Difference Between sp3d2 and d2sp3 Hybridization

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Key Difference - sp3d2 vs d2sp3 Hybridization

There are hypothetical structures known as orbitals in an atom in which electrons reside. Different scientific discoveries have proposed different shapes for these orbitals. Atomic orbitals can undergo a process known as hybridization. Hybridization of orbitals occurs in order to obtain suitable shapes required for chemical bonding. Hybridization is the mixing of atomic orbitals to form hybrid orbitals. sp^3d^2 and d^2sp^3 are such hybrid orbitals. The **key difference** between sp^3d^2 and d^2sp^3hybridization is that **sp^3d^2 hybridization involves atomic orbitals of same electron shell whereas d^2sp^3 hybridization involves atomic orbitals of two electron shells.**

What is sp3d2 Hybridization

sp^3d^2hybridization is the mixing of s, p and d atomic orbitals of the same electron shell to form sp^3d^2 hybrid orbitals. There, one s atomic orbital, three p atomic orbitals and two d atomic orbitals mix with each other. This mixing results in six hybrid orbitals of same size and shape but different from their orientation.

The sp^3d^2 hybrid orbitals are arranged in octahedral arrangement. These hybrid orbitals have 90^o angles between two orbitals in the octahedral arrangement. The octahedral arrangement displays a square plane having four hybrid orbitals and the two remaining orbitals are oriented above and below of this square plane (perpendicular to this plane).

Let us consider an example in order to understand the sp^3d^2 hybridization. Ex: SF6 molecule has an octahedral shape because the 3s, 3p and 3d atomic orbitals of the sulfur atom (S) are mixed to formsp^3d^2 hybrid orbitals.

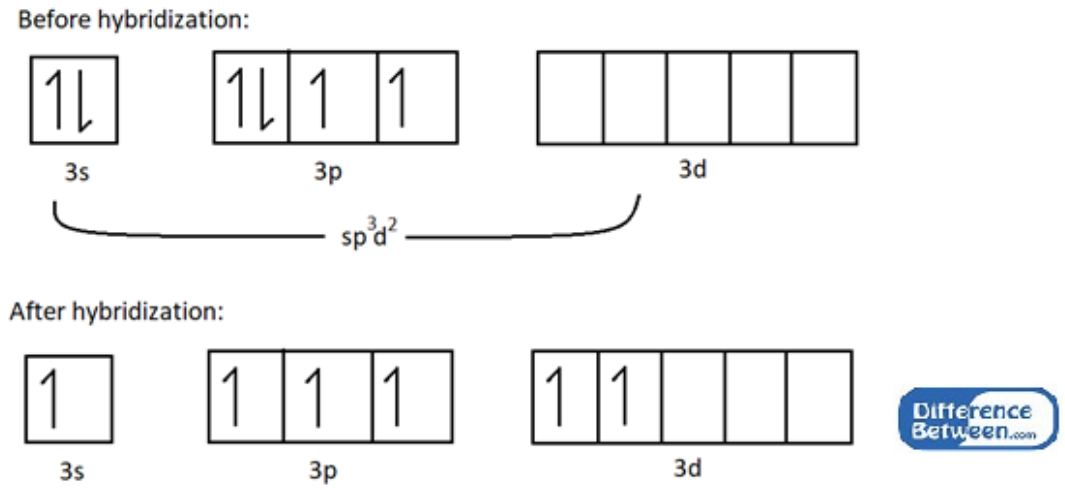

Figure 01: Electronic structure of sulfur atom before and after Hybridization.

As shown in the above image, the hybridization results in six unpaired electrons that can participate in chemical bonding with six fluorine atoms. Most importantly, all the atomic orbitals involved in this hybridization are in the same electron shell (in above example, it is n=3 electron shell).

What is d2sp3 Hybridization?

d^2sp^3 hybridization is the mixing of s and p atomic orbitals of the same electron shell with d orbitals of another electron shell to form d^2sp^3 hybrid orbitals. This hybridization results in six hybrid orbitals. These hybrid orbitals are arranged in an octahedral geometry.

Most importantly, in this hybridization, the d atomic orbitals come from a different electron shell (n-1 electron shell) whereas s and p atomic orbitals are of the same electron shell. Let us consider an example to understand this hybridization. Most of the metal ion complexes are composed of d^2sp^3 hybridized orbitals.

Ex: $Co(NH_3)^{3+}$ complex.

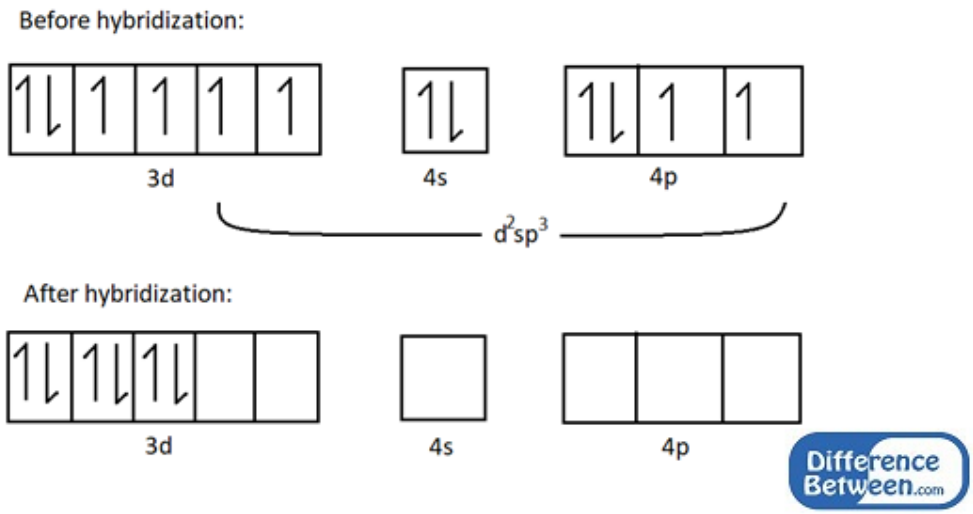

Figure 02: Electronic structure of cobalt (Co) atom before and after Hybridization.

As shown in the above image, there are six empty hybrid orbitals in cobalt atom after hybridization. These empty orbitals can participate in coordination chemical bond formation with ligands (here ammonia ligands = NH_3).

What are the Similarities Between sp3d2 and d2sp3 Hybridization?

- Both sp3d2 and d2sp3 Hybridizations result in octahedral geometry.
- Both sp3d2 and d2sp3 Hybridization geometries have 90° angle between hybrid orbitals.
- Both sp3d2 and d2sp3 Hybridization result in six hybrid orbitals.

What is the Difference Between sp3d2 and d2sp3 Hybridization?

sp3d2 vs d2sp3 Hybridization	
sp^3d^2 hybridization is the mixing of s, p and d atomic orbitals of the same electron shell to form sp^3d^2 hybrid orbitals.	d^2sp^3 hybridization is the mixing of s and p atomic orbitals of the same electron shell with d orbitals of another electron shell to form d^2sp^3 hybrid orbitals.
Nomenclature	
sp^3d^2 hybridization forms sp^3d^2hybrid	d^2sp^3 hybridization d^2sp^3 hybrid orbitals.

orbitals.	
Type of Atomic Orbitals	
sp^3d^2 hybridization involves atomic orbitals of same electron shell.	d^2sp^3 hybridization involves atomic orbitals of two electron shells.
d Orbitals	
sp^3d^2 hybridization involves d atomic orbitals of n electron shell.	d^2sp^3 hybridization involves d atomic orbitals of n-1 electron shell.

Summary - sp3d2 vs d2sp3 Hybridization

sp^3d^2 hybridization and d^2sp^3 hybridization are confusing terms that are most of the times used interchangeably by mistake. These are different in many ways. The key difference between sp^3d^2 and d^2sp^3hybridization is that, sp^3d^2 hybridization involves atomic orbitals of same electron shell whereas d^2sp^3 hybridization involves atomic orbitals of two electron shells.

Reference:

1.“8.2: Hybrid Atomic Orbitals.” Chemistry LibreTexts, Libretexts, 30 Aug. 2017. Available here