MeCaSDa: Methane Calculated Spectroscopic Database (part of VAMDC)

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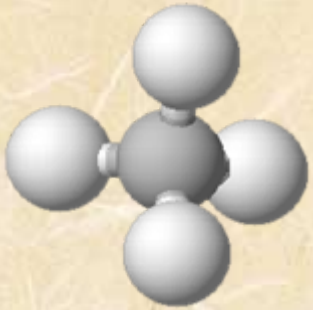
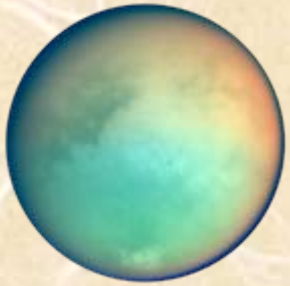
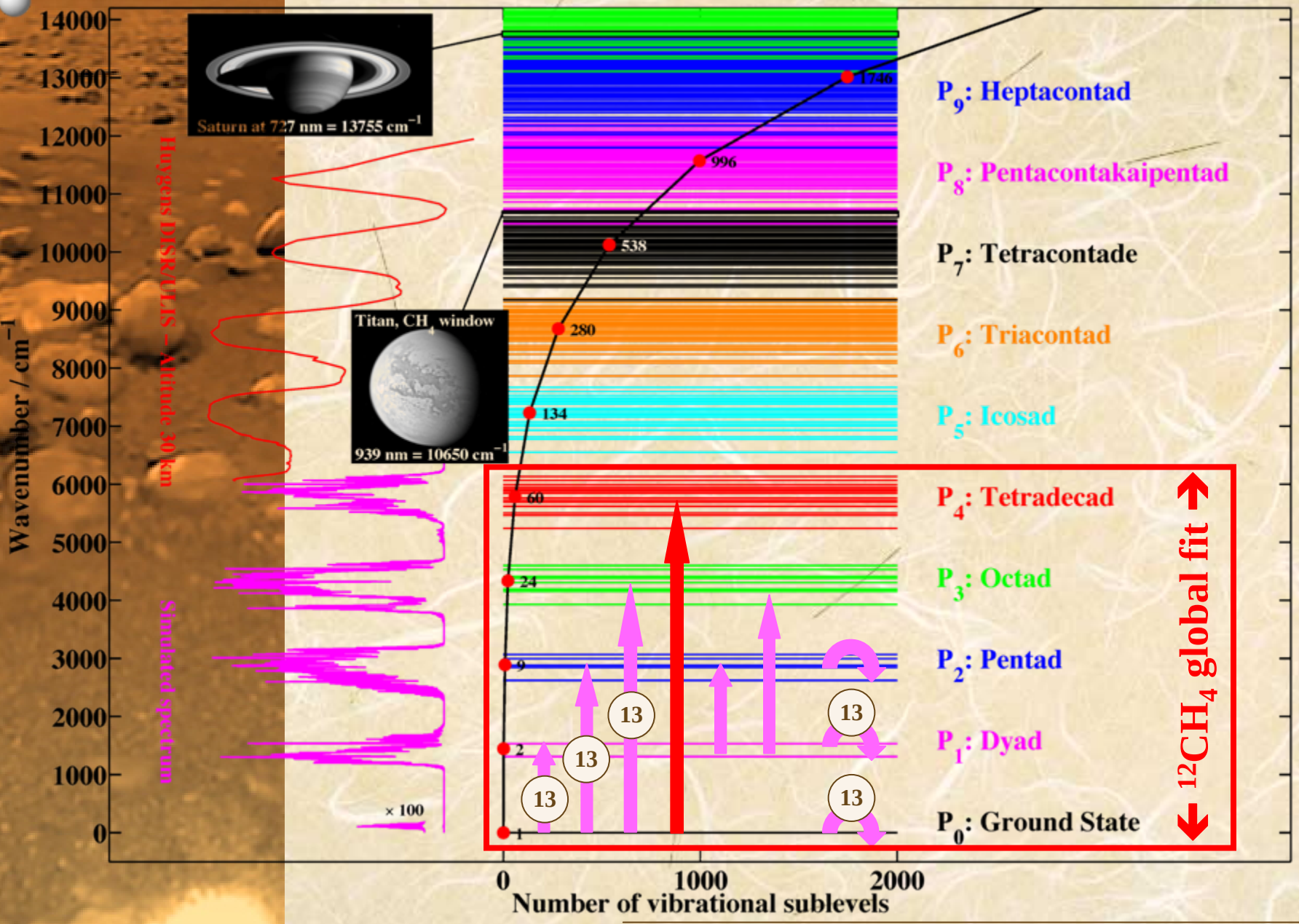
… and many collaborators in Dijon, Reims, Tomsk, Zürich, Pasadena, Meudon, …





Methane's complex spectrum



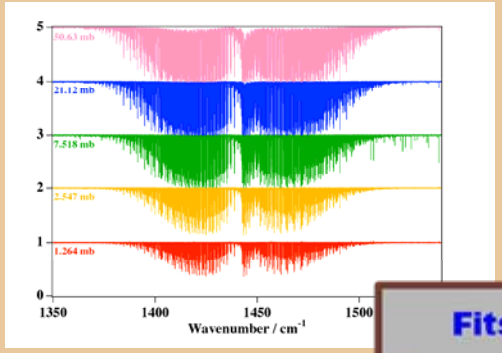
State-of-the-art for $^{12}CH_4$ (end-2012)

Polyad / Spectral region	Positions	Intensities	Profiles
1 – *Ground state* 0–200 cm^{-1} (> 5.0 μ m)	Complete analysis, $J \leq 24$	Complete analysis	Perturber: N_2
2 – *Dyad* 1000–1800 cm^{-1} (5.6–10.0 μ m)	Complete analysis, $J \leq 23$	Complete analysis, + some hot bands	Perturbers: He et N_2
3 – *Pentad* 2200–3300 cm^{-1} (3.0–4.6 μ m)	Complete analysis, $J \leq 18$	Complete analysis (cold bands)	Perturbers: He, Ar, N_2, O_2, CH_4
4 – *Octad* 3700–4800 cm^{-1} (2.0–2.7 μ m)	Very good analysis, $J \leq 21$	Very good analysis, (cold bands)	Perturbers: N_2
5 – *Tetradecad* 5400–6300 cm^{-1} (1.6–1.9 μ m)	Satisfying analysis, $J \leq 15$	Satisfying analysis (cold bands)	No calculation
6 – *Icosad* 6600–7700 cm^{-1} (1.3 – 1.5 μ m)	Very partial analysis (1 band among 20)	No analysis	No calculation
Upper polyads > 7800 cm^{-1} (< 1.28 μ m)	No analysis	No analysis	No calculation
Windows (polyad far wings, all regions)	No analysis	No analysis	No calculation

Line lists with semi-empirical line positions built for HITRAN

Virtual Atomic and Molecular Data Center

Experimental data



Since 2012 : OSU « THETA »
Terre-Homme-Environnement-Temps-Astronomie

cnrs INSU Institut national des sciences de l'Univers

UFC Université de Franche-Comté

uB Université de Bourgogne

Dadabases

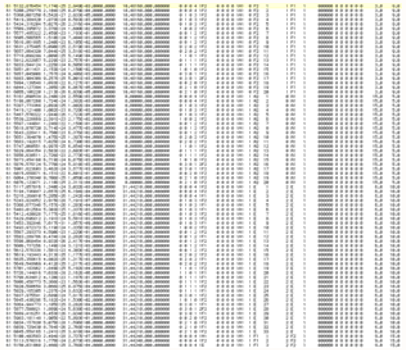
CH_4 line list has been built for **HITRAN 2013**

(with **Linda Brown**, determination of **semi-empirical upper states**)

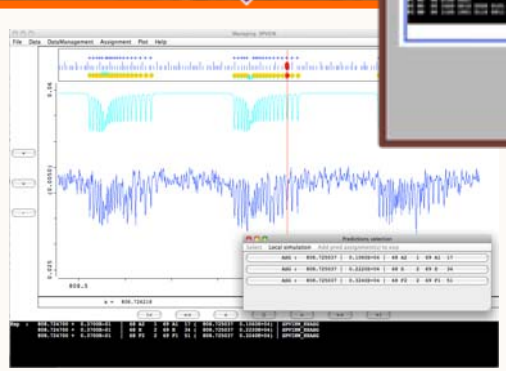
Fits and calculations

XTDS interface

Line lists



Positions, intensities, collisional parameters, accuracy



SPVIEW interface

Global modelling

Global e-Infrastructure

- European project
- Global portal
- « Modern » database
- Data traceability

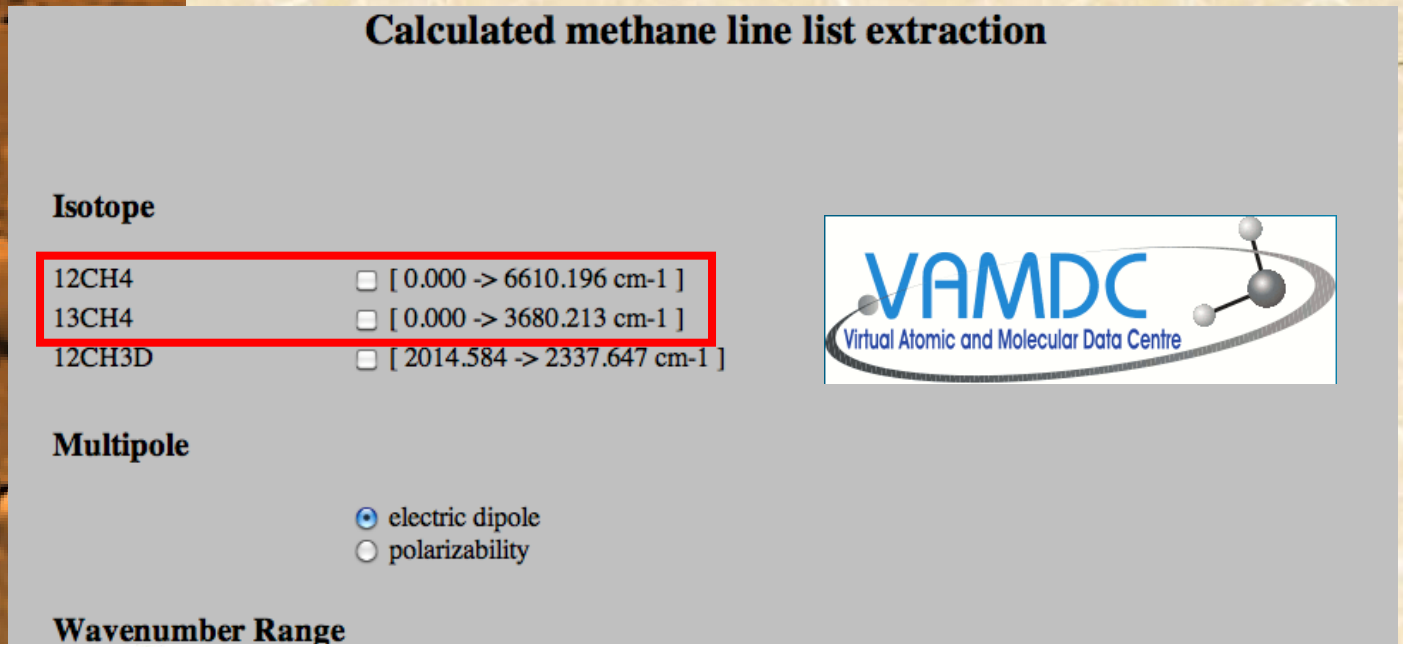
In Dijon : MeCaSDa
Server with calculated CH_4 lines

VAMDC Virtual Atomic and Molecular Data Centre

FP7 – Research Infrastructures

Virtual Atomic and Molecular Data Center

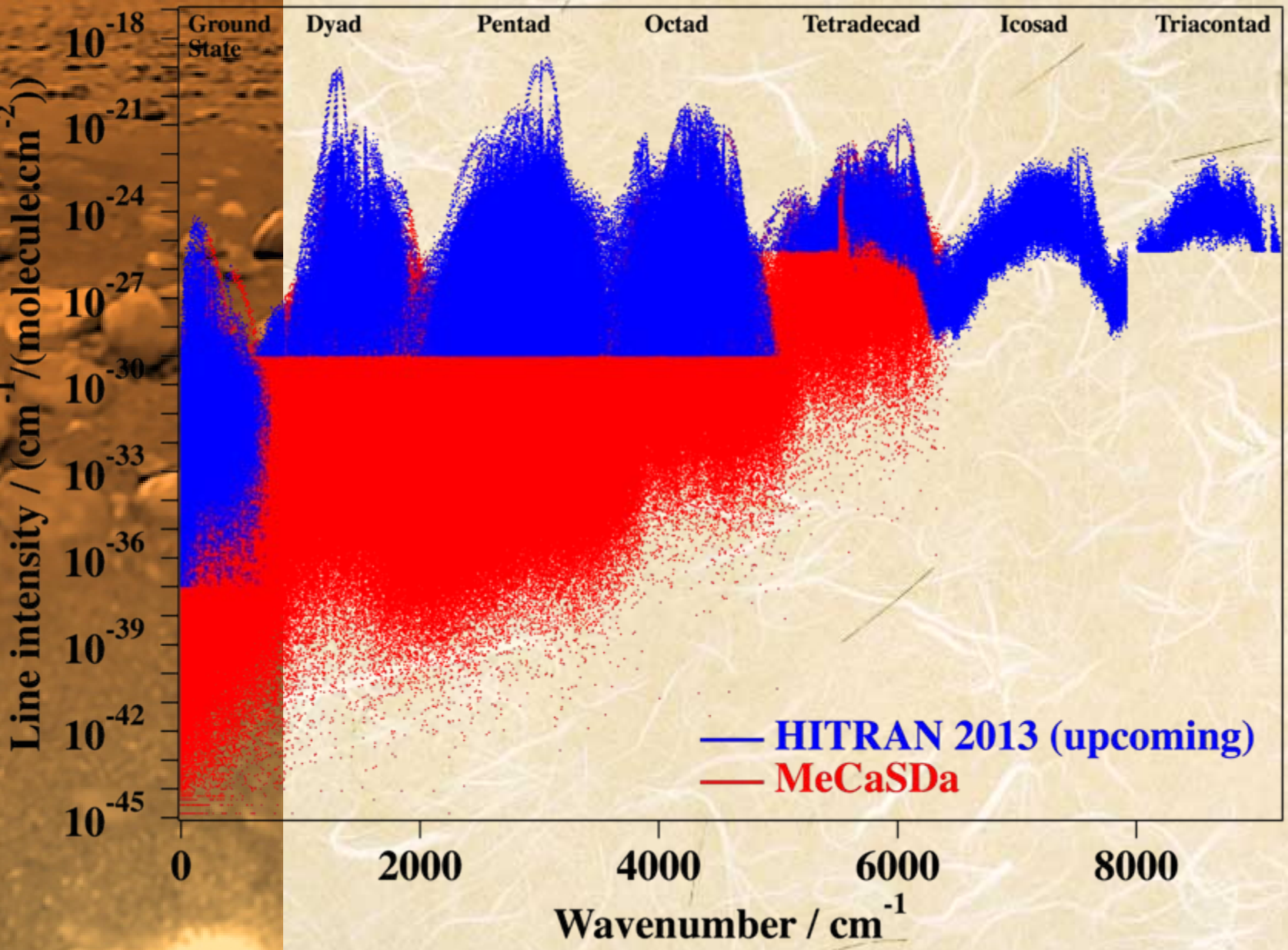
http://vamdc.icb.cnrs.fr/PHP/methane.php



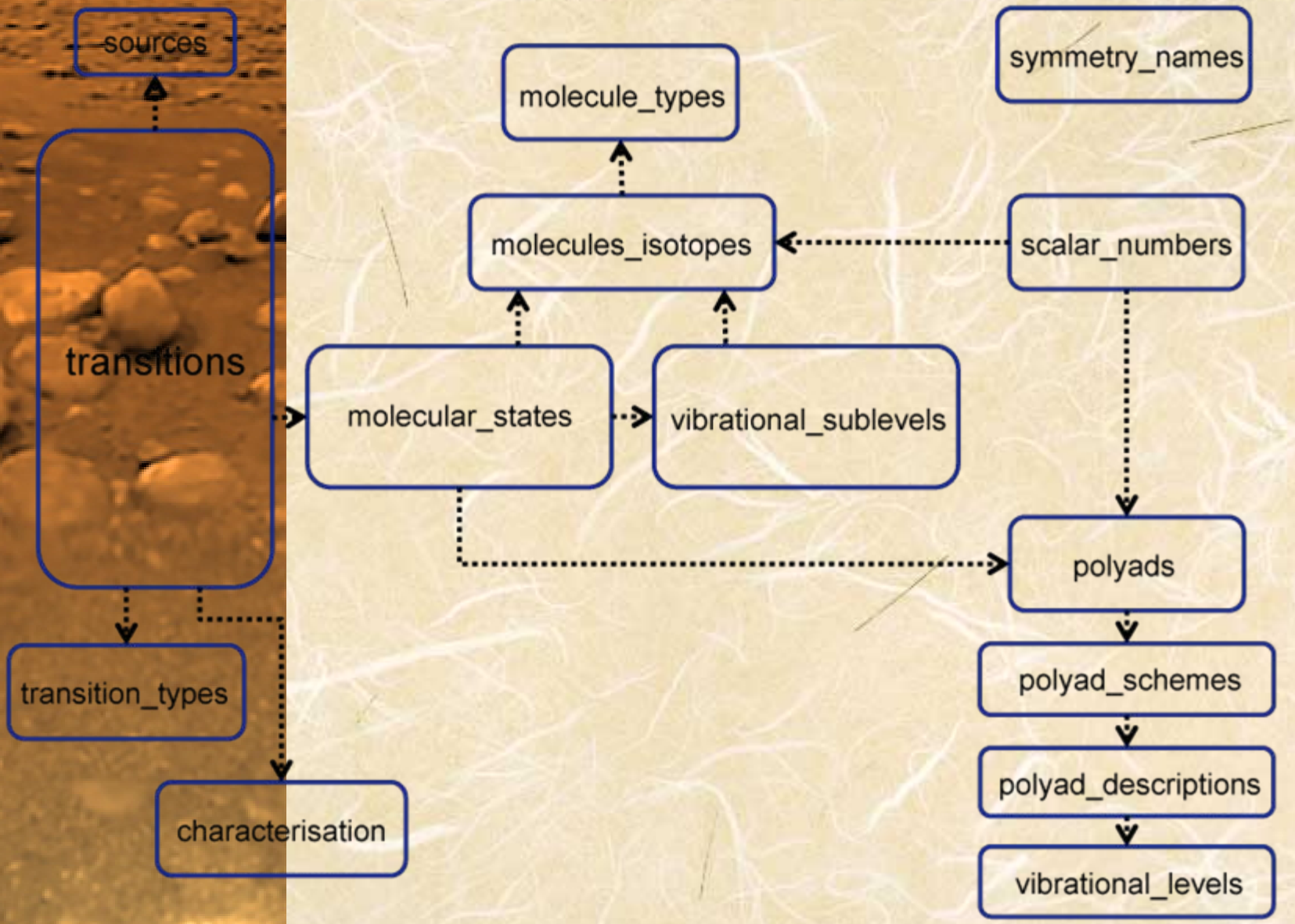
VAMDC
Virtual Atomic and Molecular Data Centre

http://portal.vamdc.eu

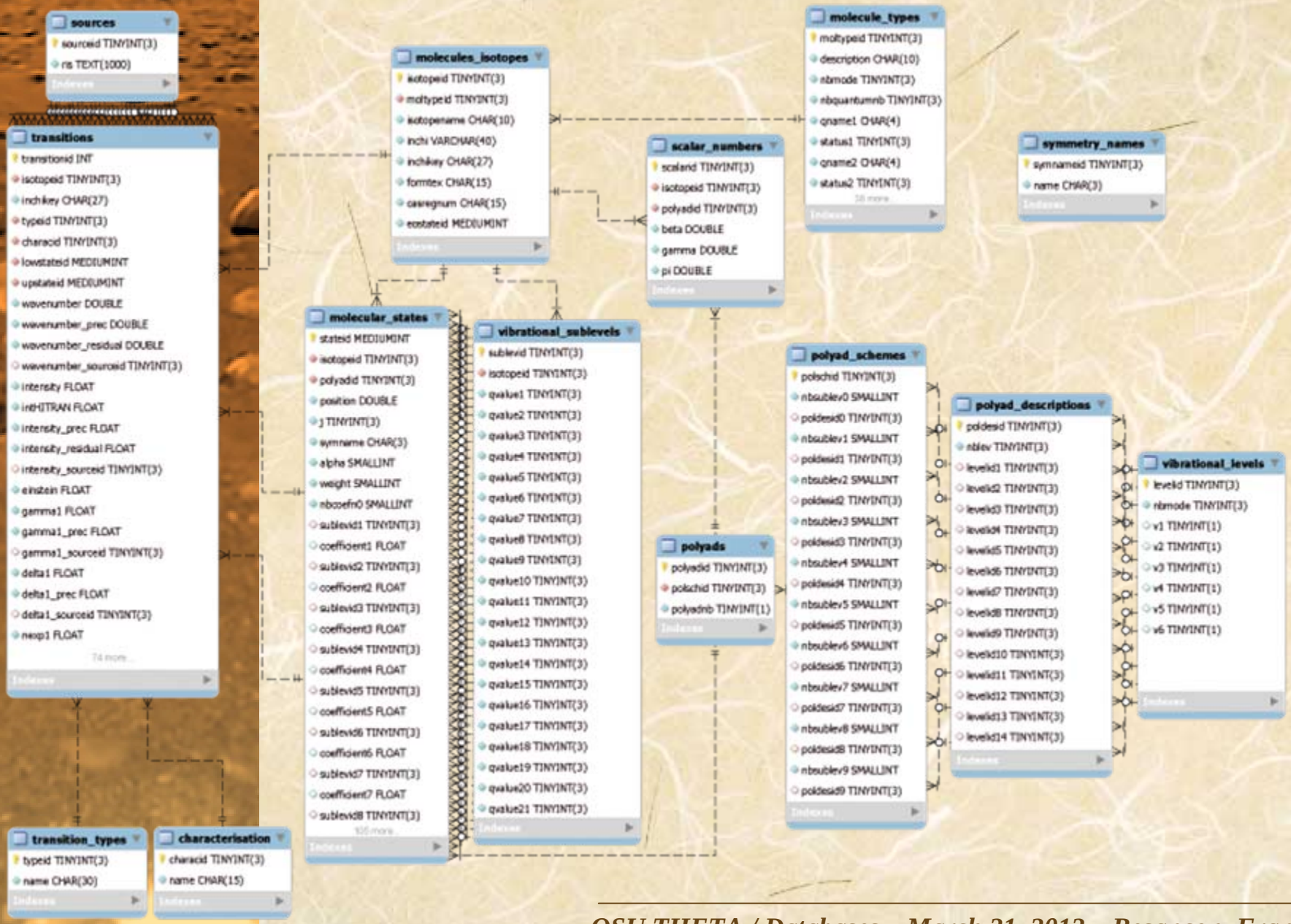
Methane lines in MeCaSDa



Relational Schema for MeCaSDa



Detailed table structure for MeCaSDa



MeCaSDa database in numbers

MeCaSDa $^{12}CH_4$ / $^{13}CH_4$	Vib. levels	Vib. sublevels	Max. J	Rovib. states
P_0 GS	1	1	25 / 25	282 / 282
P_1 Dyad	2	2	25 / 25	1408 / 1408
P_2 Pentad	5	9	25 / 25	5352 / 5352
P_3 Octad	8	24	22 / 12	12142 / 3874
P_4 Tetradecad	14	60	17 / 0	18900 / 0

MeCaSDa $^{12}CH_4$ / $^{13}CH_4$	Transitions	Nb. dipolar	Nb. Raman
	$P_0 - P_0$	1222	0
	$P_1 - P_0$	13025	19207
	$P_1 - P_1$	31510	0
	$P_2 - P_0$	49475	72954
	$P_2 - P_1$	247325	0
	$P_2 - P_2$	459276	0
	$P_3 - P_0$	97581	141446
	$P_3 - P_1$	267105	375012
	$P_3 - P_2$	1015053	0
	$P_4 - P_0$	114580	0
	$P_4 - P_1$	572747	0
	$P_4 - P_2$	2176493	3024031

MeCaSDa construction & languages

- Database developped from scratch.
- Database structure based on existing XSAMS schema (IAEA's XML Schema for Atomic, Molecular and Solid data), adapted to requests.
- XSAMS was modified for specific methane requirements.
- Fortran programs for data calculation, extraction and SQL table loading.
- The database is re-created each time data are updated (non-interactive).
- MySQL database.
- Node software written in Python under Django framework. Used to make correspondance with the XSAMS schema.
- Some Python development was needed for data extraction by requests.

FORTRAN

XSAMS
XML Schema for Atoms, Molecules, and Solids

MySQL

python™

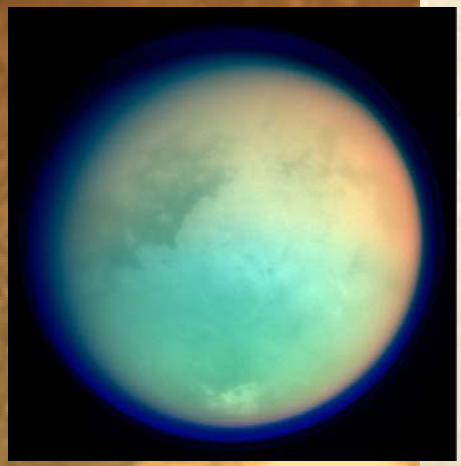
django

XML

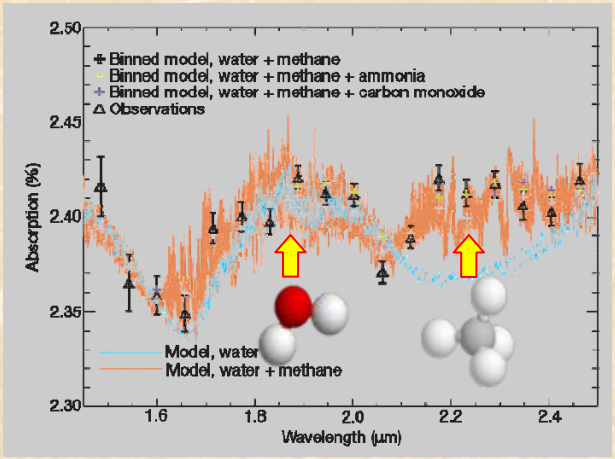
CH_4 spectroscopy: What next ?

- Continue the global fit approach
- Tetradecad (5400 – 6300 cm^{-1}) much better but still to improve
- Add new data (positions & intensities, cold & hot bands)
- Icosad, …
- Methane windows (high-*J*, far wings) for planetary atmospheres
- Hot methane (combustions, brown dwarfs, exoplanets, …)

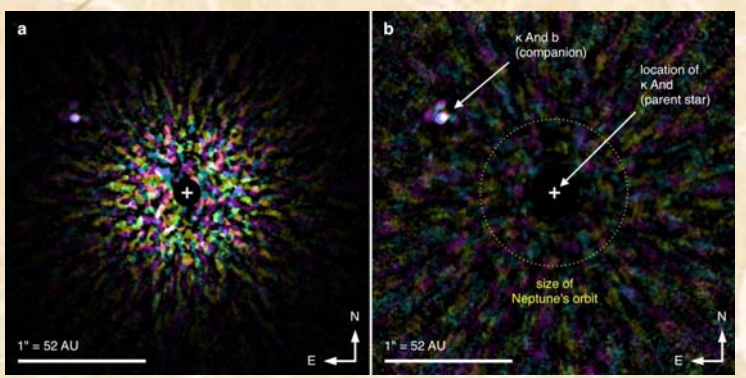
M. Louviot (ICB Dijon), R. Georges (IPR Rennes) O. Pirali (SOLEIL / Ailes), J. Vander Auwera (ULB Bruxelles), …



Titan / Cassini-Huygens



Exoplanet HD 189733 b



Exoplanet *Kappa Andromedae b*

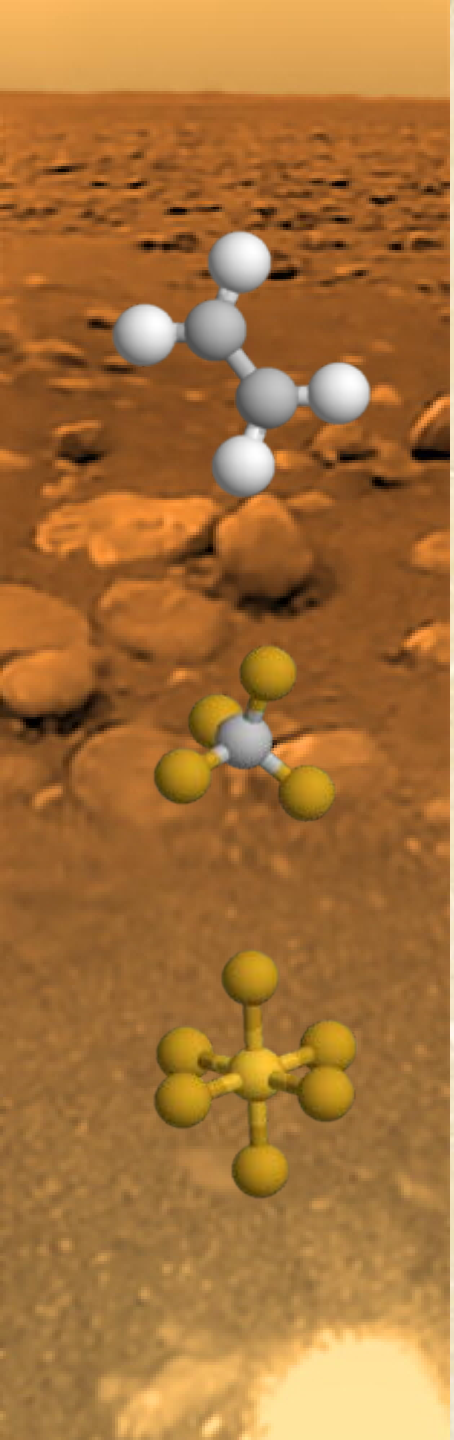
Database issues and perspectives

We have a very god server, but:

- **MySQL is not very powerful. Future SF_6 database (several Gb) may cause problems.**
- **Response delay not very satisfying.**
- **We look for another optimized SQL engine.**
- **PostgreSQL could be a solution.**

Future of VAMDC :

- **Libraries to extract data from Web sites or applications.**
- **Taverna workflow.**
- **…**



Other molecules

C_2H_4 (ethylene / ethene) – ECaSDa database:
Similar VAMDC database developped with Maud Rotger and colleagues (GSMA, Reims)

CF_4 (carbon tetrafluoride):
Many infrared and Raman bands analyzed
Database to be built

SF_6 (sulfur hexafluoride):
Many infrared and Raman bands analyzed
Database to be built
Huge data volume!