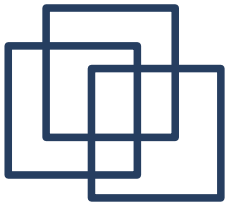


MOL-D

A COLLISIONAL DATABASE AND WEB SERVICE WITHIN THE VIRTUAL ATOMIC AND MOLECULAR DATA CENTER

Veljko Vujčić
Astronomical Observatory Belgrade

The data

- Photo-dissociation cross-sections for the individual ro-vibrational states (a pair of quantum numbers J and v) of diatomic molecular ions
- Ro-vibrational energy for the corresponding state
- 423 states for H_2^+, 833 for He_2^+
- Data for 25 discrete wavelengths (A):

50 60 70 80 90 100 200 300 400 500 600 700 800 900 1000 1100 1200 1300 1400 1500 1600 1700 1800 1900 2000

The physics

- Theoretical calculations (photon + molecular ion = atom + ion)

$$h\nu + A_2^+ \Longleftrightarrow A + A^+$$

- The cross-sections for the photodissociation of individual ro-vibration state of the considered molecular ions are determined in the dipole approximation

$$\sigma_{J,v}(\lambda) = \frac{8\pi^3}{3\lambda}\left[\frac{(J+1)|D_{E,J+1;v,J}|^2 + J|D_{E,J-1;v,J}|^2}{2J+1}\right]$$

- Mihajlov and coworkers (Mihajlov & Dimitrijevic 1986; Mihajlov et al. 1993, 2007; Ignjatovic et al. 2009, 2014b; Sreckovic et al. 2014)

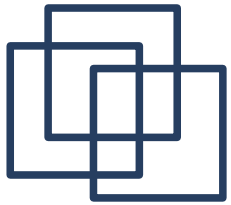
Physics (2)

- Corresponding average thermal cross-sections are given by:

$$\sigma_{\mathrm{ph}}(\lambda, T) = \frac{1}{Z} \sum_{J} \sum_{v} g_{J;v}(2J+1) e^{-\frac{E_{Jv}-E_{00}}{k_{\mathrm{B}}T}} \sigma_{J,v}(\lambda)$$

Importance

- Hydrogen and helium molecular ion data are important for calculation of solar and stellar atmosphere models and for radiative transport, as well as for kinetics of other astrophysical and laboratory plasma (i.e. early Universe).



How to get from this...

\sigma_{n,l}(\lambda) [cm^{4} s]

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0	3	0.545616E-23	0.717607E-20	0.156951E-18	0.108960E-17	0.207899E-17	0.996591E-18	0.122416E-21	0.169588E-17	0.287983E-20	0.180364E-24	0.153206E-30	0.000000E+00	0.000000E+00	0.000000E+00
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0	11	0.106395E-23	0.211846E-18	0.772224E-18	0.395282E-19	0.616475E-18	0.132813E-18	0.806793E-18	0.131352E-17	0.244558E-17	0.367176E-17	0.304861E-17	0.191902E-17	0.390149E-17	0.120941E-16
0	12	0.316589E-22	0.233828E-18	0.674704E-18	0.747455E-21	0.606459E-18	0.158131E-19	0.111401E-17	0.176948E-17	0.419954E-18	0.672522E-18	0.378910E-17	0.149535E-17	0.522588E-17	0.218437E-19
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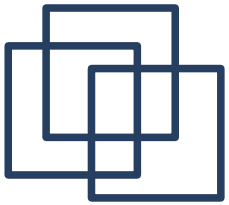

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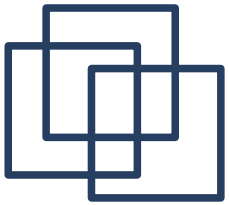


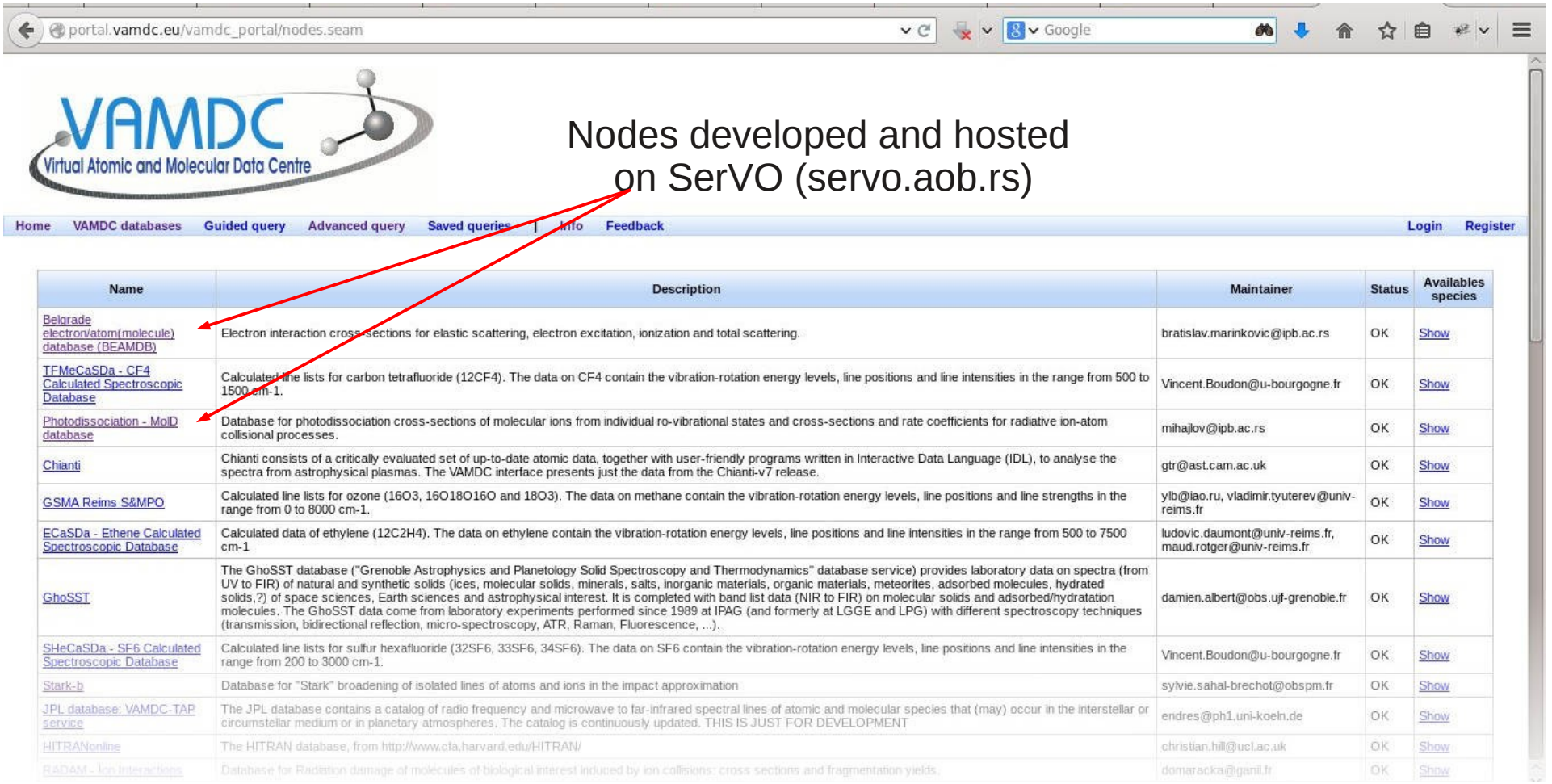
...and why?

- Fully annotated, interconnected data
- Standardized representations of species, states and their properties
- Metadata on scientific sources
- Machine readable format (human too if needed)
- Apply XSL transformations to any format (HTML, SME...)
- Convert to objects
- Interoperability

VAMDC philosophy

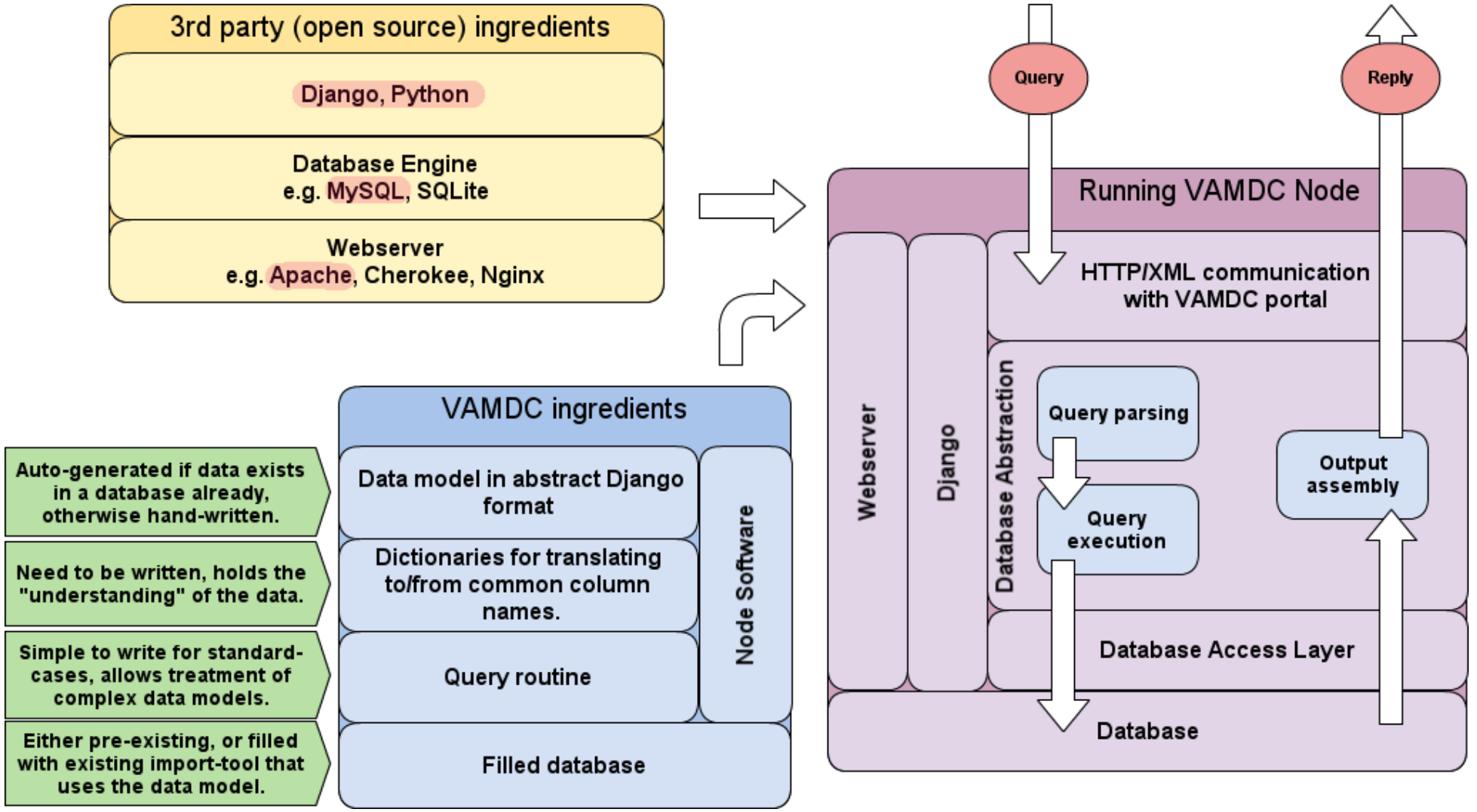
- Local providers expose data through standardized web services ('nodes')
- Central repository holds list of nodes and executes distributed, aggregate queries.
- Available as a web portal / SOAP web service / Astrogrid VODesktop / Java library
- Extensions of IVOA protocols (VAMDC-TAP), XML standard for data represantation (XSAMS)
- Transform data for further analysis (“processors”)

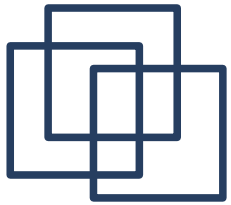
VAMDC Nodes



Name	Description	Maintainer	Status	Availables species
Belgrade electron/atom(molecule) database (BEAMDB)	Electron interaction cross-sections for elastic scattering, electron excitation, ionization and total scattering.	bratislav.marinkovic@ipb.ac.rs	OK	Show
TFMeCaSDa - CF4 Calculated Spectroscopic Database	Calculated line lists for carbon tetrafluoride (12CF4). The data on CF4 contain the vibration-rotation energy levels, line positions and line intensities in the range from 500 to 1500 cm-1.	Vincent.Boudon@u-bourgogne.fr	OK	Show
Photodissociation - MolD database	Database for photodissociation cross-sections of molecular ions from individual ro-vibrational states and cross-sections and rate coefficients for radiative ion-atom collisional processes.	mihajlov@ipb.ac.rs	OK	Show
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	Show
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	Show
ECaSDa - Ethene Calculated Spectroscopic Database	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	Show
GhoSST	The GhoSST database ("Grenoble Astrophysics and Planetology Solid Spectroscopy and Thermodynamics" database service) provides laboratory data on spectra (from UV to FIR) of natural and synthetic solids (ices, molecular solids, minerals, salts, inorganic materials, organic materials, meteorites, adsorbed molecules, hydrated solids,?) of space sciences, Earth sciences and astrophysical interest. It is completed with band list data (NIR to FIR) on molecular solids and adsorbed/hydratation molecules. The GhoSST data come from laboratory experiments performed since 1989 at IPAG (and formerly at LGGE and LPG) with different spectroscopy techniques (transmission, bidirectional reflection, micro-spectroscopy, ATR, Raman, Fluorescence, ...).	damien.albert@obs.ujf-grenoble.fr	OK	Show
SHeCaSDa - SF6 Calculated Spectroscopic Database	Calculated line lists for sulfur hexafluoride (32SF6, 33SF6, 34SF6). The data on SF6 contain the vibration-rotation energy levels, line positions and line intensities in the range from 200 to 3000 cm-1.	Vincent.Boudon@u-bourgogne.fr	OK	Show
Stark-b	Database for "Stark" broadening of isolated lines of atoms and ions in the impact approximation	sylvie.sahal-brechot@obspm.fr	OK	Show
JPL database: VAMDC-TAP service	The JPL database 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. THIS IS JUST FOR DEVELOPMENT	endres@ph1.uni-koeln.de	OK	Show
HITRANonline	The HITRAN database, from http://www.cfa.harvard.edu/HITRAN/	christian.hill@ucl.ac.uk	OK	Show
RADAM - Ion Interactions	Database for Radiation damage of molecules of biological interest induced by ion collisions: cross sections and fragmentation yields.	domaracka@ganil.fr	OK	Show

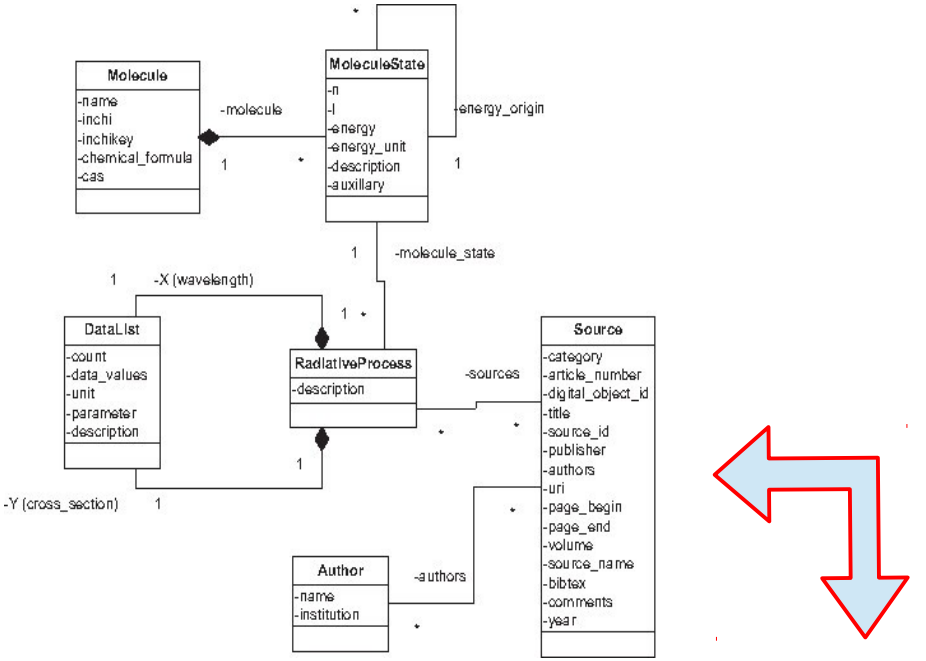
VAMDC NodeSoftware





Django is convenient

- Write static structure (models.py), django generates db for you
- OR
- Generate models from existing db
- Decide how to describe your data in XSAMS schema (dictionaries.py)
- Map models to XSAMS via queryfunc.py (it's ok for models to be incompatible with XSAMS schema)

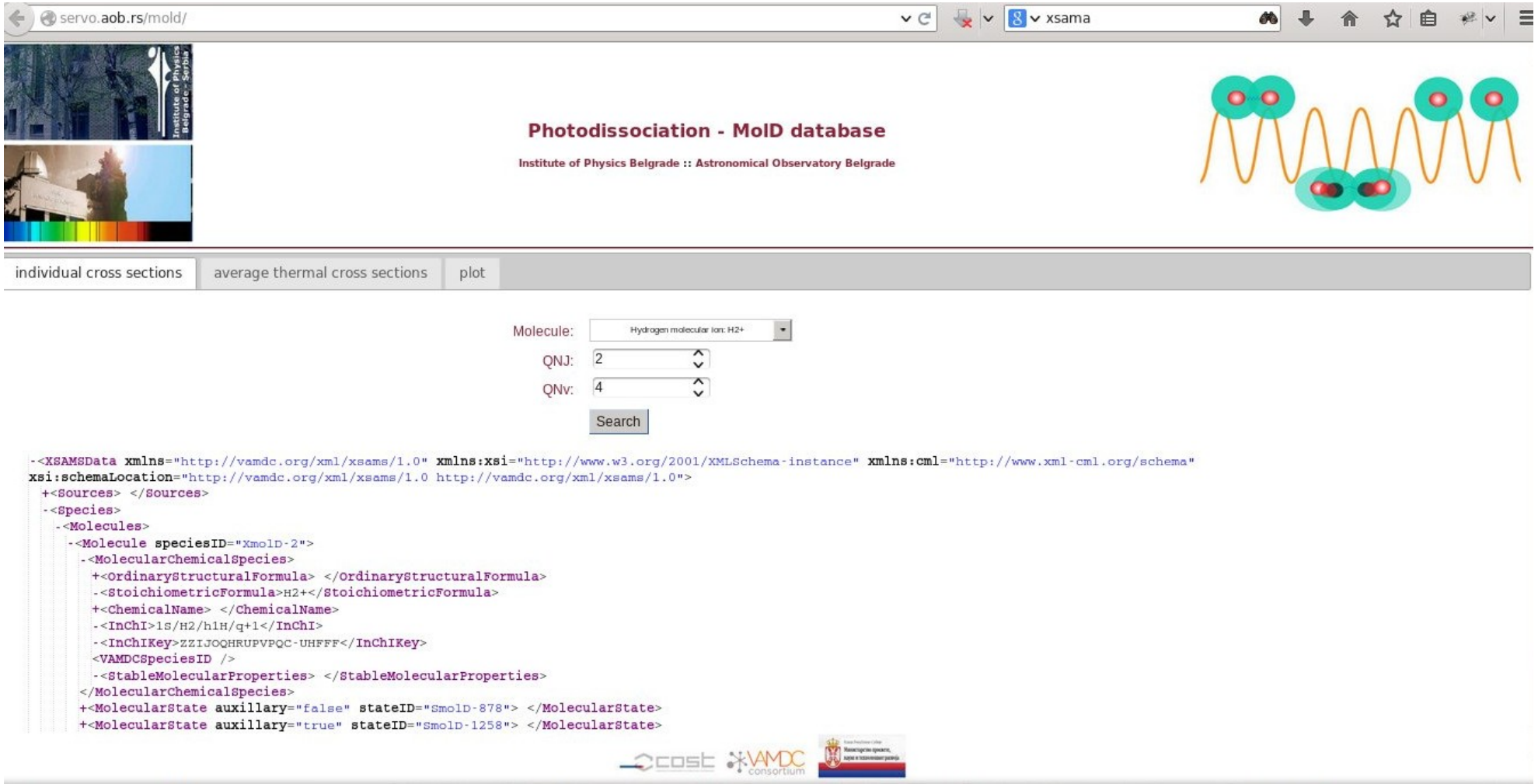



```python
from django.db import models

class Molecule(models.Model):
    name = models.CharField(max_length=32, db_index=True)
    inchi = models.CharField(max_length=256)
    inchikey = models.CharField(max_length=20)
    chemical_formula = models.CharField(max_length=128)
    cas = models.CharField(max_length=128, null=True, blank=True)
    def __unicode__(self):
        return "%s: %s" % (self.name, self.chemical_formula )
    class Meta:
        db_table = u'molecules'

class MoleculeState(models.Model):
    energy_origin = models.ForeignKey('self', null=True)
    n = models.PositiveSmallIntegerField(null=True, blank=True)
    l = models.PositiveSmallIntegerField(null=True, blank=True)
    energy = models.CharField(max_length=128, null=True, blank=True)
```

Web service & web interface

- http://servo.aob.rs/mold
- VAMDC asks only for a standard-compliant and validated web service
- Build more stuff on top of Django/Python
- Easy template / url handling
- AJAX – enabled interface

xsams


servo.aob.rs/mold/
xsama
Photodissociation - MolD database
Institute of Physics Belgrade :: Astronomical Observatory Belgrade
individual cross sections
average thermal cross sections
plot
Molecule:
Hydrogen molecular ion: H2+
QNJ:
2
QNv:
4
Search
-<XSAMSData xmlns="http://vamdc.org/xml/xsams/1.0" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns:cml="http://www.xml-cml.org/schema"
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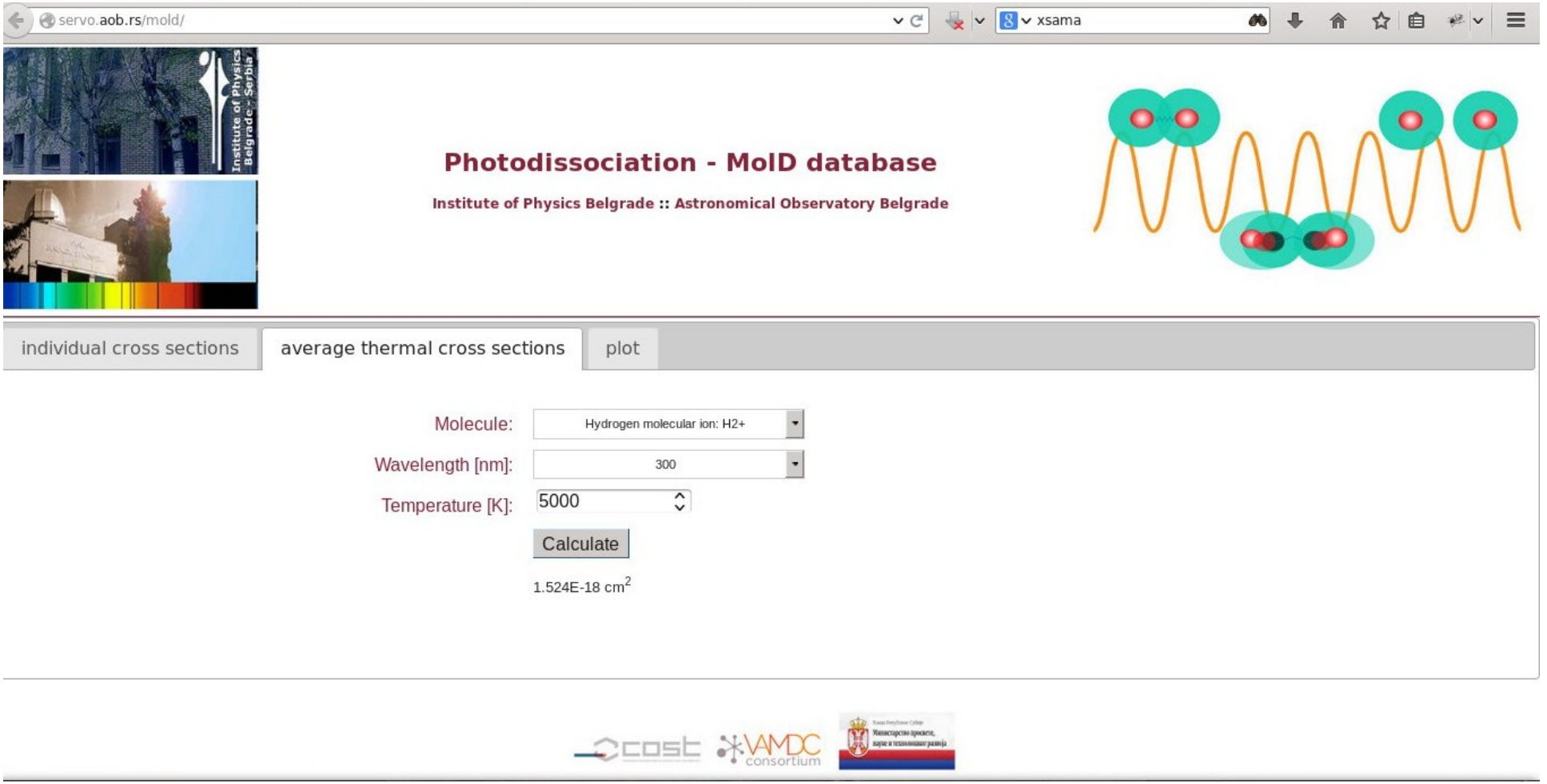
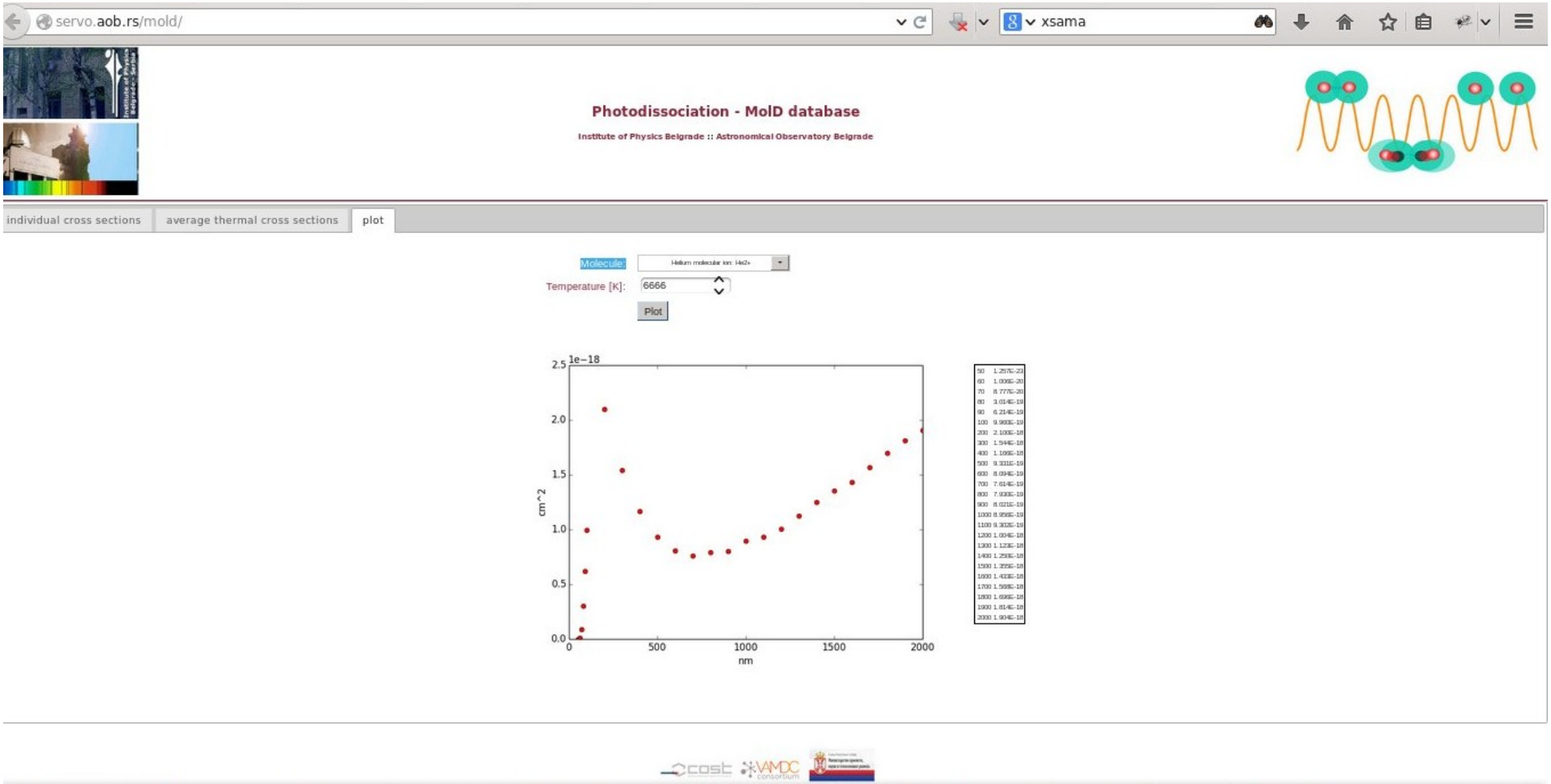
+<MolecularState auxillary="true" stateID="SmolD-1258"> </MolecularState>
cost
VAMDC
consortium

avg thermal cs's



plot


servo.aob.rs/mold/
xsama
Photodissociation - MolD database
Institute of Physics Belgrade :: Astronomical Observatory Belgrade
individual cross sections
average thermal cross sections
plot
Molecule:
Helium molecular ion: He2+
Temperature [K]:
6666
Plot
1e−18
cm^2
nm
0.0
0.5
1.0
1.5
2.0
2.5
0
500
1000
1500
2000

Further development

- Include new data about processes which involve species such as HeH^+, LiH^+, NaH^+, SiH^+ which are important for the early universe chemistry, the stellar and solar atmosphere modeling.
- Results of the rate coefficients for the ion-atom absorption processes and inverse emission processes
- Inclusion of the rate coefficients for the chemi-ionization in atom-Rydberg atom collisions (including the processes of the associative and Penning type ionization) and corresponding inverse chemi-recombination processes in electron-ion-atom collisions.