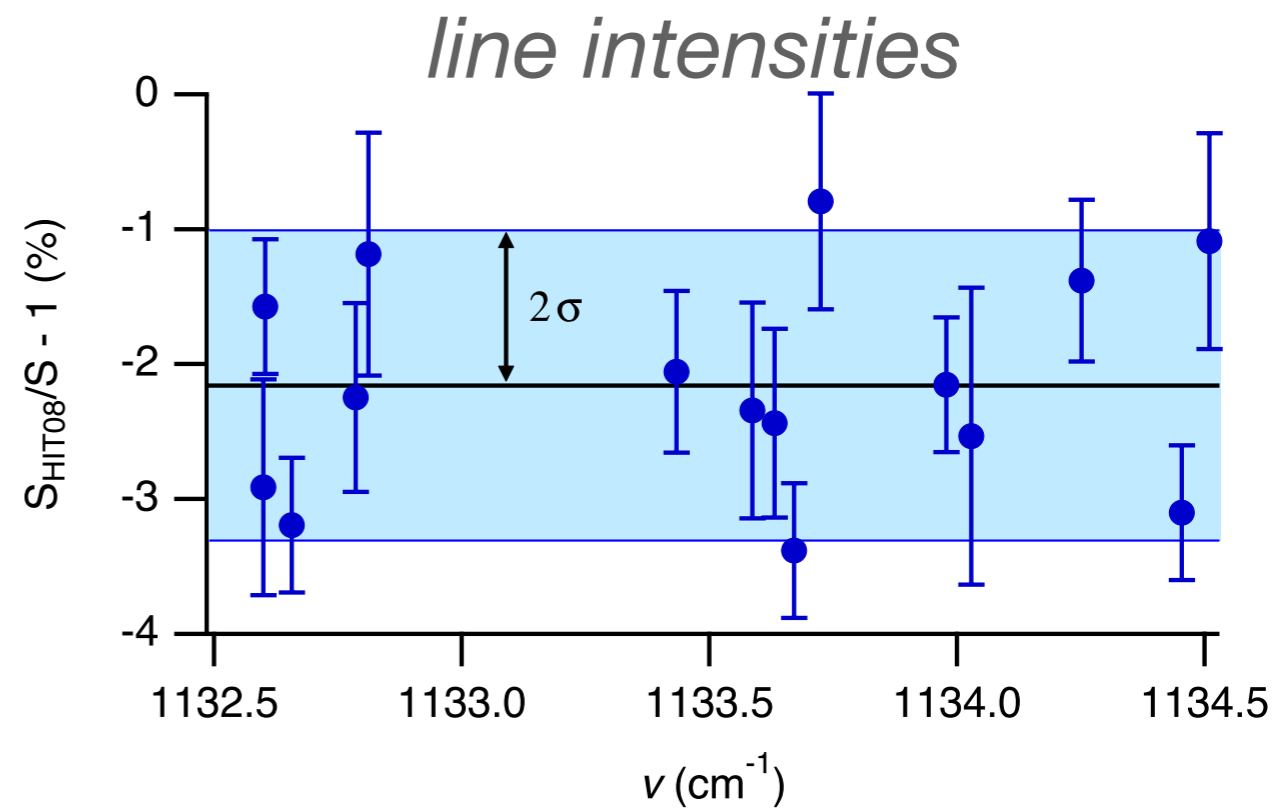
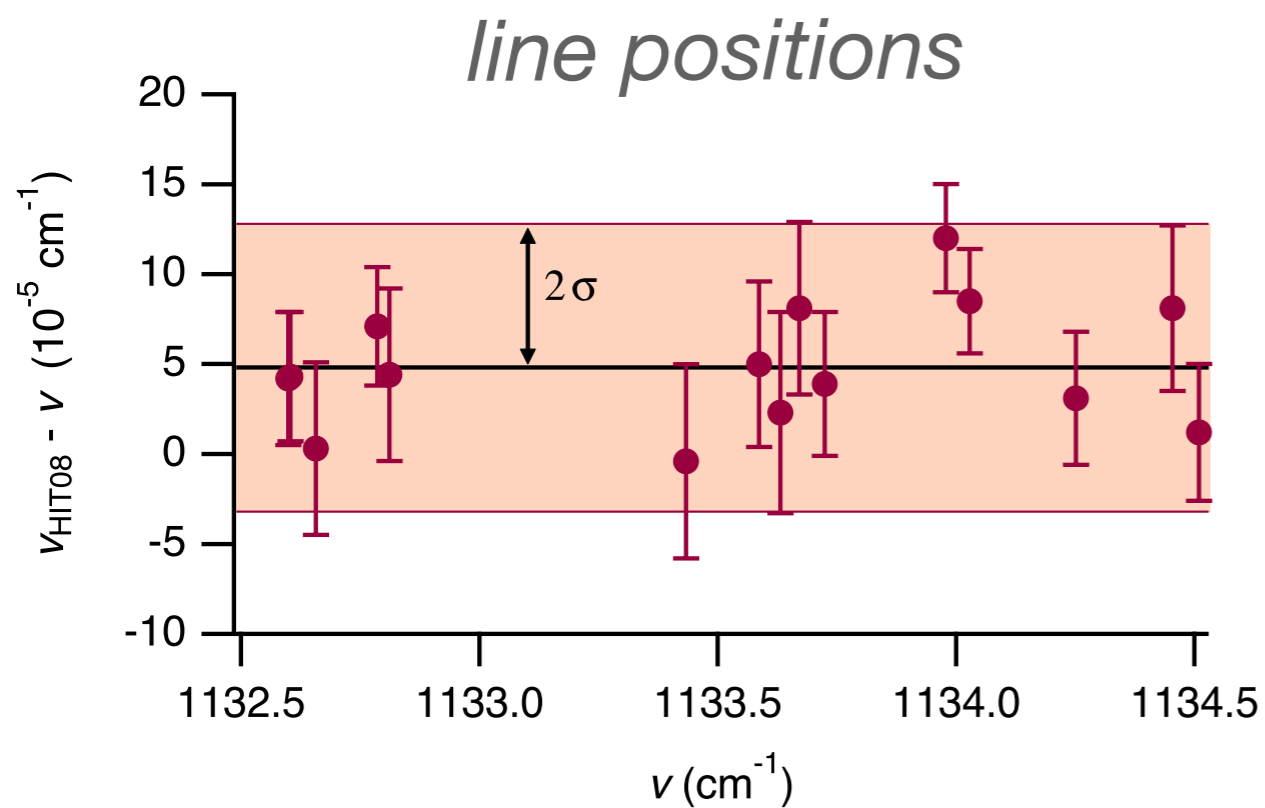
Spectra Acquisition and the Wavenumber Scale



Summary IR Spectroscopy in SWIFT Target Window

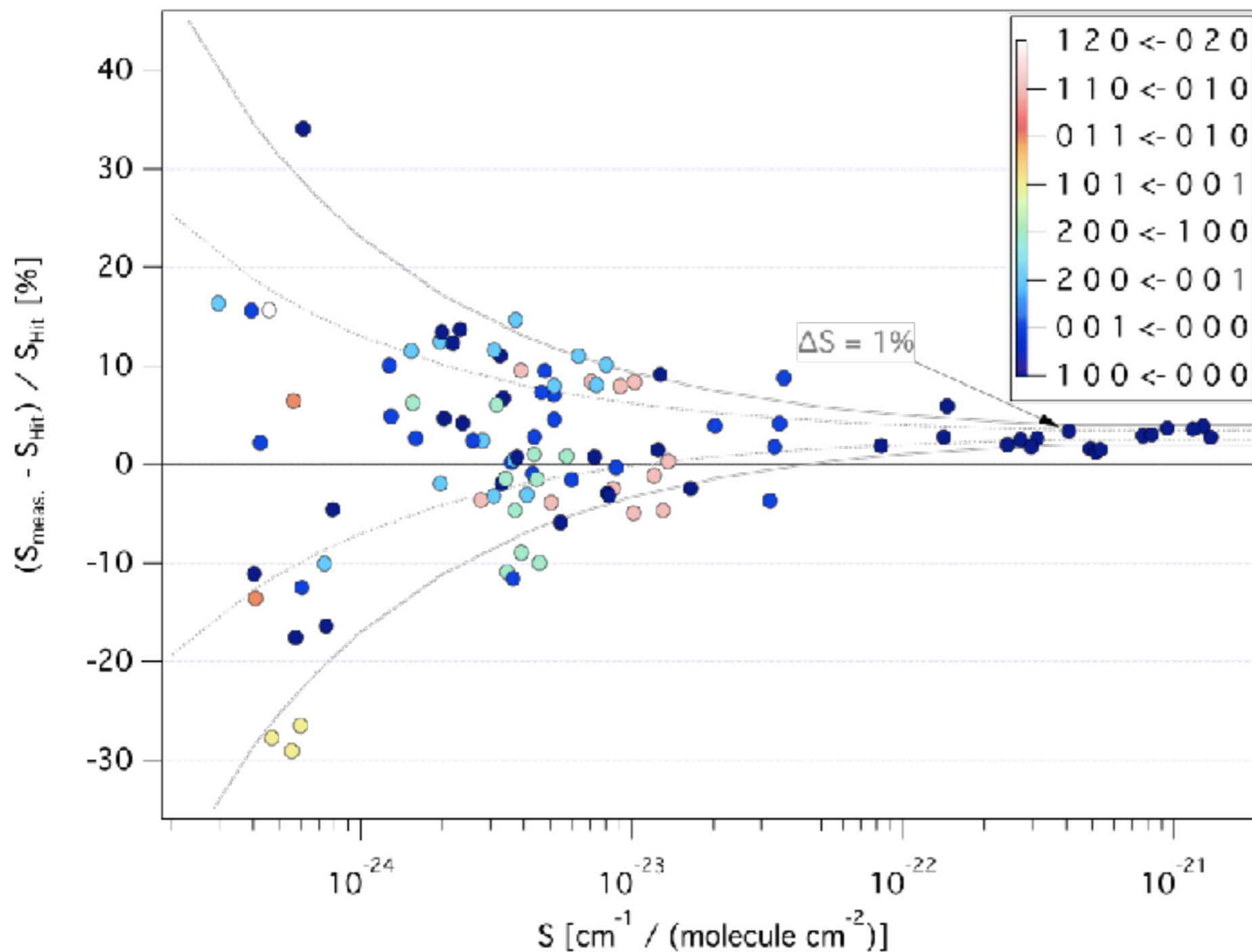


Analysis of 15 strong absorption lines in small spectral window



*Guinet et al. JQSRT **110**, 2010*

Intensities at 1130 cm⁻¹



UV - IR (10 μm) data consistency

- Confirm ~ **4% discrepancy** between UV and IR
- Both regions seem to require correction
- UV (253.7 nm): **-1.4 %**
- IR (10 μm): **+ 2.1 %**



5 & 10 μm regions
Field observations &
validation of database

Sensitivity to bias in line parameters

FTS-Paris

► sensitivity coefficient

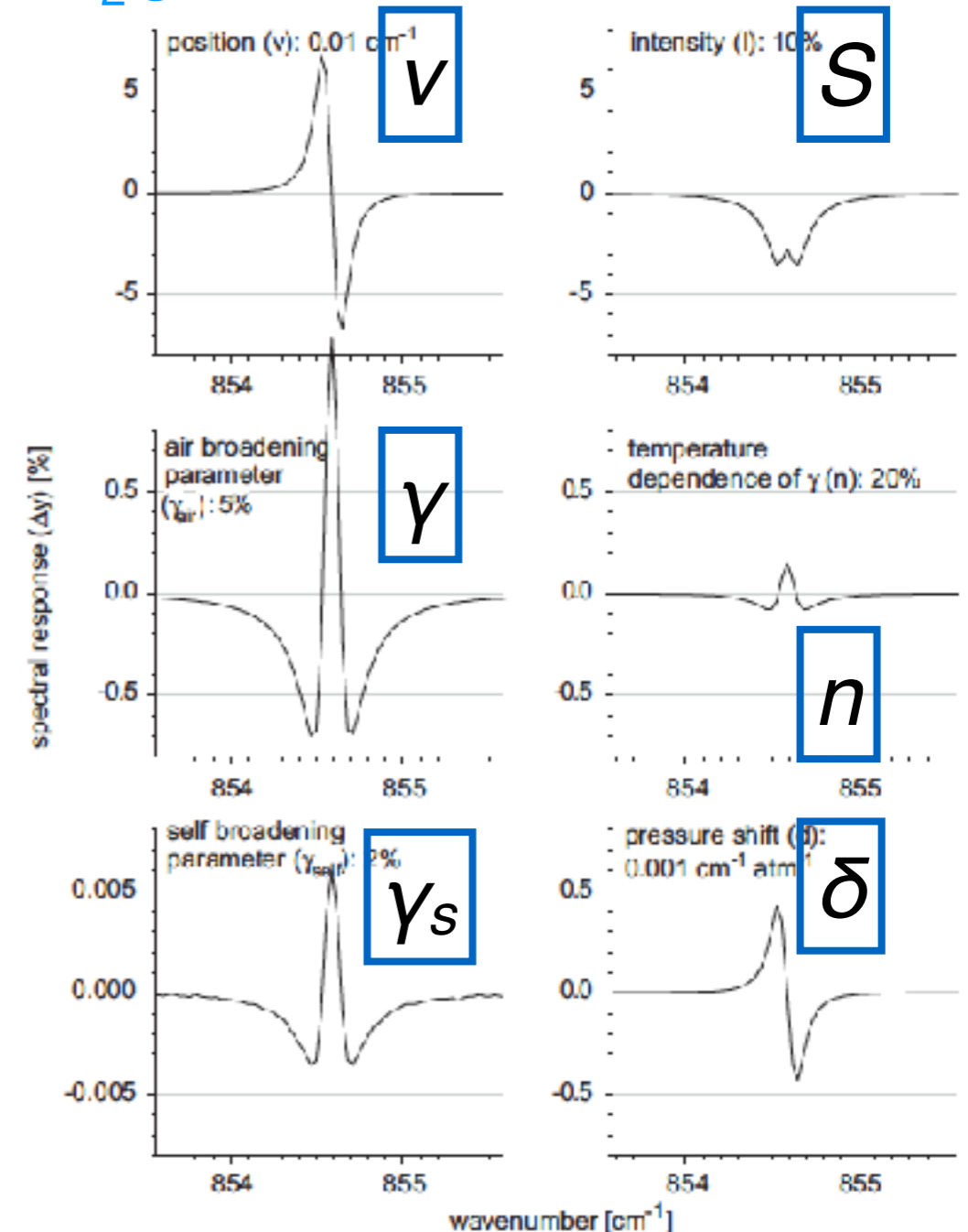
$$\alpha(x) = \frac{\Delta C_{ol}}{C_{ol}} / \frac{\Delta x}{x}$$

► O₃

Band	Weight w_i (%)	$\alpha(x)$ or $\alpha_i(x)$		
		$x = S$	$x = \gamma_{air}$	$x = \gamma_{self}$
001 ← 000	91.2	-0.94	-0.152	-0.049
011 ← 010	5.0	-1.75	0.541	0.063
100 ← 000	1.7	-0.86	0.245	0.021
002 ← 001	1.5	-1.51	0.286	0.067
Weighted sum	99.4	-0.98	-0.104	-0.035

Janssen et al, *J. Mol. Spectrosc.* **326** (2016)

► H₂O



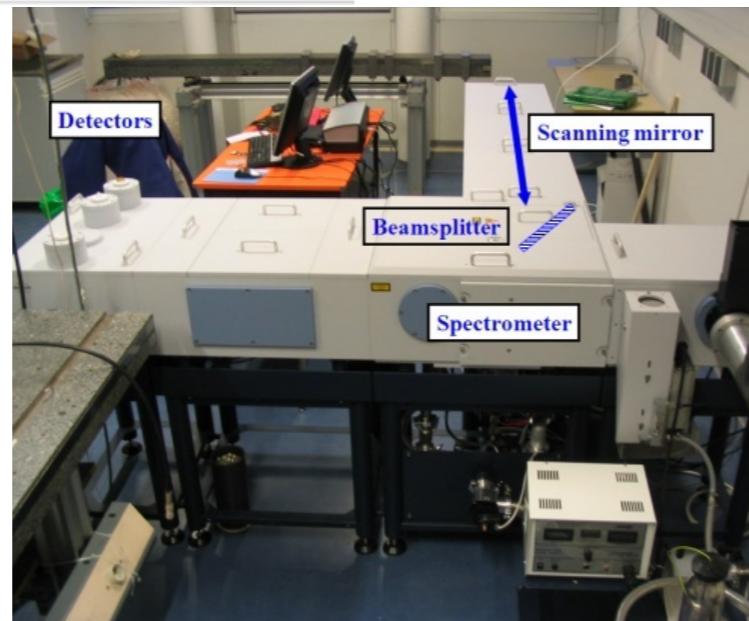
Schneider & Hase, *J. Quant. Spectrosc. Radiat. Trans.* **110** (2009)

FTS-Paris at Air Quality Station Jussieu: Remote Sensing over a Megacity



The screenshot shows the TCCON web interface. On the left is a navigation menu with categories like 'Home', 'Data', 'System/Account/Tools', 'Links', 'Four Corners', 'Glossary', 'About us', 'FAQ', 'Jobs', 'API', 'Reference', 'L1/Level 1', 'Level 2', 'Level 3', 'Level 4', 'Level 5', 'Level 6', 'Level 7', 'Level 8', 'Level 9', 'Level 10', 'Level 11', 'Level 12', 'Level 13', 'Level 14', 'Level 15', 'Level 16', 'Level 17', 'Level 18', 'Level 19', 'Level 20'. The main content area shows the 'Paris' station status. It includes a table with columns 'Site', 'User Name', 'Operational?', and 'Description'. Below the table, there is a photo of the Bruker 125 HR instrument on a rooftop. Text below the photo reads: 'Paris, France', 'TCCON status: Operational', 'Height: 11, 235 m, 40 meters above sea level', 'FTS Paris - Bruker FT120HR', 'Operated by: JEM (Laboratoire d'Etudes de Rayonnement et de la Matière en Astrophysique et Atmosphère, IMB 812), Université Pierre et Marie Curie / CNRS / Observatoire de Paris / IFR, Collaborators: '9014 (P.L. Pasca, J. Jeseck, C. Christoferson), Université Pierre et Marie Curie (http://www.ipsm.fr/), CNRS (http://www.cnrs.fr/), Observatoire de Paris (http://www.obspm.fr/), IRL (http://www.irl.fr/)'

Bruker 125 HR



- ▶ pollutant monitoring
- ▶ GHG monitoring

- ▶ TCCON (provisional) status since June 2015

- ▶ high-resolution

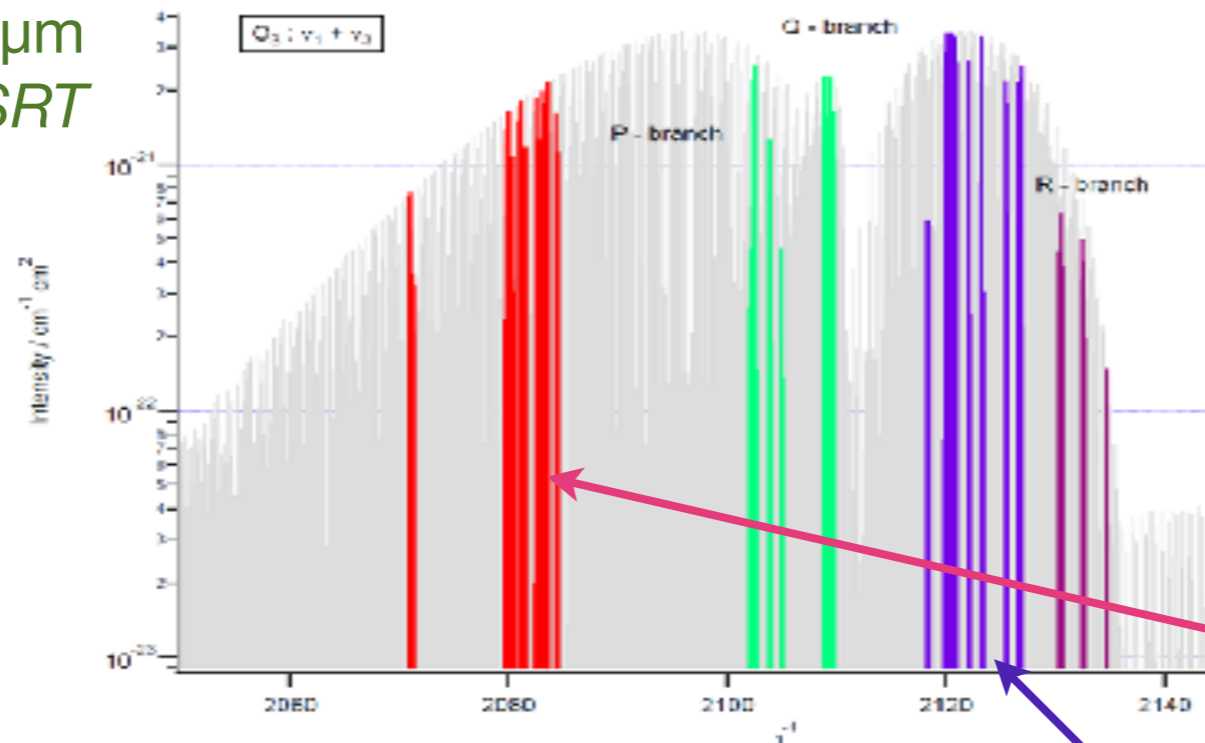
- ▶ GHG: CO₂, CH₄, N₂O, HF, CO, H₂O, HDO

- ▶ **required precision** (CO₂)
right now: 1 ppm → 0.25 %
future: 0.5 ppm → 0.125 %

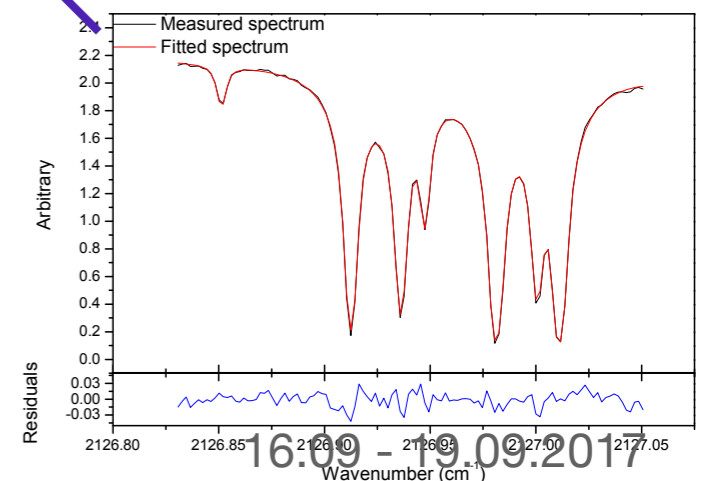
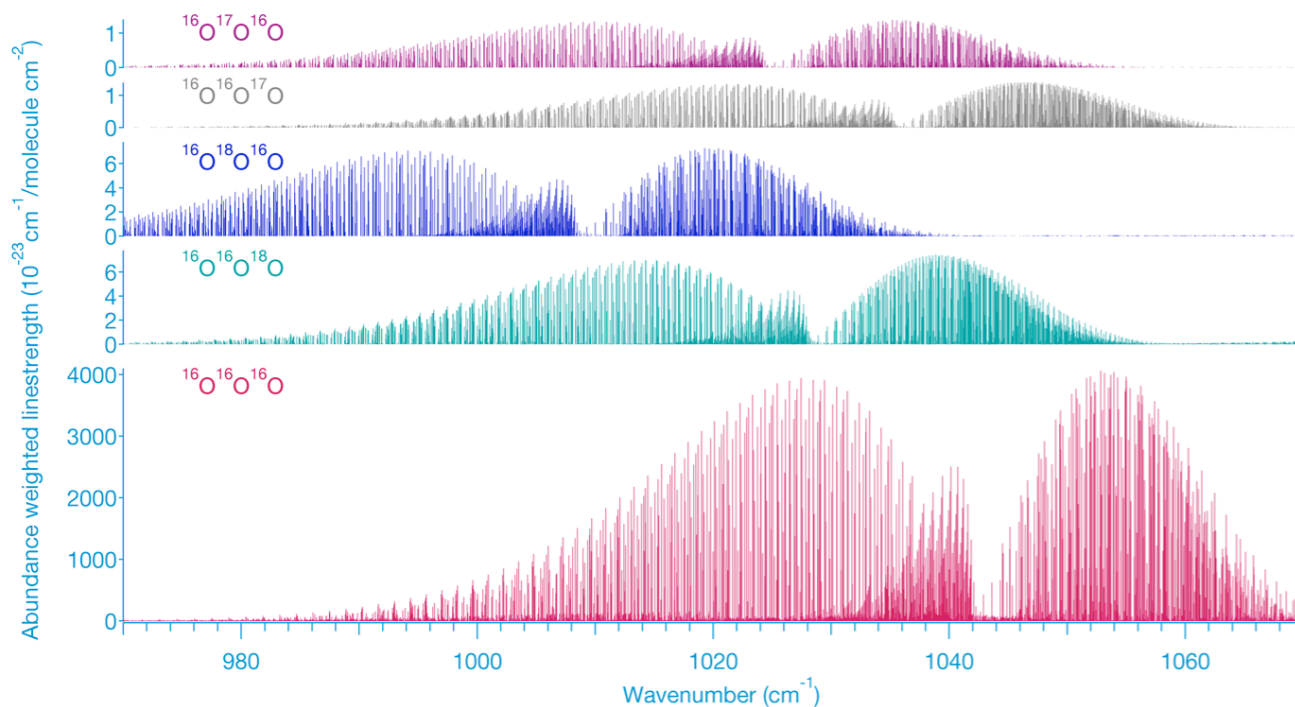
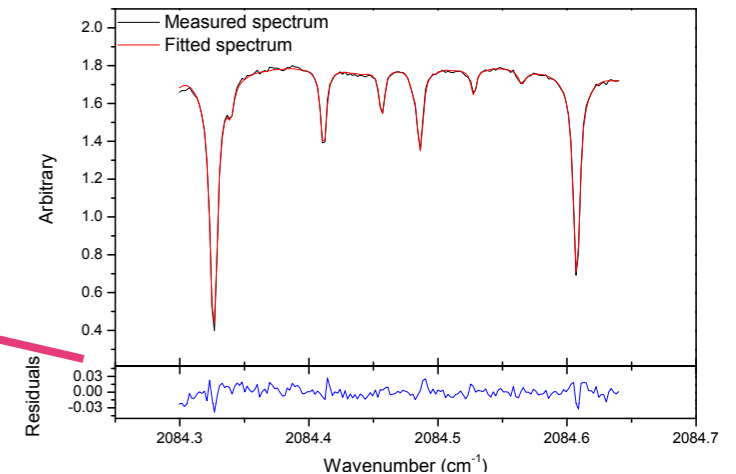
O₃ Multispectral Study 5 & 10 μm

FTS-Paris

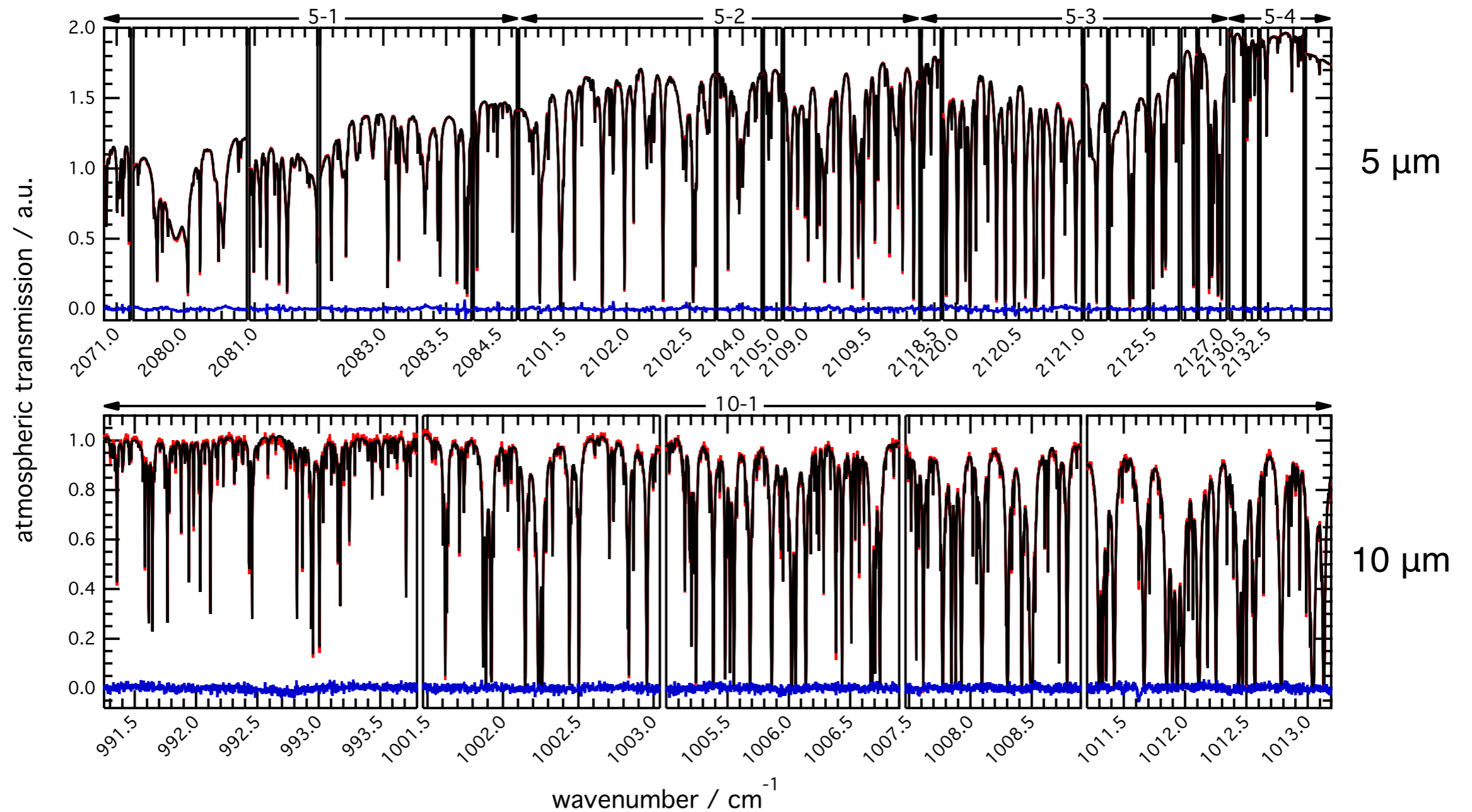
Good agreement (< 2%)
between 5 and 10 μm
(Thomas et al. *JQSRT*
111, 2010)



Problem with
evaluation of (ACE)
satellite data (Walker et
al. 2007)

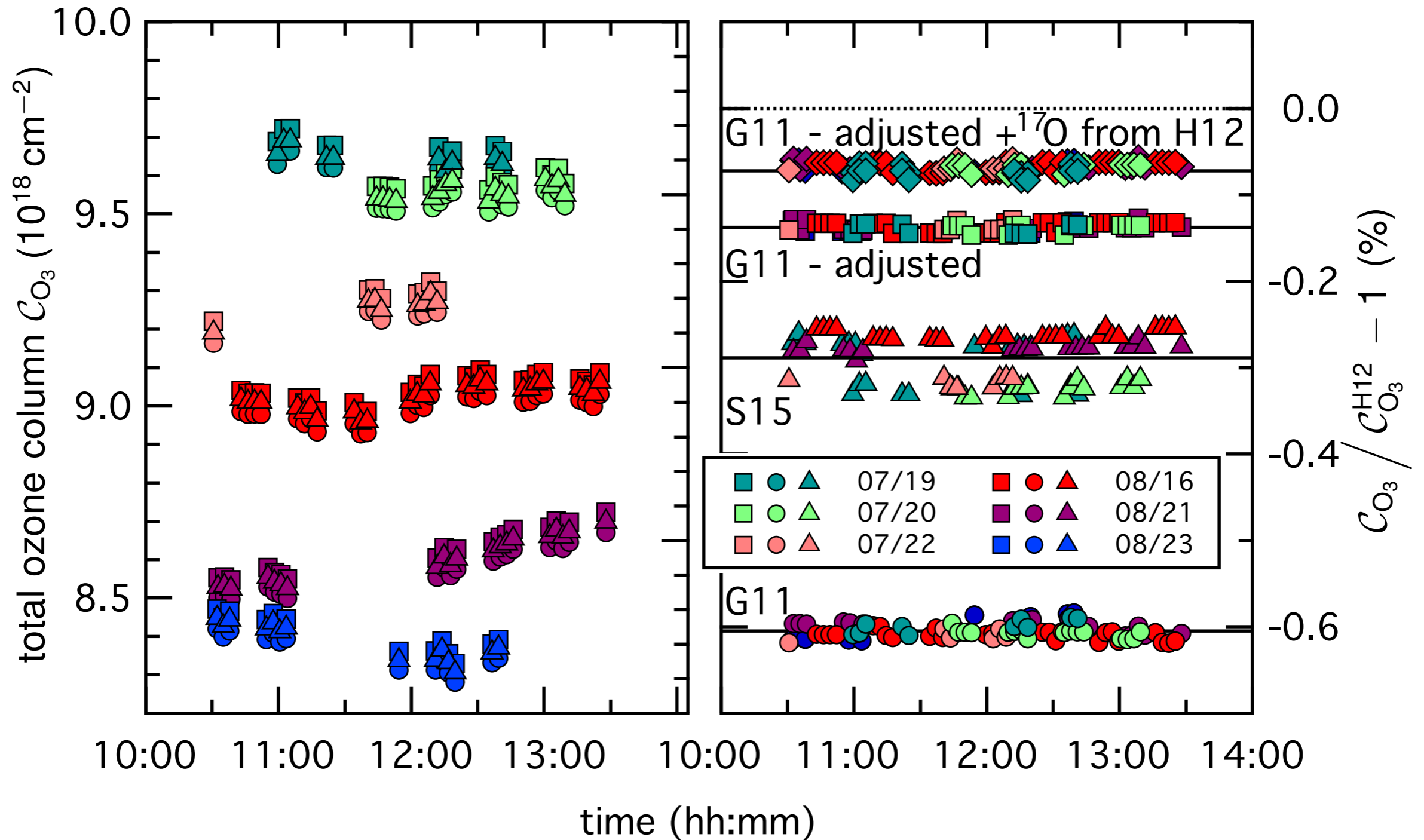


Atmospheric FT spectra over Paris



O₃ Multispectral Study - 10 μm

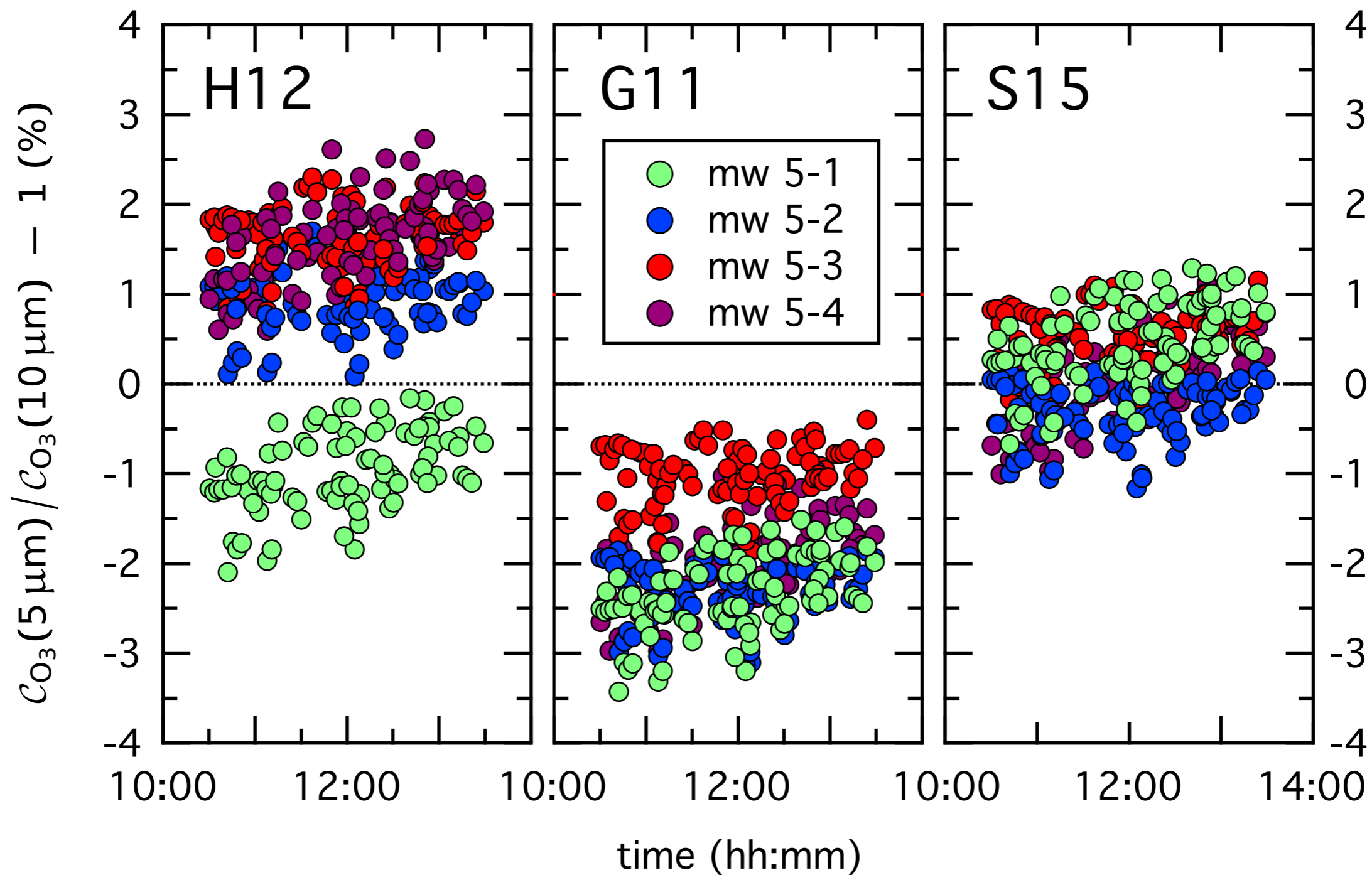
FTS-Paris



Janssen et al, *J. Mol. Spectrosc.* **326**, 48 (2016)

O₃ Multispectral Study 5 & 10 μm

FTS-Paris



Janssen et al, *J. Mol. Spectrosc.* **326**, 48 (2016)

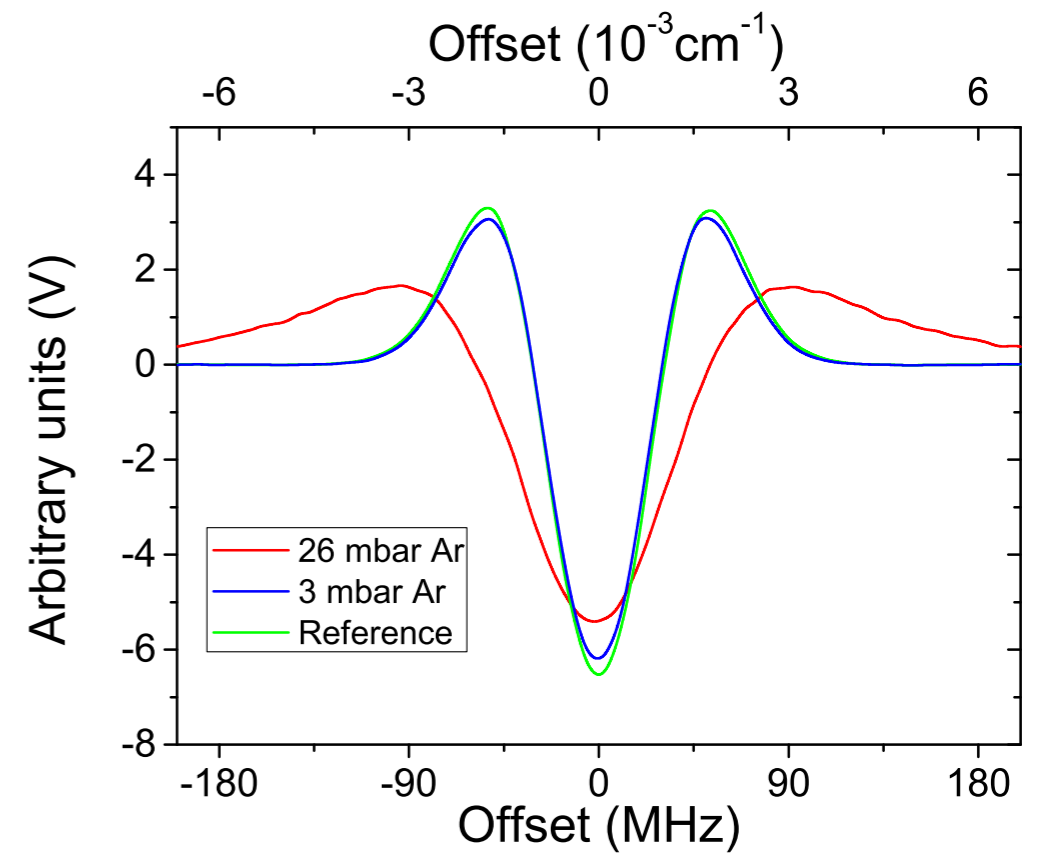
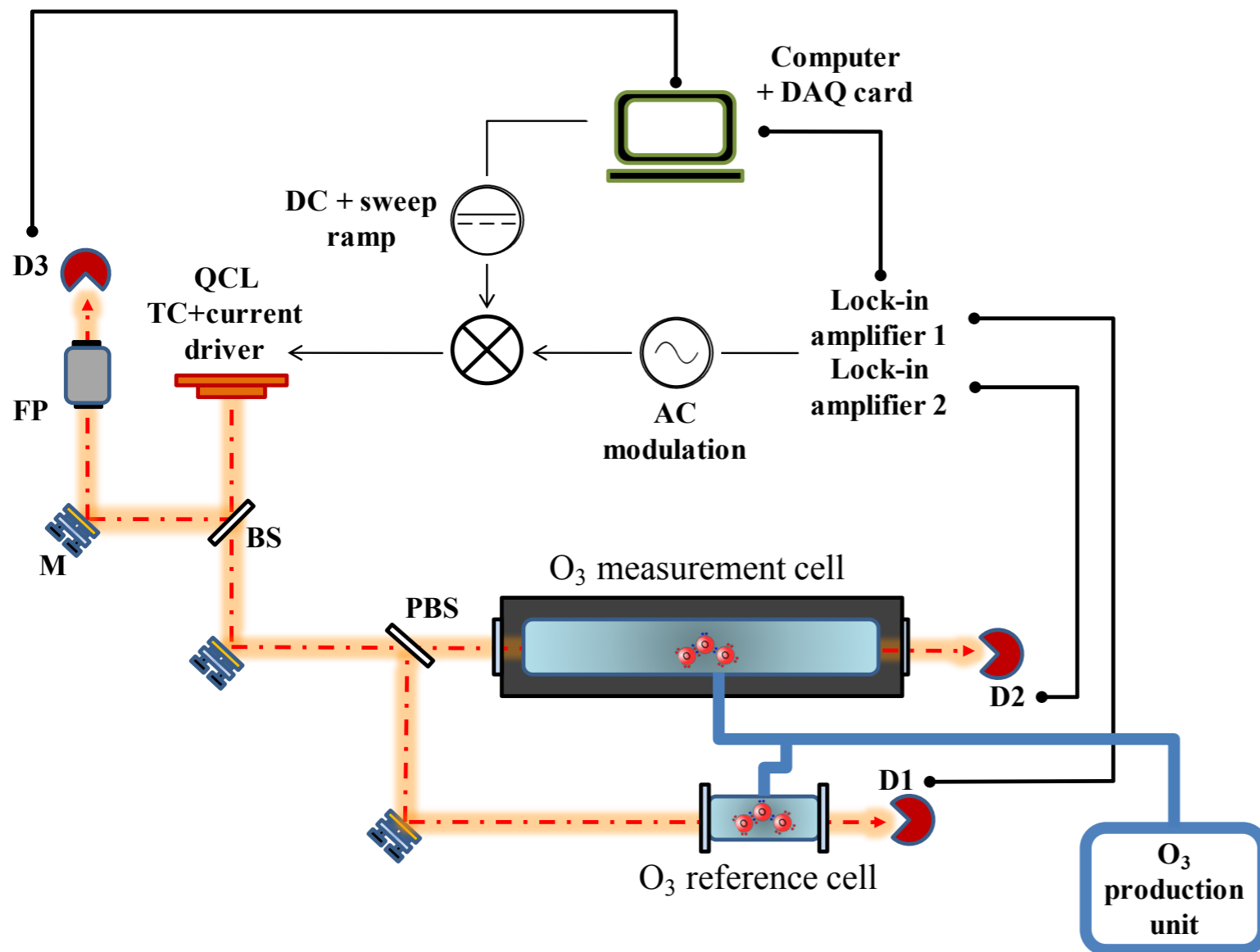
Short Summary

- At 10 μm data bases (DBs) are consistent ($< 1\%$)
- At 5 μm differences between DBs are larger ($> 1\%$)
- SM&PO data base is currently most consistent ($< 1\%$)
- obvious need to include isotopes in order to get to the $< 1\%$ accuracy level

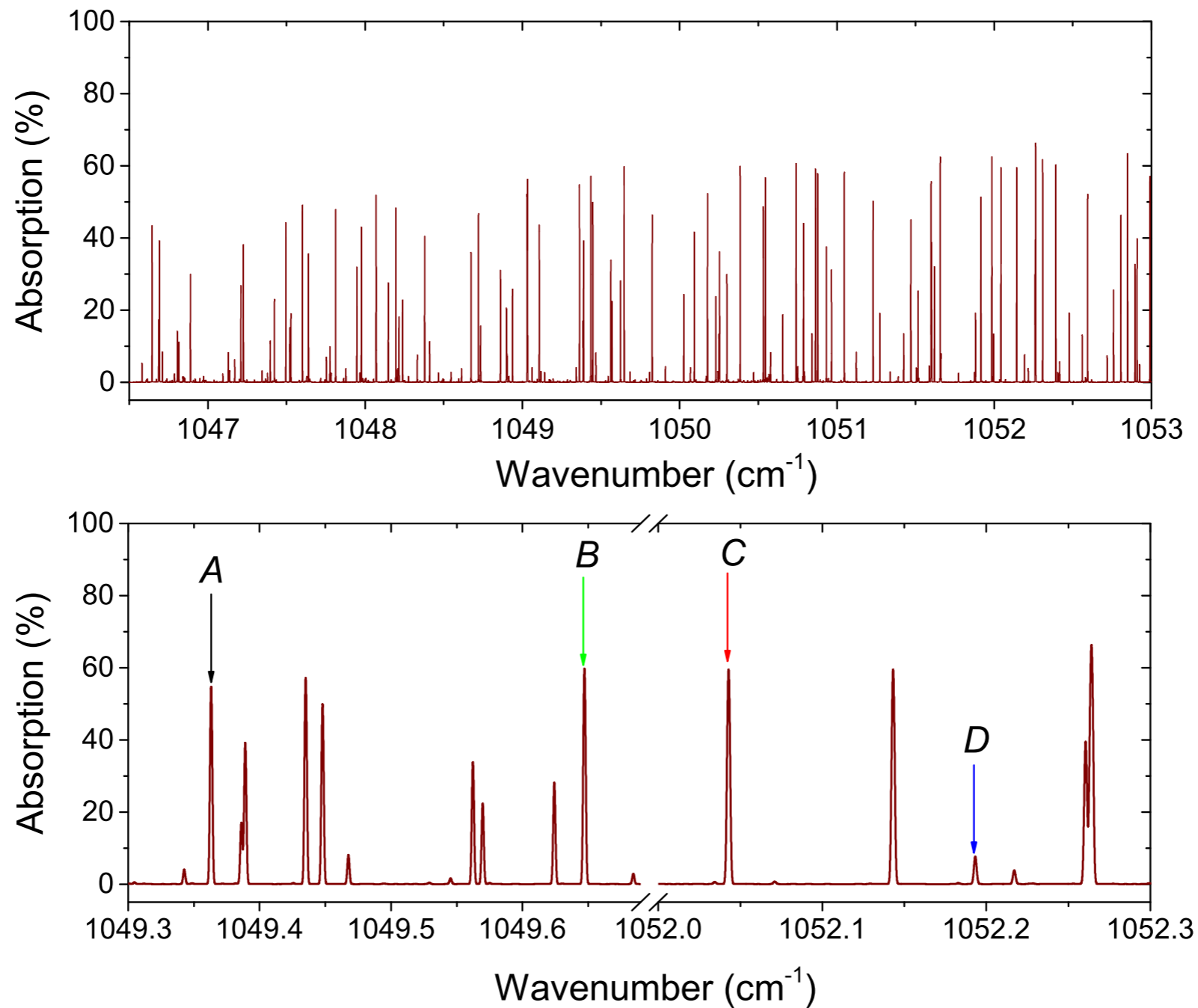
Pressure shift at 10 μm



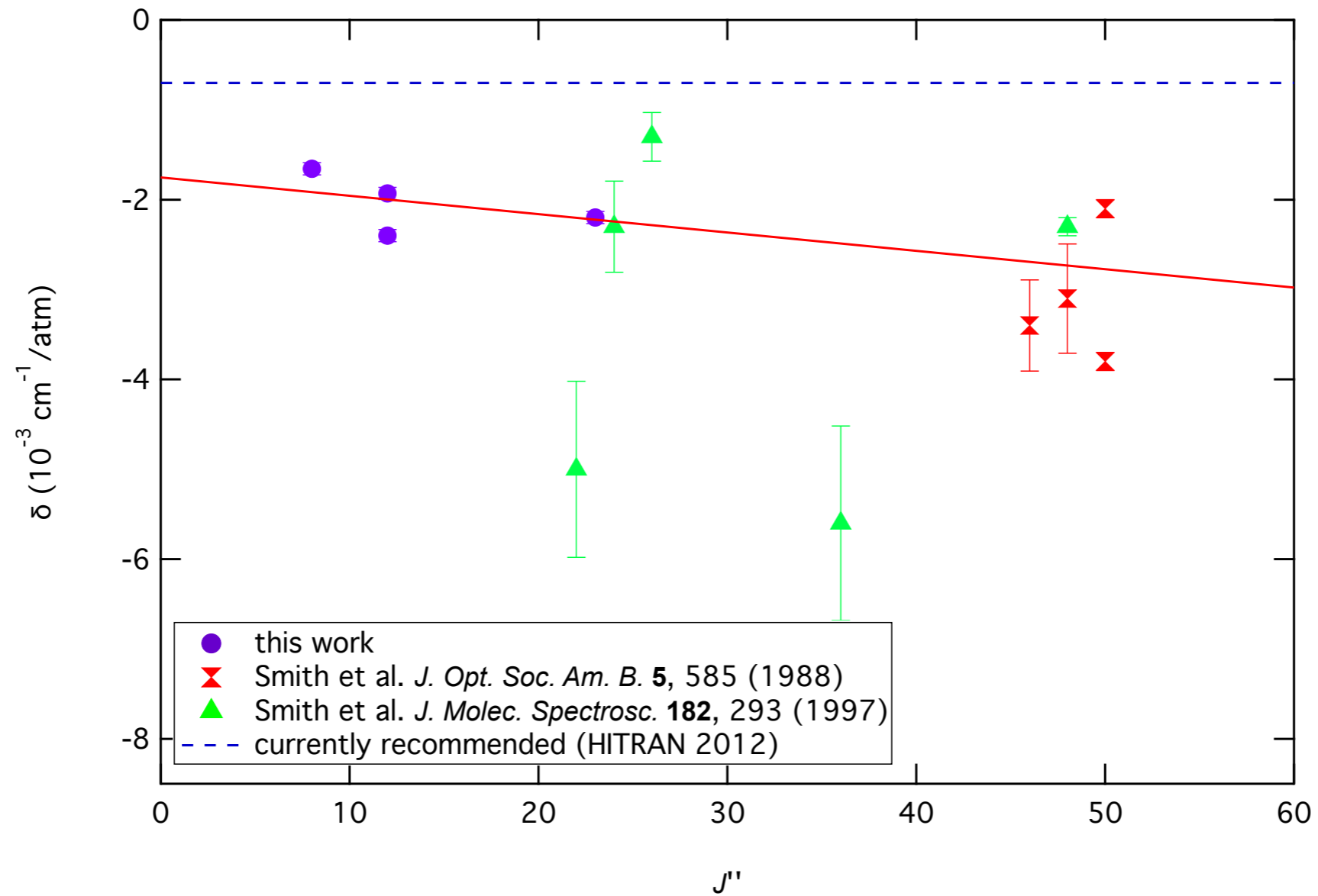
Pressure shift



Pressure shift



Pressure (air) shift



Minnissale et al, in prep. for publication in *J. Mol. Spectrosc.*

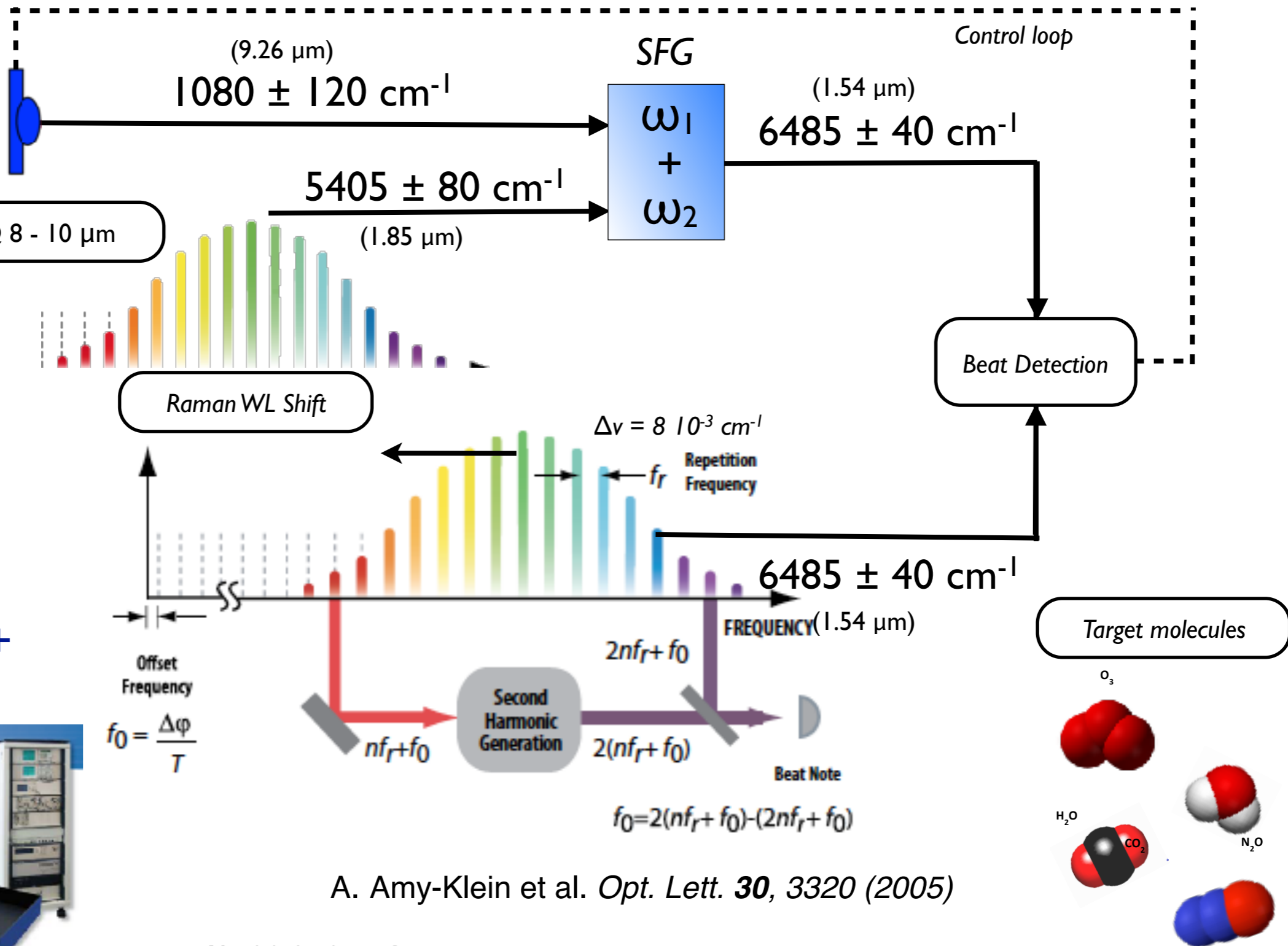
Ongoing project

l'Observatoire de Paris SYRTE
Systèmes de Référence Temps-Espace

REFIMEVE+



Menlo FCI 500-250-WG



A. Amy-Klein et al. *Opt. Lett.* **30**, 3320 (2005)

Thanks to

▶ colleagues

C. Boursier
H. Elandaloussi
P. Jeseck
D. Koshelev
C. Rouillé
Y. Té
T. Zanon

▶ former colleagues

C. Camy-Peyret
B. Daudé
M. Guinet
M. Minissale
D. Mondelain
D. Simone

▶ collaborators

A. Amy-Klein (LPL/F)
F. Néz (LKB/F)
H. Fleurbaey (LKB/F)
J. Gröbner (PMOD-WDC/CH)

▶ funding agencies



Virtual Atomic and Molecular Data Centre
(VAMDC: <http://www.vamdc.eu>)

Latest Achievements and
Prospects for Collaboration

M.L. Dubernet¹, C.M. Zwölf¹, N. Moreau¹, Y.A. Ba¹
And VAMDC Consortium Collaboration

¹LERMA Department, Paris Observatory
and Paris Observatory Data Center

History

The **VAMDC Consortium** is a technical and political framework for sharing Atomic and Molecular data

Build upon 2 FP7 European funded Projects:

- VAMDC: 2009-2012 with 25 different laboratories
 - ◆ The baseline of the Infrastructure
- SUP@VAMDC: 2012-2014 with 9 laboratories
 - ◆ Building the political framework
 - ◆ Expanding towards other communities
- Currently « VAMDC Consortium » is sustained
 - ◆ Via its members in kind (and cash via self-financing and fees for those not maintaining resources)
 - ◆ Via a small starting budget of 60kEuros for 4 years

Consortium Overview

M.L. Dubernet & al, J. Opt. Phys. B, (2016), 49, 074003

- The VAMDC consortium is:
 - ◆ Built on a Memorandum of Understanding.
 - ◆ Currently composed by 17 members who signed the MoU.
 - ◆ Officially launched on November 1, 2014.

- **Board of Directors:** Full members → Decisions

- **Science and Technical Board:** Full and Associated Members
 - ◆ Propose evolutions and Maintain the VAMDC infrastructure

- **How to join us** (accession documents)
 - ◆ Memorandum of Understanding
 - ◆ Internal Regulations
 - ◆ Roadmap

ABOUT US

Presentation

Partners



Databases



Virtual Tour

How to join us



VAMDC Consortium
MoU
Internal regulations
Roadmap
Infrastructure

Supporting Projects

Policy Citation

HOW TO JOIN THE VAMDC INFRASTRUCTURE

Step 1: If you want to share your atomic & molecular data through VAMDC infrastructure, please first contact the VAMDC team at support@vamdc.eu

Step 2: Once we agree on the terms, you might want to learn about the infrastructure

- [Tutorials](#)
- [Standards](#)

ABOUT US

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Virtual Tour

How to join us



VAMDC Consortium
MoU
Internal regulations
Roadmap
Infrastructure

Supporting Projects

Policy Citation

HOW TO JOIN VAMDC CONSORTIUM AS A MEMBER

You might become a VAMDC Consortium Member under conditions set up in the Memorandum of Understanding, Articles 3.1 and 3.2. For further details and information, contact director@vamdc.eu

MoU's Articles 3.1 and 3.2



3.1 VAMDC Consortium Full Members

- The VAMDC Consortium Full Members are institutions that hold physically a resource tagged « VAMDC », i.e. a database or a service registered in the "VAMDC" registries, or that maintain/update a documentation officially tagged « VAMDC ».
- Otherwise full members can be institutions paying annual membership fees set by the Board of Directors.

Full Members can participate in calls engaging the VAMDC infrastructure and can use the "VAMDC brand". Accession to full member status is granted by the Board of Directors and an accession document is signed.

3.2 VAMDC Consortium Associated Members

17 full members today, Full Membres candidates
+ Associated Members candidates

EUROPE

- Astronomska Opsevatorija (Serbia, [M. Dimitrijevic](#))
- Observatory of Cagliari - INAF (Italy, [G. Mulas](#))
- Observatory of Catania – INAF (Italy, [G. Leto](#))
- Observatory of Paris (France, M.L. Dubernet)
 - Legal Representative
- Queen's University Belfast (UK, T. Millar)
- Open University (UK, N. Mason)
- University of Cambridge (UK, N. Walton)
- University College London (UK, J. Tennyson)
- Uppsala Universitet (Sweden, N. Piskunov)
- Universitaet zu Koeln (Germany, S. Schlemmer)
- Université de Bordeaux (France, V. Wakelam)
- Université de Bourgogne (Dijon, V. Boudon)
- Université de Champagne-Ardenne (Reims, V. Tyuterev)
- Université Joseph Fourier (Grenoble, B. Schmitt)
- Université Paul Sabatier (Toulouse, C. Joblin)
- Université de Mons (Belgium, Quinet)
- Atomic and Molecular Data Unit (IAEA, B. Braams)

Africa

University of South Africa (D. Smits)

RUSSIA

- Institute for Astronomy RAS (T. Ryabchikova)
- Institute of Atmospheric Optics (V. Perevalov)
- Institute of Spectroscopy RAS (A. Ryabtsev) & RFNC (P. Loboda)

USA

- NIST (Y. Ralchenko, C. Gonzalez)
- The Harvard-Smithsonian Center for Astrophysics (L. Rothman)
- Jet Propulsion Laboratory from NASA, CALTECH (B. Drouin)

South America

- Universidade Federal do Paraná (Brazil, M. Fujimoto)
- Corporacion Parque tecnologico de Merida (IVIC, C. Mendoza)

ASIA- PACIFIC

- Tata Institute for Fundamental Research (India, E Krishnakumar)
- Indian School of Mines (India, B. Antony)
- Korea Atomic Energy Reserch Institute (South Korea, Y. Rhee)
- Australian National University Flinders University (Australia, M. Brunger)
- National Institute for Fusion Science (Japan, NIFS, I. Murakami)

ABOUT US

Presentation

Partners

France
UK
Germany
Sweden
Austria
Italy
Russia
USA
Australia
India
Korea
South Africa
Northern Ireland
Serbia
Venezuela

Databases

Virtual Tour

How to join us

Supporting Projects



**INAF – Cagliari
Astronomical
Observatory**
The National Institute for
Astrophysics is the leading
Italian Research Institute for
the Study of the Universe
www.oa-cagliari.inaf.it

[Read more](#)



**INAF-Catania
Astrophysical
Observatory**
The Catania Astrophysical
Observatory (OACT) is one
of the twelve observatories
which together with some
former CNR Institutes
www.oact.inaf.it/

[Read more](#)



Universitaet Wien
www.univie.ac.at/asap/main.php?s=databases

[Read more](#)



**Corporacion Parque
tecnologico de Merida**

[Read more](#)



**Institute of Atmospheric
Optics**
www.iao.ru/

[Read more](#)



**Russian Federal Nuclear
Center- All-Russian
Institute of Technical
Physics**

[Read more](#)



**Institute of Spectroscopy
RAS**
Institute for Spectroscopy
was established in 1968 as
a successor of the
Commission for
Spectroscopy within the
General physics and
astronomy Branch of the
USSR Academy of Sciences
isan.troitsk.ru/en/index.php?page=about

[Read more](#)



**Astronomical
Observatory Belgrade**
Founded jointly with the
Meteorological Observatory
on April, 7 1887,
Astronomical Observatory
of Belgrade (AOB) is one of
the oldest scientific
institutions in Serbia
www.aob.rs/

[Read more](#)

ACCESS TO THE VIRTUAL TOUR

Mapping of the VAMDC
partners and databases

[Access to
the virtual
tour](#)

MORE INFORMATION?

You have questions?
You want to participate
in our projects?

[Contact us](#)

VIRTUAL TOUR

Where we are

See our videos

- Research
- Education
- Industry
- Outreach



[All countries](#) ▾
 [All fields](#) ▾
 [All activities](#) ▾
 Databases
 Partners

PARTNERS

1/ INAF – Cagliari Astronomical Observatory
 The National Institute for Astrophysics is the leading Italian Research Institute for the Study of the Universe
www.cas-cagliari.inaf.it

[Read more](#)

2/ INAF-Catania Astrophysical Observatory
 The Catania Astrophysical Observatory (CACT) is one of the twelve observatories which together with some former CNR Institutes
www.cact.inaf.it/

[Read more](#)

DATABASE

1/ PAH
 The Theoretical Spectral Database of Polycyclic Aromatic Hydrocarbons was developed in collaboration by G. Mallocci and G. Mulas

[Read more](#)

2/ ECaSDa – Ethylene Calculated Spectroscopic Database
 Calculated data of ethylene (12C2H4). The data on ethylene contain the vibration-rotation energy levels, line positions
vamdc.univ-reims.fr/PHP/ethylene.php

[Read more](#)

ACCESS TO THE FORUM

Exchange ideas, Ask questions, Find answers

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or

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MORE INFORMATION?

You have questions?
You want to participate in our projects?

[Contact us](#)

SEE OUR BLOGS

Links to blogs related to atomic and molecular data or astronomy

[See our blogs](#)

Databases	Type of A&M Data	Partners	Application's Fields
VALD	Atomic Linelists	Uppsalla, Vienna, Moscow – N. Piskunov	Stellar - GAIA
CHIANTI	Atomic Linelists and collisions	Cambridge (UK)+MSSL/UCL – H. Mason, G. Rixon	Solar Physics
Spectr-W3	Atomic Linelists and Collisions	Russia (RFNC VNIITF) – P. Loboda	Solar/Stellar Physics + Fusion
Stark-B	Atomic LineShifts/Broadening with charged perturbers	Observatory of Belgrade (Serbia) + Observatory of Paris (LERMA) – M. Dimitrijevic/S. Sahal-Bréchet	Stellar Physics + Plasmas
TipBase, TopBase	Atomic Linelists and Collisions from Opacity Project and IRON Project	Observatory of Paris (LERMA) + CTPM (Venezuela) + CDS (Strasbourg, Fce) – C. Zeippen/ C. Mendoza/F. Delahaye	Stellar Physics
CDMS	Molecular Linelists (mm, Sub-mm)	Cologne (Germany) – S. Schlemmer	ISM + Earth
JPL	Molecular Linelists (mm, Sub-mm)	Pasadena (USA) + Cologne (Germany) – B. Drouin	ISM + Earth
SMPO	O ₃ linelists	Reims (France)+ Tomsk (Russia) – V. Tyuterev	Earth – Exo-Planets
MeCaSDa	Linelists CH ₄	Dijon (France) – V. Boudon	Earth, Planets, Exo-Planets,

Databases	Type of A&M Data	Partners	Application's Fields
HITRAN	Molecular Linelists and Broadening Coefficients	Harvard (USA) + UCL – L. Rothman+J. Tennyson	Earth, Planets, Exo-Planets
CDSO	CO ₂ Linelists	IAO, Tomsk – V. Perevalov	Earth, Planets, Brown Dwarfs
W@SIS	Water Information System	IAO, Tomsk – A. Fazliev+ UCL (J. Tennyson)	Earth and Planets
KIDA	Kinetic Data	Bordeaux (France) – V. Wakelam	ISM - Planetology
UdfA	Kinetic Data (ex-UMIST)	Belfast (UK) – T. Millar	ISM - Planetology
GhoSST	Solid Spectroscopy Data	Grenoble (France) – B. Schmitt	Planetology, ISM
LASP	Solid Spectroscopy Data	Obs. of Catania – G. Leto	Planetology, ISM
BASECOL	Low Energy Molecular Collisions	Observatory of Paris – M.L. Dubernet	ISM
PAH	PAH Theoretical Data and soon experimental Data	Observatory of Cagliari (Italy) – IRAP (Toulouse, France) – G. Mulas+C. Joblin	ISM and Planets

Databases	Type of A&M Data	Partners	Application's Fields
RADAM Ion interaction	Database for Radiation damage of molecules of biological interest induced by ion collisions: cross sections and fragmentation yields	GANIL - FRANCE	Biology – radiation Damage
IDEABD	Dissociative electron attachment upon interaction of low energy electrons with molecules.	Innsbrück	Radiation Damage, Planets, ExoPlanets,
BEAM-DB	Molecular/atom—electron collisions	Belgrade, Serbia	Biology, radiation damage
ECaSDa	Ethene Calculated LInelists	Reims – L. Daumont	Earth and Planets
ALADDIN2	Sub-Set of IAEA ALADDIN : atomic collisions	IAEA – Vienna – B. Braams	Plasmas
DESIRE	Spectroscopy of sixth row elements (Z=72-86)	Belgium – P.Quinet	Plasmas – Stellar - Solar
SESAME	Electronic Spectra of atoms and molecules	Paris Obs. – E. Roueff	ISM - Stellar

Databases	Type of A&M Data	Partners	Application's Fields
SHeCaSDa	Hexafluoride Calculated LInelists	Dijon – V. Boudon	Earth and Exo-Planets
TFMeCaSDa	Tetrafluoro-Methane calculated linelists	Dijon – V. Boudon	Earth
MOLD	Photo-Dissociation Cross-sections	Belgrade - Serbia	Stellar
LxCAT	Low temperature plasmas data	L Pitchford - Toulouse	Plasmas
NIST Atomic Spectra	Spectroscopy of Atoms –	NIST – Yuri Ralchenko	Stellar – ISM - Plasmas
IAMDB	Indian Atomic and Molecular Database (atomic collisions, A+M spectroscopy)	Tata Institute Fundamental Research, ISM, Sandar Patel Univ	Astrophysics
DREAM	Radiative data for rare earth	Belgium – P Quinet	Stellar-Solar-Plasmas – Lighting -
ExoCross	Molecular Linelists	UK – UCL – J. Tennyson	Exo, Brown Dwarf, Earth, Stellar

User Communities

➤ Atmospheric Science

- ◆ input for complex terrestrial atmosphere/climate models, determination of concentrations and radiative transport of about 100 species

➤ Astrophysics, Astrochemistry and Planetary Science

- ◆ great need for reliable A&M data because of extraordinary range of physical conditions

➤ Plasma Technologies

- ◆ plasma-assisted materials processing or surface modification, e.g. manufacture of semi-conductor chips. A&M data needed for modeling chemically active plasmas.

User Communities cont'd

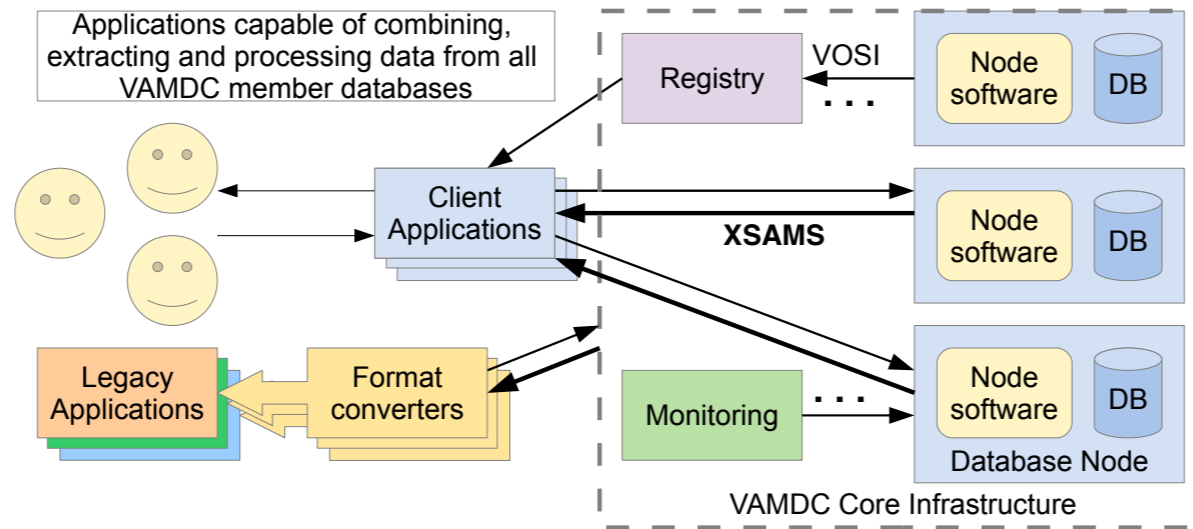
➤ Fusion Energy Research

- ◆ design and operation of vital fusion device systems require large amounts of A&M collisional and spectroscopic data

➤ Radiation Science

- ◆ radiotherapy models exploring damage of DNA by radiation need A&M data, e.g. electron collisions with DNA components and other biomolecules

How is VAMDC technically organised ?



- A set of standards (www.vamdc.eu/standards)
 - ◆ Data exchange Protocols, Data Description
 - ◆ Standard vocabulary for all exchanges, including for registration of resources
- A set of software (www.vamdc.eu/software)
- Documentation and on-line support system (www.vamdc.eu)
- Monitoring of services

RESEARCH SERVICES

Access to Data

VAMDC Research Portal
RADAM Portal

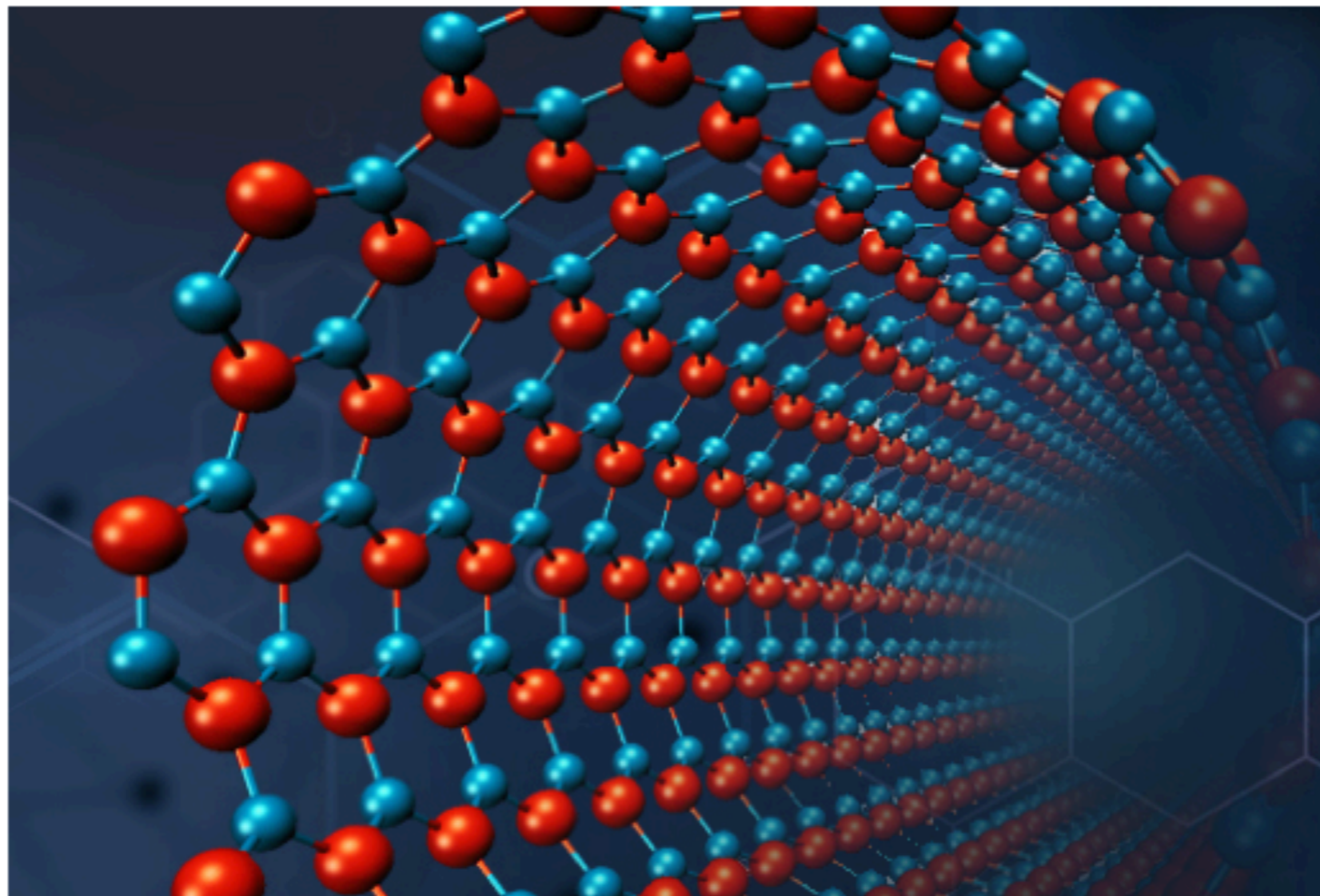
Software

SPECTCOL
SPECVIEW
XSAMS Converter
PDL-VAMDC
JavaScriptPortal
TAPValidator
Java NodeSoftware
Python NodeSoftware
Libraries
Virtual machines for node building

Documents

Standards
Science use cases
Tutorials
See our videos
FAQ

SERVICES [RESEARCH]



VAMDC aims to be an interoperable e-infrastructure that provides the international research community with access to a broad range of atomic and molecular (A&M) data compiled within a set of A&M databases accessible through the provision of a single portal and of user software. Furthermore VAMDC aims to provide A&M data providers and compilers with a large dissemination platform for their work.

ACCESS TO THE DATA

Access to VAMDC databases

[Access to the data](#)

ACCESS TO THE FORUM

Exchange ideas, Ask questions, Find answers

[Read more](#)

or

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What can we currently do with VAMDC?

Virtual Atomic and Molecular Data Centre

- Query all registered databases via the Portal (www.portal.eu) or other portals
 - ◆ Visualisation of Data
 - ◆ Download of Data
- Standalone Work with Software:
 - ◆ Query databases & Mix heterogeneous databases
 - ➔ *Example of SPECTCOL software*
- Use of our libraries in user applications in order to access the VAMDC registered databases
- Include new databases or data in the infrastructure

Welcome to the VAMDC portal!

VAMDC aims to be an interoperable e-infrastructure that provides the international research community with access to a broad range of atomic and molecular (A&M) data compiled within a set of A&M databases accessible through the provision of this portal and of user software. Furthermore VAMDC aims to provide A&M data providers and compilers with a large dissemination platform for their work.

VAMDC infrastructure was established to provide a service to a wide international research community and has been developed in conjunction with consultations and advice from the A&M user community.

[Currently we have 29 databases running and ready to serve you with the data.](#)



Citation policy

You commit to cite the authors of the specific datasets you may use for realizing any published work, the databases publishing those datasets and the VAMDC Consortium.

- Citation of data should be done via normal reference from journals and Digital Object Identifier of datasets when such DOI will be implemented
- Citation of databases should be done via citing the name of the database, the URL of the database and the reference provided by the database to cite it
- Citation of VAMDC Consortium should be done via citing both its Name: « VAMDC Consortium » and the URL: « <http://www.vamdc.org> »

2 query forms

Tutorial for Portal

Welcome to the VAMDC portal!

VAMDC aims to be an interoperable e-infrastructure that provides the international research community with access to a broad range of atomic and molecular (A&M) data compiled within a set of A&M databases accessible through the provision of this portal and of user software. Furthermore VAMDC aims to provide A&M data providers and compilers with a large dissemination platform for their work.

VAMDC infrastructure was established to provide a service to a wide international research community and has been developed in conjunction with consultations and advice from the A&M user community.

You must accept the following disclaimer to use our services (this will install a cookie in your web browser) :

Accept Decline

General Disclaimer

The VAMDC Consortium and its activities are based upon a high trust model within an academic environment. In case of an (alleged) infringement of any right of third parties, the Consortium should be contacted in writing in order to discuss the issue. In order to minimize the risks it should be clarified that the Consortium shall not provide any guarantee and/or warranty with respect to a fitness-for-purpose and furthermore that the Consortium shall not identify any party for any (alleged) infringement of any rights of third parties (including but not limited to intellectual and industrial property rights and/or rights of confidentiality).

Disclaimer for final users accessing the data and or running online services/processing (this disclaimer should be applied to all the web services provided by VAMDC in any form (TAP services, online code, etc))

Tutorials For Portal

RESEARCH SERVICES

Access to Data

VAMDC Research Portal
RADAM Portal

Software

SPECTCOL
SPECVIEW
XSAMS Converter
PDL-VAMDC
JavaScriptPortal
TAPValidator
Java NodeSoftware
Python NodeSoftware
Libraries
Virtual machines for node
building

Documents

Standards
Science use cases
Tutorials
See our videos
FAQ

TUTORIALS

We provide different tutorial addressed both to data providers and final users.
Follow the links below for further information on each item of the following list:

- [General page for Tutorials](#)
- You produce/collect atomic and molecular data and want to include them into VAMDC
 - [Outline](#)
 - [Self-Study Course](#)
- How to use the [VAMDC Portal](#)
 - [User Guide for the Portal](#)
 - [First Steps with the VAMDC Portal](#)
 - [Extracting Data from query results with the viewers](#)
- How to use VAMDC software
 - [Spectcol](#) – [Readmore](#)
 - [Specview](#) – [Readmore](#)
 - [PDL-VAMDC](#) – [Readmore](#)
 - [The XSAMS file format and TAP Validator application](#) (mainly for the data providers)
 - [Python Scripting](#)
 - [Using VAMDC Java libraries](#)
- You want to check [XSAMS files](#), [TAPValidator](#) – [ReadMore](#)

ACCESS TO THE DATA

Access to VAMDC
databases

[Access to
the portal](#)

ACCESS TO THE FORUM

Exchange Ideas, Ask
questions, Find answers

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or

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the forum](#)

- SQL-like requests
- Example : `select * where ((AtomSymbol = 'he') OR (AtomSymbol = 'li'))`
 - All quantities are well defined into a dictionary
 - <http://dictionary.vamdc.eu>



The screenshot shows the VAMDC Dictionary website interface. At the top, there is a blue header with the VAMDC logo (Virtual Atomic and Molecular Data Centre) on the left and the text "VAMDC Dictionary" on the right. Below the header, the page is organized into sections, each with a title and a "Show/Hide" link:

- Returnables**
- Atoms and atomic states**
[Show/Hide](#)
- Molecules, their states and quantum numbers**
[Show/Hide](#)
- Solids and Particles**
[Show/Hide](#)
- Processes**
[Show/Hide](#)
- Environments, Functions, Methods and Sources**
[Show/Hide](#)
- Unclassified Keywords**
[Show/Hide](#)

At the bottom of the page, there are logos for PADC (Paris Astronomical Data Centre), Observatoire de Paris, and LERMA (Laboratoire d'Etude du Rayonnement et de la Matière en Astrophysique).

Molecules, their states and quantum numbers

Show/Hide

Keyword	Short Description	Long Description	Type	*
MoleculeBasisStates	The basis states for a set of molecular states expressed as a linear combination on some basis	The basis states for a set of molecular states expressed as a linear combination on some basis		
MoleculeCASRegistryNumber	CAS registry number of molecule	CAS registry number of molecule	String	
MoleculeCNPIGroup	CNPI group of molecule	CNPI group of molecule	String	
MoleculeChemicalName	Molecule name	Conventional molecule name, e.g. CO ₂ , NH ₃ , Feh (may not be unique)	String	
MoleculeComment	Comment on molecule	Comment on molecule	String	
MoleculeIUPACName	IUPAC name of molecule	IUPAC name of molecule	String	
MoleculeInchi	Inchi of molecule	Inchi of molecule	String	
MoleculeInchiKey	InchiKey if molecule	InchiKey if molecule	String	
MoleculeIonCharge	Molecule ion charge	Molecule ion charge	Integer	
MoleculeMolecularWeight	molecular weight	molecular weight	Float	*
MoleculeNormalModeDisplacementVectorComment	Comments concerning this normal mode's displacement vectors	Comments concerning this normal mode's displacement vectors	String	
MoleculeNormalModeDisplacementVectorMethod	Method for displacement vector in molecule normal mode	Method for displacement vector in molecule normal mode	String	
MoleculeNormalModeDisplacementVectorRef	A reference to the atom in the molecule's structure to which this displacement vector applies	A reference to the atom in the molecule's structure to which this displacement vector applies	String	

Query by...

Species

Processes

Environment

Advanced

Atom 1

Clear «

Atom symbol

He

Mass number

to

Nuclear charge

to

Ion charge

to

InChIKey

State energy

to

1/cm

Equivalent to

1/cm

Molecule 1

Clear «

Chemical name

Stoichiometric formula

CO

Structural formula

CO

Spin isomer

COS

CO2

Standard InChIKey

CO+

COS+

CO2+

Find data

Reset

Legend

available, can answer

available, don't support query

unsupported keyword

- ▶ Belgrade electron/atom(molecule) database (BEAMDB)
- ▶ TFMeCaSDa - CF4 Calculated Spectroscopic Database
- ▶ Photodissociation - MolD database
- ▶ Chianti
- ▶ GSMA Reims S&MPO
- ▶ ECaSDa - Ethene Calculated Spectroscopic Database
- ▶ GhoSST
- ▶ SHeCaSDa - SF6 Calculated Spectroscopic Database
- ▶ Stark-b
- ▶ JPL database: VAMDC-TAP service
- ▶ HITRANonline
- ▶ RADAM - Ion Interactions
- ▶ MeCaSDa - Methane Calculated Spectroscopic Database
- ▶ VALD (atoms)
- ▶ VAMDC species-DB
- ▶ LXcat
- ▶ OACT - LASP Database
- ▶ TOPbase : VAMDC-TAP interface
- ▶ BASECOL: VAMDC-TAP interface
- ▶ UMIST Database for Astrochemistry
- ▶ IDEADB - Innsbruck Dissociative Electron Attachment Database
- ▶ TIPbase : VAMDC-TAP interface

- Repository of all species contained in the infrastructure, sorted by database
- <http://species.vamdc.eu>
- Browsable through a web site to find quickly where a species can be found,
- Data can be exported in a xls file, easy to sort or to convert to csv
- Queryable through an API :
 - <http://species.vamdc.eu/api/v12.07/nodes>
 - <http://species.vamdc.eu/api/v12.07/species>
- Returns JSON structured data

Search

VALD sub-set in Moscow (obs)

All nodes

Species name

Stoichiometric formula

Mass min

Mass max

Search

All nodes

Species name

Stoichiometric formula

Mass min

Mass max

Charge min

Charge max

Name	Stoichiometric formula	InChI	Mass number	InChIKey	Charge
Helium	He	InChI=1S/He/i1-1	3	SWQJXJUGLN CZEY- BJUDXGMSA- N	0
Helium	He	InChI=1S/He/i1+0	4	SWQJXJUGLN CZEY- IGMARMGPSA- N	0

BASECOL: VAMDC-TAP interface

Name	Stoichiometric formula	InChI	Mass number	InChIKey	Charge
CO	CO	InChI=1S/CO/c1-2	28	UGFAIRIUMAV XCW- UHFFFAOYSA- N	0

CDMS

Name	Stoichiometric formula	InChI	Mass number	InChIKey	Charge
Carbon Monoxide	CO	InChI=1S/CO/c1-2	28	UGFAIRIUMAV XCW- UHFFFAOYSA- N	0
Carbon Monoxide	CO	1S/CO/c1-2/i1+1	29	UGFAIRIUMAV XCW- OUBTZVSYSA- N	0
Carbon Monoxide	CO	1S/CO/c1-2/i2+1	29	UGFAIRIUMAV XCW- VQEHIDDOSA- N	0
Carbon	CO	1S/CO/c1-2/i2+	30	UGFAIRIUMAV XCW-	0

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PDL-VAMDC
JavaScriptPortal
TAPValidator
Java NodeSoftware
Python NodeSoftware
Libraries
Virtual machines for node
building

Documents

Standards

Science use cases
Tutorials
See our videos
FAQ

STANDARDS

VAMDC standards are a set of norms, protocols, regulations which are the basis of the VAMDC-infrastructure operations.

Follow the links below for further information on each item of the following list:

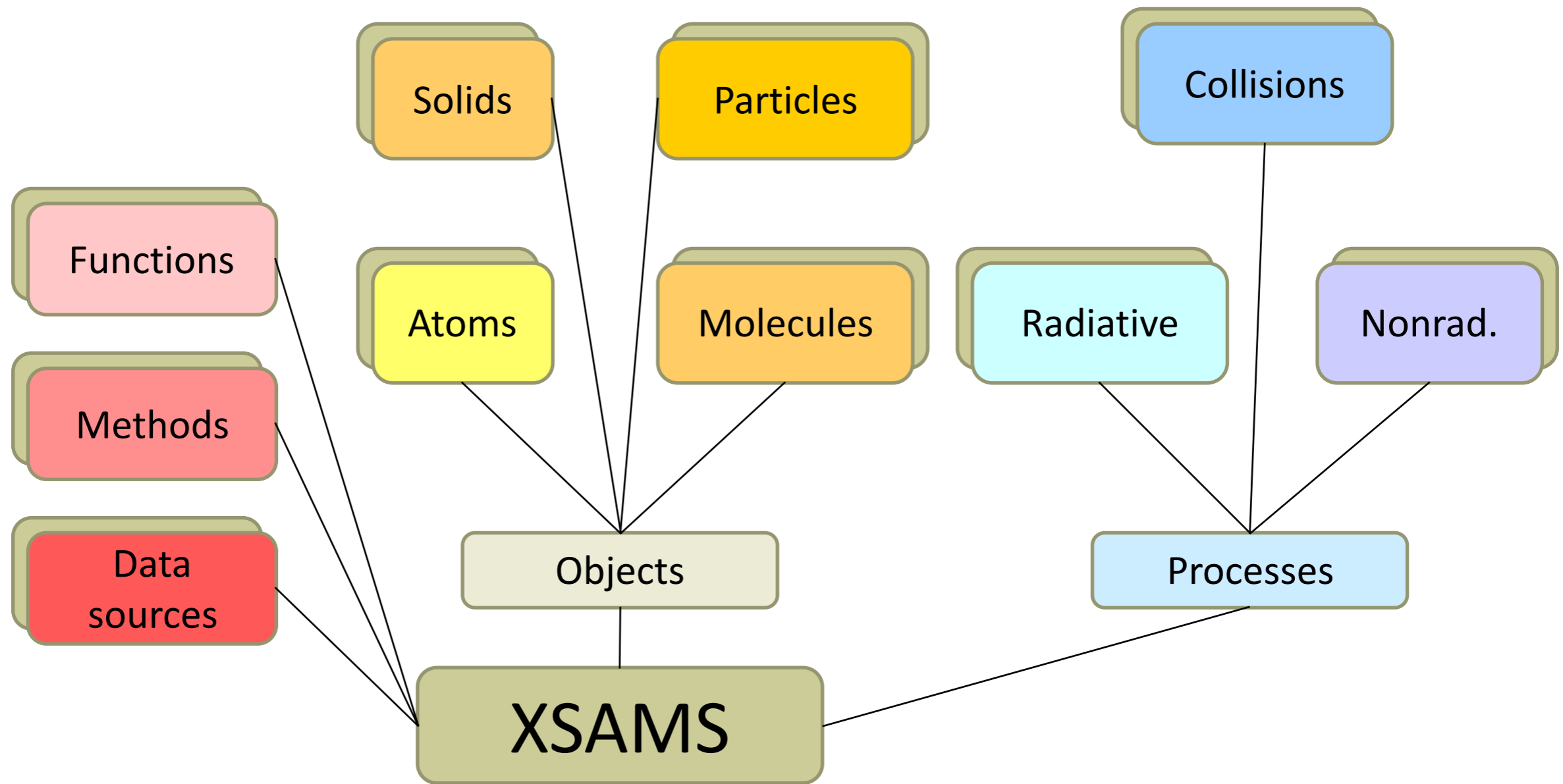
- [VAMDC standards documentation page](#)
 - [VAMDC documentation and software versioning policy](#)
 - [Data access protocol, query language and dictionaries](#)
 - [Data model](#)
 - [Registry](#)
 - [Units](#)
 - [InChI Generation](#)
 - [XSAMS Processor service](#)

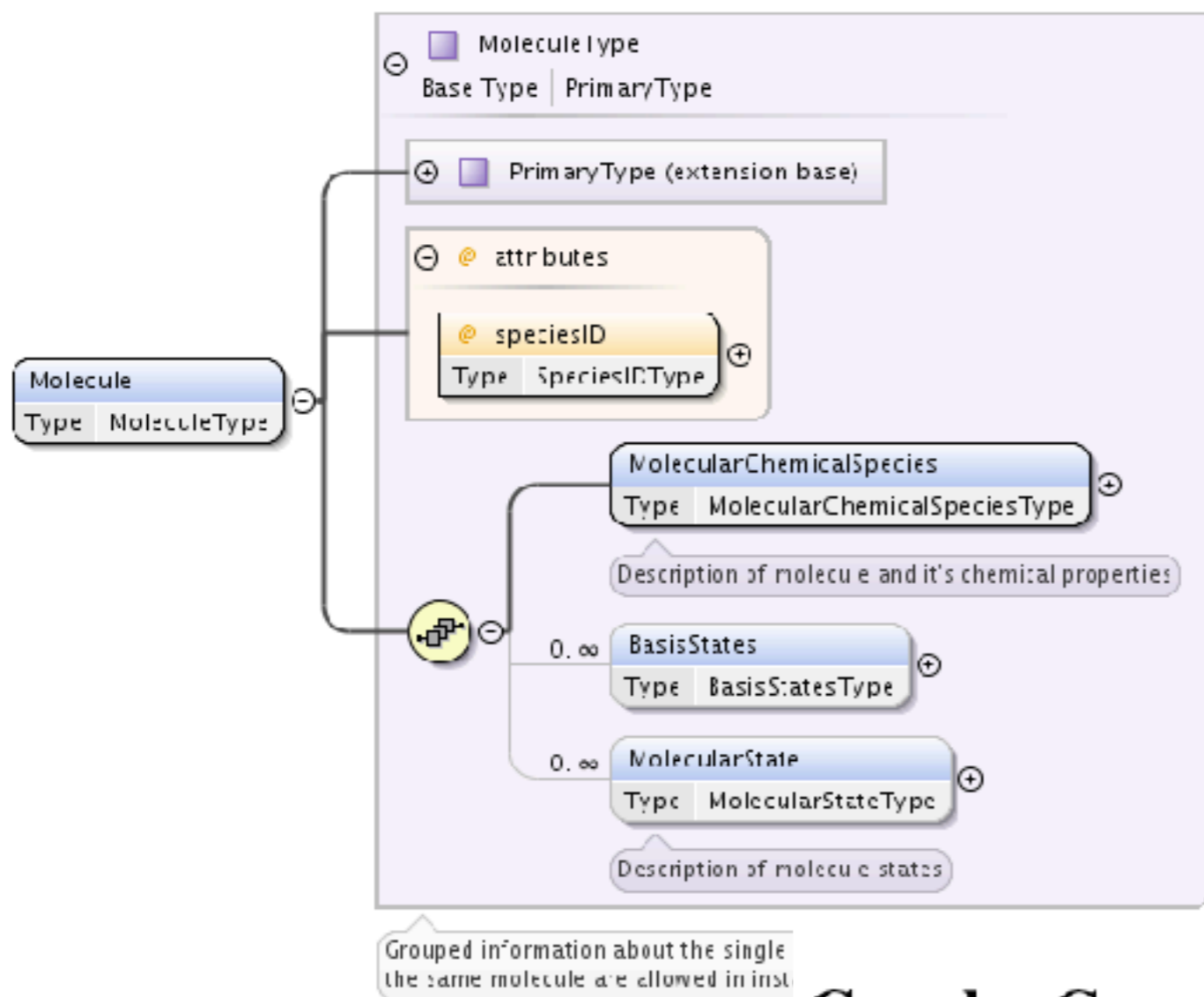
Official citation of VAMDC standards

The official citation of VAMDC standards is:

« M. L. Dubernet, M. Doronin, C. Endres, C. Hill, T. Marquart, L. Nenadovic, Y. Ralchenko, G. Rixon and K. Smith, VAMDC Standards Documentation and Reference Guides, version r12.07, Virtual Atomic and Molecular Data Centre, <http://standards.vamdc.eu> (2012) »

XSAMS tree: XML Schema for Atoms, Molecules and Solids

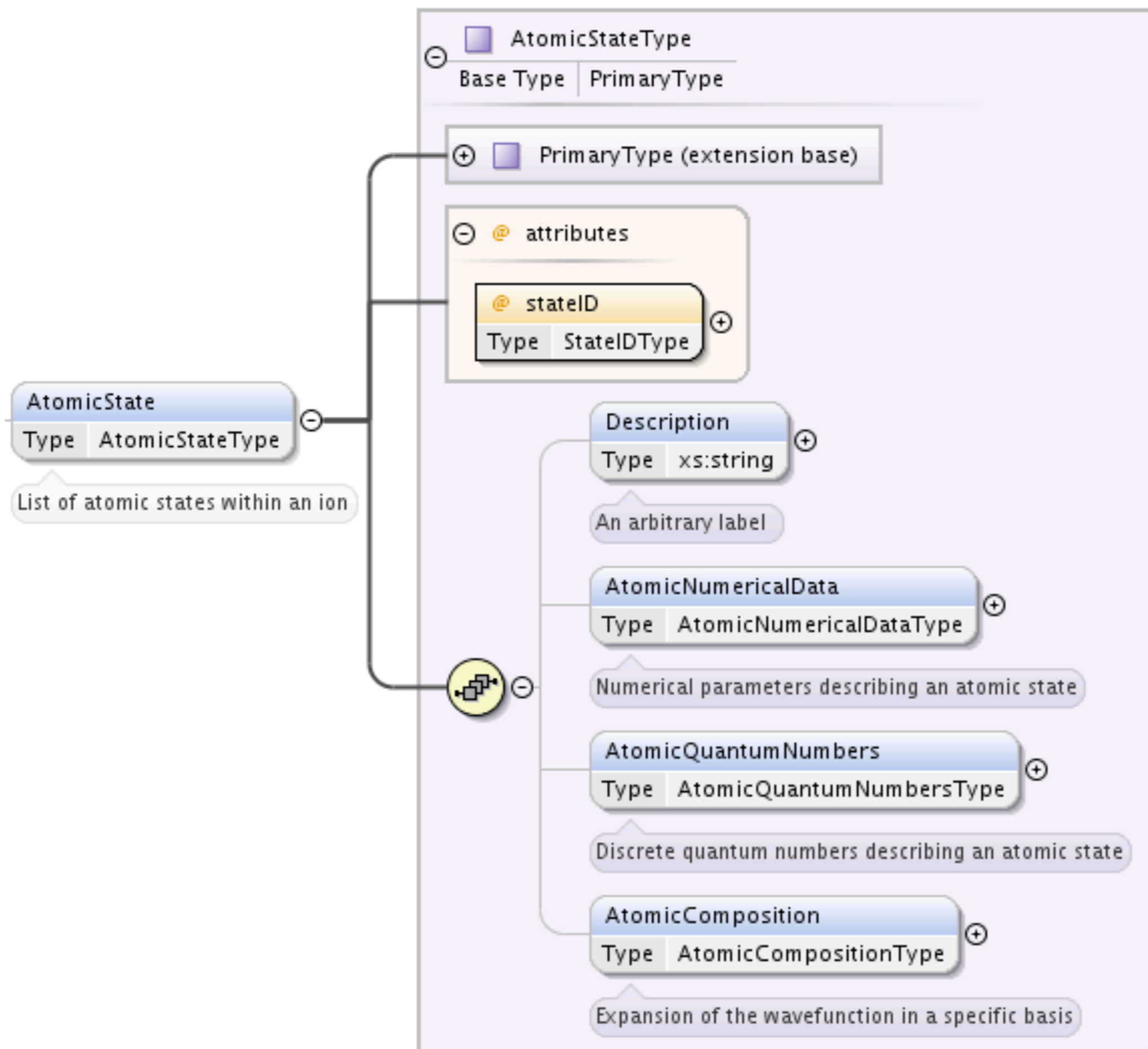




Case-by-Case Quantum Number Descriptions

1. [dcs](#): Diatomic closed-shell molecules
2. [hunda](#): Hund's case (a) diatomics
3. [hundb](#): Hund's case (b) diatomics
4. [ltes](#): Closed-shell, linear triatomic molecules
5. [nltes](#): Closed-shell, non-linear triatomics
6. [stcs](#): Closed shell, symmetric-top molecules
7. [lpcs](#): Closed-shell, linear polyatomic molecules
8. [asymcs](#): Closed-shell, asymmetric top molecules
9. [asymos](#): Open-shell, asymmetric top molecules
10. [sphcs](#): Closed-shell, spherical-top molecules
11. [sphos](#): Open-shell, spherical-top molecules
12. [ltos](#): Open-shell, linear triatomic molecules
13. [lpos](#): Open-shell, linear polyatomic molecules
14. [nlto](#): Open-shell, non-linear triatomic

AtomicState



Actions

Results from VAMDC node

1: Rotational de-excitation of CO ($v=0$) by He (Cecchi-Pestellini & al, 2002)

Rate Coefficients

Energy Table of CO

Energy Table of He

2: Vibrational de-excitation of CO by He (Cecchi-Pestellini & al., 2002)

Rate Coefficients of Rotational de-excitation of CO ($v=0$) by He (Cecchi-Pestellini & al, 2002)

<input type="button" value="Unselect all"/>	I1	I2	F1	F2	5.0	10.0	20.0	40.0	60.0	80.0	100.0	200.0	300.0
<input checked="" type="checkbox"/>	2	1	1	1	3.4E-11	3.2E-11	3.0E-11	2.8E-11	2.7E-11	2.6E-11	2.6E-11	2.5E-11	2.5E-11
<input checked="" type="checkbox"/>	3	1	1	1	1.3E-11	1.3E-11	1.2E-11	1.1E-11	1.1E-11	1.1E-11	1.1E-11	1.4E-11	1.6E-11
<input checked="" type="checkbox"/>	3	1	2	1	4.2E-11	4.5E-11	4.5E-11	4.6E-11	4.7E-11	4.6E-11	4.9E-11	5.0E-11	5.2E-11
<input checked="" type="checkbox"/>	4	1	1	1	6.2E-12	6.6E-12	7.2E-12	8.5E-12	9.5E-12	1.0E-11	1.1E-11	1.2E-11	1.3E-11
<input checked="" type="checkbox"/>	4	1	2	1	2.3E-11	2.2E-11	2.0E-11	1.8E-11	1.8E-11	1.8E-11	1.9E-11	2.2E-11	2.6E-11
<input checked="" type="checkbox"/>	4	1	3	1	4.6E-11	4.9E-11	5.0E-11	5.1E-11	5.2E-11	5.3E-11	5.4E-11	5.8E-11	6.1E-11
<input checked="" type="checkbox"/>	5	1	1	1	1.8E-12	1.9E-12	1.9E-12	2.0E-12	2.1E-12	2.1E-12	2.2E-12	2.6E-12	3.1E-12
<input checked="" type="checkbox"/>	5	1	2	1	1.3E-11	1.4E-11	1.5E-11	1.7E-11	1.8E-11	2.0E-11	2.1E-11	2.4E-11	2.7E-11
<input checked="" type="checkbox"/>	5	1	3	1	2.7E-11	2.7E-11	2.4E-11	2.2E-11	2.2E-11	2.2E-11	2.3E-11	2.7E-11	3.1E-11
<input checked="" type="checkbox"/>	5	1	4	1	5.3E-11	5.4E-11	5.4E-11	5.4E-11	5.4E-11	5.5E-11	5.6E-11	6.0E-11	6.4E-11
<input checked="" type="checkbox"/>	6	1	1	1	1.4E-12	1.5E-12	1.8E-12	2.4E-12	2.9E-12	3.3E-12	3.7E-12	4.9E-12	5.6E-12
<input checked="" type="checkbox"/>	6	1	2	1	3.4E-12	3.6E-12	3.7E-12	4.1E-12	4.4E-12	4.6E-12	4.9E-12	6.0E-12	7.0E-12
<input checked="" type="checkbox"/>	6	1	3	1	1.7E-11	1.8E-11	1.9E-11	2.1E-11	2.3E-11	2.4E-11	2.6E-11	3.0E-11	3.3E-11

To be improved: exportation for example, **we need feedback from user**

Choose a request type ([reset page](#))

- For collisional process
- For radiative process
- By species

Define collision type

- Without reaction (Elastic and Inelastic)
- With reaction

Process name

Process description

Process code

Please, enter the number of targets and colliders you wish to add

Targets

Atoms Molecules Particles

Colliders

Atoms Molecules Particles

Next ->

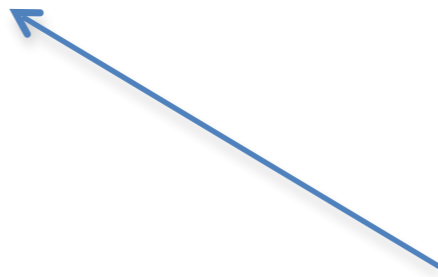
Submit query and find data

Save queries so that you can re-use them

- 1- in session
- 2 - later if you have worked being logged onto the portal

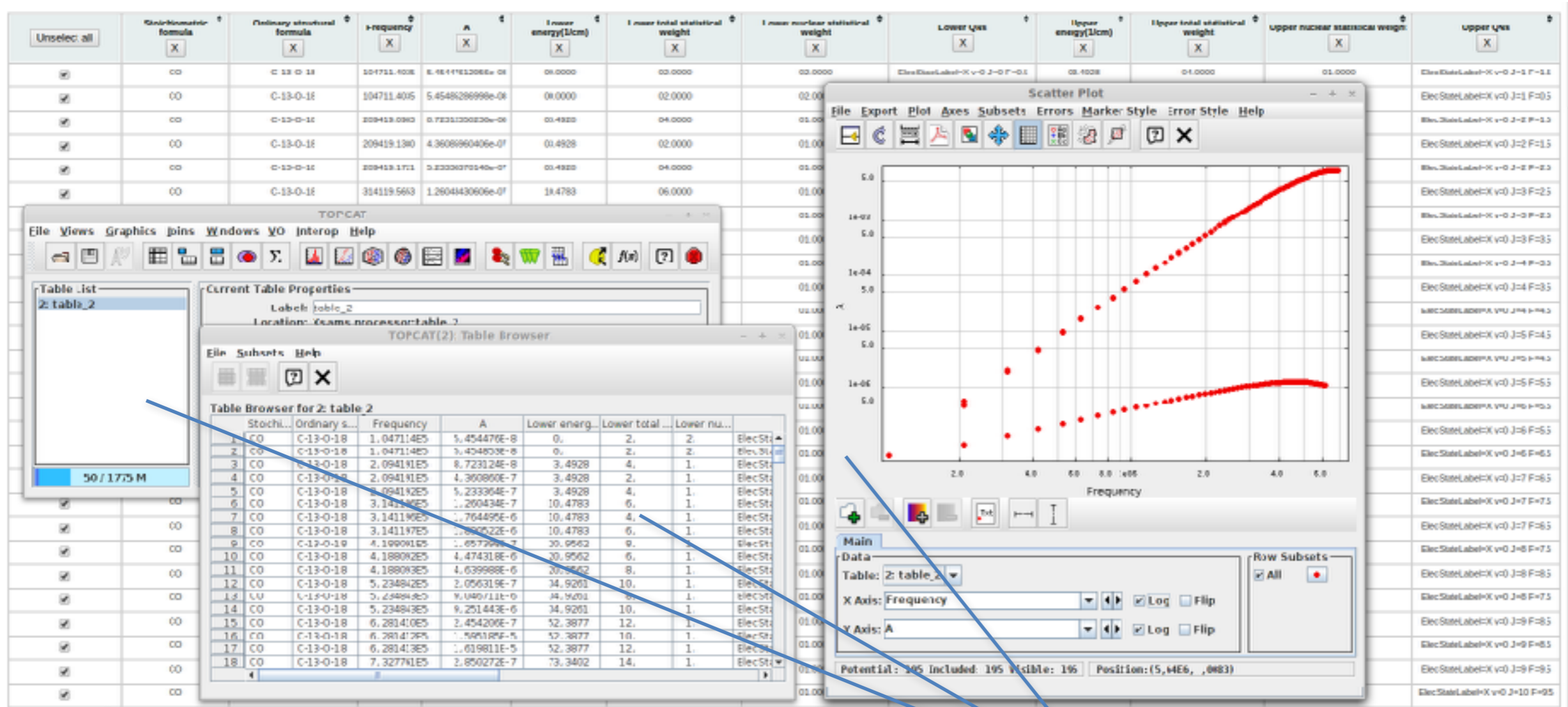
Home VAMDC databases Guided query Advanced query **Saved queries** | Disclaimer Info Feedback

No result selected



Query	Comments	Date	Database	Results	Results Status	Download
<div style="display: flex; flex-direction: column; gap: 5px;"> Edit Clone Delete </div> <pre>select * where ((target.InchiKey = 'UGFAIRIUMAVXCW-UHFFFAOYSA-N')) AND ((collider.AtomSymbol = 'He')) AND (CollisionCode = 'inel')</pre>		Jan 6, 2016	<input type="checkbox"/> BASECOL: VAMDC-TAP interface	Sp: 6 -st:0 - Pr:2	OK	XSAMS
			<input type="checkbox"/> KIDA: VAMDC-TAP interface	Sp: 3 -st:0 - Pr:0	OK	XSAMS

Data are sent to TOPCAT VO tool
Full compatibility with Virtual Observatory Tools



The screenshot displays the TOPCAT software interface. The main window shows a table with columns for chemical formula, ordinary statistical formula, frequency, A, lower energy, lower total weight, lower nuclear statistical weight, lower energy, upper energy, upper total weight, upper nuclear statistical weight, and upper energy. A 'Scatter Plot' window is overlaid on the table, showing a plot of A versus Frequency. The plot has a logarithmic x-axis labeled 'Frequency' ranging from 2.0 to 5.0, and a logarithmic y-axis labeled 'A' ranging from 1e-06 to 5.0. The data points are red dots, and a red curve is fitted to the data. The 'Main' window at the bottom shows the 'Data' section with 'Table: Z: table_2' selected, and the 'X Axis' set to 'Frequency' and the 'Y Axis' set to 'A'. The 'Row Subsets' section is also visible.

OUR NEW VISUALISATION on PORTAL

TOPCAT TOOL

What is the portal / What it is not

- Portal gives a visibility on the content of all the databases
- A single way to query all databases
- A single way to visualise the data
 - ◆ A single format description for quantities and quantum numbers
- Cannot perform the specific services that some databases might provide
 - ◆ Portal might be a first step towards finding the data

What can we currently do with VAMDC?

Virtual Atomic and Molecular Data Centre

- Query all registered databases via the Portal (www.portal.eu) or other portals
 - ◆ Visualisation of Data
 - ◆ Download of Data

- Standalone Work with Software:
 - ◆ Query databases & Mix heterogeneous databases
 - ➔ *Example of SPECTCOL software*

- Use of our libraries in user applications in order to access the VAMDC registered databases

- Include new databases or data in the infrastructure

Access to Data

VAMDC Research Portal
RADAM Portal

Software

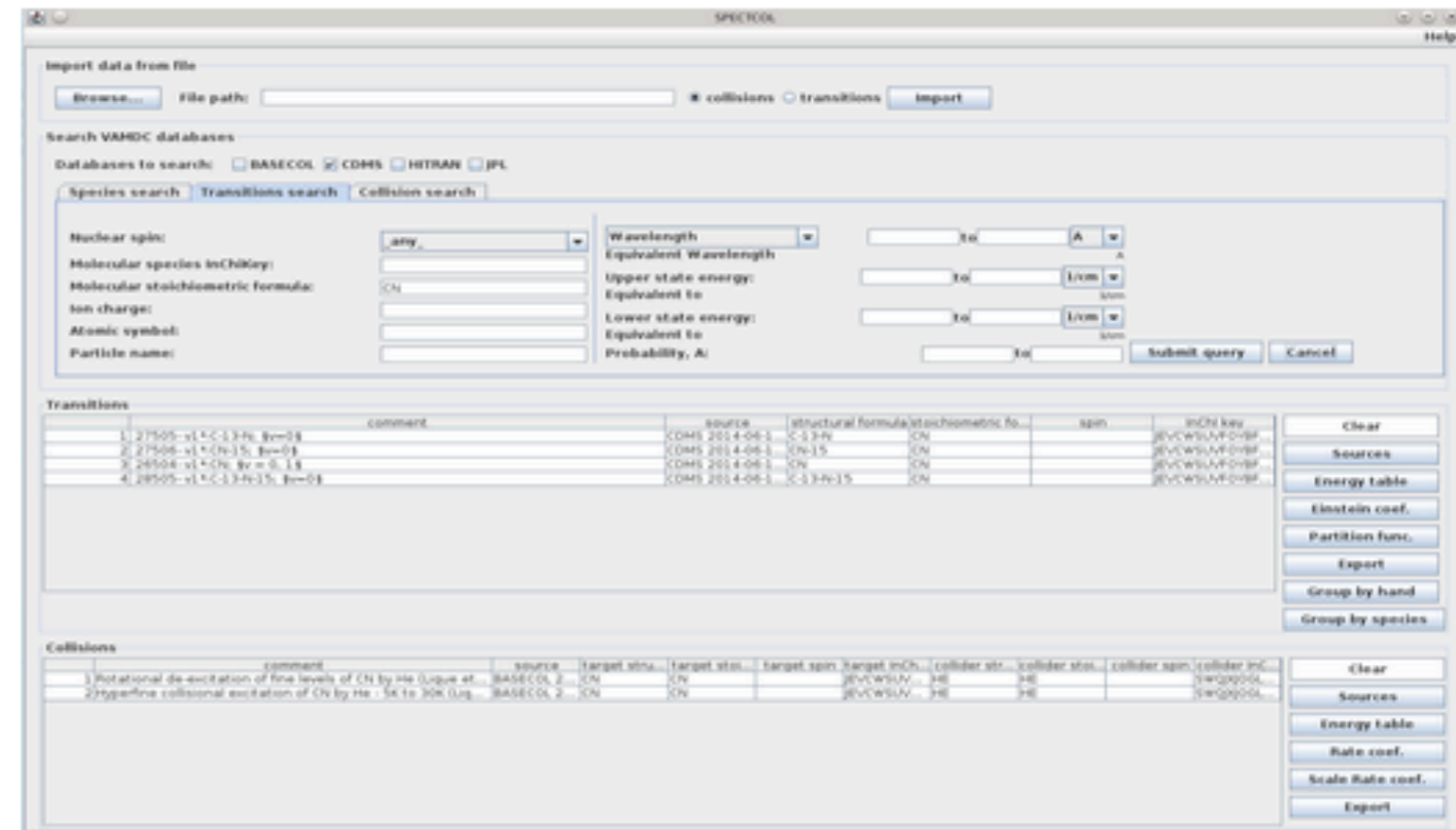
SPECTCOL

SPECVIEW
XSAMS Converter
PDL-VAMDC
JavaScriptPortal
TAPValidator
Java NodeSoftware
Python NodeSoftware
Libraries
Virtual machines for node building

Documents

Standards
Science use cases
Tutorials
See our videos
FAQ

SPECTCOL



The screenshot shows the SPECTCOL web interface. At the top, there is an 'Import data from file' section with a 'Browse...' button and a 'File path:' input field. Below this is a 'Search VAMDC databases' section with radio buttons for 'collisions' and 'transitions', and an 'Import' button. The search criteria section includes fields for 'Nuclear spin', 'Molecular species InChIKey', 'Molecular stoichiometric formula', 'ion charge', 'Atomic symbol', and 'Particle name'. There are also dropdown menus for 'Wavelength' and 'Equivalent Wavelength', and input fields for 'Upper state energy' and 'Lower state energy'. A 'Submit query' button is located at the bottom right of the search section.

The 'Transitions' table shows the following data:

	comment	source	structural formula/stoichiometric fo	spin	InChI key
1	27500-vl *C-13-N, Jv=08	CDMS 2014-06-1	C-13-N	0N	2VCWSU4P08P
2	27500-vl *C-13-N, Jv=09	CDMS 2014-06-1	CN-13	0N	2VCWSU4P08P
3	28500-vl *C-13-N, Jv=0, L8	CDMS 2014-06-1	CN	0N	2VCWSU4P08P
4	28500-vl *C-13-N-13, Jv=08	CDMS 2014-06-1	C-13-N-13	0N	2VCWSU4P08P

The 'Collisions' table shows the following data:

	comment	source	target str...	target str...	target spin	target InChI	collider str.	collider str...	collider spin	collider InChI
1	Rotational de-excitation of fine levels of CN by He (logue et...	BASECOL 2	CN	CN		2VCWSU4P08P	He	He		2VCWSU4P08P
2	27500-vl collisional excitation of CN by He - 5x to 30x (log...	BASECOL 2	CN	CN		2VCWSU4P08P	He	He		2VCWSU4P08P

SPECTCOL is a graphical tool implemented in Java. It allows to manipulate and combine spectroscopic and collisional data coming from the databases (BASECOL, CDMS, HITRAN, JPL,...) using VAMDC technology.

XSAMS(Xml Schema for Atoms, Molecules and Solids) is the VAMDC data format and SPECTCOL is able to manipulate and provides methods to convert these data into other formats(CSV, RADEX, LTE ...).

For any question or feedback use the forum link [here](#).

Credits:

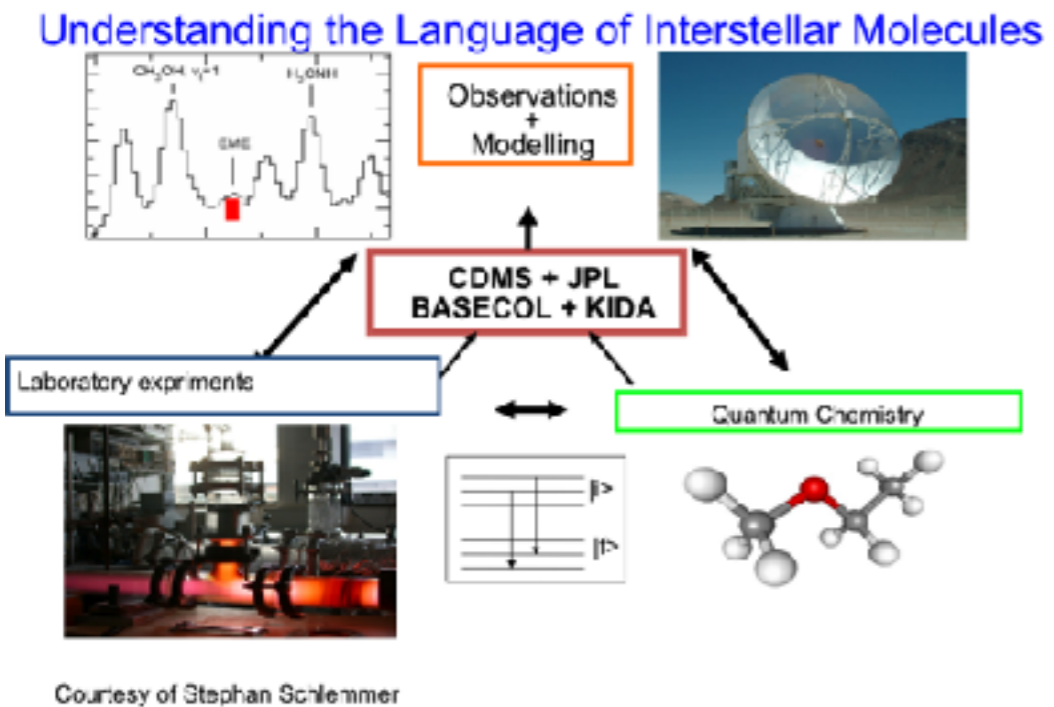
M.L. Dubernet, Y.A. Ba, L. Nenadovic, M. Doronin

BSD Licence, @VAMDC Copyright

Scientific Use Case

Provide GUI to users to solve specific user problems

SPECTCOL Tool: Y.A. Ba (Obs Paris, LERMA)



Non-LTE Analysis of Spectra requires Combined spectroscopic And collision Data

CDMS

BASECOL

Database to search: BASECOL CDMS HITRAN JPL

Species search | Transition search | **Collision search**

Target: Collider:

Nuclear spin:

Molecular species InChIKey:

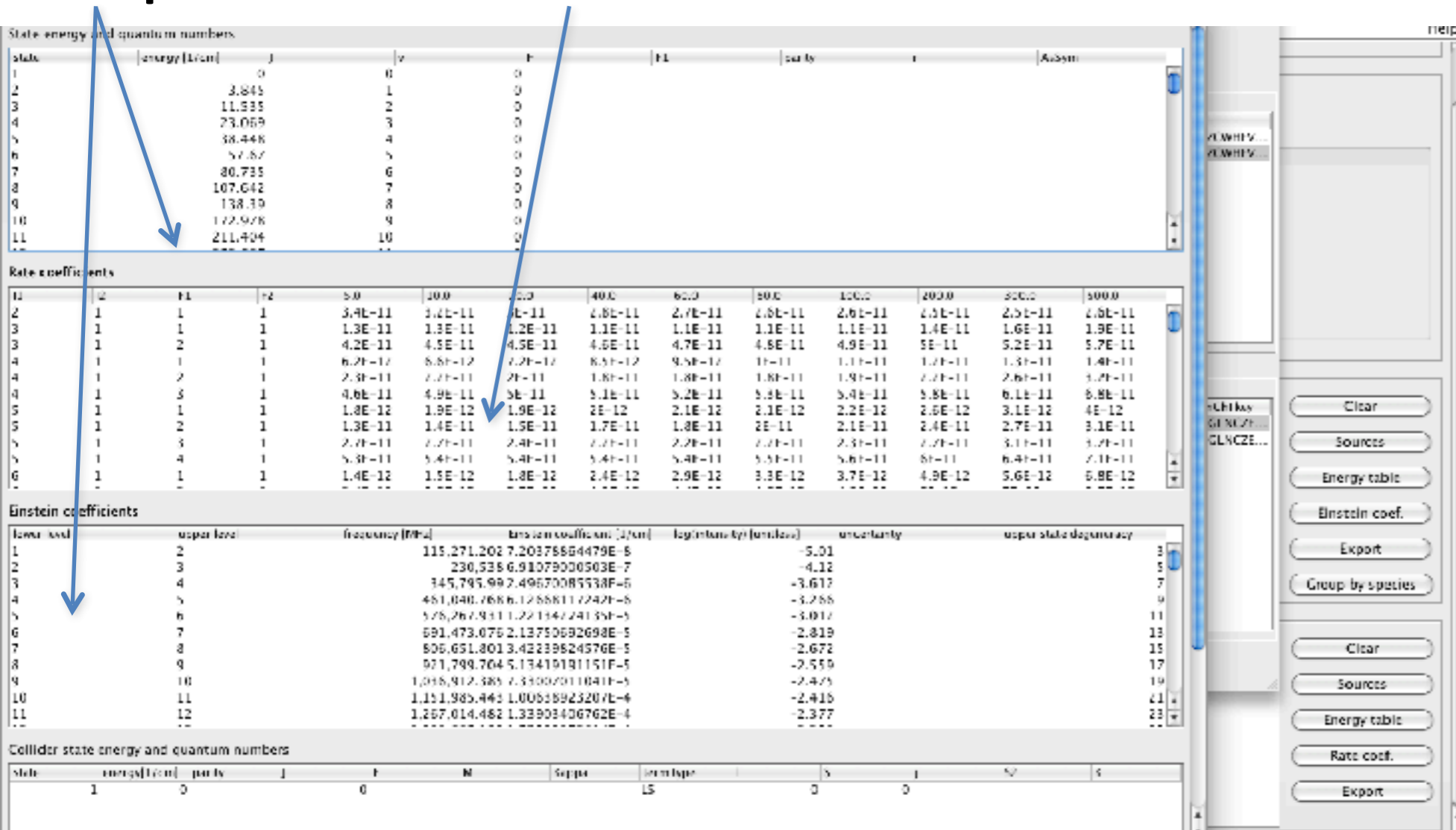
Molecular stoichiometric formula:

Atomic symbol:

Transition	comment	source	stoichiometric formula	stoichiometric formula	spin	InChI key
1 Carbon atomoxide: 13C isotope		CDMS 2012-06-1...	C-13-O	CO		UCFARILMAYXCV...
2 Carbon atomoxide: 18O isotope		CDMS 2012-06-1...	CO-18	CO		UCFARILMAYXCV...
3 Carbon atomoxide: cooly substituted isotope with 13C and 17O		CDMS 2012-06-1...	C-13-O-17	CO		UCFARILMAYXCV...
4 Carbon atomoxide: 17O isotope		CDMS 2012-06-1...	CO-17	CO		UCFARILMAYXCV...
5 Carbon atomoxide: v=0		CDMS 2012-06-1...	CO	CO		UCFARILMAYXCV...
6 Carbon atomoxide: cooly substituted isotope with 13C and 18O		CDMS 2012-06-1...	C-13-O-18	CO		UCFARILMAYXCV...
7 CO, v=1-2		CDMS 2012-06-1...	CO	CO		UCFARILMAYXCV...

Collisions	comment	source	target atom...	target stoich...	target spin	target InChI...	collider struc...	collider sto-c...	collider spin	collider InChI...
1 Rotational de-excitation of CO by H ⁺ at T < 100K (Suzuki & al. 2007)	BASECOL 23...	CO	CO	CO		UCFARILMAYXCV...	H	H		UCFARILMAYXCV...
2 Vibrational de-excitation of CO by H (Bastinier & al. 2007)	BASECOL 23...	CO	CO	CO		UCFARILMAYXCV...	H	H		UCFARILMAYXCV...
3 Rotational de-excitation of CO by H for 100K < T < 1000K (Bastinier & al. 2007)	BASECOL 23...	CO	CO	CO		UCFARILMAYXCV...	H	H		UCFARILMAYXCV...

Spectro and Collisions are combined



The screenshot displays a software interface with several data tables:

- State energy and quantum numbers:** A table with columns for state, energy [E_{atom}], J, F, FL, parity, I, and Assym.
- Rate coefficients:** A table with columns for l1, l2, f1, f2, and various rate coefficient values (e.g., 5.9E-11, 3.2E-11).
- Einstein coefficients:** A table with columns for lower level, upper level, frequency [MHz], Einstein coefficient [1/s], log(intensity) [unitless], uncertainty, and upper state degeneracy.
- Collider state energy and quantum numbers:** A table with columns for state, energy [E_{atom}], J, F, M, upper, lower, S, I, N, and S.

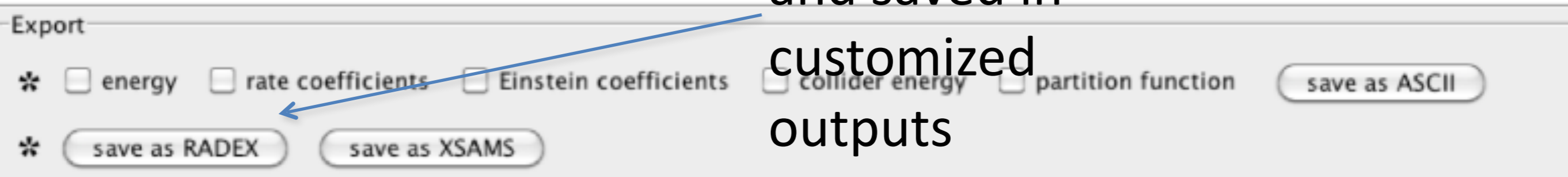
Next Version:

Same query as portal

Find all DB

Send Data to TopCat for visualisation

and saved in customized outputs



The screenshot shows the 'Export' section with the following options:

- energy
- rate coefficients
- Einstein coefficients
- collider energy
- partition function
- save as ASCII
- save as RADEX
- save as XSAMS

What can we currently do with VAMDC?

Virtual Atomic and Molecular Data Centre

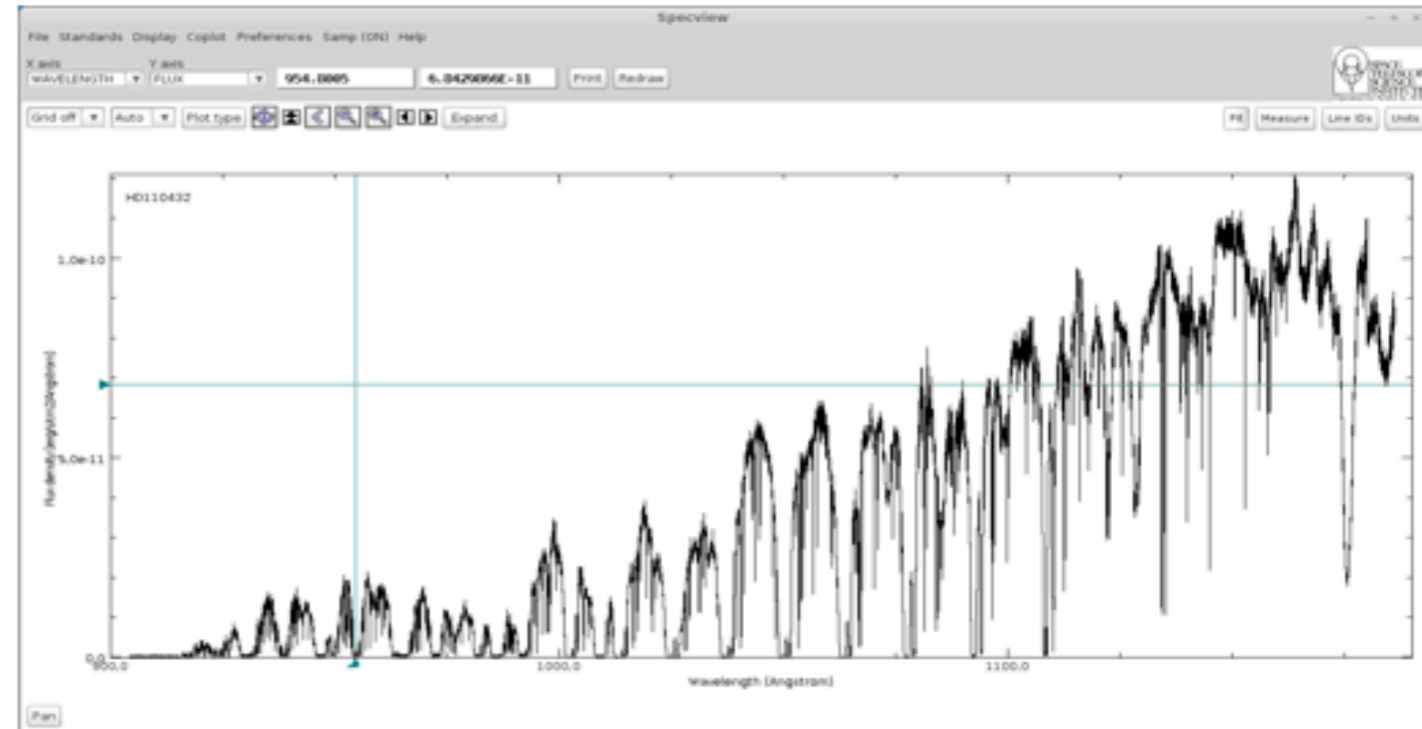
- Query all registered databases via the Portal (www.portal.eu) or other portals
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SPECVIEW
 XSAMS Converter
 PDL-VAMDC
 JavaScriptPortal
 TAPValidator
 Java NodeSoftware
 Python NodeSoftware
 Libraries
 Virtual machines for node building

Documents -
 Standards
 Science use cases
 Tutorials
 See our videos
 FAQ

SPECVIEW



Specview is a tool for 1-D spectral visualization and analysis of astronomical spectrograms. It is written in Java thus can be run anywhere Java is supported. **Specview** is capable of reading all the Hubble Space Telescope spectral data formats, as well as data from several other instruments (such as IUE, FUSE, ISO, FORS and SDSS), preview spectra from MAST, and data from generic FITS and ASCII tables. It can also read data from Virtual Observatory servers, and read and write spectrogram data in Virtual Observatory SED format. It can also read files in the SPC Galactic format used in the chemistry field.

Specview can overplot spectral line identifications taken from a variety of line lists, including user-supplied lists. Its linelists' query form has been modified to include the VAMDC Query Module, called QueryBuilder, thus providing the full capability of querying the VAMDC databases. In particular it allows to select finely the observed species and properties of linelists. Currently about 20 spectroscopic databases are inter-connected through VAMDC and accessible through VAMDC software and libraries.

Scientific Use Case +

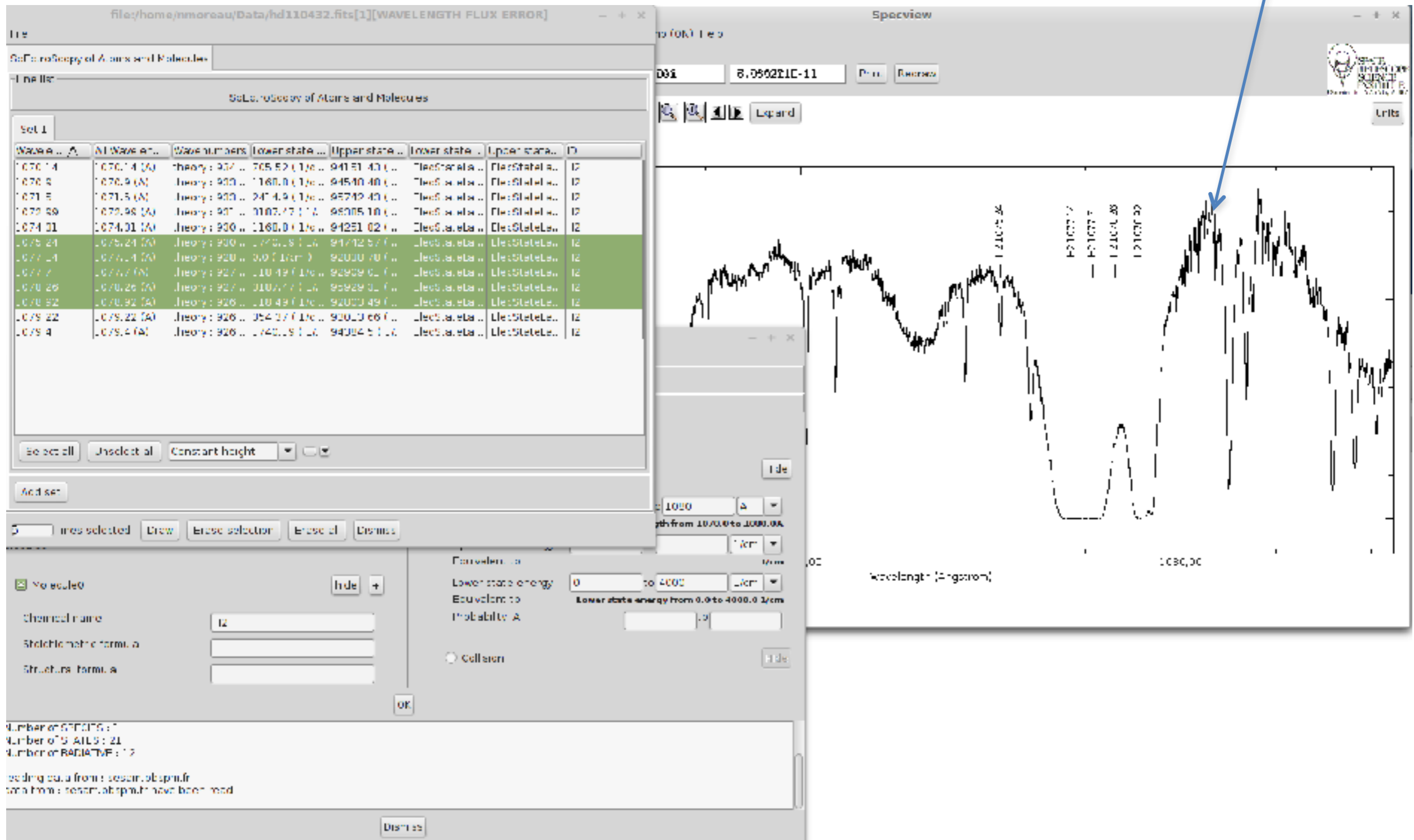
Tutorial +

Version History -

Collaboration VAMDC (N. Moreau)
 With I. Busko (STScI)

www.stsci.edu/institute/software_hardware/specview/

SSAP VO



The image shows a screenshot of the Specview software interface. On the left, a window titled 'file:/home/nmoreau/Data/hd110432.fits[1][WAVELENGTH FLUX ERROR]' displays a table of spectral line data. The table has columns for Wavelength, Wavelength (Å), Wave numbers, Lower state energy, Upper state energy, Lower state energy (cm⁻¹), Upper state energy (cm⁻¹), and ID. The table is filtered for 'Set 1' and shows 12 rows of data. Below the table are buttons for 'Select all', 'Unselect all', and 'Constant height'. At the bottom of this window, there are fields for 'Chemical name' (set to 'H2'), 'Stoichiometric formula', and 'Structural formula', along with a 'Show' button and a 'Dismiss' button.

On the right, the main Specview window displays a spectral plot of the HD 110432 star. The x-axis is labeled 'Wavelength (Angstrom)' and ranges from approximately 1000 to 10000. The y-axis represents flux. The plot shows a complex spectrum with many absorption lines. A blue arrow points to a specific feature in the spectrum, labeled 'SSAP VO'. Below the plot, there are controls for 'Zoom' (set to 1000) and 'Wavelength from 1000.00 to 10000.00'. The plot also shows several vertical lines representing theoretical transitions, with labels like 'H2 10107.1', 'H2 10107.7', 'H2 10107.8', and 'H2 10107.9'.



Previous day OK Next day

Enter a date: Ex: 28/3/2001, 28.3.1, 28-3-01, YYYYMMDD or YYMMDD

en | fr My Selection

- HOME**
 - Latest observations
 - Latest movies
 - Long term archive
 - News
 - QUERY**
 - For observations
 - For specific dates
 - For solar features
 - For synoptic
 - HELIO features
 - TOOLS**
 - Ephemeris
 - Solar spectra
 - Related to
 - Live Sun &
 - Software
 - GUIDES**
 - Instruments
 - Data
 - Software
 - Educational resources (fr)
- Collection before 1980
[Solar Web Guide](#)
[Multimedia Gallery](#)



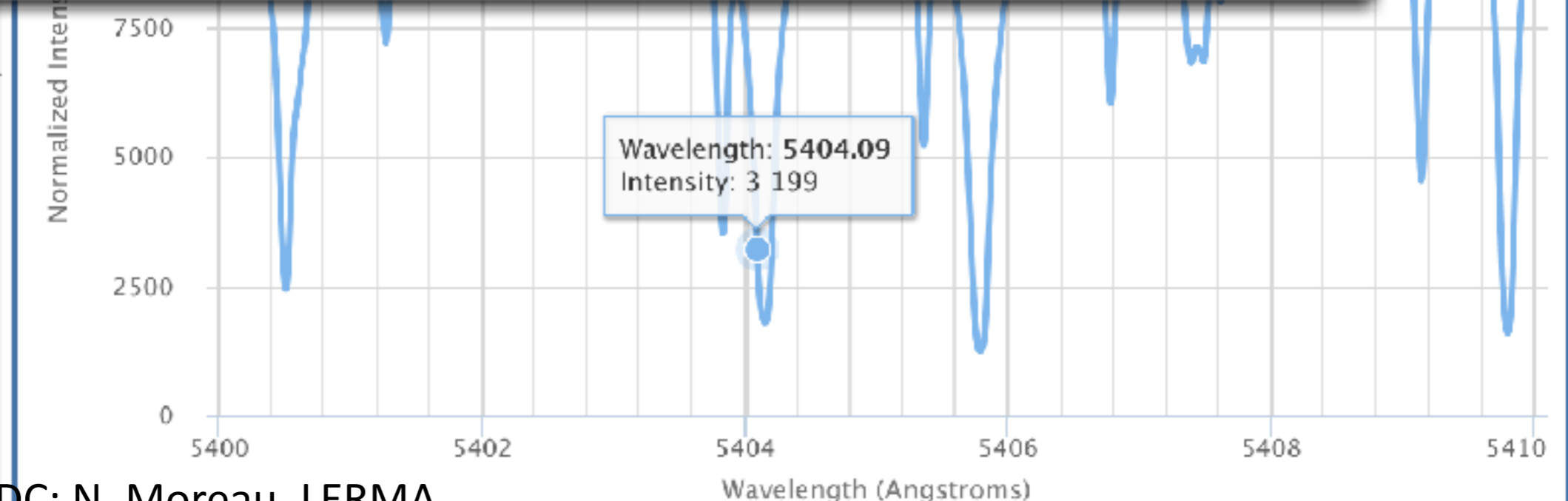
Spectrum 5404.09 Å

Results from [NIST Atomic Spectra Database](#) (National Institut of Standards and Technology):

Ion	Observed Wavelength	Air (Å)	Ritz Wavelength Air (Å)	Aki (s-1)	fik	Acc.	Ei (cm-1)	Ek (cm-1)	gi-gk
Sc II	5404.085		5 404.090				39 115.04	-57 614.40	3-5

This element is also found in [VAMDC](#) databases:

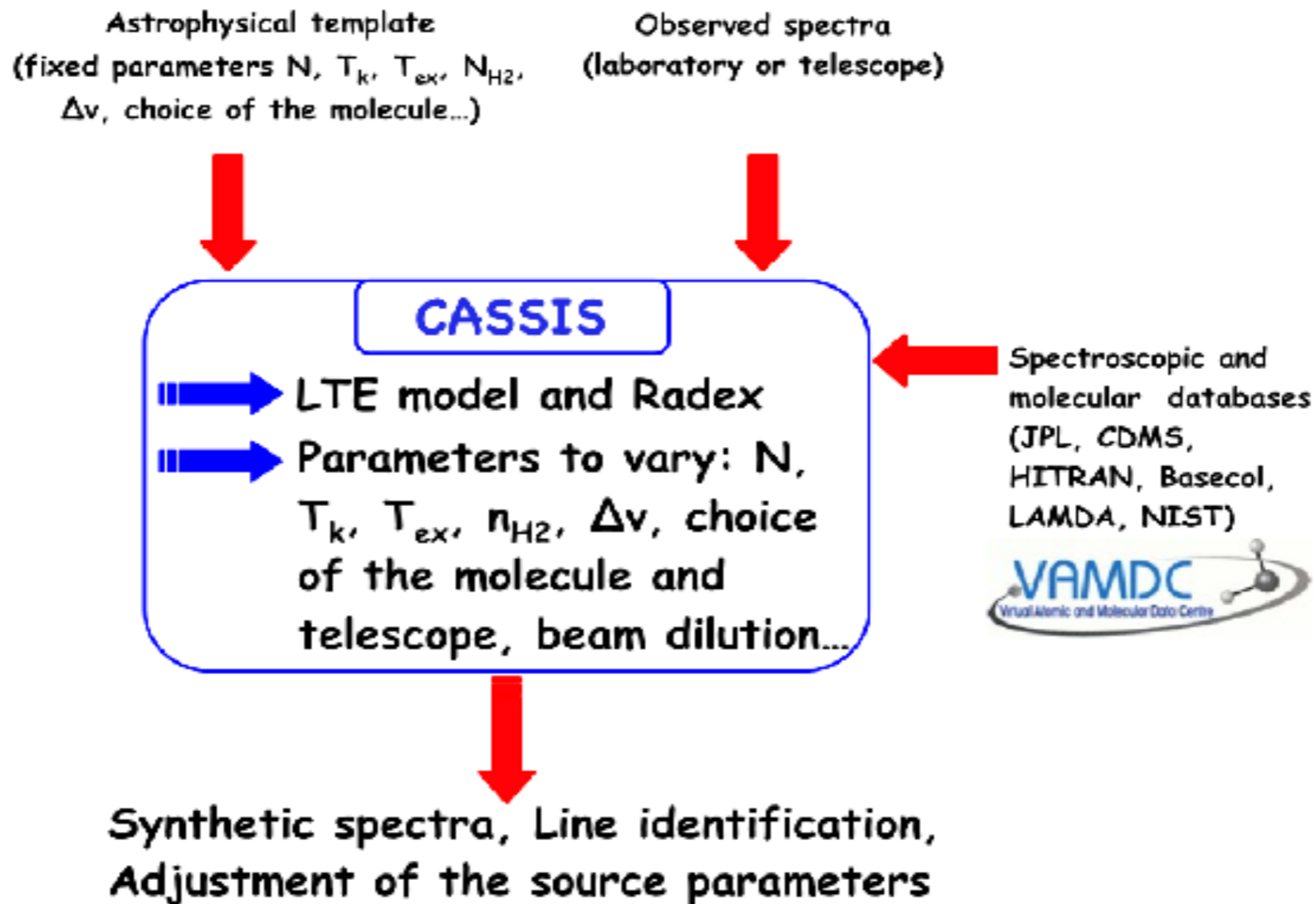
Database name	Element Symbol	Nuclear Charge	Wavelength	Upper State Energy	Upper State Energy Units	Lower State Energy	Lower State Energy Units
VALD	Sc	21	5404.0882399941	57614.4000	1/cm	39115.0400	1/cm



CASSIS Software

*M. Boiziot, S. Bottinelli, E. Caux, J.M. Glorian, C. Vastel, IRAP, Toulouse
Y. A. Ba, VAMDC Support, LERMA*

The CASSIS (Centre d'Analyse Scientifique de Spectres Instrumentaux et Synthétiques) software has been developed by CESR/IRAP since 2005. All information about it can be found on a dedicated website: <http://cassis.irap.omp.eu>. The functionalities are represented in the flow chart below:



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- **Include new databases or data in the infrastructure**

Include your data in VAMDC

- Include your data in existing Database connected to VAMDC
 - ◆ Contact the DB manager directly
 - ◆ Contact VAMDC Support: support@vamdc.eu

- Create a new DB to be connected to VAMDC
 - ◆ Contact a node in order to include your DB at their node
 - ◆ Contact VAMDC Support : support@vamdc.eu
 - To include at an existing node
 - To create a new node

Tutorials For Data Producers

RESEARCH SERVICES

Access to Data

VAMDC Research Portal
RADAM Portal

Software

SPECTCOL
SPECVIEW
XSAMS Converter
PDL-VAMDC
JavaScriptPortal
TAPValidator
Java NodeSoftware
Python NodeSoftware
Libraries
Virtual machines for node
building

Documents

Standards
Science use cases
Tutorials
See our videos
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TUTORIALS

We provide different tutorial addressed both to data providers and final users.
Follow the links below for further information on each item of the following list:

- [General page for Tutorials](#)
- You produce/collect atomic and molecular data and want to include them into VAMDC
 - [Outline](#)
 - [Self-Study Course](#)
- How to use the [VAMDC Portal](#)
 - [User Guide for the Portal](#)
 - [First Steps with the VAMDC Portal](#)
 - [Extracting Data from query results with the viewers](#)
- How to use VAMDC software
 - [Spectcol](#) – [Readmore](#)
 - [Specview](#) – [Readmore](#)
 - [PDL-VAMDC](#) – [Readmore](#)
 - [The XSAMS file format and TAP Validator application](#) (mainly for the data providers)
 - [Python Scripting](#)
 - [Using VAMDC Java libraries](#)
- You want to check [XSAMS files](#), [TAPValidator](#) – [ReadMore](#)

ACCESS TO THE DATA

Access to VAMDC databases

[Access to the portal](#)

ACCESS TO THE FORUM

Exchange ideas, Ask questions, Find answers

[Read more](#)

or

[Access to the forum](#)

Advantages of Inclusion in VAMDC

- Each Data is precisely described and referenced
 - ◆ Allows to check consistency of Databases
- Methodology to obtain data can be included

- **Uniform** query and visualisation
 - ◆ Similar Databases can be compared

- Allows **visibility of small databases, groups' work**
- Allowed new paradigm for existing DB: CDMS, HITRAN

Duties for VAMDC connected Databases' managers

- Have a technical manager and a scientific manager
- Check technical quality with respect to VAMDC
 - ◆ Be compliant with VAMDC
- Check scientific quality of databases output through VAMDC
- Provide information about your database and your group
- For those who are not members, but hold resources: be aware of VAMDC regulations

We provide on-line and face-to-face support

- ◆ To include your data and your databases
- ◆ To implement our « modules » in your software
- ◆ To use our software, our standards
- We can **organize tutorials**
- We can **support visits** for the purpose of implementation
- We have **communications channels** that are available to all

EVENTS

- Conferences
- Research
- Education
- Industry
- Outreach
- Workshops
- Research
- Industry
- Tutorials

2015/08/28 - 2015/08/29 - 2015 Annual x VAMDC Consortium x Workshop

Workshops
The 2015 Annual "VAMDC Consortium" Workshop will be held after the HRMS conference from Friday 28th August (afternoon) till Saturday 29th August. The Saturday's sessions are internal VAMDC meetings only. Friday's sessions are opened.

[Read more](#)

2015/08/24 - 2015/08/28 - 24th Colloquium on High Resolution Molecular Spectroscopy

Conferences
The Twenty Fourth Colloquium on High Resolution Molecular Spectroscopy that will take place in Dijon, France, on August 24-29, 2015.

[Read more](#)

2015/08/03 - 2015/08/14 - XXIX General Assembly IAU 2015

Conferences
XXIX General Assembly IAU (<http://astronomy2015.org>), Hawaii, August 3-14, 2015

[Read more](#)

2015/06/15 - 2015/06/19 - 10th Serbian Conference on Spectral Line Shapes in Astrophysics

Conferences
SCSLSA 2015, June 15-19, 2015 – Srabrnj jezero, Serbia

[Read more](#)

2015/06/15 - 2015/06/19 - VAMDC at spring 2015 Interop in Sesto

Conferences
The IVDA is an organisation aiming at creating interoperability standards to publish and exchange astronomical data. It will held a meeting in Sesto, Italy, between

RESEARCH NEWS

Software

2014/09/01 - SPECTCOL 4th Release

software

Version 12.07-r2

[Read more](#)

Standards

Publications

Save the figure

2013/12/01 - SPECTCOL 3rd release

software

Version 12.07-r1

[Read more](#)

2011/05/27 - Standards 1st release

standards

Version 11.05

[Read more](#)

Services

News

C

- Research
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- Industry
- Outreach
- Events
- Blogs
- Success Stories

RESEARCH P

ine for VAMDC data



AstroAtom
Partners blog
News from AstroAtom
[See the blog](#)



Populär Astronomi
Partners blog
Populär Astronomi Blog in Swedish
[See the blog](#)