

M. Biruš,  
N. Kujundžić,  
M. Pribanić and  
Z. Tabor

**Equilibrium Studies on Complexation of Iron(III) by Acet-, Glycinium and Betaine Hydroxamic Acids**

Equilibrium studies were performed to investigate the complexation of iron(III) by synthetic monohydroxamic acids: acet-, glyciniun, and betaine hydroxamic acids. Determination were made at 1.0 M ionic strength and at 25 °C by spectrophotometric methods.

The synthesis of a new compound betaine hydroxamic acid chloride is described . . . . .

313—324

H. Vogler

**Donor-Acceptor Cyclophanes with Biradical-Ionic Ground States**

Donor-acceptor cyclophanes are proposed which should be characterized by a biradical-ionic ground state  $D^{+q}A^{-q}$  with an electron transfer  $q > 1/2$  from the donor D to the acceptor A . . . . .

325—329

M. Ladika,  
D. E. Sunko and  
S. Borčić

**Solvolysis Rate of 3-Methyl-2-(3-pentynyl)-2-cyclohexenyl *p*-Nitrobenzoate. A Model System for  $\pi$ -Participation of the CC Triple Bond**

The title compound solvolyses in 97%  $CF_3CH_2OH$  without  $\pi$ -participation of the CC triple bond, showing solvolysis rate retardation in comparison with the saturated analog. This result is explained by electron-withdrawing inductive effect of the CC triple bond. . . . .

331—337

S. El-Basil,  
P. Krivka and  
N. Trinajstić

**Application of the Dualist Model. Generation of Kekulé Structures and Resonant Sextets of Benzenoid Hydrocarbons**

The dualist model of Balaban is used for the enumeration and display of Kekulé structures  $K$  and resonant sextet numbers  $r(G; k)$  of large cata-condensed benzenoid hydrocarbons.

A number of formulae for competing the number of Kekulé structures of various families of cata-condensed benzenoid hydrocarbons are derived. In addition, the above approach is applicable to large benzenoid systems consisting of cata-condensed fragments and thin peri-condensed fragments. . . . .

339—353

S. Carter and  
J. N. Murrell

**Analytical Two-valued Potential Energy Functions for the Ground State Surfaces**

of  $\text{CO}_2(\tilde{\mathbf{X}}^1\Sigma_g^+)$  and  $\text{CS}_2(\tilde{\mathbf{X}}\Sigma_g^+)$

A technique for constructing analytical two-valued potential energy functions of triatomic molecules is outlined. It is shown how these functions can be determined from the dissociation channels of the molecule, and from variational calculations of its vibrational spectrum

355—365

T. P. Živković

**Splitting of the Configuration Interaction Space  $X_n$  into Two Complementary Subspaces**

The configuration interaction space  $X_n$  generated by  $n$  particles moving over  $2n$  orbitals is considered. The formalism of the molecular orbital resonance theory (MORT) approach is used. It is shown that the space  $X_n$  can be split into subspaces  $X_n^+$  and  $X_n^-$  so that »elementary« one-particle operators connect either the states contained in the same subspace, or they connect the states contained in different subspaces. As a simple consequence the pairing theorem results. The connection with the pairing theorem as derived by other authors is discussed.

367—389

A. T. Balaban  
and I. Tomescu

**Chemical Graphs. XL. Three Relations  
Between the Fibonacci Sequence and  
the Numbers of Kekulé Structures for  
Non-branched *cata*-Condensed Polycyclic  
Aromatic Hydrocarbons**

For benzenoid or non-benzenoid catafusenes having a non-branched string of *cata*-condensed rings, the numbers K of Kekulé structures can be expressed via the recurrence relationship (1); as a corollary when each annelated segment has exactly two rings, the numbers of Kekulé structures form the Fibonacci sequence. Corollary 2 presents a second relationship with Fibonacci numbers .

391—404

M. Dumić,  
M. V. Proštenik,  
J. Fabijanić und  
I. Butula

**Chemie der 1,3-Dioxepine; III. Palladium-katalysierte Isomerisierung von 4,7- zu 6,7-Dihydro-1,3-dioxepinen**

4,7-Dihydro-1,3-dioxepine werden an verschiedenen Palladium/Träger-Katalysatoren zu 6,7-Dihydro-1,3-dioxepinen isomerisiert. Dabei zeigen Pd/Al<sub>2</sub>O<sub>3</sub> und Pd(OH)<sub>2</sub>/SiO<sub>2</sub> die grösste Aktivität, Pd/TiO<sub>2</sub>, Pd/SiO<sub>2</sub> und Pd/CaCO<sub>3</sub> die grösste Selektivität. Durch Neben- bzw. Folgereaktionen bilden sich bei Isomerisierung von 4,7-Dihydro-2-isopropyl-1,3-dioxepin 2-Isopropyl-1,3-dioxepin bzw. 4-(2-Methylpropen-1-yloxy)-butanal und 2-Isopropyl-tetrahydrofuran-3-carbaldehyd.

405—409

V. Grdinić and  
M. Jakševac-Mikša

**Microdetection of Some Biologically Active Thiol Compounds with Sodium Pentacyanoammineferrate(II) on Ion-Exchange Resin Grains**

A new test for microdetection of thiol compounds, using sodium pentacyanoammineferrate(II) as a reagent and ion-exchange resin as the reaction medium, is presented. Nineteen thiol compounds were examined. Detection limits and tolerance limits were investigated. Limits of concentration, limits of dilution and exponents of sensitivity were evaluated . . . . .

411—414

**V. Škarić,  
M. Pavela-Vrančić  
and J.  
Matulić-Adamić**

**Stereoselective Transformations in the  
Thymidine Series**

A series of stereoselective transformations of thymidine derivatives yielded a number of new compounds, characterized by ultraviolet, infrared,  $^{13}\text{C}$ -NMR and  $^1\text{H}$ -NMR spectroscopies.

**415—424**

**J. Babnik,  
T. Lah,  
V. Cotič and  
V. Turk**

**Anticathepsin D Antibody-Sepharose  
Chromatography of Human Cathepsin D**

Cathepsin D was isolated from human tissues by affinity chromatography on columns containing anticathepsin D antibodies bound to Sepharose 4B. The method yielded pure cathepsin D. It also enables quantitative determination of cathepsin D in small samples of human material taken by biopsy . . . . .

**425—432**

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Obavijest

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