

virtual orbital

An orbital from a set of MOs obtained as solutions of the SCF equations (see Hartree-Fock method) whose energies are higher than those of doubly occupied MOs producing the single determinant wavefunction of lowest energy for a given system. The virtual orbitals obtained from SCF calculations are not variationally correct approximations (see variational principle) to the excited state orbitals. Their energies are not related to electron affinities of the molecular system.

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