

Tanabe-Sugano diagram:

Tanabe-Sugano diagram is used in coordination chemistry to predict absorption in the UV, visible and IR electromagnetic spectrum of coordination compounds. The results from a Tanabe-Sugano diagram analysis of a metal complex can also be compared to experimental spectroscopic data. They can also be used to predict the size of the ligand field necessary to cause high spin to low spin transitions. In a Tanabe-Sugano diagram, the ground state is used as a constant reference, in contrast to Orgel diagram. They show both spin allowed and spin forbidden transitions. They also show both high spin and low spin complexes.

In Tanabe-Sugano diagram, the ground state is always taken as the abscissa (horizontal axis) which provides a constant reference point. The other energy states are plotted relative to this ground state. The energy of transition of electron from the ground to the excited states can be calculated by the vertical distance from the ground state. In order to make the diagram general for different metal ions with the same electronic configurations and to acknowledge for different ligands, both of which affect Dq and B or B' , the axes are plotted in units of energy/ B (i.e. E/B) and Dq/B . For examples, d^5 diagram equally applies for the both $Mn^{2+}(d^5)$ & $Fe^{3+}(d^5)$ where for each metal ion the corresponding value of B is used.

Left hand ordinate represents the energies of the Russell-Saunders terms of the free ion in units of B (E/B). Abscissa represents the crystal field strength $10Dq$ in units of B (Dq/B). The energies of states with spin multiplicity different from those of the ground states are also included in this diagram. Configuration interaction is included as bending of lines for the excited states. These states require Racah parameters B & C (inter electronic repulsion parameters) in the analytical expressions for their energies. Thus, state energies in Tanabe-Sugano diagrams are dependent on Dq , B & C and thus would need a four dimensional plot. It can be simplified by assuming that $C = 4.5B$ and to express both the state energies and Dq as multiples of B' . The value of B & C are different for different metal ions and are characteristics of a metal ion.

Hence, the ordinate is taken in units of E/B' and the abscissa is in units of Dq/B' . The position of the spectral states are function of two parameters Dq & B .

The simple relation $C = 4.5B'$ may not be true in every case, so Tanabe-Sugano diagrams have only qualitative significance, but much help in interpreting spectra and in finding approximate value of Dq . For high spin complexes, the Tanabe-Sugano diagrams are similar to Orgel diagram except states of lower spin multiplicity for d^4 , d^5 , d^6 & d^7 which have low spin and high spin forms. For d^1 , d^2 , d^3 , d^8 & d^9 , the ground state is same in both weak and strong ligand fields. With increasing ligand field, state with lower multiplicity derived from a higher free ion state become ground state.

