Vibrations and waves: exercise sheet 1

Vibrations of diatomic molecules of single elements

The purpose of this exercise is to put some data into the analysis of the vibrations of diatomic molecule developed in Lecture week 1, and to analyse the validity of a simple model for the interatomic interactions. Data are provided in the following table

Molecule	Mass (g/mol)	Bond length (Å)	Frequency (THz)	Dissociation energy (kJ/mol)
H_2	1	0.74	132	436
D_2	2	0.74	93.5	436
N_2	14	1.10	71	945
O_2	16	1.21	47	498
F_2	19	1.42	27	159
Cl_2	35.5	1.99	17	243
Br_2	79.9	2.28	9.5	193
I_2	126.9	2.67	6.2	151

1. Show from the mass and frequency values provided in the table that the force constants for stretching the bonds in the hydrogen and deuterium molecules are virtually identical. Check your numerical answers with the class demonstrator.

2. Show that the frequency change on increased mass of the halogens is not simply due to the increased mass, and that there is a gradual decrease in the bond stretching force constant with increasing atomic number.

3. From the dissociation energies and the bond lengths, calculate the parameters in the Lennard-Jones energy function for N_2 and O_2, using the following form of the potential energy function:

$$E(r) = -4\varepsilon\left[\left(\frac{\sigma}{r}\right)^6 - \left(\frac{\sigma}{r}\right)^{12}\right]$$

4. Evaluate the quality of the Lennard-Jones potential for the calculation of vibrational frequencies of N_2 and O_2.