Hund rules

- 1. Of the different multiplets resulting from different configurations of electrons in degenerate orbitals of an atom those with greatest multiplicity have the lowest energy (multiplicity rule).
- 2. Among multiplets having the same multiplicity, the lowest-energy one is that with the largest total orbital angular momentum (angular momentum rule) (valid if the total orbital angular momentum is a constant of motion).
- 3. In configurations containing shells less than half full of electrons, the term having the lowest total angular momentum *J* lies lowest in energy, whereas in those with shells more than half filled, the term having the largest value of *J* lies lowest (fine structure rule). Hund rules apply if the 'Russell–Saunders' coupling scheme is valid. Sometimes the first rule is applied with questionable validity to molecules.

Source:

PAC, 1996, 68, 2223 (Glossary of terms used in photochemistry (IUPAC Recommendations 1996)) on page 2246