MOL-D: A Collisional Database and Web Service within the Virtual Atomic and Molecular Data Center

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Received 5 June 2015; accepted 23 July 2015
DOI: 10.1007/s12036-015-9344-y

Abstract. MOL-D database is a collection of cross-sections and rate coefficients for specific collisional processes and a web service within the Serbian Virtual Observatory (SerVO) and the Virtual Atomic and Molecular Data Center (VAMDC). This database contains photo-dissociation cross-sections for the individual ro-vibrational states of the diatomic molecular ions and rate coefficients for the atom-Rydberg atom chemi-ionization and inverse electron–ion–atom chemi-recombination processes. At the moment it contains data for photodissociation cross-sections of hydrogen H2+ and helium He2+ molecular ions and the corresponding averaged thermal photodissociation cross-sections. The ro-vibrational energy states and the corresponding dipole matrix elements are provided as well. 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).

Key words. Atomic and molecular processes: photodissociation/association—chemi-ionization/recombination—astronomical databases: miscellaneous—plasmas—spectral line profiles.
1. Introduction

Mihajlov and coworkers have demonstrated that ion–atom radiative processes, the photodissociation of the diatomic molecular ion in the symmetric and non-symmetric cases, could be important in specific stellar atmosphere layers and they should be included in chemical models (Mihajlov & Dimitrijevic 1986; Mihajlov et al. 1993, 2007; Ignjatović et al. 2009, 2014b; Srećković et al. 2014). In the symmetric case, we consider the processes of molecular ion photodissociation (bound-free) and ion–atom photoassociation (free-bound):

\[ h\nu + A^+_2 \Leftrightarrow A + A^+, \]

and the corresponding free–free absorption and emission processes:

\[ h\nu + A + A^+ \Leftrightarrow A^+ + A, \]

where \( A \) and \( A^+ \) are atom and ion in their ground states, and \( A^+_2 \) is molecular-ion in the ground electronic state.

In the non-symmetric case, the similar processes of photodissociation/photoassociation are

\[ h\nu + AX^+ \Leftrightarrow A^+ + X, \]

and the corresponding absorption/emission processes

\[ h\nu + A + X^+ \Leftrightarrow A^+ + X. \]

The processes of stimulated photoassociation, characteristic for the non-symmetric case are

\[ \varepsilon_\lambda + A + X^+ \Leftrightarrow (AX^+)^*, \]

where \( X \) is an atom whose ionization potential is less than the corresponding value for atom \( A \). \( AX^+ \) is also molecular-ion in the ground electronic state and \( (AX^+)^* \) molecular-ion in the first excited electronic state.

In the general case, molecular ion \( A^+_2 \) or \( AX^+ \) can be in one of the states from the group which contains the ground electronic state. Similarly, the excited molecular ion \( (AX^+)^* \) can exist in one of the states from the group which contains the first excited electronic state of the considered molecular ion.

For the solar atmosphere, \( A \) usually denotes atom H(1s) and \( X \) one of the relevant metal atoms (Mg, Si, Ca, Na, . . .) (Mihajlov & Dimitrijevic 1986; Mihajlov et al. 1993, 2007; Ignjatović et al. 2014b; Srećković et al. 2014), but there are cases where \( A = \text{He} \) and \( X = \text{H}, \text{Mg}, \text{Si}, \text{Ca}, \text{Na} \). For the helium-rich white dwarf atmospheres, \( A \) denotes He(1s\(^2\)) and \( X \) denotes H(1s), and eventually C, O (Mihajlov & Dimitrijevic 1992; Mihajlov et al. 2013; Ignjatović et al. 2014a).

Our results show the importance of including the symmetric processes with \( A = \text{H}(1s) \) in the stellar atmosphere models (see e.g. Fontenla et al. 2009) and for the early Universe investigation (see Coppola et al. 2013). Also, our results for \( A = \text{He}(1s^2) \) have been used for modeling the DB white dwarf atmospheres (Koester 2015). Such data are also of interest for research on the corresponding weakly ionized laboratory plasmas.
The processes mentioned above are closely connected to several groups of inelastic atomic collision processes. The first few groups consist of the chemi-ionization processes in symmetric and non-symmetric atom/Rydberg-atom collisions, including the processes of associative ionization as well as the corresponding inverse electron–ion–atom chemi-recombination processes:

\[ A^*(n) + A \leftrightarrow A^+_2 + e, \]  
\[ A^*(n) + A \leftrightarrow A + A^+_2 + e, \]  
\[ A^*(n) + X \leftrightarrow A^+_2 + e, \]  
\[ A^*(n) + X \leftrightarrow A + X^+_2 + e. \]

\( A^*(n) \) is an atom in one of the highly excited (Rydberg) states with the principal quantum number \( n \gg 1 \), \( e \) is a free electron and \( A, A^+_2, X \) have the same meaning as in the previous cases. The ionization potential of the atom \( X \) is lower than that of the atom \( A \). The considered radiative processes are allowed by the dipole selection rules.

The other groups of processes consist of excitation and deexcitation processes known also as the \((n - n')\)-mixing processes:

\[ A^*(n) + A \implies \begin{cases} A^*(n') + A, \\ A + A^*(n'), \end{cases} 1 \ll n < n' \]  
\[ A^*(n) + A \implies \begin{cases} A^*(n') + A, \\ A + A^*(n'), \end{cases} 1 \ll n' < n. \]

\( A^* \) has the same meaning as in the case of chemi-ionization/chemi-recombination processes.

Chemi-ionization/chemi-recombination and \((n - n')\)-mixing processes are such that system passes through the phase where it can be treated in the form:

\( (A + A^+)_{q-m}^{\text{in,fin}} + e_{\text{out}}, \)  
\( (A + X^+)_{q-m}^{\text{in,fin}} + e_{\text{out}}. \)

\((A + A^+)_{q-m}^{\text{in,fin}}\) and \((A + X^+)_{q-m}^{\text{in,fin}}\) denote a quasi-molecular ion-atom complex in the corresponding (initial or final) electronic state, and \( e_{\text{out}} \) denotes a free electron in weakly bound or free state.

The connection of these processes with the above described radiative processes is in the following chemi-ionization/chemi-recombination and \((n - n')\)-mixing transitions:

\( (A + A^+)_{q-m}^{\text{in}} \longrightarrow (A + A^+)_{q-m}^{\text{fin}}. \)  
\( (A + X^+)_{q-m}^{\text{in}} \longrightarrow (A + X^+)_{q-m}^{\text{fin}}. \)
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.

The processes described above (equations (1)–(11)) are schematically illustrated in Figures 1–6.

The results obtained during the investigation of the processes mentioned in the present section are presented in MOL-D database which will be described in the next section. The first version of this database is available online and can be accessed directly through http://servo.aob.rs/mold or through VAMDC node within the Serbian Virtual Observatory (SerVO – http://servo.aob.rs, Jevremović et al. 2009), and the Virtual Atomic and Molecular Data Center (VAMDC – http://www.vamdc.org, Dubernet et al. 2010; Rixon et al. 2011).

2. Content of MOL-D e-service

The MOL-D is an e-service which exposes our results to the wider community. In particular, we provide:

- the cross-sections for the photodissociation of individual ro-vibrational states of the considered molecular ions as well as the cross sections for the inverse ion–atom photoassociation (equations (1) and (3)), in a wide region of photon wavelengths $\lambda$, 

Figure 2. The schematic presentation of the processes (equations (3)–(5)) for the case of the molecular ion $AX^+$ and ion–atom system $A^+ + X$.

Figure 3 (a), (b). The schematic presentation of the chemi-ionization/recombination processes (equations (6)–(9)): $n$ is the principal quantum number of the Rydberg state, $\epsilon_k$ is the energy of the free electron.
Figure 4. The schematic presentation of the chemi-ionization and \((n-n')\)-mixing processes (equations (7) and (10)): \(n\) and \(n'\) are the principal quantum numbers of the considered Rydberg states.

- the averaged thermal cross sections for the considered molecular ion photodissociation and for the reverse process, ion–atom photoassociation (equations (1) and (3)), in a wide region of \(\lambda\) and temperature \(T\),
- the rate coefficients and the corresponding averaged thermal cross sections for the ion–atom absorption processes and inverse emission processes (equations (2) and (4)), as well as for the non-symmetric ion–atom photoassociation in equation (5) in a wide region of \(\lambda\) and \(T\),
- visualization of the wavelength dependence of the averaged thermal cross sections for a given temperature input.

MOL-D is available online from the end of 2014 and for the moment it contains the data for the photodissociation processes (equation (1)) with \(A = \text{H}(1s)\) and \(A = \text{He}(1s^2)\). In the near future, we intend to include the relevant data for some other non-symmetric photodissociation processes (equation (3)).

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

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

and the corresponding averaged thermal cross sections are given by

\[
\sigma_{\text{ph}}(\lambda, T) = \frac{1}{Z} \sum_J \sum_v g_{J,v} (2J + 1) e^{-\frac{E_{J,v} - E_{0,0}}{k_B T}} \sigma_{J,v}(\lambda).
\]
Figure 5. Static structure of the MOL-D database. Relationships between entities are shown by connected lines with designated cardinalities (‘1’ and ‘*’ denote one and many, respectively), i.e. a molecule can have multiple states.

\[ D_{E,J+1;v,J} \] is the relevant dipole matrix element, \( E_{J,v} \) is the energy of the individual states with the angular and vibrational quantum numbers \( J \) and \( v \) respectively, and \( Z \) is the partition function

\[ Z = \sum_J \sum_v g_{J,v} (2J + 1) e^{- \frac{E_{J,v} - E_{0,0}}{k_B T}}. \] (18)

In this expression, the product \( g_{J,v} \cdot (2J + 1) \) is the statistical weight of the considered state and the coefficient \( g_{J,v} \) depends on the ‘spin of the nuclei’.

We also plan to include the rate coefficients for the chemi-ionization/recombination and \((n - n')\) mixing (equations (6)–(11)). The values of the rate coefficients will be determined in the semi-classical approach (see e.g. Mihajlov et al. 2011), but using a significantly improved numerical procedure with respect to the previous papers (Mihajlov et al. 2003, 2004, 2005, 2008, 2011; Srečković et al. 2013).
Figure 6. Some screen shots of the MOL-D node at the Belgrade server station.
Figure 6. (continued).
3. Technical characteristics of MOL-D database

The principal structure of the Belgrade MOL-D database is shown schematically in Figure 5 using UML notation.

MOL-D data are exposed as a web form and a web service accessible according to VAMDC specification\(^1\). VAMDC (Dubernet \textit{et al.} 2010) standards define VAMDC-TAP RESTful web-service request using VSS2 query language and results formatted as a XSAMS (XML Schema for atoms, molecules and solids) document\(^2\). Such approach enables accessing multiple databases in a single query.

Software is built on top of Django, a web-based Python framework, and represents an adaptation and extension of VAMDC Node Software. User interface is AJAX-enabled, using JQuery javascript framework and plots are generated by pyplot (matplotlib).

Besides acting as a VAMDC-compliant web service, accessible through VAMDC portal and other tools implemented on VAMDC standards, MOL-D offers on-site services such as

- user can make a selection based on molecule and quantum number \(J\) (\(QN_J\)) or quantum number \(v\) (\(QN_v\))
- calculate averaged thermal cross section based on the temperature for a specific molecule and wavelength
- make a plot of averaged thermal cross sections along all (discrete) wavelengths for a given temperature

A screenshot of MOL-D database at Belgrade server station\(^3\) is shown in Figure 6. An example of the visualization of a data set that represents the averaged cross section versus wavelength is shown in the right panel of Figure 6.

4. Future development and perspectives

In the near future, we plan to add the results of the rate coefficients for the ion–atom absorption processes and inverse emission processes. We will also include data for the non-symmetric ion–atom photoassociation. Our plans also consist of including the rate coefficients for chemi-ionization in atom-Rydberg atom collisions (including the processes of associative and Penning type ionization) and corresponding inverse chemi-recombination processes in electron–ion–atom collisions. Finally, we intend to include the rate coefficients for the excitation and deexcitation \((n \rightarrow n')\)-mixing processes in the relevant region of the principal quantum number \(n\) and \(T\).

We plan to calculate and include new data about processes which involve species such as HeH\(^+\), LiH\(^+\), NaH\(^+\), SiH\(^+\) which are important for the early Universe chemistry and for the modeling of stellar and solar atmospheres. The MOL-D database will be regularly updated with new results.

\(^1\)http://vamdc-standards.readthedocs.org/en/latest/dataAccessProtocol/vamdc.tap.html
\(^2\)http://vamdc.eu/documents/standards/dataModel/vamdc.xsams/index.html
\(^3\)http://servo.aob.rs/mold
Acknowledgements

The authors are thankful to the Ministry of Education, Science and Technological Development of the Republic of Serbia for the support of this work within the projects 176002 and III44002. A part of this work has been supported by VAMDC. VAMDC is funded under the Combination of Collaborative Projects and Coordination and Support Actions Funding Scheme of the Seventh Framework Program. The authors are also grateful to Dr. Guy Rixon for his help in all aspects of inclusion of MOLD database in VAMDC.

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