

Molecular Spectroscopy Databases in the Framework of the VAMDC and DAT@OSU Projects

V. BOUDON¹, C. RICHARD¹, M. ROTGER²

¹Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 6303, CNRS / Université Bourgogne Franche-Comté,
9 Av. A. Savary, BP 47870, F-21078 Dijon Cedex, France,

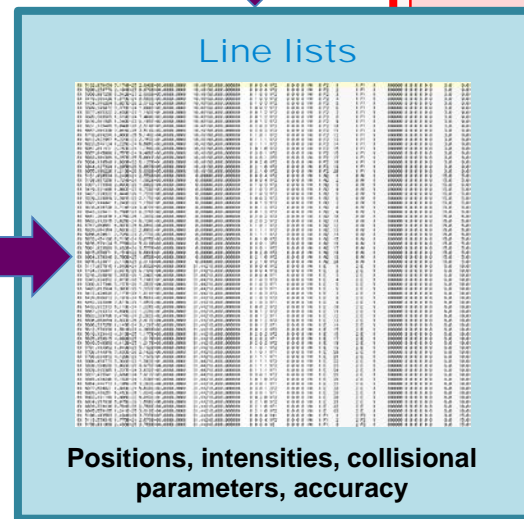
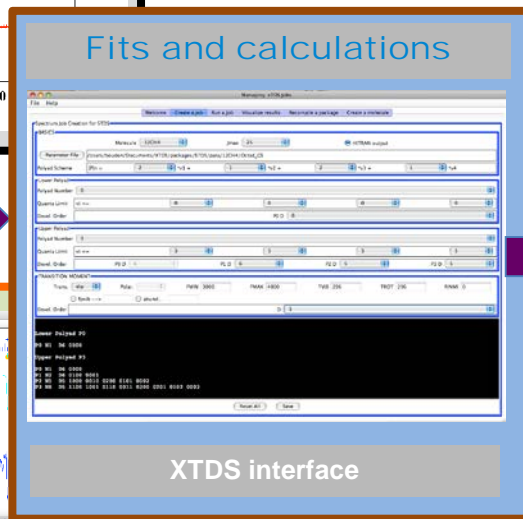
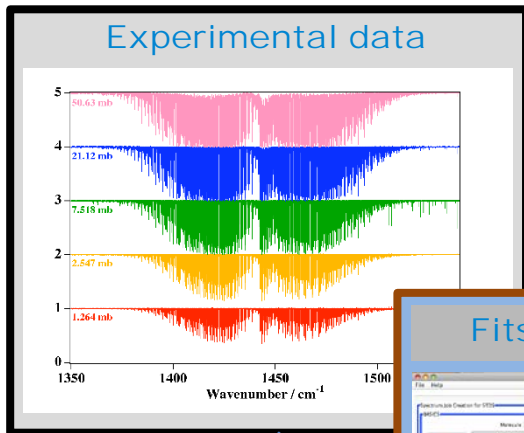
²GSMA, UMR CNRS 7331, Université de Reims Champagne-Ardenne, Moulin de la Housse B.P. 1039, F-51687 Reims
Cedex, France.



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Molecular spectroscopy databases at ICB & OSU THETA



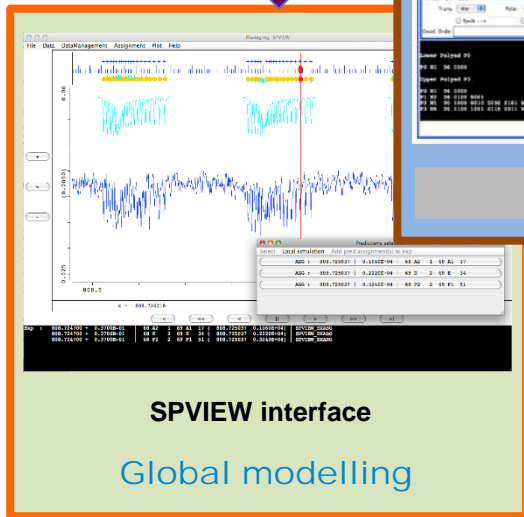
Databases

Line list construction for **HITRAN** and **GEISA**
(with **NASA/JPL**)

Global e-Infrastructure

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

In Dijon :
Server with calculated CH₄ lines



Dijon – 3 databases:

- MeCaSDa (CH₄) → VAMDC / dat@OSU
- SHeCaSDa (SF₆) → VAMDC / dat@OSU
- TFMecaSDa (CF₄) → VAMDC / dat@OSU
- RuCaSDa (RuO₄) → VAMDC / dat@OSU
- GeCaSDa (GeH₄) → VAMDC / dat@OSU

Collaboration with Reims – 2 databases:

- ECaSDa (C₂H₄) → VAMDC / dat@OSU
- S&MPO (O₃) → VAMDC

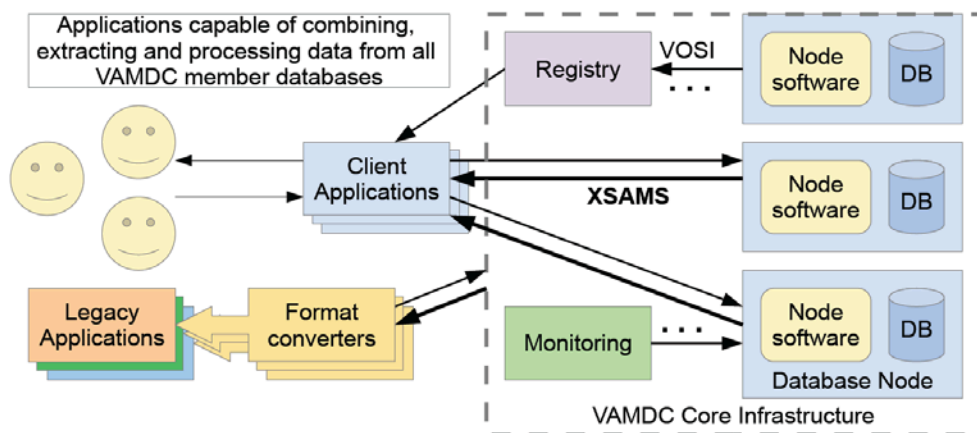
**Molecular spectroscopy data
are always freely available**

The VAMDC Consortium: vamdc.org



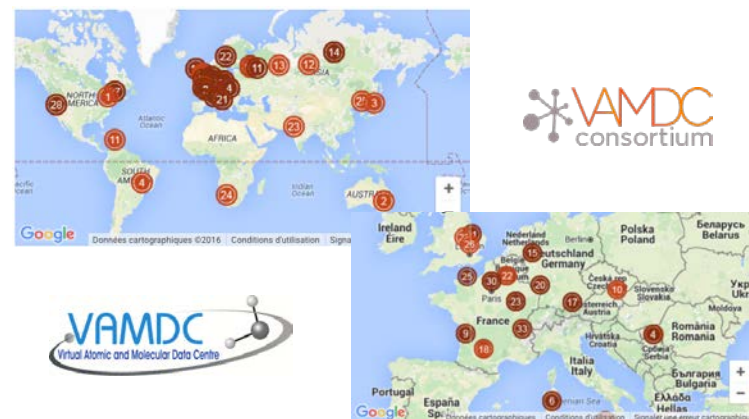
VAMDC is a technical and political framework for sharing Atomic and Molecular data

- 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 online support system (www.vamdc.eu)
- Monitoring of services



Currently 35 databases in the consortium (more to come):

ALADDIN2, BASECOL, Belgrade electron/atom(molecule) database (BEAMDB), CDMS, Carbon Dioxide Spectroscopic Databank 1000K, Carbon Dioxide Spectroscopic Databank 296K, Chianti, DESIRE, **ECaSDa**, **GeCaSDa**, GhoSST, **HITRANonline**, IDEADB, JPL database, **KIDA**, LXcat, **MeCaSDa**, OACT - LASP Database, PAH, Photodissociation - MolD database, RADAM - Ion Interactions, **RuCaSDa**, **S&MPO**, **SHeCaSDa**, SpEctroScopy of Atoms and Molecules Sesam, Spectr-W3, Stark-B, **TFMeCaSDa**, TIPbase, TOPbase, UMIST Database for Astrochemistry, VALD (atoms), VALD subset in Moscow, VAMDC species-DB, Water, ...



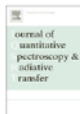
The VAMDC portal

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journal homepage: www.elsevier.com/locate/jqsrt



Virtual atomic and molecular data centre

M.L. Dubernet^{a,b,*}, V. Boudon^c, J.L. Culhane^d, M.S. Dimitrijevic^e, A.Z. Fazliev^f, C. Joblin^g, F. Kupka^h, G. Letoⁱ, P. Le Sidaner^j, P.A. Loboda^k, H.E. Mason^l, N.J. Mason^m, C. Mendozaⁿ, G. Mulas^o, T.J. Millar^p, L.A. Nuñez^q, V.I. Perevalov^r, N. Piskunov^s, Y. Ralchenko^t, G. Rixon^{bb}, L.S. Rothman^u, E. Roueff^v, T.A. Ryabchikova^w, A. Ryabtsev^y, S. Sahal-Bréchet^w, B. Schmitt^x, S. Schlemmer^z, J. Tennyson^z, V.G. Tyuterev^{aa}, N.A. Walton^{bb}, V. Wakelam^{cc}, C.J. Zeppen^{ww}

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The virtual atomic and molecular data centre (VAMDC) consortium*

M L Dubernet¹, B K Antony², Y A Ba¹, Yu L Babikov^{3,4}, K Bartschat⁵, V Boudon⁶, B J Braams⁷, H-K Chung⁸, F Daniel⁹, F Delahaye¹⁰, G Del Zanna⁹, J de Urquijo¹⁰, M S Dimitrijevic^{11,12}, A Domaracka¹², M Doronin¹³, B J Drouin¹³, C P Endres¹⁴, A Z Fazliev¹⁵, S V Gagarin¹⁵, I E Gordon¹⁶, P Gratier^{17,18}, U Heiter¹⁹, C Hill²⁰, D Jevremović¹¹, C Joblin²¹, A Kasprzak²², E Krishnakumar²³, G Leto²⁴, P A Loboda^{15,25}, T Louge²¹, S Maciel^{12,26}, B P Marinkovic²⁷, A Markwick²⁸, T Marquart¹⁹, H E Mason²⁹, N J Mason²⁹, C Mendoza³⁰, A A Mihajlov²⁷, T J Millar³¹, N Moreau³², G Mulas^{21,32}, Yu Pakhomov³³, P Palmeri³⁴, S Pancheshnyi³⁵, V I Perevalov³⁶, N Piskunov³⁷, J Postler³⁸, P Quinet³⁹, E Quintas-Sánchez⁴⁰, Yu Ralchenko³⁸, Y-J Rhee³⁹, G Rixon⁴⁰, L S Rothman⁴¹, E Roueff⁴², T Ryabchikova⁴³, S Sahal-Bréchet⁴⁴, P Scheier⁴⁵, S Schlemmer⁴⁶, B Schmitt⁴⁷, E Stempels⁴⁸, S Tashkun⁴⁹, J Tennyson⁵⁰



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Query Execution

Done

Modify query Stop waiting Save query

Comments

Your request

```
select * where (RadTransWavelength >= 82644.62809917355 AND RadTransWavelength <= 83333.33333333333) AND ((InChIKey IN ('VNWKTOKETHGBQD-UHFFFAOYSA-N','VNWKTOKETHGBQD-UOBTZVSYSAN')))
```

Results by node

Name	View data	Response	Last database update	Download	Species	States	Processes	Radiative	Collisions	Non Radiative
MeCaSDa - Methane Calculated Spectroscopic Database	-- Choose display --	OK	Not available	XSAMS file	2	9084	9294	9294	0	0
HITRANOnline	-- Choose display --	OK	Not available	XSAMS file	2	508	1169	1169	0	0
JPL database: VAMDC-TAP service		EMPTY	27/09/2017 16:45		0	0	0	0	0	0



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Query by...

Species

Processes

Environment

Advanced

Molecule 1

Chemical name

Methane

Stoichiometric formula

CH4

Structural formula

Spin isomer

Standard InChIKey

VNWKTOKETHGBQD-UHFFFAOYSA-N, VNWKTOKETHGBQD-UOBTZVSYSAN

Select All None Search by stoichiometric formula if no isotopologue is selected.

Isotopologue

Methane ¹²CH₃D₃

Methane ¹³CH₄

Methane CH₄

Methane C-13-H3D

Radiative

Wavenumber

1200

to 1210

cm⁻¹

Equivalent Wavelength

Wavelength from 82644.62809917355 to 83333.33333333333A

Upper state energy

to

1/cm

Equivalent to

1/cm

Lower state energy

to

1/cm

Equivalent to

1/s

Equivalent to

1/s

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
- Theoretical spectral database of polycyclic aromatic hydrocarbons
- Photodissociation - MolD database
- Chianti
- GSMA Reims S&MPO
- ECaSDa - Ethene Calculated Spectroscopic Database
- NIST Atomic Spectra Database
- GhoSST
- SHeCaSDa - SF6 Calculated Spectroscopic Database
- Stark-b
- JPL database: VAMDC-TAP service
- HITRANOnline
- VALD sub-set in Moscow (obs)
- 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
- CDMS
- Carbon Dioxide Spectroscopic Databank 296K (VAMDC-TAP)
- SpEctroscopy of Atoms and Molecules
- Carbon Dioxide Spectroscopic Databank 1000K (VAMDC-TAP)
- Spectr-W3
- Water internet Accessible Distributed Information System



<http://portal.vamdc.org>

Example of data: The MeCaSDa database

Calculated Methane Spectroscopic Database: <http://vamdc.icb.cnrs.fr/PHP/mecasda.php>

- **Calculated line lists** resulting from the latest spectroscopic assignments and fits for line positions, line intensities and collisional broadening parameters. **IR and Raman**.
- **Advantage: complete** for the spectral regions under consideration.
- **Drawback:** may be less accurate than databases based on experimental data (HITRAN, GEISA). But **complementary** to them.
- Full **description of eigenstates** with all quantum numbers and eigenvector decomposition.



Isotope(s)

- $^{12}\text{CH}_4$ [0.001 -> 6772.680 cm^{-1}]
- $^{13}\text{CH}_4$ [0.000 -> 4741.874 cm^{-1}]
- $^{12}\text{CH}_3\text{D}$ [2014.584 -> 2337.647 cm^{-1}]

Characterisation

- electric dipole [0.000e+0 -> 8.879e-18 $\text{cm}^{-1}/(\text{molecule cm}^{-2})$]
- polarizability [3.724e-21 -> 8.694e+0 arbitrary unit]

Wavenumber Range

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journal homepage: www.elsevier.com/locate/jqsrt



MeCaSDa and ECaSDa: Methane and ethene calculated spectroscopic databases for the virtual atomic and molecular data centre



Yaye Awa Ba^{a,1}, Christian Wenger^b, Romain Surleau^b, Vincent Boudon^{b,*},
Maud Rotger^{a,*}, Ludovic Daumont^{a,1},
Vladimir G. Tyuterev^a, Marie-Lise Dul

THE JOURNAL OF CHEMICAL PHYSICS 144, 024312 (2016)



^a Groupe de Spectrométrie Moléculaire et Atmosphérique (GSMA), UFR, Sciences Exactes et Naturelles, Moulin de la Housse B.P. 103
^b Laboratoire Interdisciplinaire Carnot de Bourgogne (ICB), CNRS I 21078 DIJON Cedex, France
^c Laboratoire de Physique Moléculaire pour l'Atmosphère et l'Astronomie, Case 76, 4 Place Jussieu, 75252 Paris Cedex 05, France

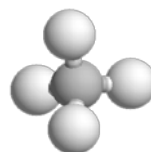
Global analysis of the high temperature infrared emission spectrum of $^{12}\text{CH}_4$ in the dyad (ν_2/ν_4) region

Badr Amyay,^{1,a)} Maud Louviot,¹ Olivier Pirali,² Robert Georges,³ Jean Vander Auwera,⁴ and Vincent Boudon^{1,a)}

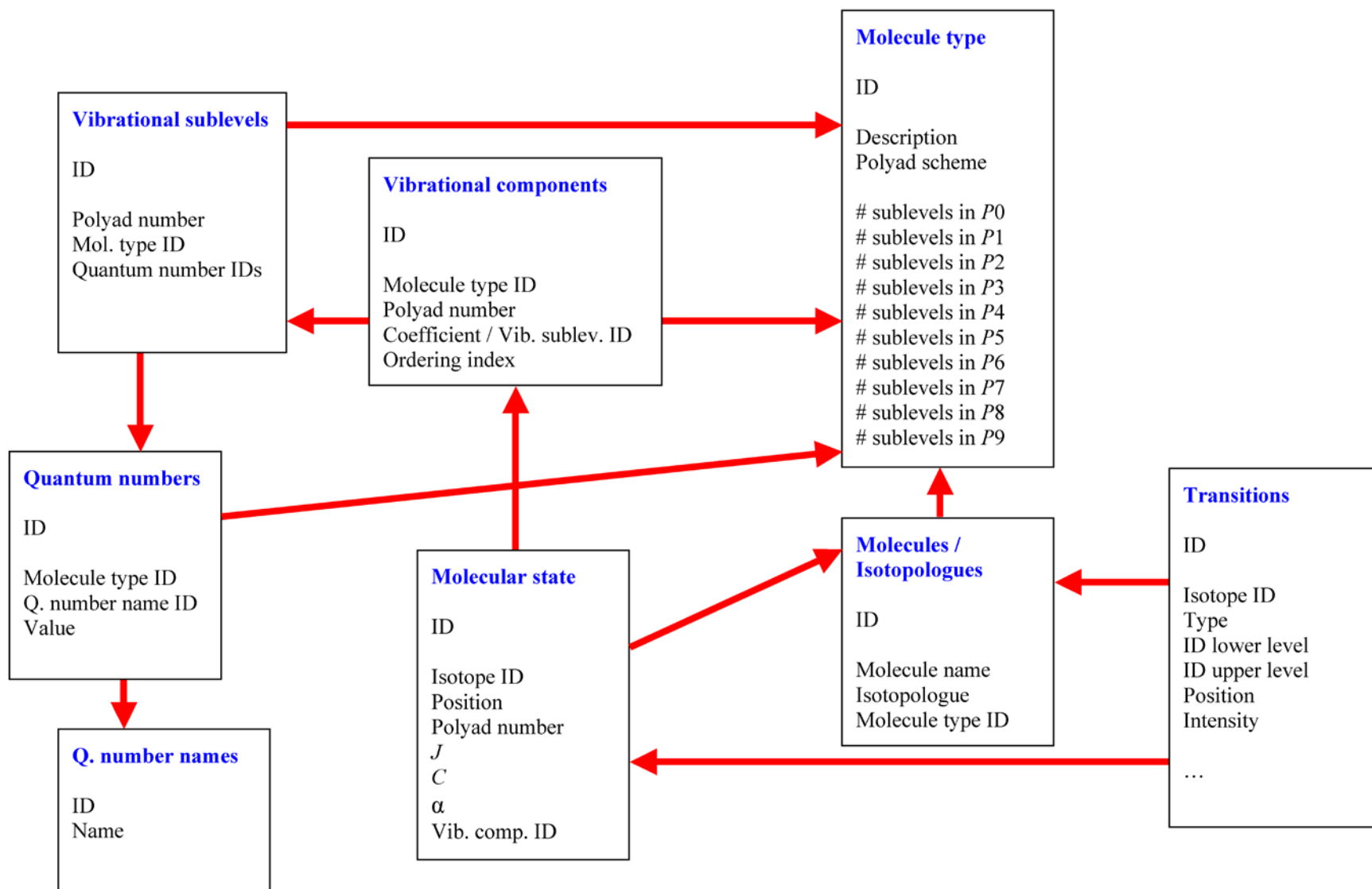
¹Laboratoire Interdisciplinaire Carnot de Bourgogne (ICB), UMR 6303 CNRS, Université Bourgogne Franche-Comté, 9 Avenue A. Savary, BP 47870, 21078 Dijon Cedex, France
²Ligne AILES, Synchrotron SOLEIL, L'Orme des Merisiers, F-91192 Gif-sur-Yvette, France
³Université Paris-Saclay, F-91405 Orsay, France
⁴Institut de Physique de Rennes, UMR 6251, Campus de Beaulieu, Université de Rennes 1/CNRS, F-35042 Rennes Cedex, France

⁵Service de Chimie Quantique et Photophysique, C.P. 16009, Université Libre de Bruxelles, 50 Avenue F. D. Roosevelt, B-1050 Brussels, Belgium

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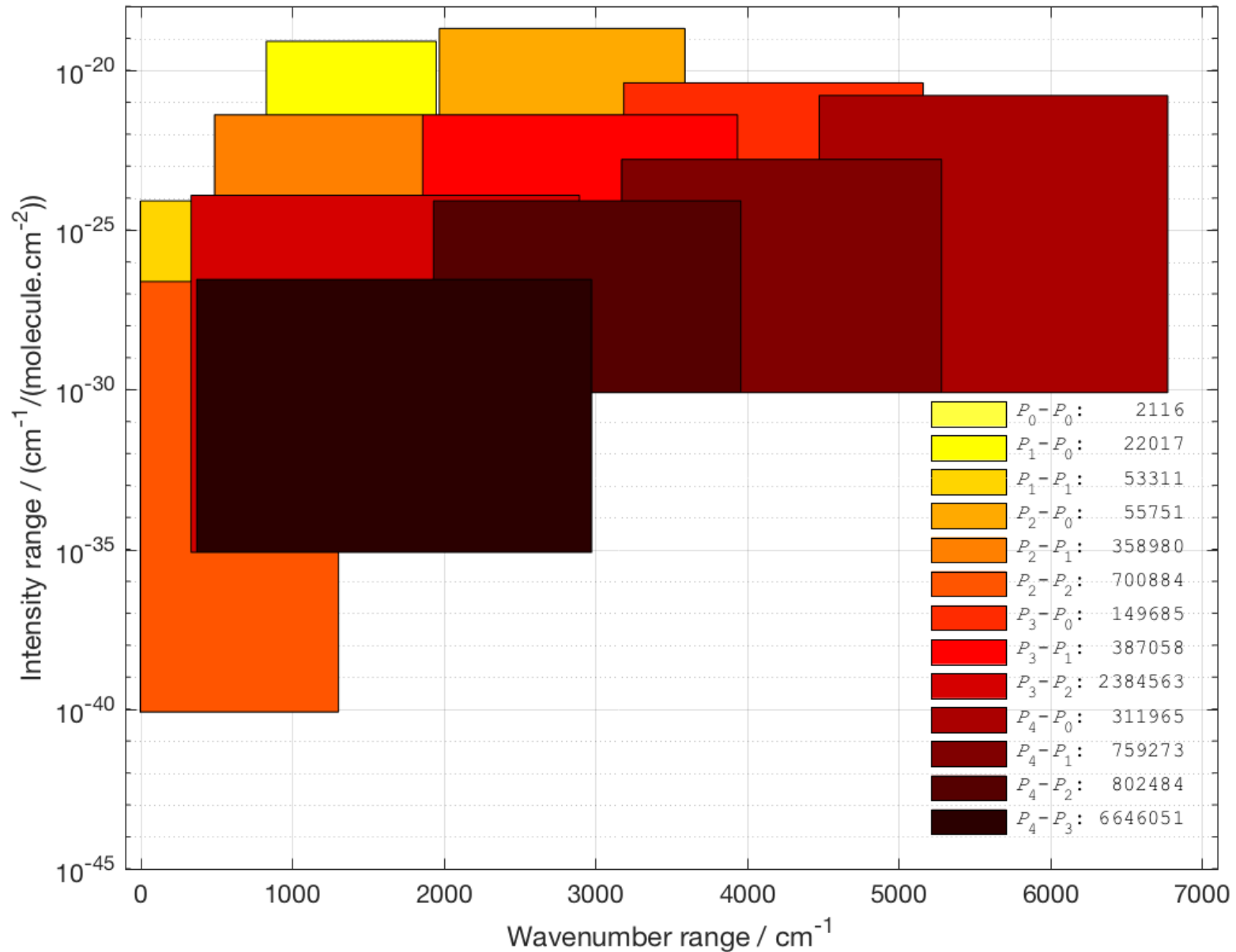


Database structure : MeCaSDa SQL tables



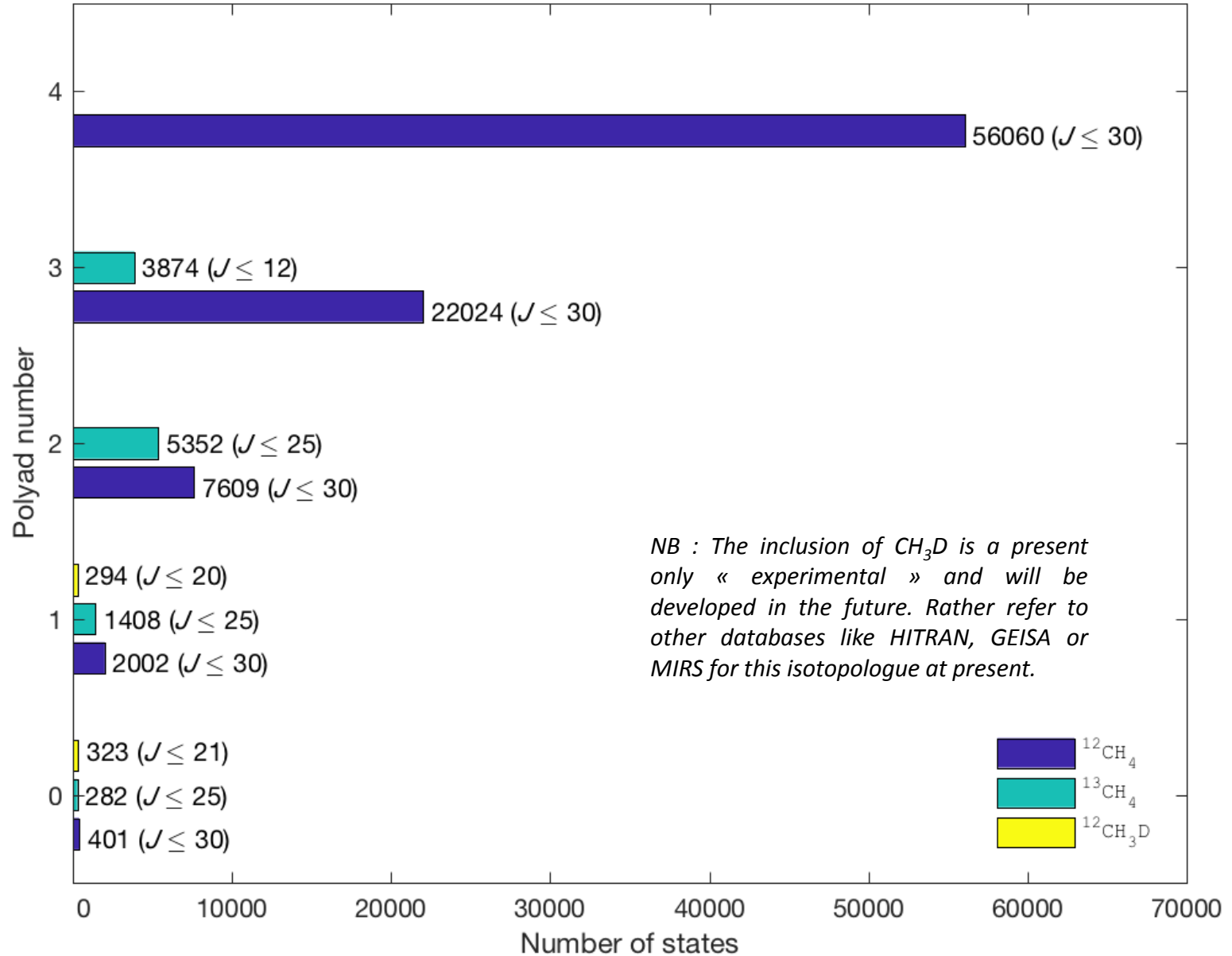
MeCaSDa spectral and intensity coverage

MeCaSDa: spectral and intensity range / number of transitions in IR for $^{12}\text{CH}_4$



MeCaSDa molecular states

MeCaSDa: number of states for each polyad



DAT@OSU database pages

Database : MeCaSDa database



Voir la fiche

Modifier

General metadata

Identifiant : local : FR-18008901306731-2015-03-06

Description : Calculated spectroscopic line lists for methane, resulting from the most recent high-resolution experimental spectrum assignments and fits.

Disciplines : [physics, atomic, molecular & chemical](#) (physics), [spectroscopy](#) (physics)

Keywords : [Greenhouse gases](#), [Methane](#), [molecular spectroscopy](#)

Dates : Data acquisition : from 1 Jan 2013 ongoing
Metadata record : Creation : 1 Jan 2015 Update : 8 Sep 2017 Issue : 1 Jan 2013

Update periodicity : [as needed](#) **Language :** [English](#) (eng)

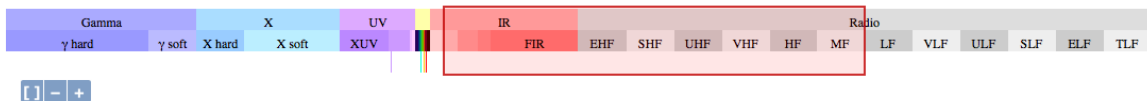
Additional information : Data update: November 2016.

Audience : Research

Coverages

Spectral coverage :

- [Methane calculated line list](#) : between $1.0E-5 \text{ cm}^{-1}$ and 6445.723 cm^{-1}



Administrative metadata

Data creators Affiliation

Vincent Boudon	LICB
Cyril Richard	LICB
Romain Surleau	LICB

Contributors Affiliation Role

Vincent Boudon	LICB	data collector
Tony Gabard	LICB	data collector

Publisher : [Laboratoire interdisciplinaire Carnot de Bourgogne](#)

Science contact : [Vincent Boudon](#) **Computing contact :** [Cyril Richard](#)

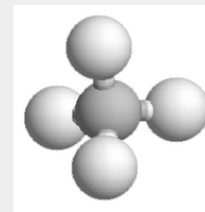
Project and funder :

- [Virtual Atomic and Molecular Data Centre \(VAMDC\)](#)
 - European Union (European project)

Access : available

Access to data

Rights



Collection

[Calculated spectroscopic databases](#)

Quotation

Vincent Boudon, Cyril Richard, Romain Surleau (2013): [MeCaSDa database](#). LICB. [FR-18008901306731-2015-03-06](#)

Future developments

Spectroscopic analyses (more data!) :

- Continue the **global analyses**
- **Hot methane** (combustions, brown dwarfs, exoplanets, ...): e-PYTHEAS
- Isotopologues like **CH₃D**
- Towards higher excited states of **ethylene**
- **New molecules**: SiF₄ (volcanos), ...

Database & software improvements:

- **Parallelization** of spectrum calculation programs

VAMDC portal improvements:

- **HITRAN & GEISA output** on portal
- **Graphical tools** on portal
- **User traceability**
- Inclusion of **GEISA in VAMDC**



<http://e-pytheas.cnrs.fr>



Isotope(s)

- ⁷⁴GeH₄ [1929.205 -> 2265.053 cm⁻¹]
- ⁷²GeH₄ [1929.670 -> 2265.368 cm⁻¹]
- ⁷⁰GeH₄ [1930.068 -> 2265.686 cm⁻¹]
- ⁷³GeH₄ [1929.503 -> 2265.234 cm⁻¹]
- ⁷⁶GeH₄ [1929.894 -> 2264.778 cm⁻¹]

Characterisation

- electric dipole [1.000e+23 -> 4.700e+19 cm⁻¹/(molecule cm²)]
- polarizability [0.000e+0 -> 0.000e+0 arbitrary unit]

Wavenumber Range

Lower wavenumber: cm⁻¹
Upper wavenumber: cm⁻¹

Intensity Threshold

Threshold:

**Work of Cyril
Richard**

