Problems for Molecular Dynamics

Circle the correct answer and explain where requested.

A. The reason that the values of the rotational quantum number, J, have "little, if any" effect on reaction cross section is that the rotational energy, even for values of J as high as 5, is negligible in comparison with minimum kinetic energy necessary for reaction.

True False

Explain

B. The maximum value of the impact parameter, b_{max}, at which a reactive collision will occur, increases with increasing relative velocity of the reactants.

True False

Explain

C. The minimum kinetic energy necessary for a reactive collision to occur is the difference between the potential energy barrier height relative to the classical ground state and the vibrational energy in the $v = 0$ quantum state.

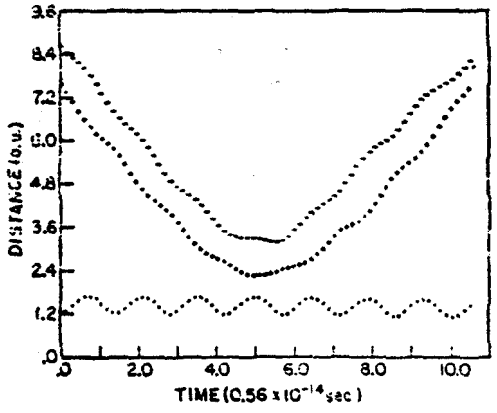
True False

Explain

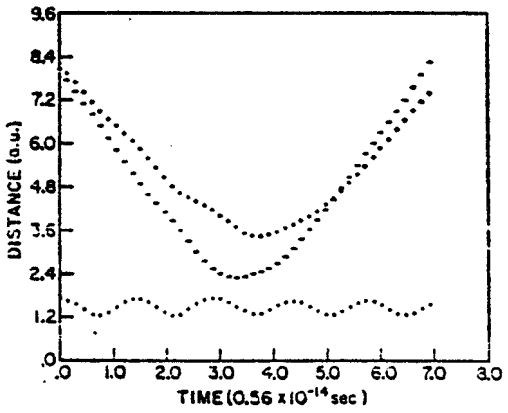
D. Each of the Figures below show a non-reactive collision for the same kinetic energy but different quantum states J, v. If the velocity were increased so that the kinetic energy were <u>very</u> much above the threshold value, which figure (A or B) represents the system which would have the greatest reaction cross section.

True False

Explain



A



B

E. The threshold velocity increases with increasing rotational quantum number but decreases with increasing vibrational quantum number.

True False

Explain

F. In the Karplus Theory the impact parameter, b, is chosen randomly in a Monte Carlo procedure in the calculation of the reaction cross section.

True False

Explain

G. The minimum kinetic energy (given in terms of the relative velocity) that two molecules (atoms) must have in order to react is equal to the height of the potential energy barrier.

True False

Explain

H. The reaction cross section is a function of the frequency of vibration of the reacting molecule.

True False

Explain

I. The molecular trajectories were calculated by systematically choosing various values of the impact parameter, rotational and vibrational quantum numbers, and the orientation of the H_2 molecule relative to the H molecule and then solving the 12 Hamiltonian Equations numerically.

True False

Explain

J. If the reaction probability calculated from the collision trajectories is found to be the following function of the impact parameter

$P_r = \left[(2 - b)/2\right]$ for $b \leq 2$ a.u.

$P_r = 0$ for $b > 2$ a.u.

where b and the number 2 are in atomic units (a.u.). The reaction cross section is

(1) 8/3 sq. a.u. $\left(a_o^2\right)$

(2) 4/3 sq. a.u.

(3) 2 sq. au.

(4) 12.56 sq. a.u.

(5) None of the above

(6) Not possible to calculate from the above information