

the geometry acquired by the molecule, are summed up in Table 1.

TABLE 1
Geometry of Covalent Molecules Involving Different Types of Hybrid Orbitals of the Central Atom

Type of Hybrid Involved	Name of the Compound	Geometry of the Molecule	Bond Angles $\angle ABA$
sp	BeF_2	Linear	180°
sp^2	BF_3	Trigonal planar	120°
sp^3	CH_4	Tetrahedral	109.5°
sp^3d	PF_5	Trigonal bipyramidal	120° and 90°
sp^3d^2	SF_6	Octahedral	90°
sp^3d^3	IF_7	Pentagonal bipyramidal	72° and 90°

It may be noted that in the above compounds, all the electron pairs are bonded and the geometry and bond angles are exactly the same as expected according to VSEPR theory.

GEOMETRY OF MOLECULES CONTAINING BOND PAIRS AS WELL AS LONE PAIRS OF ELECTRONS

So far we have seen that in a molecule in which central atom has no lone pairs of electrons in any of its hybrid orbitals, the arrangement of hybrid orbitals around the central atom and the geometry of the molecule are the same. But, as already mentioned, the presence of one or more orbitals containing lone pairs in the valency shell cause some distortion in the geometry of the molecule. A few examples of molecules containing bond pairs as well as lone pairs of electrons and involving different types of hybridisation may now be considered.

1. Geometry of $SnCl_2$ Molecule. The outer electronic configuration of the central atom, tin, in this case, is $5s^2 5p^1 5d^1$. There are two unpaired electrons in the $5p$ orbitals of tin and these are sufficient to form two bonds with chlorine atoms and, therefore, there is no need of promotion of electrons. The bond formation can take place by the overlapping of the two mutually perpendicular half-filled p_x and p_y orbitals of tin atom with the

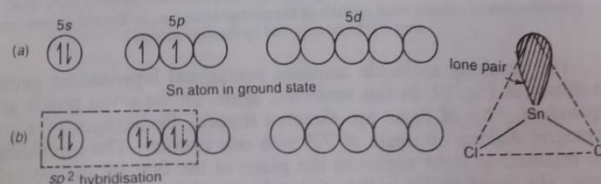


Fig. 20. V-shaped geometry of $SnCl_2$ molecule resulting from sp^2 hybridisation of the valence shell orbitals of Sn atom.

HYBRIDISATION

half-filled p orbitals of be angular with $Cl-Sn$ by X-ray analysis and close to 120° . This s orbitals and not two. orbitals of tin hybrid energy, as shown in

These sp^2 hybrid trigonal planar geometry of electrons while. These two sp^2 hybrid the half-filled $2p_z$ to form two $Sn-Cl$ atom Sn in $SnCl_2$ each containing orbitals contain contains a lone geometry of the V-shaped with. However, on pair-bond pair-bond slightly less still V-shaped

2. Ge central atom three p orbitals as shown in and these ammonia case, however have the NH_3 molecule. This is

no unpaired electron, as shown in Fig. 5.

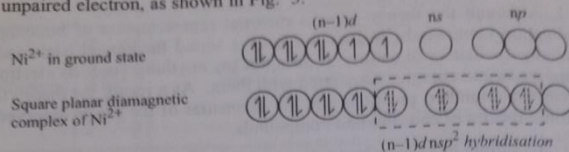


Fig. 5. The diamagnetic square planar complex of Ni(II). The complex has no unpaired electron.

This may lead to the conclusion that *all square planar complexes of Ni(II) should be diamagnetic*. But actually it is not so. We come across quite a few square planar complexes of Ni(II) which are *paramagnetic*. Valence bond theory does make an attempt to explain this observation by postulating that in such complexes one of the unpaired (n-1)d electrons of Ni²⁺ gets transferred to the vacant 4p_z orbital to vacate the (n-1)d orbital which is required for (n-1)d nsp² hybridisation to form a *square planar complex*. Such a complex would contain two unpaired electrons as shown in Fig. 6 and would thus be *paramagnetic*. But it is difficult to explain why such excitation of electron occurs in one square planar complex but not in the other.

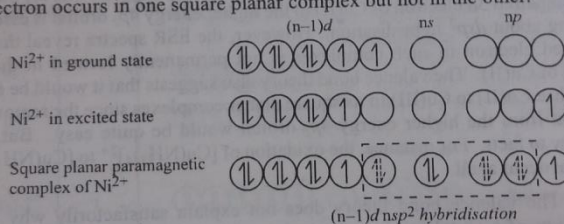


Fig. 6. The paramagnetic square planar complex of Ni(II). The complex has two unpaired electrons.

CRYSTAL FIELD (C.F.) THEORY

The crystal field theory developed by H. Bethe and V. Bleck (1935) proved to be far more successful in explaining the bonding in and the properties of coordination complexes than the valence bond theory. According to the **crystal field theory**, *bonding between a central metal ion and its ligand arises from purely electrostatic interactions*. If the ligand is an anion, the attraction towards the cation is as that between any oppositely charged particles. If the ligand is a neutral molecule such as NH₃ or H₂O, the negative end of the dipole is attracted towards the central positive ion.

Knowing the arrangement of ligands around the central metal ion, assuming the bonds between metal ion and the ligands to be purely electrostatic and considering the metal ion and the ligands as *point charges* q_1 and q_2 , separated by a distance r , the metal-ligand bond energies for various complexes can be calculated using the Coulomb's law, viz., $B.E. = -q_1q_2/r$. The values

obtained in the case of low coordination metal complexes, explained the

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obtained were found to be in close agreement with those obtained experimentally in the case of non-transition metal complexes. The values were, however, too low compared to the experimentally observed values, in the case of transition metal complexes. The cause of discrepancy, according to the crystal field theory, lies in the manner of the orientation of the d orbitals in space, as explained below.

Orientation of d orbitals and Crystal Field Splitting of Energy Levels

As shown in Chapter 1, the d orbitals can be divided into two groups depending upon the nature of their orientation in space. One of the groups consists of three orbitals which are oriented in the regions in between the coordinate axes while the other group comprises of two orbitals which are oriented along the axes. In the case of a free metal ion, all the five d orbitals have the same energy, i.e., they are **degenerate**, meaning energetically alike. Consider a hypothetical case in which the set of five d orbitals of the metal ion is spherically surrounded by a uniformly spread negative charge. The electrostatic repulsion between d electrons and this charge would result in uniform increase in the energies of d orbitals. In other words, although the orbitals acquire higher energy, they would still remain *degenerate*. Now consider that the negative charge surrounding d orbitals of the metal ion gets concentrated in a number of point charges in certain specific positions. The energy of the orbitals lying in the directions of the point charges would be raised to a larger extent than that of the orbitals lying in between the point charges because the electrons in the former type of d orbitals would experience greater repulsion from point charges than the electrons in the latter type of d orbitals. This means that some of the d orbitals would get associated with a higher energy than the other d orbitals. The splitting of five degenerate d orbitals of the metal ion into sets of orbitals having different energies is called **crystal field splitting**. The concept forms the basis of crystal field theory. In the crystal field theory we consider ligands as point charges.

The number of ligands and their arrangement around the central metal ion will naturally affect the relative energies of the five d orbitals. In other words, the magnitude and the type of the crystal field splitting will be different in complexes of different geometries in which metal ions have different coordination numbers. We would illustrate this concept by considering complexes with coordination numbers 6 and 4 which are the most common. The discussion would be restricted to the most common structures which are octahedral, square planar and tetrahedral.

Crystal Field Splitting in Octahedral Complexes. In an octahedral complex, the coordination number is 6. The metal ion is at the centre and the ligands occupy the six corners of the octahedron, as shown in Fig. 7.

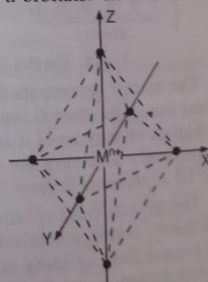


Fig. 7. Six ligands at the corners of an octahedron surrounding the metal ion, M^{n+} .

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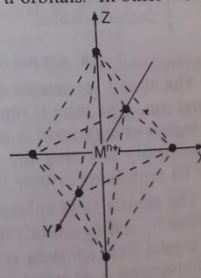


Fig. 7. Six ligands at the corners of an octahedron surrounding the metal ion, M^{n+} .

The three axes X , Y and Z pointing along the corners of the octahedron are also shown. Let us suppose that the metal ion M^{n+} has a single d electron (d^1 configuration). In the free ion, when there are no ligands, the electron can occupy any one of the d orbitals because all are of the same energy. Such orbitals having the same energy are called degenerate orbitals, as already mentioned.

However, in the octahedral complex MX_6 , all the five d orbitals will not remain of equal energy. This can be easily understood from the following discussion.

As already explained, the two orbitals, $d_{x^2-y^2}$ and d_{z^2} are oriented along the axes while the remaining three orbitals are oriented in between the axes.

In the case of octahedral complexes, the former two orbitals are designated as e_g orbitals while the latter three orbitals are designated as t_{2g} orbitals. As the six ligands approach the central ion along the axes, the electron, if present in the e_g orbitals, is repelled more by the ligand electrons than if it is present in the t_{2g} orbitals. In other words, the energy of the d_{z^2} and $d_{x^2-y^2}$ orbitals increases much more than the energy of the d_{xy} , d_{yz} and d_{zx} orbitals. (It should be remembered that when a charge is repelled by a similar charge, its potential energy increases. The greater the repulsion, the greater is the increase of energy). Thus, in octahedral complexes, the five d orbitals split up into two sets: one set consisting of two orbitals of higher energy (e_g orbitals) and the other set consisting of three orbitals of lower energy (t_{2g} orbitals). The crystal field splitting in an octahedral complex is illustrated in Fig. 8.

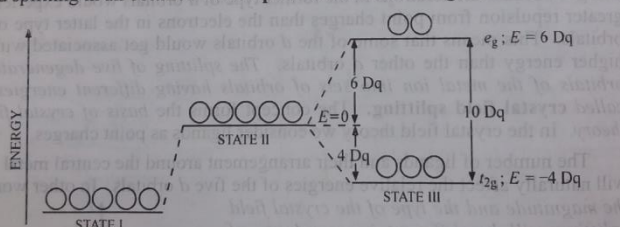


Fig. 8. Crystal field splitting in an octahedral complex.

The state I represents degeneracy of all the five d orbitals in the isolated central ion. The state II represents hypothetical degeneracy of all the orbitals at a higher energy level if the negative charge of all the ligands is assumed to be uniformly affecting the electrons in the d orbitals of the metal ion. The state III represents crystal field splitting discussed above.

The crystal field splitting is measured in terms of the energy difference between t_{2g} and e_g orbitals Δ_o (the subscript o indicating octahedral complex). The crystal field splitting is generally measured in terms of a parameter, Dq . By convention Δ_o is taken to be equal to $10 Dq$.

It can be shown that for an octahedral system, the energy of the t_{2g} orbitals is $4 Dq$ or $0.4 \Delta_o$ less than the energy of the hypothetical degenerate d orbitals which would result if crystal field splitting is ignored (Fig. 8, state II).

It follows, that of the d orbitals

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It follows, therefore, that the energy of the e_g orbitals is $6 Dq$ or $0.6 \Delta_o$ above that of the hypothetical degenerate d orbitals. (The total energy of the unsplit d orbitals must be equal to the energy of the split d orbitals).

Crystal Field Stabilization Energy (CFSE). We know that an electron always prefers to occupy an orbital of a lower energy. It is evident that if an octahedral complex contains one d electron, that electron will reside in one of the t_{2g} orbitals. This orbital has an energy $-4 Dq$ or $-0.4 \Delta_o$ compared to the energy (taken as zero) of the hypothetical degenerate orbitals of state II (Fig. 8). Thus, the complex will be $4 Dq$ or $0.4 \Delta_o$ more stable than predicted by the pure electrostatic theory. Evidently, the energy of the complex would now be less. The decrease in energy $= 0 - (-4 Dq) = 4 Dq$ is called the crystal field stabilisation energy (CFSE) of the complex under consideration. The **crystal field stabilisation energy (CFSE)** may thus be defined as *the lowering in the energy of a transition metal ion in a given ligand environment due to crystal field effects*. The splitting of d orbitals (or of energy terms which arise due to electrostatic repulsions amongst d electrons)* of a metal ion due to electrostatic crystal field potential of ligands and the consequences thereof are known as **crystal field effects**.

The qualitative procedure commonly adopted for calculating CFSEs of the complexed metal ions containing more than one d electrons is to assume that the interelectronic repulsions amongst d electrons do not affect the CFSEs much. Therefore, CFSEs are calculated by this qualitative procedure by considering the splitting of d orbitals alone. For each electron entering into a t_{2g} orbital, the crystal field stabilisation energy is $4 Dq$. Hence, for each electron entering into an e_g orbital, the destabilisation energy would be $6 Dq$. Working on this basis, it is possible to calculate crystal field stabilisation energies for various metal ions in octahedral complexes.

For example, for a d^2 system, the two electrons will occupy t_{2g} orbitals. The crystal field stabilisation energy, $CFSE = 0 - 2(-4 Dq) = 8 Dq$, provided it is assumed that the changes in the interelectronic repulsions amongst the d electrons due to crystal field effects do not appreciably alter the stabilisation energy of the complex. Similarly, for a d^3 system, $CFSE = 0 - 3(-4 Dq) = 12 Dq$.

However, for a d^4 system, there are two possibilities:

1. All the four electrons may occupy t_{2g} orbitals. One electron obviously gets paired. The electronic configuration may be written as $(t_{2g})^4$.
2. Three electrons occupy t_{2g} orbitals and one electron goes to one of the higher e_g orbitals. The configuration may then be written as $(t_{2g})^3(e_g)^1$.

The actual configuration may be decided on the basis of Δ_o and the pairing energy (P), i.e., the energy required to pair the electrons with one another. The pairing energy is evidently related to the energy of electrostatic repulsion amongst the d electrons. The configuration (1) is possible if $\Delta_o > P$, i.e., $\Delta_o >$ the energy of electrostatic repulsions amongst d electrons. In this case, the complex has less number of unpaired electrons and is called *low spin complex* or *strong field complex*. On the other hand, configuration (2) is

*A detailed discussion of energy terms is given in Chapter 27.

possible if $\Delta_0 < P$, i.e., $\Delta_0 <$ the energy of electrostatic repulsions amongst d electrons. In that case, the maximum number of electrons remain unpaired and the complex is called *high spin complex* or *weak field complex*.

A more exact procedure for calculating CFSEs of high spin complexes is to include in calculations the effects of interelectronic repulsions amongst the d electrons along with the effects of splitting of d orbitals due to crystal field effects. The results obtained with or without including the effect of interelectronic repulsions, however, are identical except for d^2 , d^7 (high spin) metal ions in weak field octahedral ligand environments and for d^3 , d^8 metal ions in tetrahedral ligand environments. In these particular cases, the more exact procedure gives CFSEs of 6 Dq instead of 8 Dq.

In low spin complexes, the effects of interelectronic repulsions amongst the d electrons are *quite small* compared to the effects of splitting of d orbitals. The CFSEs of low spin complexes are, therefore, estimated by neglecting the interelectronic repulsion factor.

The crystal field stabilisation energies for metal ions having different numbers of d electrons in octahedral complexes are given in Table 3.

TABLE 3
Crystal Field Stabilisation Energies for Metal Ions having Different
Number of d Electrons in Octahedral Complexes.

No. of d electrons in metal ions	Distribution of Electrons (High Spin)		CFSE*	Distribution of electrons (Low Spin)		CFSE
	t_{2g}	e_g		t_{2g}	e_g	
1	↑ ○ ○ ○ ○		4 Dq			
2	↑ ↑ ○ ○ ○		6 Dq**			
3	↑ ↑ ↑ ○ ○		12 Dq			
4	↑ ↑ ↑ ↑ ○		6 Dq	↑ ↑ ↑ ○ ○		16 Dq
5	↑ ↑ ↑ ↑ ↑		0	↑ ↑ ↑ ○ ○		20 Dq
6	↑ ↑ ↑ ↑ ↑		4 Dq	↑ ↑ ↑ ↑ ○		24 Dq
7	↑ ↑ ↑ ↑ ↑		6 Dq**	↑ ↑ ↑ ↑ ↑		18 Dq
8	↑ ↑ ↑ ↑ ↑		12 Dq			
9	↑ ↑ ↑ ↑ ↑		6 Dq			
10	↑ ↑ ↑ ↑ ↑		0			

* Calculated by including the effects of interelectronic repulsions amongst the d electrons and the effects of d orbital splitting.

** CFSEs of these configurations are 8 Dq if we consider the effects of d orbital splitting alone and neglect the effects of interelectronic repulsions amongst the d electrons.

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Crystal Field Splitting in Tetrahedral Complexes. The coordination number for tetrahedral complexes is 4. The tetrahedral arrangement of four ligands surrounding a metal ion may be visualized by placing ligands at the alternate corners of a cube, as shown in Fig. 9.

It can be shown that in a tetrahedral structure, none of the d orbitals points exactly towards the ligands.

The three d orbitals d_{xy} , d_{yz} and d_{zx} are pointing close to the direction in which ligands are approaching while the two orbitals $d_{x^2-y^2}$ and d_{z^2} are lying in between the ligands. As a result of this, the energy of the former three orbitals increases compared to the energy of the latter two orbitals because the electrons in the former orbitals would be repelled by ligand electrons more strongly than electrons in the latter orbitals. Thus, the d orbitals are again split into two groups but in a reverse order. The three orbitals, d_{xy} , d_{yz} and d_{zx} , designated as t_2 orbitals, now have higher energy than the two orbitals $d_{x^2-y^2}$ and d_{z^2} , designated as e orbitals. This is diagrammatically shown in Fig. 10.

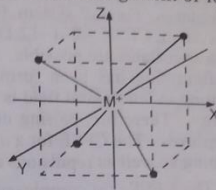


Fig. 9. Tetrahedral arrangement of four ligands around the metal ion.

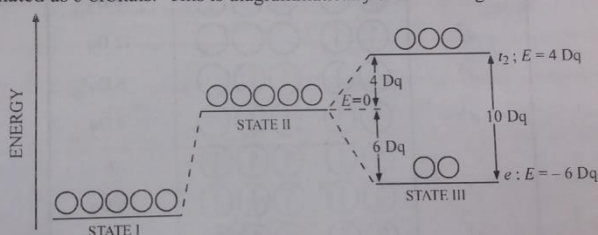


Fig. 10. Crystal field splitting in tetrahedral complexes. State II represents a hypothetical state if it is assumed that negative charge of ligands uniformly affects the charge of d electrons.

The crystal field splitting (*i.e.*, the energy difference between the two sets of orbitals), in this case, is denoted by Δ_t , the subscript t indicating tetrahedral complexes. It is less than Δ_o observed in the case of octahedral complexes, discussed earlier. It has been estimated that $\Delta_t \approx -4/9 \Delta_o$; the minus sign denotes that the order of splitting in tetrahedral complexes is the reverse of that in octahedral complexes. The smaller value Δ_t as compared to Δ_o is partly due to lesser number of ligands in the tetrahedral field.

Since an electron prefers to move into a region of lower energy for reasons of stability, it follows that if a tetrahedral complex contains a d electron, that electron will reside in one of the $d_{x^2-y^2}$ and d_{z^2} orbitals.

An electron going into either of the $d_{x^2-y^2}$ and d_{z^2} orbitals is stabilised by 6 Dq (or $0.6 \Delta_t$) while that going into any of the other three orbitals is destabilised by 4 Dq (or $0.4 \Delta_t$).

The CFSEs for tetrahedral complexes having different electronic configurations can also be calculated by following the same procedure as for octahedral complexes. For a d^1 system, for example, $\text{CFSE} = 0 - (-6 \text{ Dq}) = 6 \text{ Dq}$ and for a d^2 system, $\text{CFSE} = 0 - (-12 \text{ Dq}) = 12 \text{ Dq}$. For a d^3 system, both low spin and high spin states are possible. However, no tetrahedral complex with low spin configuration has been formed. This is due to the fact that crystal field splitting in tetrahedral field is quite small and it is always less than the pairing energy. Therefore, pairing does not occur and the complexes are high spin complexes. The CFSE for a d^3 system, taking into consideration the d orbital splitting as well as repulsions amongst d electrons, is 6 Dq .

The CFSEs for complexes with metal ions having different configurations of d orbitals in tetrahedral field are given in Table 4.

TABLE 4
Crystal Field Stabilisation Energies for Tetrahedral Complexes with Metal Ions having different Electronic Configurations

Electronic configuration	Distribution of Electrons e t_2	CFSE
d^1	\uparrow \circ \circ \circ \circ	6 Dq
d^2	\uparrow \uparrow \circ \circ \circ	12 Dq
d^3	\uparrow \uparrow \uparrow \circ \circ	6 Dq^*
d^4	\uparrow \uparrow \uparrow \uparrow \circ	4 Dq
d^5	\uparrow \uparrow \uparrow \uparrow \uparrow	0
d^6	$\uparrow\downarrow$ \uparrow \uparrow \uparrow \circ	6 Dq
d^7	$\uparrow\downarrow$ $\uparrow\downarrow$ \uparrow \uparrow \uparrow	12 Dq
d^8	$\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$ \uparrow \uparrow	6 Dq^*
d^9	$\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$ \uparrow	4 Dq
d^{10}	$\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$	0

* CFSEs of these configurations are 8 Dq if we consider the effect of d orbital splitting alone and neglect the effects of interelectronic repulsions amongst the d electrons.

Crystal Field Splitting in Tetragonal and Square planar Complexes. The splitting of d orbitals in tetragonal and square planar complexes can be understood by gradually withdrawing two ligands lying along the Z axis from an octahedral complex.

As the ligands lying on the Z axis are moved away, the ligands in the XY plane tend to approach the central ion more closely. As a result of this, the electrons in d orbitals in the XY plane experience greater repulsion from the

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electrons of ligands in a tetragonal complex than in an octahedral complex. This causes an increase in the energy of d orbitals in XY plane, i.e., an increase in the energy of $d_{x^2-y^2}$ and d_{xy} orbitals in tetragonal complexes compared to their energies in octahedral complexes, as illustrated in Fig. 11.

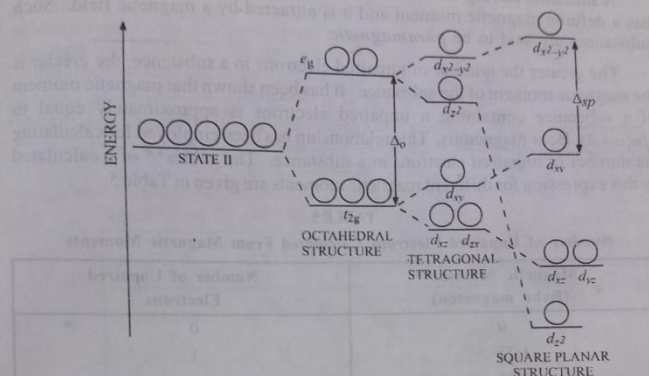


Fig. 11. Crystal field splitting in octahedral, tetragonal and square planar complexes.

Further, since the ligands lying on the Z axis have been moved away, the electrons in the d orbitals along the Z axis as well as in the XZ and YZ planes experience relatively smaller repulsions from the electrons of the ligands. This results in appreciable fall in the energy of d_{z^2} orbital as well as d_{xz} and d_{yz} orbitals. These changes are shown in Fig. 11. The structure in which the two trans ligands are at larger distance as compared to the other four ligands in XY plane is called **tetragonal structure**.

As the trans ligands lying along the Z axis drop out completely, a **square planar complex ML_4** is formed. This is accompanied by a further rise in the energies of $d_{x^2-y^2}$ and d_{xy} orbitals and a further fall in the energies of d_{z^2} , d_{xz} and d_{yz} orbitals, as illustrated in Fig. 11. The crystal field splitting in the case of the square planar complex is indicated by Δ_{sp} .

Magnetic Properties of Metal Complexes and Crystal Field Theory. An important application of crystal field theory has been in understanding magnetic properties of transition metal complexes. As already discussed in Chapter 19, an electron, because of its orbital and spin motions, produces magnetic field whose strength is measured in units of Bohr magneton (B.M.)

$$\text{B.M.} = \frac{eh}{4\pi mc}$$

where h is Planck's constant, c is the velocity of light, e is the charge on the electron and m is its mass.

The value of B.M. as obtained by the above expression is 9.274×10^{-21} erg gauss $^{-1}$. If an orbital contains paired electrons, the magnetic moment of one

