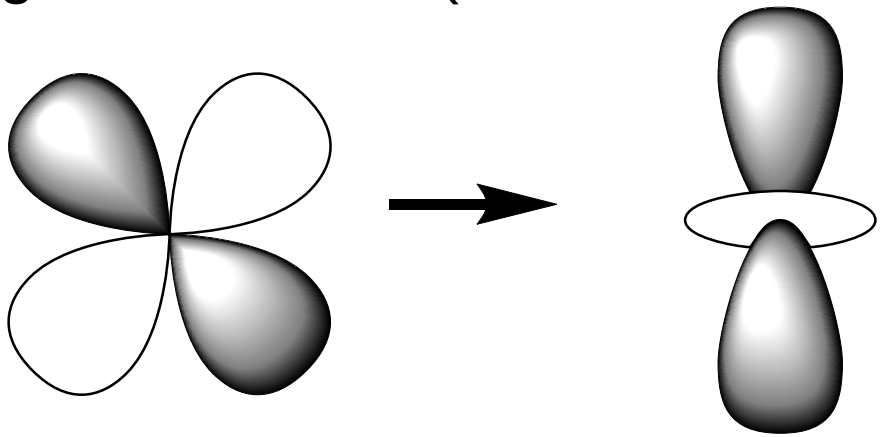
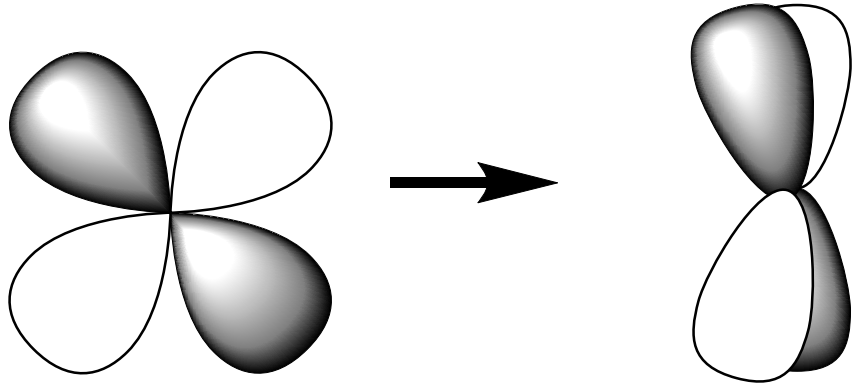
Transition dipole moment

The transition dipole moment for a $Fe(H_2O)_6^{3+}$ 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.



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Neither of these transitions is allowed. The number of nodes is equal in both the ground and excited state. However, there is an energy difference in the top set of orbitals because of the ligand field of the H_2O molecules. These present an octahedral ligand field, which splits the d-orbitals into two sets. In this case splitting leads to the following energy level diagram.