

Wade's rules

The electron-counting rules for prediction of stable structures of polyhedral inorganic, organometallic, and organic compounds. So-called "skeletal" electrons, i.e., valence electrons of atoms positioned in the vertices of a molecular polyhedron that form bonding electron pairs of the framework bonds, are taken into account, their number being determined as follows

$$\text{Main-group elements } k = v + x - 2$$

$$\text{Transition metals } k = v + x - 12$$

where v is the full number of valence electrons of an atom or group in a vertex and x is the number of one-electron ligands. For deltahedral closo (closed) structures (characterized by triangle faces) with m vertices there exist $(m + 1)$ bonding molecular orbitals which may be filled with not more than $2m + 2$ skeletal electrons ($m = 4, 5, \dots$). For nido (nest-like) structures derived from the closo-forms through truncation of one apex there are $(m + 2)$ bonding MOs which may be occupied with not more than $2m + 4$ skeletal electrons. For arachno (web-like) structures derived from nido-forms through truncation of one apex, there are $(m + 3)$ bonding MOs that may be occupied by $2m + 6$ electrons. The extension of Wade's rules is the polyhedral skeletal electron pair approach that makes allowance for the total electron count in condensed polyhedra derived by the condensation of smaller tetrahedral, octahedral, and trigonal-prismatic fragments. The total electron count in a condensed polyhedron is equal to the sum of the electron counts for the parent polyhedra A and B minus the electron count characteristic of the atom, pair of atoms, or face of atoms common to both polyhedra.

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