

Plateforme e-science Pour la Physique Atomique et Moléculaire "Virtual Atomic & Molecular Data Center"

**M.L. Dubernet
VOParis Data Centre**



**Equipe VOParis-molecular: M.L. Dubernet, N. Moreau, E.
Roueff**

Motivation Générale

■ 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

VO: Interoperability of ressources 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, UMST, 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

Historique

- ❑ ***Turning Besançon Observatory on-line facilities into the VO - Galactic Model Simulation, Binary Star, Molecular Collisional and TNO data bases.*** B. Debray, M.L. Dubernet, A. Grosjean, E. Oblak, J.M. Petit, C. Reylé, A. Robin, Proceedings ADASS XII, 2002, Baltimore.
- ❑ **“ACI/ANR Masse de Données en Astrophysique” de F. Génova - 2003-2006**
- ❑ **Organisation Forum en 2004 par M.L. Dubernet à Meudon**
- ❑ **Définition UCDs en 2004, ML Dubernet & E Roueff**
- ❑ **Début Collaboration avec ESAC en 2004**
- ❑ **Début collaboration NIST/IAEA/ORNL en 2005**
- ❑ **Implémentations standards à partir de 2006 (N. Moreau)**

Make available laboratory data

- Scientific work 1
 - Collect data
 - Documentation of data on methods and references
- Scientific work 2 (UML, XML expertise)
 - Structure information
 - Common set of metadata
 - Data Model/XML Schema
- Software development of databases and access

Motivation for standardisation

- Allow transparent exchange of data

Avantages

- “Good” Standardisation obliges documentation
- No time wasted on format by scientist

Inconvenients

- Huge work ahead for some scientists (documentation, metadata)

Current Projects

voparis-molecular.obspm.fr

- Data Model on linelists (IVOA):
 - version 0.5: limited
 - version 0.6: more features (currently in discussion)
- Data Model & XML Schema for all data
 - collaboration NIST/ONRL/IAEA/Obs. Paris
 - Atoms, Molecules, “Solide”
 - Processus: radiative, autoionization, reactive
 - Documentation, References
- Implementations:
 - CDMS & BASECOL & H2 Data of Roueff & Abgrall

Basecol Database (basecol.obspm.fr)

Implementation: N. Moreau, G. Souesmes, B. Debray

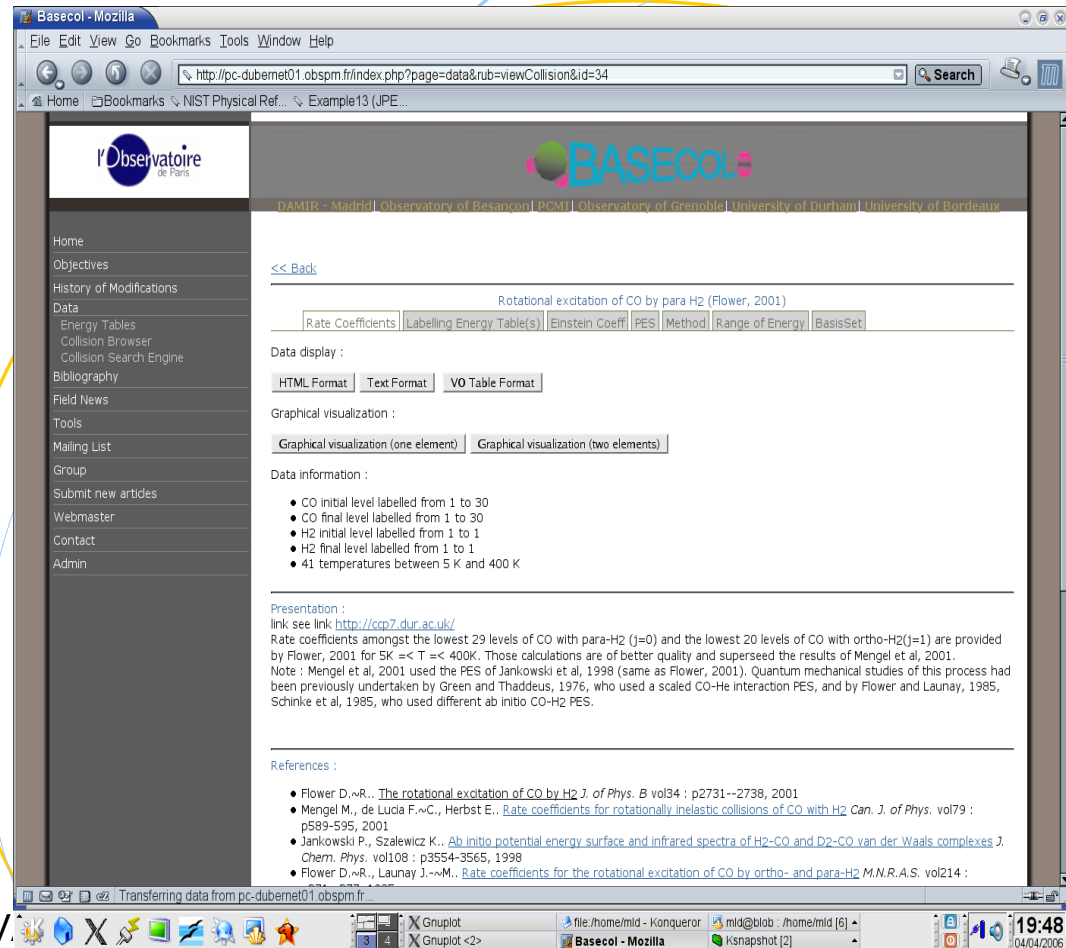
Design: M.L. Dubernet

FP6: "Molecular Universe" Collaboration
Corresponds to a Need for Community

Linked to CDMS and JPL

– Published (de)-excitation rate coefficients

- Rotational (fine, hyperfine), Ro-vib., Vib.
- Currently: 21 Target molecules; Perturbers : He, H, H₂
- 119 collisional systems
- Fully documented and referenced (630 ref.)
- Fitting coefficients, visualisation tools
- Energy levels, Einstein coefficients, QN
- Fully checked and evaluated



Basecol - Mozilla

File Edit View Go Bookmarks Tools Window Help

http://pc-dubernet01.obspm.fr/index.php?page=data&rub=viewCollision&id=34

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l'Observatoire de Paris

BASECOL

DAMIR - Madrid | Observatory of Besancon | PCMI | Observatory of Grenoble | University of Durham | University of Bordeaux

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Rotational excitation of CO by para H2 (Flower, 2001)

Rate Coefficients | Labelling Energy Table(s) | Einstein Coeff | PES | Method | Range of Energy | BasisSet

Data display :

HTML Format | Text Format | VO Table Format

Graphical visualization :

Graphical visualization (one element) | Graphical visualization (two elements)

Data information :

- 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
- 41 temperatures between 5 K and 400 K

Presentation :

link see link <http://ccp7.dur.ac.uk/>

Rate coefficients amongst the lowest 29 levels of CO with para-H2 (j=0) and the lowest 20 levels of CO with ortho-H2(j=1) are provided by Flower, 2001 for 5K ≤ T ≤ 400K. Those calculations are of better quality and supersede the results of Mengel et al, 2001. Note : Mengel et al, 2001 used the PES of Jankowski et al, 1998 (same as Flower, 2001). Quantum mechanical studies of this process had been previously undertaken by Green and Thaddeus, 1976, who used a scaled CO-He interaction PES, and by Flower and Launay, 1985, Schinke et al, 1985, who used different ab initio CO-H2 PES.

References :

- Flower D.~R.. The rotational excitation of CO by H2 J. of Phys. B vol34 : p2731--2738, 2001
- Mengel M., de Lucia F.~C., Herbst E., Rate coefficients for rotationally inelastic collisions of CO with H2 Can. J. of Phys. vol79 : p589-595, 2001
- Jankowski P., Szalewicz K.. Ab initio potential energy surface and infrared spectra of H2-CO and D2-CO van der Waals complexes J. Chem. Phys. vol108 : p3554-3565, 1998
- Flower D.~R., Launay J.~M.. Rate coefficients for the rotational excitation of CO by ortho- and para-H2 M.N.R.A.S. vol214 :

Transferring data from pc-dubernet01.obspm.fr

GNuplot

file:/home/mid - Konqueror

mid@blob : /home/mid [6]

Basecol - Mozilla

Ksnapshot [2]

19:48
04/04/2006

Basecol - Mozilla

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http://pc-dubernet01.obspm.fr/index.php?pag

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DAMIR - Madrid Observa

[<< Back to collision's details](#)

CO initial levels :

H2 initial levels :

CO final levels :

H2 final levels :

Temperatures :

Enter numbers (separated by ';') or/and an interval
 Example : 1;9-21;23

1 : CO
 2 : H2

	I1	F1	I2	F2	5	10	20	30	40	50	60	70	80
1	1	1	1	1	+3.55e-09	+2.72e-09	+2.02e-09	+1.9e-09	+1.94e-09	+2.02e-09	+2.13e-09	+2.19e-09	+2.28e-09
1	2	1	1	1	+2.53e-11	+4.85e-11	+6.45e-11	+7.48e-11	+7.98e-11	+8.4e-11	+8.86e-11	+9.32e-11	+9.62e-11
1	3	1	1	1	+3.82e-12	+2.17e-11	+5.54e-11	+7.73e-11	+9.4e-11	+1.04e-10	+1.14e-10	+1.18e-10	+1.26e-10
1	4	1	1	1	+5.84e-14	+1.63e-12	+8.89e-12	+1.65e-11	+2.39e-11	+3.06e-11	+3.74e-11	+4.29e-11	+4.9e-11
1	5	1	1	1	+2.67e-16	+7.21e-14	+1.3e-12	+3.64e-12	+6.34e-12	+9.09e-12	+1.18e-11	+1.42e-11	+1.67e-11
1	6	1	1	1	+3.99e-19	+1.83e-15	+1.4e-13	+6.74e-13	+1.62e-12	+2.96e-12	+4.62e-12	+6.58e-12	+8.8e-12
1	7	1	1	1	+1.72e-22	+2.15e-17	+8.39e-15	+6.87e-14	+2.14e-13	+4.51e-13	+7.71e-13	+1.16e-12	+1.61e-12
1	8	1	1	1	+1.44e-26	+1.21e-19	+4.11e-16	+7.31e-15	+3.58e-14	+1.04e-13	+2.29e-13	+4.26e-13	+7.06e-13
1	9	1	1	1	+2.58e-30	+1.18e-21	+2.9e-17	+9.49e-16	+5.96e-15	+1.94e-14	+4.53e-14	+8.69e-14	+1.47e-13
1	10	1	1	1	+3.39e-35	+2.54e-24	+7.97e-19	+6.22e-17	+6.31e-16	+2.88e-15	+8.75e-15	+2.09e-14	+4.26e-14
1	11	1	1	1	+6.6e-40	+1.17e-26	+5.18e-20	+9.39e-18	+1.39e-16	+7.52e-16	+2.47e-15	+6.1e-15	+1.25e-14
1	12	1	1	1	+1.4e-45	+9.01e-30	+8.99e-22	+4.63e-19	+1.16e-17	+8.78e-17	+3.69e-16	+1.11e-15	+2.7e-15
1	13	1	1	1	+0e+00	+1.19e-32	+3.65e-23	+5.49e-20	+2.28e-18	+2.28e-17	+1.12e-16	+3.7e-16	+9.45e-16

Mozilla

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http://pc-dubernet01.obspm.fr/match34_Einstein_CDM5_2006-02-14.txt

number of lines : 29

Initial level	Final level	Frequency	Einstein coefficient	Log(A)	Uncertainty
2	1	115271.2018	7.2034148e-8	-7.1425	0.0005
3	2	230538.0000	6.9103080e-7	-6.1605	0.0005
4	3	345795.9899	2.4965589e-6	-5.6027	0.0005
5	4	461040.7882	6.1263650e-6	-5.2128	0.0005
6	5	576267.9305	1.2212740e-5	-4.9132	0.0005
7	6	691473.0783	2.1374069e-5	-4.6701	0.0005
8	7	806651.8060	3.4222452e-5	-4.4657	0.0050
9	8	921799.7000	5.1339745e-5	-4.2895	0.0050
10	9	1036912.3930	7.3298304e-5	-4.1349	0.0050
11	10	1151985.4520	1.0063605e-4	-3.9972	0.0110
12	11	1267014.4860	1.3390036e-4	-3.8732	0.0050
13	12	1381995.1050	1.7353034e-4	-3.7606	0.0130
14	13	1496922.9090	2.2003922e-4	-3.6575	0.0120
15	14	1611793.5180	2.7390517e-4	-3.5624	0.0110
16	15	1726602.5057	3.3536041e-4	-3.4745	0.0024
17	16	1841345.5060	4.0500226e-4	-3.3925	0.0110
18	17	1956018.1390	4.8289379e-4	-3.3161	0.0110
19	18	2070615.9930	5.6952029e-4	-3.2445	0.0140
20	19	2185134.6800	6.6502238e-4	-3.1772	0.0130
21	20	2299569.8420	7.6955157e-4	-3.1138	0.0100
22	21	2413917.1130	8.831834e-4	-3.0539	0.0110
23	22	2528172.0600	1.0064098e-3	-2.9972	0.0110
24	23	2642330.3439	1.1389669e-3	-2.9435	0.0039
25	24	2756387.5840	1.2806260e-3	-2.8926	0.0170
26	25	2870339.4070	1.4318806e-3	-2.8441	0.0130
27	26	2984181.4550	1.5920820e-3	-2.7980	0.0140
28	27	3097909.3610	1.7614786e-3	-2.7541	0.0170
29	28	3211518.7506	1.9397870e-3	-2.7122	0.0047
30	29	3325005.2827	2.1265850e-3	-2.6723	0.0051

Taskbar and System Tray

























































System Clock: 19:52, 04/04/2006

System Tray: Gnuplot, file:/home/mlid - Konqueror, mld@blob : /home/mlid [6], Mozilla, Ksnapshot [5]

Automatic script to get data from Basecol: **BASECOL Tool for MOLPOP** (Implementation: N. Moreau, Design: M. Elitzur, ML Dubernet)

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 :

 c-C3H2-ortho_He_ rotation.aj	 c-C3H2-ortho_He_ rotation.kij	 c-C3H2-ortho_He_ rotation.le	 c-C3H2-para_He_ rotation.aj	 c-C3H2-para_He_ rotation.kij	 c-C3H2-para_He_ rotation.le	 CO_H2-ortho_ rotation.aj
 CO_H2-ortho_ rotation.kij	 CO_H2-ortho_ rotation.le	 CO_H2-para_ rotation.aj	 CO_H2-para_ rotation.kij	 CO_H2-para_ rotation.le	 CO_He_ rotation.aj	 CO_He_ rotation.kij
 CO_He_ rotation.le	 CO_H_ rotation.aj	 CO_H_ rotation.kij	 CO_H_ rotation.le	 CO_H_ rotation_2.aj	 CO_H_ rotation_2.kij	 CO_H_ rotation_2.le
 collision_tables.dat	 CS_H2-para_ rotation.aj	 CS_H2-para_ rotation.kij	 CS_H2-para_ rotation.le	 CS_H2-para_ rotation_2.aj	 CS_H2-para_ rotation_2.kij	 CS_H2-para_ rotation_2.le
 CS_He_ rotation.aj	 CS_He_ rotation.kij	 CS_He_ rotation.le	 H2CO-ortho_He_ rotation.aj	 H2CO-ortho_He_ rotation.kij	 H2CO-ortho_He_ rotation.le	 H2CO-para_He_ rotation.aj
 H2CO-para_He_ rotation.kij	 H2CO-para_He_ rotation.le	 H2O-ortho_H2_ortho_ rotation.aj	 H2O-ortho_H2_ortho_ rotation.kij	 H2O-ortho_H2_ortho_ rotation.le	 H2O-ortho_H2-para_ rotation.aj	 H2O-ortho_H2-para_ rotation.kij
 H2O-ortho_H2-para_ rotation.le	 H2O-ortho_He_ rotation.aj	 H2O-ortho_He_ rotation.kij	 H2O-ortho_He_ rotation.le	 H2O-para_H2-ortho_ rotation.aj	 H2O-para_H2-ortho_ rotation.kij	 H2O-para_H2-ortho_ rotation.le
 H2O-para_H2-para_ rotation.aj	 H2O-para_H2-para_ rotation.kij	 H2O-para_H2-para_ rotation.le	 H2O-para_He_ rotation.aj	 H2O-para_He_ rotation.kij	 H2O-para_He_ rotation.le	 HC3N_He_ rotation.aj

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

```

Energy table

1 Einstein coefficients A_{ij} for c-C3H2
2 Reference : JPL

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

1 Rotational Excitation of ortho-cyclopropendyle by He (Chandra & al., 2000)
2 Reference : JPL

3	4	N	g	Energy in cm ⁻¹	Level details...
4	5	1	9	1.6332	Ka=0 Kc=1 N=1 epsilon=1 tau=1
6	5	2	15	1.6332	Ka=1 Kc=0 N=1 epsilon=1 tau=1
7	3	1	15	2.2451	Ka=1 Kc=2 N=2 epsilon=1 tau=1
8	4	1	15	4.4798	Ka=2 Kc=1 N=2 epsilon=1 tau=1
9	5	1	15	4.4798	Ka=0 Kc=3 N=3 epsilon=1 tau=3
10	6	1	21	6.5296	Ka=1 Kc=2 N=3 epsilon=1 tau=1
11	7	1	21	8.3875	Ka=2 Kc=1 N=3 epsilon=1 tau=1
12	8	1	21	4.4798	Ka=1 Kc=4 N=4 epsilon=1 tau=3
13	9	1	21	11.155	Ka=3 Kc=0 N=3 epsilon=1 tau=3
14	10	1	27	8.3875	Ka=2 Kc=3 N=4 epsilon=1 tau=1
15	11	1	21	6.3153	Ka=0 Kc=5 N=5 epsilon=1 tau=5
16	12	1	21	8.3875	Ka=3 Kc=2 N=4 epsilon=1 tau=1
17	13	1	21	12.6262	Ka=4 Kc=1 N=4 epsilon=1 tau=3
18	14	1	27	11.155	Ka=1 Kc=4 N=5 epsilon=1 tau=3
19	15	1	27	13.4194	Ka=1 Kc=6 N=6 epsilon=1 tau=5
20	16	1	27	13.5296	Ka=2 Kc=3 N=5 epsilon=1 tau=1
21	17	1	33	13.4194	Ka=3 Kc=2 N=5 epsilon=1 tau=1
22	18	1	27	8.3875	Ka=4 Kc=1 N=5 epsilon=1 tau=3
23	19	1	27	12.6262	Ka=2 Kc=5 N=6 epsilon=1 tau=3
24	20	1	27	17.3465	Ka=5 Kc=0 N=5 epsilon=1 tau=5
25	21	1	27	11.155	Ka=0 Kc=7 N=7 epsilon=1 tau=7
26	22	1	27	13.4194	Ka=3 Kc=4 N=6 epsilon=1 tau=1
27	23	1	27	13.5296	Ka=4 Kc=3 N=6 epsilon=1 tau=1
28	24	1	27	20.2037	Ka=1 Kc=6 N=7 epsilon=1 tau=5
29	25	1	33	17.3465	Ka=1 Kc=8 N=8 epsilon=1 tau=7
30	26	1	33	19.5679	Ka=5 Kc=2 N=6 epsilon=1 tau=3
31	27	1	33	22.3944	Ka=6 Kc=1 N=6 epsilon=1 tau=3
32	28	1	39	19.5679	Ka=2 Kc=5 N=7 epsilon=1 tau=3
33	29	1	33	13.4194	Ka=2 Kc=7 N=8 epsilon=1 tau=5
34	30	1	33	20.2037	Ka=3 Kc=4 N=7 epsilon=1 tau=1
35	31	1	33	24.6162	Ka=0 Kc=9 N=9 epsilon=1 tau=9
36	32	1	33	26.8337	Ka=4 Kc=3 N=7 epsilon=1 tau=1
37	33	1	33	17.3465	Ka=5 Kc=2 N=7 epsilon=1 tau=3
38	34	1	33	19.5679	Ka=3 Kc=6 N=8 epsilon=1 tau=3
39	35	1	33	22.3944	Ka=6 Kc=1 N=7 epsilon=1 tau=5
40	36	1	33	28.5113	Ka=7 Kc=0 N=7 epsilon=1 tau=7
41	37	1	33	13.4194	Ka=1 Kc=8 N=9 epsilon=1 tau=1
42	38	1	33	20.2037	Ka=4 Kc=5 N=8 epsilon=1 tau=1
43	39	1	33	24.6162	Ka=1 Kc=10 N=10 epsilon=1 tau=9
44	40	1	33	31.093	Ka=5 Kc=4 N=9 epsilon=1 tau=1
45	41	1	39	24.6162	Ka=2 Kc=7 N=9 epsilon=1 tau=5
46	42	1	39	26.8337	Ka=6 Kc=3 N=8 epsilon=1 tau=3
47	43	1	39	31.093	Ka=2 Kc=9 N=10 epsilon=1 tau=7
48	44	1	33	17.3465	Ka=7 Kc=2 N=8 epsilon=1 tau=5
49	45	1	33	22.3944	Ka=0 Kc=11 N=11 epsilon=1 tau=11
50	46	1	33	28.5113	Ka=3 Kc=6 N=9 epsilon=1 tau=3

Collision rates

1 Rotational Excitation of ortho-cyclopropendyle by He (Chandra & al., 2000)
2 Number of temperature columns : 4

3	4	I	J	Temperature (K)...	30	60	90	120
4	2	1	1	8.032e-12	8.321e-12	8.281e-12	8.16e-12	8.16e-12
6	3	1	1	2.091e-11	2.096e-11	2.091e-11	2.098e-11	2.098e-11
7	4	2	1	1.609e-12	1.895e-12	2.102e-12	2.17e-12	2.17e-12
8	4	1	1	1.251e-11	1.33e-11	1.454e-11	1.581e-11	1.581e-11
9	5	3	1	8.336e-12	8.54e-12	8.632e-12	8.6e-12	8.6e-12
10	6	2	1	1.329e-11	1.33e-11	1.341e-11	1.357e-11	1.357e-11
11	7	1	1	2.067e-12	2.334e-12	2.485e-12	2.526e-12	2.526e-12
12	8	1	1	2.55e-11	2.346e-11	2.287e-11	2.284e-11	2.284e-11
13	9	1	1	8.323e-12	8.103e-12	7.968e-12	7.822e-12	7.822e-12
14	10	1	1	2.784e-12	3.241e-12	3.485e-12	3.607e-12	3.607e-12
15	11	1	1	4.456e-12	3.715e-12	3.559e-12	3.529e-12	3.529e-12
16	12	1	1	1.497e-12	1.363e-12	1.357e-12	1.331e-12	1.331e-12
17	13	1	1	1.348e-11	1.381e-11	1.477e-11	1.582e-11	1.582e-11
18	14	1	1	2.135e-11	2.109e-11	2.097e-11	2.098e-11	2.098e-11
19	15	1	1	6.256e-12	6.754e-12	6.977e-12	7.066e-12	7.066e-12
20	16	1	1	7.275e-12	6.789e-12	7.051e-12	7.442e-12	7.442e-12
21	17	1	1	5.075e-13	5.046e-13	5.221e-13	5.291e-13	5.291e-13
22	18	1	1	1.23e-11	1.193e-11	1.189e-11	1.19e-11	1.19e-11
23	19	1	1	5.586e-12	6.061e-12	6.513e-12	6.91e-12	6.91e-12
24	20	1	1	1.763e-12	2.053e-12	2.257e-12	2.382e-12	2.382e-12
25	21	1	1	1.572e-11	1.647e-11	1.68e-11	1.708e-11	1.708e-11
26	22	1	1	1.858e-11	1.498e-11	1.399e-11	1.366e-11	1.366e-11
27	23	1	1	2.586e-12	2.673e-12	2.715e-12	2.728e-12	2.728e-12
28	24	1	1	7.54e-12	7.841e-12	8.159e-12	8.324e-12	8.324e-12
29	25	1	1	1.614e-11	1.449e-11	1.4e-11	1.388e-11	1.388e-11
30	26	1	1	9.92e-12	1.011e-11	1.027e-11	1.029e-11	1.029e-11
31	27	1	1	4.762e-12	5.756e-12	6.291e-12	6.593e-12	6.593e-12
32	28	1	1	8.483e-12	9.172e-12	9.5e-12	9.776e-12	9.776e-12
33	29	1	1	3.956e-12	3.846e-12	3.935e-12	3.955e-12	3.955e-12
34	30	1	1	1.534e-11	1.415e-11	1.46e-11	1.537e-11	1.537e-11
35	31	1	1	4.222e-12	3.74e-12	3.731e-12	3.798e-12	3.798e-12
36	32	1	1	6.05e-12	5.493e-12	5.381e-12	5.346e-12	5.346e-12
37	33	1	1	1.79e-11	1.727e-11	1.715e-11	1.724e-11	1.724e-11
38	34	1	1	2.746e-12	3.175e-12	3.262e-12	3.756e-12	3.756e-12
39	35	1	1	9.252e-12	1.015e-11	1.049e-11	1.061e-11	1.061e-11
40	36	1	1	2.024e-12	2.84e-12	3.246e-12	3.466e-12	3.466e-12
41	37	1	1	1.417e-12	1.121e-12	1.052e-12	1.024e-12	1.024e-12
42	38	1	1	1.466e-11	1.13e-11	1.041e-11	1.008e-11	1.008e-11
43	39	1	1	3.25e-12	2.951e-12	2.934e-12	2.92e-12	2.92e-12
44	40	1	1	2.139e-12	2.311e-12	2.457e-12	2.51e-12	2.51e-12
45	41	1	1	2.012e-11	2.018e-11	2.134e-11	2.264e-11	2.264e-11
46	42	1	1	7.822e-12	7.294e-12	7.128e-12	7.024e-12	7.024e-12
47	43	1	1	3.14e-12	3.551e-12	3.793e-12	3.904e-12	3.904e-12

Automatic Access to CDMS data

(N. Moreau & ML Dubernet)

Request into CDMS database

Wavelength interval (meters)

Frequency interval (Mhz)

Element name

Element stoichiometry

Element symmetry

Output format

<input type="text"/>	(format : min value1/max value1 ,min value2/max value2, ...)
<input type="text"/>	(format : min value1/max value1 ,min value2/max value2, ...)
<input type="text"/>	(format : element1 ,element2,...)
<input type="text"/>	(format : element1 ,element2,...)
<input type="text" value="All symmetries"/>	
<input type="text" value="HTML"/>	

[parameters description](#)

Service sur les données de CDMS
Récupération des données
Traitement scientifique des données
Inclusion dans base MySql
Couche VO sur la base: Service



- CDMS**
- What's New
- Catalog
- General Entries
- Search
- partition functions
- 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_{μ^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	

Automatic Access to CDMS data

VOClient to access services (N. Moreau & M.L. Dubernet)

The screenshot shows the VOClient application window with a configuration dialog box open. The dialog box has two sections: 'General parameters' and 'Services configuration'. The 'General parameters' section includes three checkboxes: 'Add header in text file', 'Load default configuration file at startup', and 'Default configuration file'. The 'Services configuration' section contains a table with the following data:

Name	Type	URL	Reachable
basecol	SLAP	http://linelists.obspm.fr/transitions.php?base...	yes

At the bottom of the dialog box, there are four buttons: 'Add service', 'Remove service', 'Test activity', and 'OK'. The background application window shows a menu bar with 'File', 'Columns', 'Lines', 'Spectro', 'Interoperability', and 'Help'. The status bar at the bottom of the application window displays the user 'dubernet@PC-MLD', a mail icon with '[INBOX (915 total, 91 non lu...)', and several open files including 'DIJON_08 - Navigateur de fic...', 'DIJON_08.ppt - OpenOffice.o...', and 'VOClient'.

Parameters

List of services: **basecol-SLAP**

wavelength (meter)	
frequency (Mhz)	25000/40000
chemical_element	
symmetry	
stoichiometry	

Data

wavelength (meter)	frequency (Mhz)	intensity (nm2MHz)	title	chemicaleleme
0.0105916	28304.63	-5.8038	H2C34S; symmetry: ortho; dat...	H2C34S
0.0104103	28797.5987	-6.7379	H2C34S; symmetry: para; date...	H2C34S
0.00887858	33765.8	-5.472	H2C34S; symmetry: para; date...	H2C34S
0.00878461	34127.0188	-6.665	H2C34S; symmetry: para; date...	H2C34S
0.00823877	36388.01	-5.6591	H2C34S; symmetry: ortho; dat...	H2C34S
0.0110044	27242.9101	-4.3387	HC13CCN, v7 = 1; symmetry: ...	HC13CCN, v7 = 1
0.0109885	27282.3636	-4.3375	HC13CCN, v7 = 1; symmetry: ...	HC13CCN, v7 = 1
0.00825333	36323.8178	-3.943	HC13CCN, v7 = 1; symmetry: ...	HC13CCN, v7 = 1
0.0082414	36376.4206	-3.9417	HC13CCN, v7 = 1; symmetry: ...	HC13CCN, v7 = 1
0.0109703	27327.7285	-6.1779	HC3N, (1,0,0,1) -v4-v7; symm...	HC3N, (1,0,0,1) -v4
0.0109539	27368.4733	-6.1766	HC3N, (1,0,0,1) -v4-v7; symm...	HC3N, (1,0,0,1) -v4
0.00822772	36436.8982	-5.7822	HC3N, (1,0,0,1) -v4-v7; symm...	HC3N, (1,0,0,1) -v4
0.00821547	36491.22	-5.7809	HC3N, (1,0,0,1) -v4-v7; symm...	HC3N, (1,0,0,1) -v4
0.00970731	30883.1632	-4.9706	MgF; symmetry: none; date of i...	MgF
0.00967454	30987.7619	-4.5021	MgF; symmetry: none; date of i...	MgF
0.00966956	31003.7206	-4.5019	MgF; symmetry: none; date of i...	MgF
0.00966671	31012.887	-4.2685	MgF; symmetry: none; date of i...	MgF
0.0113212	26480.5842	-5.3716	C4D; symmetry: none; date of i...	C4D
0.0113059	26516.5732	-5.5253	C4D; symmetry: none; date of i...	C4D
0.0112676	26606.5498	-6.6685	C4D; symmetry: none; date of i...	C4D
0.00848949	35313.3648	-5.011	C4D; symmetry: none; date of i...	C4D
0.00848085	35349.3523	-5.1228	C4D; symmetry: none; date of i...	C4D
0.00845073	35475.3178	-6.5511	C4D; symmetry: none; date of i...	C4D
	37044.7385	-4.316	CaC; symmetry: none; date of i...	CaC
	25058.4483	-8.0923	HDCO; symmetry: none; date o...	HDCO
	25421.539	-7.9599	HDCO; symmetry: none; date o...	HDCO
	25761.8555	-7.096	HDCO; symmetry: none; date o...	HDCO
	26149.9297	-5.1434	HDCO; symmetry: none; date o...	HDCO
	26863.968	-9.5941	HDCO; symmetry: none; date o...	HDCO
	27593.3941	-7.1293	HDCO; symmetry: none; date o...	HDCO
	28088.9996	-7.4436	HDCO; symmetry: none; date o...	HDCO
	28143.8175	7.1842	HDCO; symmetry: none; date o...	HDCO
	29225.7457			
	29867.02			
	30678.8058			
	32072.2			
	33374.85			

Title	Displayed
wavelength	<input checked="" type="checkbox"/>
frequency	<input checked="" type="checkbox"/>
intensity	<input checked="" type="checkbox"/>
title	<input checked="" type="checkbox"/>
chemicalelement_name	<input checked="" type="checkbox"/>
chemicalelement_symmetry	<input checked="" type="checkbox"/>
initial_quantum_numbers	<input checked="" type="checkbox"/>
final_quantum_numbers	<input checked="" type="checkbox"/>
initial_level_energy	<input checked="" type="checkbox"/>
final_level_energy	<input checked="" type="checkbox"/>
einstein_coefficient	<input checked="" type="checkbox"/>
log10_einstein_coefficient	<input checked="" type="checkbox"/>
initial_statistical_weight	<input checked="" type="checkbox"/>
final_statistical_weight	<input checked="" type="checkbox"/>
quantum_number_tag	<input checked="" type="checkbox"/>
id_chemical_element	<input checked="" type="checkbox"/>
data_source	<input checked="" type="checkbox"/>

Deselect all **Validate**

Title	Keep value
H2C34S; symmetry: ortho; date of import: 2007...	<input checked="" type="checkbox"/>
H2C34S; symmetry: para; date of import: 2007...	<input checked="" type="checkbox"/>
HC13CCN, v7 = 1; symmetry: none; date of imp...	<input checked="" type="checkbox"/>
HC3N, (1,0,0,1) -v4-v7; symmetry: none; date o...	<input checked="" type="checkbox"/>
MgF; symmetry: none; date of import: 2007-12...	<input checked="" type="checkbox"/>
C4D; symmetry: none; date of import: 2007-12...	<input checked="" type="checkbox"/>
CaC; symmetry: none; date of import: 2007-12...	<input checked="" type="checkbox"/>
HDCO; symmetry: none; date of import: 2007-1...	<input checked="" type="checkbox"/>
NaF; symmetry: none; date of import: 2007-12-...	<input checked="" type="checkbox"/>
I-C13CC2H2; symmetry: ortho; date of import: ...	<input checked="" type="checkbox"/>
I-C13CC2H2; symmetry: para; date of import: 2...	<input checked="" type="checkbox"/>
C13CCCH; symmetry: none; date of import: 200...	<input checked="" type="checkbox"/>

Deselect all **Validate**

- 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:
 - chemicalelement_name, chemicalelement_symmetry
 - final_level_energy, einstein_coefficient, g_up
 - quantum_number_tag.id_chemical_element,
 - data_source, creation_date
 - Link to quantum numbers (URL)
 - Link to partition function values

```

- <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.uri" datatype="char" arraysize="*/>
    <FIELD name="partition_function_link" ucd="meta.ref.uri" datatype="char" arraysize="*/>
  - <DATA>
    + <TABLEDATA></TABLEDATA>
    </DATA>
  </TABLE>
</RESOURCE>
</VOTABLE>

```

Automatic Access to H2 Data of Roueff & Abgrall

(N. Moreau & E. Roueff, H. Abgrall)

Request into Molat database

Wavelength interval	<input type="text"/>	Angstrom	(format : min value1/max value1,min value2/max value2, ...)
Wavenumber interval (cm-1)	<input type="text"/>		(format : min value1/max value1,min value2/max value2, ...)
Lower energy (cm-1)	<input type="text"/>		(format : min value1/max value1,min value2/max value2, ...)
Oscillator strength	<input type="text"/>		(format : min value1/max value1,min value2/max value2, ...)
Element name	<input type="text"/>		(format : element1,element2,...)
Output format	HTML		

Submit

[parameters description](#)

Service identique dans fonctionnement/outils que pour CDMS
Récupération des données sur le site MOLAT
Inclusion dans base MySql
Couche VO sur la base: Service

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

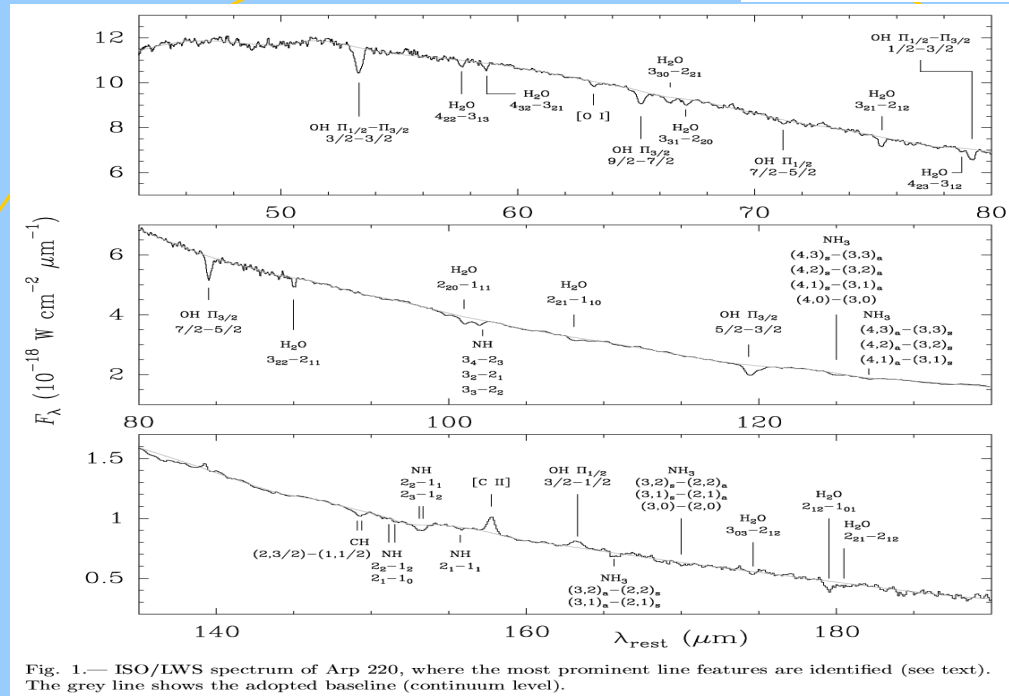
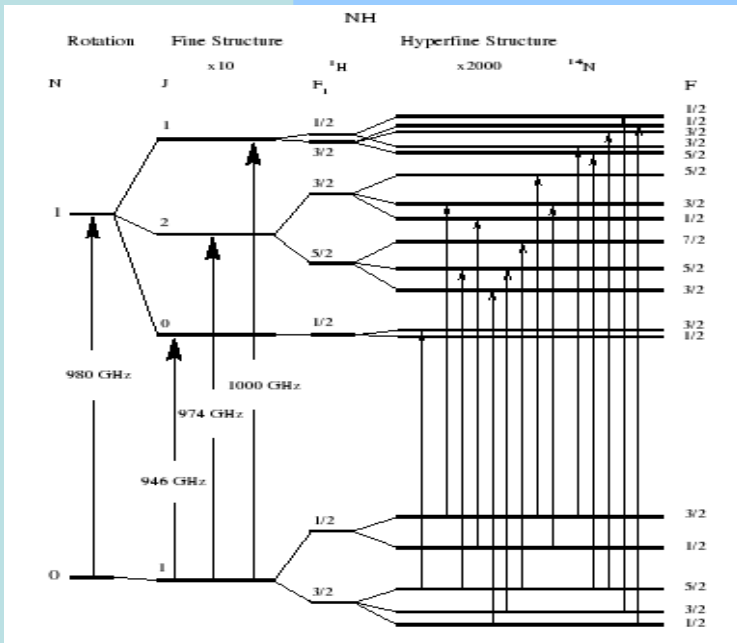
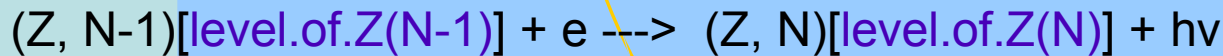
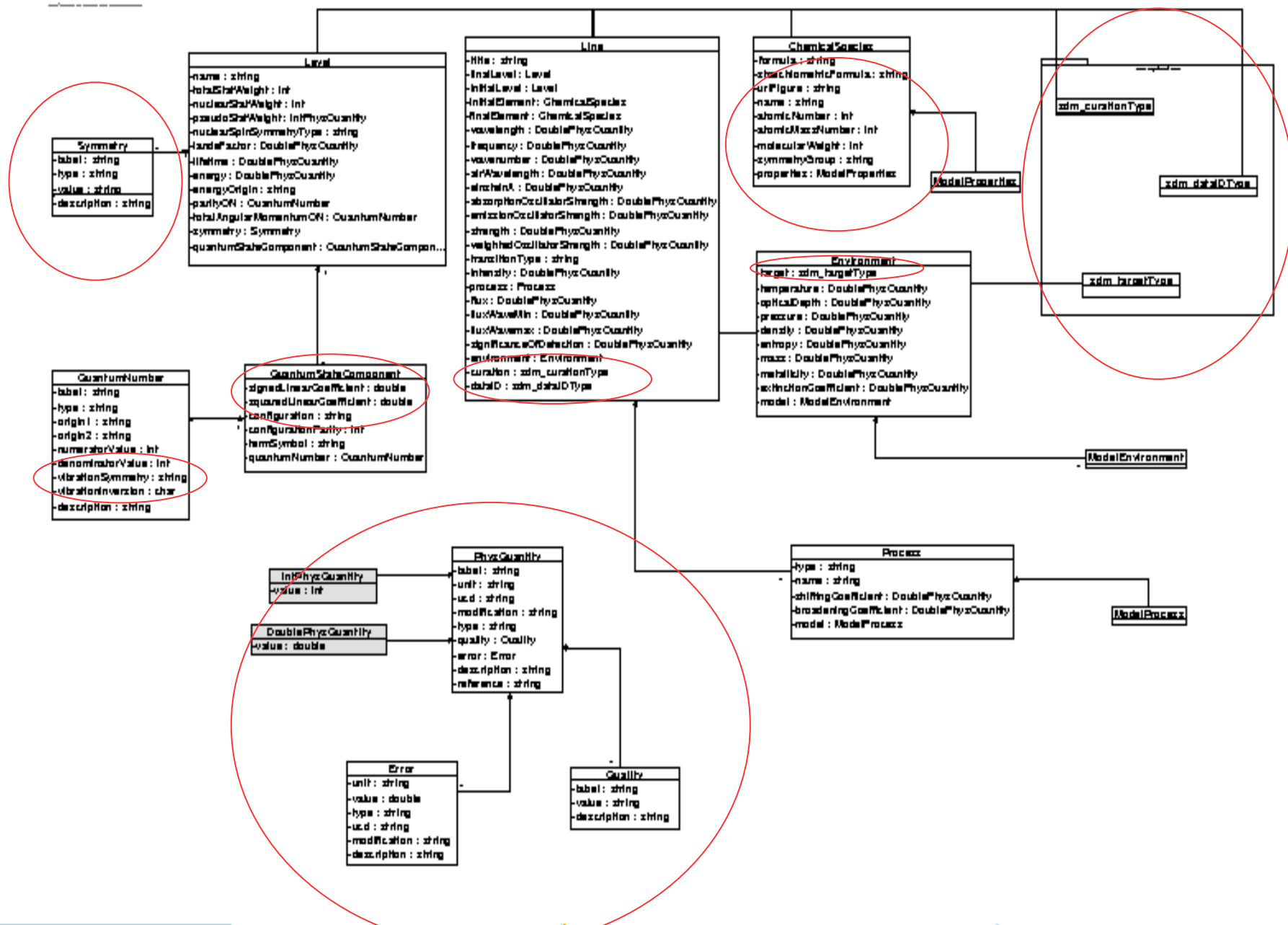


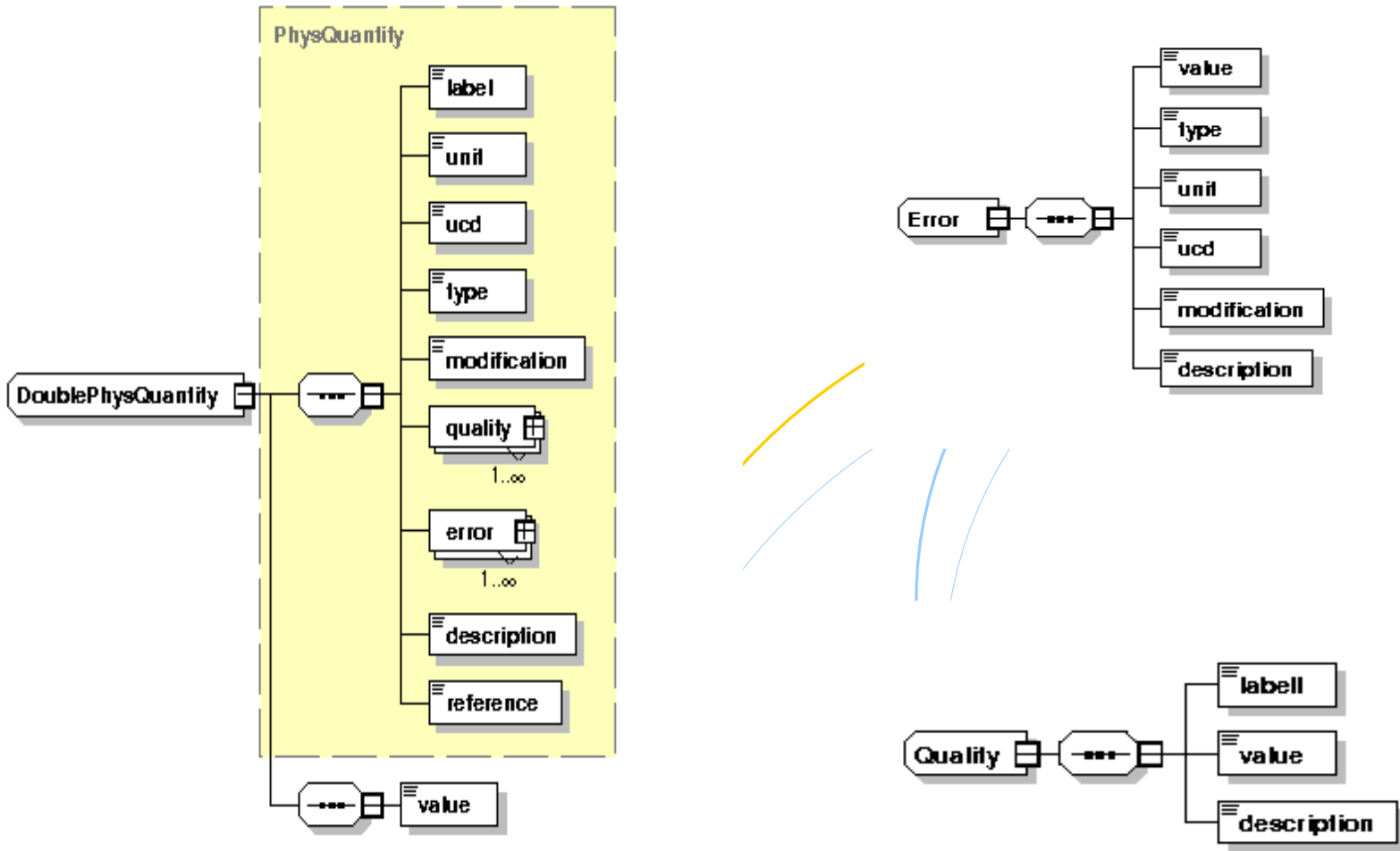
Fig. 1.— ISO/LWS spectrum of Arp 220, where the most prominent line features are identified (see text). The grey line shows the adopted baseline (continuum level).

Radiative recombinaison



- Data Model on linelists (IVOA):
 - version 0.5: limited (*Ed. P. Osuna & M. Guanazzi*)
 - version 0.6: more features (currently in discussion) –
- Version 0.6 (*Ed. ML Dubernet & E. Roueff*)
 - DataID, Curation --> link to IVOA Spectral DM
 - Target --> link to IVOA Spectral DM
 - PhysQuantity
 - Documentation, Error, Quality
 - ChemicalSpecies, Symmetry, etc.. --> Physics



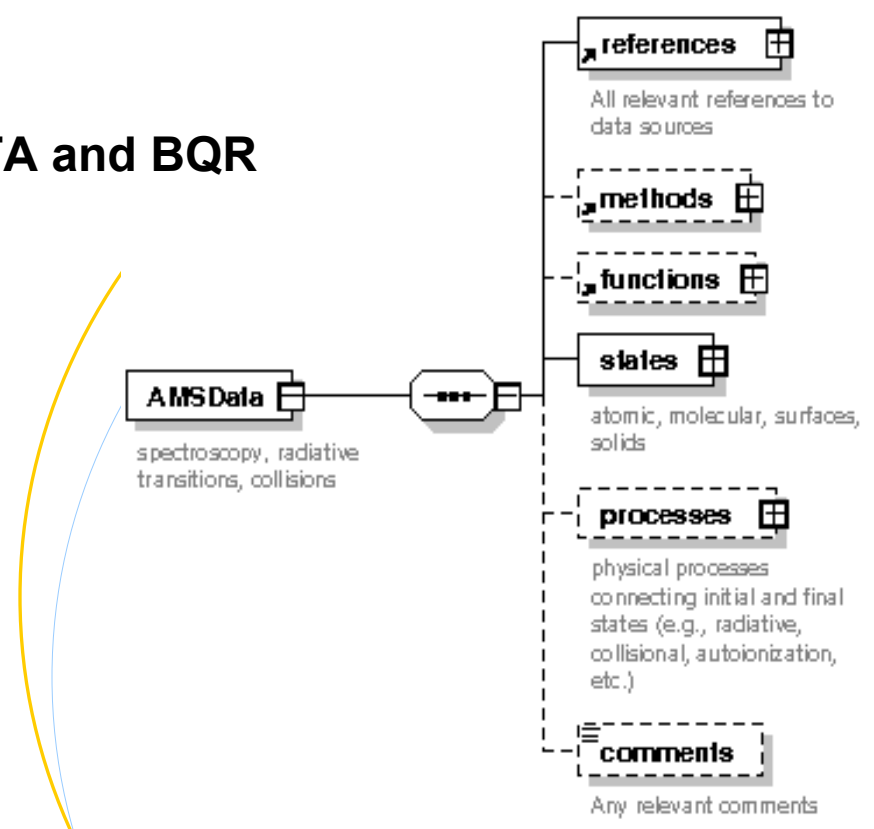


XML schema for Atomic, Molecular and Particule-Surface Interaction

NIST/ORNL/IAEA/Paris Observatory

2 à 3 meetings par an: Vienne/Paris et Conf: Washington, Beijing

Paris Observatory:
 ML Dubernet & E Roueff
 2 meetings à paris: ICAMDATA and BQR



XML schema for Atomic, Molecular and Particle Surface Interaction Data: Description of Molecular States

Version 0.1

Draft Document 01 October 2007

This version-01 October 2007

Latest version:

Previous versions:

Editors:

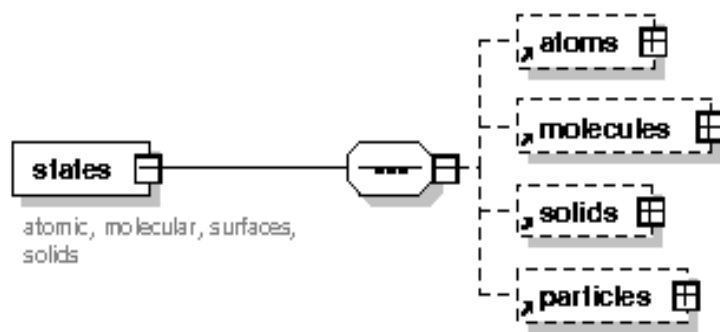
M.L. Dubernet

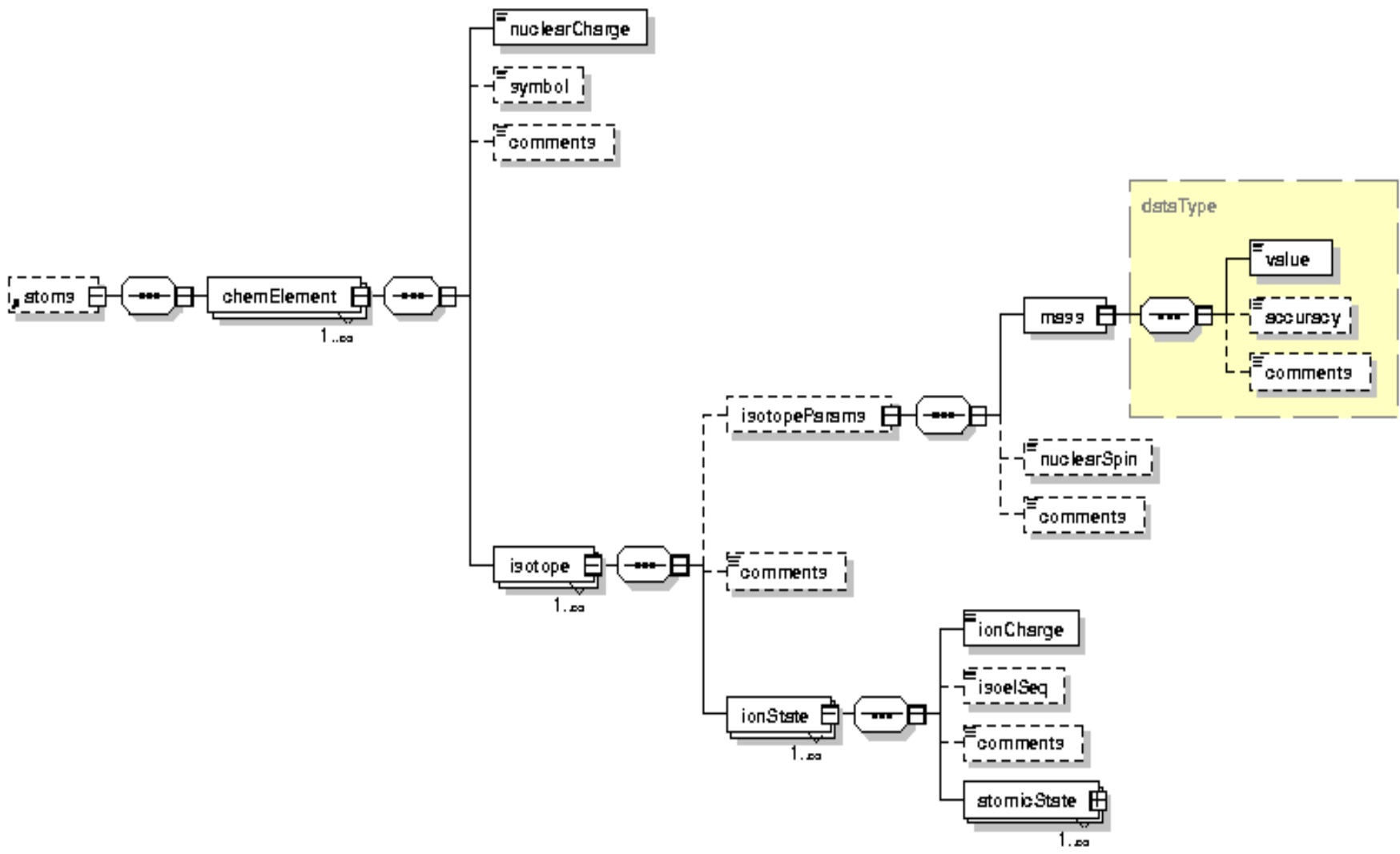
Contributors:

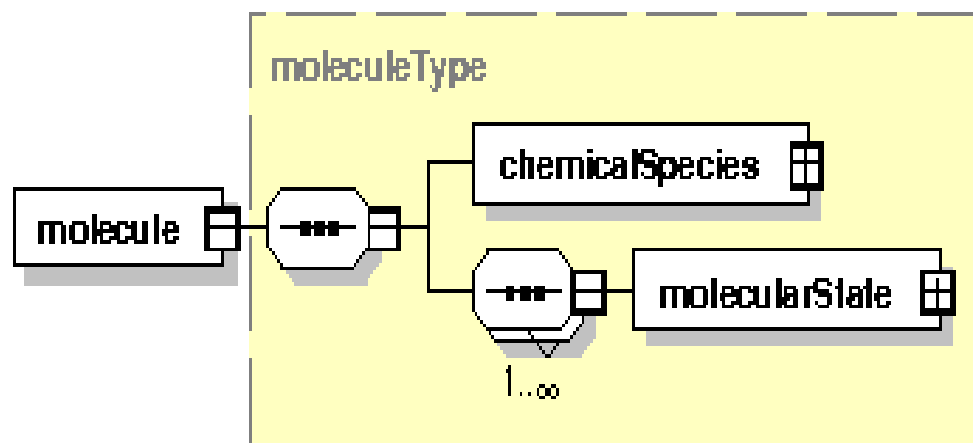
Marie-Lise Dubernet, Evelyne Roueff

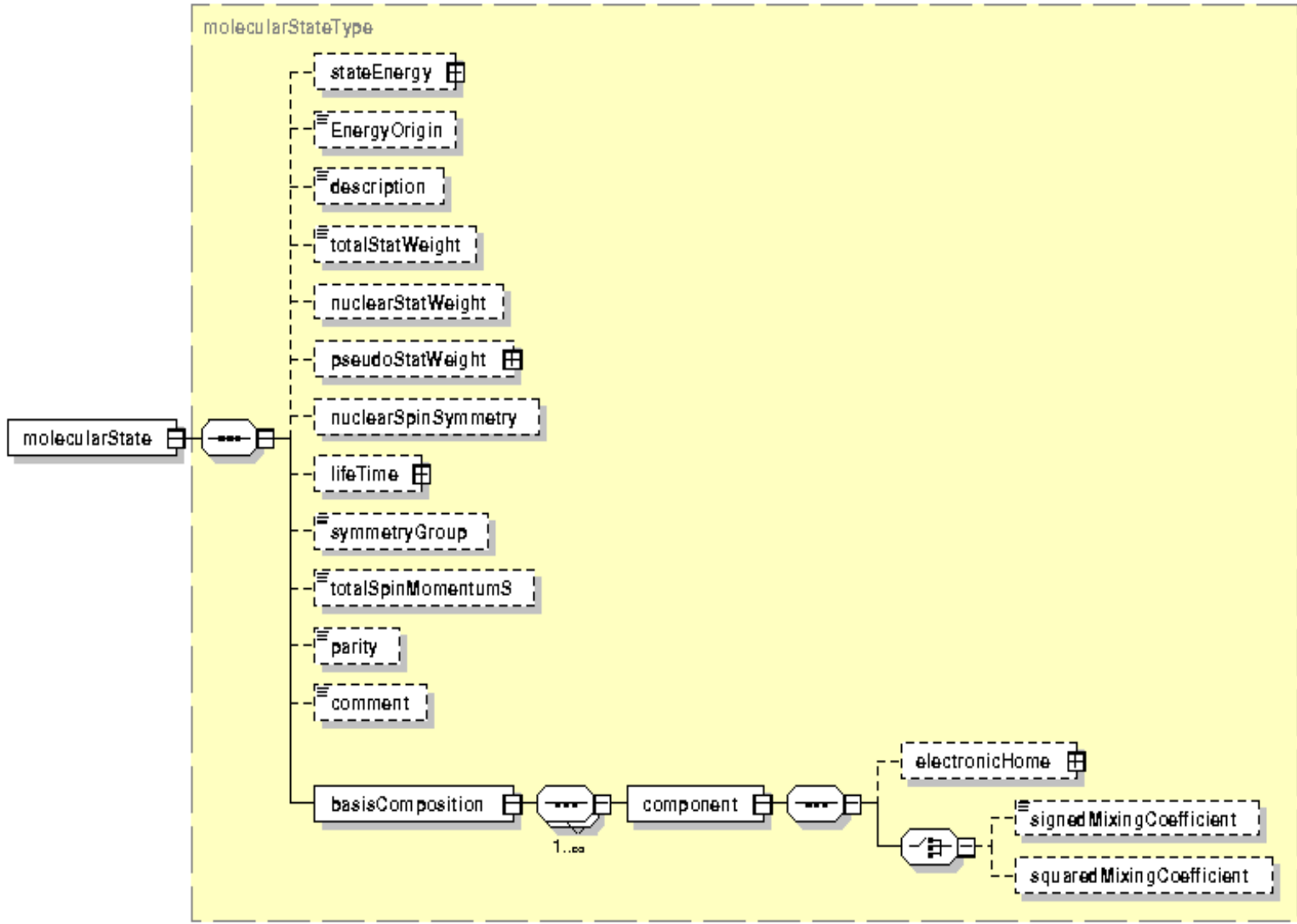
Abstract

This document presents a proposal for a XML schema to describe Molecular States. It is part of a wider XML schema aimed at describing Atomic, Molecular and Particle Surface Interaction Data in distributed databases around the world. This general XML schema is a collaborative project between NIST, Oackridge University, IAEA and Paris Observatory.









3.4.5 `MolecularStateType.totalStatWeight`

Statistical weight associated to the level including all degeneracies (including nuclear spins).

3.4.6 `MolecularStateType.nuclearStatWeight`

The same as "totalStatWeight" for nuclear spin states only.

3.4.7 `MolecularStateType.pseudoStatWeight`

Statistical weight associated to the level including some degeneracies, but not all. This "pseudoStatWeight" must be **absolutely** documented. It does not include all degeneracies and is used in fractions where the common factor "totalStatWeight" has been removed. As an example, CDMS database provides such "pseudoStatWeight".

3.4.8 `MolecularStateType.nuclearSpinSymmetryType`

A string indicating the type of nuclear spin symmetry. Possible values can be "para", "ortho", "meta", "A", "E". This element is a comfort element very often used to classify levels.

3.4.9 `MolecularStateType.lifetime`

Intrinsic lifetime of a level due to its total radiative decay. When only discrete radiative decay is involved, it is given by

$$\tau_i = \frac{1}{\sum_k A_{ik}} \quad (3.1)$$

(see object "DataType")

3.4.10 `MolecularStateType.conformation`

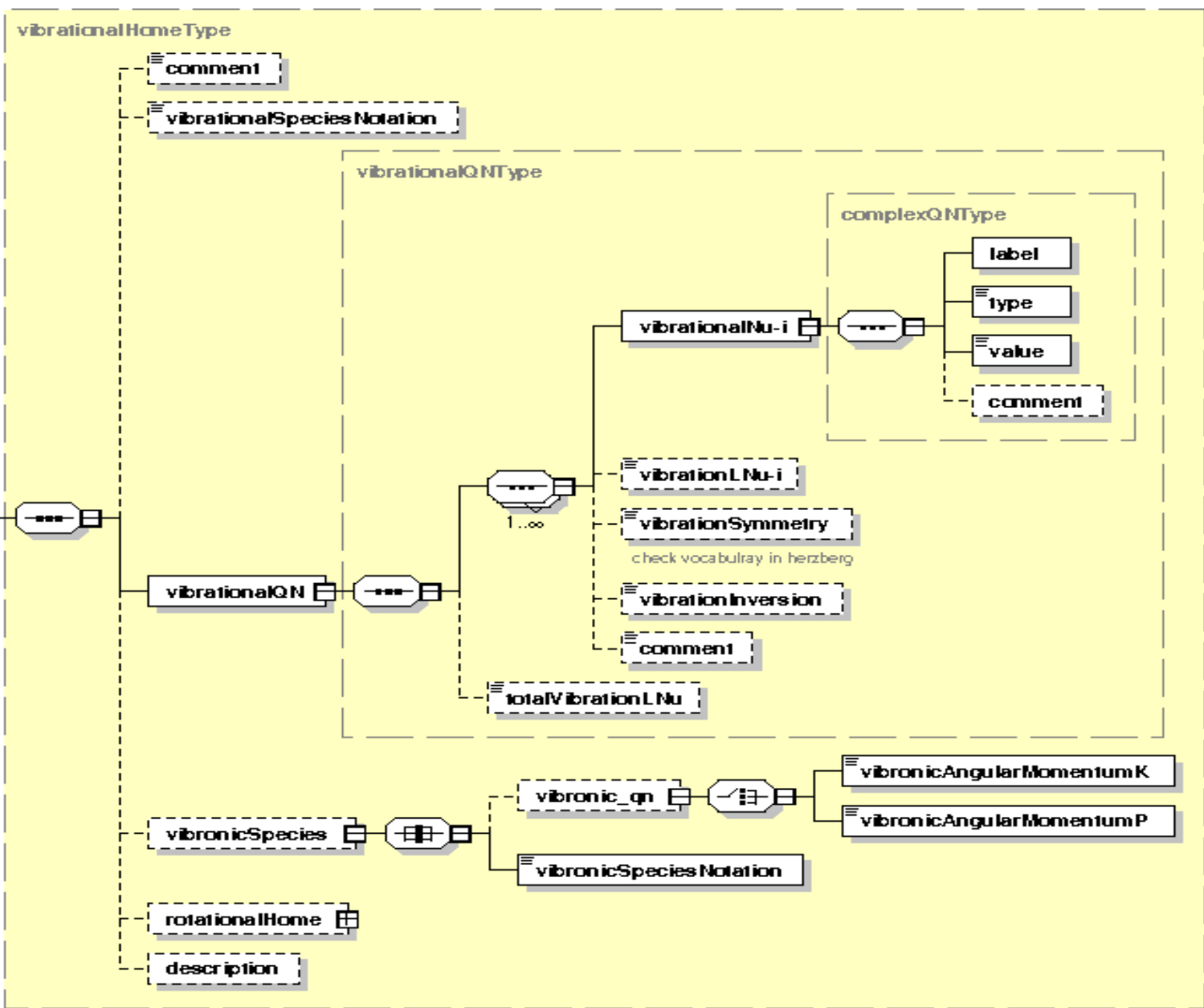
a string giving the conformation, such as *cis*, *trans*, etc..

3.4.11 `MolecularStateType.symmetryGroup`

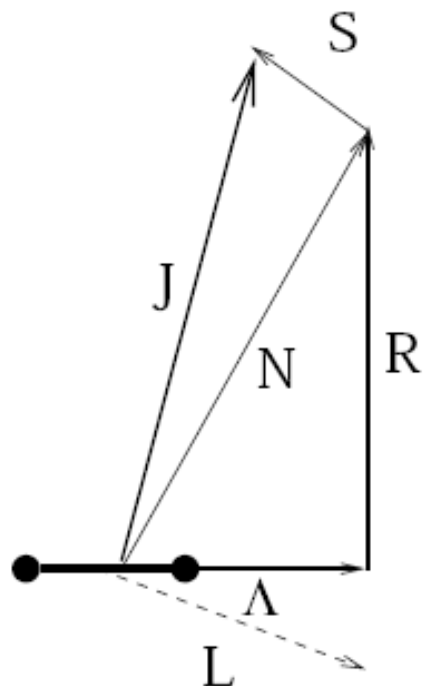
It is the Molecular Point Group. A description can be found in "Notations and Conventions in Molecular Spectroscopy: Part 2. Symmetry notation", ?).

3.4.12 `MolecularStateType.parity`

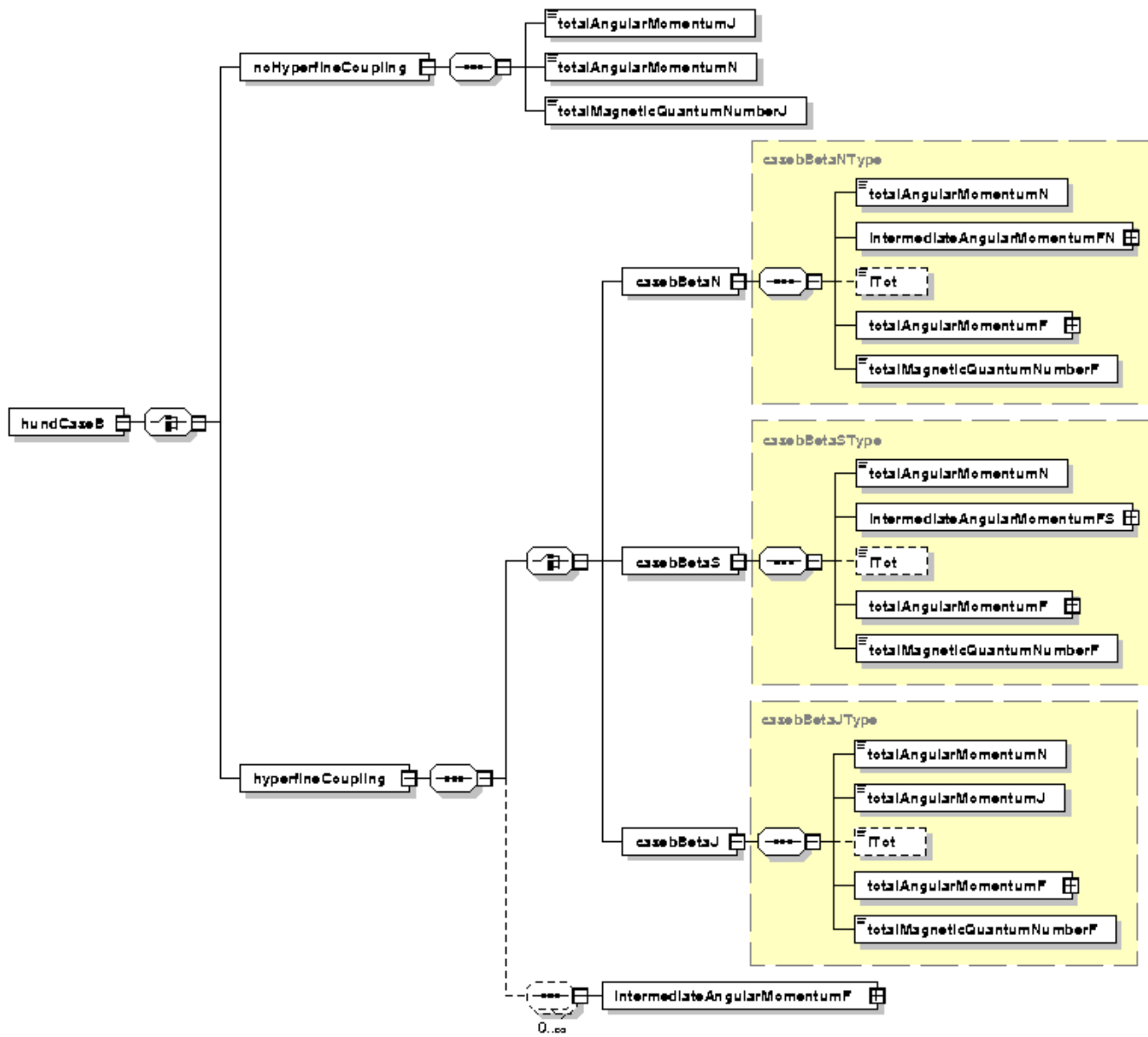
"MolecularStateType.parity" gives the total parity of the level (see Appendix B). It is of type "angularMomentumType"



Hund's case (b)



Symbol in Diagram	Type in DM
Λ	<code>totalMolecularProjectionL</code>
R	<code>rotationR</code>
N	<code>totalAngularMomentumN</code>
S	<code>totalSpinMomentumS</code>
J	<code>totalAngularMomentumJ</code>
L (not defined)	<code>totalElectronicOrbitalMomentumL</code>



Conclusion

- Huge scientific work with scientists having some XML, UML expertise and ready to spend time on the subject
- **XML schema for Atomic, Molecular and Particule-Surface Interaction (NIST/ORNL/IAEA/Paris Observatory)**
- Implementation spring 2008 on NIST/IAEA/BASECOL
- Version 1.0 June 2008
- **Linelists DataModel (Paris Observatory/ESAC)**
- Version 0.5 already implemented on CDMS **with extensions**
- Version 0.6 to be discussed

Groupe de Travail National

- **Fédérer et Organiser la Communauté Française sur**
 - Standards et Outils
 - Soutien financier ASOV
 - Soutien "moral" GDR Spectroscopie
 - Année Prochaine: PN INSU: LEFE/Astro
- **1ere Réunion en Juillet 2008**
- **Inscription de "Virtual Atomic and Molecular Data Center" dans Euro-VO DCA**

Answer Call for I3

- Interoperability of Atomic and Molecular Resources
 - Standards quite advanced (to be continued)
 - Registry, Query Languages
- Interdisciplinary Applications
 - Astronomy & Astrophysics
 - Environment
 - Planetology, Plasmas
 - Industry
- Worldwide connection: USA, China, Korea, Japan, Russia

VO Collaborations

- LERMA: F. Boone (PI of the DALIA project)
- LUTH: 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, JPL: J. Pearson
- HITRAN: L. Rothman, GEISA: J. Husson-Jacquinet
- Institut Carnot, Bourgogne: V. Boudon
- LPG: B. Schmitt, O. Dutuit, Observatory of Bordeaux: V. Wakelam, LPMAA: Base CO₂, Reims: Base O₃

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