doi:10.1351/goldbook.BT06999

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.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1925

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