水素・ヘリウムの衝突輻射モデルと中性粒子輸送コードの開発

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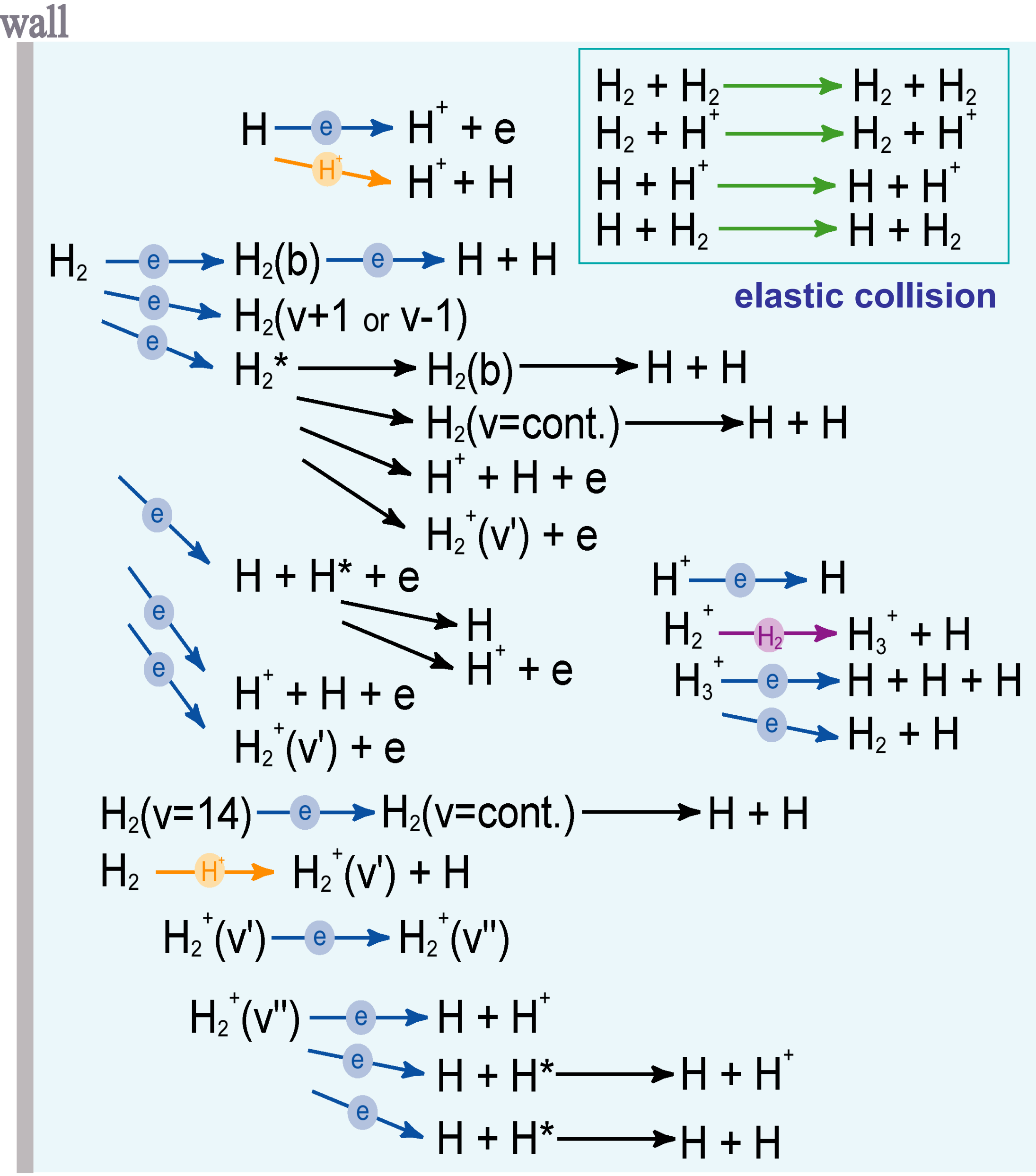
筑波大学プラズマ研究センターシンポジウム
双方向型共同研究「磁化プラズマ中の壁不純物粒子挙動とプラズマ特性への影響」
平成25年8月29日(木)8:50～17:50　30日(金) 9:00～17:10
つくばサイエンスインフォメーションセンター大会議室

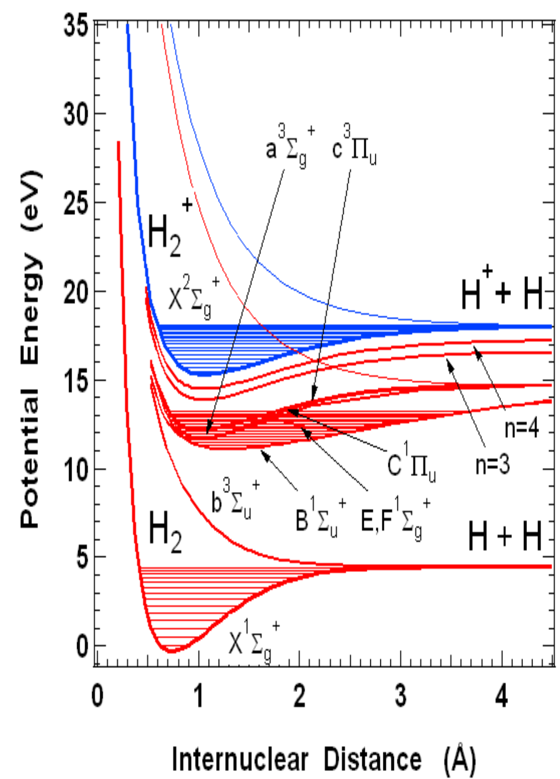
Introduction : Our models



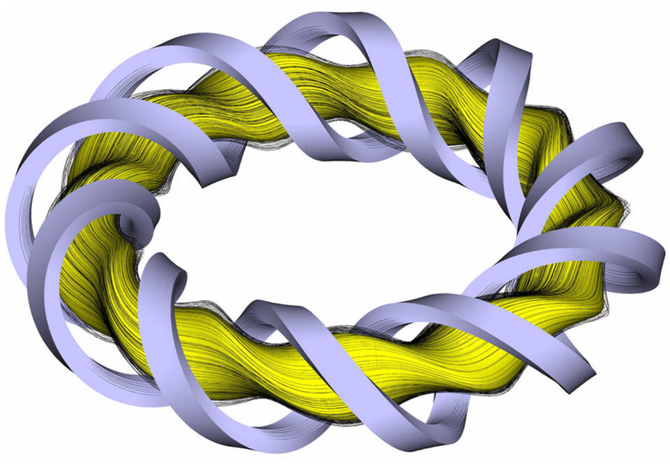
Collisional–Radiative Models

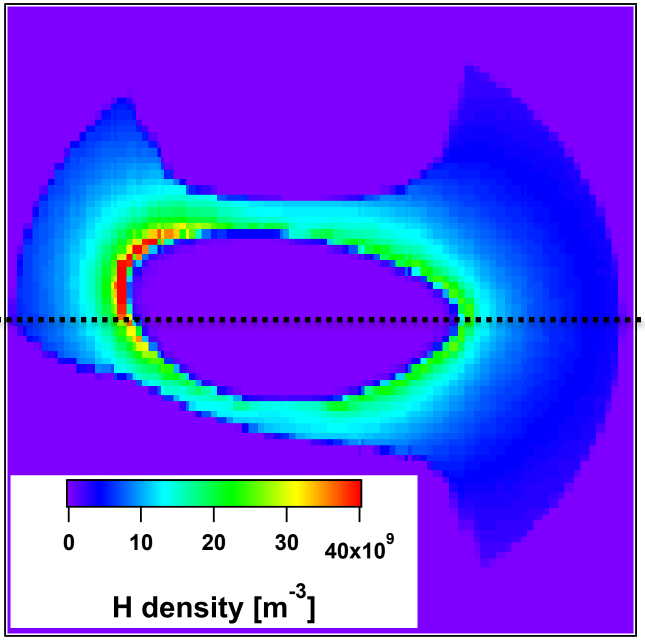
Hydrogen atom
Hydrogen molecule (H2)
Helium atom (M. Goto)

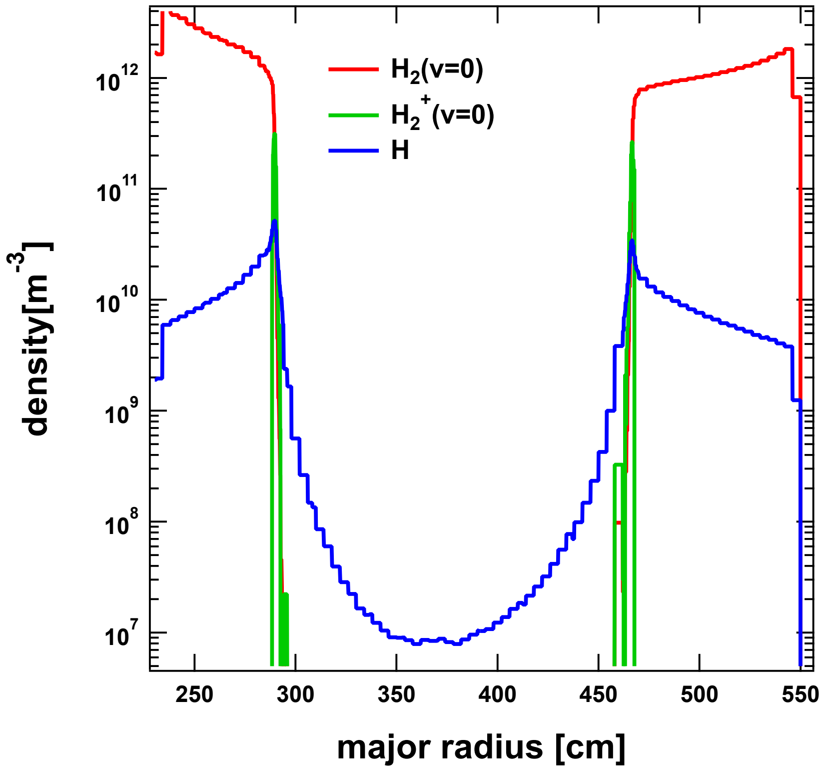
Neutral-Transport Code

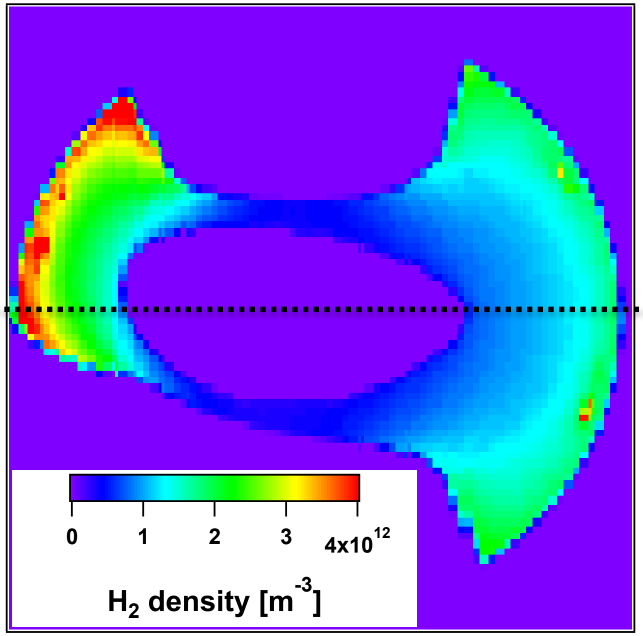


LHD 中性粒子輸送コードの計算結果

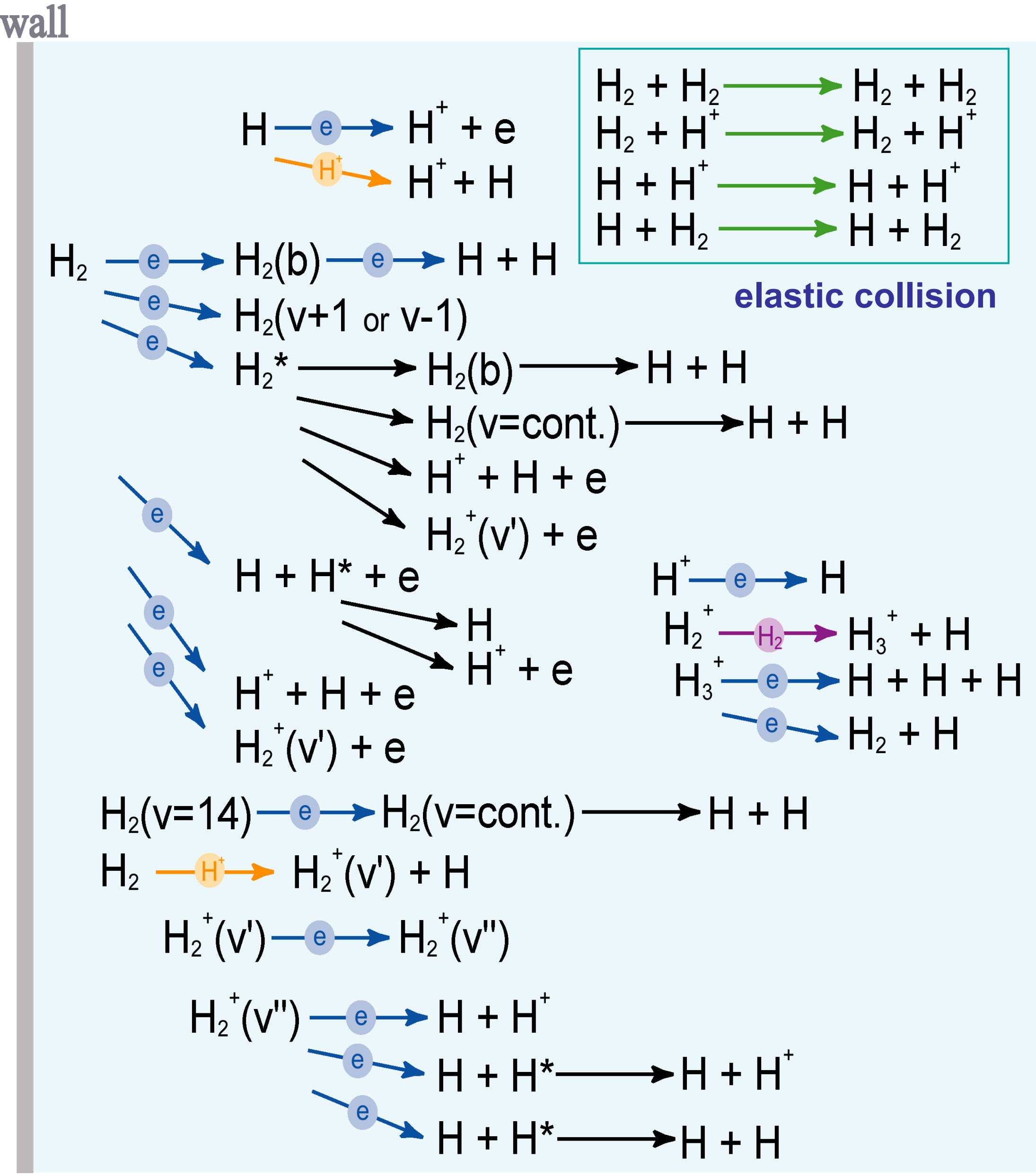








Introduction ： Our models



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Hydrogen molecule (H2)
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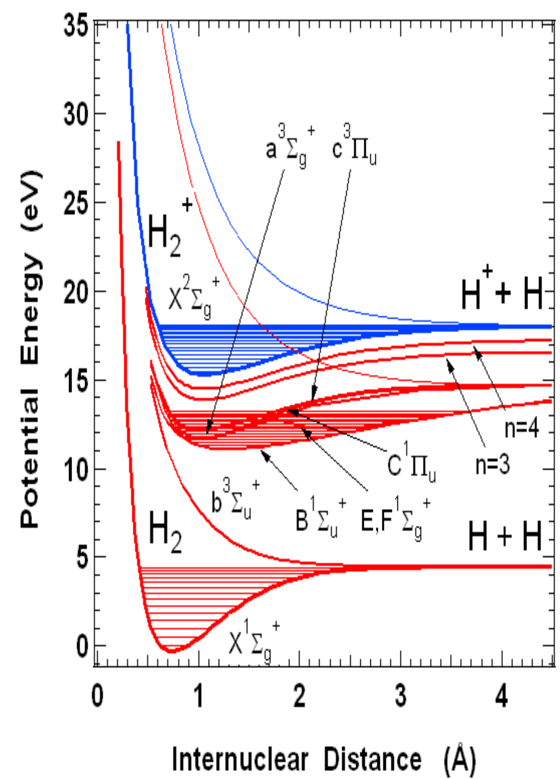
Neutral-Transport Code



H 衝突輻射モデル

H Collisional-Radiative Model

inflow

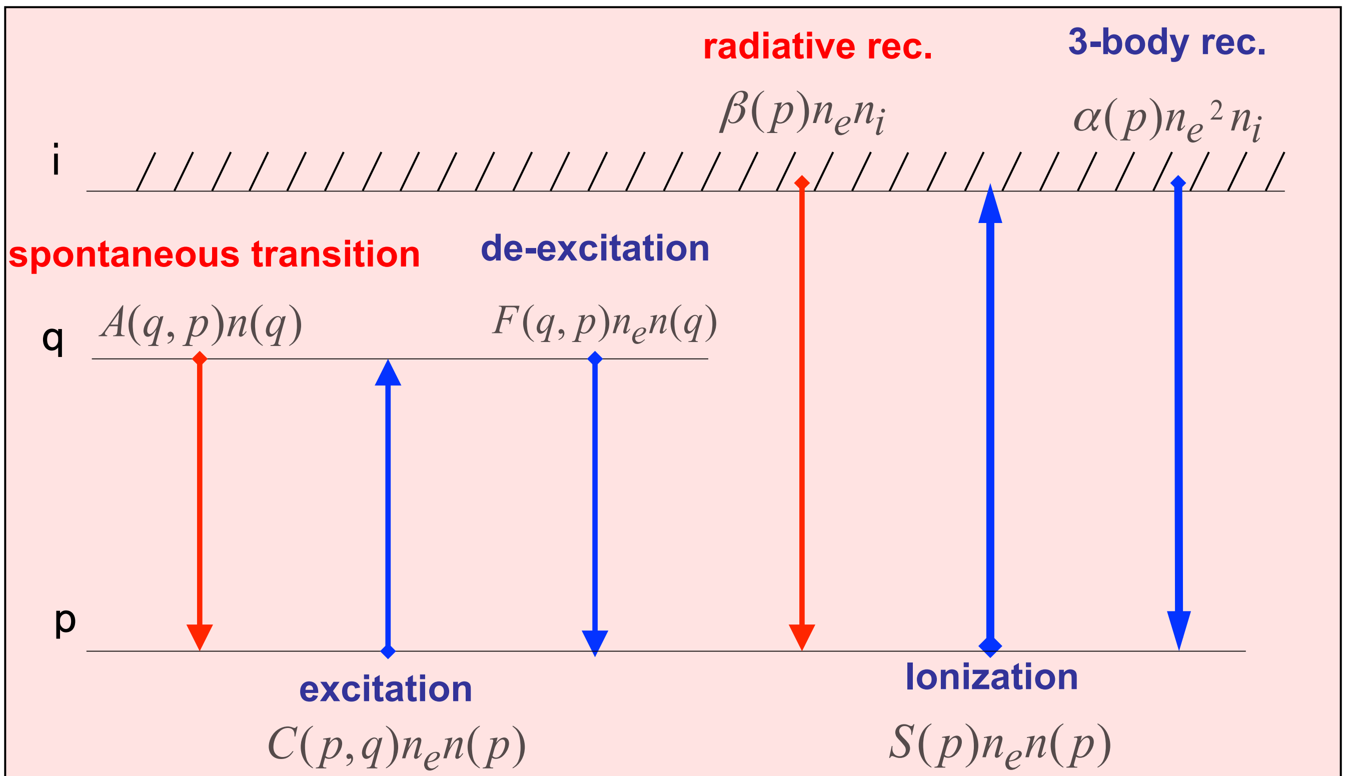
$$\frac{dn(p)}{dt} = \sum_{q<p} C(q,p) n_e n(q) + \sum_{q>p} \{F(q,p) n_e + A(q,p)\} n(q) + \alpha(p) n_e^2 n_i + \beta(p) n_e n_i$$

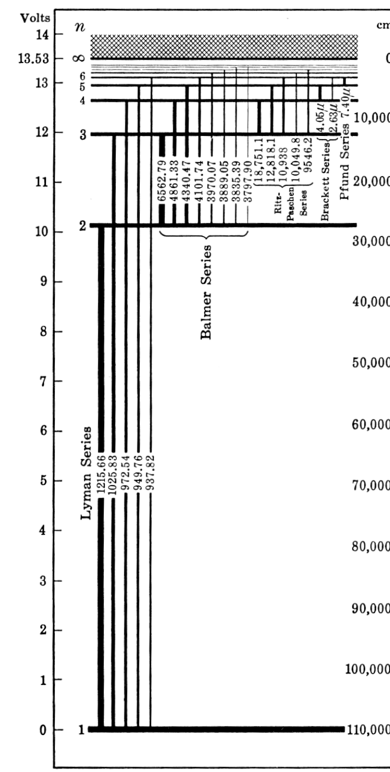
$$-[\{\sum_{q<p} F(p,q) + \sum_{q>p} C(p,q) + S(p)\} n_e + \sum_{q<p} A(p,q)] n(p)$$

outflow

PLASMA

e H$^+$ H





Solving Rate equations

$$\frac{dn(p)}{dt} = \sum_{q<p} C(q,p) n_e n(q) + \sum_{q>p} \{F(q,p) n_e + A(q,p)\} n(q) + \alpha(p) n_e^2 n_i + \beta(p) n_e n_i$$
$$- [\{\sum_{q<p} F(p,q) + \sum_{q>p} C(p,q) + S(p)\} n_e + \sum_{q<p} A(p,q)] n(p)$$

p>=2

unknown

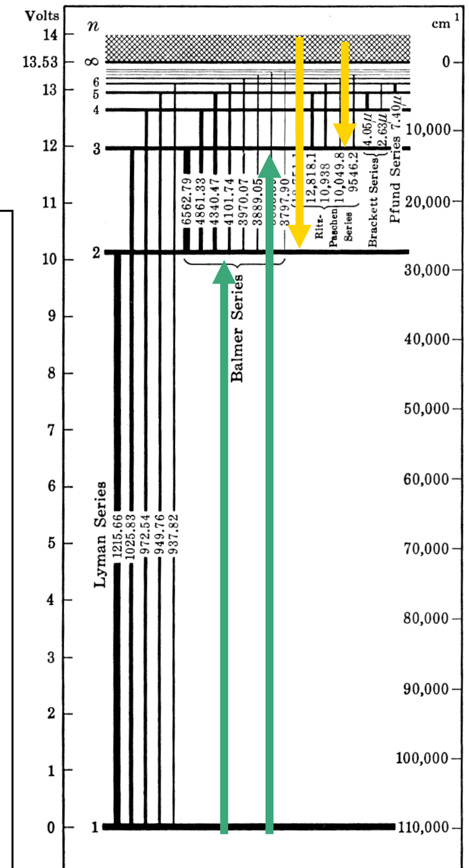
$$\frac{d}{dt}\begin{pmatrix} \cdot \\ \cdot \\ n(3) \\ n(2) \end{pmatrix} = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}\begin{pmatrix} \cdot \\ \cdot \\ n(3) \\ n(2) \end{pmatrix} + \begin{pmatrix} \cdot \\ \cdot \\ \alpha(3)n_e + \beta(3) \\ \alpha(2)n_e + \beta(2). \end{pmatrix} n_i n_e + \begin{pmatrix} \cdot \\ \cdot \\ C(1,3) \\ C(1,2) \end{pmatrix} n(1) n_e$$

0

quasi-steady-state approximation (QSS)

$$n(p) = \underline{R_0(p) n_i n_e} + \underline{R_1(p) n(1) n_e}$$

Recombining component　　Ionizing component

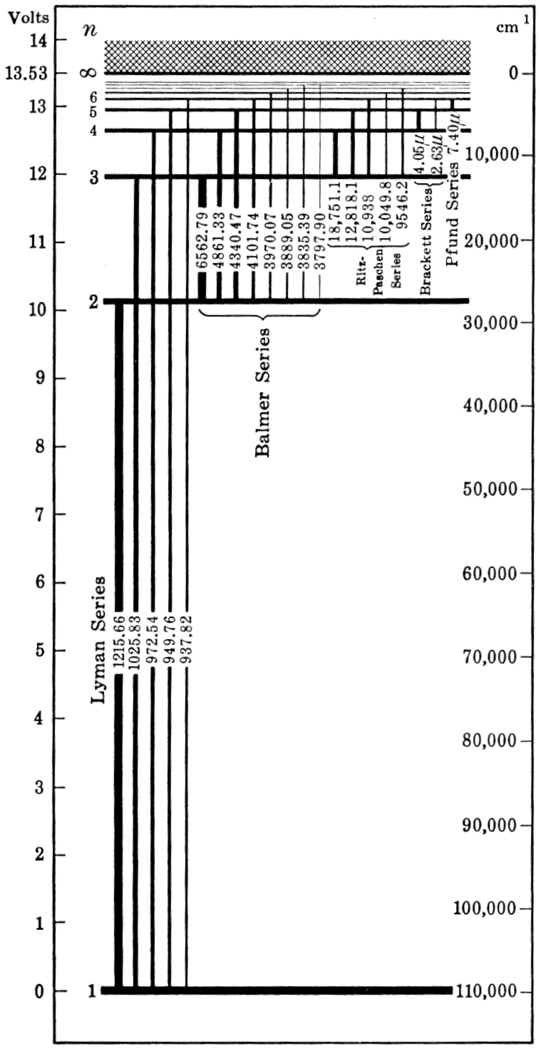


p=1 $$\frac{dn(1)}{dt} = -S_{CR} n(1) n_e + \alpha_{CR} n_{H^+} n_e$$

S_{CR} effective ionization rate coefficient

α_{CR} effective recombination rate coefficient

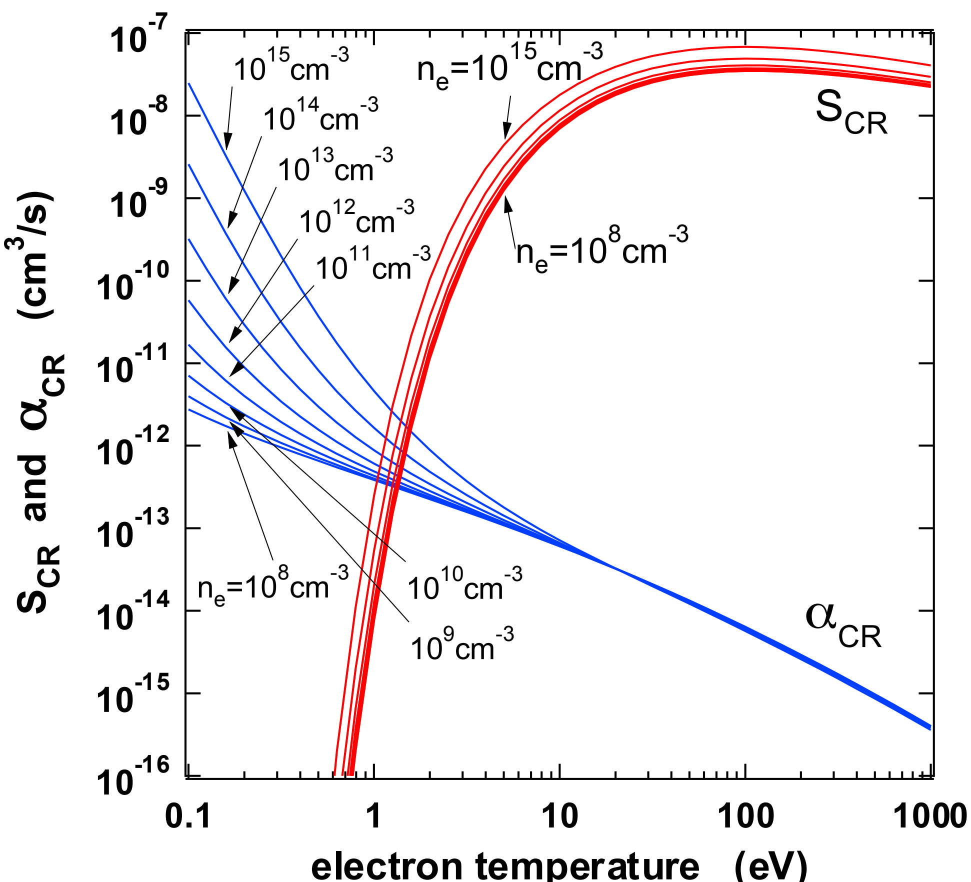
Effective Ionization and Recombination Rate coefficients



S_{CR} Effective Ionization Rate Coefficient

α_{CR} Effective Recombination Rate Coefficient

$$\frac{dn(1)}{dt} = -S_{CR}\, n(1) n_e + \alpha_{CR}\, n_{H^+} n_e$$

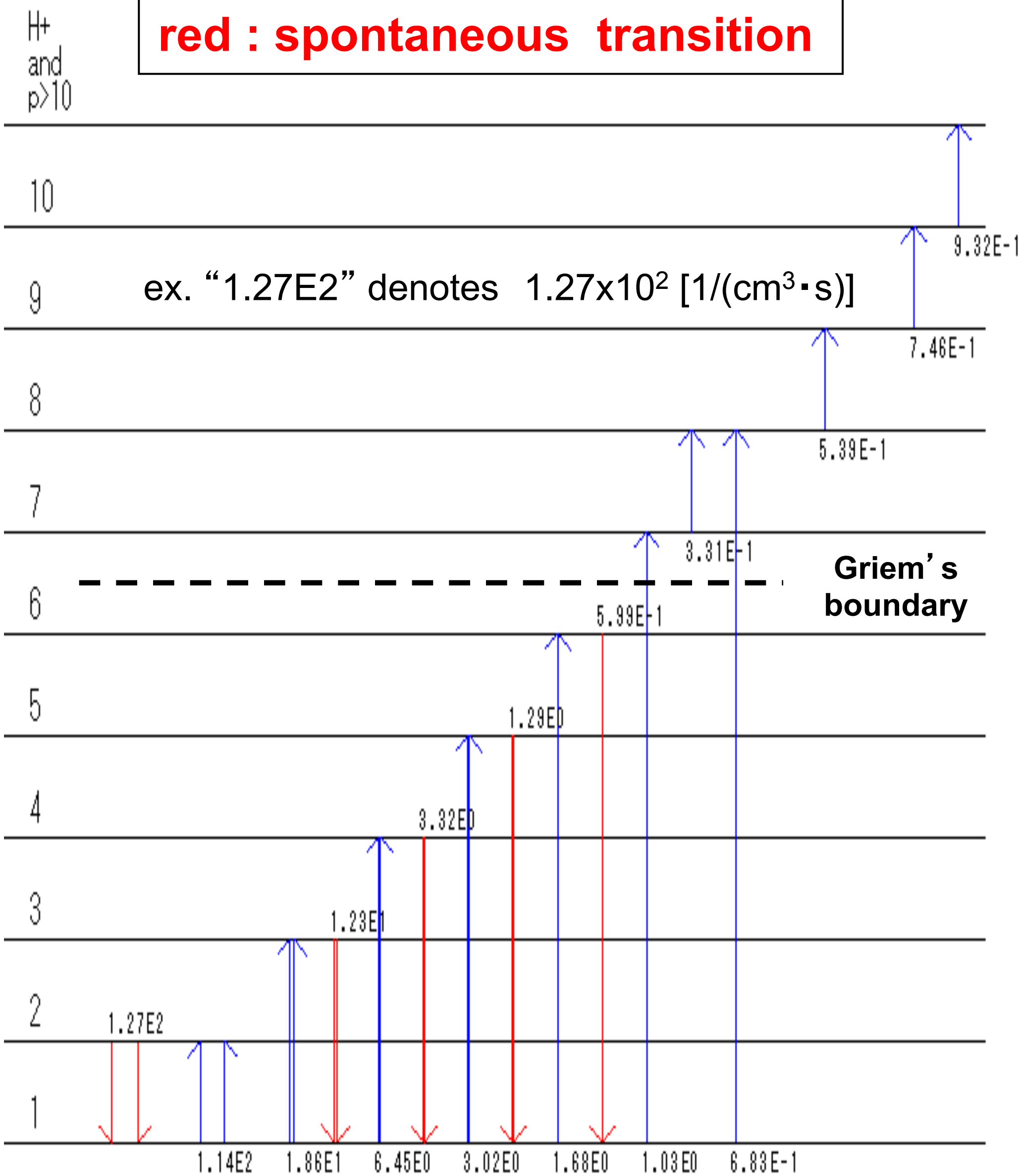


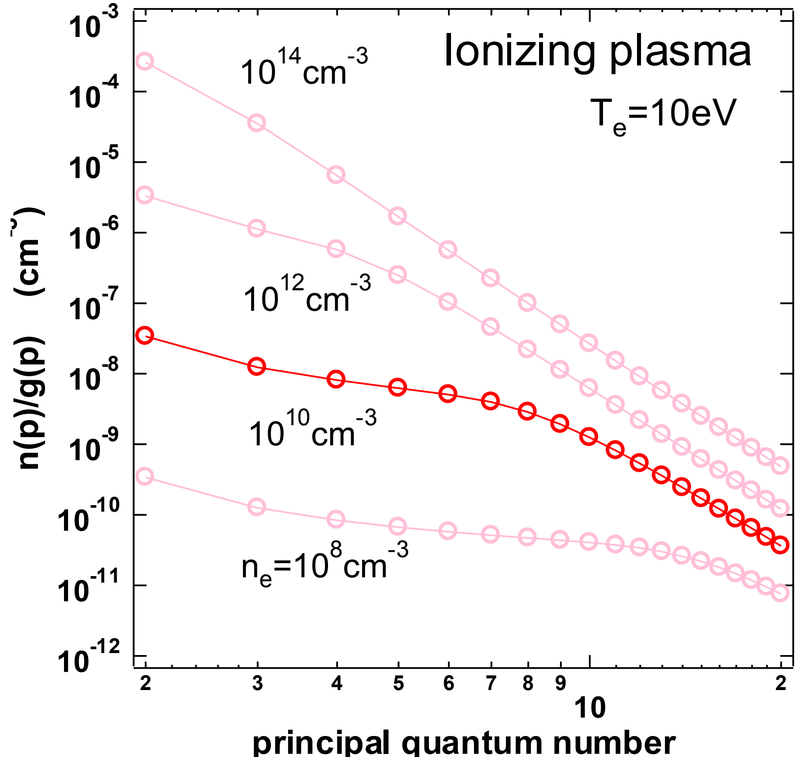
Ionizing component T_e=10eV n_e=10^{10}cm^{-3} n(1)=1cm^{-3}

blue : electron impact

red : spontaneous transition

ex. "1.27E2" denotes 1.27x10^2 [1/(cm^3・s)]

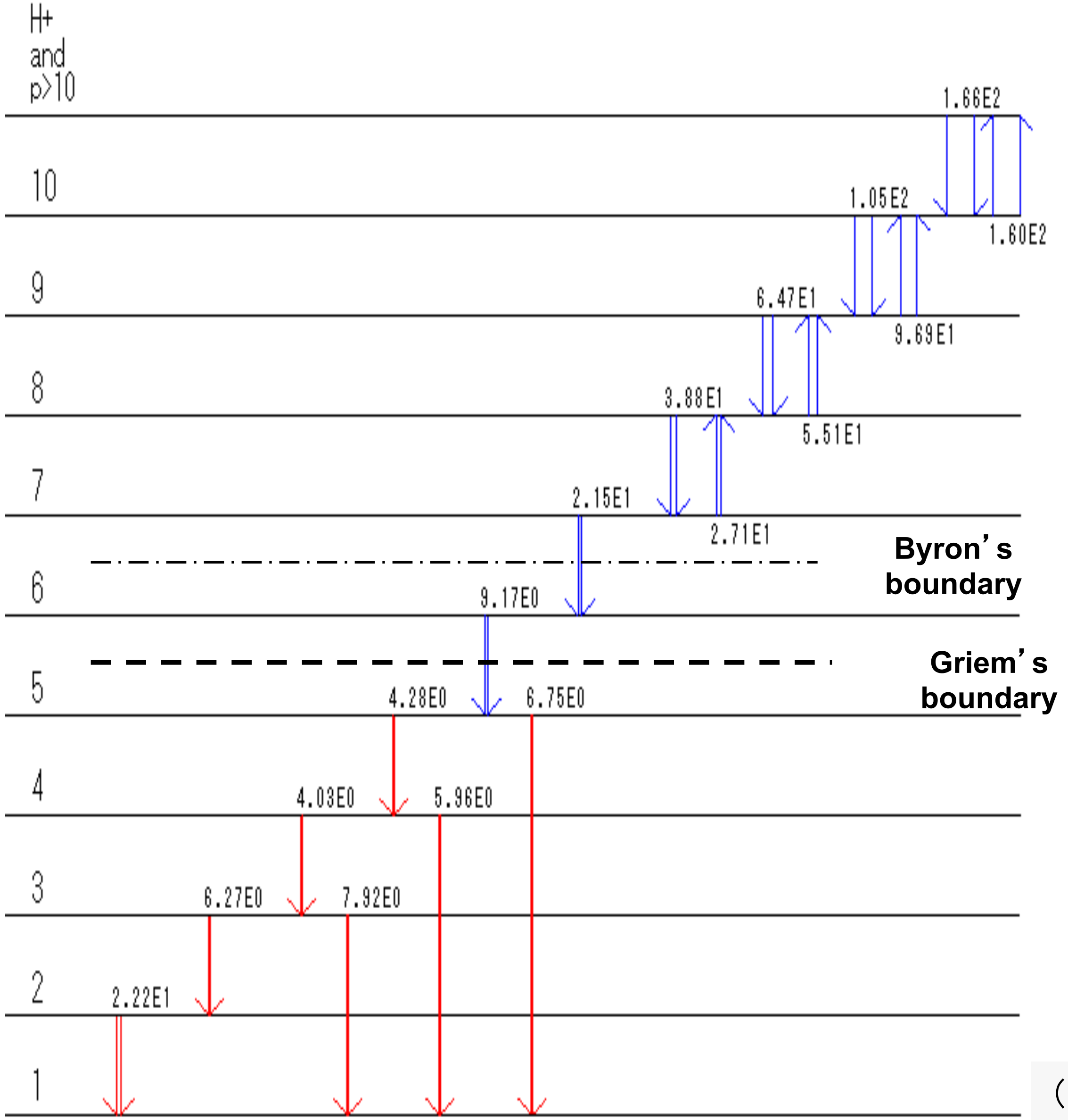


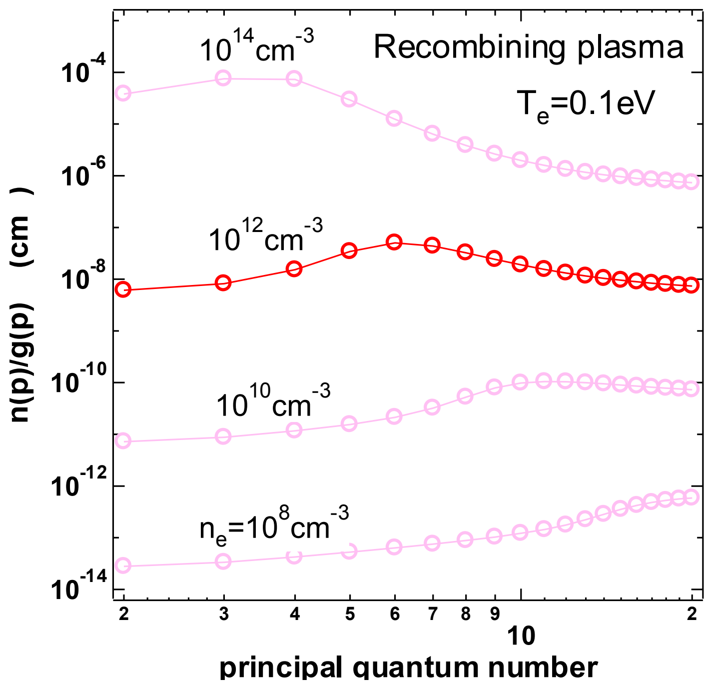


S(1)n(1)ne=6.92E1 [1/(cm^3・s)]

Recombining component

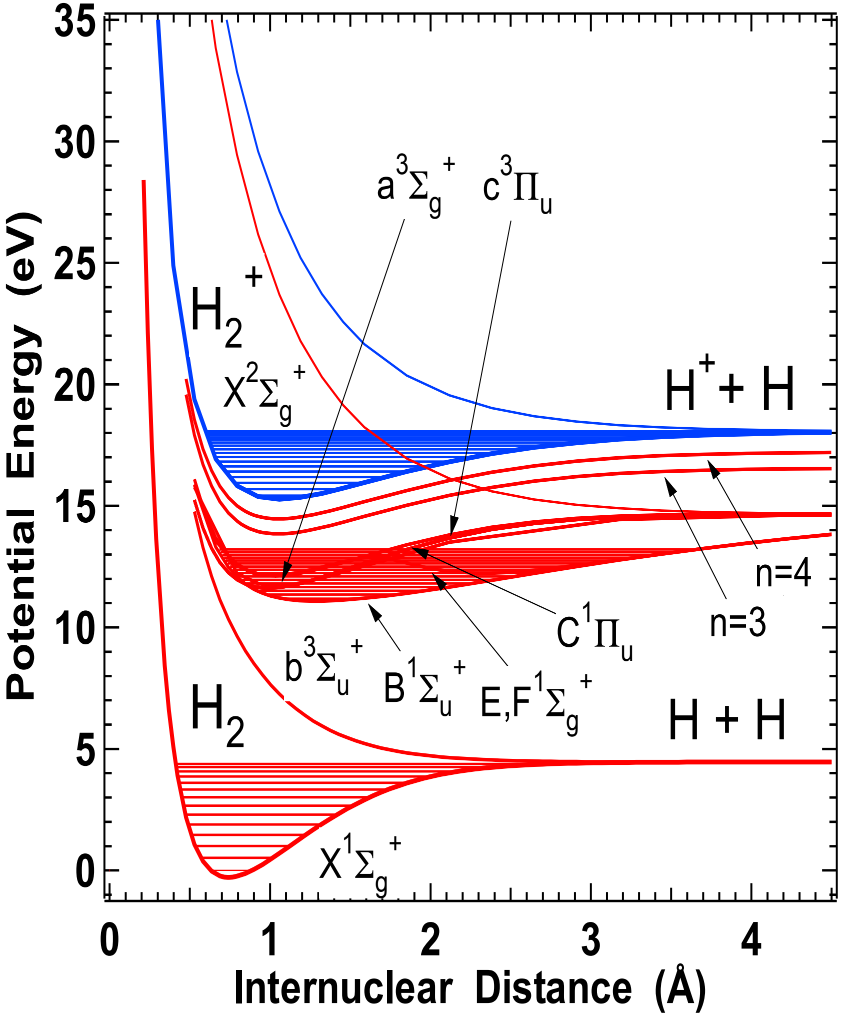
T_e=0.1eV n_e=10^{12}cm^{-3} ni=1cm^{-3}



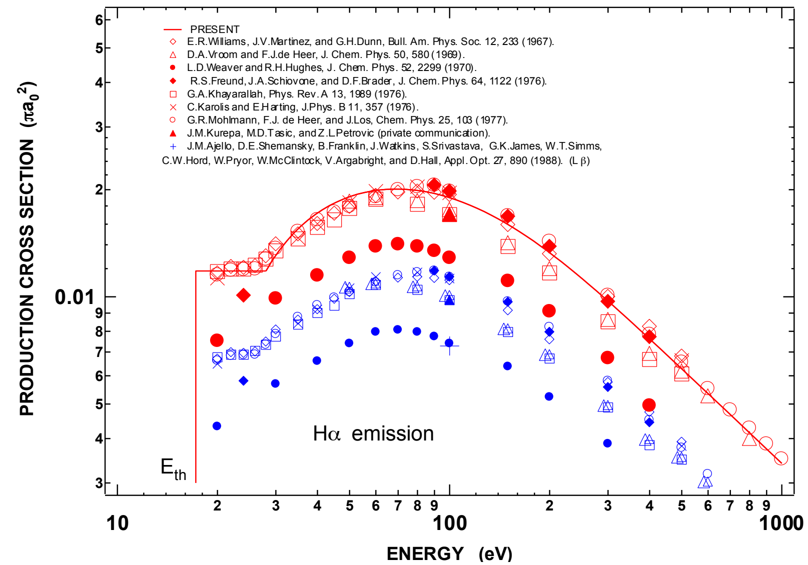


$(\alpha(1)ne+\beta(1))nzne$=4.69E-1 [1/(cm^3・s)]

H_2 + e -> H + H(p) + e



Potential Energy (eV)
Internuclear Distance (Å)
H_2^+
$X^2\Sigma_g^+$
$H^+ + H$
$a^3\Sigma_g^+$
$c^3\Pi_u$
$C^1\Pi_u$
n=4
n=3
$b^3\Sigma_u^+$
$B^1\Sigma_u^+$
$E,F^1\Sigma_g^+$
H_2
H + H
$X^1\Sigma_g^+$



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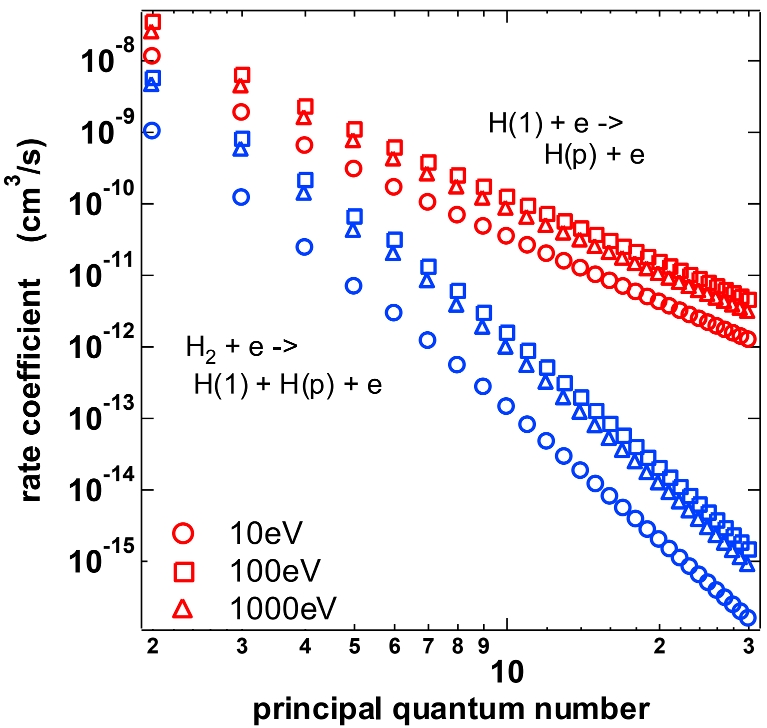
PRODUCTION CROSS SECTION (πa_0^2)
Hα emission
E_{th}
ENERGY (eV)



rate coefficient (cm^3/s)
H(1) + e -> H(p) + e
H_2 + e -> H(1) + H(p) + e
10eV
100eV
1000eV
principal quantum number

Collisional-Radiative Model : Inclusion of $H_2 + e \rightarrow H + H(p) + e$

$$\frac{dn(p)}{dt} = \sum_{q<p} C(q,p) n_e n(q) + \sum_{q>p} \{F(q,p) n_e + A(q,p)\} n(q) + \alpha(p) n_e^2 n_i + \beta(p) n_e n_i$$

$$+ C_{H2}(p) n_{H2} n_e$$

$$- [\{\sum_{q<p} F(p,q) + \sum_{q>p} C(p,q) + S(p)\} n_e + \sum_{q<p} A(p,q)] n(p)$$

p>=2

unknown

$H_2 + e \rightarrow H + H(p) + e$

$$\frac{d}{dt}\begin{pmatrix} \cdot \\ \cdot \\ n(3) \\ n(2) \end{pmatrix} = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}\begin{pmatrix} \cdot \\ \cdot \\ n(3) \\ n(2) \end{pmatrix} + \begin{pmatrix} \cdot \\ \cdot \\ \alpha(3) n_e + \beta(3) \\ \alpha(2) n_e + \beta(2). \end{pmatrix} n_i n_e + \begin{pmatrix} \cdot \\ \cdot \\ C(1,3) \\ C(1,2) \end{pmatrix} n(1) n_e + \begin{pmatrix} \cdot \\ \cdot \\ C_{H2}(3) \\ C_{H2}(2) \end{pmatrix} n_{H2} n_e$$

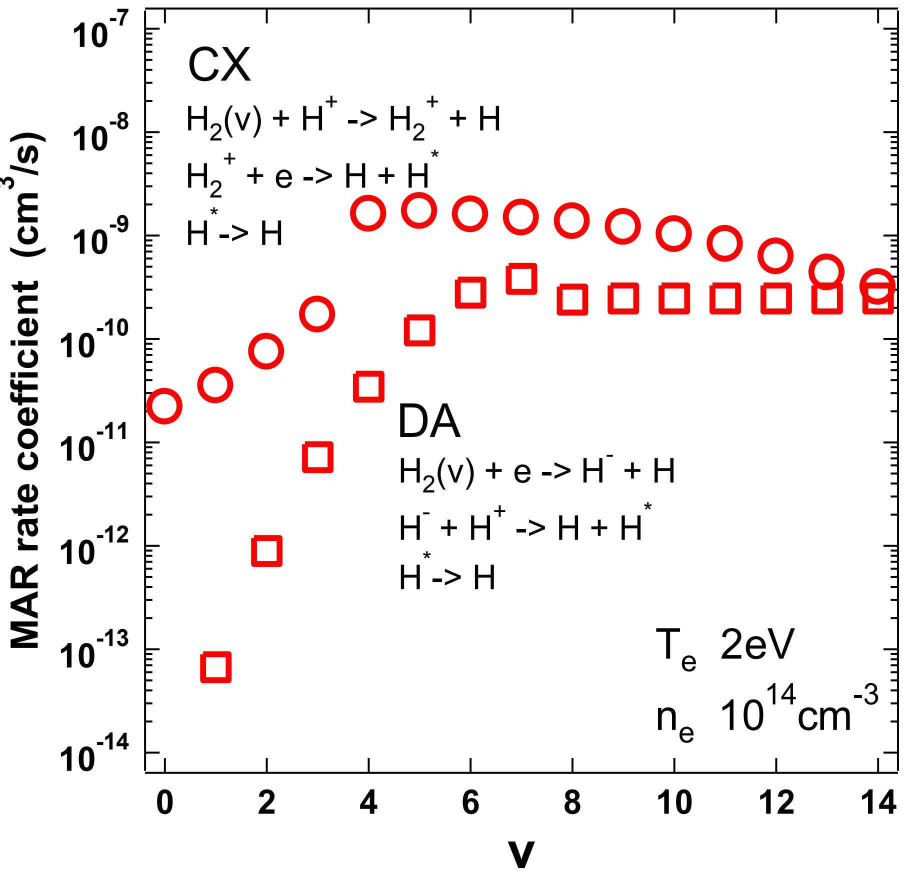
0

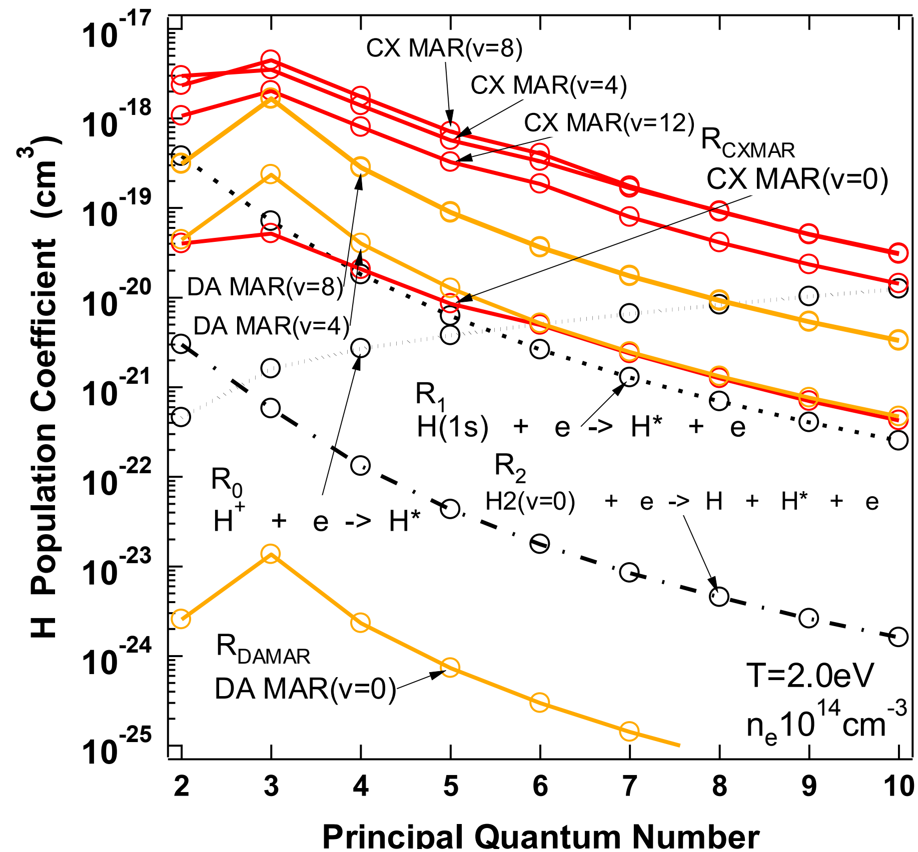
(QSS)

$$n(p) = \underline{R_0(p) n_i n_e} + \underline{R_1(p) n(1) n_e} + \underline{R_2(p) n_{H2} n_e}$$

Recombining component — Ionizing component — New term

MAR (Molecular Assisted Recombination)

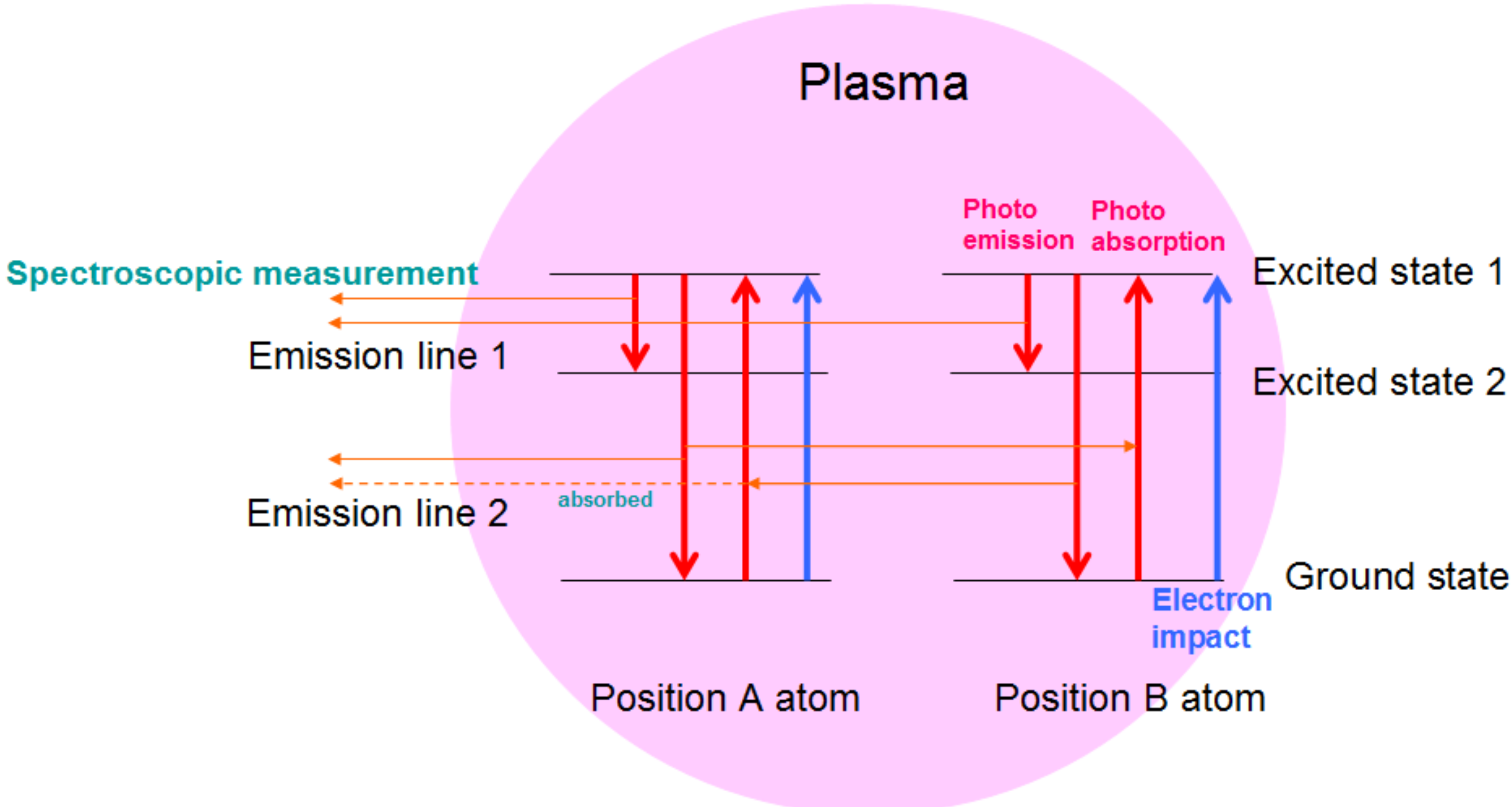




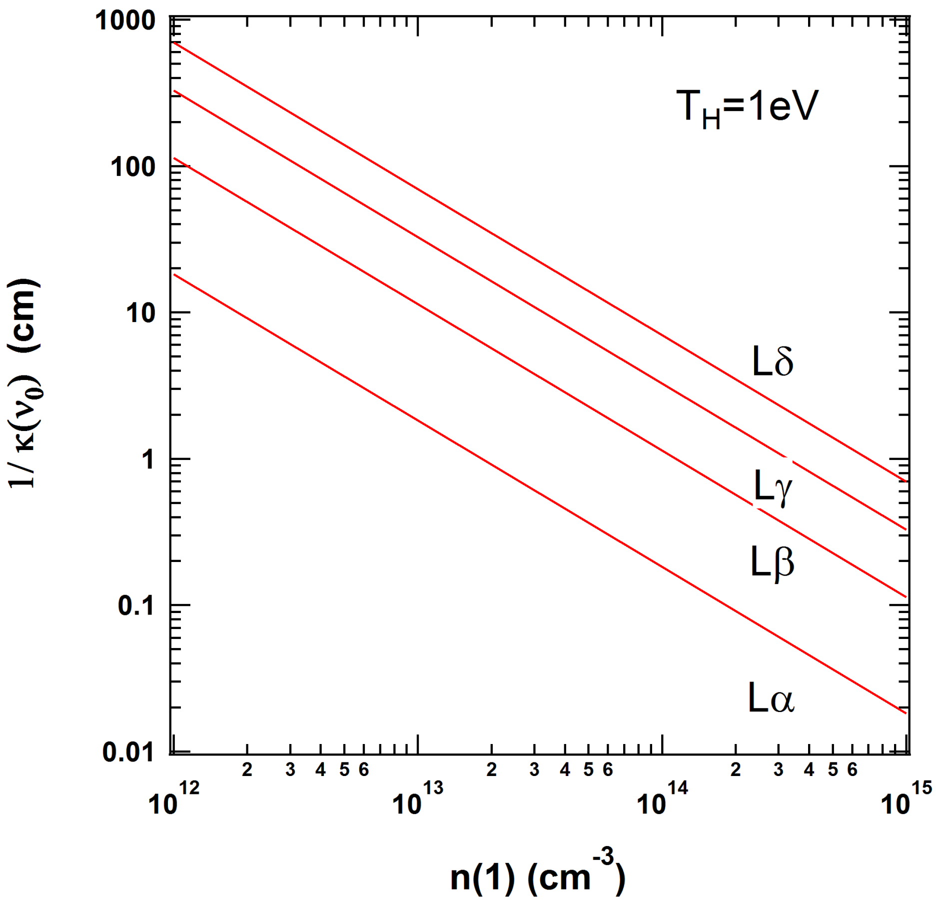
$$n(p) = R_0(p)n_e n_{H^+} + R_1(p)n_e n_H + R_2(p)n_e n_{H_2} + R_{MAR}(p)n_e n_{H_2}$$

輻射輸送

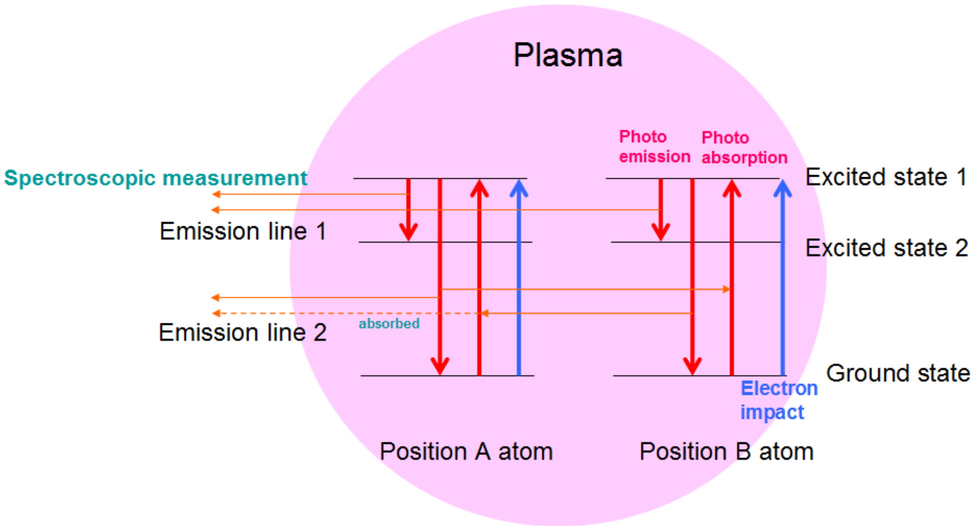
輻射輸送


Plasma
Spectroscopic measurement
Emission line 1
Emission line 2
absorbed
Photo emission
Photo absorption
Excited state 1
Excited state 2
Ground state
Electron impact
Position A atom
Position B atom

ライマン線吸収長



1000
100
10
1
0.1
0.01
$1/\kappa(\nu_0)$ (cm)
T_H=1eV
Lδ
Lγ
Lβ
Lα
10^{12}
10^{13}
10^{14}
10^{15}
n(1) (cm^{-3})



Plasma
Spectroscopic measurement
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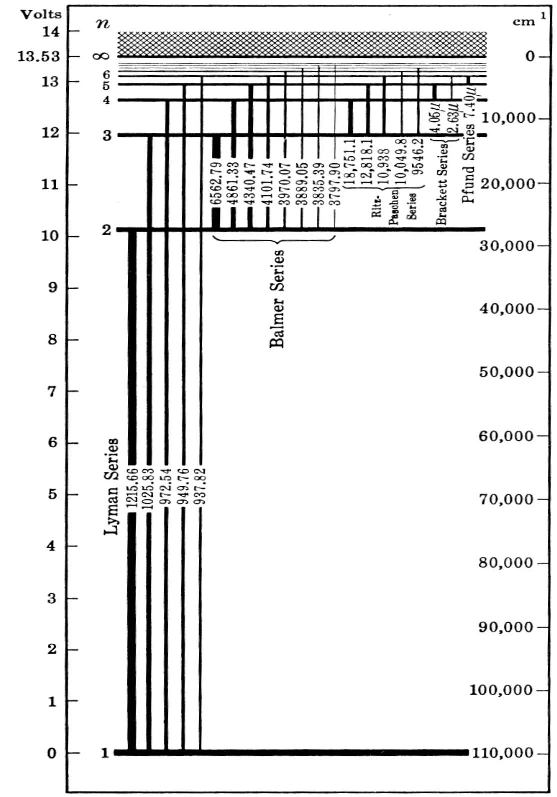
Position A atom
Position B atom



Volts
n
cm⁻¹
Lyman Series
1215.66
1025.83
972.54
949.76
937.82
Balmer Series
6562.79
4861.33
4340.47
4101.74
3970.07
3889.05
3835.39
3797.90
Ritz-Paschen Series
18,751.1
12,818.1
10,938
10,049.8
9546.2
Brackett Series
4.05μ
2.63μ
Pfund Series 7.40μ

H Collisional-Radiative Model

inflow

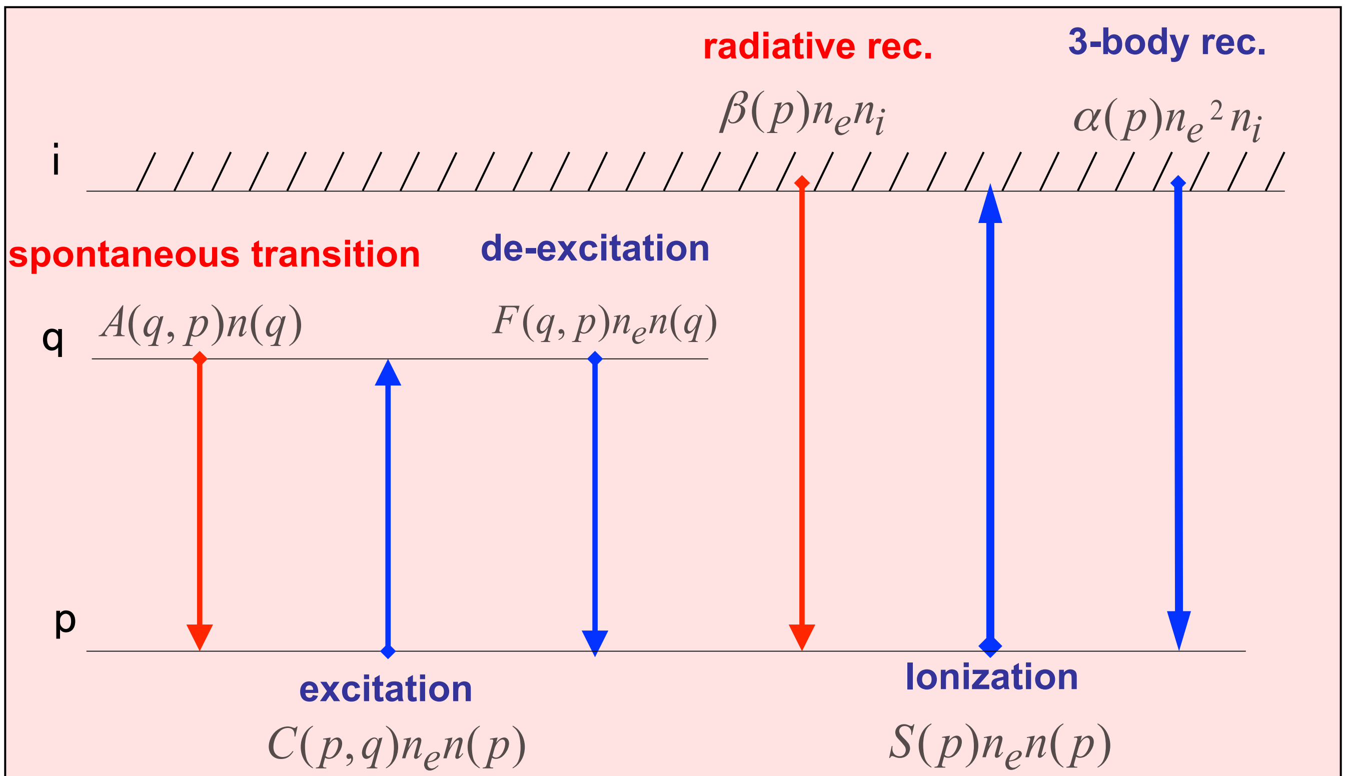
$$\frac{dn(p)}{dt} = \sum_{q<p} C(q,p)n_e n(q) + \sum_{q>p} \{F(q,p)n_e + A(q,p)\} n(q) + \alpha(p)n_e^2 n_i + \beta(p)n_e n_i$$

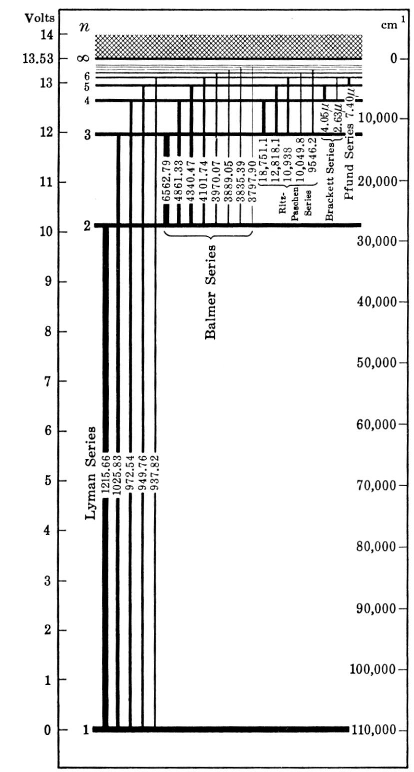
$$-[\{\sum_{q<p} F(p,q) + \sum_{q>p} C(p,q) + S(p)\} n_e + \sum_{q<p} A(p,q)] n(p)$$

outflow

PLASMA

e H$^+$ H



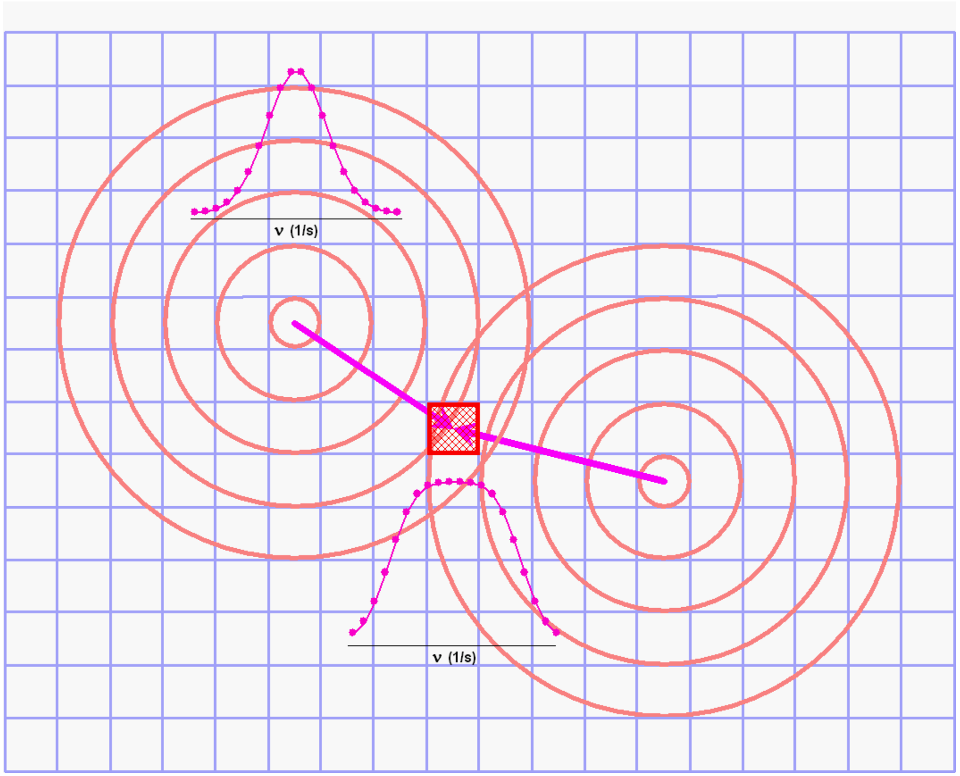


輻射輸送の計算手法

(1)　空間を微小セルに分割し、各場所に

- ・原子スペクトルプロファイル$g(\nu)$　：中性粒子輸送コード水素原子温度（ドップラー広がり）
- ・基底状態原子密度$n(1)$　：中性粒子輸送コード
- ・電子密度n_e
- ・電子温度T_e

を与える。



(2)　初めに輻射輸送を考慮せず、各場所の励起準位ポピュレーションを衝突輻射モデルにより計算する。

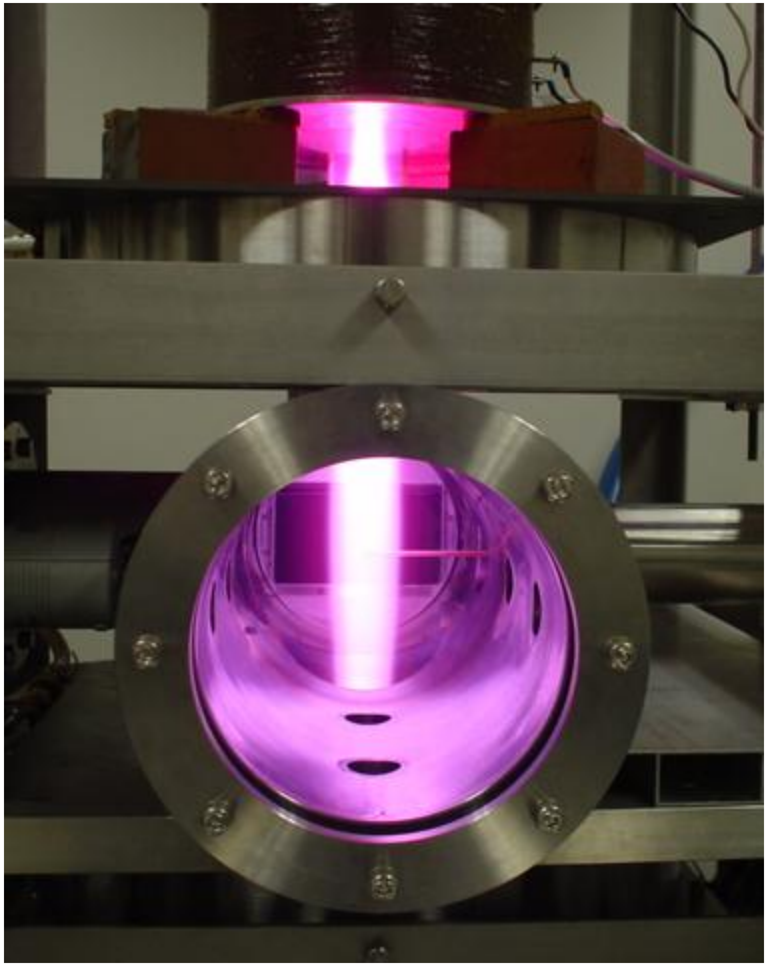
(3)　(2)の励起準位ポピュレーションから各場所の光の放出と吸収を計算し、光強度の空間分布を計算する。

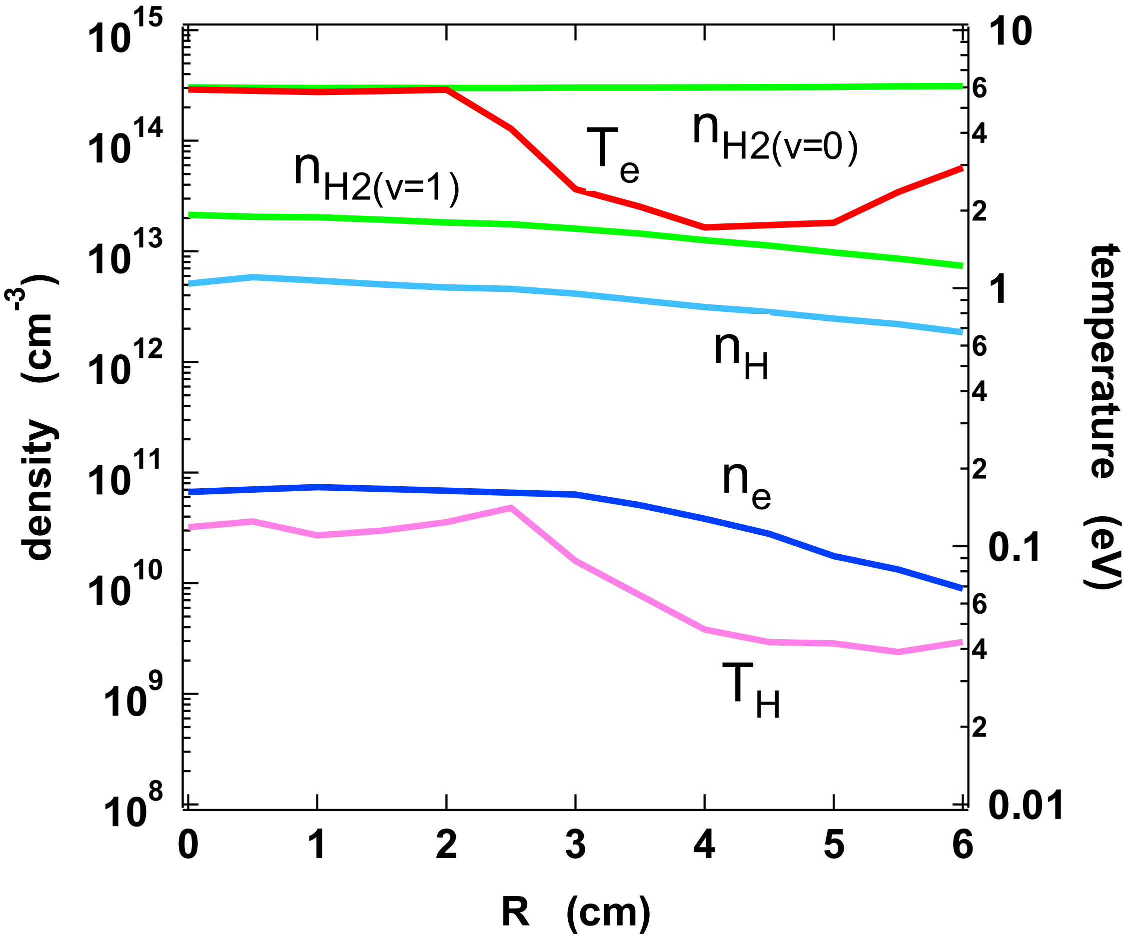
(4)　(3)の光強度を用いて、光吸収を考慮して各場所の励起準位ポピュレーションを計算する。

(5)　このような計算を各場所の光強度と励起準位ポピュレーションの値が収束するまで繰り返す。

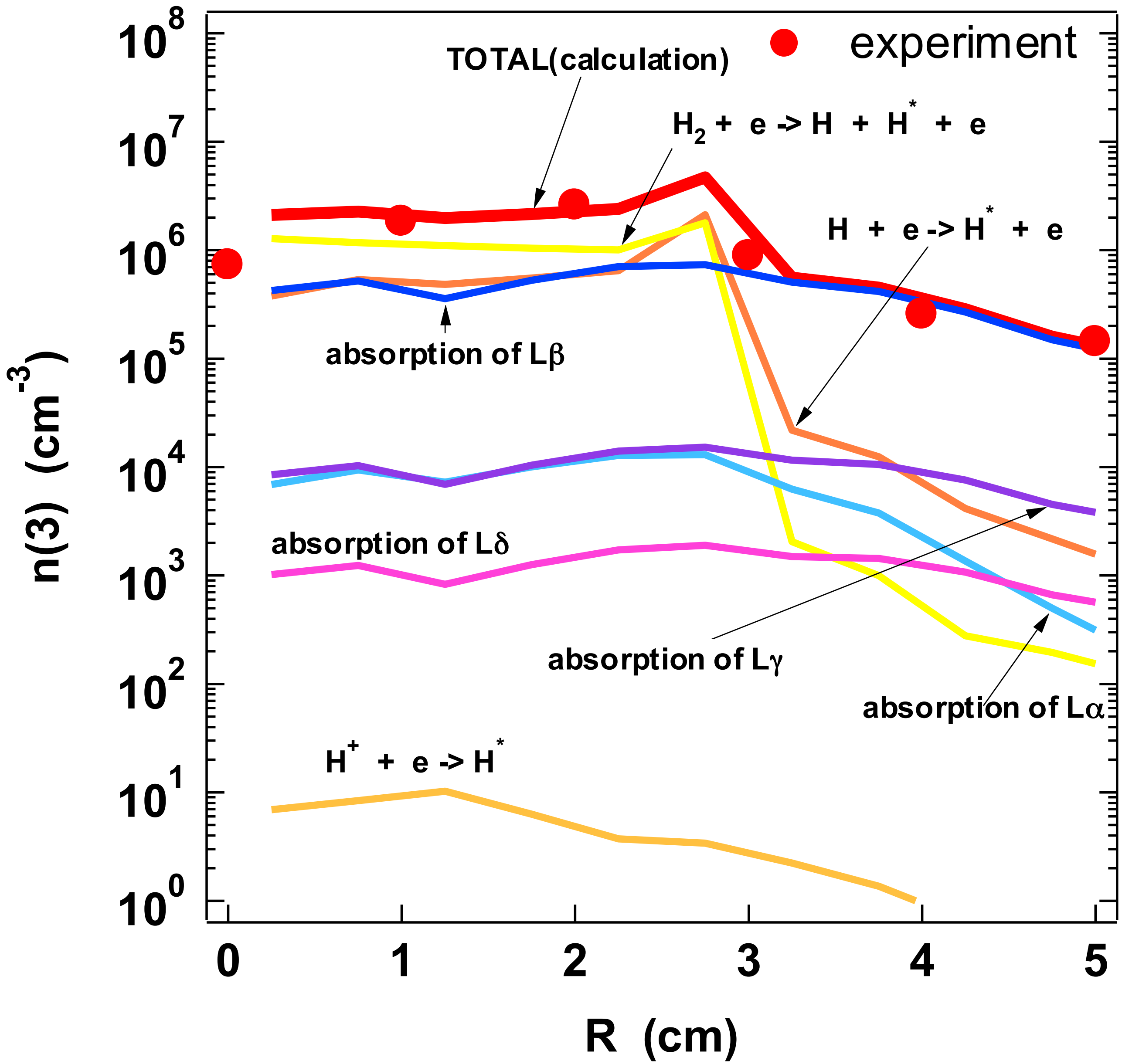
中性粒子輸送コード計算結果

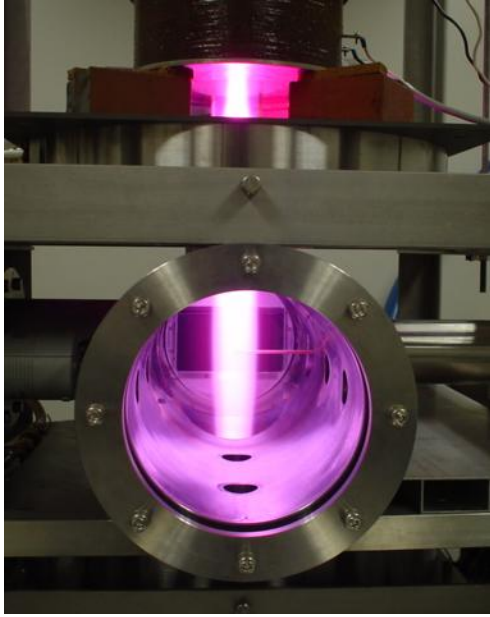
水素原子･分子密度 ＆ 水素原子温度

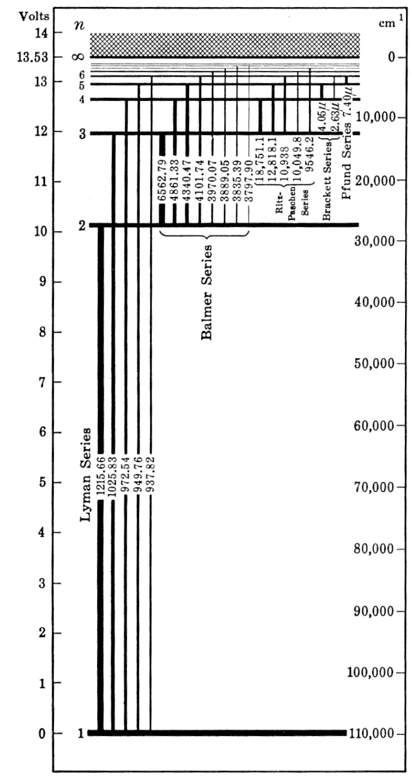




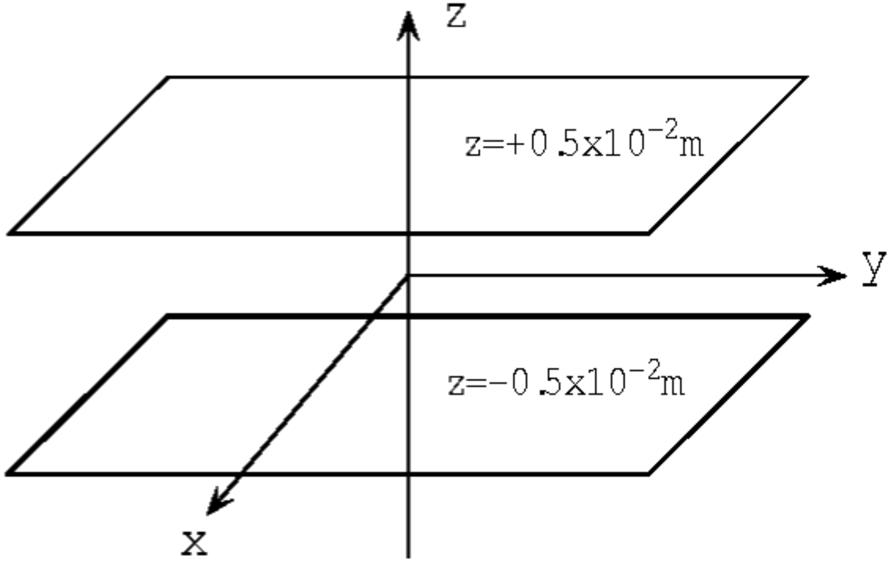
輻射輸送計算　RFプラズマ







輻射輸送の簡単な計算例　　計算条件



$T_e = 1$ eV

$n_e = n_{H+} = 10^{21}$ m^{-3}

$n(1) = 10^{20}$ m^{-3}

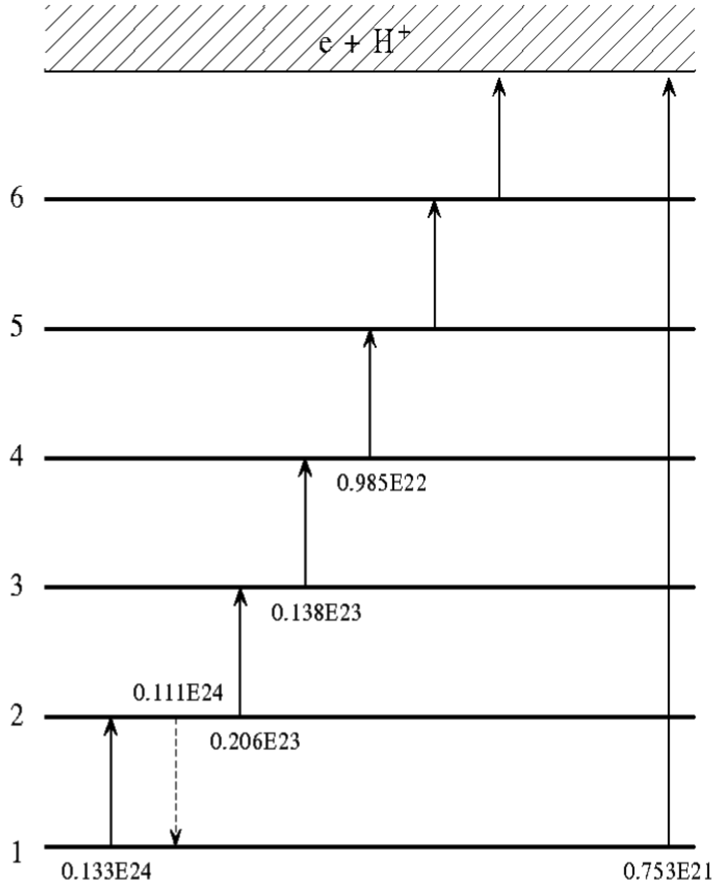
$T_H = 1$ eV

輻射輸送を考慮しない場合

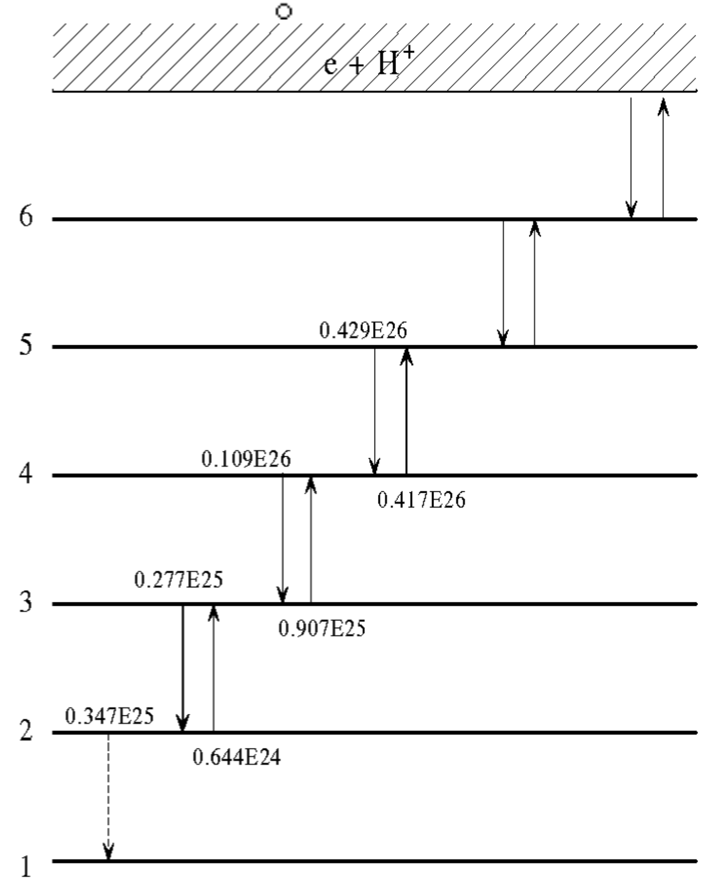
$$S_{CR} = 2.5 \times 10^{-19}, \quad \alpha_{CR} = 4.6 \times 10^{-18} \quad \left[\frac{\mathrm{m}^3}{\mathrm{s}}\right]$$

$$\frac{dn(1)}{dt} = -S_{CR}n(1)n_e + \alpha_{CR}n_{H^+}n_e$$

$$= -2.5 \times 10^{22} + 4.6 \times 10^{24} \quad \left[\frac{1}{\mathrm{m}^3\mathrm{s}}\right]$$



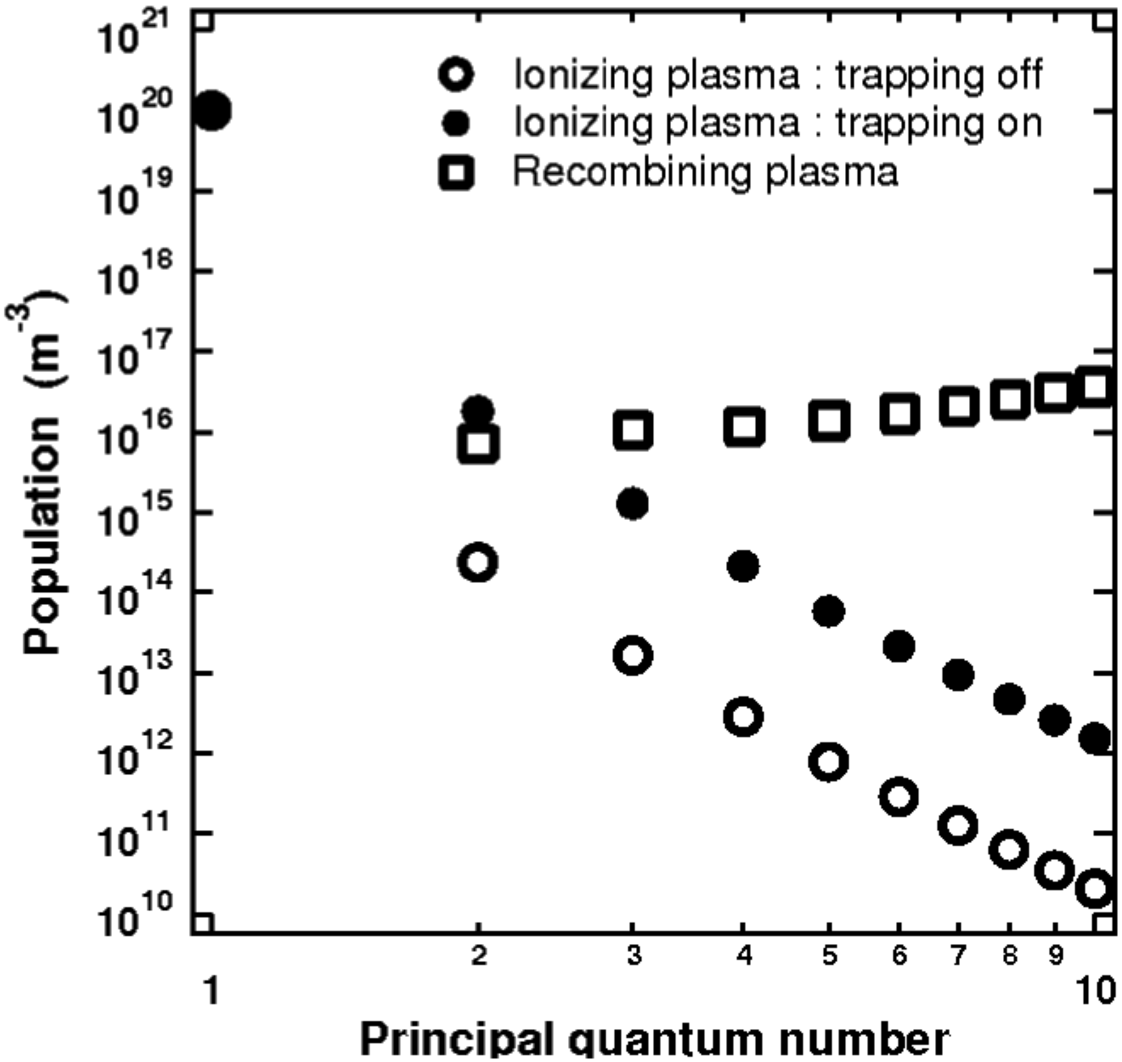
The excitation and de-excitation flow of ionizing plasma component. The figures denote the quantities of the fluxes. For example, 0.133E24 denotes $0.133 \times 10^{24} [\mathrm{m}^{-3}\mathrm{s}^{-1}]$. The solid line denotes the transition by electron collision, and the broken line denotes the spontaneous radiative transition.

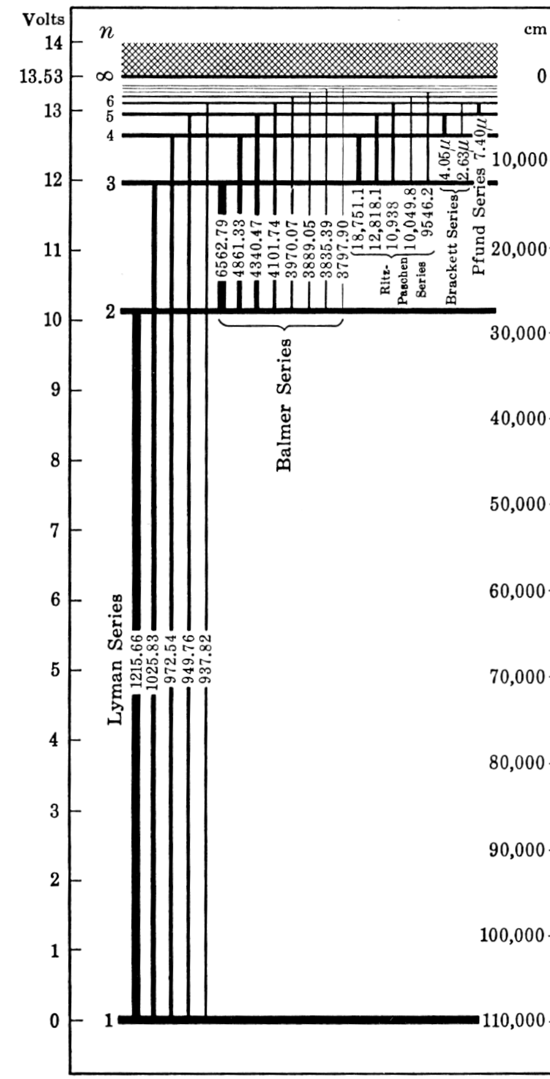


The excitation and de-excitation flow of recombining plasma component. The figures denote the quantities of the fluxes. For example, 0.347E25 denotes $0.347 \times 10^{25} [\mathrm{m}^{-3}\mathrm{s}^{-1}]$. The solid line denotes the transition by electron collision, and the broken line denotes the spontaneous radiative transition.

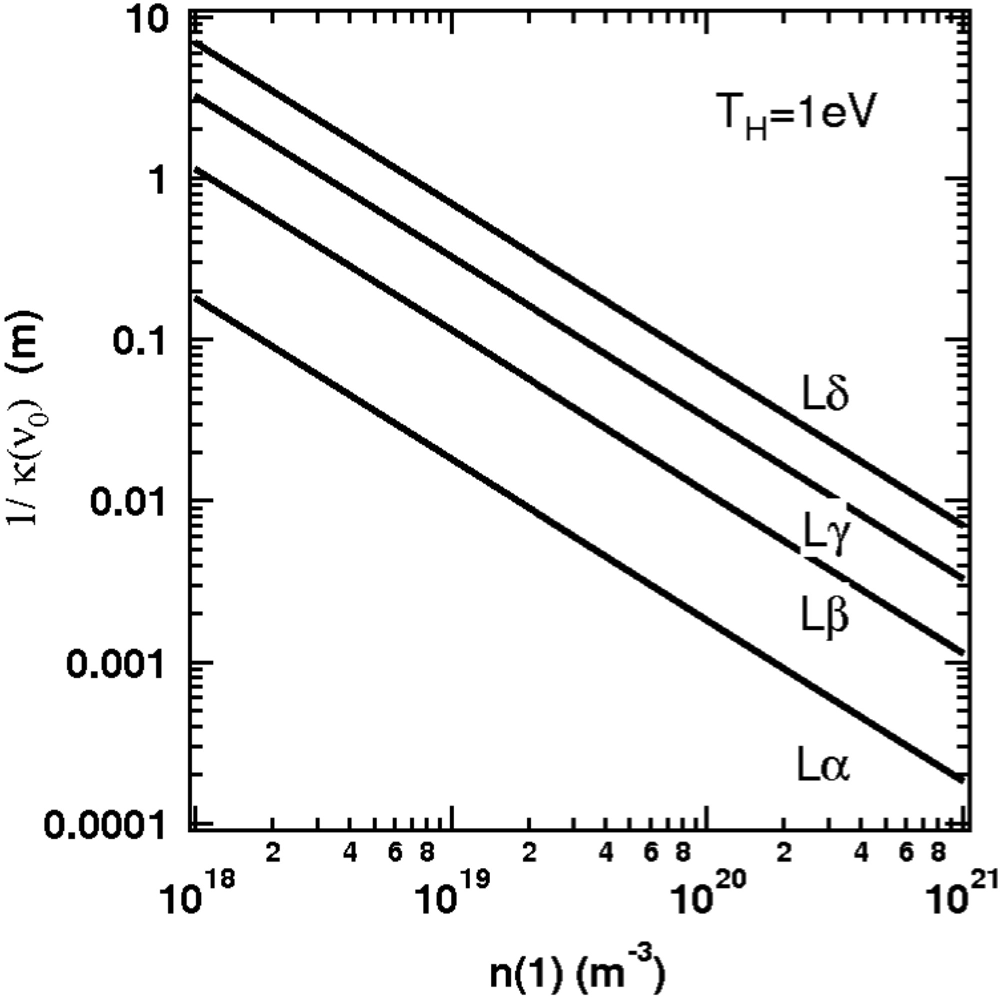
ポピュレーション

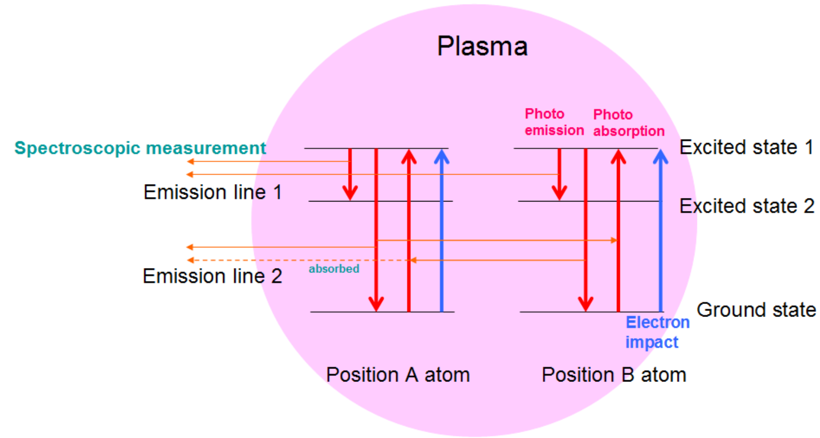
$$n(p) = \underbrace{R_0(p) n_i n_e}_{\text{recombining}} + \underbrace{R_1(p) n(1) n_e}_{\text{ionizing}}$$

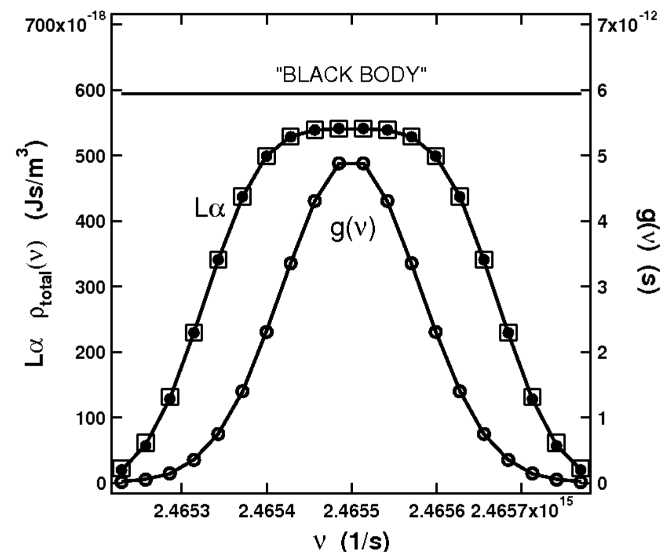




光の減衰長

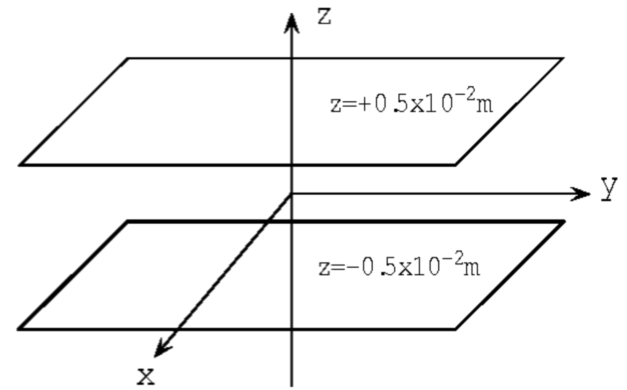


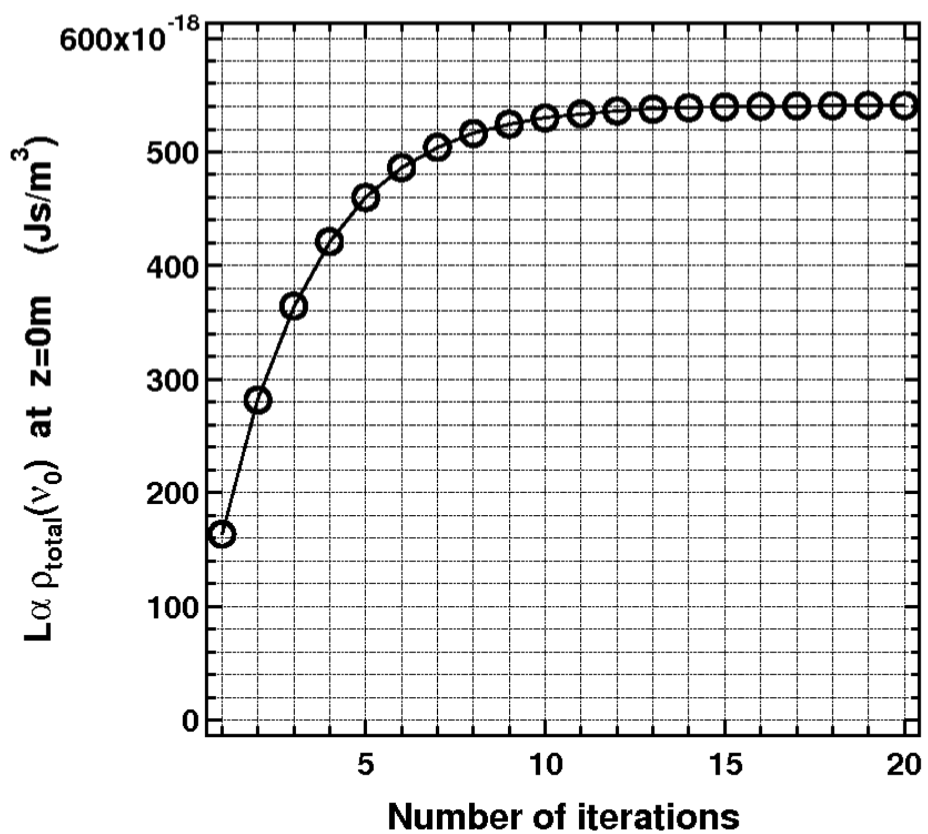




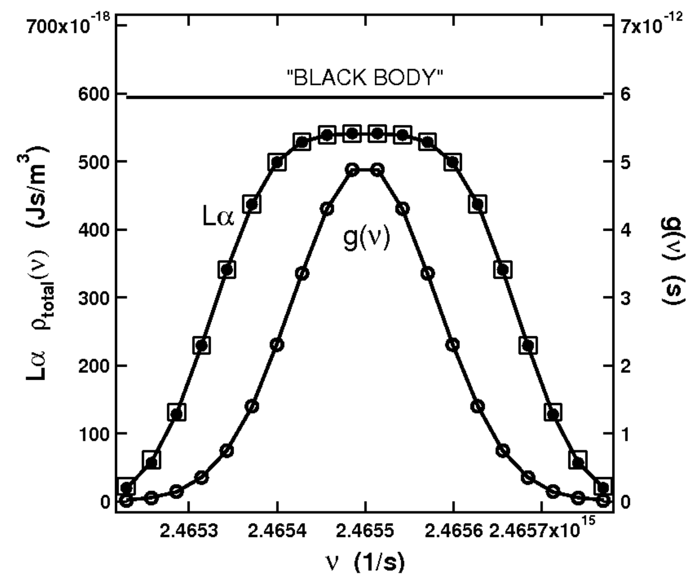
L_α spectrum at the center $z = 0$m of the slab which is achieved after convergence. The closed circles and the open squares denote results for $R_{LIMIT} = 4.0 \times 10^{-2}$m and $R_{LIMIT} = 8.0 \times 10^{-2}$m, respectively. The emission line profile of the Doppler broadening $g(\nu)$ is also shown. The line of "BLACK BODY" is a reference value which is calculated assuming a uniform infinite volume plasma whose population density is the same as that at $z = 0$m.

輻射輸送の計算　　収束の様子



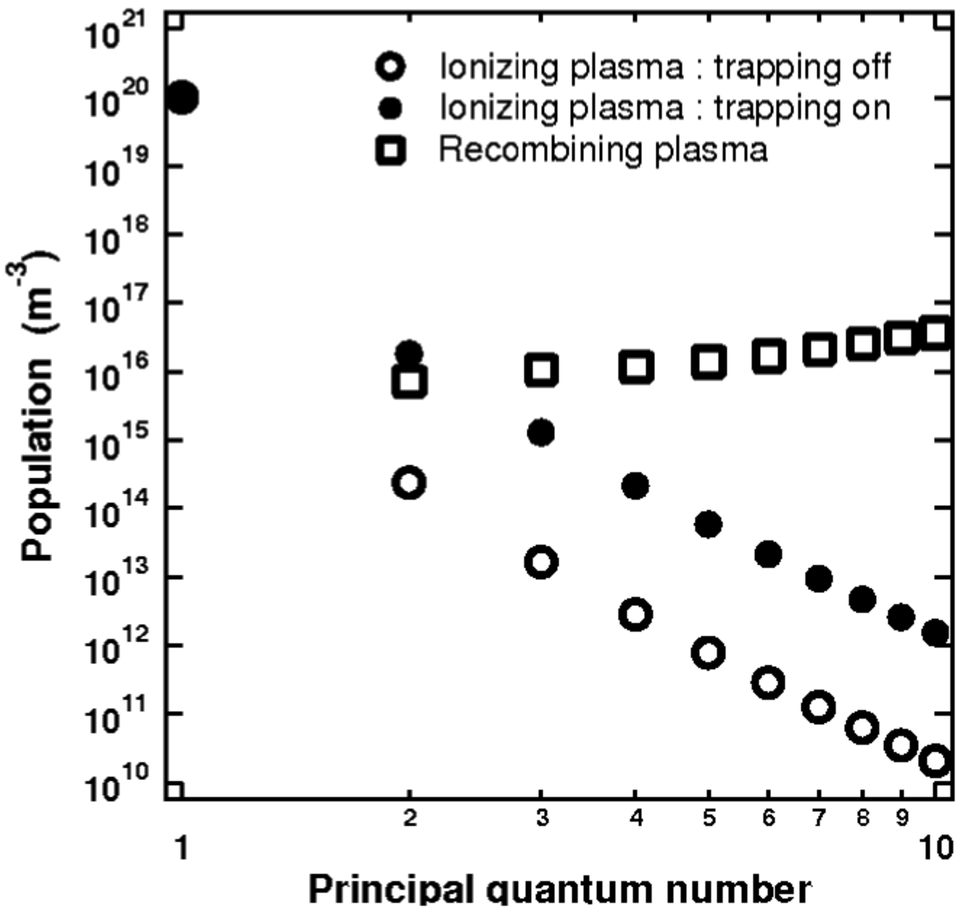


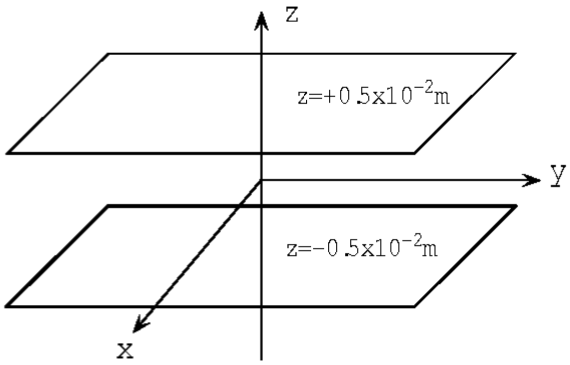
The $\rho_{total}(\nu_0)$ of L_α at the center $z = 0$m of the slab is shown as a function of the number of iterations.

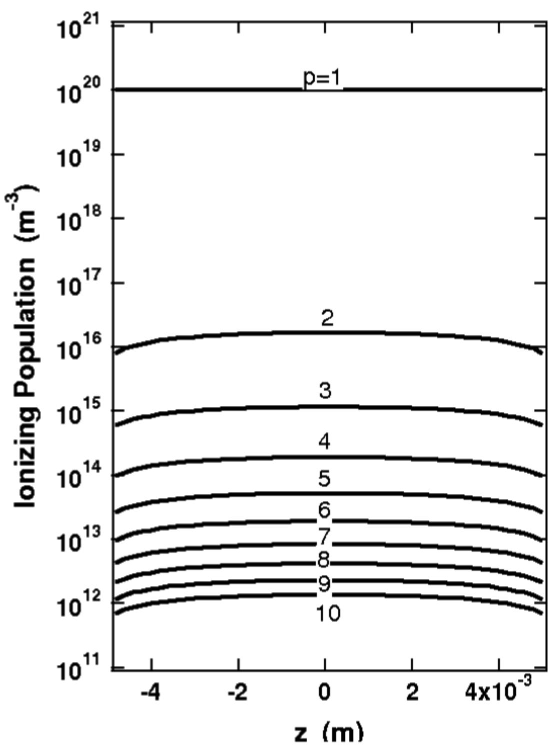


L_α spectrum at the center $z = 0$m of the slab which is achieved after convergence. The closed circles and the open squares denote results for $R_{LIMIT} = 4.0 \times 10^{-2}$m and $R_{LIMIT} = 8.0 \times 10^{-2}$m, respectively. The emission line profile of the Doppler broadening $g(\nu)$ is also shown. The line of "BLACK BODY" is a reference value which is calculated assuming a uniform infinite volume plasma whose population density is the same as that at $z = 0$m.

輻射輸送の計算　　収束の様子







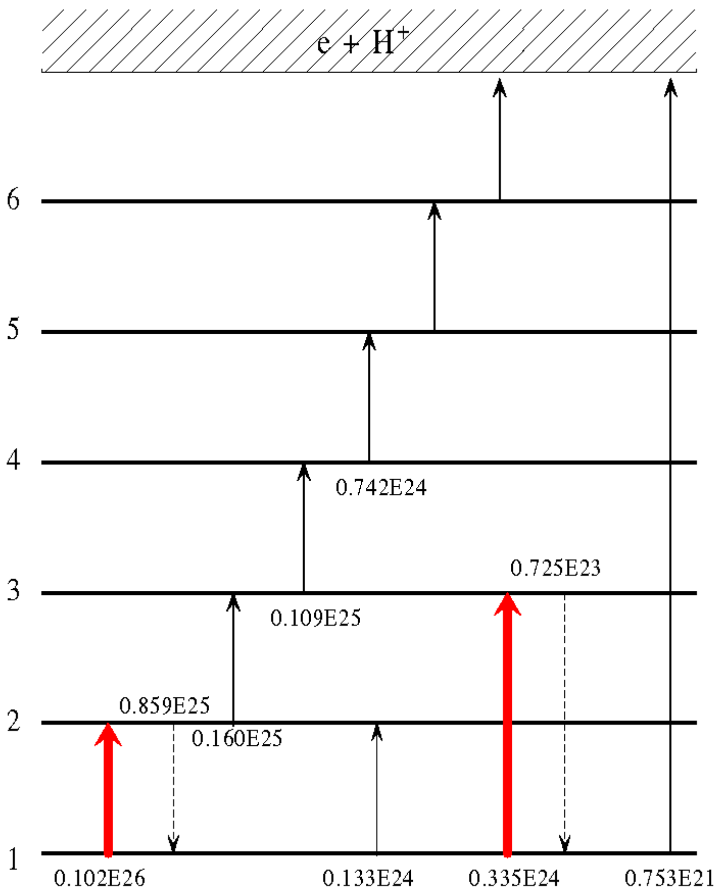
Population densities of the excited levels of the ionizing plasma. $n(1)$ is $10^{20}[\mathrm{m}^{-3}]$.

輻射輸送を考慮した場合

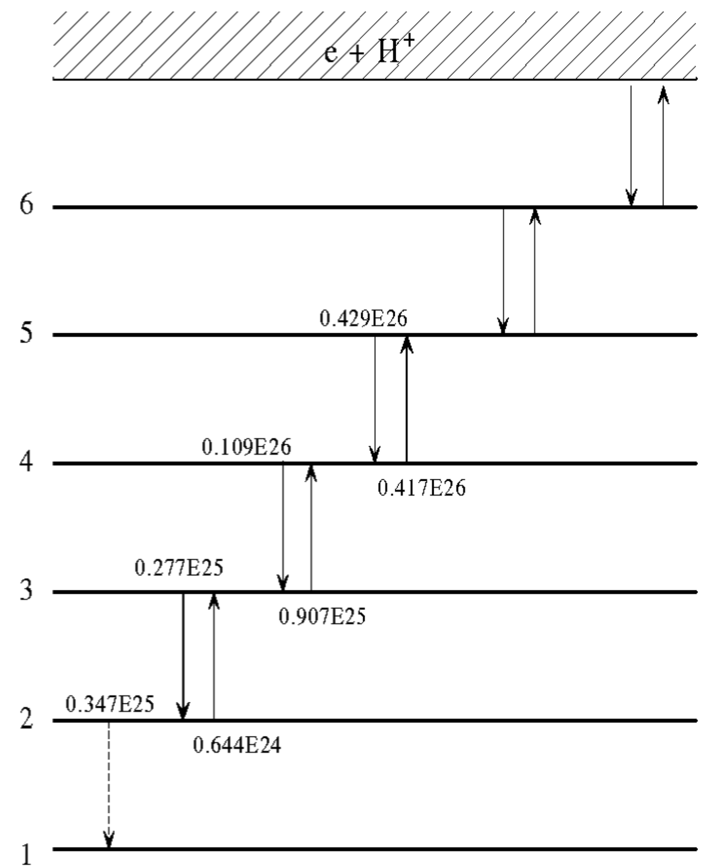
$$S_{CR} = 1.9 \times 10^{-17}, \quad \alpha_{CR} = 4.6 \times 10^{-18} \quad \left[\frac{m^3}{s}\right]$$

$$\frac{dn(1)}{dt} = -S_{CR}n(1)n_e + \alpha_{CR}n_{H^+}n_e$$

$$= -1.9 \times 10^{24} + 4.6 \times 10^{24} \quad \left[\frac{1}{m^3 s}\right]$$

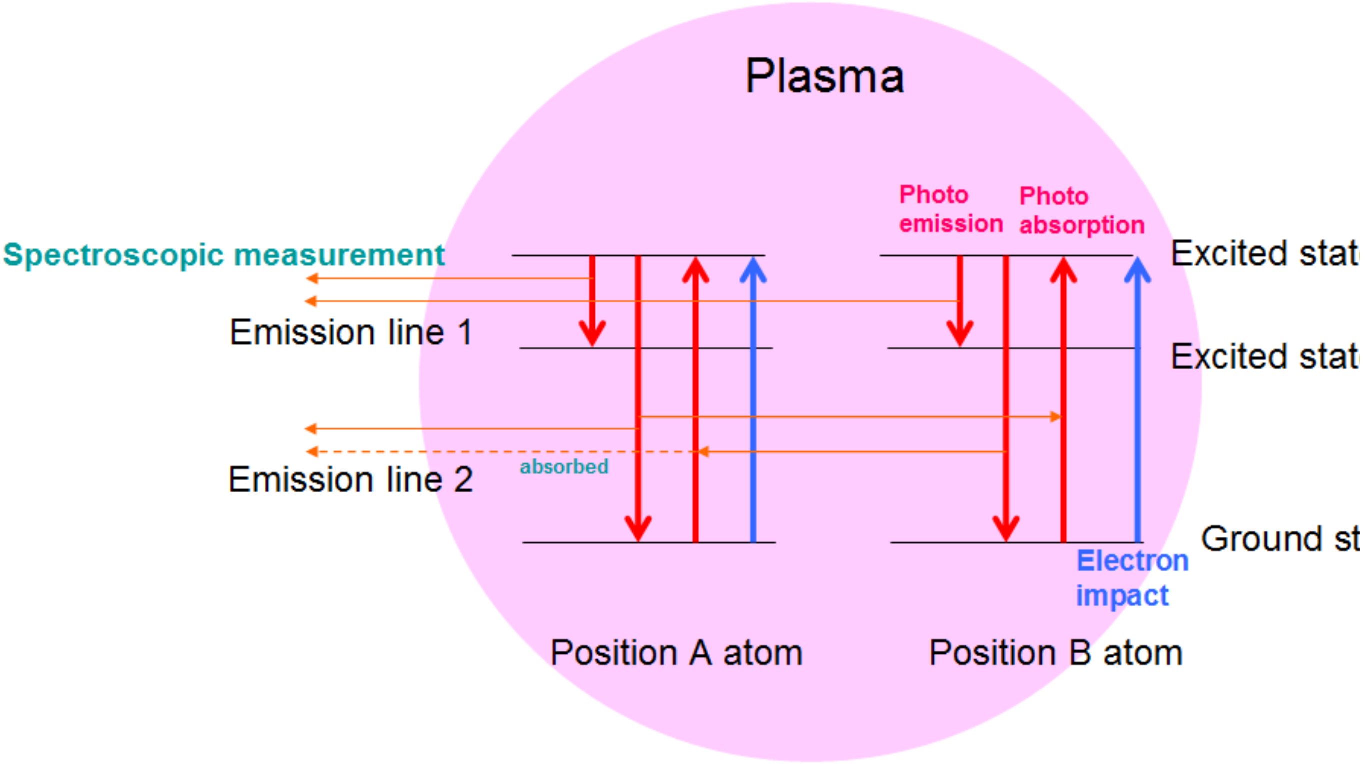


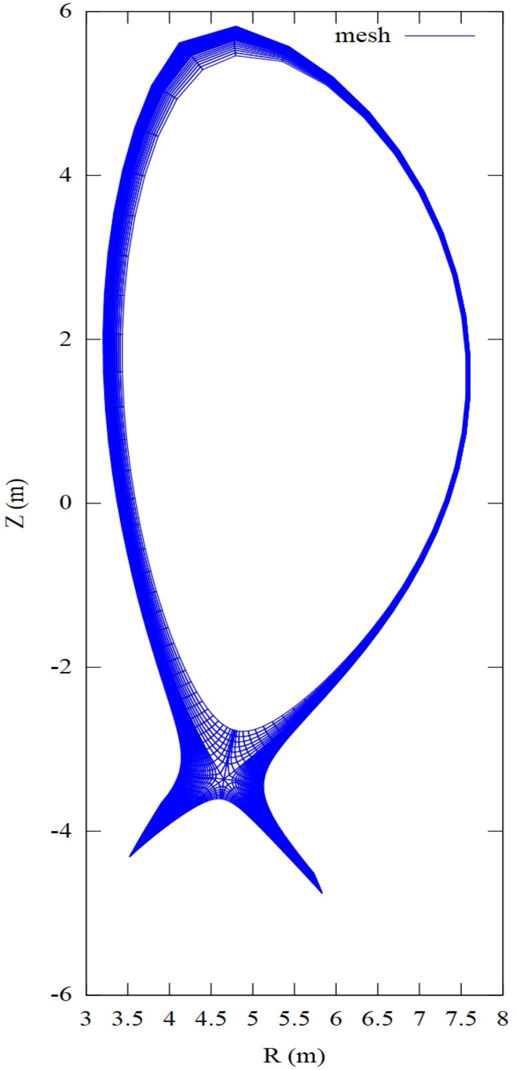
The excitation and de-excitation flow ionizing plasma component at the center $z = 0$m of the slab. The thick solid line (red) denotes the absorption of photon. The thin solid line denotes the transition by electron collision, and the broken line denotes the spontaneous radiative transition.



The excitation and de-excitation flow of recombining plasma component. The figures denote the quantities of the fluxes. For example, 0.347E25 denotes $0.347 \times 10^{25} [m^{-3}s^{-1}]$. The solid line denotes the transition by electron collision, and the broken line denotes the spontaneous radiative transition.

原型炉SlimCSでの輻射輸送の計算

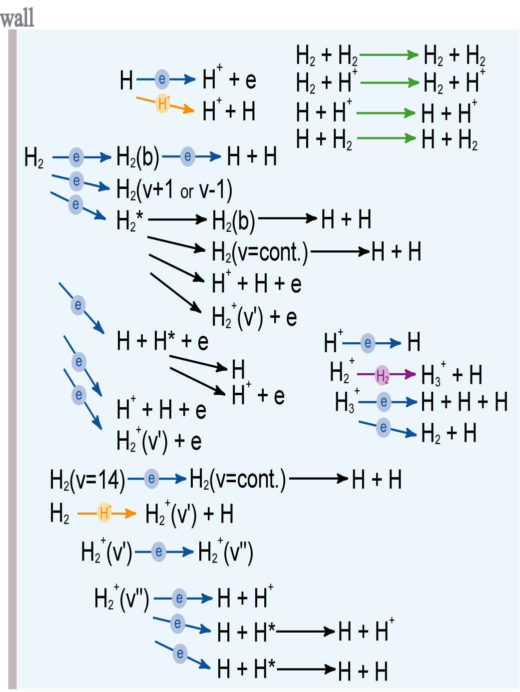


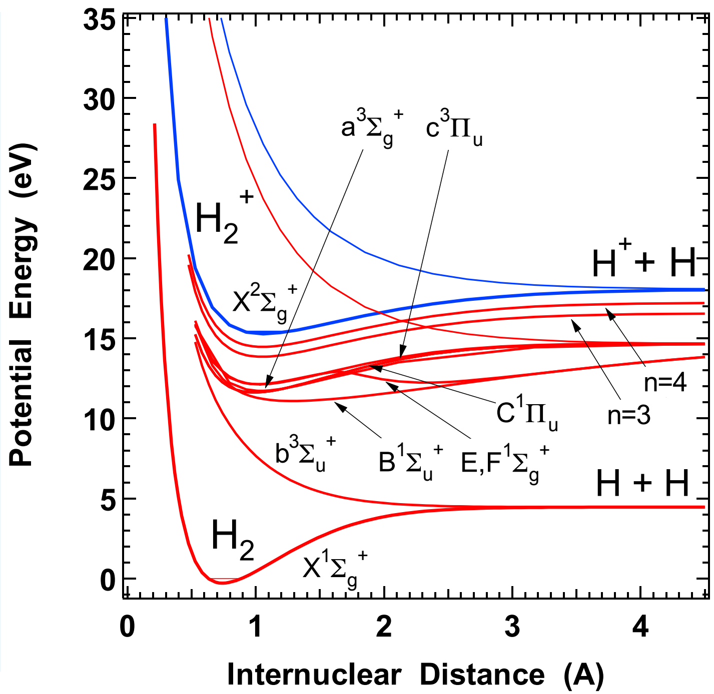


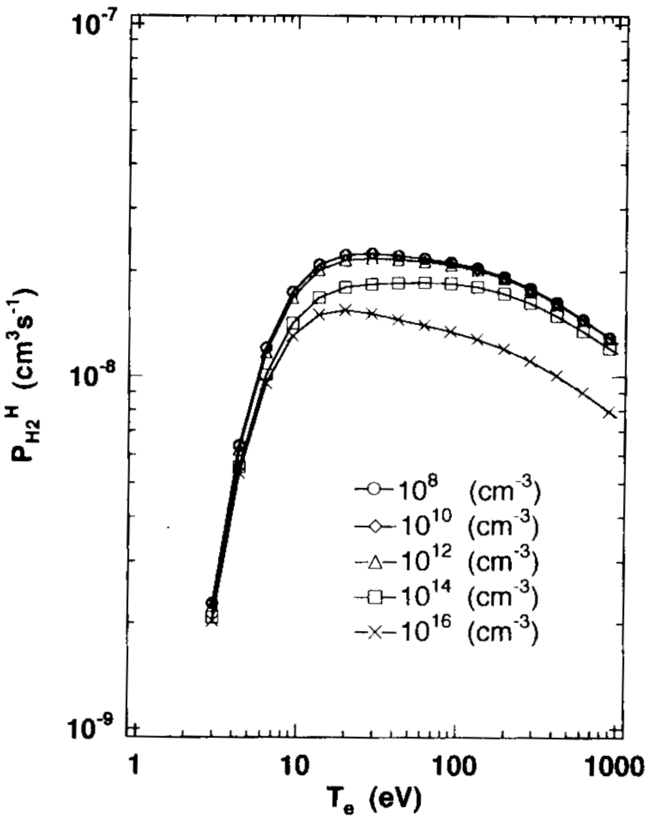
H_2 衝突輻射モデル

H_2 Collisional-Radiative Model (ver.1)

Calculation of effective reaction rate coefficients



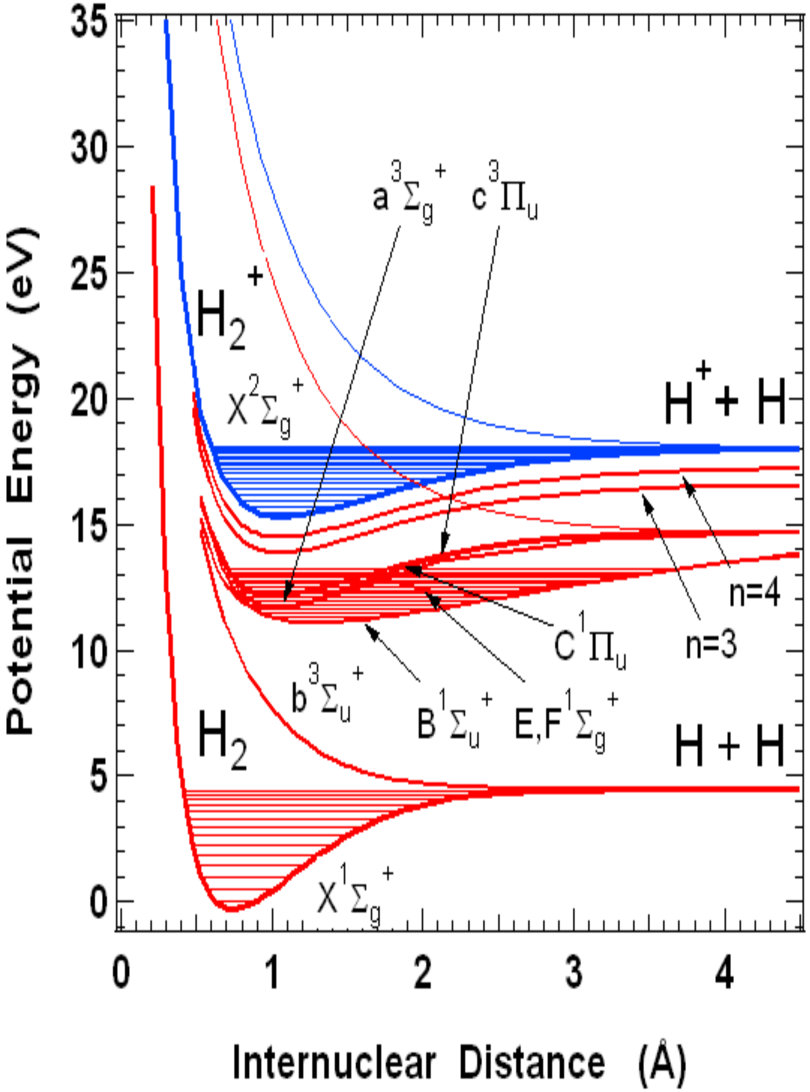




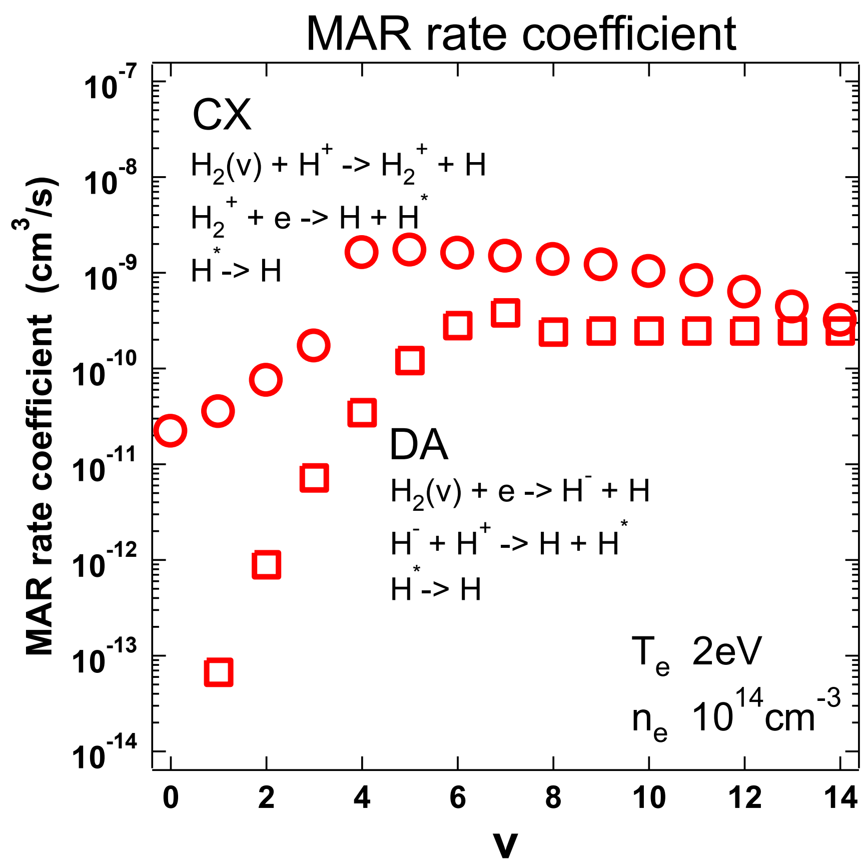
※K. Sawada, K. Eriguchi, T. Fujimoto:
Hydrogen–atom spectroscopy of the ionizing plasma containing molecular hydrogen: line intensities and ionization rate; J. Appl. Phys. 73, 8122–8125, 1993.

※K. Sawada, T. Fujimoto:
Effective ionization and dissociation rate coefficients of molecular hydrogen in plasma; J. Appl. Phys. 78, 2913–2924, 1995.

H_2 Collisional-Radiative Model (ver.2)

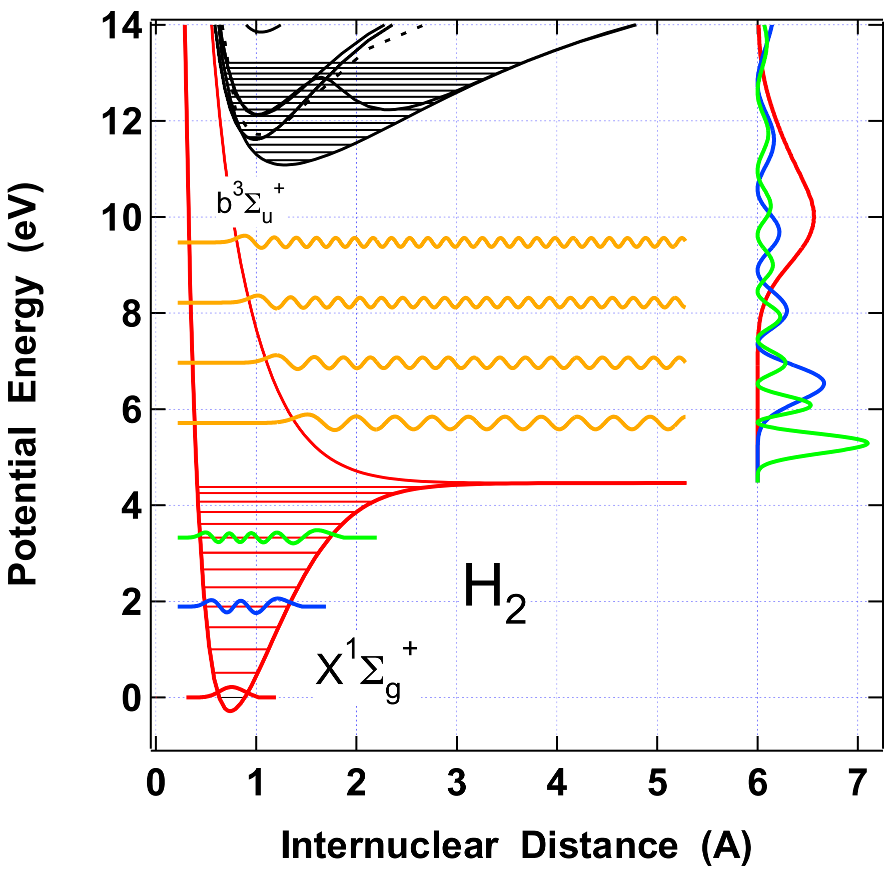


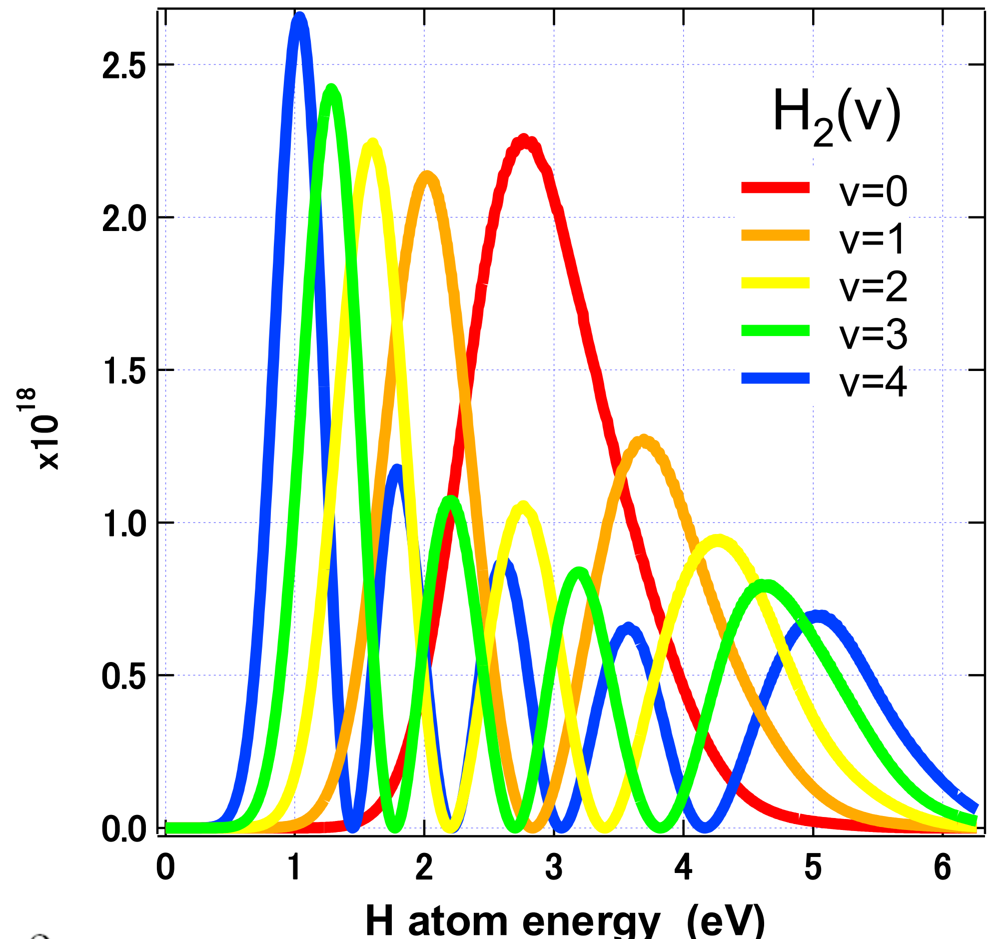
Vibrational levels for n<=2 electronic state are considered.



※K. Sawada and T. Fujimoto:
Effect of initial vibrational excitation of molecular hydrogen on molecular assisted recombination in divertor plasmas;
Contrib. Plasma Phys. 42, 603–607, 2002.

速度分布の計算例　$H_2(X) \rightarrow H_2(b) \rightarrow H + H$

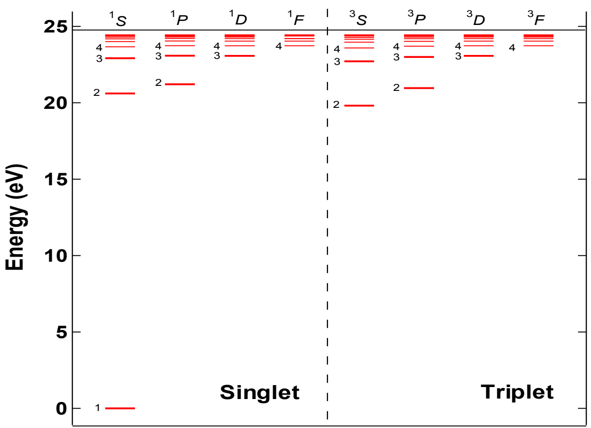




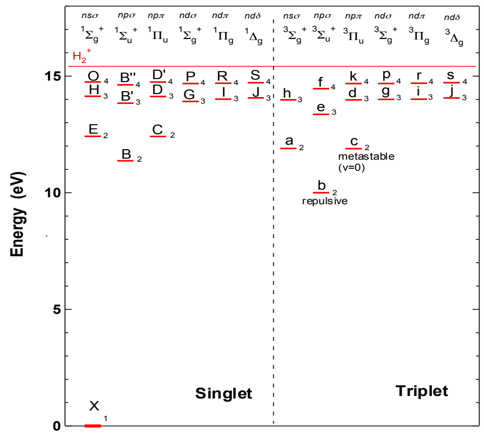
$$q_{\kappa v} = \left| \int \chi_{\kappa}^{b}(R)\chi_{v}^{X}(R)dR \right|^2$$

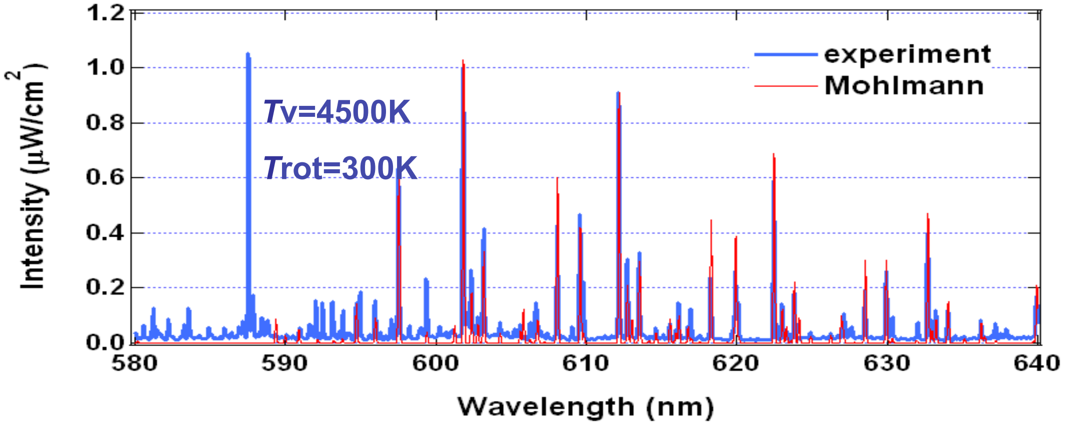
Construction of electronically and rovibrationally state-resolved collisional-radiative model of molecular hydrogen

He atom



H_2

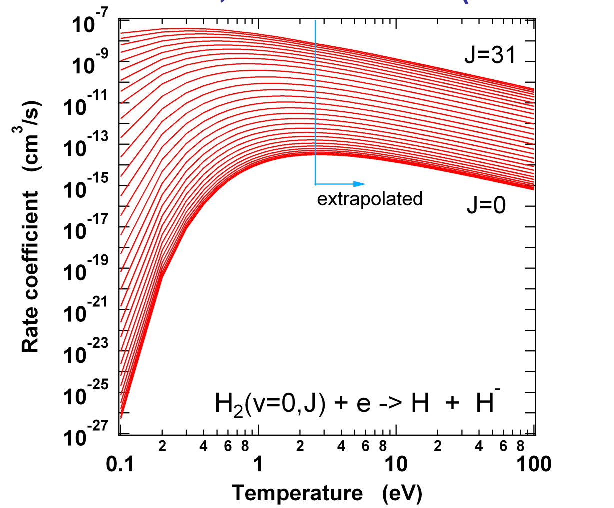


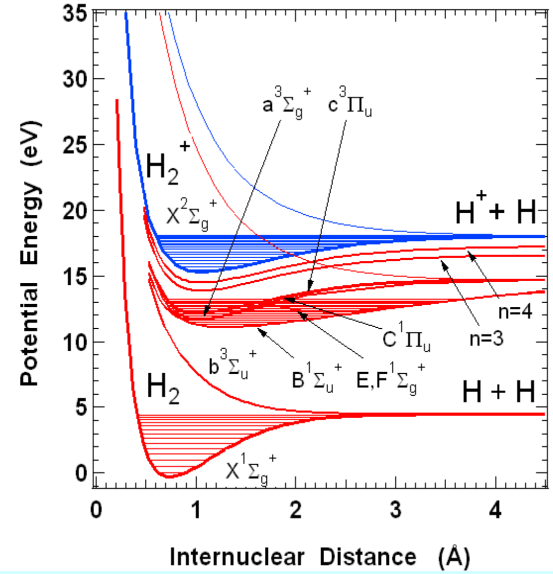


Determination of *n*e, *T*e, *T*v, *T*rot from observed spectra

***T*v, *T*rot -> Population $X^1\Sigma_g^+(v,J)$**

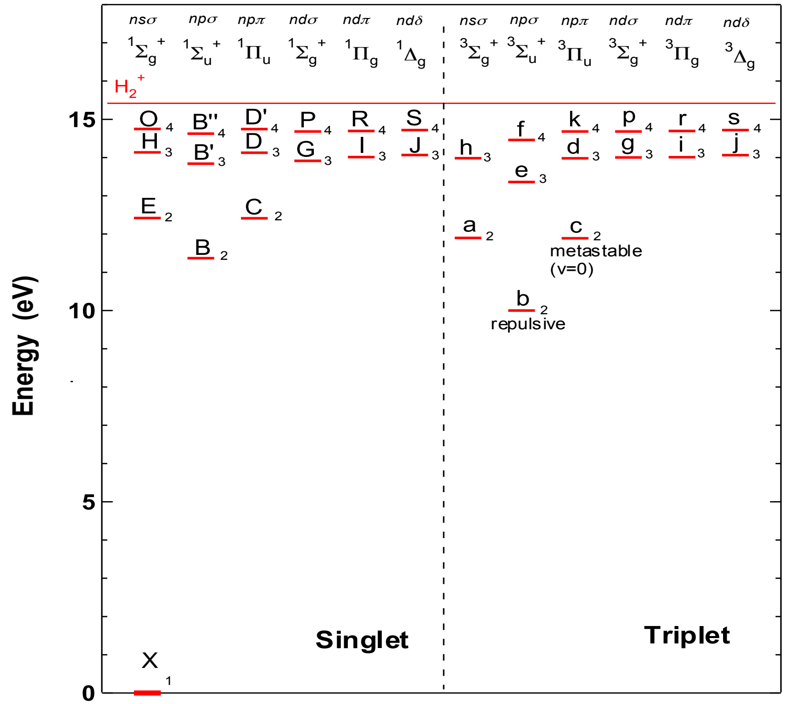
J. Horacek et al., NIFS-DATA-73 (Feb. 2003)





Calculation of effective reaction rate coefficients

H_2 energy levels



Thanks to Professor C. JUNGEN

$EF^1\Sigma_g^+$, $GK^1\Sigma_g^+$, $H^1\Sigma_g^+$, $B^1\Sigma_u^+$, $C^1\Pi_u$,

$B'^1\Sigma_u^+$, $D^1\Pi_u$, $I^1\Pi_g$, $J^1\Delta_g$

D.Bailly et al. , Molecular Physics 108, 827, (2010)

others

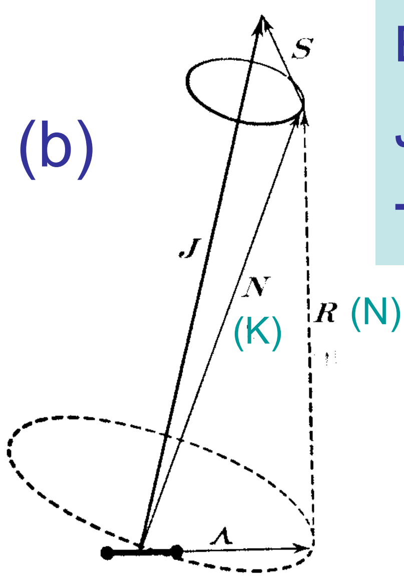
The Hydrogen Molecule Wavelength Tables of GERHARD HEINRICH DIEKE,

Edited by H. M. Crosswhite,

John Wiley & Sons Inc (1972)

Triplet : - 149.6 cm^{-1}

Hund's case (b)



n < 7

4133 levels are included in H_2 CR model.

$H_2(X)$ + e -> H_2^* + e

R.K.Janev, D.Reiter, U.Samm,

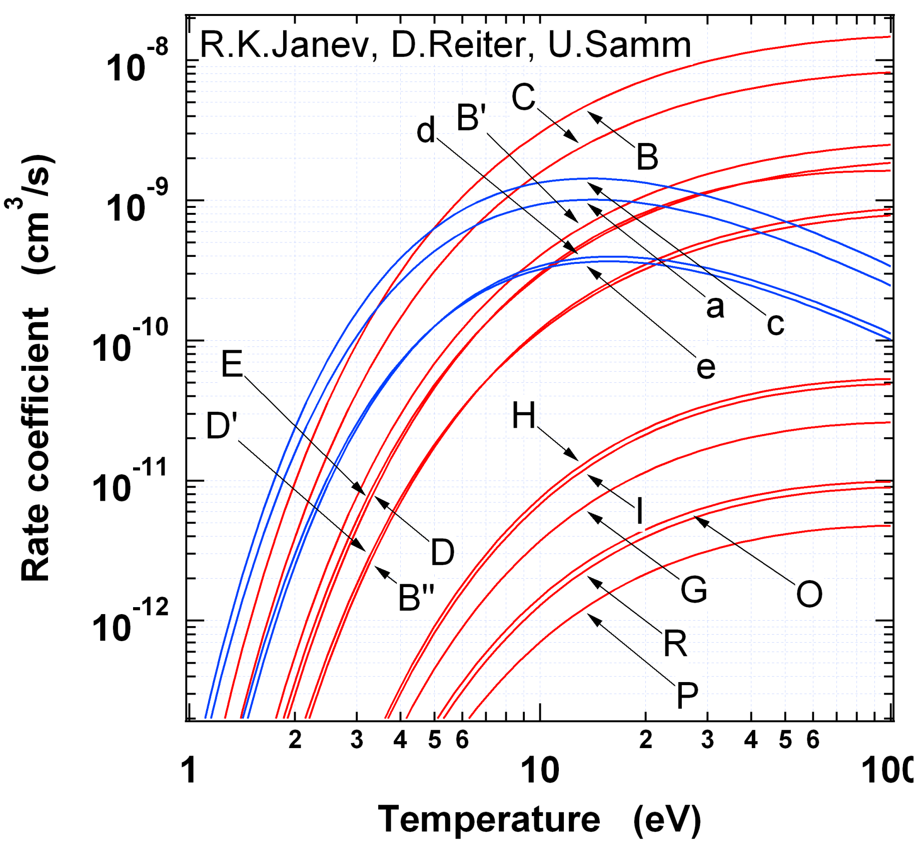
Collision Processes in Low-Temperature Hydrogen Plasmas,

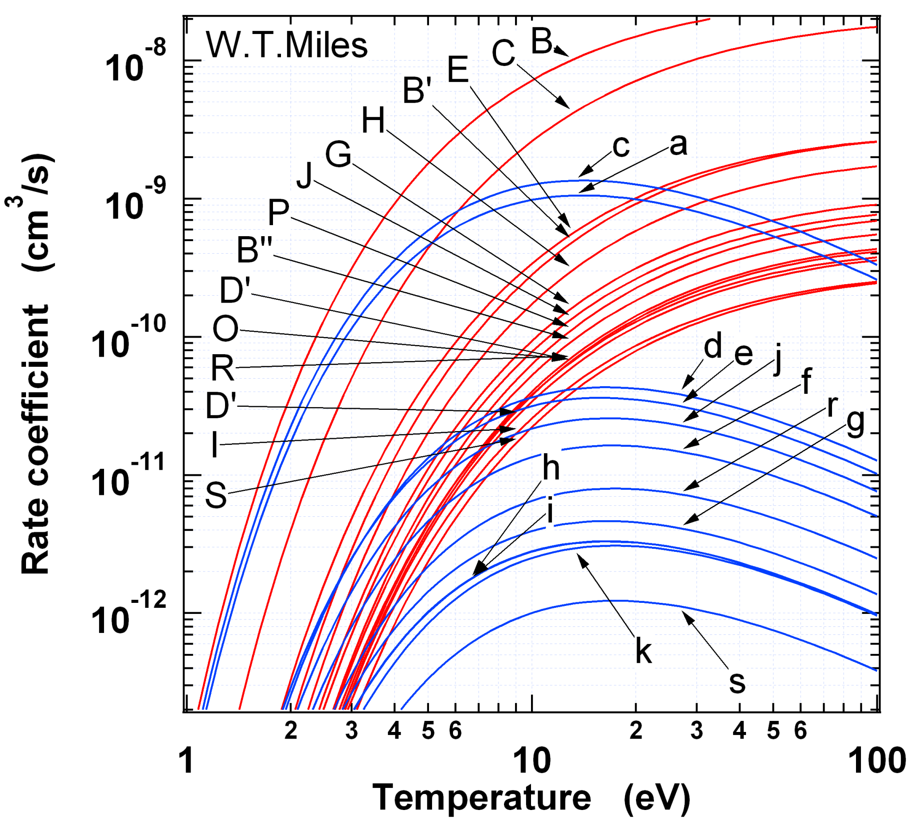
http://www.eirene.de/report_4105.pdf

W.T. Miles, R. Thompson, and A.E.S. Green, J. Appl. Phys. 43, 678 (1972).

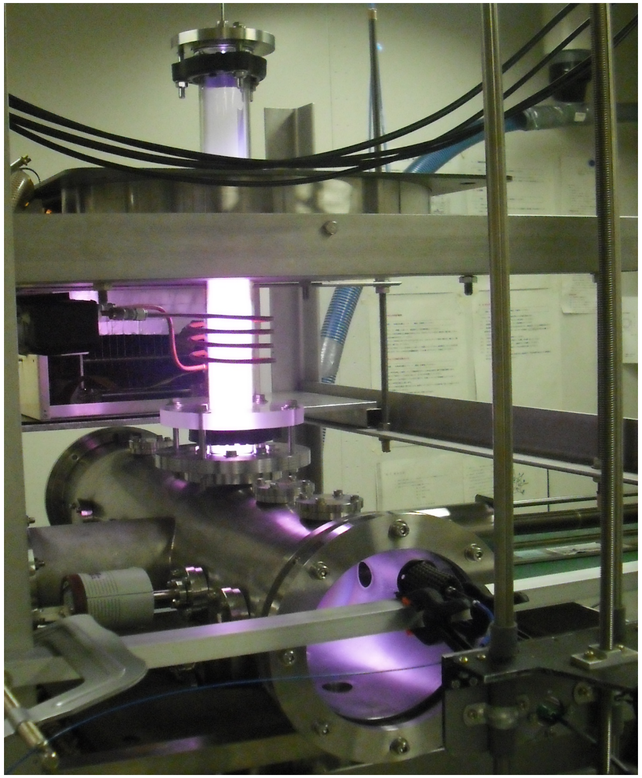
Born-Bethe approximation modified at low energies by phenomenological techniques

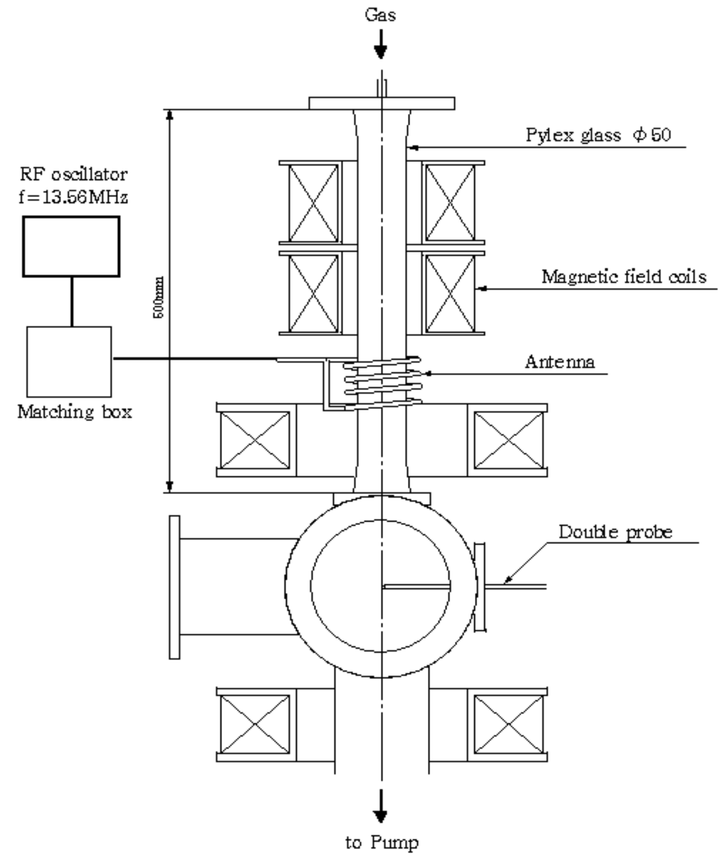
All cross sections are given for n<=4.

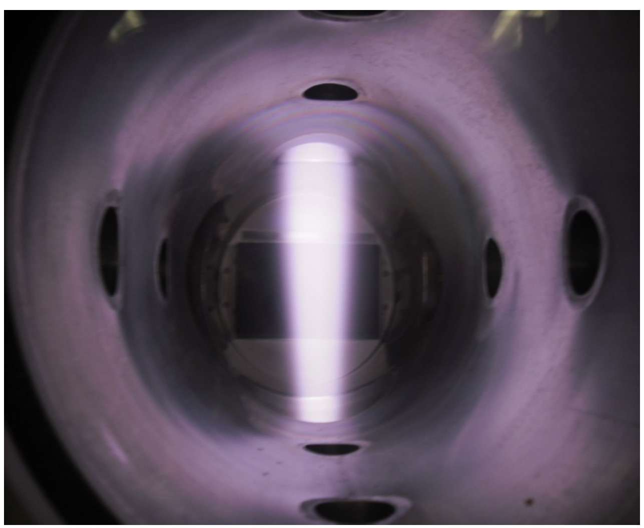


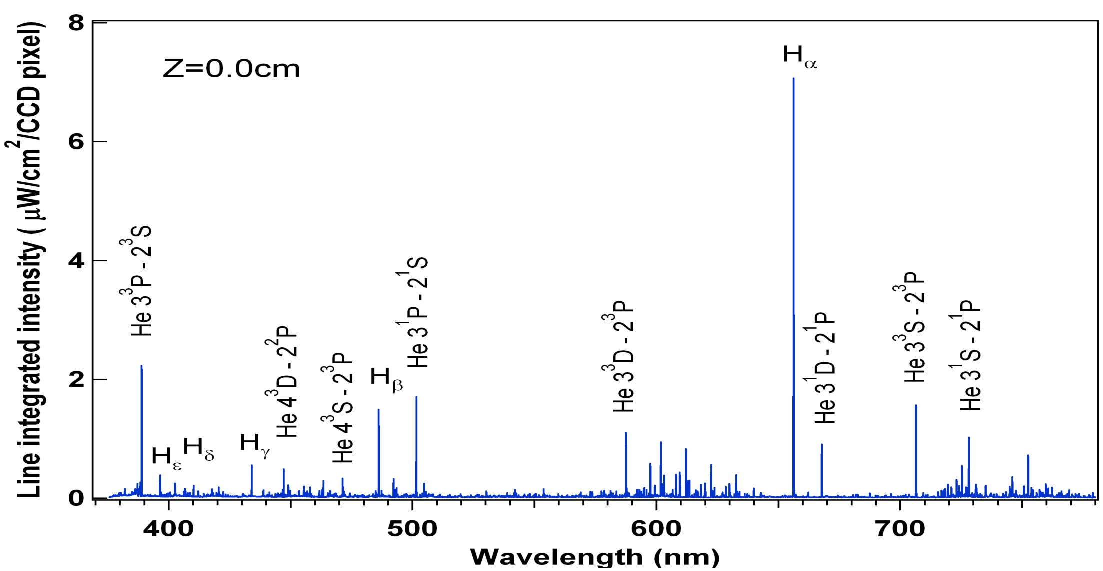


RF plasma

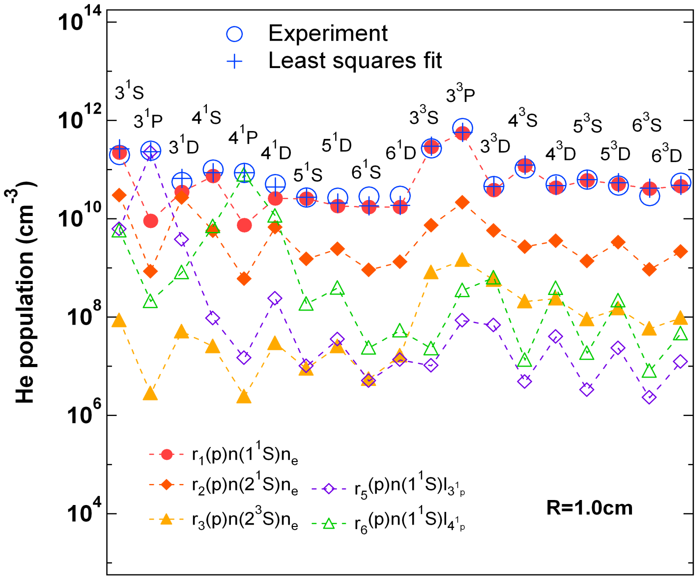


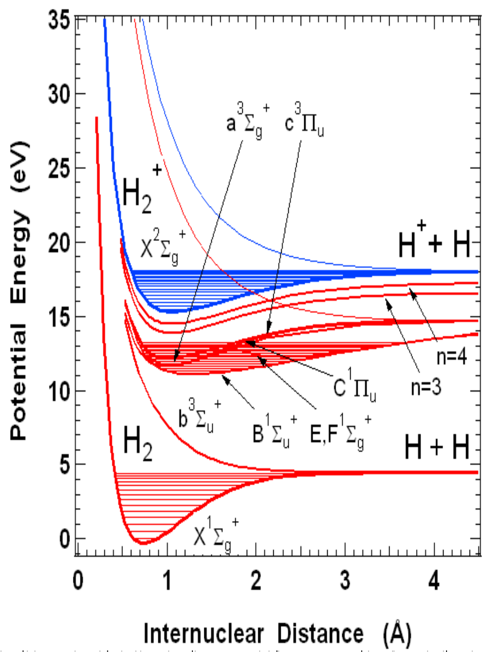

Gas
Pylex glass φ50
RF oscillator
f=13.56MHz
500mm
Magnetic field coils
Antenna
Matching box
Double probe
to Pump

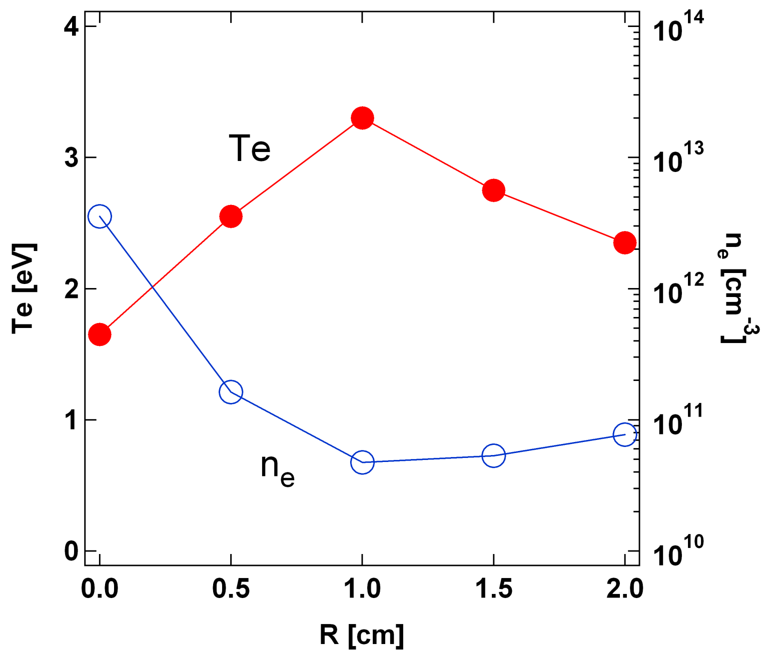


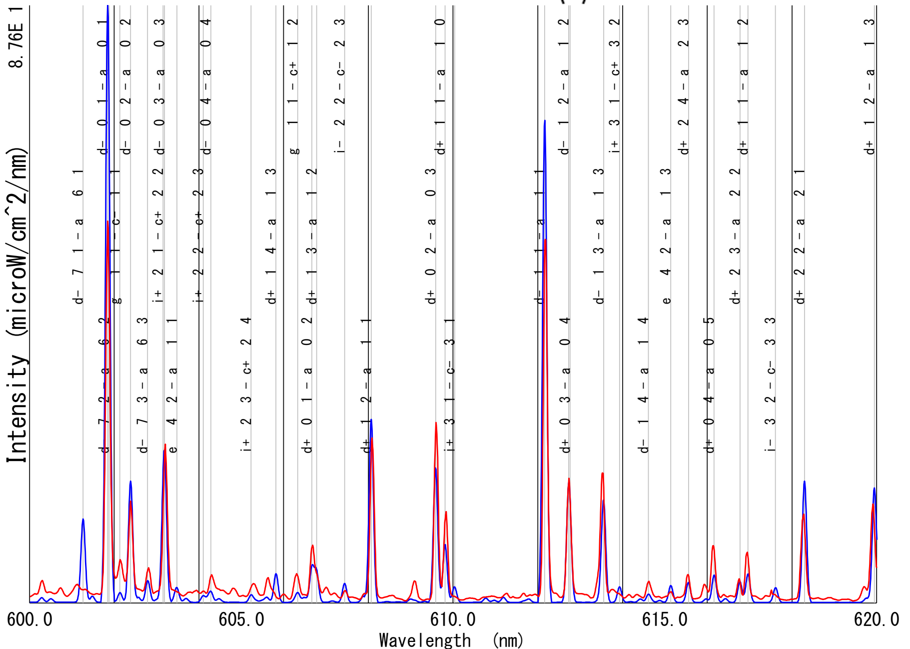

Z=0.0cm
Line integrated intensity (μW/cm²/CCD pixel)
Wavelength (nm)
Hα
He 3³P - 2³S
Hε
Hδ
Hγ
He 4³D - 2²P
He 4³S - 2³P
Hβ
He 3¹P - 2¹S
He 3³D - 2³P
He 3¹D - 2¹P
He 3³S - 2³P
He 3¹S - 2¹P
0
2
4
6
8
400
500
600
700

Determination of *ne*, *Te*, *Tv*, *Trot* from observed spectra

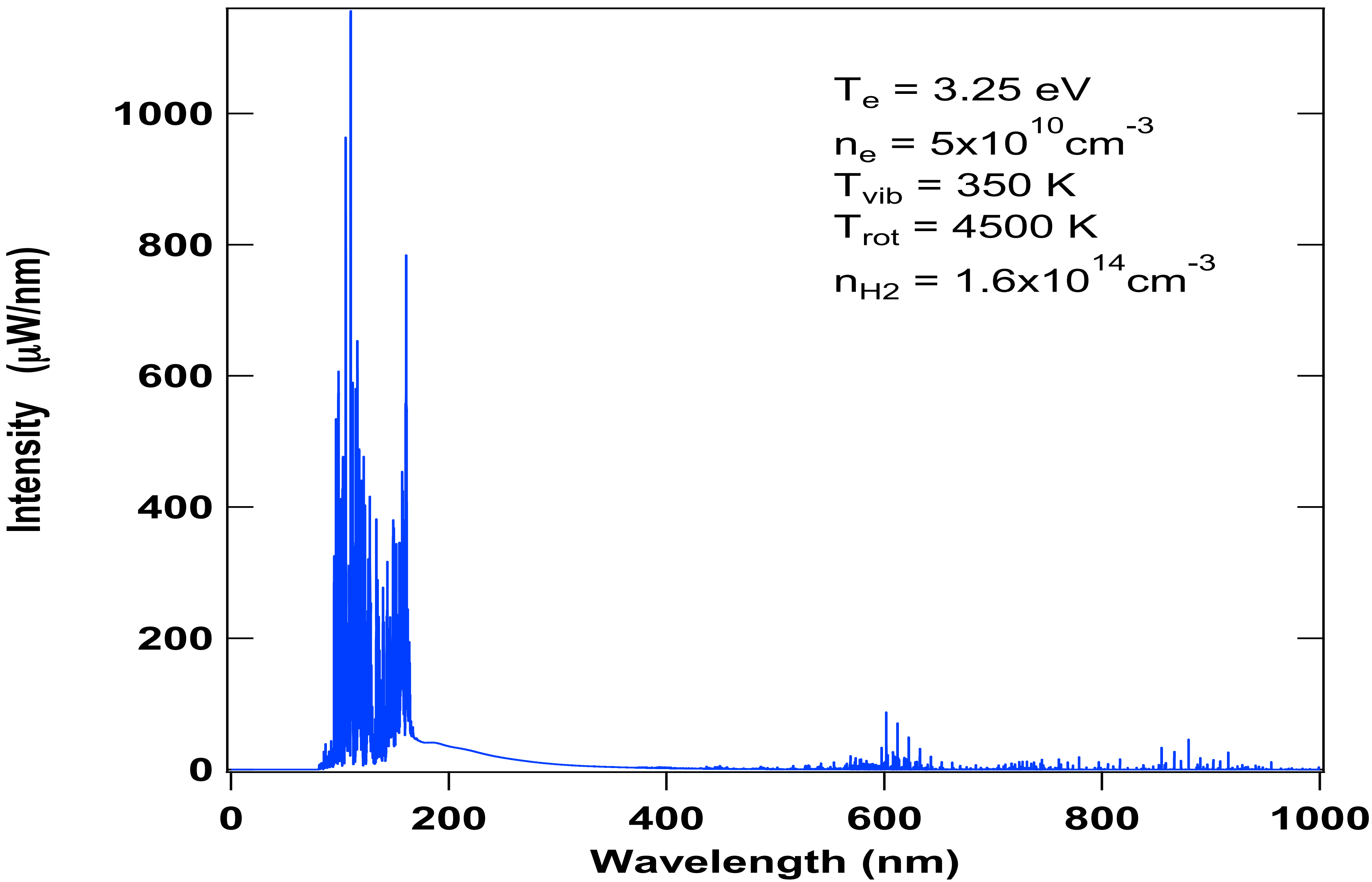




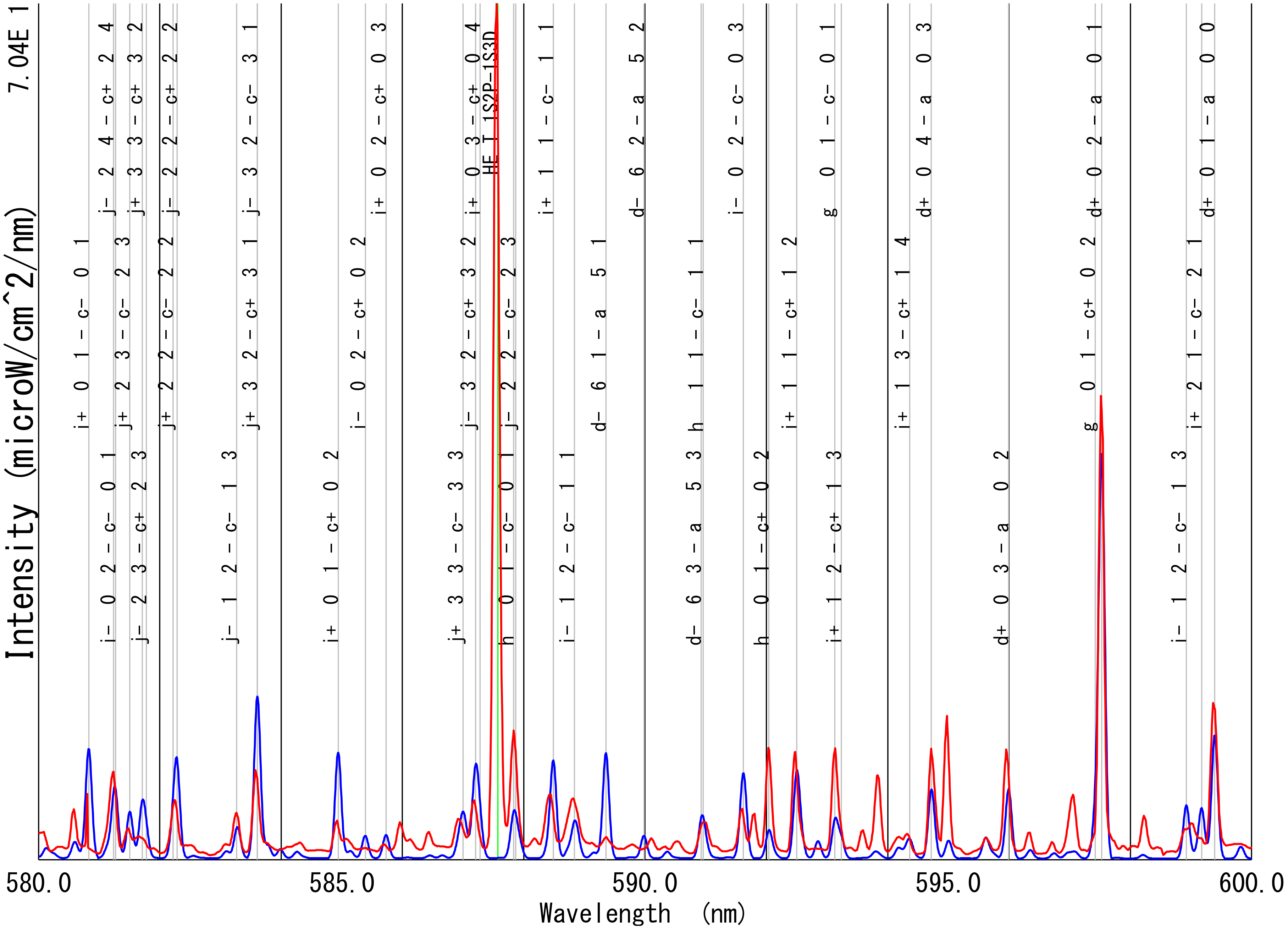




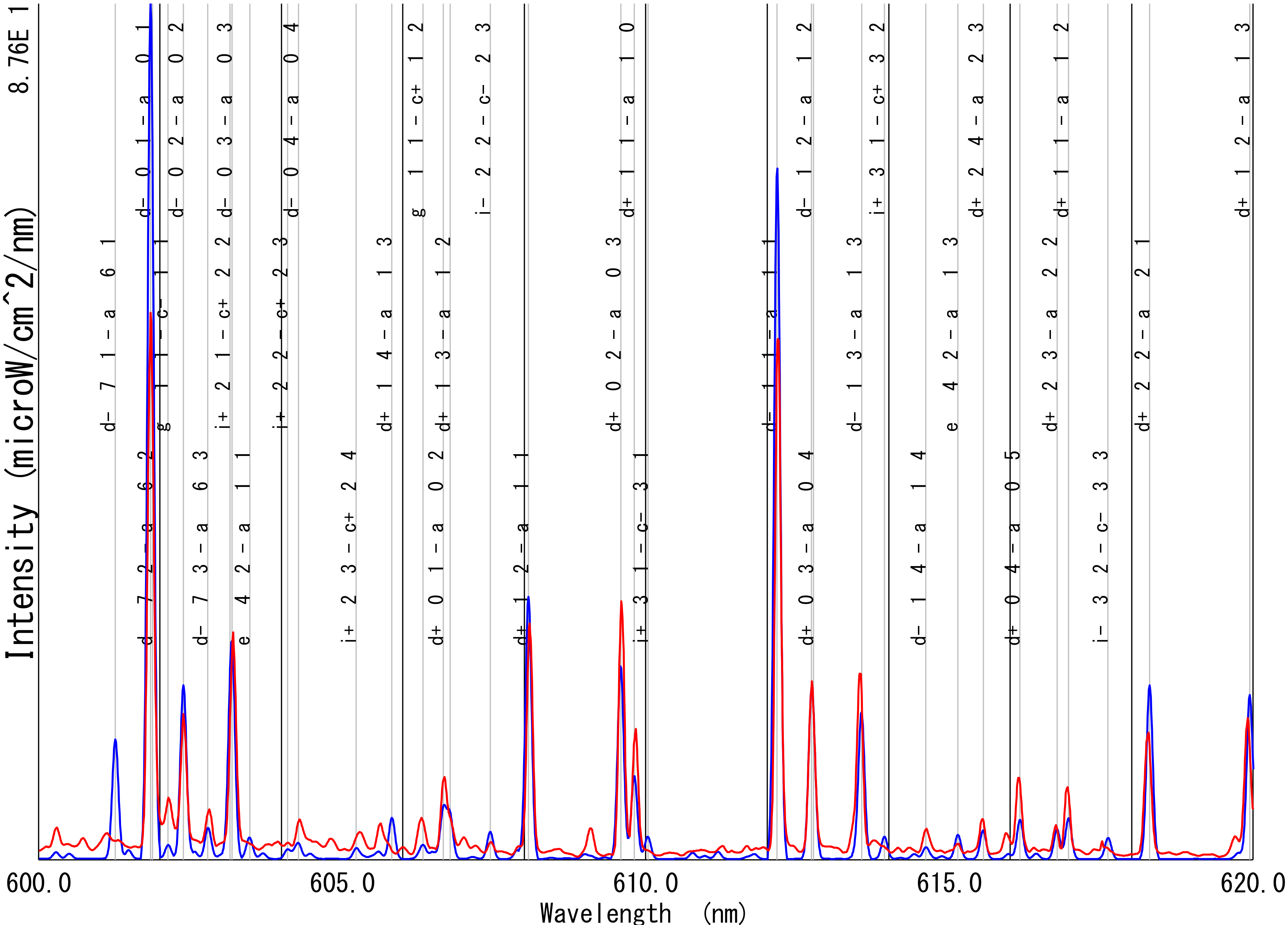
H_2 CR model calculation : H_2 spectra



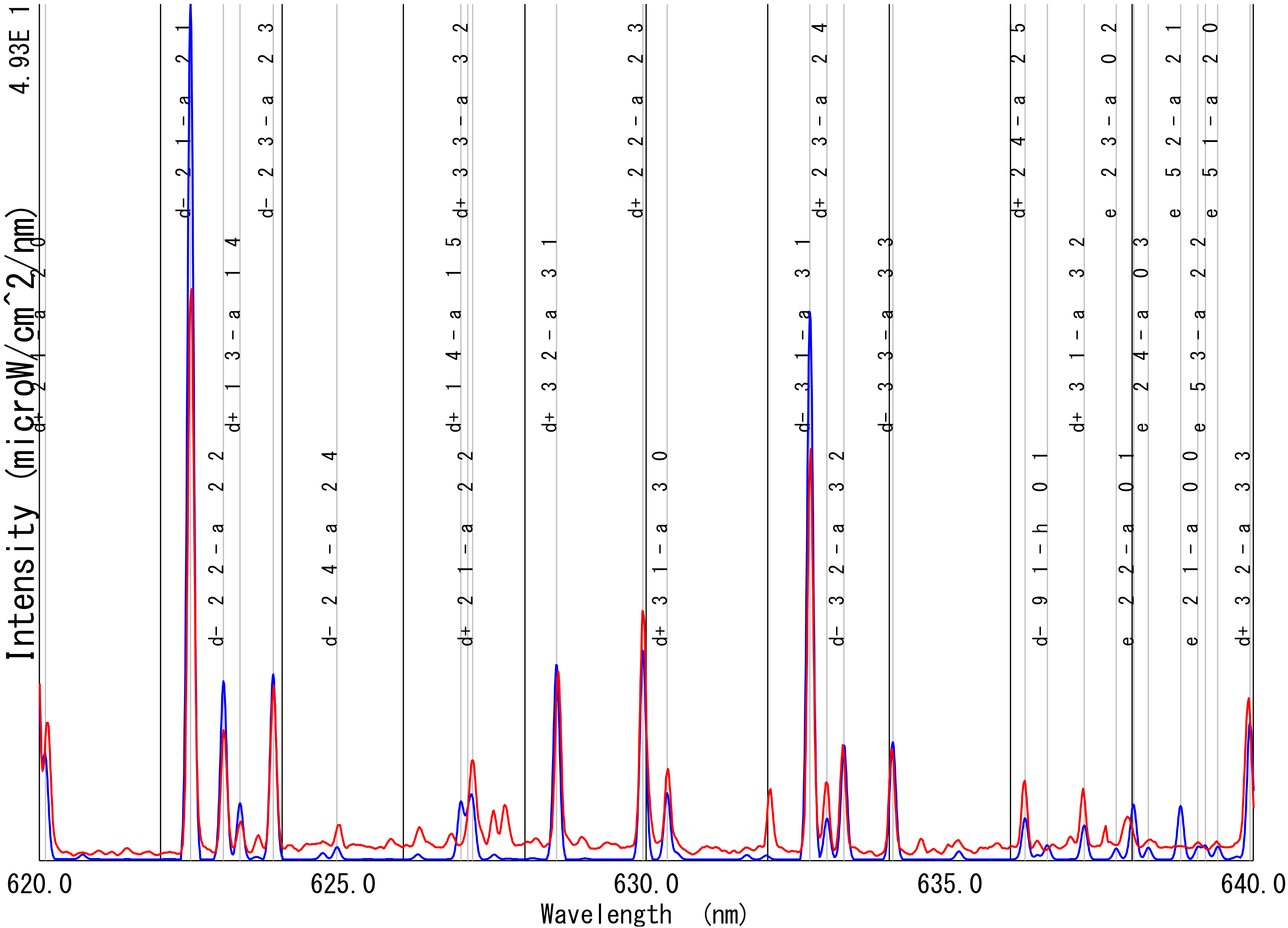
580-600 nm red (exp.) blue (calc.)



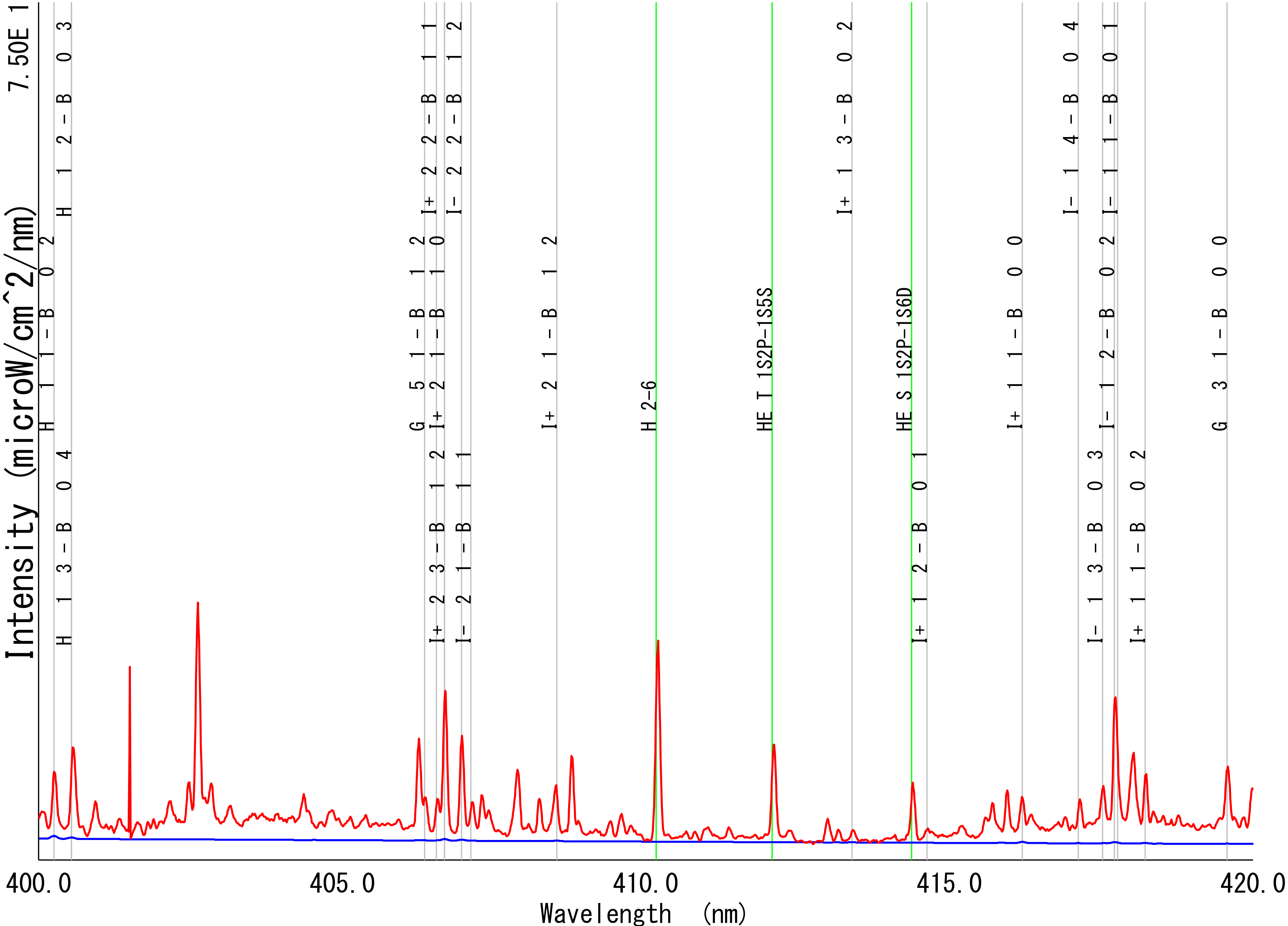
600-620 nm red (exp.) blue (calc.)



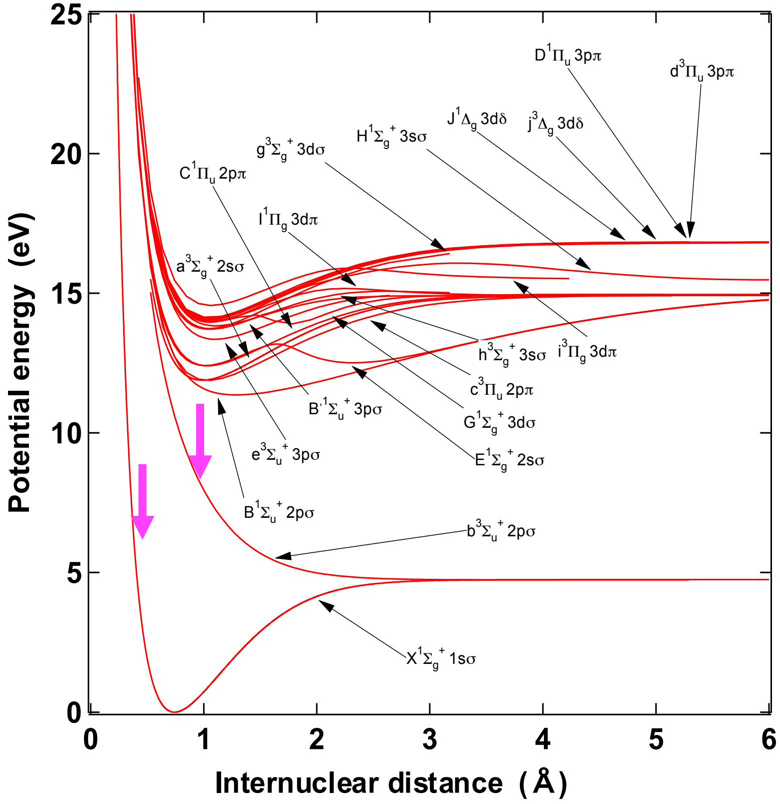
620-640 nm red (exp.) blue (calc.)

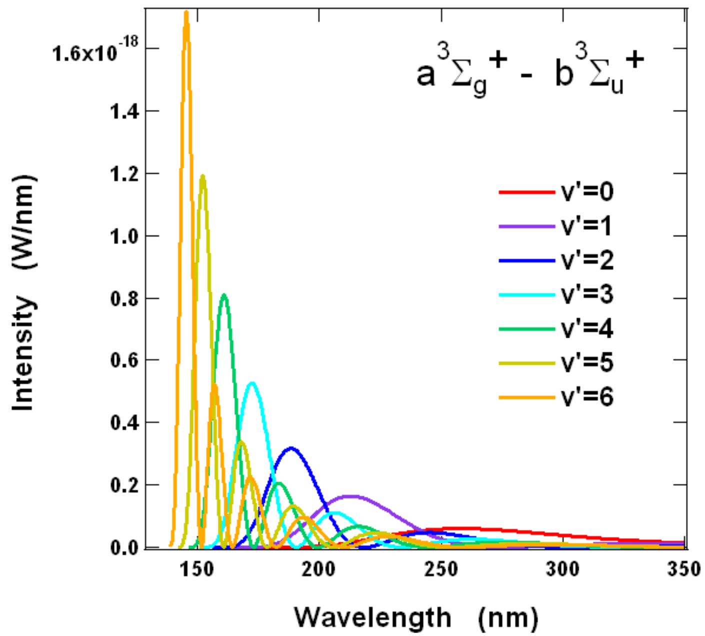


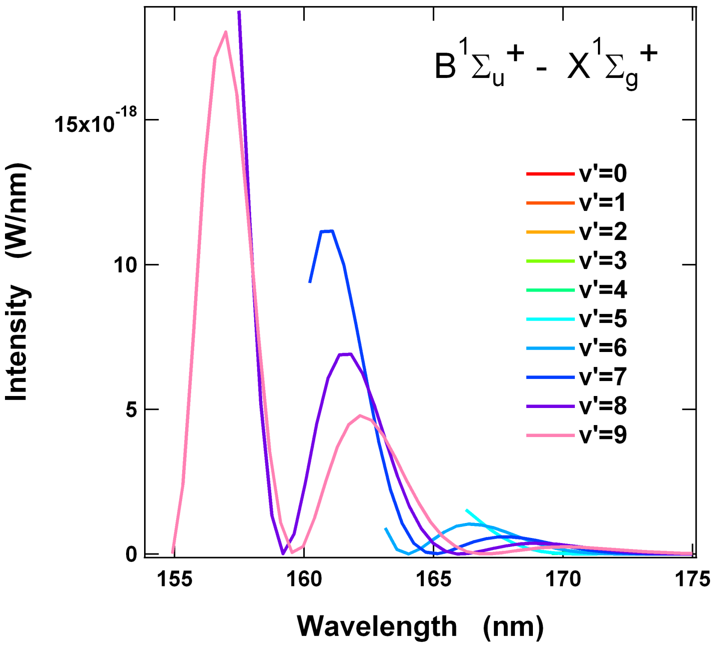
400-420 nm red (exp.) blue (calc.)



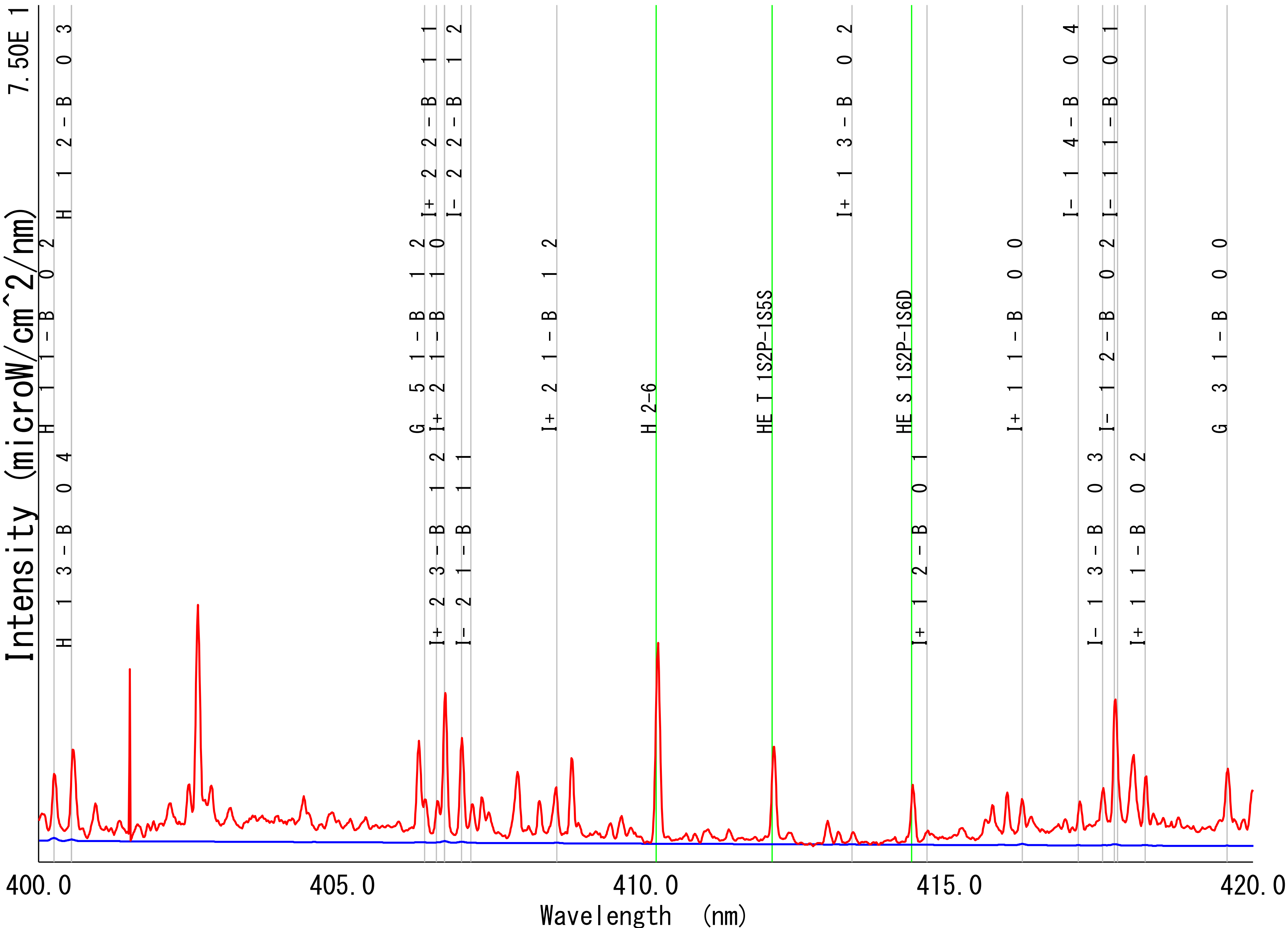
H_2 Transition Probability to Continuum states



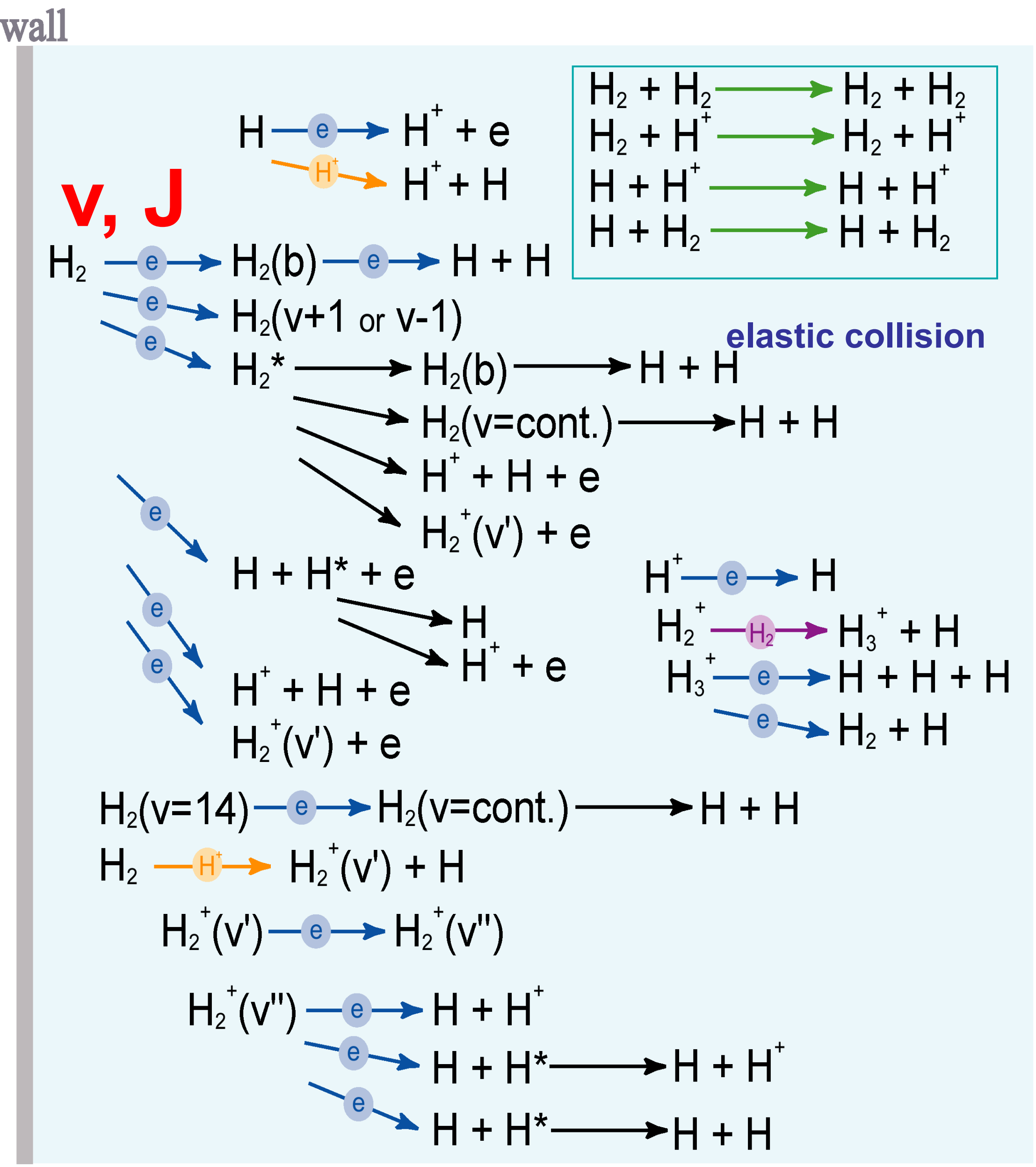




400-420 nm red (exp.) blue (calc.)



Our models



Collisional–Radiative Models

Hydrogen atom
Hydrogen molecule (H_2)
Helium atom (Dr. Goto)

Neutral-Transport Code