Wavelengths

The quantity called $\bar{\nu}$, which is the wavenumber, but divided by 2π, i.e. not k, $\bar{\nu} = 1/\lambda$, while $\bar{\lambda} = \frac{\lambda}{2\pi} = \frac{1}{k}$
It is customary to give the energy in terms of $\bar{\nu}$, i.e. one of the units of energy is cm^{-1}

$$1eV = 8065.48cm^{-1} = 806548m^{-1}$$

$$1a.u.energy \rightarrow 219475cm^{-1}$$

To show the relations, we introduce k_0^γ, which is the photon (γ) wavenumber, when the photon has energy 1 a.u.; It is thus *not* the k_0, which is $1/a_0$!!

$$k_0^\gamma = \frac{\omega_0}{c} = \frac{E_0}{\hbar c} = \frac{e^2}{a_0}\frac{1}{\hbar c} = \frac{e^2}{\hbar c}\frac{1}{a_0}$$

We can thus write

$$\bar{\lambda}_0 = \frac{\lambda_0}{2\pi} = \frac{1}{k_0^\gamma} = 137a_0$$

so that

$$\lambda_0 = 2\pi\ 137\ a_0 = 6.28 \times 137 \times 0.529\ \text{Å}$$

which can be summarized as

$$1a.u. = 27.2eV \rightarrow 540\ \text{Å}$$
$$1\ \text{eV} \rightarrow 27.2 \times 540\ \text{Å} = 12\ 386\ \text{Å}$$

A simple general relation is

$$\lambda\ [\ \text{Å}\ ]\ =\ \frac{12\ 386}{E[eV]}\ \text{Å}$$