Collisional–radiative model

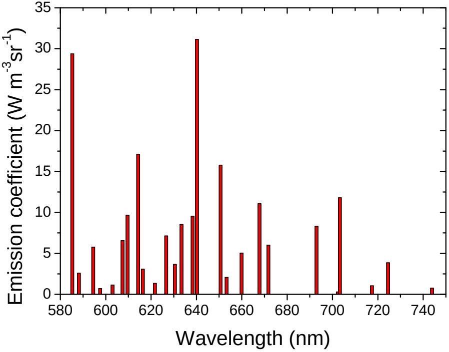
Lenka Dosoudilová

Emission coefficient

$$J_{ij} = \frac{1}{4\pi} n_j A_{ij} h\nu_{ij}, \quad i < j$$

Particles

- atoms in ground state
- atoms in excited states
  - resonance
  - metastable
- ions in ground and excited states
- molecules in ground and excited states
- electrons



Continuity equation

$$\frac{\partial n_i}{\partial t} + \nabla(n_i\vec{v}) = \left(\frac{\partial n_i}{\partial_t}\right)_{\text{coll,rad}}$$

- collisional and radiative processes much faster than transport processes

$$0 = \left(\frac{\partial n_i}{\partial_t}\right)_{\text{coll,rad}}$$

- particles with long lifetimes

$$\nabla(n_i\vec{v}) = -D\nabla^2 n_i$$

- balance equation

$$\left(\frac{\partial n_i}{\partial_t}\right)_{\text{coll,rad}} = R_{\text{prod}} - R_{\text{loss}}$$

Equation for ground state

$$n_{\text{gs}} = \frac{p}{kT_{\text{g}}}$$

Approximative models

- weakly ionized plasma: $n_g > n_e, n_+$
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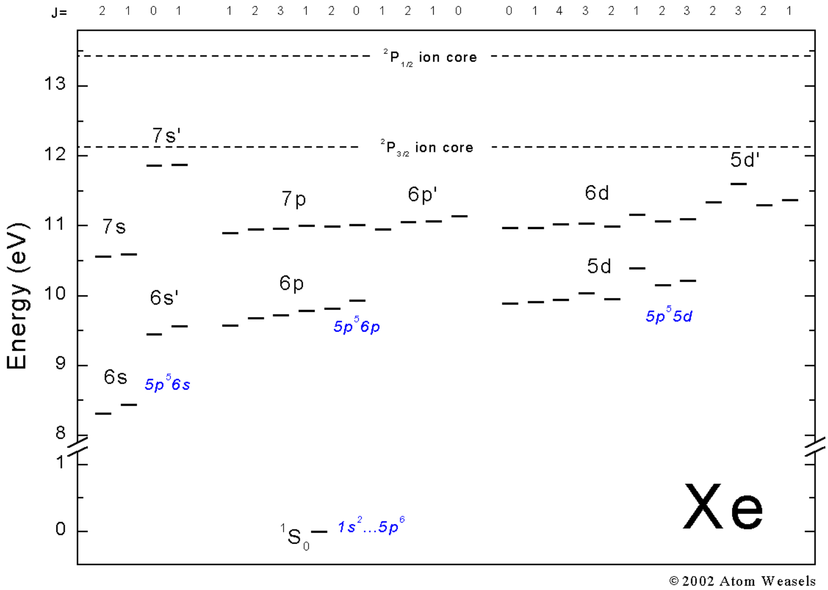
  - for lowest lying energy levels with short radiative lifetimes
- Saha/thermodynamic equilibrium
  - applicable at high n_e
  - (de)excitation by electron collisions
  - for levels close E_{ion} with long radiative lifetimes
  - recombination $\simeq$ ionization $\gg$ excitation


J=
2 1 0 1 1 2 3 1 2 0 1 2 1 0 0 1 4 3 2 1 2 3 2 3 2 1
Energy (eV)
13
12
11
10
9
8
1
0
²P1/2 ion core
²P3/2 ion core
7s'
7s
6s'
6s
5p⁵6s
7p
6p
5p⁵6p
6p'
6d
5d
5p⁵5d
5d'
¹S0
1s²...5p⁶
Xe
© 2002 Atom Weasels

Elementary processes

- electron-impact excitation and de-excitation

$$\mathrm{e} + \mathrm{Xe}(i) \leftrightarrow \mathrm{e} + \mathrm{Xe}(j), \qquad i < j$$

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$$Xe(i) + Xe_m \rightarrow e + Xe + Xe^+$$

$$Xe_2^* + Xe_2^* \rightarrow e + Xe + Xe + Xe_2^+$$

- electron collisional recombination for atomic and molecular ions

$$e + e/Xe + Xe^+ \rightarrow e/Xe + Xe(j)$$

$$e + Xe_2^+ \rightarrow Xe(j) + Xe_{gs}$$

- three-body collisional association

$$\mathrm{Xe_m} + \mathrm{Xe} + \mathrm{Xe} \rightarrow \mathrm{Xe}_2^* + \mathrm{Xe}$$
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- electron-impact/atom-collision dissociation of excimers and molecular ions

$$\mathrm{e/Xe} + \mathrm{Xe}_2^* \longrightarrow \mathrm{e/Xe} + \mathrm{Xe_{gs}} + \mathrm{Xe_m}$$
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- quenching: diffusion-controlled at the wall, collisions with neutral species and metastables

Rate coefficient

- e.g. excitation from ground state

$$\left(\frac{\partial n_i}{\partial_t}\right)_{\text{coll,rad}} = k_{1i}\, n_\text{e} n_\text{gs}$$

- calculation

$$k = \langle \sigma(v)\, v \rangle = \int_0^\infty \sigma(v) v f(v) \mathrm{d}v = \sqrt{\frac{2}{m_e}} \int_0^\infty \sigma(E) E f(E) \mathrm{d}E$$

- distribution function

$$f(v) = 4\pi \left(\frac{m_\text{e}}{2\pi k T_\text{e}}\right)^{3/2} v^2 \exp\left(-\frac{m_\text{e} v^2}{2kT_\text{e}}\right)$$

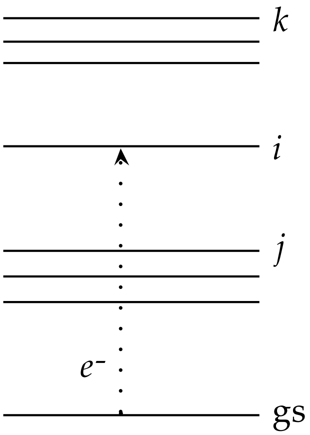
$$f(E) = \frac{2\sqrt{E}}{\sqrt{\pi (kT_\text{e})^3}} \exp\left(-\frac{E}{kT_\text{e}}\right)$$

- measurements: cross sections

Types of cross sections σ

- optical emission

$$\sigma_{i \to j}^{\text{opt}} \sim \Phi_{i \to j}^{\text{obs}}$$



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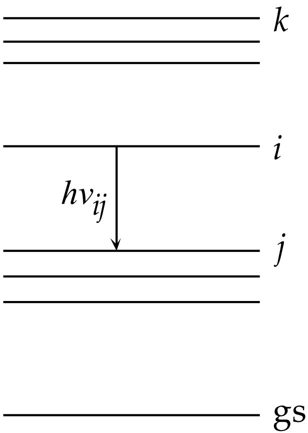

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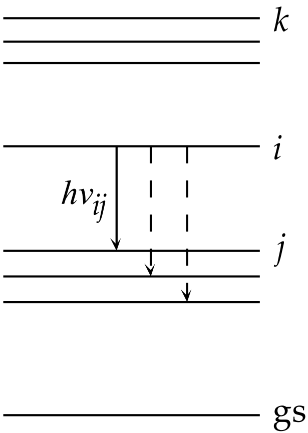
$$\sigma_{i\to j}^{\mathrm{opt}} = \frac{A_{ij}}{\sum_{l<i} A_{il}} \sigma_{i}^{\mathrm{app}}$$



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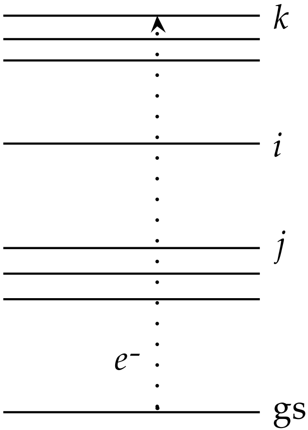
- cascade

$$\sigma^{\text{cas}}_{i} = \sum_{k>i} \sigma^{\text{opt}}_{k\to i}$$



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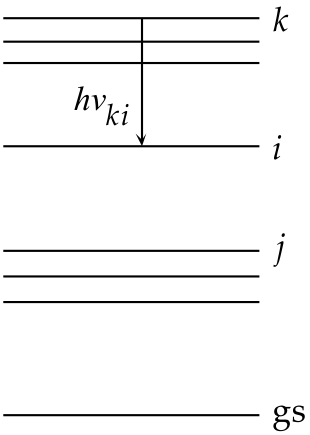

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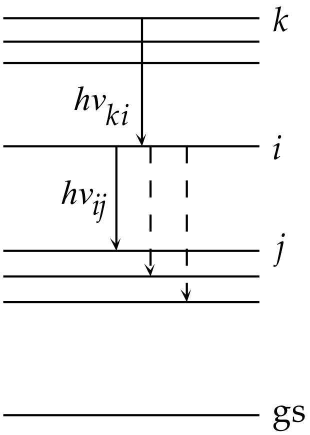
- cascade

$$\sigma_i^{\mathrm{cas}} = \sum_{k>i} \sigma_{k\to i}^{\mathrm{opt}}$$

- direct

$$\sigma_i^{\mathrm{dir}} = \sigma_i^{\mathrm{app}} - \sigma_i^{\mathrm{cas}}$$



Measurements of cross section

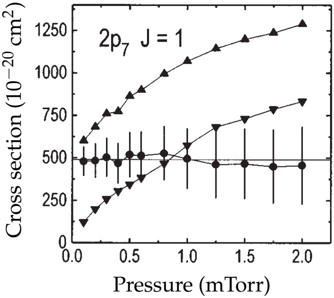
- optical emission cross section
  - vacuum chamber, ultrahigh purity gas, monoenergetic beam of e^-
  - measuring electron current and photon emission rate

$$\sigma_{i \to j}^{\mathrm{opt}} = \frac{\Phi_{ij}}{n_0 (I/e)}$$

- direct excitation cross sections
  - electron energy loss as function of scattering angle
  - differential cross section

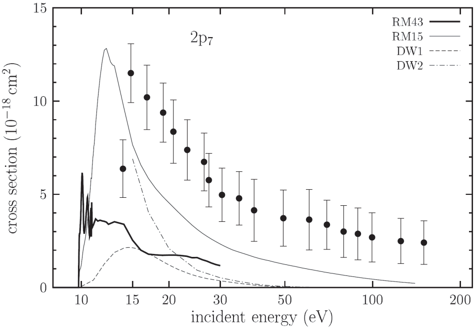
Theoretical calculations

- Born approximation
- R-matrix
- distorted-wave approximation

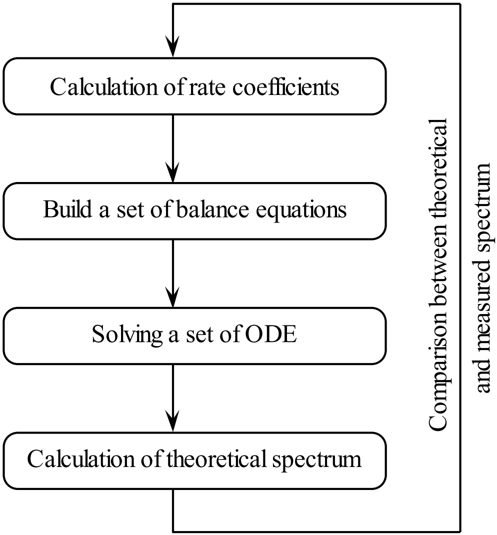


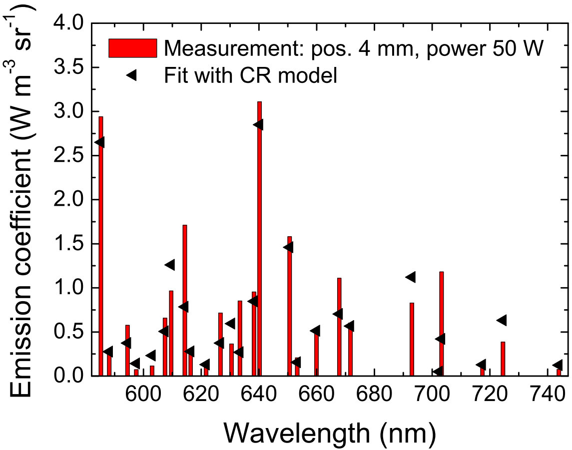
Incident electron energy 30 eV

J. T. Fons, C. C. Lin, Phys. Rev. A **58**, 4603 (1998)



K. Bartschat *et al.*, Phys. Rev. A **69**, 062706 (2004)


Calculation of rate coefficients
Build a set of balance equations
Solving a set of ODE
Calculation of theoretical spectrum
Comparison between theoretical
and measured spectrum



Z. Navrátil *et al.*, Journal of Physics D: Applied Physics, **43** (50), 505203 (2010)

Thank you for your attention!