The Electronic Structure of Some Polyatomic Molecules

N. Trinajstić

Institute »Ruder Bošković«, Zagreb, Croatia, Yugoslavia

The first weak band in the UV spectra of the mononegative ions of naphthalene, anthracene and tetracene has been assigned to the symmetry forbidden $B_{3g}$ transition. The simplified Pariser-Parr method proposed by Longuet-Higgins and Salem gives the best agreement with expt. as compared with Hückel theory, Pariser-Parr method, and the SCF Pople method.

The aromatic character of (18) annulene trioxide has been discussed in terms of its bond orders. The results indicate less aromatic character in (18) annulene trioxide than in (18) annulene, and also that the C$_6$—C$_6$ bond is similar to a double bond. This is in good agreement with expt.

A new simple method for deriving equiv. orbitals based on a stepwise usage of the max. overlap procedure is described and applied to water, ammonia, HCN and formaldehyde. The results obtained using this procedure are as good as the results obtained from more complicated and sophisticated methods (e.g., the procedure of Foster and Boys, or that of Reudenberg). Equiv. orbitals have been used to calc. the partial dipole moment contributions to the total dipole moment of the mol. The results infer that the main contributions to the total dipole moment of small mol. arise from the lone pair moments, since the bond moment is approx. cancelled by the nuclear moment. For example, the lone pair on nitrogen in HCN has a dipole moment of 1.678 a.u., the bond moments for the C—N and C—H bonds are 0.066 a.u. and —0.715 a.u., resp., and the total dipole moment of HCN is 0.429 a.u.

The s- and p-character of the N—H and lone pairs on nitrogen in NH, NH$_2$ and NH$_3$ have been investigated using equiv. orbitals.

The thesis was partly published in:
J. Chem. Soc. (A), 1966, 1924;

Examiners: Prof. M. Randić, Prof. B. Težak, and Dr. S. Borčić.


Thesis deposited at the University Library and Institute »Ruder Bošković«, Zagreb.

(128 pages, 15 figures, 19 tables, 78 references, original in Croatian)
1. The Electronic Structure of Some Polyatomic Molecules

I. Trinajstić N.
II. Institute «Ruđer Bošković», Zagreb, Croatia, Yugoslavia

Bond moments
Equivalent orbitals
Lone pair moments
Molecular orbital calculations of,
- anthracene, mono- and di-negative ions
- naphthalene, mono- and di-negative ions
- tetracene, mono-, di- negative and mono-positive ions
Determinati on of Thorium and Uranium in Biological Materials by Activation Analysis

M. Picer

Institute for Medical Research, Yugoslav Academy of Sciences and Arts, Zagreb, Croatia, Yugoslavia

For many elements, quant. anal. methods have not been sufficiently sensitive for the measurement of trace elements in biol. materials. Consequently, little is known of the role of such elements in the etiology and in the treatment of various diseases.

The recent availability of high—flux nuclear reactors has made possible the application of neutron activation techniques to trace element analysis. The method described was devised for the quant. detn. of thorium and uranium in human blood, bone, urine and faeces. Ashed samples of biol. material were placed in the reactor and exposed to a neutron flux of \(1 \times 10^{13}\) n/cm.\(^2\)/sec. for approx. 5 days.

The nuclear reactions and transformations on both elements where as follows:

\[
{^{232}Th} + n = {^{233}Th} \quad \beta^- \quad 22.1\ min \quad {^{233}Pa} \quad \beta^- \quad {^{234}U} \\
{^{234}U} + n = {^{235}U} \quad \beta^- \quad 23.5\ min \quad {^{235}NP} \quad \beta^- \quad {^{239}Pu}
\]

After bombardment the radiochemical sepns. of {\(^{233}Pa\)} and {\(^{235}NP\)} were completed, and the resulting radioisotopes were simultaneously measured against their respective standards.

Radioisotope identification can be accomplished, both by half-life or by gama-spectra analysis. The normal values for thorium and uranium in the analysed materials are presented. The proposed anal. procedures are suitable for the study of metabolism of these elements in biol. equil. conditions.

Examiners: Prof. H. Ivecovic, Dr. P. Strohal, and Prof. O. Weber.


Thesis submitted at the University Library, Zagreb, and at the Institute for Medical Research, Zagreb.

(82 pages, 29 figures, 123 references, original in Croatian)
MCC-27

1. Determination of Thorium and Uranium in Biological Materials by Activation Analysis

I. Picec M.

II. Institute for Medical Research, Yugoslav Academy of Sciences and Arts, Zagreb, Croatia, Yugoslavia

<table>
<thead>
<tr>
<th>Thorium, in human blood</th>
<th>—, in bones</th>
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<th>Uranium, in human blood</th>
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Electrochemical Study of $\text{UO}_2^{2+} - \text{H}_2\text{O}_2 - 1\text{M Na}_2\text{CO}_3$ Aqueous Solutions

V. Žutić

Institute «Ruder Bošković», Zagreb, Croatia, Yugoslavia

Reduction of uranil peroxodicarbonate in 1M Na$_2$CO$_3$ soln. has been studied by means of polarography, cyclic voltammetry and controlled-potential electrolysis at the mercury electrodes. Only one reduction wave with the half-wave potential at $-1.15$ V vs. S. C. E. has been observed. The overall electron change was found to equal 3, and the final product of the electrode reaction has been identified as uranium(V) carbonate complex. Interaction of uranium(V) carbonate and uranyl peroxodicarbonate to form uranyl tricarbonate has been studied in macro-scale and a mechanism for the reduction of uranyl tricarbonate and uranyl peroxodicarbonate mixts. at the dropping mercury electrode has been proposed, as well as the mechanism for the simultaneous reduction of hydrogen peroxide and uranyl peroxodicarbonate.


Examiners: Prof. C. Đorđević, Dr. M. Branica, and Dr. Z. Pučar.


Thesis deposited at the University Library and Institute «Ruder Bošković», Zagreb.

(90 pages, 22 figures, 7 tables, 115 references, original in Croatian)

V. ŽUTIĆ
MCC-28

1. Electrochemical Study of UO₂²⁺ — H₂O₂ — 1M Na₂CO₃ Aqueous Solutions
I. Zutić V.
II. Institute »Ruder Bošković«, Zagreb, Croatia, Yugoslavia

Polarography, of uranyl complexes Uranyl carbonate complexes, reduction of Uranyl peroxodicarbonate complex, reduction of Voltammetry, cyclic, of uranyl complexes
Precipitation and Hydrolysis of Rare Earth Elements in Distilled Water and in Sea Water

B. Pokrić

Institute "Ruder Bošković", Zagreb, Croatia, Yugoslavia

The pptn. diagrams of rare earth hydroxides show that the rare earth elements exist in same hydrolytic species in the acid range both in dist. water and in sea water. The studied elements are entirely hydrolyzed at pH about 8 which exist in normal sea water. The pptn. pH values of all rare elements studied in sea water are lower than the pH values in dist. water. In some cases the observed shift of the pptn. pH values in sea water is in the order of magnitude of several pH units in comparison with the pptn. pH values of rare earth hydroxides in sea water.

All elements studied in natural sea water are dissolved in the form of uncharged assoc. and one may expect a very effective fixation on other solid particles or surfaces. That indicates why such elements occur in sea water in a greater extent in the particulate form.


Examiners: Dr. M. Branica, Dr. Z. Pučar, and Dr. B. Kunst.


Thesis deposited at the University Library and Institute "Ruder Bošković", Zagreb.

(65 pages, 15 figures, 2 tables, 47 references, original in Croatian)

B. POKRIĆ
MCC-29

I. Precipitation and Hydrolysis of Rare Earth Elements in Distilled Water and in Sea Water

I. Pokrić B.
II. Institute "Ruder Bošković", Zagreb, Croatia, Yugoslavia

Precipitation, of rare earth Rare earth, precipitation of Sea water, precipitation of rare earth in
BIBLIOGRAPHIA CHEMICA CROATICA

1960

BCC-346
S. Ašperger, I. Murati, and D. Pavlović
Institute of Inorganic and Physical Chemistry, Faculty of Pharmacy, University of Zagreb and Department of Physical Chemistry, Institute »Ruder Bošković«, Zagreb, Croatia, Yugoslavia

Kinetics and Mechanism of the Decomposition of Complex Cyanides of Iron(II) and Molybdenum(IV)

BCC-347
S. Ašperger and N. Ilačevac
Department of Physical Chemistry, Institute »Ruder Bošković«, Zagreb, and Institute of Inorganic and Physical Chemistry, Faculty of Pharmacy, University of Zagreb, Zagreb, Croatia, Yugoslavia

Secondary Isotope Effect in the Hydrolysis of a Sulphonium Ion

BCC-348
A. Bežjak and D. Grdenić
Department of Structural and Inorganic Chemistry, Institute »Ruder Bošković«, Zagreb, Yugoslavia

The Crystal Structure of Mellitic Acid

BCC-349
D. Grdenić and D. Pavković-Devdić
ˇOdjel za strukturnu i anorgansku kemiju Instituta »Ruder Bošković«, Zagreb, Jugoslavija

Galij u jugoslavenskim boksitima

1961

BCC-350
S. Ašperger, D. Pavlović, and M. Orhanović
Department of Physical Chemistry, Institute »Ruder Bošković«, Zagreb, and Department of Inorganic and Physical Chemistry, Faculty of Pharmacy, University of Zagreb, Zagreb, Yugoslavia

Mechanism of Substitution of Chlorine in cis- and trans-Chloronitrobis (ethylenediamine) cobalt(III) Ions by Thiocyanate in Methanol

BCC-351
S. Ašperger, N. Ilačevac, and D. Pavlović
Department of Physical Chemistry, Institute »Ruder Bošković«, Zagreb, and Department of Inorganic and Physical Chemistry, Faculty of Pharmacy, University of Zagreb, Zagreb, Yugoslavia

Secondary Deuterium Isotope Effects in Bimolecular Elimination of 2-Phenylethyl-1, 1-d2 Bromide and 2-Phenylethyl dimethylsulfonium-1, 1-d2 Bromide
BCC-352
C. Djordjević
Department of Structural and Inorganic Chemistry, Institute
»Ruder Bošković«, Zagreb, Yugoslavia
Metal-Oxygen Vibration Modes in the Infrared Spectra of
Aluminium, Gallium and Indium Tris-Acetylacetonates

BCC-353
D. Grdenić and B. Kamenar
Department of Structural and Inorganic Chemistry, Institute
»Ruder Bošković«, Zagreb, Yugoslavia
Structures Involving Unshared Electron Pair: Pyramidal
Configuration of Trichlorostannite Ion

BCC-354
B. Kamenar and D. Grdenić
Department of Structural and Inorganic Chemistry, Institute
»Ruder Bošković«, Zagreb, Yugoslavia
The Crystal Structure of Stannous Chloride Dihydrate

BCC-355
I. Murati and S. Asperger
Department of Inorganic and Physical Chemistry, Faculty of Pharmacy,
University of Zagreb, and Department of Physical Chemistry, Institute
»Ruder Bošković«, Zagreb, Yugoslavia
Colorimetric Determination of Small Amounts of
Aquopentacyanoferrate(II) in the Presence of Ferro- and
Ferricyanide

BCC-356
Z. Ban and M. Sikirica
Institute »Ruder Bošković«, Zagreb, Yugoslavia
Crucible-Free Synthesis of Silicides and Borides
New Nuclear Materials including Non-metallic Fuels, Vol. II,
IAEA, Vienna, 1963, p. 175.

BCC-357
R. Blinc, I. Zupančič, S. Maričić, and Z. Veksli
Nuclear Institute »Jožef Stefan«, Ljubljana, and Institute
»Ruder Bošković«, Zagreb, Yugoslavia
Anisotropy of Fluorine Chemical Shift Tensor in XeF₄

BCC-358
D. Irutek, E. Jungman, S. Maričić, and M. Zovko
Institute of Light Metals, Zagreb, and Institute »Ruder Bošković«, Zagreb,
Yugoslavia
Solubilities of Boehmite from Yugoslav Bauxites
I. Intern. Symp. on Bauxites, Alum. Hydroxides and Oxides,
E. Jungaman, K. Klarić, S. Maričić, and Z. Meić
Institute "Ruder Bošković", Zagreb, and Institute of Light Metals, Zagreb, Yugoslavia

A Proton Magnetic Resonance and Infrared Study in the Series: Aluminium Hydroxide Gel, Pseudoboehmite, Boehmite

M. Sikirica and Z. Ban
Institute "Ruder Bošković", Zagreb, Yugoslavia

New Phase in the System Uranium-Molybdenum-Silicon

L. Träger, A. Kornhauser, and A. Wacker
Institut für Therapeutische Biochemie der Universität Frankfurt, Frankfurt am Main, Germany

The Tritium Isotope Effect in Pyrimidines

J. Čaja and V. Pravdić
Institute "Ruder Bošković", Zagreb, Yugoslavia

Electrochemical Reduction of Uranium(VI) at Mercury Electrodes in Carbonate Solutions
J. Electroanal. Chem. 8 (1964) 390.

D. Grdenić and B. Korpar-Čolig
Laboratory of General and Inorganic Chemistry, Faculty of Science, University of Zagreb, Zagreb, Yugoslavia

Another Preparation Method of Vanadium(III) and Uranium(IV) 1,3-Diketone Complexes
Inorg. Chem. 3 (1964) 1328.

S. Maričić, G. Pifat, and V. Pravdić
Institute "Ruder Bošković", Zagreb, Yugoslavia

Hydration of Haemoglobin and its Reversible Oxygenation

V. Pravdić, M. Branica, and Z. Pučar
Institute "Ruder Bošković", Zagreb, Yugoslavia

Uranium Dioxide Production. A Survey of Electrochemical Reduction and Precipitation from Carbonate Solutions
3rd Int. Conf. PUAE (Geneve) 1964, P/703.

M. Randić
Department of Chemistry, University of Sheffield, England

The Splitting of d-Orbitals in Less Symmetrical Molecules Containing a Cyclopentadienyl Ligand
BCC-367
A. Wacker, H. Dellweg, L. Träger, A. Kornhauser, E. Lodemann, G. Türck, R. Selzer, P. Chandra, and M. Ishimoto
Institut für Therapeutische Biochemie der Universität Frankfurt, Frankfurt am Main, Germany
Organic Photochemistry of Nucleic Acids
Photochem. and Photobiol. 3 (1964) 369.

BCC-368
S. Asperger, D. Pavlović, L. Klasinc, and I. Murati
Department of Inorganic and Physical Chemistry, Faculty of Pharmacy, University of Zagreb, and Department of Physical Chemistry, Institute „Ruder Bošković“, Zagreb, Yugoslavia
α-Hydrogen Exchange in the Reaction of 2-Phenylethyldimethylsulphonium Bromide with Deuteroxide in Deuterium Oxide Solution

BCC-369
Z. Ban and M. Sikirica
Institute „Ruder Bošković“, Zagreb, Yugoslavia
The Crystal Structure of Ternary Silicides ThM₂Si₂
(M = Cr, Mn, Fe, Co, Ni and Cu)

BCC-370
C. Djordjević
Institute „Ruder Bošković“, Zagreb, Yugoslavia

BCC-371
C. Djordjević
Institute „Ruder Bošković“, Zagreb, Yugoslavia
Metal-Oxygen Stretching Frequencies in Some Metal-Nitroacetylacetonates in Solid and Solution Infrared Spectra

BCC-372
W. F. Espenscheid, E. Willis, E. Matijević, and M. Kerker
Department of Chemistry, Clarkson College of Technology, Potsdam, New York, USA

BCC-373
D. Grdenić
Laboratory of General and Inorganic Chemistry, Faculty of Science, University of Zagreb, Zagreb, Yugoslavia
The Structural Chemistry of Mercury
Quart. Rev. 19 (1965) 303.
BCC-374
D. Grdenić and B. Kamenar
Laboratory of General and Inorganic Chemistry, Faculty of Science, University of Zagreb, Zagreb, Yugoslavia
Structure Involving Unshared Electron Pair: Coordination of Antimony in Racemic Potassium Antimonyl Tartrate

BCC-375
M. Grdinić and V. Hahn
Department of Organic Chemistry and Biochemistry, Institute »Ruder Bošković«, Zagreb, and Laboratory of Organic Chemistry, Faculty of Technology, University of Zagreb, Zagreb, Yugoslavia
Chemistry of Imidoyl and Amide Chlorides. II. On the Preparation and Properties of the N-Mono- and N,N-Dialkyl-Substituted Amide Halides

BCC-376
M. J. Herak and M. Mirnik
Laboratory of Radiochemistry, Institute »Ruder Bošković«, Zagreb, and Laboratory of Physical Chemistry, Faculty of Science, University of Zagreb, Zagreb, Yugoslavia
Determination of the Ion Adsorption by the Radioactive Tracer Technique. V. Influence of the Dispersity of AgI, of the Valency of Counter Ions, of the Dilution of the Mother Liquor and of pH
Kolloid-Z. Polymere 205 (1965) 129.

BCC-377
B. Kamenar, B. F. Hoskins, and C. K. Prout
Chemical Crystallography Laboratory, University of Oxford, Oxford, England
The Molecular Structure of Eschenmoser's »pseudo-corrin«

BCC-378
B. Kamenar, and C. K. Prout
Chemical Crystallography Laboratory, University of Oxford, Oxford, England
Molecular Complexes. Part I. The Crystal and Molecular Structure of the 1:1 Adduct of Benzo trifuroxan and 13,14-Dithiatricyclo (8, 2, 1, 14) tetradeca-4,6,10,12-tetraene

BCC-379
B. Kamenar, C. K. Prout, and J. D. Wright
Chemical Crystallography Laboratory, University of Oxford, Oxford, England
Molecular Complexes. Part II. The Crystal Structure of the 1:1 Complex of Bis-8-hydroxyquinolinatopalladium(II) and Chloranil

BCC-380
W. Kemula, Lj. Jeftić, and Z. Galus
Department of Inorganic Chemistry, University of Warsaw, Warsaw, Poland
Electrochemistry of Nickel Complexes with Clathrate Forming Agents
Electrochemical Investigation of Nickel Pyridine and Nickel-Picoline Complexes
J. Electroanal. Chem. 10 (1965) 387.

A. Kornhauser and R. F. Nyström
Radiocarbon Laboratory, University of Illinois, Urbana, Ill., U.S.A.
Determination of Carbon-14 and/or Tritium in the Methyl Group of Organic Compounds. Isotopic C-methyl Analysis
J. Labelled Comds. 1 (1965) 201.

S. Kveder and S. Iskrić
Institute »Ruder Bošković«, Zagreb, Yugoslavia
5-Hydroxytryptamine Metabolism by the Nuclear Fraction of Rat-Liver Homogenate

B. Ladešić and D. Keglević
Institute »Ruder Bošković«, Zagreb, Yugoslavia
Biochemical Studies in Tobacco Plants II. The Metabolism of the Optical Isomers of α- and β-Methionine in Nicotiana Rustica

J. N. Murrell, M. Randić, and D. R. Williams
University of Sheffield, Sheffield, England
The Theory of Intramolecular Forces in the Region of Small Orbital Overlap

N. Pravdić and D. Keglević
Institute »Ruder Bošković«, Zagreb, Yugoslavia
Glucuronic Esters III. The Synthesis of the Fully Benzylated C-1 Hydroxyl Free Glucuronic Acid
Tetrahedron 21 (1965) 1897.

M. Randić and Z. Maksić
Institute »Ruder Bošković«, Zagreb, Yugoslavia
Maximum Overlap Hybridization in Cyclopropane and Some Related Molecules

C. Smart, R. Jacobsen, M. Kerker, J. P. Kratoňvil, and E. Matijević
Clarkson College of Technology, Potsdam, N. Y., U.S.A.
Experimental Study of Multiple Light Scattering
The Crystal Structure of Double Nitrate Octahydrates of Thorium and Bivalent Metals
Acta Cryst. 18 (1965) 698.

Maximum Overlap Hybridization in Methyl Substituted Cyclopropanes

Chemical State of Radiobromine Formed by the Rb$^{85}$ (n, α) Br$^{82}$ Reaction

Isotopeneffekte bei der chemischen Umwandlung von Tritiummarkiertem Uracil

Heterogeneous Exchange of Precipitates. V. Exchange between an Aqueous Ferric Chloride Solution and Ferric (Hydr)oxides Differently Treated after the Precipitation
Kolloid-Z. Polymere 205 (1965) 111.

Heterogeneous Exchange of Precipitates. VI. Exchange of Ferric Ion between an Aqueous Ferric Chloride Solution and Colloidal Beta Ferric Oxide Monohydrate Obtained by Slow Hydrolysis
Kolloid-Z. Polymere 205 (1965) 118.

Heterogeneous Exchange of Precipitates. VII. Fraction Exchange Calculation when the Composition of the System Changes During the Experiment
Kolloid-Z. Polymere 205 (1965) 120.