Physical and Chemical Kinetics
Final Examination
04-12-2013

Please use the provided paper sheets to write down the solutions of the problems. Write your name and student ID number on a first page and enumerate all subsequent pages. Do not forget to hand in your paperwork after the examination.

Problem 1

Hydrogen atom interacts with argon atom which is at rest in the laboratory frame of reference. The velocity of the hydrogen atom has (x, y, z) components of $(1 \times 10^3\,\mathrm{m/s},\ 0,\ 0)$. Molecular weights of hydrogen and argon are 2 g/mol and 40 g/mol, respectively.

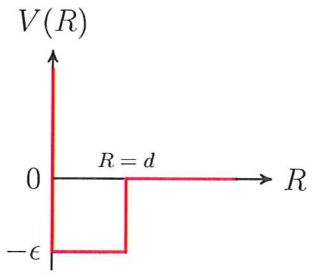
a. Find the velocities of the atoms in the center-of-mass frame of reference.

b. Find the kinetic energy of relative movement of the atoms.

c. Find the total angular momentum of atoms relative to the origin of the center-of-mass frame of reference when distance between atoms $\mathbf{r} = (1\,\mathrm{cm}, 1\,\mathrm{cm}, 0)$.

Problem 2

Interaction of particles is described by an attractive square-well potential with depth ϵ at a distance d between particles (see fig.). The relative velocity of the particles before collision is v, impact parameter is b and their relative mass is μ.



a. What is magnitude of the relative velocity after collision?

b. Sketch the trajectory of the particle moving in a field with this potential.

c. Find the distance of the closest approach between the particles as a function of v, b, μ, ϵ, and d.

Problem 3

Consider hydrogen cyanide HCN at temperature $T = 300\,\mathrm{K}$. Molecular weight of HCN is $27\,\mathrm{g/mol}$.

a. Find the magnitude of the average velocity of HCN molecules at this temperature.

b. How many times faster or slower will be mixing HCN with air after increasing the temperature 2 times?

c. Find the sound velocity in HCN gas at $T = 300\,\mathrm{K}$.

Problem 4

Formation of the nitrogen oxide proceeds in the flame front through the so-called "prompt" mechanism:

$$\mathrm{CH} + \mathrm{N_2} \xrightarrow{k_1} \mathrm{HCN} + \mathrm{N}$$

$$\mathrm{N} + \mathrm{O_2} \xrightarrow{k_2} \mathrm{NO} + \mathrm{O}$$

$$\mathrm{HCN} + \mathrm{O_2} \xrightarrow{k_3} \mathrm{NO} + \mathrm{CHO}$$

a. Assuming that rate coefficients k_2 and k_3 are much larger than k_1, derive the expression for the rate of formation of the nitric oxide.

b. Where is a higher concentration of CH molecules expected: in mixtures with excess of oxidizer or mixtures with excess of fuel?

c. Find the mole fraction of NO molecules in the combustion products after their passing the flame front. The combustion gases can be treated as air at temperature 2000 K and pressure $10\,\mathrm{atm} \approx 1 \times 10^6\,\mathrm{Pa}$. The residence time of combustion products in the flame front is $\sim 1\,\mathrm{ms}$. The rate coefficient $k_1 = 3.0 \times 10^{12} T^{0.88} e^{-10130/T}\ \mathrm{cm^3/mol\,s}$ and the concentration of CH molecules in the flame front is 10 ppm.