ATOMIC AND MOLECULAR PROCESSES FOR INVESTIGATION OF AGN AND STARS

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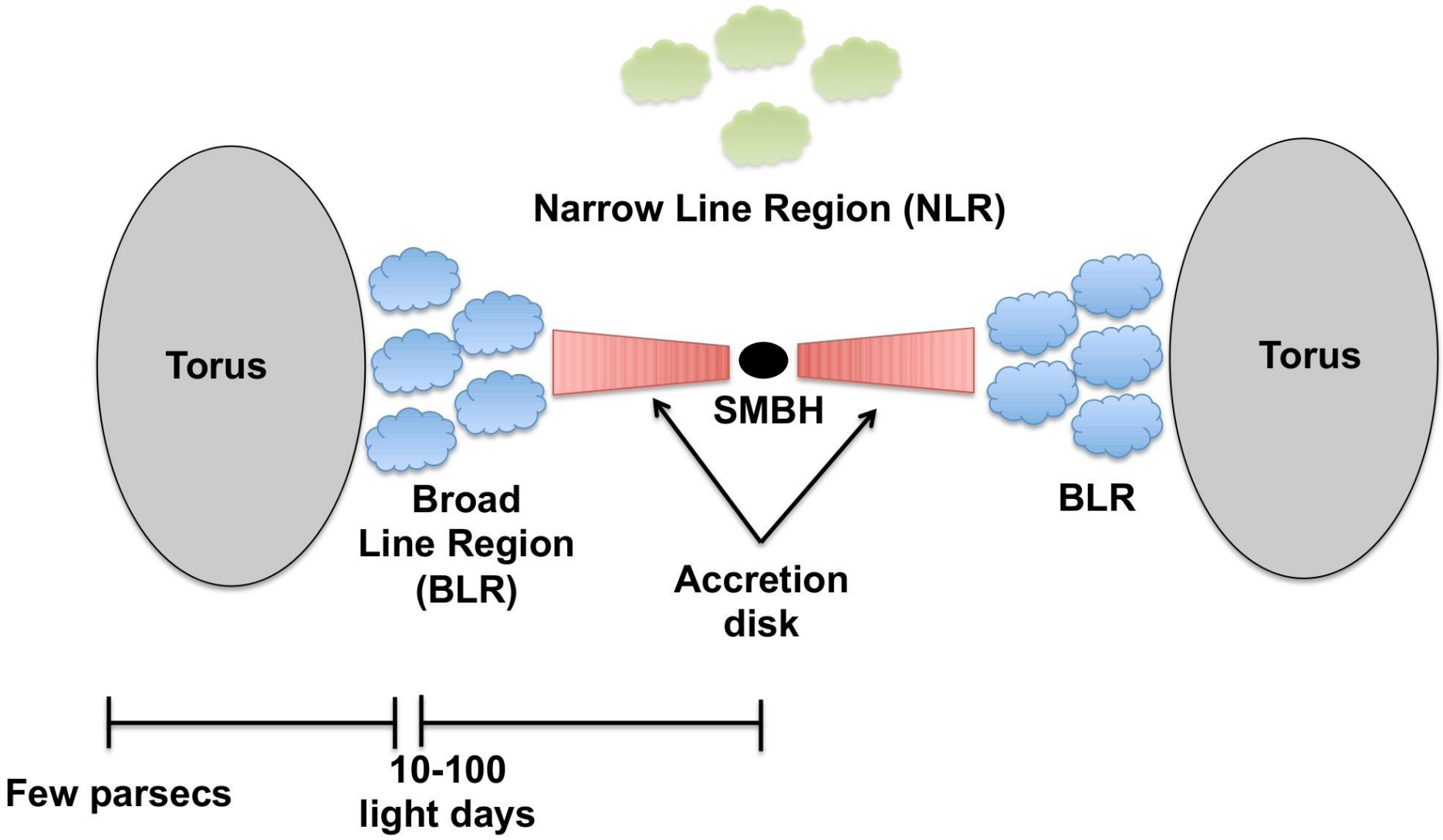
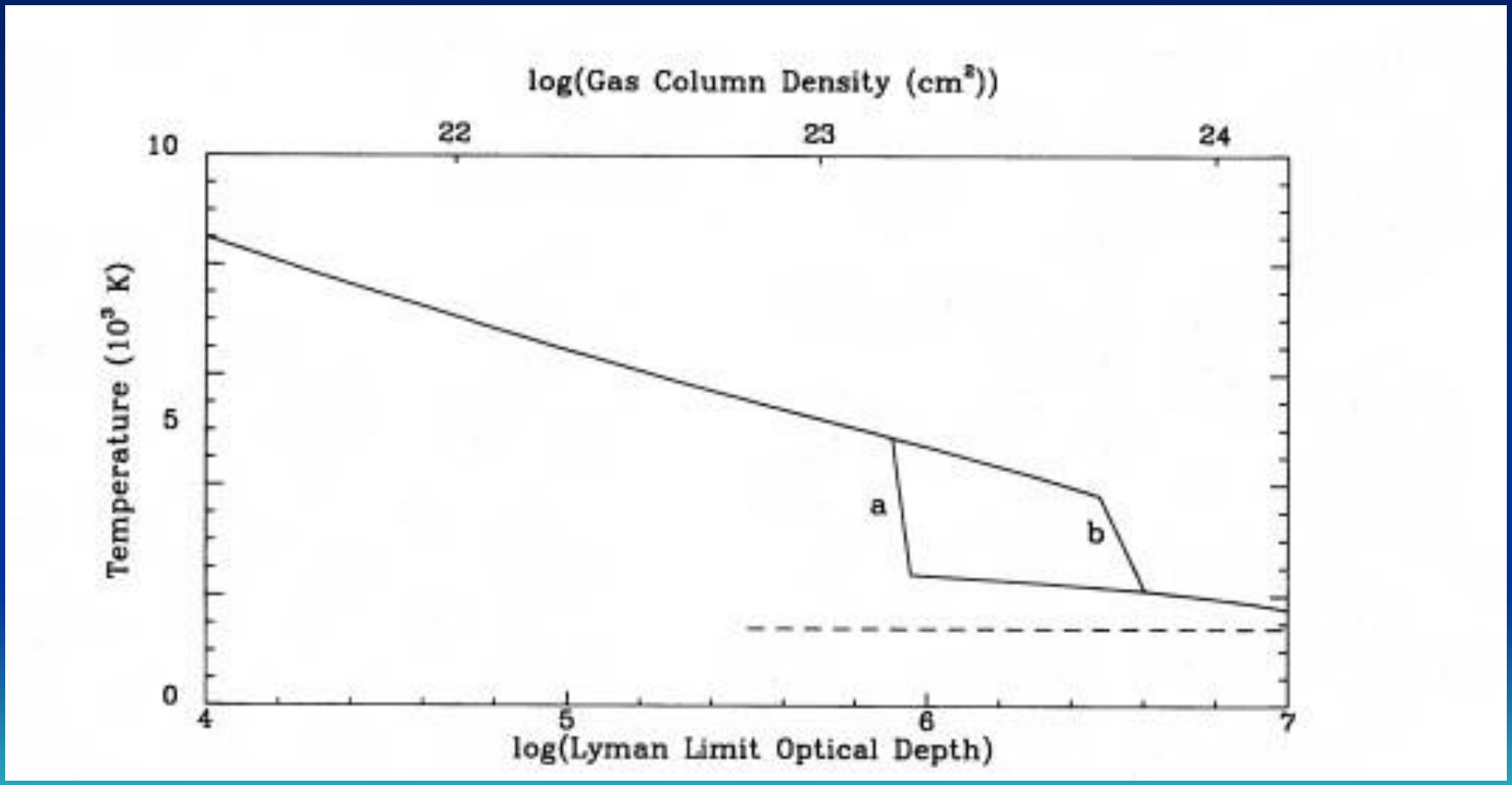

Narrow Line Region (NLR)
Torus
Torus
SMBH
Broad
Line Region
(BLR)
BLR
Accretion
disk
Few parsecs
10-100
light days

The illuminated surface of the clouds is highly ionized by UV and X radiation. Inside the degree of ionization decreases up to the gas column density of $N = 10^{22} cm^{-2}$ when gas becomes neutral. Deep into the coud the temperature is 8000 – 5000 K and than sharply decrease up to 2000 K.

Mercè Crosas and Jon C. Weisheit, Hydrogen molecules in quasar broad-line regions MNRAS, 1993, 262, 359.



C. Alenka Negrette et al. ApJ 2012, 756, Po62

- A high density of – 10^{11} – 10^{13} cm^{-3} is needed in order to explain the existence of particular spectral lines of Fe II, Al III, C III

Mercè Crosas and Jon C. Weisheit, Hydrogen molecules in quasar broad-line regions, MNRAS, 1993, 262, 359.

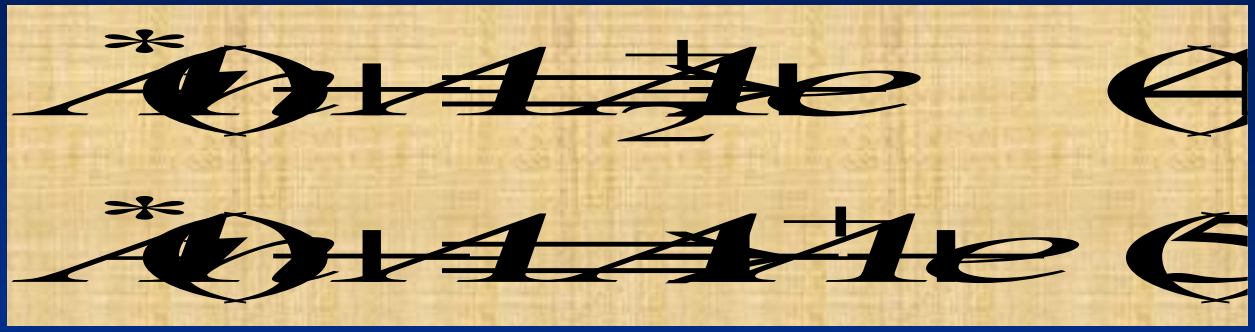
Table 2. Collisional reactions.

Reaction	Rate Coefficient (cm^3/s)		Ref
1. $H^+ + e^- \rightarrow H + h\nu$	$K_1 = 1.59 \times 10^{-13} T_4^{-0.5} e^{-\tau_{LL}} + 2.6 \times 10^{-13} T_4^{-0.85}$		1
2. $H + e^- \rightarrow H^- + h\nu$	$K_2 = 2.65 \times 10^{-15} T_4 + 1.22 \times 10^{-15}$		2
3. $H^- + H \rightarrow H_2 + e^-$	$K_3 = 2.7 \times 10^{-9}$		3
4. $H^- + H^+ \rightarrow H + H$	$K_4 = 7.0 \times 10^{-9} T_4^{-0.5}$		4
5. $H^- + H_2^+ \rightarrow H + H + H$ $\rightarrow H_2 + H$	$K_5 = 5.0 \times 10^{-8} T_4^{-0.5}$		4
6. $H^+ + H \rightarrow H_2^+ + h\nu$	$K_6 = 2.9 \times 10^{-16} T_4^{-1.8}$,	$T < 6700K$	5
	$K_6 = 5.8 \times 10^{-16} (T_4/5.6)^{-0.66 \log 10 (T_4/5.6)}$,	$T > 6700K$	5
7. $H_2^+ + H \rightarrow H_2 + H^+$	$K_7 = 6.4 \times 10^{-10}$		6
8. $H_2 + H^+ \rightarrow H_2^+ + H$	$K_8 = 2.4 \times 10^{-9} e^{-2.12/T_4}$		7
9. $H_2^+ + e^- \rightarrow H^+ + H + e^-$	$K_9 = 2.0 \times 10^{-8}$		8
10. $H_2 + e^- \rightarrow 2H + e^-$	$K_{10} = 1.1 \times 10^{-8} e^{-10.2/T_4} T_4^{0.35}$		5
11. $H_2 + e^- \rightarrow H^- + H$	$K_{11} = 9.69 \times 10^{-13} e^{-11.323/(\ln 10^4 T_4 - 7.28)}$		5
12. $H + H + H \rightarrow H_2 + H$	$K_{12} = 5.5 \times 10^{-33} T_4^{-1}$		5
13. $H_2 + H \rightarrow H + H + H$	$K_{13} = 6.53 \times 10^{-9} e^{-5.24/T_4}$		5
14. $H_2 + H + H \rightarrow H_2 + H_2$	$K_{13} = K_{10}/8$		5
15. $H_2 + H_2 \rightarrow H_2 + H + H$	$K_{15} = 11.3 \times 10^{-9} e^{-5.33/T_4}$		5
16. $H(n=1) + H^*(n=2) \rightarrow H_2^* \rightarrow H_2 + h\nu$	$K_{16} = 5.0 \times 10^{-14}$		9
17. $H(n=1) + H^*(n=2) \rightarrow H_2^+ + e^-$	$K_{17} = 8.73 \times 10^{-12} T_4^{0.95}$,	$T < 5000K$	10
	$K_{17} = 2.9 \times 10^{-11} T_4^{2.69}$,	$T > 5000K$	10
18. $H(n=1) + H^*(n=3) \rightarrow H_2^+ + e^-$	$K_{18} = 4.42 \times 10^{-11} T_4^{0.95} e^{0.87/T_4}$,	$T < 5000K$	11
	$K_{18} = 1.47 \times 10^{-10} T_4^{2.69} e^{0.87/T_4}$,	$T > 5000K$	11

- The **chemi-ionization** processes in atom - Rydberg atom collisions, as well as the corresponding **chemi-recombination** processes are considered as factors of influence on the atom excited-state populations

-The obtained results demonstrate the fact that the considered chemi ionization/recombination processes must have a very significant influence on the **optical properties of weakly ionized lyers.** Thus, it is shown that these processes and their importance for non-local thermodynamic equilibrium modeling of BLR clouds should be investigated further.

- **Chemi-ionization** processes in principle include the processes of **associative ionization**



where A, X and X^+ are atoms and the atom ion in their ground states, $A^*(n)$ atom in a highly excited (Rydberg) state with the principal quantum number n >>1 and AX^+ is the corresponding molecular ion in its ground electronic state.

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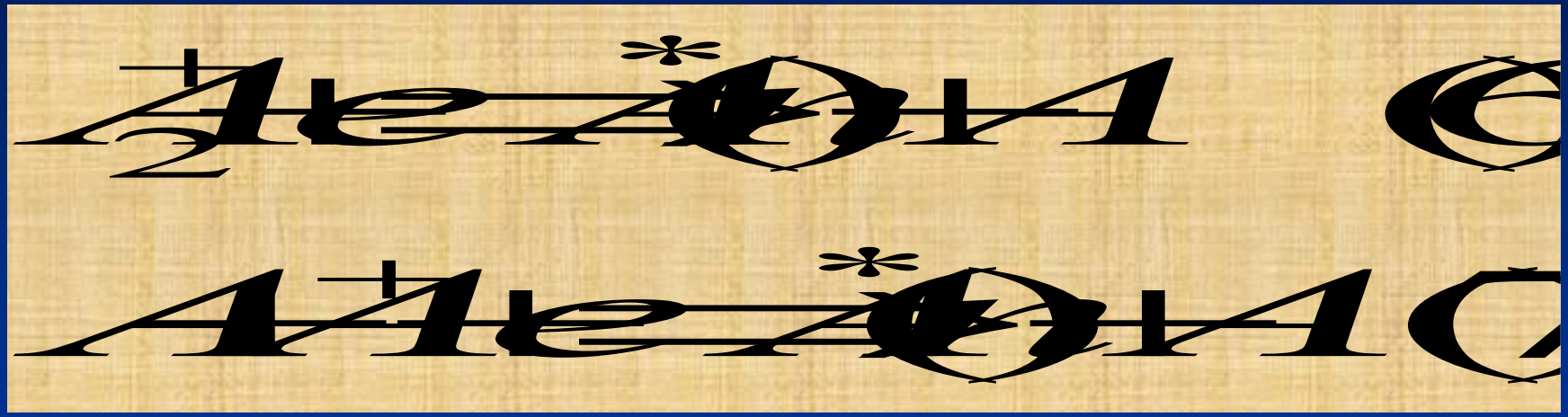


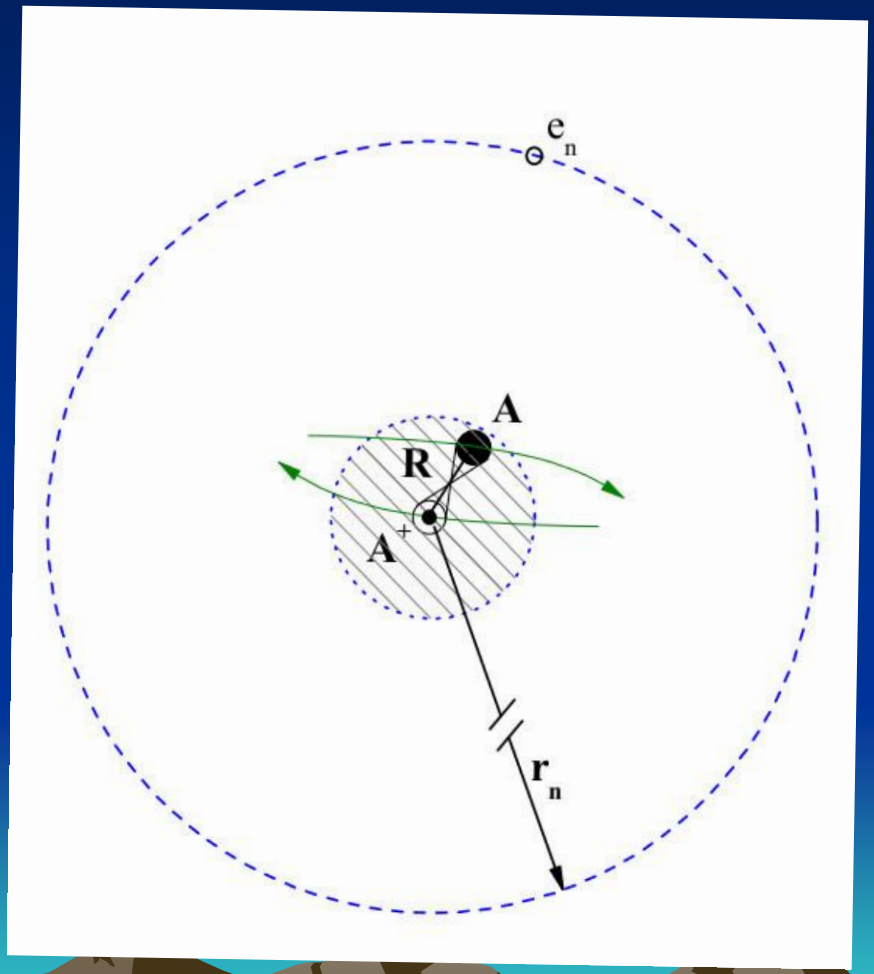
and the corresponding **inverse recombination processes**,

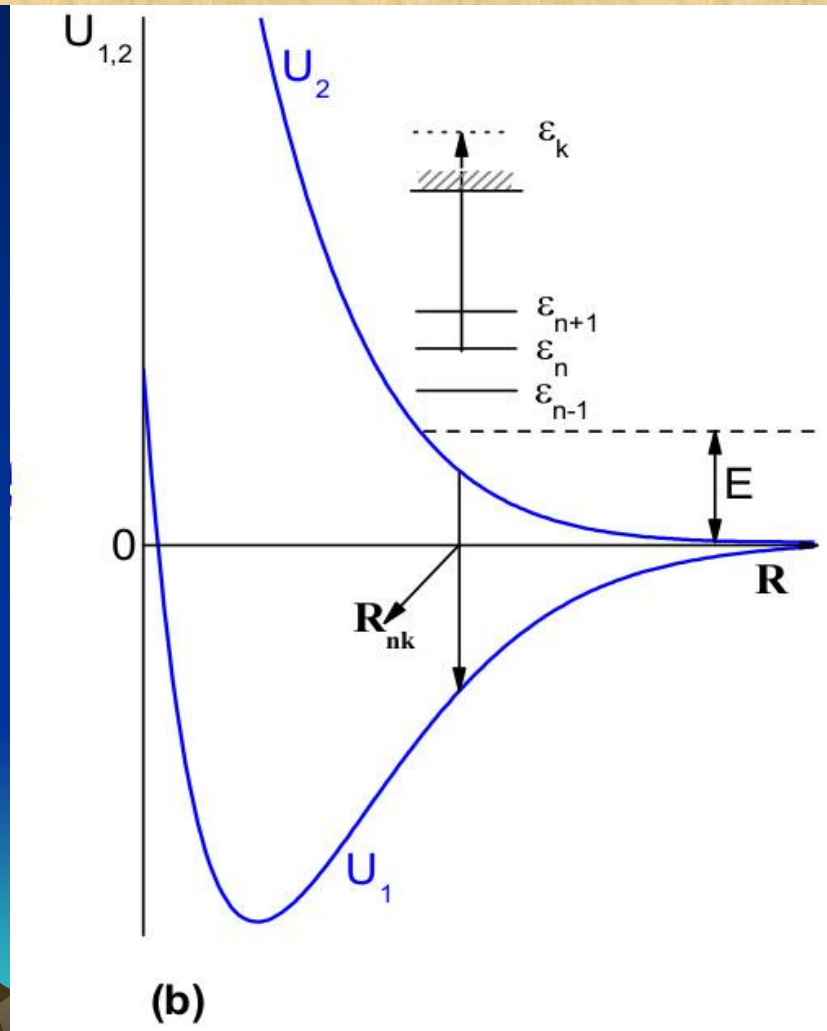
$$A^*(n) + e \Rightarrow A^+ + 2e,$$

$$A^+ + 2e \Rightarrow A^*(n) + e,$$

$$A^+ + e \Rightarrow A^*(n) + \varepsilon_\lambda,$$

A*(n) +A is represented as [A^{+}+ *A(1s)] + e





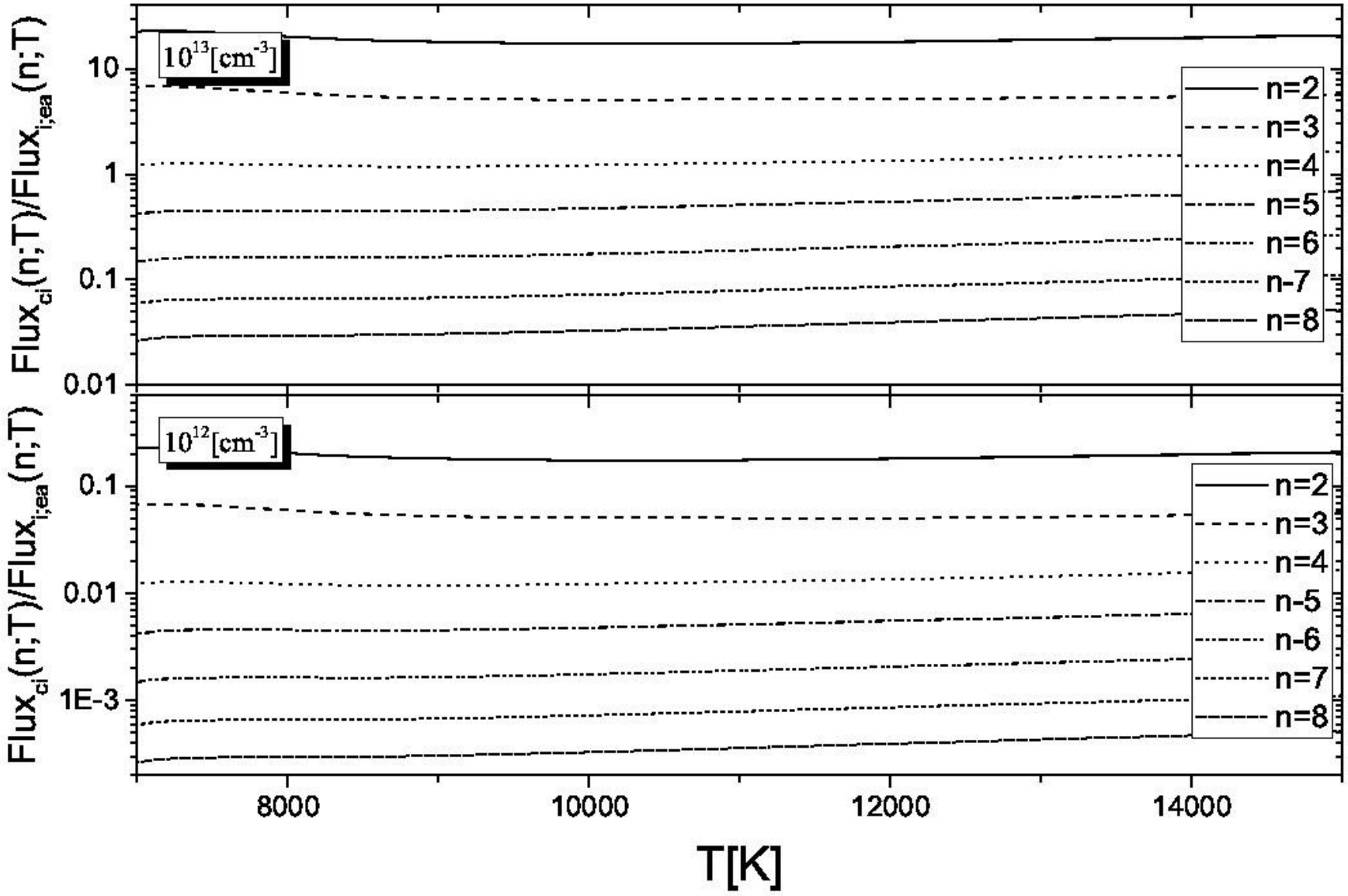
(b)

$$\sigma_{\mathrm{ci}}^{(a,b)}(n, E) = 2\pi \int_0^{\rho_{\max}^{(a,b)}(E)} P_{\mathrm{ci}}^{(a,b)}(n, \rho, E)\rho d\rho,$$

$$K_{\mathrm{ci}}^{(a,b)}(n, T) = \int_{E_{\min}^{(a,b)}(n)}^{E_{\max}} v\sigma_{\mathrm{ci}}^{(a,b)}(n, E) f(v; T) dv,$$

$$K_{\mathrm{ci}}(n, T) = K_{\mathrm{ci}}^{(a)}(n, T) + K_{\mathrm{ci}}^{(b)}(n, T),$$

$$I_{\mathrm{ci}}(n, T) = K_{\mathrm{ci}}(n, T) \cdot N_n N_1,$$
$$I_{\mathrm{cr}}(n, T) = K_{\mathrm{cr}}(n, T) \cdot N_1 N_i N_e,$$


10^{13}[cm^{-3}]
10^{12}[cm^{-3}]
n=2
n=3
n=4
n=5
n=6
n-7
n=8
n-5
n-6
n=7
10
1
0.1
0.01
1E-3
8000
10000
12000
14000
T[K]
Flux$_{ci}$(n;T)/Flux$_{i;ea}$(n;T)

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Atom–Rydberg atom chemi-ionization/recombination processes in the hydrogen clouds in broad-line region of AGNs

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ABSTRACT

The possibility that the chemi-ionization processes in atom–Rydberg atom collisions, as well as the corresponding chemi-recombination processes, may be useful for the diagnostics, modelling, and confirmation of existence or non-existence of very dense weakly ionized domains in clouds in broad-line region of active galactic nuclei, has been considered. The obtained results demonstrate the fact that the considered chemi-ionization/recombination processes, which influence on the ionization level and atom excited-state populations, must have a very significant influence on the optical properties of the weakly ionized regions where the neutral hydrogen densities are larger than $10^{12}\,\mathrm{cm}^{-3}$ since in such conditions they dominate over the relevant concurrent electron–atom collision processes. This can be used as a diagnostic method to find out if the domains with such densities exist or not. Additionally, our previous results obtained for principal quantum number $2 \leq n \leq 8$ and $4000\,\mathrm{K} \leq T \leq 10\,000\,\mathrm{K}$ are extended for principal quantum number $9 \leq n \leq 20$ and $10\,000\,\mathrm{K} < T \leq 20\,000\,\mathrm{K}$ and also for low-temperature region ($T < 4000$ K) for $2 \leq n \leq 20$.

Key words: atomic processes – galaxies: active – galaxies: nuclei.

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The role of some collisional processes in AGNs: Rate coefficients needed for modeling

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Molecular processes
Atomic processes
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Galaxies: active
Galaxies: nuclei

ABSTRACT

The importance of some atom hydrogen collisions in AGN has been investigated. The results are useful for better estimation of the hydrogen Balmer lines fluxes, which usage for effective temperature diagnostics in astrophysical plasma is limited by errors from the line formation models. The data could be also useful for modeling cooler and denser parts of AGN BLR clouds, as well as for the investigation of Rydberg states of hydrogen and for the study of their influence during the cosmological recombination epoch. The results of the present work suggest that the investigated processes are of interest for the research and modeling of such media.

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The influence of collisional-ionization and recombination processes on spectral line shapes in stellar atmospheres and in the hydrogen clouds in broad-line region of AGNs

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Abstract. In this paper, the importance of $H^*(n) + H(1s)$ collisional ionization as well as the influence of inverse recombination processes in different environments has been investigated within the regions $2 \leq n \leq 20$ and 4 000 K $\leq T \leq$ 20 000 K. The interpretation of this influence is based on existing method of describing inelastic processes in symmetrical atomRydberg-atom collisions. These processes have effect on ionization and the populations of hydrogen excited atoms in moderately ionized plasma layers. From the results it follows that the investigation of these processes is of interest for the research and modelling of such medium.

Key words: Atomic processes – Galaxies: active – Line: profiles – Plasmas

VAMDC Idea

- Problems in A&M data community
- -LACK OF STANDARDS AND COMMON GUIDELINES
- -INTEROPERABILITY problem – prevents productive search and data mining
- -DATA EXCHANGE problem – informal, e-mails, ASCII files…
- -OVERLAPING OF EFFORTS

VAMDC IDEA

- -Majority of developers are Astronomers, Physicists, Chemicists – NEED OF HIRING COMPUTER ENGINEERS
- -DATA IDENTIFICATION PROBLEM -XML schemata keys not only for data exchange but also for data identification
- -CRITICAL EVALUATION OF DATA

Extensible Markup Language (XML) lets you define and store data in a shareable manner. XML supports information exchange between computer systems such as websites, databases, and third-party applications.

DICTIONARY

XML - eXtensible Markup Language.

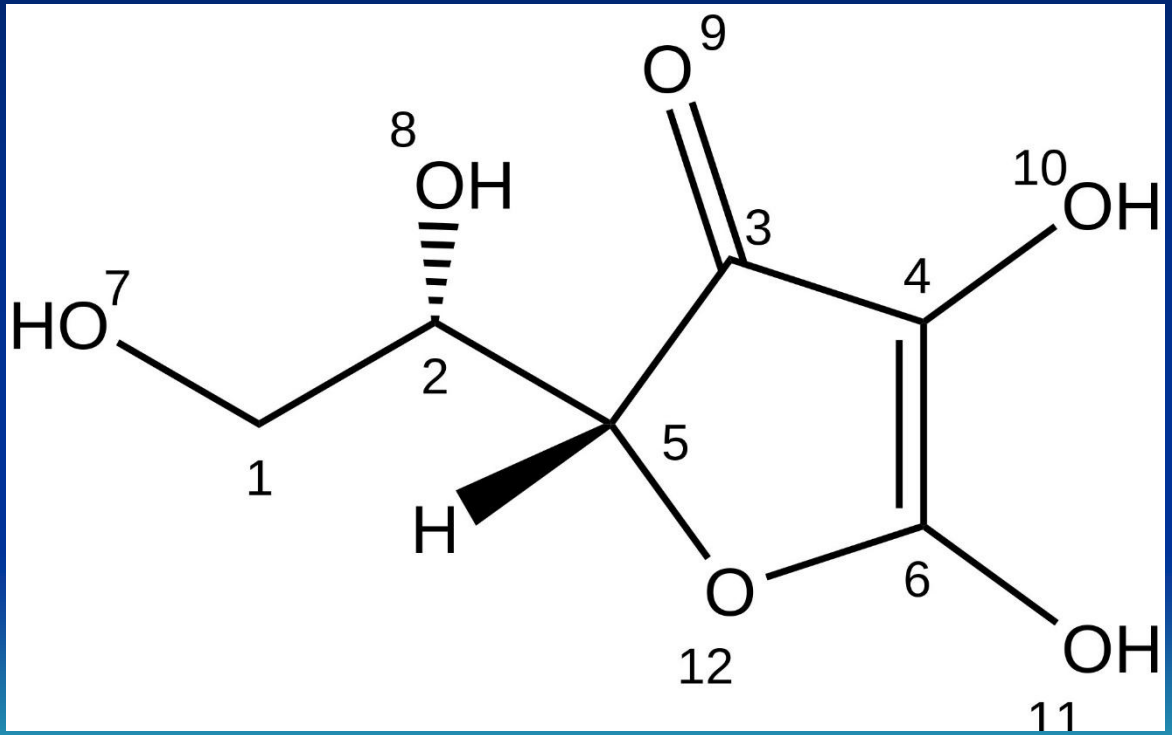
Designed to store and transport data

XSAMS: XML Schema for Atoms, Molecules and Solids

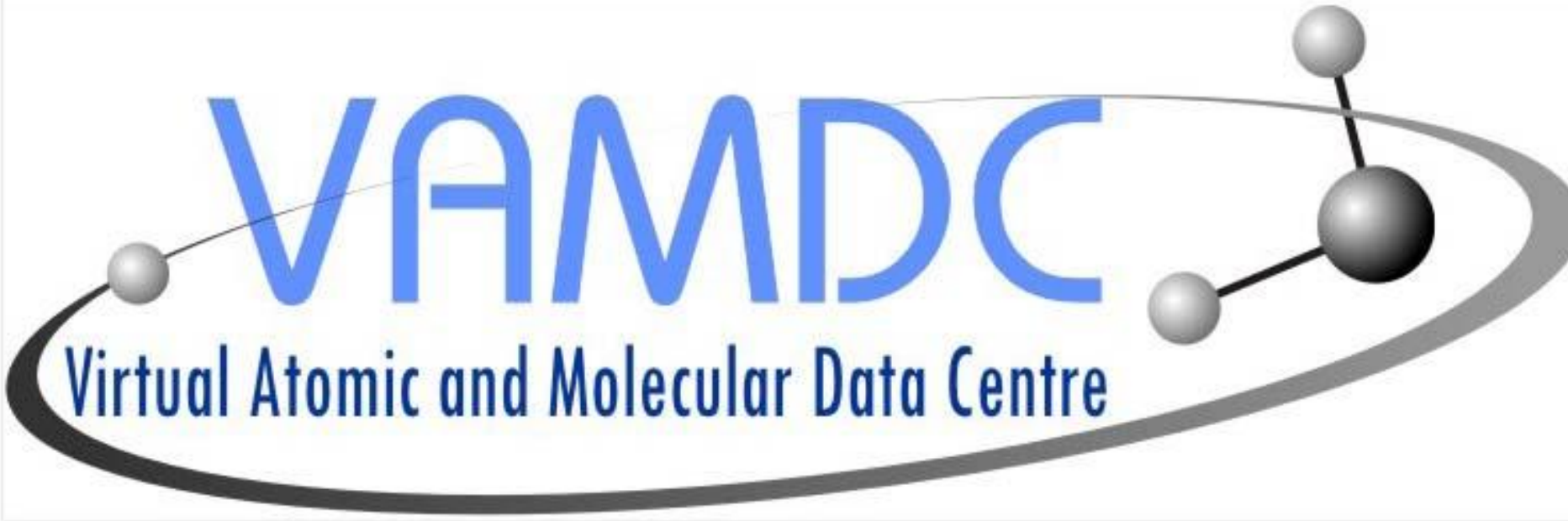
InChI- International Chemical Identifier is a textual identifier for chemical substances, designed to provide a standard way to encode molecular information and to facilitate the search for such information in databases and on the web

InchKey - International Chemical Identifier

InChI=1/C6H8O6/c7-1-2(8)5-3(9)4(10)6(11)12-5/h2,5,7-10H,1H2/t2-,5+/m0/s1



The InChIKey, is a fixed length (27 character) condensed digital representation of the InChI that is not human-understandable. The InChIKey specification was released in September 2007 in order to facilitate web searches for chemical compounds, since these were problematic with the full-length InChI



VAMDC

Virtual Atomic and Molecular Data Centre

Virtual Atomic and Molecular Data Center

Virtual Atomic and Molecular Data Center (VAMDC) connects 39 database which can be searched simultaneously and its partners are from Australia, Austria, France, Germany, India, Italy, Japan, Korea, Russia, Serbia, South Africa, Sweden, UK, USA and Venezuela.

AMDIS Ionization

Ionization cross sections and rate coefficients by electron impact.

emoto.masahiko@nifs.ac.jp

CHIANTI

CHIANTI is an atomic database for spectroscopic diagnostics of astrophysical plasmas.

TIPTOP

TIPTOPbase

Atomic data computed in the Opacity Project and Iron Project, energy levels, *gf*-values, *A*-values, photoionization cross sections and electron impact cross sections and rates for light chemical elements with atomic number, Z = 1 - 28.

The NIST (National Institute of Standards and Technology) Atomic Database

Atomic Spectra Database contains evaluated data on about 77,000 energy levels and 144,000 spectral lines from atoms and ions of 99 elements.

Vienna Atomic Line Database (VALD)

The VALD database of atomic data for analysis of radiation from astrophysical objects. The nodes are in Montpelier, Uppsala and Moscow. A vast collection of spectral line parameters (central wavelengths, energy levels, statistical weights, transition probabilities, line broadening parameters) for all chemical elements of astronomical importance

STARK-B

This is a database of calculated widths and shifts of isolated lines of atoms and ions due to electron and ion collisions.

SESAM SpEctroScopy of Atoms and Molecules(Paris)

- Atomic and molecular spectra database

Photodissociation - MolD database (Belgrade)

- 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.

Collisional Atomic Processes (Excitation-Ionization) - ACol database (Serbia)

- Database for collisional processes of excitation/deexcitation and ionization/recombination in hydrogen, helium, and alkali plasmas.

Belgrade electron/atom(molecule) database (BEAMDB), Serbia

- Electron interaction cross-sections for elastic scattering, electron excitation, ionization and total scattering.

AMBDAS

- The Atomic and Molecular Bibliographic Data System (AMBDAS) is a bibliographic database of literature on fundamental atomic and molecular processes for fusion applications maintained by the International Atomic Energy Agency.

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