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

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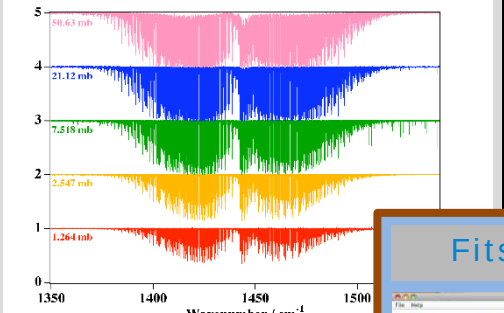
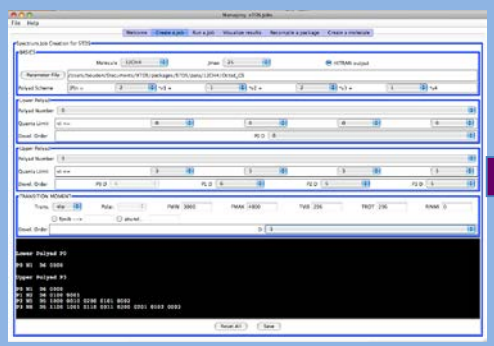
Molecular spectroscopy databases

at ICB & OSU THETA

Experimental data

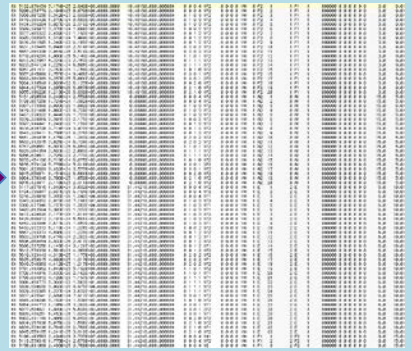


Fits and calculations



XTDS interface

Line lists



Positions, intensities, collisional parameters, accuracy

Databases

Line list construction for **HITRAN** and **GEISA**

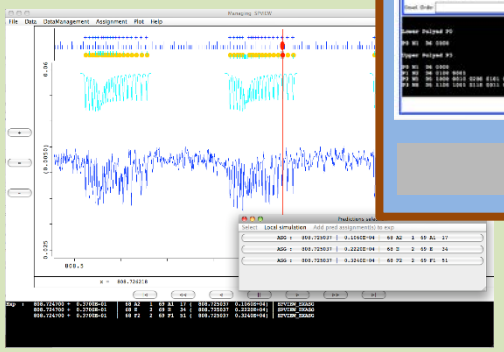
(with **NASA/JPL**)

Global e-Infrastructure

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

In Dijon :
Server with calculated CH_4 lines

VAMDC
Virtual Atomic and Molecular Data Centre



SPVIEW interface

Global modelling

Dijon – 3 databases:

- MeCaSDa (CH_4) → VAMDC / dat@OSU
- SHeCaSDa (SF_6) → VAMDC / dat@OSU
- TFMeCaSDa (CF_4) → VAMDC / dat@OSU
- RuCaSDa (RuO_4) → VAMDC / dat@OSU
- GeCaSDa (GeH_4) → VAMDC / dat@OSU

Collaboration with Reims – 2 databases:

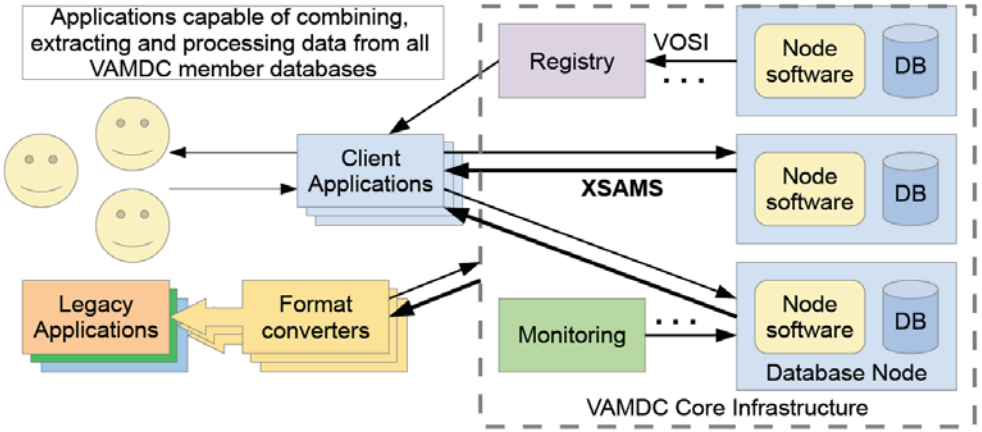
- ECaSDa (C_2H_4) → VAMDC / dat@OSU
- S&MPO (O_3) → VAMDC

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

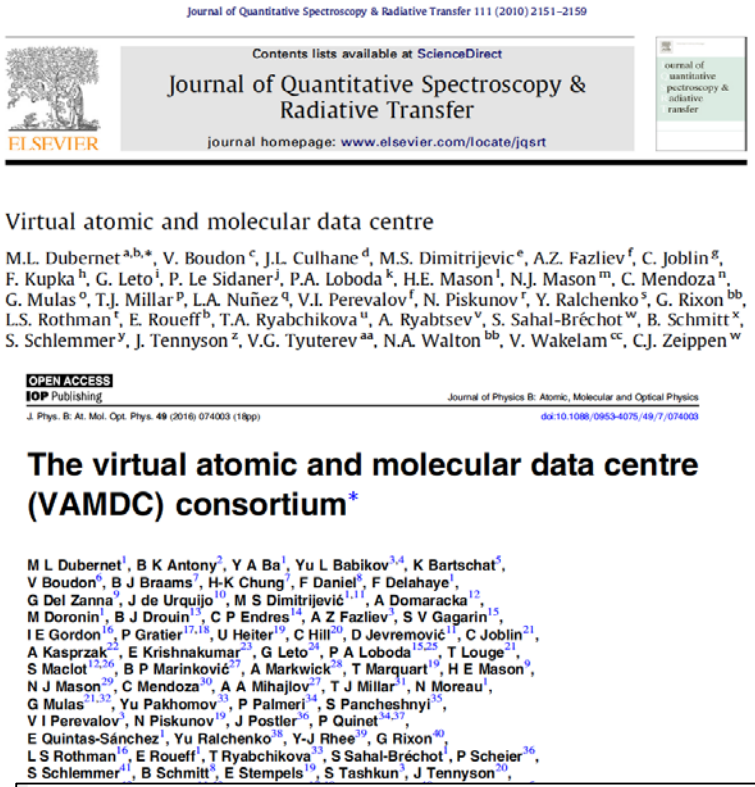
- A set of standards (www.vamdc.eu/standards)
  - Data exchange protocols, data description
  - Standard vocabulary for all exchanges, including for registration of ressources
- A set of software (www.vamdc.eu/software)
- Documentation and online support system (www.vamdc.eu)
- Monitoring of services



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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Virtual atomic and molecular data centre

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

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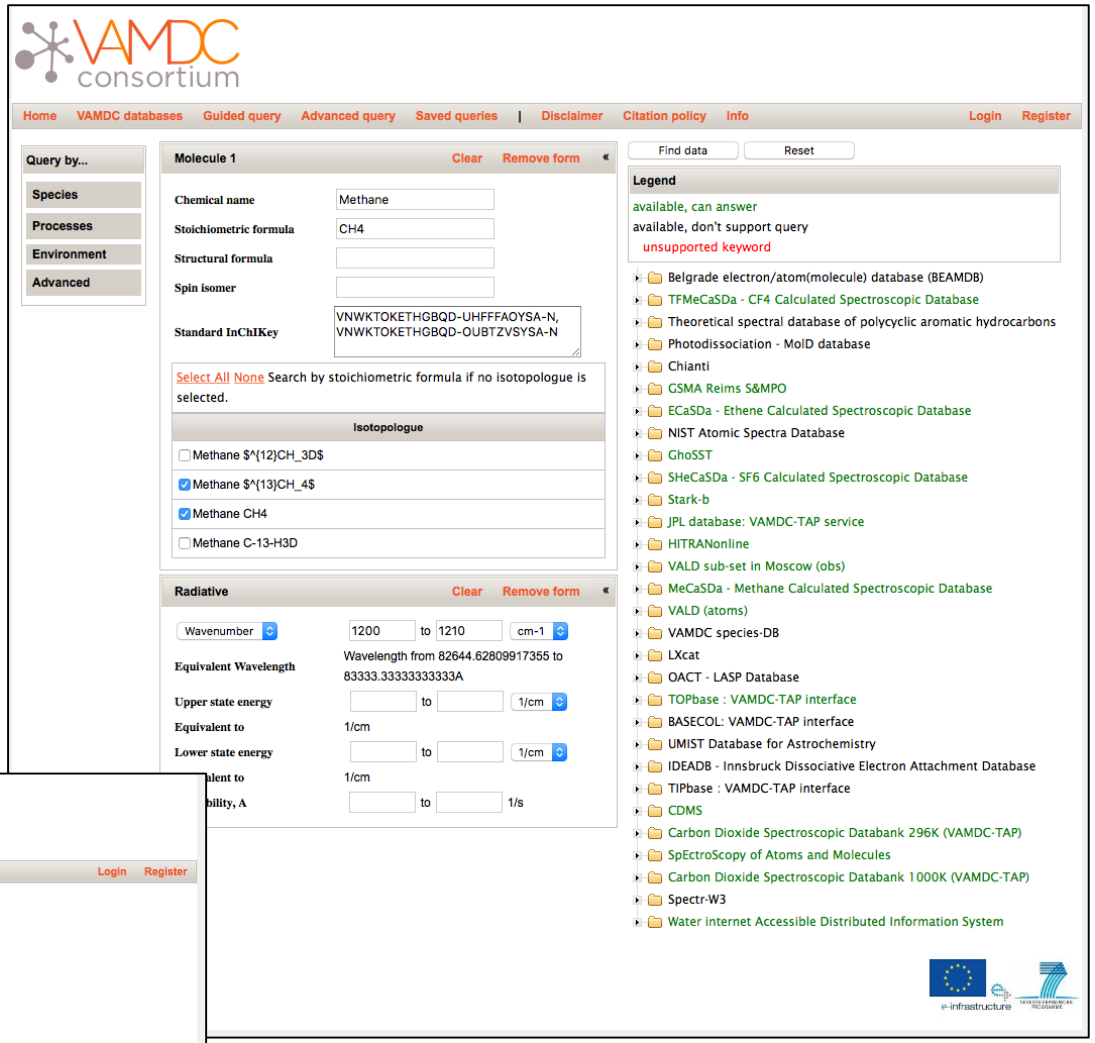
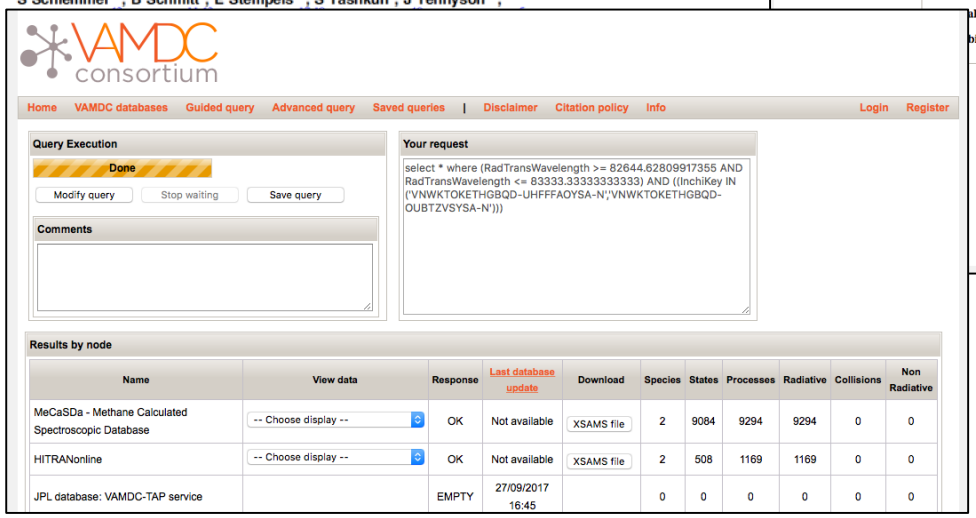


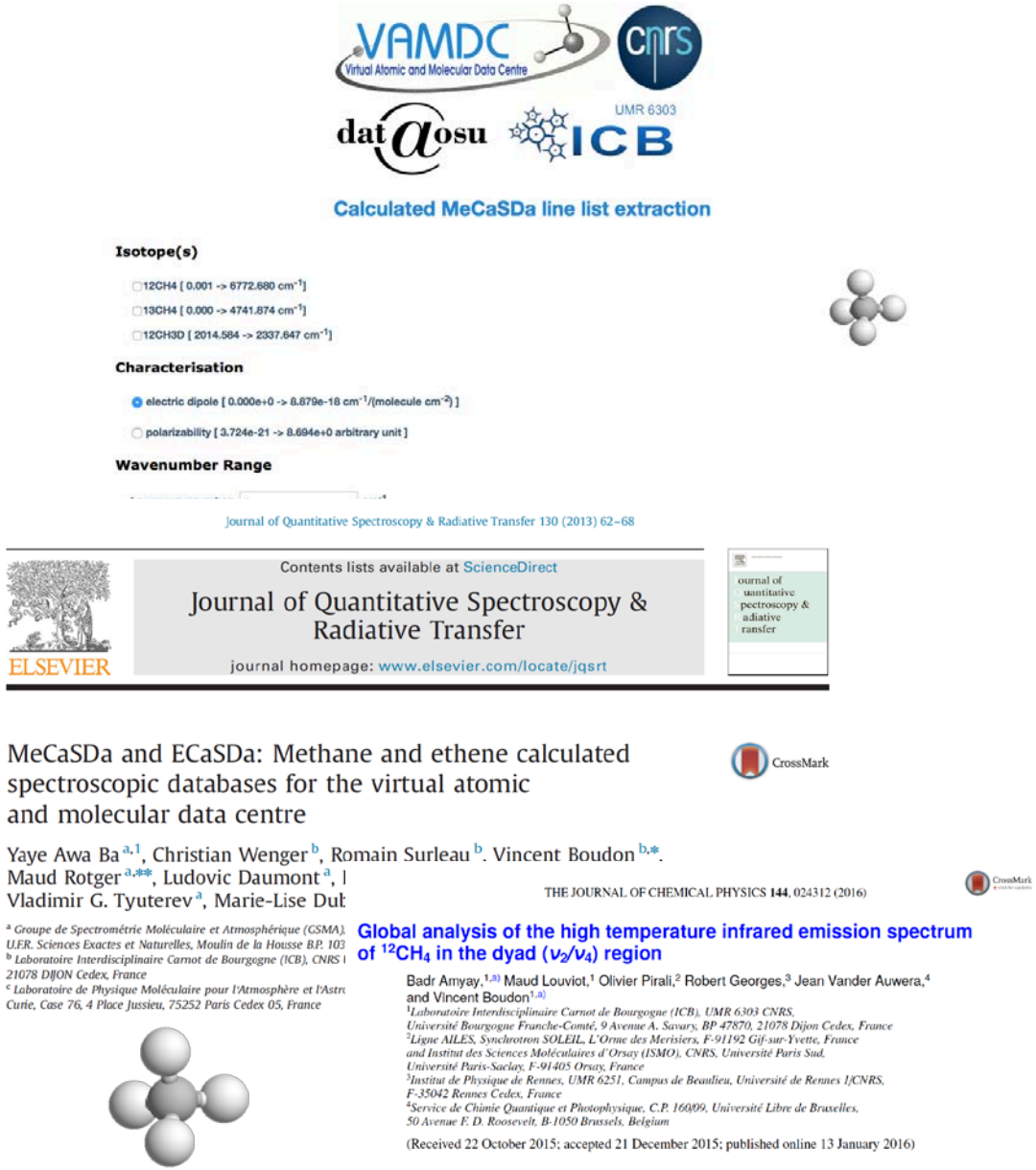


http://portal.vamdc.org

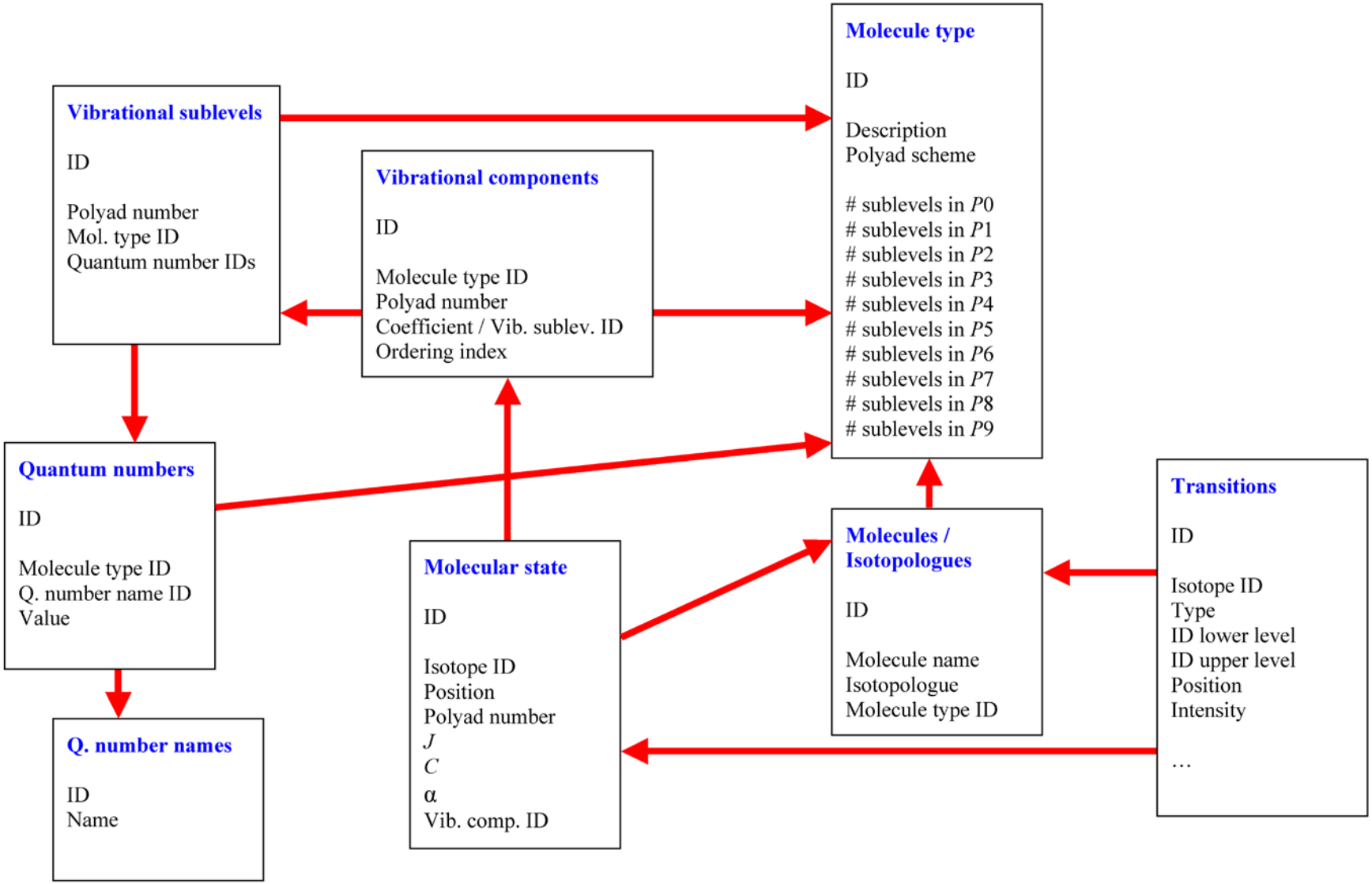
Example of data: The MeCaSDa database

Calculated **Me**thane **S**pectroscopic **Da**tabase: http://vamdc.icb.cnrs.fr/PHP/mecasda.php

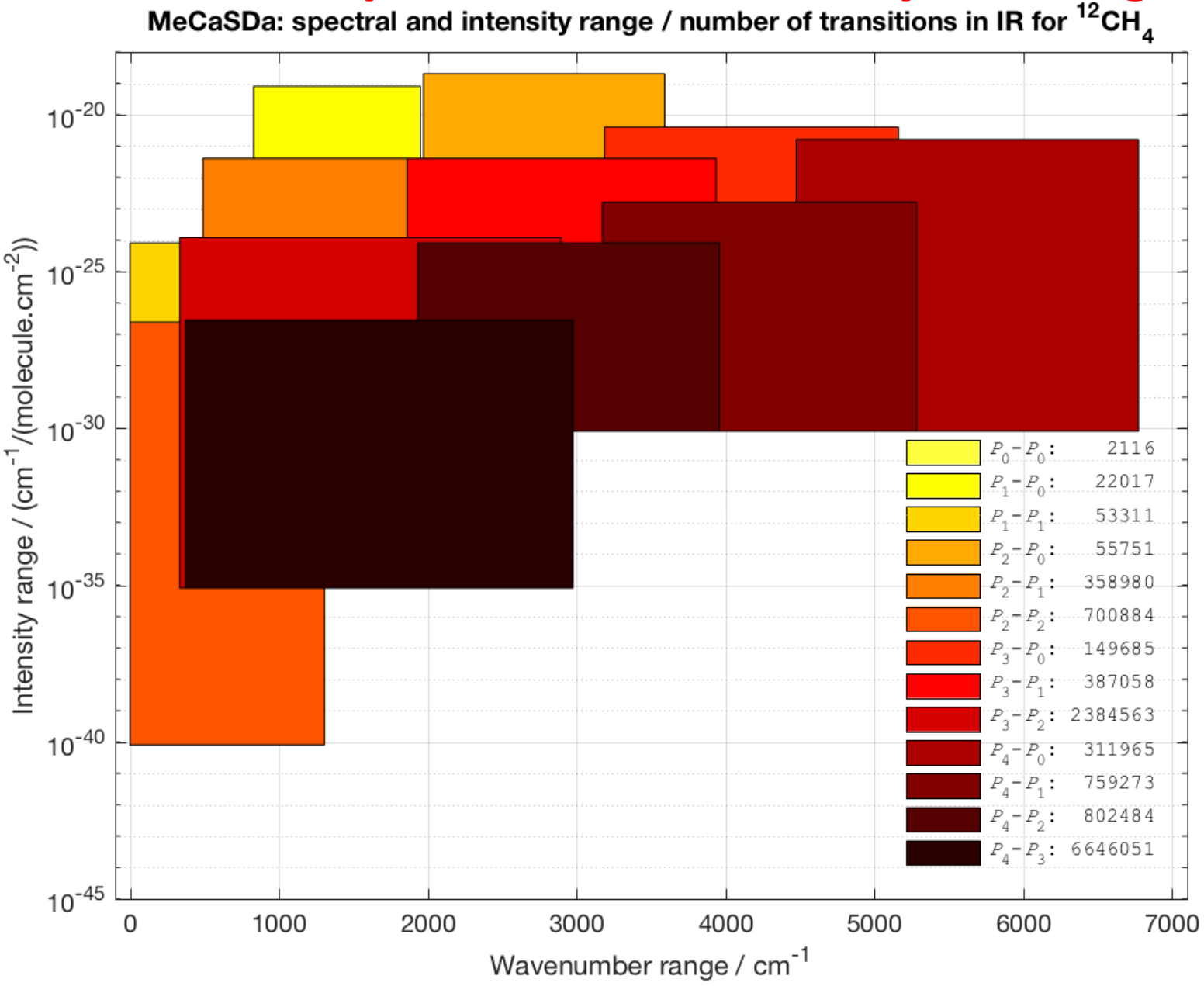
- **Calculated line lists** resulting from the latest spectroscopic assignments and fits for line positions, line intensities and collisional broadening parameters. IR and Raman.
- **Advantage**: complete for the spectral regions under consideration.
- **Drawback:** may be less accurate than databases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



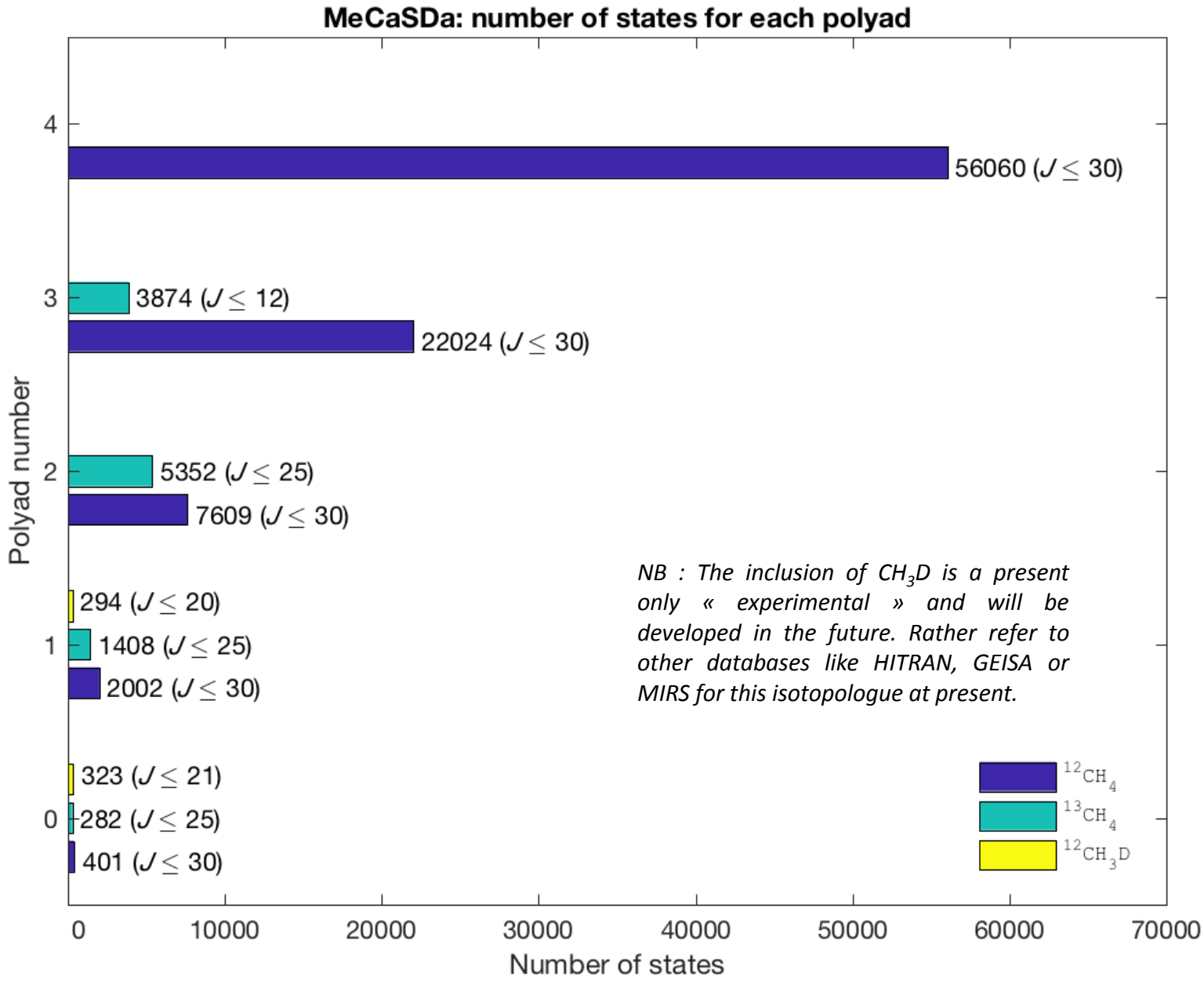
Database structure : MeCaSDa SQL tables



MeCaSDa spectral and intensity coverage



MeCaSDa molecular states



DAT@OSU database pages

dat@osu — vboudon Your interface Logout Help

Database : MeCaSDa database

Accueil de l'accès réservé | Voir la fiche | Modifier

General metadata

Identifier : 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)

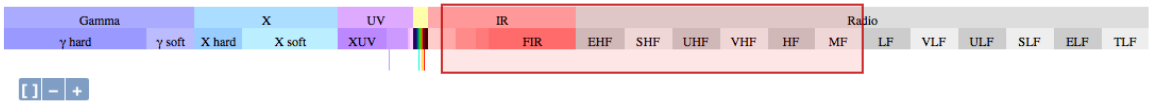
Additional information : Data update: November 2016.

Audience : Research

Coverages

Spectral coverage :

- Methane calculated line list : between 1.0E-5 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

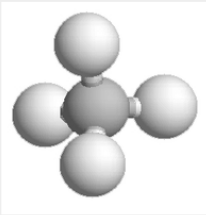
Project and funder :

- Virtual Atomic and Molecular Data Centre (VAMDC)
  - European Union (European project)

Access : available

Access to data

Rights CC BY NC ND



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 CH_3D
- Towards higher excited states of ethylene
- New molecules: SiF_4 (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