Online database services for atomic and molecular data

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Atomic and molecular data resources

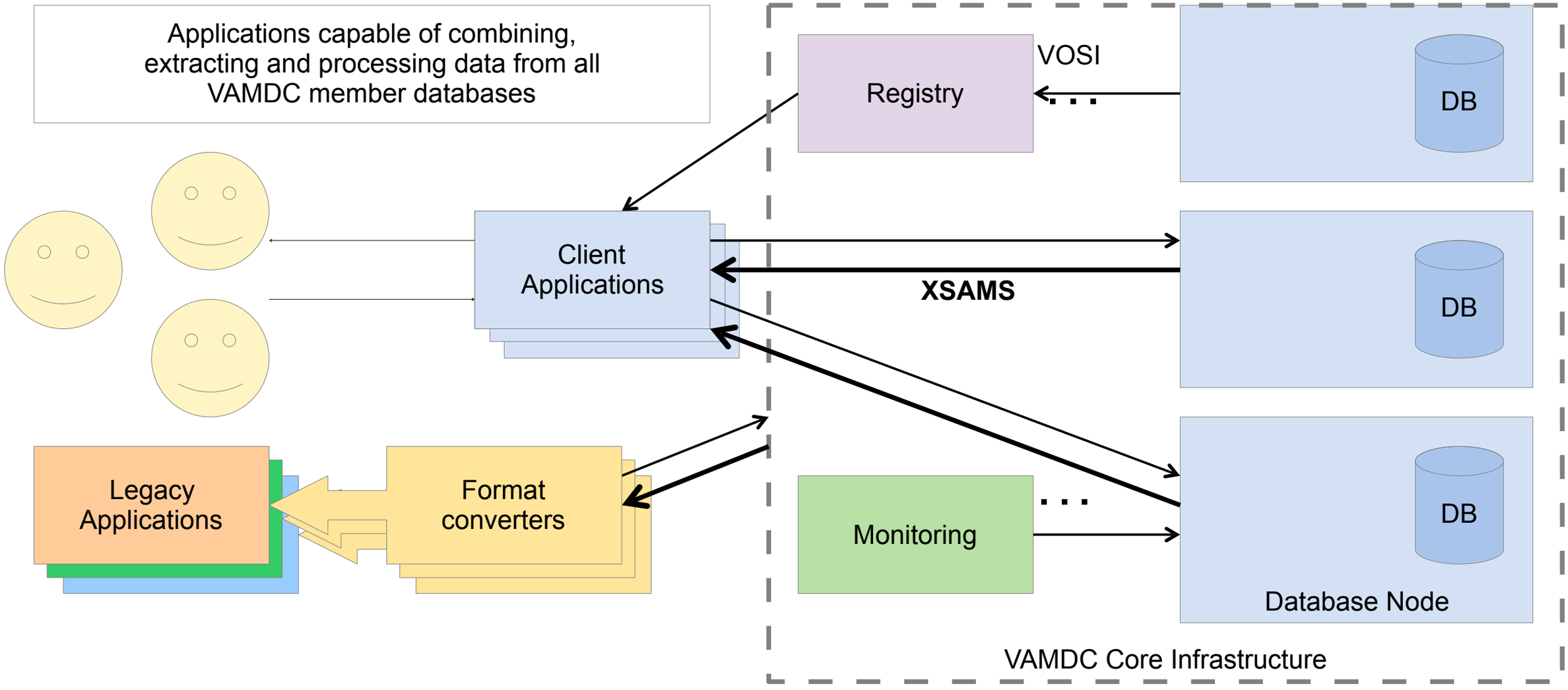
- **VAMDC** — Virtual Atomic and Molecular Data Centre
- **ExoMol** — High-temperature molecular line lists for exoplanet and cool star atmospheres
- **Aladdin** — IAEA database of electron / photon / heavy particle / surface collisional cross sections
- **QDB** — Quantemol database of chemistries for low-temperature plasma research
- **HITRANonline** — Transition line lists for atmospheric molecular spectroscopy

VAMDC — Virtual Atomic and Molecular Data Centre

http://vamdc.eu/

- Standards and services for interchange of AM data
- “Portal” service for online access to multiple databases with a single query
- XSAMS data format for standardised representation of AM data
- “Node” software for hosting AM data

VAMDC Infrastructure



VAMDC — Queries with VSS2

- VSS2 is an “SQL-like” query language for requesting data from VAMDC-compliant databases

- Example 1: Data on Mn^{+}, Mn, Mn^{-}, Mn^{-2}, …

```
SELECT Species WHERE AtomNuclearCharge = 25 AND
                     AtomIonCharge < 2
```

- Example 2: All data on He^{z} + $O^{z'}$ → Products

```
SELECT * WHERE reactant0.atomsymbol="He" and
               reactant1.atomsymbol="O"
```

VAMDC — The VSS2 API

- Submitting VSS2 queries to an online database as a “GET” request.

- Example: All data on He^{z} + $O^{z'}$ → Products

```
http://aladdin2.xnx.webfactional.com/node/tap/sync//
                    node/tap/sync/?
REQUEST=doQuery&LANG=VSS2&FORMAT=XSAMS&QUERY=SELECT *
          WHERE reactant0.atomsymbol="He" AND
                reactant1.atomsymbol="O"
```

Returns an XSAMS document to the user

VAMDC — The VAMDC Portal

http://portal.vamdc.eu/

- Building VSS2 queries through a user-friendly interface in a browser
- Recent developments: “Guided Query” http://portal.vamdc.org/vamdc_portal/queryTree.seam
- Example: CO_2 absorption in 15 μm band
  - Select “For radiative process”
  - Select Wavelength=“14 — 16 um”
  - Select “Number of molecules”=1
  - Search for “Stoichiometric Formula”=CO2
  - Click “Submit query and find data”

VAMDC — The XSAMS format

http://standards.vamdc.org/

- An XML-based format for the transmission of AM data
- Originally conceived at the IAEA
- Developed and refined over 5 years of the VAMDC project
- “A consistent, self-describing format designed to promote good practice”:
  - units
  - uncertainties
  - data source attribution
  - time-stamping
  - …

VAMDC — The XSAMS format

- Atomic States
- Molecular States
- Radiative Processes
- Collisional Processes
- “Environments”
- Functions with parameters and arguments
- Sources
- “Methods” (experimental, theoretical, …)
- Data tables, references to external files

VAMDC — The XSAMS format

- Example XSAMS snippet:

```
<AtomicState stateID="Schianti-1001006">
<Description>2s2 2p</Description>
<AtomicNumericalData>
   <StateEnergy methodRef="Mchianti-EXP">
      <Value units="1/cm">63.4</Value>
      <Evaluation recommended="true">
          <Quality>A+</Quality>
      </Evaluation>
      <Accuracy type="statistical" relative="False">0.2</Accuracy>
   </StateEnergy>
</AtomicNumericalData>
<AtomicQuantumNumbers>
   <TotalAngularMomentum>1.5</TotalAngularMomentum>
</AtomicQuantumNumbers>
<AtomicComposition>
...
```

VAMDC — The XSAMS format

- Example XSAMS snippet (molecular state):

```
<MolecularState stateID="S14-H2O-1">
   <Description>A state of H2(16O)</Description>
   <MolecularStateCharacterisation>
      <StateEnergy>
         <Value units="1/cm”>1813.223400</Value>
      </StateEnergy>
      <TotalStatisticalWeight>69</TotalStatisticalWeight>
   </MolecularStateCharacterisation>
   <nltcs:QNs>
      <nltcs:ElecStateLabel>X</nltcs:ElecStateLabel>
      <nltcs:J>11</nltcs:J>
      <nltcs:Ka>3</nltcs:Ka>
      <nltcs:Kc>8</nltcs:Kc>
      <nltcs:v1>0</nltcs:v1>
      <nltcs:v2>0</nltcs:v2>
      <nltcs:v3>0</nltcs:v3>
   </nltcs:QNs>
</MolecularState>
```

VAMDC — Databases producing XSAMS output

- Atomic Spectroscopy:
  - NIST
  - VALD
- Molecular Spectroscopy
  - CDMS
  - HITRAN
- Scattering and Reactions
  - KIDA
  - BASECOL
  - IDEADB
  - LXcat
  - UMIST

VAMDC — The XSAMS format

- Advantages
  - Self-validating (to some extent)
  - Text-based: no encoding issues
  - XML-parsing tools exist

- Disadvantages
  - Verbose, large files
  - Complex to write and read
  - Conversion tools?
  - Adoption by AM community?

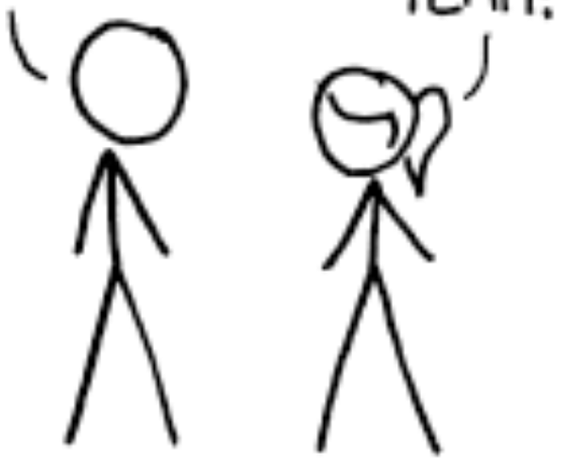
VAMDC — More recent developments

- **29 databases** connected to the portal, including: BASECOL, CDMS, HITRAN, Chianti, LXCat, NIST Atomic Spectra Database, VALD
- **New output formats** from XSAMS:
  - BibTeX citations
  - HTML table view
  - XSAMS2SME (“Spectroscopy Made Easy”)
- **Time-stamping** (Last database update)
- **Direct editing** of VSS2 query

HOW STANDARDS PROLIFERATE:
(SEE: A/C CHARGERS, CHARACTER ENCODINGS, INSTANT MESSAGING, ETC)

SITUATION: THERE ARE 14 COMPETING STANDARDS.

14?! RIDICULOUS! WE NEED TO DEVELOP ONE UNIVERSAL STANDARD THAT COVERS EVERYONE'S USE CASES.



SOON:

SITUATION: THERE ARE 15 COMPETING STANDARDS.

ExoMol — High-temperature molecular line lists

http://exomol.com/

- Ab initio calculations of energy levels and Einstein *A* coefficients
- For high-*T*, one has to consider many transitions, even for small molecules:
  - $^{12}C^{32}S$: 1.99×10^5 transitions
  - $^{51}V^{16}O$: 2.77×10^6 transitions
  - $^{12}C^{1}H_4$: 9.82×10^9 transitions
  - $^{31}P^{1}H_3$: 1.68×10^{10} transitions
  - … and more to come (SO_3, H_2CO, …)

ExoMol — Data Format

- XSAMS is a non-starter with 10^{10} transitions
- Data provided in compressed, plain-text files
- Separate out the states from the transitions, e.g. CH_4:

States
[8.19×10^6]

ID	*E*	*J*	*g*	QNs
1	…			
2	…			
3	…			

Transitions
[9.82×10^{10}]

ID’	ID”	*A*
1	2	…
1	3	…
2	3	…
1	4	…

ExoMol — API

- All ExoMol-calculated data is available at URLs with a defined format:

  http://www.exomol.com/db/<molec>/<iso>/<dataset>/<iso>__<dataset>.<ext>

  - <molec>: Molecular formula
  - <iso>: Isotopologue formula in “slug” form
  - <dataset>: Name of the calculation dataset
  - <ext>: File extension indicating data type

e.g. Partition function for $^{12}C^{1}H_4$ (“YT10to10” data set)

http://www.exomol.com/db/CH4/12C-1H4/YT10to10/12C-1H4__YT10to10.pf

ExoMol — API

- Machine-readable definitions files:
  - `exomol.all`:
    - always available at http://www.exomol.com/db/exomol.all
    - summarises current status of data availability
    - can be easily checked for updates, new line lists, etc.
  - "Definitions" files (`<iso>__<dataset>.def`) provide definitions for fields in dataset files
    - Quantum numbers used
    - Maximum temperature
    - Wavenumber range
    - Availability of cooling functions, broadening coefficients, …

ExoMol — Derived Data

- Astronomers often can't use very large line lists, so we provide:
  - Calculated absorption cross sections at 0.01 cm^{-1} grid spacing …
  - … and an online service for binning down to lower resolutions
  - *k*-coefficient tables

ExoMol — High-temperature molecular line lists

- Uncertainties are only estimates…
- … except where energy levels can be replaced by experimental values (e.g. MARVEL) …
- … and in many cases the intensities are expected to be more accurate than experiment
- As yet, no attempt has been made to quantify uncertainties in cross sections or *k*-coefficients.

QDB — Quantemol database of “chemistries” for plasma research

- Under development as a commercial product…
- … with a free data-access component and paid-for “value-added” content
- Calculated and experimental data on:
  - Electron collision cross sections
  - Heavy-particle collisional processes
  - Radiative processes in plasmas (to come)

QDB — Quantemol database of “chemistries” for plasma research

- Validation of data sets by:
  - Experimental benchmarking from open sources
  - Calculations performed for a range of models (HPEM, Global_Kin, ChemKin, …)
  - User-contributed assessment and comments
  - Validation of entire chemistries by comparison with experiment

QDB — Quantemol database of “chemistries” for plasma research

- Data formats
  - Where possible, collision cross sections are provided as a function of electron energy (text table format)
  - Heavy-particle processes described by a set of Arrhenius-like parameters:

$$k(T) = A\left(\frac{T}{T_{\mathrm{ref}}}\right)^{n} \exp\left(-\frac{E}{k_{\mathrm{B}}T}\right)$$

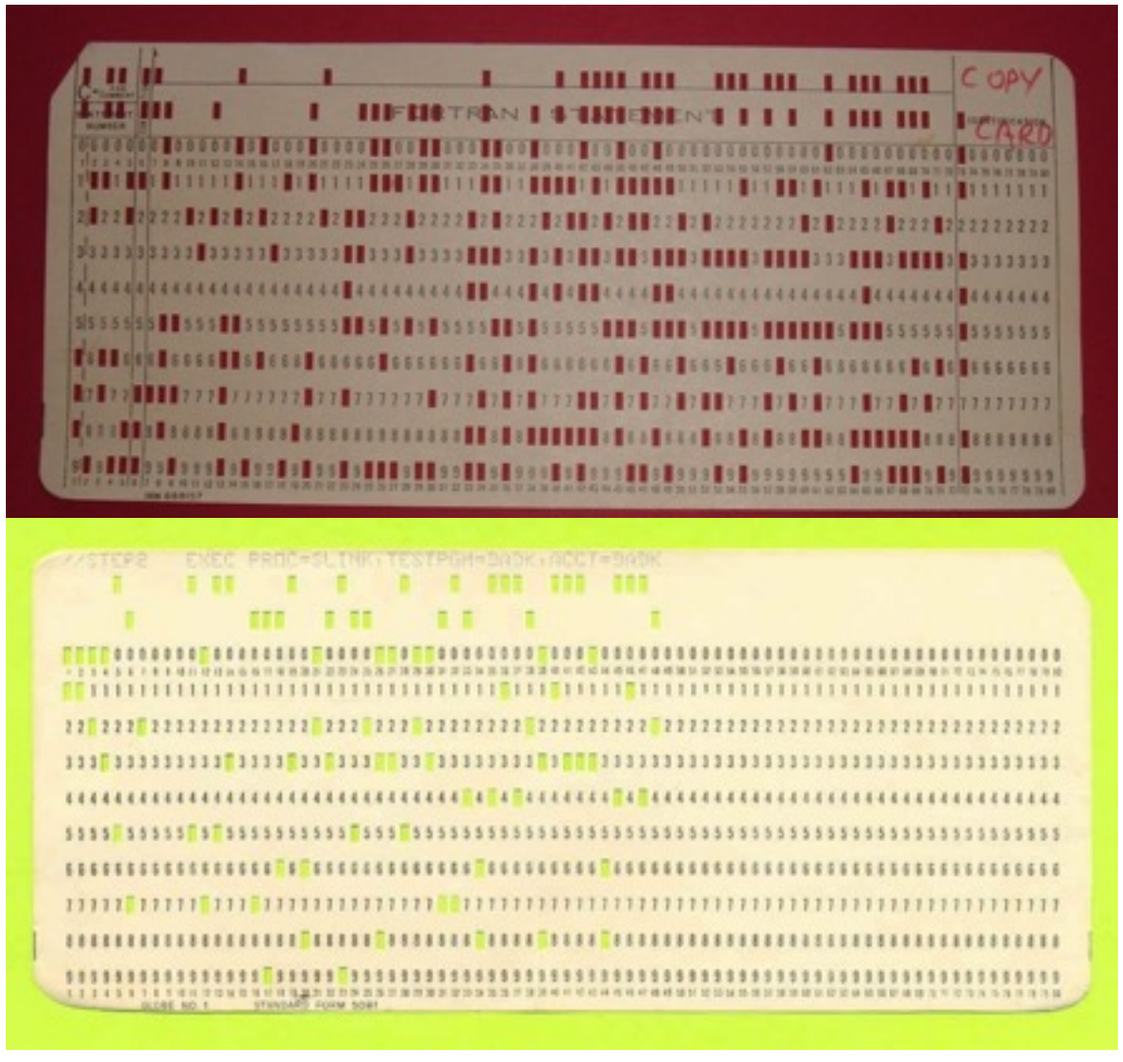
  - Individual data sets are not large…
  - … but there may be a great many of them (especially for state-resolved processes involving molecules)

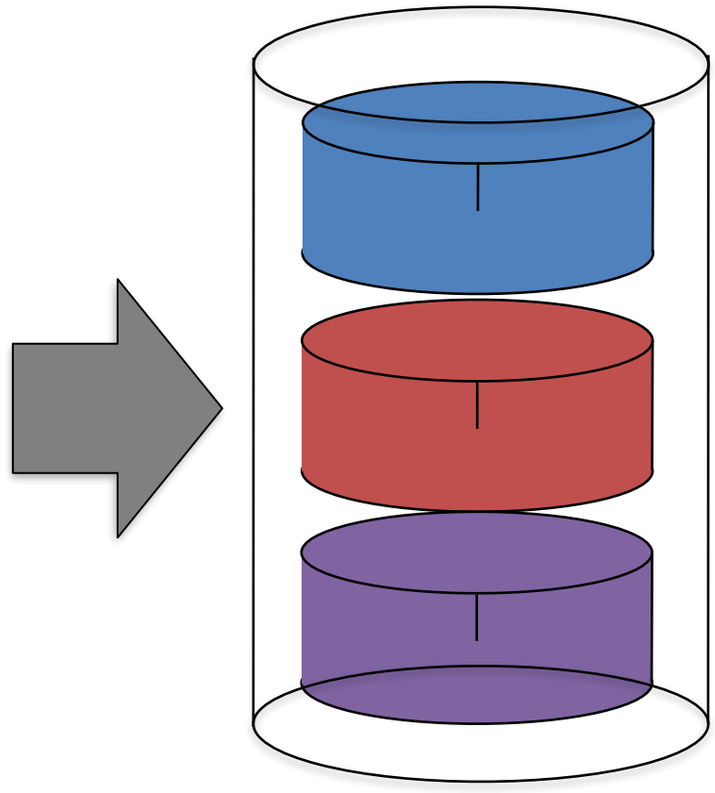
HITRAN*online*

http://hitran.org/

- Molecular transition line lists for modelling planetary atmospheres (especially Earth's)
- Fixed-width 160 character format since 2004
- Data moved to relational database format during VAMDC project
- New format allows an arbitrary number of parameters, quantum assignments, etc.
- Original references / sources

HITRAN*online*





HITRAN*online*

http://hitran.org/

- New interface allows users to create, edit and save their own output formats
- HITRANonline also functions as a VAMDC node, and produces valid XSAMS documents
- HAPI (HITRAN Application Programming Interface) provides a Python library for manipulating HITRAN data, creating plots, etc. programmatically

Conclusions

- You can’t force users to adopt new standards
- Sustainability is crucial
- Provide software tools for interconversion between data formats that are actually used
- Visualisation is nice
- Data should have provenance and be easy to cite / attribute