

- J. J. Aaron, A. Tine, C. Villiers, C. Párkányi and D. Bouin**     **Electronic Absorption and Fluorescence Spectra of Indole Derivatives. Quantitative Treatment of the Substituent Effects and a Theoretical Study**
- The electronic absorption and fluorescence spectra of nine substituted indoles are discussed. Satisfactory linear Hammett correlations have been established for the electronic absorption and fluorescence maxima. PPP (LCI-SCF-MO) calculations for the indoles have been carried out and the results used to interpret the experimental data. . . . . 157—168
- J. Bertrán, J. Anguiano, and A. Oliva**     **The Electrophile Desolvation Process in Nucleophile-Electrophile Combination Reactions**
- The protonation and methylation of ethylene in different solvents are studied, by means of the MINDO/3 method, in order to check the hypothesis of partial desolvation of the electrophile at the transition state. It has been found that degree of desolvation depends on both the electrophile and the solvent. The consequences of these results are discussed. . . . . 169—174
- N. Bodor, A. J. Harget and E. Phillips**     **Structure — Activity Relationships in the Antiinflammatory Steroids: A Pattern Recognition Approach**
- A pattern recognition method was applied to a set of steroids for which experimental results using two different bioassays were known. The resulting structure-activity relationships are discussed. The method predicts a synergistic effect to be in operation between certain pairs of substituents. . . . . 175—183

G. Frenking and H. Schwarz	<b>SCF-Calculations as Tool to Interpret Reaction Pathes — The Cases of CO<sub>2</sub> Loss from Ionized ClCH<sub>2</sub>—COOCH<sub>3</sub> and C<sub>2</sub>H<sub>4</sub> Loss from Ionized (CH<sub>3</sub>)<sub>2</sub>N—COCH<sub>2</sub>X</b>	185—190
Ā. Furka	<b>An Empirical Formula Expressing the Mutual Dependence of C—C Bond Distances</b> An empirical formula is suggested to describe the mutual dependence of the length of the bonds formed by a central atom with other equivalent carbon atoms. Reference and deduced systems: diamond, graphite, cumulene and polyene chains, and intermediate structures between them. A geometrical representation of the formula is also discussed. . . . .	191—197
Ā. Furka	<b>Comparison of the Heats of Formation of Hydrocarbons</b> An equation is suggested to convert heats of formation of hydrocarbons into relative enthalpies which numerically demonstrate the structure dependent stabilizing and destabilizing effects. . . . .	199—201
P. Ilić and N. Trinajstić	<b>Structural Normalization of the Topological Resonance Energy</b> Normalizing method for topological resonance energy values of conjugated compounds is presented. It is based on a graph-theoretical procedure which observes the number, the size, and the organization of circles of the respective conjugated compound. . . . .	203—213
A. Jurić and N. Trinajstić	<b>Topological Resonance Energies of Thiocoumarins</b> Topological resonance energies of thiocoumarin, thiochromone, and related structures are reported. Comparison of the calculated values gave information about the degree of distortion of benzene rings in these compounds. . . . .	215—219

- E. C. Kirby**      **The Use of a Micro-Computer as an Aid to Theoretical Calculations.**  
 Some programs have been written in the computer language BASIC to help in the applications of simple Hückel theory. . . . . 221—223
- G. Marconi and G. Orlandi**      **Vibronic Coupling in Carbonyl Compounds**  
 The vibronic coupling integrals for Formaldehyde, Glyoxal, and Biacetyl, calculated using MINDO/3 and CNDO/S programs, are found to provide a satisfactory basis for the explanation of the radiative and radiationless behavior of carbonyl compounds. . . . . 225—235
- Ov. Mekenyan, D. Bonchev, and N. Trinajstić**      **Structural Complexity and Molecular Properties of Cyclic Systems with Acyclic Branches**  
 The degree of structural complexity of cyclic molecules with acyclic branches is expressed by means of rules based on the sum of the distances in the corresponding graphs. It is shown that these topological rules are well reflected in the properties of isomeric alkyl-benzenes. . . . . 237—261
- M. Mintas, K. Jakopčić, and L. Klasinc**      **Photoelectron Spectroscopy of Some trans-2,2'-Disubstituted Stilbenes**  
 The He I photoelectron spectra of trans-stilbene, -2,2'-dichlorostilbene, -2-amino-2'-chlorostilbene, -2,2'-diaminostilbene, and -2,2'-dinitrostilbene are recorded. Their electronic structure can well be described on the basis of the composite molecule method and simple Hückel molecular orbital calculations. . . . . 263—267
- U. Norinder, D. Tanner, and O. Wennerström**      **Dianions from Cyclophanes with Unsaturated Bridges; Cyclic Conjugation in 22—38  $\pi$ -Electron Perimeter Systems**  
 A series of cyclophanes with unsaturated bridges has been synthesized. Several of these cyclophanes containing  $4n$  perimeters can be reversibly reduced to their dianions, a process which conveniently can be studied by cyclic voltammetry. A

good correlation between calculated energies of the LUMO orbitals and the reversible reduction potentials has been obtained. Recent theories of resonance energies in neutral molecules and dianions with conjugated perimeters have been tested on the unsaturated cyclophanes. . . . . 269—280

**I. Novak,  
L. Klasinc, G.  
Karminski-Zamola  
and K. Jakopčić**

**Photoelectron Spectroscopy of Heterocycles. 1-(2-Furyl)-2-arylethenes**

HeI photoelectron spectra of 2-ethenylfuran, cis-2-(2-phenylethenyl)-furan, trans-2-(2- $\alpha$ -naphthylethenyl)-furan, cis-2-(2-phenylethenyl)-5-methylfuran and trans-2-(2- $\alpha$ -naphthylethenyl)-5-methylfuran were recorded. Their assignment is attempted. . . . . 281—287

**P. R. Surján**

**Conformation Analysis in Light of Localization and Delocalization**

The origin of barriers to internal rotations around single bonds is discussed in terms of localized molecular orbitals and through space and through bond delocalization interactions. Bond-bond pair potentials for giving rise to barrier forces are analysed. . . . . 289—295

**H. Vogler**

**On the Existence of Biradical-Ionic States of Donor-Acceptor Cyclophanes. A Simple MO-Theoretical Study**

The ground and lowest excited states of donor-acceptor cyclophanes are investigated by means of MO-theory. Conditions for the occurrence of biradical-ionic ground states are derived. . . . . 297—313

CROATICA  
CHEMICA ACTA

Croat. Chem. Acta Vol. 56 No. 2

157—314 (1983)

Zagreb, 30. lipanj, 1983

## SADRŽAJ

Elektronski apsorpcijski i fluorescencijski spektri indolnih derivata. Kvantitativna obradba utjecaja supstituenata i teorijsko razmatranje ... <b>J. J. Aaron, A. Tine, C. Villiers, C. Párkányi i D. Bouin</b>	157—168
Proces desolvatacije elektrofila u reakcijama kombinacije nukleofil-elektrofil ... <b>J. Bertrán, J. Anguiano i A. Oliva</b>	169—174
Odnos strukture i aktivnosti u antiupalnim steroidima: Pristup prepoznavanjem obrasca ... <b>N. Bodor, A. J. Harget i E. Phillips</b>	175—183
SCF-proračuni kao sredstva za interpretaciju reakcijskih mehanizama — slučajevi otpuštanja CO <sub>2</sub> iz ioniziranog ClCH <sub>2</sub> —COOCH <sub>3</sub> i C <sub>2</sub> H <sub>4</sub> iz ioniziranog (CH <sub>3</sub> ) <sub>2</sub> N—COCH <sub>2</sub> X ... <b>G. Frenking i H. Schwarz</b>	185—190
Empirijska formula koja prikazuje međusobnu ovisnost duljine C—C veza ... <b>A. Furka</b>	191—197
Usporedba toplina stvaranja ugljikovodika ... <b>A. Furka</b>	199—201
Strukturalno normiranje topologijske rezonancijske energije ... <b>P. Ilić i N. Trinajstić</b>	203—213
Topologijske rezonancijske energije tiokumarina ... <b>A. Jurić i N. Trinajstić</b>	215—219
Upotreba mikrokompjutera kao pomagala u teorijskim računima ... <b>E. C. Kirby</b>	221—223
Vibronsko sprezanje u karbonilnim spojevima ... <b>G. Marconi i G. Orlandi</b>	225—235
Strukturalna sastavljenost i molekularna svojstva cikličkih sistema s acikličkim ograncima ... <b>Ov. Mekenyan, D. Bonchev i N. Trinajstić</b>	237—261
Fotoelektronski spektri nekih trans-2,2'-disupstituiranih stilbena ... <b>M. Mintas, K. Jakopčić i L. Klasinc</b>	263—267
Dianioni ciklofana s nezasićenim mostovima; ciklička konjugacija u sistemima s 22—38 π-elektrona na perimetru ... <b>U. Norinder, D. Tanner i O. Wennerström</b>	269—280
Fotoelektronska spektroskopija heterocikličkih spojeva. 1-(2-furil)-2-ari-leteni ... <b>I. Novak, L. Klasinc, G. Karminski-Zamola i K. Jakopčić</b>	281—287
Konformacijska analiza s aspekta lokalizacije i delokalizacije ... <b>P. R. Surján</b>	289—295
O postojanju biradikal-ionskih stanja donor-akceptor ciklofana. Jednostavna MO-teorijska studija ... <b>H. Vogler</b>	297—313

CROATICA  
CHEMICA ACTA

Croat. Chem. Acta Vol. 56 No. 2

157—314 (1983)

Zagreb, June 30, 1983

The contents of CCA may be reproduced citing the original form  
in any medium without prior permission

## CONTENTS

Electronic Absorption and Fluorescence Spectra of Indole Derivatives. Quantitative Treatment of the Substituent Effects and a Theoretical Study ... J. J. Aaron, A. Tine, C. Villiers, C. Párkányi, and D. Bouin	157—168
The Electrophile Desolvation Process in Nucleophile-Electrophile Combination Reactions . . . . . J. Bertán, J. Anguiano, and A. Oliva	169—174
Structure-Activity Relationships in the Antiinflammatory Steroids: A Pattern Recognition Approach . . . N. Bodor, A. J. Harget, and E. Phillips	175—183
SCF-Calculations as Tool to Interpret Reaction Pathes — The Cases of CO <sub>2</sub> Loss from Ionized ClCH <sub>2</sub> -COOCH <sub>3</sub> and C <sub>2</sub> H <sub>4</sub> Loss from Ionized (CH <sub>3</sub> ) <sub>2</sub> N-COCH <sub>2</sub> X . . . . . G. Frenking and H. Schwarz	185—190
An Empirical Formula Expressing the Mutual Dependence of C—C Bond Distances . . . . . A. Furka	191—197
Comparison of the Heats of Formation of Hydrocarbons . . . A. Furka	199—201
Structural Normalization of Topological Resonance Energy . . . P. Ilić and N. Trinajstić	203—213
Topological Resonance Energies of Thiocoumarins . . . A. Jurić and N. Trinajstić	215—219
The Use of a Micro-Computer as an Aid to Theoretical Calculations . . . E. C. Kirby	221—223
Vibronic Coupling in Carbonyl Compounds . . . G. Marconi and G. Orlandi	225—235
Structural Complexity and Molecular Properties of Cyclic Systems with Acyclic Branches . . . Ov. Mekenyan, D. Bonchev, and N. Trinajstić	237—261
Photoelectron Spectroscopy of Some trans-2,2'-Disubstituted Stilbenes . . . M. Mintas, K. Jakopčić, and L. Klasinc	263—267
Dianions from Cyclophanes with Unsaturated Bridges; Cyclic Conjugation in 22—38 $\pi$ -Electron Perimeter Systems . . . U. Norinder, D. Tanner, and O. Wennerström	269—280
Photoelectron Spectroscopy of Heterocycles. 1-(2-Furyl)-2-arylethenes . . . I. Novak, L. Klasinc, G. Karminski-Zamola, and K. Jakopčić	281—287
Conformation Analysis in Light of Localization and Delocalization . . . P. R. Surján	289—295
On the Existence of Biradical-Ionic States of Donor-Acceptor Cyclophanes. A Simple MO-Theoretical Study . . . . . H. Vogler	297—313