SP-1(B) :ORGEL Diagram

Orgel diagrams are correlation diagrams showing the relative energies of electronic terms in transition metal complexes.

Orgel diagrams are restricted to only weak field (high spin) cases, and offer no information about strong field (low spin) cases.

Orgel diagrams are **qualitative**, no energy calculations can be performed from these diagrams.

Orgel diagrams only show the symmetry states of the highest spin multiplicity instead of all possible terms, unlike a Tanabe-Sugano diagram.

Orgel diagrams will, however, show the number of spin allowed transitions, along with their respective symmetry designations.

In an Orgel diagram, the parent term (P, D, or F) in the presence of no ligand field is located in the center of the diagram, with the terms due to that electronic configuration in a ligand field at each side.

There are **TWO** Orgel diagrams (D & F):

D Orgel diagram: d^1, d^4, d^6, and d^9 configurations.

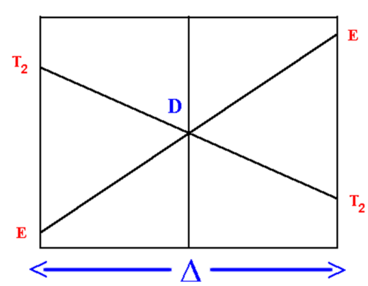
F Orgel diagram: d^2, d^3, d^7, and d^8 configurations.

In an Orgel diagram lines with the same Russell – Saunders terms will diverge due to the non-crossing rule, but all other lines will be linear.

D Orgel diagram

The left side contains d^1 and d^6 tetrahedral and d^4 and d^9 octahedral complexes. The right side contains d^4 and d^9 tetrahedral and d^1 and d^6 octahedral complexes.

For complexes with D ground terms only one electronic transition is expected and the transition energy corresponds directly to D.



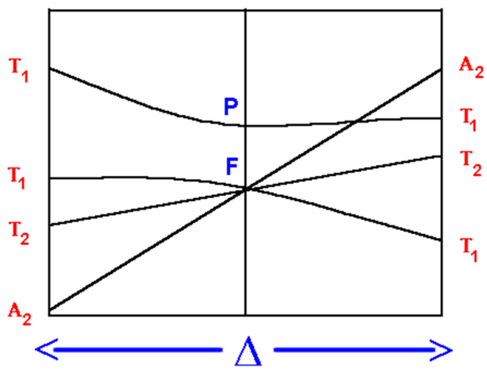
d^1, d^6 Tetrahedral (Td)	D Orgel diagram	d^4 , d^9 Tetrahedral (Td)
d^4 , d^9 Octahedral (Oh)		d^1 , d^6 Octahedral (Oh)

****For simplicity, the g subscripts required for the octahedral complexes are not shown.*

F Orgel diagram

The left side contains d^2 and d^7 tetrahedral and d^3 and d^8 octahedral complexes. The right side contains d^3 and d^8 tetrahedral and d^2 and high spin d^7 octahedral complexes.

For complexes with F ground terms, three electronic transitions are expected and D may not correspond directly to a transition energy. The following configurations are dealt with: d^2, d^3, high spin d^7 and d^8.



F Orgel diagram

d^2, d^7 Tetrahedral (Td)	d^3, d^8 Tetrahedral (Td)
d^3, d^8 Octahedral (Oh)	d^2, d^7 Octahedral (Oh)

****For simplicity, the g subscripts required for the octahedral complexes are not shown.*

F Orgel diagram

LHS:

High spin d^3, d^8 octahedral (Oh)
High spin d^2, d^7 Tetrahedral (Td)

Depending on the ligand field energy of the complexes, the possible transitions are

$^4A_{2g} \rightarrow {}^4T_{2g}$
$^4A_{2g} \rightarrow {}^4T_{1g}(F)$
$^4A_{2g} \rightarrow {}^4T_{1g}(P)$

RHS: Depending on the ligand field energy,

d^3, d^8 Tetrahedral (Td)
d^2, d^7 Octahedral (Oh)

Depending on the ligand field energy of the complexes, the possible transitions are

$^3T_{1g} \rightarrow {}^3T_{2g}$
$^3T_{1g} \rightarrow {}^3A_{2g}$
$^3T_{1g} \rightarrow {}^3T_{1g}(P)$

The last two transitions can occur in a reverse way at higher Δ values

Electronic spectra of

(i) high spin tetrahedral $[Co(Cl)_4]^{2-}$ …………d^7 metal ion (**LHS**)

(ii) high spin octahedral $[Co(H_2O)_6]^{3+}$ ………… d^7 metal ion (**RHS**)