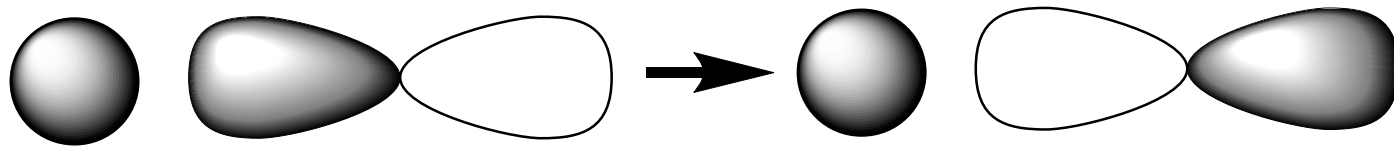


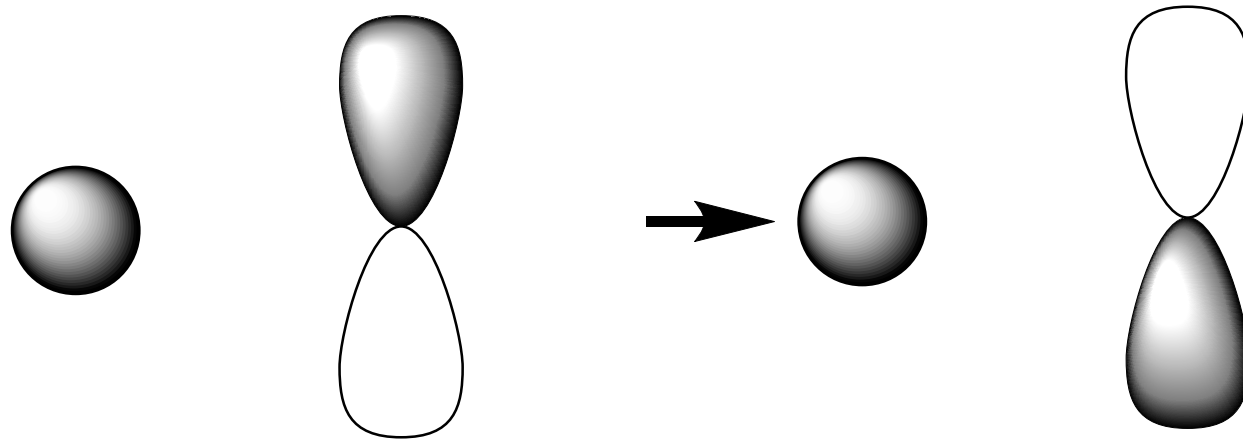
Transition dipole moment

The transition dipole moment for a molecule such as HF can be understood by examining potential initial and final states using molecular orbitals. Please identify if either of the two possible combinations of atomic orbitals shown could potentially lead to an electronic transition. What polarization of the electric vector would be appropriate for inducing the transition (vertical or horizontal)?

A.



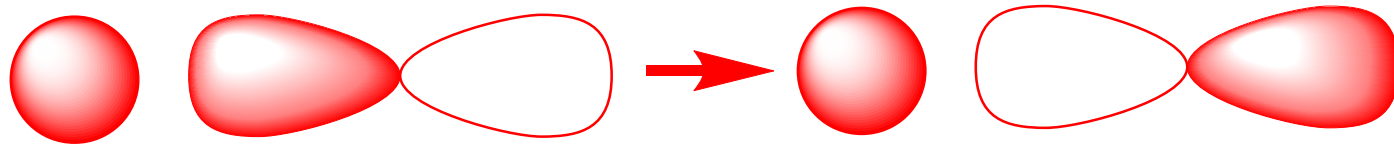
B.



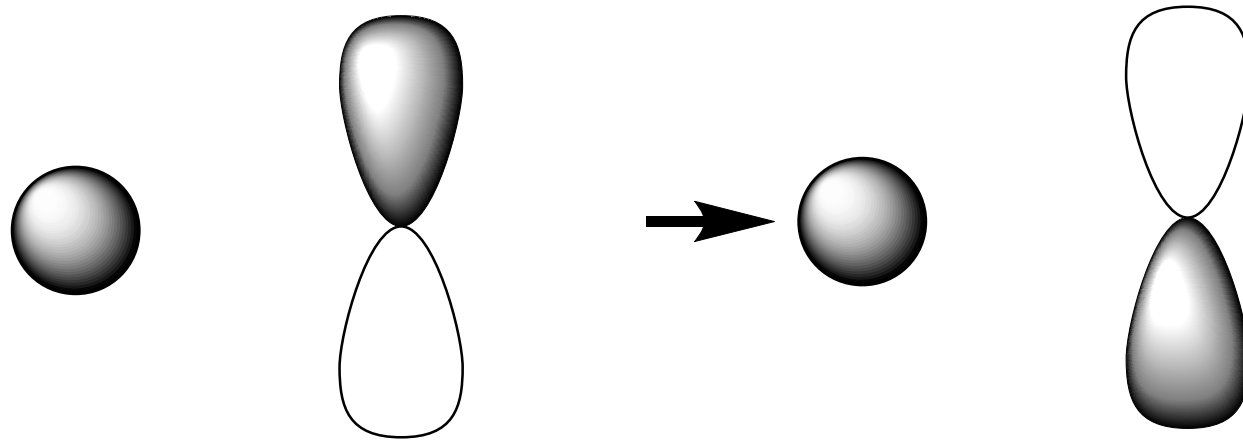
Transition dipole moment

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A.



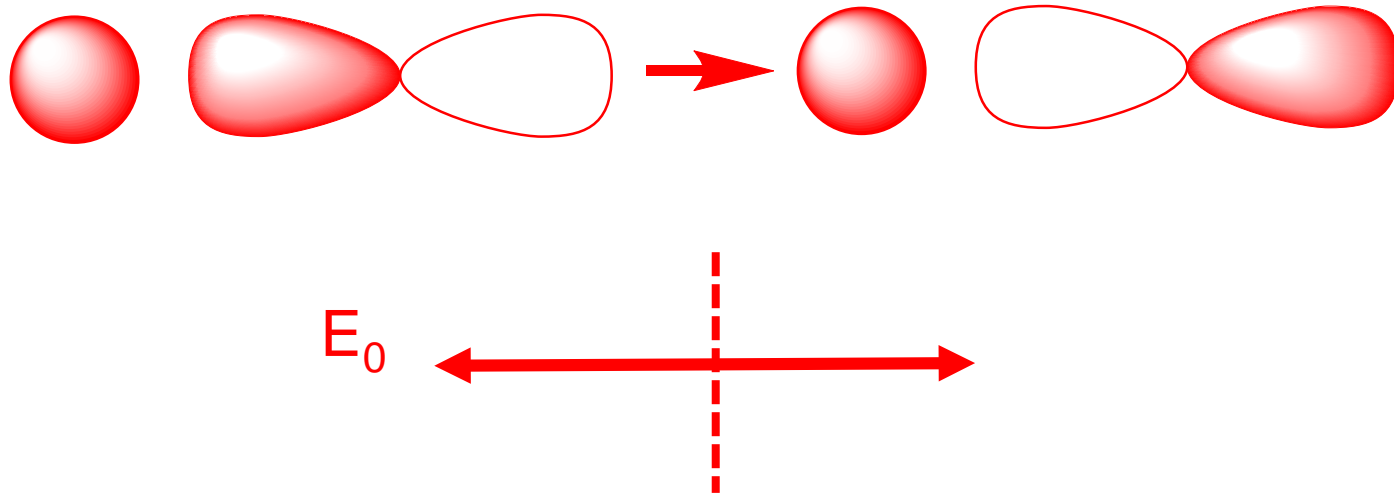
B.



Transition dipole moment

The transition dipole moment for a molecule such as HF can be understood by examining potential initial and final states using molecular orbitals. Please identify if either of the two possible combinations of atomic orbitals shown could potentially lead to an electronic transition. What polarization of the electric vector would be appropriate for inducing the transition (vertical or horizontal)?

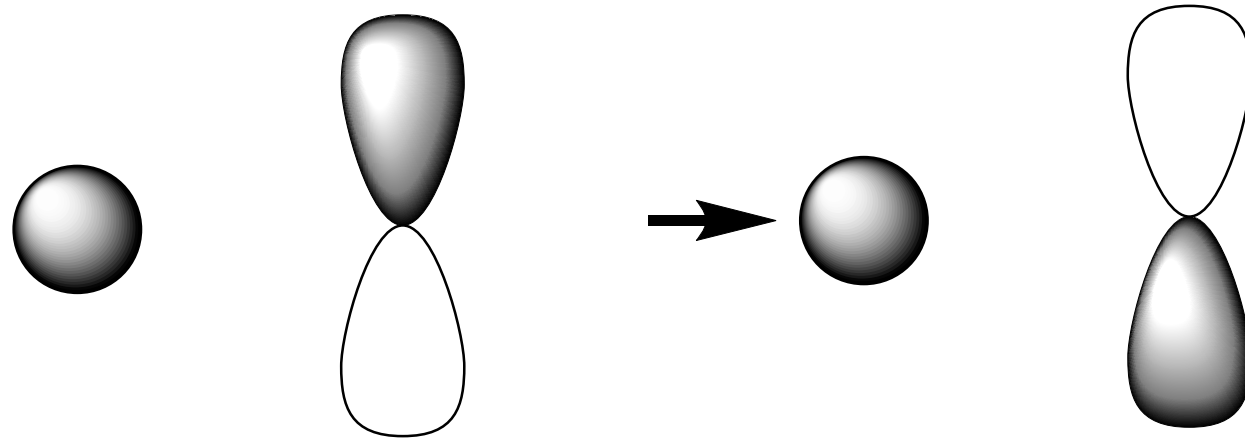
A.



Transition dipole moment

The transition dipole moment for a molecule such as HF can be understood by examining potential initial and final states using molecular orbitals. Please identify if either of the two possible combinations of atomic orbitals shown could potentially lead to an electronic transition. What polarization of the electric vector would be appropriate for inducing the transition (vertical or horizontal)?

B.



This is a non-bonding combination. Therefore, there is no energy difference.