Low-energy collisions between two indistinguishable tritium-bearing hydrogen molecules: HT+HT and DT+DT

Renat A. Sultanov

Odessa College, Department of Mathematics, 201 W. University Blvd, Odessa,

Texas 79764, USA

25th European Conference on Few-Body Problems in Physics

MAINZ, GERMANY

July 30 - August 4, 2023

emails: rsultanov@odessa.edu (private r.sultanov2@yahoo.com)

Financial support from the **Alexander von Humboldt Foundation** and the **EFB25 Conference Organizing Committee** is gratefully acknowledged.

1. In the interstellar medium **(ISM)**, in cool stellar and in various planetary atmospheres, astronomers extensively observe and identify different atoms and molecules.
2. These molecules are detected through emission and adsorption of electromagnetic radiation.
3. The radiation and its interpretation provide astronomers with valuable information about astronomical objects.

1. In order to obtain correct interpretation of different physical and chemical processes in the areas of interest in ISM it is important to know: **cross sections and thermal rate coefficients** of all microscopical processes in the population of emitting and adsorbing atoms and molecules.

$$\Lambda_{\mathrm{HD}}(T) = n_{j_1}(\mathrm{H_2}) n_{j_2}(\mathrm{HD}) \times k_{j_1 j_2 \to j_1' j_2'}(T) \times h\nu_{j_2 j_2'}$$

$$\Lambda'_{\mathrm{HD}} = \Lambda_{\mathrm{HD}}(T) - \Lambda_{\mathrm{HD}}(T_{CMB}), \quad T < 100 \text{ K}$$

Few - Body Atomic Collisions

1. $\mathrm{H} + \mathrm{H}_2(v,j) \rightarrow \mathrm{H}_2(v',j') + \mathrm{H}$

2. $\mathrm{H} + \mathrm{HD}(v,j) \rightarrow \mathrm{HD}(v',j') + \mathrm{H}$ **PES for** H_3**.**

3. $\mathrm{He} + \mathrm{H}_2(v,j) \rightarrow \mathrm{H}_2(v',j') + \mathrm{He}$

4. $\mathrm{He} + \mathrm{HD}(v,j) \rightarrow \mathrm{HD}(v',j') + \mathrm{He}$ **PES for** $\mathrm{He} + \mathrm{H}_2$**.**

5) $\mathrm{H}_2(v_1,j_1) + \mathrm{H}_2(v_2,j_2) \rightarrow \mathrm{H}_2(v_1',j_1') + \mathrm{H}_2(v_2',j_2')$

6) $\mathrm{H}_2(v_1,j_1) + \mathrm{HD}(v_2,j_2) \rightarrow \mathrm{H}_2(v_1',j_1') + \mathrm{HD}(v_2',j_2')$ **PES for** $\mathrm{H}_2 - \mathrm{H}_2$ **or** H_4**.**

7. **Water:** $\mathrm{H_2O} + \mathrm{H_2}$; $\mathrm{H_2O} + \mathrm{HD}$; $\mathrm{HDO} + \mathrm{H_2}$ **at 2K - 1000K.**

8. **3-Body Recombination:** $\mathrm{H} + \mathrm{H} + \mathrm{H} \rightarrow \mathrm{H_2} + \mathrm{H}.$

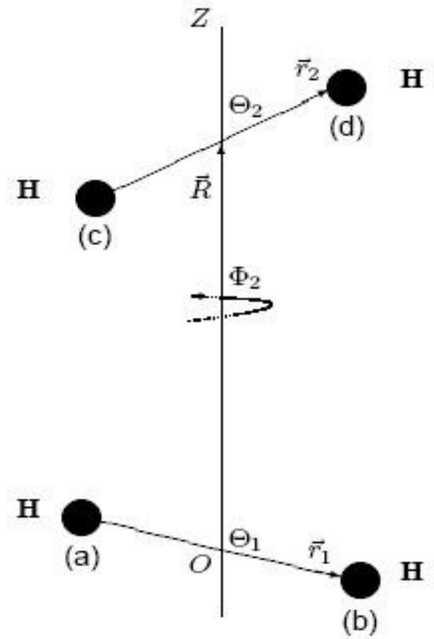
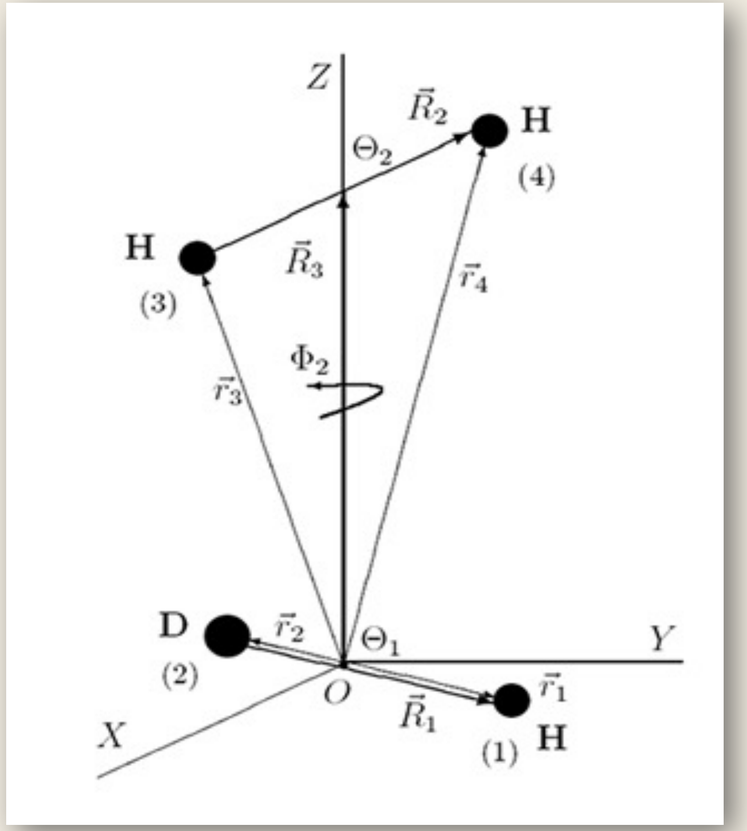


Fig. 1. 4-body coordinates for the H_2–H_2 system used in this work.



$$V(\vec{r}_1, \vec{r}_2, \overrightarrow{R}) = V(r_1, \theta_1, r_2, \theta_2, R, \phi_2) = V(\theta_1, \theta_2, R, \phi_2)$$

A Pure Quantum-Mechanical Approach:
rigid rotor model

$$(H_0 + V(\vec{r}_1, \vec{r}_2, \vec{R}) - E)\Psi(\vec{r}_1, \vec{r}_2, \vec{R}) = 0$$

$$\left(\frac{\hat{P}^2_{\vec{R}}}{2M_{12}} + \frac{\hat{L}^2_{\hat{r}_1}}{2\mu_1 r_1^2} + \frac{\hat{L}^2_{\hat{r}_2}}{2\mu_2 r_2^2} + V(\vec{r}_1, \vec{r}_2, \vec{R}) - E \right) \Psi(\hat{r}_1, \hat{r}_2, \vec{R}) = 0$$

$$M_{12} = 2m_h(m_h + m_d)/(3m_h + m_d)$$

$$\mu_1 = m_h/2\mu_2 = m_h m_d/(m_h + m_d)$$

$$\Psi(\hat{r}_1, \hat{r}_2, \vec{R}) = \sum_{JM j_1 j_2 j_{12} L} \frac{U^{JM}_{j_1 j_2 j_{12} L}(R)}{R} \phi^{JM}_{j_1 j_2 j_{12} L}(\hat{r}_1, \hat{r}_2, \vec{R})$$

$$\phi^{JM}_{j_1 j_2 j_{12} L}(\hat{r}_1, \hat{r}_2, \vec{R}) = \sum_{m_1 m_2 m_{12} m} C^{j_{12} m_{12}}_{j_1 m_1 j_2 m_2} C^{JM}_{j_{12} m_{12} l m} Y_{j_1 m_1}(\hat{r}_1) Y_{j_2 m_2}(\hat{r}_2) Y_{Lm}(\hat{R})$$

$$\left(\frac{d^2}{dR^2} - \frac{L(L+1)}{R^2} + k_\alpha^2\right) U_\alpha^{JM}(R) = 2M_{12} \sum_{\alpha'} \int < \phi_\alpha^{JM}(\hat{r}_1, \hat{r}_2, \vec{R})$$

$$|V(\vec{r}_1, \vec{r}_2, \vec{R})| \phi_{\alpha'}^{JM}(\hat{r}_1, \hat{r}_2, \vec{R}) > U_{\alpha'}^{JM}(R) d\hat{r}_1 d\hat{r}_2 d\hat{R}$$

$$\alpha \equiv (j_1 j_2 j_{12} L)$$

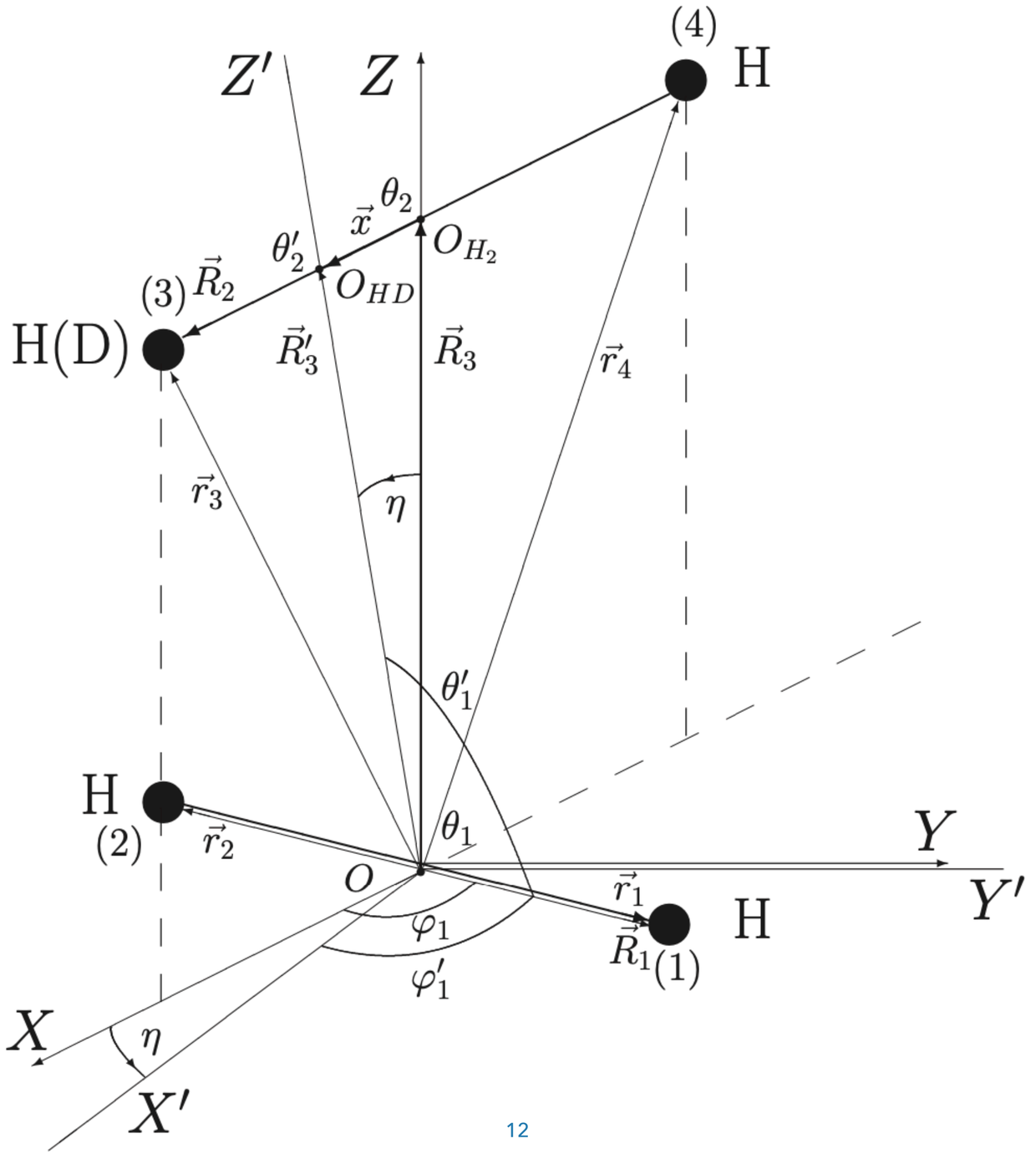
$$U_{\alpha}^{J} \underset{R\to+\infty}{\sim} \delta_{\alpha\alpha'} e^{-i(k_{\alpha\alpha}R-(l\pi/2))} - \sqrt{\left(\frac{k_{\alpha\alpha}}{k_{\alpha\alpha'}}\right)} S_{\alpha\alpha'}^{J} e^{-i(k_{\alpha\alpha'}R-(l'\pi/2))}$$

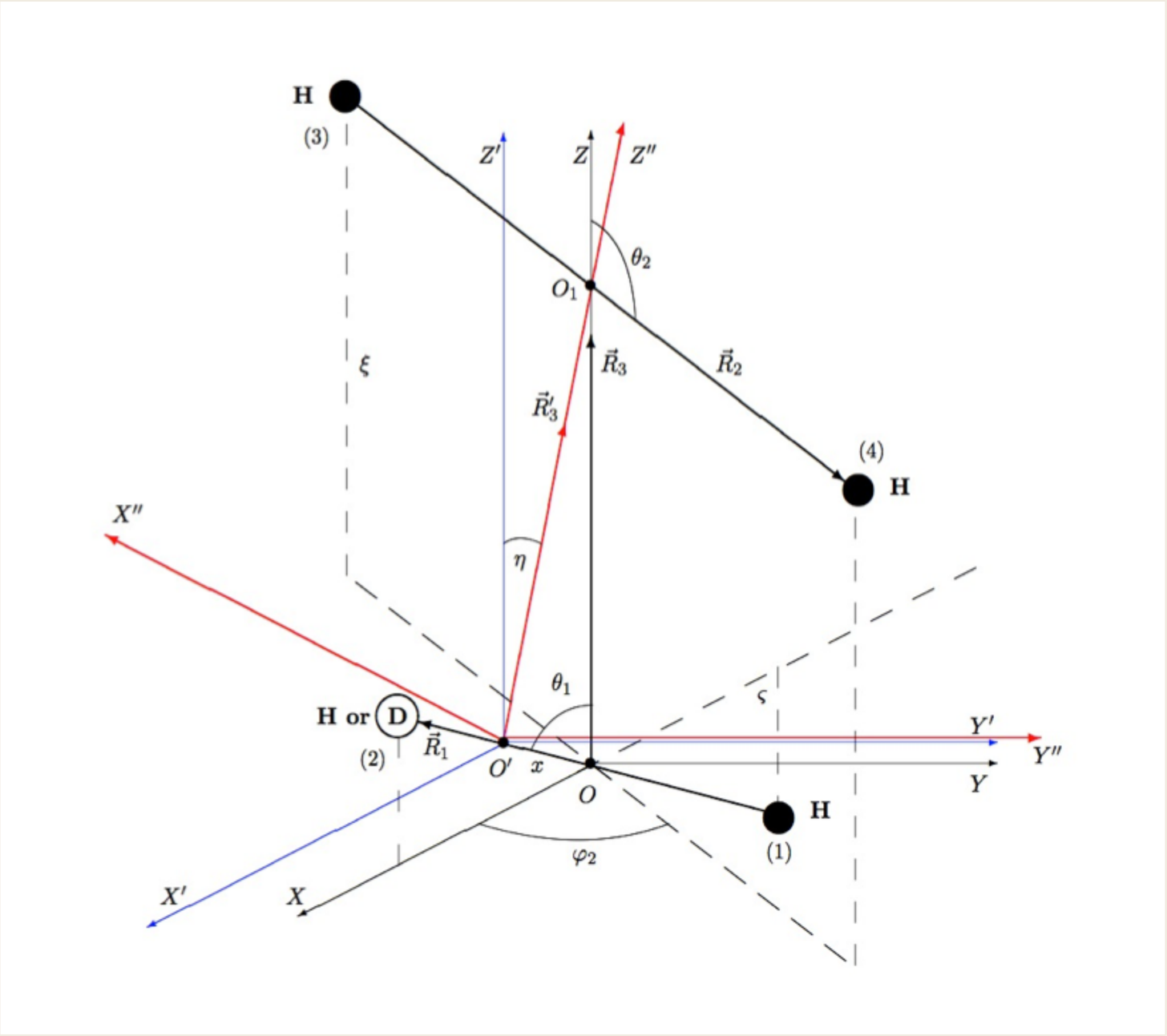
$$k_{\alpha\alpha'} = \sqrt{2M_{12}(E + E_{\alpha} - E_{\alpha'})}$$

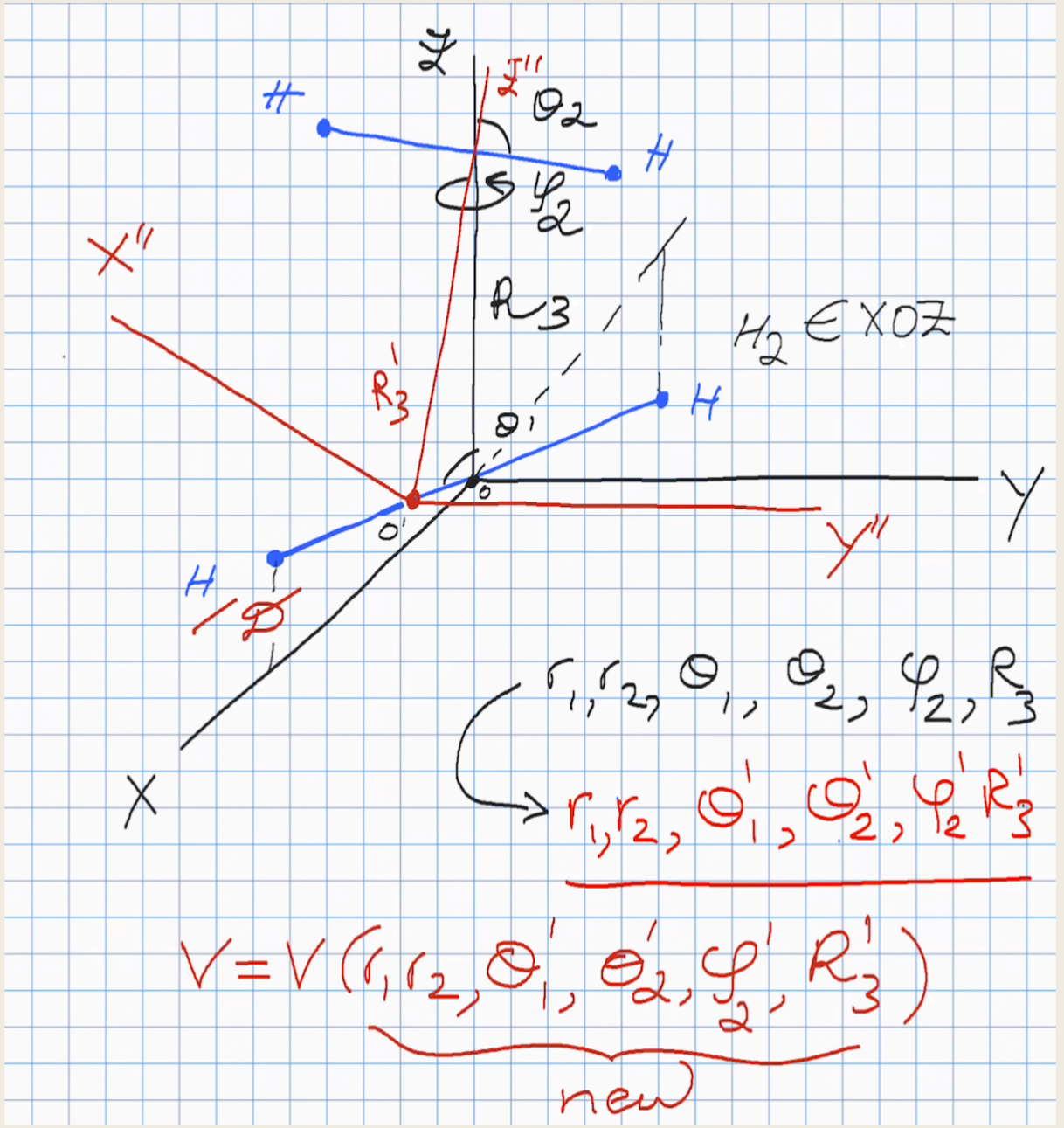
$$\sigma(j_1', j_2'; j_1 j_2, \epsilon) = \frac{\pi}{(2j_1+1)(2j_2+1)k_{\alpha\alpha'}} \sum_{J j_{12} j_{12}' L L'} (2J+1)|\delta_{\alpha\alpha'} - S^J(j_1', j_2', j_{12}' L'; j_1, j_2, j_{12}, L; E)|^2$$

$$\epsilon = E - B_1 j_1(j_1+1) - B_2 j_2(j_2+1)$$

$$k_{j_1 j_2 \to j_1' j_2'}(T) = \sqrt{\frac{8k_B T}{\pi M_{12}}} \frac{1}{(k_B T)^2} \int_{\epsilon_s}^{\infty} \sigma_{j_1 j_2 \to j_1' j_2'}(\epsilon) e^{-\epsilon/k_B T} \epsilon d\epsilon$$


(4)
H
Z'
Z
θ_2
$\vec{x}$
O_{H_2}
θ'_2
O_{HD}
(3)
$\vec{R}_2$
H(D)
$\vec{R}'_3$
$\vec{R}_3$
$\vec{r}_4$
$\vec{r}_3$
η
θ'_1
H
(2)
$\vec{r}_2$
θ_1
Y
O
$\vec{r}_1$
Y'
H
φ_1
$\vec{R}_1$
(1)
φ'_1
X
η
X'


H
(3)
Z′
Z
Z″
θ2
O1
ξ
R⃗3
R⃗2
R⃗′3
(4)
H
X″
η
θ1
H or D
R⃗1
(2)
O′
x
ς
Y′
Y″
Y
O
H
(1)
φ2
X′
X


Z
Z''
θ2
H
H
φ2
X''
R3
H2 ∈ XOZ
R'3
O'
H
O
Y
O'
Y''
H
φ2
X
r1, r2, θ1, θ2, φ2, R3
r1, r2, θ'1, θ'2, φ'2 R'3
V = V (r1, r2, θ'1, θ'2, φ'2, R'3)
new

$$\cos\eta = \frac{R_3'^2 + R_3^2 - x^2}{2R_3'R_3}$$

$$\sin\eta = \frac{x}{R_3'\sin\theta_1}$$

$$\theta_1' = \arccos(\cos\theta_1 \cos\eta + \sin\theta_1 \sin\eta),$$
$$\theta_2' = \arccos(\cos\theta_2 \cos\eta + \sin\theta_2 \sin\eta \cos\Phi_2),$$
$$\varphi_2' = \arccos\left(\cot\phi_2 \cos\eta + \frac{\cot\theta_1 \sin\eta}{\sin\phi_2}\right).$$

RESULTS

HD + *ortho*-H_2 , HD + *para*-H_2 , $H_2 + H_2$

Original H_2-H_2 *PESs*: DJ (2000), **BMKP (2002),** R. Hinde (2008).

1) A. I. Boothroyd, P. G. Martin, W. J. Keogh, and M. J. Peterson, *J. Chem. Phys. 116, 666 (2002).*

2) J. Schaefer, *Astron. Astrophys. Suppl. Ser. 85 (1990) 1101.*

3) D. R. Flower, E. Roueff, *Mon. Not. R. Astron. Soc. 309 (1999) 833.*

4) D. R. Flower, *J. Phys. B: At. Mol. Opt. Phys. 32 (1999) 1755.*

5) D. R. Flower, *Mon. Not. R. Astron. Soc. 318 (2000) 875.*

RECENT RESULTS: HD + H_2, H_2 + H_2

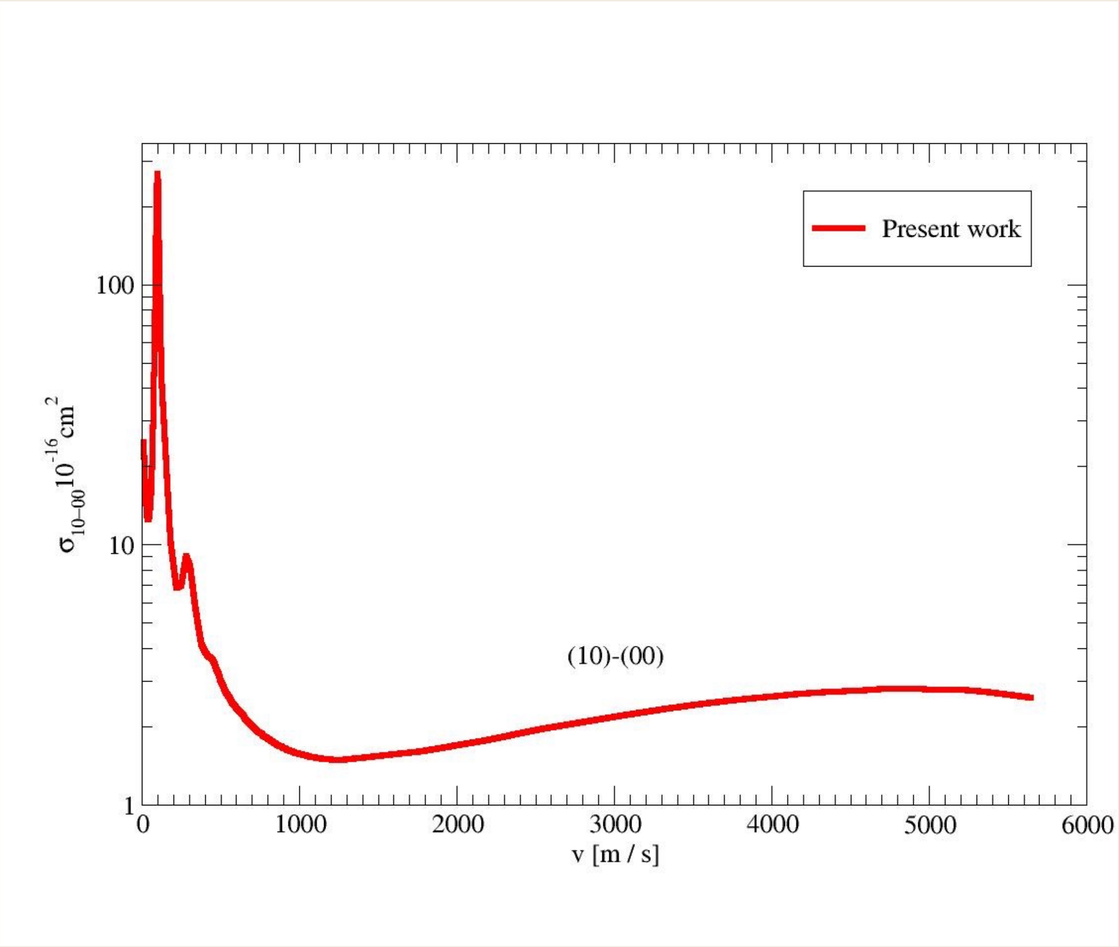
1) Balakrishnan N, Croft J F E, Yang B H, Forrey R C, and Stanci P C, **ApJ 2018** 866 : 95.

2) Wan Y, Balakrishnan N, Yang B H, Forrey R C, and Stancil P C, **MNRAS 2019** 488, 381.

3) Wan Yier, **PhD Dissertation 2019**, The University of Georgia, Athens, Georgia:

http://getd.libs.uga.edu/pdfs/wan_yier_201908_phd.pdf.

HD (j_1=1) + *para* - H_2 (j_2=0): (10) - (00) with BMKP PES (CPL 436 (2007) 19-24).



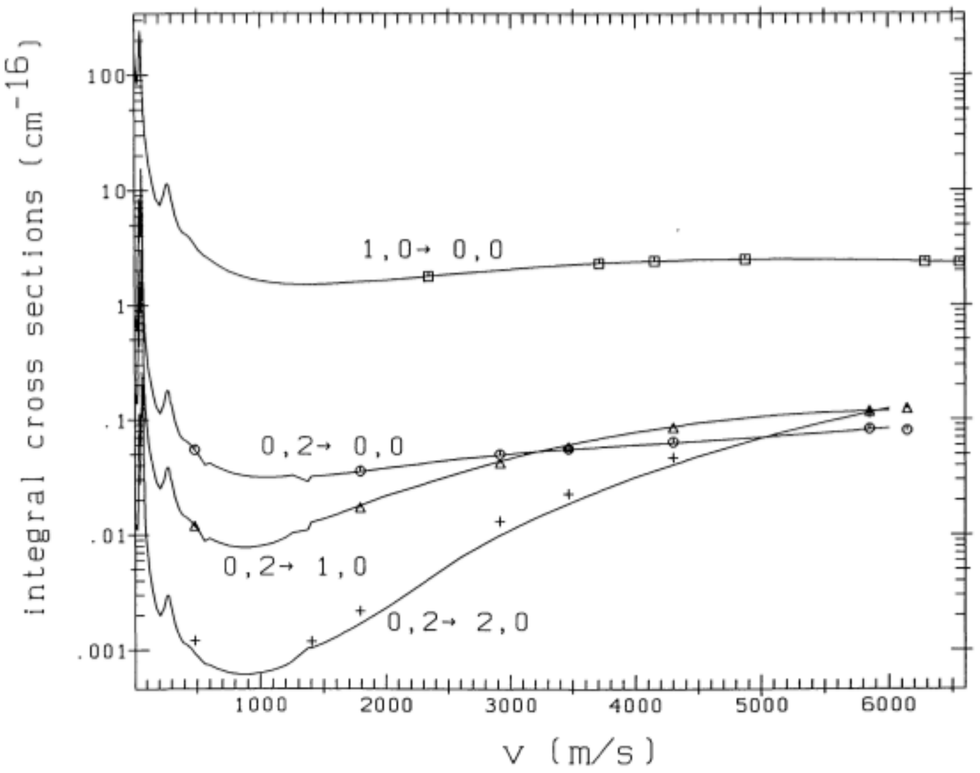
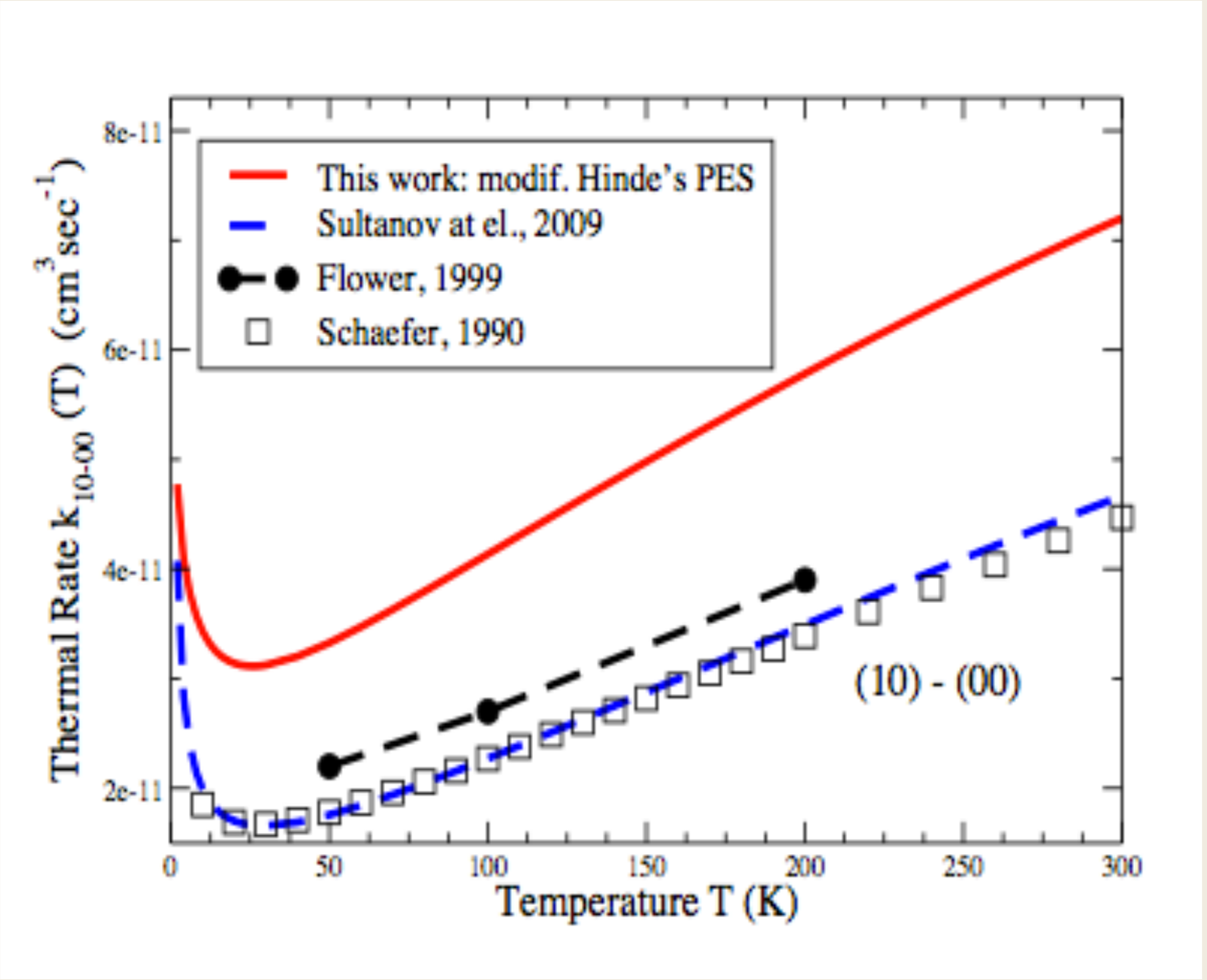
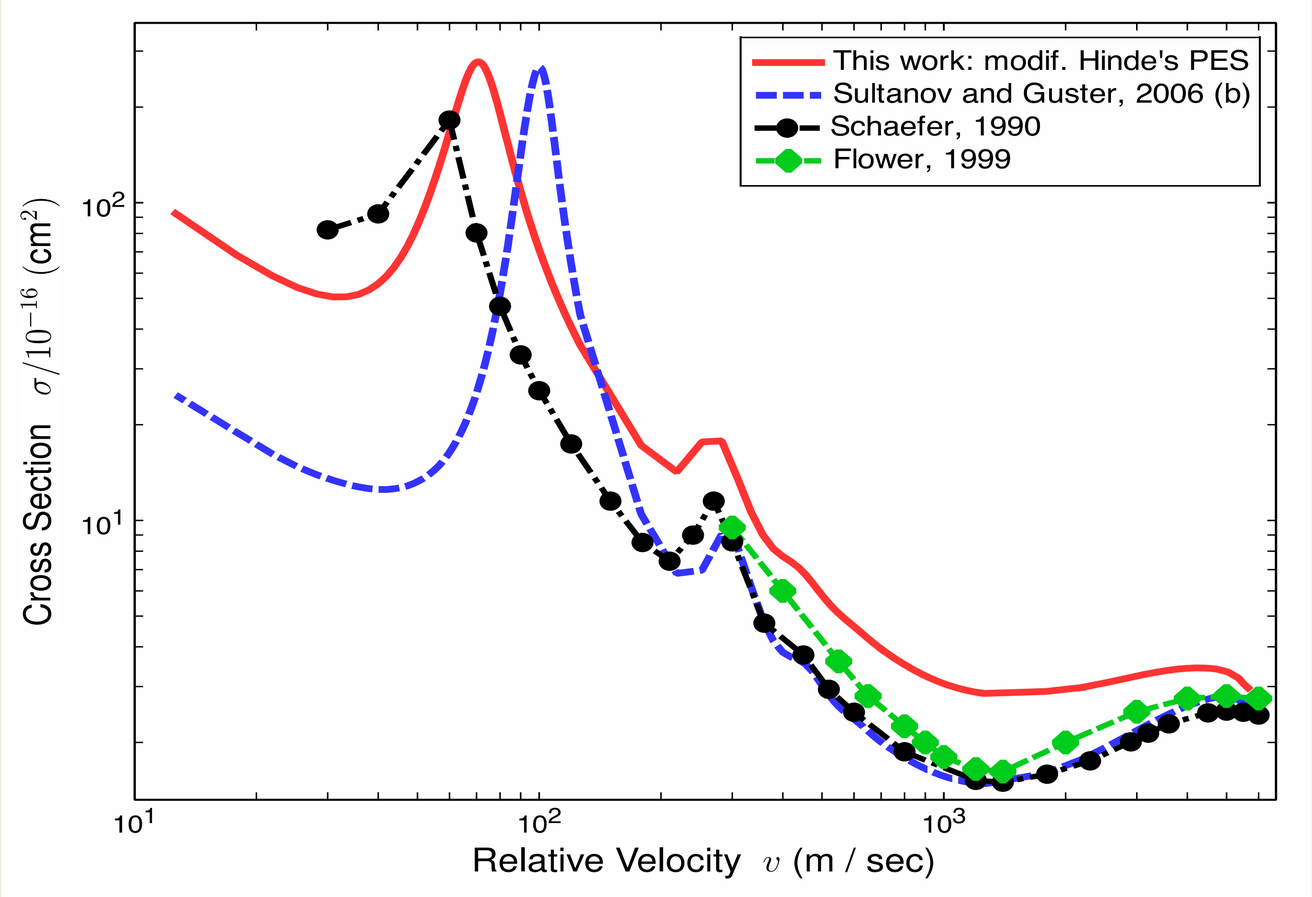
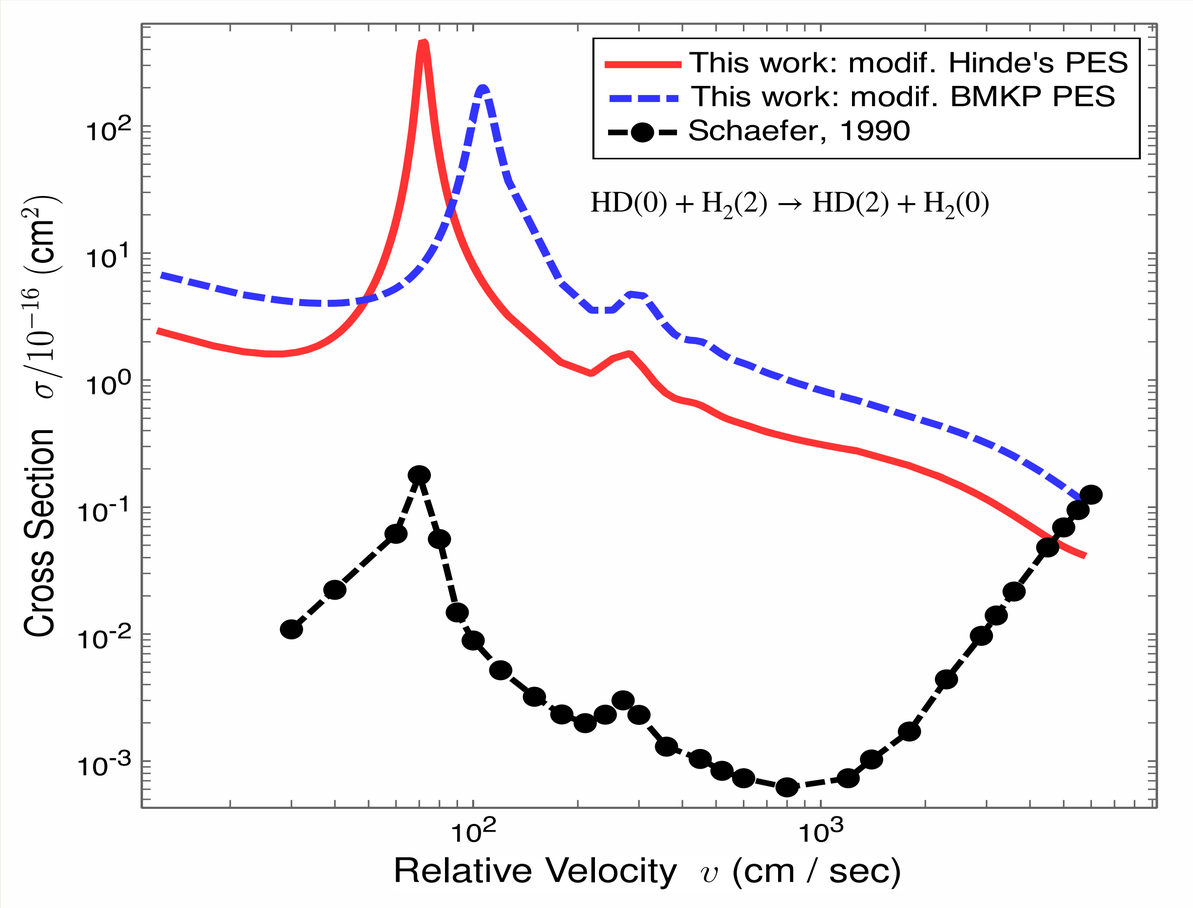


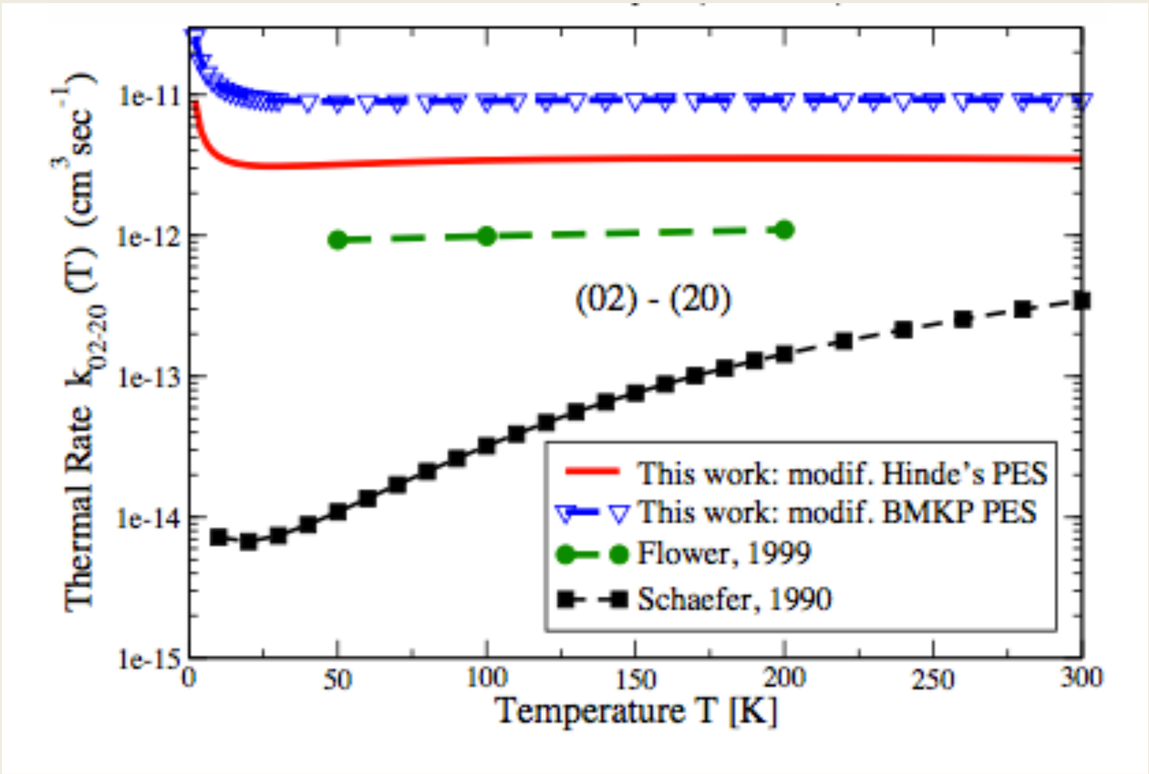
FIGURE 6. Calculated de-excitation cross sections of HD-H2 for transitions from j'_{HD}, $j'_{H2} = 1, 0$ and 0,2. The extra points on the curves are test results obtained from extended basis sets as explained in the text.


This work: modif. Hinde's PES
Sultanov at el., 2009
Flower, 1999
Schaefer, 1990
(10) - (00)
Thermal Rate k_{10-00} (T) ($cm^3 sec^{-1}$)
Temperature T (K)
8e-11
6e-11
4e-11
2e-11
0
50
100
150
200
250
300

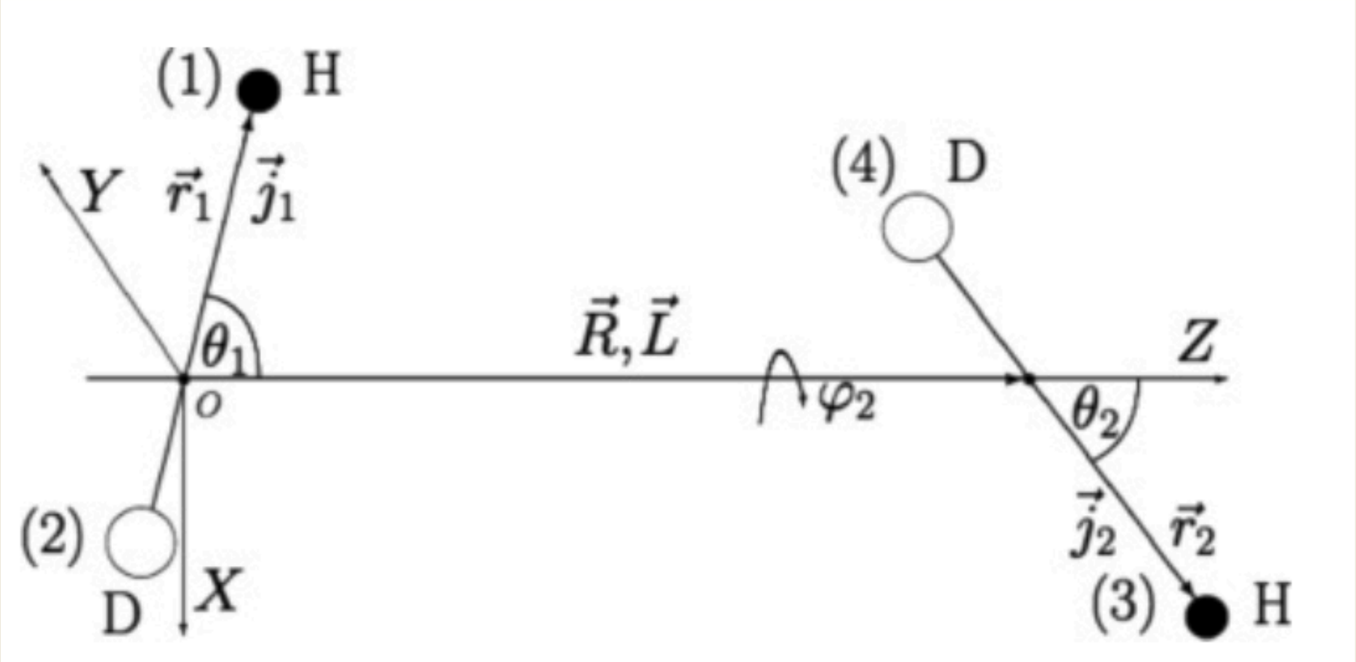
10-00
(J. Phys. B 49 (2016) 015203)

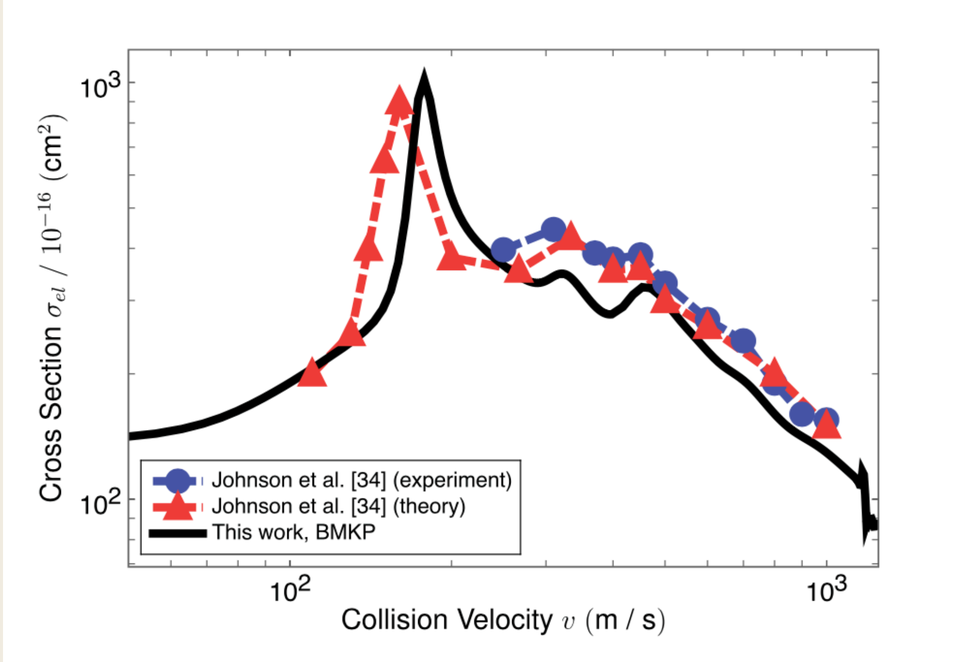


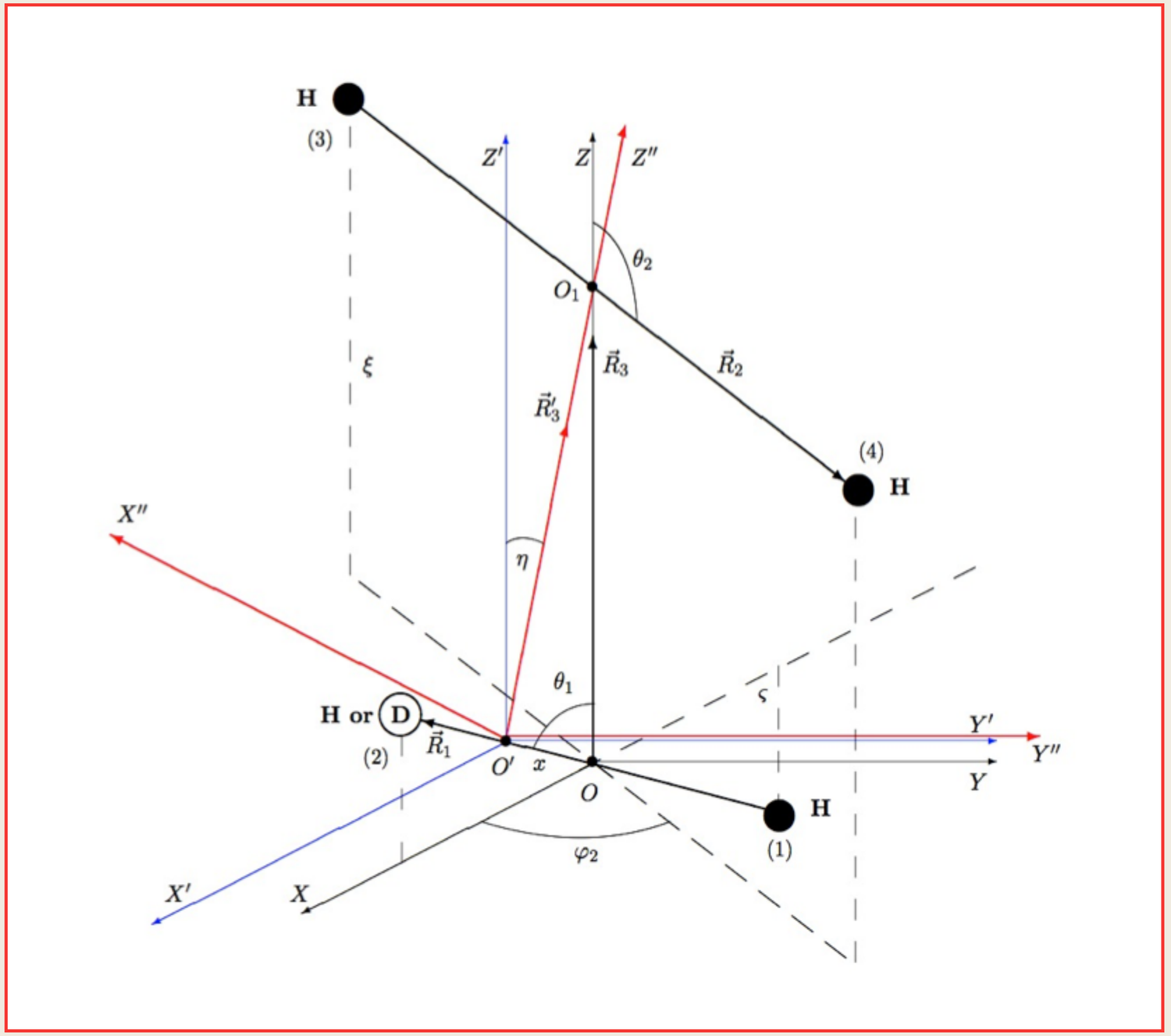

This work: modif. Hinde's PES
This work: modif. BMKP PES
Schaefer, 1990
$HD(0) + H_2(2) \rightarrow HD(2) + H_2(0)$
Cross Section $\sigma/10^{-16}$ (cm^2)
10^2
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
10^2
10^3
Relative Velocity v (cm / sec)

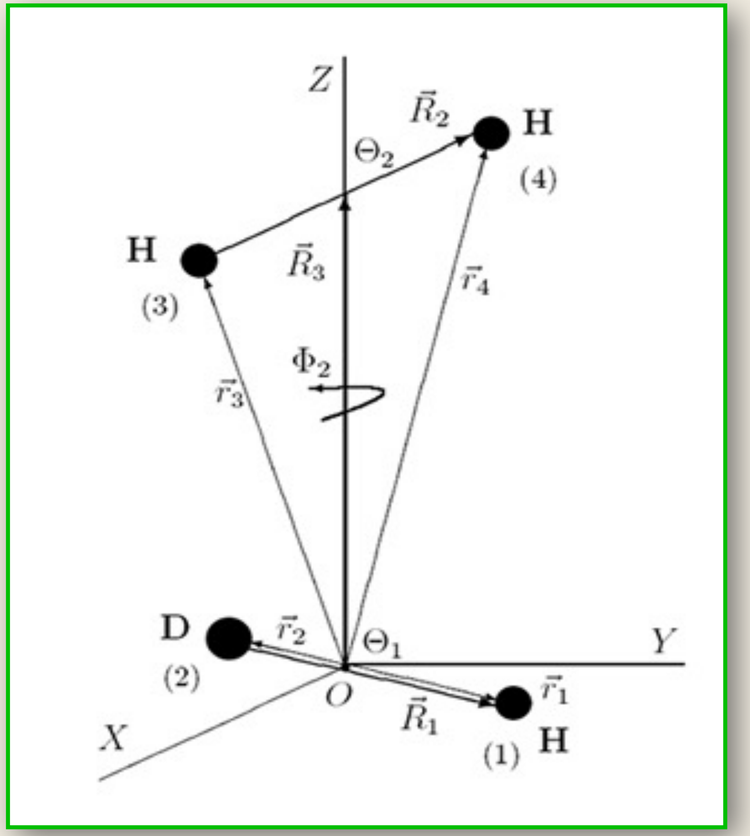

Thermal Rate k_{02-20} (T) (cm^3 sec^{-1})
1e-11
1e-12
1e-13
1e-14
1e-15
0
50
100
150
200
250
300
Temperature T [K]
(02) - (20)
This work: modif. Hinde's PES
This work: modif. BMKP PES
Flower, 1999
Schaefer, 1990

HD + HD Collision

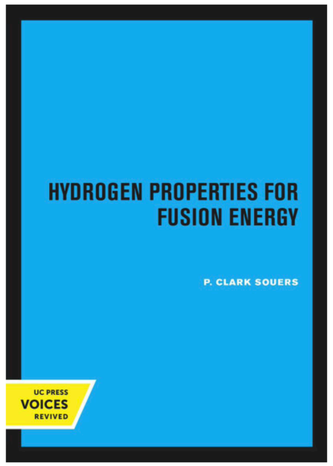





H
(3)
Z'
Z
Z''
θ2
O1
ξ
R3
R2
R'3
(4)
H
X''
η
θ1
H or D
(2)
R1
O'
x
O
Y'
Y''
Y
H
(1)
φ2
X'
X


Z
R2
H
(4)
Θ2
H
(3)
R3
r4
Φ2
r3
D
(2)
r2
Θ1
Y
O
r1
R1
(1)
H
X

HT + HT and DT + DT Collisions



Requires Authentication Published by University of California Press 1986

Hydrogen Properties for Fusion Energy

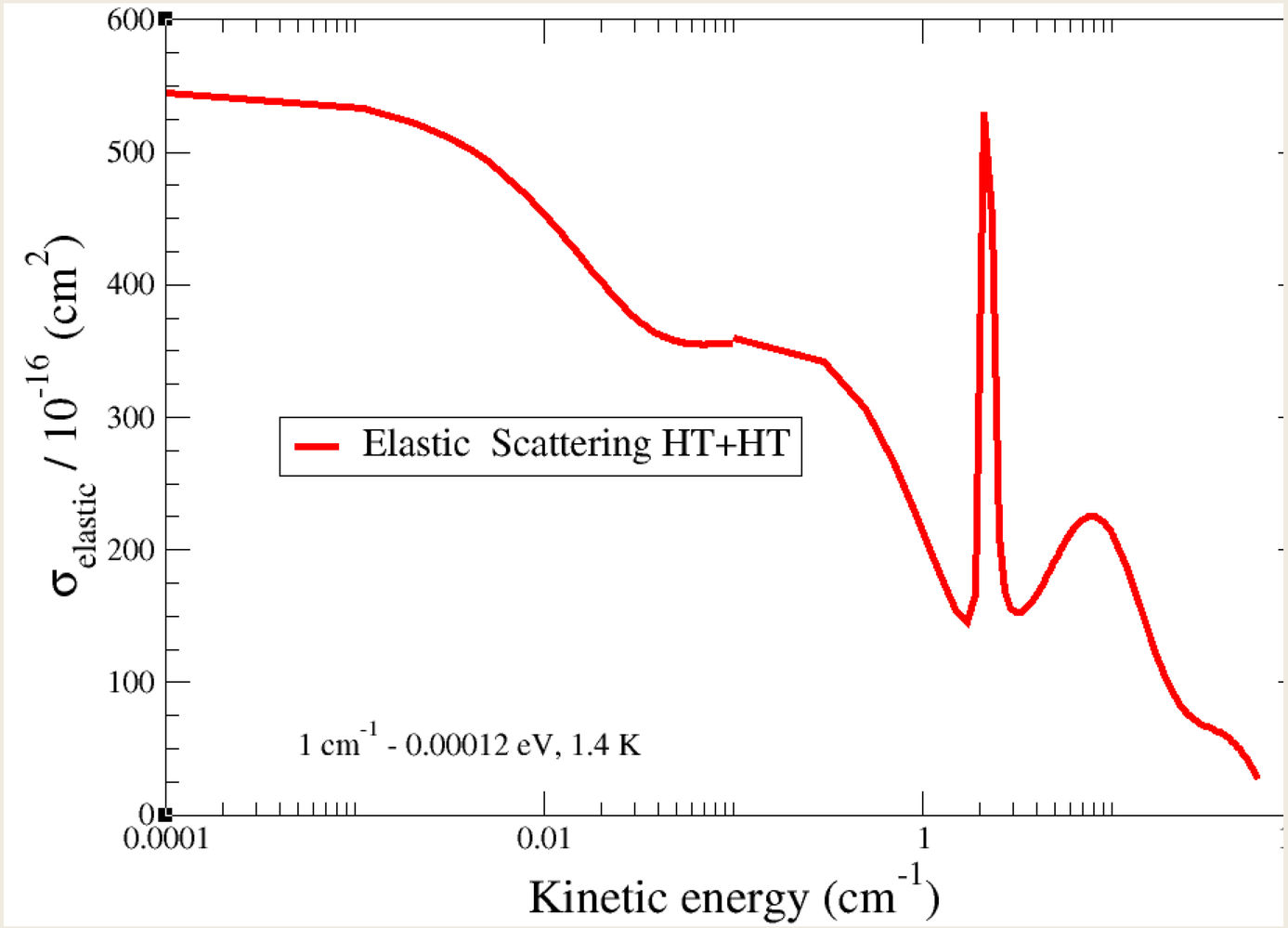
P. Clark Souers

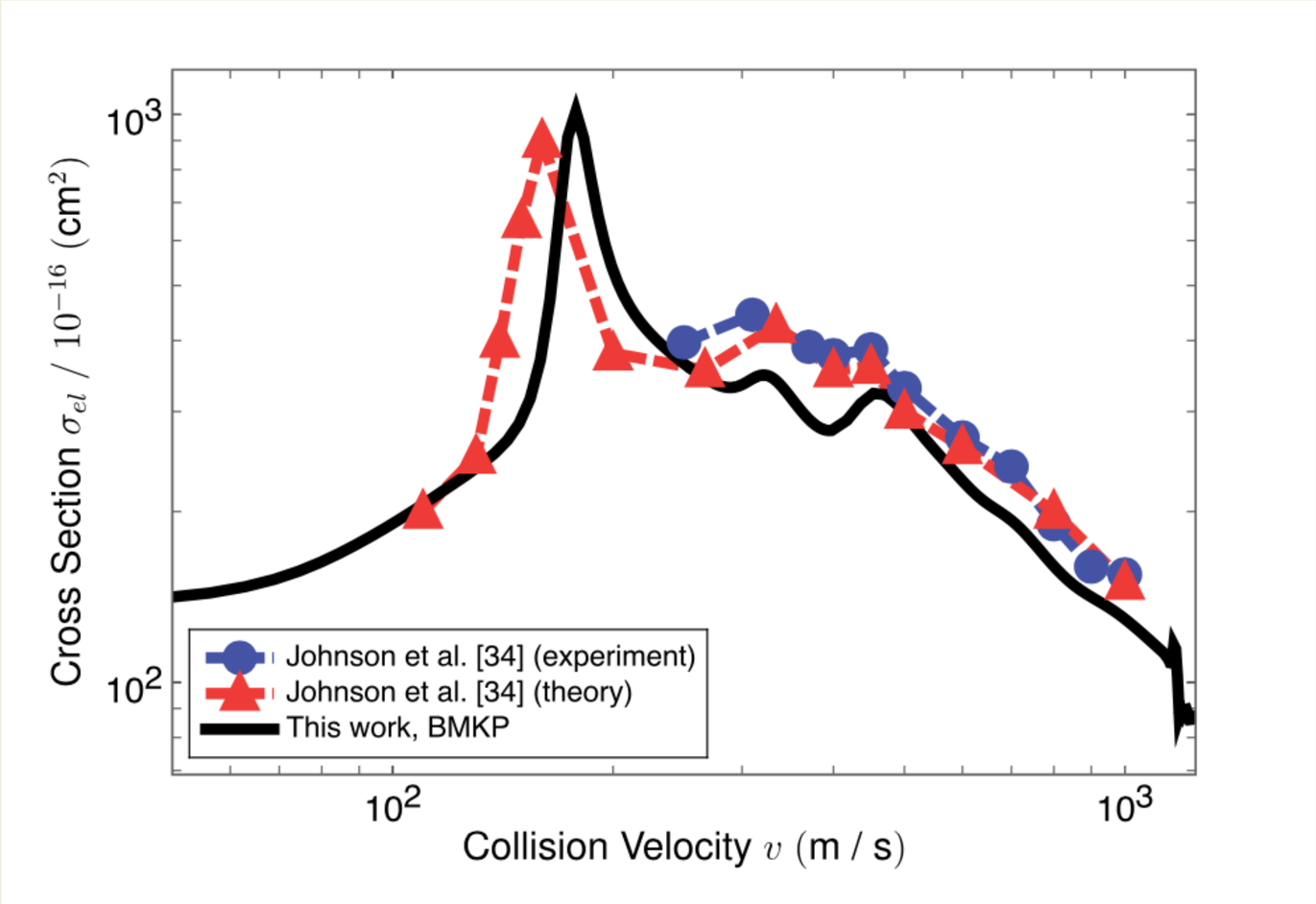
https://doi.org/10.1525/9780520338401

UNIVERSITY of CALIFORNIA PRESS

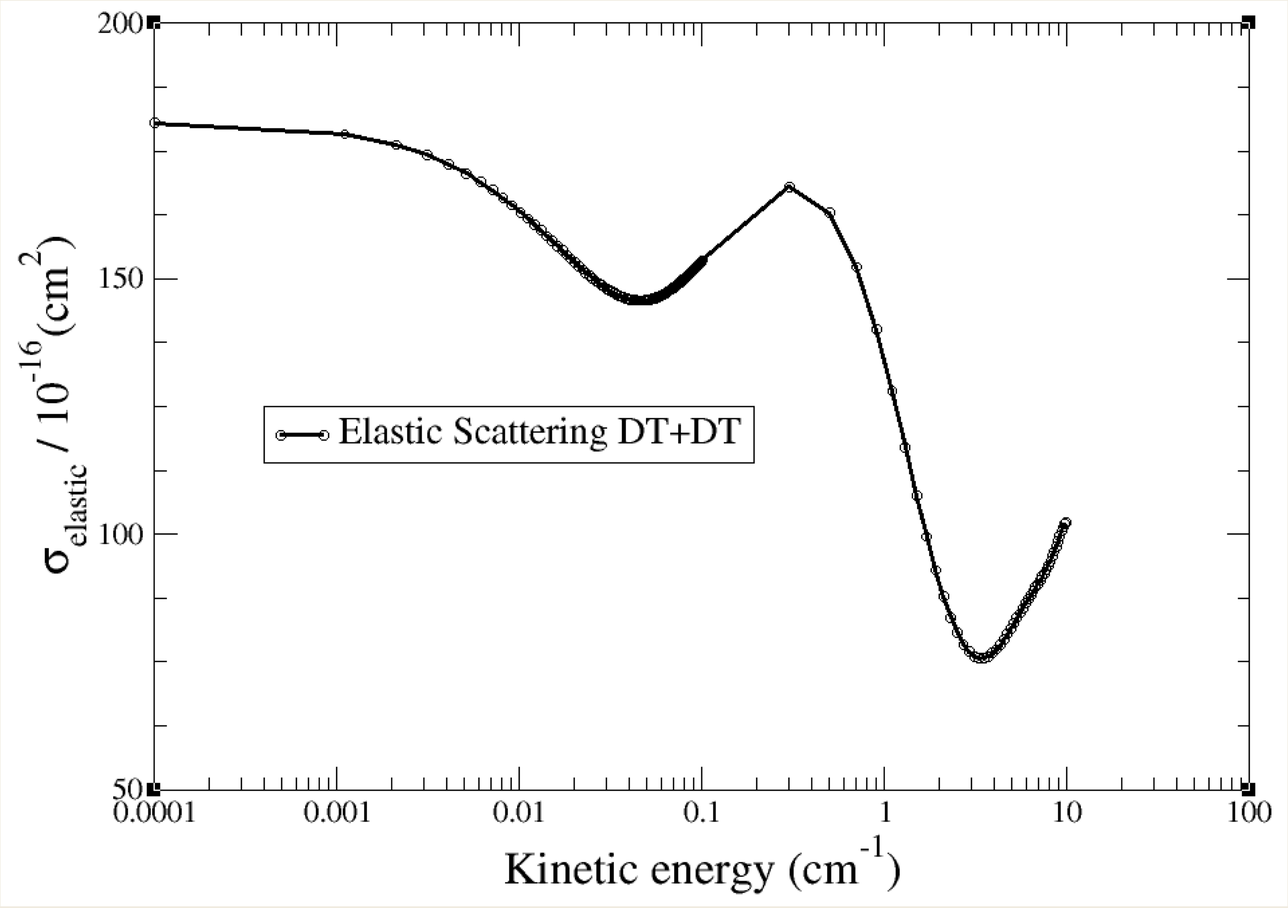
Language: English
Publisher: University of California Press
Copyright year: 1986
Edition: Reprint 2020
Audience: College/higher education;
Pages
Main content: 408
Keywords: physics; nuclear power; thermodynamics; energy technology; ceramic; low temperature physics; mechanical engineering; materials science

HT + HT Elastic / Inelastic Scattering




Cross Section σ_{el} / 10^{-16} (cm^2)
10^3
10^2
10^2
10^3
Collision Velocity v (m / s)
Johnson et al. [34] (experiment)
Johnson et al. [34] (theory)
This work, BMKP

DT + DT Elastic / Inelastic Scattering
(calculations in progress...so far)



Thank You for Your Time & Attention!

- PLEASE LET ME KNOW IF YOU HAVE QUESTIONS!
- Thank you very much!
- EMAIL #1: rsultanov@odessa.edu
- EMAIL #2: r.sultanov2@yahoo.com