

- Z. B. Maksić** **Prologue**
 The nature, the scope and limitations of quantum models of the molecular electronic structure and properties are thoroughly discussed. The gnoseological importance of models is noted. Their role in bridging the gap between the phenomenological concepts and rigorous quantum theory is stressed. I—III
- Z. S. Herman
and L. Pauling** **Hybrid Bond Orbitals and Bond Strengths for Pentacovalent Bonding**
 A brief history of the theory of hybrid bond orbitals is presented. Bond strengths and hybrid bond orbitals are derived for pentacovalent systems and the experimental implications of the obtained results are discussed. 765—778
- W. E. Palke** **On Determining Orbital Hybridization**
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- G. Del Re
and C. Barbier** ***In Situ* Atomic Orbitals and Extended Basis Molecular Calculations**
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- K. H. Aufderheide** **A Localized Atomic Orbital Description of the Rotational Barrier in Ethane**
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- P. R. Surján** **The Representation of the Chemical Bond in Quantum Chemical Calculations**
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- A. Garcia-Leigh
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M. Klessinger

Fragment Molecular Orbitals for Molecules and Interacting Systems

Different approaches to describe the structure and properties of molecules, as well as their reactions in terms of localized fragment orbitals, are briefly reviewed and the method of fragments-in-molecules (FIM) is thoroughly discussed. A partitioning of the energy of interaction between molecular fragments yields definition of inductive and mesomeric effects in agreement with experience.

887—899

G. Náray-Szabó

Chemical Fragmentation for Molecular Orbital Calculations on Proteins

The conceptual and mathematical basis of a MO method which enables the calculation of conformational energy changes and properties of proteins is presented. The basis of strictly localized MOs and the information inherent in the chemical formulae of the polypeptide backbone and side chains were exploited.

901—910

F. Bernardi,
A. Bottoni,
and G. Tonachini

A Quantitative Analysis of the Role of Non-Bonded and Geminal Interactions in H_2N-X Molecules

Quantitative analysis of the role of the nonbonded and geminal interactions in the molecules of the type H_2N-X ($X = H, F, Cl, OH, SH$) is presented. The computations were performed within the *ab initio* SCF—MO framework and the various types of orbital interactions were estimated by using either a total energy approach or a quantitative PMO treatment.

911—925

L. S. Bartell

Do the VSEPR Points-on-a-Sphere Repulsions Simulate Quantum Interactions?

The VSEPR theory in its points-on-a-sphere (POS) variant is applied to the potential energy surface study of molecular bending deformations. A form of the simple effective force between repelling points is determined.

927—939

Electron Transmission Spectra of Fluorinated Benzenes

The overlapping spheres multiple scattering $X\alpha$ method is used to investigate the ionization potentials, electron affinities and elastic cross sections for electron scattering of benzene and its fluoro-derivatives. The results agree well with available experimental data. 1011—1030

**N. D. Epiotis,
J. R. Larson,
and H. H. Eaton**

»Common Denominators« by the MOVB Method: The Structures of H_2O , H_2O_2 and their Derivatives

The qualitative MOVB method is applied to elucidate the structural properties of H_2O and H_2O_2 systems and their derivatives. It is shown that factors governing their geometries are the same to the first approximation. 1031—1053

**P. Politzer
and B. A. Zilles**

Some Observations Concerning Electronic Densities, Electrostatic Potentials and Chemical Potentials

The hypothesis that the electronic density distribution in a molecule is qualitatively similar to the nuclear potential, holds true for a number of molecular systems. It is, however, in error in at least two cases: oxirane and cubane, which are thoroughly discussed in the paper. 1055—1064

**D. Hadži,
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D. Kocjan,
T. Šolmajer,
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The Molecular Electrostatic Potential as a Determinant of Receptor-Drug Recognition

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M. Kibler

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The Wigner-Racah algebra of an arbitrary finite or compact continuous group is given in a new original way which represents a straightforward extension of the corresponding algebra of the rotation group. Some illustrative examples are considered. 1075—1095

C. J. Ballhausen

The $E \otimes E$ Jahn-Teller Coupling: Models and Manifestations

The state of the art of the Jahn-Teller coupling is presented. It is concluded that this problem has not been satisfactorily solved yet.

1097—1106

M. L. Ellzey, Jr.

Derivation of the AOM Parametrization from the Effective Hamiltonian for Complexed Transition Metal Ions with Application to Effectively Tetragonal Four-Coordinate Systems

The formalism of the angular overlap model for complexed transition metal ions is developed entirely from the effective Hamiltonian over appropriate MOs. Results obtained for tetrabromo and tetrachloro Pd(II) and Pt(II) complexes are discussed.

1107—1124

M. Grodzicki

The Applicability of Point-Charge Approximations to the Calculation of Molecular Expectation Values

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B. Galabov,
B. Nikolova,
and W. J. Orville-Thomas

Infrared Band Intensities, Electric Charge Distribution in Molecules and Polar Properties of Valence Bonds

The description of molecular charge distributions in terms of empirical bond parameters extracted from vibrational intensities in the IR spectra is thoroughly discussed. The theoretical prerequisites of the approach and some of its applications are presented.

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R. C. Haddon
and H. D. Roth

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H. Vogler

A Theoretical Study of the ^1H -Chemical Shifts of $[4n]$ - and $[4n+2]$ -Annulenes and their Di- and Tetraanions

The relationship between ^1H -chemical shifts and ring currents, local anisotropies and net charges is considered by using MO methods at various levels of sophistication. The results are in accordance with experience.

1177—1191

J. K. Burdett,
S. Lee,
and W. C. Sha

The Method of Moments and the Energy Levels of Molecules and Solids

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N. Raos
and V. Simeon

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A. Koukoulas and
M. A. Whitehead

Penetration in the CNDO Theory

The problem of penetration integrals in the semiempirical CNDO formalism is briefly discussed.

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