**Molecular Reaction Dynamics: Applications to Triatomic systems.**

# Discussion of the exercises

The central objective of this exercise was to study triatomic reactivity.

You should now understand and be able to discuss:

a) re-crossing the transition state region

b) vibrational energy release in an exothermic reaction.

## Methods and Results

For each exercise, you should summarise the results as suggested on the wiki: include the data as suggested, in the data sheet, together with diagrams selected to illustrate the trajectories you have run along with a short text summary.

Discuss the points specifically indicated in the data sheet.

**Exercise 1: H + H2 potential energy surface**

**Exercise 2: F + H2 potential energy surface**

## Conclusions

Summarise your findings overall and very briefly explain what you did and why.

**Data Sheet and Discussion Points:**

***Exercise 1: H + H2 potential energy surface***

Tutorial summary: For discussion - what value does the total gradient of the potential energy surface have at a minimum and at a transition structure? Briefly explain how minima and transition structures can be distinguished using the curvature of the potential energy surface.

Determination of the TS geometry

**rts** = \_\_\_

Trajectories from TS

positions and average momenta at large t

**r1 r2** **p1 p2**

\_\_\_\_ \_\_\_\_ \_\_\_\_ \_\_\_\_

Reactive and unreactive trajectories

Conditions Reactive? Y/N Description / discussion

(screenshot + notes)

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**r1 = 0.74** **r2** = **2.0**

**p2= -2.5**  **-0.8 < p1 < -1.5**

**a) p1=\_\_\_\_**

**b) p1=\_\_\_\_**

**c) p1=\_\_\_\_**

Conditions Reactive? Y/N Description / discussion

(screenshot + notes)

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**r1 = 0.74 r2 = 2.0**

**p1= -1.25 p2 = -2.5**

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**r1 = 0.74 r2 = 2.0**

**p1 = -1.5 p2 = -2.0**

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**r1 = 0.74 r2 = 2.0**

**p1 = 1.5 p2 = -2.5**

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**r1 = 0.74 r2 = 2.0**

**p1 = -2.5 p2 = -5.0**

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**r1 = 0.74 r2 = 2.0**

**p1 = -2.5 p2 = -5.2**

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*For discussion: In the transition state theory of reaction rates it is assumed that once the system reaches the transition structure, with sufficient energy, it goes on to produce products. However transition state theory can overestimate the reaction rate. Why?*

***Exercise 2: F + H2 potential energy surface***

Illustrate and briefly describe the **mep** from the TS

Discuss the mechanism of release of the reaction energy of F + H2.

How could this be confirmed experimentally?

**Overall Conclusion**