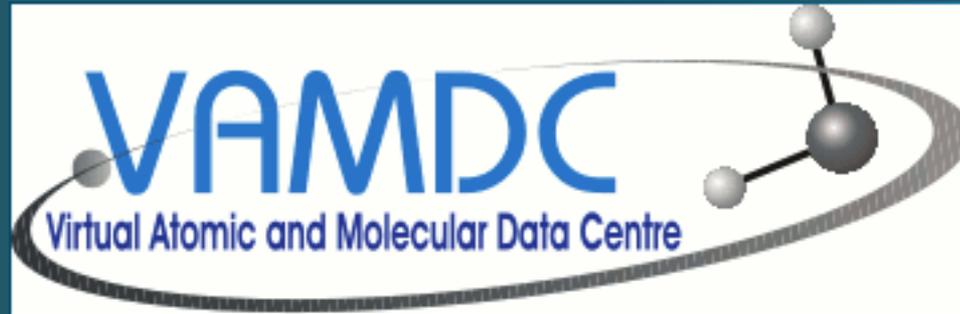


# A methane data base

for



Vincent BOUDON, Romain SURLEAU, Christian WENGER<sup>(1)</sup>  
and Yaye Awa BA<sup>(2)</sup>

(1)- Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 5209 CNRS-Université de Bourgogne

(2)- Groupe de Spectrométrie Moléculaire et Atmosphérique, UMR CNRS 6089, Université de Reims

# Polyads

Table 1: The normal modes of methane

$\nu_1$	$\nu_2$	$\nu_3$	$\nu_4$
$A_1$	$E$	$F_2$	$F_2$
Stretching	Bending	Stretching	Bending
Raman	Raman	IR	IR
$2916 \text{ cm}^{-1}$	$1533 \text{ cm}^{-1}$	$3019 \text{ cm}^{-1}$	$1311 \text{ cm}^{-1}$

We have approximately:  $\nu_1 \approx \nu_3 \approx 2\nu_2 \approx 2\nu_4$

Definition of polyad  $P_n$ :

$$n = 2\nu_1 + \nu_2 + 2\nu_3 + \nu_4$$

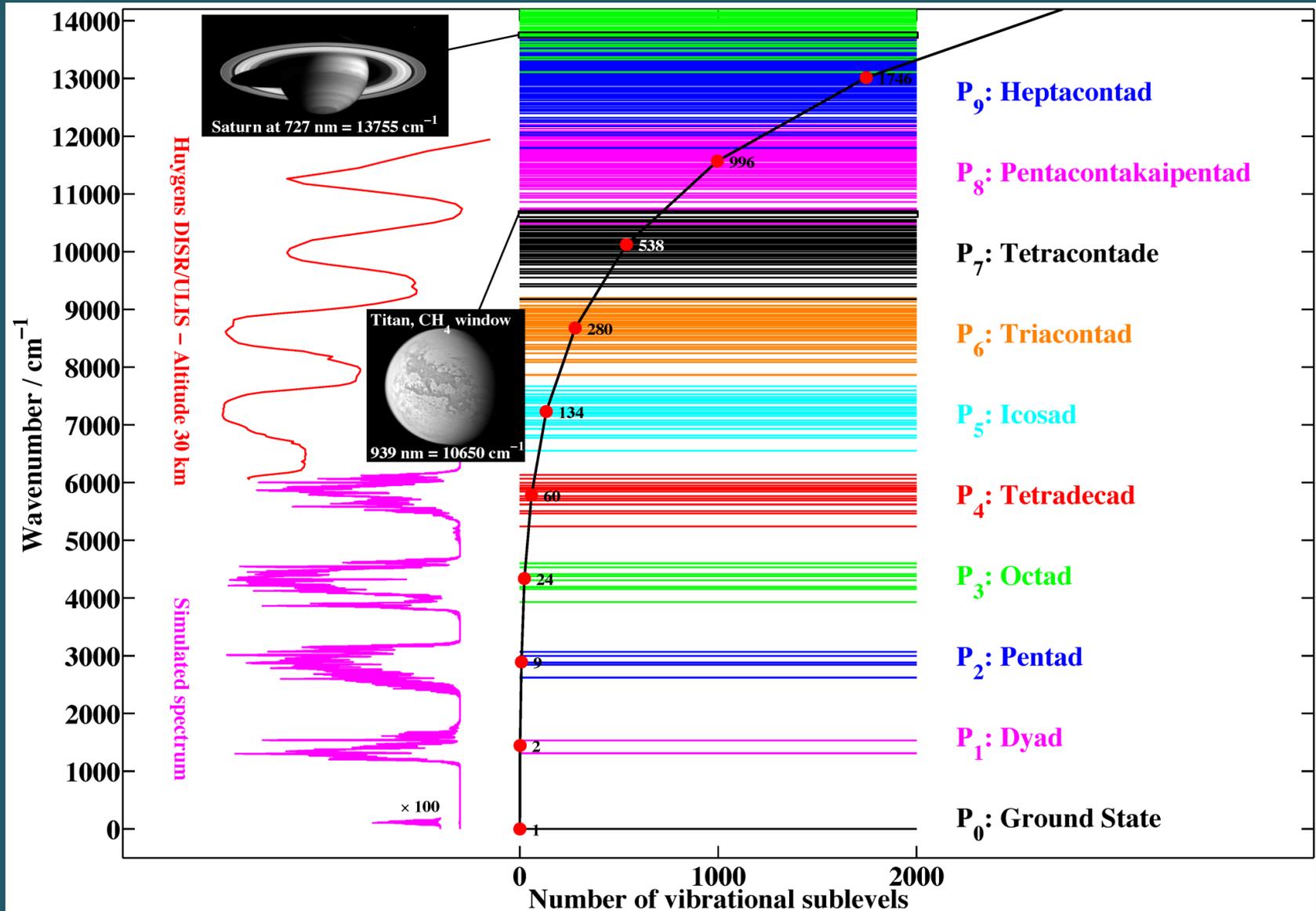
methane

$$n = \sum_k i_k \nu_k$$

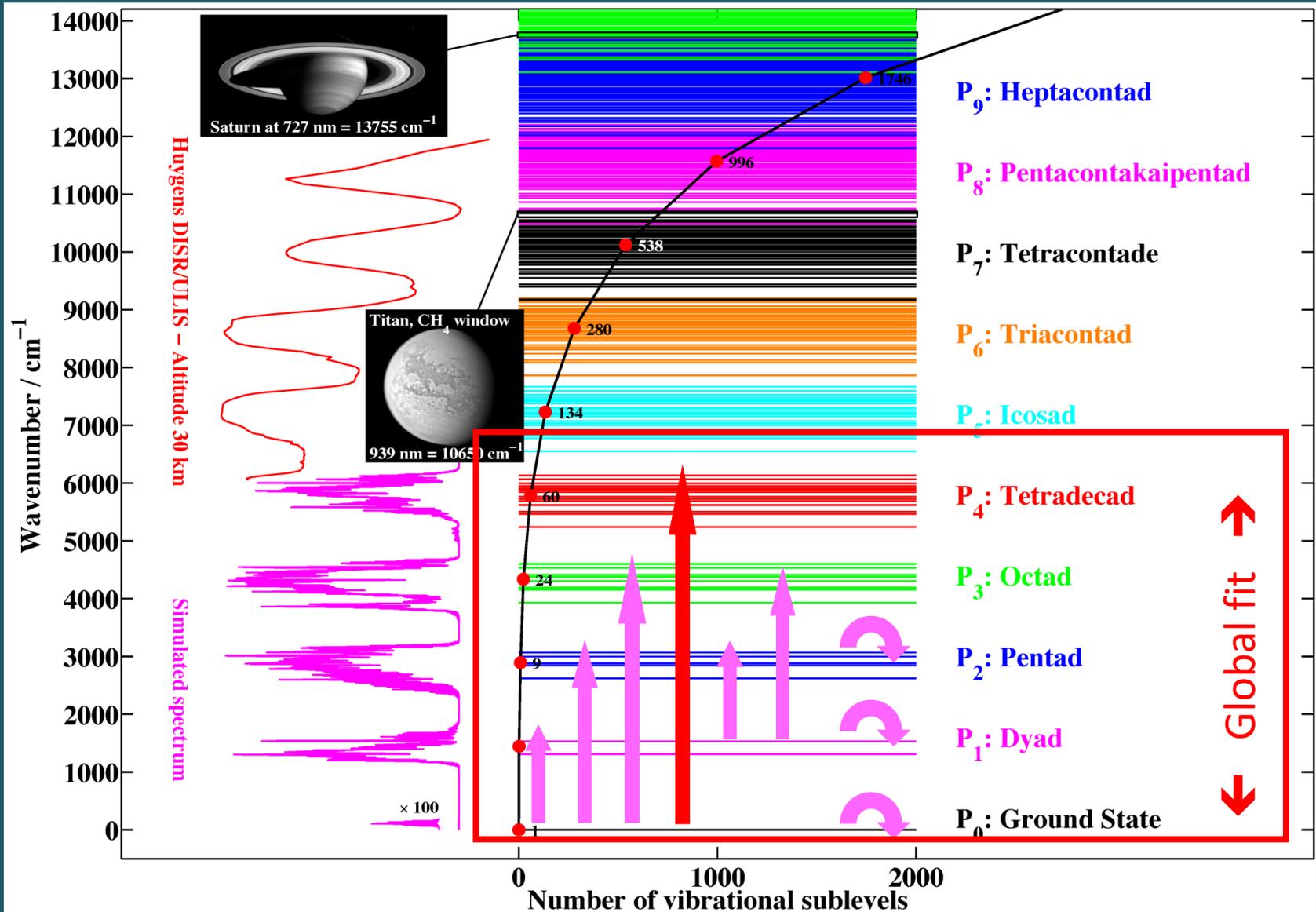
general case

set of  $i_k$  coefficients: polyad scheme

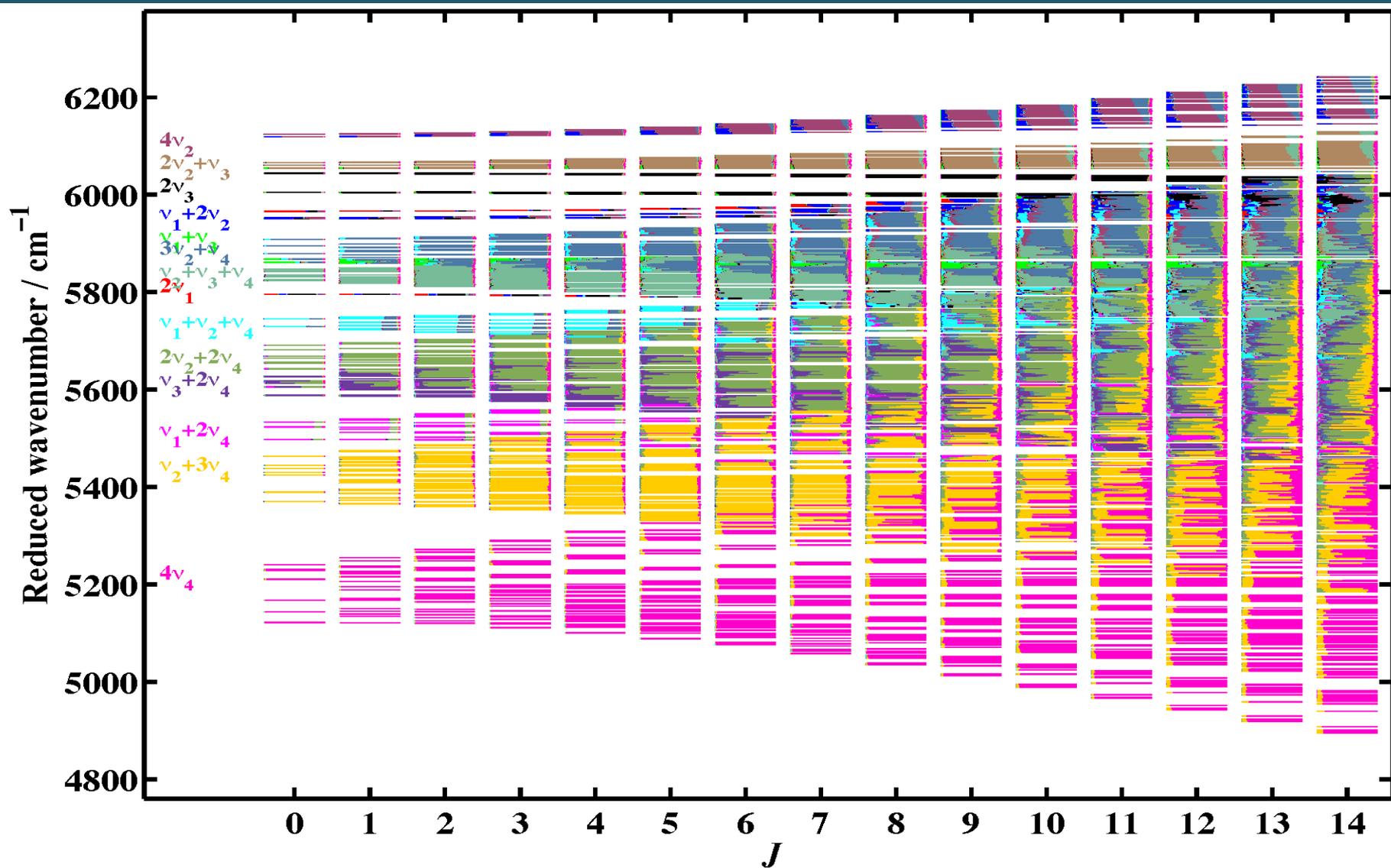
# The polyads of methane



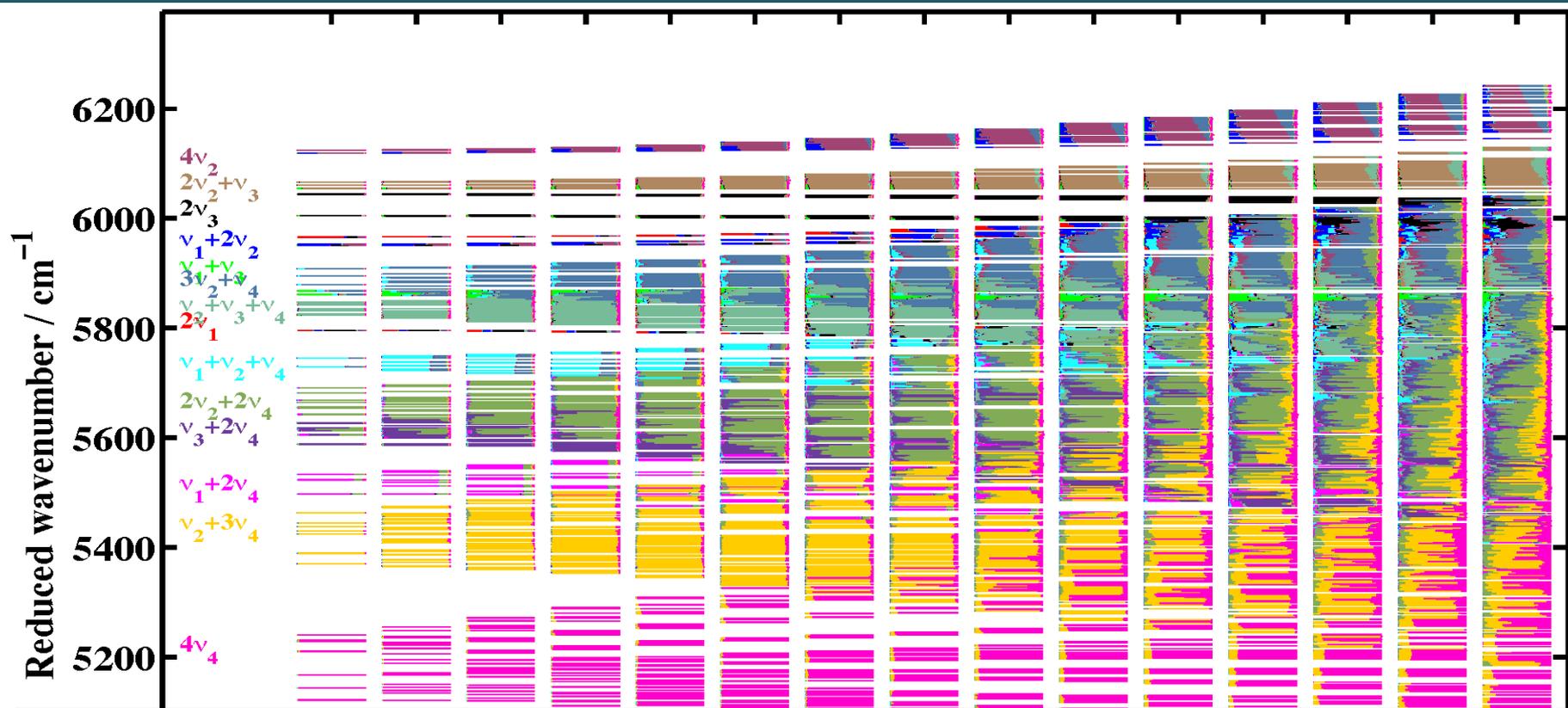
# The polyads of methane



# Tetradecad calculated levels and mixings



# Tetradecad calculated levels and mixings



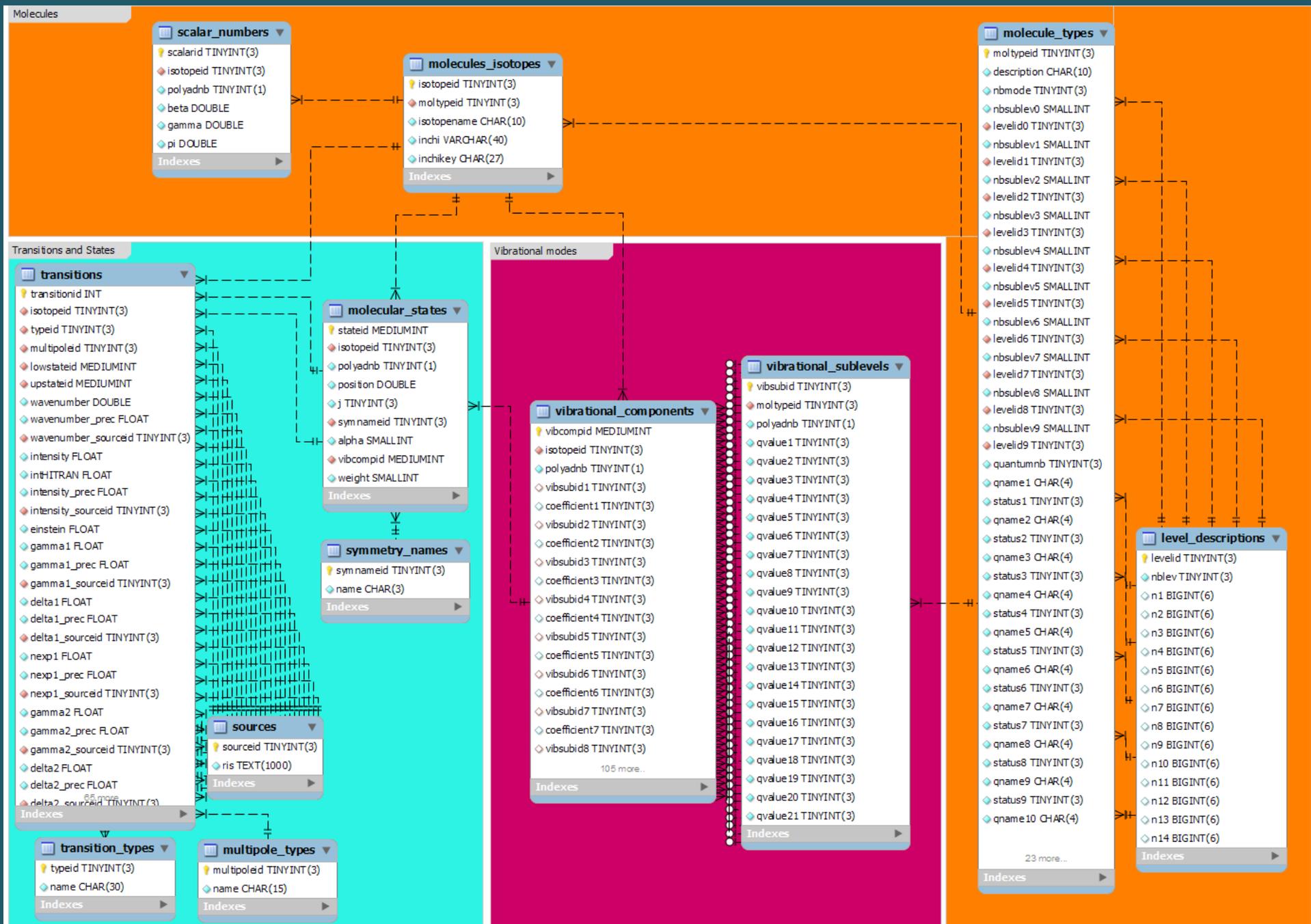
High resolution spectroscopy and first global analysis  
of the Tetradecad region of methane  $^{12}\text{CH}_4$

A. Nikitin, V. Boudon, Ch. Wenger, S. Albert, L.R. Brown, S. Bauerecker and M. Quack

# Creating the data base

Identical for methane and ethylene:

- Line assignment
- Fit of the model parameters (accuracy)
- Calculate all transitions
- Create the tables (text format) and the sql script
- Source this script which creates and feeds the base



# Transitions

isotopologue

type

lower level

upper level

wavenumber

accuracy+source

intensity

intHITRAN

accuracy+source

Einstein coefficient

collisional parameters: self, N2, O2, air, H2O, CO2, H2, He, Ar

broadening

shift

temperature exponent



accuracy+source

# Levels

isotopologue

$P_n$

position

$J$

$C$

$\alpha$

vibrational components

weight

polyad number

energy

rotational quantum number

rovibrational symmetry

multiplicity (ranking) index

increasing energy order

mixings

statistical weight of the level

# Tables of the data base

transitions

molecular\_states

transition\_types

MW, IR, visible, Raman, ...

sources

RIS format

multipole\_types

electric dipole, polarizability

symmetry\_names

A1, A2, E, F1, F2, ...

molecule\_types

XY4, XY3Z

molecules\_isotopes

$^{12}\text{CH}_4$ ,  $^{13}\text{CH}_4$ ,  $^{12}\text{CH}_3\text{D}$       Inchi

level\_descriptions

sets of modes

scalar\_numbers

used for levels drawing calibration

vibrational\_components

mixing percentages

vibrational\_sublevels

intermediate quantum number values

# 41 920 molecular states

## XY<sub>4</sub>

### 12CH<sub>4</sub>

P0 : 327  
P1 : 1408  
P2 : 5352  
P3 : 8274  
P4 : 18900

### 13CH<sub>4</sub>

P0 : 282  
P1 : 1408  
P2 : 5352

## XY<sub>3</sub>Z

### 12CH<sub>3</sub>D

P0 : 323  
P1 : 294

6 249 558 transitions: 2 595 740 absorption  
3 653 818 Raman

	wave number cm <sup>-1</sup>	intensity cm <sup>-2</sup> *atm <sup>-1</sup>	intensity arb. unit		J <sub>max</sub>
<u>12CH4</u>					
1547	0. / 275.	8.E-32 / 2.E-05		GS_GS	27
13025	911. / 1868.	2.E-18 / 2.E+00		Dyad_GS	25
19207	671. / 2076.		4.E+00 / 4.E+18	Dyad_GS_raman	25
31510	0. / 688.	2.E-41 / 2.E-05		Dyad_Dyad	25
49475	2076. / 3484.	1.E-22 / 5.E+00		Pentad_GS	25
72954	1842. / 3685.		5.E-03 / 2.E+20	Pentad_GS_raman	25
247325	455. / 2304.	6.E-29 / 1.E-02		Pentad_Dyad	25
459275	0. / 1133.	4.E-42 / 6.E-08		Pentad_Pentad	25
53439	3434. / 4902.	3.E-17 / 1.E-01		Octad_GS	18
75027	3276. / 5032.		2.E+02 / 1.E+17	Octad_GS_raman	18
267105	1854. / 3685.	3.E-20 / 6.E-03		Octad_Dyad	18
375012	1696. / 3804.		5.E+00 / 3.E+17	Octad_Dyad_raman	18
1015053	274. / 2473.	3.E-26 / 3.E-05		Octad_Pentad	18
114580	4670. / 6446.	2.E-19 / 4.E-02		Tetradecad_GS	17
3024031	1378. / 4097.		8.E-07 / 9.E+14	Tetradecad_Pentad_raman	17
<u>13CH4</u>					
1222	0. / 253.	2.E-29 / 2.E-05		GS_GS	25
13025	901. / 1865.	2.E-19 / 3.E+00		Dyad_GS	25
31525	0. / 694.	9.E-42 / 2.E-05		Dyad_Dyad	25
49475	2057. / 3478.	7.E-22 / 5.E+00		Pentad_GS	25
14636	2325. / 3219.		2.E+01 / 2.E+20	Pentad_GS_raman	25
72951	1823. / 3680.		8.E-01 / 3.E+19	Pentad_GS_raman_ani	25
247325	439. / 2307.	2.E-29 / 1.E-02		Pentad_Dyad	25
<u>12CH3D</u>					
834	2015. / 2338.	1.E-03 / 2.E+02		nu2	21

# Accuracy

RMS deviation for 12CH4

	wave number	intensity
Dyad-GS	0.13 mk	} 9.6 %
Pentad-GS	0.60 mk	
Octad-GS	3.5 mk	
Tetradecad-GS	23.0 mk	13.9 %

# Accuracy

RMS deviation for 13CH4

	wave number	intensity
GS-GS	38.1 KHz	na
Dyad-GS	0.06 mk	na
Pentad-GS	0.46 mk	4.4 %
Dyad-Dyad	36.3 KHz	na

# Extraction

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

methane line lists2 - Mozilla Firefox

Eichier Édition Affichage Historique Marque-pages Outils ?

methane line lists2

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

Google

### Calculated methane line list extraction

**Isotope**



12CH4  [ 0.000 -> 6445.721 cm-1 ]

13CH4  [ 0.000 -> 3680.047 cm-1 ]

12CH3D  [ 2014.584 -> 2337.647 cm-1 ]

**Multipole**

electric dipole

polarizability

**Wavenumber Range**

Lower wavenumber  cm-1      Upper wavenumber  cm-1

**Intensity Threshold**

Threshold  cm-1/(molecule cm-2)

**The extraction can last several minutes**

## The File contents :

[Retour](#)

61	2300.008030	6.797e-31	4.119e-5	.0000.0000	2951.25600.000.000000	0 0 0 3 1F2	0 0 0 1 1F2 16 E	11	17 E	7	460000	0 0 0 0 0 0	66.0	70.0
61	2300.028963	6.725e-29	2.191e-3	.0000.0000	2796.99810.000.000000	0 0 0 3 1F1	0 0 6 0 1S+ 14 E	26	15 E	10	380000	0 0 0 0 0 0	58.0	62.0
61	2300.033074	2.606e-27	9.417e-4	.0000.0000	1754.88550.000.000000	0 0 0 3 1F2	0 0 6 0 1S+ 5 F1	8	6 F2	6	480000	0 0 0 0 0 0	33.0	39.0
61	2300.039497	9.420e-29	9.702e-3	.0000.0000	3143.77560.000.000000	0 0 0 3 1F1	0 0 6 0 1S+ 16 F1	46	17 F2	17	380000	0 0 0 0 0 0	99.0	105.0
62	2300.040613	1.933e-29	1.226e-4	.0000.0000	2624.74680.000.000000	0 0 0 2 1A1	0 0 6 0 1S+ 21 F2	14	22 F1	3	240000	0 0 0 0 0 0	258.0	270.0
61	2300.058421	7.838e-30	9.146e-4	.0000.0000	3169.46930.000.000000	0 0 0 3 1F2	0 0 6 0 1S+ 16 F2	52	17 F1	22	270000	0 0 0 0 0 0	99.0	105.0
61	2300.068847	1.773e-31	2.689e-4	.0000.0000	3697.06920.000.000000	0 1 1 0 1F2	0 0 0 2 1F2 16 F2	209	15 F1	3	060000	0 0 0 0 0 0	99.0	93.0
61	2300.081279	6.486e-29	1.409e-3	.0000.0000	2796.99810.000.000000	0 0 0 3 1F1	0 0 6 0 1S+ 14 F2	38	15 F1	15	380000	0 0 0 0 0 0	87.0	93.0
61	2300.088723	5.880e-27	1.856e-3	.0000.0000	1976.57420.000.000000	0 0 0 2 1F2	0 0 6 0 1S+ 18 F2	7	19 F1	4	470000	0 0 0 0 0 0	111.0	117.0
61	2300.096543	1.143e-28	7.064e-3	.0000.0000	3143.84140.000.000000	0 1 0 2 1F1	0 0 6 0 1S+ 16 A2	16	17 A1	6	380000	0 0 0 0 0 0	165.0	175.0
62	2300.097764	8.093e-32	1.802e-7	.0000.0000	2399.59020.000.000000	0 0 0 2 1A1	0 0 6 0 1S+ 20 F2	12	21 F1	5	230000	0 0 0 0 0 0	246.0	258.0
61	2300.101919	3.587e-33	1.936e-5	.0000.0000	4039.88970.000.000000	0 2 0 0 1E	0 0 0 1 1F2 24 F1	115	23 F2	5	350000	0 0 0 0 0 0	147.0	141.0
61	2300.112025	4.822e-29	2.199e-4	.0000.0000	2475.83940.000.000000	0 0 0 3 1F1	0 0 0 1 1F2 14 F1	2	15 F2	3	470000	0 0 0 0 0 0	87.0	93.0
61	2300.112230	1.693e-30	1.798e-3	.0000.0000	3610.97670.000.000000	0 3 0 0 1A1	0 0 0 2 1F2 15 F2	206	14 F1	5	060000	0 0 0 0 0 0	93.0	87.0
63	2300.113170	6.146e-19	5.013e+2	.0000.0000	753.08960.000.000000	010000 1S+	000000 1S+ 14 A1	3	13 A2	3	000000	0 0 0 0 0 0	116.0	108.0
63	2300.113170	6.146e-19	5.013e+2	.0000.0000	753.08960.000.000000	010000 1S+	000000 1S+ 14 A2	2	13 A1	2	000000	0 0 0 0 0 0	116.0	108.0
61	2300.114793	3.644e-29	1.640e-4	.0000.0000	2473.17810.000.000000	0 0 0 3 1F1	0 0 0 1 1F2 14 F2	2	15 F1	1	470000	0 0 0 0 0 0	87.0	93.0
61	2300.120262	4.218e-31	1.706e-6	.0000.0000	2353.07290.000.000000	0 0 0 3 1F1	0 0 6 0 1S+ 13 E	2	12 E	7	460000	0 0 0 0 0 0	54.0	50.0
61	2300.128865	9.509e-30	8.841e-5	.0000.0000	2539.03060.000.000000	0 0 0 3 1F2	0 0 0 1 1F2 14 E	4	15 E	4	480000	0 0 0 0 0 0	58.0	62.0
61	2300.137467	7.206e-28	6.908e-2	.0000.0000	3141.10280.000.000000	0 0 0 3 1F1	0 0 6 0 1S+ 17 F2	23	17 F1	16	380000	0 0 0 0 0 0	105.0	105.0
61	2300.145935	3.657e-29	3.768e-3	.0000.0000	3143.86290.000.000000	0 1 0 2 1F1	0 0 6 0 1S+ 16 F2	48	17 F1	18	380000	0 0 0 0 0 0	99.0	105.0
61	2300.154131	4.881e-32	2.635e-4	.0000.0000	4039.59000.000.000000	0 2 0 0 1E	0 0 0 1 1F2 24 F2	117	23 F1	5	350000	0 0 0 0 0 0	147.0	141.0
61	2300.166522	2.474e-27	9.115e-4	.0000.0000	1596.68540.000.000000	0 0 0 3 1F2	0 0 6 0 1S+ 2 F1	1	3 F2	3	480000	0 0 0 0 0 0	15.0	21.0
61	2300.177424	1.254e-26	7.237e-3	.0000.0000	1915.04040.000.000000	0 0 0 3 1F2	0 0 6 0 1S+ 7 F1	13	8 F2	9	480000	0 0 0 0 0 0	45.0	51.0
61	2300.185852	9.497e-32	5.535e-5	.0000.0000	3473.71210.000.000000	0 3 0 0 1E	0 0 0 2 1F2 14 F2	199	13 F1	5	070000	0 0 0 0 0 0	87.0	81.0
61	2300.187314	9.911e-29	1.365e-3	.0000.0000	2716.96480.000.000000	0 0 0 3 1F2	0 0 0 1 1F2 15 F2	9	16 F1	7	480000	0 0 0 0 0 0	93.0	99.0
61	2300.188674	1.079e-31	3.184e-4	.0000.0000	3846.06120.000.000000	0 1 1 0 1F1	0 0 0 2 1F2 17 F1	211	16 F2	1	060000	0 0 0 0 0 0	105.0	99.0
61	2300.191795	2.030e-27	1.385e-1	.0000.0000	3164.06090.000.000000	0 1 0 2 1F2	0 0 6 0 1S+ 16 A1	18	17 A2	7	280000	0 0 0 0 0 0	165.0	175.0
61	2300.194997	4.070e-34	1.755e-6	.0000.0000	3924.13620.000.000000	0 3 0 0 1E	0 0 0 2 1F2 17 F1	226	16 F2	7	060000	0 0 0 0 0 0	105.0	99.0
61	2300.196938	2.056e-33	4.076e-7	.0000.0000	3359.85610.000.000000	0 0 0 2 1A1	0 0 6 0 1S+ 24 F1	19	25 F2	2	330000	0 0 0 0 0 0	147.0	153.0
61	2300.202403	2.556e-33	5.068e-7	.0000.0000	3359.84710.000.000000	0 0 0 2 1A1	0 0 6 0 1S+ 24 F2	21	25 F1	3	330000	0 0 0 0 0 0	147.0	153.0
61	2300.215087	1.678e-29	2.595e-3	.0000.0000	3143.91120.000.000000	0 1 0 2 1F2	0 0 6 0 1S+ 16 E	31	17 E	12	380000	0 0 0 0 0 0	66.0	70.0
61	2300.217692	1.259e-29	5.405e-4	.0000.0000	2963.65530.000.000000	0 0 0 3 1F1	0 0 6 0 1S+ 16 F1	20	16 F2	15	380000	0 0 0 0 0 0	99.0	99.0
61	2300.219000	1.619e-27	1.280e-3	.0000.0000	2172.79620.000.000000	0 0 0 3 1F2	0 0 0 1 1F2 11 A1	1	12 A2	3	480000	0 0 0 0 0 0	115.0	125.0
61	2300.233738	1.270e-27	8.192e-4	.0000.0000	2112.14410.000.000000	0 0 0 3 1F1	0 0 6 0 1S+ 10 A1	3	10 A2	3	480000	0 0 0 0 0 0	105.0	105.0
61	2300.238658	1.495e-29	8.507e-5	.0000.0000	2506.65140.000.000000	0 0 0 3 1F2	0 0 6 0 1S+ 13 F2	16	13 F1	15	380000	0 0 0 0 0 0	81.0	81.0
61	2300.241272	2.909e-26	2.232e-2	.0000.0000	2166.58450.000.000000	0 0 0 3 1F2	0 0 0 1 1F2 11 A2	2	12 A1	3	480000	0 0 0 0 0 0	115.0	125.0
61	2300.264018	3.130e-26	3.724e-4	.0000.0000	1252.04630.000.000000	0 0 0 2 1F2	0 0 6 0 1S+ 14 F1	2	15 F2	4	570000	0 0 0 0 0 0	87.0	93.0
61	2300.296364	1.649e-31	9.930e-6	.0000.0000	3106.01840.000.000000	0 0 0 2 1E	0 0 6 0 1S+ 23 F2	18	24 F1	3	340000	0 0 0 0 0 0	141.0	147.0
62	2300.306349	8.933e-27	1.151e-3	.0000.0000	1780.83300.000.000000	0 0 0 2 1E	0 0 6 0 1S+ 17 F2	7	18 F1	4	360000	0 0 0 0 0 0	210.0	222.0
61	2300.307201	2.540e-32	2.702e-6	.0000.0000	3162.47940.000.000000	0 0 0 3 1F2	0 0 6 0 1S+ 17 F1	24	17 F2	19	360000	0 0 0 0 0 0	105.0	105.0
62	2300.309431	2.893e-31	6.436e-7	.0000.0000	2399.38510.000.000000	0 0 0 2 1A1	0 0 6 0 1S+ 20 F1	12	21 F2	4	200000	0 0 0 0 0 0	246.0	258.0
61	2300.315099	1.023e-30	7.759e-4	.0000.0000	3646.64290.000.000000	0 3 0 0 1A2	0 0 0 2 1A1 15 A1	70	14 A2	3	070000	0 0 0 0 0 0	155.0	145.0
62	2300.321766	3.501e-34	6.950e-8	.0000.0000	3360.01480.000.000000	0 0 0 2 1A1	0 0 6 0 1S+ 24 F1	21	25 F2	2	200000	0 0 0 0 0 0	294.0	306.0
61	2300.325513	4.351e-29	1.320e-1	.0000.0000	3851.82620.000.000000	0 1 1 0 1F2	0 0 0 2 1F2 17 F2	213	16 F1	3	070000	0 0 0 0 0 0	105.0	99.0
61	2300.328866	4.200e-26	1.459e-1	.0000.0000	2305.97170.000.000000	0 0 0 3 1F2	0 0 0 1 1F2 12 E	5	13 E	6	480000	0 0 0 0 0 0	50.0	54.0
61	2300.333086	2.540e-28	3.855e-3	.0000.0000	2639.78300.000.000000	0 0 0 3 1F2	0 0 6 0 1S+ 14 E	10	14 E	9	480000	0 0 0 0 0 0	58.0	58.0
61	2300.335328	6.112e-27	3.535e-3	.0000.0000	1915.38020.000.000000	0 0 0 3 1F1	0 0 6 0 1S+ 7 F2	12	8 F1	9	480000	0 0 0 0 0 0	45.0	51.0

# Technical resources

Dell poweredge R610

2x Intel Xeon X5570 quad core

12 GB RAM

150 GB disk (SSD)

18 GB calculation jobs

2 GB MySql data base

OS : Debian Squeeze 64bits

Thanks to: VAMDC European network  
ANR Project 'CH4@Titan'

# To do

- Collisional parameters  
Tony Gabard, ICB Dijon
- $^{13}\text{CH}_4$  Octad  
H.M. Niederer, S. Albert, ETH Zürich
- $\text{CH}_3\text{D}$  fit with  $\text{C}_3\text{vTDS}$   
presently MIRS, A. Nikitin, LTS Tomsk
- Several polyad schemes for one molecule type

# Communication between VAMDC and the databases: NodeSoftware

Software (Django or java version) using the standards and protocols defined by VAMDC :

models.py

queryfunc.py

dictionaries.py

Restrictables

Returnables

Requestables => not yet implemented

# Models.py

Database is redefined in Python code: each table is defined as a python code class.

molecules_isotopes	
isotopeid	TINYINT(3)
moltypeid	TINYINT(3)
formula	CHAR(10)
isotopename	CHAR(10)
inchi	VARCHAR(40)
inchikey	CHAR(27)



Class Molecules_isotopes	
List of attributes	

# Queryfunc.py

SetupResult (main function) : query the database and pass the output to the generator.

SQL Query

Run query in the data model

Create and stock the results

# Dictionaries.py

Link between the database informations and the global names of VAMDC.

- **Restrictables** : elements used to put some constraints on the table columns.

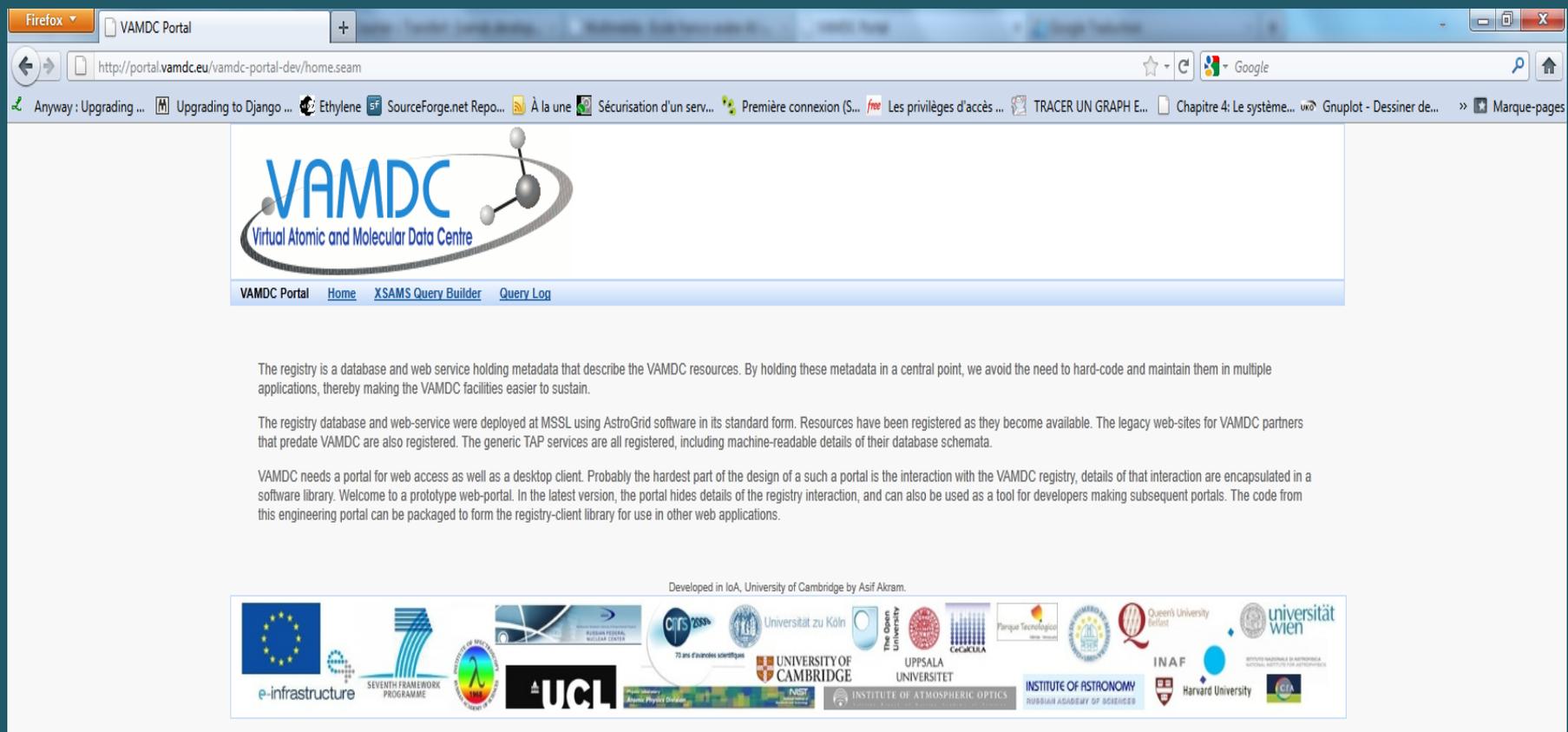
```
RESTRICTABLES = {\n    'RadTransWavenumber':'wavenumber',\n    'RadTransProbabilityLineStrength':'intensity'\n}
```

- **Returnables** : list of elements available in the database.

```
RETURNABLES = {\n    'RadTransWavenumber':'RadTran.wavenumber',\n    'RadTransWavenumberUnit':'1/cm',\n    'MoleculeChemicalName':'Molecule.isotopename',\n}
```

# VAMDC portal

<http://portal.vamdc.eu/vamdc-portal-dev/>



The screenshot shows a Firefox browser window with the address bar displaying <http://portal.vamdc.eu/vamdc-portal-dev/home.seam>. The page features the VAMDC logo, which includes the text "VAMDC Virtual Atomic and Molecular Data Centre" and a molecular structure graphic. Below the logo is a navigation menu with links for "VAMDC Portal", "Home", "XSAMS Query Builder", and "Query Log".

The main content area contains three paragraphs of text:

The registry is a database and web service holding metadata that describe the VAMDC resources. By holding these metadata in a central point, we avoid the need to hard-code and maintain them in multiple applications, thereby making the VAMDC facilities easier to sustain.

The registry database and web-service were deployed at MSSL using AstroGrid software in its standard form. Resources have been registered as they become available. The legacy web-sites for VAMDC partners that predate VAMDC are also registered. The generic TAP services are all registered, including machine-readable details of their database schemata.

VAMDC needs a portal for web access as well as a desktop client. Probably the hardest part of the design of a such a portal is the interaction with the VAMDC registry, details of that interaction are encapsulated in a software library. Welcome to a prototype web-portal. In the latest version, the portal hides details of the registry interaction, and can also be used as a tool for developers making subsequent portals. The code from this engineering portal can be packaged to form the registry-client library for use in other web applications.

Developed in IoA, University of Cambridge by Asif Akram.

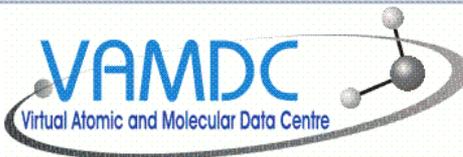
The footer of the page displays a row of logos for various partner institutions and programs, including the European Union's e-infrastructure, the Seventh Framework Programme, UCL, the University of Cambridge, Uppsala Universitet, the Institute of Atmospheric Optics, the Institute of Astronomy, INAF, Harvard University, and the Russian Academy of Sciences.

# Query the databases

Firefox VAMDC Portal

http://portal.vamdc.eu/vamdc-portal-dev/xsamsForm.seam?actionMethod=home.xhtml%3ANavigator.defaultQueryBuilder()&cid=524

urca



VAMDC Portal Home XSAMS Query Builder Query Log

**Query Parameters**

Atoms

Molecules

Transitions

Collisions

Free Form

[X Close](#)

**Molecules**

Chemical Name:

Stoichiometric Formula:

Molecule Ion Charge: Range

Molecule InChI:

InChI Key:

Formula	InChI	InChI Key
<input checked="" type="checkbox"/>	InChI=1S/C2H4/c1-2/h1-2H2/f1+0H2,2+0H2	VGGSQFUCUMXWEO-XKSUVOSDSA-N
<input checked="" type="checkbox"/>	InChI=1S/C2H4/c1-2/h1-2H2/f1+0H2,2+1H2	VGGSQFUCUMXWEO-NARUAAMMSA-N

[Select All](#)

Resource	Query Parameters
<a href="#">BASECOL: development VAMDC-TAP interface</a>	<a href="#">atomsymbol</a> <a href="#">collisioncode</a> <a href="#">inchikey</a> <a href="#">moleculeinchikey</a> <a href="#">moleculestoichiometricformula</a> <a href="#">moleculestateenergy</a> <a href="#">moleculestatenuclearspinisomer</a> <a href="#">sourceyear</a> <a href="#">temperature</a>
<a href="#">KIDA: VAMDC-TAP interface</a>	<a href="#">moleculeioncharge</a> <a href="#">moleculechemicalname</a> <a href="#">moleculeinchi</a> <a href="#">moleculeinchikey</a>
<a href="#">TOPbase: VAMDC-TAP interface</a>	<a href="#">atomioncharge</a> <a href="#">radtranswavelength</a> <a href="#">atomnuclearcharge</a> <a href="#">atomsymbol</a>
<a href="#">Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)</a>	<a href="#">radtranswavenumber</a>
<a href="#">TIPbase: VAMDC-TAP interface</a>	<a href="#">atomioncharge</a> <a href="#">atomnuclearcharge</a> <a href="#">atomsymbol</a>
<a href="#">HITRAN-UCL resource</a>	<a href="#">radtranswavenumber</a> <a href="#">radtranswavelength</a> <a href="#">moleculeinchikey</a> <a href="#">moleculestoichiometricformula</a> <a href="#">moleculechemicalname</a> <a href="#">radtransprobabilitya</a>
	<a href="#">radtranswavenumber</a>

# Select databases

Firefox VAMDC Portal

http://portal.vamdc.eu/vamdc-portal-dev/xsamsForm.seam?actionMethod=home.xhtml%3Anavigator.defaultQueryBuilder()&cid=524



VAMDC Portal Home XSAMS Query Builder Query Log

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Molecule Ion Charge: Range

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Formula	InChI	InChI Key
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<input checked="" type="checkbox"/>	InChI=1S/C2H4/c1-2/h1-2H2 /1+0H2,2+1H2	VGGSQFUCUMXWEO-NARUAAMMSA-N

[Select All](#)

[Refine the Submitted Query](#)

XSAMS Query: SELECT ALL WHERE MoleculeInChIKey='VGGSQFUCUMXWEO-XKSUVOSDSA-N' OR MoleculeInChIKey='VGGSQFUCUMXWEO-NARUAAMMSA-N'

Resource Title	Status	Species	States	Radiative	Collisions	Non Radiative	Sources
<input type="checkbox"/> KIDA: VAMDC-TAP interface	Erreur Interne de Servlet	0	0	0	0	0	0
<input type="checkbox"/> HITRAN-UCL resource	OK	0	368	200	0	0	0
<input type="checkbox"/> SMPO VAMDC/TAP interface	BAD REQUEST	0	0	0	0	0	0
<input checked="" type="checkbox"/> Ethylene Database	OK	0	197	248833	0	0	1
<input type="checkbox"/> TAP-XSAMS for GhoSST database	OK	0	0	0	0	0	1
<input type="checkbox"/> Cologne Database for Molecular Spectroscopy: VAMDC-TAP service	OK	0	0	0	0	0	0
<input type="checkbox"/> UMIST Database for Astrochemistry	OK	0	0	0	0	0	0
<input type="checkbox"/> Methane line lists	NO CONTENT	0	0	0	0	0	0

[Cancel](#) [Get data](#)

Developed in IoA, University of Cambridge by Asif Akram.



# Results

VAMDC results: radiative transitions - Mozilla Firefox

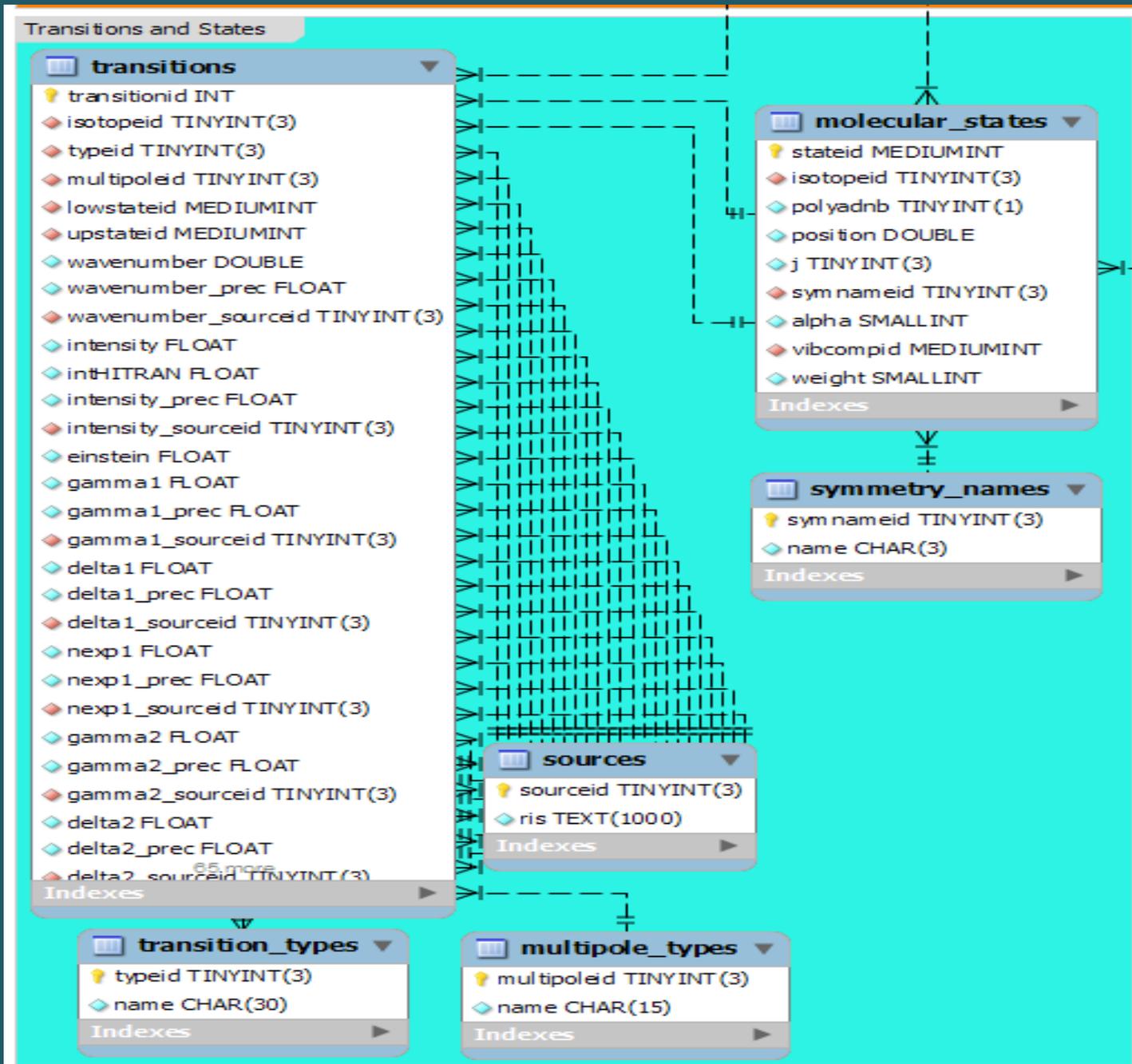
VAMDC results: radiative transitions

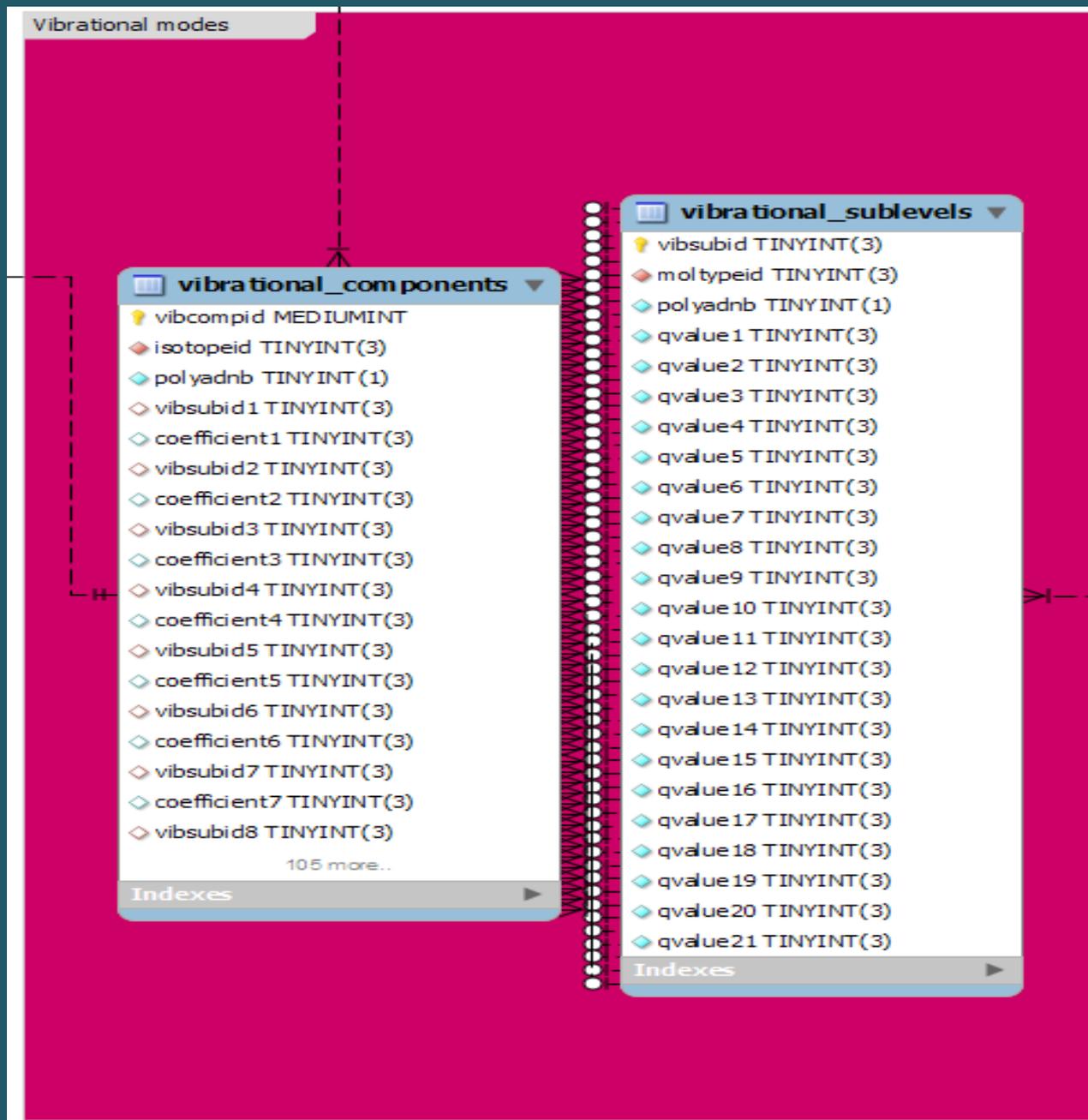
http://apm37.ast.cam.ac.uk:9080/vamdcstatic/line-list?url=/opt/quer

## Query results: radiative transitions

(Switch to display of states.)

Specie	Ion charge	$\lambda/\nu/n/E$	Probability	Initial state	Final state	Broadening
12C2H4 -		n=500.020989 1/cm	A=0.0001367	<a href="#">1881.464268 1/cm</a>	<a href="#">2381.485258 1/cm</a>	
12C2H4 -		n=500.05231 1/cm	A=4.175e-05	<a href="#">5854.304224 1/cm</a>	<a href="#">6354.356535 1/cm</a>	
12C2H4 -		n=500.05231 1/cm	A=4.175e-05	<a href="#">5854.304224 1/cm</a>	<a href="#">6354.356535 1/cm</a>	
12C2H4 -		n=500.121047 1/cm	A=3.584e-07	<a href="#">981.195525 1/cm</a>	<a href="#">1481.316572 1/cm</a>	
12C2H4 -		n=500.126133 1/cm	A=4.953e-07	<a href="#">2128.674221 1/cm</a>	<a href="#">2628.800354 1/cm</a>	
12C2H4 -		n=500.138506 1/cm	A=0.01751	<a href="#">5368.188086 1/cm</a>	<a href="#">5868.326592 1/cm</a>	
12C2H4 -		n=500.138506 1/cm	A=0.01751	<a href="#">5368.188086 1/cm</a>	<a href="#">5868.326592 1/cm</a>	
12C2H4 -		n=500.138875 1/cm	A=1.007	<a href="#">4924.456193 1/cm</a>	<a href="#">5424.595068 1/cm</a>	
12C2H4 -		n=500.138875 1/cm	A=1.007	<a href="#">4924.456193 1/cm</a>	<a href="#">5424.595068 1/cm</a>	
12C2H4 -		n=500.153619 1/cm	A=0.002153	<a href="#">2415.515797 1/cm</a>	<a href="#">2915.669416 1/cm</a>	
12C2H4 -		n=500.15362 1/cm	A=0.002153	<a href="#">2415.515797 1/cm</a>	<a href="#">2915.669416 1/cm</a>	
12C2H4 -		n=500.162059 1/cm	A=2.706e-12	<a href="#">1732.831365 1/cm</a>	<a href="#">2232.993424 1/cm</a>	
12C2H4 -		n=500.196867 1/cm	A=0.003941	<a href="#">3772.023925 1/cm</a>	<a href="#">4272.220792 1/cm</a>	
12C2H4 -		n=500.196867 1/cm	A=0.003941	<a href="#">3772.023925 1/cm</a>	<a href="#">4272.220792 1/cm</a>	
12C2H4 -		n=500.215914 1/cm	A=1e-12	<a href="#">461.987121 1/cm</a>	<a href="#">962.203035 1/cm</a>	
12C2H4 -		n=500.219741 1/cm	A=1.199e-10	<a href="#">2112.567084 1/cm</a>	<a href="#">2612.786825 1/cm</a>	
12C2H4 -		n=500.219741 1/cm	A=1.199e-10	<a href="#">2112.567084 1/cm</a>	<a href="#">2612.786825 1/cm</a>	
12C2H4 -		n=500.26591 1/cm	A=0.002338	<a href="#">3649.714768 1/cm</a>	<a href="#">4149.980678 1/cm</a>	
12C2H4 -		n=500.26591 1/cm	A=0.002338	<a href="#">3649.714768 1/cm</a>	<a href="#">4149.980678 1/cm</a>	
12C2H4 -		n=500.274967 1/cm	A=5.342e-05	<a href="#">1442.163391 1/cm</a>	<a href="#">1942.438358 1/cm</a>	
12C2H4 -		n=500.282492 1/cm	A=2.179e-12	<a href="#">440.035394 1/cm</a>	<a href="#">940.317886 1/cm</a>	
12C2H4 -		n=500.302177 1/cm	A=1.053e-05	<a href="#">1628.824634 1/cm</a>	<a href="#">2129.126811 1/cm</a>	
12C2H4 -		n=500.304743 1/cm	A=3.5e-05	<a href="#">1212.982071 1/cm</a>	<a href="#">1713.286814 1/cm</a>	
12C2H4 -		n=500.304894 1/cm	A=3.5e-05	<a href="#">1212.982071 1/cm</a>	<a href="#">1713.286965 1/cm</a>	
12C2H4 -		n=500.325688 1/cm	A=9.13e-07	<a href="#">1218.963266 1/cm</a>	<a href="#">1719.288954 1/cm</a>	
12C2H4 -		n=500.371713 1/cm	A=2.208e-06	<a href="#">1326.896247 1/cm</a>	<a href="#">1827.26796 1/cm</a>	
12C2H4 -		n=500.384799 1/cm	A=0.000115	<a href="#">2051.748058 1/cm</a>	<a href="#">2552.132856 1/cm</a>	
12C2H4 -		n=500.390306 1/cm	A=2.698e-05	<a href="#">1677.563212 1/cm</a>	<a href="#">2177.953518 1/cm</a>	
12C2H4 -		n=500.395769 1/cm	A=1.003e-08	<a href="#">586.062402 1/cm</a>	<a href="#">1086.458171 1/cm</a>	





**scalar\_numbers**

- scalarid TINYINT(3)
- isotopeid TINYINT(3)
- polyadnb TINYINT(1)
- beta DOUBLE
- gamma DOUBLE
- pi DOUBLE

Indexes

**molecules\_isotopes**

- isotopeid TINYINT(3)
- moltypeid TINYINT(3)
- isotopename CHAR(10)
- inchi VARCHAR(40)
- inchikey CHAR(27)

Indexes

**molecule\_types**

- moltypeid TINYINT(3)
- description CHAR(10)
- nbmode TINYINT(3)
- nbsublev0 SMALLINT
- levelid0 TINYINT(3)
- nbsublev1 SMALLINT
- levelid1 TINYINT(3)
- nbsublev2 SMALLINT
- levelid2 TINYINT(3)
- nbsublev3 SMALLINT
- levelid3 TINYINT(3)
- nbsublev4 SMALLINT
- levelid4 TINYINT(3)
- nbsublev5 SMALLINT
- levelid5 TINYINT(3)
- nbsublev6 SMALLINT
- levelid6 TINYINT(3)
- nbsublev7 SMALLINT
- levelid7 TINYINT(3)
- nbsublev8 SMALLINT
- levelid8 TINYINT(3)
- nbsublev9 SMALLINT
- levelid9 TINYINT(3)
- quantumnb TINYINT(3)
- qname1 CHAR(4)
- status1 TINYINT(3)
- qname2 CHAR(4)
- status2 TINYINT(3)
- qname3 CHAR(4)
- status3 TINYINT(3)
- qname4 CHAR(4)
- status4 TINYINT(3)
- qname5 CHAR(4)
- status5 TINYINT(3)
- qname6 CHAR(4)
- status6 TINYINT(3)
- qname7 CHAR(4)
- status7 TINYINT(3)
- qname8 CHAR(4)
- status8 TINYINT(3)
- qname9 CHAR(4)
- status9 TINYINT(3)
- qname10 CHAR(4)

23 more...

Indexes

**level\_descriptions**

- levelid TINYINT(3)
- nblev TINYINT(3)
- n1 BIGINT(6)
- n2 BIGINT(6)
- n3 BIGINT(6)
- n4 BIGINT(6)
- n5 BIGINT(6)
- n6 BIGINT(6)
- n7 BIGINT(6)
- n8 BIGINT(6)
- n9 BIGINT(6)
- n10 BIGINT(6)
- n11 BIGINT(6)
- n12 BIGINT(6)
- n13 BIGINT(6)
- n14 BIGINT(6)

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