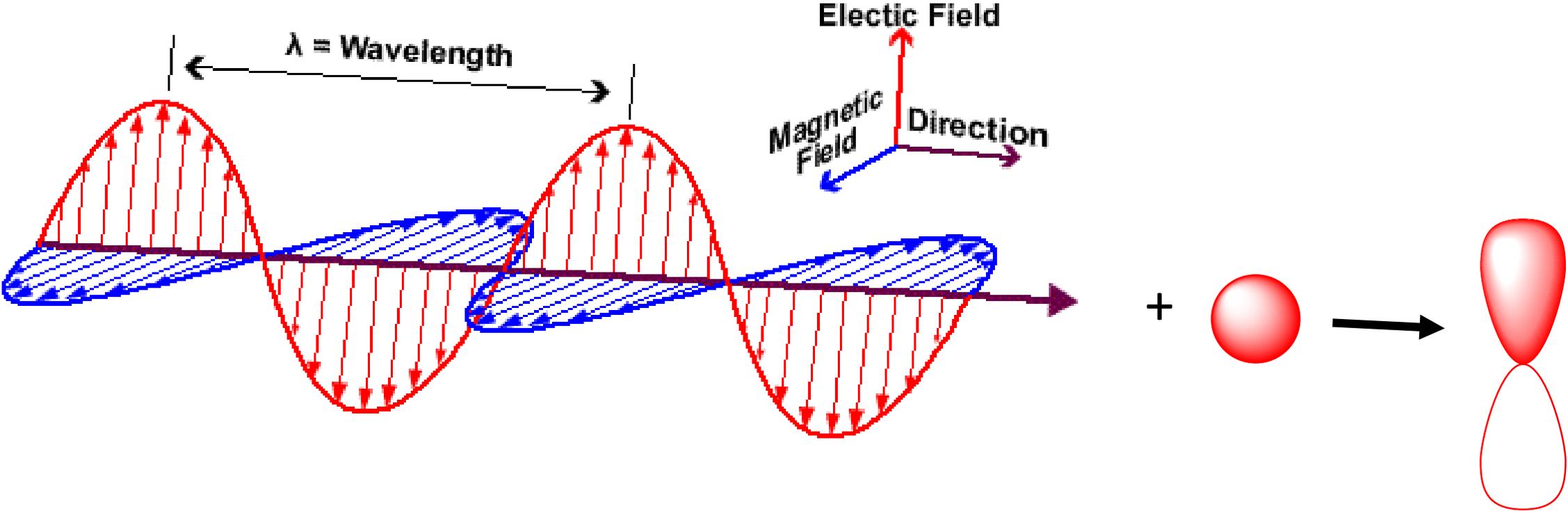


Ground state dipole moment for HF



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We consider the ground state 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 state molecular orbital:

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

where, for the ground state, the mixing angle $\theta_g = 40^\circ$. Assuming that the charge asymmetry is equal to the difference between the coefficient on $1s_H$ and $2p_{z,F}$ calculate the ground state dipole moment. You may assume that all resonance or overlap integrals are zero. You may also assume that the Coulomb integrals have the value:

$$e \int 1s_H z 1s_H dz = e z_H \quad \text{and} \quad e \int 2p_{z,F} z 2p_{z,F} dz = e z_F$$

which refers to one charge at position z_H and a charge at position z_F . Finally, the bond length is $|z_H - z_F| = 0.95 \text{ \AA}$.