Copy of a printed diagram referenced as "Molecular orbitals for O2 showing the triplet nature of the ground state"

Contributors

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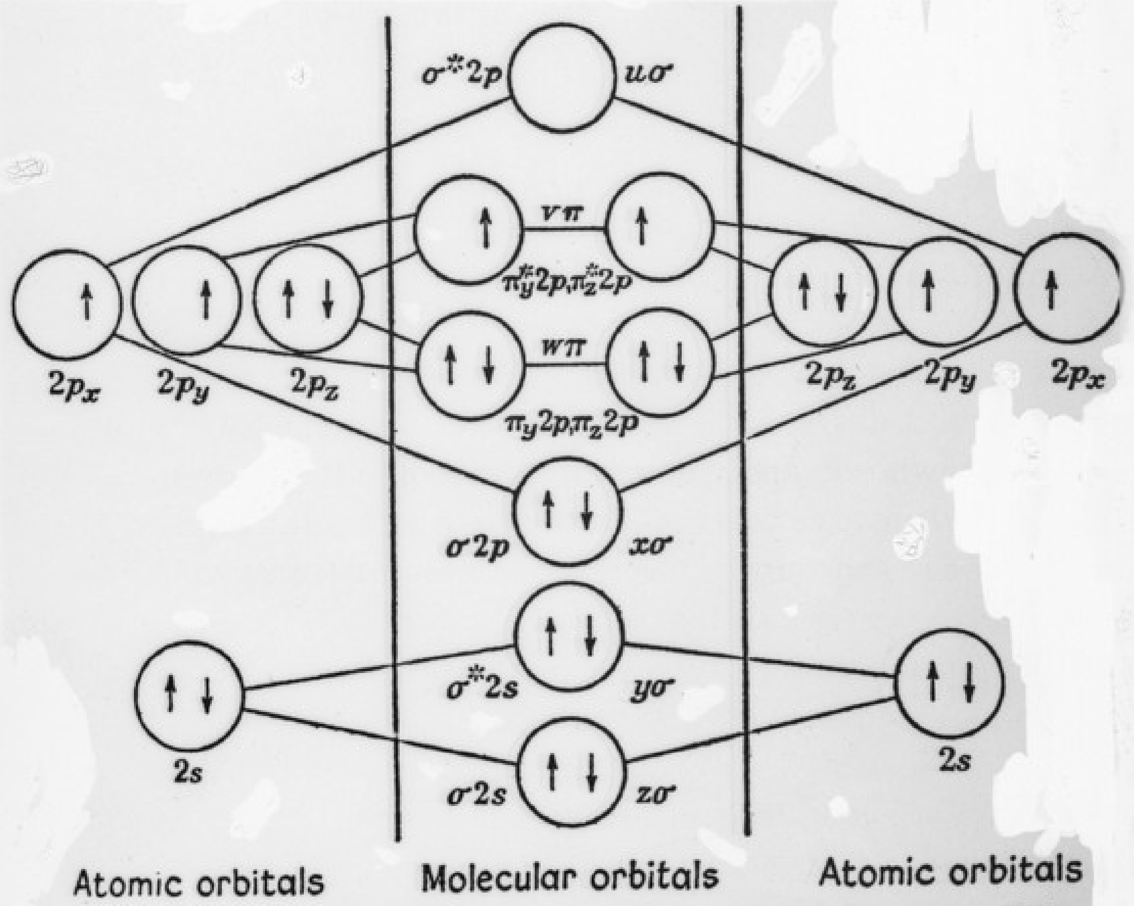
are less common than those of heteropolar binding, in which atoms A and B are different. However, the greater part of our previous discussion will still apply. Thus, in heteronuclear diatomics we can still apply the LCAO approximation (§ 4.3) writing for the m.o. an expression

$$\psi = \psi_A + \lambda\psi_B, \tag{31}$$



Molecular orbitals for O_2, showing the triplet nature of the ground state.

as in (3): but λ is no longer equal to ± 1. Nor is the energy given by the simple values (6) and (7), but we are obliged to solve the quadratic secular equations (5). The conditions (a)–(c) of § 3, viz. nearly equal energies, maximum overlapping, and the same symmetry around the bond axis, generally allow us to infer quite easily which a.o.'s ψ_A and ψ_B may be compounded together. It is