

On Rüdenberg's Integral Approximations and Their Unrestricted and Combined Use in Crystal Orbital Theories of Hartree-Fock Type

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The analysis based on Rüdenberg's well-known letter of 1951, which has been outlined for molecules in a preceding contribution, now will be transferred to translational periodic systems in one, two, or three dimensions. Again, when applied unrestrictedly to "Linear Combination of Atomic Orbitals" representations (LCAO) of both "Unrestricted" and "Restricted Hartree-Fock" pictures (UHF and RHF), Rüdenberg's integral approximations of Mulliken type lead to a thorough interpretation of "Extended Hückel" crystal orbital theories (EHT). Moreover, Rüdenberg's ideas provide us with "Unrestricted and Combined" extensions (U&C) of the widely-used approximation schemes "Zero Differential Overlap" (ZDO) and "Neglect of Diatomic Differential Overlap" (NDDO). An improved variant of EHT is also presented. Corresponding "Restricted and Combined" concepts (R&C), which overcome some shortcomings inherent in Rüdenberg's original recipes, will be sketched.

Key words: Unrestricted (and Restricted) Hartree-Fock Crystal Orbitals; Integral Approximations According to Mulliken and Rüdenberg; Zero Differential Overlap (ZDO); Neglect of Diatomic Differential Overlap (NDDO); Extended Hückel Theory (EHT).