Tutorial 1: Spectroscopic units

Constants: $h = 6.6256 \cdot 10^{-34}\ \mathrm{J \cdot s} = 6.6256 \cdot 10^{-27}\ \mathrm{erg \cdot s} = 4.135667 \cdot 10^{-15}\ \mathrm{eV \cdot s}$
$c = 2.998 \cdot 10^{8}\ \mathrm{m/s} = 2.998 \cdot 10^{10}\ \mathrm{cm/s}$

Conversion: $E_{erg} = E_{eV} \cdot 1.6022 \cdot 10^{-12}$

Exercise 1

The total energy of a molecule is a sum of several contributions (electronic, vibrational, rotational, electronic spin, nuclear spin ...) which are quantified. The spacing of the different levels is such that the radiation emitted or absorbed by the molecule is located in very different regions of the electromagnetic spectrum. The table below shows the various domains of the electromagnetic spectrum and the corresponding spectroscopic phenomena.

λ	Spectral domain	Phenomenon	Spectroscopic techniques
10^{-1} to 10^{3} Å	X-rays Far U.V.	Transitions of internal electrons in atoms/molecules	X-ray fluorescence
10^{3} to 10^{4} Å	U.V. (10^{3} to 4×10^{3} Å) Visible Near I.R. (>7.5 Å)	Transitions of external (valence) electrons of atoms or molecules	Electronic spectroscopy U.V. – visible
1 to 10^{2} µm	I.R.	Molecular vibrations	I.R. spectroscopy
10^{2} to 10^{5} µm	Far I.R. (10^{2}-10^{3}µm) Microwave	Molecular rotations	Microwave spectroscopy
10 to 30 cm	Microwave		
0.3 to 300 m	Radio waves	Transitions between electronic spin states in the presence of magnetic field Transitions between nuclear spin states in the presence of magnetic field	Electronic paramagnetic resonance Nuclear magnetic resonance

1a) Determine the transition relationships between the usual spectroscopic units: energy E (eV), wavelength λ (Å) and wavenumber $\bar{\nu}$ (cm^{-1}).

1b) Establish a correspondence table between the energy units: erg, eV, cm^{-1}, Hz.

2) Tell which spectrum domain the following energy, wave number, wavelength or frequency radiations belong to:

E=2 eV, $\bar{\nu}$=2500 cm^{-1}, 50000 cm^{-1}, 100 cm^{-1} ;

λ=25*10^{4} Å, ν=6*10^{7} Hz.

3) Sort in ascending order, the energy differences between two electronic levels, two vibrational levels and two rotational levels.