B.Sc. Semester-IV
Core Course-VIII (CC-VIII)
Inorganic Chemistry

I. Coordination Chemistry
9. The Angular Overlap Method

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I. Coordination Chemistry: 20 Lectures

Werner's theory, valence bond theory (inner and outer orbital complexes), electroneutrality principle and back bonding. Crystal field theory, measurement of 10 Dq (Δo), CFSE in weak and strong fields, pairing energies, factors affecting the magnitude of 10 Dq (Δo, Δt). Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry Jahn-Teller theorem, square planar geometry. Qualitative aspect of Ligand field and MO Theory.

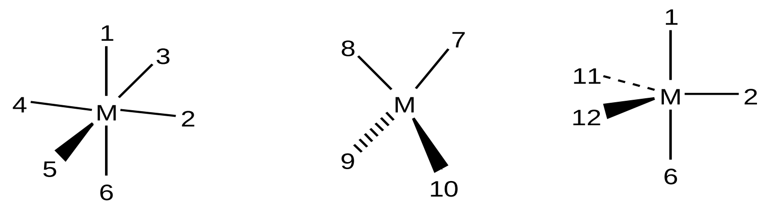
IUPAC nomenclature of coordination compounds, isomerism in coordination compounds. Stereochemistry of complexes with 4 and 6 coordination numbers. Chelate effect, polynuclear complexes, Labile and inert complexes.

Coverage:

1. The Angular Overlap Method

Angular Overlap Method

An attempt to systematize the interactions for all geometries.



The various complexes may be fashioned out of the ligands above

Linear: 1,6

Trigonal: 2,11,12

T-shape: 1,3,5

Tetrahedral: 7,8,9,10

Square planar: 2,3,4,5

Trigonal bipyramid: 1,2,6,11,12

Square pyramid: 1,2,3,4,5

Octahedral: 1,2,3,4,5,6

Angular Overlap Method

All σ interactions with the ligands are stabilizing to the ligands and destabilizing to the d orbitals. The interaction of a ligand with a d orbital depends on their orientation with respect to each other, estimated by their overlap which can be calculated.

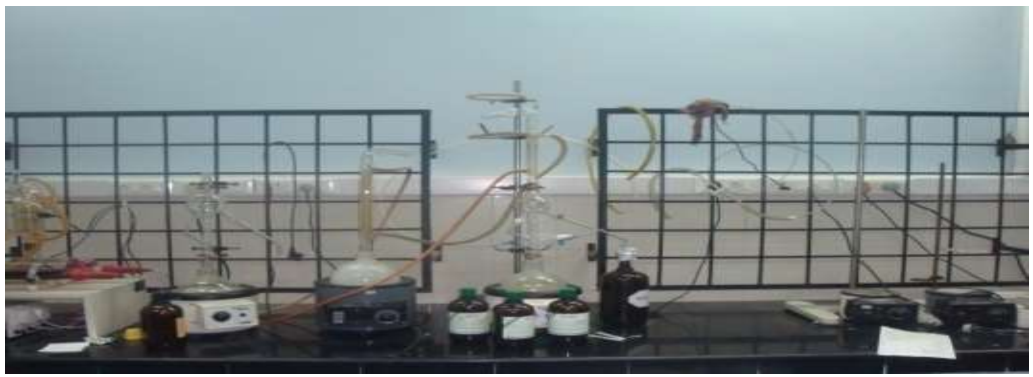
The total destabilization of a d orbital comes from all the interactions with the set of ligands.

For any particular complex geometry we can obtain the overlaps of a particular d orbital with all the various ligands and thus the destabilization.

ligand	d_{z2}	d_{x2-y2}	d_{xy}	d_{xz}	d_{yz}
1	1 e_σ	0	0	0	0
2	¼	¾	0	0	0
3	¼	¾	0	0	0
4	¼	¾	0	0	0
5	¼	¾	0	0	0
6	1	0	0	0	0
7	0	0	1/3	1/3	1/3
8	0	0	1/3	1/3	1/3
9	0	0	1/3	1/3	1/3
10	0	0	1/3	1/3	1/3
11	¼	3/16	9/16	0	0
12	1/4	3/16	9/16	0	0

Thus, for example a d_{x2-y2} orbital is destabilized by (3/4 +6/16) e_σ = 18/16 e_σ in a trigonal bipyramid complex due to σ interaction. The d_{xy}, equivalent by symmetry, is destabilized by the same amount. The d_{z2} is destabililzed by 11/4 e_σ.

Thank You



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