DESTRUCTION OF SOME MOLECULAR IONS OF ASTROPHYSICAL INTEREST

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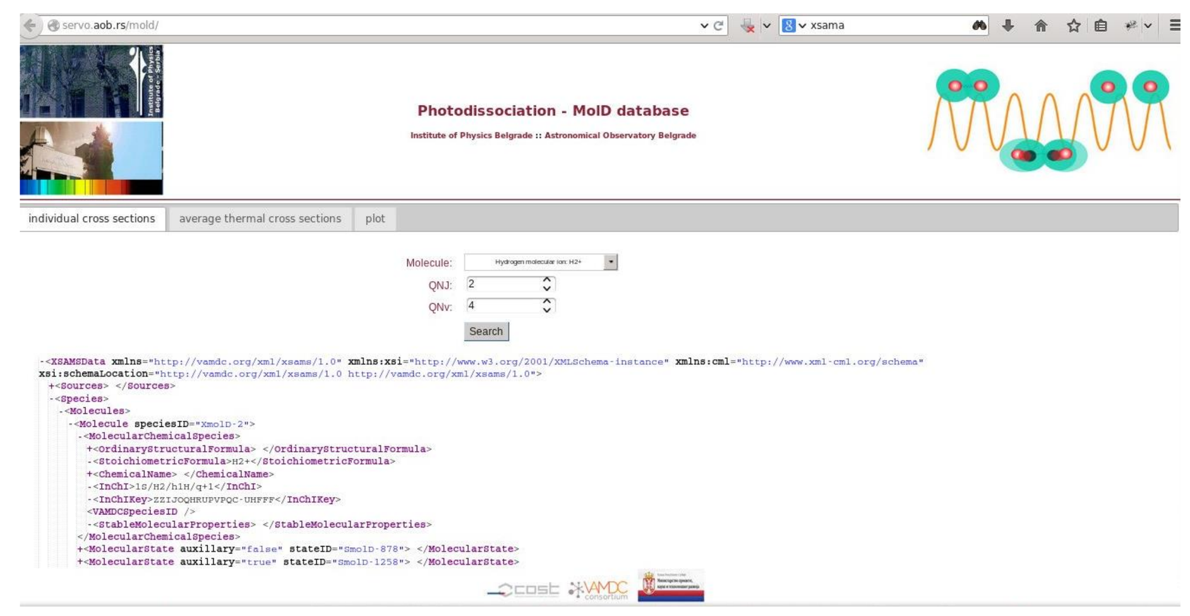
Opacities of stellar atmospheres are caused by a huge number of radiative processes. As part of the development of more sophisticated stellar atmosphere models, we can further explore known processes and include all processes not previously discussed. The average cross-section for the photodissociation and the corresponding spectral absorption coefficients of the molecular ions Li2+, Na2+, LiNa+, H2+ and HeH+ are calculated for the wide region of temperatures and wavelengths ready for further use with a particular accent to the applications for astro plasma research and low temperature laboratory plasma research.
The results for the average photodissociation cross-sections and rate coefficients of the diatomic molecular ions as examples are presented in this poster.
Belgrade **MOL-D** database is a collection of cross-sections and rate coefficients for specific collisional processes [1]. It can be accessed via website of Serbian Virtual Observatory [2,3] or as a web service which is part of the Virtual Atomic and Molecular Data Center (VAMDC [4,5]) network. The database contains photodissociation cross-sections for the individual ro-vibrational states of the diatomic molecular ions, averaged thermal photodissociation cross-sections (see Fig.1) and rate coefficients for the atom-Rydberg atom chemi-ionization and inverse electron-ion-atom chemi-recombination processes. At this moment MOL-D is in the second stage of development. We are including new cross-section and rate coefficients data for processes which involve species such as MgH^+, HeH^+, LiH^+, NaH^+[6,7],eta. .

Our data:

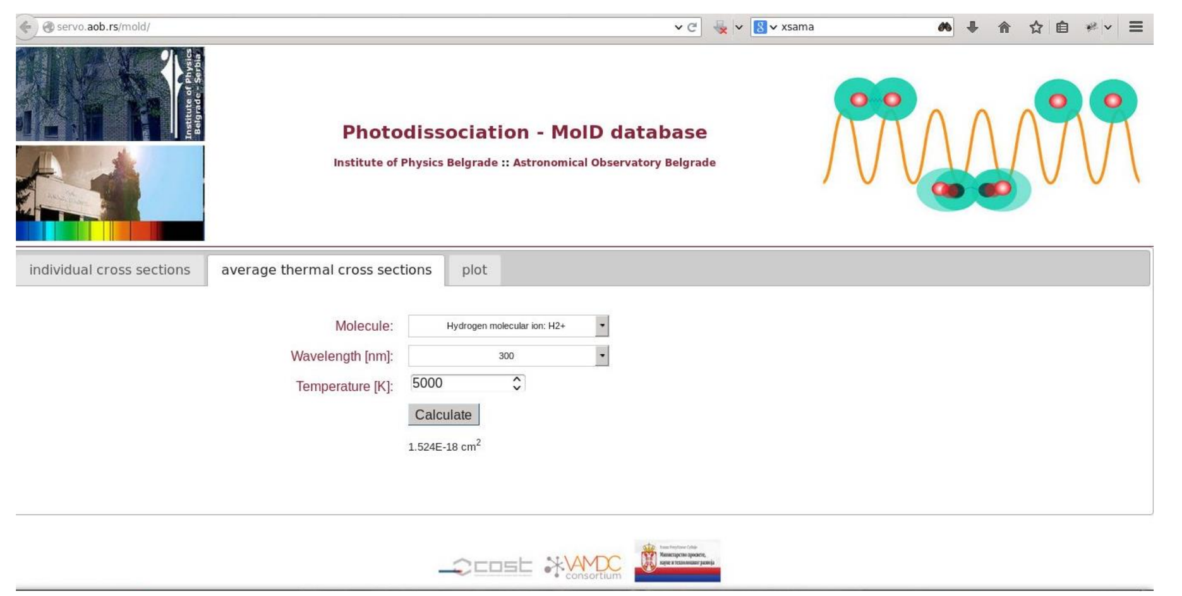
- Photo-dissociation cross-sections for the individual ro-vibrational states (a pair of quantum numbers J and v) of diatomic molecular ions and cations
- Ro-vibrational energy for the corresponding state
- 400 states for H_2^+, 800 for He_2^+, 600 for MgH^+, 60 for LiH^+, 50 NaH^+ (roughly) ...
- Data for few hundred discrete wavelengths (A)

Web service & interface

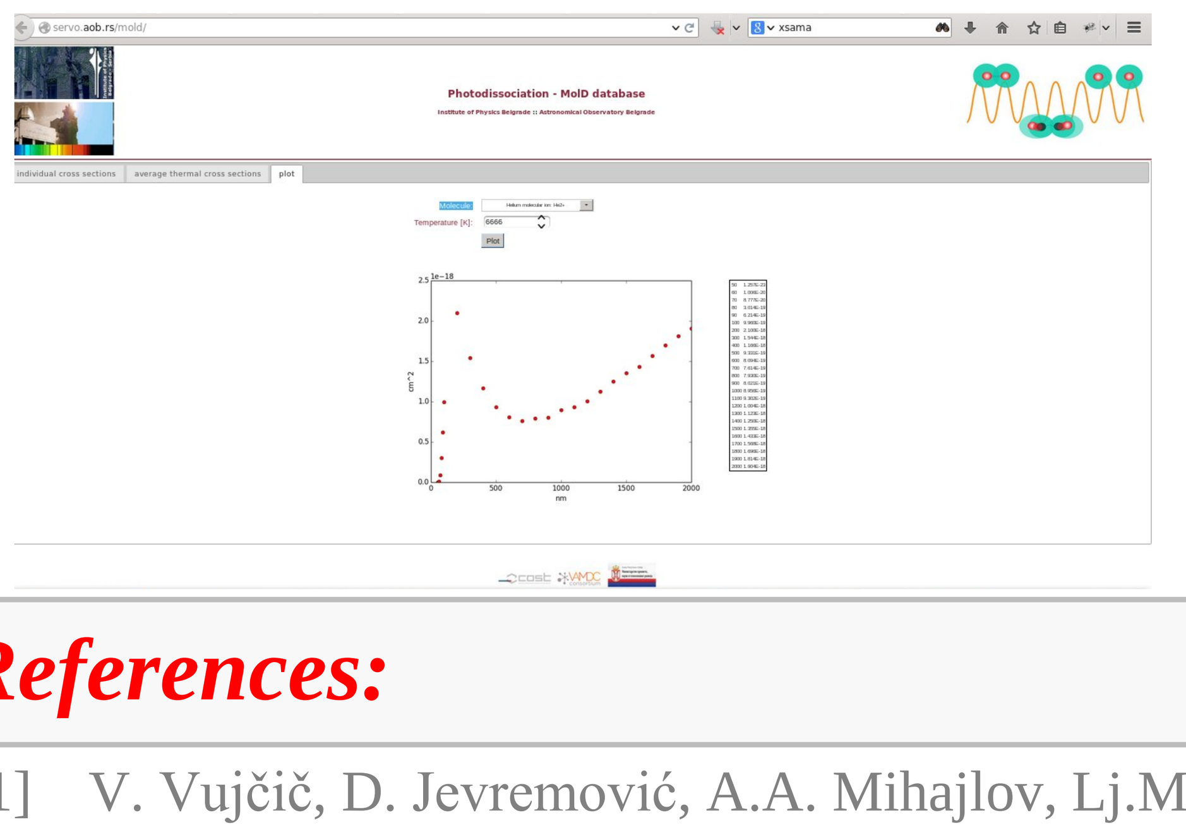
-XSAMS output



-Average thermal cross sections



-Plot



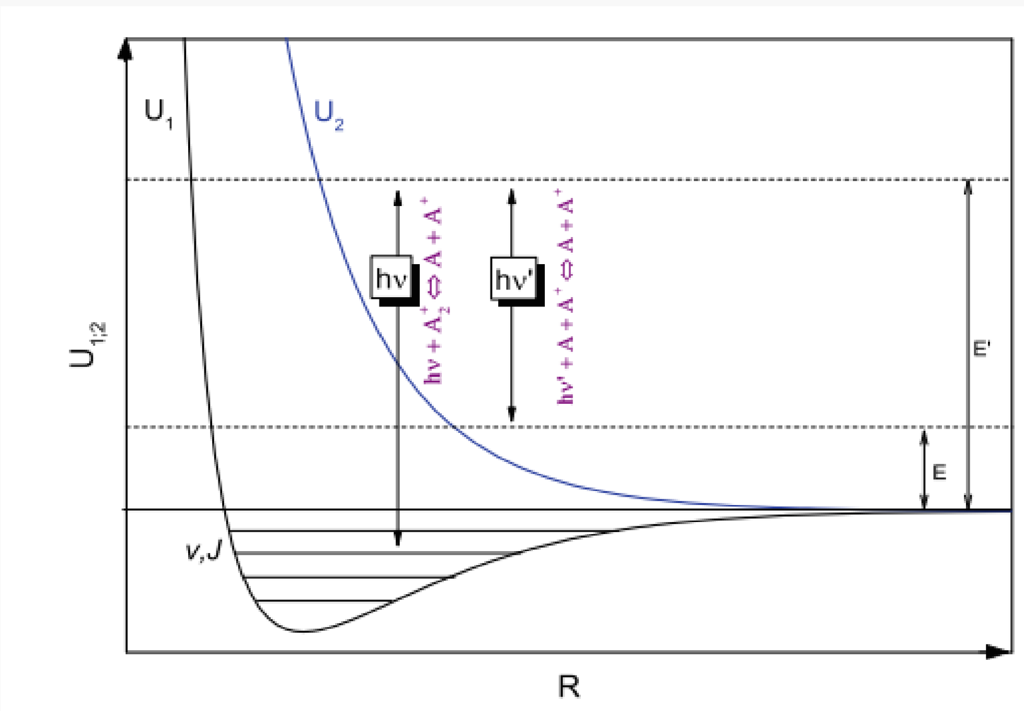


Figure 1. The schematic presentation of the photo-dissociation/association processes (equation (1)) and free–free processes (equation (2)): R is the internuclear distance, $U_1(R)$ and $U_2(R)$ are the potential energy curves of the initial(lower) and final(upper) electronic state of molecular ion A_2^+, J and v are individual ro-vibrational states, E and E' are the total energies of the system $A + A^+$, $h\nu$ and $h\nu'$ are the photon energies.

Further development:

- Incremental inclusion of data from our papers concerning atomic and molecular processes important for modeling different stellar atmospheres and laboratory plasmas as they become published.
- New web utilities and interfaces for SerVO MOL-D website.

Theory:

- Theoretical calculations for processes of molecular-ion photodissociation and ion-atom photoassociation

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

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

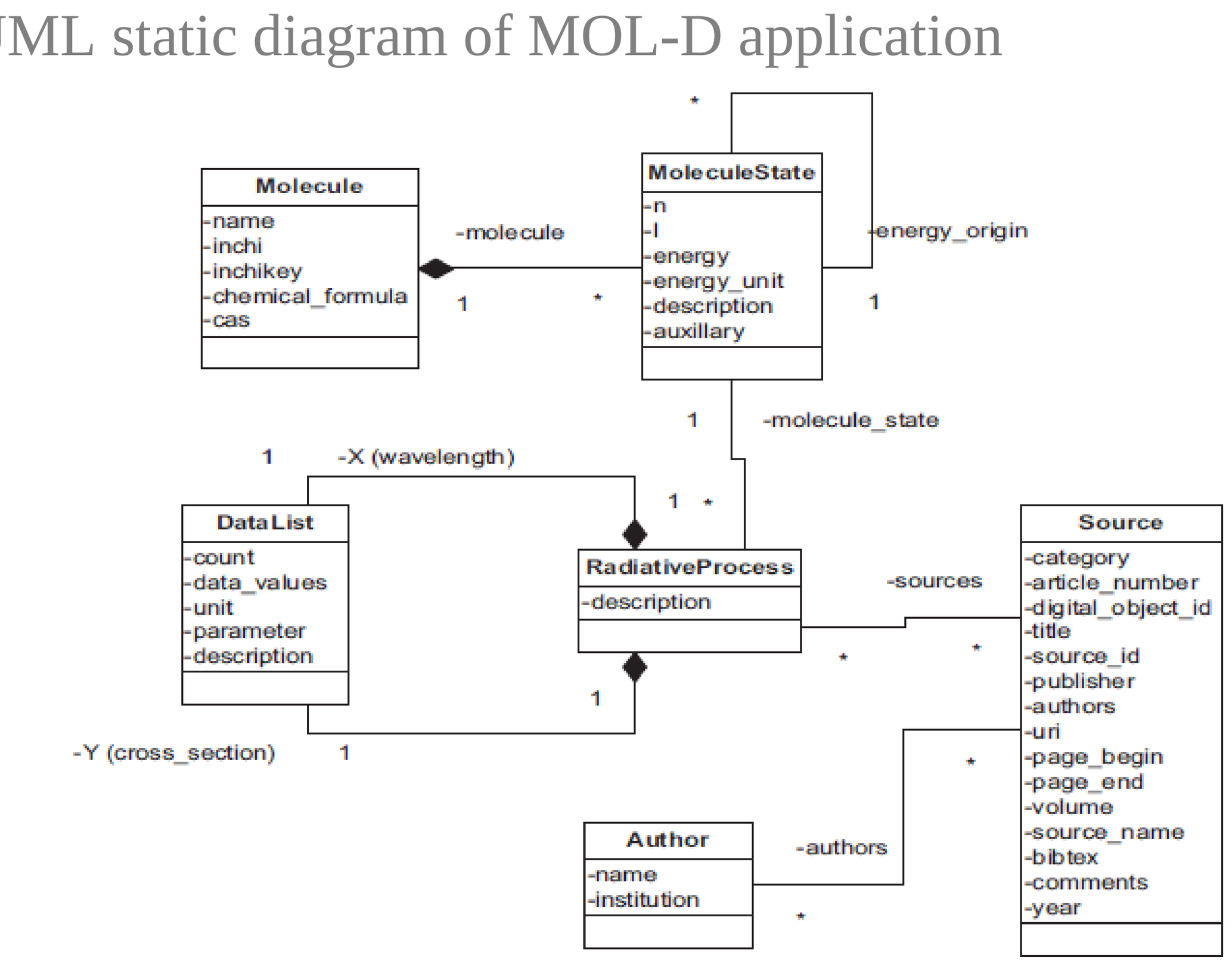
$$\sigma_{J,v}(\lambda) = \frac{8\pi^3}{3\lambda}\left[\frac{(J+1)|D_{E,J+1;v,J}|^2 + J|D_{E,J-1;v,J}|^2}{2J+1}\right]$$

- Corresponding average thermal cross-sections are given by:

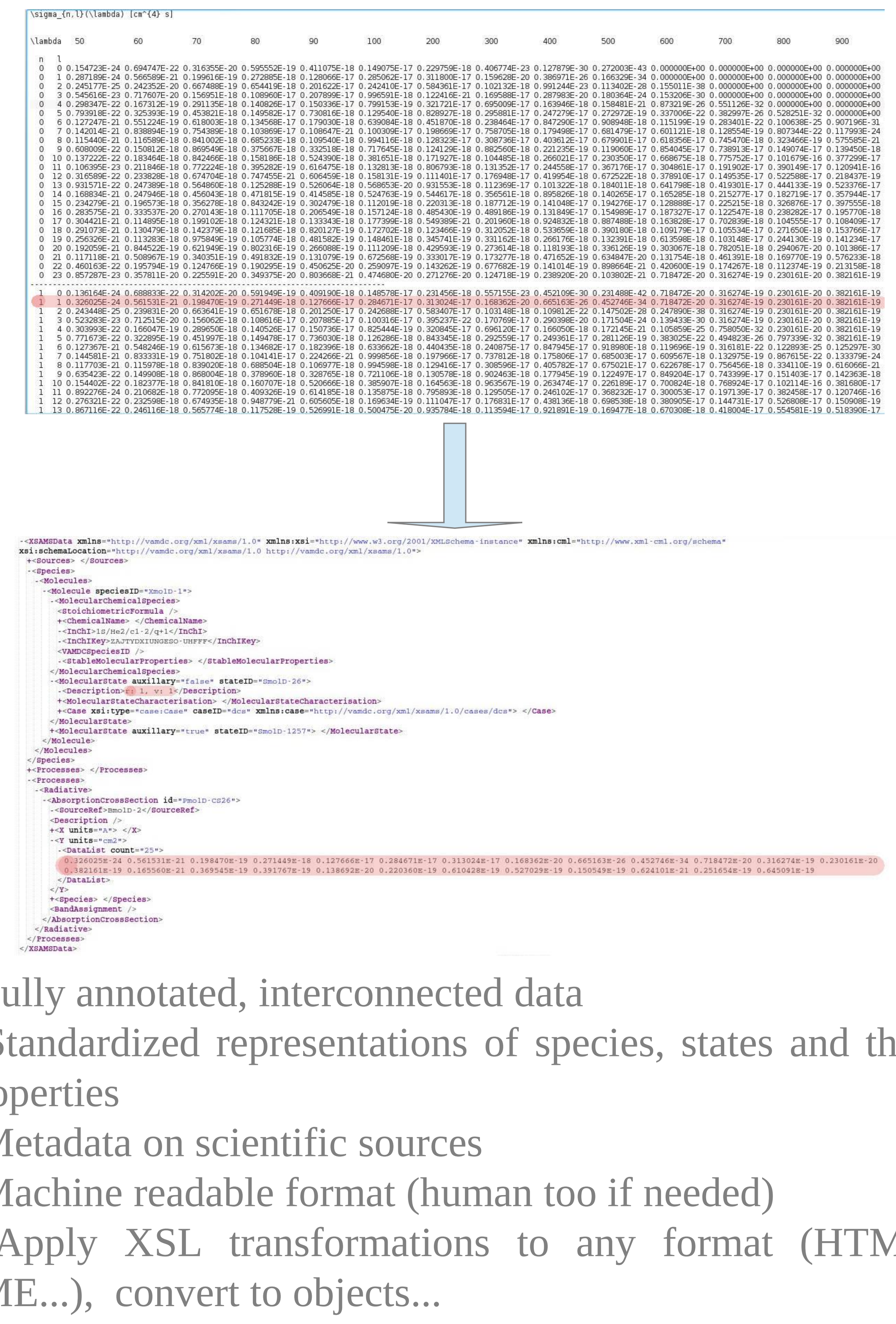
$$\sigma_{\rm ph}(\lambda,T) = \frac{1}{Z}\sum_J\sum_v g_{J;v}(2J+1)e^{-\frac{E_{Jv}-E_{00}}{k_BT}}\sigma_{J,v}(\lambda)$$

Database structure:

UML static diagram of MOL-D application



-From ascii to XML



- 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...

References:

[1] V. Vujčič, D. Jevremović, A.A. Mihajlov, Lj.M. Ignjatović, V.A. Srećković, M.S. Dimitrijević, M. Malović, Journal of Astrophysics and Astronomy, Volume 36, Issue 4, pp. 693-703 (2015).
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[3] http://servo.aob.rs/mold/
[4] M.L. Dubernet, B.K. Antony, Y.A. Ba et al., Journal of Physics B Atomic Molecular Physics, 49, 074003, (2016).
[5] http://portal.vamdc.eu/
[6] B.P. Marinković, D. Jevremović, V. Srećković et al., EPJD, 71, 158 (2017).
[7] Srećković, V. A., et al. Proc. of the International Astronomical Union 12.S325 (2017): 393-396.