

Level-1 release

VAMDC PMI
April 2010



Purpose of release

- Internal use:
 - “practice” infrastructure tech
 - Limited user feedback
- External review in Month 10 (July 2010)

Goals

- Access “all” data from common UI. “All” =
 - DBs with existing web interface
 - Sample DBs with tables interface
 - Sample DBs with XSAMS interface
- Discover data / interfaces to data from registry

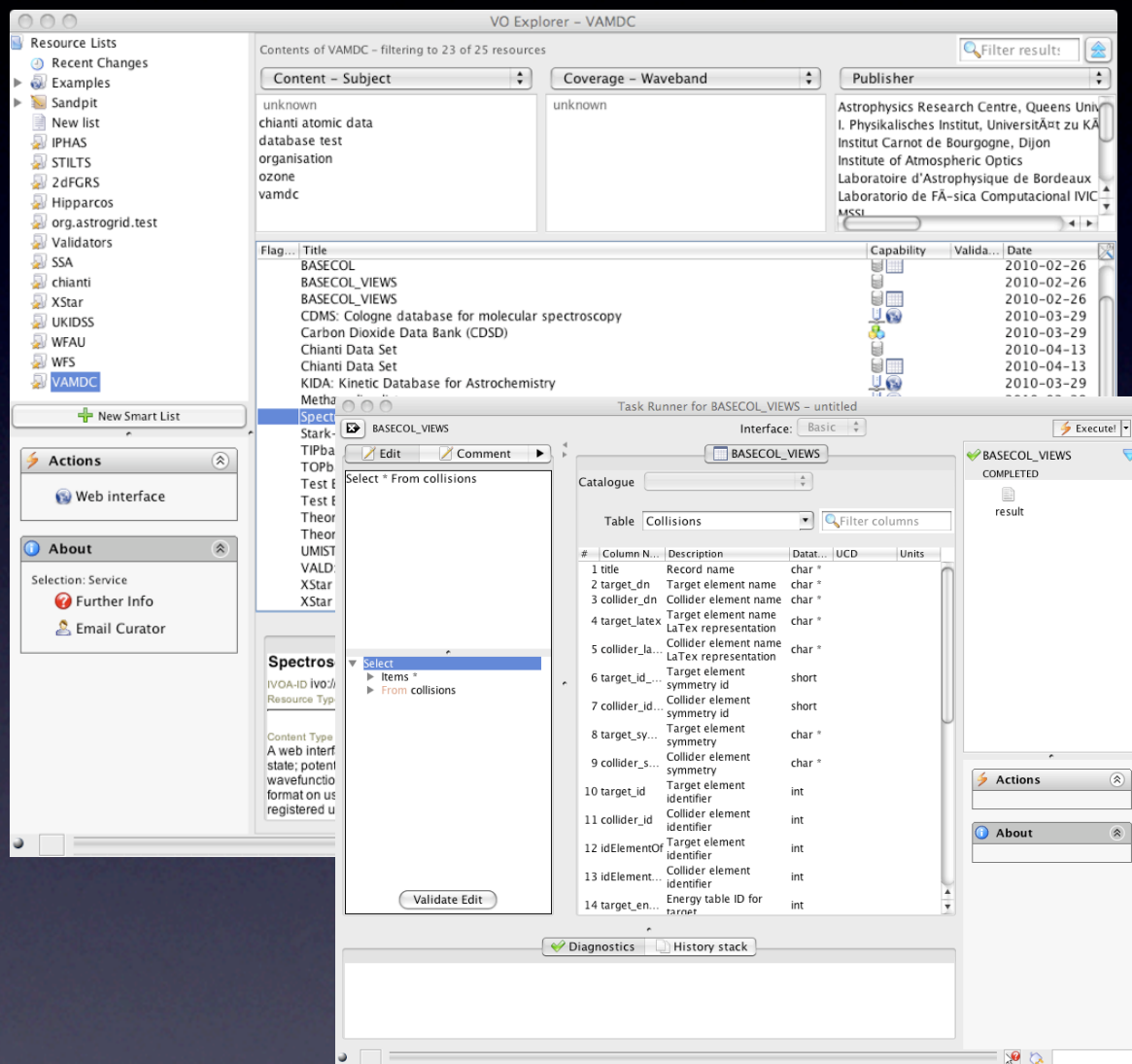
Deferred goals (to Year 2)

- Uniform format for all query results
- Send same query to many DB as one operation
- Execution of codes as services (may be dropped)
- Workflows with significant processing of data

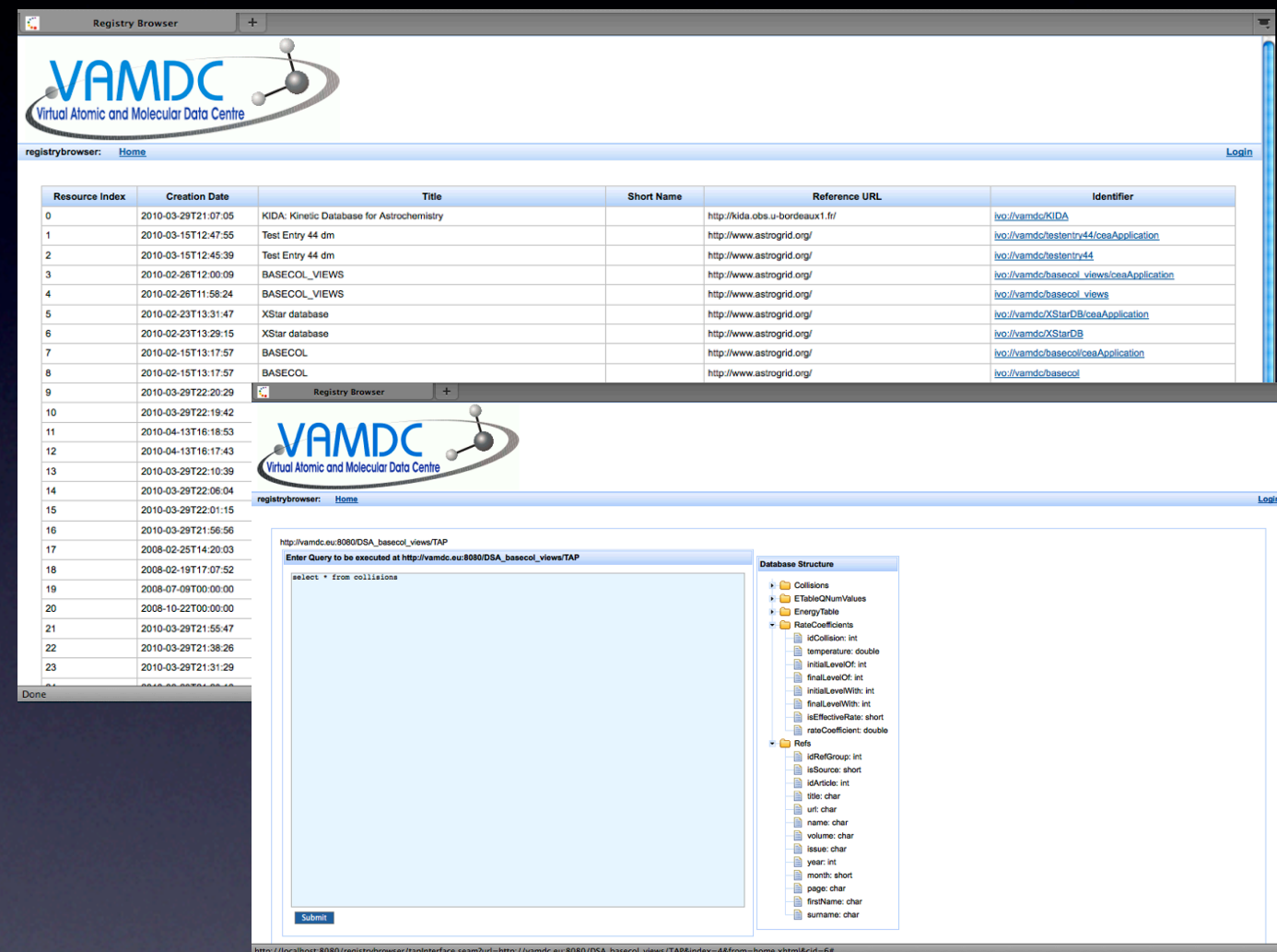
Components

- Registry
- Basic portal
- VODesktop
- Few TAP services on data
- Few XSAMS services on data
- Legacy web-sites

Two UIs



VODesktop



VAMDC web-portal

They have/will have the same basic features

Using a legacy web UI

1. Choose data

VO Explorer - VAMDC

Contents of VAMDC - filtering to 23 of 25 resources

Content - Subject Coverage - Waveband Publisher

unknown unknown Astrophysics Research Centre, Que
I. Physikalisches Institut, UniversitÄ
Institut Carnot de Bourgogne, Dijon
Institute of Atmospheric Optics
Laboratoire d'Astrophysique de Bo
Laboratorio de FÄ-sica Computaci
MSSI

Flag...	Title	Capability	Valida...	Date
	BASECOL			2009-12-17
	BASECOL			2010-02-26
	BASECOL_VIEWS			2010-02-26
	BASECOL_VIEWS			2010-02-26
	CDMS: Cologne database for molecular spectroscopy			2010-03-29
	Carbon Dioxide Data Bank (CDSD)			2010-03-29
	Chianti Data Set			2010-04-13
	Chianti Data Set			2010-04-13
	KIDA: Kinetic Database for Astrochemistry			2010-03-29
	Methane line lists			2010-03-29
	Spectroscopy and Molecular Properties of Ozone			2010-03-29
	Stark-B			2010-03-29
	TIPbase			2010-03-29
	TOPbase			2010-03-29
	Test Entry 44 dm			2010-03-15
	Test Entry 44 dm			2010-03-15
	Theoretical spectral database of polycyclic aromatic hydrocarbons			2010-03-29

BASECOL

IVOA-ID ivo://vamdc/basecol
Resource Type CatalogService Created 2010-02-15 Updated 2010-02-26

Content Type other Subject vamdc Level research [Further Information...](#)

Relationships service-for [ivo://vamdc/basecol/ceaApplication](#)

Show Table Metadata

Annotate
☐ Flag ☒
Highlight
Alternative title
Notes

Using a legacy web UI

1. Choose data

VO Explorer - VAMDC

Contents of VAMDC - filtering to 1 of 25 resources

Filter result!

Content - Subject Coverage - Waveband Publisher

unknown unknown VAMDC

chianti atomic data
database test
organisation
ozone
vamdc

Flag...	Title	Capability	Valida...	Date
	Spectroscopy and Molecular Properties of Ozone			2010-03-29

Flag... Title Capability Valid... Date

Spectroscopy and Molecular Properties of Ozone

Information Table Metadata XML

Spectroscopy and Molecular Properties of Ozone

IVOA-ID ivo://vamdc/SMPO
Resource Type Service Created 2010-03-29

Content Type other Subject ozone Level research

A web interface to a database comprising: molecular structure and spectroscopic constants in the ground electronic state; potential function; dipole moment surface; transition moments; vibration and vibration-rotation energies and wavefunctions; isotopic effects; simulated and experimental spectra from MW to Infrared; downloading results in text format on user's computer and sending them via e-mail; gas and/or isotopic species mixture preparation by

Annotate

Flag

Highlight

Alternative title

Notes

Using a legacy web UI

VO Explorer - VAMDC

Contents of VAMDC - filtering to 1 of 25 resources

Filter result!

Content - Subject Coverage - Waveband Publisher

unknown unknown VAMDC

chianti atomic data

database test

organisation

ozone

vamdc

Flag...	Title	Capability	Valida...	Date
	Spectroscopy and Molecular Properties of Ozone			2010-03-29

+ New Smart List

Actions

Web interface

About

Selection: Service

Further Info

Email Curator

Information Table Metadata XML

Spectroscopy and Molecular Properties of Ozone

IVOA-ID ivo://vamdc/SMPO

Resource Type Service Created 2010-03-29

Content Type other Subject ozone Level research

A web interface to a database comprising: molecular structure and spectroscopic constants in the ground electronic state; potential function; dipole moment surface; transition moments; vibration and vibration-rotation energies and wavefunctions; isotopic effects; simulated and experimental spectra from MW to Infrared; downloading results in text format on user's computer and sending them via e-mail; gas and/or isotopic species mixture preparation by

Annotate

Flag

Highlight

Alternative title

Notes

2. Follow link to legacy web-site

Using a legacy web UI

Spectroscopy & Molecular Properties of Ozone

http://smpo.iao.ru/

New deployed artifacts IVOA Documents 2mm Scale Association Computing blogs Hudson All builds Failures

russian english

Spectroscopy & Molecular Properties of Ozone

Home Molecule Energy Levels Transitions Spectra Simulation Experiment Cross-Sections Auxiliary data References Help

Log In	General Info	News
<p>Nick name : <input type="text"/></p> <p>Password : <input type="password"/></p> <p>Log in New User</p> <p>Forgot password?</p>	<p>Scope</p> <ul style="list-style-type: none">molecular structure and spectroscopic constants in the ground electronic statepotential functiondipole moment surfacetransition momentsvibration and vibration-rotation energies and wavefunctions, isotopic effectssimulated and experimental spectra from MW to InfraredDownloading results in text format on user's computer and sending them via e-mail.Gas and/or isotopic species mixture preparation by user (for registered users only).Saving results on server side and comparison of them (for registered users only).Uploading of user spectra to sever side and comparison of them to spectra obtained with the system (for registered users only).	<p>04/03/2010 Announcement of ANR research IR position in Reims University More...</p> <p>17/01/2010 Proceedings of the HighRus-2009 symposium are available now More...</p> <p>28/12/2009 Spectral line parameters of O₂ and SO₂ molecules of HITRAN source correspond to updates of 2009 More...</p>
<p>Remarks</p> <ul style="list-style-type: none">You are not obliged to log in the system but the registration allows you to achieve some extra functionalityThe registration in the system is free. Just click the button "New user" and fill in the form that appears.	<p>System developed by</p> <ul style="list-style-type: none">G.S.M.A, Université de Reims, CNRS UMR 8069, Reims, FranceL.T.S, Institute of Atmospheric Optics, Russian Academy of Sciences, Tomsk, Russia	
<p>Usage agreement</p> <p>Users of this system agree to reference SMPO Information System and the publication on used databases (HITRAN, GEISA etc) in scientific communications if the present resources may be considered as helpful to their investigations.</p>	<p>Authors, Contributors, Acknowledgements</p>	
<p>Usage statistics</p> <p>SMPO Information System SMPO Guide</p>		

3. Use web-site
as normal



Using TAP

1. Choose data

The screenshot shows the VO Explorer - VAMDC interface. On the left, a sidebar lists various resources, with 'VAMDC' selected. Red arrows point from the text '1. Choose data' to the 'VAMDC' entry in the sidebar and the 'BASECOL_VIEWS' entry in the main table. The main table displays a list of resources with columns for Flag, Title, Capability, Validation, and Date. The 'BASECOL_VIEWS' entry is highlighted. Below the table, there is a section for 'BASECOL_VIEWS' with details such as IVOA-ID, Resource Type, Content Type, Subject, Level, and Relationships. A 'Show Table Metadata' button is also visible.

Flag...	Title	Capability	Valida...	Date
	BASECOL			2010-02-26
	BASECOL			2010-02-26
	BASECOL_VIEWS			2010-02-26
	BASECOL_VIEWS			2010-02-26
	KIDA: Kinetic Database for Astrochemistry			2010-03-29
	Methane line lists			2010-03-29
	Theoretical spectral database of polycyclic aromatic hydrocarbons			2010-03-29
	Theoretical spectral database of pure carbon clusters			2010-03-29
	VALD: Vienna Atomic Line Database			2010-03-29
	XStar database			2010-02-23
	XStar database			2010-02-23

BASECOL_VIEWS

IVOA-ID ivo://vamdc/basecol_views
Resource Type CatalogService Created 2010-02-26

Content Type other Subject vamdc Level research [Further Information...](#)

Relationships service-for ivo://vamdc/basecol_views/ceaApplication

[Show Table Metadata](#)

Using TAP

VO Explorer - VAMDC

Contents of VAMDC - filtering to 11 of 25 resources

Content - Subject Coverage - Waveband Publisher

unknown unknown Institut Carnot de Bourgogne, Dijon
chianti atomic data Laboratoire d'Astrophysique de Bordeaux
database test Osservatorio Astronomico di Cagliari
organisation VALD consortium
ozone VAMDC
vamdc

Flag...	Title	Capability	Valida...	Date
	BASECOL			2010-02-26
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	KIDA: Kinetic Database for Astrochemistry			2010-03-29
	Methane line lists			2010-03-29
	Theoretical spectral database of polycyclic aromatic hydrocarbons			2010-03-29
	Theoretical spectral database of pure carbon clusters			2010-03-29
	VALD: Vienna Atomic Line Database			2010-03-29
	XStar database			2010-02-23
	XStar database			2010-02-23

2. Choose action → Table Query

Actions: Table Query

About: Selection: CatalogService, Further Info

Information Table Metadata XML

BASECOL_VIEWS

IVOA-ID ivo://vamdc/basecol_views
Resource Type CatalogService Created 2010-02-26

Content Type other Subject vamdc Level research [Further Information...](#)

Relationships service-for ivo://vamdc/basecol_views/ceaApplication

Show Table Metadata

Annotate
☐ Flag
Highlight
Alternative title
Notes

Using TAP

3. Enter query

The screenshot shows the 'Task Runner for BASECOL_VIEWS - untitled' window. The 'Interface' is set to 'Basic'. The 'Catalogue' is empty, and the 'Table' is set to 'Collisions'. The 'Filter columns' button is visible. The 'Select * From collisions' query is entered in the query editor. The 'Validate Edit' button is at the bottom of the query editor. The 'Diagnostics' and 'History stack' buttons are at the bottom of the window. The 'Actions' and 'About' buttons are on the right side.

Interface: Basic

Execute!

BASECOL_VIEWS

Edit Comment

Select * From collisions

Validate Edit

Catalogue

Table Collisions Filter columns

#	Column N...	Description	Datat...	UCD	Units
1	title	Record name	char *		
2	target_dn	Target element name	char *		
3	collider_dn	Collider element name	char *		
4	target_latex	Target element name LaTeX representation	char *		
5	collider_la...	Collider element name LaTeX representation	char *		
6	target_id_...	Target element symmetry id	short		
7	collider_id...	Collider element symmetry id	short		
8	target_sy...	Target element symmetry	char *		
9	collider_s...	Collider element symmetry	char *		
10	target_id	Target element identifier	int		
11	collider_id	Collider element identifier	int		
12	idElementOf	Target element identifier	int		
13	idElement...	Collider element identifier	int		
14	target_en...	Energy table ID for target	int		

Diagnostics History stack

Actions

About

Using TAP

4. Submit query

The screenshot shows the 'Task Runner for BASECOL_VIEWS - untitled' window. The interface is set to 'Basic'. On the left, the 'Edit' tab is active, showing a query editor with the text 'Select * From collisions'. Below the editor is a 'Validate Edit' button. A red arrow points from the text '4. Submit query' to the 'Execute!' button in the top right corner. The central pane displays a table named 'Collisions' with 14 columns. The right sidebar contains 'Actions' and 'About' sections. The bottom status bar shows 'Diagnostics' and 'History stack' tabs.

#	Column N...	Description	Datat...	UCD	Units
1	title	Record name	char *		
2	target_dn	Target element name	char *		
3	collider_dn	Collider element name	char *		
4	target_latex	Target element name LaTeX representation	char *		
5	collider_la...	Collider element name LaTeX representation	char *		
6	target_id_...	Target element symmetry id	short		
7	collider_id...	Collider element symmetry id	short		
8	target_sy...	Target element symmetry	char *		
9	collider_s...	Collider element symmetry	char *		
10	target_id	Target element identifier	int		
11	collider_id	Collider element identifier	int		
12	idElementOf	Target element identifier	int		
13	idElement...	Collider element identifier	int		
14	target_en...	Energy table ID for target	int		

Using TAP

5. Request results

The screenshot shows the 'Task Runner for BASECOL_VIEWS - untitled' application window. The interface is set to 'Basic'. On the left, a text area contains the SQL query 'Select * From collisions'. Below this is a 'Validate Edit' button. In the center, a table titled 'BASECOL_VIEWS' displays the results of the query. The table has columns: #, Column N..., Description, Datat..., UCD, and Units. The results are as follows:

#	Column N...	Description	Datat...	UCD	Units
1	title	Record name	char *		
2	target_dn	Target element name	char *		
3	collider_dn	Collider element name	char *		
4	target_latex	Target element name LaTeX representation	char *		
5	collider_la...	Collider element name LaTeX representation	char *		
6	target_id_...	Target element symmetry id	short		
7	collider_id...	Collider element symmetry id	short		
8	target_sy...	Target element symmetry	char *		
9	collider_s...	Collider element symmetry	char *		
10	target_id	Target element identifier	int		
11	collider_id	Collider element identifier	int		
12	idElementOf	Target element identifier	int		
13	idElement...	Collider element identifier	int		
14	target_en...	Energy table ID for target	int		

On the right side of the application, there is a panel showing the status of the task. It indicates 'BASECOL_VIEWS COMPLETED' with a green checkmark. Below this, there is a 'result' button. Further down, there is an 'Actions' panel with 'View' and 'Download...' options. At the bottom of the application window, there are tabs for 'Diagnostics' and 'History stack'.

Using TAP

6. View results in TopCat

TOPCAT(1): Table Browser

Table Browser for 1: result

	title	target_dn	collider...	target_latex	collider...	target_i...	collider...	targe
1	Rotational excitation of ortho-H ₂ O by He (Gre...	H ₂ O	He	H ₂ O	He	4	0	ortho
2	Rotational excitation of CS by para-H ₂ , 20K...	CS	H ₂	CS	H ₂	0	5	none
3	Rotational excitation of HCO ⁺ by para-H ₂ ...	HCO ⁺	H ₂	HCO ⁺	H ₂	0	5	none
4	Rotational excitation of OCS by He (Flower, 2001)	OCS	He	OCS	He	0	0	none
5	Rotational excitation of HCl by He (Neufeld & al.,...	HCl	He	HCl	He	0	0	none
6	Excitation of the hyperfine levels of HCl by He (Ne...	HCl	He	HCl	He	0	0	none
7	Rotational excitation of SiO by collisions with para...	SiO	H ₂	SiO	H ₂	0	5	none
8	Rotational de-excitation of CO by para-H ₂ (j...	CO	H ₂	CO	H ₂	0	5	none
9	Rotational excitation of HF(v=0) by He (Reese et...	HF	He	HF	He	0	0	none
10	Rotational Excitation of para-H ₂ CO by He (Gr...	H ₂ CO	He	H ₂ CO	He	5	0	para
11	Rotational Excitation of ortho-H ₂ CO by He (Gr...	H ₂ CO	He	H ₂ CO	He	4	0	ortho
12	Rotational Excitation of HCS ⁺ by He (Monteiro...	HCS ⁺	He	HCS ⁺	He	0	0	none
13	Rotational excitation of SO ₂ by He (Green 199...	SO ₂	He	SO ₂	He	0	0	none
14	Rotational excitation of HDO by He (Green 1989)	HDO	He	HDO	He	0	0	none
15	Rotational excitation of para-H ₂ O by He (Gre...	H ₂ O	He	H ₂ O	He	5	0	para
16	Rotational excitation of SiO by para-H ₂ , 20K...	SiO	H ₂	SiO	H ₂	0	5	none
17	Ro-vibrational excitation of ortho-H ₂ by He (F...	H ₂	He	H ₂	He	4	0	ortho
18	Ro-vibrational excitation of para-H ₂ by He (F...	H ₂	He	H ₂	He	5	0	para
19	Ro-vibrational excitation of ortho-H ₂ by H (Fl...	H ₂	H	H ₂	H	4	0	ortho
20	Ro-vibrational excitation of para-H ₂ by H (Flo...	H ₂	H	H ₂	H	5	0	para
21	Ro-vibrational excitation of ortho-H ₂ by ortho...	H ₂	H ₂	H ₂	H ₂	4	4	ortho
22	Ro-vibrational excitation of ortho-H ₂ by para...	H ₂	H ₂	H ₂	H ₂	4	5	ortho
23	Ro-vibrational excitation of para-H ₂ by ortho...	H ₂	H ₂	H ₂	H ₂	5	4	para
24	Ro-vibrational excitation of para-H ₂ by para...	H ₂	H ₂	H ₂	H ₂	5	5	para
25	Excitation of the fine structure of SO by para-H ₂ ...	SO	H ₂	SO	H ₂	0	5	none
26	Rotational excitation of CO by ortho-H ₂ (Flow...	CO	H ₂	CO	H ₂	0	4	none
27	Rotational excitation of CO by para H ₂ (Flower...	CO	H ₂	CO	H ₂	0	5	none
28	Rotational excitation of OCS by para-H ₂ (Gree...	OCS	H ₂	OCS	H ₂	0	5	none
29	Rotational excitation of HC ₃ N by He (Green &...	HC ₃ N	He	HC ₃ N	He	0	0	none
30	Vibrational de-excitation of SiO by para-H ₂ ...	SiO	H ₂	SiO	H ₂	0	5	none
31	Rotational excitation of A-methanol in its ground t...	CH ₃ OH	He	CH ₃ OH	He	1	0	A
32	Rotational excitation of E-methanol in its ground...	CH ₃ OH	He	CH ₃ OH	He	2	0	E
33	Rotational excitation of ortho-H ₂ O by ortho-H...	H ₂ O	H ₂	H ₂ O	H ₂	4	4	ortho
34	Rotational excitation of ortho-H ₂ O by para-H...	H ₂ O	H ₂	H ₂ O	H ₂	4	5	ortho
35	Rotational excitation of para-H ₂ O by ortho-H...	H ₂ O	H ₂	H ₂ O	H ₂	5	4	para
36	Rotational collisional de-excitation rate coefficient...	N ₂ H ⁺	He	N ₂ H ⁺	He	0	0	none
37	Rotational excitation of para-H ₂ O by para-H...	H ₂ O	H ₂	H ₂ O	H ₂	5	5	para
38	Rotational excitation of SiC ₂ by He (Chandra...	SiC ₂	He	SiC ₂	He	4	0	ortho

Access with XSAMS

- Like TAP, but the results are more uniform
- Different query language: details not fixed yet

Registered web UIs

- CDMS
- CDSD
- KIDA
- Dijon methane line-lists
- S&MPO
- Stark-B
- TIPBase
- TOPBase
- OAC PAH
- OAC carbon-clusters
- UDfA
- VALD

Registered codes

- None so far (not a cycle-I/level-I task)
- Should we register the legacy web-UIs for codes?

Data-sets with TAP

- BASECOL
- XStarDB
- CHIANTI

XSAMS services

- None so far.
- Hope to get a few prototypes into LI system
- Candidates:
 - BASECOL
 - VALD
 - Others? Suggestions? Volunteers?

Is that all?

Probably.

Fancier use-cases need tech we haven't finished yet

e.g.

richer metadata

uniform query interfaces

common format for results

Make it *work* before making it *rich*.

Pimp my VAMDC

- Making it more attractive in year 1
 - Worked examples of queries
 - Implement sample science-cases (from WP2)
 - Work with early users to design custom queries
 - Write some useful workflow apps that use the services