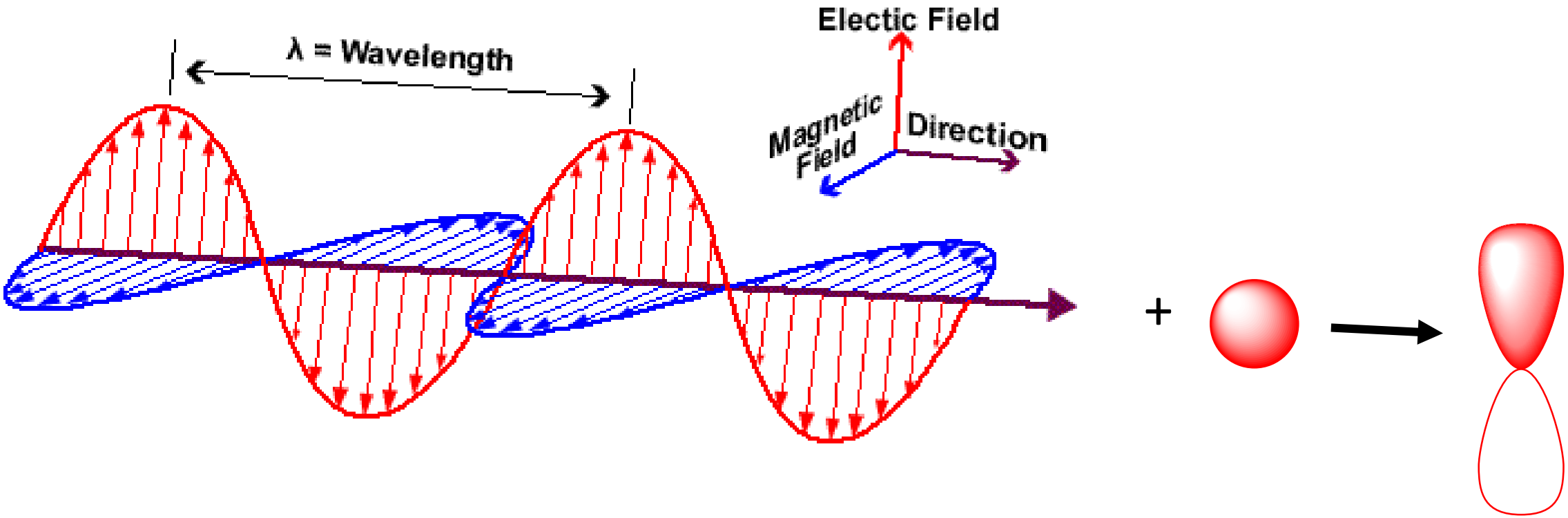
Transition dipole moment for HF



Transition dipole moment for HF

We consider the transition dipole moment of HF. The model is based on the idea that there is an electronegativity difference between the H and F atoms that introduces an asymmetry into the molecule. If we consider the ground and excited state molecular orbitals:

$$\Psi_{\sigma} = \sin\theta_g \ 1s_H + \cos\theta_g \ 2p_{z,F}$$
$$\Psi_{\sigma*} = \sin\theta_e \ 1s_H - \cos\theta_e \ 2p_{z,F}$$

Where the mixing angle $\theta_g = 30^o$ and $\theta_e = 60^o$. You may assume that all resonance or overlap integrals are zero. The Coulomb integrals have the value

$$\int 1s_H z 1s_H dz = z_H = 0.95R_0 \ and \int 2p_{z,F} z 2p_{z,F} dz = z_F = -0.05R_0$$

as defined in the calculation of the ground state dipole moment. Finally, the bond length is $R_0 = |z_H - z_F| = 0.95$ Å.