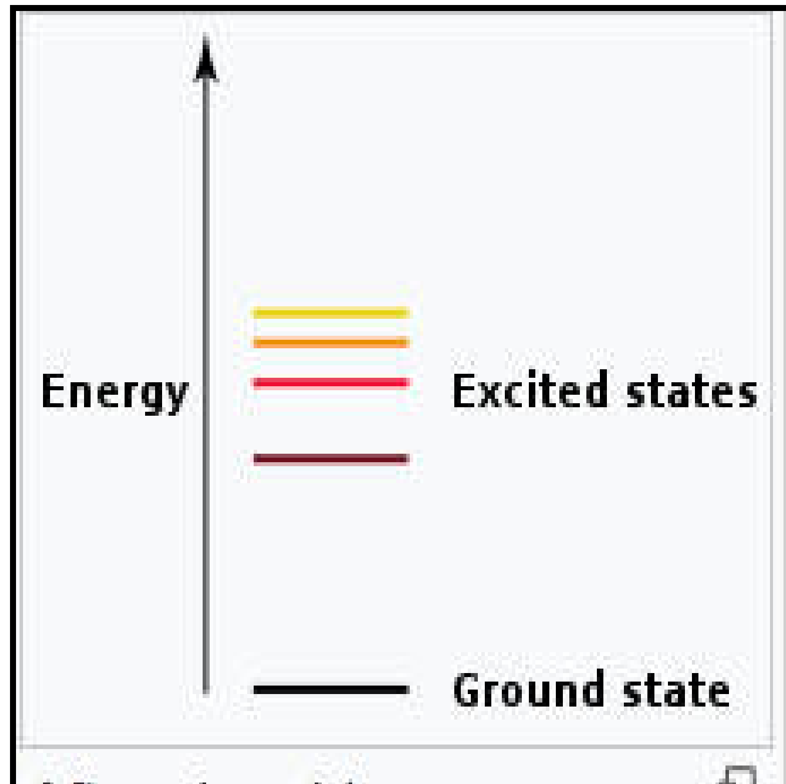
JABLONSKI DIAGRAM

Dr.R.Satheesh,
Assistant Professor in Chemistry,
Mannar Thirumalai Naicker College,
Madurai-4

What is Jablonski diagram?

A Jablonski diagram is an energy level diagram arranged with energy on a verticle axis. It shows a portion of possible consequences of applying photons from visible light to a the molecule under consideration.

When the radiations are incident on some substances, some of the electrons may absorb energy and jump to higher energy level. The electrons may return to ground state or may bring about a chemical Change



Various Processes associated with Jablonski diagram

- Internal Conversion
- Fluorescence
- Intersystem Crossing
- Phosphorescence

Spin multiplicity

- ❖**Spin multiplicity is a quantity.**
- ❖**It is calculated by the formula 2S+1**
- ❖**S stands for total electron spin**

Singlet Ground State

- ➢ Most of the molecules have even number of electrons in the ground state. Hence they are spin paired.
- ➢ *When the spins are paired, the upward orientation of the electron spin gets cancelled by downward* orientation. i.e) S = 0
- ➢ Let S1 = +1/2 ; S2 = -1/2

  S = S1 + S2 = +1/2 -1/2 = 0
- ➢ Hence 2S+1 = 2(0) +1 = 1. Therefore spin multiplicity of the molecule =1
- ➢ Therefore the molecule is in singlet ground state

Triplet Excited state

When a molecule absorbs light of a suitable energy hv, one of the paired electrons goes to excited state. The spin orientation of the two electrons may be either parallel (↑↑) or antiparallel(↑↓).

Spin calculation

- If the spins are **parallel**, then total spin is calculated as
- S = S1+ S2
- S = +1/2 + 1/2 = 1
- 2S+1 = 2x1 +1 = 3
- Spin multiplicity of the molecule = 3
- Hence the molecule is in the triplet excited state

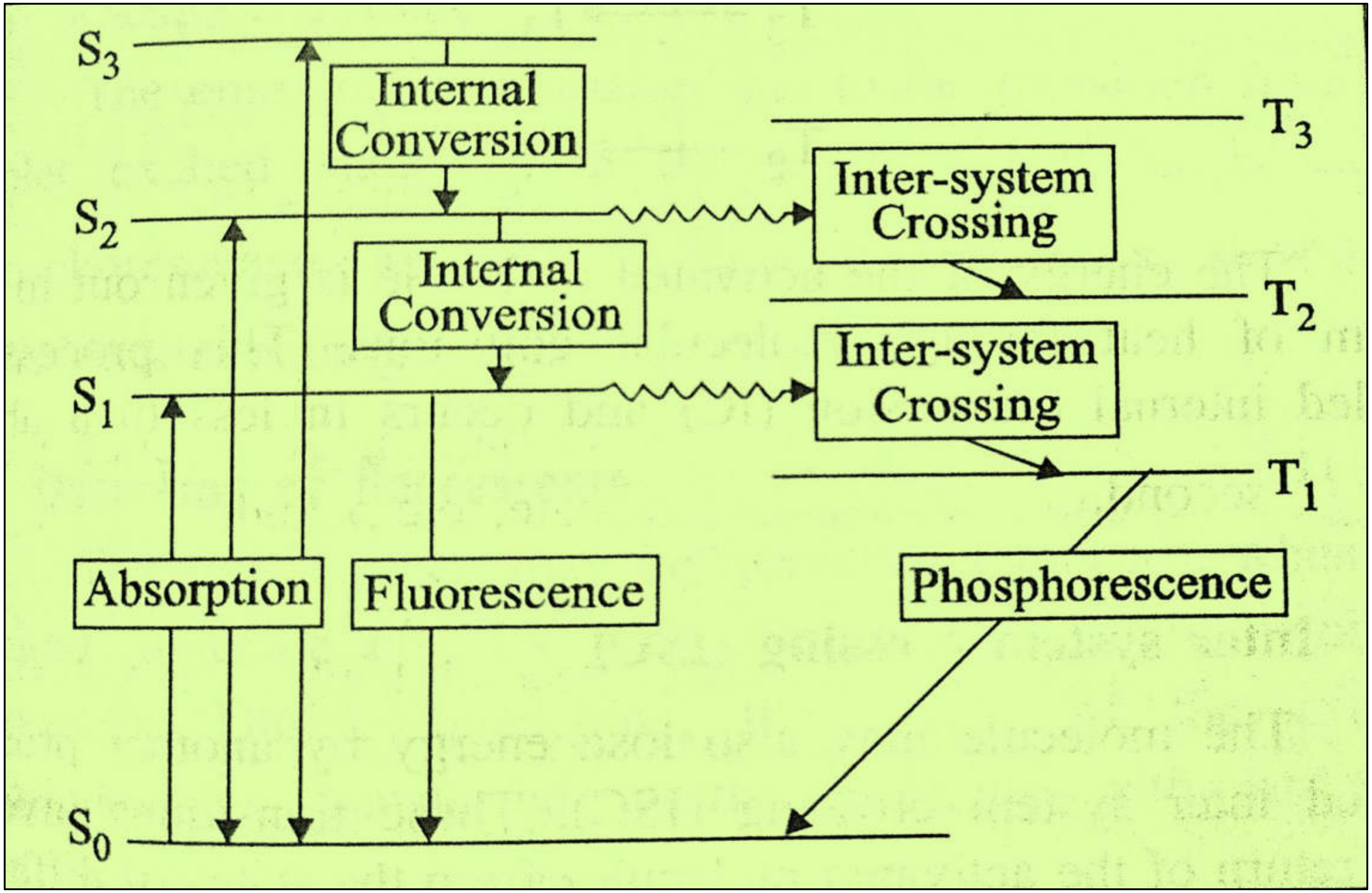
Singlet Excited state

When a molecule absorbs light of a suitable energy hv, one of the paired electrons goes to excited state. The spin orientation of the two electrons may be either parallel (↑↑) or antiparallel(↑↓).

Spin calculation

- ❖ If the spins are **antiparallel,** then total spin is calculated as
- ❖ S = S1+ S2
- ❖ S = +1/2 -1/2 = 0
- ❖2S+1 = 2x0 +1 = 1
- ❖ Spin multiplicity of the molecule = 1
- ❖Hence the molecule is in the singlet excited state

Schematic Representation of Jablonski diagram



Explanation

An electron can jump from the ground state to any of the higher electronic states depending upon the energy of the photon absorbed, we get a series of

- ❖ Singlet excited states i.e) S1, S2, S3
- ❖ Triplet excited states i.e) T1, T2, T3
- ❖ Generally singlet excited state has higher energy than the corresponding triplet excited state Therefore, the energy sequence is given as follows:

i) $E_{S1} > E_{T1}$

ii) $E_{S2} > E_{T2}$

iii) $E_{S3} > E_{T3}$

Types Of Transitions

❖ When a molecule absorbs light radiation, the electrons may jump from S0 to S1, S2 Or S3 singlet excited state depending upon the energy of light radiation as shown in Jablonski diagram.

❖ For each singlet excited state, there is a corresponding triplet excited state.

❖ The molecule in singlet or triplet excited state is said to be activated.

$$A_0 + hv \Rightarrow A^*$$

❖ The activated molecule returns to the ground state by emitting its energy through the following types of transitions.

i) Non-radiative transitions ii) radiative transitions

Non-radiative transitions

- **Internal Conversion (IC)**
- **Intersystem crossing(ISC)**

Internal Conversion

- These transitions involve the return of the activated molecule from the higher excited states to the first excited state. Thes are represented as follows.

S3 → S1
S2 → S1

(or)

T3 → T1
T2 → T1

- The energy of the activated molecule is given out in the form of heat through the molecular collisons. This process is called internal conversion(IC) and occurs in less than 10^{-11} second

Intersystem Crossing

❖The molecule also loses energy by Intersystem crossing(ISC).

❖These transitions involve the return of the activated molecules from the states of different spins i.e) different multiplicity

S2 → T2

S1 → T1

❖ These transitions are forbidden.

❖ It occurs relatively at slow rates

Radiative transitions

- These transitions involve the return of activated molecules from the singlet excited state S1 and triplet excited state T1 to the ground state S0. These accompanied by the emission of radiations.
- These radiative transitions involve the following two radiations.
  i) Fluorescence ii) Phosphorescence

Fluorescence

- Fluorescence emission originates due to transition from singlet excited state to the ground state.
- It is an allowed transition
- This transition is fast & occurs in 10^{-8} second.
- Fluorescence stops as soon as the incident radiation is cut off.
- Examples : Fluorite, Eosin, Fluorescein

Phosphorescence

- ❖ It arises due to the transition from triplet excited state to the ground state
- ❖ It is a forbidden transition
- ❖ It is a slow process
- ❖ Phosphorescence continues for some time even after the incident radiation is cut off.
- ❖ Examples : ZnS and alkaline earth sulphides

References

I. B.R. Puri, L.R. Sharma and S. Pathania, Principles of Physical Chemistry, 47th Edition, Shoban Lal Nagin Chand & Co., 2017.

2. P.L.Soni and Dharmarha, Text book of Physical Chemistry, S. Chand & Co., New Delhi, 1991