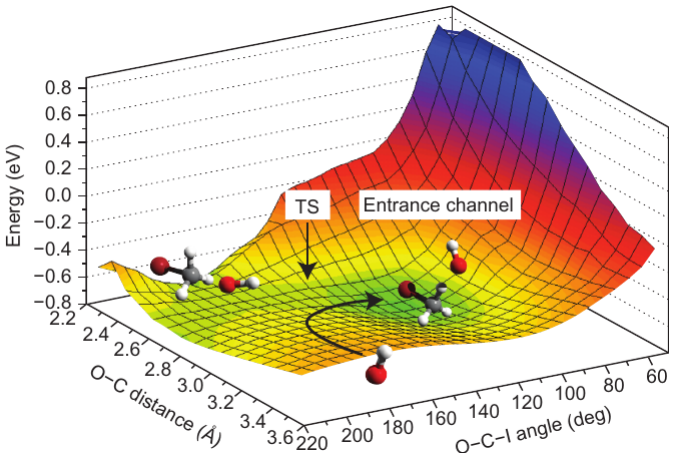
optional assignment 4 (due on 14 Nov 2020 before 12 noon)

1. Shown below is a PES for the reaction OH^-+CH_3I→products.



(a) What are the likely products?

(b) The curved arrow indicates how a co-linear approach starting at large distances is steered towards the non-co-linear entrance channel complex. Explain how this statement can be derived from the figure.

(c) What are the magnitudes of O-C distance and O-C-I angle after the system has landed in in the exit valley? If the C-I distance was monitored as the reaction progressed, what is its likely value in the exit valley?

(d) Estimate the activation energy for the reaction from the graph.

2. For a reaction A+B_2 →AB+B, the following parameters are reported:

Dissociation energy, $D_{A-B} = 591.1$kJ/mol; $D_{B-B} = 458.2$kJ/mol;

equilibrium distance, $R_{A-B} = 0.917$Å ; $R_{B-B} = 0.742$Å

Using this data and activation energy= 300 kJ/mol, draw the contour diagram for the variation of potential energy with distances between atoms.

3. Derive expressions for $\frac{d(\ln k)}{d\left(\frac{1}{T}\right)}$ for the rate constant from the Arrhenius equation and from collision theory and compare the two. Comment on the difference.

4. Rutherford scattering experiment : For the case of classical scattering of two particles with a repulsive Coulomb potential, $V(r) = \frac{B}{r}$,

scattering angle, $\chi(E,\, b) = 2\text{cosec}^{-1}\left[1 + \left(\frac{2bE}{B}\right)^2\right]^{\frac{1}{2}}$.

Show that the differential scattering cross-section,

$\frac{d\sigma}{d\Omega}(E,\, \chi) = \left(\frac{B}{4E}\right)^2 \text{cosec}^4\left(\frac{\chi}{2}\right)$