



Valency and Bonding: A Natural Bond Orbital Donor-Acceptor Perspective

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 Summary: Part I. Introduction and Theoretical Background: 1. The Schrödinger equation and models of chemistry; 2. Hydrogen atom orbitals; 3. Many-electron systems; 4. Perturbation theory for orbitals in the Hartree-Fock framework: the donor-acceptor paradigm; 5. Density matrices, natural localized and delocalized orbitals and the Lewis structure picture; 6. Natural resonance structures and weightings; 7. Pauli exchange antisymmetry and steric repulsions; 8. Summary; Part II. Electrostatic and Ionic Bonding: 9. Introduction; 10. Atomic and ionic orbitals; 11. Charge transfer and hybridization changes in ionic bonding; 12. Donor-acceptor theory of hybridization changes in ionic bonding; 13. Ionic/covalent transitions; 14. Ion-dipole and dipole-dipole bonding; 15. Beta ionic compounds of heavy alkaline earths; 16. Ionic bonding in D-block elements; 17. Summary; Part III. Molecular Bonding in the S/P-Block Elements: 18. Introduction; 19. Covalent and polar covalent bonding; 20. Conjugation and aromaticity; 21. Hyperconjugation; 22. Hypervalency; 23. Hypovalency; 24. Summary; Part IV. Molecular Bonding in the D-Block Elements: 25. Introduction; 26. Lewis-like structures for the D-block; 27. Hybridization and molecular shape; 28. Covalent and polar covalent bonding; 29. Coordinative metal-ligand bonding; 30. Hypervalent bonding; 31. Hypovalency and agostic...



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