VAMDC: The Virtual Atomic and Molecular Data Centre: Recent Advances and Future Prospects

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Virtual Atomic and Molecular Data Centre (VAMDC)

• A set of standards and services for obtaining atomic and molecular data

• Focus (for now) on:
  • gas-phase spectroscopy,
  • collisions and
  • reactions

• Provides a single, online point of access to multiple database “nodes” (the portal)

www.vamdc.eu
VAMDC Standards

1. A standardized **query language** (**VSS2**)  

- Based on Structured Query Language (SQL)  
- Used as a parameter to a “GET” query in a URL, e.g.  
  http://www.example.com/?query=SELECT States WHERE StoichiometricFormula="CO2"  
- Defines “keywords” for types of data (**returnables**) and search parameters (**restrictables**)
VAMDC Standards

2. A standardized **data format** *(XSAMS 1.0)*

- Data from different databases can be compared, aggregated, etc.
- An XML-based format: a valid XSAMS document must conform to the XSAMS **Schema**
- *Requires* data to have units and sources (for citation): **data provenance**
- *Encourages* specification of errors and uncertainties: **data integrity**
VAMDC Standards

2. A standardized **data format** (**XSAMS**) 

- Standard overseen by the **IAEA** (Atomic and Molecular Data Division)
- Verbose (because XML) ...
- .... but compresses well (typically 40x)
- “self-describing”
- “self-validating” (to some extent)
VAMDC Standards

3. Standards for identifying species - i.e. specific isotopes of atoms or ions; specific isotopologues of molecules

- InChI = IUPAC International Chemical Identifier, e.g. $^{13}$C$^{16}$O$_2$ is:
  \[
  \text{InChI}=1S/\text{CO2}/c2-1-3/i1+1
  \]
- The InChIKey is a 27-character hash on the species’ InChI identifier: this InChI becomes \text{CURLTUGMZYLDI-OUBTZVSYSA-N}
- Allows **unambiguous** and **unique** identification of species
VAMDC Standards

4. Standards for describing database nodes

• An (XML) Registry (meta-database)
• Each database can communicate:
  • what data it contains
  • what search query parameters it supports
  • when it was last updated
  • who maintains it
  • where it is hosted
  • etc.
A VAMDC database node is an online service which:

1. Can understand the VAMDC query language, VSS2
2. Will return data in valid XSAMS format
3. Is listed with the VAMDC registry
Database “Nodes”

There are currently 27 active database nodes, including:

• **VALD** - a major database of atomic and small-molecule spectroscopic line parameters (focus: astronomy and astrophysics)

• **HITRAN** - the major database of molecular spectroscopic line parameters for planetary atmospheres

• **BASECOL** - database of atomic and molecular collisional cross sections

• **CDMS / JPL** - microwave/ FIR line parameters for interstellar spectroscopy

• **KIDA** - astrochemical kinetic database
Data Permanence

transID

L1-H2O-1
L2-H2O-1
L3-H2O-1
L8124-H2O-1
L4-H2O-1
L5-H2O-1
L8125-H2O-1
L6-H2O-1
L7-H2O-1
L8-H2O-1
L9-H2O-1

Wednesday, 4 September 13
Data Permanence

“ValidOn” = “4 Feb 13”
Data Permanence

“ValidOn” = “14 Jul 13”

transID

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<th>Dec 12</th>
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</tbody>
</table>
User makes query at portal website.

VAMDC Portal

Databases
VAMDC Portal

User

XSAMS data files

VAMDC Portal

XSAMS data files

[No Data]

Databases

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VAMDC Portal

User

e.g. csv data files

Portal Data Processor

VAMDC Portal

XSAMS data files

Databases

[No Data]
### Line-list view of XSAMS

(Switch to view of states or collisions)

Assume* all wavelengths are in vacuum and Convert to air (at IAU STP).

Assume all wavelengths are in air (at IAU STP) and Convert to vacuum.

<table>
<thead>
<tr>
<th>Species</th>
<th>$\lambda/v/n/E$</th>
<th>Probability</th>
<th>Upper state</th>
<th>Lower state</th>
<th>Broadening/shifting</th>
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<tbody>
<tr>
<td>(12C)(16O)</td>
<td>n=2002.115 1/cm</td>
<td>A=28.85</td>
<td>5582.0901 1/cm — X $v = 2 J = 26$</td>
<td>3579.9751 1/cm — X $v = 1 J = 27$</td>
<td>Detail</td>
</tr>
<tr>
<td>(12C)(16O)</td>
<td>n=2003.6679 1/cm</td>
<td>A=14.46</td>
<td>4027.0394 1/cm — X $v = 1 J = 31$</td>
<td>2023.3715 1/cm — X $v = 0 J = 32$</td>
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<tr>
<td>(12C)(16O)</td>
<td>n=2006.7836 1/cm</td>
<td>A=29.08</td>
<td>5484.3687 1/cm — X $v = 2 J = 25$</td>
<td>3477.5851 1/cm — X $v = 1 J = 26$</td>
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<td>(12C)(16O)</td>
<td>n=2008.5254 1/cm</td>
<td>A=14.57</td>
<td>3909.6562 1/cm — X $v = 1 J = 30$</td>
<td>1901.1308 1/cm — X $v = 0 J = 31$</td>
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<td>n=2011.4211 1/cm</td>
<td>A=29.29</td>
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<td>A=14.68</td>
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<td>A=29.51</td>
<td>5300.1117 1/cm — X $v = 2 J = 23$</td>
<td>3284.0845 1/cm — X $v = 1 J = 24$</td>
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<td>A=14.79</td>
<td>3686.1197 1/cm — X $v = 1 J = 28$</td>
<td>1667.9709 1/cm — X $v = 0 J = 29$</td>
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<td>(12C)(16O)</td>
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<td>A=29.73</td>
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</table>
Advanced VAMDC Services

User \( \rightarrow \) Sets Parameters \( \rightarrow \) Code

Databases
Advanced VAMDC Services

User → Sets Parameters → Code

VSS2 queries

Databases
Advanced VAMDC Services

User  Sets Parameters  Code

Data Returned

Databases
Advanced VAMDC Services

User → Sets Parameters → Code → Databases

Data Returned

Flowchart:
- Start
- Process step 1
- Decision?
  - Choice 1
  - Choice 2
- Process step 2
- Process step 3
- Process step 4
- Process step 5
- Process step 6
- A
- End

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Advanced VAMDC Services

User Sets Parameters → Code

Databases

Start
→
Process step 1

Decision?
→
Choice 1
→
Process step 2

Choice 2
→
Process step 4
→
Process step 5
→
Process step 6

End

A
→
Process step 3

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Spectroscopy Made Easy

• Steps involved:
  1. Query VAMDC databases
  2. Convert XSAMS to SME line list format
  3. Start SME
  4. Import Observed stellar spectra
  5. Import SME line list
  6. Run SME
  7. Visualize the results
  8. Store fitted atomic abundances, etc.
Spectroscopy Made Easy

• For fitting spectra of stellar atmospheres

• Goal: Deriving stellar parameters from observations

• Data and tools involved:
  - Atomic and molecular data
  - Stellar models
  - Spectral synthesis
  - RT solver
  - SME
  - EOS
  - Opacities
  - VAMDC

Stellar parameters
Spectral synthesis

14/05/2013
Further Progress: SUP@VAMDC

• More databases (e.g. ALADDIN, coming soon)
• More users!
• More tools for converting between data formats (and units)
• Easier tools for reading XSAMS and using in existing codes
• Further data validation
• Expand standards to:
  • particle-surface interactions
  • solid-state properties of materials
  • theoretical calculations
SUP@VAMDC: Goals

• Dissemination
  • Non-EU research community
  • Education
  • Citizen Scientists

• Tutorials
  • Implementing a database node
  • Using the VAMDC infrastructure

• Expansion to other areas of Physics:
  • electron-molecule collisions
  • surface-particle interactions
  • radiation damage
Acknowledgements

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