Ground state dipole moment for HF

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 $\theta_g = 40^o$. 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 Ccoulomb integrals have the value:

$$e\int 1s_H z 1s_H dz = ez_H \quad and \quad e\int 2p_{z,F} z 2p_{z,F} dz = ez_F$$

which refers to one charge at position z_H and a charge at position z_F. Finally, the bond length is $|z_H - z_F| = 0.95$ Å.

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Solution: The definition of the dipole moment for this case involves two electrons since we are considering two atomic orbitals that mix.

$$M_{ground} = 2e \int \Psi_\sigma z \Psi_\sigma dz$$

We substitute the linear combinations for each orbital.

$$2e \int \Psi_\sigma z \Psi_\sigma dz = 2e \int \left(\sin\theta_g \ 1s_H + \cos\theta_g \ 2p_{z,F}\right) z \left(\sin\theta_g \ 1s_H + \cos\theta_g \ 2p_{z,F}\right) dz$$

Assuming

$$\int 1s_H z 2p_{z,F} dz = \int 2p_{z,F} z 1s_H dz = 0$$

We obtain the squared coefficients

$$M_{ground} = 2e\left[sin^2\,\theta_g \int 1s_H z 1s_H dz + cos^2\,\theta_g \int 2p_{z,F} z 2p_{z,F} dz\right]$$

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Given the definitions of the Coulomb integrals. We have

$$M_{ground} = 2e\left[sin^2\,\theta_g\, z_H + cos^2\,\theta_g\, z_F\right] = 2e\left[sin^2\,\theta_g\, z_H + cos^2\,\theta_g\, z_F\right]$$

And when we substitute θ_g= 40º, which was given in the problem we have the following dipole moment

$$M_{ground} = 2e|0.5868 - 0.4131|(0.95\text{ Å}) = 1.58\,D$$