DCC-24 (Univ. Zagreb)

Croat. Chem. Acta **39** (1967)

The Electronic Structure of Some Polyatomic Molecules

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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_5—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 mols. 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 1.078 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.

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Croat. Chem. Acta **37** (1965) 307;
Trans. Faraday Soc. **62** (1966) 1362;
J. Chem. Soc. (A), **1966**, 1624;
Croat. Chem. Acta **38** (1966) 283;
Croat. Chem. Acta **38** (1966) 287.
Examiners: Prof. M. Randić, Prof. B. Težak, and Dr. S. Borčić.
Oral examination: January 6, 1967.

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

(128 pages, 15 figures, 19 tables, 78 references, original in Croatian)

N. TRINAJSTIĆ

DCC-24

1. The Electronic Structure of Some Polyatomic Molecules

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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

MCC-27 (Univ. Zagreb)

Master of Science Thesis

Croat. Chem. Acta **39 (1967)**

Determination of Thorium and Uranium in Biological Materials by Activation Analysis

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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 1×10^{13} n/cm.^{2}/sec. for approx. 5 days.

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

$$^{232}\mathrm{Th} + {}^{1}\mathrm{n} = {}^{233}\mathrm{Th} \xrightarrow[22.1\ \mathrm{min}]{\beta^-} {}^{233}\mathrm{Pa} \xrightarrow[27.0\ \mathrm{d}]{\beta^-} {}^{233}\mathrm{U}$$

$$^{238}\mathrm{U} + {}^{1}\mathrm{n} = {}^{239}\mathrm{U} \xrightarrow[23.5\ \mathrm{min}]{\beta^-} {}^{239}\mathrm{Np} \xrightarrow[2.36\ \mathrm{d}]{\beta^-} {}^{239}\mathrm{Pu}$$

After bombardment the radiochemical sepns. of ^{233}Pa and ^{239}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. Iveković, Dr. P. Strohal, and Prof. O. Weber.

Oral examination: October 5, 1966.

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

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

M. PICER

MCC-27

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

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Thorium, in human blood
—. in bones
—, in faeces
—, in urine
Uranium, in human blood
—, in bones
—, in faeces
—, in urine

B4

MCC-28 (Univ. Zagreb)
Master of Science Thesis

Croat. Chem. Acta **39** (1967)

Electrochemical Study of UO_2^{2+} — H_2O_2 — $1M$ Na_2CO_3 Aqueous Solutions

V. Žutić

Institute »Ruđer Bošković«, Zagreb, Croatia, Yugoslavia

Reduction of uranil peroxodicarbonate in $1M$ Na_2CO_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 over-all electrone 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 peroxidicarbonate 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.

Thesis is partly published: *J. Polarog. Soc.* **13** (1967) (in press).

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

Oral examination: December 23, 1966.

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

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

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MCC-28

1. Electrochemical Study of UO_2^{2+} — H_2O_2 — 1M Na_2CO_3 Aqueous Solutions

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Polarography, of uranyl complexes
Uranyl carbonate complexes, reduction of
Uranyl peroxodicarbonate complex, reduction of
Voltammetry, cyclic, of uranyl complexes

MCC-29 (Univ. Zagreb)
Master of Science Thesis

Croat. Chem. Acta **39** (1967)

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

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Institute »Ruđer 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 *p*H about 8 which exist in normal sea water. The pptn. *p*H values of all rare elements studied in sea water are lower than the *p*H values in dist. water. In some cases the observed shift of the pptn. *p*H values in sea water is in the order of magnitude of several *p*H units in comparison with the pptn. *p*H values of rare carth 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.

The thesis was partly published: *Croat. Chem. Acta* **39** (1967) 11—23.

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

Oral examination: November 28, 1966.

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

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

B. POKRIĆ

MCC-29

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

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Precipitation, of rare earth
Rare earth, precipitation of
Sea water, precipitation of rare earth in

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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 »Ruđer Bošković«, Zagreb, Croatia, Yugoslavia

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S. Ašperger and N. Ilakovac

Department of Physical Chemistry, Institute »Ruđer Bošković«, Zagreb, and Institute of Inorganic and Physical Chemistry, Faculty of Pharmacy, University of Zagreb, Zagreb, Croatia, Yugoslavia

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Department of Structural and Inorganic Chemistry, Institute »Ruđer Bošković«, Zagreb, Yugoslavia

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Nature (London) **185** (1960) 756.

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BCC-350

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Department of Physical Chemistry, Institute »Ruđer 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

J. Chem. Soc. **1961,** 2142.

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Department of Physical Chemistry, Institute »Ruđer Bošković«, Zagreb, and Department of Inorganic and Physical Chemistry, Faculty of Pharmacy, University of Zagreb, Zagreb, Yugoslavia

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»Ruđer Bošković«, Zagreb, Yugoslavia

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»Ruđer Bošković«, Zagreb, Yugoslavia

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Department of Inorganic and Physical Chemistry, Faculty of Pharmacy,
University of Zagreb, and Department of Physical Chemistry, Institute
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Institut für Therapeutische Biochemie der Universität Frankfurt, Frankfurt am Main, Germany

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J. Electroanal. Chem. **8** (1964) 390.

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Laboratory of General and Inorganic Chemistry, Faculty of Science, University of Zagreb, Zagreb, Yugoslavia

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

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Institut für Therapeutische Biochemie der Universität Frankfurt,
Frankfurt am Main, Germany

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Laboratory of General and Inorganic Chemistry, Faculty of Science,
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Laboratory of General and Inorganic Chemistry, Faculty of Science,
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Department of Organic Chemistry and Biochemistry, Institute
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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 *p*H

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Chemical Crystallography Laboratory, University of Oxford,
Oxford, England

The Molecular Structure of Eschenmoser's »pseudo-corrin«

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Oxford, England

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W. Kemula, Lj. Jeftić, and Z. Galus

Department of Inorganic Chemistry, University of Warsaw,
Warsaw, Poland

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Warsaw, Poland

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Radiocarbon Laboratory, University of Illinois, Urbana, Ill., U.S.A.

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Institute »Ruđer Bošković«, Zagreb, Yugoslavia

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University of Sheffield, Sheffield, England

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Institute »Ruđer Bošković«, Zagreb, Yugoslavia

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Clarkson College of Technology, Potsdam, N. Y., U.S.A.

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S. Šćavničar and B. Prodić

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University of Zagreb, Zagreb, Yugoslavia

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Maximum Overlap Hybridization in Methyl Substituted Cyclopropanes

J. Chem. Soc. A **1965,** 5621.

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M. Vlatković and S. Kaučić

Institute »Ruđer Bošković«, Zagreb, Yugoslavia

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

Chemical Effects of Nuclear Transformations, Vol. II, IAEA, Vienna, 1965, p. 3.

BCC-392

A. Wacker, A. Kornhauser, and L. Träger

Institut für Therapeutische Biochemie der Universität Frankfurt,
Frankfurt am Main, Germany

Isotopeneffekte bei der chemischen Umwandlung von Tritiummarkiertem Uracil

Z. Naturforschg. **20b** (1965) 1043.

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R. H. H. Wolf, M. Mirnik, and B. Težak

Laboratory of Radiochemistry, Institute »Ruđer Bošković«, Zagreb,
and Department of Physical Chemistry, Faculty of Science,
University of Zagreb, Zagreb, Yugoslavia

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.

BCC-394

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Laboratory of Radiochemistry, Institute »Ruđer Bošković«, Zagreb,
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University of Zagreb, Zagreb, Yugoslavia

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BCC-395

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University of Zagreb, Zagreb, Yugoslavia

Heterogeneous Exchange of Precipitates. VII. Fraction Exchange Calculation when the Composition of the System Changes During the Experiment

Kolloid-Z. Polymere **205** (1965) 120.