

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

信州大学工学部 澤田圭司

平成25年度合同会合:

第1回プラズマ物理クラスター・スクレープオフ層とダイバータサブクラスター

第3回炉工学クラスター・ブランケットサブクラスター

第1回炉工学クラスター・ダイバータサブクラスター

筑波大学プラズマ研究センターシンポジウム

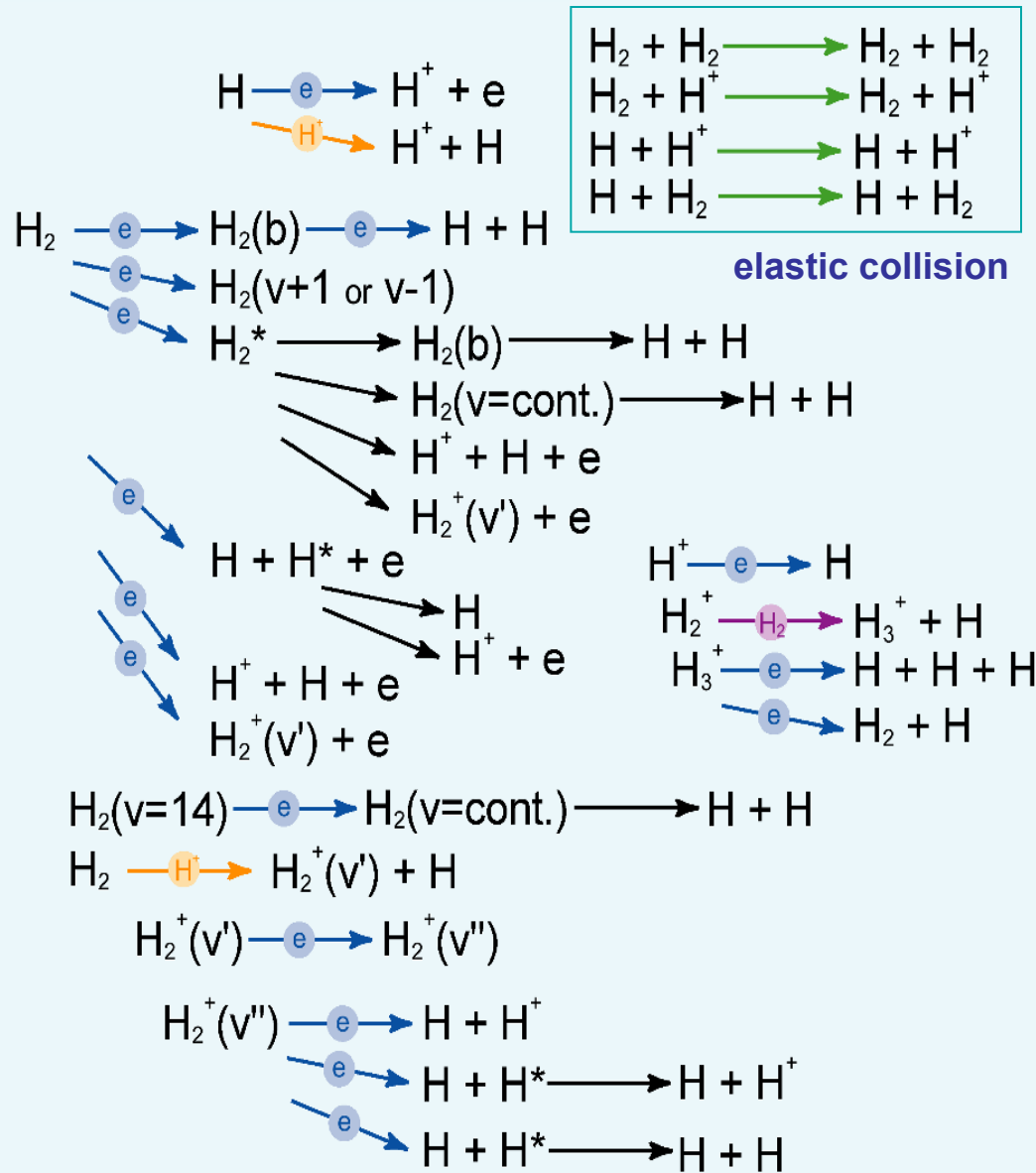
双方向型共同研究「磁化プラズマ中の壁不純物粒子挙動とプラズマ特性への影響」

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

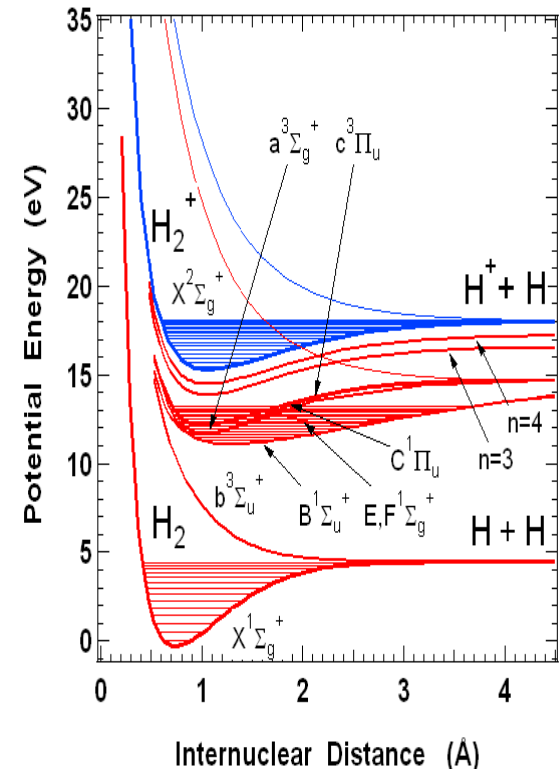
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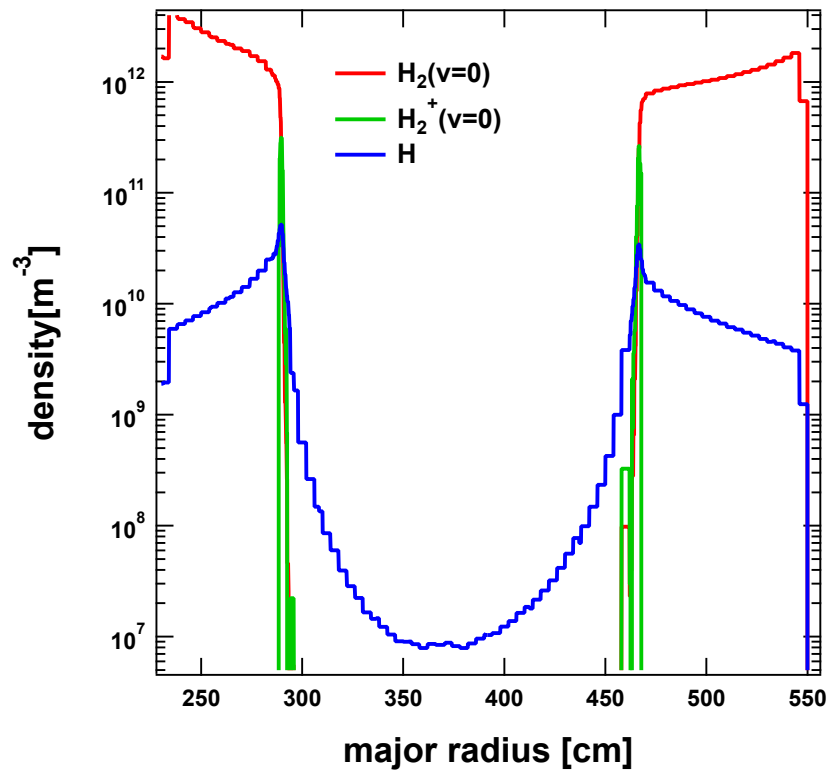
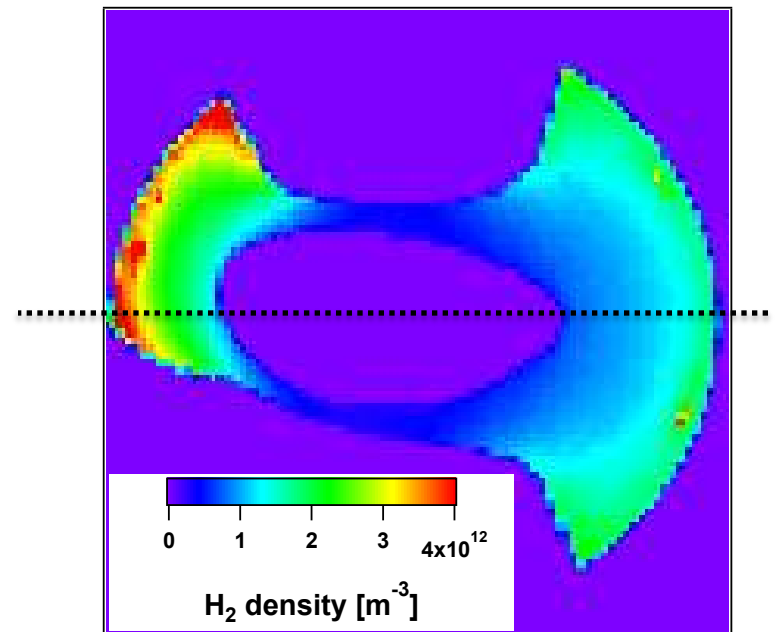
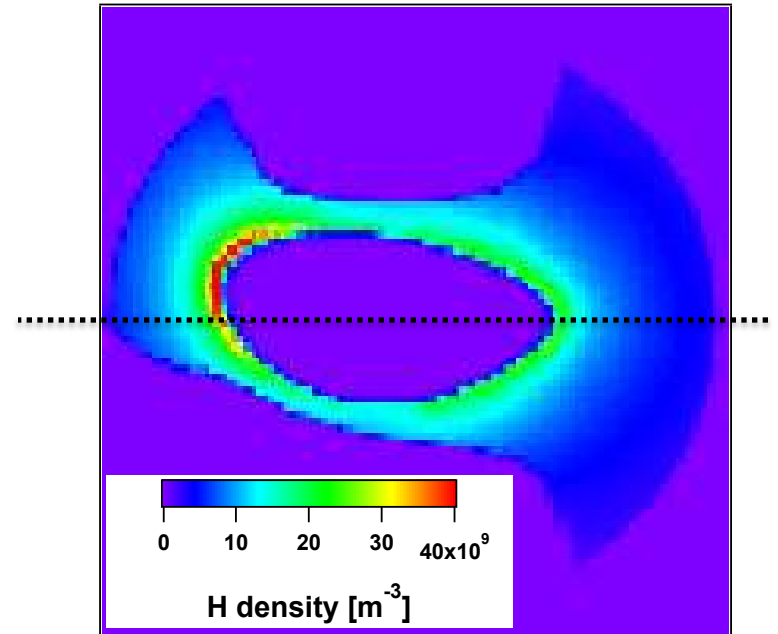
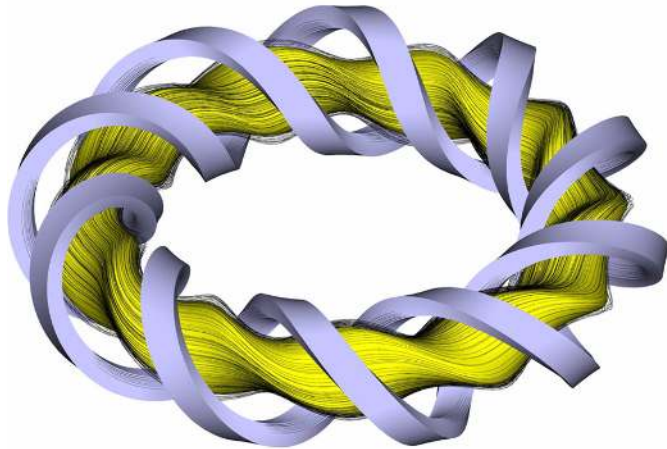
Collisional–Radiative Models

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

Neutral-Transport Code

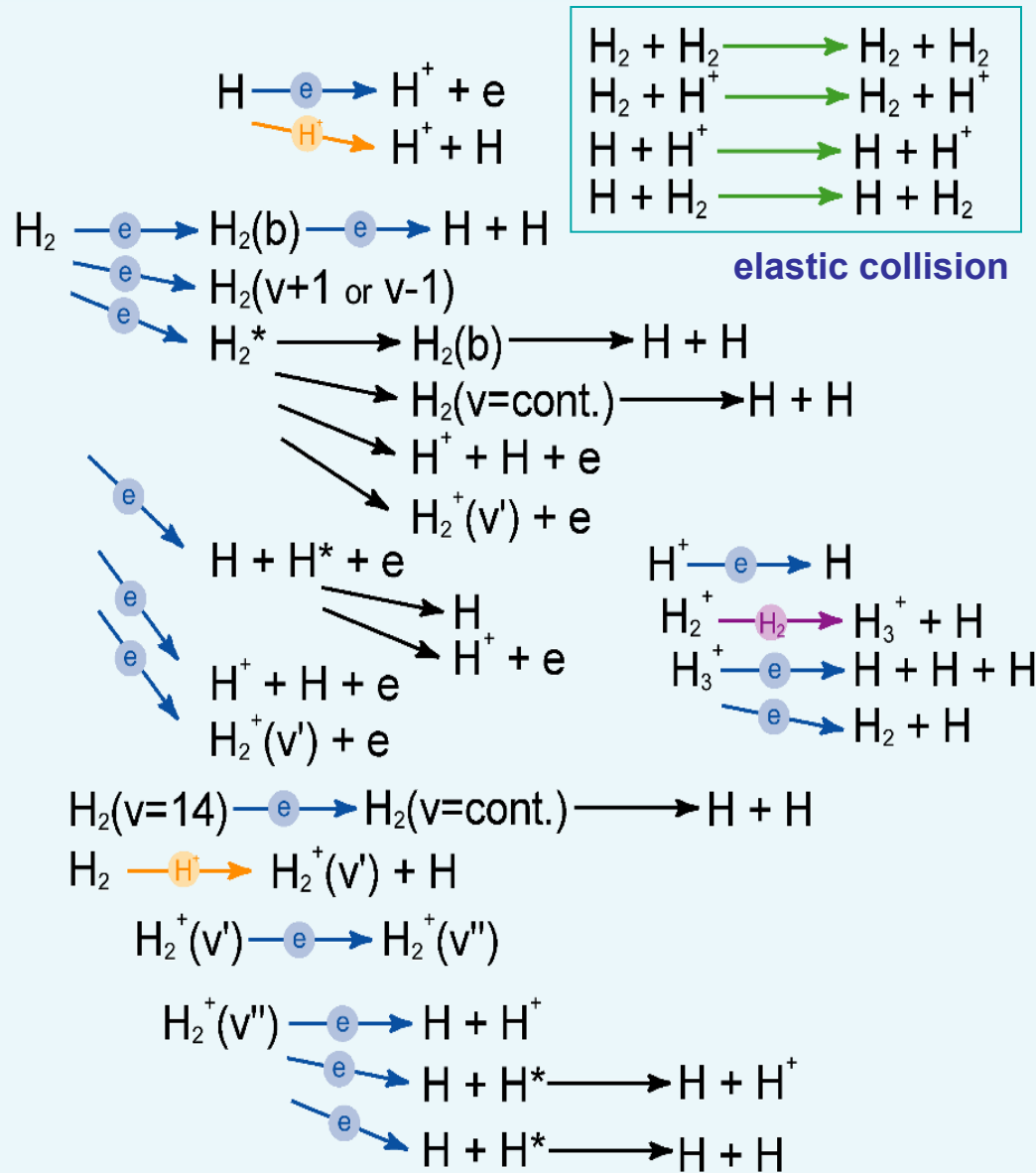


LHD 中性粒子輸送コードの計算結果



Introduction : Our models

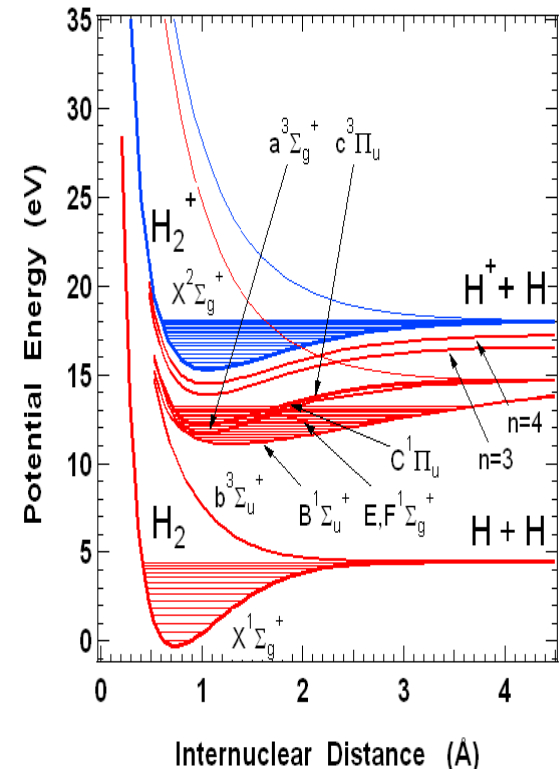
wall



Collisional–Radiative Models

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

Neutral-Transport Code



H 衝突輻射モデル

H Collisional-Radiative Model

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

inflow

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

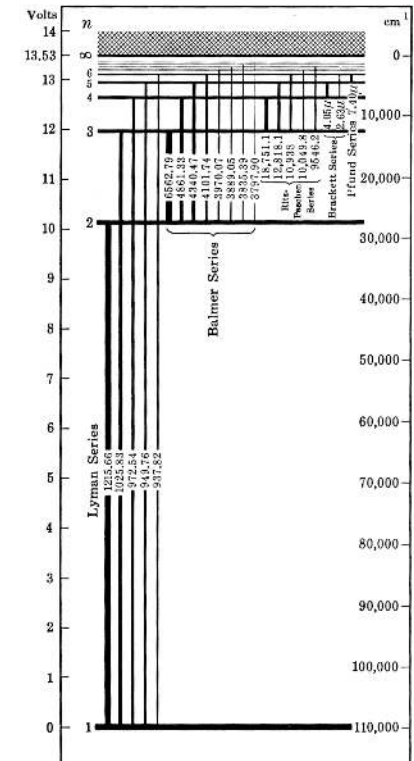
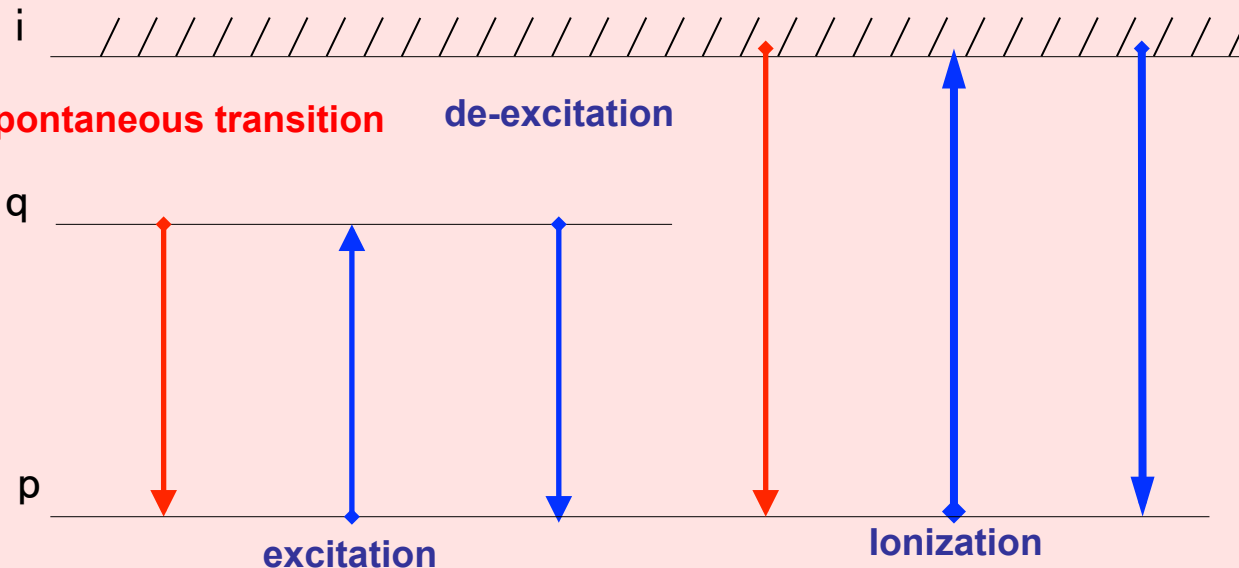
outflow

PLASMA

e H⁺ H

radiative rec.

3-body rec.



Solving Rate equations

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

$p \geq 2$

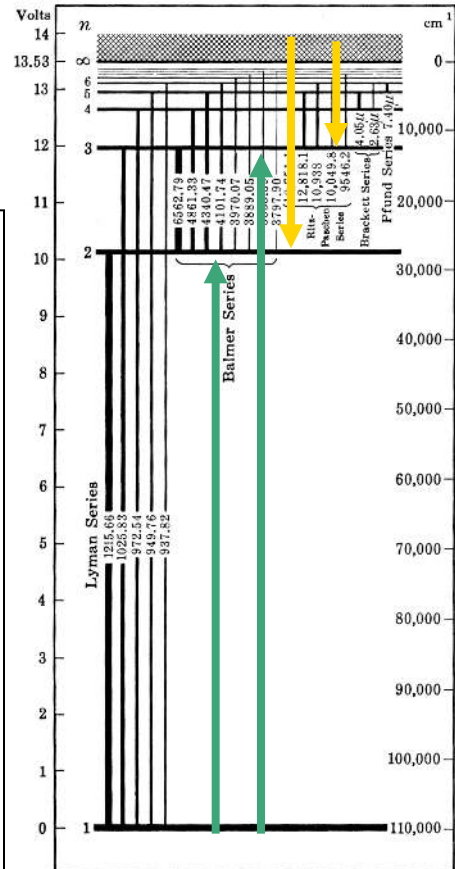
unknown

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

0

0
quasi-steady-
state
approximation
(QSS)

$$n(p) = \underbrace{R_0(p)n_i n_e}_{\text{Recombining component}} + \underbrace{R_1(p)n(1)n_e}_{\text{Ionizing component}}$$



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

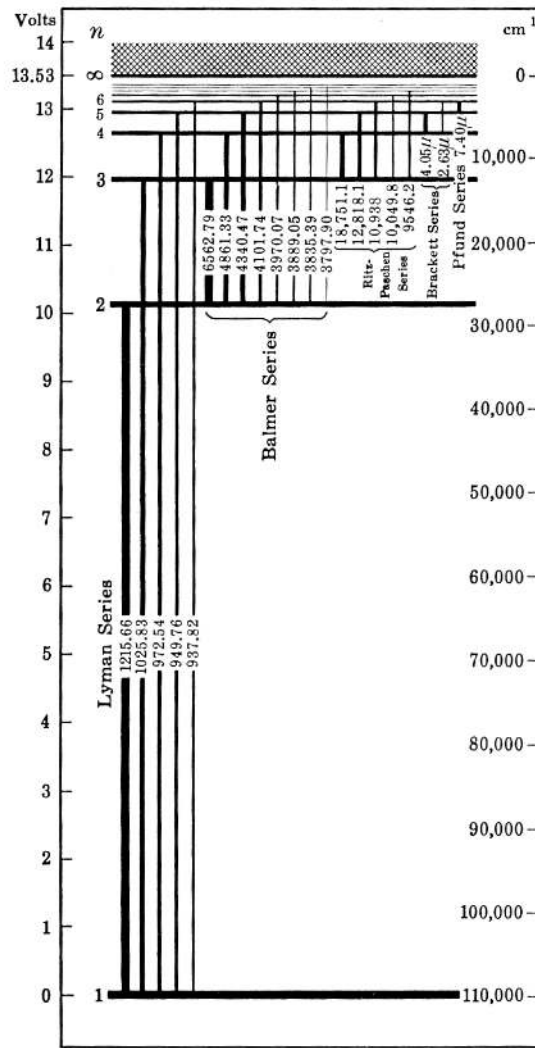
S_{CR} effective ionization rate coefficient

α_{CR} effective recombination rate coefficient

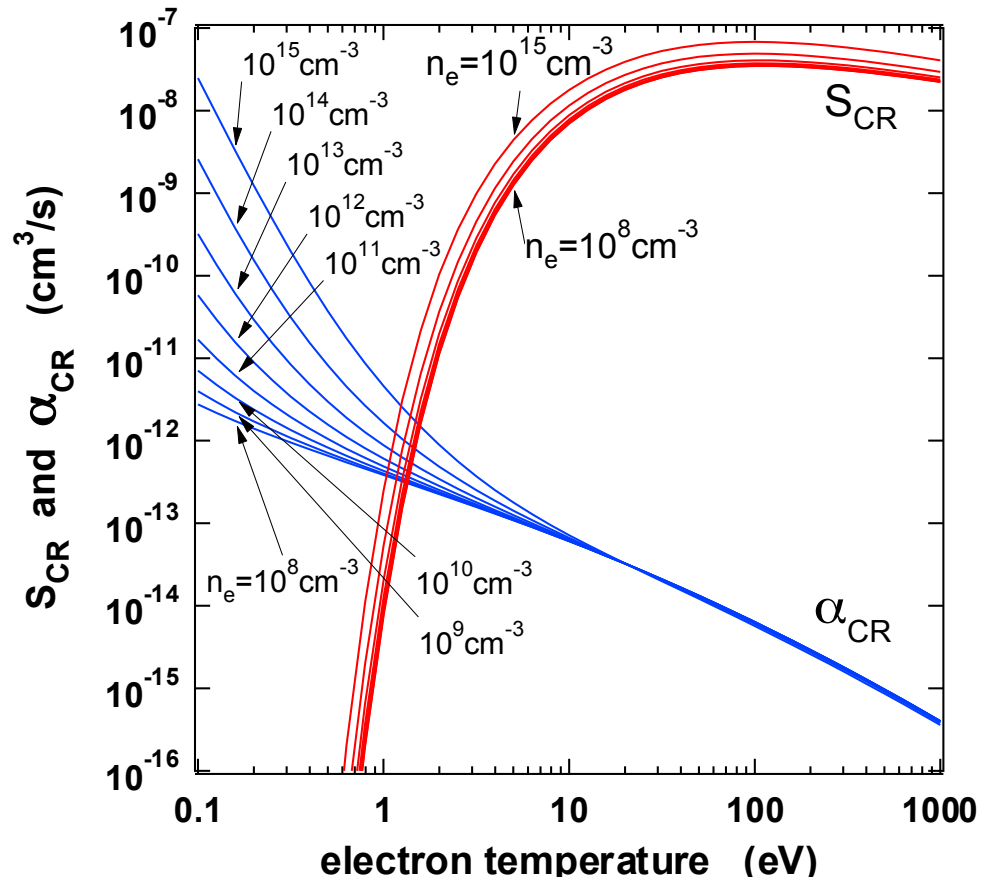
Effective Ionization and Recombination Rate coefficients

SCR Effective Ionization Rate Coefficient

αCR Effective Recombination Rate Coefficient



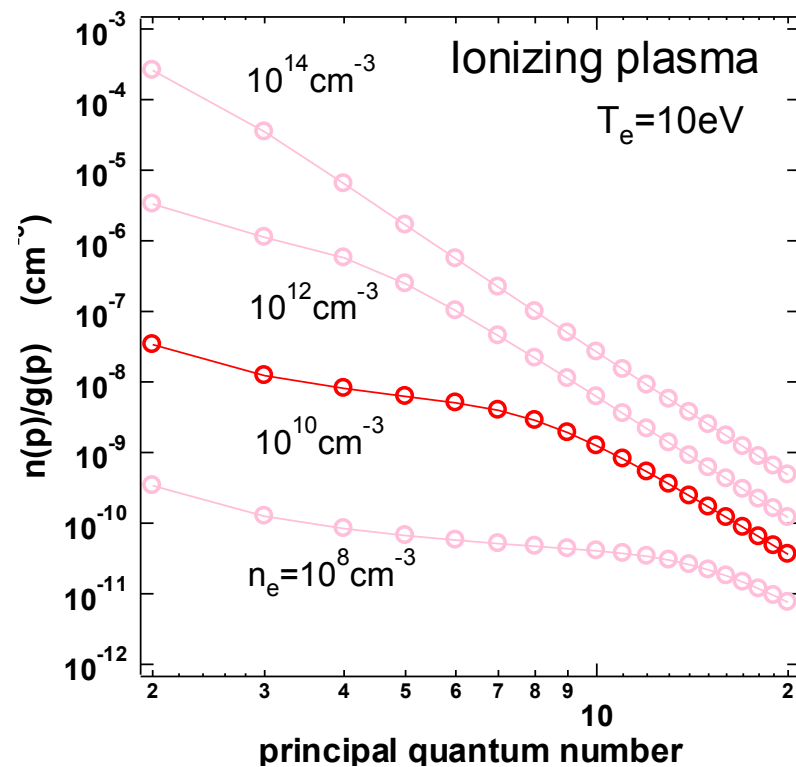
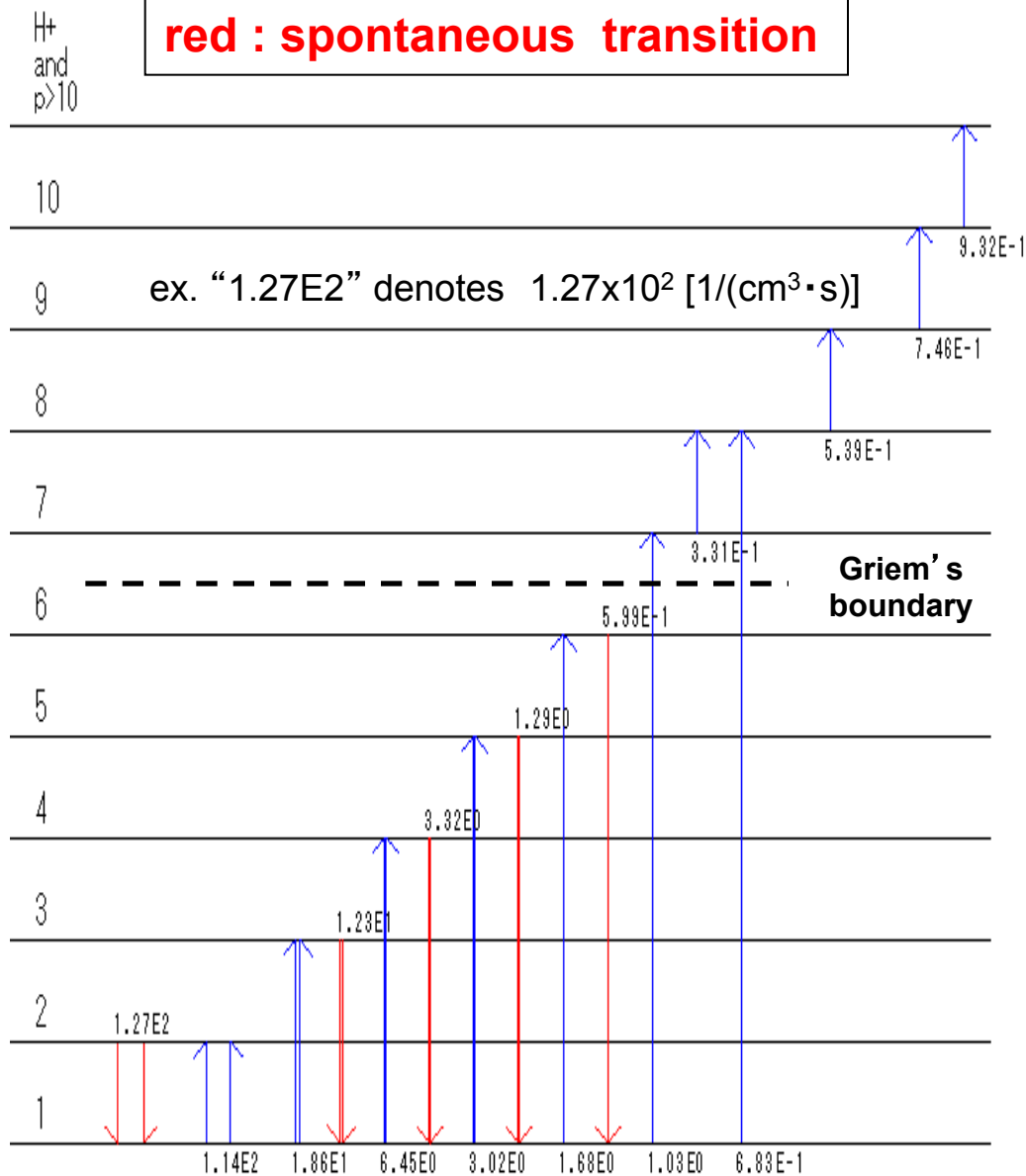
$$\frac{dn(1)}{dt} = -S_{\text{CR}} n(1)n_e + \alpha_{\text{CR}} n_{H^+} n_e$$



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

blue : electron impact

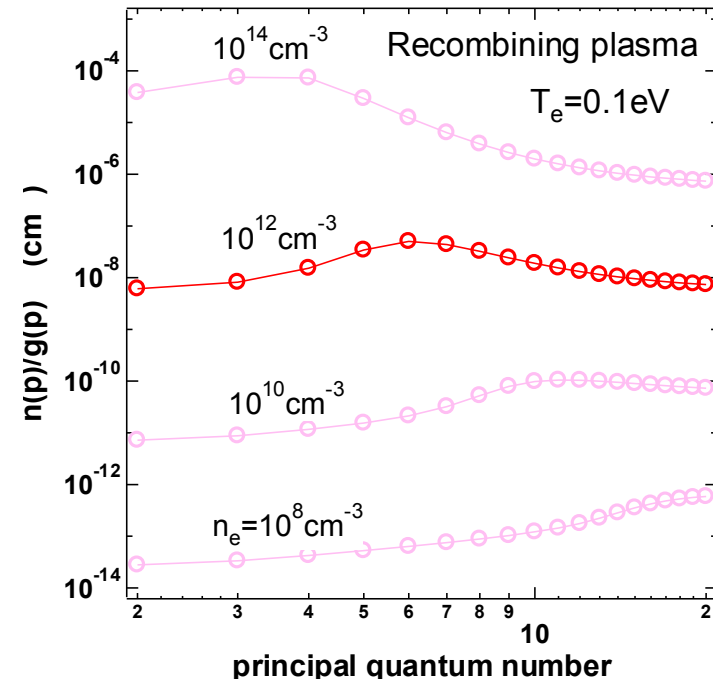
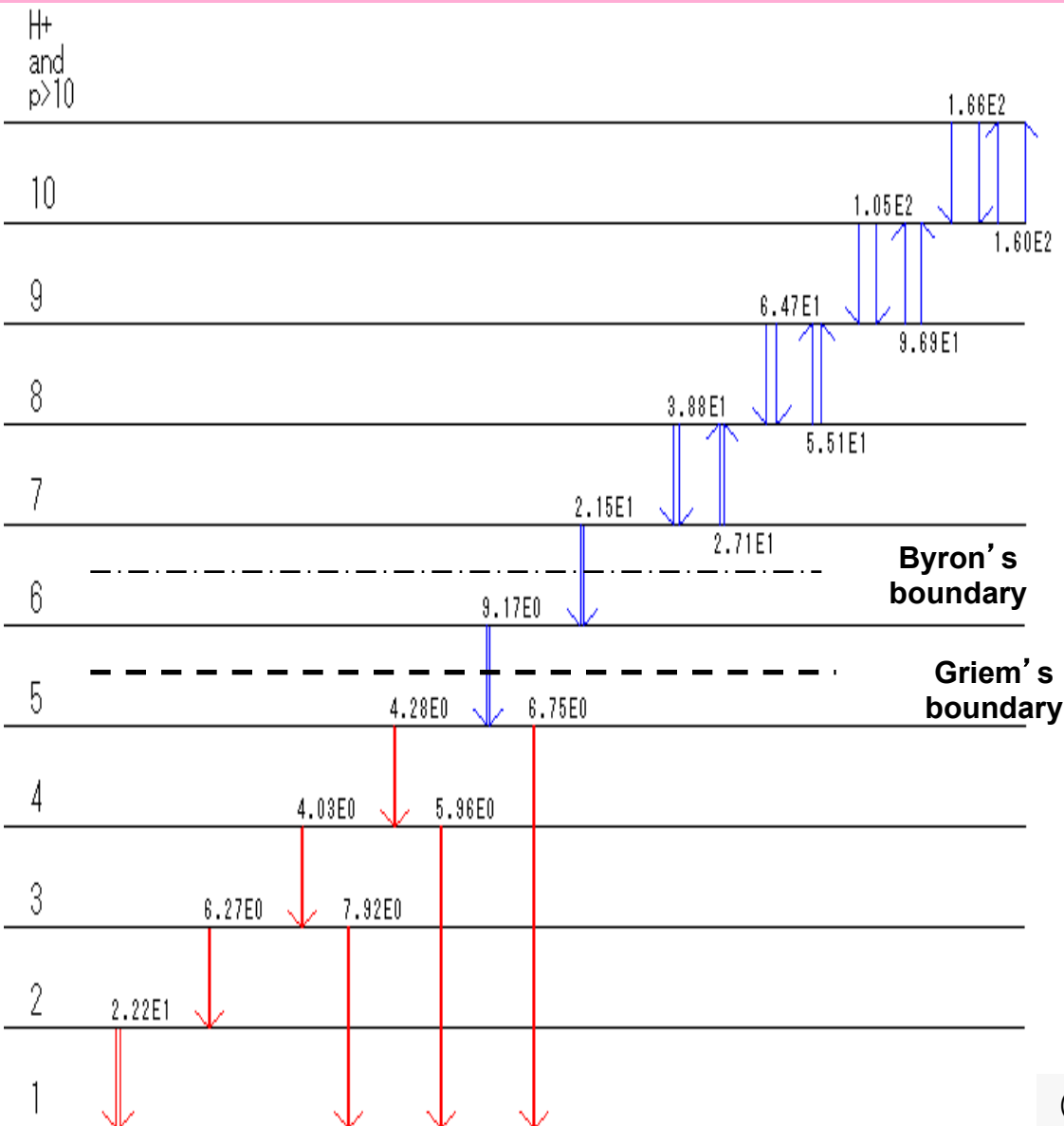
red : spontaneous transition



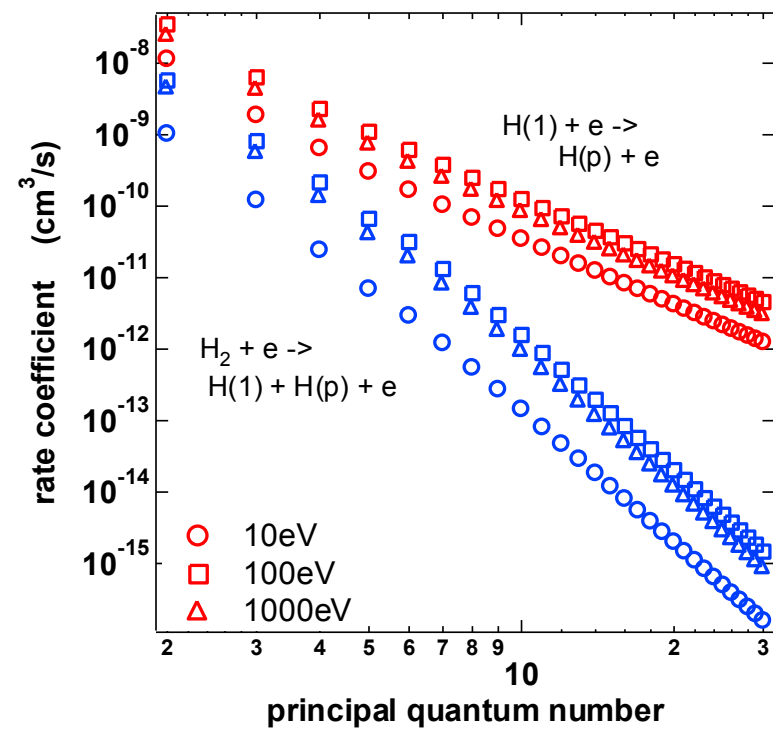
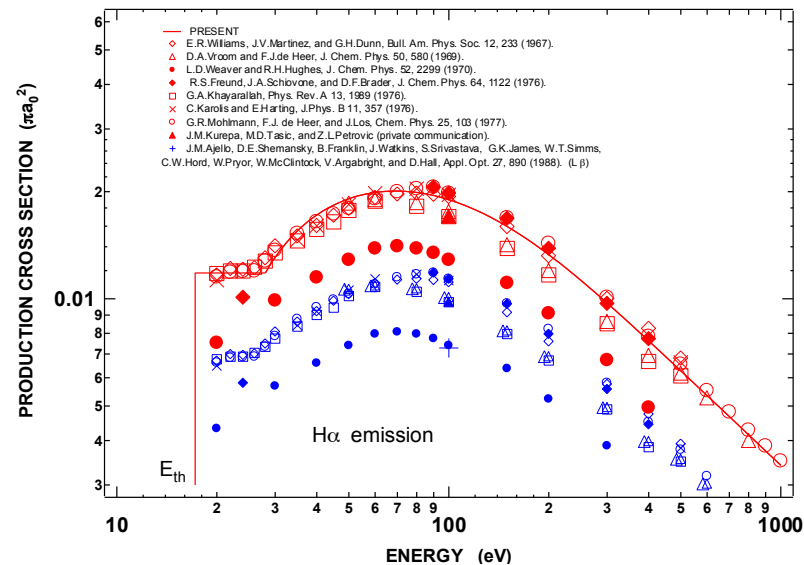
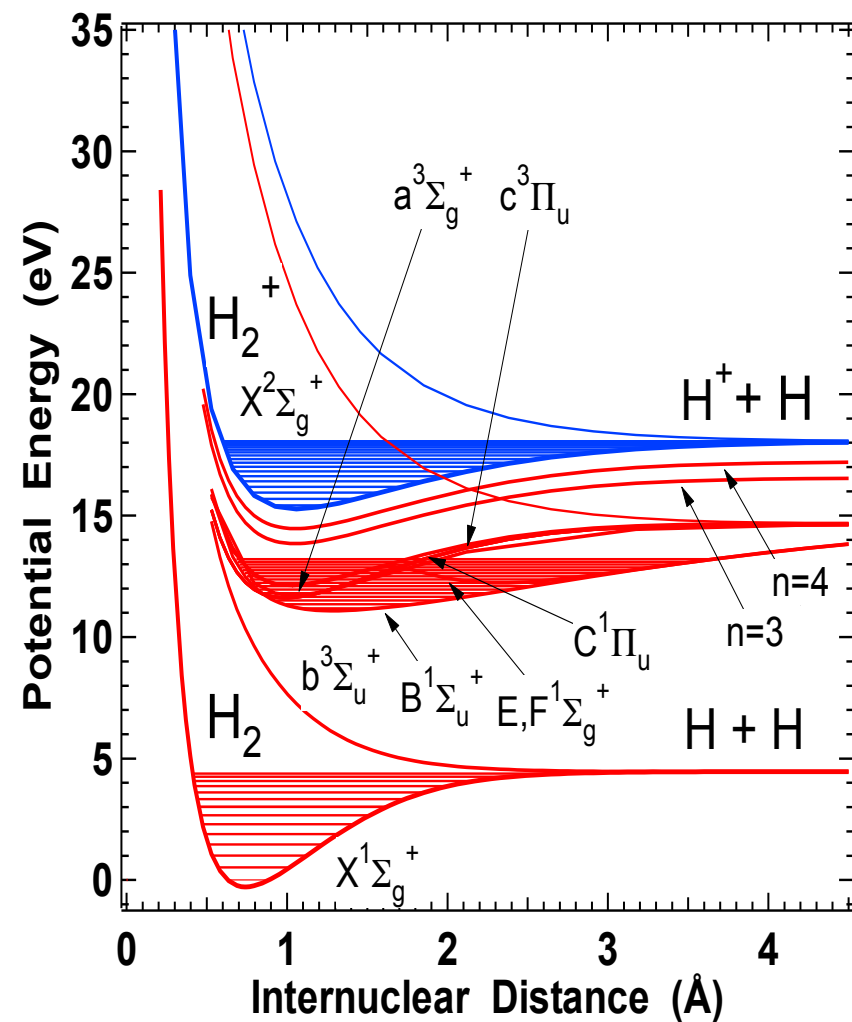
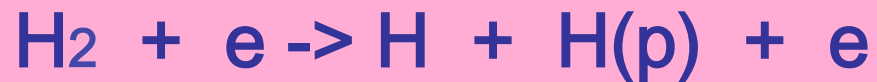
$$S(1)n(1)n_e=6.92\text{E1} \text{ [1/(\text{cm}^3 \cdot \text{s})]}$$

Recombining component

$$T_e=0.1\text{eV} \quad n_e=10^{12}\text{cm}^{-3} \quad n_i=1\text{cm}^{-3}$$



$$(\alpha(1)n_e + \beta(1))n_z n_e = 4.69\text{E-}1 \quad [1/(\text{cm}^3 \cdot \text{s})]$$



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

$$\begin{aligned} \frac{dn(p)}{dt} = & \sum_{q < p} C(q, p) n_e n(q) + \sum_{q > p} \{ F(q, p) n_e + A(q, p) \} n(q) + \alpha(p) n_e^2 n_i + \beta(p) n_e n_i \\ & + C_{H_2}(p) n_{H_2} n_e \\ & - [\{ \sum_{q < p} F(p, q) + \sum_{q > p} C(p, q) + S(p) \} n_e + \sum_{q < p} A(p, q)] n(p) \end{aligned}$$

$p \geq 2$ unknown $H_2 + e \rightarrow H + H(p) + e$

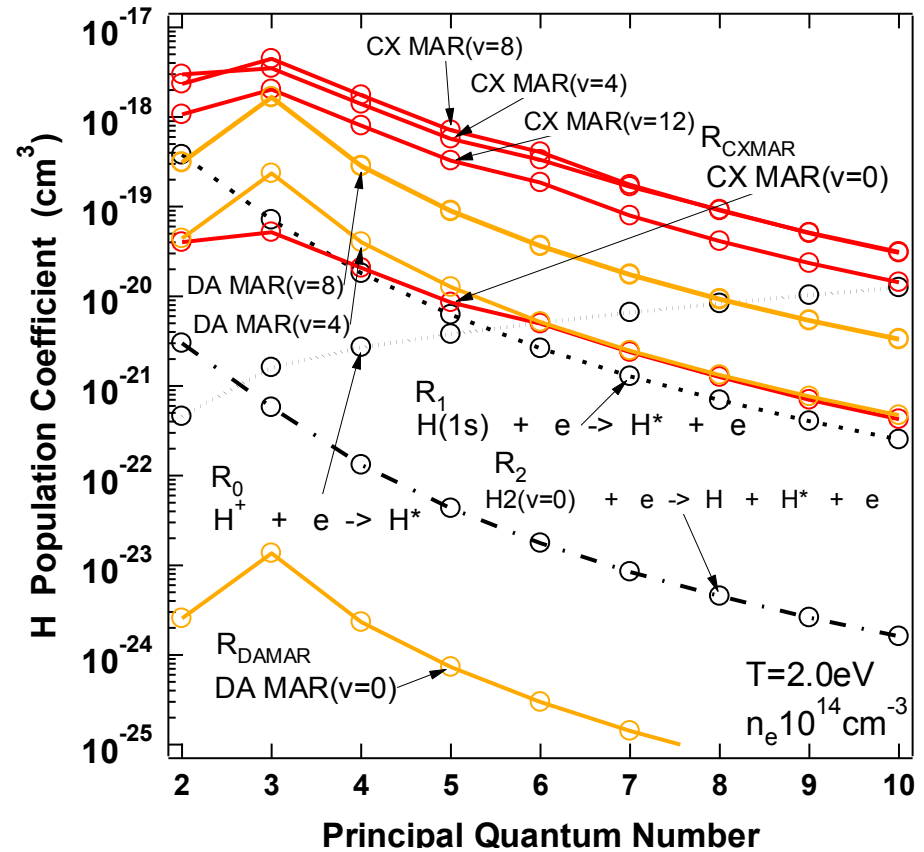
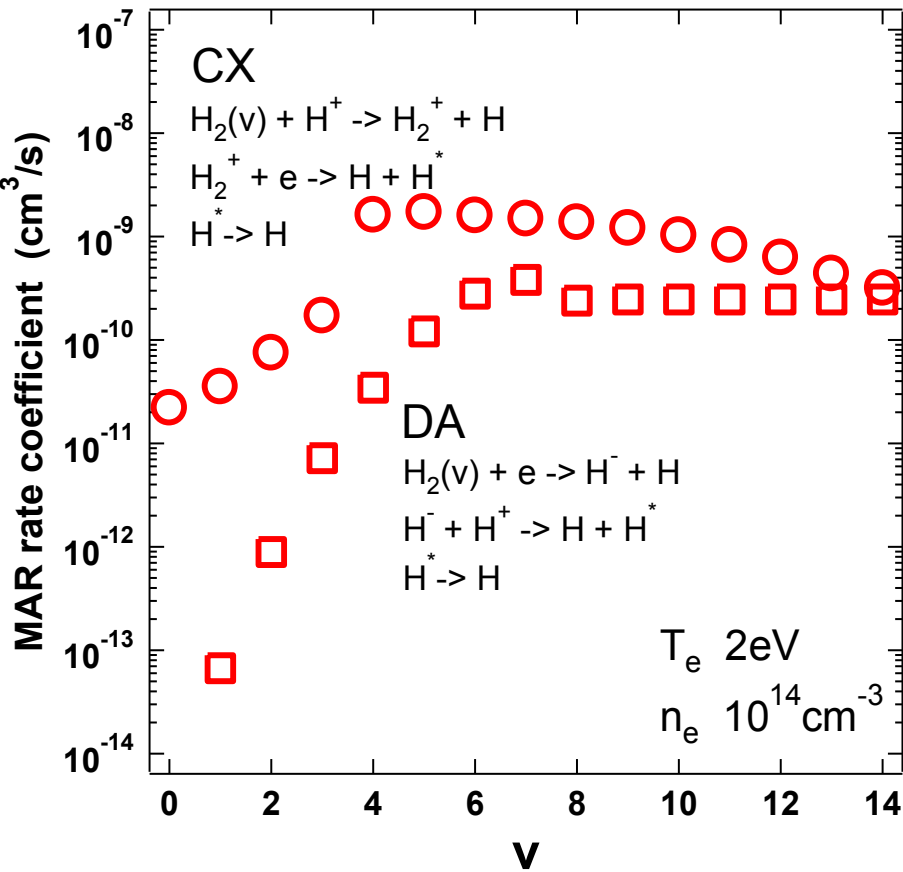
$$\frac{d}{dt} \begin{pmatrix} \cdot \\ \cdot \\ n(3) \\ n(2) \end{pmatrix} = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix} \begin{pmatrix} \cdot \\ \cdot \\ n(3) \\ n(2) \end{pmatrix} + \begin{pmatrix} \cdot \\ \cdot \\ \alpha(3)n_e + \beta(3) \\ \alpha(2)n_e + \beta(2) \end{pmatrix} n_i n_e + \begin{pmatrix} \cdot \\ \cdot \\ C(1,3) \\ C(1,2) \end{pmatrix} n(1) n_e + \begin{pmatrix} \cdot \\ \cdot \\ C_{H_2}(3) \\ C_{H_2}(2) \end{pmatrix} n_{H_2} n_e$$

0

(QSS)

$$n(p) = \underbrace{R_0(p) n_i n_e}_{\text{Recombining component}} + \underbrace{R_1(p) n(1) n_e}_{\text{Ionizing component}} + \underbrace{R_2(p) n_{H_2} n_e}_{\text{New term}}$$

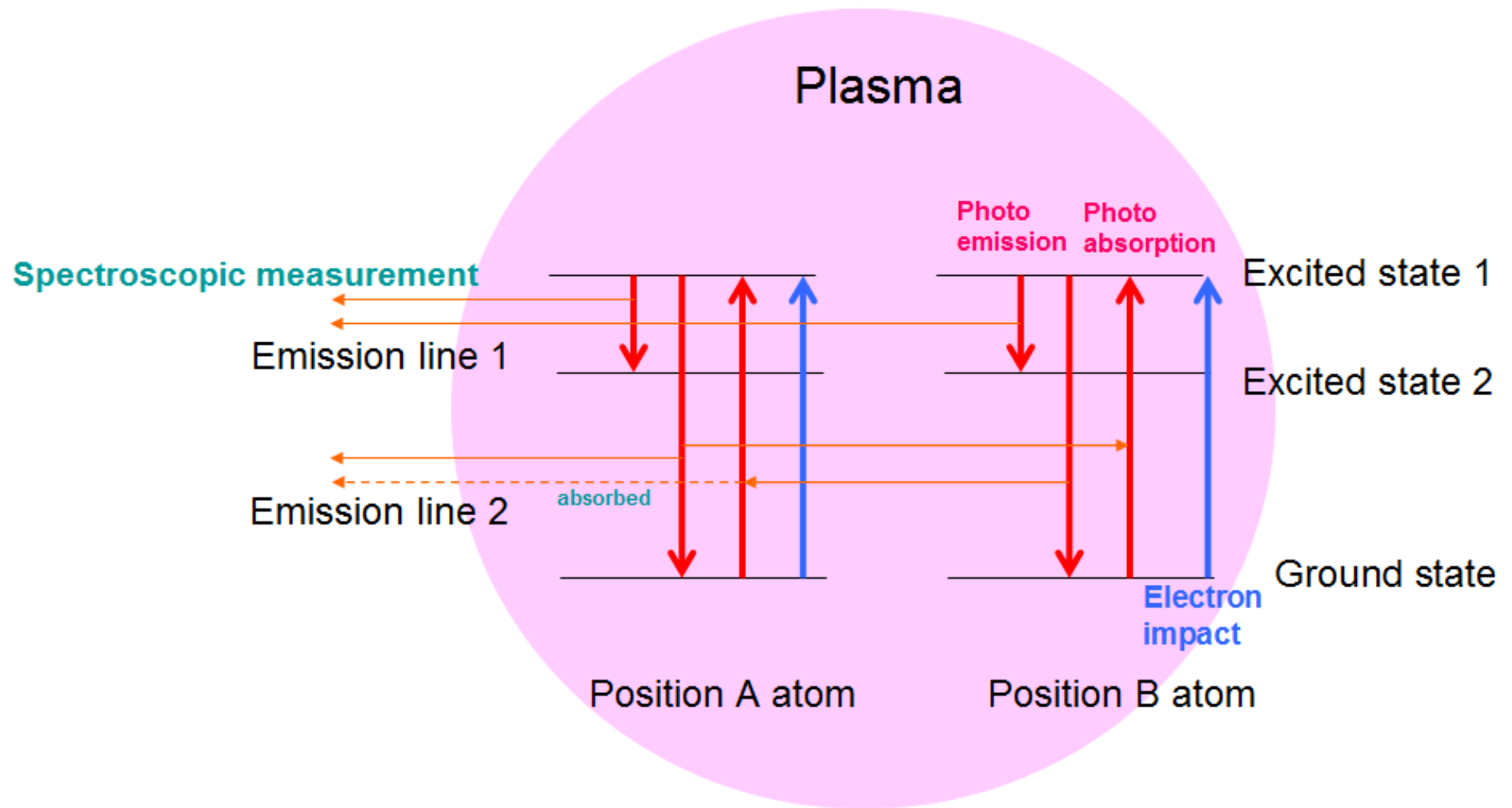
MAR (Molecular Assisted Recombination)



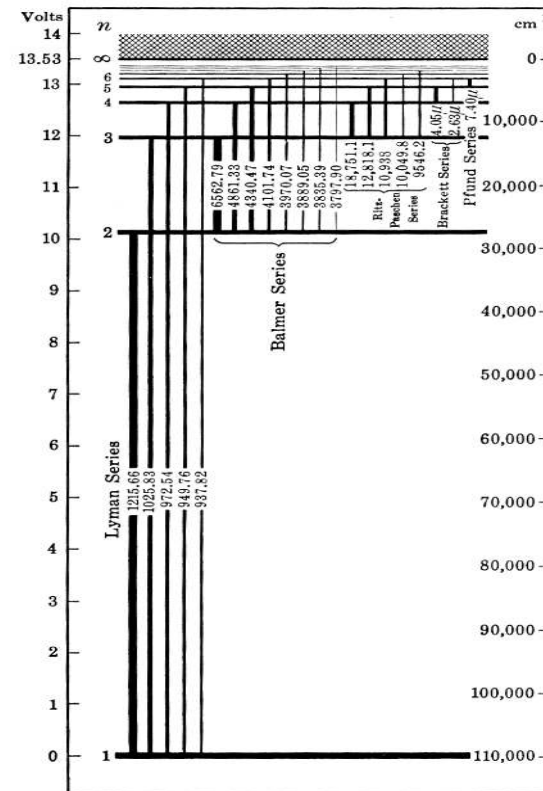
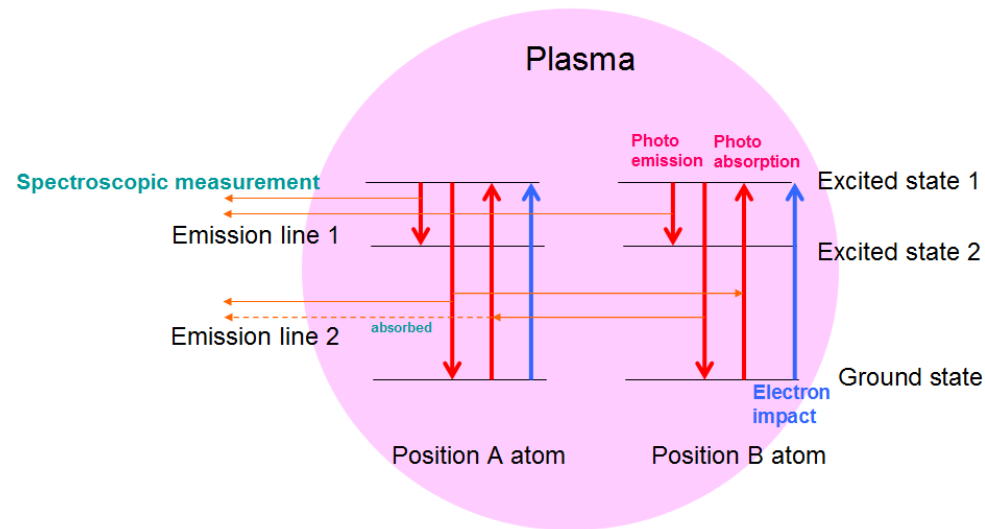
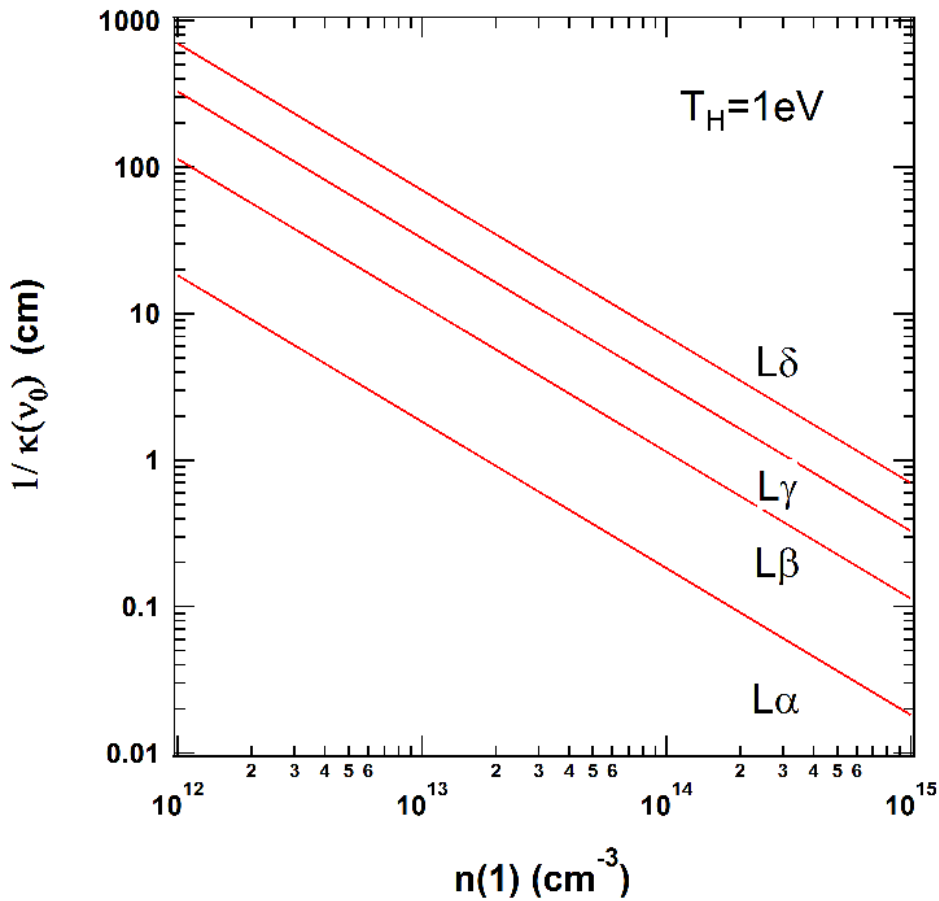
$$n(p) = R_0(p)n_en_{H^+} + R_1(p)n_en_H + R_2(p)n_en_{H_2} + R_{MAR}(p)n_en_{H_2}$$

輻射輸送

輻射輸送



ライマン線吸収長



H Collisional-Radiative Model

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

inflow

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

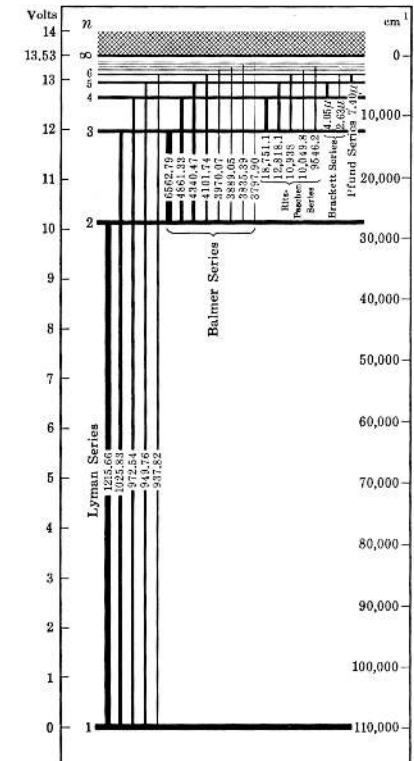
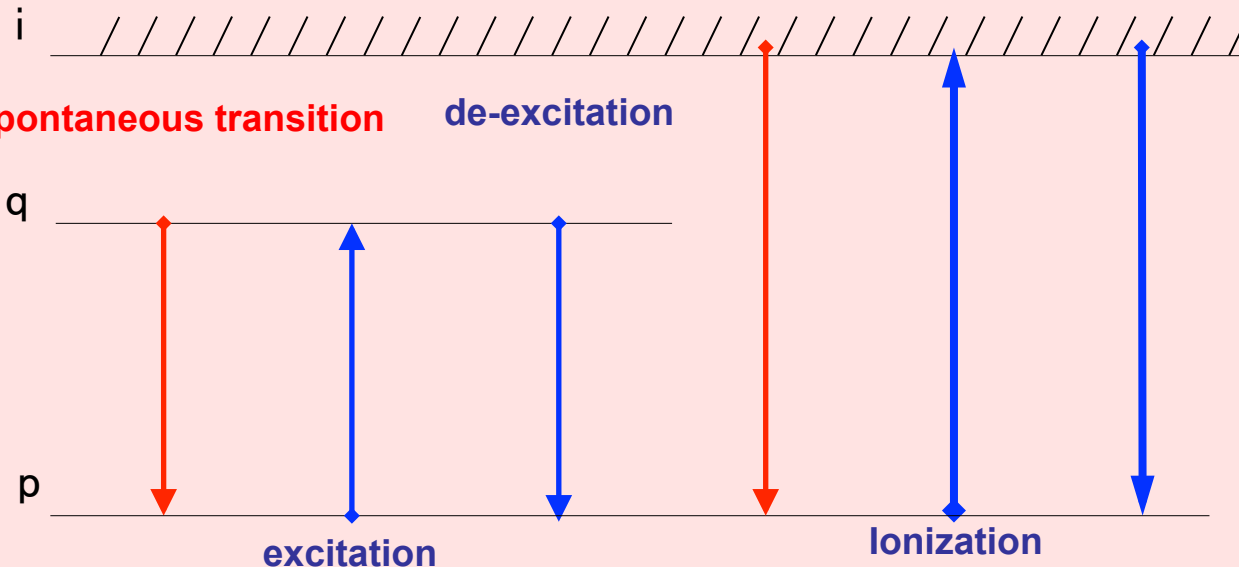
outflow

PLASMA

e H⁺ H

radiative rec.

3-body rec.



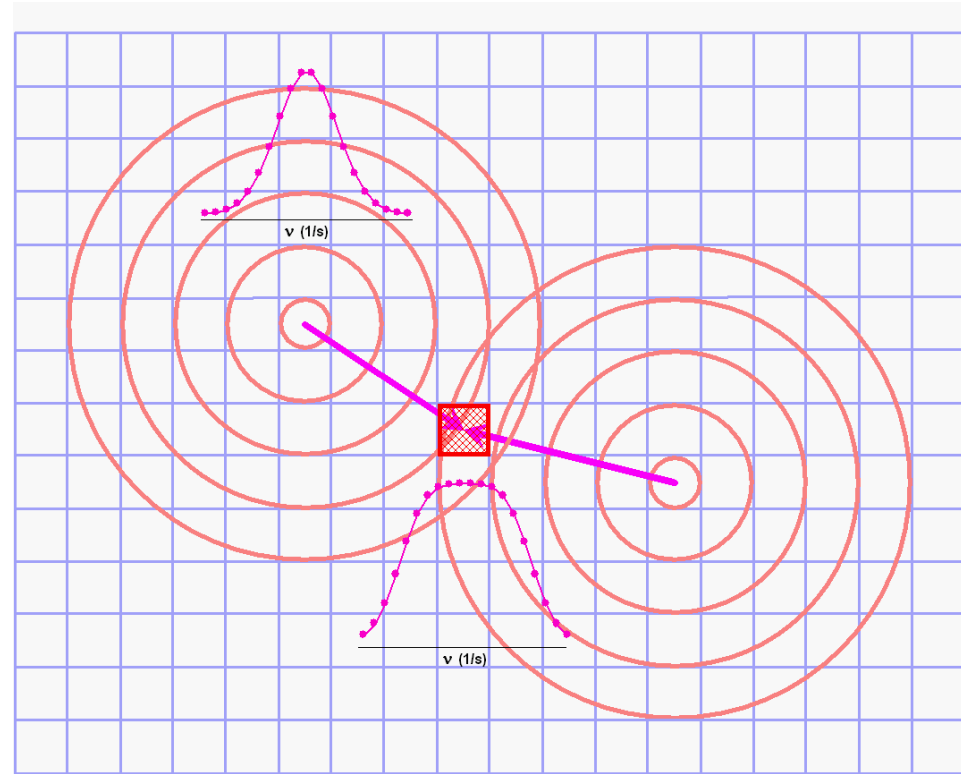
輻射輸送の計算手法

(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

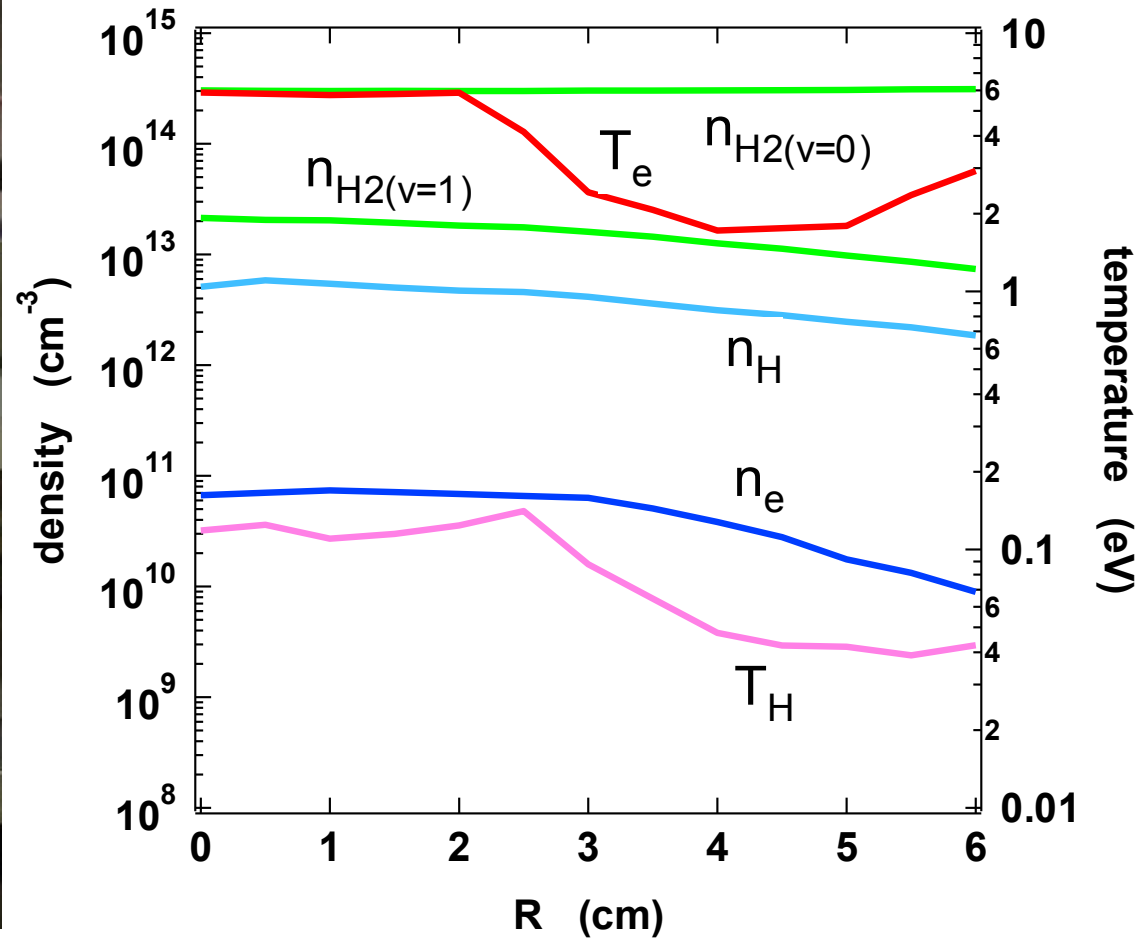
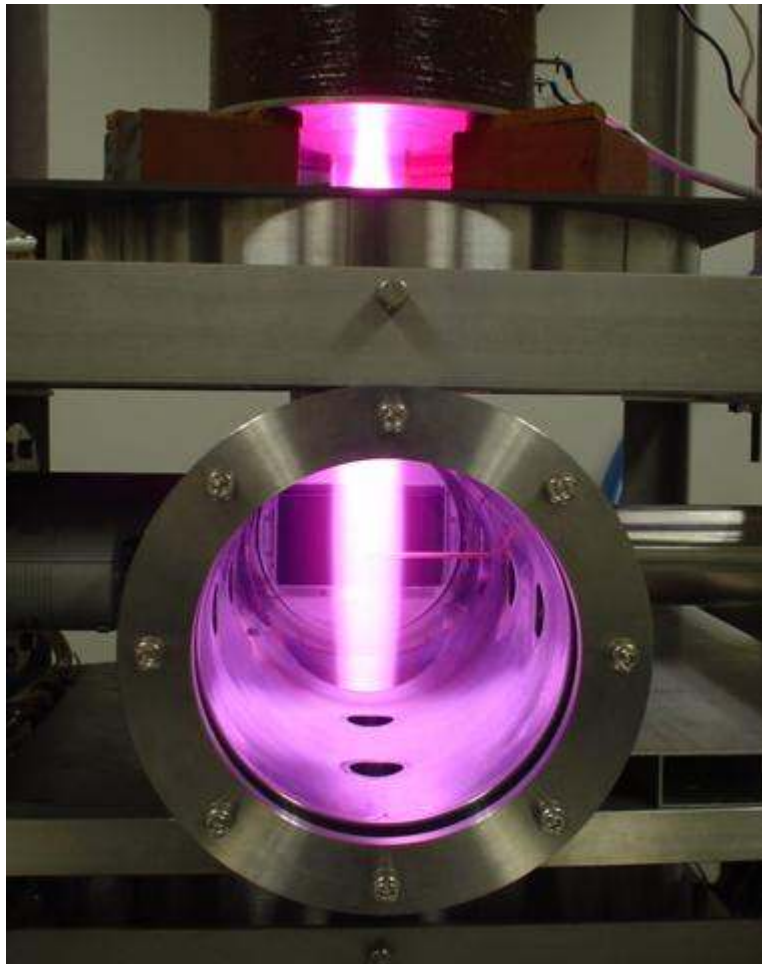
を与える。

- (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。

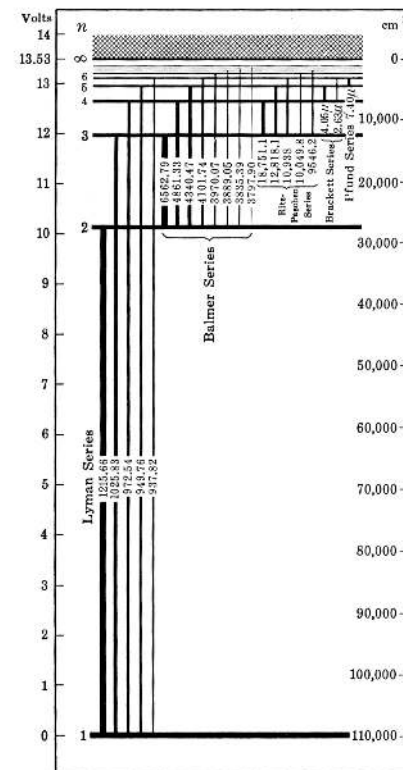
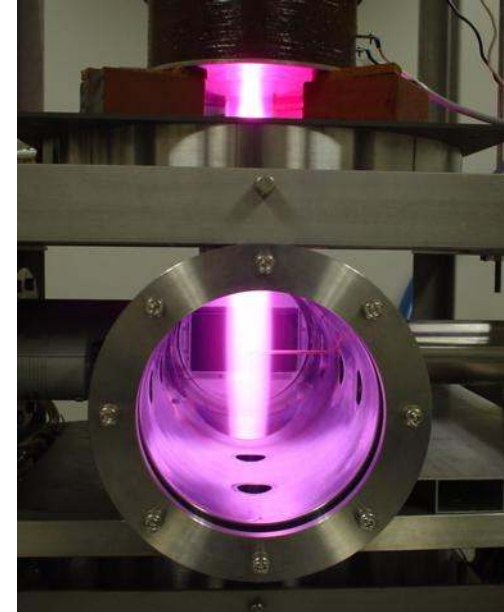
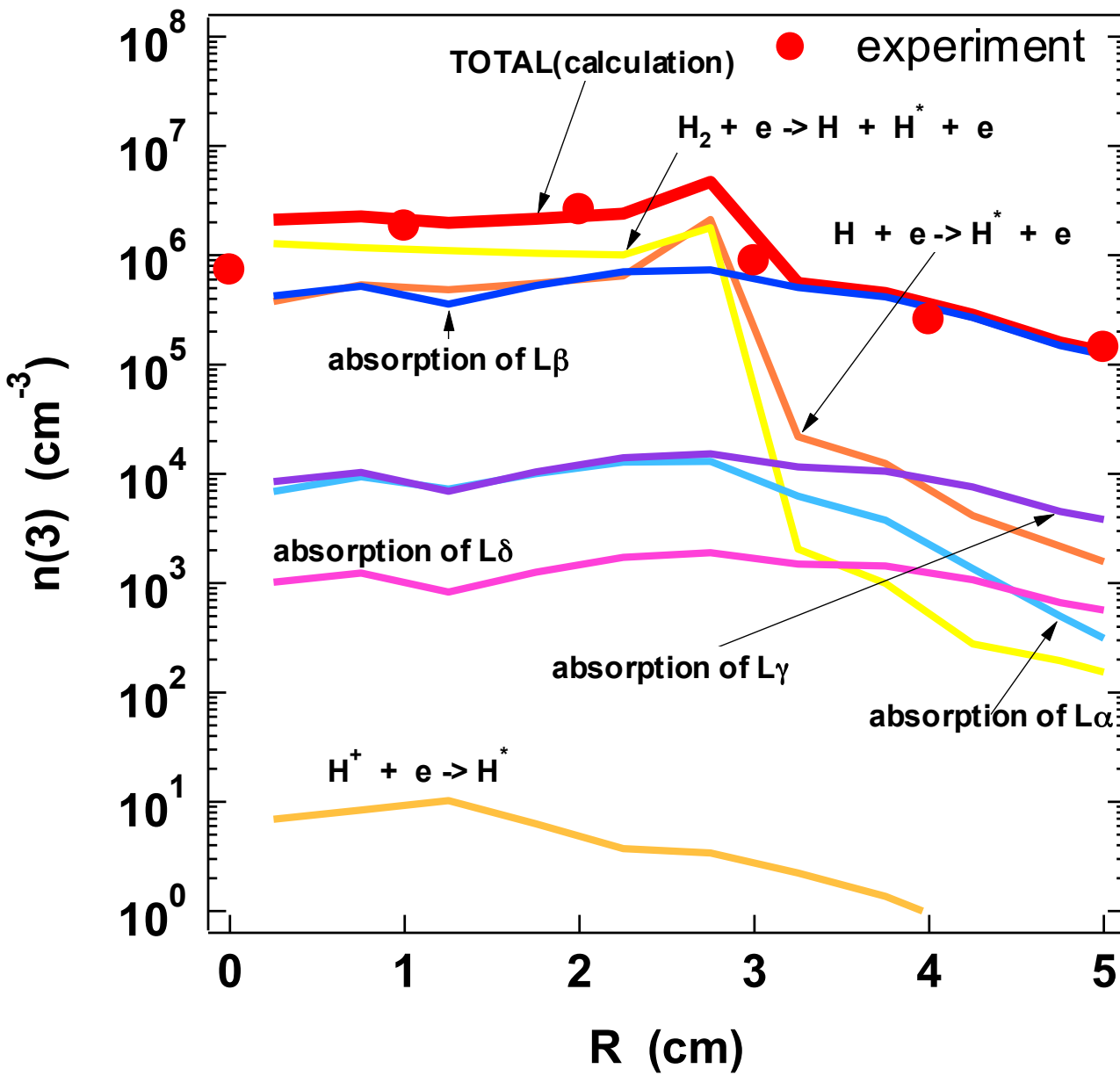


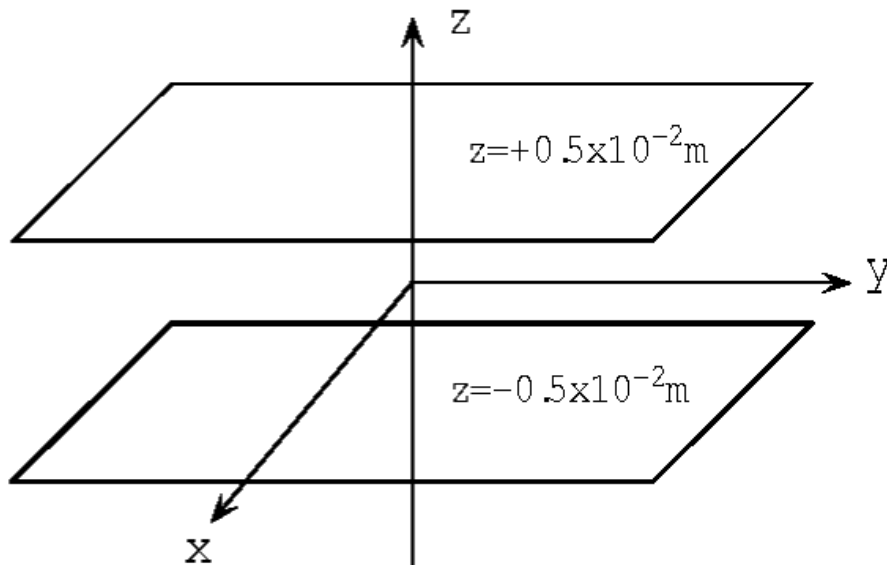
中性粒子輸送コード計算結果

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





$$T_e = 1 \text{ eV}$$

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

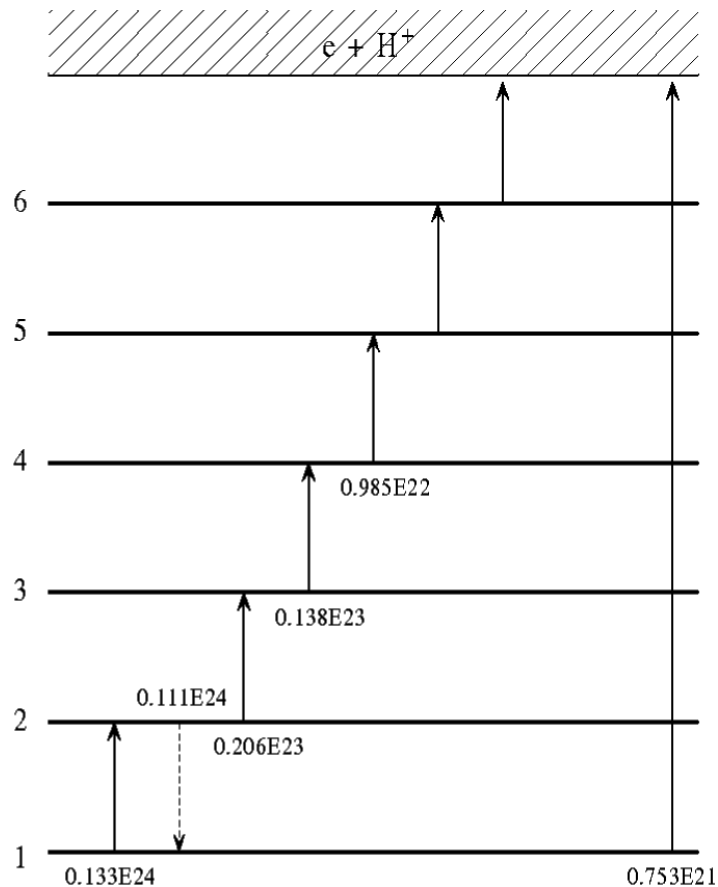
$$n(1) = 10^{20} \text{ m}^{-3}$$

$$T_H = 1 \text{ eV}$$

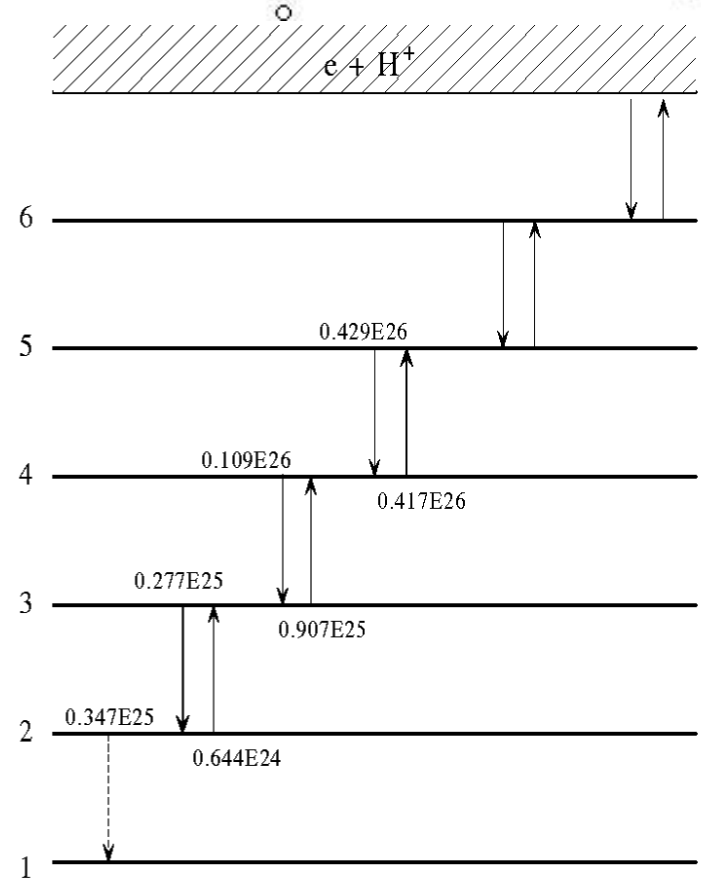
輻射輸送を考慮しない場合

$$S_{CR} = 2.5 \times 10^{-19}, \quad \alpha_{CR} = 4.6 \times 10^{-18} \quad \left[\frac{\text{m}^3}{\text{s}} \right] \quad \frac{dn(1)}{dt} = -S_{CR}n(1)n_e + \alpha_{CR}n_{H^+}n_e$$

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



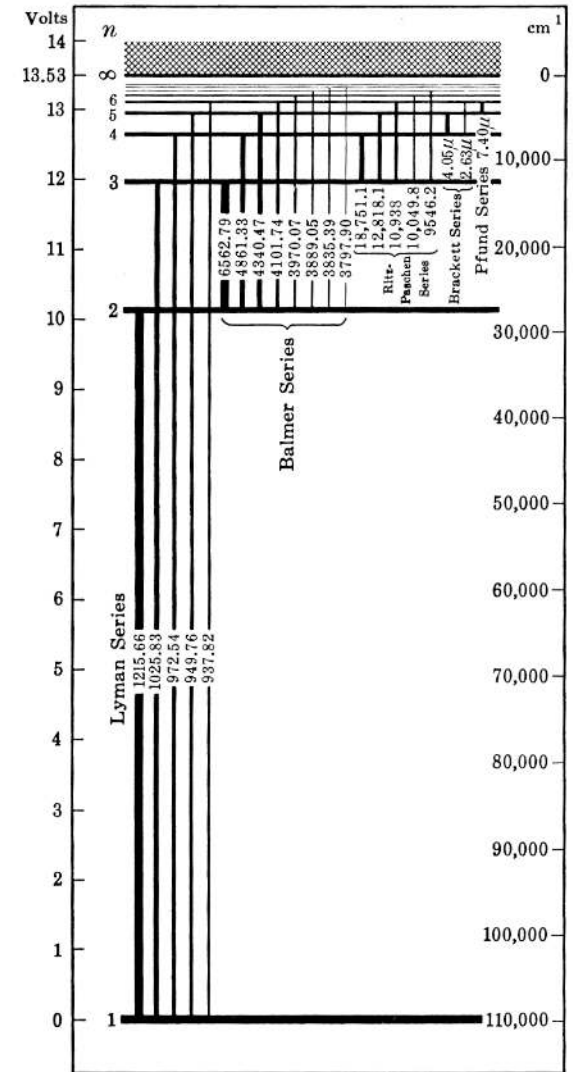
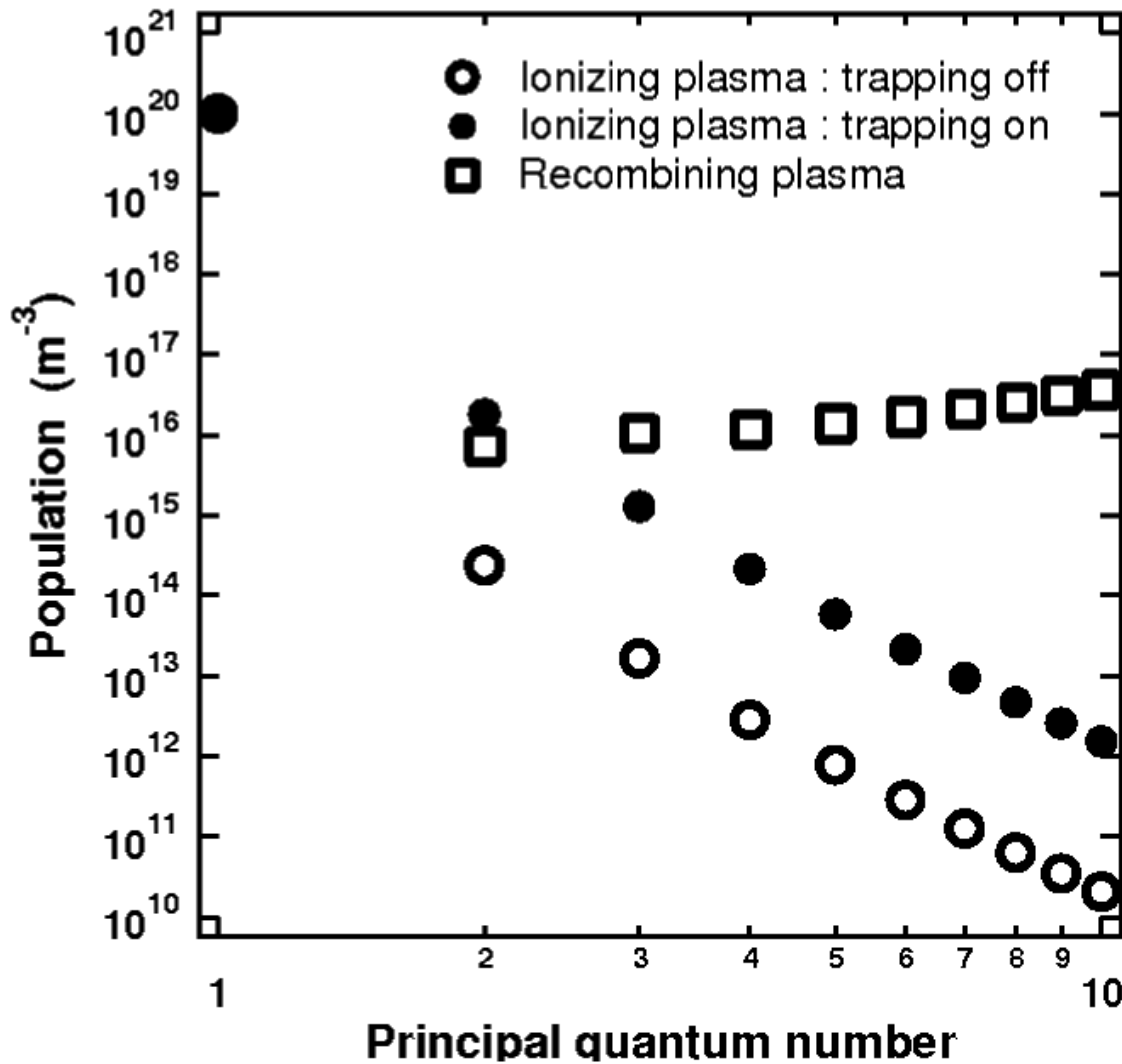
The excitation and de-excitation flow of ionizing plasma component. The figures denote the quantities of the fluxes. For example, $0.133\text{E}24$ denotes $0.133 \times 10^{24} [\text{m}^{-3}\text{s}^{-1}]$. The solid line denotes the transition by electron collision, and the broken line denotes the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



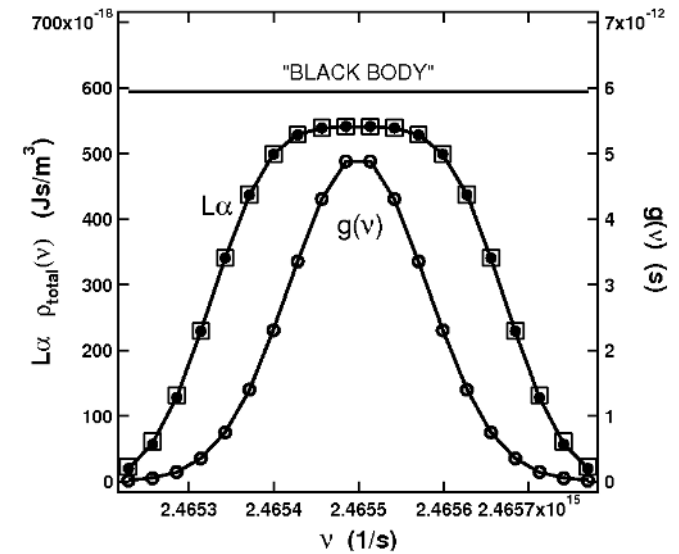
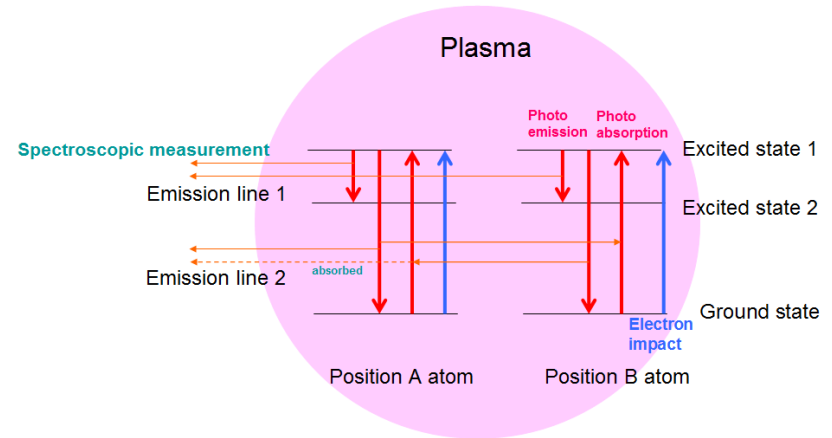
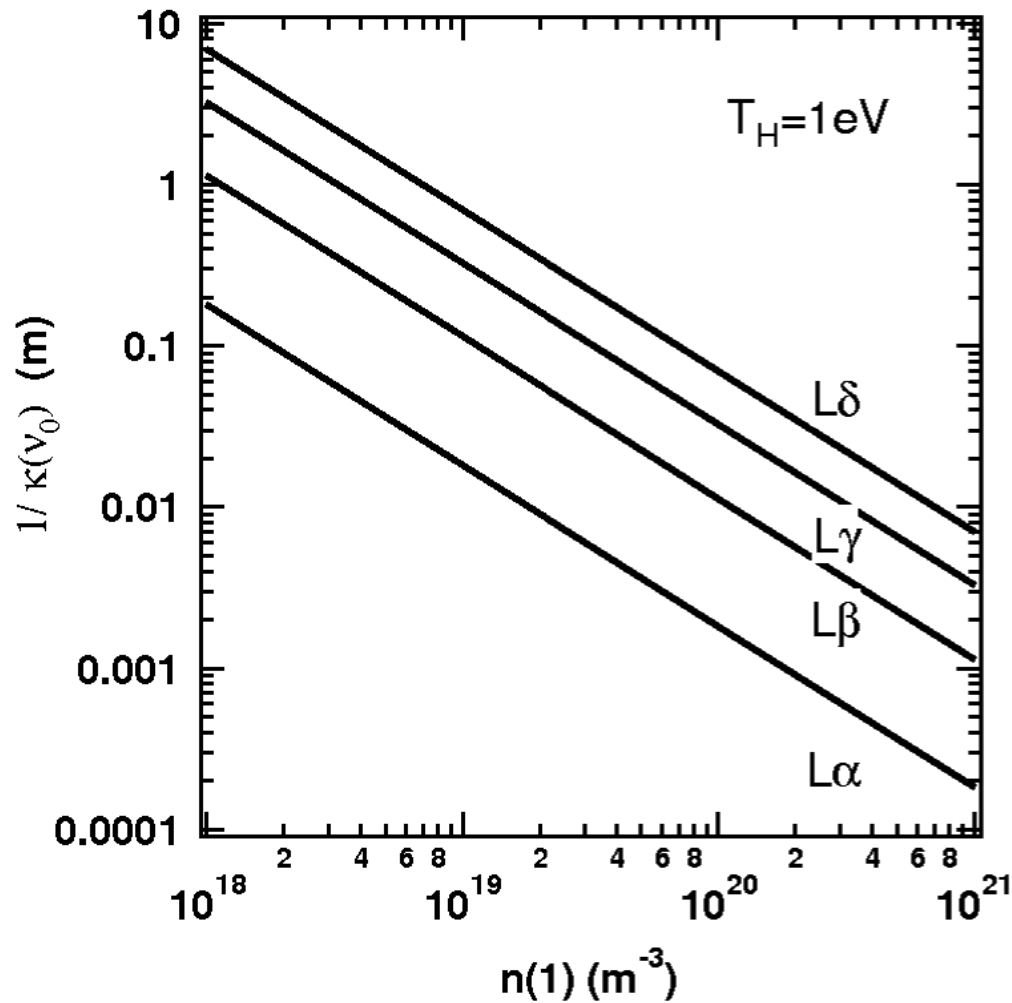
The excitation and de-excitation flow of recombining plasma component. The figures denote the quantities of the fluxes. For example, $0.347\text{E}25$ denotes $0.347 \times 10^{25} [\text{m}^{-3}\text{s}^{-1}]$. The solid line denotes the transition by electron collision, and the broken line denotes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

ポピュレーション

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



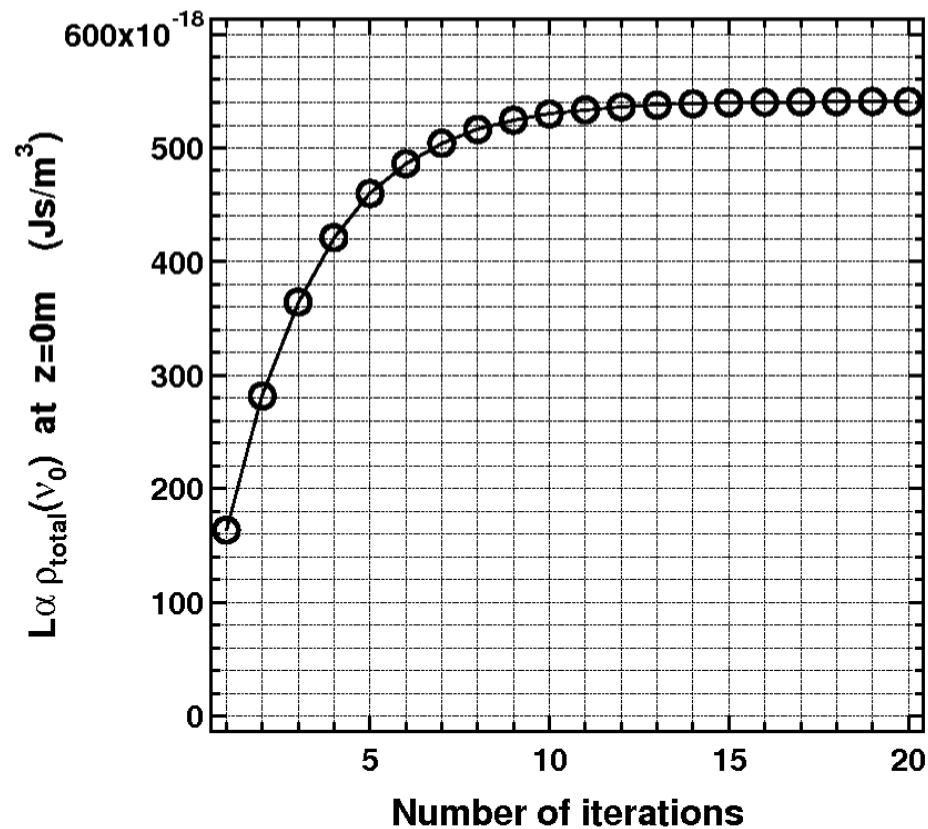
光の減衰長



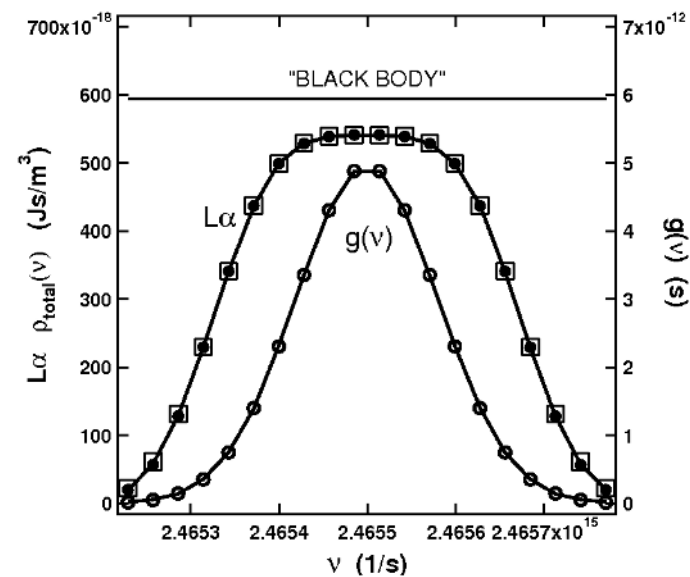
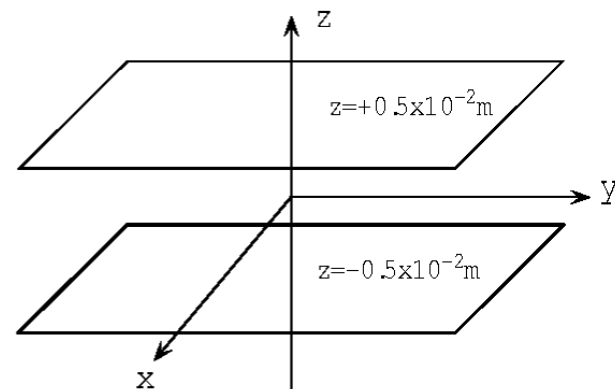
$L\alpha$ spectrum at the center $z = 0\text{m}$ of the slab which is achieved after convergence. The closed circles and the open squares denote results for $R_{\text{LIMIT}} = 4.0 \times 10^{-2}\text{m}$ and $R_{\text{LIMIT}} = 8.0 \times 10^{-2}\text{m}$, respectively. The emission line profile of 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 $z = 0\text{m}$.

輻射輸送の計算

収束の様子



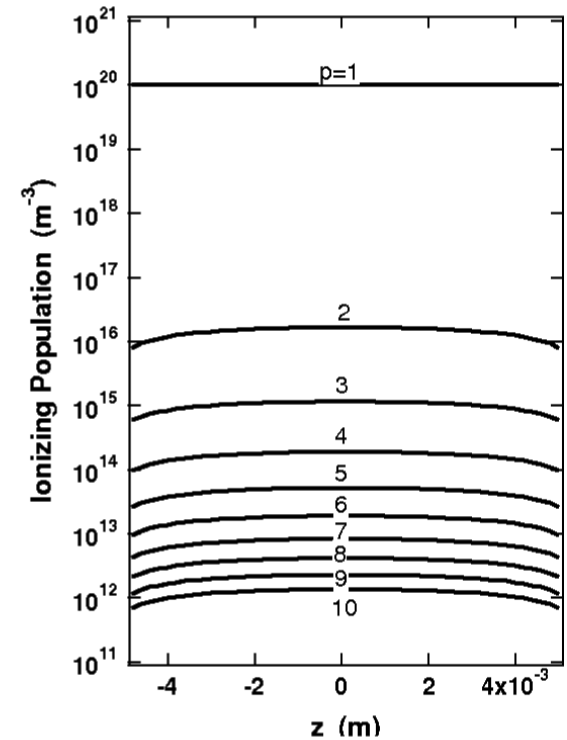
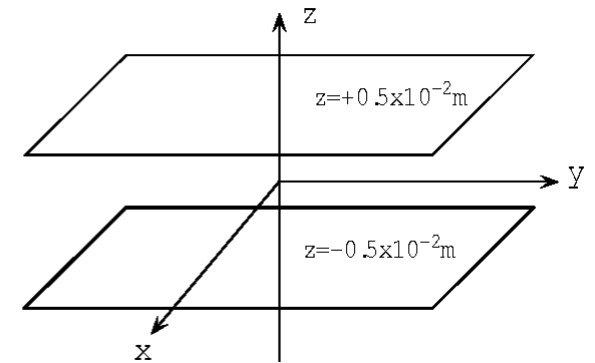
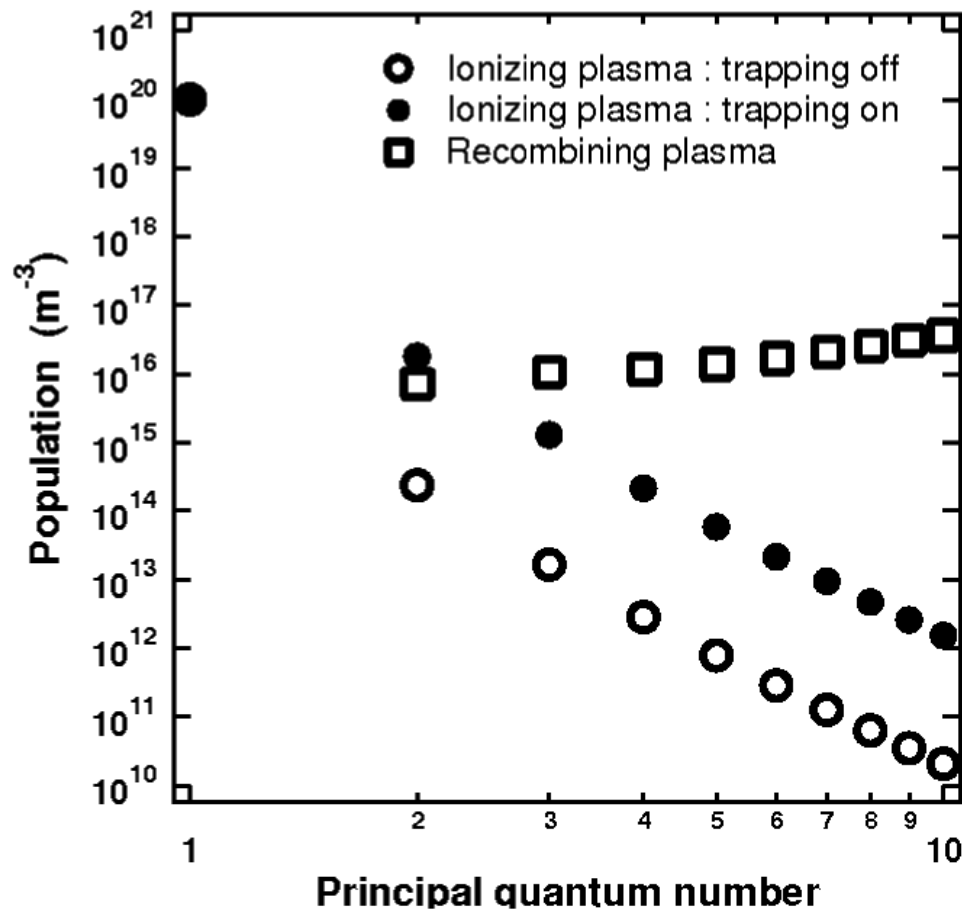
The $\rho_{\text{total}}(v_0)$ of L_α at the center $z = 0\text{m}$ of the slab is shown as a function of the number of iterations.



L_α spectrum at the center $z = 0\text{m}$ of the slab which is achieved after convergence. The closed circles and the open squares denote results for $R_{\text{LIMIT}} = 4.0 \times 10^{-2}\text{m}$ and $R_{\text{LIMIT}} = 8.0 \times 10^{-2}\text{m}$, respectively. The emission line profile of the Doppler broadening $g(v)$ 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 $z = 0\text{m}$.

輻射輸送の計算

収束の様子

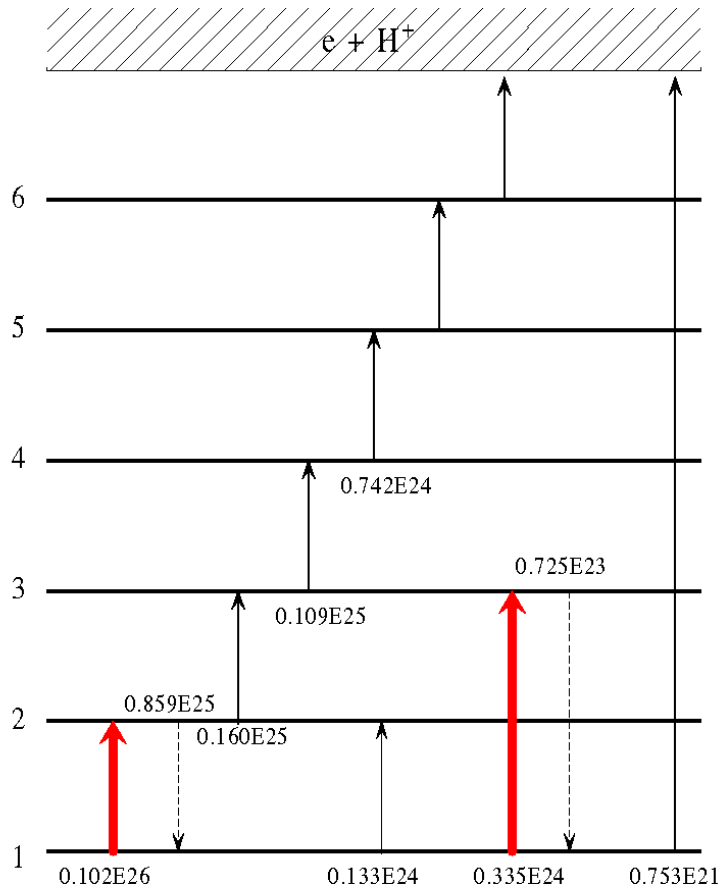


Population densities of the excited levels of the ionizing plasma.
 $n(1)$ is $10^{20} [\text{m}^{-3}]$.

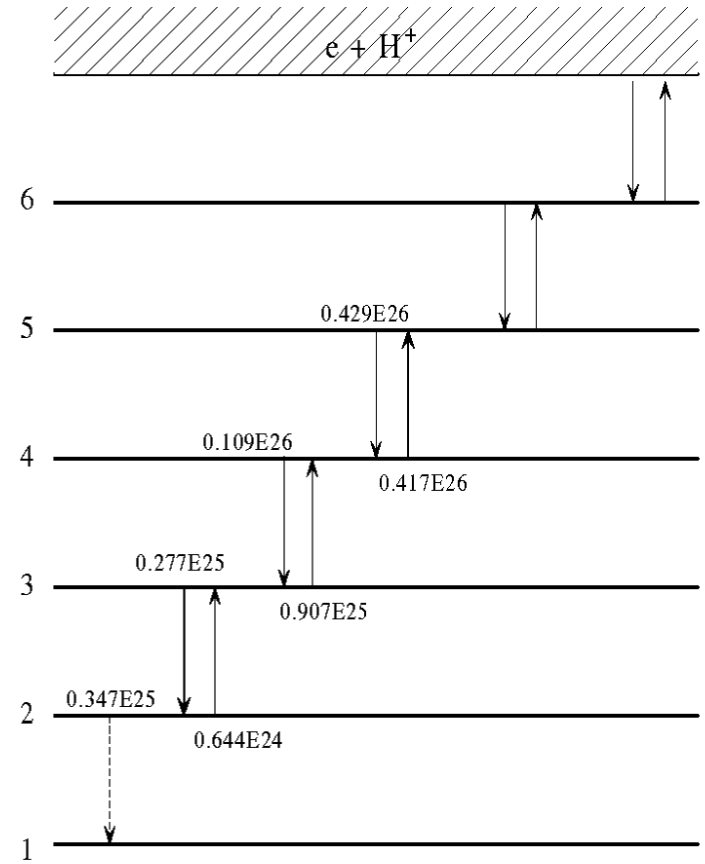
輻射輸送を考慮した場合

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

$$\begin{aligned} \frac{dn(1)}{dt} &= -S_{CR}n(1)n_e + \alpha_{CR}n_H n_e \\ &= -1.9 \times 10^{24} + 4.6 \times 10^{24} \quad \left[\frac{1}{\text{m}^3 \text{s}} \right] \end{aligned}$$

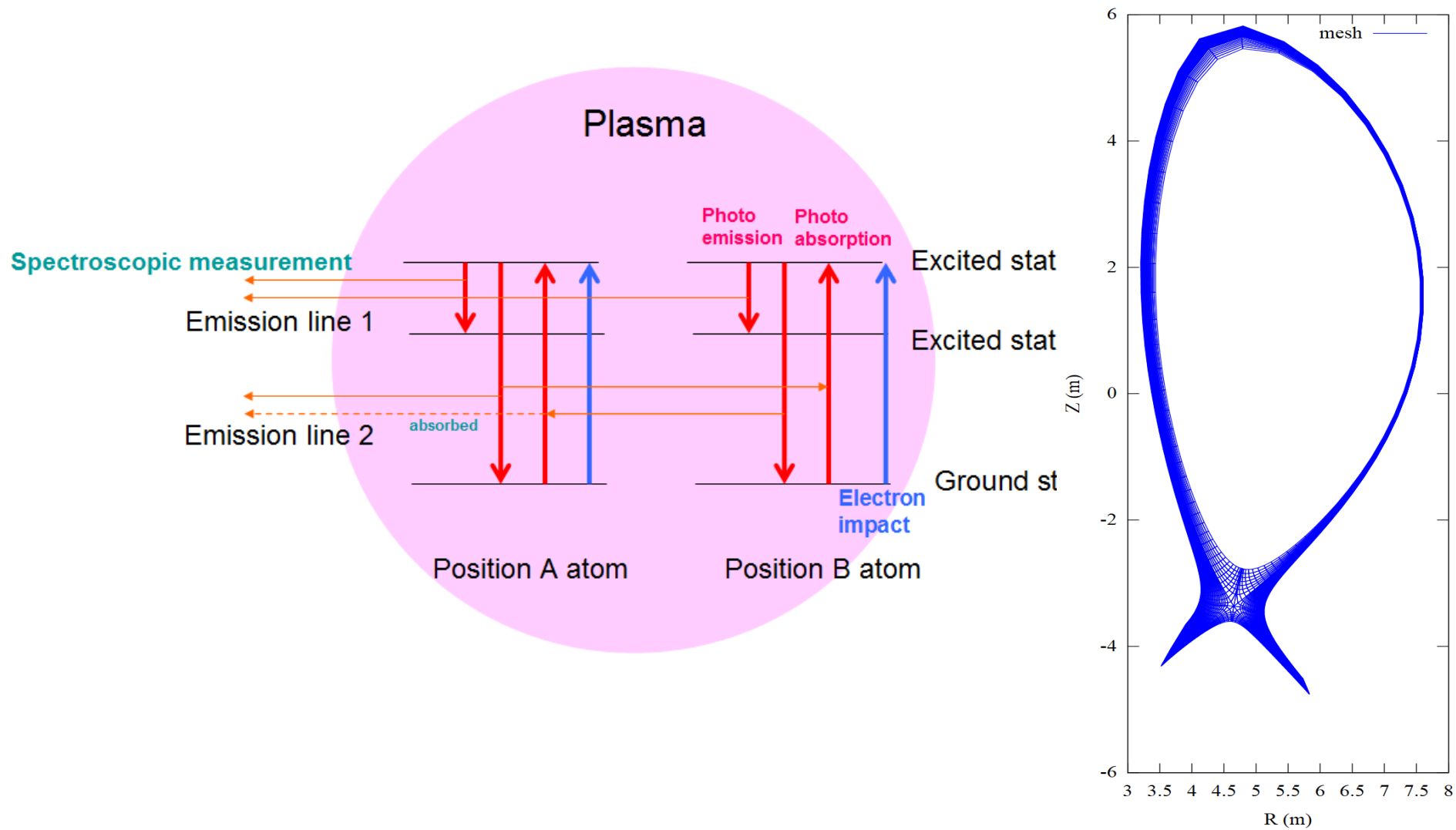


The excitation and de-excitation flow ionizing plasma component at the center $z = 0\text{m}$ of the slab. The thick solid line (red) denotes the absorption of photon. The thin solid line denotes the transition by electron collision, and the broken line denotes the spontaneous radiative transition.



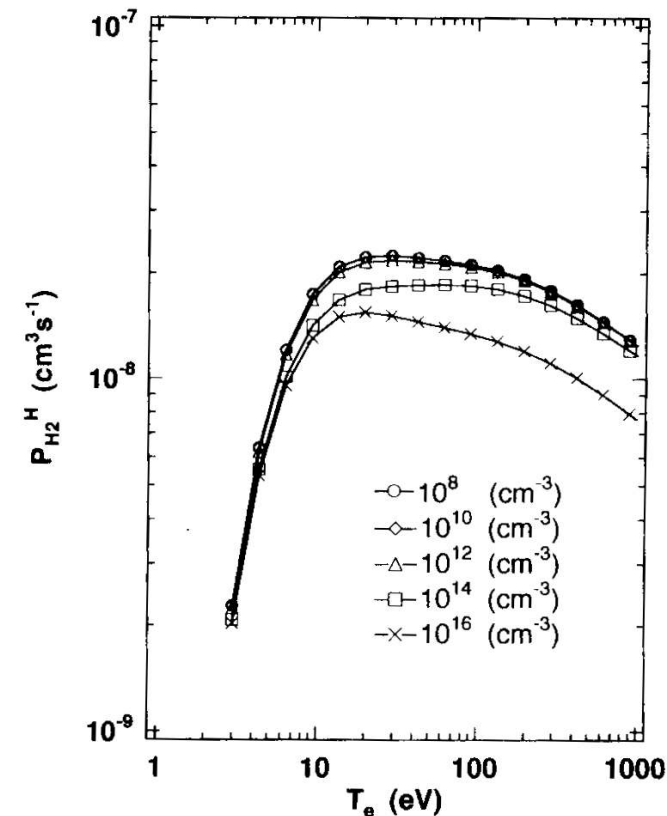
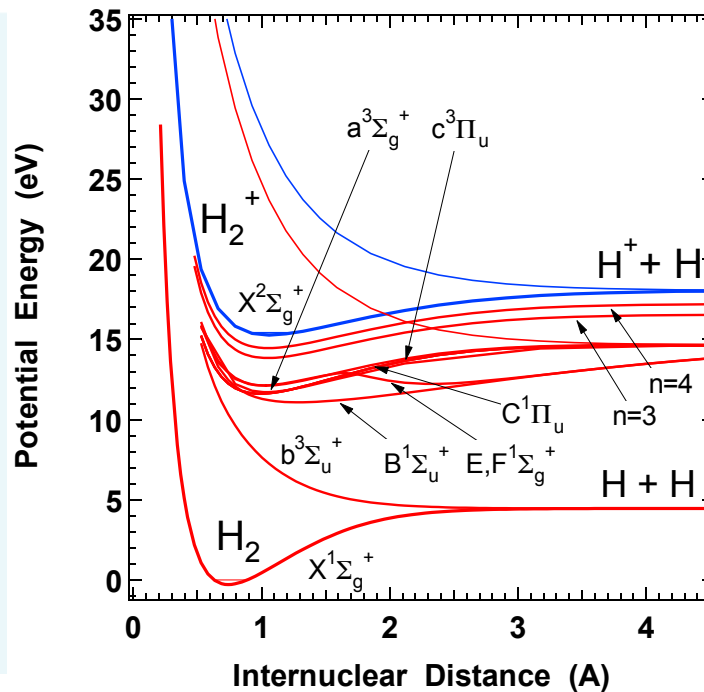
The excitation and de-excitation flow of recombining plasma component. The figures denote the quantities of the fluxes. For example, $0.347\text{E}25$ denotes $0.347 \times 10^{25} [\text{m}^{-3}\text{s}^{-1}]$. The solid line denotes the transition by electron collision, and the broken line denotes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

原型炉SlimCSでの輻射輸送の計算



H₂ 衝突輻射モデル

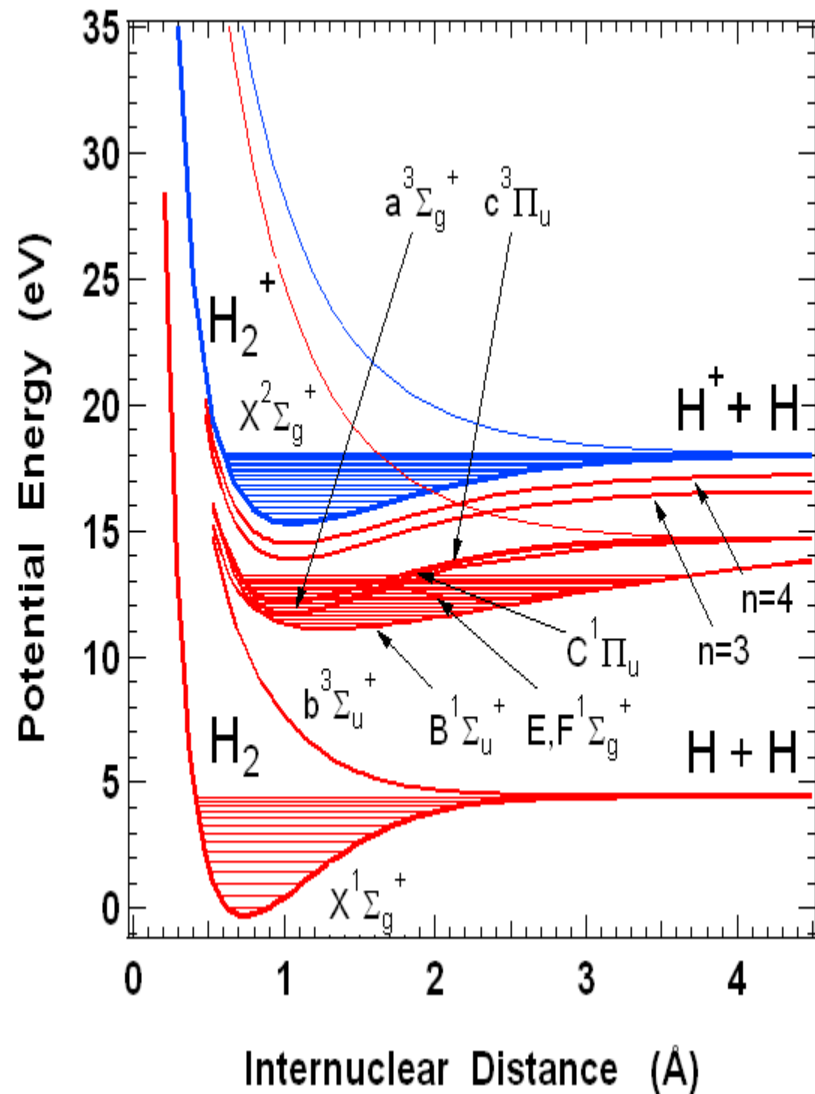
Calculation of effective reaction rate coefficients



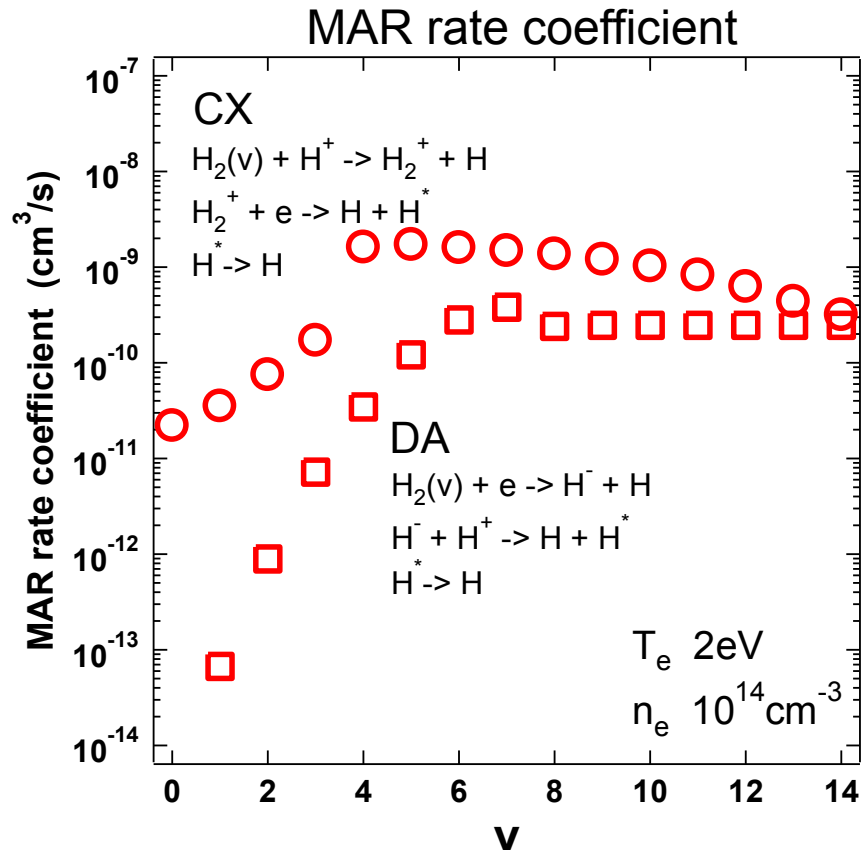
Hydrogen-atom spectroscopy of the ionizing plasma containing molecular hydrogen: line intensities and ionization rate; J. Appl. Phys. 73, 8122–8125, 1993.

Effective ionization and dissociation rate coefficients of molecular hydrogen in plasma; J. Appl. Phys. 78, 2913–2924, 1995.

H₂ Collisional-Radiative Model (ver.2)

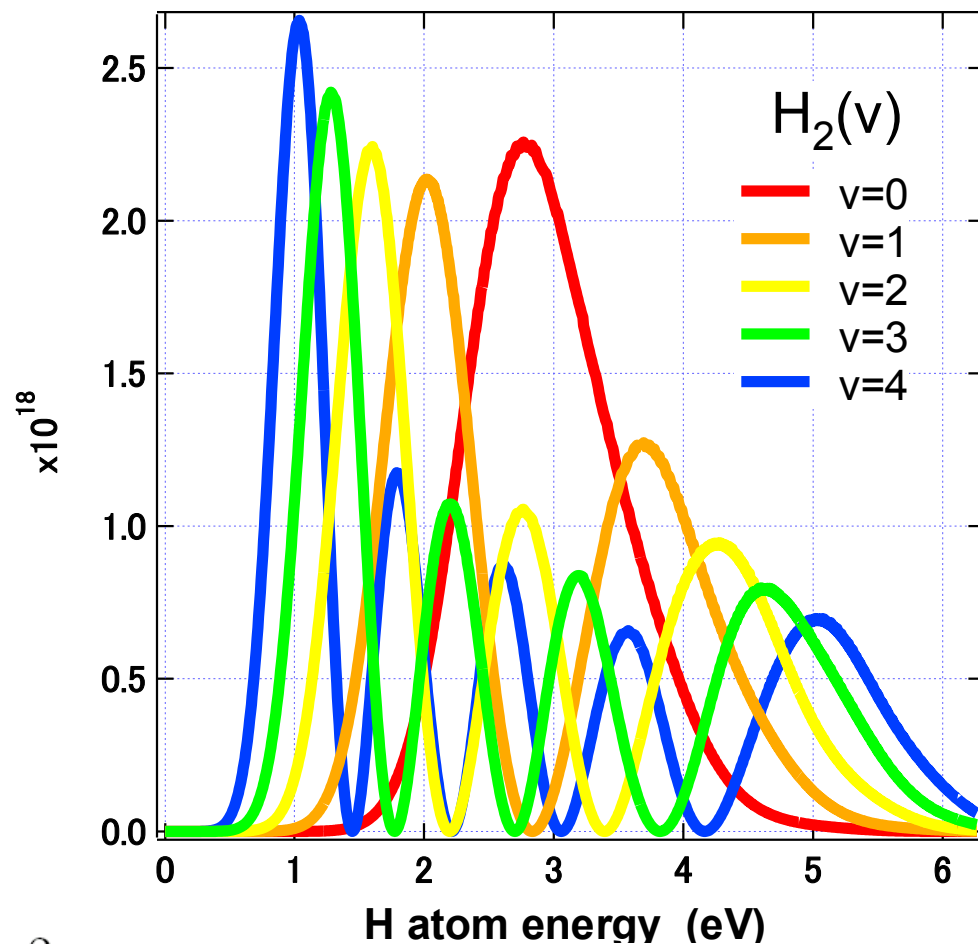
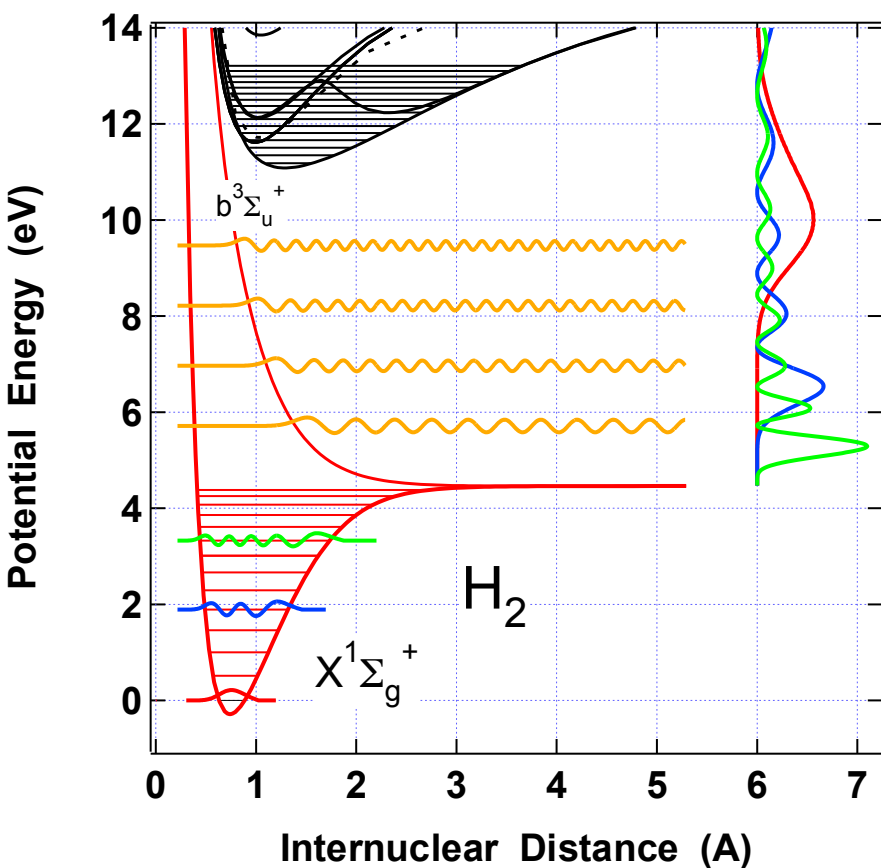


Vibrational levels for $n \leq 2$ electronic state are considered.



✧ 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.

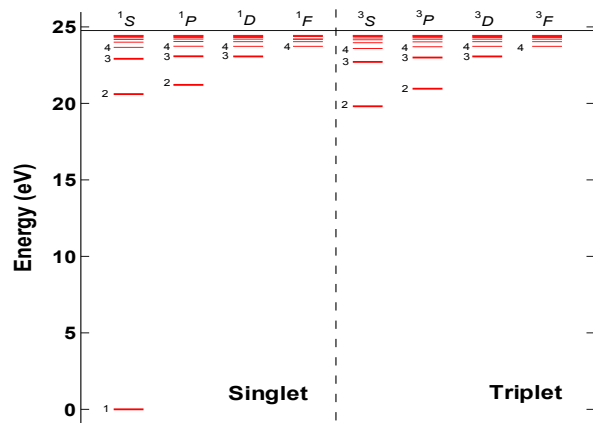
速度分布の計算例 $\text{H}_2(\text{X}) \rightarrow \text{H}_2(\text{b}) \rightarrow \text{H} + \text{H}$



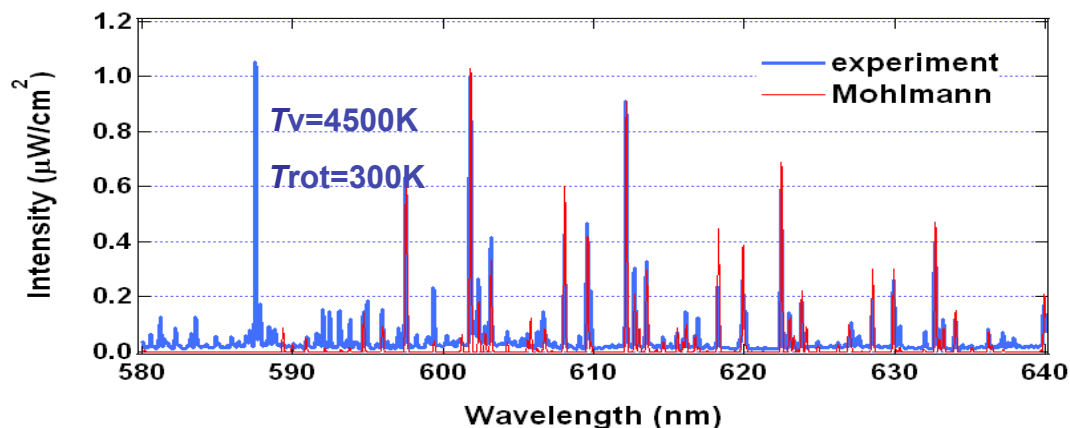
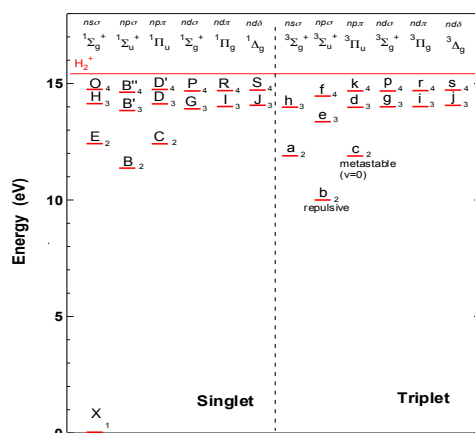
$$q_{\kappa v} = \left| \int \chi_{\kappa}^b(R) \chi_v^X(R) dR \right|^2$$

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

He atom



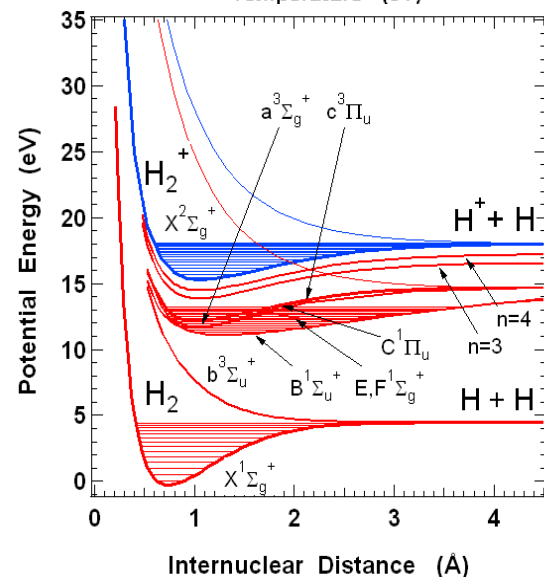
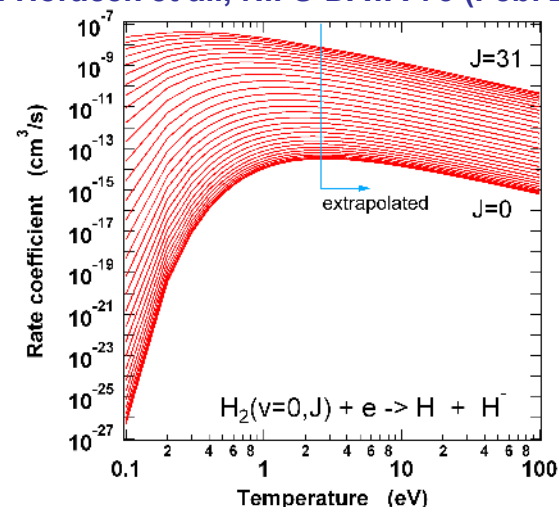
H₂



Determination of n_e , T_e , T_v , T_{rot} from observed spectra

$T_v, T_{rot} \rightarrow$ Population $X^1\Sigma_g^+(v, J)$

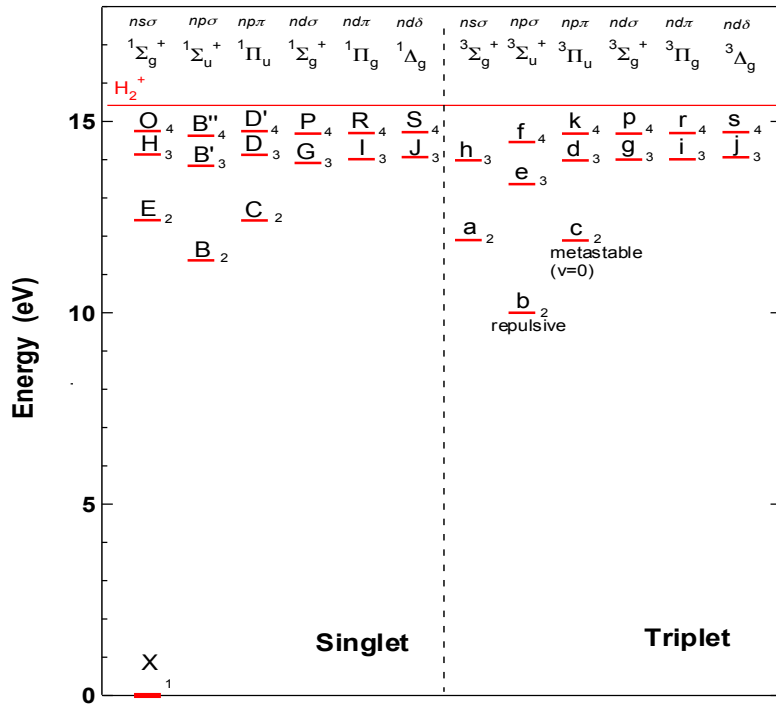
J. Horacek et al., NIFS-DATA-73 (Feb. 2003)



Calculation of effective reaction rate coefficients

H₂ 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

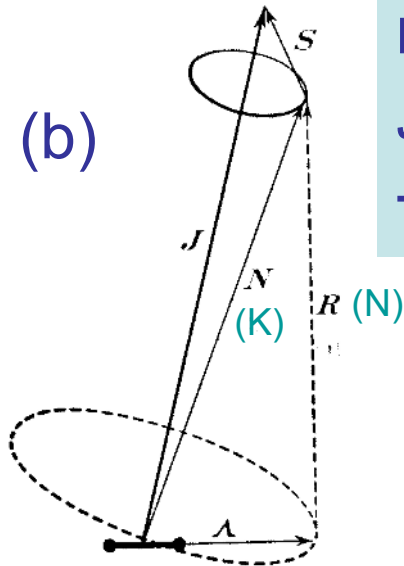
The Hydrogen Molecule Wavelength Tables of GERHARD HEINRICH DIEKE,

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

H₂ CR model.



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

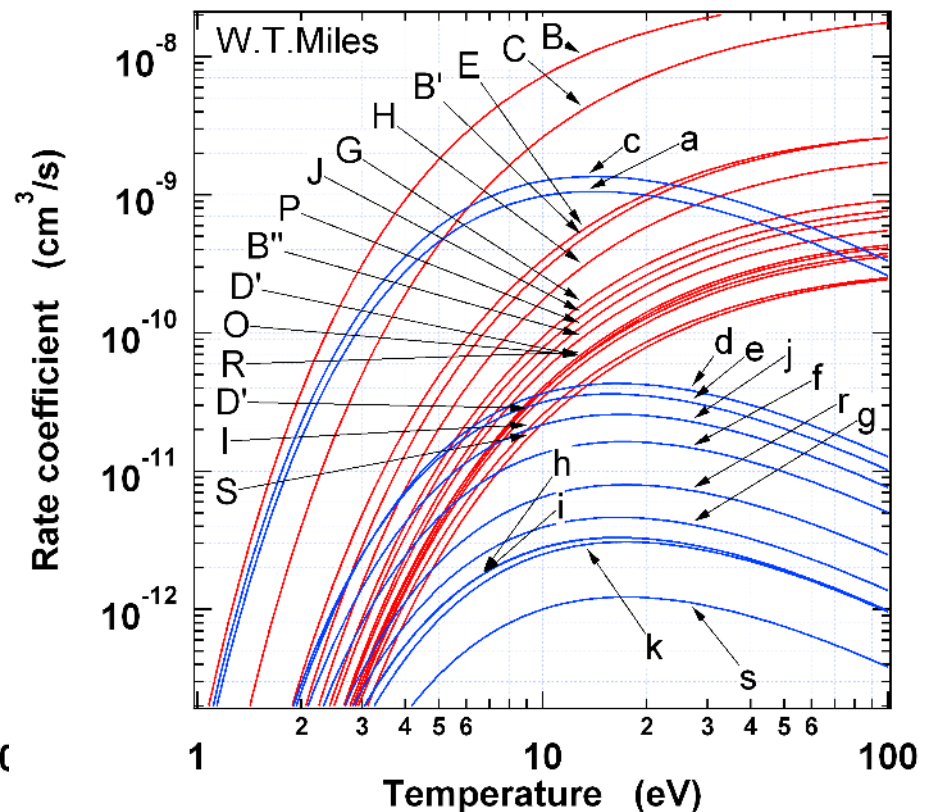
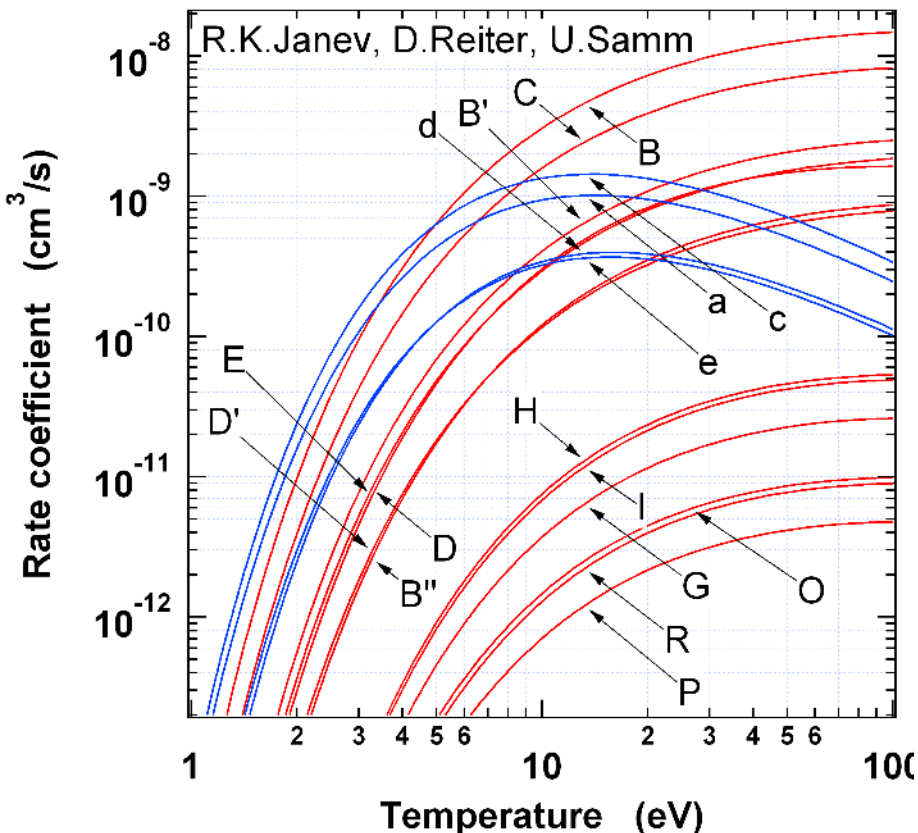
Collision Processes in Low-Temperature
Hydrogen Plasmas,

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

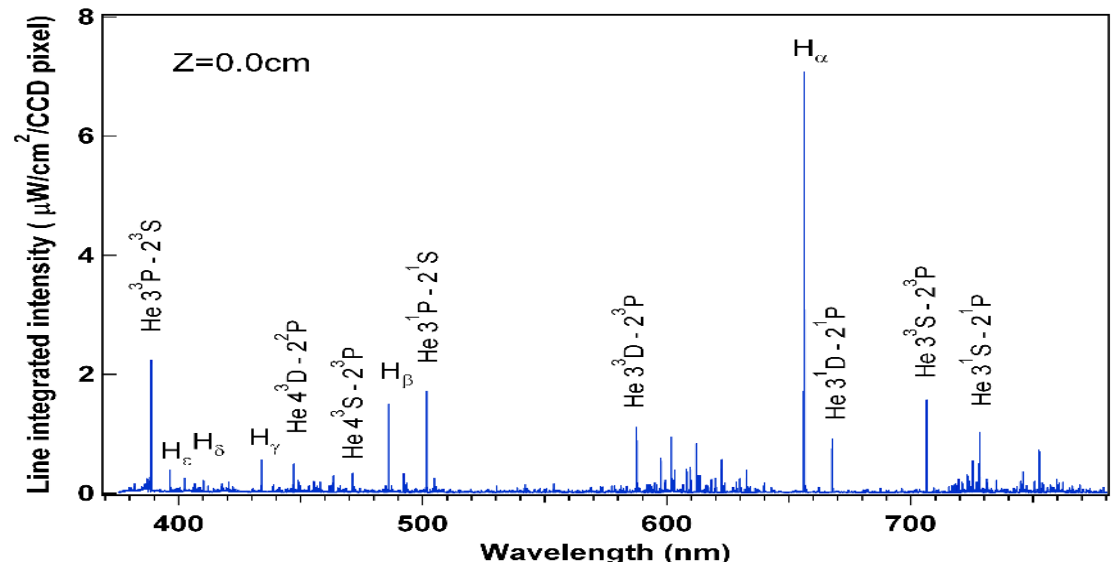
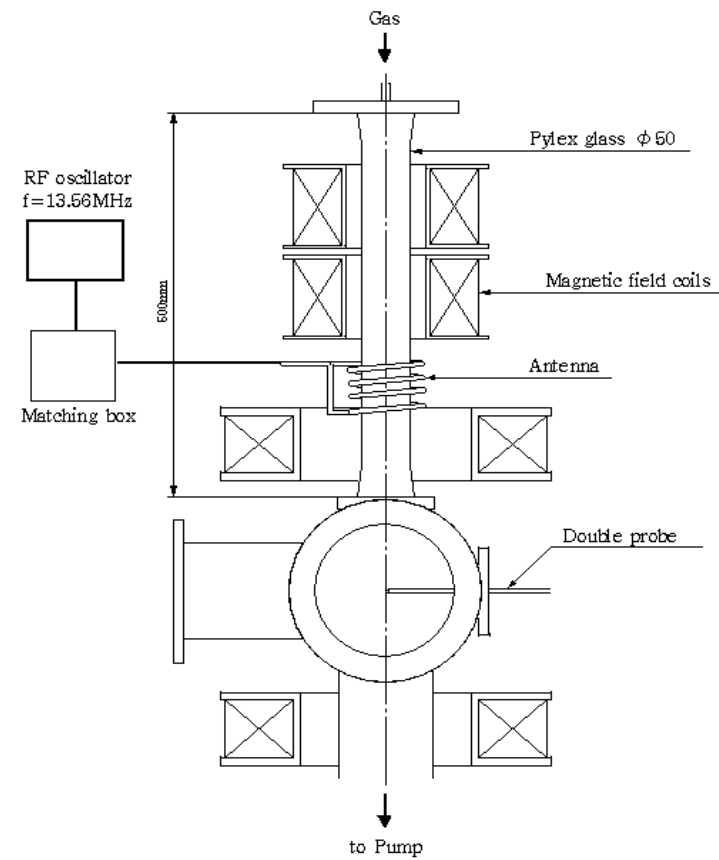
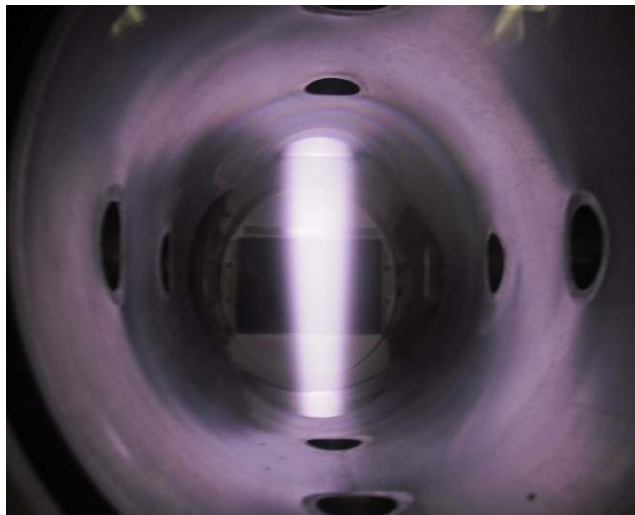
W.T. Miles, R. Thompson, and A.E.S. Green,
J. Appl. Phys. 43, 678 (1972).

Born-Bethe approximation modified at low
energies by phenomenological techniques

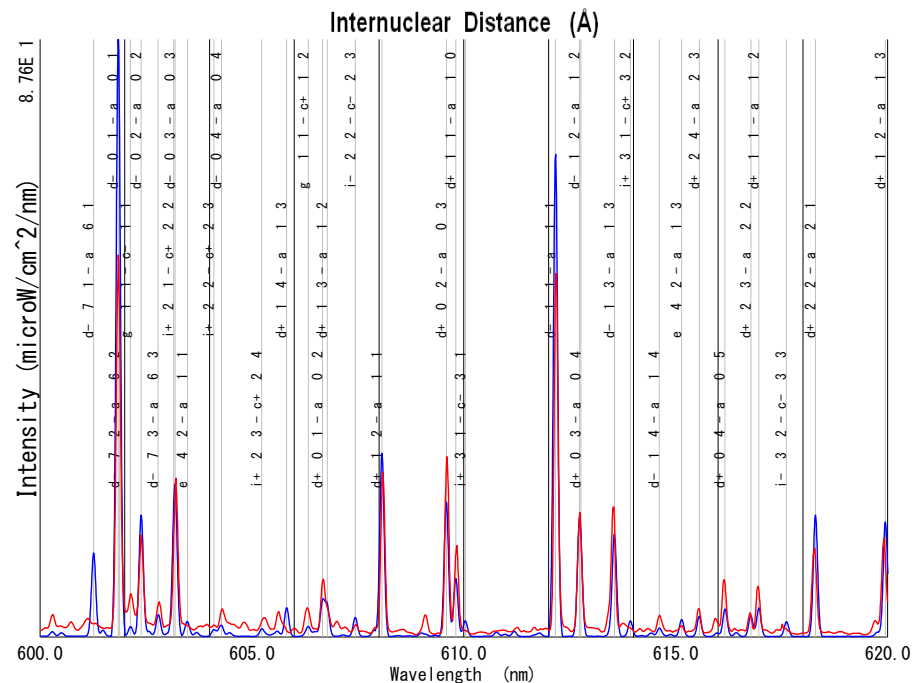
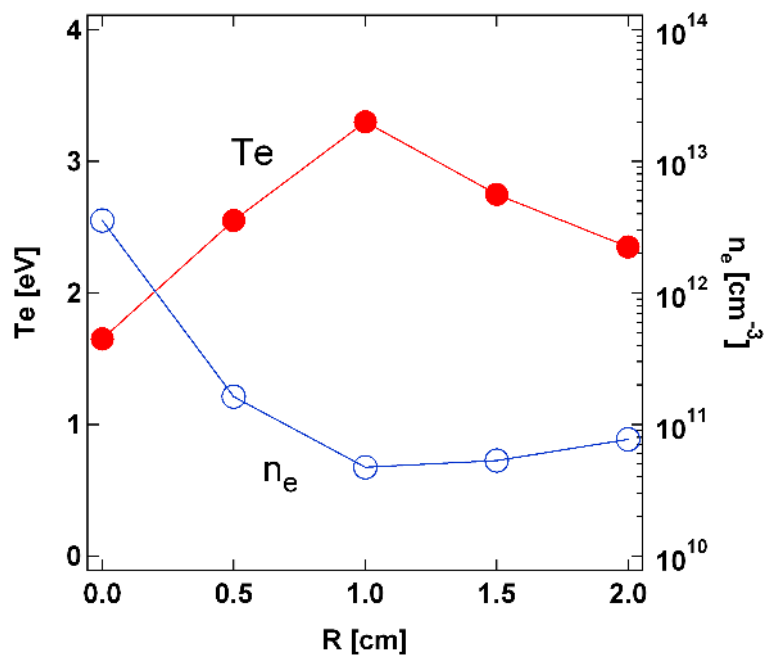
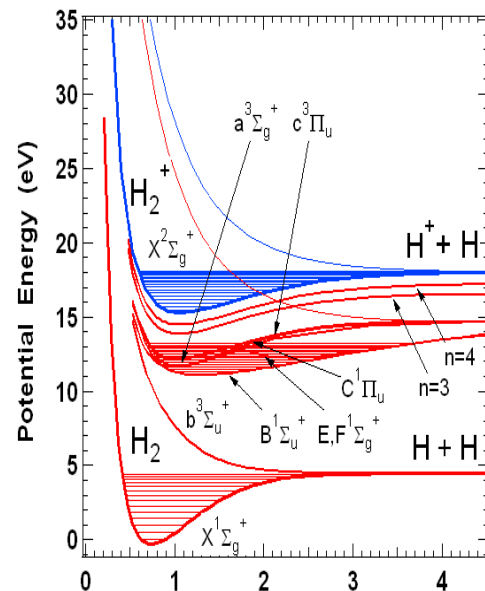
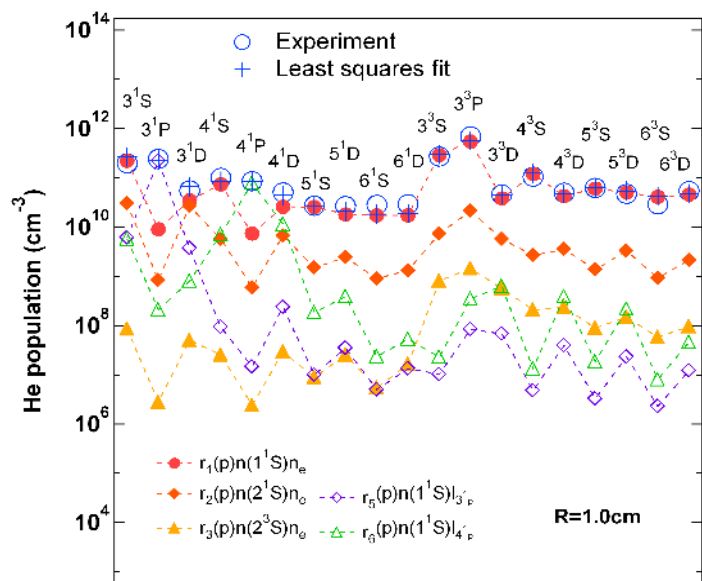
All cross sections are given for $n \leq 4$.



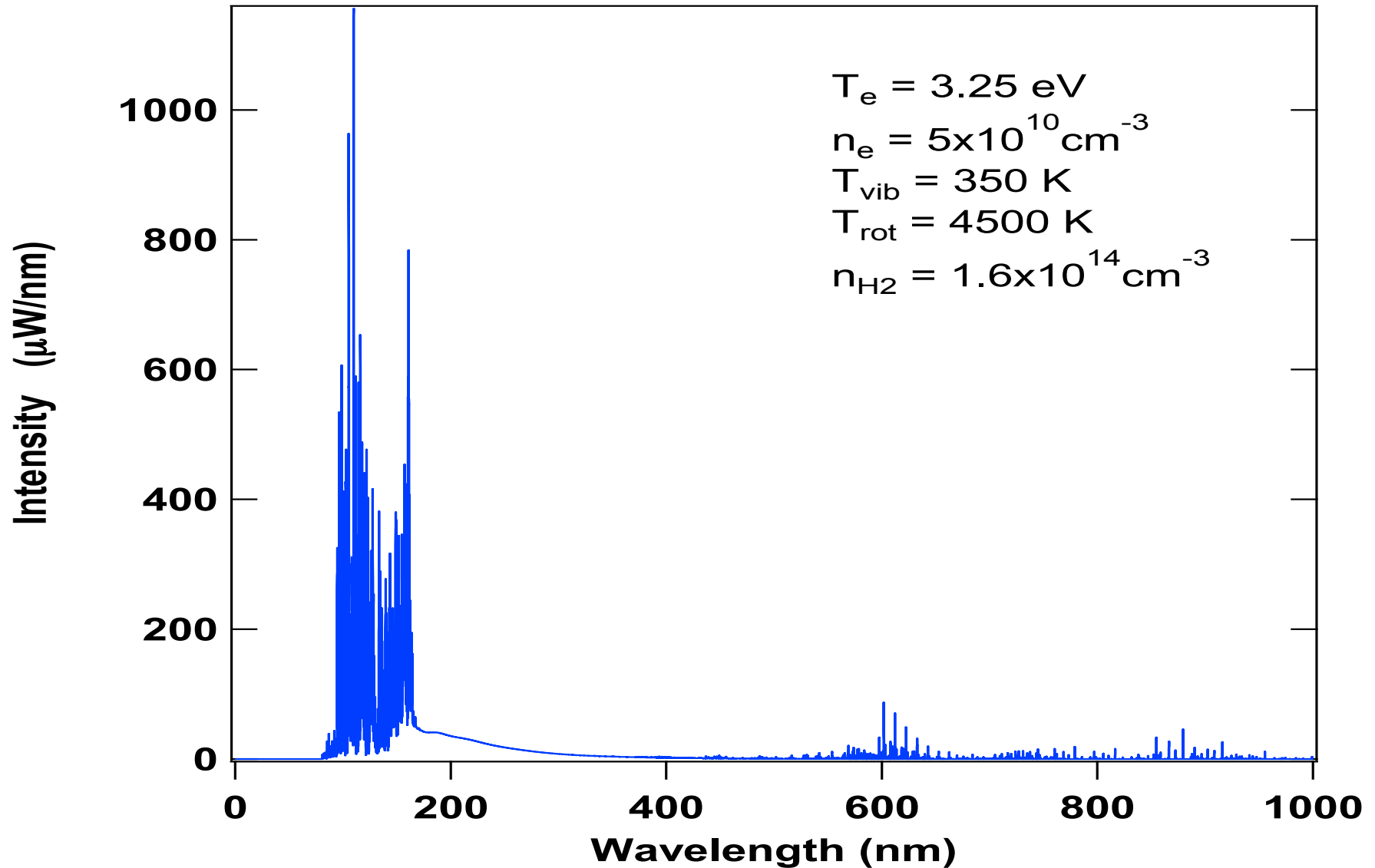
RF plasma



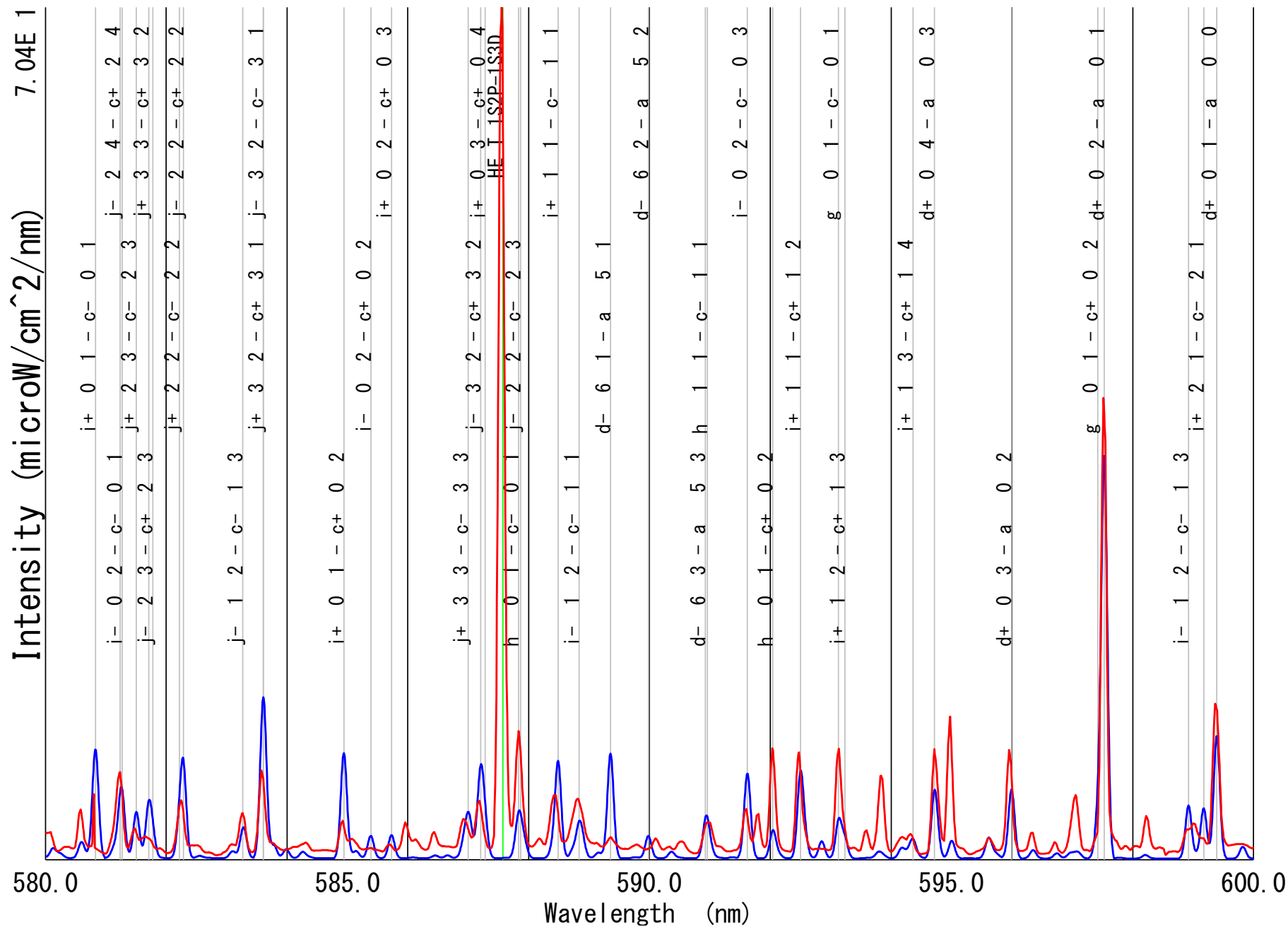
Determination of n_e , T_e , T_v , T_{rot} from observed spectra



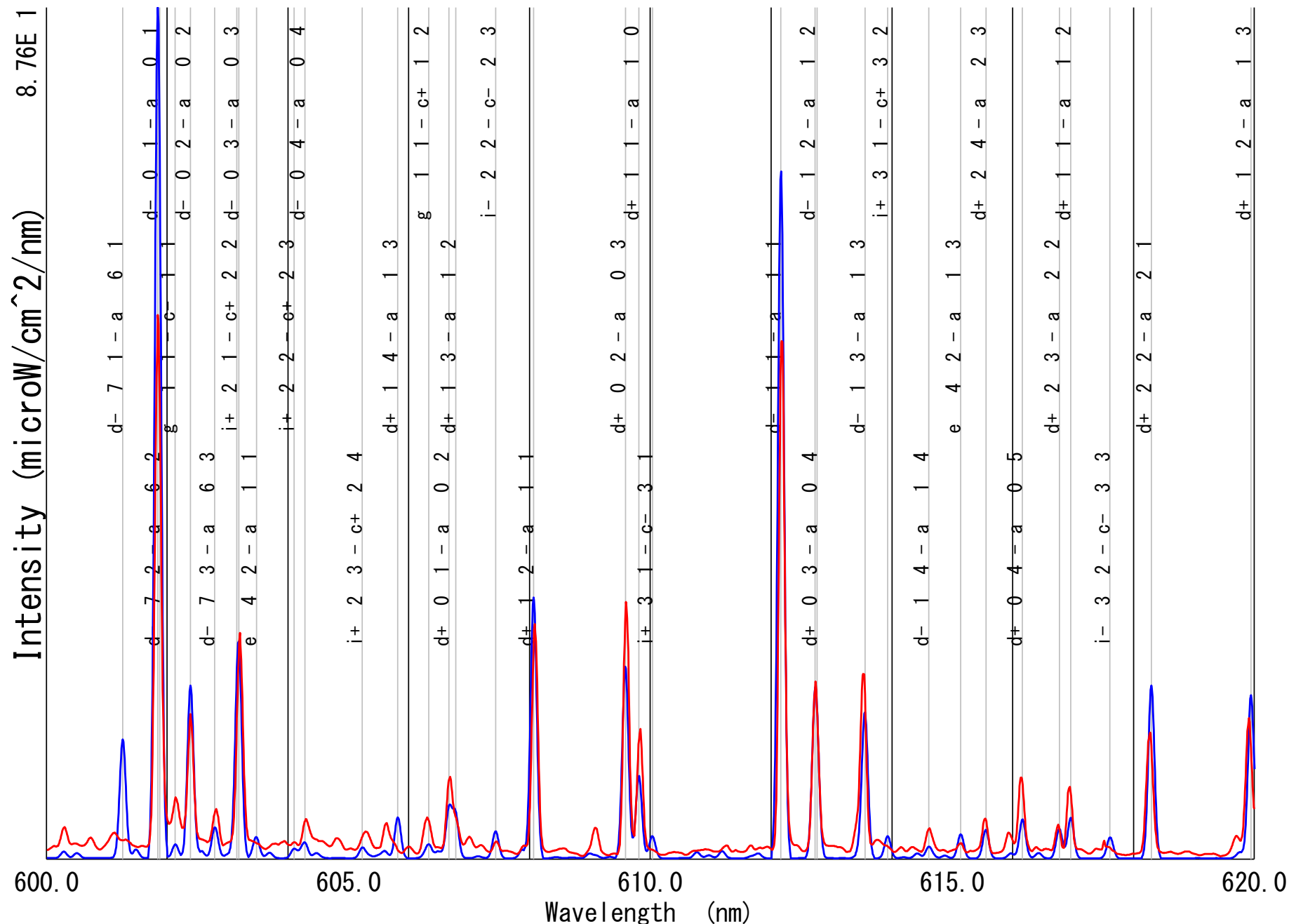
H₂ CR model calculation : H₂ spectra



blue (calc.)



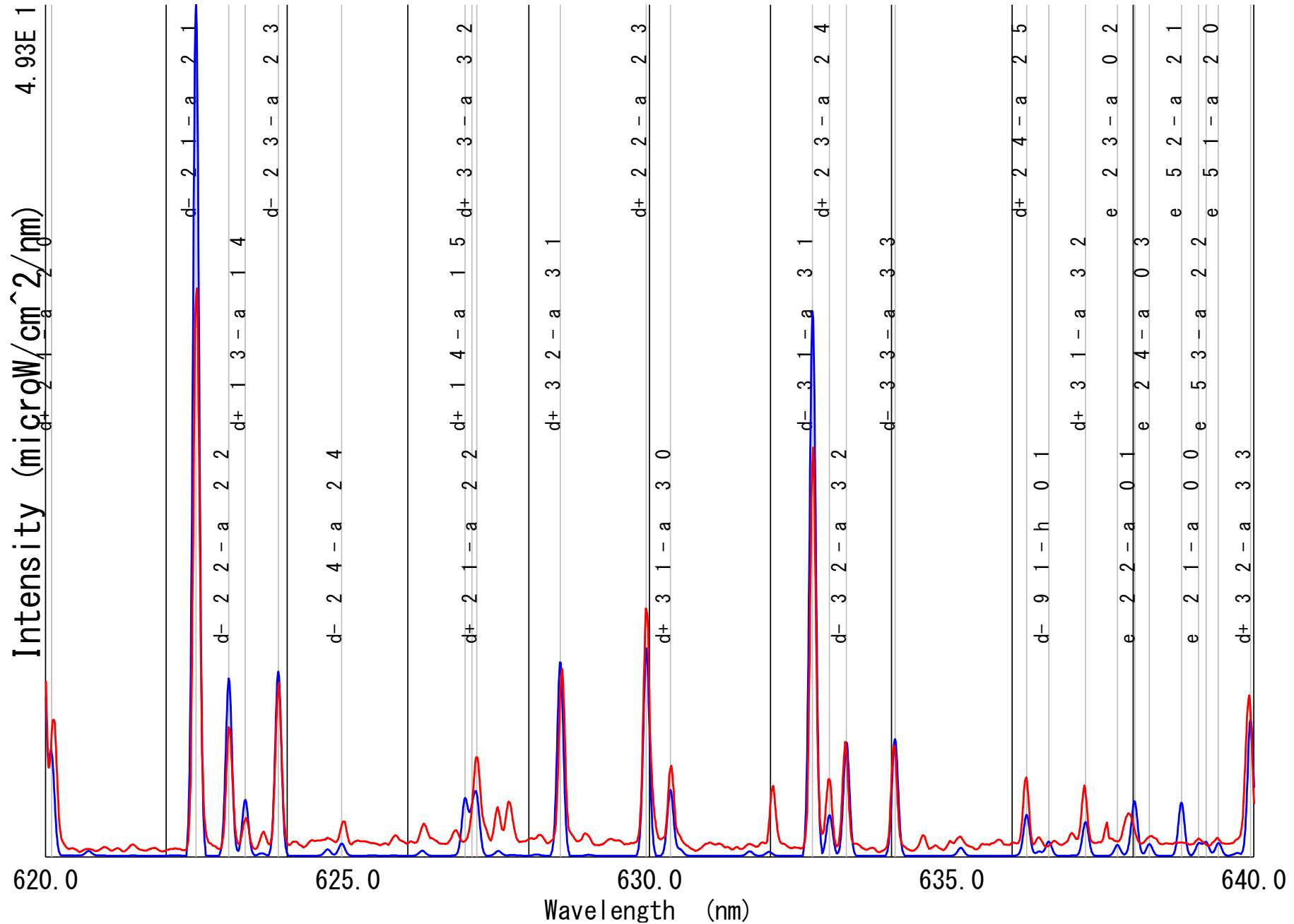
blue (calc.)



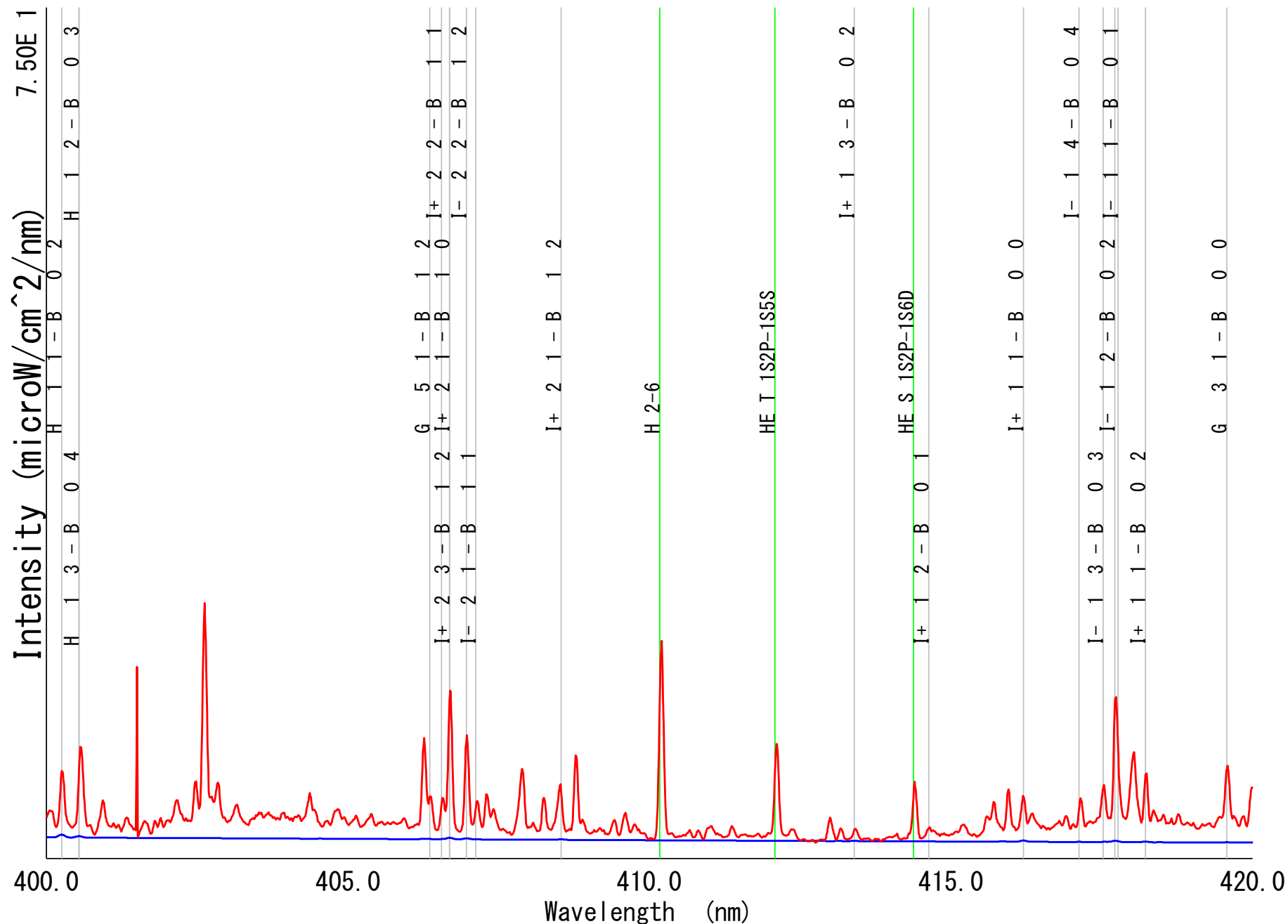
620-640 nm

red (exp.)

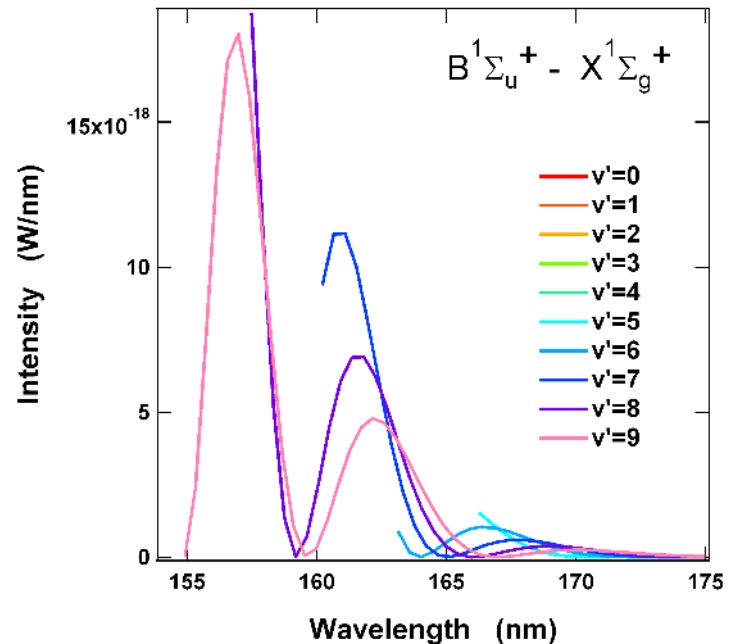
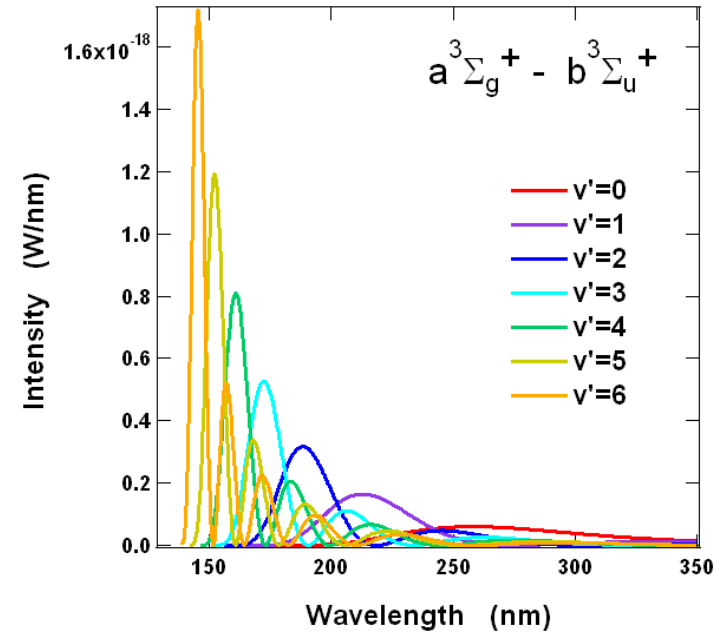
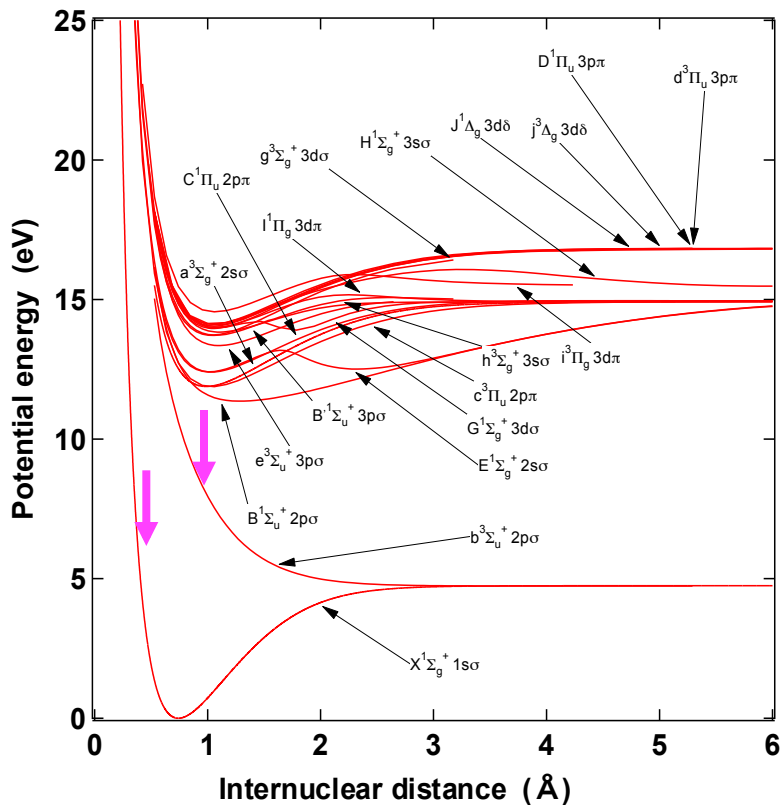
blue (calc.)



blue (calc.)



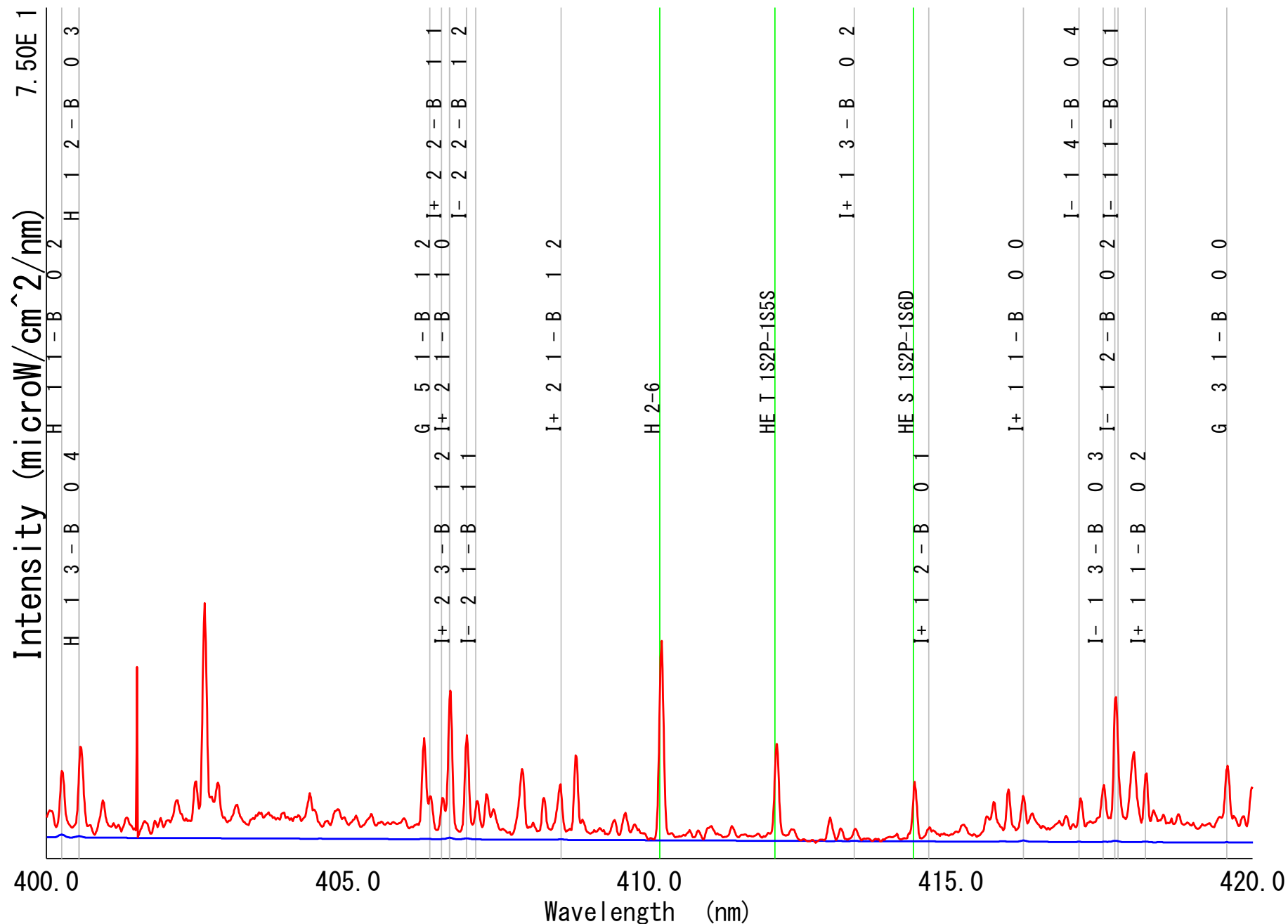
H₂ Transition Probability to Continuum states



400-420 nm

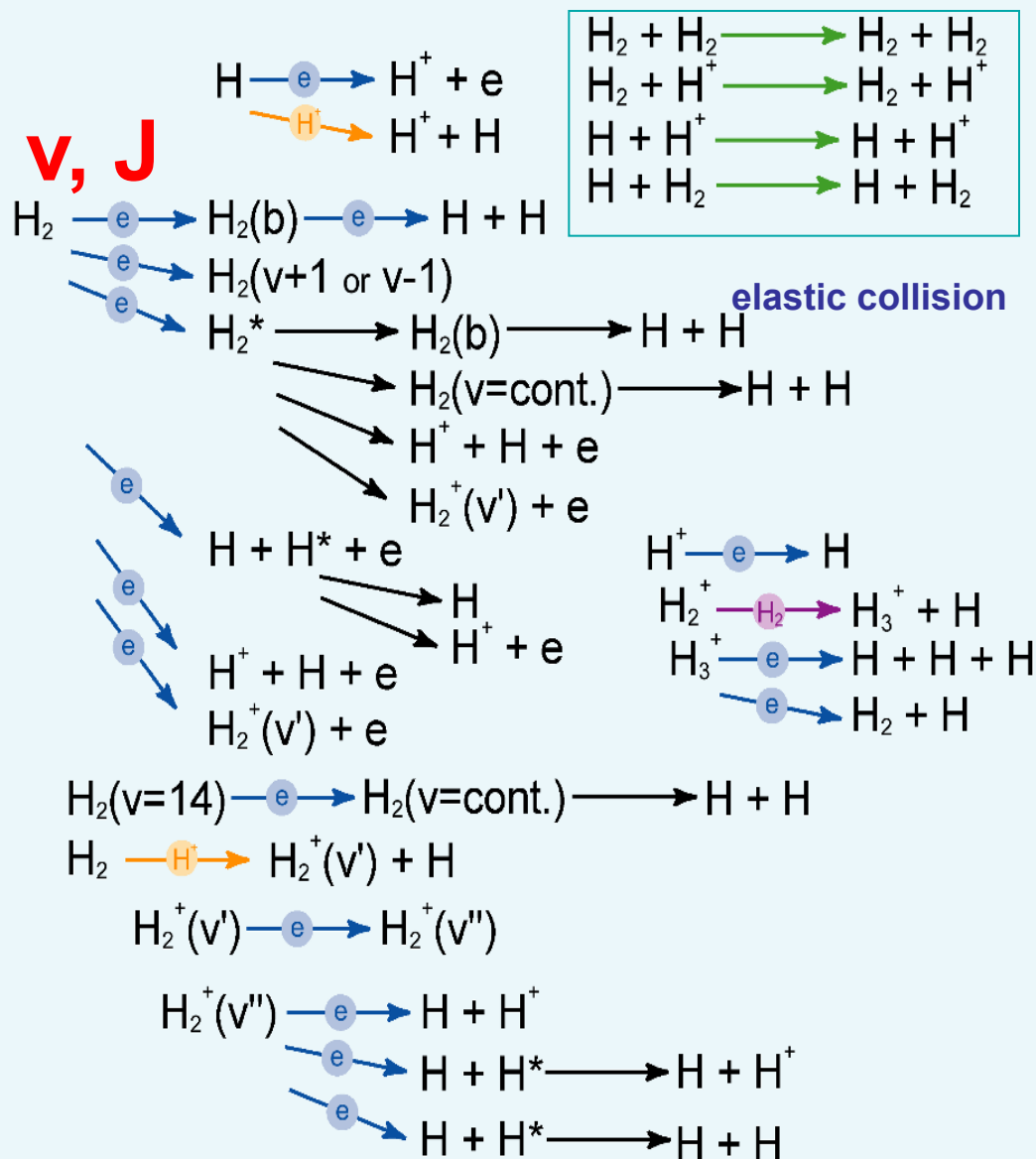
red (exp.)

blue (calc.)



Our models

wall



Collisional–Radiative Models

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

Neutral-Transport Code

