

Virtual Observatory and Relevance to Atomic and Molecular Data

M.L. Dubernet
LERMA, Paris Observatory

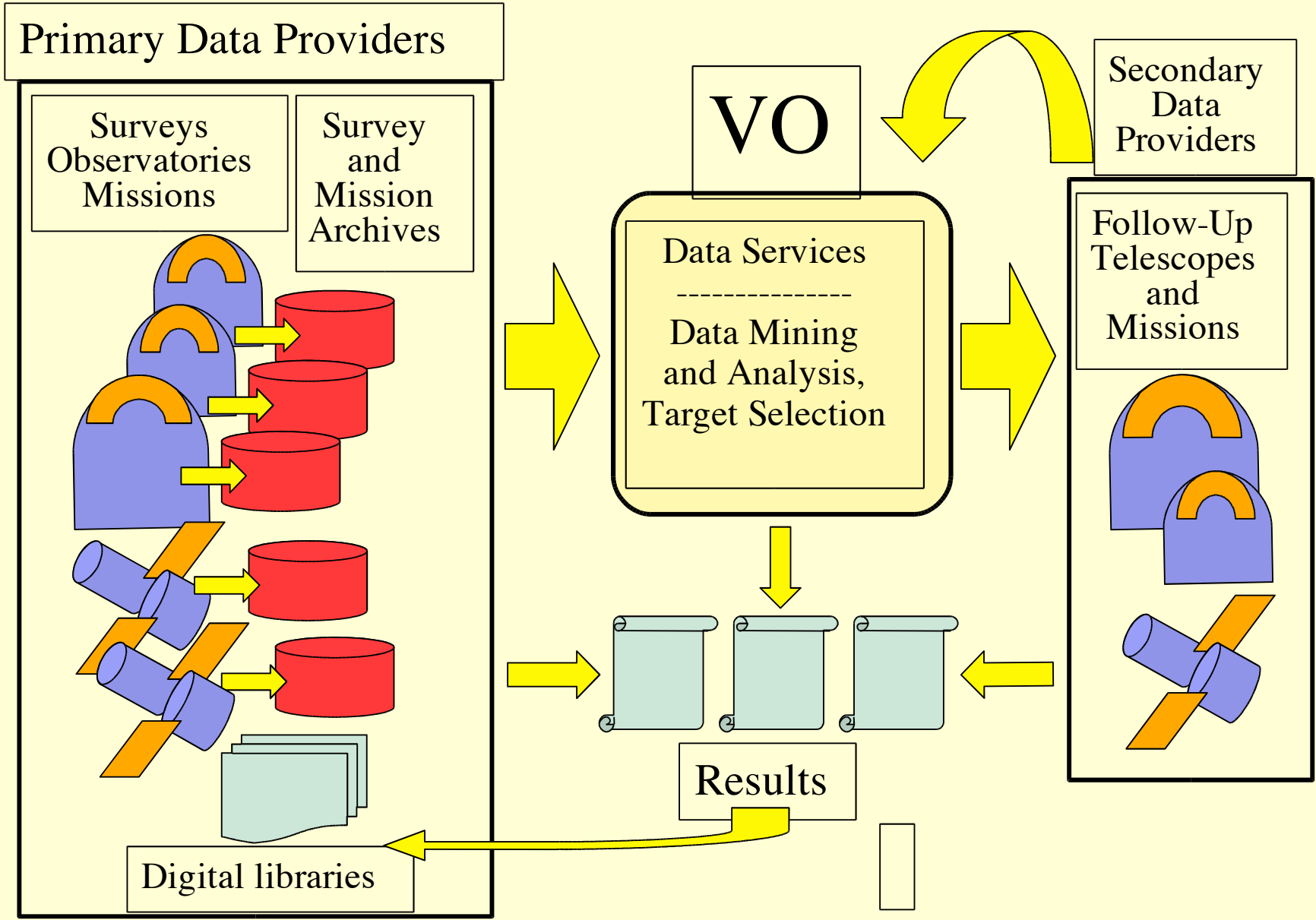


IVOA (www.ivoa.net)

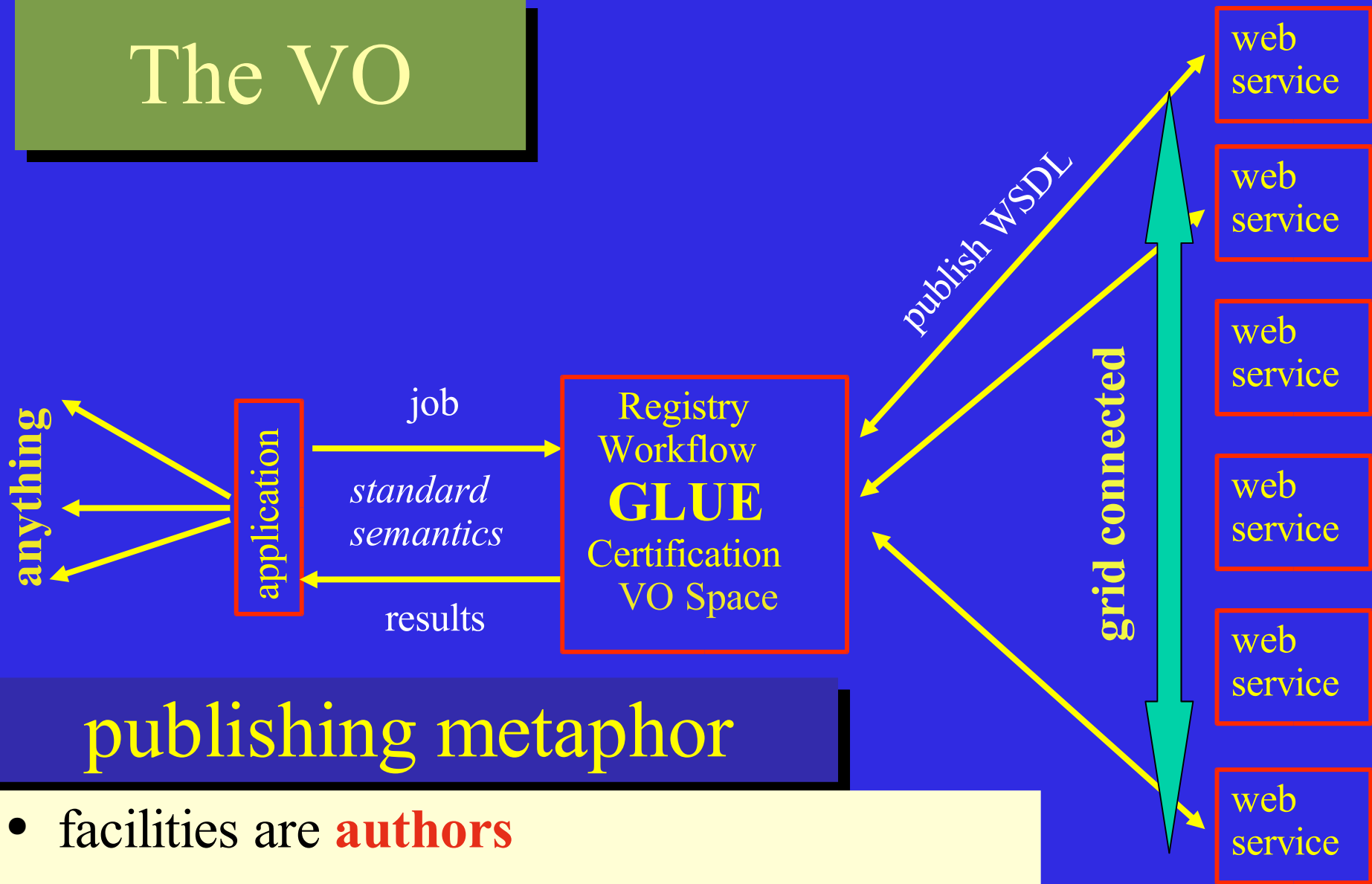
From observed data to published data including very large survey

« an enabling and coordinating entity to foster the development of tools, protocols, and collaborations necessary to realize the full scientific potential of astronomical databases in the coming decade »

NVO White Paper, juin 2000



The VO



publishing metaphor

- facilities are **authors**
 - data centres are **publishers**
 - VO portals are **shops**
 - end-users are **readers**
- VO infrastructure is **distribution system**

History

- Launch : "Virtual Observatories of the Future", 13-16 june 2000, Caltech Pasadena
- Since, many national programs : NVO, AstroGrid, GAVO, ... and AVO (Europe)
- Launch of the International Virtual Observatory Alliance in Garching on the 10-14 June 2002



Interoperability Working Groups

- Resource Registry
- Data Modeling
- Content Description
- Data Access Layer
- VOTable
- VO Query Language
- Grid & Web Service
- Standards & Processes

2 Interoperability meetings a year

Next one in China



Standards

- **VOTable**: a way to represent a table of data in XML with good metadata about the semantic meaning of the data
- **ConeSearch**: to find out about sky-located objects such as stars or images: the input is a cone of space with center and radius, the output is a VOTable that has RA and Dec columns
- **Simple Image/Spectra Access**: protocol that allows publication and query of image sets/spectra

Euro-VO

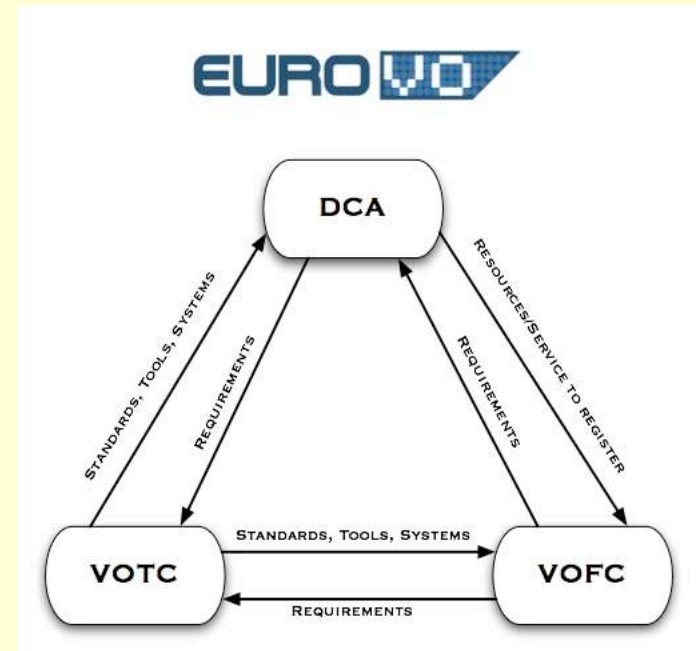
The EURO-VO project aims at deploying an **operational Virtual Observatory in Europe**.

Its objectives are

- technology take-up and VO compliant resource provision
- building the technical infrastructure
- support its utilization by the scientific community.



<http://eurovotech.org/>



<http://cds.u-strasbg.fr/twikiDCA/bin/view/EuroVODCA/WebHome>

VO-France

www.vo-france.org

Contact:

ovfrance@astro.u-strasbg.fr

Tutorials

Collaborations

Conferences




OV-France > Main > WebHome

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OV France / VO France [Inscrivez-vous sur la liste de diffusion](#)

[Du 27 juin au 1er juillet 2005: Euro VO Workshop](#)
[Du 4 au 7 avril 2005: Colloque d'ouverture de l'Action Spécifique OV France](#)
[Second Appel d'Offre 2005 Date limite: 5 juin 2005](#)
[Recensement des actions OV La date limite est dépassée mais contactez-nous si vous souhaitez envoyer un texte](#)
[...autres nouvelles et annonces / ... other news and announcements](#)



Les rubriques du TWiki OV France	Contenu	
L'action Spécifique OV France	Conseil Scientifique, charte, ...	Changements Chercher
Cas Scientifiques	Exemples d'utilisations scientifiques de l'OV	Changements Chercher
Groupes de travail	Les groupes de travail de l'OV France	Changements Chercher
Exposés	Exposés OV France, exposés aux réunions Interopérabilité	Changements Chercher
Réunions	Comptes-rendu, prochaines dates, ...	Changements Chercher
Liens STIC	Liens avec la communauté STIC	Changements Chercher
Liens	Liens utiles	Changements Chercher
Espace privé	Espace réservé nécessitant un nom d'utilisateur et un mot de passe	

Si vous voulez être inscrit sur la liste de diffusion des informations, envoyez un message à ovfrance@astro.u-strasbg.fr

Pour proposer un ajout de rubrique dans cette liste : twikiOV@astro.u-strasbg.fr

OV-France > ASOVFrance > Tutoriel2004

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ASOVFrance . ([Changes](#) | [Index](#) | [Search](#) | Go)

Tutoriel Standards et Outils de l'Observatoire Virtuel

Stasbourg 11-13 octobre 2004

L'Action Spécifique Observatoires Virtuels France organise un tutoriel à Strasbourg du 11 au 13 octobre 2004.

Ce tutoriel est destiné à aider les chercheurs et ingénieurs qui développent des services et souhaitent les rendre compatible avec l'Observatoire Virtuel International. Les standards et les outils disponibles dans le domaine de l'astronomie seront présentés, ainsi que l'état des lieux dans les disciplines Physique des plasmas spatiaux et Etude du Soleil.

Les frais de déplacement seront pris en charge par l'AS OV. Le nombre limite de participants est atteint. Vous pouvez être inscrit sur une liste supplémentaire.

Contact: tutoriel2004@astro.u-strasbg.fr

On peut consulter le [tutoriel](#) organisé en octobre 2003 en marge de la réunion ADASS sur seulement une demi-journée.

[Liste des participants](#)

[Photo](#)

[Documentation et liens](#)

[Acronymes](#)

[Programme](#)

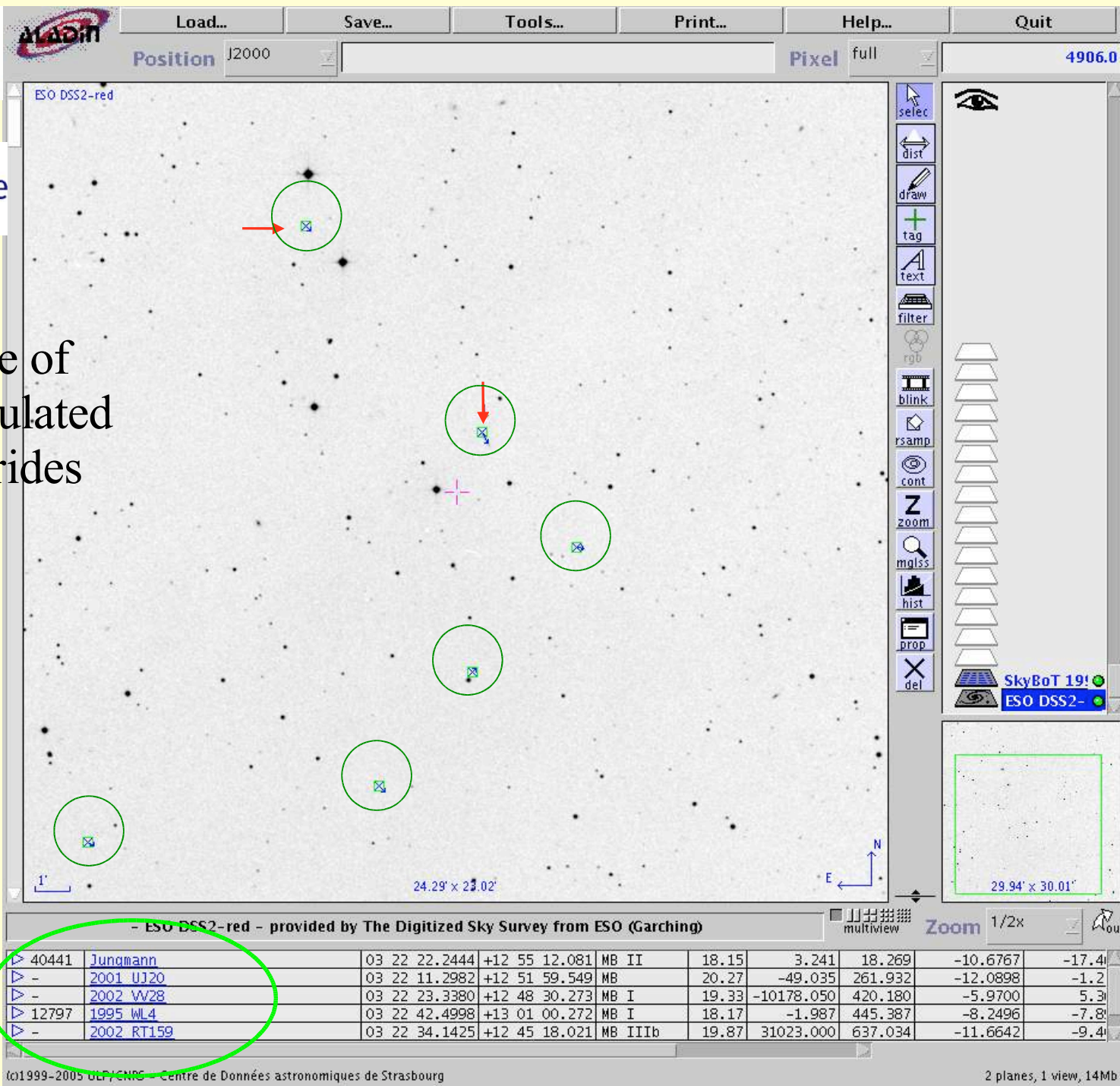




Paris VO Data Center

<http://vo.obspm.fr/>

- Federation: Paris Observatory, IAP and IPSL
- Very different products
 - Small objects of the solar system, Exoplanets
 - Planetary atmospheres
 - Simulations in the VO
 - Spectra and Images Databases (surveys, instrument archives)
 - Atomic & Molecular Physics
- Implementation of VO Standards
- Tools Development
- Central team of engineers + dedicated R&D in lab



ESO DSS2-red

Position J2000 Pixel full 4906.0

24.29' x 23.02'

29.94' x 30.01'

ESO DSS2-red - provided by The Digitized Sky Survey from ESO (Garching)

40441	Jungmann	03 22 22.2444	+12 55 12.081	MB II	18.15	3.241	18.269	-10.6767	-17.4
-	2001 UJ20	03 22 11.2982	+12 51 59.549	MB	20.27	-49.035	261.932	-12.0898	-1.2
-	2002 W28	03 22 23.3380	+12 48 30.273	MB I	19.33	-10178.050	420.180	-5.9700	5.3
12797	1995 WL4	03 22 42.4998	+13 01 00.272	MB I	18.17	-1.987	445.387	-8.2496	-7.8
-	2002 RT159	03 22 34.1425	+12 45 18.021	MB IIIb	19.87	31023.000	637.034	-11.6642	-9.4

©1999-2005 OLP/CNRS - Centre de Données astronomiques de Strasbourg 2 planes, 1 view, 14Mb

Catalogues
of other bodies

Identification
of other
celestial bodies

- **Identification of the Solar System bodies**

Some VO Simulation Projects at Paris Observatory



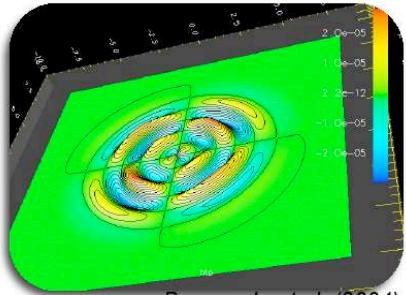
Codes

• Lorene

Relativistic team (LUTH)

- Libraries to solve partial differential equations
Multi-domain spectral methods

Applications : - Compact objects
- Relativistic jets (Zakaria Meliani)



Bonazzola et al. (2004)

• The Meudon PDR code

MIS team (LUTH)

Applications :
- Interpretation of observations in molecular regions

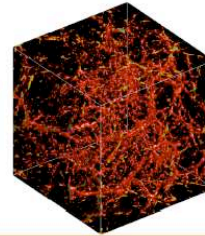
Examples : FUSE, ISO, HST(STIS)
Herschel, ALMA, ...



Ongoing projects

• Codes de cosmologie

Jean-Michel Alimi, André Füzfa & collaborators

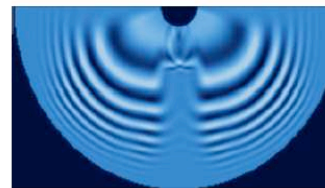


Applications : Formation of structures / galaxies
- N-body
- Hydrodynamic
- non-equilibrium chemistry

Courtesy of F. Le Petit
(LUTH, Obs. Paris)

• code MHD

Roland Grappin, Filippo Pantellini (LESIA)

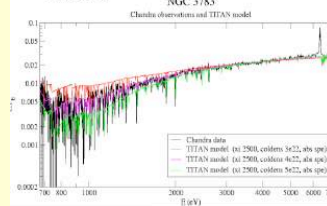


Resolution of MHD equations 1D/2D/3D
Particularities : open bounds

Applications : - stellar atmospheres, corona, winds
- stellar formation

• Titan

Anabela Gonçalves, Loïc Chevallier, René Goosman

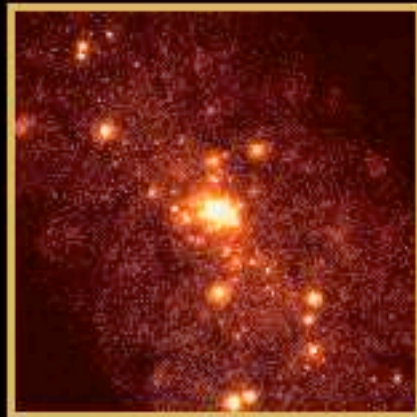


Radiative transfer in optical thick medium
Applications : Interpretation of X observations
(Chandra, XMM, XEUS, ...)

Science: Multi-wavelength Analysis

M31 – The Andromeda Galaxy

Distance: 2,900,000 light-years (900 kpc) Image Size = 2.5 x 2.5 degrees Visual Magnitude = 3.4



X-Ray: ROSAT



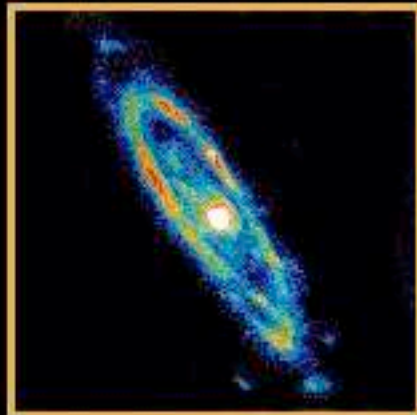
Ultraviolet: GALEX



Visible: DSS



Visible: © Jason Ware



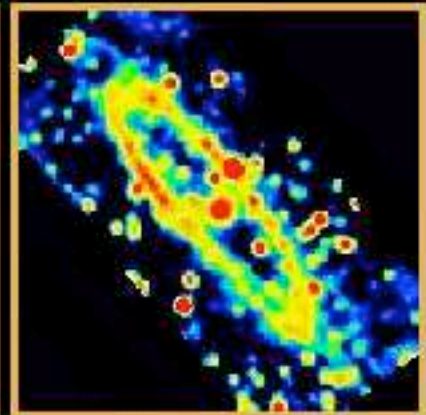
Mid-Infrared: IRAS



Mid-Infrared: Spitzer



Far-Infrared: ISO

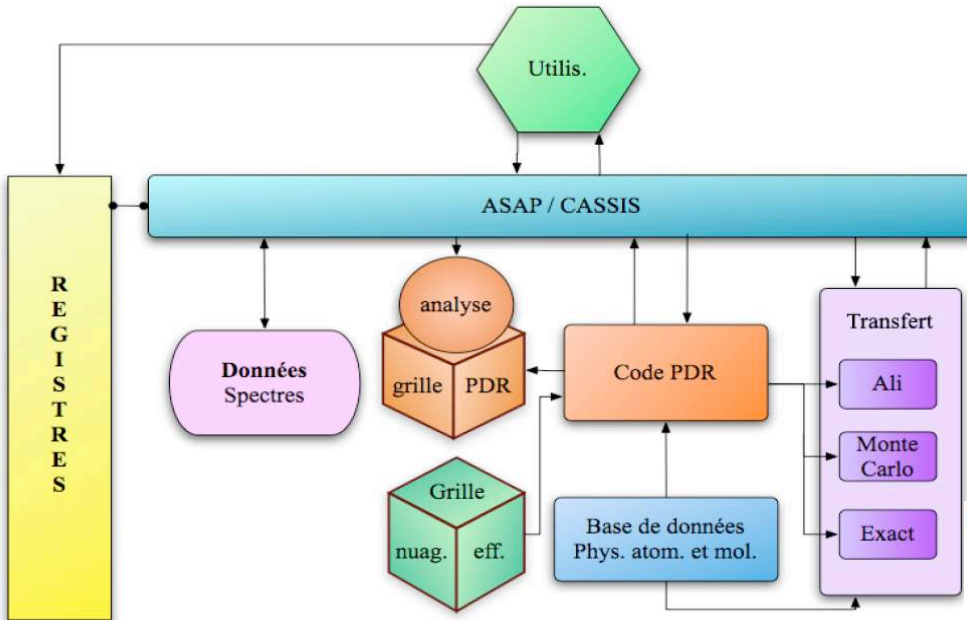


Radio: Effelsberg

Science: Comparison Models/Observations

Usecase

Next generation of instruments : huge amount of data
 ↪ need efficient tools to analyse and interpret the observations



Step 1 : Use of the VO :

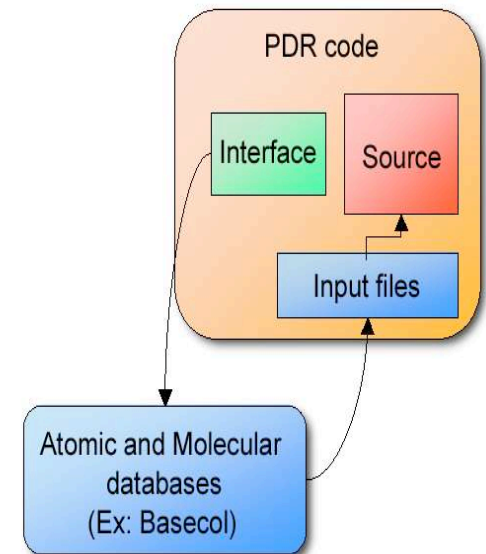
Link : PDR code / databases (1)

Courtesy of F. Le Petit
 (LUTH, Obs. Paris)

<http://aristote.obspm.fr/MIS>

Data used by PDR codes :

- Atomic and molecular properties :
 - Energy levels
 - Einstein coefficients
- Reactions between elements
 - collision rates
 - chemical reaction
 - gas phase reactions
 - surface reactions
 - photo-process cross sections



MAGIX Application Concept

Courtesy of
F. Boone



Observations

Graphical
User
Interface

*Use existing formats and
visualization tools*

model
codes

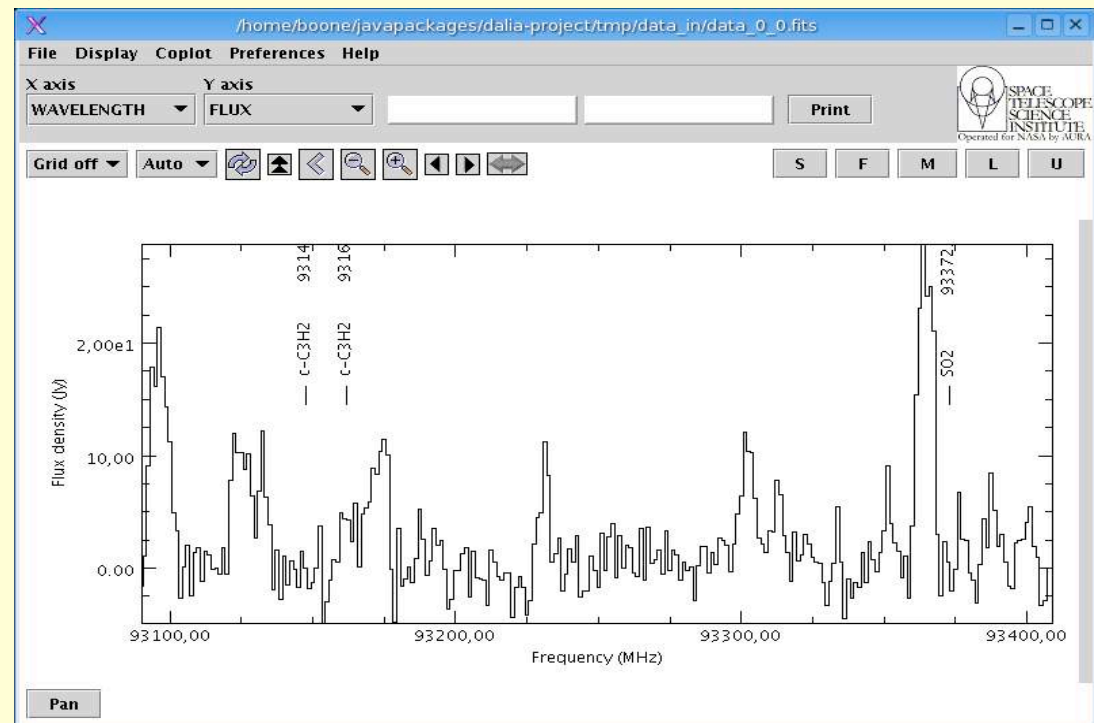
spectroscopic
data

Optimization engine

**Best fit parameters
with error bars**

Query existing databases

Science Synthetic Spectra



VO: Interoperability of resources in order to produce science

- **Observational Data**

- Archives: well taken care in IVOA, cross correlation (ALMA working group)

- **Theoretical/Observed Microphysics Data in Databases**

- Ex : NIST, CDMS/JPL, BASECOL, LOVAS catalogues, UMIST, etc

- **Numerical Codes**

- Ex : Radiative transfert codes, Modeling codes

- **Analysis tools/Visualisation**

- Analysis software (reduction pipeline, optimization algorithms, synthetic spectra): VoSpec, CASSIS, ASAP/MAGIX, etc

Requirements for Tools Implementation



- Full description of all data
 - Microphysics:
 - references, methods, accuracy
 - Identify measurements/calculations from extrapolation
 - Codes:
 - Identify hypothesis, algorithms, parameters
- Use standardized exchange language
- Long term maintenance of applications
- Deal with various resources

Access Atomic/Molecular DB starting with line lists

- Theoretical (measured or calculated) DB
 - Observed line lists DB

■ Numerous DB are available

- Atomic lines: NIST DBs, Kurucz's CD-ROM, Atomic Line List of P. Van Hoof, TOPbase, Kelly Atomic Line DB, VALD, MCHF/MCDHF Collection, D.R.E.A.M, KAERI AMODS
- Molecular Lines: JPL Spectroscopic DB, CDMS, HITRAN, GEISA, NIST
- Other DB: IEAE, NIFS, CHIANTI, UMIST, BASECOL, small compilations
- Observed databases: ATOMDB, NIST, ...

■ Identification of Pbs

- Different DB have similar datasets
 - DB have different levels of update
 - Lengthy to identify origin of datasets, find all relevant description of data
- Useful data for a single astrophysical application are dispersed in various DB
 - No homogeneous description of data

Atomic & Molecular Lines Data



Model

Paris Observatory and ESA/ESAC

ML Dubernet, P. Osuna, M. Guanazzi, J. Salgado, E. Roueff



Light – Matter Interaction : bound-bound

$$A(j) + h\nu \rightarrow A(j') \quad \text{or} \quad A(j') \rightarrow A(j) + h\nu$$

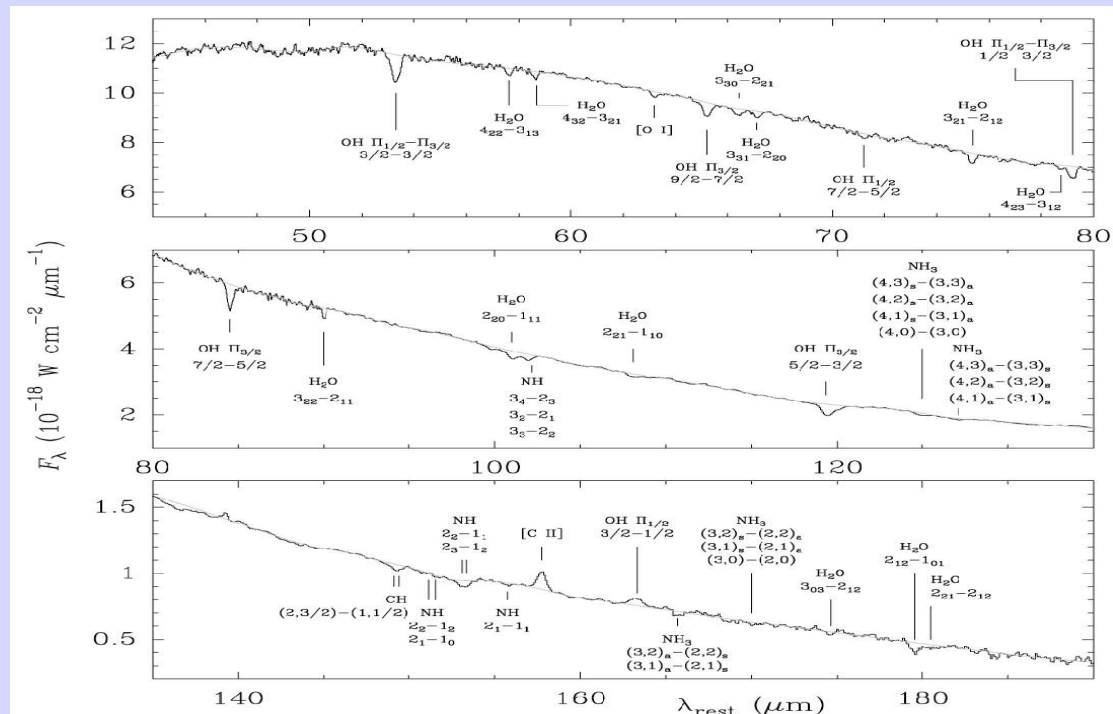
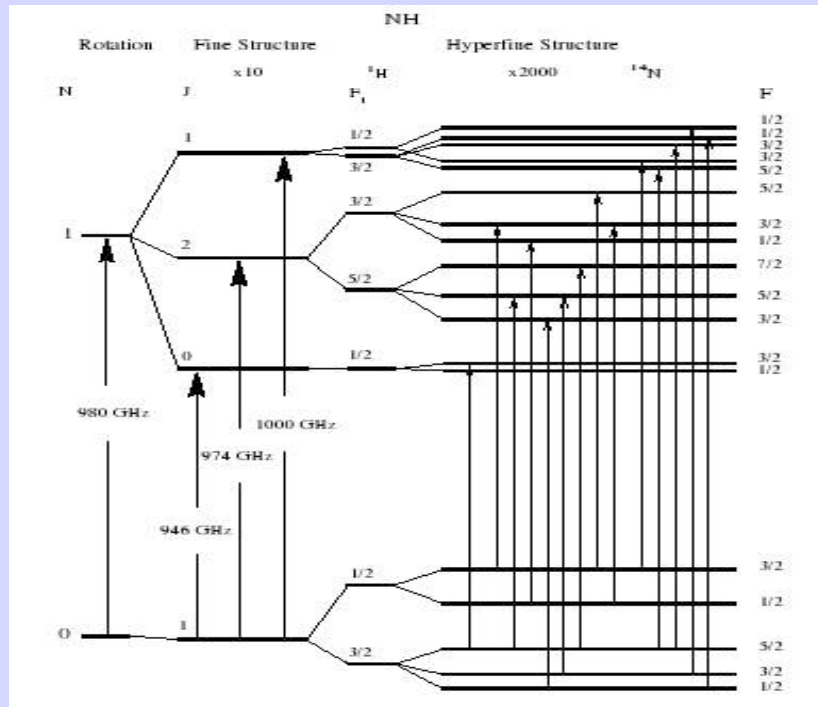
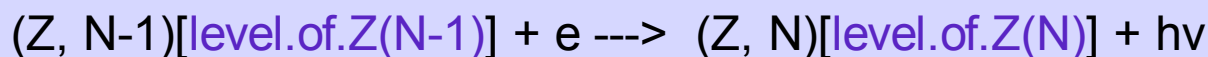


Fig. 1.— ISO/LWS spectrum of Arp 220, where the most prominent line features are identified (see text). The grey line shows the adopted baseline (continuum level).

Radiative recombinaison



MLD acknowledges support from VO-France, MDA project (F. Genova), Paris Observatory

Documents status and perspectives



International
Virtual
Observatory
Alliance

Atomic and Molecular Lines Data Model

Version 0.5

Draft Document 30 January 2006

This version:

ThisVersion-30Jan2006

Latest version:

http://www.ivoa.net/Documents/latest/LDM_v0.5

Previous versions:

Editors: Pedro Osuna, Matteo Guainazzi

Authors:

Marie-Lise Dubernet
Pedro Osuna
Matteo Guainazzi
Jesus Salgado
Evelyne Roueff

Status of This Document

This is an IVOA Working Draft for review by IVOA members and other interested parties. It is a draft document and may be updated, replaced, or obsoleted by other documents at any time. It is inappropriate to use IVOA Working Drafts as reference materials or to cite them as other than "work in progress".

A list of current IVOA Recommendations and other technical documents can be found at <http://www.ivoa.net/Documents/>.

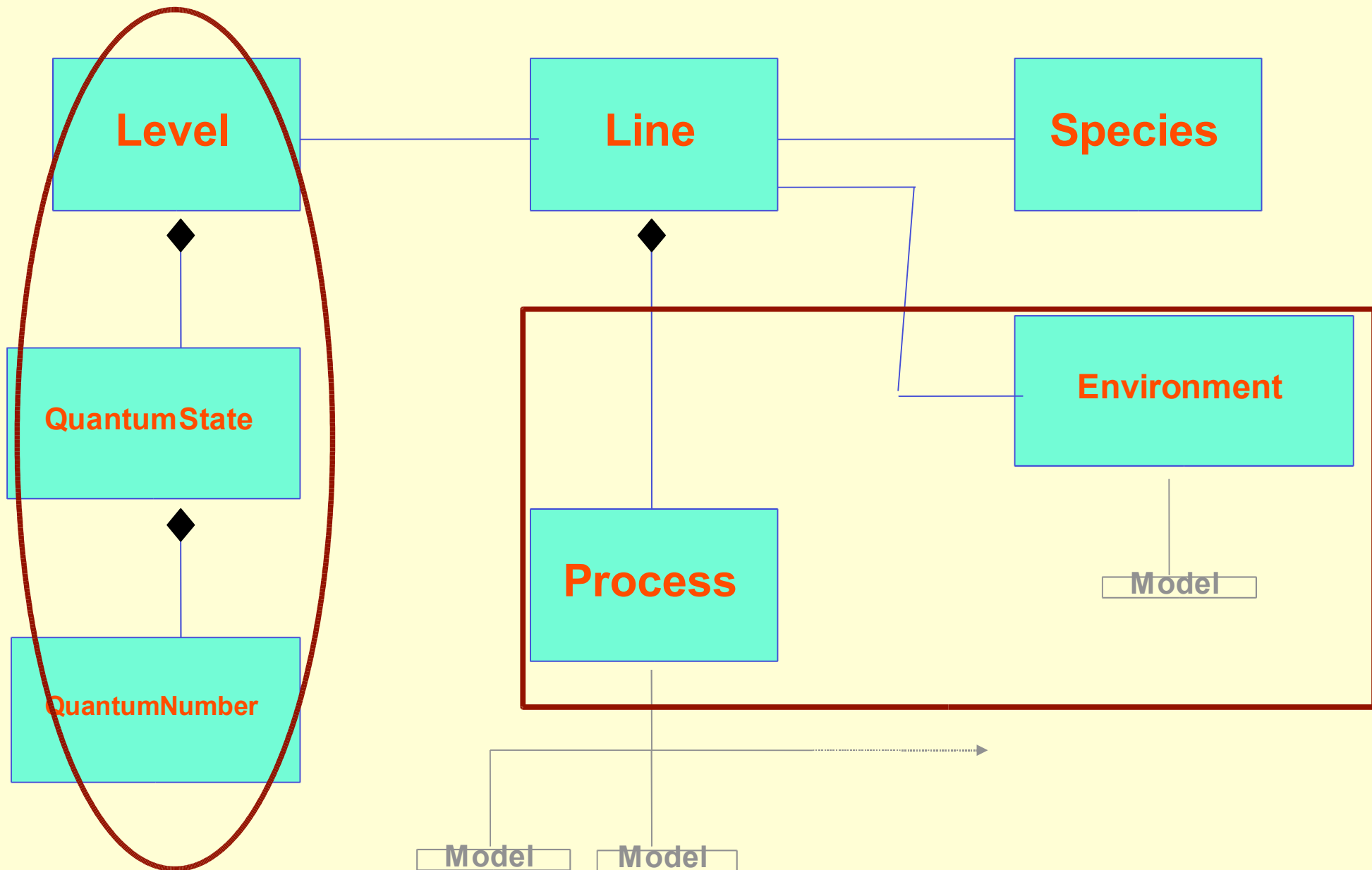
- **AML DM Current version: 0.5 (30/1/2006)**
- **circulated to the DM and DAL groups, as well as to atomic and molecular astrophysicists for comments**
- **Goal: achieve the status of a proposed recommendation in the next 4 months.**
- **Useful for ETL studies and calibration**
- **Requirements: to be implemented by the AM databases communities**

Requirements: MUST DESCRIBE

- Laboratory measured & fitted linelists
 - Based on A&M Theoretical Spectroscopy
- Linelists obtained from observed/simulated spectra
 - Environment, Process
- Atomic and Molecular Species
- **Precise enough** in order to do science
- **Unprecise enough** in order to cover observational databases

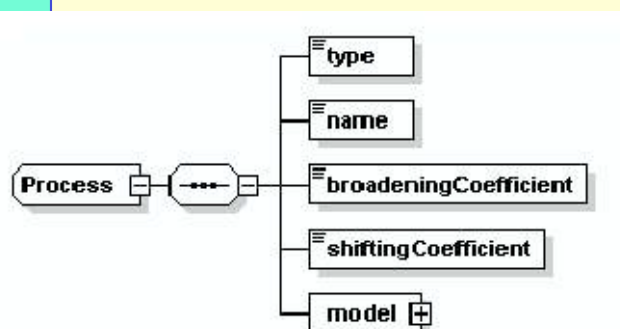
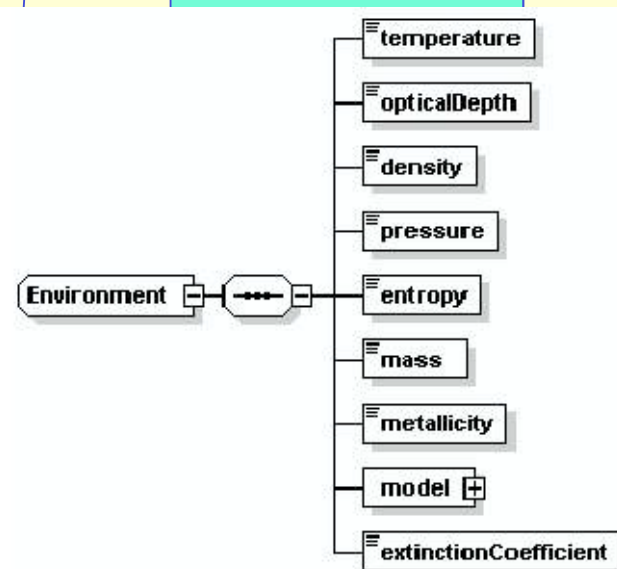
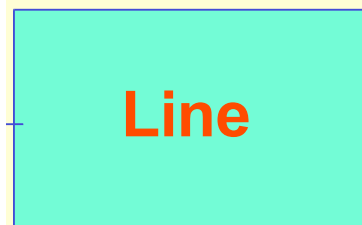
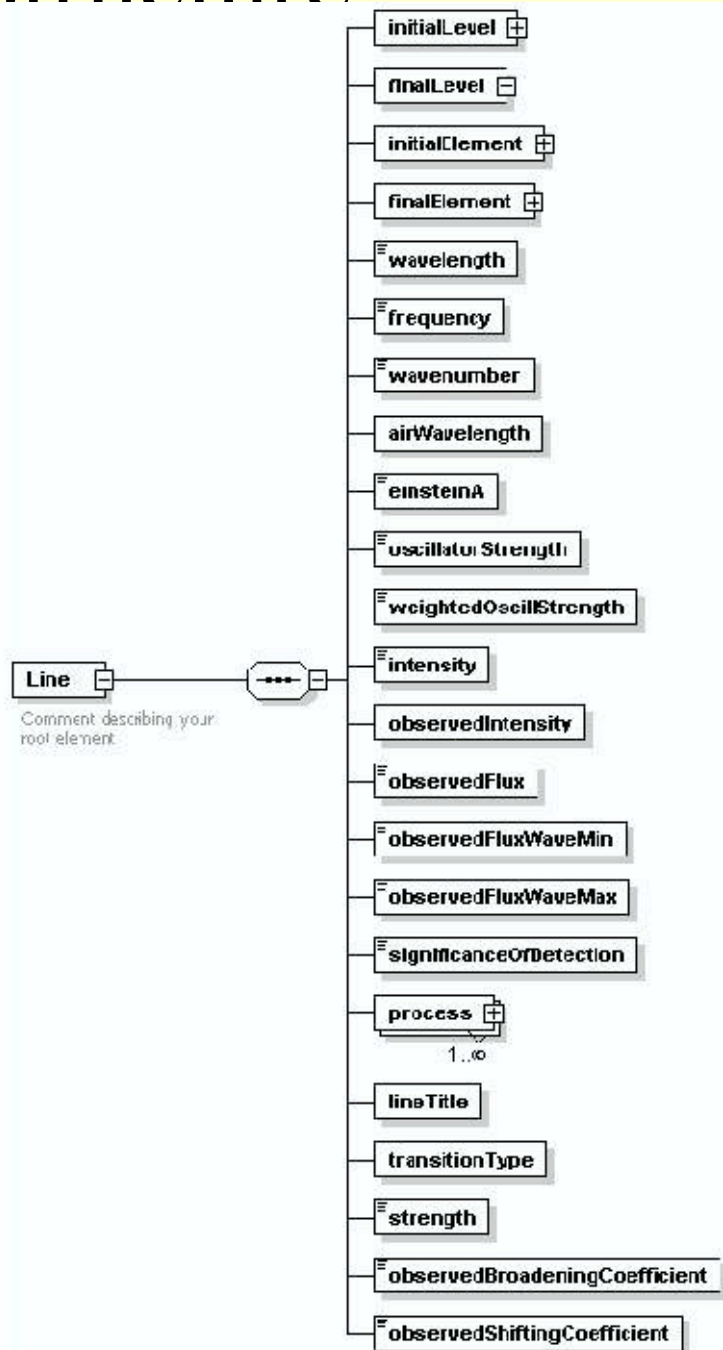
Structure

Laboratory & Observed Lines



Structure

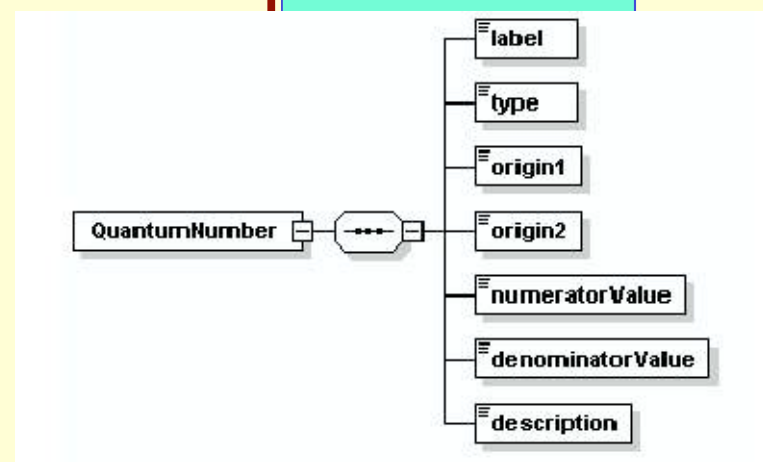
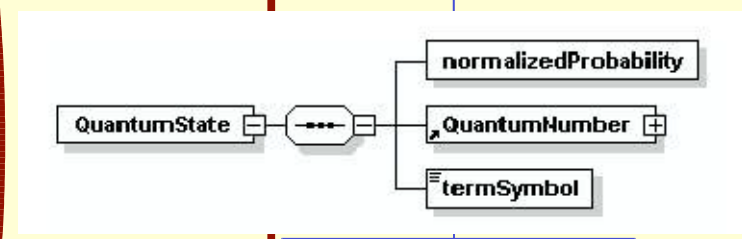
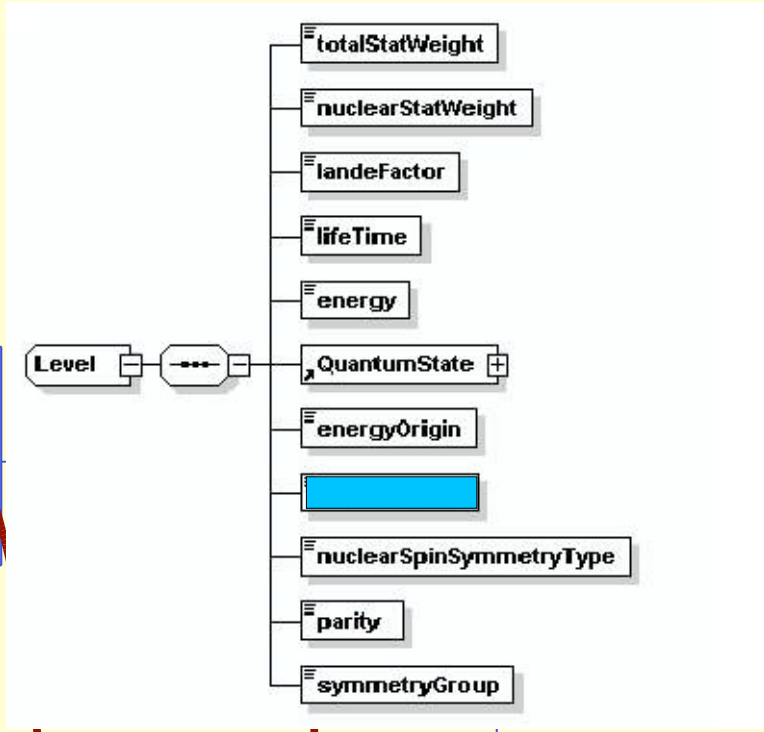
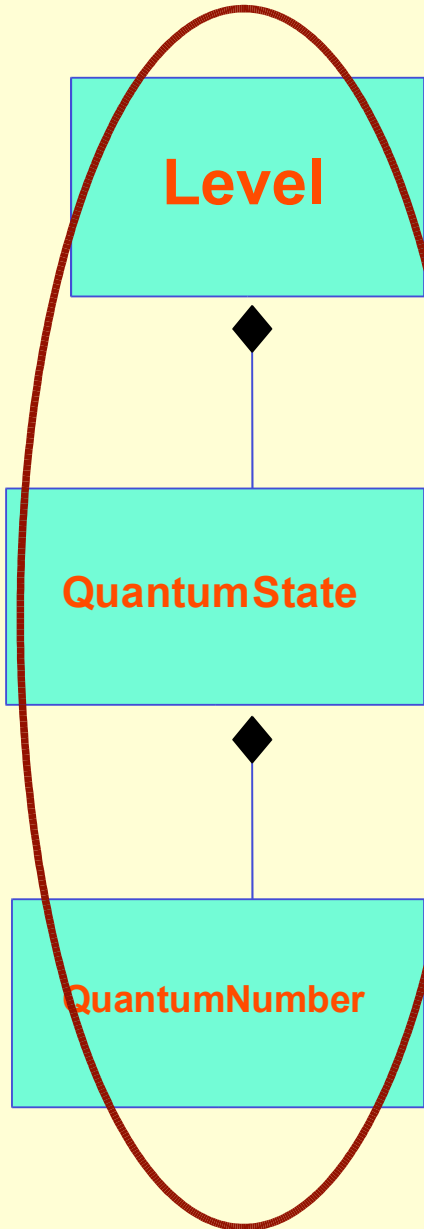
Laboratory & Observed Lines



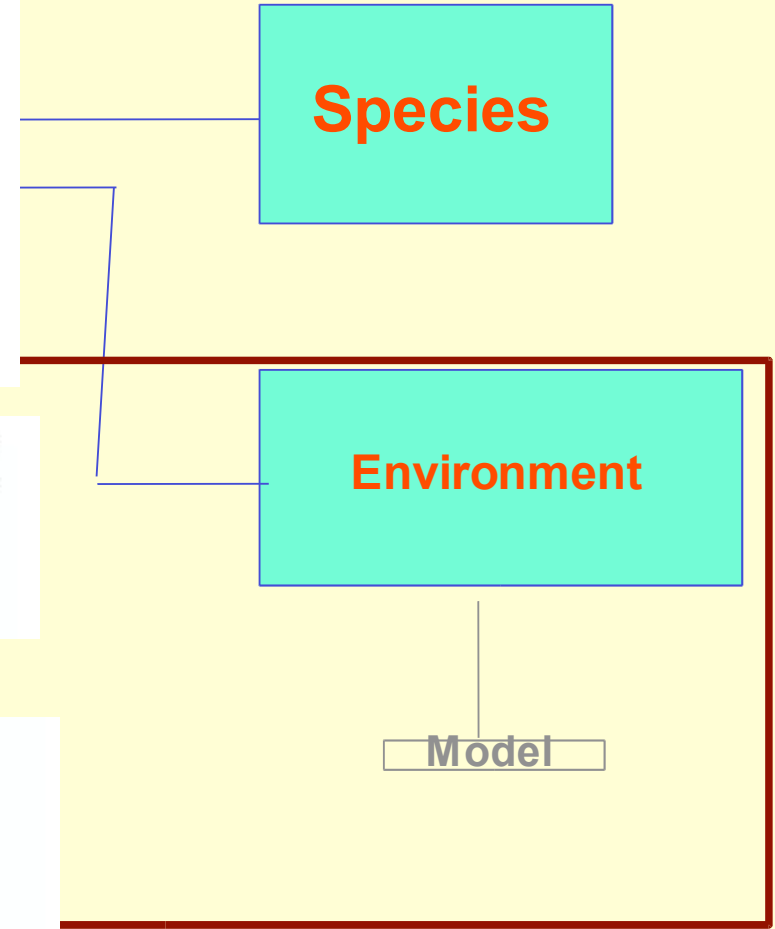
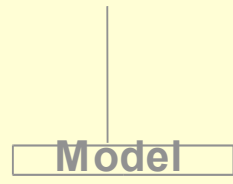
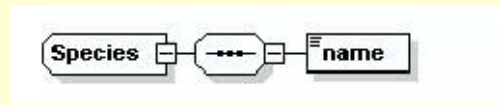
model

Model

Structure



ES



List of Quantum Numbers

- nprincipal
- lElectronicOrbitalAngularMomentum
- sAngularMomentum
- JtotalAngularMomentum
- LmagneticQuantumNumber
- SmagneticQuantumNumber
- nuclearSpinI_I
- totalNuclearSpinI
- totalSpinMomentumS
- totalMagneticQuantumNumberS
- totalMolecularProjectionS
- totalElectronicOrbitalMomentumL
- totalMagneticQuantumNumberL
- totalMolecularProjectionL
- totalAngularMomentumJ
- totalMagneticQuantumNumberJ
- totalMolecularProjectionJ
- totalAngularMomentumF
- totalMagneticQuantumNumberF
- totalAngularMomentumJa
- RotationR , MolecularProjectionR
- asymmetricTau
- asymmetricKa , asymmetricKc
- vibrationNu_i
- vibrationLNu_i
- totalVibrationLNu
- vibronicAngularMomentumK
- VibronicAngularMomentumP
- vibrationSymmetry_i
- HinderedK1, hinderedK2



*International
Virtual
Observatory
Alliance*

Simple Line Access Protocol

Version 0.5

Draft Document 17 May 2006

This version:

0.5 17May2006

Latest version:

<http://www.ivoa.net/Documents/latest/latest-version-name>

Previous version(s):

Editor(s):

Pedro Osuna
Jesus Salgado

Author(s):

Jesus Salgado
Pedro Osuna
Matteo Guainazzi
Isa Barbarisi
Marie-Lise Dubernet
Doug Tody

Abstract

This specification defines a protocol for retrieving spectral lines from different spectral line databases through a uniform interface.

SLAP

Collaboration:
ESA/ESAC
Paris Observatory

Document status

• Goal: achieve the status of a *proposed recommendation* in the next 4 months.

Query by Wavelength

Necessary steps before Proposed Recommendation

- Few explanations to modify
- Standardize molecule names
- **Quantum State**: Symmetry types such as vibronic_Species
rovibronic_Species
- Accuracy, Quality, Documentation, Versioning
 - ➔ Connection to other VO Data Models

Basecol Database (www.obspm.fr/basecol)

Useful for astrophysicists and physicists

Linked to CDMS and JPL

– Published (de)-excitation rate coefficients

- Rotational (fine, hyperfine)
- Ro-vibrational, Vibrational
- Currently: 21 Target molecules
- Perturbers : He, H, H₂
- 76 collisional systems
- Fully documented and referenced (630 ref.)
- Fitting coefficients, visualisation tools
- Energy levels, Einstein coefficients, QN

The screenshot shows a Mozilla browser window displaying the Basecol database interface. The URL in the address bar is <http://pc-dubernet01.obspm.fr/index.php?page=data&rub=viewCollision&id=34>. The page features the Basecol logo and navigation links for various observatories. The main content area is titled "Rotational excitation of CO by para H2 (Flower, 2001)" and includes tabs for "Rate Coefficients", "Labelling Energy Table(s)", "Einstein Coeff", "PES", "Method", "Range of Energy", and "BasisSet". The "Data display" section offers "HTML Format", "Text Format", and "VO Table Format" options. The "Graphical visualization" section has tabs for "Graphical visualization (one element)" and "Graphical visualization (two elements)". The "Data information" section lists: CO initial level labelled from 1 to 30, CO final level labelled from 1 to 30, H2 initial level labelled from 1 to 1, H2 final level labelled from 1 to 1, and 41 temperatures between 5 K and 400 K. The "Presentation" section provides a link to <http://ccp7.dur.ac.uk/> and a detailed description of the data. The "References" section lists several scientific papers related to the topic. The browser's taskbar at the bottom shows the system time as 19:48 on 04/04/2006.



Home

CDMS

What's New

Catalog

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archive

Molecules

in Space

Fitting Spectra

Cologne

Spectroscopy

Data

Links

Contact

Catalog Directory

See the [General](#) part for a description of the content and the [home](#) page for citation!

Entries having an asterisk after the version number have been included in the database after acceptance of our [new article on the CDMS, J. Mol. Struct., 742](#) 215–227 (2005), in January, 2005. It can not be ruled out completely that recent entries contain errors.

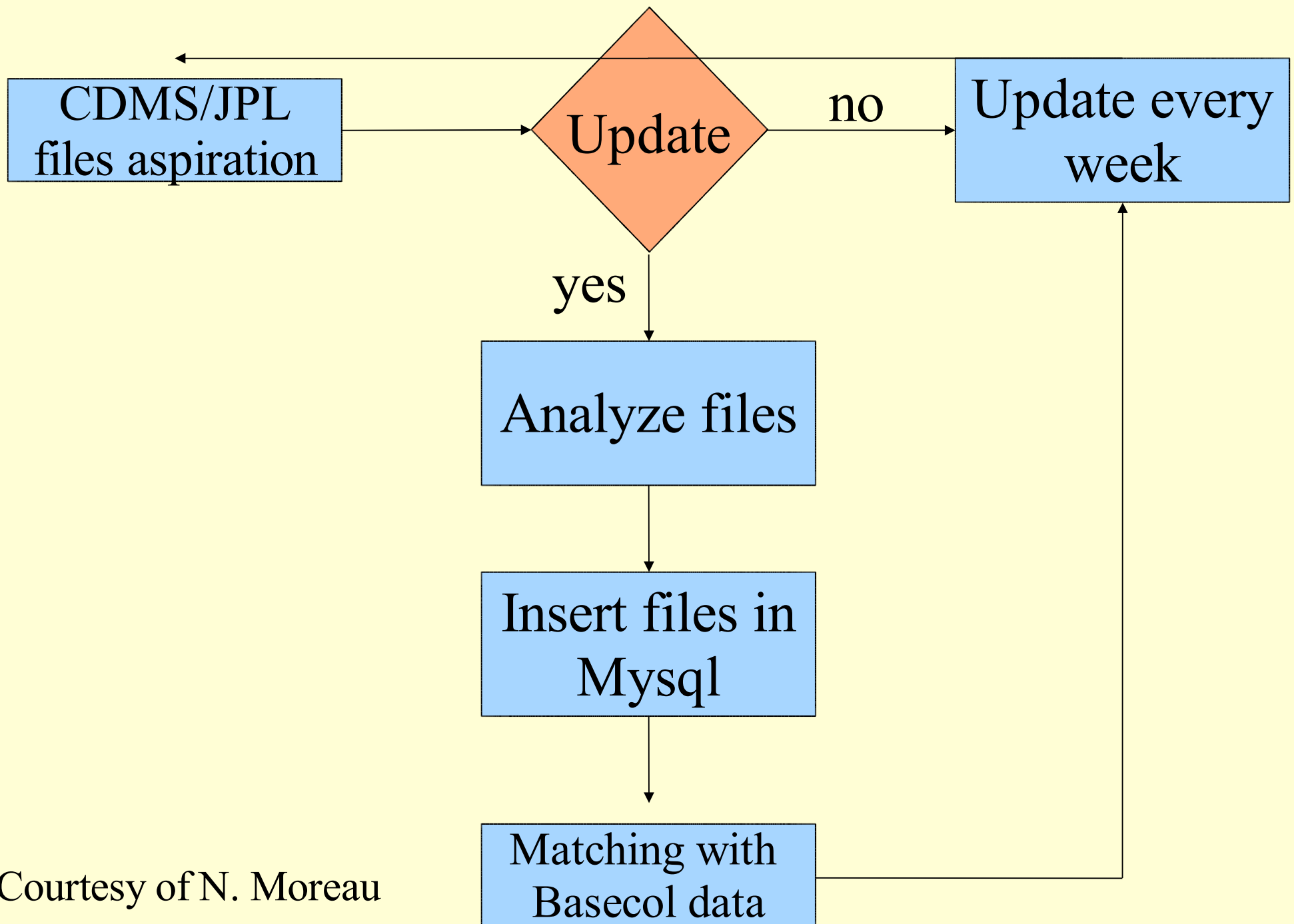
Note: Entries having an asterisk after the tag state the temperature independent $S_{\mu 2}$ instead of the intensity I at 300 K !!

For some entries, where, for example, hyperfine splitting was important for the laboratory data, but is expected to be of minor importance for radioastronomical observations, separate predictions are available. Values of the partition function given in the respective documentation refer to the vibrational ground state only – unless stated otherwise.

Get one [list of partition functions](#) for the price of a half.
Currently 387 entries.

Tag	Name	# lines	Ver.	Catalog	Documentation	Date of entry	Entry in cm ⁻¹
003501 HD, $v = 0, 1$		21	1*	HTML ASCII	e003501.cat	Sep. 2005	w003501.cat
004501 H ₂ D+		137	1*	HTML ASCII	e004501.cat	Aug. 2005	w004501.cat
005501 HD ₂ +		163	1*	HTML ASCII	e005501.cat	Aug. 2005	w005501.cat
012501 C		2	1*	HTML ASCII	e012501.cat	Sep. 2005	w012501.cat
013501 13C		7	1*	HTML ASCII	e013501.cat	Sep. 2005	w013501.cat
013502 CH		385	2*	HTML ASCII	e013502.cat	Sep. 2006	w013502.cat
014501 CH ₂		1400	1*	HTML ASCII	e014501.cat	Sep. 2005	w014501.cat
015501 NH		1948	1	HTML ASCII	e015501.cat	May 2004	w015501.cat
016501 NH ₂		18513	2	HTML ASCII	e016501.cat	Oct. 2001	w016501.cat
016502 ND		2020	1	HTML ASCII	e016502.cat	Feb. 2004	w016502.cat
016503 CH ₂ D+		222	1	HTML ASCII	e016503.cat	July 2004	w016503.cat
017501 OH+		209	1	HTML ASCII	e017501.cat	Apr. 2003	w017501.cat
018501 NH ₂ D		3343	1	HTML ASCII	e018501.cat	May 2004	w018501.cat
019501 NHD ₂		4442	1	HTML ASCII	e019501.cat	Aug. 2004	w019501.cat
020501 ND ₃		698	1	HTML ASCII	e020501.cat	June 2002	w020501.cat
024501 NaH		172	1	HTML ASCII	e024501.cat	Jan. 2001	w024501.cat
025501 CCH, $v = 0$		109	1	HTML ASCII	e025501.cat	Apr. 2004	
025502 MgH		96	1	HTML ASCII	e025502.cat	May 2001	w025502.cat
025503 CCH, $v_2 = 1$		374	1	HTML ASCII	e025503.cat	Apr. 2004	
026501 CCD		198	1	HTML ASCII	e026501.cat	Apr. 2000	
026502 13CCH		232	1	HTML ASCII	e026502.cat	May 2000	
026503 C13CH		223	1	HTML ASCII	e026503.cat	May 2000	
026504 CN, $v = 0, 1$		646	1*	HTML ASCII	e026504.cat	May. 2005	





Courtesy of N. Moreau

Service for MAGIX

- Query Parameters

- Frequency_min (instead of wavelength_min)
- Frequency_max (instead of wavelength_max)
- *Chemical_element* (SLAP non compulsory parameter)
- *Chemical_element_symmetry* (specific to this service)

- Return list of transitions with:

```
- <VOTABLE version="1.1" xsi:schemaLocation="http://www.ivoa.net/xml/VOTable/v1.1 http://www.ivoa.net/xml/VOTable/v1.1">
- <RESOURCE type="results">
  <INFO name="QUERY_STATUS" value="OK"/>
  <TABLE>
    <FIELD name="frequency" ucd="em.freq" utype="Idm:Line.frequency" datatype="int"/>
    <FIELD name="chemicalelement_name" ucd="phys.atmol.element" utype="Idm:Line.initialElement.name" datatype="char" arraysize="*/>
    <FIELD name="chemicalelement_symmetry" ucd="phys.atmol.element" datatype="char" arraysize="*/>
    <FIELD name="final_level_energy" ucd="phys.energy;phys.atmol.final;phys.atmol.level" utype="Idm:Level.energy" datatype="double"/>
    <FIELD name="einstein_coefficient" ucd="phys.atmol.transProb" utype="Idm:Line.einsteinA" datatype="double"/>
    <FIELD name="statistical_weight" ucd="" datatype="double"/>
    <FIELD name="quantum_number_tag" ucd="meta.id" datatype="int"/>
    <FIELD name="id_chemical_element" ucd="meta.id" datatype="int"/>
    <FIELD name="data_source" ucd="meta.table" datatype="char" arraysize="*/>
    <FIELD name="creation_date" ucd="" datatype="char" arraysize="*/>
    <FIELD name="quantum_numbers_link" ucd="meta.ref.url" datatype="char" arraysize="*/>
    <FIELD name="partition_function_link" ucd="meta.ref.url" datatype="char" arraysize="*/>
  <DATA>
    + <TABLEDATA></TABLEDATA>
  </DATA>
</TABLE>
</RESOURCE>
</VOTABLE>
```

SLAP Server choice



Other servers :
- NIST
- ESA

Result of a simple request

Spectral lines Dialog

File Request Display Server

Filters

Minimum frequency value (in MHz): 45000 Maximum frequency value (in MHz): 45100
Minimum energy value (in cm⁻¹): none Maximum energy value (in cm⁻¹): none
Minimum A value: none Maximum A value: none

Lines

Molecule name	Transition quantum numbers (J,F)	Wavelength	Frequency	Initial energy	Final energy	Einstein coefficients	Source DB
34SO2; symmetry: none; date of import: 2006-09-12							
34SO2	[N=19.0 Ka=2.0 Kc=18.0][N=18.0 Ka=3.0 Kc=15.0]		0.00665027919453				45079.67999998945
41KCl, v = 0, 1; symmetry: none; date of import: 2006-09-12							
41KCl, v = 0, 1	[N=6.0 v1=30.0][N=5.0 v1=30.0]		0.00665185496346				45069.00099999494
aa-(C2H5)2O; symmetry: none; date of import: 2006-09-12							
aa-(C2H5)2O	[N=8.0 Ka=2.0 Kc=6.0][N=8.0 Ka=1.0 Kc=7.0]		0.0066608678184				45008.01789998782
aa-(C2H5)2O	[N=79.0 Ka=13.0 Kc=67.0][N=80.0 Ka=12.0 Kc=68.0]		0.0066578546256				45028.387499972334
aa-(C2H5)2O	[N=79.0 Ka=13.0 Kc=66.0][N=80.0 Ka=12.0 Kc=69.0]		0.00665785456645				45028.387900015485
aa-(C2H5)2O	[N=14.0 Ka=4.0 Kc=11.0][N=15.0 Ka=3.0 Kc=12.0]		0.006651433554				45071.856399995544
c-C2H4O; symmetry: ortho; date of import: 2006-09-12							
c-C2H4O	[N=18.0 Ka=3.0 Kc=15.0][N=19.0 Ka=2.0 Kc=18.0]		0.00665008997246				45080.96269998296
c-C2H4O; symmetry: para; date of import: 2006-09-12							
c-C2H4O	[N=18.0 Ka=4.0 Kc=15.0][N=19.0 Ka=1.0 Kc=18.0]		0.00665008997246				45080.96269998296
c-C6H4; symmetry: para; date of import: 2006-09-12							
c-C6H4	[N=4.0 Ka=3.0 Kc=2.0][N=3.0 Ka=2.0 Kc=1.0]		0.0066578322546				45028.53879997784
c-C6H4	[N=21.0 Ka=12.0 Kc=9.0][N=21.0 Ka=11.0 Kc=10.0]		0.00665725755037				45032.42600000326
c-HCOOH; symmetry: none; date of import: 2006-09-12							
c-HCOOH	[N=30.0 Ka=2.0 Kc=29.0][N=29.0 Ka=3.0 Kc=26.0]		0.00666061444936				45009.73000003119
c-SiC3; symmetry: none; date of import: 2006-09-12							
c-SiC3	[N=22.0 Ka=4.0 Kc=18.0][N=23.0 Ka=2.0 Kc=21.0]		0.00665048909655				45078.2571999885
C5N; symmetry: none; date of import: 2006-09-12							

OK Apply filters

Filtered request result

The screenshot shows the 'Spectral lines Dialog' window with the following filters applied:

- Minimum frequency value (in MHz): 45000
- Maximum frequency value (in MHz): 45100
- Minimum energy value (in cm⁻¹): 100
- Maximum energy value (in cm⁻¹): none
- Minimum A value: none
- Maximum A value: none

The 'Lines' section displays a list of spectral lines with the following columns: Molecule name, Transition quantum numbers (J,F), Wavelength, and Final energy. The list includes:

Molecule name	Transition quantum numbers (J,F)	Wavelength	Final energy
34SO2; symmetry : none; date of import : 2006-09-12			
34SO2	[N=19.0 Ka=2.0 Kc=18.0][N=18.0 Ka=3.0 Kc=15.0]	0.00665027919453	124.864
aa-(C2H5)2O; symmetry : none; date of import : 2006-09-12			
aa-(C2H5)2O	[N=79.0 Ka=13.0 Kc=67.0][N=80.0 Ka=12.0 Kc=68.0]	0.0066578546256	545.5839
aa-(C2H5)2O	[N=79.0 Ka=13.0 Kc=66.0][N=80.0 Ka=12.0 Kc=69.0]	0.00665785456645	545.5839
c-C2H4O; symmetry : ortho; date of import : 2006-09-12			
c-C2H4O	[N=18.0 Ka=3.0 Kc=15.0][N=19.0 Ka=2.0 Kc=18.0]	0.00665008997246	196.4839
c-C2H4O; symmetry : para; date of import : 2006-09-12			
c-C2H4O	[N=18.0 Ka=4.0 Kc=15.0][N=19.0 Ka=1.0 Kc=18.0]	0.00665008997246	196.4839
c-HCOOH; symmetry : none; date of import : 2006-09-12			
c-HCOOH	[N=30.0 Ka=2.0 Kc=29.0][N=29.0 Ka=3.0 Kc=26.0]	0.00666061444936	345.601
c-SiC3; symmetry : none; date of import : 2006-09-12			
c-SiC3	[N=22.0 Ka=4.0 Kc=18.0][N=23.0 Ka=2.0 Kc=21.0]	0.00665048909655	114.6436
H2CCCHCN; symmetry : none; date of import : 2006-09-12			
H2CCCHCN	[N=66.0 Ka=6.0 Kc=60.0][N=65.0 Ka=7.0 Kc=59.0]	0.00665746645908	408.155
H2CO; symmetry : ortho; date of import : 2006-09-12			
H2CO	[N=19.0 Ka=3.0 Kc=16.0][N=19.0 Ka=3.0 Kc=17.0]	0.00665273665143	535.9368
HDCO; symmetry : none; date of import : 2006-09-12			
HDCO	[N=38.0 Ka=6.0 Kc=32.0][N=38.0 Ka=6.0 Kc=33.0]	0.00665059515905	1797.9431
HDCS; symmetry : none; date of import : 2006-09-12			
HDCS	[N=35.0 Ka=3.0 Kc=32.0][N=35.0 Ka=3.0 Kc=33.0]	0.00665195822091	707.6589
t-H13COOH; symmetry : none; date of import : 2006-09-12			

minimum energy value = 100

SLAP request to NIST server

Spectral lines Dialog

File Request Display Server

Filters

Minimum wavelength value (in meters) : 0.00001 Maximum wavelength value (in meters) : 0.0001
Minimum energy value (in cm-1) : none Maximum energy value (in cm-1) : none
Minimum A value : none Maximum A value : none

Lines

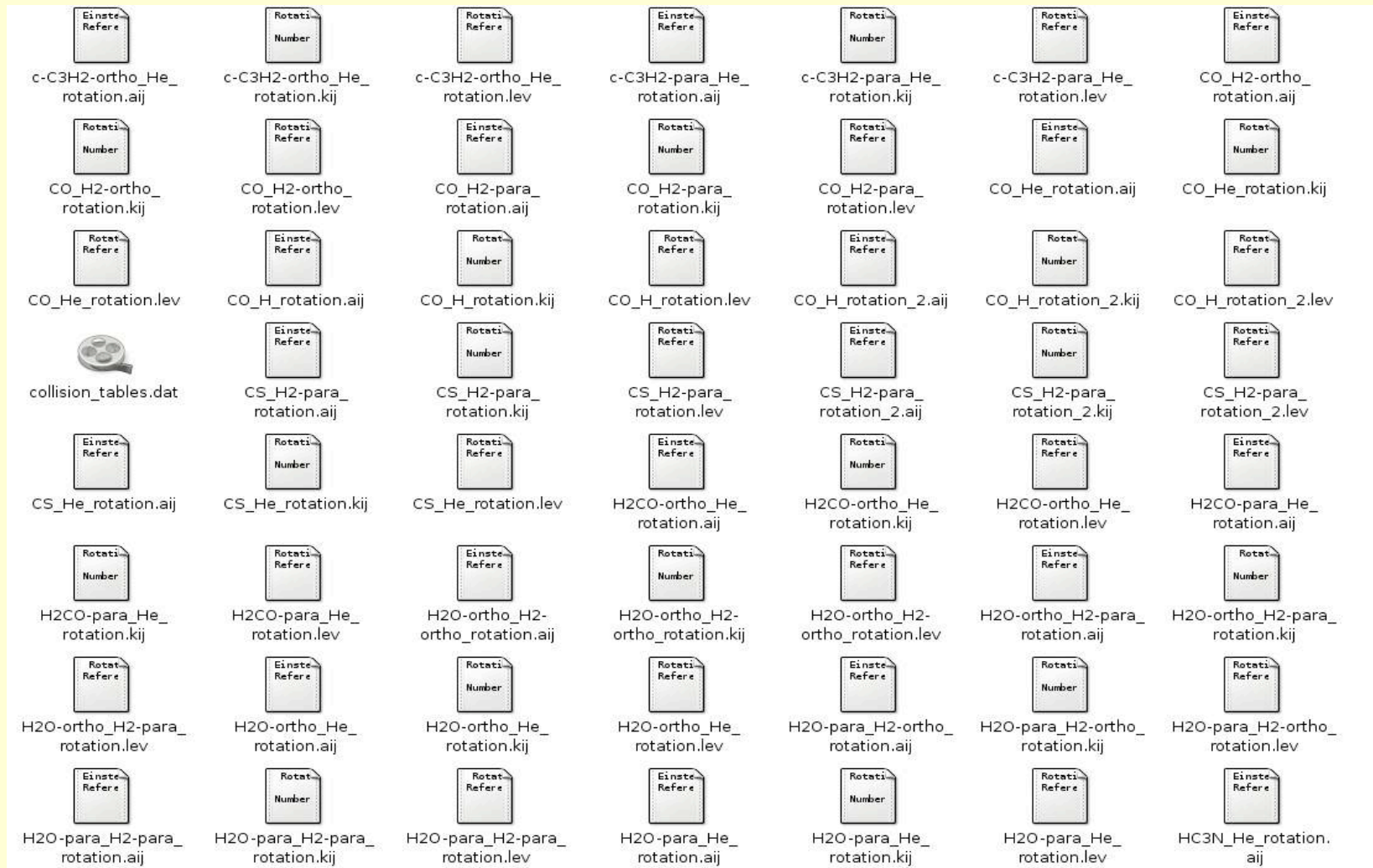
- Molecule name -	- Transition quantum numbers (J,F) -	- Wavelength -	- Frequency -	- Initial energy -	- Final energy -	- Einstein coefficients -	- Source DB -
<input checked="" type="checkbox"/> Al I 108886.8 A							
<input checked="" type="checkbox"/> Al		not available				1.088868E-5	2.7532488602842588E7
<input checked="" type="checkbox"/> Al I 109369.3 A							
<input checked="" type="checkbox"/> Al		not available				1.093693E-5	2.7411024665971164E7
<input checked="" type="checkbox"/> Al I 120282.8 A							
<input checked="" type="checkbox"/> Al		not available				1.202828E-5	2.4923967350277845E7
<input checked="" type="checkbox"/> Al I 120343.2 A							
<input checked="" type="checkbox"/> Al		not available				1.203432E-5	2.4911458063272376E7
<input checked="" type="checkbox"/> Al I 892371 A							
<input checked="" type="checkbox"/> Al		not available				8.92371E-5	3359504.712725985
<input checked="" type="checkbox"/> Al II 807230 A							
<input checked="" type="checkbox"/> Al		not available				8.0723E-5	3713841.8790183715
<input checked="" type="checkbox"/> Al VII 375900 A							
<input checked="" type="checkbox"/> Al		not available				3.759E-5	7975324.767225327
<input checked="" type="checkbox"/> Al		not available				3.759E-5	7975324.767225327
<input checked="" type="checkbox"/> Al XIII 244400 A							
<input checked="" type="checkbox"/> Al		not available				2.444E-5	1.2266467184942717E7
<input checked="" type="checkbox"/> Ar III 218315 A							
<input checked="" type="checkbox"/> Ar		not available				2.18315E-5	1.3732105352357833E7
<input checked="" type="checkbox"/> Ar IV 564600 A							
<input checked="" type="checkbox"/> Ar		not available				5.646E-5	5309820.368402409
<input checked="" type="checkbox"/> Ar		not available				5.646E-5	5309820.368402409
<input checked="" type="checkbox"/> Ar IV 775700 A							

OK Apply filters

Automatic script to get data from Basecol

Script in Python, Use the SLAP service
Store the data in VOTable or in ascii files
Get all the collisions available in Basecol

Example of a query result :



File listing all downloaded collisions

```
1 List of available tables of collision rates. After five header lines,
2 each entry consists of three lines: name of the file containing the table,,
3 description of the data and a separator line
4
5
6 H2O-ortho_He_rotation.kij
7 Rotational excitation of ortho-H2O by He (Green & al., 1993)
8 *****
9
10
11 CS_H2-para_rotation.kij
12 Rotational excitation of CS by para-H2, 20K < T < 300K, lowest 21 levels (Turner & al, 1992)
13 *****
14
15
16 HCO+_H2-para_rotation.kij
17 Rotational excitation of HCO+ by para-H2, 10K < T < 400K (Flower, 1999)
18 *****
19
20
21 OCS_He_rotation.kij
22 Rotational excitation of OCS by He (Flower, 2001)
23 *****
24
25
26 HCl_He_hyperfine.kij
27 Excitation of the hyperfine levels of HCl by He (Neufeld & al. 1994)
28 *****
29
30
31 HF_He_rotation.kij
32 Rotational excitation of HF(v=0) by He (Reese et al, 2005)
33 *****
34
35
36 H2CO-para_He_rotation.kij
37 Rotational Excitation of para-H2CO by He (Green, 1991)
38 *****
39
40
41 H2CO-ortho_He_rotation.kij
42 Rotational Excitation of ortho-H2CO by He (Green, 1991)
43 *****
44
45
```

Einstein coefficients

```

1 Einstein coefficients A_ij for c-C3H2
2 Reference : JPL
3
4      i      j      A_ij,....
5
6      2      1      4.2263065752e-07
7      3      1      2.55334550477e-05
8      4      2      7.46365079557e-05
9      4      3      3.80296644732e-06
10     5      3      7.67030052301e-05
11     6      4      7.44204214473e-05
12     6      5      1.0907409924e-05
13     7      3      6.49147849116e-05
14     7      6      3.51497796146e-06
15     8      5      0.0001800850413
16     9      4      0.000281274770668
17     9      5      4.09019577389e-07
18     9      7      1.07159096204e-06
19     10     6      0.000239338358103
20     10     8      2.46408072369e-05
21     10     9      3.8977132555e-07
22     11     8      0.000346901479579
23     12     5      8.90722201873e-05
24     12     7      0.000342485688259
25     12     10     1.67297462027e-05
26     13     6      0.000130700524776
27     13     8      1.45695026515e-07
28     13     9      0.000799273098548
29     13     12     7.57505463427e-06
30     14     10     0.000442683072
31     14     11     4.3505634887e-05
32     14     13     7.18729155496e-09
33     15     11     0.000593376026698
34     16     8      0.000125491181256
35     16     12     0.000457272678169
36     16     14     3.66887521178e-05
37     16     15     4.89008576098e-10
38     17     10     0.0002941249067
39     17     11     1.86320242591e-07
40     17     13     0.000177015839039
41     17     16     1.54060633156e-05
42     18     8      9.11569309474e-07
43     18     12     0.000661124626506
44     18     14     1.05257205244e-06
45     18     17     4.07161990011e-06
46     19     14     0.000742320443638
    
```

Energy table

```

1 Rotational Excitation of ortho-cyclopropenyl by He (Chandra & al., 2000)
2 Reference : JPL
3
4      N      g      Energy in cm^-1      Level details...
5      1      9      1.6332      Ka=0 Kc=1 N=1 epsilon=1 tau=1
6      2      15      1.6332      Ka=1 Kc=0 N=1 epsilon=1 tau=1
7      3      15      2.2451      Ka=1 Kc=2 N=2 epsilon=1 tau=1
8      4      15      4.4798      Ka=2 Kc=1 N=2 epsilon=1 tau=1
9      5      21      4.4798      Ka=0 Kc=3 N=3 epsilon=1 tau=3
10     6      21      6.3153      Ka=1 Kc=2 N=3 epsilon=1 tau=1
11     7      21      8.3875      Ka=2 Kc=1 N=3 epsilon=1 tau=1
12     8      21      4.4798      Ka=1 Kc=4 N=4 epsilon=1 tau=3
13     9      21      11.155      Ka=3 Kc=0 N=3 epsilon=1 tau=3
14     10     27      8.3875      Ka=2 Kc=3 N=4 epsilon=1 tau=1
15     11     27      6.3153      Ka=0 Kc=5 N=5 epsilon=1 tau=5
16     12     27      8.3875      Ka=3 Kc=2 N=4 epsilon=1 tau=1
17     13     21      12.6262      Ka=4 Kc=1 N=4 epsilon=1 tau=3
18     14     27      11.155      Ka=1 Kc=4 N=5 epsilon=1 tau=3
19     15     27      13.4194      Ka=1 Kc=6 N=6 epsilon=1 tau=5
20     16     27      13.5296      Ka=2 Kc=3 N=5 epsilon=1 tau=1
21     17     33      13.4194      Ka=3 Kc=2 N=5 epsilon=1 tau=1
22     18     27      8.3875      Ka=4 Kc=1 N=5 epsilon=1 tau=3
23     19     27      12.6262      Ka=2 Kc=5 N=6 epsilon=1 tau=3
24     20     27      17.3465      Ka=5 Kc=0 N=5 epsilon=1 tau=5
25     21     27      11.155      Ka=0 Kc=7 N=7 epsilon=1 tau=7
26     22     27      13.4194      Ka=3 Kc=4 N=6 epsilon=1 tau=1
27     23     27      13.5296      Ka=4 Kc=3 N=6 epsilon=1 tau=1
28     24     27      20.2037      Ka=1 Kc=6 N=7 epsilon=1 tau=5
29     25     33      17.3465      Ka=1 Kc=8 N=8 epsilon=1 tau=7
30     26     33      19.5679      Ka=5 Kc=2 N=6 epsilon=1 tau=3
31     27     33      22.3944      Ka=6 Kc=1 N=6 epsilon=1 tau=5
32     28     39      19.5679      Ka=2 Kc=5 N=7 epsilon=1 tau=3
33     29     39      13.4194      Ka=2 Kc=7 N=8 epsilon=1 tau=5
34     30     33      20.2037      Ka=3 Kc=4 N=7 epsilon=1 tau=1
35     31     33      24.6162      Ka=0 Kc=9 N=9 epsilon=1 tau=9
36     32     33      26.8337      Ka=4 Kc=3 N=7 epsilon=1 tau=1
37     33     33      17.3465      Ka=5 Kc=2 N=7 epsilon=1 tau=3
38     34     33      19.5679      Ka=3 Kc=6 N=8 epsilon=1 tau=3
39     35     33      22.3944      Ka=6 Kc=1 N=7 epsilon=1 tau=5
40     36     33      28.7 Kc=0 N=7 epsilon=1 tau=7
41     37     33      13.4194      Ka=1 Kc=8 N=9 epsilon=1 tau=7
42     38     33      20.2037      Ka=4 Kc=5 N=8 epsilon=1 tau=1
43     39     33      24.6162      Ka=1 Kc=10 N=10 epsilon=1 tau=9
44     40     33      31.083      Ka=5 Kc=4 N=8 epsilon=1 tau=1
45     41     39      24.6162      Ka=2 Kc=7 N=9 epsilon=1 tau=5
46     42     39      26.8337      Ka=6 Kc=3 N=8 epsilon=1 tau=3
47     43     39      31.083      Ka=2 Kc=9 N=10 epsilon=1 tau=7
48     44     33      17.3465      Ka=7 Kc=2 N=8 epsilon=1 tau=5
49     45     33      22.3944      Ka=0 Kc=11 N=11 epsilon=1 tau=11
50     46     33      28.5113      Ka=3 Kc=6 N=9 epsilon=1 tau=3
    
```

Collision rates

```

1 Rotational Excitation of ortho-cyclopropenyl by He (Chandra & al., 2000)
2
3 Number of temperature columns : 4
4
5      I      J      Temperature (K)....
6      30      60      90      120
7
8      2      1      8.032e-12      8.321e-12      8.281e-12      8.16e-12
9      3      1      2.091e-11      2.096e-11      2.091e-11      2.098e-11
10     3      2      1.609e-12      1.895e-12      2.102e-12      2.17e-12
11     4      1      1.251e-11      1.33e-11      1.454e-11      1.581e-11
12     4      2      8.336e-12      8.54e-12      8.632e-12      8.6e-12
13     4      3      1.329e-11      1.33e-11      1.341e-11      1.357e-11
14     5      1      2.067e-12      2.334e-12      2.485e-12      2.526e-12
15     5      2      2.55e-11      2.346e-11      2.287e-11      2.284e-11
16     5      3      8.323e-12      8.103e-12      7.968e-12      7.822e-12
17     5      4      2.784e-12      3.241e-12      3.485e-12      3.607e-12
18     6      1      4.456e-12      3.715e-12      3.559e-12      3.529e-12
19     6      2      1.497e-12      1.363e-12      1.257e-12      1.331e-12
20     6      3      1.348e-11      1.381e-11      1.477e-11      1.582e-11
21     6      4      2.135e-11      2.109e-11      2.097e-11      2.098e-11
22     6      5      6.256e-12      6.754e-12      6.977e-12      7.066e-12
23     7      1      7.275e-12      6.789e-12      7.051e-12      7.442e-12
24     7      2      5.075e-13      5.046e-13      5.221e-13      5.291e-13
25     7      3      1.23e-11      1.193e-11      1.189e-11      1.19e-11
26     7      4      5.586e-12      6.061e-12      6.513e-12      6.91e-12
27     7      5      1.763e-12      2.053e-12      2.257e-12      2.382e-12
28     7      6      1.572e-11      1.647e-11      1.68e-11      1.708e-11
29     8      1      1.858e-11      1.498e-11      1.399e-11      1.366e-11
30     8      2      2.586e-12      2.673e-12      2.715e-12      2.728e-12
31     8      3      7.54e-12      7.841e-12      8.159e-12      8.324e-12
32     8      4      1.614e-11      1.449e-11      1.4e-11      1.388e-11
33     8      5      9.92e-12      1.011e-11      1.027e-11      1.029e-11
34     8      6      4.762e-12      5.756e-12      6.291e-12      6.593e-12
35     8      7      8.483e-12      9.172e-12      9.5e-12      9.776e-12
36     9      1      3.956e-12      3.846e-12      3.935e-12      3.955e-12
37     9      2      1.534e-11      1.415e-11      1.46e-11      1.537e-11
38     9      3      4.222e-12      3.74e-12      3.731e-12      3.798e-12
39     9      4      6.05e-12      5.493e-12      5.381e-12      5.346e-12
40     9      5      1.79e-11      1.727e-11      1.715e-11      1.724e-11
41     9      6      2.746e-12      3.175e-12      3.526e-12      3.756e-12
42     9      7      9.252e-12      1.015e-11      1.049e-11      1.061e-11
43     9      8      2.024e-12      2.84e-12      3.246e-12      3.466e-12
44     10     1      1.417e-12      1.121e-12      1.052e-12      1.024e-12
45     10     2      1.466e-11      1.13e-11      1.041e-11      1.008e-11
46     10     3      3.25e-12      2.951e-12      2.934e-12      2.92e-12
47     10     4      2.139e-12      2.311e-12      2.457e-12      2.51e-12
48     10     5      2.012e-11      2.018e-11      2.134e-11      2.264e-11
49     10     6      7.822e-12      7.294e-12      7.128e-12      7.024e-12
50     10     7      3.14e-12      3.551e-12      3.793e-12      3.904e-12
    
```

Future

- Homogenisation of output for all molecular data
- Currently AMDML for Fusion Physics: NIST, IAEA, Oakridge ([see Y. Ralchenko's talk](#) at 15:30 + following Discussion Panel)
- More general approach to AMDML with inclusion [molecular physics](#)
 - [New Collaboration](#) with Paris Observatory
 - Link to IVOA for astrophysical application

Do not confuse AMDML and AMLDM !!! :-)

VO Collaborations

- LERMA: N. Moreau (PI for engineering), F. Boone (PI of the MAGIX project)
- LUTH: E. Roueff (DM), F. Le Petit (PI of PDR code in the VO)
- M. Elitzur (Kentucky Univ.): MOLPOP code
- ESAC-VO Team (spain): P. Osuna & coll. (IVOA collaboration for AMLDM, SLAP)
- CDMS: H. Mueller
- HITRAN: L. Rothman

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