

basis set

A set of basis functions employed for the representation of molecular orbitals. One may distinguish the minimal basis set (includes one *basis function* for each SCF occupied atomic orbital with distinct principal and angular momentum quantum numbers); split valence basis set (includes two or more sizes of basis function for each valence orbital); double zeta (DZ) basis set (a split valence basis set that includes exactly twice as many functions as the minimal basis set); extended basis set (the set larger than the double zeta basis set); polarized basis set (incorporates basis functions of higher angular quantum number beyond what is required by the atom in its electronic ground state; allows orbitals to change not only a size, but also a shape); basis set with diffuse functions and others.

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