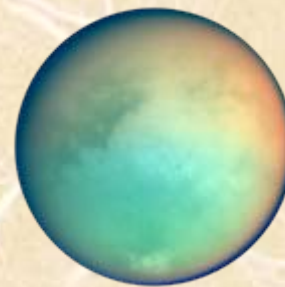
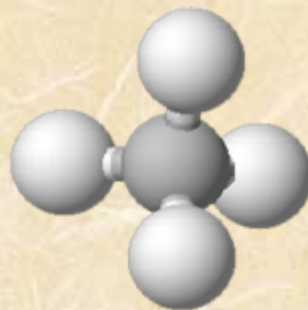


MeCaSDa: Methane Calculated Spectroscopic Database (part of VAMDC)

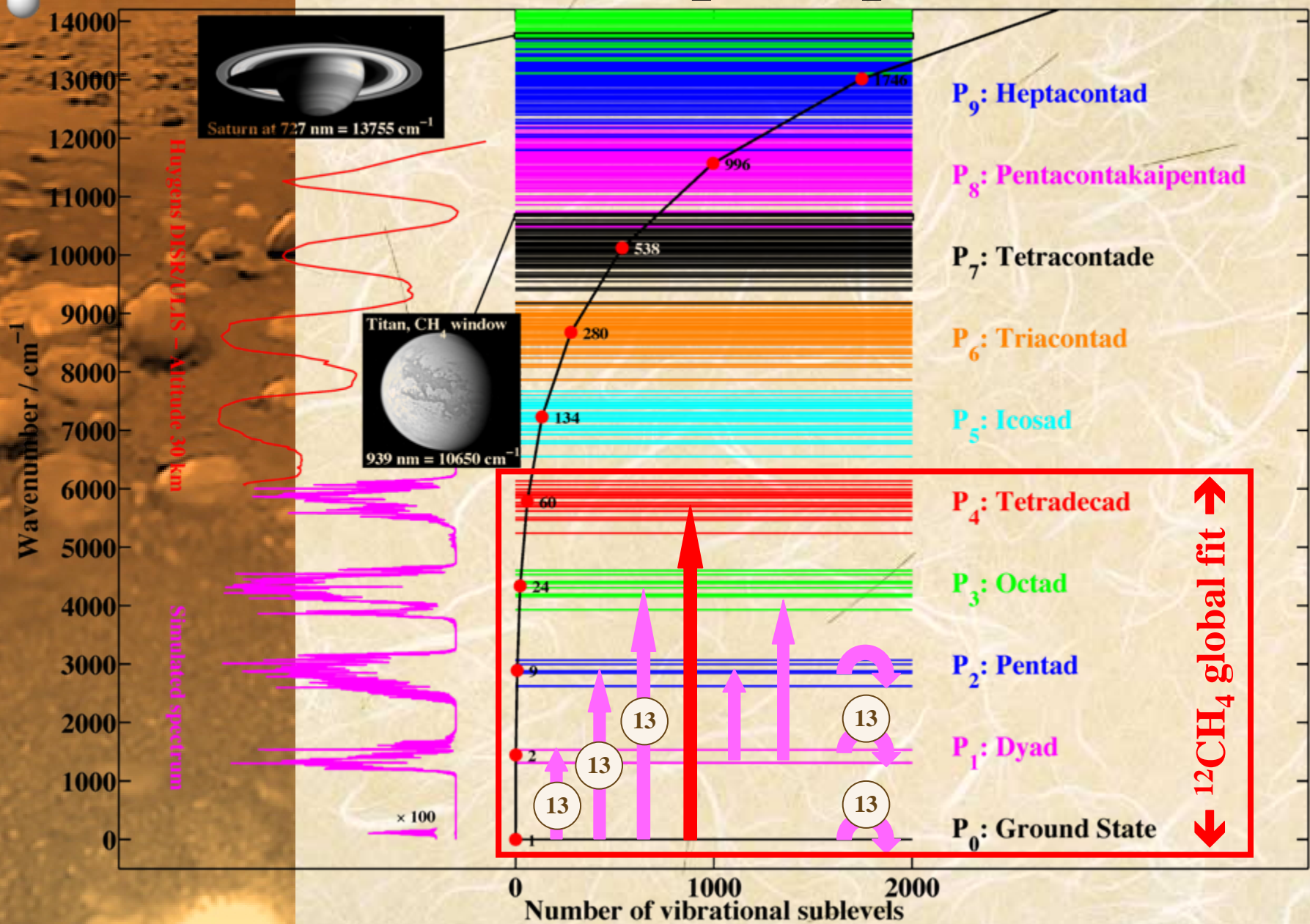
Vincent BOUDON, Christian WENGER, Romain SURLEAU (SMPCA Group)

*Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 6303 CNRS–Université de Bourgogne,
9 Av. A. Savary, BP 47870, F-21078 DIJON, FRANCE*

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



Methane's complex spectrum





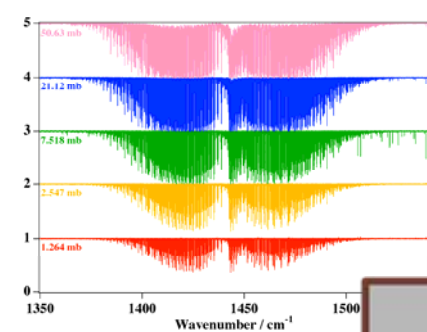
State-of-the-art for $^{12}\text{CH}_4$ (end-2012)

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



INSU
Institut national des sciences de l'Univers



Fits and calculations



XTDS interface

Line lists

Wavenumber (cm⁻¹)	Intensity	Collisional parameters	Accuracy
1350.00	1.00	0.00	0.01
1350.01	1.00	0.00	0.01
1350.02	1.00	0.00	0.01
1350.03	1.00	0.00	0.01
1350.04	1.00	0.00	0.01
1350.05	1.00	0.00	0.01
1350.06	1.00	0.00	0.01
1350.07	1.00	0.00	0.01
1350.08	1.00	0.00	0.01
1350.09	1.00	0.00	0.01
1350.10	1.00	0.00	0.01
1350.11	1.00	0.00	0.01
1350.12	1.00	0.00	0.01
1350.13	1.00	0.00	0.01
1350.14	1.00	0.00	0.01
1350.15	1.00	0.00	0.01
1350.16	1.00	0.00	0.01
1350.17	1.00	0.00	0.01
1350.18	1.00	0.00	0.01
1350.19	1.00	0.00	0.01
1350.20	1.00	0.00	0.01
1350.21	1.00	0.00	0.01
1350.22	1.00	0.00	0.01
1350.23	1.00	0.00	0.01
1350.24	1.00	0.00	0.01
1350.25	1.00	0.00	0.01
1350.26	1.00	0.00	0.01
1350.27	1.00	0.00	0.01
1350.28	1.00	0.00	0.01
1350.29	1.00	0.00	0.01
1350.30	1.00	0.00	0.01
1350.31	1.00	0.00	0.01
1350.32	1.00	0.00	0.01
1350.33	1.00	0.00	0.01
1350.34	1.00	0.00	0.01
1350.35	1.00	0.00	0.01
1350.36	1.00	0.00	0.01
1350.37	1.00	0.00	0.01
1350.38	1.00	0.00	0.01
1350.39	1.00	0.00	0.01
1350.40	1.00	0.00	0.01
1350.41	1.00	0.00	0.01
1350.42	1.00	0.00	0.01
1350.43	1.00	0.00	0.01
1350.44	1.00	0.00	0.01
1350.45	1.00	0.00	0.01
1350.46	1.00	0.00	0.01
1350.47	1.00	0.00	0.01
1350.48	1.00	0.00	0.01
1350.49	1.00	0.00	0.01
1350.50	1.00	0.00	0.01
1350.51	1.00	0.00	0.01
1350.52	1.00	0.00	0.01
1350.53	1.00	0.00	0.01
1350.54	1.00	0.00	0.01
1350.55	1.00	0.00	0.01
1350.56	1.00	0.00	0.01
1350.57	1.00	0.00	0.01
1350.58	1.00	0.00	0.01
1350.59	1.00	0.00	0.01
1350.60	1.00	0.00	0.01
1350.61	1.00	0.00	0.01
1350.62	1.00	0.00	0.01
1350.63	1.00	0.00	0.01
1350.64	1.00	0.00	0.01
1350.65	1.00	0.00	0.01
1350.66	1.00	0.00	0.01
1350.67	1.00	0.00	0.01
1350.68	1.00	0.00	0.01
1350.69	1.00	0.00	0.01
1350.70	1.00	0.00	0.01
1350.71	1.00	0.00	0.01
1350.72	1.00	0.00	0.01
1350.73	1.00	0.00	0.01
1350.74	1.00	0.00	0.01
1350.75	1.00	0.00	0.01
1350.76	1.00	0.00	0.01
1350.77	1.00	0.00	0.01
1350.78	1.00	0.00	0.01
1350.79	1.00	0.00	0.01
1350.80	1.00	0.00	0.01
1350.81	1.00	0.00	0.01
1350.82	1.00	0.00	0.01
1350.83	1.00	0.00	0.01
1350.84	1.00	0.00	0.01
1350.85	1.00	0.00	0.01
1350.86	1.00	0.00	0.01
1350.87	1.00	0.00	0.01
1350.88	1.00	0.00	0.01
1350.89	1.00	0.00	0.01
1350.90	1.00	0.00	0.01
1350.91	1.00	0.00	0.01
1350.92	1.00	0.00	0.01
1350.93	1.00	0.00	0.01
1350.94	1.00	0.00	0.01
1350.95	1.00	0.00	0.01
1350.96	1.00	0.00	0.01
1350.97	1.00	0.00	0.01
1350.98	1.00	0.00	0.01
1350.99	1.00	0.00	0.01
1351.00	1.00	0.00	0.01

Positions, intensities, collisional parameters, accuracy

Databases

CH₄ line list has been built for **HITRAN 2013**



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



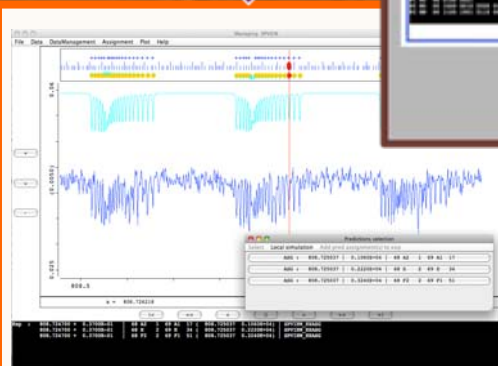
Global e-Infrastructure

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

In Dijon : **MeCaSDa**
Server with calculated CH₄ lines



FP7 - Research Infrastructures



SPVIEW interface

Global modelling



Virtual Atomic and Molecular Data Center

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

Calculated methane line list extraction

Isotope

- | | |
|---|--|
| <input checked="" type="checkbox"/> 12CH4 | <input type="checkbox"/> [0.000 -> 6610.196 cm-1] |
| <input checked="" type="checkbox"/> 13CH4 | <input type="checkbox"/> [0.000 -> 3680.213 cm-1] |
| <input type="checkbox"/> 12CH3D | <input type="checkbox"/> [2014.584 -> 2337.647 cm-1] |



Multipole

- electric dipole
 polarizability

Wavenumber Range



<http://portal.vamdc.eu>

Home VAMDC databases Query Saved queries | Info Known issues

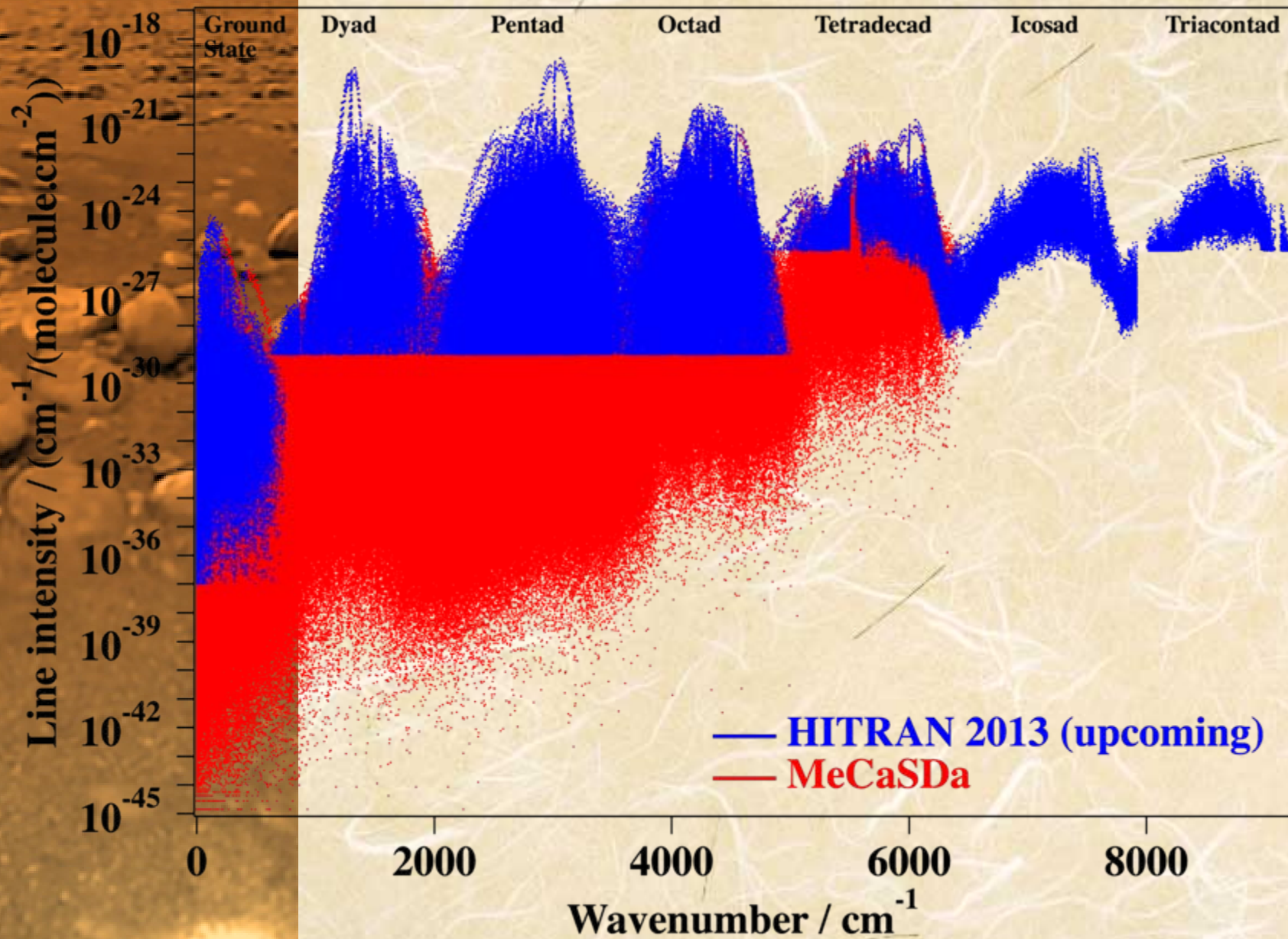
Login Register

Welcome to the VAMDC portal!

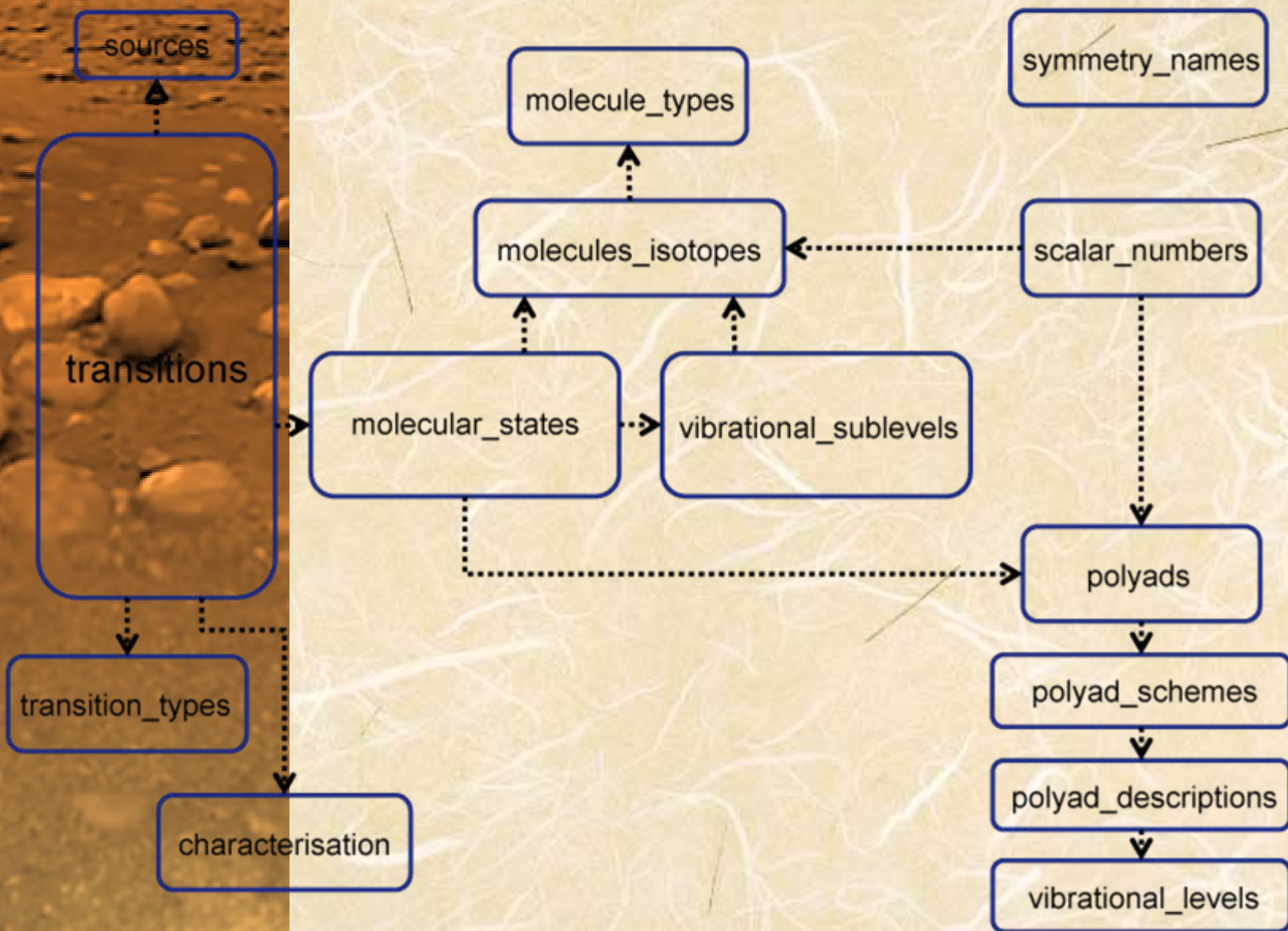
Currently we have 22 databases running and ready to serve you with the data.



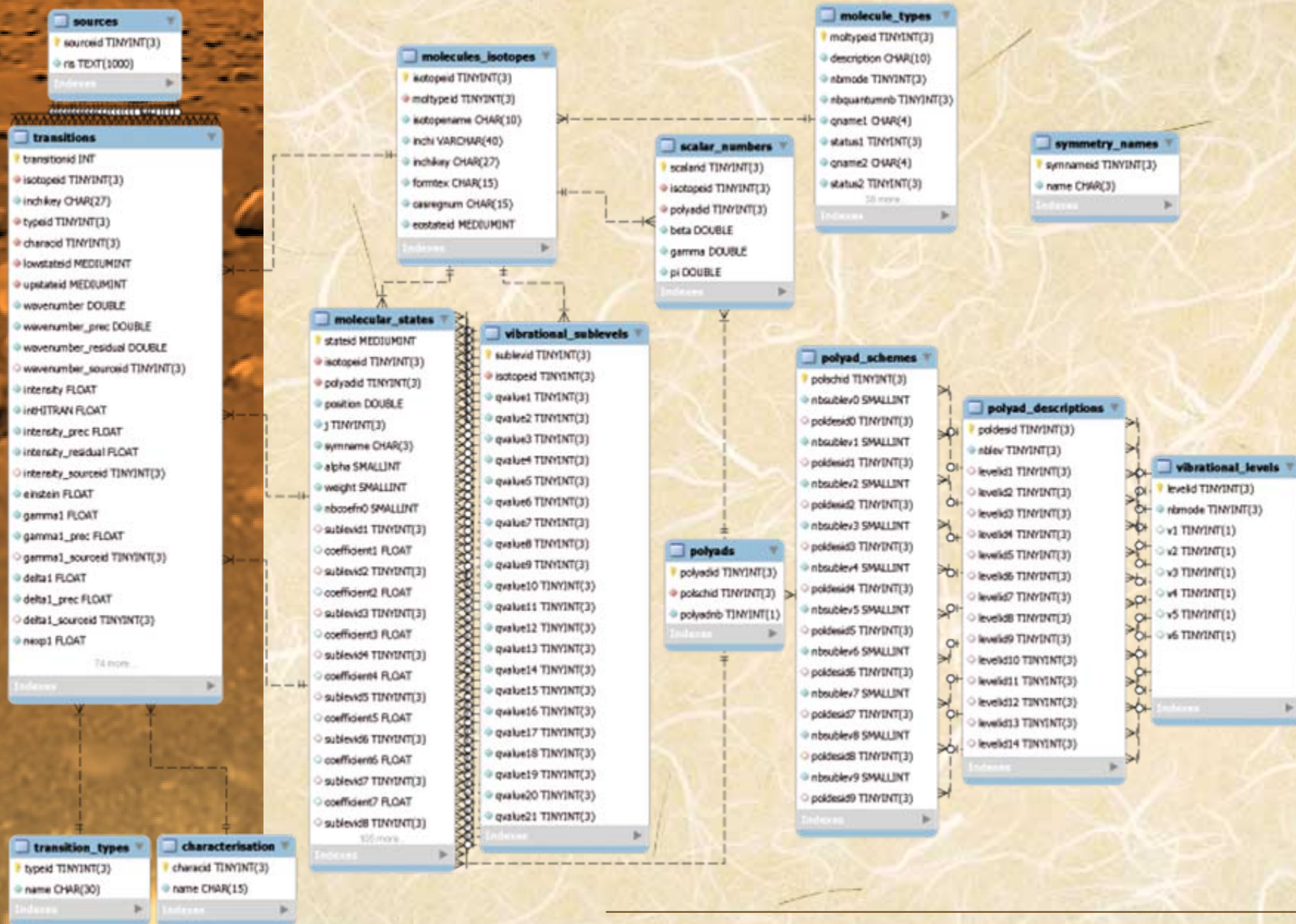
Methane lines in MeCaSDa



Relational Schema for MeCaSDa



Detailed table structure for MeCaSDa



MeCaSDa database in numbers

MeCaSDa	$^{12}\text{CH}_4 / ^{13}\text{CH}_4$	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	Transitions	Nb. dipolar	Nb. Raman
$^{12}\text{CH}_4 / ^{13}\text{CH}_4$			
	$P_0 - P_0$	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 developed 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.

FORTTRAN

XSAMS
XML Schema for Atoms, Molecules, and Solids

MySQL

python™

django

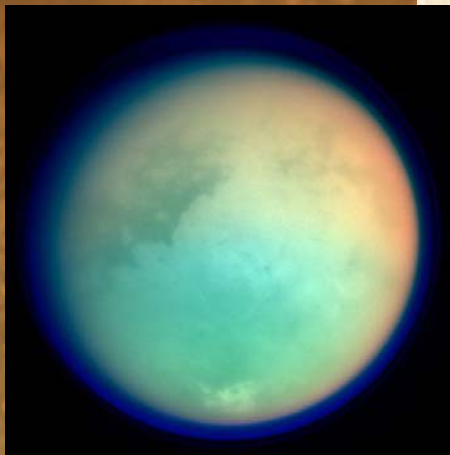
XML



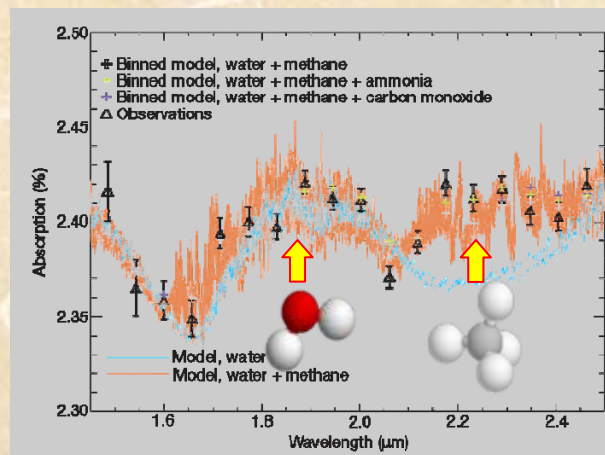
CH₄ spectroscopy: What next ?

- 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, ...)

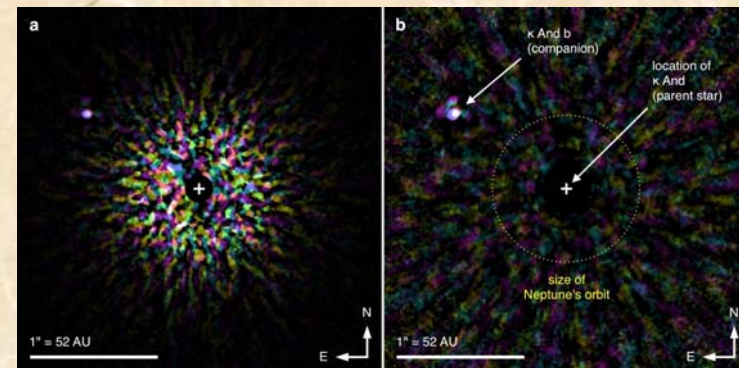
M. Louviot (ICB Dijon), R. Georges (IPR Rennes) O. Pirali (SOLEIL / Ailes), J. Vander Auwera (ULB Bruxelles), ...



Titan / Cassini-Huygens



Exoplanet HD 189733 b



Exoplanet *Kappa Andromedae b*

Database issues and perspectives

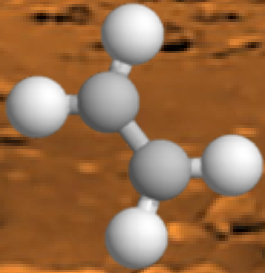
We have a very good server, but:

- MySQL is not very powerful. Future SF₆ database (several Gb) may cause problems.
- Response delay not very satisfying.
- We look for another optimized SQL engine.
- PostgreSQL could be a solution.

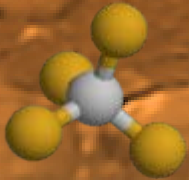
Future of VAMDC :

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

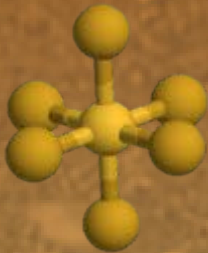
Other molecules



C₂H₄ (ethylene / ethene) – ECaSDa database:
Similar **VAMDC database** developed with
Maud Rotger and colleagues (GSMA, Reims)



CF₄ (carbon tetrafluoride):
Many infrared and Raman bands analyzed
Database to be built



SF₆ (sulfur hexafluoride):
Many infrared and Raman bands analyzed
Database to be built
Huge data volume!