Crystal field theory, ligand field splitting, low spin, high spin complexes, J. Teller Effect

The most striking aspect of coordination compounds is their vivid colors. The other aspect of coordination complexes is their magnetism. Which can also be linked to d-orbital like the colors of these complexes.

First the magnetism of coordination complexes, can be directly linked to the electron configuration of their d-orbitals. The spin-only moment can be calculated from the number of unpaired electrons in the d-orbitals.

The number of unpaired electrons in the d-orbitals, is derived from the crystal field splitting of the metal and the splitting energy between the d-orbitals in comparison to the spin pairing energy.

The two basic crystal fields are the octahedral and the tetrahedral field, which split the d-orbitals according to their symmetries. The energy of the splitting between the d-orbitals is based on 2 constraints the type of ligand and the central atom (element and it's oxidation state). The ligands are organized according to their effect in the spectrochemical series.

In the octahedral fields this splitting divides the complexes into 2 types, high and low spin complexes. The high spin complexes occur when the $\Delta_0$ is low, this means that the splitting energy is low, while low spin complexes occur in the opposite situation.

Asymmetric occupation of degenerate orbitals, arises a different kind of splitting, known as the Jahn-Teller effect. This effect is based on the theory that degenerated orbitals will change their energies when they are asymmetrically occupied. This splitting of the orbitals leads to distortions of the symmetry of the crystal field. This distortion is caused by the tendency of the metal atom to lower its energy due to the occupation of the orbitals, but this distortion always raises the energy of the molecule, so the metal atom tend to compromise between the two effects. The Jahn-Teller effect can be observed for the electronic configurations $d^4$ high spin, $d^7$ low spin and $d^9$ because for these configurations the eg orbitals are occupied asymmetrically. A special case of the Jahn –Teller effect is the square planar coordination of $d^{10}$-ions.

Questions

1) Explain the Jahn-Teller effect and sketch the splitting of the d-orbitals for a compressed octahedron.
2) Discuss the square planar coordination and sketch the d-orbital splitting.
3) Give the formula of typical Fe$^{3+}$ high spin and low spin complex, respectively. Sketch the ligand field splitting and the distribution of the electrons for both complexes.