Polytechnic of Bari,
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Institute of Inorganic
Methodologies and Plasmas
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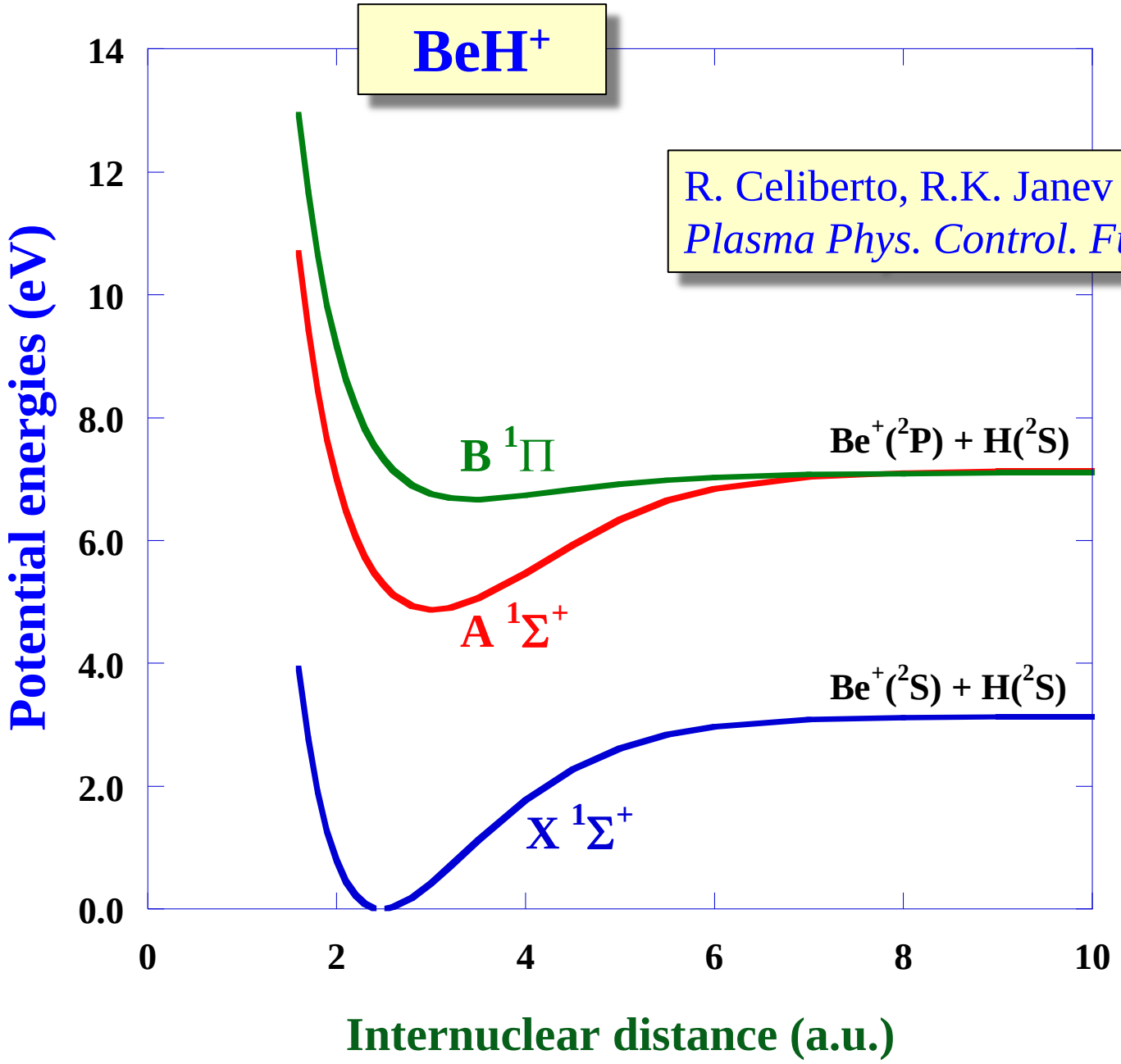
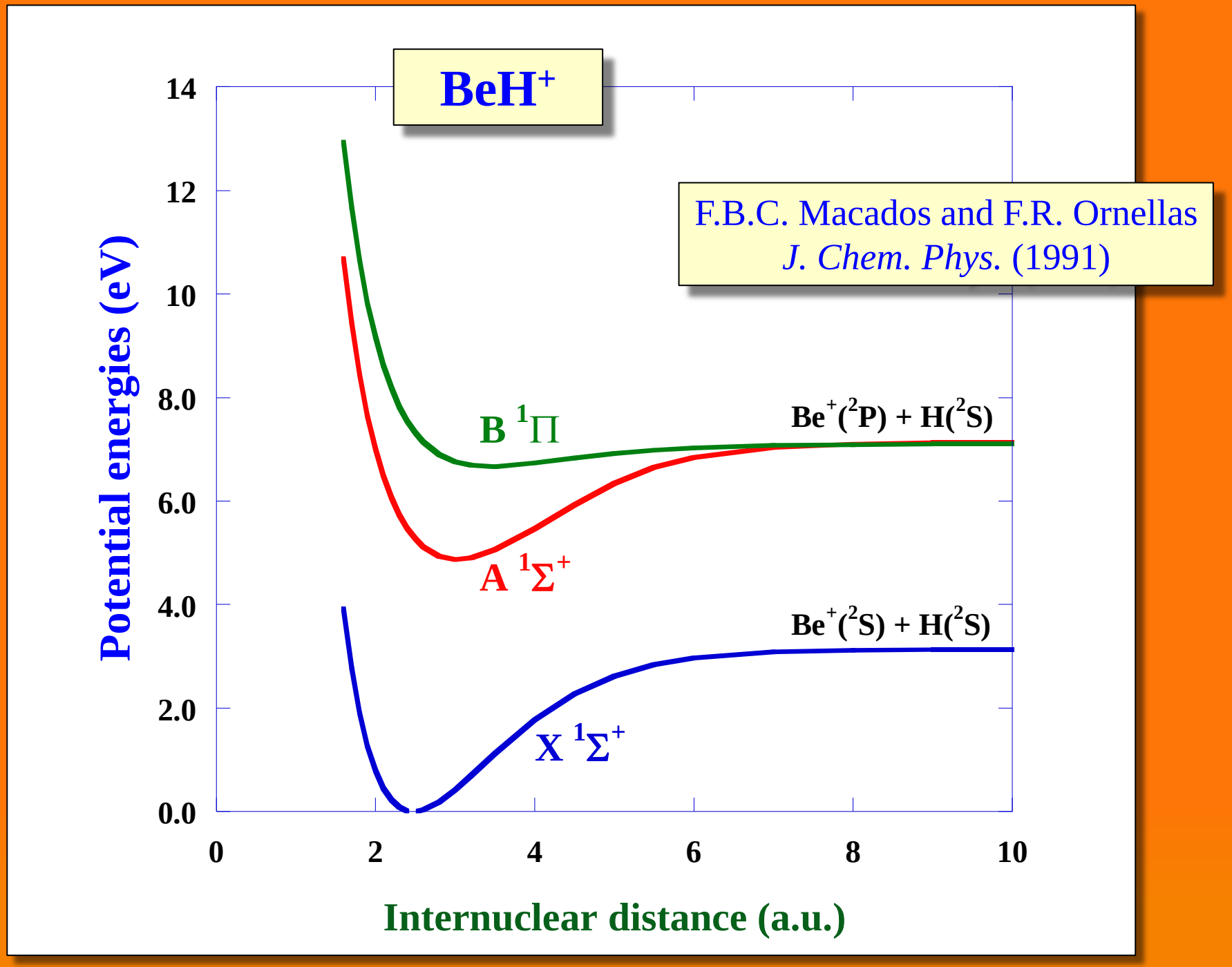
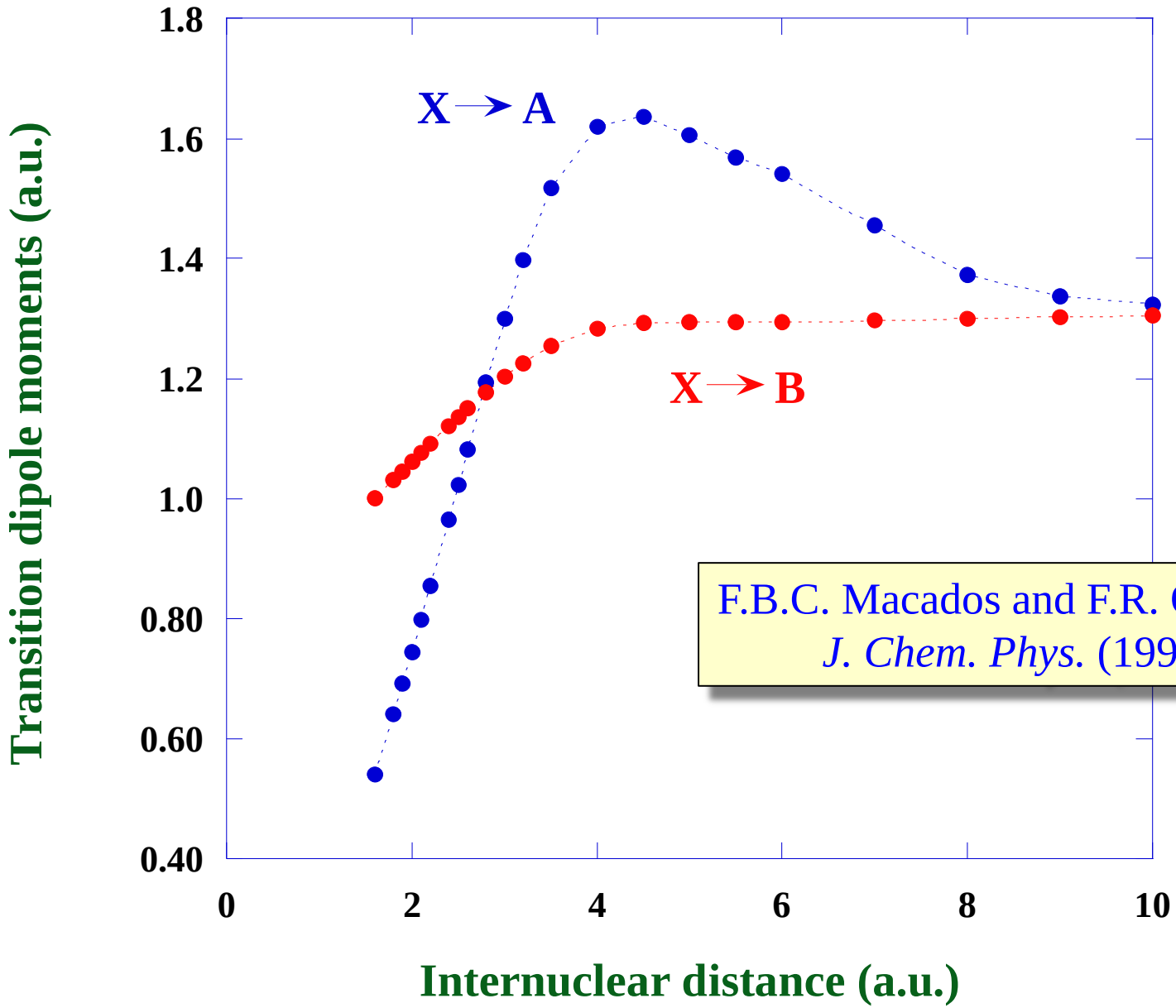
# Electron-molecule collisions in fusion plasmas

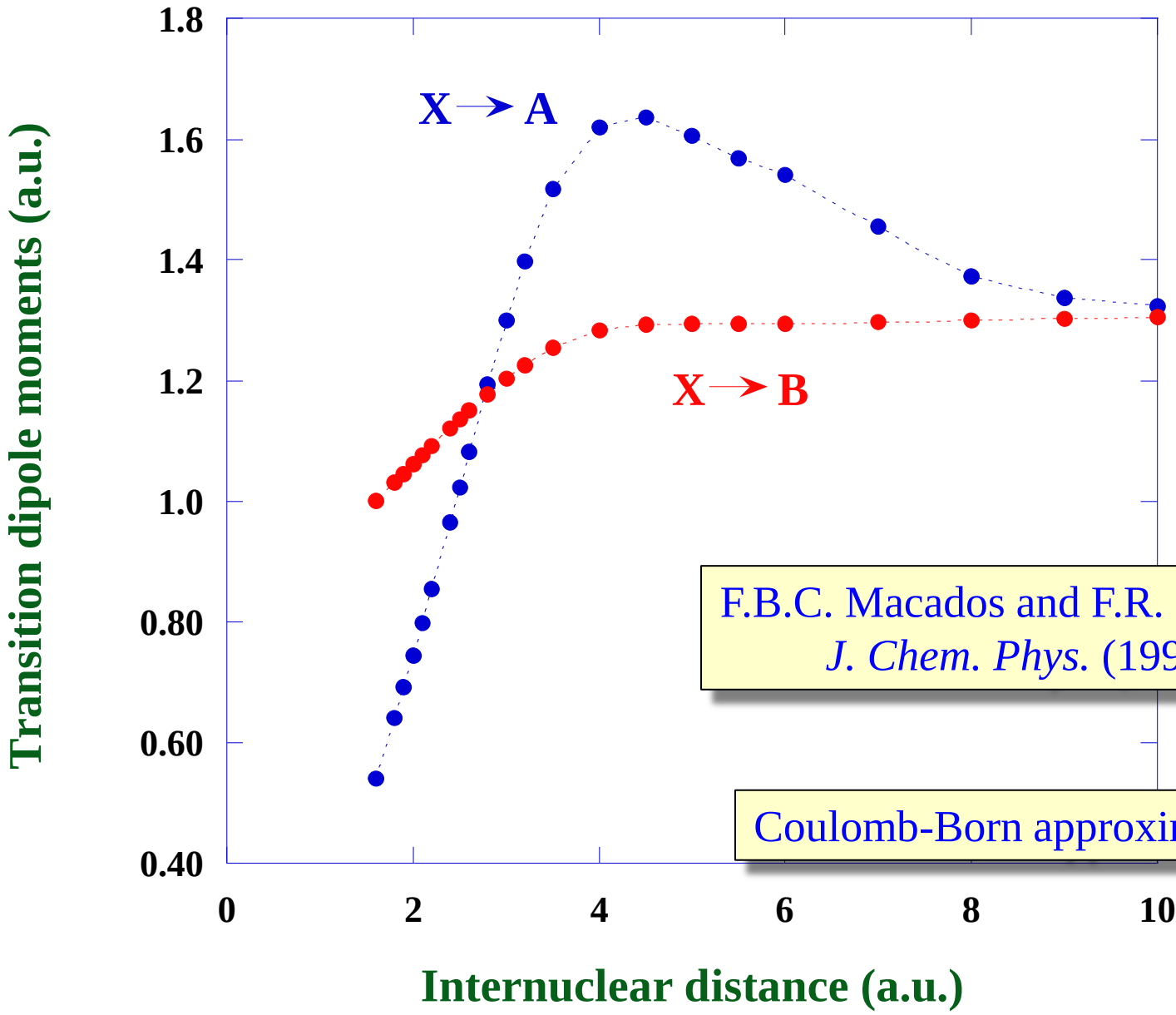
Roberto Celiberto

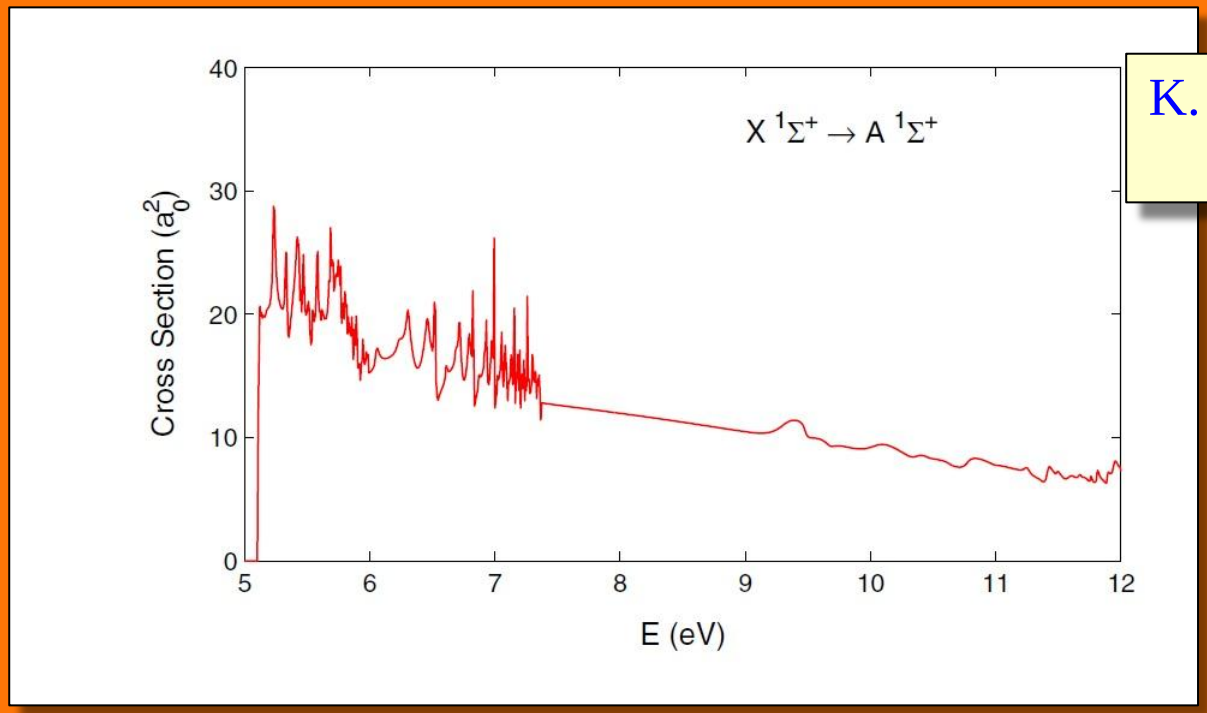
ADAS Workshop
Cadarache, 23-25 September 2012


BeH+
R. Celiberto, R.K. Janev & D. Reiter
Plasma Phys. Control. Fus. (2012)
Potential energies (eV)
Internuclear distance (a.u.)
0.0
2.0
4.0
6.0
8.0
10
12
14
0
2
4
6
8
10
B 1Π
A 1Σ+
X 1Σ+
Be+(2P) + H(2S)
Be+(2S) + H(2S)


BeH+
F.B.C. Macados and F.R. Ornellas
J. Chem. Phys. (1991)
Potential energies (eV)
Internuclear distance (a.u.)
14
12
10
8.0
6.0
4.0
2.0
0.0
0
2
4
6
8
10
B 1Π
A 1Σ+
X 1Σ+
Be+(2P) + H(2S)
Be+(2S) + H(2S)

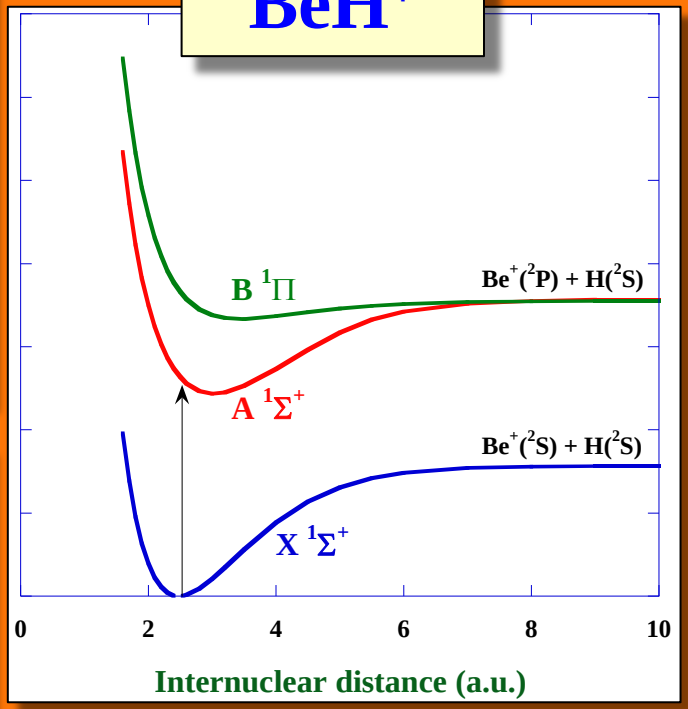

Transition dipole moments (a.u.)
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0
2
4
6
8
10
Internuclear distance (a.u.)
X → A
X → B
F.B.C. Macados and F.R. Ornellas
J. Chem. Phys. (1991)

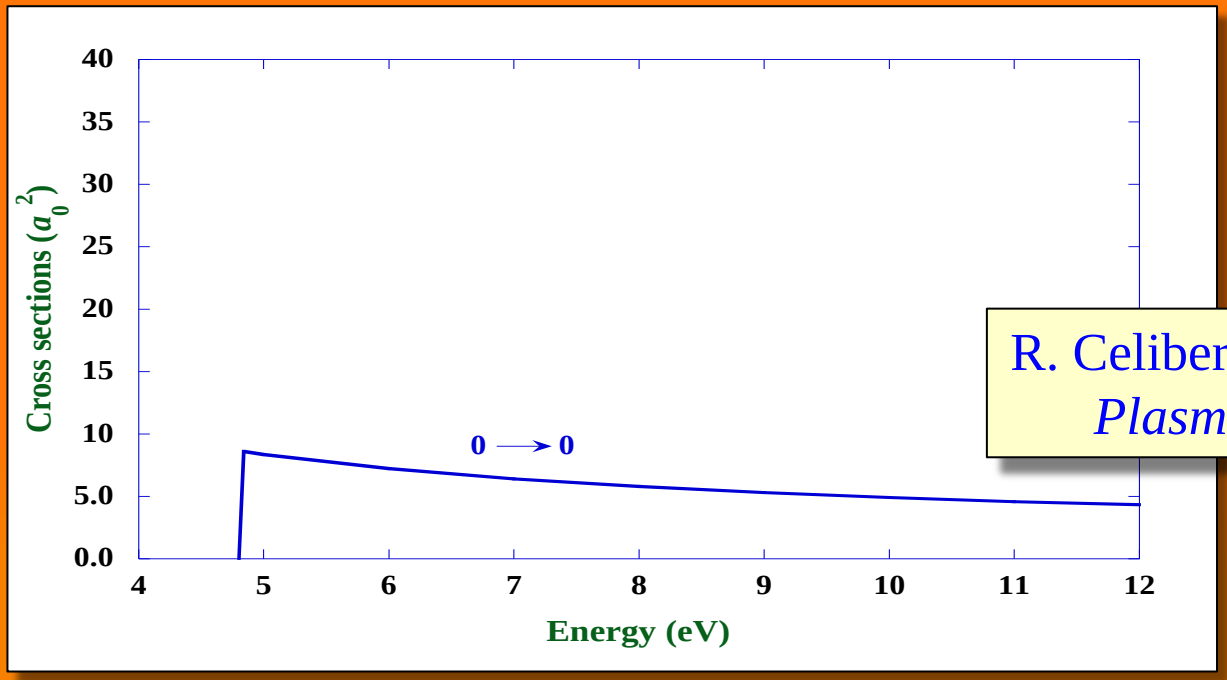

Transition dipole moments (a.u.)
1.8
1.6
1.4
1.2
1.0
0.80
0.60
0.40
0
2
4
6
8
10
Internuclear distance (a.u.)
X → A
X → B
F.B.C. Macados and F.R. Ornellas
J. Chem. Phys. (1991)
Coulomb-Born approximation



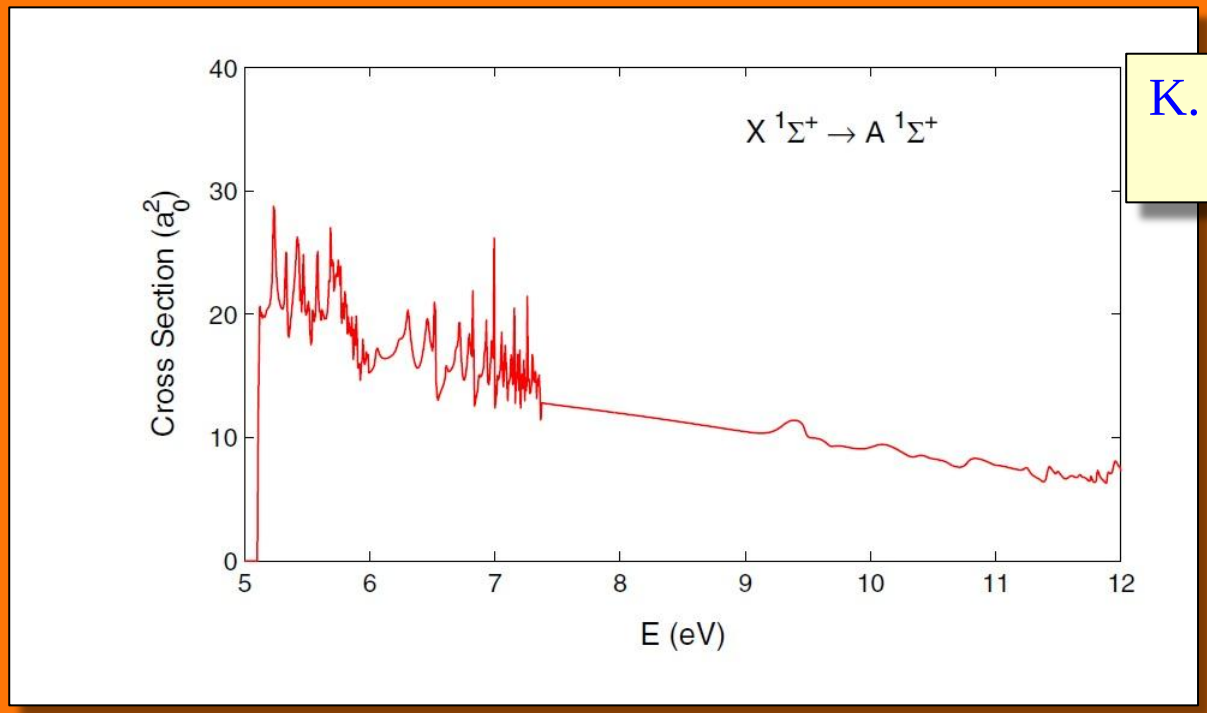

K. Chakrabarti and J. Tennyson
*Eur. Phys. J. D* (2012)

**$BeH^+$**



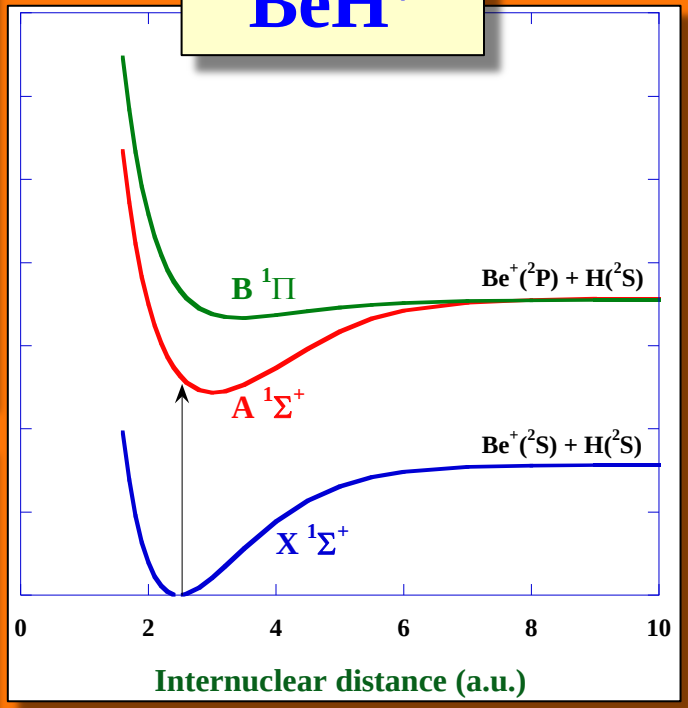



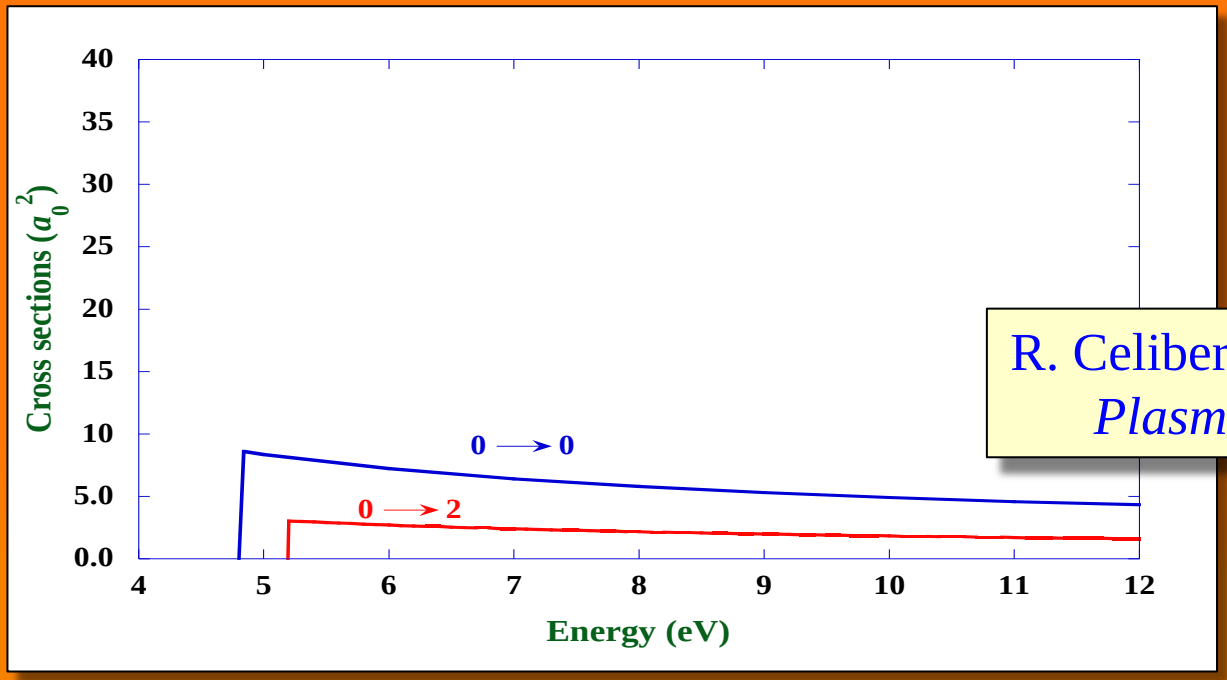

R. Celiberto, R. K. Janev and D. Reiter
*Plasma Phys. Con. Fus.* (2012)



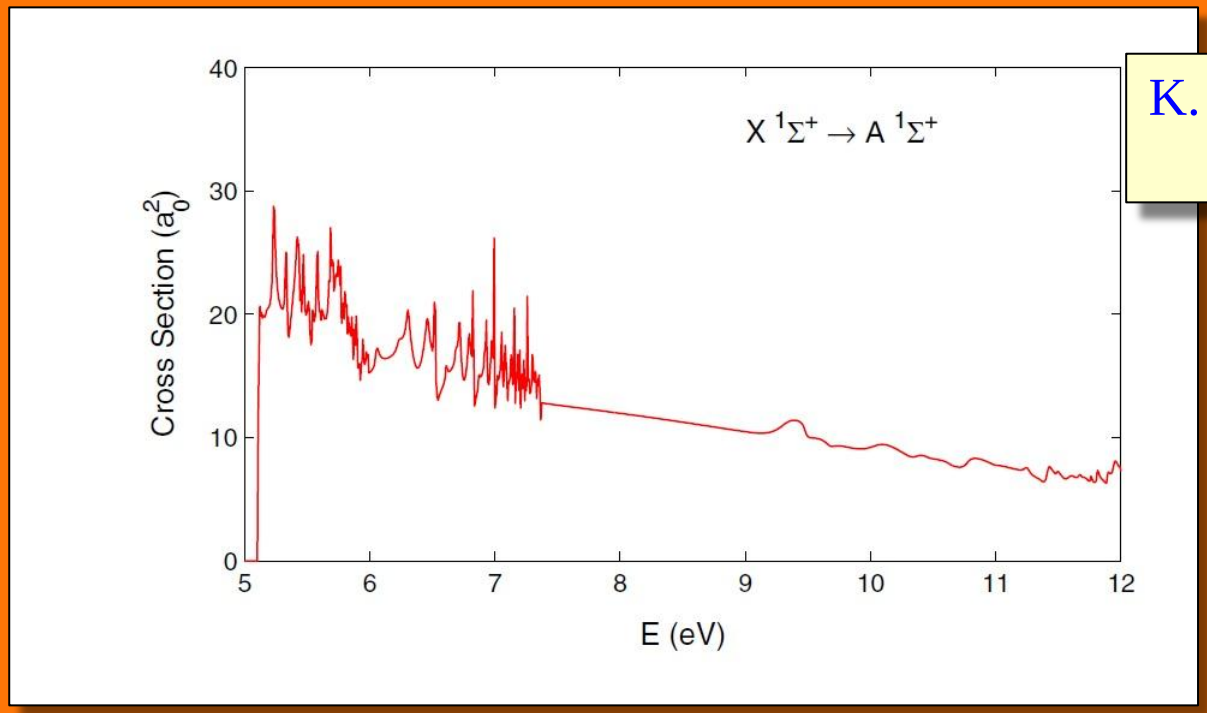

K. Chakrabarti and J. Tennyson
*Eur. Phys. J. D* (2012)

**$BeH^+$**




R. Celiberto, R. K. Janev and D. Reiter
*Plasma Phys. Con. Fus.* (2012)




K. Chakrabarti and J. Tennyson
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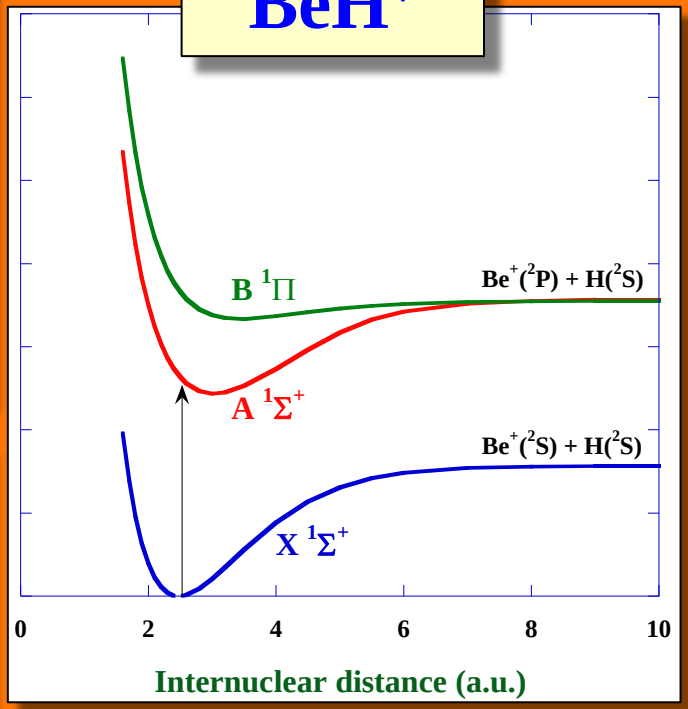
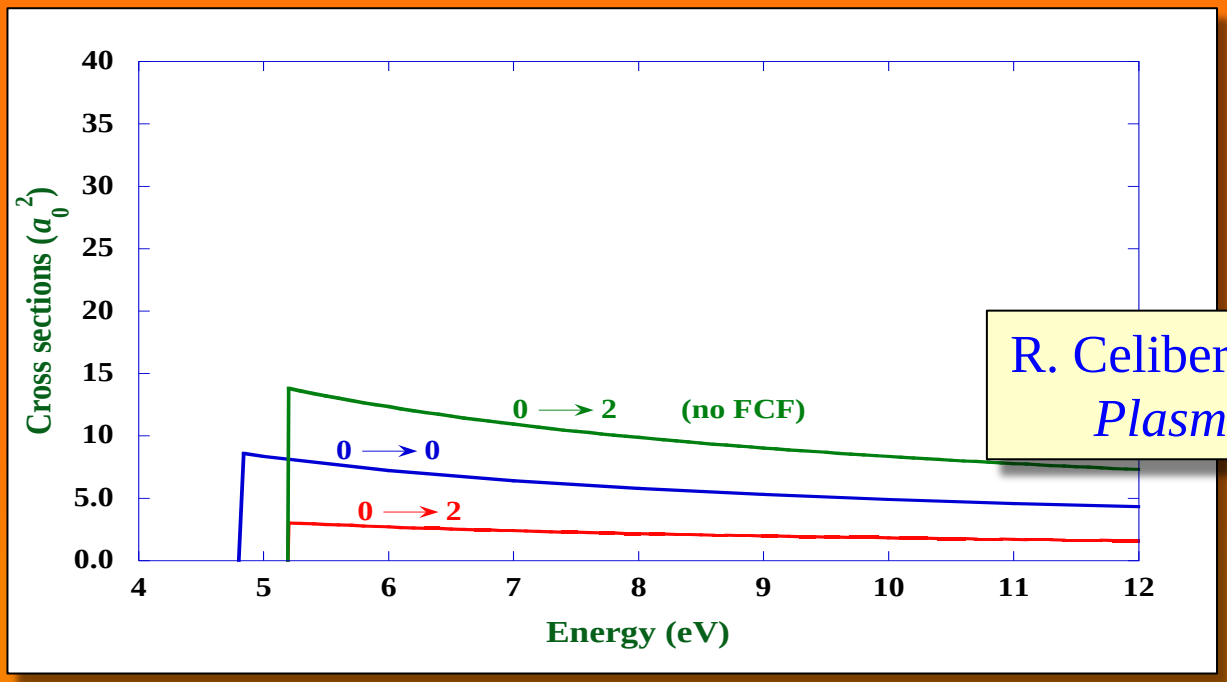
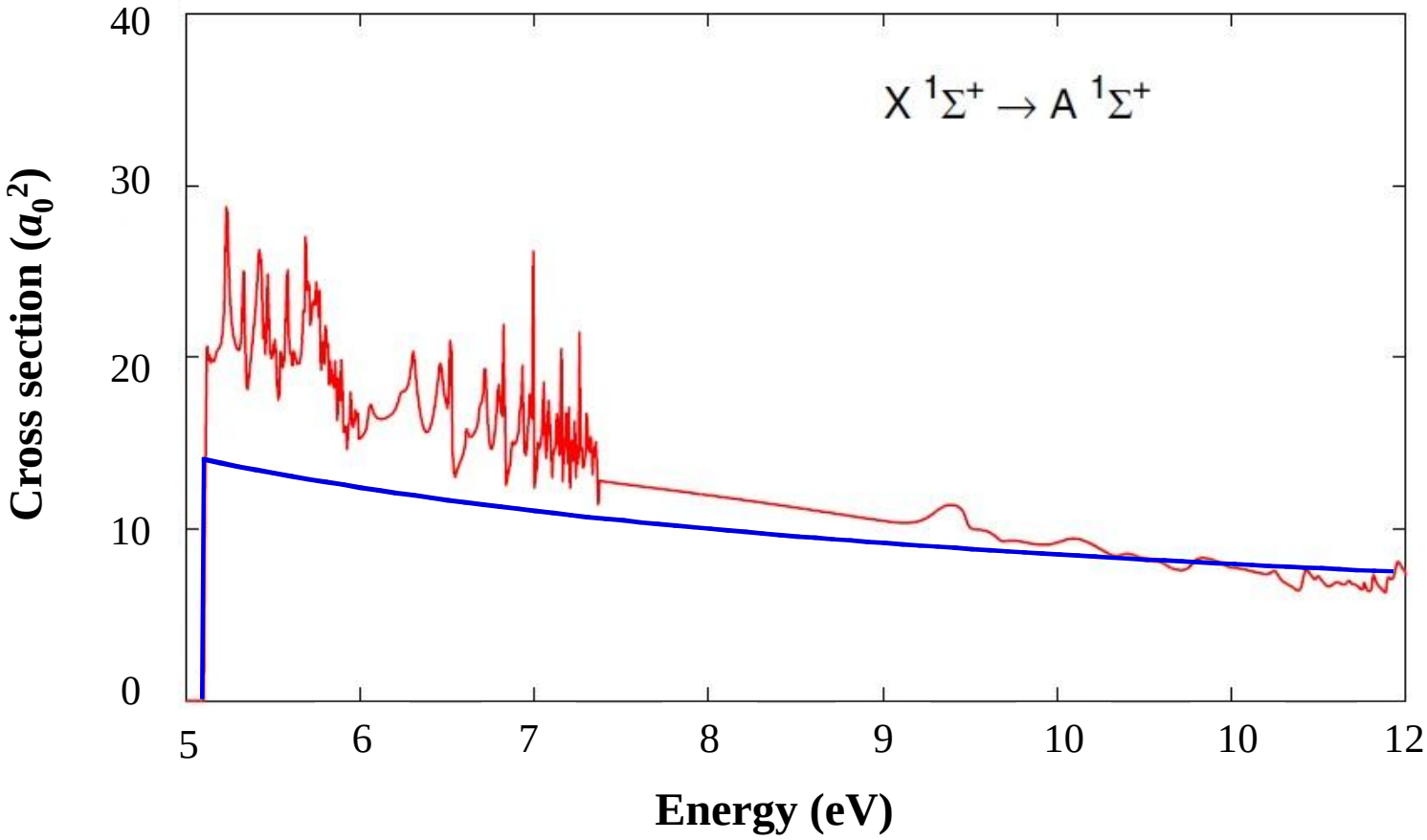
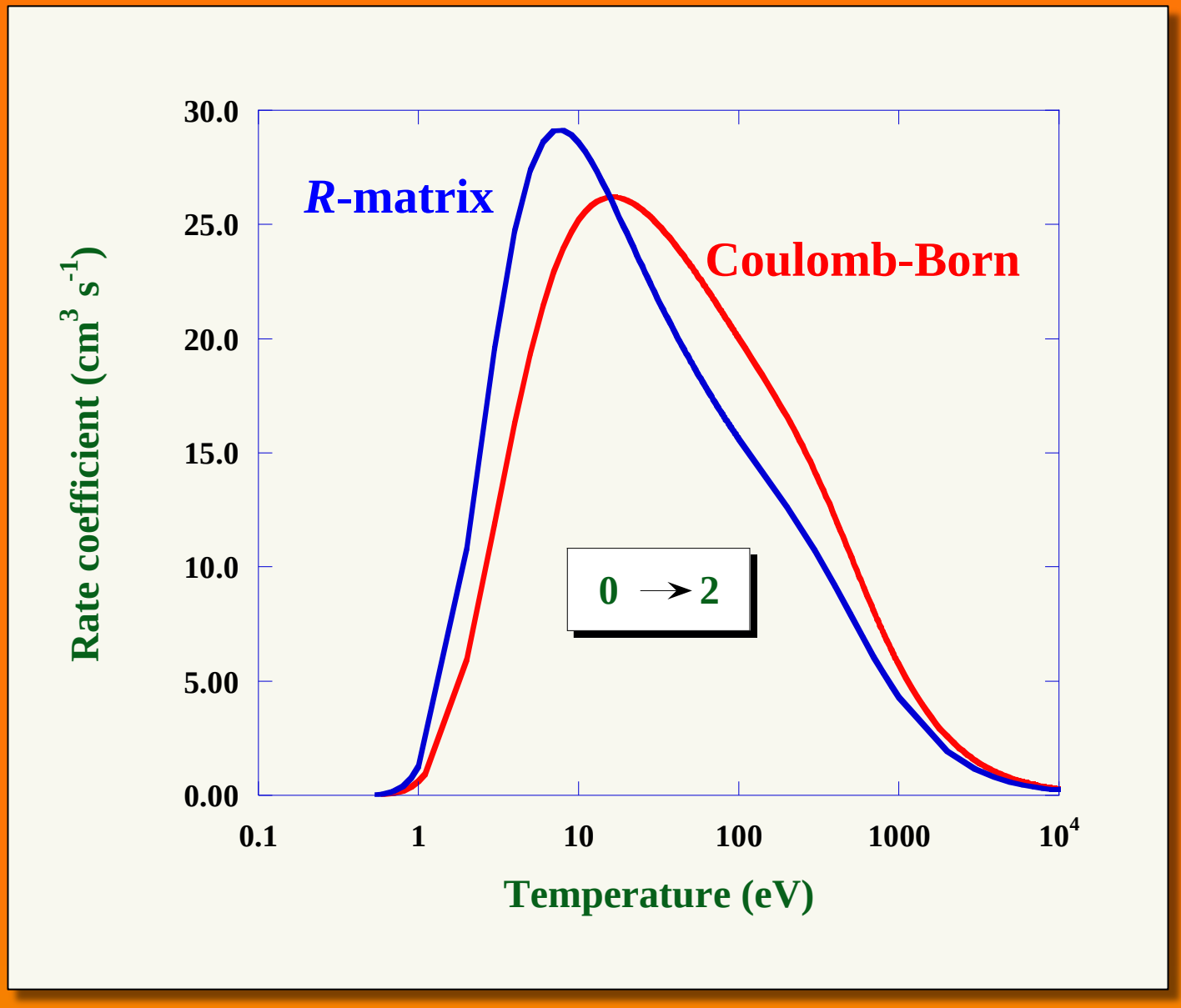
**$BeH^+$**

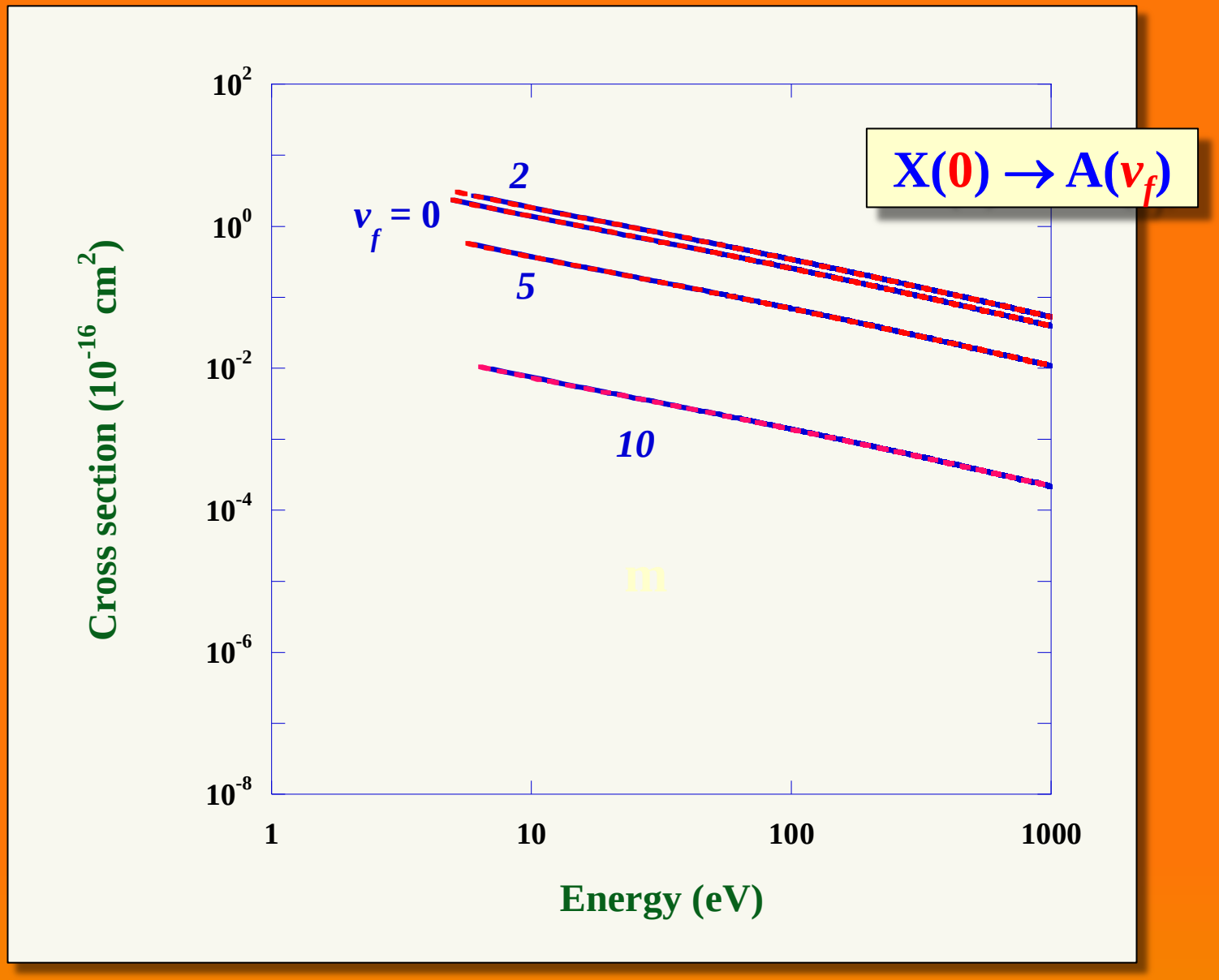


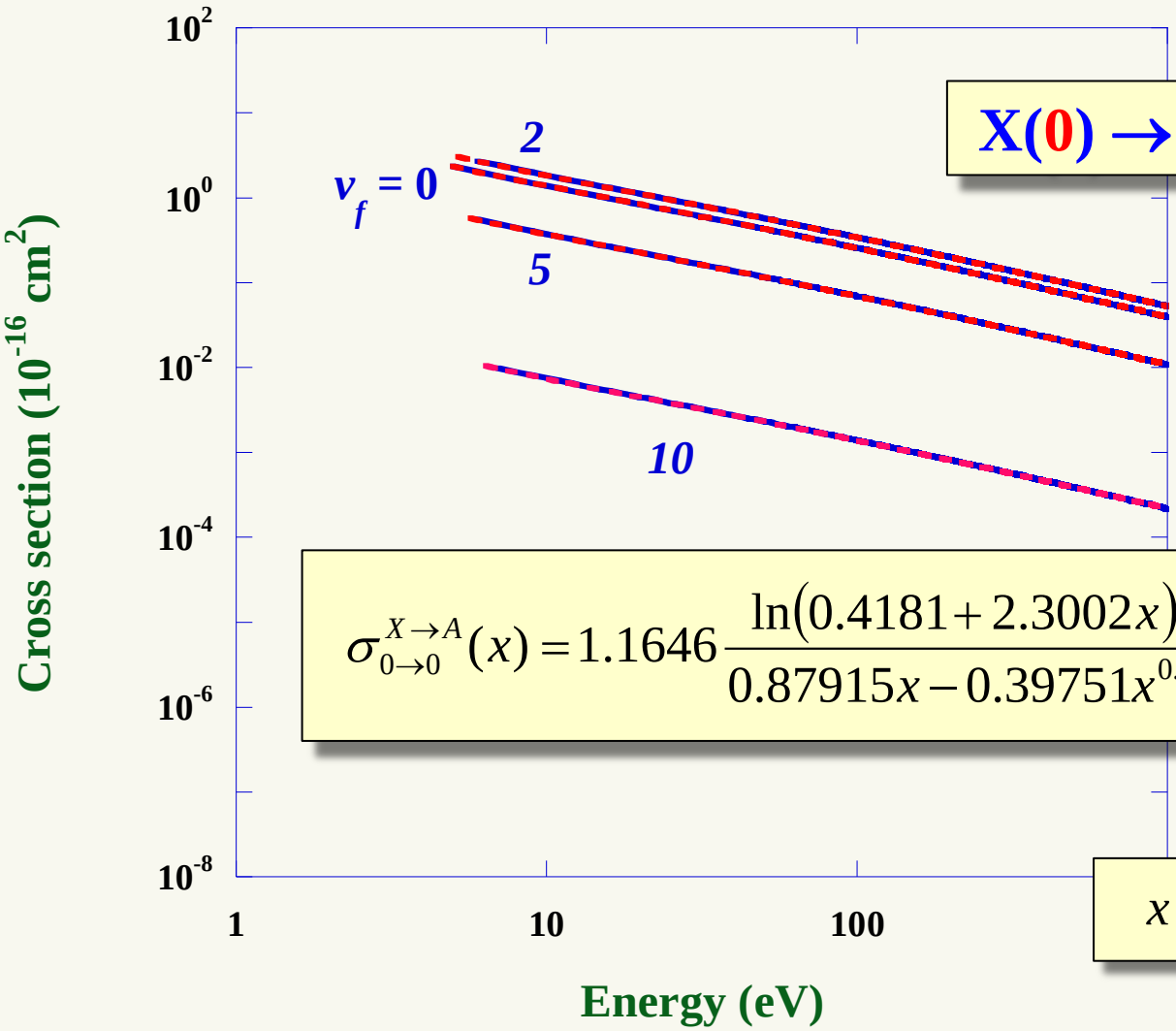




R. Celiberto, R. K. Janev and D. Reiter
*Plasma Phys. Con. Fus.* (2012)


X $^1\Sigma^+ \rightarrow$ A $^1\Sigma^+$
Cross section ($a_0^2$)
40
30
20
10
0
5
6
7
8
9
10
10
12
Energy (eV)


30.0
25.0
20.0
15.0
10.0
5.00
0.00
Rate coefficient (cm$^3$ s$^{-1}$)
R-matrix
Coulomb-Born
0 → 2
0.1
1
10
100
1000
10$^4$
Temperature (eV)

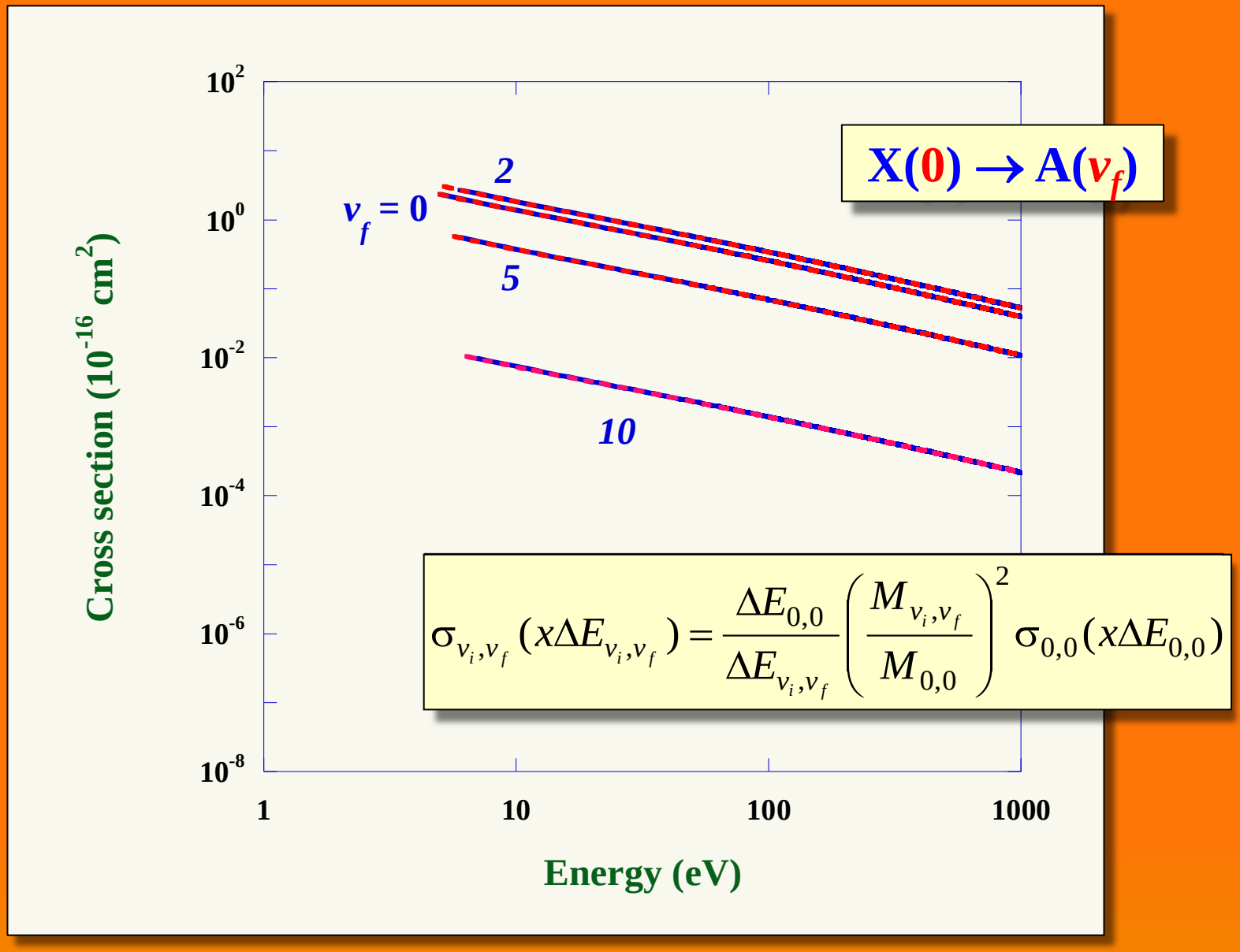

X(0) → A($v_f$)
$v_f$ = 0
2
5
10
Cross section ($10^{-16}$ cm$^2$)
$10^2$
$10^0$
$10^{-2}$
$10^{-4}$
$10^{-6}$
$10^{-8}$
1
10
100
1000
Energy (eV)

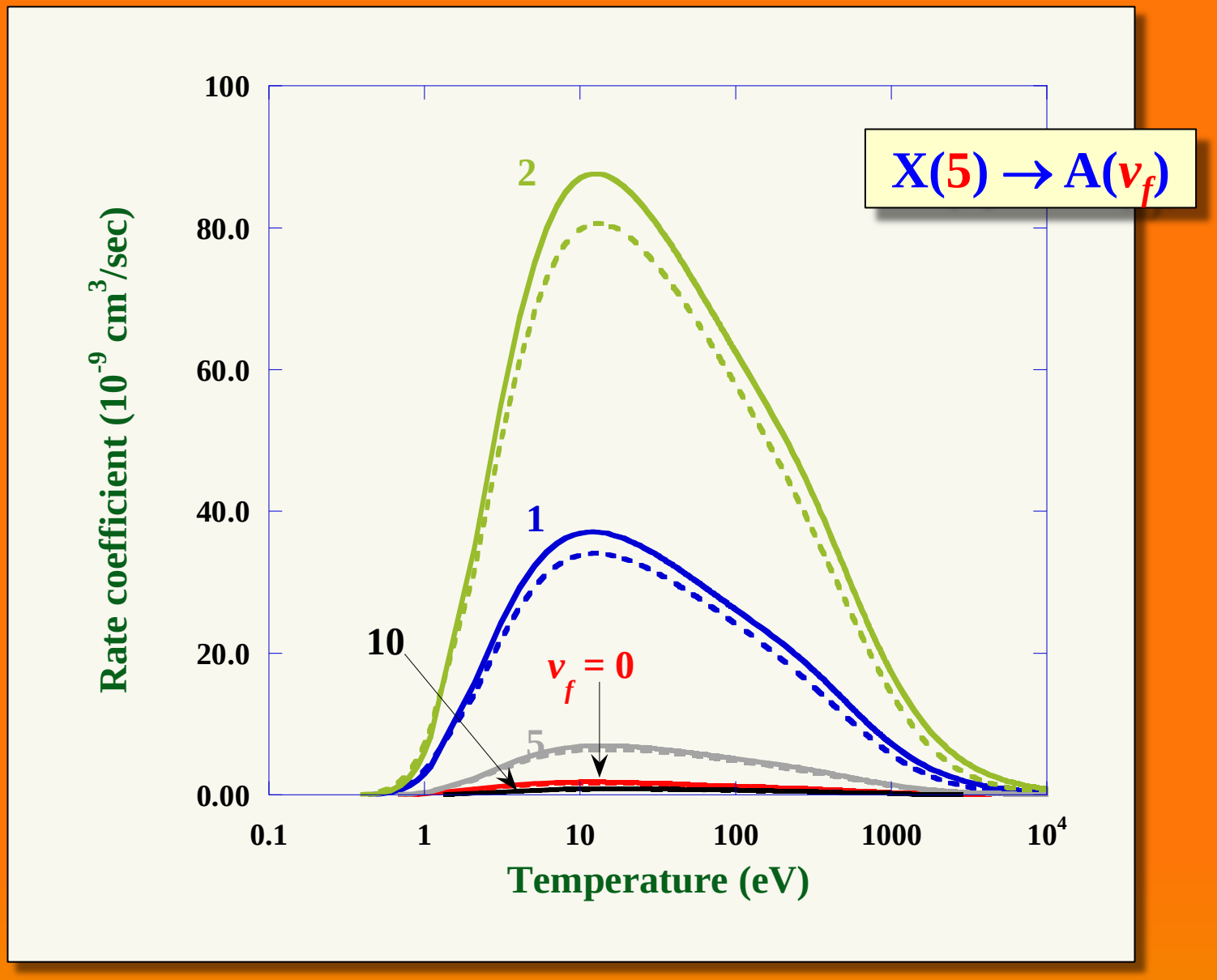


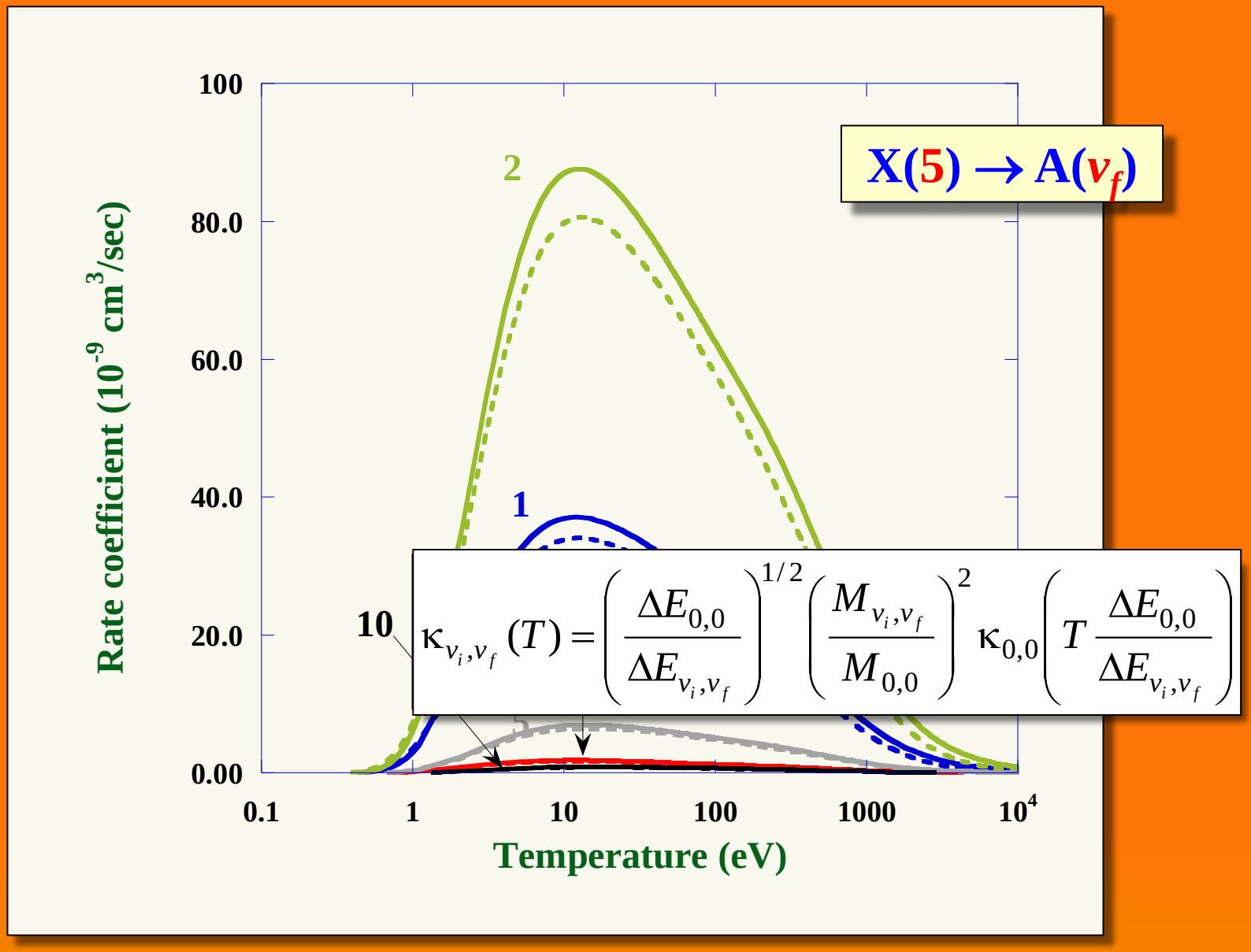

$\mathbf{X(0) \rightarrow A(}v_f\mathbf{)}$

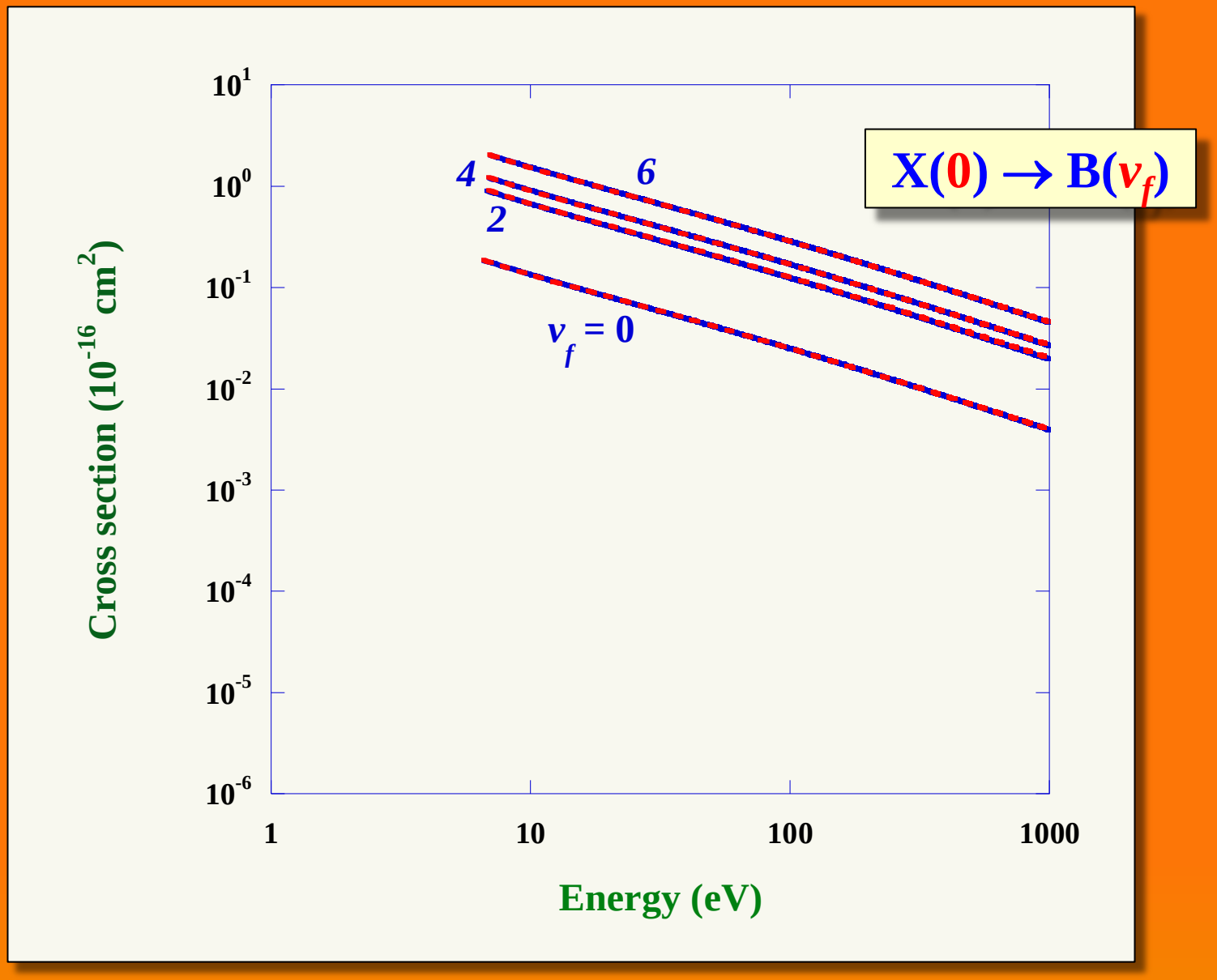
$$\sigma_{0\to 0}^{X\to A}(x) = 1.1646\,\frac{\ln(0.4181 + 2.3002x)}{0.87915x - 0.39751x^{0.1}}\,(10^{-16}\,cm^2)$$

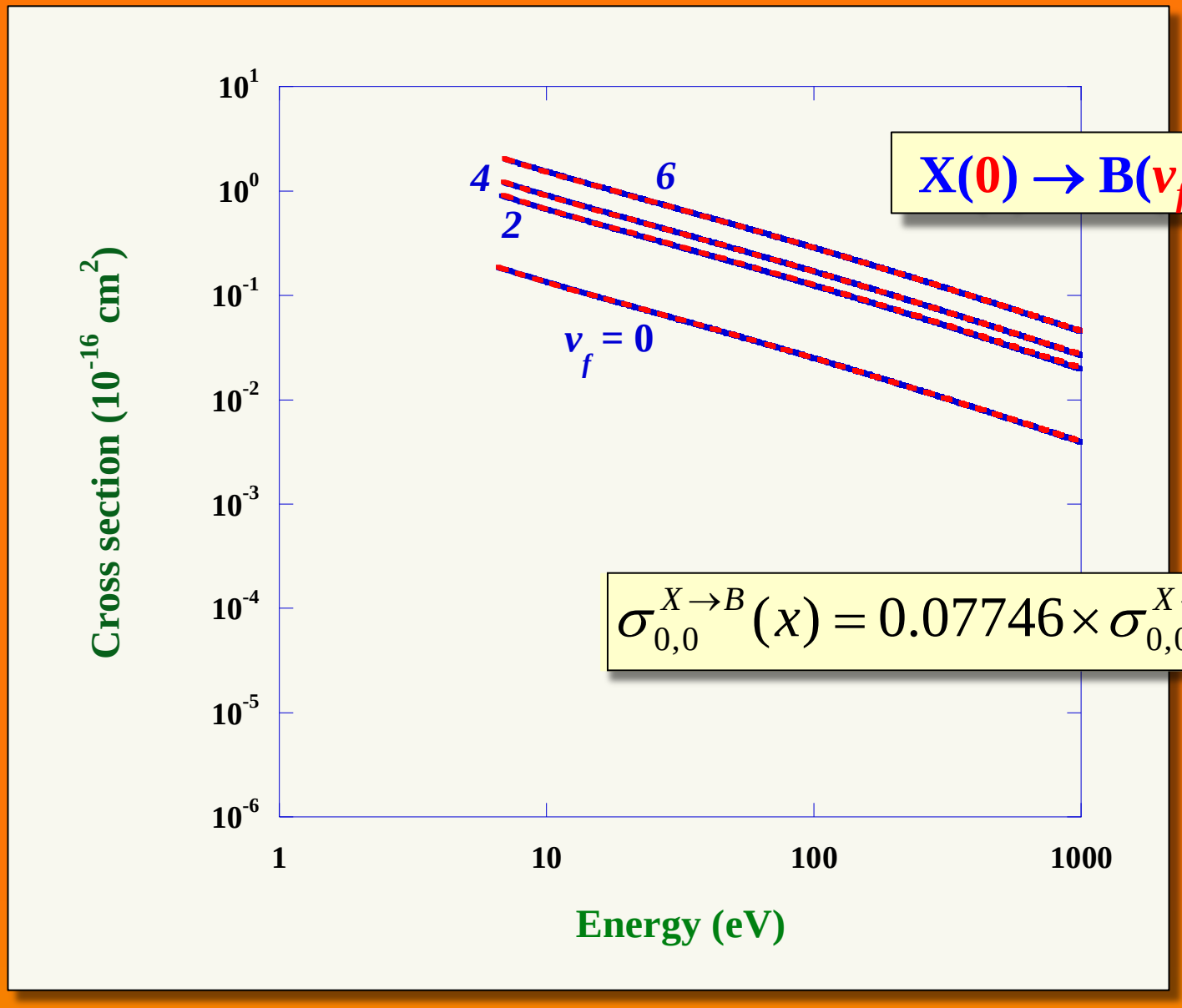
$$x = E / \Delta E_{0,0}$$

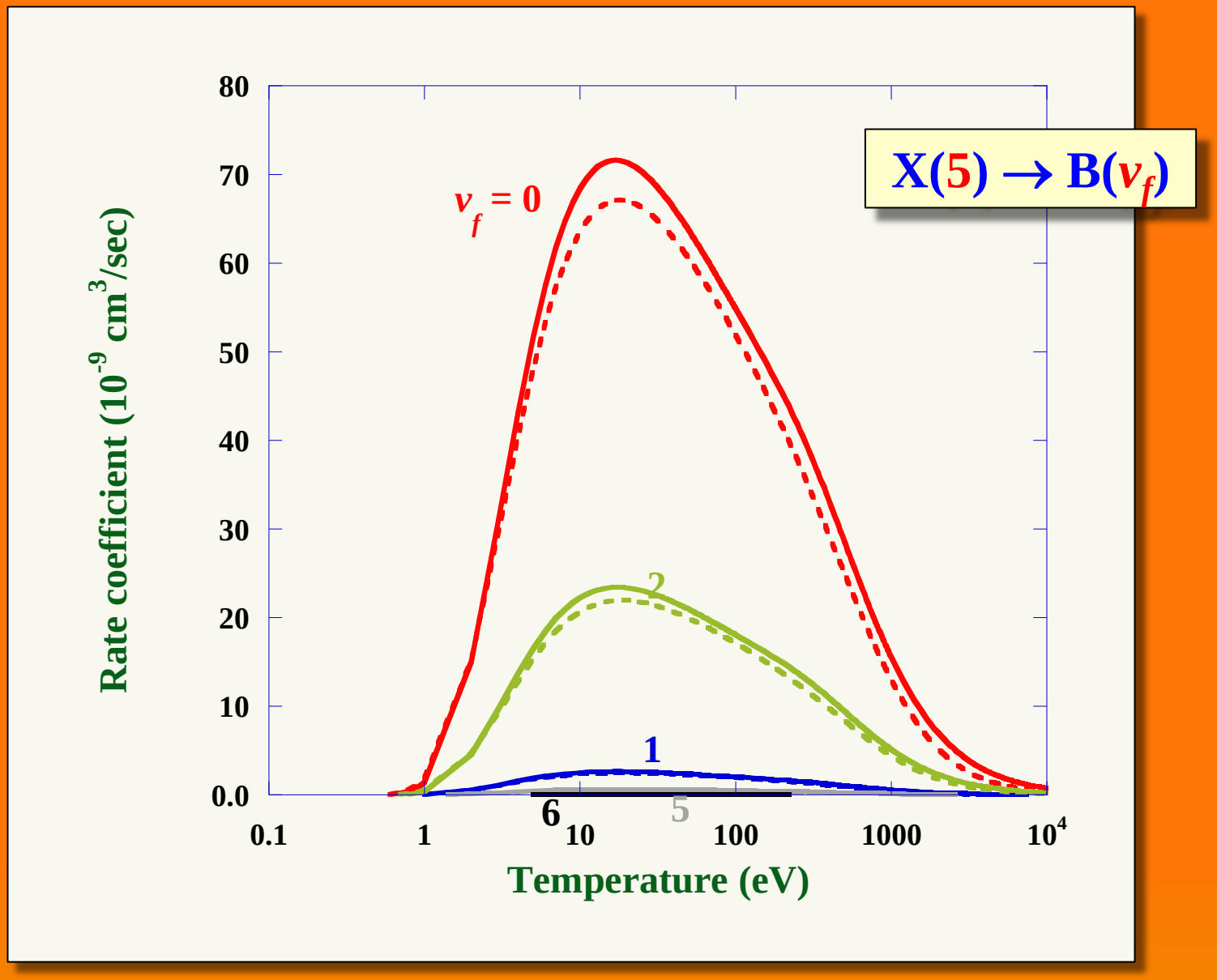

$10^2$
$10^0$
$10^{-2}$
$10^{-4}$
$10^{-6}$
$10^{-8}$
Cross section ($10^{-16}$ cm$^2$)
1
10
100
1000
Energy (eV)
$v_f = 0$
2
5
10
X(0) → A($v_f$)
$\sigma_{v_i,v_f}(x\Delta E_{v_i,v_f}) = \frac{\Delta E_{0,0}}{\Delta E_{v_i,v_f}} \left( \frac{M_{v_i,v_f}}{M_{0,0}} \right)^2 \sigma_{0,0}(x\Delta E_{0,0})$

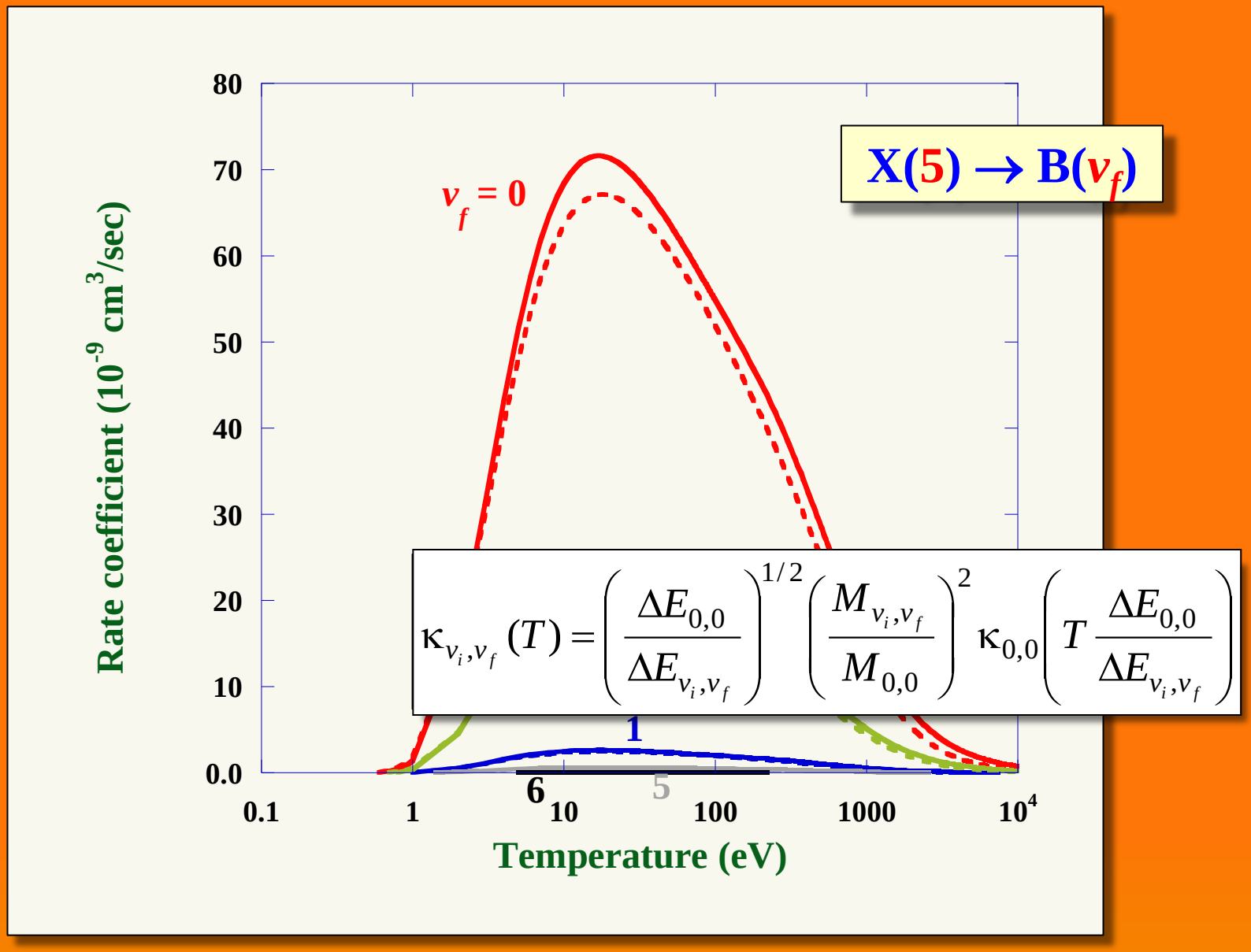

X(5) → A($v_f$)
Rate coefficient ($10^{-9}$ cm$^3$/sec)
100
80.0
60.0
40.0
20.0
0.00
0.1
1
10
100
1000
$10^4$
Temperature (eV)
2
1
10
5
$v_f$ = 0


X(5) → A($v_f$)
Rate coefficient ($10^{-9}$ cm$^3$/sec)
Temperature (eV)
100
80.0
60.0
40.0
20.0
0.00
0.1
1
10
100
1000
$10^4$
2
1
10
$\kappa_{v_i,v_f}(T) = \left(\frac{\Delta E_{0,0}}{\Delta E_{v_i,v_f}}\right)^{1/2} \left(\frac{M_{v_i,v_f}}{M_{0,0}}\right)^2 \kappa_{0,0}\left(T\frac{\Delta E_{0,0}}{\Delta E_{v_i,v_f}}\right)$

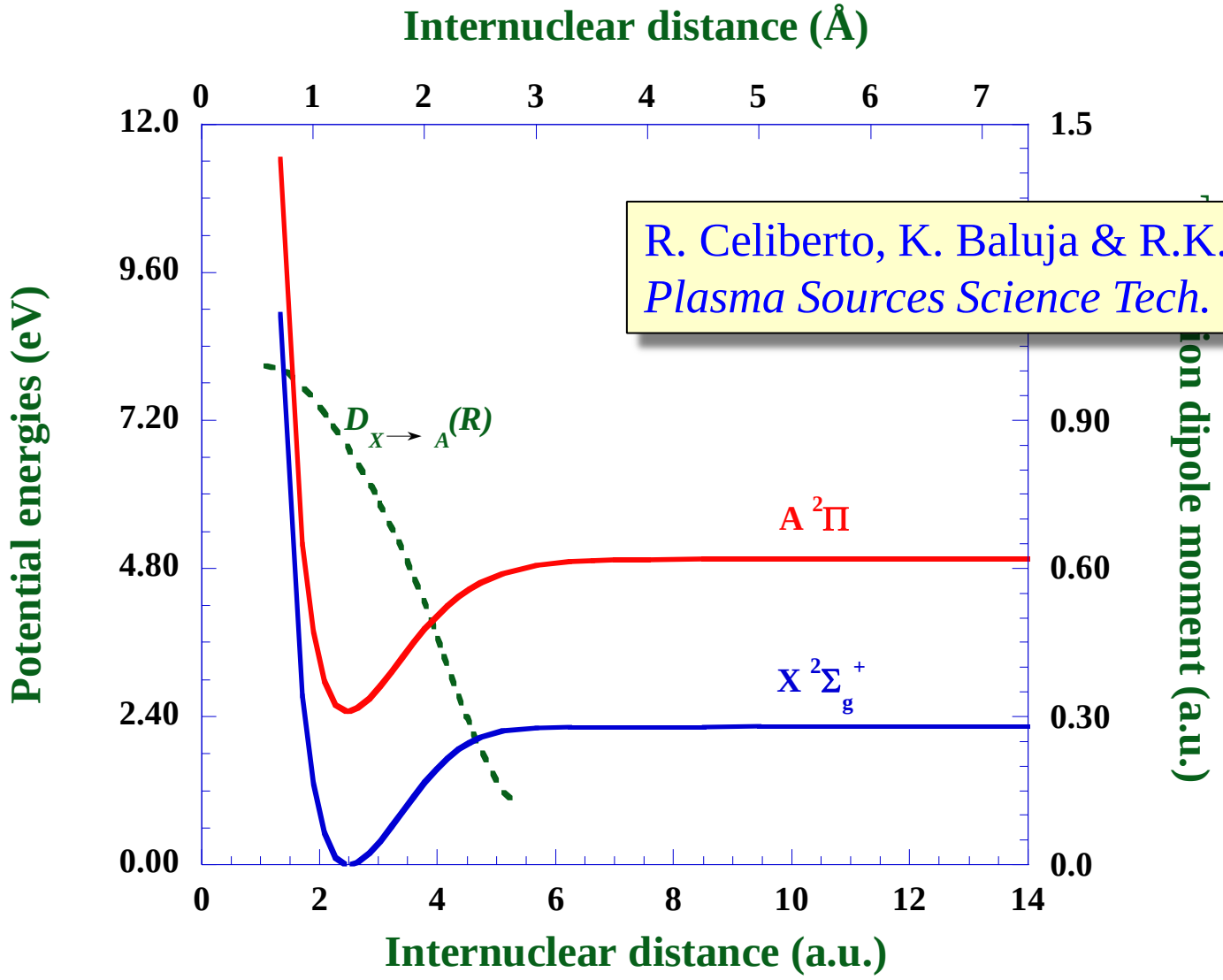

X(0) → B($v_f$)
Cross section ($10^{-16}$ cm$^2$)
$10^1$
$10^0$
$10^{-1}$
$10^{-2}$
$10^{-3}$
$10^{-4}$
$10^{-5}$
$10^{-6}$
1
10
100
1000
Energy (eV)
4
6
2
$v_f$ = 0


Cross section ($10^{-16}$ cm$^2$)
$10^{1}$
$10^{0}$
$10^{-1}$
$10^{-2}$
$10^{-3}$
$10^{-4}$
$10^{-5}$
$10^{-6}$
1
10
100
1000
Energy (eV)
4
6
2
$v_f = 0$
X(0) → B($v_f$)
$\sigma_{0,0}^{X\to B}(x) = 0.07746 \times \sigma_{0,0}^{X\to A}(x)$


X(5) → B($v_f$)
Rate coefficient ($10^{-9}$ $cm^3$/sec)
Temperature (eV)
$v_f$ = 0
1
2
5
6
80
70
60
50
40
30
20
10
0.0
0.1
1
10
100
1000
$10^4$

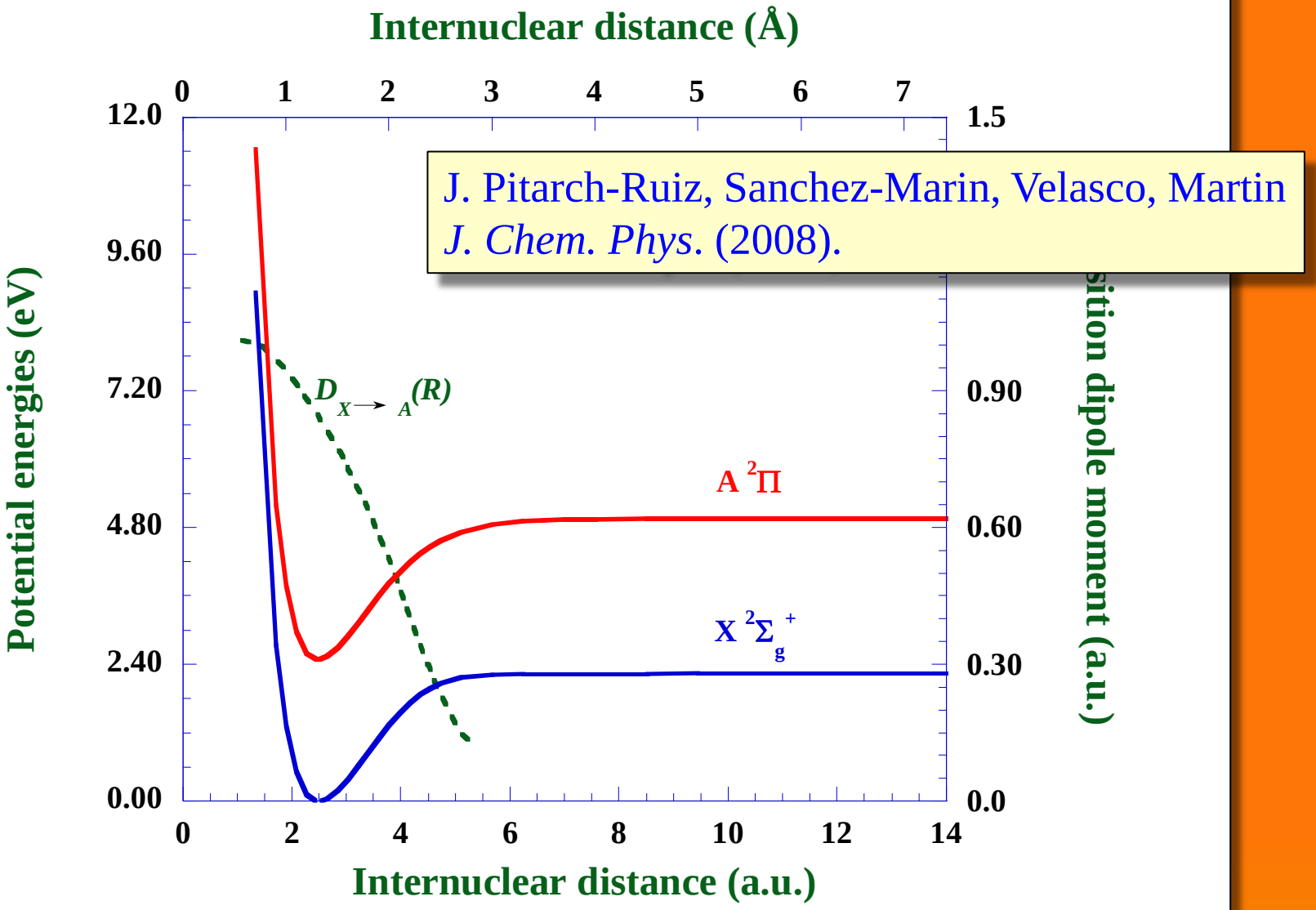

X(5) → B($v_f$)
$v_f$ = 0
Rate coefficient ($10^{-9}$ cm$^3$/sec)
Temperature (eV)
80
70
60
50
40
30
20
10
0.0
0.1
1
10
100
1000
$10^4$
1
6
5
$\kappa_{v_i,v_f}(T) = \left(\frac{\Delta E_{0,0}}{\Delta E_{v_i,v_f}}\right)^{1/2} \left(\frac{M_{v_i,v_f}}{M_{0,0}}\right)^2 \kappa_{0,0}\left(T\frac{\Delta E_{0,0}}{\Delta E_{v_i,v_f}}\right)$

# BeH

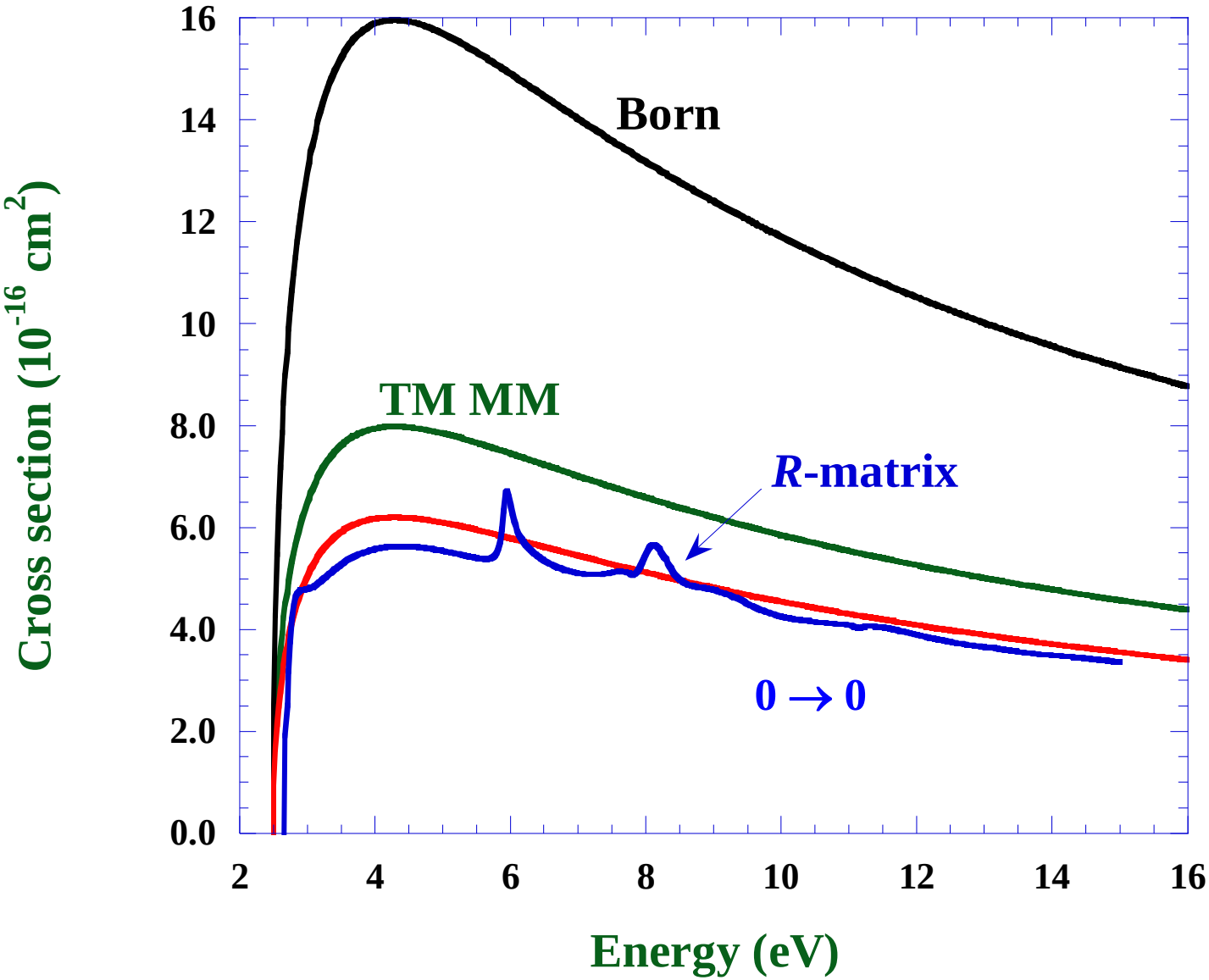


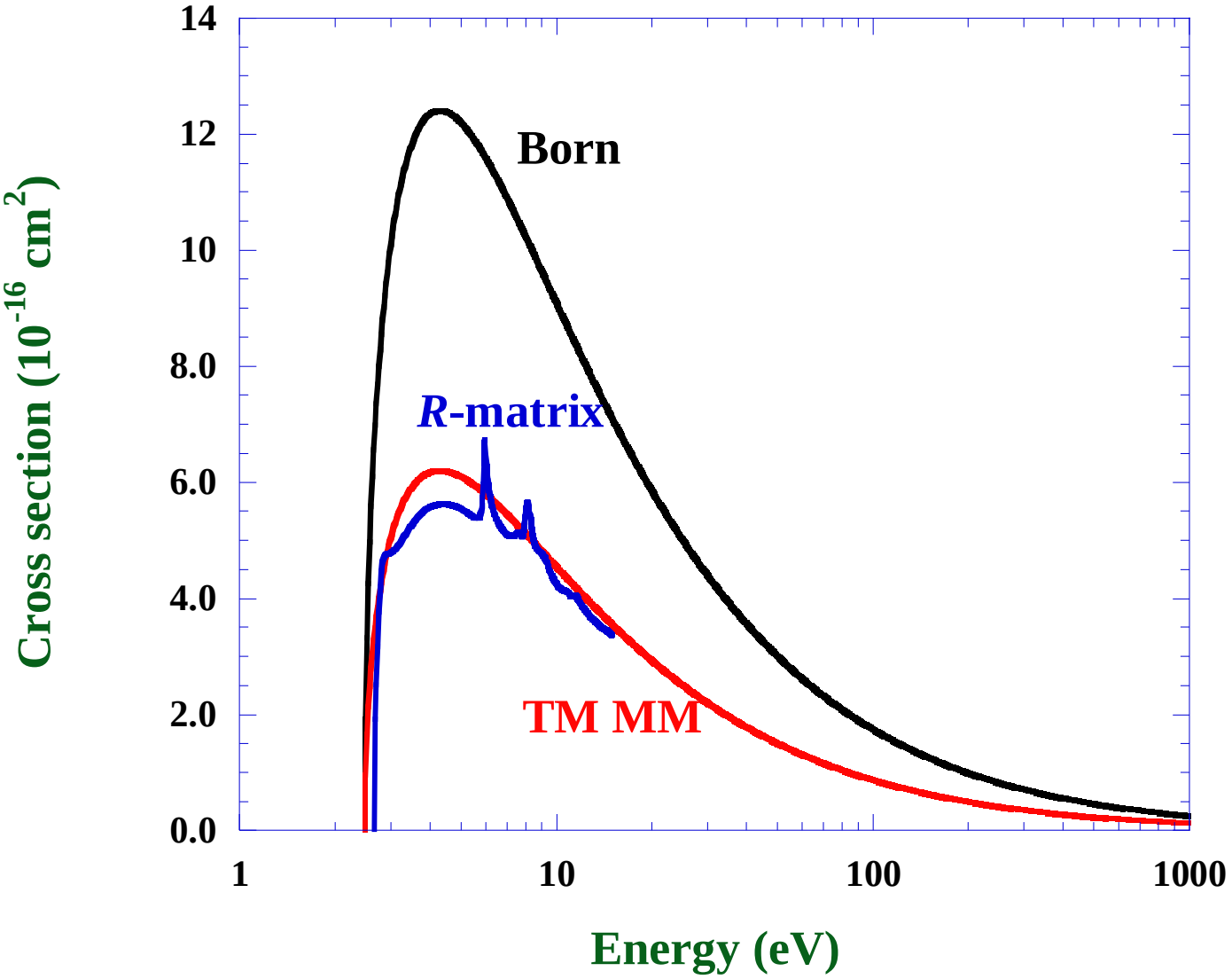

R. Celiberto, K. Baluja & R.K. Janev
*Plasma Sources Science Tech.* (submitted)

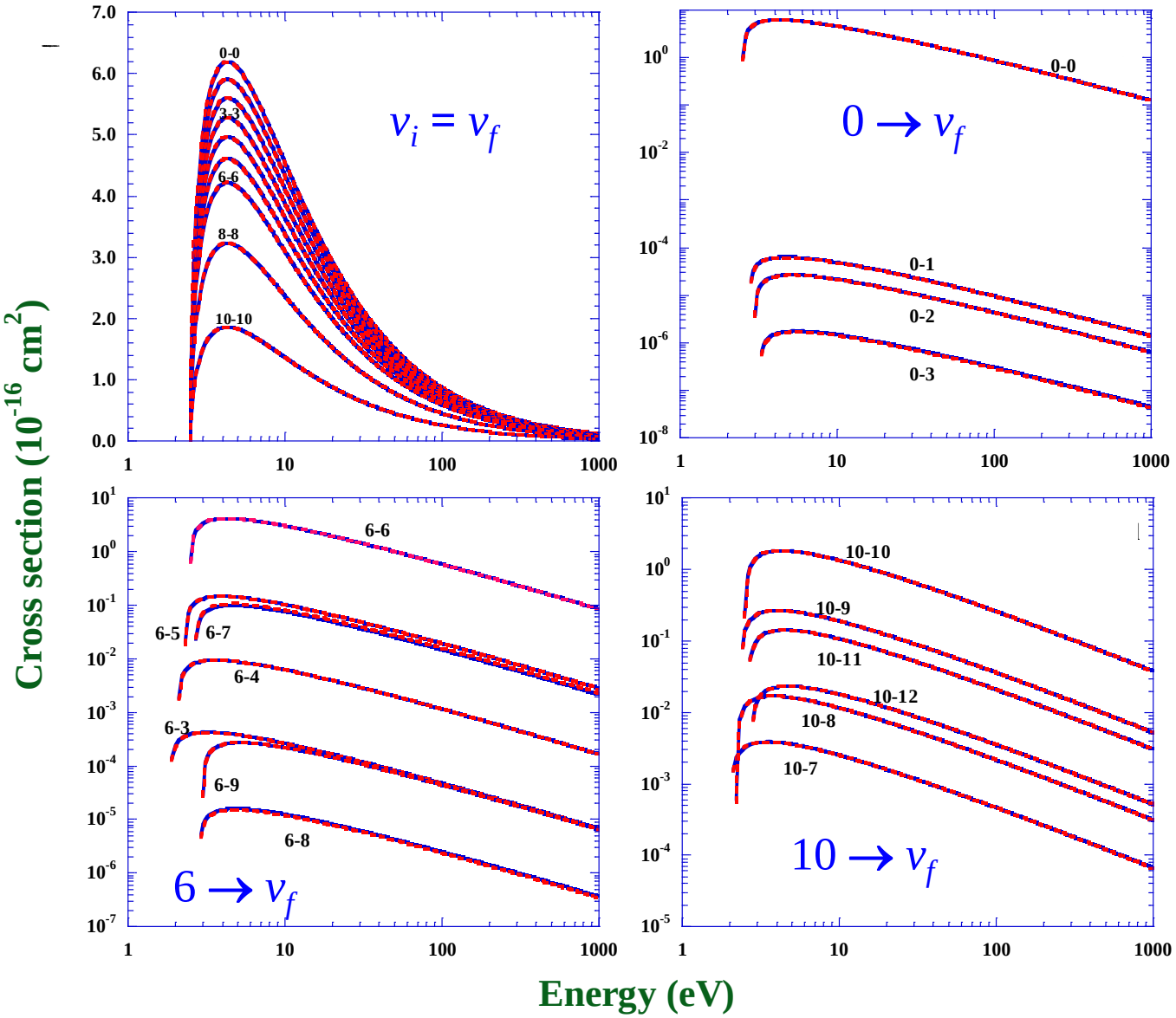
# BeH

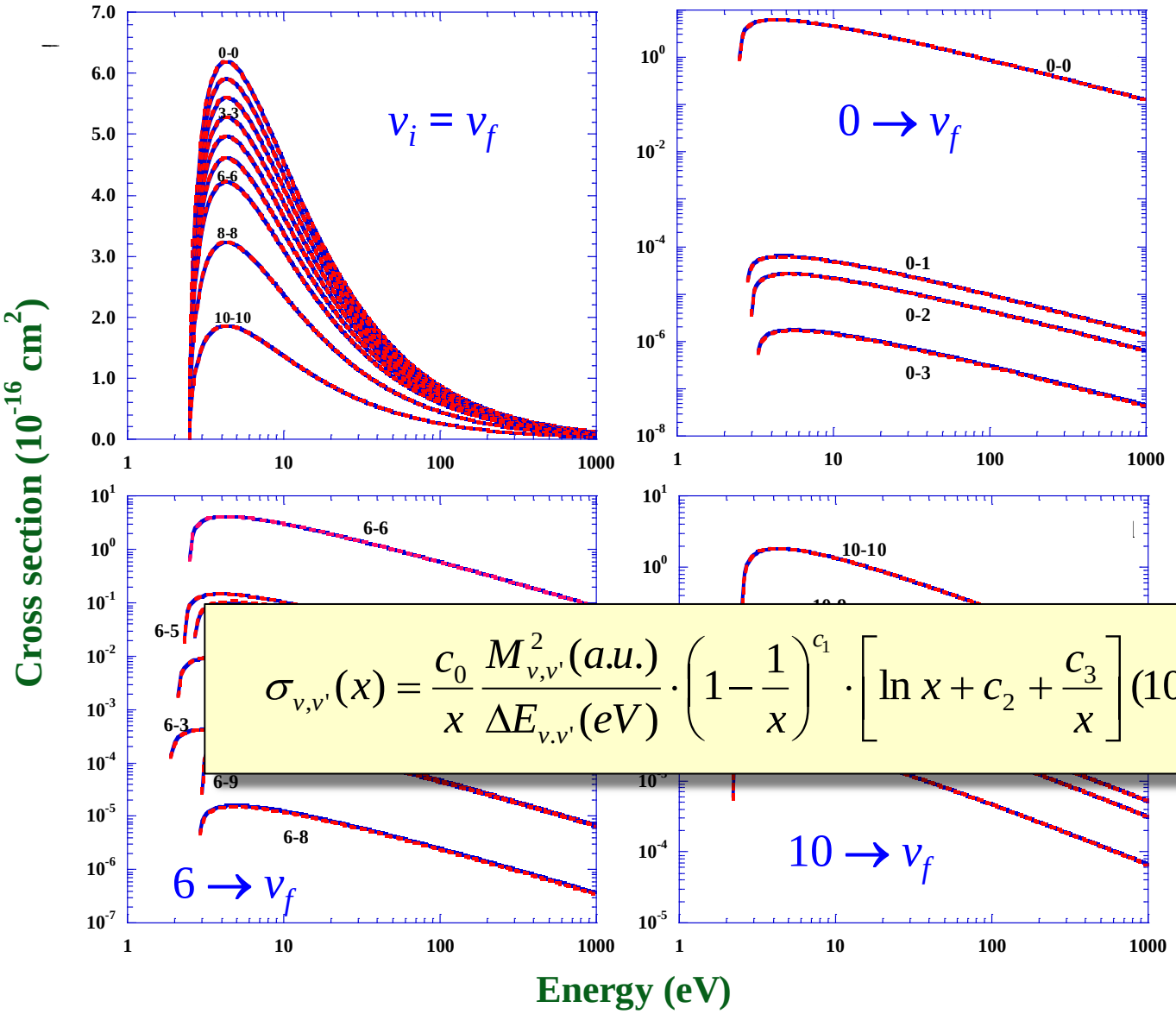



J. Pitarch-Ruiz, Sanchez-Marin, Velasco, Martin
*J. Chem. Phys.* (2008).

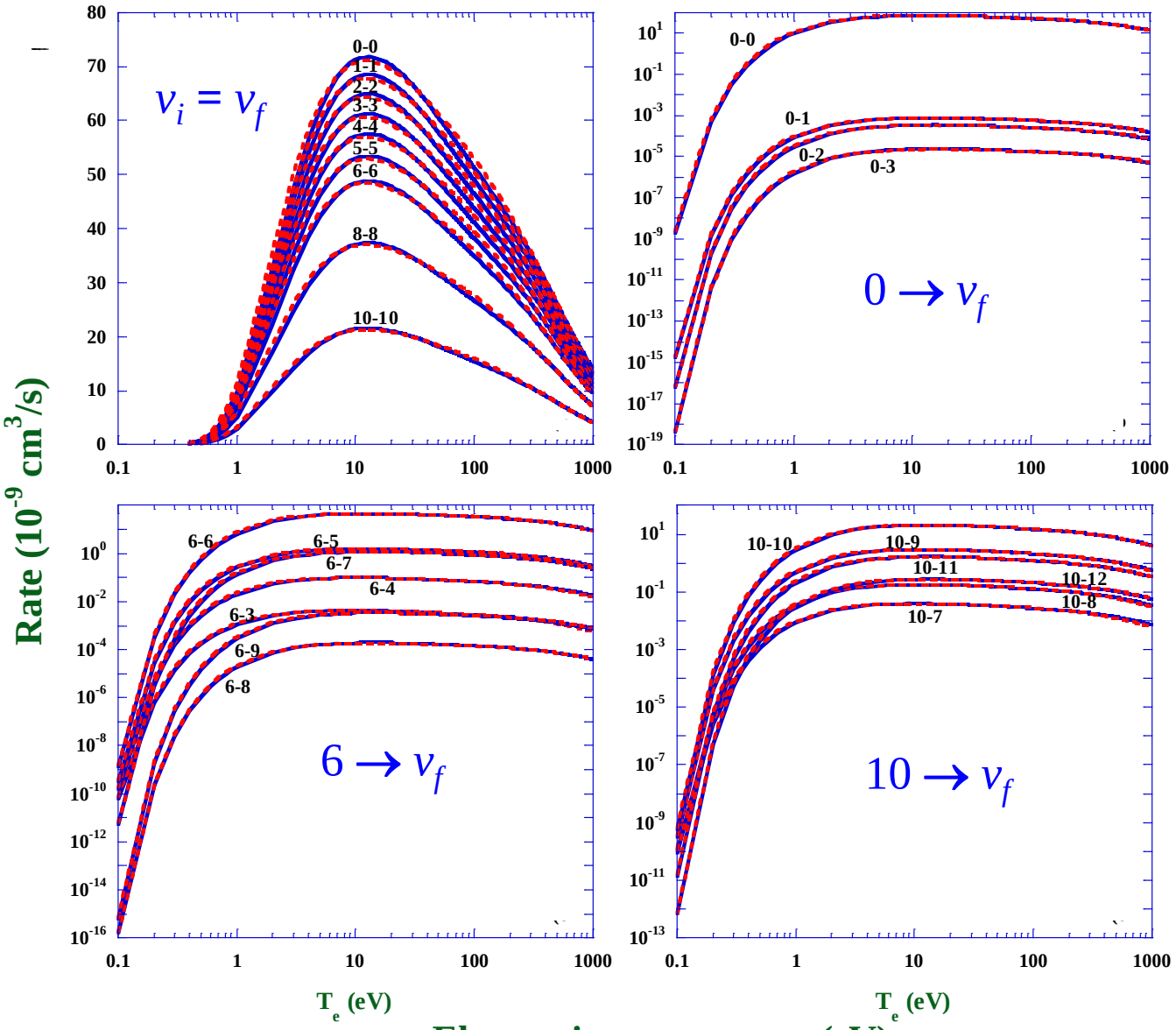

Cross section ($10^{-16}$ cm$^2$)
16
14
12
10
8.0
6.0
4.0
2.0
0.0
2
4
6
8
10
12
14
16
Energy (eV)
Born
TM MM
*R*-matrix
$0 \rightarrow 0$

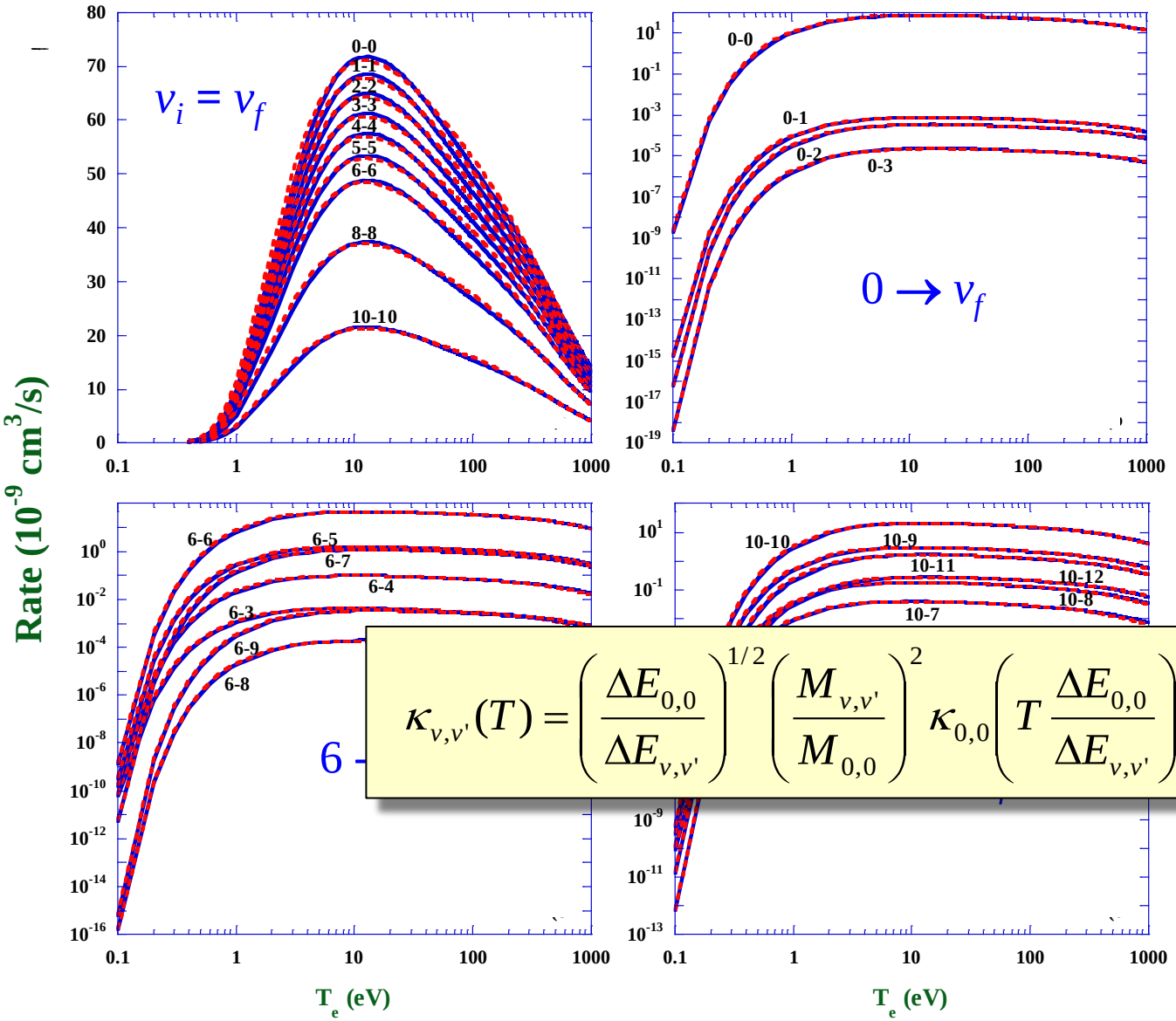

Cross section ($10^{-16}$ cm$^2$)
14
12
10
8.0
6.0
4.0
2.0
0.0
1
10
100
1000
Energy (eV)
Born
*R*-matrix
TM MM


Cross section ($10^{-16}$ cm$^2$)
Energy (eV)
$v_i = v_f$
0-0
3-3
6-6
8-8
10-10
$0 \rightarrow v_f$
0-0
0-1
0-2
0-3
$6 \rightarrow v_f$
6-6
6-5
6-7
6-4
6-3
6-9
6-8
$10 \rightarrow v_f$
10-10
10-9
10-11
10-12
10-8
10-7




$$\sigma_{v,v'}(x) = \frac{c_0}{x}\frac{M^2_{v,v'}(a.u.)}{\Delta E_{v,v'}(eV)} \cdot \left(1 - \frac{1}{x}\right)^{c_1} \cdot \left[\ln x + c_2 + \frac{c_3}{x}\right](10^{-16} cm^2)$$


Rate ($10^{-9}$ cm$^3$/s)
$v_i = v_f$
0-0
1-1
2-2
3-3
4-4
5-5
6-6
8-8
10-10
$0 \rightarrow v_f$
0-1
0-2
0-3
$6 \rightarrow v_f$
6-5
6-7
6-4
6-3
6-9
6-8
$10 \rightarrow v_f$
10-9
10-11
10-12
10-8
10-7
$T_e$ (eV)
Electronic temperature (eV)



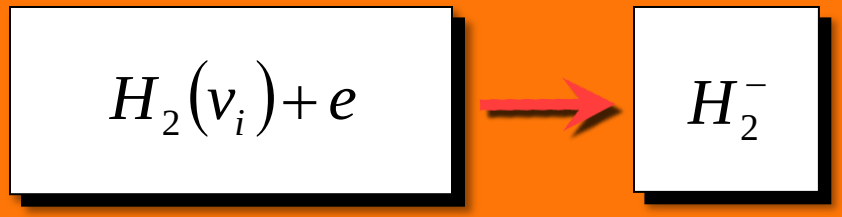

$$\kappa_{v,v'}(T) = \left(\frac{\Delta E_{0,0}}{\Delta E_{v,v'}}\right)^{1/2} \left(\frac{M_{v,v'}}{M_{0,0}}\right)^{2} \kappa_{0,0}\left(T\,\frac{\Delta E_{0,0}}{\Delta E_{v,v'}}\right) \left(10^{-9}\, cm^3 s^{-1}\right)$$

# Resonant processes

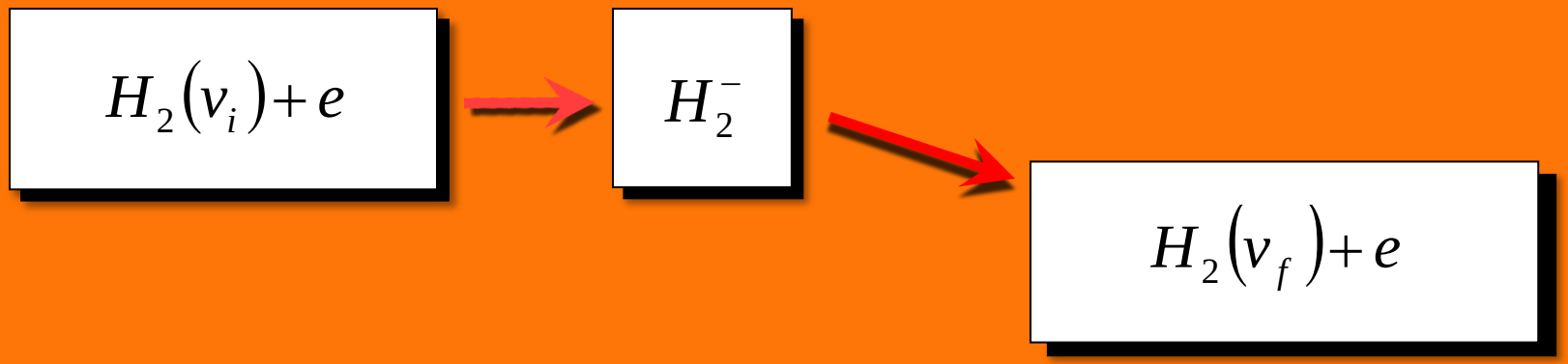
# Resonant processes

$H_2(v_i) + e$

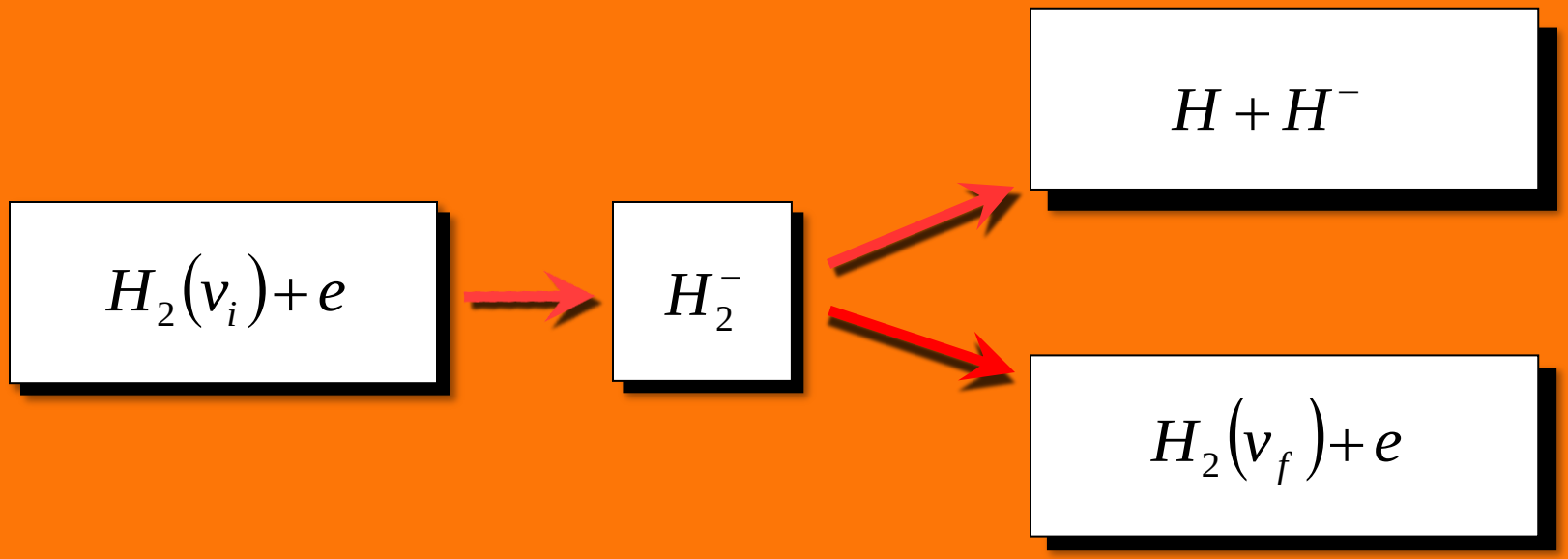
# Resonant processes



# Resonant processes



# Resonant processes



## DEA Negative ion sources

$$H_2(v) + e \rightarrow H_2^- \rightarrow H + H^-$$

$$H_2(v') + e \rightarrow H_2^- \rightarrow H_2(v'') + e$$

## DEA Negative ion sources

$$H_2(v) + e \rightarrow H_2^- \rightarrow H + H^-$$

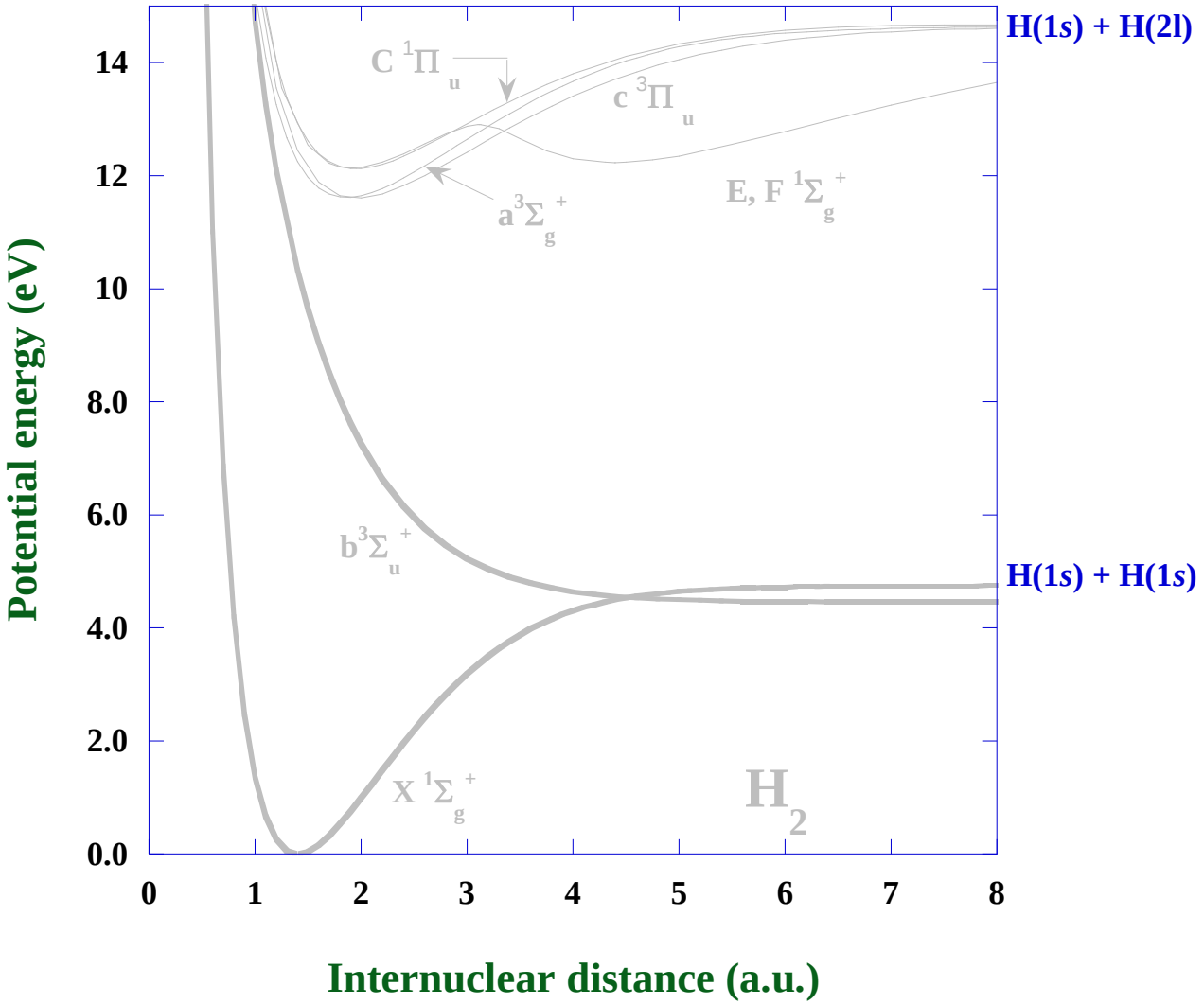
$$H_2(v') + e \rightarrow H_2^- \rightarrow H_2(v'') + e$$

## Molecular Assisted Recombination (MAR)

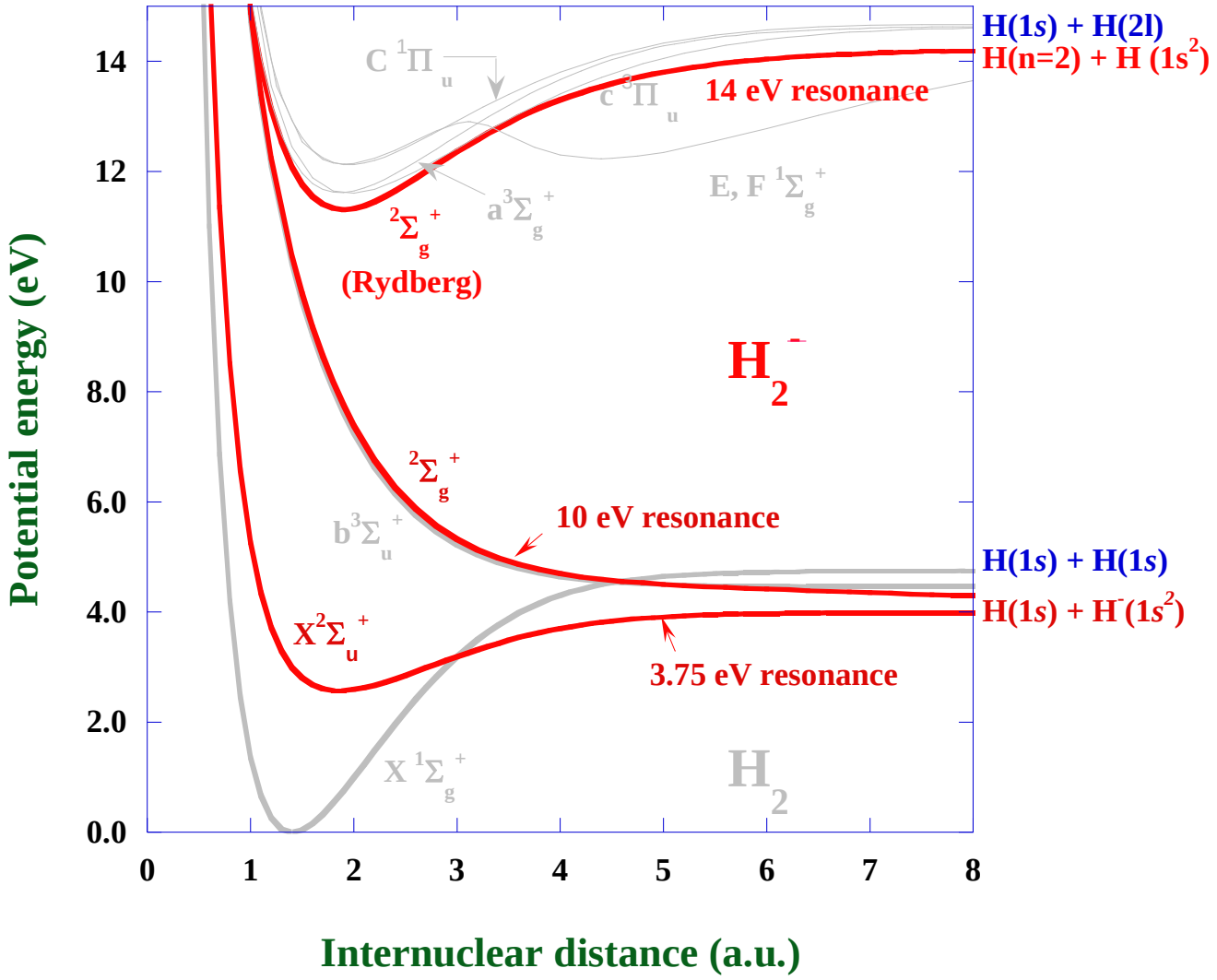
$$H_2(v \geq 4) + e \rightarrow H_2^- \rightarrow H + H^-$$

$$H^+ + H^- \rightarrow H + H$$

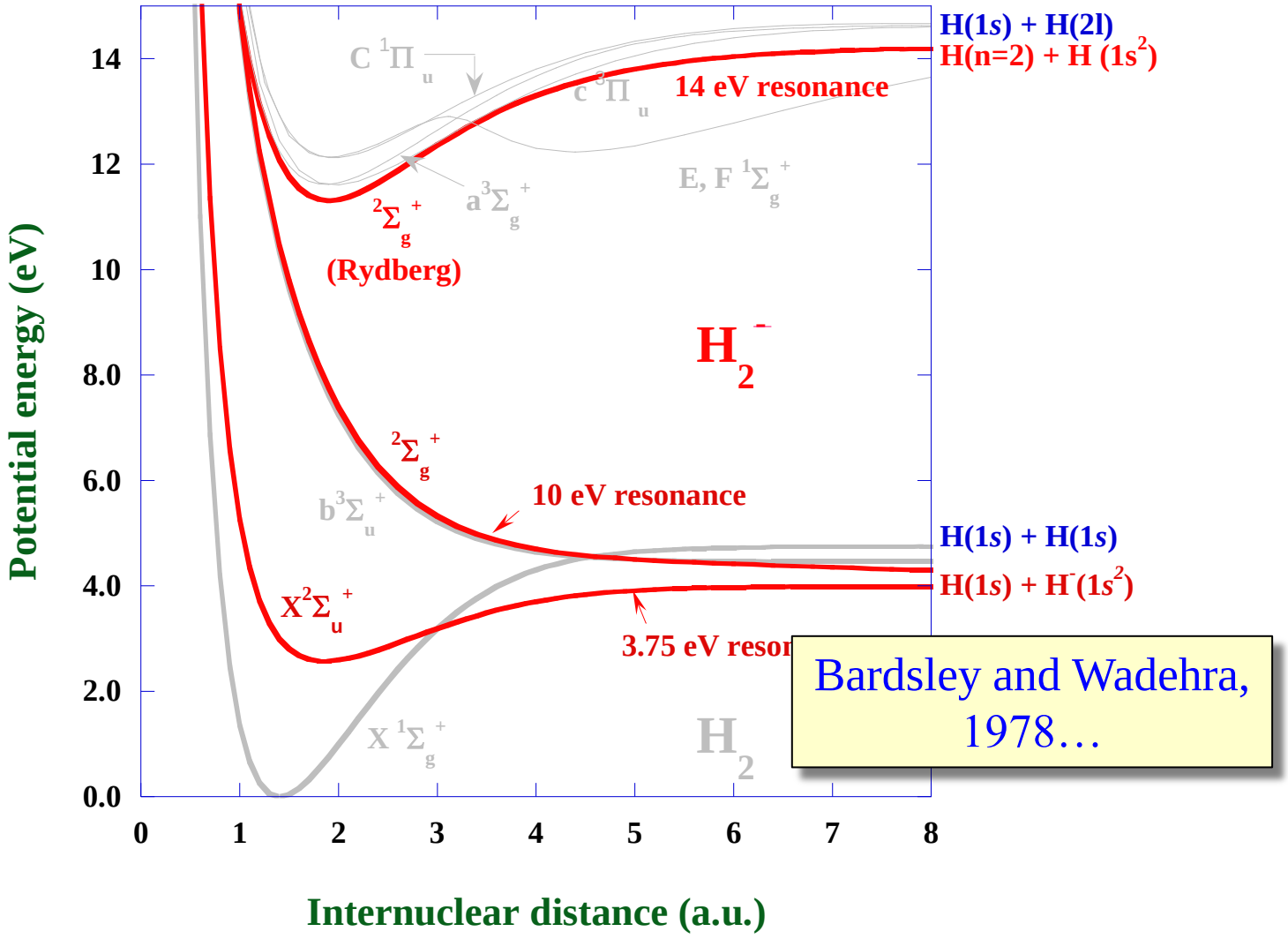
# Resonant processes



# Resonant processes

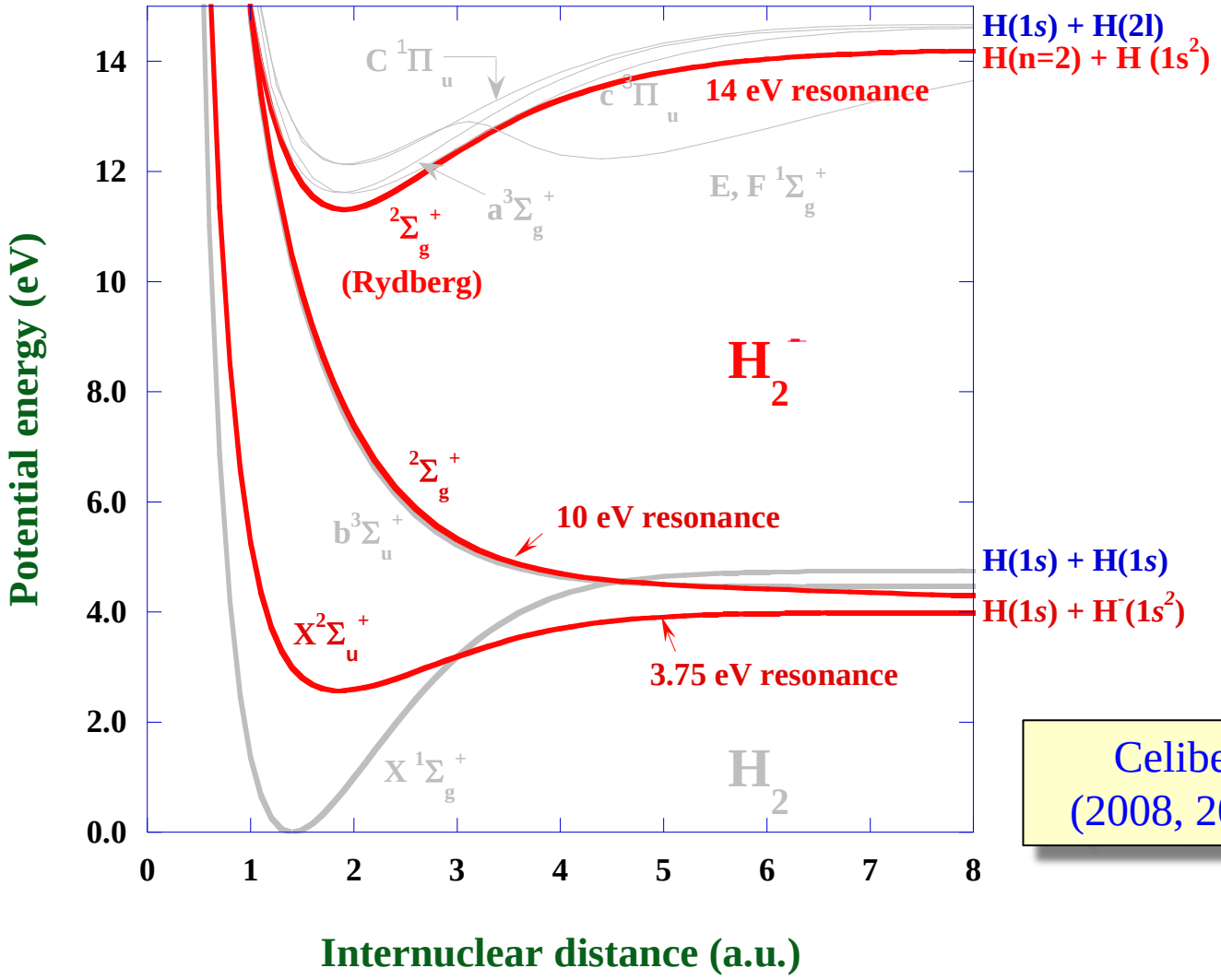


# Resonant processes




Bardsley and Wadehra, 1978…

# Resonant processes

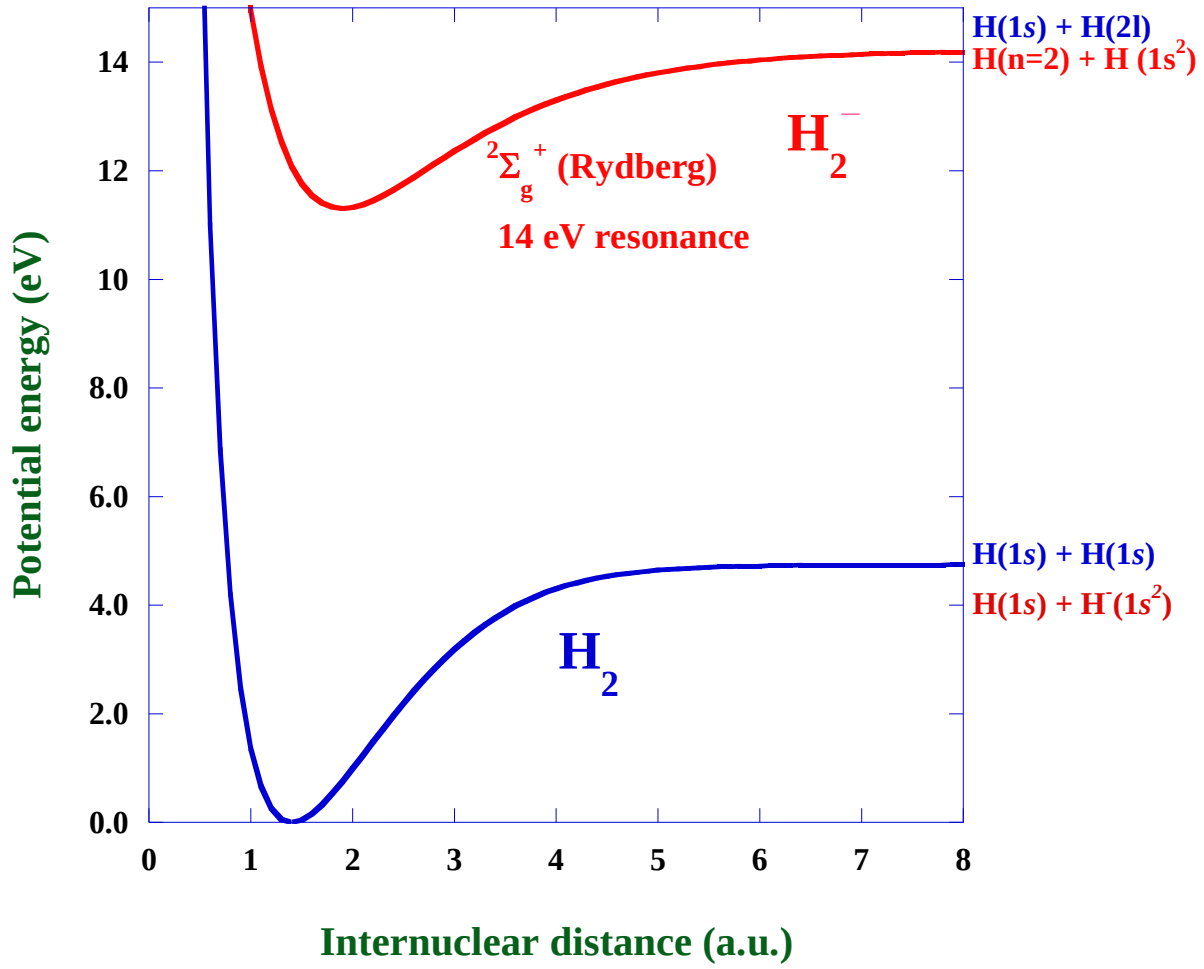


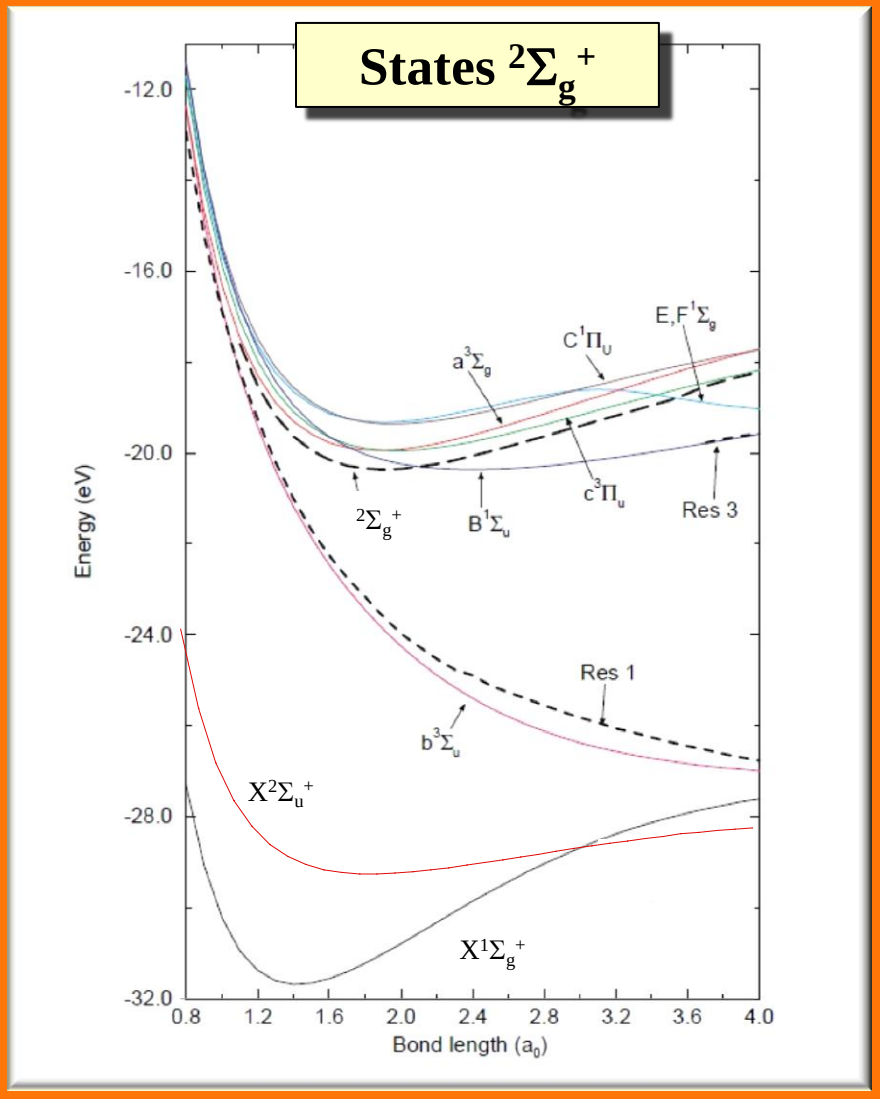

Celiberto et al
(2008, 2009, 2012)

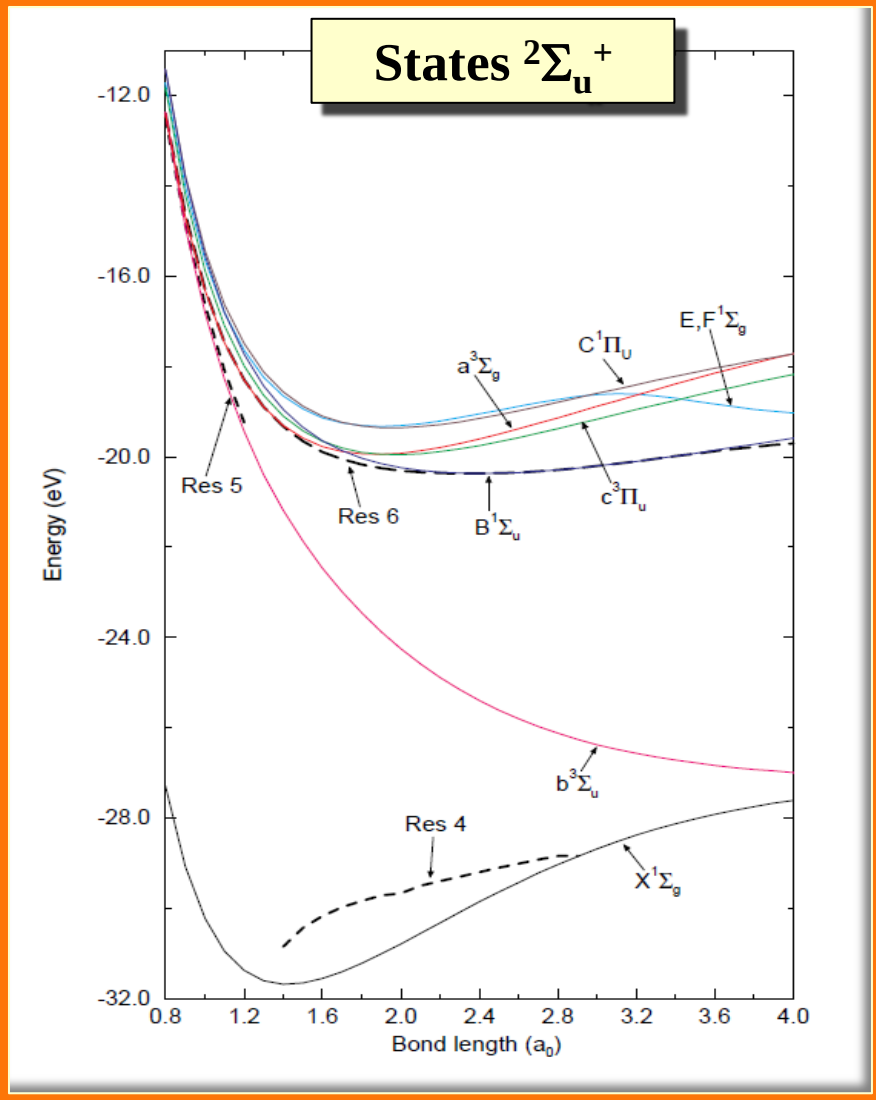
$H_2(v_i) + e \rightarrow H_2^-(^2\Sigma_g^+)^*$

$\rightarrow H^*(n = 2) + H^-(1s^2)$ Dissociative Electron Attachment

$\rightarrow H_2(v_f) + e$ Resonant Vibrational Excitation

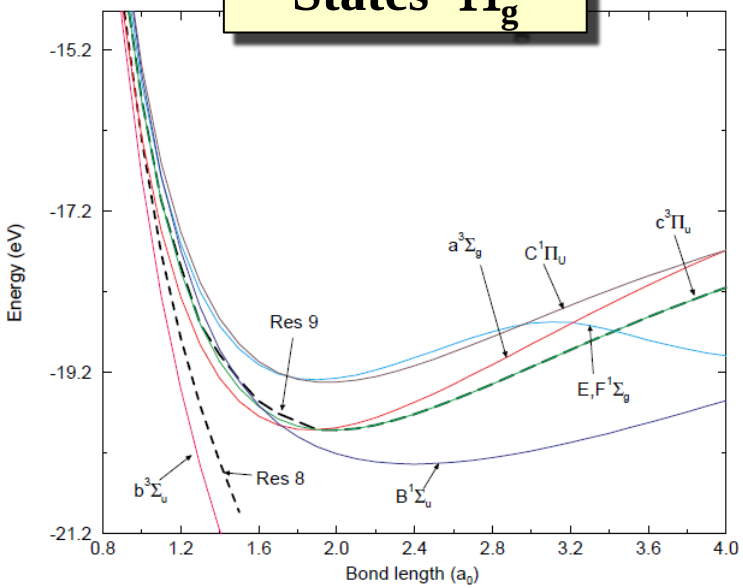




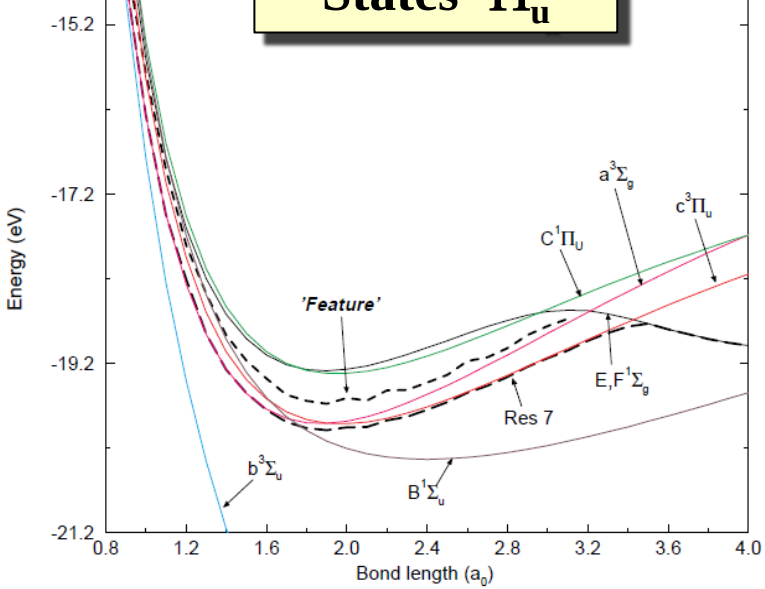




**D. Stibbe & J. Tennyson**
***J. Phys. B: At. Mol. Opt. Phys.* (1998)**

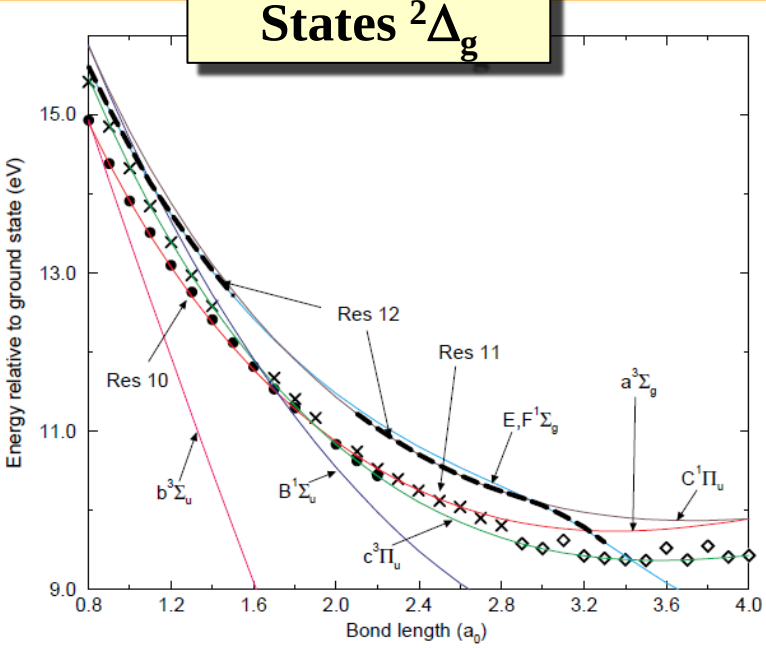
## States $^2\Pi_g$



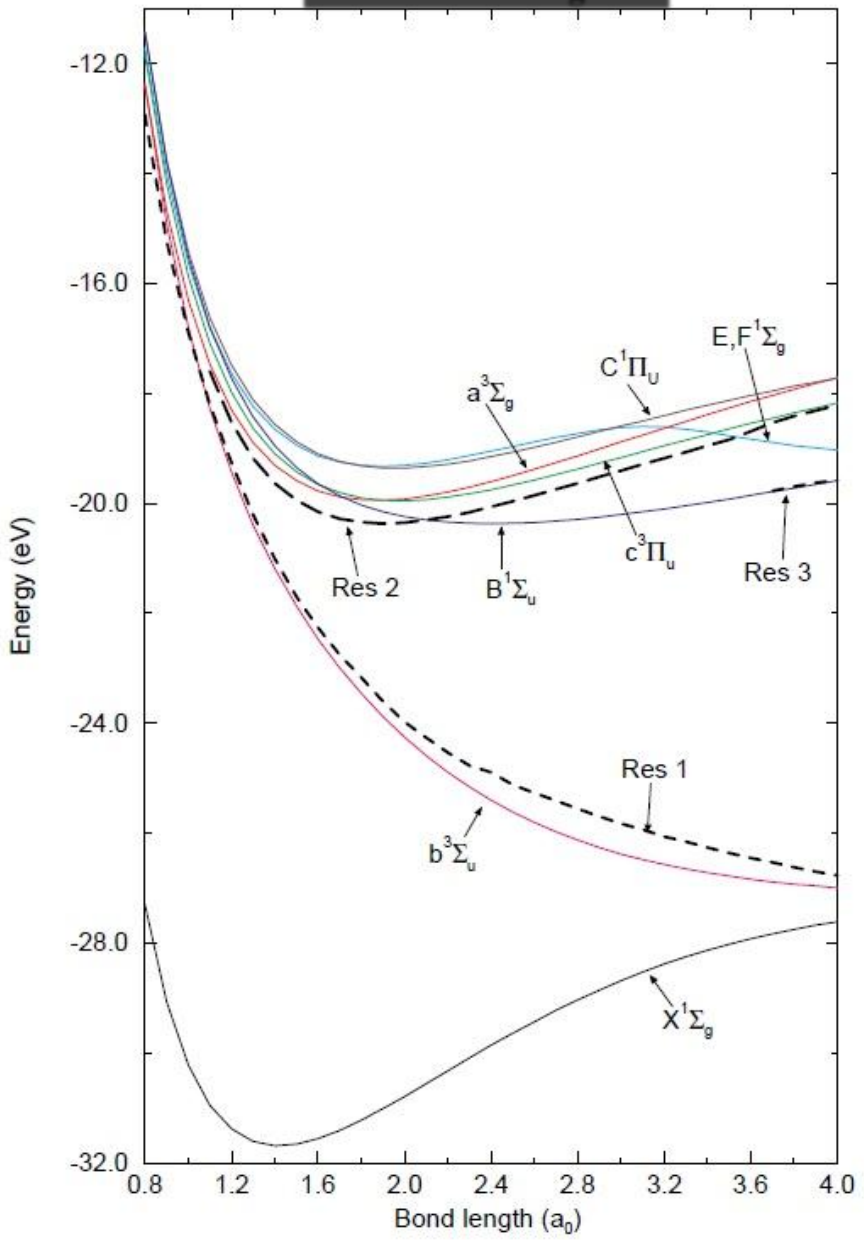

## States $^2\Pi_u$



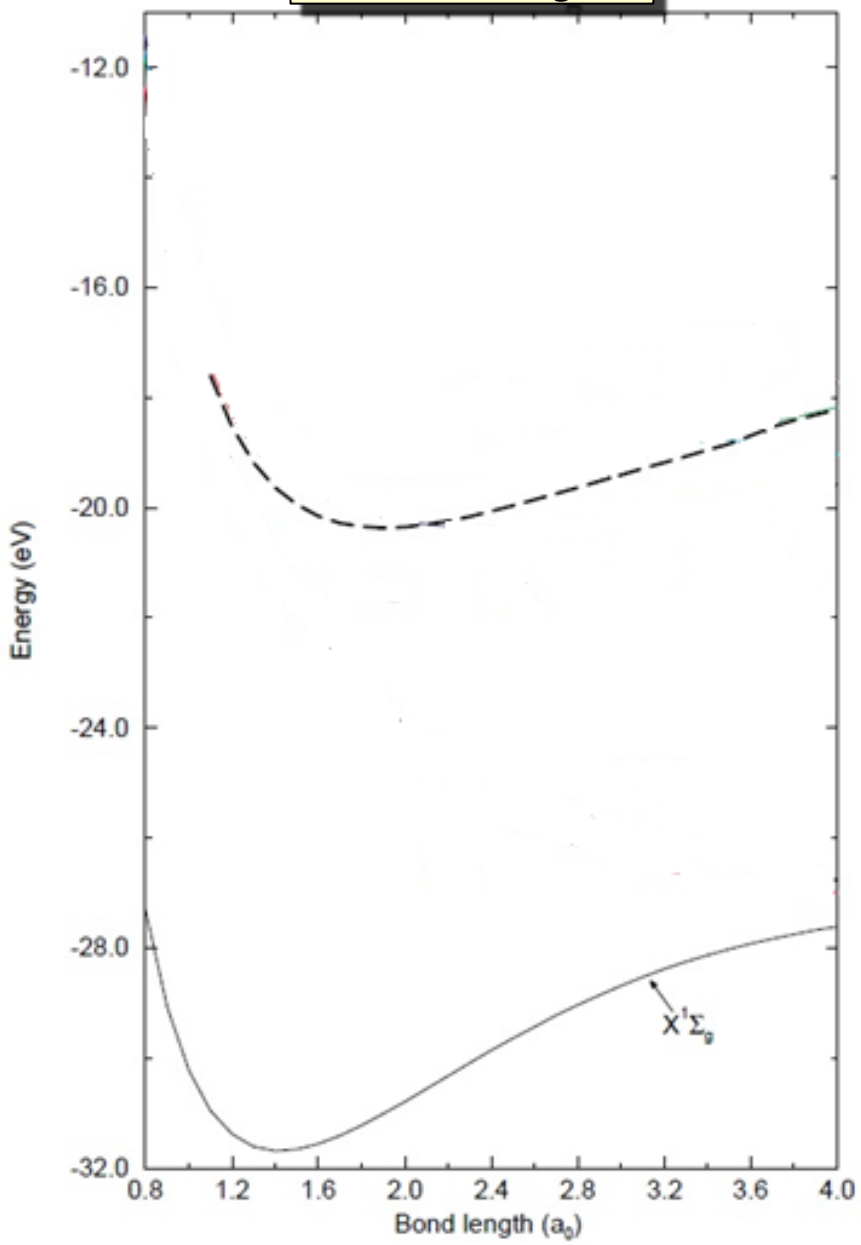

## States $^2\Delta_g$



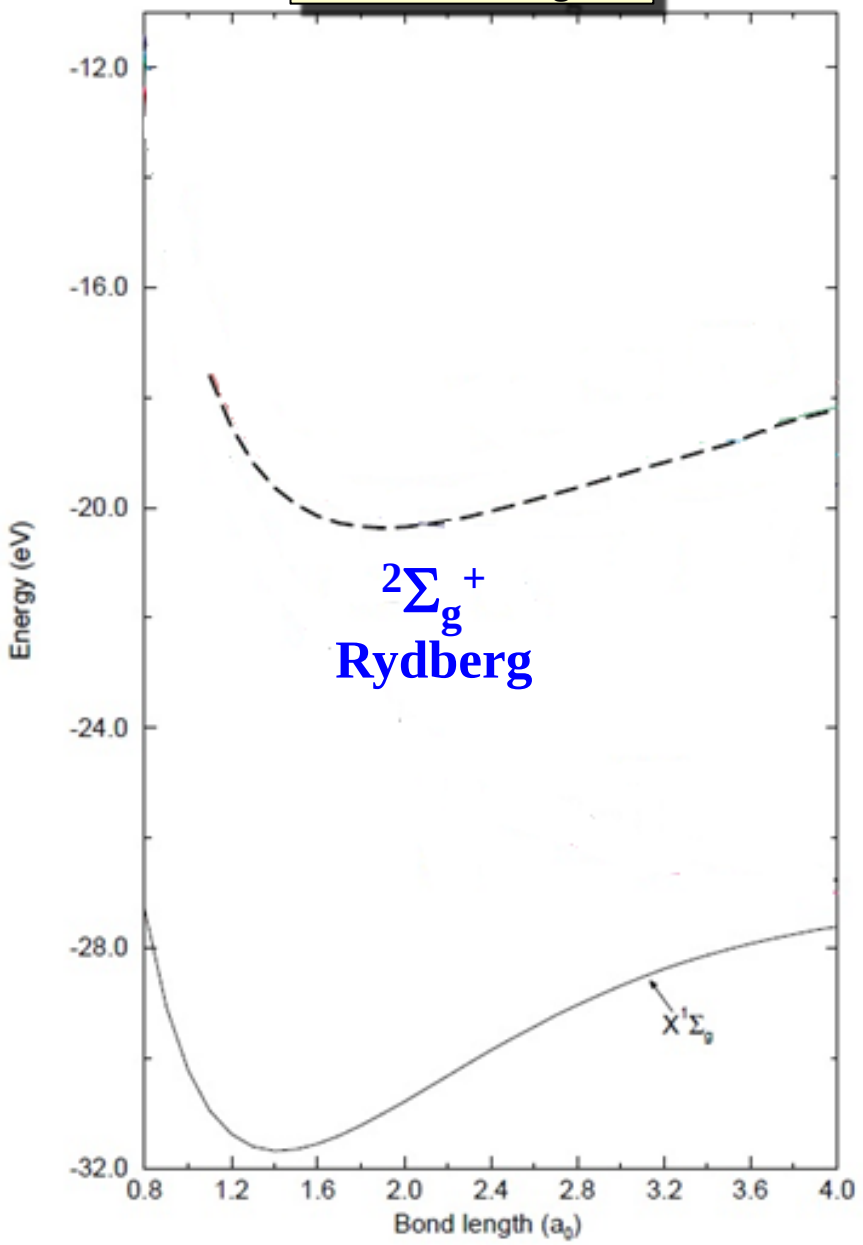
# States $^2\Sigma_g^+$



# States $^2\Sigma_g^+$

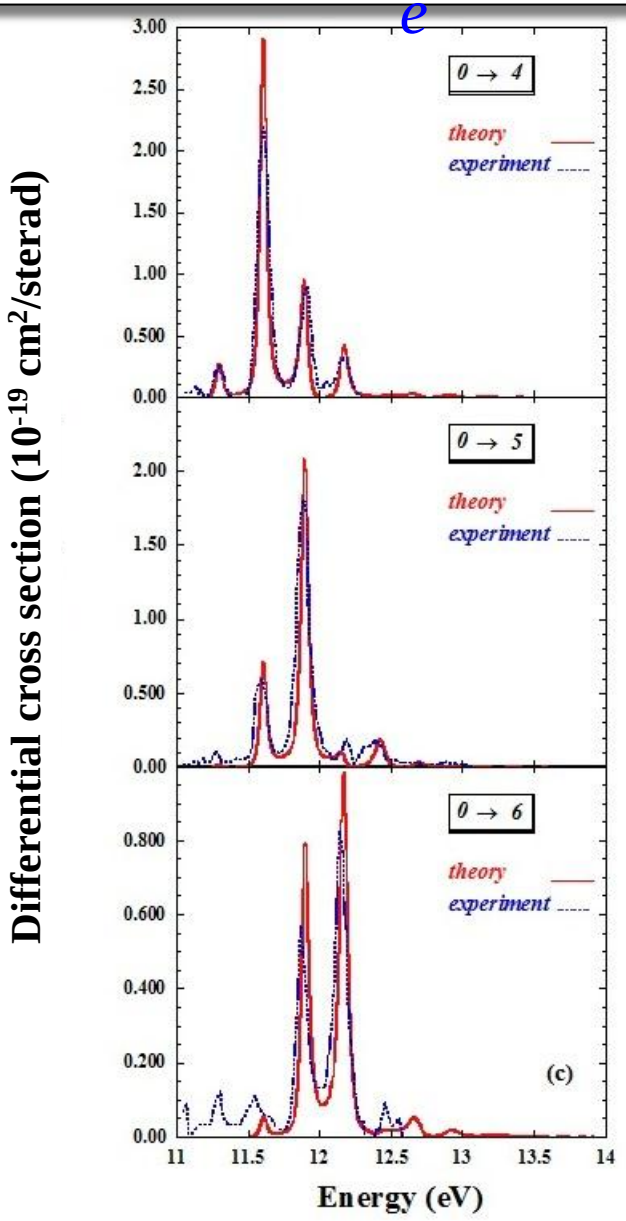


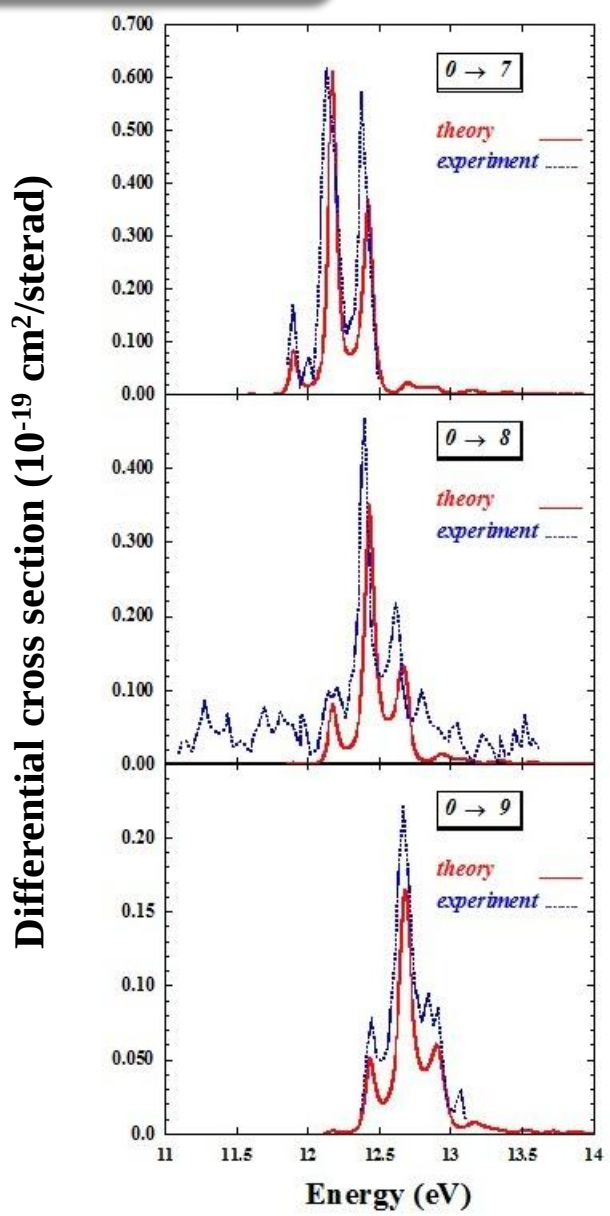
# States $^2\Sigma_g^+$



$H_2(v_i = 0) + e \rightarrow H_2^-(^2\Sigma_g^+)^* \rightarrow H_2(v_f) + e$

θ = 85°

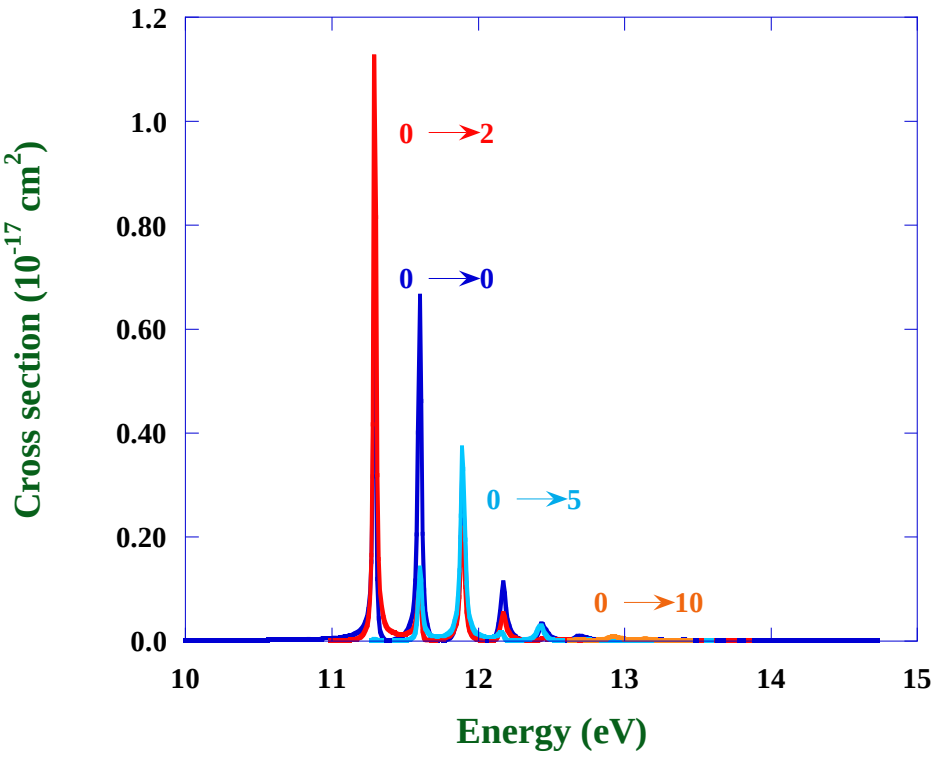


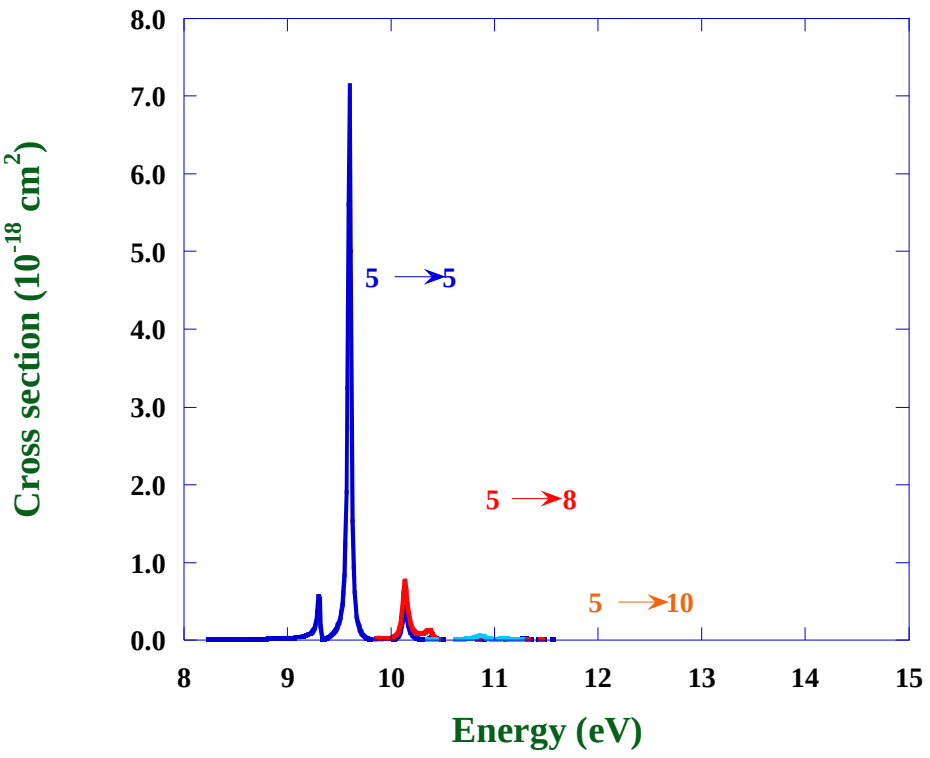




Comer & Read (1971)

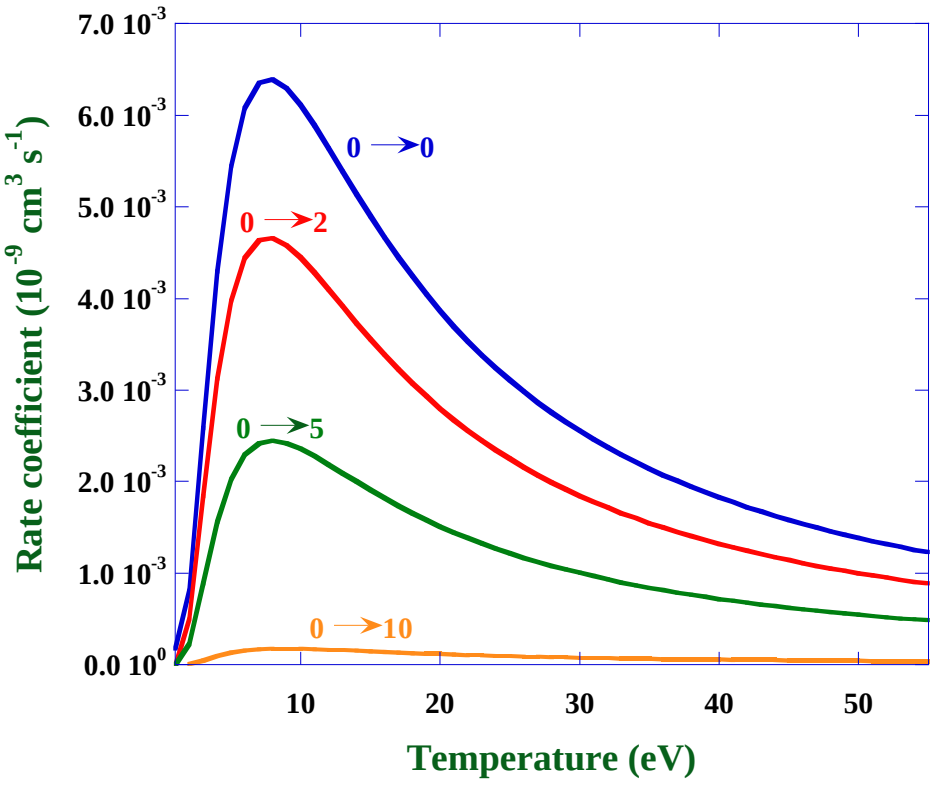
Celiberto et al (2008)

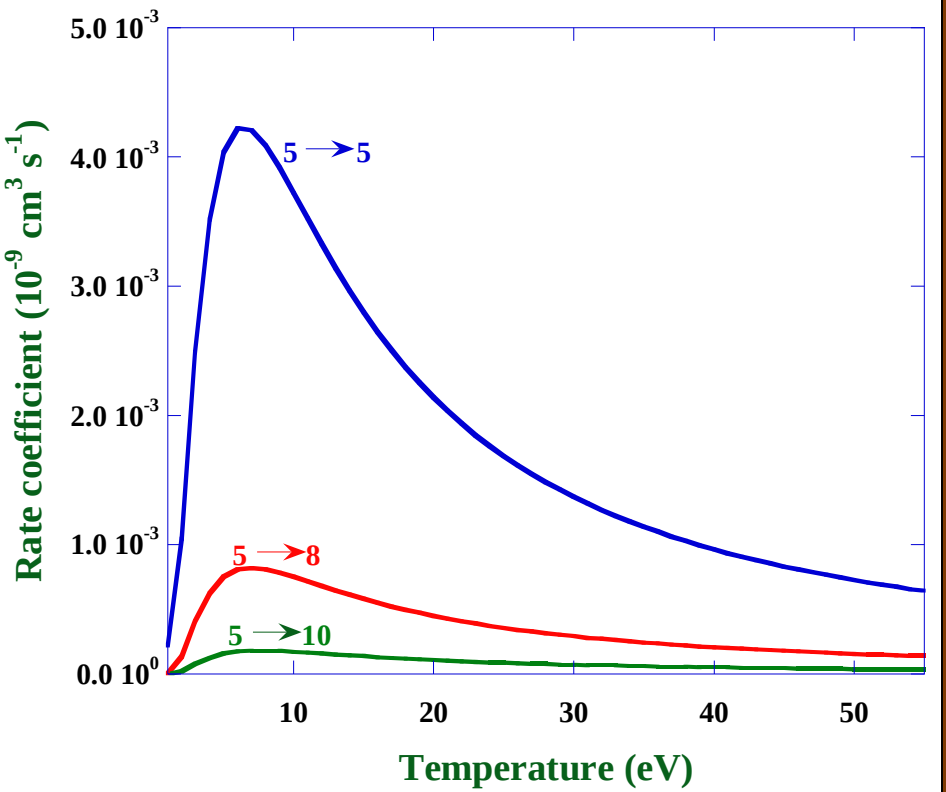
$$H_2(v_i) + e \rightarrow H_2^-(^2\Sigma_g^+)^* \rightarrow H_2(v_f) + e$$



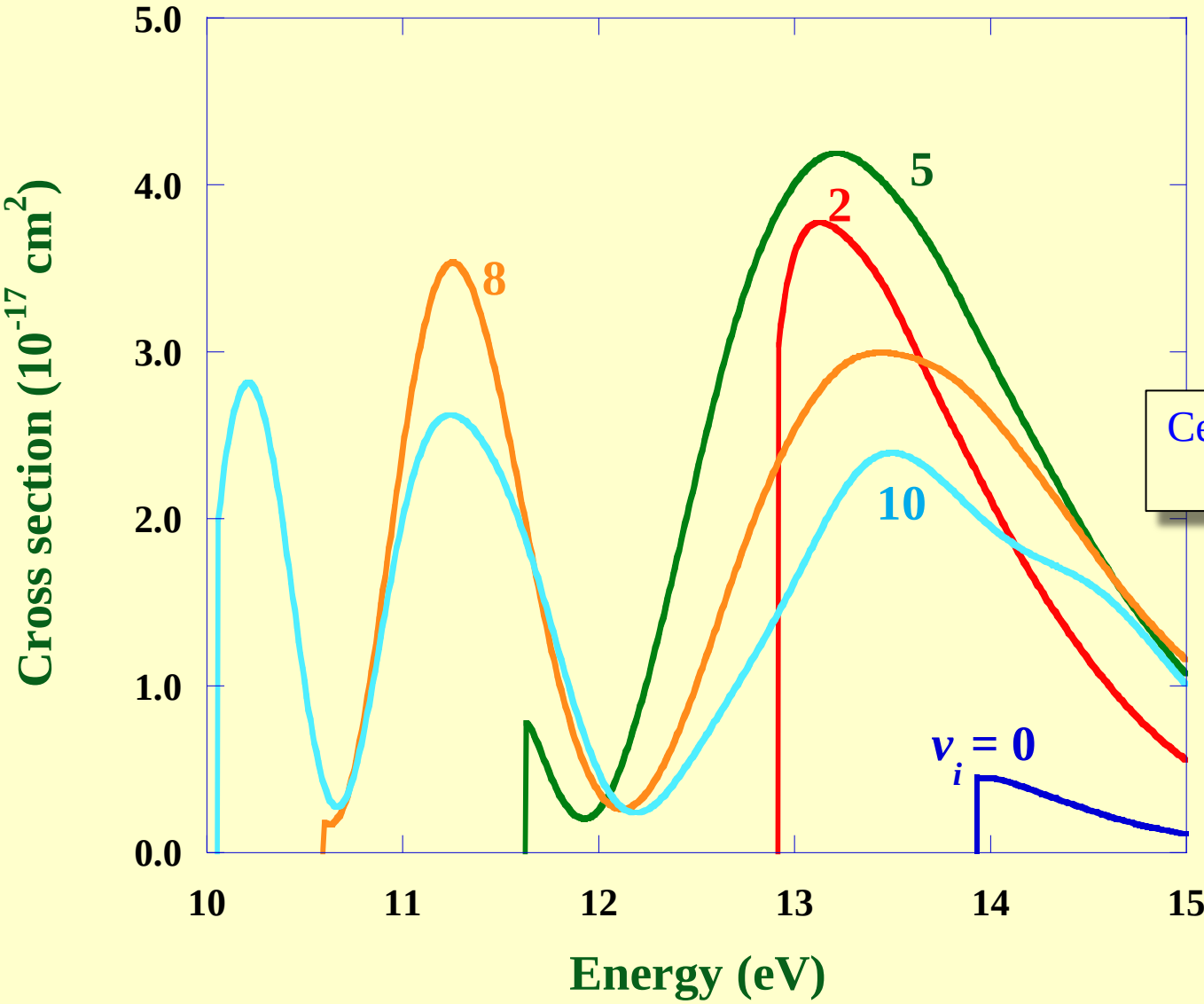



$$H_2(v_i) + e \rightarrow H_2^-(^2\Sigma_g^+)^* \rightarrow H_2(v_f) + e$$



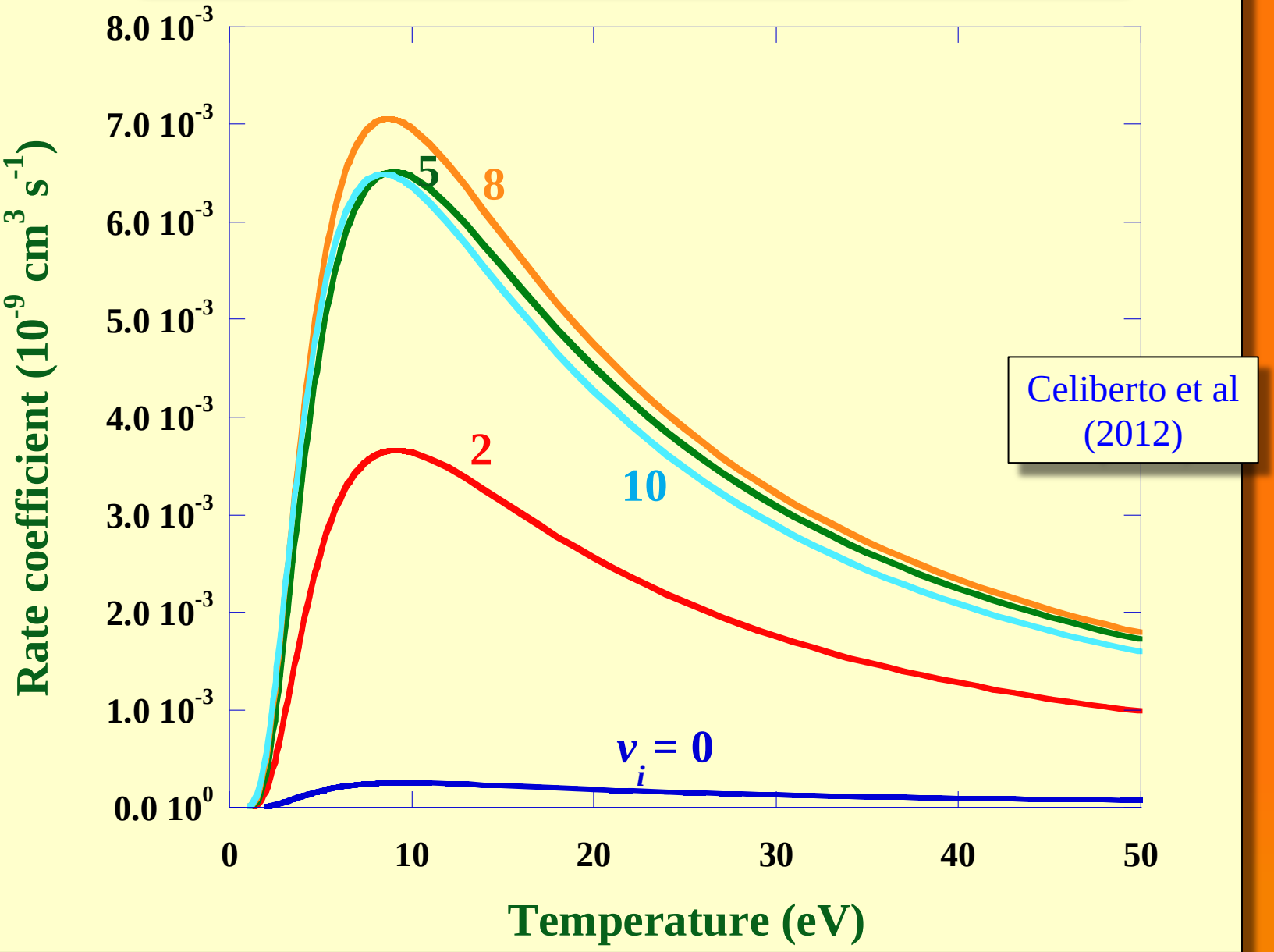



$$H_2(v_i) + e \rightarrow (H_2^-)^* \rightarrow H^*(n = 2) + H^-$$




Celiberto et al (2012)

$$H_2(v_i) + e \rightarrow (H_2^-)^* \rightarrow H^*(n = 2) + H^-$$



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THE PHYS4ENTRYDB TEAM

PHYS4ENTRY *database design*

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