

- *Russell Saunders coupling.*
- *Orgel diagram.*

Russell Saunders coupling

- In atomic spectroscopy, **Russell–Saunders coupling**, also known as **LS coupling**, specifies a **coupling** scheme of electronic spin- and orbital-angular momenta.
- In light atoms, the interactions between the orbital angular momenta of individual electrons is stronger than the spin-orbit **coupling** between the spin and orbital angular momenta. These cases are described by **L-S coupling**.
- The interactions that can occur are of three types.
 - spin-spin coupling
 - orbit-orbit coupling
 - spin-orbit coupling

- There are two principal coupling schemes used:
 - i. Russell-Saunders (or L - S) coupling
 - ii. jj coupling.
- In the Russell Saunders scheme it is assumed that:
spin-spin coupling $>$ orbit-orbit coupling $>$ spin-orbit coupling.
- This is found to give a good approximation for first row transition series where spin-orbit (J) coupling can generally be ignored, however for elements with atomic number greater than thirty, spin-orbit coupling becomes more significant and the j-j coupling scheme is used.

Spin-Spin Coupling

- S - the resultant spin quantum number for a system of electrons. The overall spin S arises from adding the individual m_s together and is as a result of coupling of spin quantum numbers for the separate electrons

Orbit-Orbit Coupling

- L - the total orbital angular momentum quantum number defines the energy state for a system of electrons. These states or term letters are represented as in later.

Spin-Orbit Coupling

- Coupling occurs between the resultant spin and orbital momenta of an electron which gives rise to J the total angular momentum quantum number. Multiplicity occurs when several levels are close together and is given by the formula $(2S+1)$. The Russell Saunders term symbol that results from these considerations is given by: $(2S+1)L$
- $S = +\frac{1}{2}$, hence $(2S+1) = 2$

For $L=2$, the Ground Term is written as 2D

The Russell Saunders term symbols for the other free ion configurations are given in the Table below.

Terms for $3d^n$ free ion configurations			
Configuration	# of energy levels	Ground Term	Excited Terms
d^1, d^9	1	2D	-
d^2, d^8	5	3F	$^3P, ^1G, ^1D, ^1S$
d^3, d^7	8	4F	$^4P, ^2H, ^2G, ^2F, 2 \times ^2D, ^2P$
d^4, d^6	16	5D	$^3H, ^3G, 2 \times ^3F, ^3D, 2 \times ^3P, ^1I, 2 \times ^1G, ^1F, 2 \times ^1D, 2 \times ^1S$
d^5	16	6S	$^4G, ^4F, ^4D, ^4P, ^2I, ^2H, 2 \times ^2G, 2 \times ^2F, 3 \times ^2D, ^2P, ^2S$

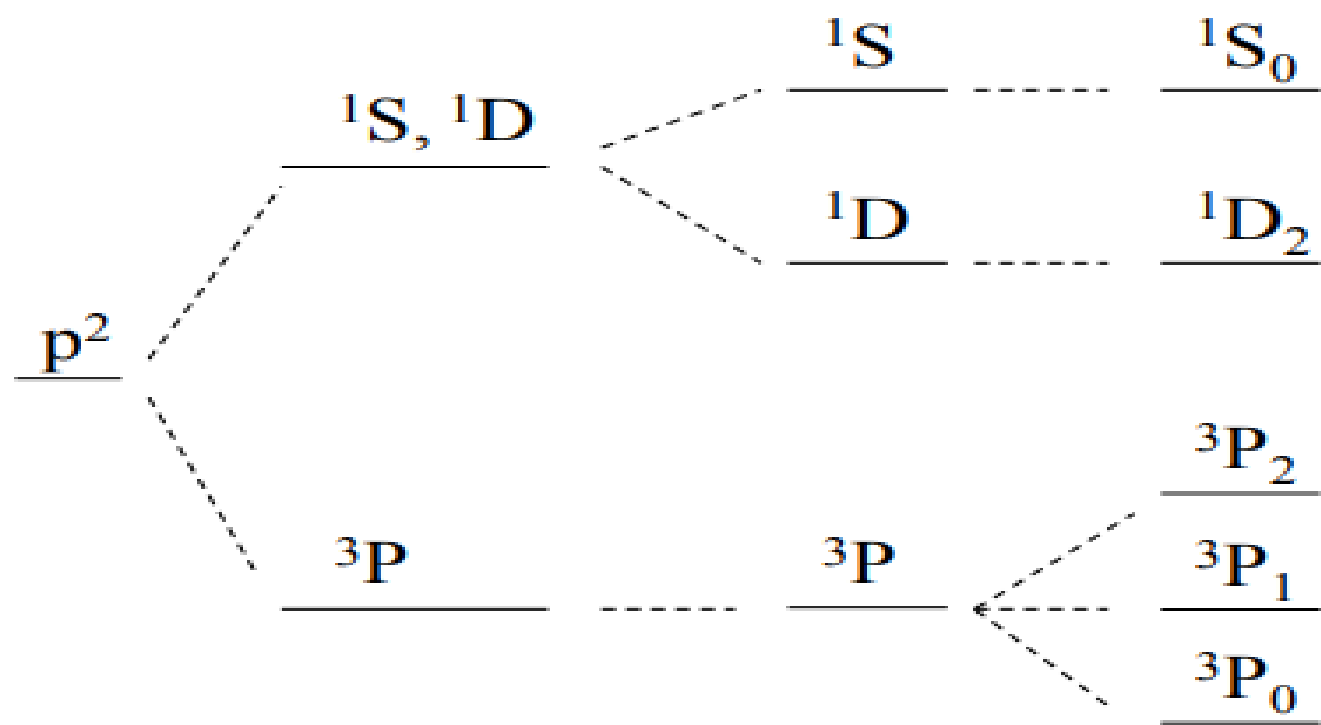
- **Hund's Rules**

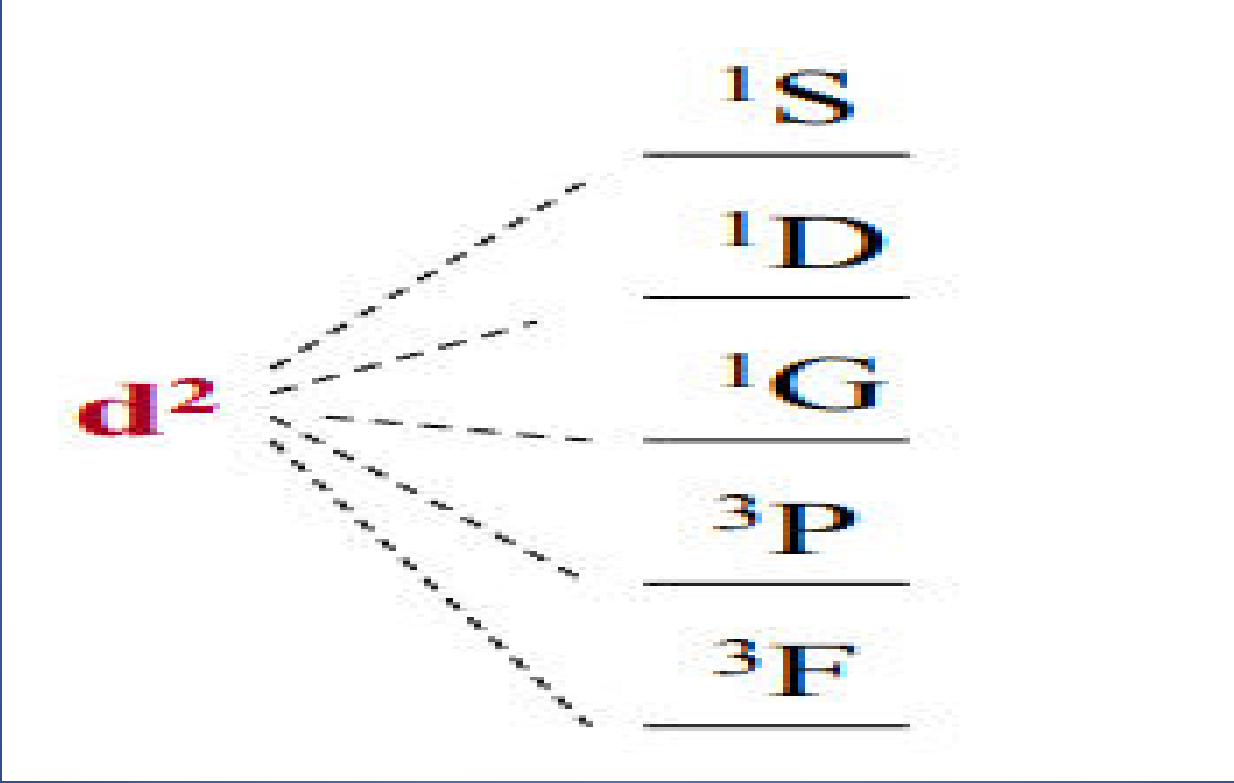
The Ground Terms are deduced by using Hund's Rules.

The two rules are:

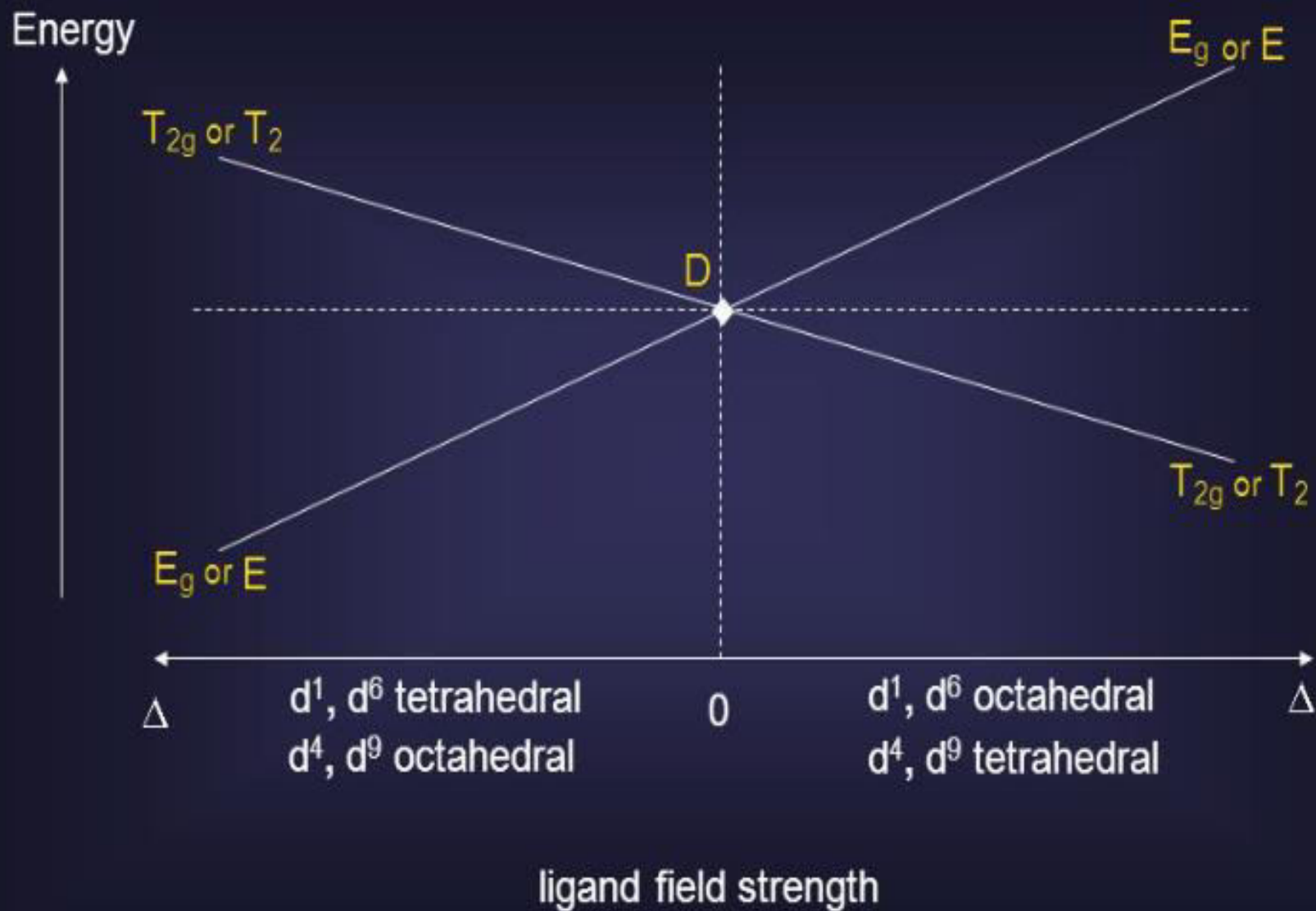
- 1) The Ground Term will have the maximum multiplicity
- 2) If there is more than 1 Term with maximum multiplicity, then the Ground Term will have the largest value of L .

d^n	2	1	0	-1	-2	L	S	Ground Term
d^1	↑					2	1/2	2D
d^2	↑	↑				3	1	3F
d^3	↑	↑	↑			3	3/2	4F
d^4	↑	↑	↑	↑		2	2	5D
d^5	↑	↑	↑	↑	↑	0	5/2	6S
d^6	↑↓	↑	↑	↑	↑	2	2	5D
d^7	↑↓	↑↓	↑	↑	↑	3	3/2	4F
d^8	↑↓	↑↓	↑↓	↑	↑	3	1	3F
d^9	↑↓	↑↓	↑↓	↑↓	↑	2	1/2	2D

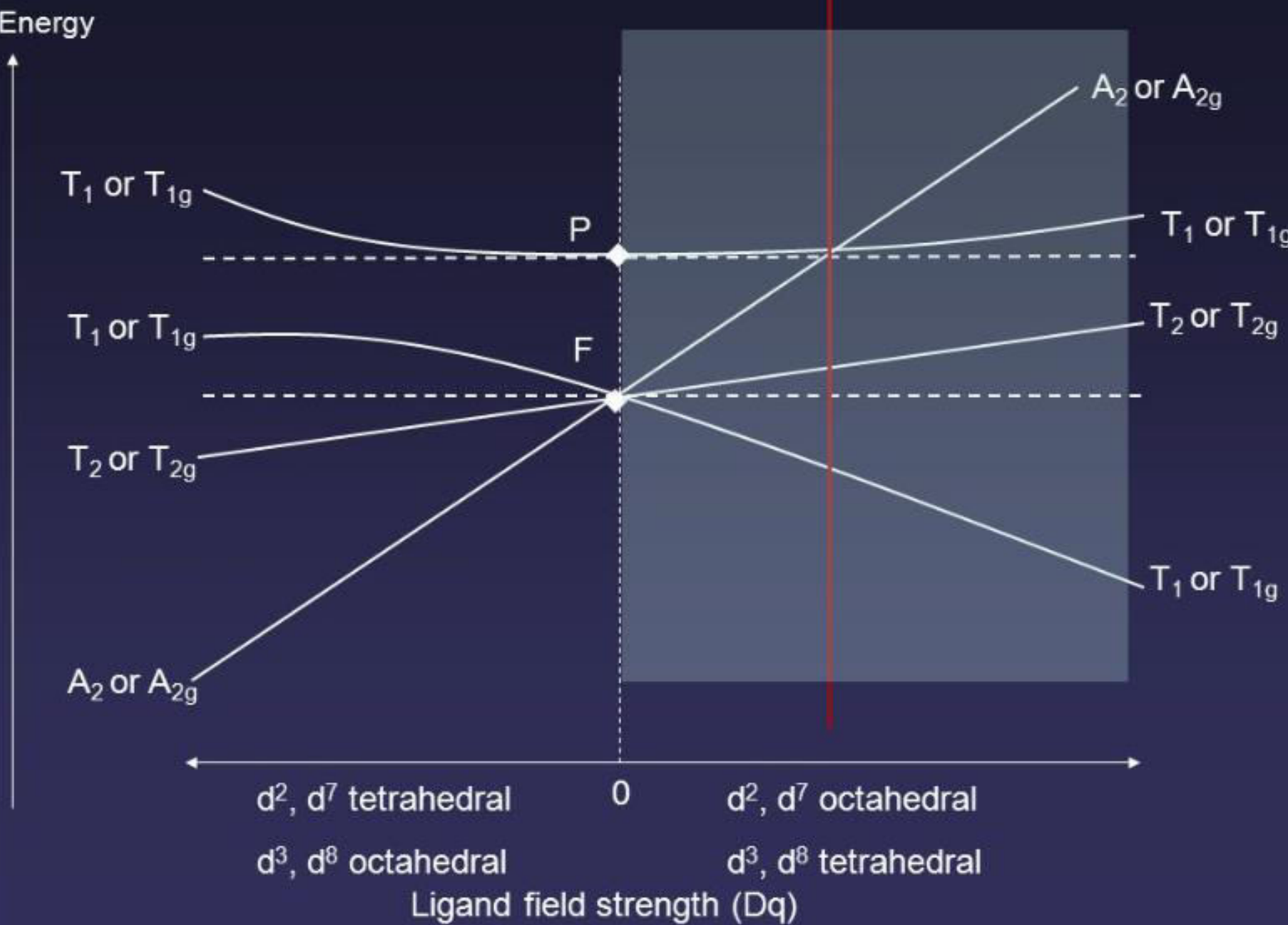




Orgel diagram for d^1 , d^4 , d^6 , d^9



Orgel diagram for d^2, d^3, d^7, d^8 ions



- For a d^7 configuration :
- in the +2 box are 2 electrons, so L for that box is $2*2= 4$
- in the +1 box are 2 electrons, so L for that box is $1*2= 2$
- in the 0 box is 1 electron, L is 0
- in the -1 box is 1 electron, L is $-1*1= -1$
- in the -2 box is 1 electron, L is $-2*1= -2$
- Total value of L is therefore $+4 +2 +0 -1 -2$ or $L=3$.
Note that for 5 electrons with 1 electron in each box then the total value of L is 0. This is why L for a d^1 configuration is the same as for a d^6 .

- The other thing to note is the idea of the "hole" approach. A d^1 configuration can be treated as similar to a d^9 configuration. In the first case there is 1 electron and in the latter there is an absence of an electron i.e., a hole.
- The overall result shown in the Table above is that:
- 4 configurations (d^1, d^4, d^6, d^9) give rise to D ground terms,
- 4 configurations (d^2, d^3, d^7, d^8) give rise to F ground terms
- and the d^5 configuration gives an S ground term.