Overview on the VAMDC Project

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and the **VAMDC Collaboration (P.I. M.-L. Dubernet)**

M.L. Dubernet et al. 2010, JQSRT 111, 2152

Special thanks to

Nigel Mason and T.A. Ryabchikova
for providing the originals of many of the transparencies
shown in the following

Further input has been taken from the VAMDC homepage at
http://www.vamdc.eu/ as well as from presentations by
N. Mason, N. Piskunov, and G. Rixon at the 2nd and 3rd annual
VAMDC Conferences.

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OUTLINE

- VAMDC
  - Node members
  - What is it ? Idea behind it ? Expected outcome ?
  - Clientele
  - Technology, available databases
  - Astronomical Examples
  - Current Release of VAMDC
  - Need for VAMDC when working with VALD (slides courtesy of T.A. Ryabchikova)

VAMDC Vienna Node Team Members

Friedrich Kupka → **Institute of Mathematics**

Theresa Rank-Lüftinger → **Institute for Astronomy**

Werner W. Weiss → **Institute for Astronomy**

and until May 2011

Christian Stütz → **Computer Centre of the University**

What is VAMDC ?

The Virtual Atomic and Molecular Data Centre (VAMDC) is an international project aimed to create an interoperable interface to existing Atomic and Molecular (A&M) databases. In general, each database within VAMDC has been organised in its own way.

It consists of 8 work packages. 15 administrative partners which represent 23 teams from 6 countries within the EU (Austria, France, Germany, Italy, Sweden, and the UK) as well as from Russia, Serbia, and Venezuela have entered the VAMDC consortium.

Presently, the **VAMDC project** includes 24 A&M DBs, among others: **BASECOL, CDMS, CDSD, CHIANTI, Ethelyne, GhoSST, HITRAN, KIDA, PAH, SPECTR-W^3, StarkB, TIPbase, TOPbase, VALD.**

A detailed description of VAMDC is given by ***Dubernet et al. (2010), JQSRT 111, 2151.***

The VAMDC Collaboration I

- CNRS in France: LPMAA (Paris), LUTH (Paris), VO-Paris Data Centre, LERMA (Paris), LAB (Bordeaux), ICB (Burgogne), GSMA (Champagne-Ardenne), CESR (Toulouse), IPAG (Grenoble)
- Cambridge University (CMSUC)
- University College London (UCL)
- Open University (OU)
- Universität Wien (UNIVIE)
- Uppsala Universitet (UU)
- Universität zu Köln (Köln)
- Istituto Nazionale di Astrofisica (INAF)

The VAMDC Collaboration II

- Queen's University Belfast (QUB)
- Astronomska Opservatorija (AOB)
- Institute of Spectroscopy RAS (ISRAN)
- Russian Federal Nulcear Center - All-Russian Institute of Technical Physics (RFNC-VNIITF)
- Institute of Atmospheric Optics (IAO)
- Corporacion Parque tecnologico de Merida (CeCalCULA/IVIC)
- Institute for Astronomy RAS (INASAN)

The Idea behind VAMDC

- A&M data have been collected and assessed in a various databases. They underpin a wide range of physics in applied research and industrial development.
- Many databases have been built to serve specific needs. VALD is one such example with its own advantages, special tools, and limitations.
- Various kinds of data, formats, completeness, etc. and
- specialized extraction tools exist for each of the A&M databases.
- Problems:
  - data duplication
  - different user interfaces
  - restricted access
  - often fragmentary, ...

Expected VAMDC outcomes

- Develop/extend standards for interoperability of A&M resources
- Implementation of selected databases
- Find resources easily
- Query those resources with dedicated protocols/languages
- Transfer large amounts of data asynchronously
- Create a safe environment for publishing latest sets of A&M data
- Linking producers with users

- Key benefits from using VAMDC:
  - find any type of AM data with a click, provide uniform access
  - cross-matching different data sets, wide access to latest published data

A & M Users: The VAMDC Clientele

- Astrophysics / Astronomy / Planetary Science
- Atmospheric Science
- Fusion Science
- Plasma Science
- Radiation Science

and their applications in research and industrial development

Technology I: VAMDC Components

"Grand Central" in Paris

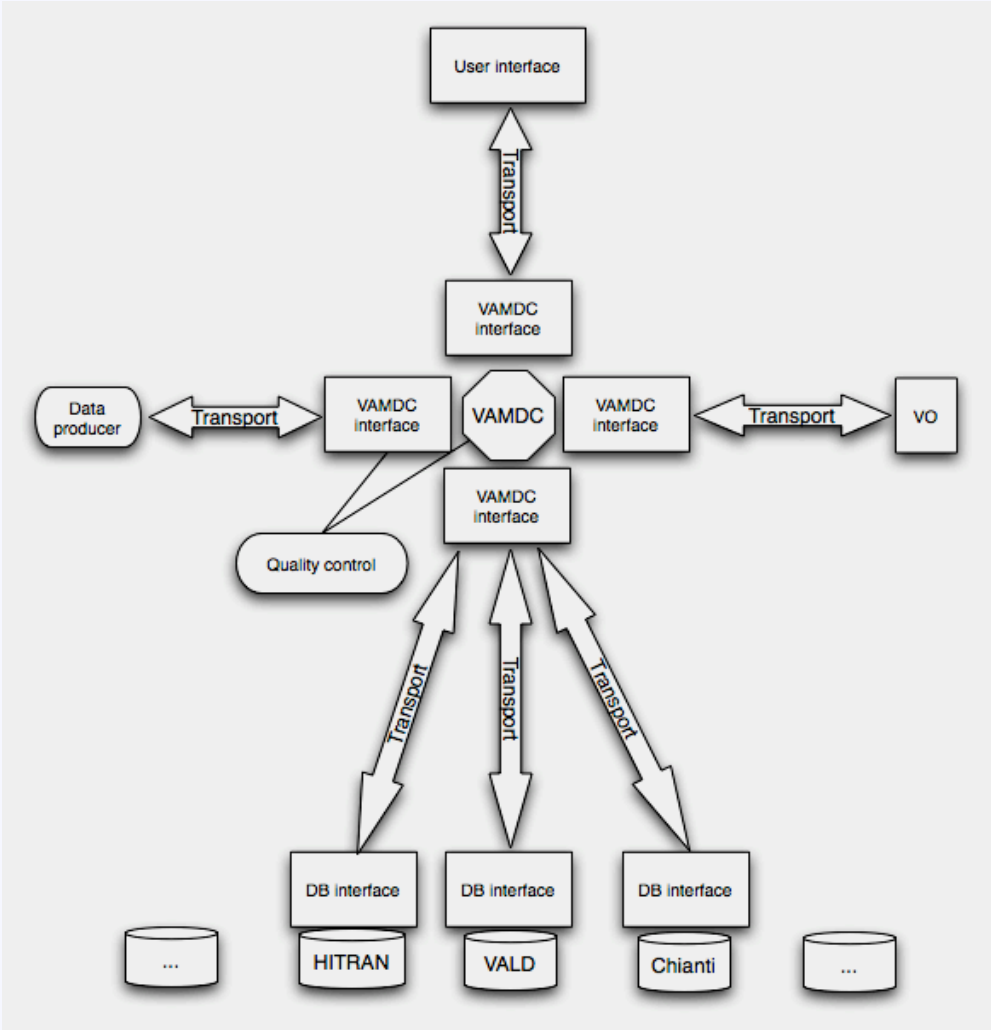
Web-based transport protocol

Interface(s) to DBs

User interface

Automatic interface (e.g. to VO)

Data publishing tools



Technology II: VAMDC Components

VAMDC in action:

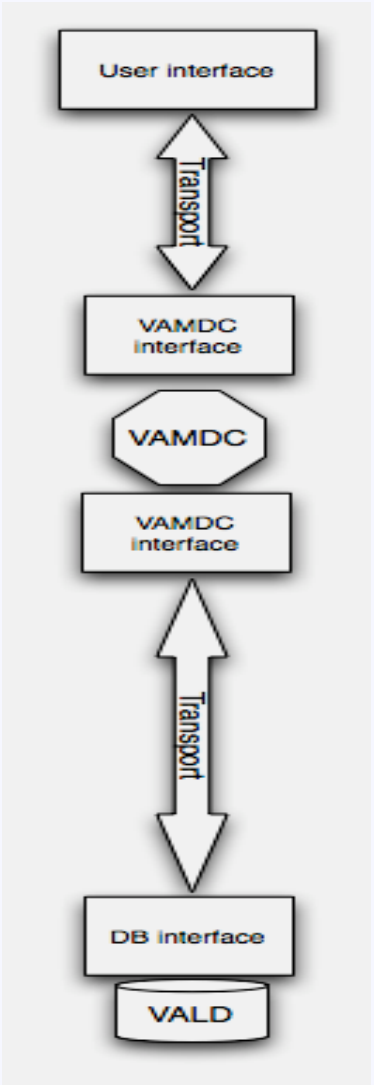
user accessing a database,

for instance VALD, through

VAMDC. The general interface

now is the VAMDC Portal at

http://portal.vamdc.eu/



Technology III: Web-Based Transport Protocol

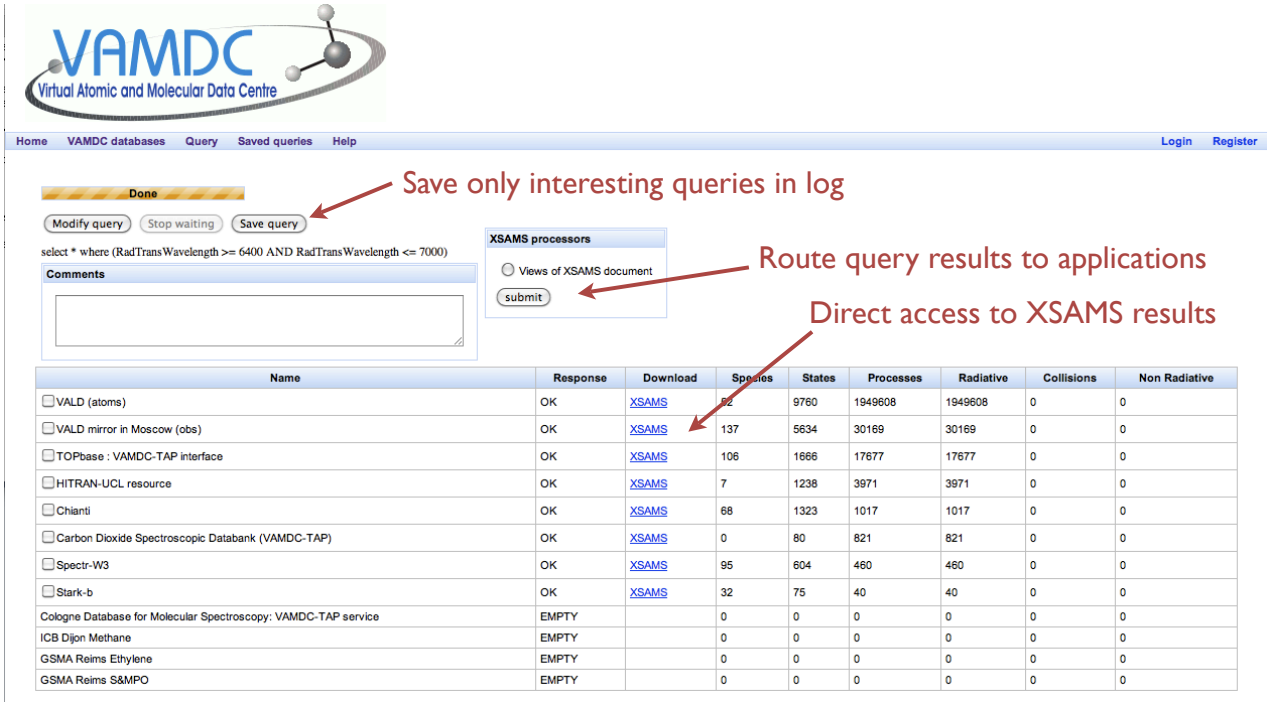
- The transport protocol handles:
  - database (DB) queries for status and data content (registry update)
  - query / data transfer between user and Grand Central
  - query / data transfer between a DB and Grand Central
- The transport protocol using VAMDC-XSAMS 0.3 (expected to be equal to the XSAMS 1.0 standard) is:
  - self-descriptive (XML description of what is sent including units, formats etc., use of XSAMS data format)
  - efficient for large data sets (compressed binary tables)

Technology IV: Interface to Databases

- Fully compatible with the VAMDC transport on the outside
- Tuned to the specific DB on the inside:
  - converting incoming queries to the internal query format
  - converting the DB extraction to the transport-compatible format
- Capable of responding to VAMDC-specific queries (registry update)
- Capable of collecting the accounting information

Technology V: Registry Browser

Portal (2)

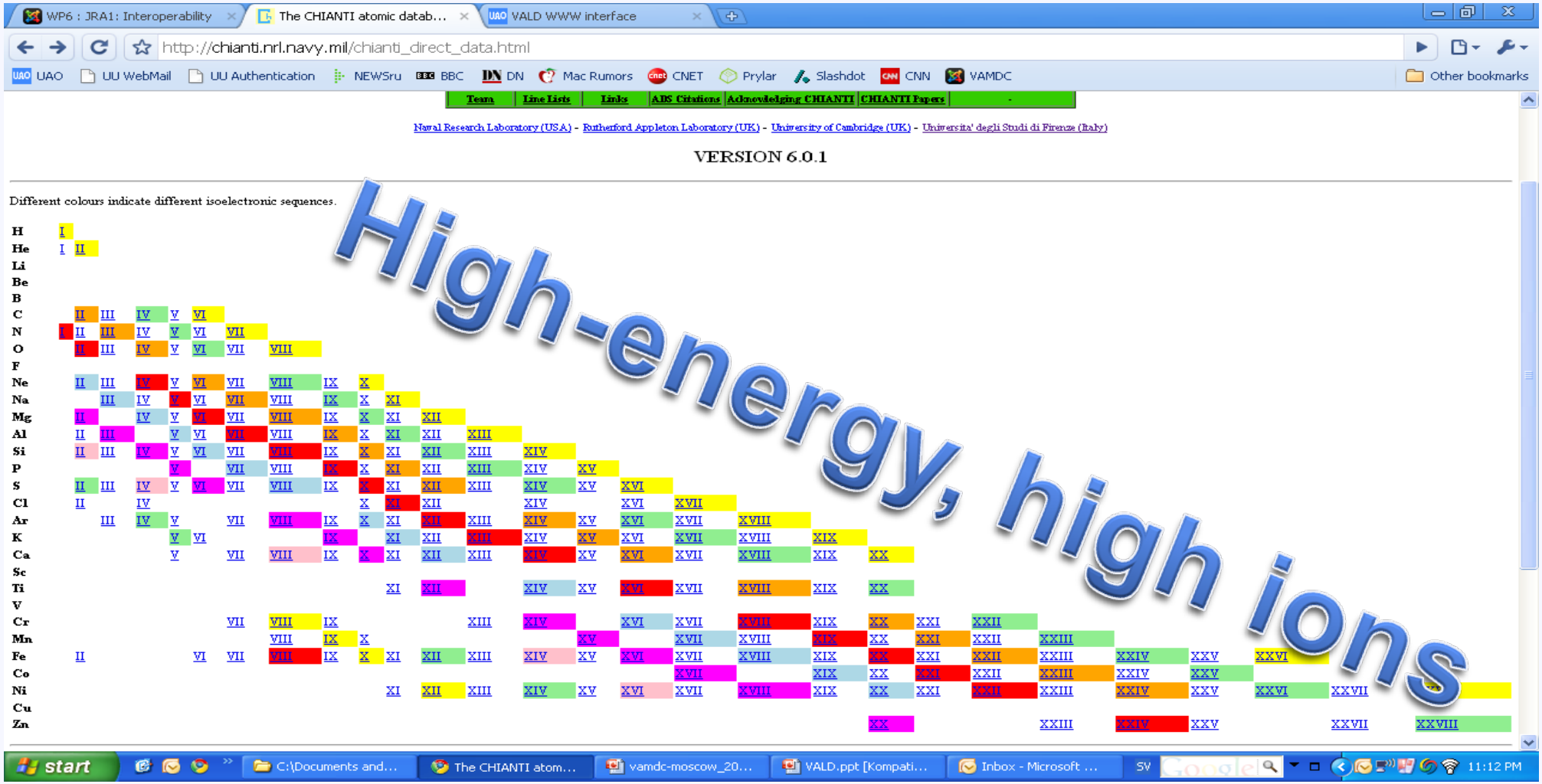


Improved view of results from nodes

from: Guy Rixon, WP4/SA1: deployment, report to VAMDC PM3, February 2012

Astronomical Examples I

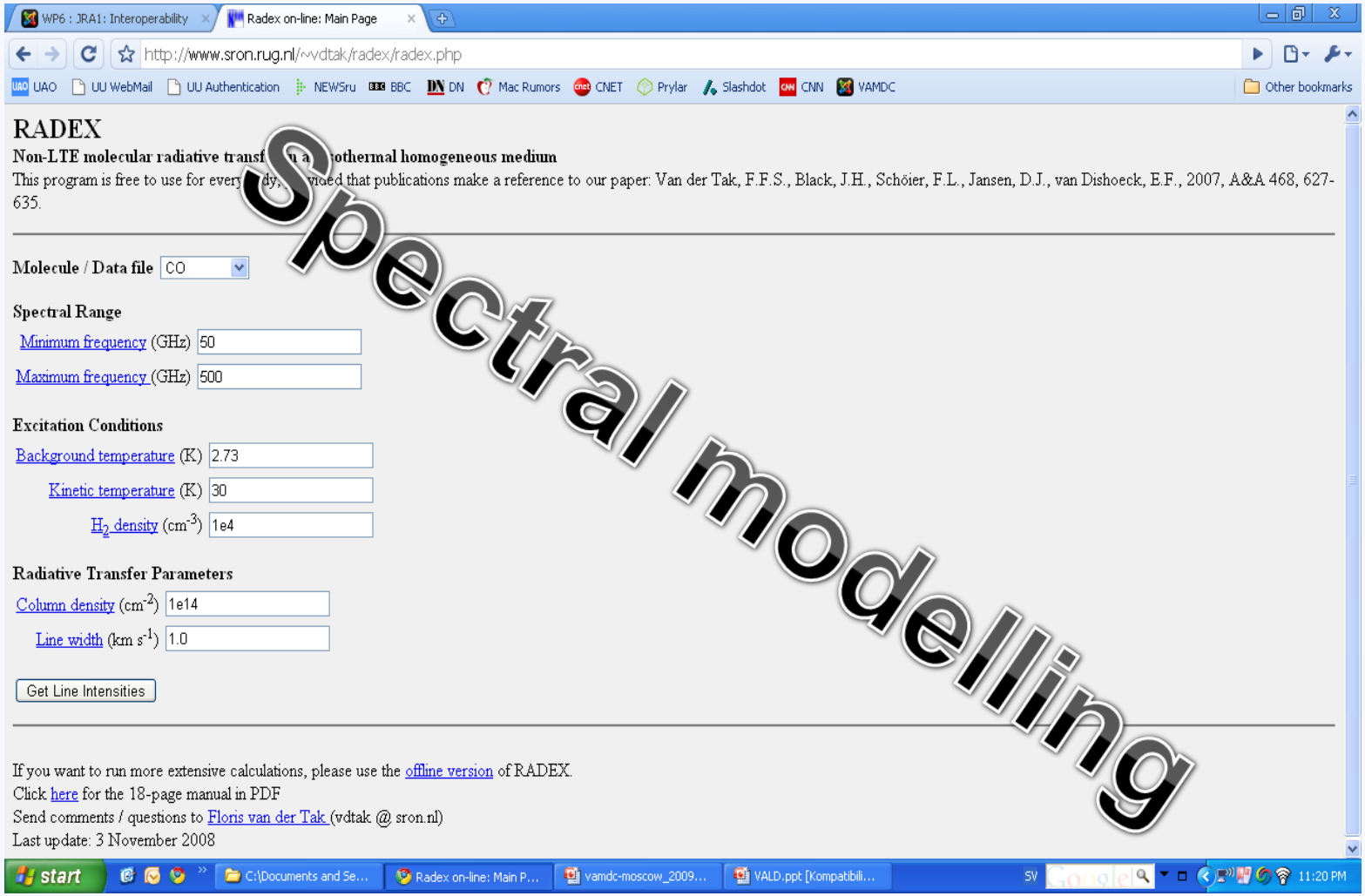
Chianti atomic line database (example courtesy of N. Piskunov)



Astronomical Examples II

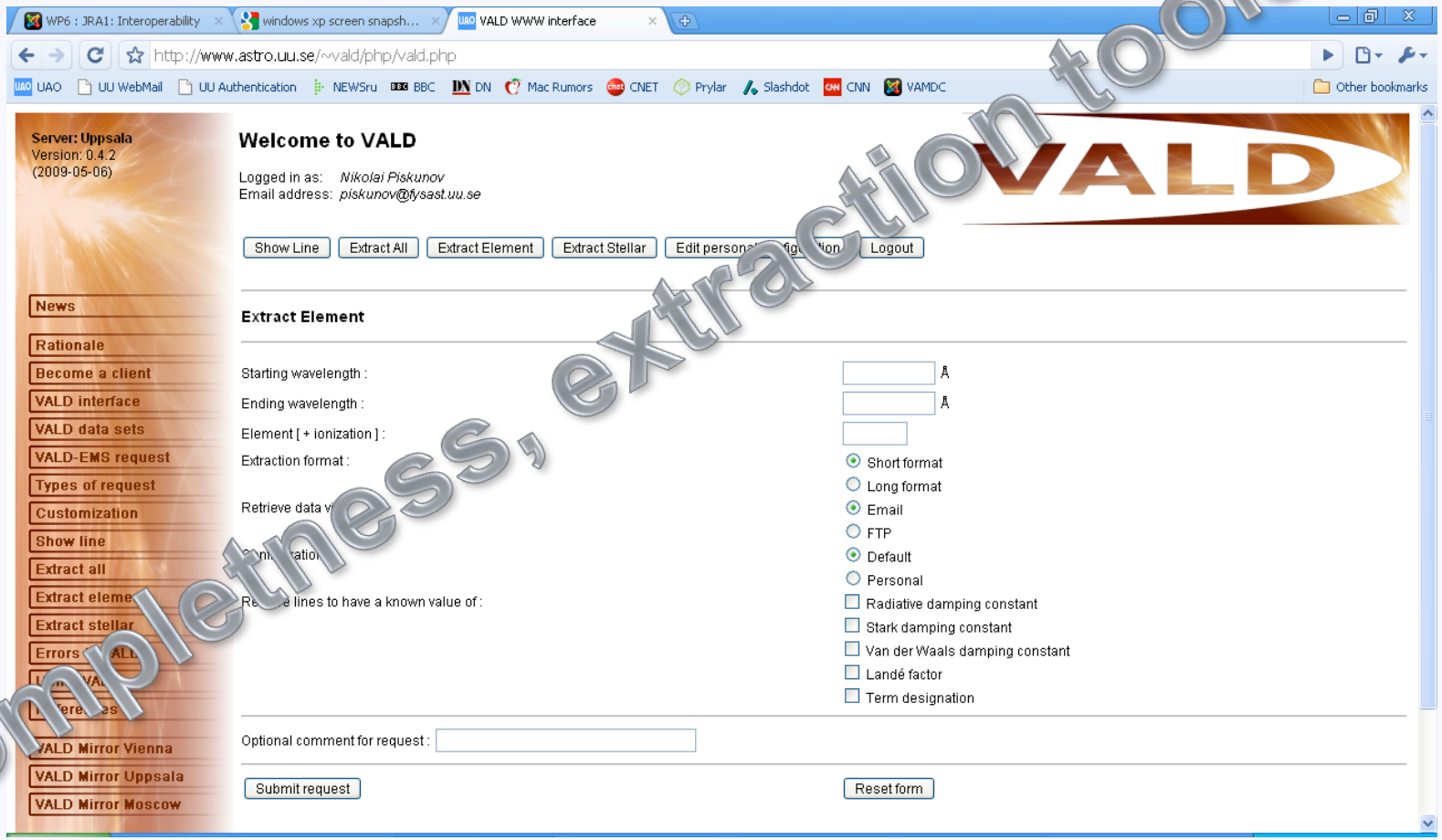
Leiden Atomic and Molecular Database

(example courtesy of N. Piskunov)



Astronomical Examples III

Vienna Atomic Line Database



(example courtesy of N. Piskunov)

Databases for Current Release

Current nodes

DB	Std. version	S/w version	Valid XSAMS 0.3?
Stark-b	11.12	11.12	N
BASECOL	11.12	Java VAMDC-TAP implementation 12.02	Y
KIDA	11.10	Java VAMDC-TAP implementation 11.10	N
TOPbase	11.12	11.12	Y
Carbon Dioxide Spectroscopic Databank	11.12	11.12	Y
TIPbase	11.12	11.12	Y
HITRAN-UCL resource	11.12	11.12	Y
Spectr-W3	11.12	11.12	Y
GSMA Reims S&MPO	11.12	11.12	Y
GSMA Reims Ethylene	11.12	11.12r1	Y
GhoSST	11.12	Unknown	Y
Chianti	11.12	11.12	Y
Cologne Database for Molecular Spectroscopy	11.12	11.12	Y
Vienna Atomic Line Database (Uppsala)	11.12	11.12-rc1	Y
Vienna Atomic Line Database (Moscow)	11.12	11.12	Y
UMIST Database for Astrochemistry	11.12	11.12r1	N
Theoretical spectral database of PAH	11.12	11.12	Y
ICB Dijon Methane	11.12	11.12r1	Y
Lund	11.12	11.12r1	Y

- 19 nodes (including 2 versions of VALD)
- 18 visible to portal in registry (UdFA not showing up yet)
- 16 working (i.e. valid XSAMS v0.3 output)

from: Guy Rixon, WP4/SA1: deployment, report to VAMDC PM3, February 2012

Name	Description	Maintainer	Status
Cologne Database for Molecular Spectroscopy: VAMDC-TAP service	The Cologne Database for Molecular Spectroscopy (CDMS) contains a catalog of radio frequency and microwave to far-infrared spectral lines of atomic and molecular species that (may) occur in the interstellar or circumstellar medium or in planetary atmospheres. The catalog is continuously updated.	endres@ph1.uni-koeln.de	OK
ICB Dijon Methane	Calculated line lists for methane (12CH4, 13CH4 and 12CH3D). The data on methane contain the vibration-rotation energy levels, line positions and line intensities in the range from 0 to 6200 cm-1.	Christian.Wenger@u-bourgogne.fr	OK
VALD (atoms)	The Vienna Atomic Line Database (VALD) is a collection of atomic line parameters (wavelengths, transition energies and quantum numbers, oscillator strengths, Lande factors, radiative and collisional broadening). This resource is the VAMDC-TAP representation of the atomic data in VALD3.	thomas.marquart@fysast.uu.se	OK
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)	The current version of CDSD-296 consists of 7 most abundant in the Earth's atmosphere isotopic species of the carbon dixoide molecule: 626, 636, 628, 627, 638, 637, 828, covers 5.9 - 12784.1 cm-1 spectral range and contains 419610 lines.	vip@lts.iao.ru	OK
BASECOL: VAMDC-TAP interface	This database, called BASECOL is devoted to collisional ro-vibrational excitation of molecules by colliders such as atom, ion, molecule or electron. It is supervised by an international working group of molecular physicists and astrophysicits involved in the calculations and use of ro-vibrational cross-sections, in order to ensure the continuity and the quality of the database.	misha@doronin.org	OK
TOPbase : VAMDC-TAP interface	TOPbase lists LS-coupling energy levels, gf-values and photoionization cross sections for astrophysically abundant ions (Z=1,14; Z=16; Z=18; Z=20; Z=26) computed in the Opacity Project.	nicolas.moreau@obspm.fr - franck.delahaye@obspm.fr	OK
Theoretical spectral database of polycyclic aromatic hydrocarbons	The Cagliari/Toulouse PAH database is a collection of theoretical spectroscopic data about Polycyclic Aromatic Hydrocarbons and carbon clusters. It provides basic geometric characteristics, energetics, harmonic analyses and electronic photoabsorption data. It is maintained by the Astrochemistry group at INAF-Observatory of Cagliari and the Institut de Recherche en Astrophysique et PlanÃ©tologie in Toulouse.	gmulas@oa-cagliari.inaf.it	OK
Chianti	Chianti consists of a critically evaluated set of up-to-date atomic data, together with user-friendly programs written in Interactive Data Language (IDL), to analyse the spectra from astrophysical plasmas. The VAMDC interface presents just the data from the Chianti-v7 release.	gtr@ast.cam.ac.uk	OK
TIPbase : VAMDC-TAP interface	TIPbase lists fine-structure levels, A-values, collision strengths and effective collision strengths for astrophysically abundant ions, mainly from the Fe isonuclear sequence computed in the Iron Project.	nicolas.moreau@obspm.fr - franck.delahaye@obspm.fr	OK
GSMA Reims S&MPO	Calculated line lists for ozone (16O3, 16O18O16O and 18O3). The data on methane contain the vibration-rotation energy levels, line positions and line strengths in the range from 0 to 8000 cm-1.	ylb@iao.ru, vladimir.tyuterev@univ-reims.fr	OK
GSMA Reims Ethylene	Calculated data of ethylene (12C2H4). The data on ethylene contain the vibration-rotation energy levels, line positions and line intensities in the range from 500 to 7500 cm-1	ludovic.daumont@univ-reims.fr, maud.rotger@univ-reims.fr	OK
TAP-XSAMS for GhoSST database		bernard.schmitt@obs.ujf-grenoble.fr	OK
Lund laboratory spectroscopy database	Experimental data for transitions and lifetimes	hampus@astro.lu.se	OK
Stark-b	Database for "Stark" broadening of isolated lines of atoms and ions in the impact approximation	sylvie.sahal-brechot@obspm.fr	OK
Spectr-W3	The information accumulated in the SPECTR-W3 ADB contains over 450,000 records and includes factual experimental and theoretical data on ionization potentials, energy levels, wavelengths, radiation transition probabilities, oscillator strengths, and (optionally) the parameters of analytical approximations of electron-collisional cross-sections and rates for atoms and ions. Those data were extracted from publications in physical journals, proceedings of the related conferences, special-purpose publications on atomic data, and provided directly by authors. The information is supplied with references to the original sources and comments, elucidating the details of experimental measurements or calculations, where necessary and available. To date, the SPECTR-W3 ADB is the largest factual database in the world containing the information on spectral properties of multicharged ions.	p_a_loboda@mail.ru	OK
Water internet Accessible Distributed Information System	Database containing information on water spectras, notably data on H216O, HDO, D2O, H217O and H218O.	faz@iao.ru	OK
HITRAN-UCL resource	The HITRAN database - truncated version for beta testing, from http://www.cfa.harvard.edu/HITRAN/	christian.hill@ucl.ac.uk	OK
VALD sub-set in Moscow (obs)	The part of Vienna Atomic Line Database (VALD) with accurate wavelength and energy levels. It also provides laboratory and calculated transition probabilities, Lande factors and broadening parameters. It is used for line identification and spectral synthesis.	pakhomov@inasan.ru	OK
KIDA: VAMDC-TAP interface	KIDA is a database of kinetic data interesting for astrochemical (interstellar medium and planetary atmospheres) studies. In addition to the available referenced data, KIDA provides recommendations over a number of important reactions. Chemists and physicists can add their data to the database.	Valentine.Wakelam@obs.u-bordeaux1.fr	OK

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Atoms Clear Remove

Atom symbol

InChIKey

Mass number to

Nuclear charge to

Ion charge to

State energy to 1/cm

Equivalent to null to null1/cm

Transitions Clear Remove

Wavelength 11000 to 11500 A

Upper state energy to 1/cm

Equivalent to null to null1/cm

Lower state energy to 1/cm

Equivalent to null to null1/cm

Probability, A to 1/s

Find data Save query

Legend

available, can answer
available, don't support query
unsupported keyword

- Cologne Database for Molecular Spectroscopy: VAMDC-TAP service
- ICB Dijon Methane
- VALD (atoms)
- Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)
- BASECOL: VAMDC-TAP interface
- TOPbase : VAMDC-TAP interface
- Theoretical spectral database of polycyclic aromatic hydrocarbons
- Chianti
- TIPbase : VAMDC-TAP interface
- GSMA Reims S&MPO
- GSMA Reims Ethylene
- TAP-XSAMS for GhoSST database
- Stark-b
- Spectr-W3
- HITRAN-UCL resource
- VALD mirror in Moscow (obs)
- KIDA: VAMDC-TAP interface

VAMDC
Virtual Atomic and Molecular Data Centre

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Done

Modify query | Stop waiting | Save query

select * where (RadTransWavelength >= 11000 AND RadTransWavelength <= 11500)

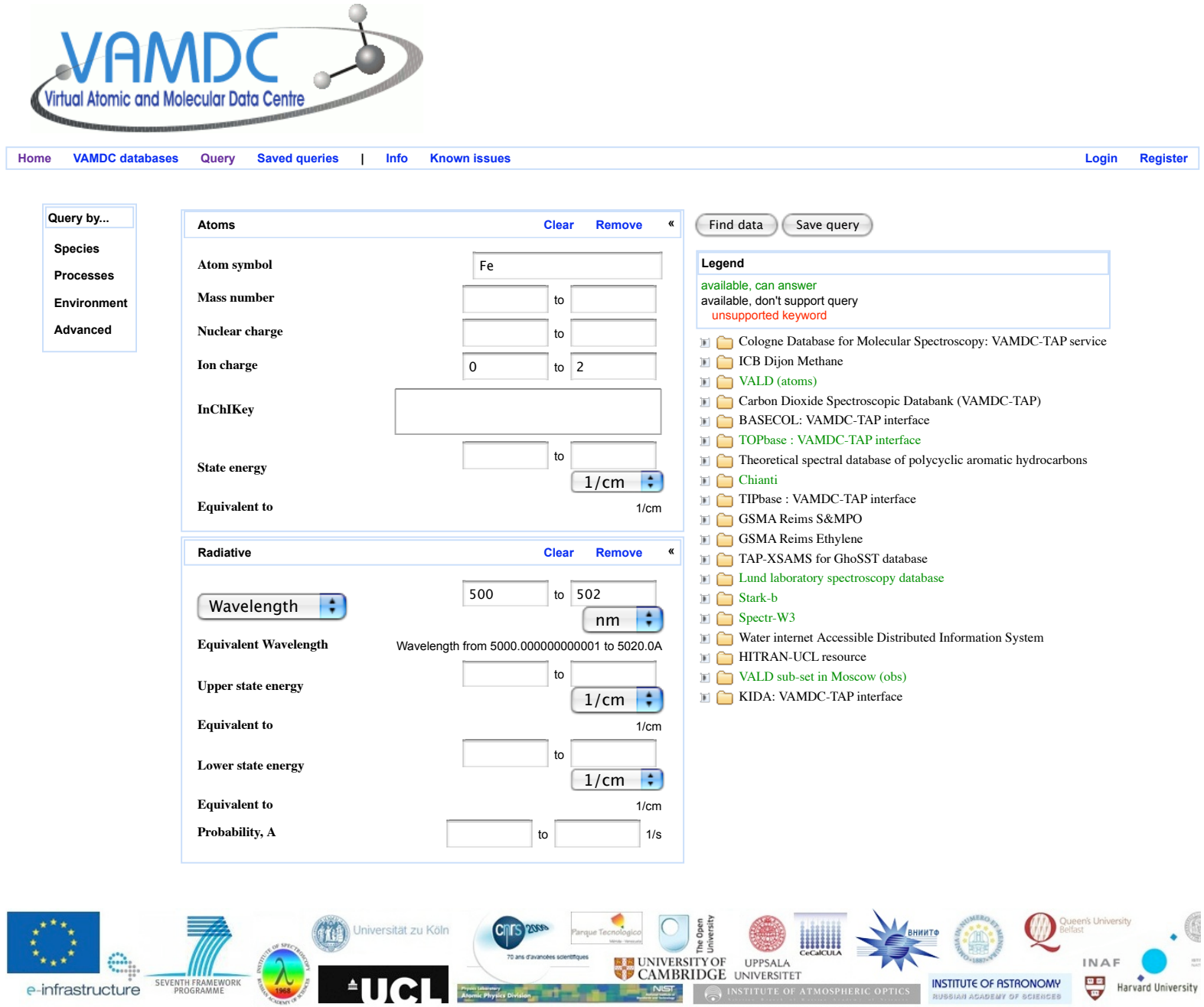
Comments

XSAMS processors

Views of XSAMS document

submit

Name	Response	Download	Species	States	Processes	Radiative	Collisions	Non Radiative
VALD (atoms)	OK	XSAMS	46	9423	585459	585459	0	0
HITRAN-UCL resource	OK	XSAMS	7	1280	10505	10505	0	0
VALD mirror in Moscow (obs)	OK	XSAMS	91	5190	8602	8602	0	0
TOPbase : VAMDC-TAP interface	OK	XSAMS	104	1468	6596	6596	0	0
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)	OK	XSAMS	0	80	2945	2945	0	0
Chianti	OK	XSAMS	52	494	305	305	0	0
Spectr-W3	OK	XSAMS	39	186	133	133	0	0
Stark-b	OK	XSAMS	18	39	21	21	0	0
Cologne Database for Molecular Spectroscopy: VAMDC-TAP service	EMPTY		0	0	0	0	0	0
ICB Dijon Methane	EMPTY		0	0	0	0	0	0
GSMA Reims Ethylene	EMPTY		0	0	0	0	0	0
GSMA Reims S&MPO	EMPTY		0	0	0	0	0	0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Clear
Remove
Atom symbol
Fe
Mass number
Nuclear charge
Ion charge
0
2
InChIKey
State energy
1/cm
Equivalent to
1/cm
Radiative
Clear
Remove
Wavelength
500
502
nm
Equivalent Wavelength
Wavelength from 5000.000000000001 to 5020.0A
Upper state energy
1/cm
Equivalent to
1/cm
Lower state energy
1/cm
Equivalent to
1/cm
Probability, A
1/s
Find data
Save query
Legend
available, can answer
available, don't support query
unsupported keyword
Cologne Database for Molecular Spectroscopy: VAMDC-TAP service
ICB Dijon Methane
VALD (atoms)
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)
BASECOL: VAMDC-TAP interface
TOPbase : VAMDC-TAP interface
Theoretical spectral database of polycyclic aromatic hydrocarbons
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GSMA Reims S&MPO
GSMA Reims Ethylene
TAP-XSAMS for GhoSST database
Lund laboratory spectroscopy database
Stark-b
Spectr-W3
Water internet Accessible Distributed Information System
HITRAN-UCL resource
VALD sub-set in Moscow (obs)
KIDA: VAMDC-TAP interface

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Done

Modify query | Stop waiting | Save query

select * where (RadTransWavelength >= 5000.000000000001 AND RadTransWavelength <= 5020.0) AND ((AtomSymbol = 'Fe' AND IonCharge >= 0 AND IonCharge <= 2))

Comments

XSAMS processors

- BibTeX from XSAMS
- Table views of XSAMS
- Xsams2SME

Process | Result

XSAMS processor that converts XML document into the CSV-format wanted by Spectroscopy Made Easy (SME). This is one instance of a generic service for applying XSLT-stylesheets to XSAMS.

Name	Response	Download	Species	States	Processes	Radiative	Collisions	Non Radiative
VALD sub-set in Moscow (obs)	OK	XSAMS	3	406	301	301	0	0
TOPbase : VAMDC-TAP interface	OK	XSAMS	1	162	109	109	0	0
Spectr-W3	OK	XSAMS	2	8	4	4	0	0
Chianti	OK	XSAMS	1	4	2	2	0	0
Lund laboratory spectroscopy database	OK	XSAMS	0	0	0	0	0	0
VALD (atoms)	TRUNCATED (37%)	XSAMS	3	6076	15811	15811	0	0
Stark-b	EMPTY		0	0	0	0	0	0

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Done

Modify query | Stop waiting | Save query

select * where (RadTransWavelength >= 5000.0000000000001 AND RadTransWavelength <= 5020.0) AND ((AtomSymbol = 'Fe' AND IonCharge >= 0 AND IonCharge <= 2))

Comments

XSAMS processors

- BibTeX from XSAMS
- Table views of XSAMS
- Xsams2SME

Process | Result

General views of data in XSAMS format. The display is tabular and textual. Initial display is a list of states, with links to details of each state. An alternate display of radiative transitions is available.

Name	Response	Download	Species	States	Processes	Radiative	Collisions	Non Radiative
VALD sub-set in Moscow (obs)	OK	XSAMS	3	406	301	301	0	0
TOPbase : VAMDC-TAP interface	OK	XSAMS	1	162	109	109	0	0
Spectr-W3	OK	XSAMS	2	8	4	4	0	0
Chianti	OK	XSAMS	1	4	2	2	0	0
Lund laboratory spectroscopy database	OK	XSAMS	0	0	0	0	0	0
VALD (atoms)	TRUNCATED (37%)	XSAMS	3	6076	15811	15811	0	0
Stark-b	EMPTY		0	0	0	0	0	0

Single-state view of XSAMS

XSAMS Result:

Bvald-2012-06-13-12-6-50

Species

Isotope: ^{56}Fe

InChI=1S/Fe (XEEYBQQBJWHFJM-UHFFFAOYSA-N)

Ion charge: 0

State

State description:

Energy above ground state: 704.0070 1/cm

Lande factor: 1.50 unitless

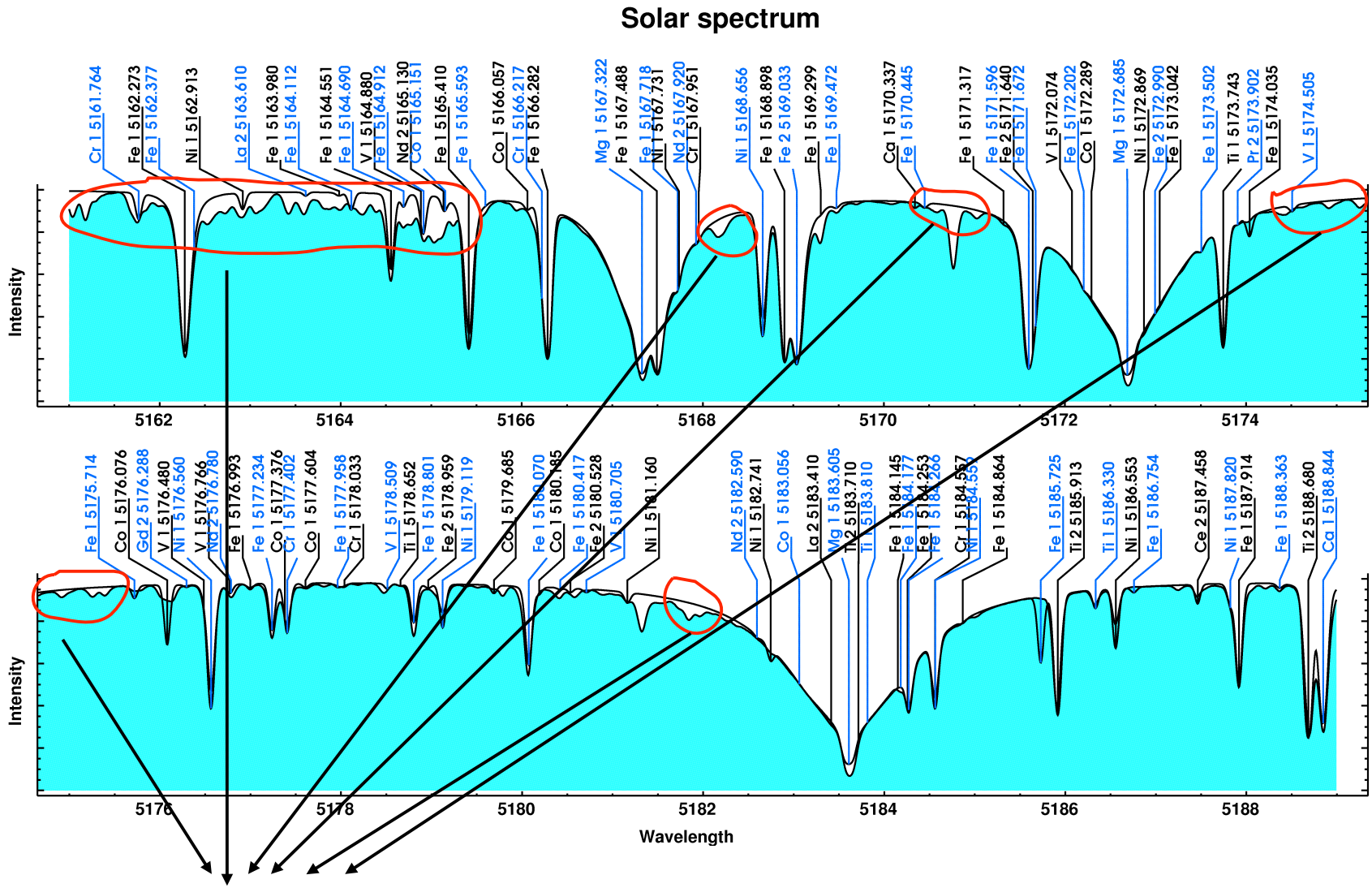
Quantum numbers for entire state: J = 2.0 parity = even

Electronic composition: $^{5}D_{2.0}$

SME Result:

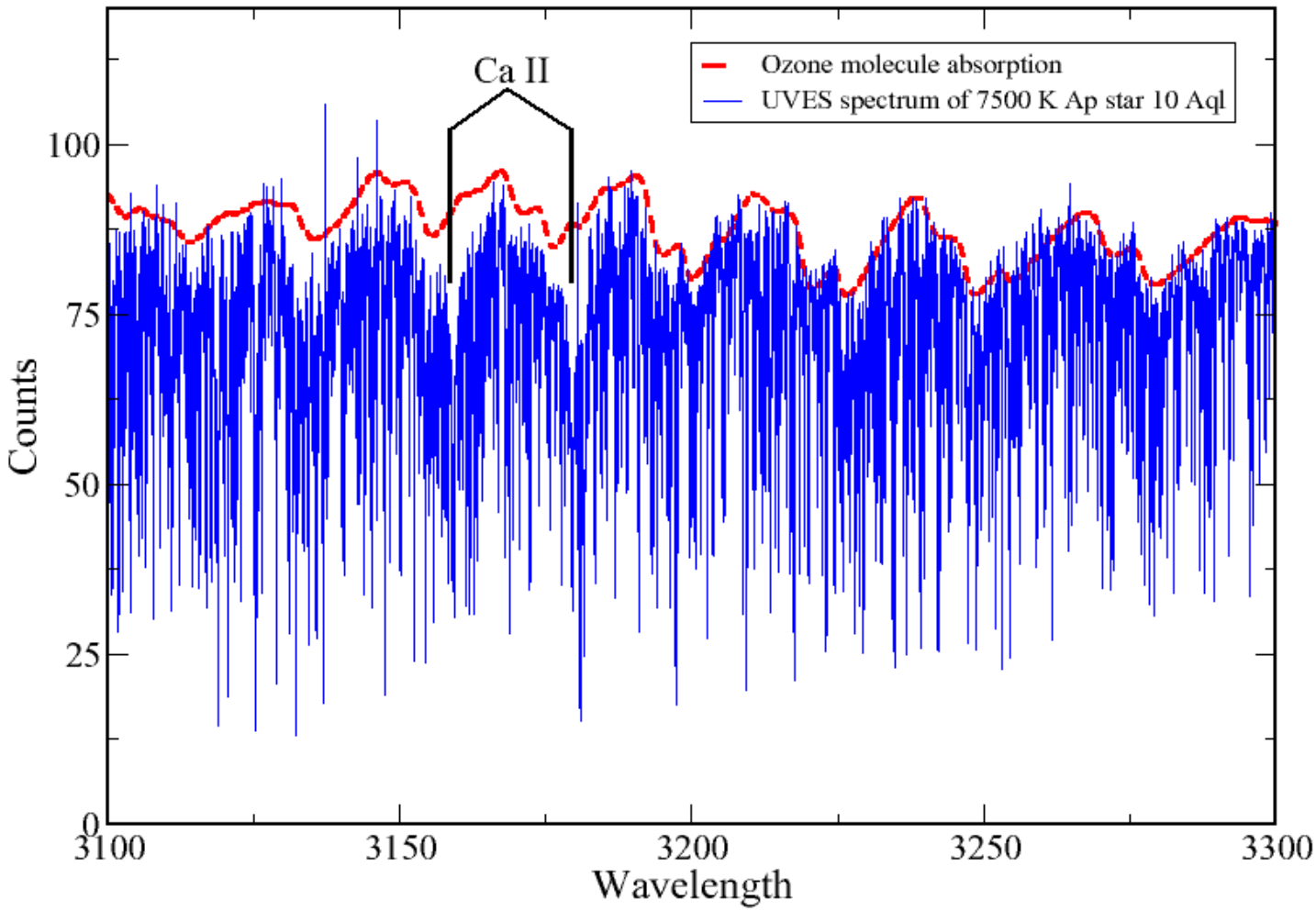
```
5001.9000, 5019.5000, 4,

'Fe 1', 5001.9000, 03.8810, 0.0, 0,0,0,    0.000, 0.000, 0.000, ''
'Fe 1', 5014.9000, 03.9426, 0.0, 0,0,0,    0.000, 0.000, 0.000, ''
'Fe 2', 5018.4000, 02.8903, 0.0, 0,0,0,    0.000, 0.000, 0.000, ''
'Fe 2', 5019.5000, 05.5681, 0.0, 0,0,0,    0.000, 0.000, 0.000, ''
```

Examples of mutual use of both atomic and molecular data in stellar spectroscopy.



C_2 → HITRAN? , atomic data → VALD

One needs to know ozone absorption (**S&MPO** database) to place properly a continuum level in A-type star.



... for more on VAMDC stay tuned for the next talk by Nigel Mason ...

...THANK YOU FOR YOUR TIME !