Ionization & Excitation Rate Coefficient Calculations for Plasma Emitting in EUV Range

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Abstract

❖**A method for calculation of cross-sections and rate coefficients of inelastic electron-atom interaction processes, such as excitation, ionization and dielectronic recombination, is proposed and examined in this report. The system of equations in the first order collisional theory is solved directly by using one-electron wave functions of discrete and continuous spectra calculated in Hartree-Fock-Slater potential. Obtained cross-sections and rates are compared with experimental data and different approximations based on the Bethe-Born approach. Contribution of various terms and dependency of rates on plasma temperature and density is analyzed. The suggested method permits to describe experimental cross-sections near the edges, that is essential for the plasma, effectively emitting in EUV range. The calculations were made, in particular, for Xe plasma.**

Model

❖ **Opacity and emissivity are calculated at given free electron temperature T_e , matter density ρ and spectral radiation intensity I_ω**

❖ **One-electron wave functions, oscillator strengths and cross sections are calculated by using the average atom model with self-consistent field: Hartree-Fock-Slater model with given occupancies and ionization stage**

❖ **The average occupancies and ionization stage are calculated from level kinetics equations in Collisional Radiative Steady State (CRSS) case**

❖ **Close lines are unified into clusters with accounting for reabsorption effects**

Level Kinetics Equations

$$\frac{dN_\nu}{dt} = (1 - \frac{N_\nu}{g_\nu})\, S_\nu - N_\nu L_\nu$$

$$S_\nu = \sum_{\mu<\nu} N_\mu (\alpha_{\mu\nu}^{abs} + \alpha_{\mu\nu}^{ex}) + \sum_{\mu>\nu} N_\mu (\alpha_{\mu\nu}^{em} + \alpha_{\mu\nu}^{dex}) + Z_0 (\alpha_\nu^{r} + \alpha_\nu^{phr} + \alpha_\nu^{dr})$$

$$L_\nu = \sum_{\mu<\nu} (1 - \frac{N_\mu}{g_\mu})(\alpha_{\mu\nu}^{em} + \alpha_{\mu\nu}^{dex}) + \sum_{\mu>\nu} (1 - \frac{N_\mu}{g_\mu})(\alpha_{\mu\nu}^{abs} + \alpha_{\mu\nu}^{ex}) + \alpha_\nu^{i} + \alpha_\nu^{phi} + \alpha_\nu^{ai}$$

Atom Process Rates

$$W_{if} = \frac{2\pi}{\hbar} |< f \, | V' | \, i >|^2 \, \rho_i(E)$$

van Regemorter, 1962 – excitation
Lotz, 1968 – ionization.

The cross sections of collisional processes by Vainstein:

$$\sigma'_{a_0 a} = \sum_{\kappa} \left[Q_{\kappa} \sigma'_{\kappa}(\ell_0, \ell) + Q''_{\kappa} \sigma''_{\kappa}(\ell_0, \ell) \right],$$

$$\sigma'_{\kappa}(\ell_0, \ell) = \pi a_0^2 \frac{16}{2(2\ell_0 + 1)\varepsilon} \left(\frac{\pi}{2} \right)^2 \sum_{\lambda_0, \lambda} P_{\kappa}^d \left(P_{\kappa}^d - \sum_{\kappa'} P_{\kappa' \kappa}^e \right),$$

$$\sigma''_{\kappa}(\ell_0, \ell) = \pi a_0^2 \frac{16}{2(2\ell_0 + 1)\varepsilon} \left(\frac{\pi}{2} \right)^2 \sum_{\lambda_0, \lambda} \left(\sum_{\kappa'} P_{\kappa' \kappa}^e \right)^2.$$

Here *ε* is the electron energy. Factor Q_κ depends on angular momentum of ion in the states a_0 and *a*. Direct and exchange terms P^d_κ, $P^e_{\kappa'\kappa}$ can be written by using *3jm* and *6j* symbols:

$$P^d_\kappa = \sqrt{\frac{(2\ell_0+1)(2\ell+1)(2\lambda_0+1)(2\lambda+1)}{2\kappa+1}} \begin{pmatrix} \kappa & \ell_0 & \ell \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \kappa & \lambda_0 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \times$$

$$\times R^{(\kappa)}_{n_0\ell_0,n\ell;\varepsilon\lambda_0,\varepsilon'\lambda},$$

$$P^e_{\kappa'\kappa} = (-1)^{\kappa+\kappa'} \sqrt{(2\kappa+1)(2\ell_0+1)(2\ell+1)(2\lambda_0+1)(2\lambda+1)} \times$$

$$\times \begin{pmatrix} \kappa' & \ell_0 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \kappa' & \lambda_0 & \ell \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} \kappa' & \ell_0 & \lambda \\ \kappa & \lambda_0 & \ell \end{Bmatrix} R^{(\kappa')}_{\varepsilon\lambda_0,n\ell;n_0\ell_0,\varepsilon'\lambda},$$

where $R^{(\kappa)}_{\alpha,\beta;\gamma,\delta}$ is the Slater integral:

$$R^{(\kappa)}_{\alpha,\beta;\gamma,\delta} = \int\int R_\alpha(r')R_\beta(r')\frac{r^\kappa_<}{r^{\kappa+1}_>}R_\gamma(r'')R_\delta(r'')dr'dr''.$$

Dielectronic Recombination

$$\gamma^{(ai)} = 2\pi \sum_{n_2=1}^{n_2=n_{max}} \sum_{n_3=1}^{n_3=n_{max}} \sum_{\ell_2=0}^{\ell_2=n_2-1} \sum_{\ell_3=0}^{\ell_3=n_3-1} \sum_{\ell_4=0}^{\ell_4=\ell_{max}} \times$$

$$\times N_{n_1\ell_1} N_{n_2\ell_2} \left(1 - \frac{N_{n_3\ell_3}}{2(2\ell_3+1)}\right) \left(1 - \frac{1}{1+exp[(E-\mu)/\theta]}\right) \times$$

$$\times (2\ell_3+1)(2\ell_4+1)(B_1+B_2+B_{12}),$$

where

$$B_1 = \sum_{k=0}^{k=\infty} \frac{1}{2k+1} \begin{pmatrix} \ell_2 & k & \ell_3 \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{pmatrix} \ell_1 & k & \ell_4 \\ 0 & 0 & 0 \end{pmatrix}^2 R^2(n_1, \ell_1, n_2, \ell_2, n_3, \ell_3, E, \ell_4, k),$$

$$B_2 = \sum_{p=0}^{p=\infty} \frac{1}{2p+1} \begin{pmatrix} \ell_1 & p & \ell_3 \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{pmatrix} \ell_2 & p & \ell_4 \\ 0 & 0 & 0 \end{pmatrix}^2 R^2(n_2, \ell_2, n_1, \ell_1, n_3, \ell_3, E, \ell_4, p),$$

$$B_{12} = (-1)^{\ell_1+\ell_2+\ell_3+\ell_4+1} \sum_{k=0}^{k=\infty} \sum_{p=0}^{p=\infty} \begin{pmatrix} \ell_2 & k & \ell_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_1 & k & \ell_4 \\ 0 & 0 & 0 \end{pmatrix} \times$$

$$\times \begin{pmatrix} \ell_1 & p & \ell_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_2 & p & \ell_4 \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} \ell_2 & \ell_3 & k \\ \ell_1 & \ell_4 & p \end{Bmatrix} \times$$

$$\times R(n_1, \ell_1, n_2, \ell_2, n_3, \ell_3, E, \ell_4, k) R(n_2, \ell_2, n_1, \ell_1, n_3, \ell_3, E, \ell_4, p),$$

$$R(n_1, \ell_1, n_2, \ell_2, n_3, \ell_3, E, \ell_4, k) = \int\int R_{n_1\ell_1}(r_1) R_{n_2\ell_2}(r_2) \frac{r_<^k}{r_>^{k+1}} R_{n_2\ell_2}(r_2) R_{E\ell_4}(r_1) dr_1 dr_2.$$

The rate of dielectronic recombination

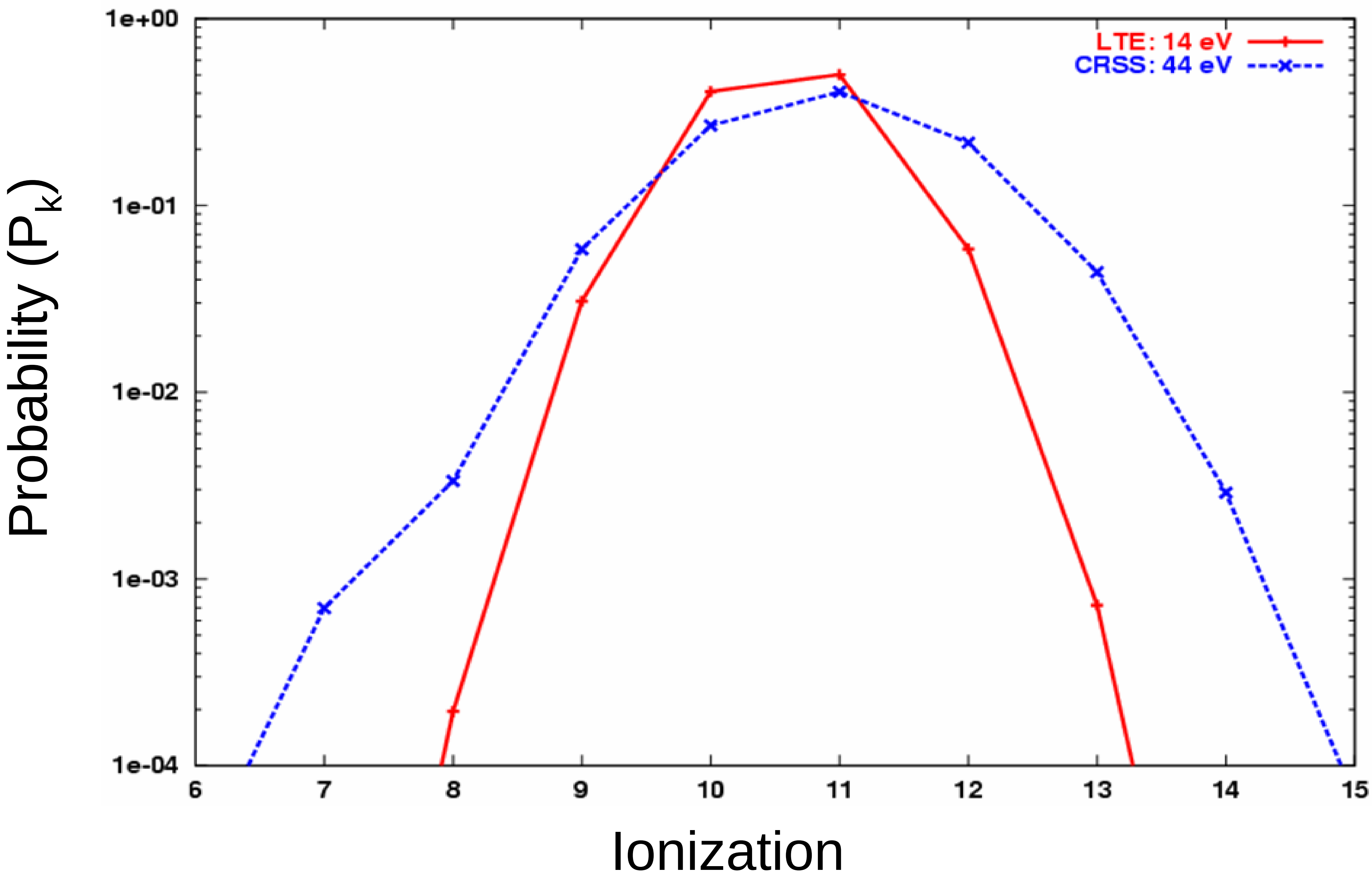
$$\gamma_{n\ell}^{(dr)} = \sum_{pq} \frac{\gamma^{(rad)}(pq \to n\ell)}{\sum_{n'\ell'} \gamma^{(rad)}(pq \to n'\ell') + \gamma_{pq}^{(ai)}} \gamma_{pq}^{(dc)},$$

where $\gamma^{(rad)}(pq \to n\ell)$ is the rate of spontaneous emission.

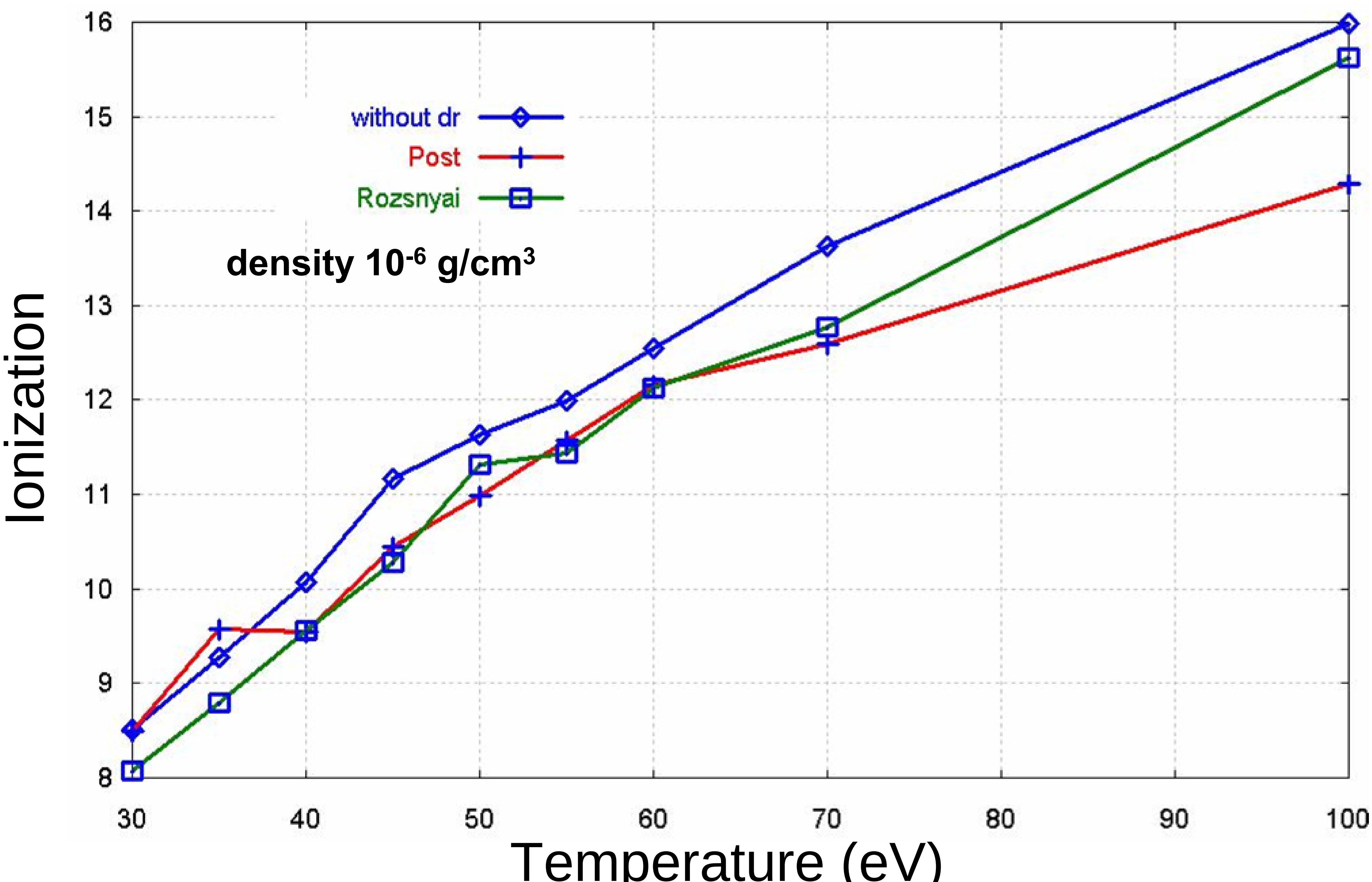
Ionization Energies for Xe: Experiment, GRASP, THERMOS

Ion	Experiment	GRASP	THERMOS
Xe I	*12.13*	*11.89*	*12.42*
Xe II	*21.21*	*21.16*	*19.89*
Xe III	*32.12*	*30.51*	*30.20*
Xe IV	-	*41.42*	*40.85*
Xe V	-	*52.28*	*51.66*
Xe VI	-	*64.71*	*63.37*
Xe VII	-	*89.69*	*89.11*
Xe VIII	-	*104.3*	*103.6*
Xe IX	-	*179.2*	*179.6*
Xe X	-	*205.1*	*204.8*

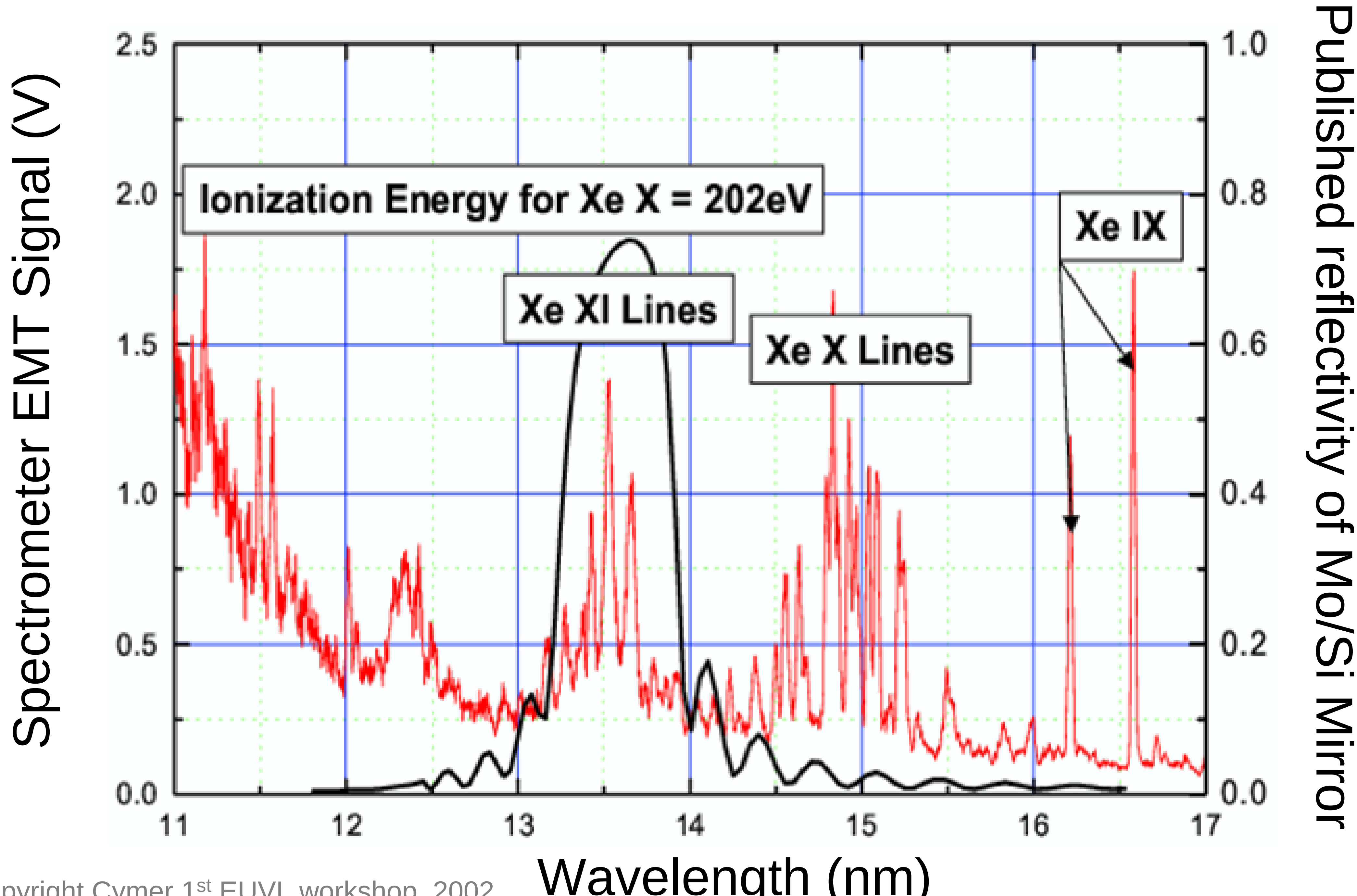
Ion Probabilities of Xe for Saha (LTE) and CRSS Models



Average Ionization Stage for Xe
at different dielectronic recombination rate

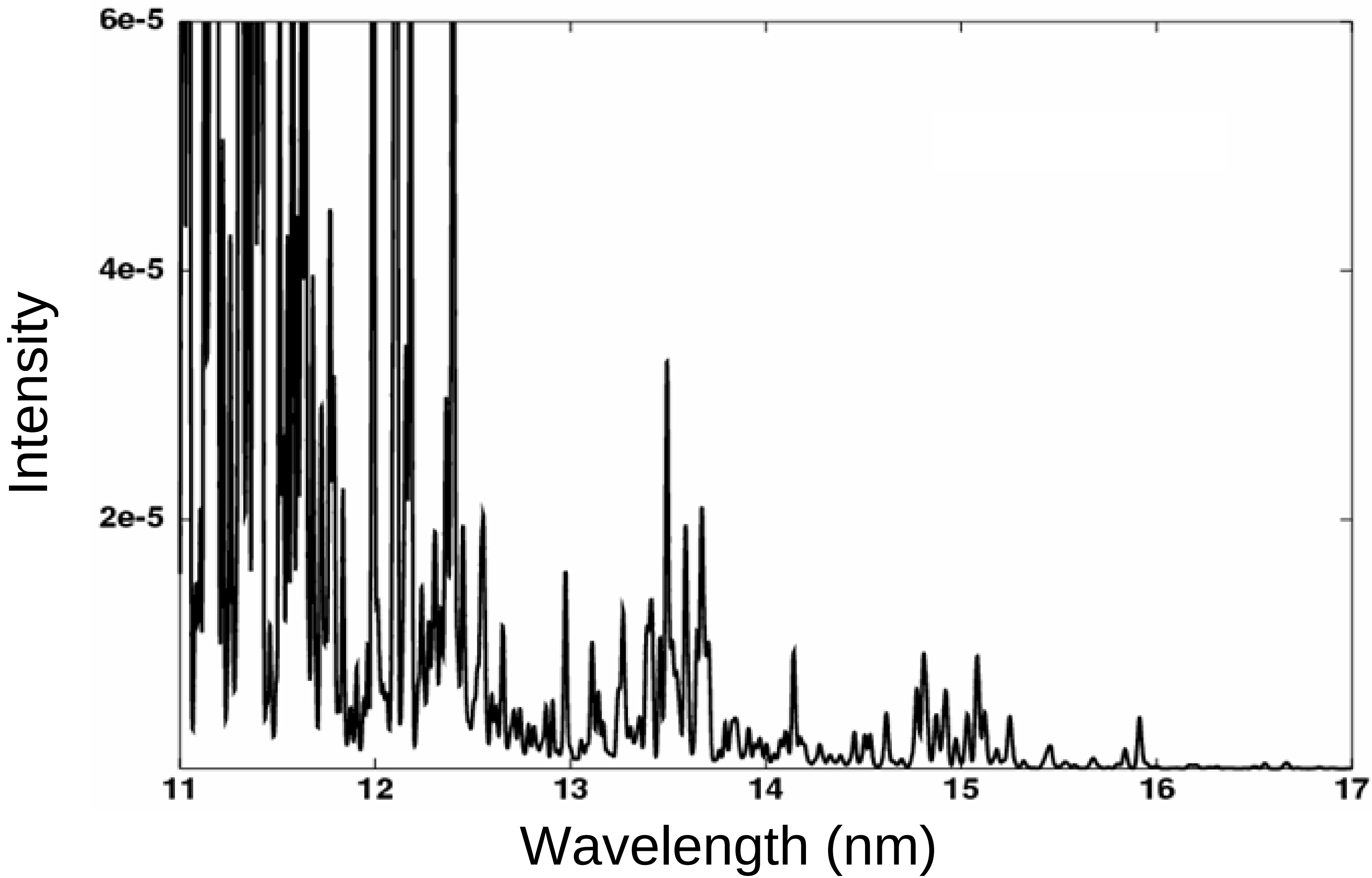


Measured EUV Spectrum of Xenon



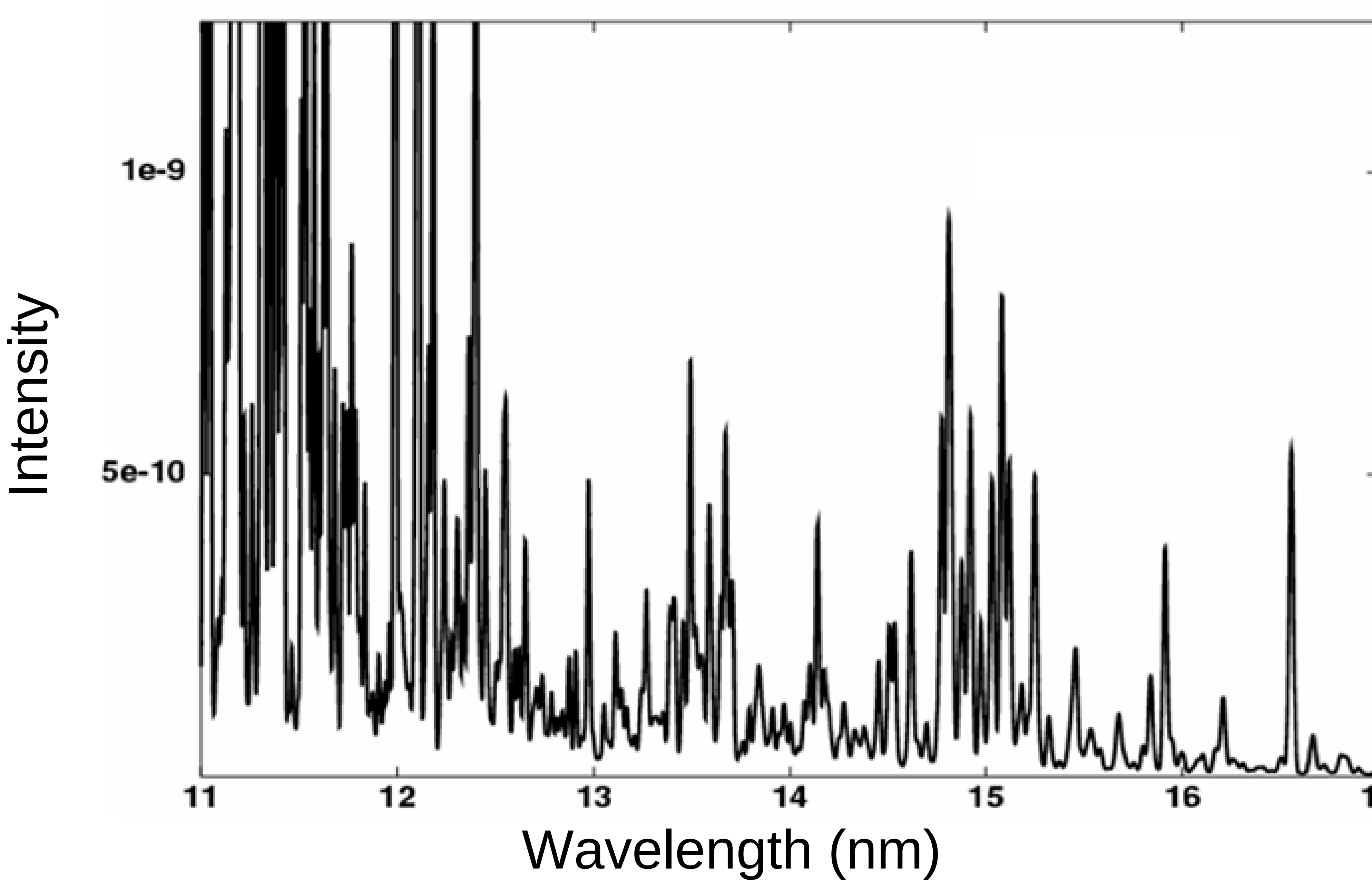
Emission Spectrum of Xe for LTE (Saha) Model

density 10^{-6} g/cm^3, temperature 14 eV (Z_0=10.5)



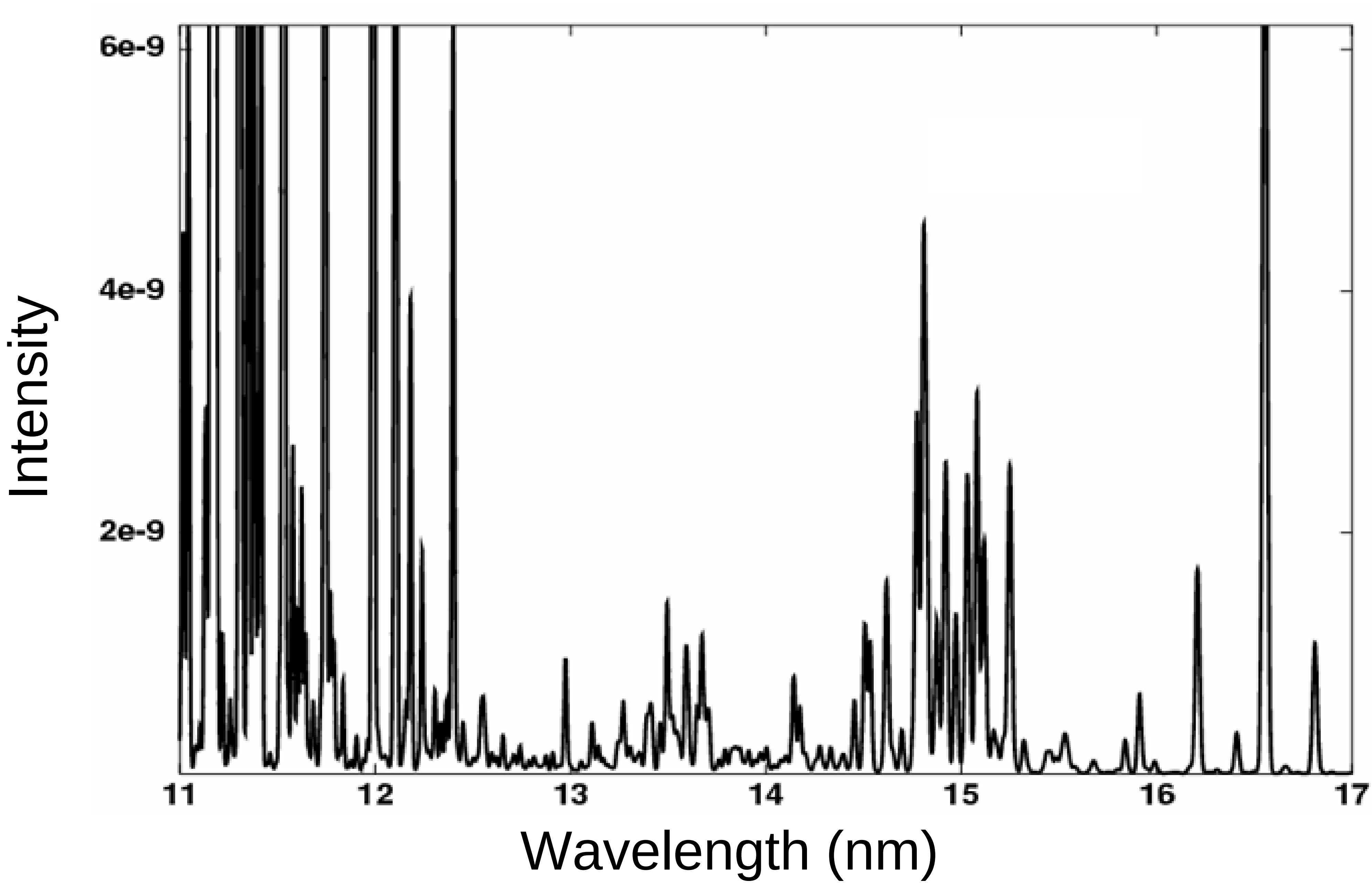
Emission Spectrum of Xe for Corona Equilibrium Model

density 10^{-6} g/cm^3, temperature 35 eV (Z_0=10.5)



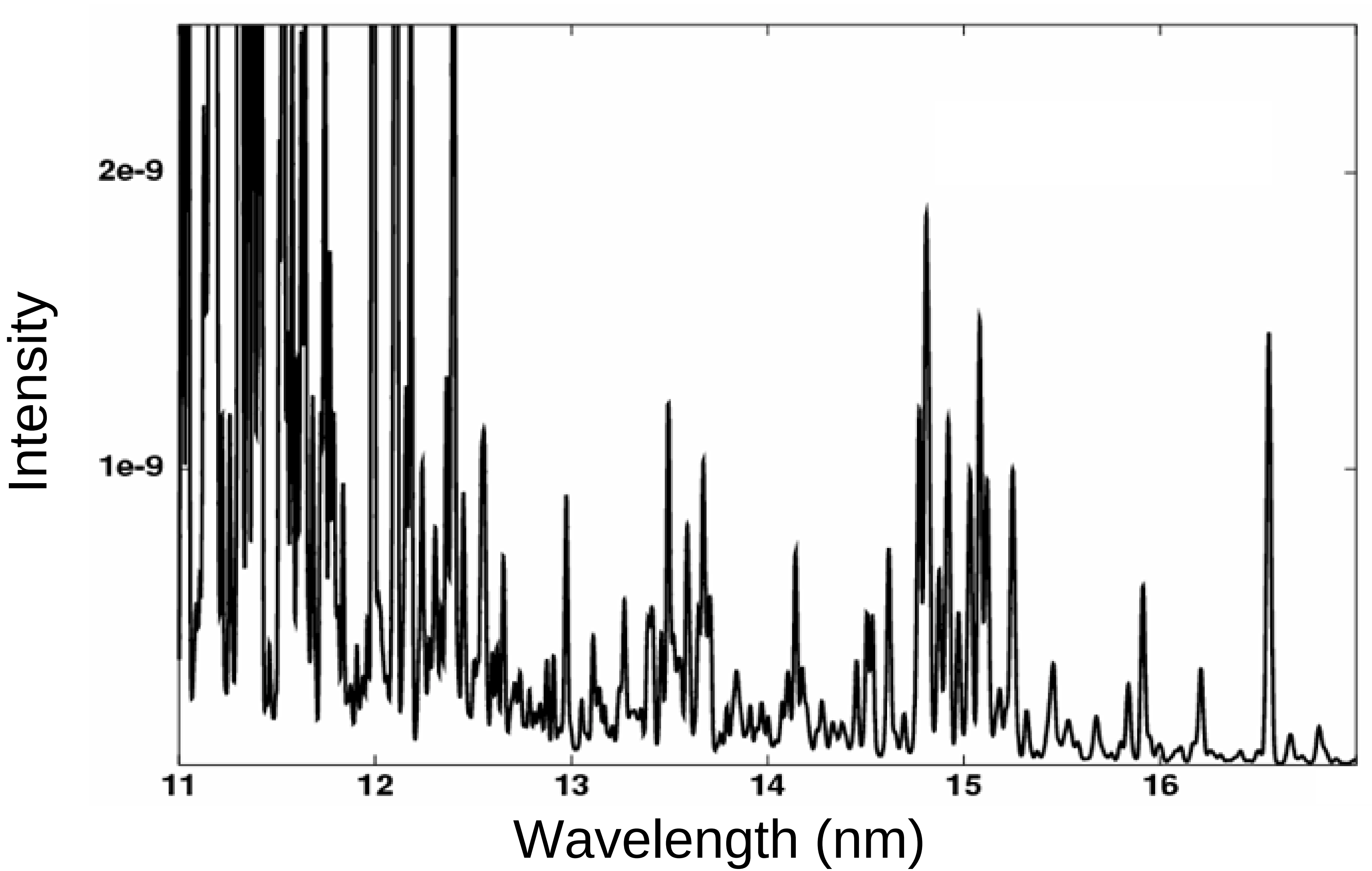
Emission Spectrum of Xe for CRSS Model

density 10^{-6} g/cm^3, temperature 40 eV (Z_0=9.6)



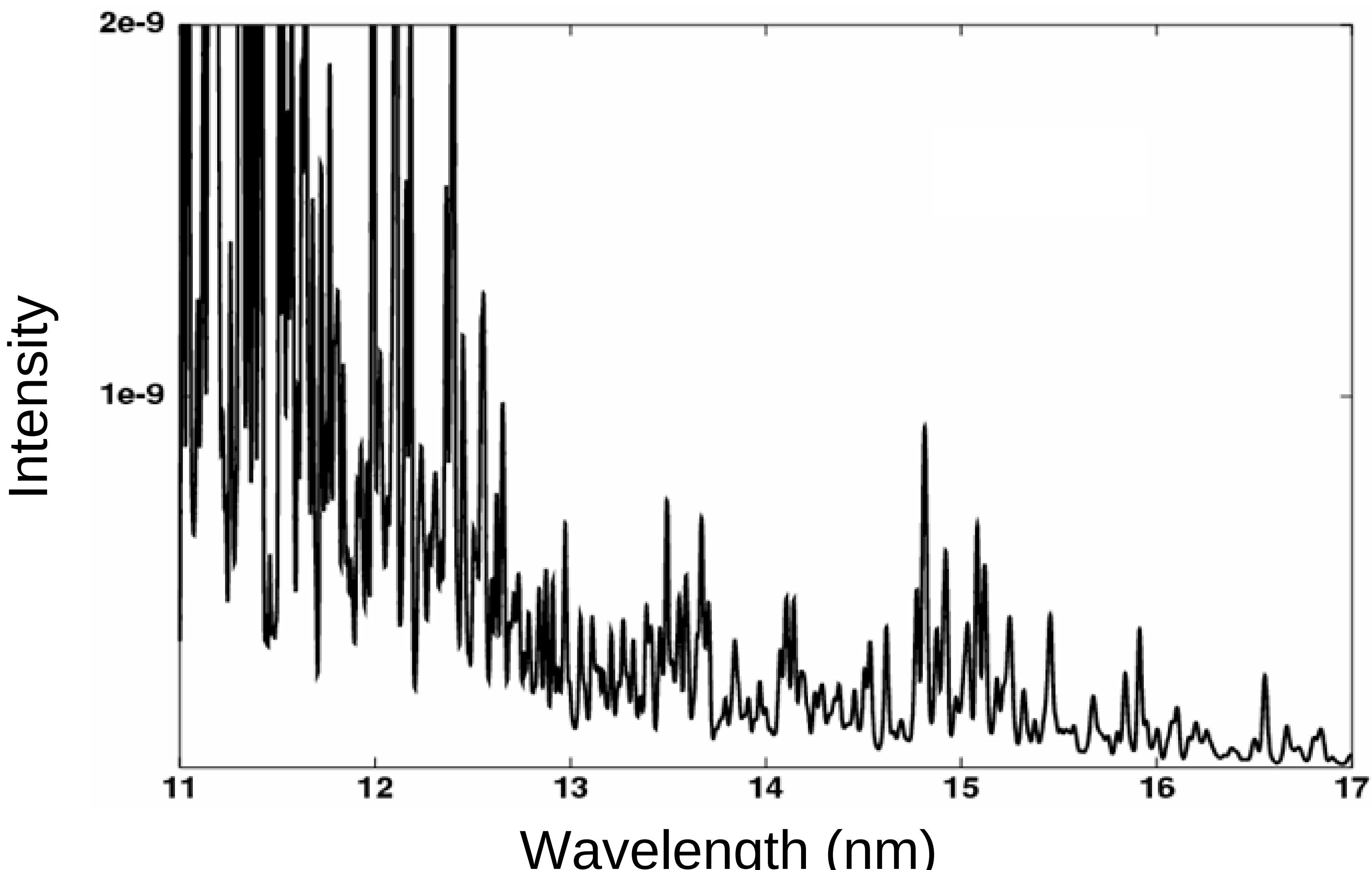
Emission Spectrum of Xe for CRSS Model

density 10^{-6} g/cm^3, temperature 44 eV (Z_0=10.5)



Emission Spectrum of Xe for CRSS Model

density 10^{-6} g/cm^3, temperature 50 eV (Z_0=11)



Summary

- ❖ **Influence of various kinetic models onto high Z plasma ion stage and EUV emission is considered**

- ❖ **EUV emission is conditioned by numerous transitions inside one atom shell ($\Delta n=0$) unified into clusters**

- ❖ **Narrow ionization stage interval for generation of EUV restricts the necessary plasma temperature region**

- ❖ **Dielectronic recombination plays an important role in ionization stage definition and must be examined accurately in non-LTE plasma**