Fourier Transforms of Lattice Sums in Hartree-Fock Calculations for Simple Crystals

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An efficient method is presented to compute the Fourier transforms of lattice sums over Slater-type orbitals (STO) products that arise on crystal Hartree-Fock calculations. Introduction of one-dimensional integral representations for the Fourier transforms of the STO's enables a separation of the three infinite sums under the two-dimensional integral sign. This, in turn, makes it possible to calculate and store quantities associated with the three Fourier transform components separately. Beside infinite sums can be recognized as fast convergent theta functions, both for large and small arguments. The orbital transform integrations are then performed numerically. The method is very advantageous when lattice sum transforms are needed for a large number of transform vectors.

Formulas for simple-cubic crystals are presented when 1s, 2s, 2p, 3s, 3p and 3d STO's are involved but they can be easily generalized for orbitals of higher quantum numbers.

The numerical results are given for the lattice sums in which 1s, 2s and 2p STO's are entering. The method ensures an accuracy of at least one in 10^4.

A relationship between molecular and crystal quantities is established too.

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A. GRAOVAC
Crystal Hartree-Fock calculations, the Fourier transforms of lattice sums over Slater-type orbitals, Theta functions, numerical transforms integrations.

Simple-cubic crystals, ls, 2s, 2p, 3s, 3p, 3d Slater-type orbitals.

Generalization for orbitals of higher quantum numbers, a relationship between molecular and crystal quantities.
BIBLIOGRAPHIA CHEMICA CROATICA

1973

BCC-1485

L. Eriksson, E. Matijević and S. Friberg

The Swedish Institute of Surface Chemistry, Stockholm, Sweden

Desorption of Hydrolyzed Metal Ions from Hydrophobic Interfaces. I. Latex-Aluminium Nitrate Systems

J. Colloid Interface Sci. 43 (1973) 591.

BCC-1486

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Numerical Treatment in Determining Stability Constants by the Spectrophotometric Method of Corresponding Solutions


BCC-1487

A. Graovac, H. J. Monkhorst and T. Zivković

Institute »Ruder Bošković«, Zagreb, Croatia, Yugoslavia

Slater Orbital Molecular Integrals with Numerical Fourier Transform Methods. I (Coplanar) Multicenter Exchange Integrals over 1s Orbitals

Int. J. Quantum Chem. 7 (1973) 233.

BCC-1488

I. Gutman and N. Trinajstić

Institute »Ruder Bošković«, Zagreb, Croatia, Yugoslavia

Graph Theory and Molecular Orbitals


BCC-1489

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A New Type of Liquid Crystal


BCC-1490

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Partition of Hexafluoroacetylacetone in the System: Water-Tri-n-Butyl Phosphate-Organic Solvent and the Extraction of Sodium by Various Fluorinated β-Diketones and Tri-n-Butyl Phosphate

BCC-1491
B. B. Tomazić and J. W. O'Laughlin
Ames Laboratory — USAEC and Department of Chemistry, Iowa State University, Ames, Iowa 50010
Synergic Extraction of Iron with Hexafluoroacetylacetone and Tri-n-Butyl Phosphate

1974

BCC-1492
A. Bell and E. Matijević
Institute of Colloid and Surface Science and Department of Chemistry, Clarkson College of Technology, Potsdam, New York 13676
Growth Mechanism of Hydrous Chromium(III) Oxide Spherical Particles of Narrow Size Distribution

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M. Bravarić, J. Rolich, N. Ban and V. Gnjatović
Institute of Organic Chemical Technology, Faculty of Technology, University of Zagreb, and INA Institute, Zagreb, Yugoslavia
Studies of Alcoholysis of Poly (vinyl Acetate) to Poly (vinyl Alcohol)

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Lj. Buttula and M. Malnar
Faculty of Pharmacy and Biochemistry, University, Zagreb, A. Kovačića 1
Aminoalkane Sulfonic Acids, Reaction with Acetic Anhydride

BCC-1495
D. L. Catone and E. Matijević
Institute of Colloid and Surface Science, and Department of Chemistry, Clarkson College of Technology, Potsdam, New York 13676
Aluminium Hydrous Oxide Sols II. Preparation of Uniform Spherical Particles by Hydrolysis of Al sec-Butoxide

BCC-1496
T. S. Chou, J. R. Burgdorf, A. L. Ellis, S. R. Lammert and S. P. Kukolja
The Lilly Research Laboratories, Eli Lilly and Company, Indianapolis, Indiana 46206
Azetidinone Sulfenic Acids. Isolation of Crystalline Sulfenic Acids from Penicillin Sulfoxides and a Study of their Reactivities

BCC-1497
D. Cvetković, I. Gutman and N. Trinajstić
Faculty of Electrical Engineering, University of Belgrade, P.O.B. 816, 11001 Belgrade, Serbia, Yugoslavia, and Institute «Ruder Bošković», P.O.B. 1016, 41001 Zagreb, Croatia, Yugoslavia
Graph Theory and Molecular Orbitals. VII. The Role of Resonance Structures
BCC-1498
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Faculty of Electrical Engineering, University of Belgrade, Belgrade, Serbia, Yugoslavia and Institute P.O.B. 816, 11001 Belgrade, Serbia, Yugoslavia and Institute "Ruder Bošković", P.O.B. 1016, 41001 Zagreb, Croatia, Yugoslavia
Conjugated Molecular Having Integral Spectra

BCC-1499
H. Čačković, J. Loboda-Čačković, R. Hosemann and D. Weich
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin-Dahlem
Recrystallization Process of Branched Polyethylene During Stretching and a Statistical Explanation

BCC-1500
V. Čaplar, V. Šunjić and F. Kajfež
Compagnia de Ricerca Chimica SA., Chiasso, Switzerland and Institute of Organic Chemistry and Biochemistry, University of Zagreb, Croatia, Yugoslavia
N1-Substitution in 2-Methyl-4(5)nitroimidazole III. (1) New Syntheses of 1-(2-(Ethylsulfonyl)ethyl)-2-methyl-5-nitroimidazole

BCC-1501
R. Despotović, V. Horvat, S. Popović and Z. Selir
"Ruder Bošković" Institute, 41001 Zagreb, Croatia, Yugoslavia
The Aging of Silver Iodide
J. Colloid Interface Sci. 49 (1974) 147.

BCC-1502
Gj. Deželić, N. Šegudović and J. J. Petres
Andrija Stampar School of Public Health, Medical Faculty, University of Zagreb, and Department of Physical Chemistry, Institute "Ruder Bošković", 41000 Zagreb, Croatia, Yugoslavia
Light Scattering in Optically Active Systems
J. Colloid Interface Sci. 49. (1974) 481.

BCC-1503
V. Fintić i G. Špoljarić
Zavod za ispitivanje i kontrolu lijekova SRH, Zagreb and Zavod za farmaceutsku kemiju, Farmaceutsko-biokemijski fakultet, Zagreb
Reakcija fluorescnecije za identifikaciju soli pralidoksima

BCC-1504
V. Fintić i G. Špoljarić
Zavod za ispitivanje i kontrolu lijekova SRH, Zagreb and Zavod za farmaceutsku kemiju Farmaceutsko-biokemijski fakultet, Zagreb
Reakcije termijske razgradnje za dokazivanje i razlikovanje pralidoksim-klorida i pralidoksim-jodida

BCC-1505
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Institut za medicinska istraživanja i medicinu rada Jugoslavenske akademije znanosti i umjetnosti, Zagreb
Prikaz metoda za određivanje sumporova dioksida u atmosferi
BCC-1506
B. Grabarić, B. Mayer, I. Piljac and I. Filipović
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Croatia, Yugoslavia
Spectrophotometric Determination of Stability Constants of n-butyrate and 2-, 3- and 4-hydroxybutyrate of Cobalt(II), Nickel(II) and Copper(II)

BCC-1507
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Institute »Ruder Bošković«, Zagreb, Croatia, Yugoslavia
The Nonexistence of Topological Formula for Total π-Electron Energy

BCC-1508
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British Columbia, Canada V6T 1W5
ENDOR Study of the Minority Radicals Formed in X-Ray-Irradiated Single Crystals of Thymidine

BCC-1509
J. Jednacak, V. Pravdic and W. Haller
Electrochemistry Laboratory, »Ruder Bošković« Institute, 41001 Zagreb,
Croatia, Yugoslavia
The Electrokinetic Potential of Glasses in Aqueous Electrolyte Solutions
J. Colloid Interface Sci. 43 (1974) 16.

BCC-1510
D. Keglević and Š. Valenteković
Tracer Laboratory, Institute »Ruder Bošković«, Zagreb (Yugoslavia)

BCC-1511
J. Loboda-Čačković, H. Čačković and R. Hosemann
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin-Dahlem (Germany)
Structural Changes in Paracrystallites of Drawn Polyethylene by Irradiation

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R. B. Mallion, N. Trinajstić and A. J. Schwenk
Department of Theoretical Chemistry, University of Oxford, United
Kingdom and Mathematical Institute, University of Oxford, United Kingdom
Graph Theory in Chemistry — Generalization of Sachs’ Formula
BCC-1513
B. Matković, B. Ribar, B. Prelesnik and R. Herak
Institute »Ruder Bošković«, 41001 Zagreb, Department of Physics and Mathematics, University of Novi Sad, 21000 Novi Sad and Institute Boris Kidrič, Vinča, 11001 Beograd, Yugoslavia
Crystal Structure of Mercury(II) Hydroxide Nitrate. Refinement by Neutron Diffraction

BCC-1514
Z. Meić, W. Braun, H. Knehr and W. Zeil
Institute »Ruder Bošković«, Zagreb (Yugoslavia)
Kraftkonstanten und Zentrifugalverzerrungskonstanten des Methylchlorsilans

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Institute Rudor Bošković, Odjel fizičke kemije, Zagreb
Određivanje žive metodom besplamene atomske apsorpcije

BCC-1516
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Growth of Calcium Phosphate on Hydroxyapatite Crystals. Effect of Supersaturation and Ionic Medium

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Department of Physical Chemistry, University of Zagreb, Faculty of Science, Zagreb, Croatia (Yugoslavia)
The Precipitation of Mercurous Halides in the Nitric Acidic Medium
Colloid Interface Sci. 252 (1974) 46.

BCC-1518
R. Perkins, R. Brace and E. Matijević
Institute of Colloid and Surface Science and Department of Chemistry, Clarkson College of Technology, Potsdam, New York 13676
Colloid and Surface Properties of Clay Suspension. I. Laponite CP

BCC-1519
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Institute of Pharmacognosy, Faculty of Pharmacy and Biochemistry, University of Zagreb
The Genus Helleborus: Chemistry of Subterranean Parts

BCC-1520
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Institute of Pharmacognosy, Faculty of Pharmacy and Biochemistry, University of Zagreb
Phytochemical Examination of Viburnum tinus L
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M. Pokorny, E. Zissis, H. G. Fletcher, Jr. and N. Pravdić
The Inhibitory Activity of 2-Acetamido-2-Deoxy-\(\text{\textgreek{n}}\)-Gluconolactones and their Isopropylidene Derivatives on 2-Acetamido-2-Deoxy-\(\beta\)-\(\text{\textgreek{n}}\)-Glucosidase

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The Oxidation of Partially Protected 2-Acetamido-2-Deoxypyranoses with Silver Carbonate on Celite

BCC-1523
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Mode of Action of 2-Ethylisonicotinaldehyde Thiosemicarbazone on Mycobacterium tuberculosis

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Photochemical Bleaching of Hematoporphyrin

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M. Randić and J. W. H. Sutherland
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Construction of Nonequivalent Hybrids in Hydrocarbon Polymers: Polybutadiene, Polyisoprene and Related Systems

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Institut für physikalische Chemie der Universität Freiburg i. Br., Institute «Ruder Bošković», Zagreb, Jugoslawien und Kernforschungszentrum Karlsruhe, Institut für Radiochemie
Vergleich der Photoelektronenspektren und Photoionenspektren von Vinylfluorid

BCC-1527
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Istituto di Chimica delle Macromolecole del CNR, Via Alfonso Corti 12, Milan, Italy
Dynamics and Poly(vinyl chloride). I. Infinite Perfect Model
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Department of Chemistry, Northwestern University Evanston, Illinois 60201 (U. S. A.)
On the Influence of Electrode Curvature and Growth in D. C. and A. C. Polarography: The E. E. Mechanism with Amalgam Formation

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Microdetermination of Lead by a Fluorescent Ring-oven Technique

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Izmjenjivači iona i produženo djelovanje lijekova

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The Influence of Amphoretic Polyelectrolyte Gelatin on the Formation of Cobalt(II), Nickel(II), Magnesium(II), Manganese(II), Iron(III), and Aluminium(III) Hydroxide

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Titrimetric Application of Multiparametric Curve Fitting. III. Evaluation of the Parameters Characterizing Acidimetric Potentiometric Titrations of Laurate Ion
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V. Zutić, C. Poty and L. Gierst
Centre for Marine Research, "Ruder Bošković" Institute, Zagreb (Yugoslavia) and Université Libre de Bruxelles, Faculté des Sciences, Brussels (Belgium)
The Behaviour of Electrogogenerated Hydrogen Peroxide in the Presence of Chemical Acceptors. I. Uranyl Tricarbonate Aqueous Solutions

1975

BCC-1536
N. Avdalović
Zavod za fiziologiju, Medicinski fakultet Sveučilišta u Zagrebu, Salata 3, pp. 925, 41001 Zagreb
Uptake of Radioactive Orotic Acid and Cycloleucine into Normal Castrated Kidneys of Mice Adapted to a Controlled Feeding Schedule

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N. Avdalović and M. Bates
Zavod za fiziologiju Medicinskog fakulteta, Sveučilišta u Zagrebu, Salata 3, pp. 925, 41001 Zagreb
Some New Aspects in the Pathway of RNA Synthesis in Mouse Tissues Following Castration

BCC-1538
N. Avdalović, M. Bates and T. Rončević
Zavod za fiziologiju Medicinskog fakulteta, Sveučilišta u Zagrebu, Salata 3, pp. 925, 41001 Zagreb
Some New Aspects in the Pathway of RNA Synthesis in Mouse Tissues Following Castration

BCC-1539
N. Avdalović, M. Bates and T. Rončević
Zavod za fiziologiju Medicinskog fakulteta, Sveučilišta u Zagrebu, Salata 3, pp. 925, 41001 Zagreb
Some New Aspects in the Pathway of RNA Biosynthesis in Mouse Tissues Following Castration

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A. Bell and E. Matijević
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Complex Chemistry of Hydrous Chromium(III) Oxide Sols Formation

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Theory of a General Method for Phase Analysis
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H. Bilinski
Department of Physical Chemistry, »Ruder Bošković« Institute, Zagreb
Is the Total Concentration of Lead in Blood a Significant Test for Lead Poisoning?

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Department of Chemistry, Faculty of Pharmacy and Biochemistry, University of Zagreb, and Institute »Ruder Bošković«, Zagreb, Croatia, Yugoslavia
Mechanism of Base Methanolysis of trans-chlorocyanobis(ethylenediamine)cobalt(III)

BCC-1544
N. Blažević, M. Žinić, T. Kovač, V. Šunjić and F. Kajfžež
CRC, Compagnia di Ricerca Chimica, Chiasso, Switzerland and Institute of Organic Chemistry and Biochemistry, University of Zagreb
Identification Methods for (±)-alpha-(3-Benzoylphenyl)-propionic Acid (Ketoprofen) and its Enantiomers Based on Physico-Chemical Properties

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General Properties of the Hartree-Fock Problem Demonstrated on the Frontier Orbital Model I. Relation among Various Types of Extrema

BCC-1546
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General Properties of the Hartree-Fock Problem Demonstrated on the Frontier Orbital Model. II. Analysis of the Customary Iterative Procedure

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Kinetics and Mechanism of Replacements in Pentacyano(ligand)ferrate(II) Ions

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Oxalato Complexes of Niobium and Tantalum. I. Oxo-oxalatophosphine and -Arsine Oxide
BCC-1549
V. Čaplar, V. Šunjić, F. Kajfež and T. Kovač
CRC, Compagnia di Ricerca Chimica S. A. Chiasso, Switzerland and Institute of Organic Chemistry and Biochemistry, University of Zagreb,
N(1)-Substituted 4(5)-Nitroimidazoles. IV. Syntheses of 1-(2’-Morpholino-ethyl)-5-Nitroimidazole

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R. Despotović, N. Filipović and J. Katanec
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The Structure of the Interface Layer in Silver Iodide/Tenside Systems

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V. Drenkic, A. Dajac, J. Kufinec and Z. Stefanac
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Metal Complexes with Thio Derivatives of n-Salicylidene-ethylamine

BCC-1552
I. Filipović, I. Piljac, B. Grabarić and B. Mayer
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Polarographic Determination of Stability Constants of 2-, 3- and 4-hydroxybutyrate Complexes of Copper(II)

BCC-1553
Department of Chemistry, Indiana University, Bloomington, Indiana, 47401, the »Ruder Bošković« Institute and the Department of Chemistry, Faculty of Natural Sciences and Mathematics, University of Zagreb, 41000 Zagreb, Yugoslavia
Methyl-d3 Isotope Effects, α-Methyl Hydrogen Rate Effects, and the Analysis of Some Solvolytic Reaction Mechanisms

BCC-1554
H. Füredi-Milhofer, E. Oljica-Žabčić, B. Purgarić, B. Kosar-Grašić and N. Pavković
Department of Physical Chemistry »Ruder Bošković« Institute, Zagreb, Croatia, Yugoslavia
Precipitation of Calcium Phosphates from Electrolyte Solutions. IV. Precipitation Diagrams of the System Calcium Chloride-Sodium Phosphate 0.15 M Sodium Chloride

BCC-1555
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Contribution to the Ring Oven Methodology. XI
BCC-1556
A. Gertner und V. Grdinić
Chemisches Institut, Pharmazeutisch-Biochemische Fakultät, Universität Zagreb
Betachtungen über gewisse, für die chemische Mikroanalyse massgebliche, Eigenschaften von Kapillarträgern

BCC-1557
A. Gertner, D. Kodrnja, D. Pavišić und V. Grdinić
Chemisches Institut, Pharmazeutisch-Biochemische Fakultät, Universität Zagreb
Ultramikrobestimmung von Al(III) in Gegenwart von Fe(III) nach vorheriger Trennung der Ionen im Ringofenverfahren

BCC-1558
B. Grabarić, M. Tkalčec, I. Piljac, I. Filipović und Vl. Simeon
Laboratory of Inorganic Chemistry, Faculty of Technology and Institute for Inorganic and Analytical Chemistry, University of Zagreb, Croatia (Yugoslavia) and Institute for Medical Research and Occupational Health, Yugoslav Academy of Sciences and Arts, 41000 Zagreb, Croatia, (Yugoslavia)
Numerical Evaluation of Complex Stability Constants from Polarographic Data for Quasi-Reversible Processes
Anal. Chem. 74 (1975) 147.

BCC-1559
A. Graovac, H. J. Monkhorst and M. L. Glasser
Department of Physics, University of Utah, Salt Lake City, Utah 84112, USA and Battelle Memorial Institute, Columbus, Ohio 43210, USA
Computation of Fourier Transform Quantities in Hartree-Fock Calculations for Simple Crystals
Int. J. Quantum Chem. 9 (1975) 243.

BCC-1560
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Contributions to the Ring Oven Methodology XIII

BCC-1561
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Beiträge zur Ringofenmethodik. XIV. Komplexbildung mit einem Füllungsreagens auf Kapillarträgern

BCC-1562
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Radiometrisch verfolgte Ionenelution durch Wasser auf Zellstoffhaltigen Kapillarträgern
BCC-1563
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Contributions to the Ring Oven Methodology, XII

BCC-1564
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Radiometrische Löslichkeitsbestimmung von $^{59}$Fe(OH)$_3$ in Äthyldiamintetraessigsäure

BCC-1565
V. Grdinić, Z. Tabor and A. Gertner
Institut für Chemie, Pharmazeutisch-Biochemische Fakultät der Universität Zagreb, 41000 Zagreb, A Kovačića 1, Jugoslawien
Beiträge zur Ringofenmethodik. XV. Kationentrennung mit Dithiooxamid und radiometrische Prüfung des Trennungsverfahrens

BCC-1566
I. Gutman, N. Trinajstić, and C. P. Wilcox
Institute »Ruder Bošković«, P. O. B. 1016, 41001 Zagreb, Croatia, Yugoslavia
Graph Theory and Molecular Orbitals. X. The Number of Kekulé Structures and the Thermodynamic Stability of Conjugated Systems
Tetrahedron 31 (1975) 143.

BCC-1567
O. Hadžija and M. Tonković
»Ruder Bošković« Institute, Zagreb, Yugoslavia
Gravimetric Microdetermination of Alkoxy Groups in Sulphur Containing Compounds

BCC-1568
K. Kljač, A. Gojmerac and M. Proštenik
Institute of Chemistry and Biochemistry, Faculty of Medicine, University of Zagreb
Thin Layer Chromatographic Differentiation of Sphingolipid Bases and Complex Sphingolipids Oxidized with Osmium Tetraxide

BCC-1569
D. Kodrnja und A. Gertner
Chemisches Institut, Pharmazeutisch-Biochemische Fakultät, Universität Zagreb
Einfluss von Mg(II)-, Ca(II)- und Ba(II)-Ionen auf Fluoreszenzspektren von Tetrazyklinderivaten

BCC-1570
G. A. Koppel and S. Kukolja
The Lilly Research Laboratories, Eli Lilly and Company, Indianapolis, Indiana 46206
The Oxoazetidinesulphenic Acid Anion: s- vs O-Alkylation
BCC-1571
N. Kujundžić, Lj. Butula and M. Pečar
Faculty of Pharmacy and Biochemistry, Department of Chemistry
University of Zagreb, Zagreb, A. Kovačića 1, Croatia
Mitodepressive Substances. I. Effects of Some Heterocyclic
Aminohydroxamic Acids on the Growth of Lapidium Sativum L.

BCC-1572
S. Kukolja, S. R. Lammert, M. R. Gleissner and A. I. Ellis
The Lilly Research Laboratories, Eli Lilly and Company, Indianapolis, Indiana 46206
Chemical Transformations of Penicillins and Cephalosporins. Me­
chanism and Stereochemistry of the Interconversions of Penam and Cepham Systems

BCC-1573
A. D. Lindsay, E. Matijević and J. P. Krato­hvil
Institute of Colloid and Surface Science and Department of Chemistry, Clarkson College of Technology, Potsdam, N. Y. 13676, USA
Interaction of Nonionic Dextran with Silver Bromide Hydrosols

BCC-1574
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Zavod za fiziologiju, Medicinski fakultet, Sveučilište, Zagreb, und Institut für Physiologische Chemie der Universität, Düsseldorf, Deutschland
Characterization of Glycogen from the Liver of Chinese Hamster

BCC-1575
Z. B. Maksić, K. Kovačević and M. Eckert-Maksić
Institute »Ruder Bošković«, 41001 Zagreb, Croatia, Yugoslavia and Department of Physical Chemistry, The University of Zagreb, 41000 Zagreb, Croatia
The Calculation of Strain Energies in Cyclic and Polycyclic
Hydrocarbons by the Maximum Overlap Approximation

BCC-1576
F. J. Mangravite, T. D. Buzzell, E. A. Cassell, E. Matijević and G. B. Saxton
Institute of Colloid and Surface Science, Departments of Civil Engineering and Chemistry, Clarkson College of Technology, Potsdam, N. Y.
Removal of Humic Acid by Coagulation and Microflotation

BCC-1577
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Kinetics of Aaquation and Formation of the Tetra-aqua(2,2'-bipyridyl)-chromium(III) Ion

BCC-1578
E. Matijević, R. S. Sapieszko and J. B. Melville
Institute of Colloid and Surface Science, and Department of Chemistry, Clarkson College of Technology, Potsdam, New York 13676
Ferric Hydrous Oxide Sols. I. Monodisperzed Basic Iron(III)
Sulfate Particles
J. Colloid Interface Sci. 50 (1975) 567.
BCC-1579
E. Matijević
Institute of Colloid and Surface Science, Clarkson College of Technology, Potsdam, New York, U.S.A.
Kolloider en försummad värld
Kem. Tidskr. 87 (1975) 34.

BCC-1580
L. Meites and E. Matijević
Department of Chemistry and Institute of Colloid and Surface Science, Clarkson College of Technology, Potsdam, New York 13676 (U.S.A.)
Automatic Classification of Chemical Behavior by Sequential Hypothesization and Multiparametric Curve-Fitting. Part II. The Fully Automated Elucidation of Data Obtained in Acidimetric Potentiometric Titrations of the Anions of Long-Chain Acids

BCC-1581
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CRC, Compagnia di Ricerca Chimica, Chiasso, Switzerland and Institute of Organic Chemistry and Biochemistry, University of Zagreb, Zagreb, Croatia, Yugoslavia
Regio- and Stereoselectivity in β-Participation of a Vinilogous-Amide Nitrogen

BCC-1582
K. Moskaliuk, V. Marjanović, K. Mažuranić and A. Horvat
Institut für anorganische und analytische Chemie der Universität Zagreb und Institut für analytische Chemie KTO der technologischen Fakultät der Universität Zagreb, Jugoslawien
Photometrische Kationenbestimmung mit Gelatinifolien. Kupferbestimmung mit Diathyldithiocarbamat

BCC-1583
M. Orhanović and J. E. Early
Department of Chemistry, Georgetown University, Washington DC 20057
Kinetics of Reduction of Co(NH₃)₅Cl⁺ and cis- and trans-Co(en)₂Cl₂⁺ by Ti(III)

BCC-1584
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Reduction of Co(III) Oxidants by Ti(III)

BCC-1585
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Chemisches Institut, Pharmazeutisch-Biochemische Fakultät, Universität Zagreb
Zusammenwirken von maskierendem und Fällungs-Reagens zwecks Trennung von Ni(II)-Ionen aus Fe(III)-Co(II)-Ni(II)-Gemischen auf Kapillarrträgern
BIBLIOGRAPHIA CHEMICA CROATICA

BCC-1586
J. J. Petres and Gj. Deželić
Department of Physical Chemistry, Institute «Ruder Bošković» and Department of Biochemical Chemistry, Andrija Stampar School of Public Health, Faculty of Medicine, University of Zagreb, 41000 Zagreb, Croatia, Yugoslavia

Light Scattering by Large Ellipsoidal Particles. I. Rayleigh-Debye Approach
J. Colloid Interface Sci. 50 (1975) 296.

BCC-1587
I. Piljač, M. Tkalić and B. Grabarić
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Use of Optically Transparent Thin-Layer Cells for Determination of Composition and Stability Constants of Metal Ion Complexes with Electrode Reaction Products

BCC-1588
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Oxidations with Selenoxides. VIII. A New Method for the Preparation of N-Oxides

BCC-1589
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The Mechanism of Olefinic Cyclizations. A Case of π-Participation

BCC-1590
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Institute for Medical Research, Yugoslav Academy of Sciences and Arts, Moše Pijade 158, 41000 Zagreb (Yugoslavia)

Quantitative Thin-Layer Chromatographic Assay of Amino Acid Decarboxylase Activity
J. Chromatogr. 105 (1975) 418.

BCC-1591
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Kristallstrukturen von Au₄In₄ (h) und Au₃In₂

BCC-1592
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Synthesis and Polymerization of Optically Active Trans-(R) (-)-5-Phenyl-1,3-hexadiene and Trans-(R) (-)-6-Phenyl-1,3-heptadiene

BCC-1593
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On Rearrangement of the Connectivity Matrix of a Graph
BIBLIOGRAPHIA CHEMICA CROATICA

BCC-1594
M. Randić
Department of Chemistry, Harvard University, Cambridge, MA. 02138, U.S.A.
Graph Theoretical Approach to Local and Overall Aromaticity of Benzenenoid Hydrocarbons
_Tetrahedron_ 31 (1975) 1477.

BCC-1595
M. Randić and L. Kumar
Department of Physics, University of Utah, Salt Lake City, Utah 84112 (U.S.A.)
Hybridization in Highly Strained Small Ring Hydrocarbons. V. Methylene and Isopropylene Substituted Spiropentanes

BCC-1596
B. Raspor and M. Branica
Center for Marine Research, »Ruder Bošković«, Institute, Zagreb, Croatia, (Yugoslavia)
Polarographic Reduction of Cd(II)-Nitrilotriacetic Acid in Chloride Solutions of pH about 8

BCC-1597
B. Raspor and M. Branica
»Ruder Bošković« Institute, Center for Marine Research, Zagreb, Croatia, Yugoslavia
Comparison of the Polarographic Reduction of Cd-NTA, -EDTA and -DTPA Chelates in Chloride Solutions
_J. Electroanal. Chem._ 60 (1975) 335.

BCC-1598
E. Reiner, B. Krauthacker, V. Simeon and M. Skrinjarić-Spoljar
Institute for Medical Research, Yugoslav Academy of Sciences and Arts, Zagreb, Croatia, Yugoslavia
Mechanism of Inhibition in vitro of Mammalian Acetylcholinesterase and Cholinesterase in Solutions of O,O-Dimethyl 2,2,2-Trichloro-1-Hydroxyethyl Phosphate(Trichlorphon)

BCC-1599
S. Rendić, V. Šunjić, F. Kajfež, N. Blažević and T. Alebić-Kolbah
CRC, Compagnia di Ricerca Chimica, 6330 Chiasse, Switzerland and Institute of Organic Chemistry and Biochemistry, University of Zagreb, Zagreb, Yugoslavia
Resolution of (±)-α-(3-benzoylphenyl-)-propionic Acid (Ketoprofen) and Diastereomeric Interaction of its Enantiomers with Some Biological Systems
_Chimia_ 29 (1975) 170.

BCC-1600
S. Rendić, V. Šunjić, F. Kajfež, N. Blažević and P. Mildner
CRC, Compagnia di Ricerca Chimica S.A., Chiasse, Switzerland and Institut für organische Chemie und Biochemie, Universität Zagreb
_Biotransformation der 1,4-Benzodiazepine_ 
BCC-1601
A. Rubčić and G. Zerbi
University of Zagreb, Faculty of Science, Zagreb, Yugoslavia and Istituto di Chimica delle Macromolecole, CNR, Milan, Italy
**Dynamics of Structurally Disordered Poly(vinyl chloride)**

BCC-1602
A. Rubčić and G. Zerbi
Istituto di Chimica delle Macromolecole, CNR, Via Alfonso Corti 12, Milan, Italy
**Dynamics of Poly(vinyl chloride). II. Model with Conformational and Configurational Disorder**
Macromolecules 7 (1975) 759.

BCC-1603
I. Ružić and S. W. Felsberg
Department of Chemistry, Northwestern University, Evanston, Ill. 60201 (U.S.A.) and Division of Molecular Science, Department of Applied Science, Brookhaven National Laboratory, Upton, N. Y., 11973 (U.S.A.)
**Computer Simulation of Electrochemical Phenomena at the Dropping Mercury Electrode**

BCC-1604
I. Ružić and D. E. Smith
Department of Chemistry, Northwestern University, Evanston, Ill. 60201
**Reexamination of Experimental Data on the Time-Dependence of Alternating Current Polarographic Waves with Metal Ion-Metal Amalgam Redox Couples**

BCC-1605
I. Ružić and D. E. Smith
Department of Chemistry, Northwestern University, Evanston, Ill. 60201
**On the Influence of Coupled Homogeneous Redox Reactions on Electrode Processes in D. A. and A. C. Polarography. II. The E. E. Mechanism with a Coupled Homogeneous Redox Reaction**

BCC-1606
D. Sevdic, Lj. Jovanovac and H. Meider-Goričan
Institut »Ruder Bošković«, Zagreb, Jugoslawien
**Die Extraktion und Trennung von Mikromengen Silber(I) und Quecksilber(II) mit Makrocyclischen Polythioathern**

BCC-1607
S. L. Swartzen-A llen and E. Matijević
Institute of Colloid and Surface Science and Department of Chemistry, Clarkson College of Technology, Potsdam, New York 13676
**Colloid and Surface Properties of Clay Suspensions. II. Electrophoresis and Cation Adsorption of Montmorillonite**
J. Colloid Interface Sci. 50 (1975) 143.

BCC-1608
N. Stojanac, A. Sood, Z. Stojanac and Z. Valenta
Department of Chemistry, University of New Brunswick, Fredericton, New Brunswick E3B 5A3
**A Synthetic Approach to Quassin. Introduction of Functionality and Stereochemistry by a Diels-Alder Reaction**
BCC-1609
Z. Stojanac, R. A. Dickinson, N. Stojanac, R. J. Woznow and Z. Valenta
Department of Chemistry, University of New Brunswick, Fredericton, New Brunswick, E3B 5A3
Catalyzed Orientation Reversals in Diels-Alder Reactions

BCC-1610
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Department of Chemistry, University of Texas at El Paso, El Paso, Texas 79968 and Institute »Ruder Bošković«, P. O. Box 1016, Zagreb, Croatia, Yugoslavia
Kekulé Structures and Resonance Energies of Benzenoid Hydrocarbons

BCC-1611
M. Široki, Lj. Marić, Z. Štefanac and M. Herak
Laboratory of Analytical Chemistry, Faculty of Science, The University of Zagreb, (Yugoslavia)
Characterization of Complexes Involved in the Spectrophotometric Determination of Cobalt with 4-(2-Fyridylazo)Resorcinol

BCC-1612
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Institute for Medical Research and Occupation Health, Yugoslav Academy of Sciences and Arts, Zagreb, Yugoslavia
Autoradiographic Studies of 3H-Uridine Uptake by Human Cells in Tissue Culture Treated with Puromycin (Puro and Pan) and X-Radiation
Arh. Hig. Rada Toksikol. 26 (1975) 3.

BCC-1613
I. Šoštarić and Vl. Simen
Institut für Medizinforschung und Arbeitsmedizin, Jugoslawische Akademie der Wissenschaften und Künste, Zagreb, Kroatien, Jugoslawien
Die Stabilität der Kobalt(II)- und Kupfer(II)-Komplexe mit α-, β- und γ-Aminobutyrat

BCC-1614
B. Šrepel i D. Mijatović
Zavod za farmakognosiju, Farmaceutsko-biokemijski fakultet, Zagreb
Rezervni polisaharidi plodova roda Berberis
Arh. Hig. Rada Toksikol. 25 (1975) 189.

BCC-1615
V. Šunjić, J. Kufinec and F. Kajfež
CRC, Compagnia di Ricerca Chimica SA., Chiasso (Switzerland) Institute of Organic Chemistry and Biochemistry, University of Zagreb, and Institute for Drug Control, Zagreb (Yugoslavia)
Chiral 1,4-Benzodiazepine. VII. Cyclization Rates of 2-(N-α-ammuniumacyl)-amino-5-chloro-benzophenones in the Chiral 1,4-benzo­ diazepin-2-ones
BIBLIOGRAPHIA CHEMICA CROATICA

BCC-1616
B. Tamhina and M. J. Herak
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Spectrophotometric Determination of Vanadium(V) with 2-Carboxy-5-hydroxy-1-(4-tolyl)-4-pyridone

BCC-1617
B. Tamhina, M. J. Herak and V. Jagodić
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Spectrophotometric Determination of Molybdenum as a Mixed Thiocyanate-Mono(n-octyl)α-Anilinobenzylphosphonate Complex

BCC-1618
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Chemistry Department, State University of New York at Buffalo, Buffalo, New York 14214

The Seeded Growth of Calcium Phosphates. Surface Characterization and the Effect of Seed Material
J. Colloid Interface Sci. 50 (1975) 451.

BCC-1619
Lj. Tušek, P. R. Danesi and R. Chiarizia
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A Cyclic Polyether Suitable for Alkali Cations Solvent Extraction Procedures

BCC-1620
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Cyclic Chronopotentiometry of Nickel(II) at Mercury Electrodes in Acidic Perchlorate Solutions: Case of Higher Order Nonregenerative Reactions Following Electron Transfer

BCC-1621
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Synthesis and Characterization of Optically Active Poly(2-Phenylvinyl Alkyl Ethers) and Corresponding Monomers

BCC-1622
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Graph Theory and Molecular Orbitals. XI. Aromatic Substitution
Tetrahedron 31 (1975) 147.

BCC-1623
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Determination of 2-Ethylisonicotinaldehyde Thiosemicarbazone in Biological Material
BCC-1624

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On Conjugated Molecules with Identical Topological Spectra