Wade's rule:

K. Wade provided the rule to corelate the number of frame work electrons with the structure of borane and carborane clusters. This rule is concerned with "Polyhedral skeletal electron pair theory (PSEPT)". The type of structure adopted by clusters is related to total number of electron count (TEC).

* Rules/steps of finding structure of clusters through Wade's rule:

1. Total electron count (TEC) is known as follows:
   TEC = Valence electron of transition metal + Electrons of ligand + Charge + Electrons of interstitial atom (non-metal)
   e.g. for $[Rh_6(CO)_{16}]$: Valence electrons of Rh = 9, Electrons of one ligand (CO) = 2
   So, TEC = 9×6 + 2×16 = 54+32 = 86
2. Each metal atom is using 12 electrons for non-skeletal bonds or non-framework bond. Total no. of electrons for non-skeletal bonds (B) = No. of metal atoms × 12.
   e.g. for $[Rh_6(CO)_{16}]$: B = 6×12 [Since no. of metal (Rh) atoms = 6]
3. Calculate PEC (Polyhedral electron count) or framework electrons as follows:
   PEC = TEC − B
   e.g. for $[Rh_6(CO)_{16}]$: PEC = 86 − 72 = 14
4. Calculate framework electron pairs by dividing PEC by 2, i.e., PEC/2. This value gives structure of the cluster on the basis of satisfying the specify relation given by Wade (Table-1)

Table-1

Relation	Predicted Structure
(n+1)	Closo
(n+2)	Nido
(n+3)	Arachano
(n+4)	Hypo
n	Hypercloso
(n−1)	Supercloso
n = No. of atoms (metal)	

Table-2

No. of atoms (Vertex)	Geometry
4	Tetrahedral
5	Trigonal bipyramidal
6	Octahedral
7	Pentagonal bipyramidal
8	Dodecahedron
9	Tricapped triangular prism
10	Bicapped trigonal prism
11	Icosahedron (Octadecahedron)
12	Icosahedron (bicapped pentagonal antiprism)

Above rules can be understand by following examples:

1. $[Os_5(CO)_{16}]$: No. of Os atoms (n) = 5; Valence electrons of Os = 8, one CO (ligand) has 2 e⁻.
   TEC = VE of Os + Total no. of electrons of CO = 5×8 + 16×2 = 40+32 = 72
   Value of B = No. of metal atoms × 12 = 5×12 = 60
   PEC = TEC − B = 72 − 60 = 12 ; PEC/2 = 12/2 = 6. Thus, framework electron pairs = 6
   Here, no of metal (Os) atoms = 5 (n). It satisfy relation (n+1) = 5+1 = 6 (i.e., PEC/2)
   So, it has Closo structure. Geometry: Trigonal bipyramidal (Since n = 5)
2. $[Co_6(CO)_{15}H]^-$: No. of Co atoms (n) = 6, Valence electrons of Co = 9, One CO (ligand) has 2e⁻
   TEC = Valence electron (VE) of Co + No. of electrons of CO + Charge + No. of electron in H.
   = 6×9 + 15×2 + 1 + 1 = 54+30+1+1 = 86 (Eighty Six)
   Value of B = No. of metal atoms × 12 = 6 × 12 = 72
   PEC = TEC − B = 86 − 72 = 14 ; PEC/2 = 14/2 = 7. Thus, frame work electron pairs = 7
   No. of Co atoms (n) = 6. It satisfy relation (n+1) = 6+1 = 7 (i.e., PEC/2)
   So, it has Closo structure. Geometry: Octahedral (Since n = 6)