VAMDC
Virtual Atomic and Molecular Data Centre
http://www.vamdc.eu (.org)

Coordinator: Marie Lise Dubernet
Observatoire de Paris,
Université Pierre et Marie Curie

- General Overview of VAMDC Programme
  - Partners
  - Objectives
  - Program of Work
- Infrastructure
  - Portal

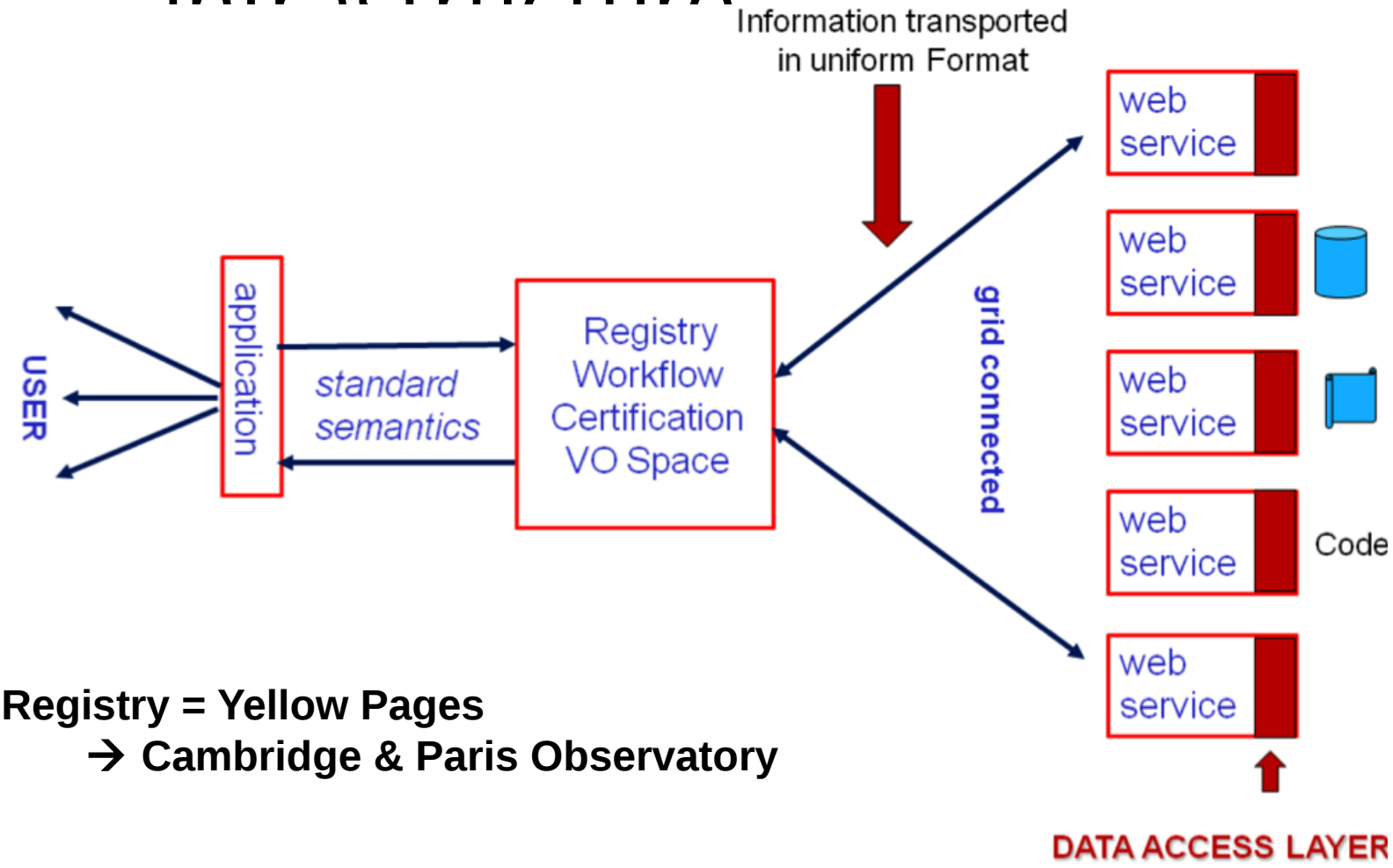
VAMDC - The Mission

- An international collaboration between groups involved in the generation, evaluation, and use of atomic and molecular data (A&M data).
- Aims: creating a well-documented interoperable interface to existing A&M data resources.
- Funded by EU-FP7 E-Science Infrastructures programme, started July 2009, until end 2012. The Sup@VAMDC 2012 to 2014 (Extend to outside EU)
- Consortium: 15 partner institutes from six EU and six non-EU countries

VAMDC - The mission

- Connecting Europe to Russia, Central Europe, South America, North America → Aim at worldwide connection
- Connecting Different Fields of Producers of Atomic and Molecular Physics and Chemistry
- Connecting A.& M. Producers to A. & M. Users
- Connecting to Research/E-Infrastructures: Euro-VO (IVOA), Europlanet

Schematic diagram of the VAMDC infrastructure



Registry = Yellow Pages

→ Cambridge & Paris Observatory

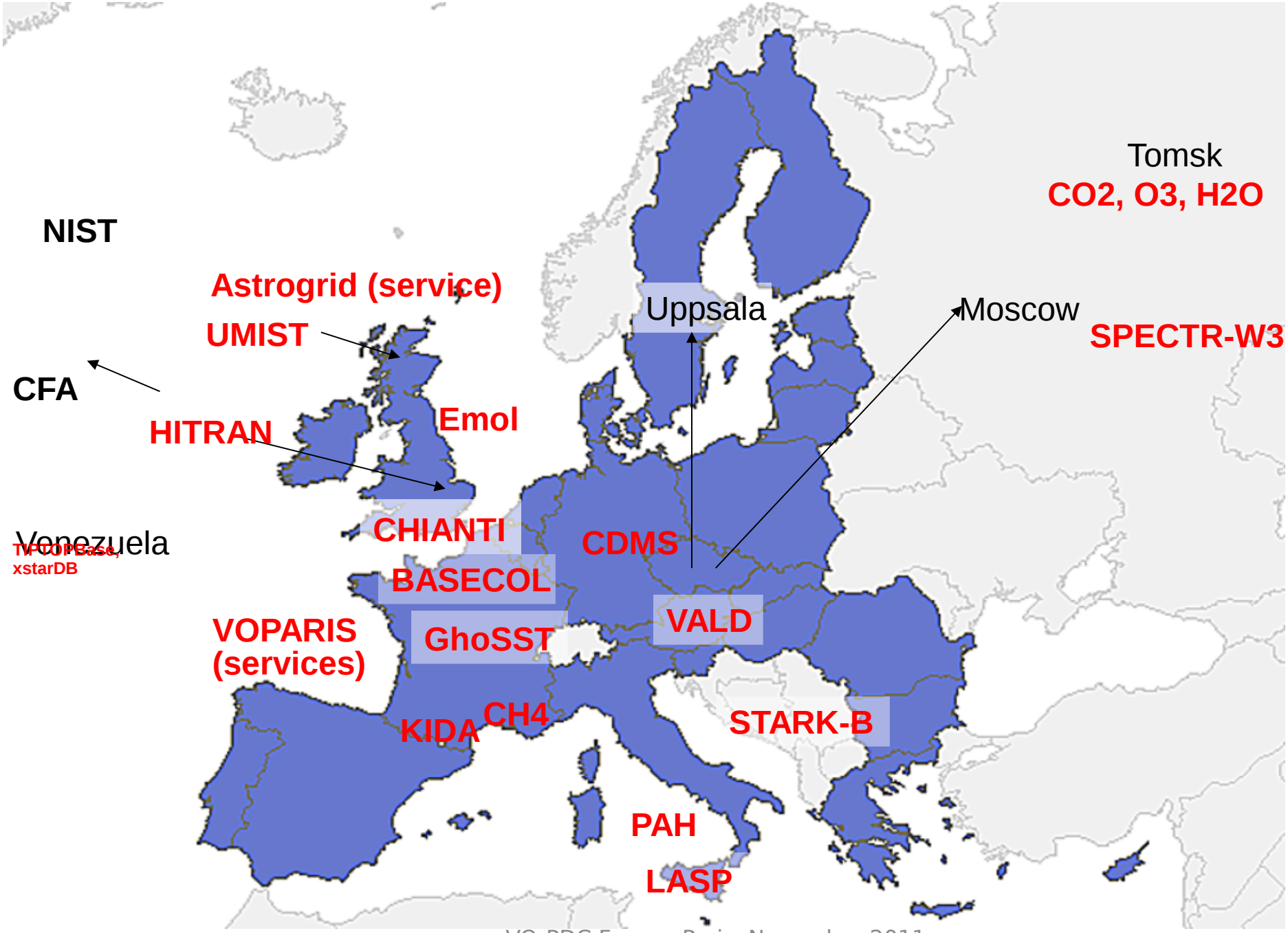
Core databases

- Developed and maintained at partner institutes, >28 databases
- Atomic data for astrophysics − 8 databases
- Molecular data − 9 databases
- Solid Spectroscopy data − 2 databases

Technological Nodes

Institute of Astronomy: Cambridge University

VO-Paris Data Center: Paris Observatory


NIST
Astrogrid (service)
UMIST
CFA
HITRAN
Emol
Venezuela
TIPTOPBase,
xstarDB
CHIANTI
CDMS
BASECOL
VOPARIS
(services)
GhoSST
VALD
KIDA
CH4
STARK-B
PAH
LASP
Uppsala
Moscow
Tomsk
CO2, O3, H2O
SPECTR-W3

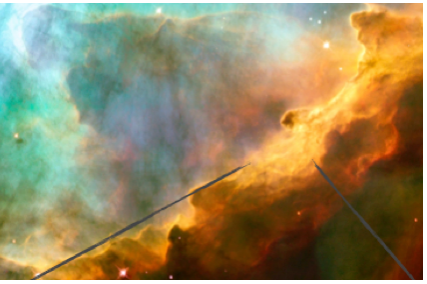
Basecol Database (basecol.obspm.fr)
Paris Observatory

Collaboration: Bordeaux, Besançon, Grenoble, Madrid, Durham

P.I. = ML Dubernet

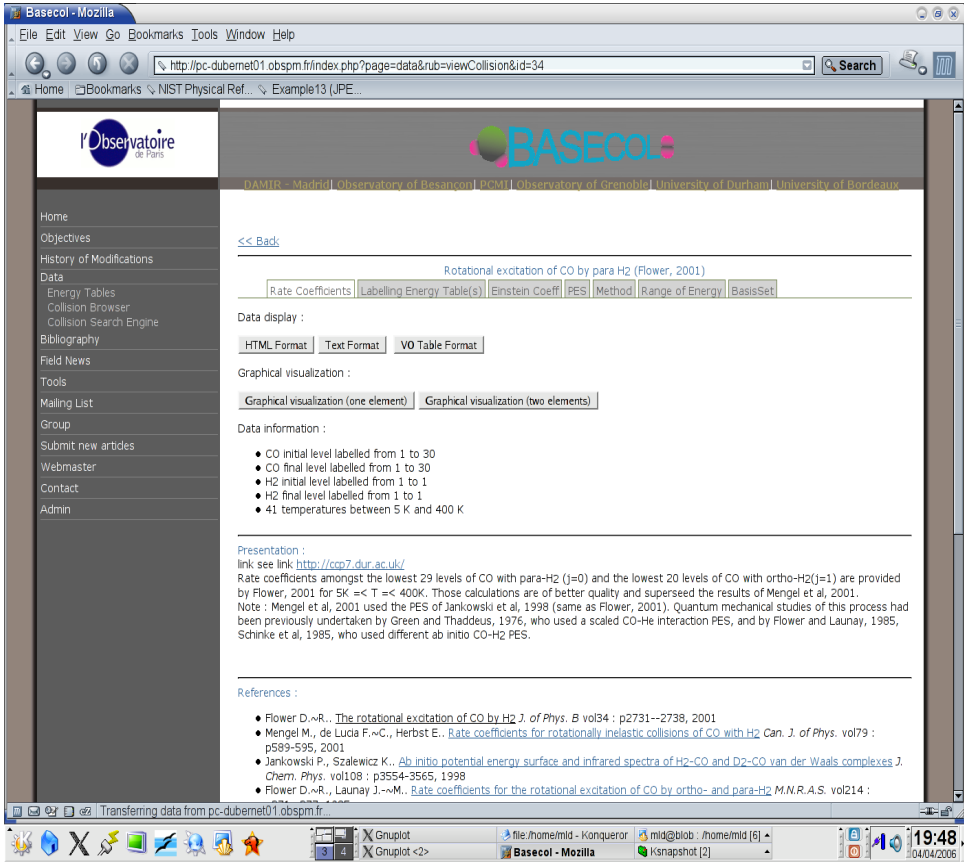
Published (de)-excitation rate coefficients

- Rotational (fine, hyperfine), Ro-vib., Vib.
- Currently: 47 Target molecules; Perturbers : electrons, He, H, H_2
- 130 collisional systems
- Fully documented and referenced (759 ref.)
- Fitting coefficients, visualisation tools
- Energy levels, Einstein coefficients, QN
- Fully checked and evaluated



Linked to CDMS and JPL

Astrophysical Applications



GhoSST

Observatory of Grenoble (B. Schmitt)

http://ghosst.obs.ujf-grenoble.fr

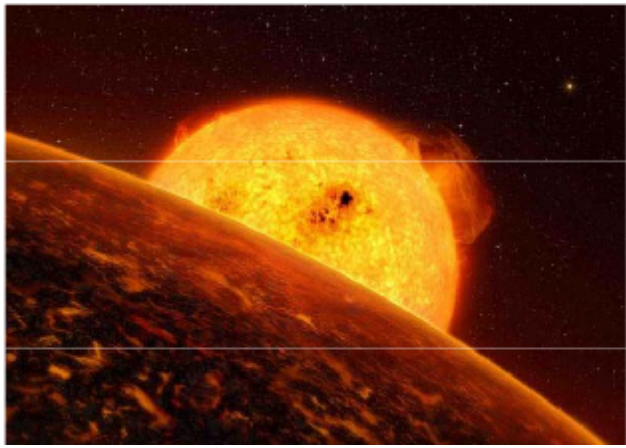
- GhoSST (Grenoble astrophysics and planetology Solid Spectroscopy and Thermodynamics,) database service, offers spectroscopic laboratory data on molecular and atomic solids from the near UV to the far-infrared.
- **Now to upgrade to 'SSHADE' as part of new**
- **Europlanet RI**

KIDA

Observatory of Bordeaux (V. Wakelam)

http://kida.obs.u-bordeaux1.fr

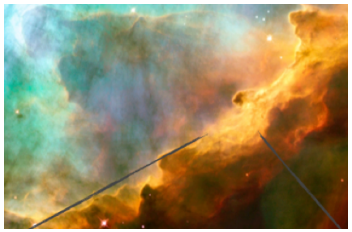
- KIDA - KInetic Database for Astrochemistry contains data on chemical reactions used in the modelling of the chemistry in the interstellar medium and in planetary atmospheres
- **ISM and Planetology Applications**

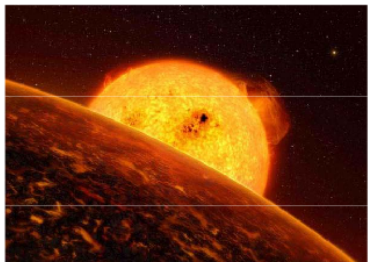


PAH

Observatory of Cagliari (G. Mulas) and « ex-CESR » (C. Joblin)

http://astrochemisty.ca.astro.it/database/





- **PAHs (Polycyclic Aromatic Hydrocarbon) and carbon clusters spectral database provides a number of properties for a sample of presently about 60 species in four charge states: anion, neutral, cation and dications.**
- The properties include general energetic such as electron affinity and ionisation energies, static polarizability, permanent dipole moment, van der Waals coefficients, symmetry, multiplicity, and optimised geometry of the ground electronic state; harmonic vibrational analyses, i. e. normal modes, their frequencies and IR activities; and vertical electronic photoabsorption cross-sections and complex frequency-dependent electronic polarisabilities in the linear regime.

Stark-B

- This is a database of the theoretical widths and shifts of isolated lines of atoms and ions due to collisions with charged perturbers, obtained within the impact approximation.
- This database is devoted to modelling and spectroscopic diagnostics of stellar atmospheres and envelopes. In addition, it is also relevant to laboratory plasmas, laser equipment and technological plasmas. The database is currently developed in Paris, and a mirror is planned in Belgrade
- **Astronomical Observatory of Belgrade and Paris Observatory**

TIPTOPBASE, OPSERVER

C. Mendoza (IVIC), N. Nunez (CPTM) in collaboration with Paris Observatory (C. Zeippen, F. Delahaye, N. Moreau)

TIPTOPbase located at the Centre de Données astronomiques de Strasbourg, France contains:

- **TOPbase** (http://cdsweb.u-strasbg.fr/topbase/topbase.html), listing atomic data computed in the Opacity Project, namely LS-coupling energy levels, gf-values and photoionization cross sections for light elements ($Z \leq 26$) of astrophysical interest.
- **TIPbase** (http://cdsweb.u-strasbg.fr/tipbase/home.html). Intermediate-coupling energy levels, A-values and electron impact excitation cross sections and rates for astrophysical applications ($Z \leq 28$), computed by the IRON Project.

Opserver, located at the Ohio Supercomputer Center, USA, (http://opacities.osc.edu/), a remote, interactive server for the computation of mean opacities for stellar modelling using the monochromatic opacities computed by the Opacity Project.

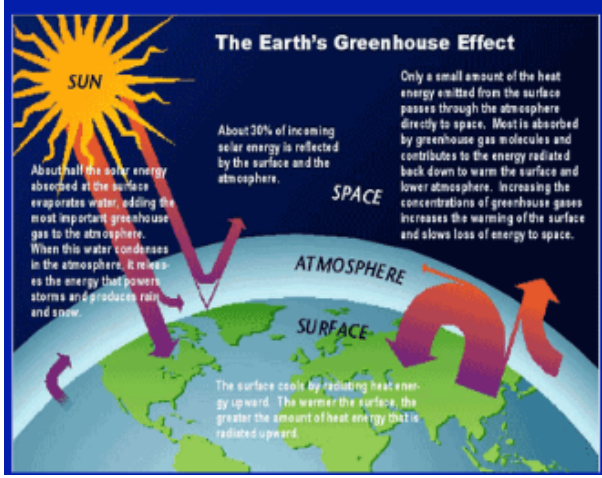
Stellar Physics

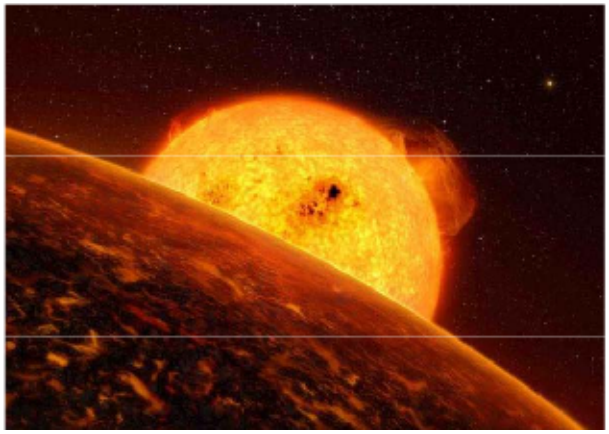
S&MPO AND Ethylene

- Spectroscopy & Molecular Properties of Ozone) relational database (http://ozone. iao.ru and http://ozone.univ-reims.fr/) contains spectral line parameters for the ozone molecule, experimental UV cross-sections, information on ozone's molecular properties, updated reference lists classified by type as well as programs and extended facilities for user applications.
- **Earth, Exo-Planets**
- **IAO-Tomsk (V. Perevalov) and University of Reims (V. Tyuterev)**

CH_4 Database

Institut Carnot de Bourgogne (V. Boudon)





- Database of line parameters for the three isotopologues of methane ($^{12}CH_4$, $^{13}CH_4$ and CH_3D) with positions, intensities, lineshape parameters from FIR to Visible
- Methane is a major greenhouse pollutant on Earth and an important constituent of many astrophysical bodies (giant planets, Titan, dwarf planets, brown dwarfs, methane stars, exoplanets).
- Modelling methane absorption over a wide spectral range is essential to retrieve methane vertical profiles, minor species abundances and surface propertie.

User Communities

Originally developed for

Astrophysics, Astrochemistry and Planetary Science communities

Since it was seen that there was a great need for reliable A&M data because of extraordinary range of physical conditions and such data needed to be collected in one place

VAMDC is a one stop shop

User Communities

- Atmospheric Science
  - input for complex terrestrial atmosphere/climate models, determination of concentrations and radiative transport of about 100 species, e.g. water

- Plasma Technologies
  - plasma-assisted materials processing or surface modification, e.g. manufacture of semi-conductor chips. A&M data needed for modeling chemically active plasmas.

User Communities cont'd

- Lighting
  - A&M databases needed for development of future light sources – new working gas species, e.g. Xe, and metal alloys such as InSb (Indium antimonide)
- Fusion Energy Research (IAEA)
  - design and operation of vital fusion device systems require large amounts of A&M collisional and spectroscopic data
- Radiation Science (RADAM portal)
  - radiotherapy models exploring damage of DNA by radiation need A&M data, e.g. electron collisions with DNA components and other biomolecules

VAMDC – the future

- Community to use the tool !

- Development will be through new projects eg

Europlanet Research Infrastructure

- But needs your input for Data needs (and format etc)

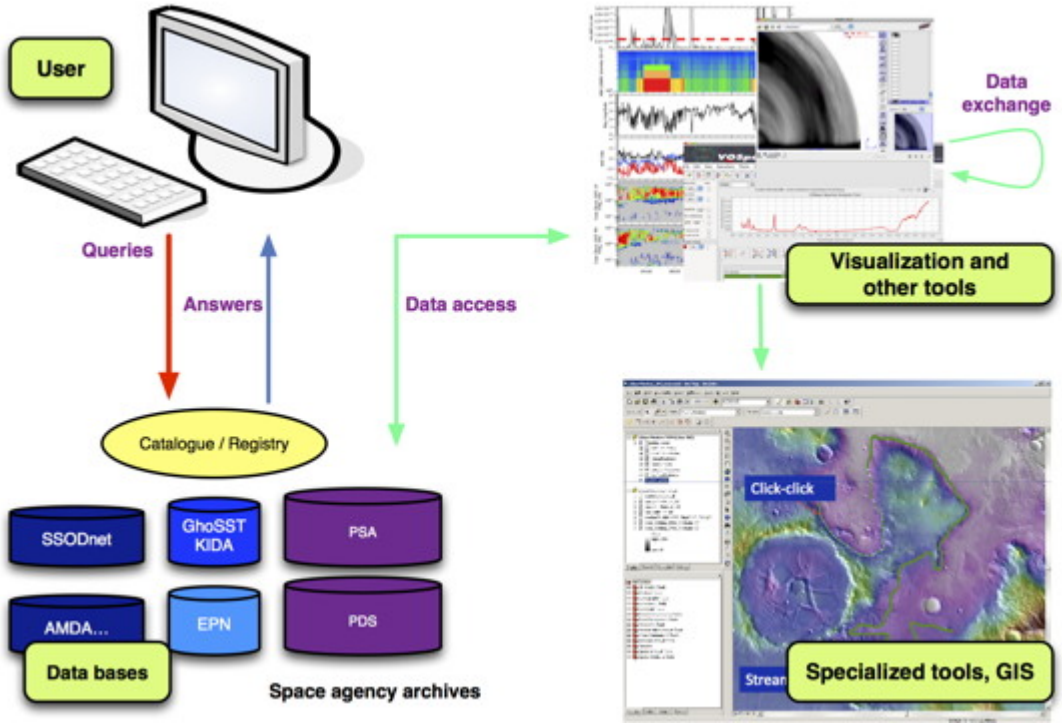
http://www.europlanet-2020-ri.eu/

europlanet 2020

- **Databases and data tools**
- **Large effort to develop databases for astronomy and planetary science**

- **Europlanet to provide ‘virtual access’ to databases and tools (link to IVOA)**
- **VESPA (Virtual European Solar and Planetary Access) is to build a Virtual Observatory for Solar System Sciences**
- **http://vespa.obspm.fr**

The Virtual Observatory in Planetary Science



VESPA New tools

- Solid Spectroscopy Hosting Architecture of Databases and Expertise – SSHADE
- Planetary surfaces (including machine learning tools- CATNAP)
- Magnetospheres (models) Atmospheres
- Small Bodies (MATISSE – comets)
- Atmospheres (models – eg Titan ionosphere/ Mars)

- Also to link to CATNAP Comet proposal (if funded)

Finally….

- Welcome

  and

  We look forward to hearing your data needs

  and

  How we can coordinate response to meet them

VAMDC PORTAL

VAMDC Virtual Atomic and Molecular Data Centre

VAMDC Portal | Home | XSAMS Query Builder | Query Log

Query Parameters

- Atoms
- Molecules
- Transitions
- Collisions
- Free Form

Resource	Query Parameters
TOPbase : VAMDC-TAP interface	atomioncharge radtranswavelength atomnuclearcharge atomsymbol
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)	radtranswavenumber
TIPbase : VAMDC-TAP interface	atomioncharge atomnuclearcharge atomsymbol
HITRAN-UCL resource	radtranswavenumber radtranswavelength moleculeinchikey moleculestoichiometricformula moleculechemicalname radtransprobabilitya
Lund laboratory spectroscopy database	radtranswavenumber radtranswavelength atomstateenergy radtransprobabilitylog10weightedoscillatorstrength atomnuclearcharge atomsymbol atomioncharge
Spectr-W3	atomnuclearcharge radtranswavelength atomioncharge radtransprobabilityoscillatorstrength atomsymbol

Common way of specifying a data extract
Standard web-service parameters
Common query language
Common dictionary of terms

VAMDC Portal | Home | XSAMS Query Builder | Query Log

Query Parameters

- Atoms
- Molecules
- Transitions
- Collisions
- Free Form

Molecules X Close

Chemical Name:

Stoichiometric Formula: CO

Molecule Ion Charge:

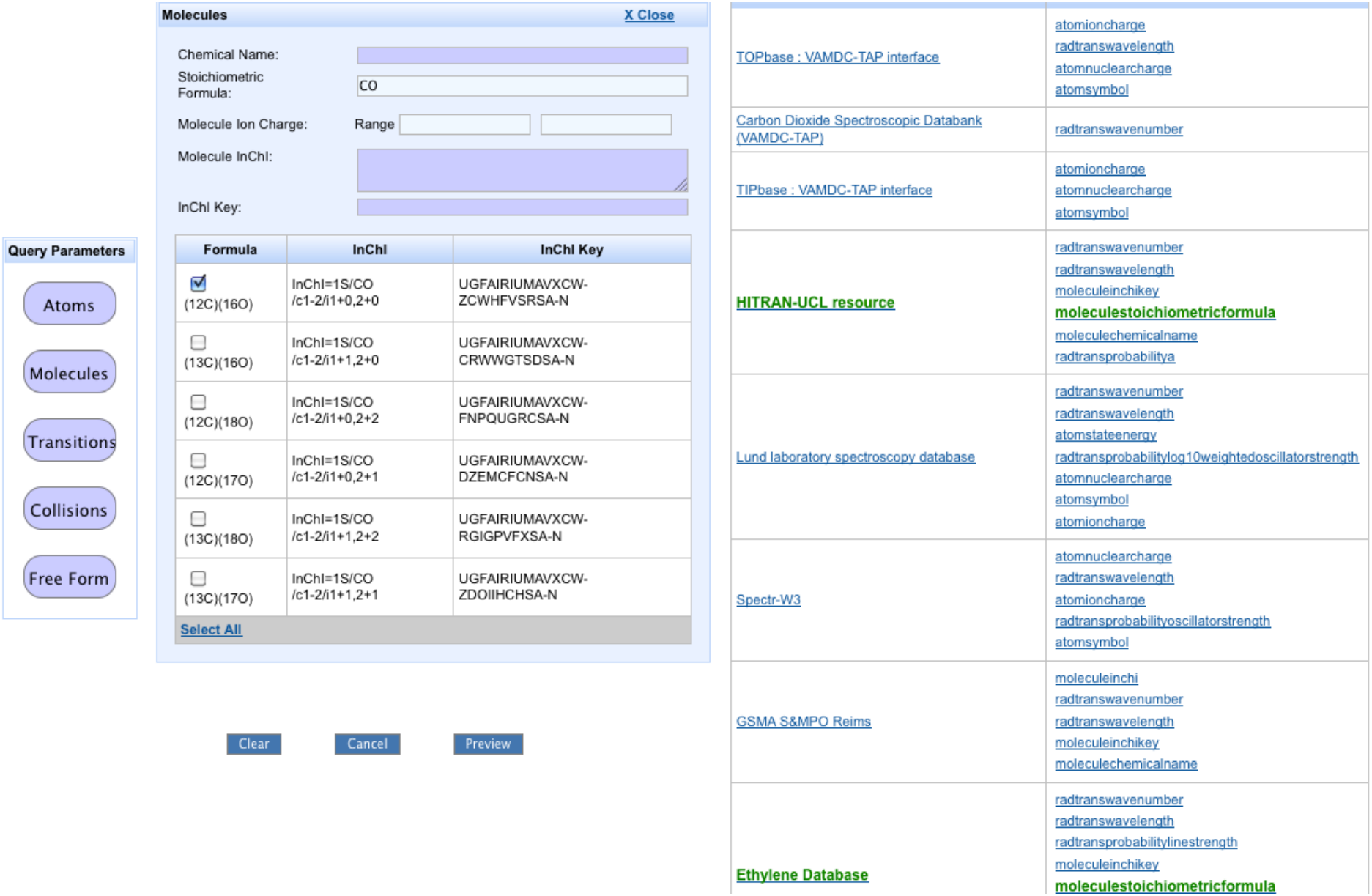
Molecule InChI:

InChI Key:

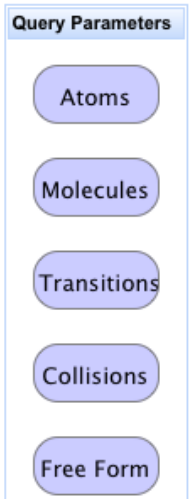
CO2
CO
COS
COF2
CO+
COFe
CONi

Clear

Resource	Query Parameters
TOPbase : VAMDC-TAP interface	atomioncharge radtranswavelength atomnuclearcharge atomsymbol
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)	radtranswavenumber
TIPbase : VAMDC-TAP interface	atomioncharge atomnuclearcharge atomsymbol
HITRAN-UCL resource	radtranswavenumber radtranswavelength moleculeinchikey **moleculestoichiometricformula** moleculechemicalname radtransprobabilitya
Lund laboratory spectroscopy database	radtranswavenumber radtranswavelength atomstateenergy radtransprobabilitylog10weightedoscillatorstrength atomnuclearcharge atomsymbol atomioncharge
Spectr-W3	atomnuclearcharge radtranswavelength atomioncharge radtransprobabilityoscillatorstrength



TOPbase : VAMDC-TAP interface	atomioncharge radtranswavelength atomnuclearcharge atomsymbol
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)	radtranswavenumber
TIPbase : VAMDC-TAP interface	atomioncharge atomnuclearcharge atomsymbol
HITRAN-UCL resource	radtranswavenumber radtranswavelength moleculeinchikey **moleculestoichiometricformula** moleculechemicalname radtransprobabilitya
Lund laboratory spectroscopy database	radtranswavenumber radtranswavelength atomstateenergy radtransprobabilitylog10weightedoscillatorstrength atomnuclearcharge atomsymbol atomioncharge
Spectr-W3	atomnuclearcharge radtranswavelength atomioncharge radtransprobabilityoscillatorstrength atomsymbol
GSMA S&MPO Reims	moleculeinchi radtranswavenumber radtranswavelength moleculeinchikey moleculechemicalname
Ethylene Database	radtranswavenumber radtranswavelength radtransprobabilitylinestrength moleculeinchikey **moleculestoichiometricformula**



Molecules

Chemical Name:

Stoichiometric Formula: co

Molecule Ion Charge: Range

Molecule InChI:

InChI Key:

Formula	InChI	InChI Key
☑ (12C)(16O)	InChI=1S/CO /c1-2/i1+0,2+0	UGFAIRIUMAVXCW-ZCWHFVSRSA-N
☐ (13C)(16O)	InChI=1S/CO /c1-2/i1+1,2+0	UGFAIRIUMAVXCW-CRWWGTSDSA-N
☐ (12C)(18O)	InChI=1S/CO /c1-2/i1+0,2+2	UGFAIRIUMAVXCW-FNPQUGRCSA-N
☐ (12C)(17O)	InChI=1S/CO /c1-2/i1+0,2+1	UGFAIRIUMAVXCW-DZEMCFCNSA-N
☐ (13C)(18O)	InChI=1S/CO /c1-2/i1+1,2+2	UGFAIRIUMAVXCW-RGIGPVFXSA-N
☐ (13C)(17O)	InChI=1S/CO /c1-2/i1+1,2+1	UGFAIRIUMAVXCW-ZDOIIHCHSA-N

Select All

XSAMS Query: SELECT ALL WHERE MoleculeInchiKey='UGFAIRIUMAVXCW-ZCWHFVSRSA-N'

Resource Title	Status	Species	States	Radiative	Collisions	Non Radiative	Sources
☑ HITRAN-UCL resource	OK	0	172	100	0	0	0
☐ Ethylene Database	NO CONTENT	0	0	0	0	0	0
☑ TAP-XSAMS for GhoSST database	OK	1	0	0	0	0	1
☑ BASECOL: VAMDC-TAP interface	OK	6	0	0	11	0	0
☑ Cologne Database for Molecular Spectroscopy: VAMDC-TAP service	OK	2	186	182	0	0	4

Cancel Get data

Refine the Submitted Query

Query results: atomic and molecular states

(Switch to display of radiative transitions.)

Specie	Ion charge	State energy	Description	Quantum numbers	More information
Carbon Monoxide - CO		0.0 1/cm		Label=X^1\Sigma^+, v=0, J=0, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		3.845033 1/cm		Label=X^1\Sigma^+, v=0, J=1, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		11.534953 1/cm		Label=X^1\Sigma^+, v=0, J=2, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		23.069466 1/cm		Label=X^1\Sigma^+, v=0, J=3, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		38.448131 1/cm		Label=X^1\Sigma^+, v=0, J=4, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		57.67036 1/cm		Label=X^1\Sigma^+, v=0, J=5, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		80.735419 1/cm		Label=X^1\Sigma^+, v=0, J=6, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		107.642427 1/cm		Label=X^1\Sigma^+, v=0, J=7, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		138.390355 1/cm		Label=X^1\Sigma^+, v=0, J=8, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		172.978029 1/cm		Label=X^1\Sigma^+, v=0, J=9, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		211.404127 1/cm		Label=X^1\Sigma^+, v=0, J=10, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		253.667181 1/cm		Label=X^1\Sigma^+, v=0, J=11, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		299.765576 1/cm		Label=X^1\Sigma^+, v=0, J=12, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		349.69755 1/cm		Label=X^1\Sigma^+, v=0, J=13, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		403.461194 1/cm		Label=X^1\Sigma^+, v=0, J=14, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		461.054454 1/cm		Label=X^1\Sigma^+, v=0, J=15, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		522.475129 1/cm		Label=X^1\Sigma^+, v=0, J=16, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		587.720871 1/cm		Label=X^1\Sigma^+, v=0, J=17, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		656.789186 1/cm		Label=X^1\Sigma^+, v=0, J=18, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		729.677434 1/cm		Label=X^1\Sigma^+, v=0, J=19, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		806.382828 1/cm		Label=X^1\Sigma^+, v=0, J=20, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		886.902435 1/cm		Label=X^1\Sigma^+, v=0, J=21, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		971.233178 1/cm		Label=X^1\Sigma^+, v=0, J=22, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		1059.371831 1/cm		Label=X^1\Sigma^+, v=0, J=23, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		1151.315024 1/cm		Label=X^1\Sigma^+, v=0, J=24, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		1247.059241 1/cm		Label=X^1\Sigma^+, v=0, J=25, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		1346.60082 1/cm		Label=X^1\Sigma^+, v=0, J=26, F1=, F2=, parity=, symmetry=	Detail

Available data for selected state

Specie

Structural formula: CO

Stoichiometric formula: CO

Molecule name: Carbon Monoxide

InChI: 1S/CO/c1-2/i1+0,2+0 (UGFAIRIUMAVXCW-ZCWHFVSRSA-N)

State

State description:

State energy above ground state: 38.448131 1/cm

Total statistical weight: 9

Quantum description of state as closed-shell, diatomic molecule: Label=X^1\Sigma^+, v=0, J=4, F1=, F2=, parity=, symmetry=

Closed-shell, diatomic molecules

- case prefix: dcs
- case ID: 1

`ElecStateLabel`

XML Element
`dcs:ElecStateLabel`

Description
`ElecStateLabel` is a label identifying the electronic state: X, A, a, B, etc..

Attributes
None

Restrictions
string

v

XML Element
`dcs:v`

Description
v is the vibrational quantum number.

Attributes
None

Restrictions
non-negative integer

J

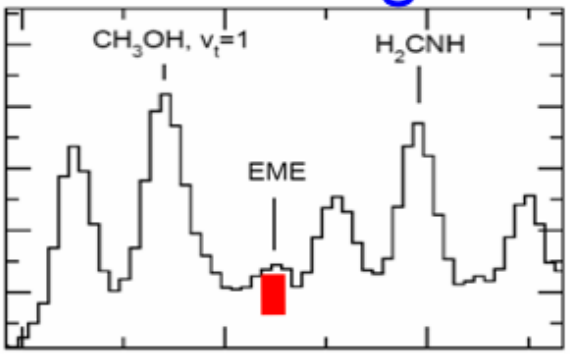
XML Element
`dcs:J`

Query results: radiative transitions

(Switch to display of states.)

Specie	Ion charge	λ/v/n/E	Probability	Initial state	Final state
Carbon Monoxide - CO		v=115271.2021 MHz	A=7.20378864479e-08 1/cm $\log_{10}$gf=-5.0105	- 0.0 1/cm	- 3.845033 1/cm
Carbon Monoxide - CO		v=230538.0 MHz	A=6.91079000503e-07 1/cm $\log_{10}$gf=-4.1197	- 3.845033 1/cm	- 11.534953 1/cm
Carbon Monoxide - CO		v=345795.9899 MHz	A=2.49670085538e-06 1/cm $\log_{10}$gf=-3.6118	- 11.534953 1/cm	- 23.069466 1/cm
Carbon Monoxide - CO		v=461040.7681 MHz	A=6.12668117242e-06 1/cm $\log_{10}$gf=-3.2657	- 23.069466 1/cm	- 38.448131 1/cm
Carbon Monoxide - CO		v=576267.931 MHz	A=1.22134274135e-05 1/cm $\log_{10}$gf=-3.0118	- 38.448131 1/cm	- 57.67036 1/cm
Carbon Monoxide - CO		v=691473.076 MHz	A=2.13750692698e-05 1/cm $\log_{10}$gf=-2.8193	- 57.67036 1/cm	- 80.735419 1/cm
Carbon Monoxide - CO		v=806651.8008 MHz	A=3.42239824576e-05 1/cm $\log_{10}$gf=-2.6716	- 80.735419 1/cm	- 107.642427 1/cm
Carbon Monoxide - CO		v=921799.7039 MHz	A=5.13419191151e-05 1/cm $\log_{10}$gf=-2.559	- 107.642427 1/cm	- 138.390355 1/cm
Carbon Monoxide - CO		v=1036912.3846 MHz	A=7.33007011041e-05 1/cm $\log_{10}$gf=-2.4751	- 138.390355 1/cm	- 172.978029 1/cm
Carbon Monoxide - CO		v=1151985.4434 MHz	A=0.000100638923207 1/cm $\log_{10}$gf=-2.4156	- 172.978029 1/cm	- 211.404127 1/cm
Carbon Monoxide - CO		v=1267014.4817 MHz	A=0.000133903406762 1/cm $\log_{10}$gf=-2.3773	- 211.404127 1/cm	- 253.667181 1/cm
Carbon Monoxide - CO		v=1381995.1022 MHz	A=0.000173532853014 1/cm $\log_{10}$gf=-2.3581	- 253.667181 1/cm	- 299.765576 1/cm
Carbon Monoxide - CO		v=1496922.9091 MHz	A=0.000220040322442 1/cm $\log_{10}$gf=-2.3561	- 299.765576 1/cm	- 349.69755 1/cm
Carbon Monoxide - CO		v=1611793.5079 MHz	A=0.00027390476357 1/cm $\log_{10}$gf=-2.3699	- 349.69755 1/cm	- 403.461194 1/cm
Carbon Monoxide - CO		v=1726602.5057 MHz	A=0.000335356678509 1/cm $\log_{10}$gf=-2.3987	- 403.461194 1/cm	- 461.054454 1/cm
Carbon Monoxide - CO		v=1841345.5116 MHz	A=0.000404993044566 1/cm $\log_{10}$gf=-2.4413	- 461.054454 1/cm	- 522.475129 1/cm
Carbon Monoxide - CO		v=1956018.1363 MHz	A=0.000482878531678 1/cm $\log_{10}$gf=-2.4973	- 522.475129 1/cm	- 587.720871 1/cm
Carbon Monoxide - CO		v=2070615.9924 MHz	A=0.000569495347659 1/cm $\log_{10}$gf=-2.5659	- 587.720871 1/cm	- 656.789186 1/cm
Carbon Monoxide - CO		v=2185134.6949 MHz	A=0.000664985100589 1/cm $\log_{10}$gf=-2.6467	- 656.789186 1/cm	- 729.677434 1/cm
Carbon Monoxide - CO		v=2299569.8609 MHz	A=0.000769499240577 1/cm $\log_{10}$gf=-2.7393	- 729.677434 1/cm	- 806.382828 1/cm
Carbon Monoxide - CO		v=2413917.1097 MHz	A=0.000883246473397 1/cm $\log_{10}$gf=-2.8433	- 806.382828 1/cm	- 886.902435 1/cm

Understanding the Language of Interstellar Molecules

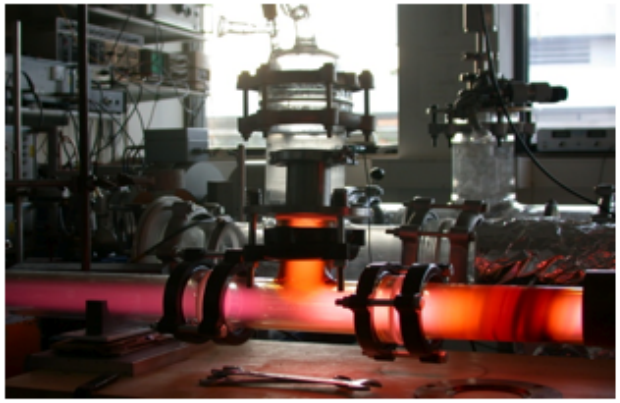


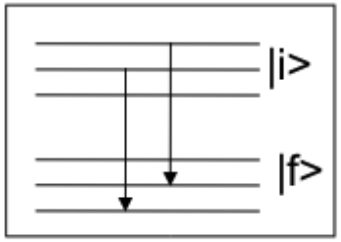
Observations
+
Modelling

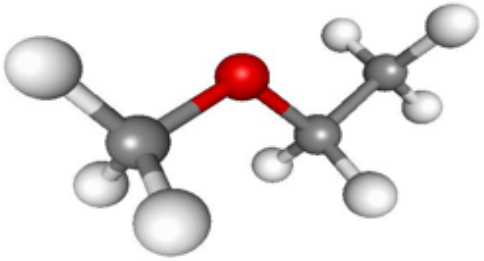
CDMS + JPL
BASECOL + KIDA

Laboratory expriments

Quantum Chemistry







Courtesy of Stephan Schlemmer

Open to Any Producers & Users **from July 2012**

- Open to Producers to include their data within VAMDC environment
  - In existing databases
  - Building their own database (Django publishing tools for example) and registring it to VAMDC registries
- Open to users to include VAMDC developed software into their own applications
  - Licencing will allow any use
- All Softwares & Documentation From June 2012

at http://www.vamdc.eu (org)