

# Important Questions on Cages and Metal Clusters

## Important Questions on Cages and Metal Clusters

- Calculate the no. of skeletal electron pairs in  $[\text{Pd}_5(\text{CN})_{12}]^{2-}$ ?  
A. 6  
B. 7  
C. 8  
D. 9
- Determine the geometry of the complex  $[\text{Rh}_6\text{N}(\text{CO})_{17}]^{3+}$ .  
A. Trigonal Prism  
B. Trigonal Bipyramidal  
C. Square pyramidal  
D. Pentagonal bipyramidal
- Determine the geometry of the complex  $[\text{Os}_5\text{C}(\text{CO})_{15}]$ .  
A. Trigonal Prism  
B. Trigonal Bipyramidal  
C. Square pyramidal  
D. Pentagonal bipyramidal
- $\text{Os}_6(\text{CO})_{18}$  has a monocapped TBP structure. On addition of 2 electrons, the structure changes to:  
A. Trigonal Prism  
B. Octahedron  
C. Square pyramidal  
D. Pentagonal bipyramidal
- Calculate the Bonding molecular orbital of the following cage structure  $[\text{Fe}_4(\text{CO})_{12}\text{C}]^{2-}$ .  
A. 35  
B. 32  
C. 44  
D. 31
- Determine type of cluster of compound  $[\text{Os}_6\text{C}(\text{CO})_{17}]$ .  
A. Arachno  
B. Nido  
C. hypo  
D. Closo
- Determine type of cluster of compound  $[\text{Os}_6\text{C}(\text{CO})_{17}\{\text{P}(\text{OMe})_3\}_3]$ .  
A. Arachno  
B. Nido  
C. hypo  
D. Closo
- Determine type of cluster of compound  $[\text{Ru}_5\text{N}(\text{CO})_{14}]^-$ .  
A. Arachno  
B. Nido  
C. hypo  
D. Closo
- Determine type of cluster of compound  $[\text{Ni}_5(\text{CO})_{12}]^{2-}$ .  
A. Arachno  
B. Nido  
C. hypo  
D. Closo
- Calculate the M-M- Bond present in  $[(\text{Fe}_3(\text{CO})_{12})]$ .  
A. 3  
B. 0  
C. 2  
D. 1

## Answer Key

1. C	2. A	3. C	4. B	5. D	6. D	7. C
8. D	9. A	10. A				

## Solutions

### Solution 1.

Determination of structure for Skeletal Electron Pair:

Step I → Calculate TVE (Total Valence e- count.)

Step II → Add the value of the valence electron of interstitial atoms.

E.g., H → 1 e-

H<sub>2</sub> → 2 e-

Carbon family → 4 e-

Nitrogen family → 5 e-

Step III → Calculate skeletal electron Pair (S) as:

$$S = (\text{TVE} - n \times 12) / 2$$

Electronic configuration of Pt = 4d<sup>10</sup>4s<sup>0</sup>

Pd is a 10 e<sup>-</sup> contributor whereas CN is a 2e<sup>-</sup> contributor in nature method.

$$\text{TVE} = 5 \times 10 + 12 \times 2 + 2 = 76$$

$$S = (76 - 12 \times 5) / 2$$

$$= (76 - 60) / 2$$

Skeletal electron pair = 8

### Solution 2.

Determination of structure for Geometry: -

Step I → Calculate TVE (Total Valence e- count.)

Step II → Add the value of the valence electron of interstitial atoms.

E.g., H → 1 e-

H<sub>2</sub> → 2 e-

Carbon family → 4 e-










Nitrogen family → 5 e-

Step II → Compare with table of geometries.

Electronic configuration of Rh = 4d<sup>8</sup>5s<sup>1</sup>

Hence electronic configuration by Ru = 9 e<sup>-</sup>

$$\begin{aligned} \text{TVE} &= (9 \times 6) + 5 + (17 \times 2) - 3 \\ &= 54 + 5 + 34 - 3 \\ &= 90 \end{aligned}$$

Cluster framework	Diagrammatic representation of the cage	Valence electron count
Triangle		48
Tetrahedron		60
Butterfly, or planar raft of four atoms	 	62
Square		64
Trigonal bipyramid		74
Octahedron		86
Trigonal prism	 	90

**Solution 3.**

Determination of structure for Geometry: -

Step I → Calculate TVE (Total Valence e- count.)

Step II → Add the value of the valence electron of interstitial atoms.

E.g., H → 1 e<sup>-</sup>

H<sub>2</sub> → 2 e<sup>-</sup>

Carbon family → 4 e<sup>-</sup>

Nitrogen family → 5 e<sup>-</sup>

Step II → Compare with table of geometries.

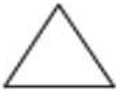








[Os<sub>5</sub>C(CO)<sub>15</sub>]

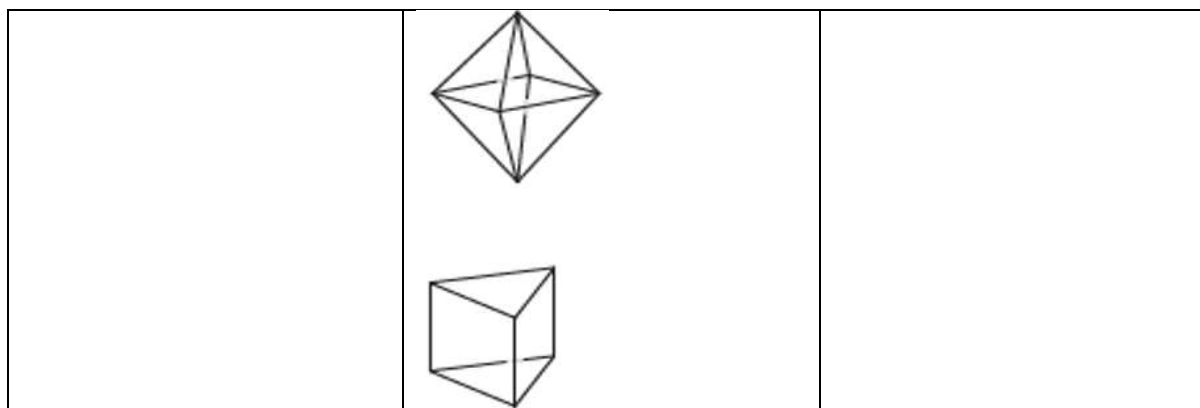
Electronic configuration of Os = 5d<sup>6</sup>6s<sup>2</sup>

Hence, electronic configuration by Os = 8 e<sup>-</sup>

$$\begin{aligned} \text{TVE} &= (8 \times 5) + 4 + (15 \times 2) \\ &= 40 + 4 + 30 \\ &= 74 \end{aligned}$$

Compare TVE with table as:

Cluster framework	Diagrammatic representation of the cage	Valence electron count
Triangle		48
Tetrahedron		60
Butterfly, or planar raft of four atoms	 	62
Square		64
Trigonal bipyramid		72
Square-based pyramid		74
Octahedron		86
Trigonal prism		90



It is square Pyramidal.

**Solution 4.**

Determination of structure for Geometry: -

Step I → Calculate TVE (Total Valence e- count.)

Step II → Add the value of the valence electron of interstitial atoms.

E.g., H → 1 e-

H<sub>2</sub> → 2 e-

Carbon family → 4 e-

Nitrogen family → 5 e-

Step II → Compare with table of geometries.

We know that Os<sub>6</sub>(CO)<sub>18</sub> has a monocapped TBP structure.

Calculate total valence electrons as:

Electronic configuration of Os = 5d<sup>6</sup>6s<sup>2</sup>

Hence, electronic configuration by Os = 8 e<sup>-</sup>


$$\text{TVE} = (8 \times 6) + (18 \times 2)$$

$$= 48 + 36$$

$$= 84$$

On adding 2 electrons, the total valence electron becomes 86.

Compare TVE with table as:

Cluster framework	Diagrammatic representation of the cage	Valence electron count
Triangles		48
Tetrahedron		60

Butterfly, or planar raft of four atoms		62
Square		64
Trigonal bipyramid		72
Square-based pyramid		74
Octahedron		86
Trigonal prism		90

It is an octahedron in shape.

**Solution 5.**

Determination of Bonding molecular orbital: -

Step I → Calculate TVE (Total Valence e- count.)

Step II → Add the value of the valence electron of interstitial atoms.

E.g., H → 1 e-

H<sub>2</sub> → 2 e-

Carbon family → 4 e-

Nitrogen family → 5 e-

Step III → Calculate Bonding molecular orbital

$$\text{BMO} = (\text{TVE})/2$$

Calculate T.V.E as:

C = 4 e<sup>-</sup> Contribution because it is encapsulated atom

$$\begin{aligned}\text{Os} &= 3d^64s^2 = 8 \text{ e}^- \text{ contribution} \\ &= 4+(8 \times 4) + (12 \times 2) +2 \\ &= 62 \text{ e}^-\end{aligned}$$

$$\text{BMO} = \text{Total valence electron} /2$$

$$=62/2$$

$$= 31$$

### Solution 6.

Determination of structure for HNCC: -

Step I → Calculate TVE (Total Valence e- count.)

Step II → Add the value of the valence electron of interstitial atoms.

E.g., H → 1 e-

H<sub>2</sub> → 2 e-

Carbon family → 4 e-

Nitrogen family → 5 e-

Step III → Calculate Skeletal electron Pair (S)

$$S = (\text{TVE} - n \times 12)/2$$

n = Number of metals in the given cluster.

Step IV

The structure is arranged according to the wade rule, if skeletal electron pair is,

S=n -1 Super closo

S=n Hyper closo

S=n +1 Closo

S=n+2 Nido

S=n +3 Arach no

S=n +4 Hypho

Calculate T.V.E as:

C = 4 e<sup>-</sup> Contribution because it is encapsulated atom

$$\text{Os} = 3d^64s^2 = 8 \text{ e}^- \text{ contribution}$$



$$= 4 + (8 \times 6) + (17 \times 2)$$

$$= 86 e^-$$

$$\text{Skeletal Electron pair} = (\text{TVE} - 12 \times n) / 2$$

$$= (86 - 12 \times 6) / 2$$

$$= 7$$

$S = n + 1$  hence, it is an example of Closo

### Solution 7.

Determination of structure for HNCC: -

Step I → Calculate TVE (Total Valence e- count.)

Step II → Add the value of the valence electron of interstitial atoms.

E.g., H → 1 e-

H<sub>2</sub> → 2 e-

Carbon family → 4 e-

Nitrogen family → 5 e-

Step III → Calculate Skeletal electron Pair (S)

$$S = (\text{TVE} - n \times 12) / 2$$

n = Number of metals in the given cluster.

Step IV

The structure is arranged according to the Wade rule, If skeletal electron pair is,

$S = n - 1$  Super closo

$S = n$  Hyper closo

$S = n + 1$  Closo

$S = n + 2$  Nido

$S = n + 3$  Arachno

$S = n + 4$  Hypo

Ligand	Electronic configuration
Co	2
P(OMe) <sub>3</sub>	2

Calculate T.V.E of [Os<sub>6</sub>C(CO)<sub>17</sub>{P(OMe)<sub>3</sub>}]<sub>3</sub> as:

C = 4 e<sup>-</sup> Contribution because it is encapsulated atom

Os = 5d<sup>6</sup>6s<sup>2</sup> = 8 e<sup>-</sup> contribution

$$= 4 + (8 \times 6) + (17 \times 2) + (2 \times 3)$$

$$= 92$$

$$\text{Skeletal Electron pair} = (\text{TVE} - 12 \times \text{N}) / 2$$

$$= (92 - 12 \times 6) / 2$$

$$= 10$$

$$10 = 6 + 4$$

$S = n + 4$  hence, it is an example of Hypo

### Solution 8.

Determination of structure for HNCC: -

Step I → Calculate TVE (Total Valence e- count.)

Step II → Add the value of the valence electron of interstitial atoms.

E.g., H → 1 e-

H<sub>2</sub> → 2 e-

Carbon family → 4 e-

Nitrogen family → 5 e-

Step III → Calculate Skeletal electron Pair (S)

$$S = (\text{TVE} - n \times 12) / 2$$

n = Number of metals in the given cluster.

Step IV

The structure is arranged according to the Wade rule, if skeletal electron pair is,

$S = n - 1$  Super closo

$S = n$  Hyper closo

$S = n + 1$  Closo

$S = n + 2$  Nido

$S = n + 3$  Arach no

$S = n + 4$  Hypo

Ligand	Electronic configuration
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Co	2
----	---

Calculate T.V.E of [Ru<sub>5</sub>N(CO)<sub>14</sub>]<sup>-</sup> as:

N = 5 e<sup>-</sup> Contribution because it is encapsulated atom

Ru = 4d<sup>7</sup>5s<sup>1</sup> = 8 e<sup>-</sup> contribution

$$= 5 + (8 \times 5) + (14 \times 2) + 1$$

$$= 74$$

$$\text{Skeletal Electron pair} = (\text{TVE} - 12 \times \text{N}) / 2$$

$$= (74 - 12 \times 5) / 2$$

$$S = 7$$

$$7 = 6 + 1$$

$S = n + 1$  hence, it is an example of Closo

### Solution 9.

Determination of structure for  $\text{HNCC}$ : -

Step I  $\rightarrow$  Calculate TVE (Total Valence e- count.)

Step II  $\rightarrow$  Add the value of the valence electron of interstitial atoms.

E.g.,  $\text{H} \rightarrow 1 \text{ e}^-$

$\text{H}_2 \rightarrow 2 \text{ e}^-$

Carbon family  $\rightarrow 4 \text{ e}^-$

Nitrogen family  $\rightarrow 5 \text{ e}^-$

Step III  $\rightarrow$  Calculate Skeletal electron Pair (S)

$$S = (\text{TVE} - n \times 12) / 2$$

$n$  = Number of metals in the given cluster.

Step IV

The structure is arranged according to the Wade rule, if skeletal electron pair is,

$S = n - 1$  Super closo

$S = n$  Hyper closo

$S = n + 1$  Closo

$S = n + 2$  Nido

$S = n + 3$  Arach no

$S = n + 4$  Hypo

Ligand	Electronic configuration
--------	--------------------------

Co	2
----	---

Calculating T.V.E of  $[\text{Ni}_5(\text{CO})_{12}]^{2-}$

$$\text{Ni} = 3d^8 5s^2 = 10 \text{ e}^- \text{ contribution}$$

$$= (10 \times 5) + (12 \times 2) + 2$$

$$= 76$$

$$\text{Skeletal Electron pair} = (\text{TVE} - 12 \times \text{N})/2$$

$$= (76 - 12 \times 5)/2$$

$$S = 8$$

$$8 = 5 + 3$$

$S = n + 3$  hence, it is an example of arachno

**Solution 10.**

Ligand	Electronic configuration
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CO	2
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Fe =  $3d^6 5s^2 \rightarrow 8 e^-$  contributor

$$\text{T.V.E} = 12 \times 2 + 3 \times 8$$

$$= 24 + 24$$

$$= 48$$

$$\text{Total M-M Bond} = (18 \times n - \text{T.V.E})/2$$

$$= (54 - 48)/2 = 3$$

No. M-M Bond present in compound = 3

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