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TANABE SUGANO DIAGRAM

Tanabe–Sugano diagrams are used in coordination chemistry to predict absorptions 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 are qualitatively useful and can be used to approximate the value of $10Dq$, the ligand field splitting energy. Tanabe–Sugano diagrams can be used for both high spin and low spin complexes, unlike Orgel diagrams, which apply only to high spin complexes. Tanabe–Sugano diagrams 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 diagrams. The energy of the ground state is taken to be zero for all field strengths, and the energies of all other terms and their components are plotted with respect to the ground term.

Parameters

The x-axis of a Tanabe–Sugano diagram is expressed in terms of the ligand field splitting parameter, Dq , or Δ , divided by the Racah parameter B . The y-axis is in terms of energy, E , also scaled by B . Three Racah parameters exist, A , B , and C , which describe various aspects of interelectronic repulsion. A is an average total interelectron repulsion. B and C correspond with individual d-electron repulsions. A is constant among d-electron configuration, and it is not necessary for calculating relative energies, hence its absence from Tanabe and Sugano's studies of complex ions. C is necessary only in certain cases. B is the most important of Racah's parameters in this case. One line corresponds to each electronic state. The bending of certain lines is due to the mixing of terms with the same symmetry. Although electronic transitions are only "allowed" if the spin multiplicity remains the same (i.e. electrons do not change from spin up to spin down or vice versa when moving from one energy level to another), energy levels for "spin-forbidden" electronic states are included in the diagrams, which are also not included in Orgel diagrams. Each state is given its symmetry label (e.g. A_{1g} , T_{2g} , etc.), but "g" and "u" subscripts are usually left off because it is understood that all the states are *gerade*. Labels for each state are usually written on the right side of the table, though for more complicated diagrams (e.g. d^6) labels may be written in other locations for clarity. Term symbols (e.g. 3P , 1S , etc.) for a specific d^n free ion are listed, in order of increasing energy, on the y-axis of the diagram. The relative order of energies is determined using Hund's rules. For an octahedral complex, the spherical, free ion term symbols split accordingly:

Splitting of Term Symbols from Spherical to Octahedral Symmetry

Term	Degeneracy	States in an octahedral field
S	1	A_{1g}
P	3	T_{1g}

D	5	$E_g + T_{2g}$
F	7	$A_{2g} + T_{1g} + T_{2g}$
G	9	$A_{1g} + E_g + T_{1g} + T_{2g}$
H	11	$E_g + T_{1g} + T_{1g} + T_{2g}$
I	13	$A_{1g} + A_{2g} + E_g + T_{1g} + T_{2g} + T_{2g}$

Certain Tanabe–Sugano diagrams (d^4 , d^5 , d^6 , and d^7) also have a vertical line drawn at a specific Dq/B value, which corresponds with a discontinuity in the slopes of the excited states' energy levels. This pucker in the lines occurs when the spin pairing energy, P , is equal to the ligand field splitting energy, Dq . Complexes to the left of this line (lower Dq/B values) are high-spin, while complexes to the right (higher Dq/B values) are low-spin. There is no low-spin or high-spin designation for d^2 , d^3 , or d^8 .

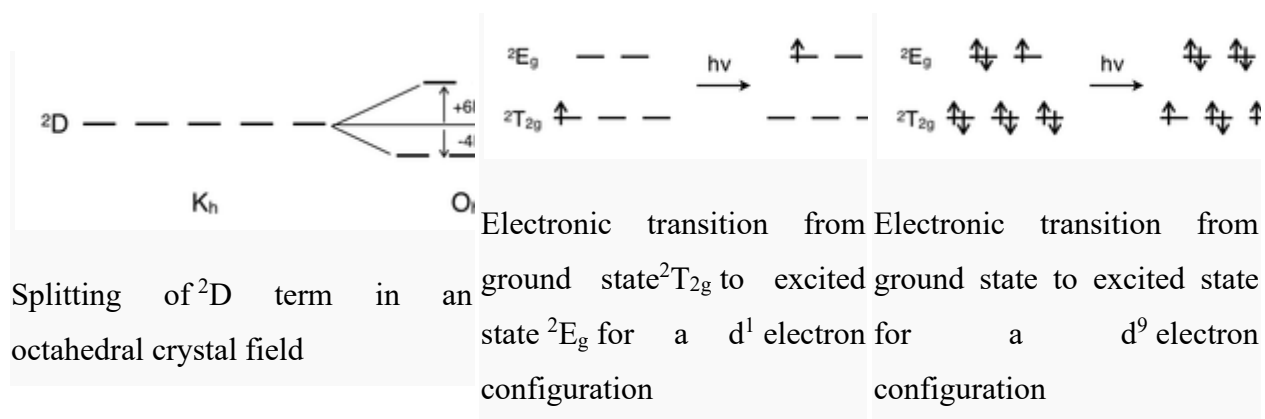
Unnecessary diagrams: d¹, d⁹ and d¹⁰

d¹

There is no electron repulsion in a d¹ complex, and the single electron resides in the t_{2g} orbital ground state. A d¹ octahedral metal complex, such as [Ti(H₂O)₆]³⁺, shows a single absorption band in a UV-vis experiment.^[5] The term symbol for d¹ is ²D, which splits into the ²T_{2g} and ²E_g states. The t_{2g} orbital set holds the single electron and has a ²T_{2g} state energy of -4Dq. When that electron is promoted to an e_g orbital, it is excited to the ²E_g state energy, +6Dq. This is in accordance with the single absorption band in a UV-vis experiment. The prominent shoulder in this absorption band is due to a Jahn-Teller distortion which removes the degeneracy of the two ²E_g states. However, since these two transitions overlap in a UV-vis spectrum, this transition from ²T_{2g} to ²E_g does not require a Tanabe–Sugano diagram.

d⁹

Similar to d¹ metal complexes, d⁹ octahedral metal complexes have ²D spectral term. The transition is from the (t_{2g})⁶(e_g)³ configuration (²E_g state) to the (t_{2g})⁵(e_g)⁴ configuration (²T_{2g} state). This could also be described as a positive "hole" that moves from the e_g to the t_{2g} orbital set. The sign of Dq is opposite that for d¹, with a ²E_g ground state and a ²T_{2g} excited state. Like the d¹ case, d⁹ octahedral complexes do not require the Tanabe–Sugano diagram to predict their absorption spectra.



d¹⁰

There are no d-d electron transitions in d¹⁰ metal complexes because the d orbitals are completely filled. Thus, UV-Vis absorption bands are not observed and a Tanabe–Sugano diagram does not exist.