DCC-48 (Univ. Zagreb)

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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.

A part of this work was published in *Intern. J. Quantum Chem.* 7 (1973) 233, *Annales de la Société Scientifique de Bruxelles* **89**, II (1975) 252 and *Intern. J. Quantum Chem.* 9 (1975) 243.

Examiners: Prof. Z. B. Maksić, Prof. N. Trinajstić and Dr. A. Ažman

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DDC-48 (Univ. Zagreb)

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

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II. Institute »Ruđer Bošković«, P. O. B. 1016, 41001 Zagreb, Croatia, Yugoslavia

Crystal Hartree-Fock calculations, the Fourier transforms of lattice sums over Slater-type orbitals
Theta functions, numerical transforms integrations
Simple-cubic crystals, 1s, 2s, 2p, 3s, 3p, 3d Slater-type orbitals
Generalization for orbitals of higher quantum numbers, a relationship between molecular and crystal quantities

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BCC-1556

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BCC-1557

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Chemisches Institut, Pharmazeutisch-Biochemische Fakultät, Universität Zagreb

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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)

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BCC-1559

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Int. J. Quantum Chem. **9** (1975) 243.

BCC-1560

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University of Zagreb, Pharmaceutico-Biochemical Faculty, Institute of Chemistry A. Kovačića 1, Zagreb

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Mikrochim. Acta (1975) 253.

BCC-1561

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Institut für Chemie, Pharmazeutisch-Biochemische Fakultät der Universität Zagreb, 41000 Zagreb, A Kovačića 1, Jugoslawien

Beiträge zur Ringofenmethodik. XIV. Komplexbildung mit einem Fällungsreagens auf Kapillarträgern

Mikrochim. Acta (1975) 425.

BCC-1562

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Chemisches Institut, Pharmazeutisch-Biochemische Fakultät, Universität Zagreb

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BCC-1563

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BCC-1564

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BCC-1565

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BCC-1566

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Mikrochim. Acta (1975) 213.

BCC-1568

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BCC-1570

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The Lilly Research Laboratories, Eli Lilly and Company, Indianapolis, Indiana 46206

The Oxoazetidinesulphenic Acid Anion: s- vs O-Alkylation

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BCC-1573

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BCC-1575

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Tetrahedron Lett. (1975) 101.

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BCC-1579

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BCC-1580

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BCC-1581

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BCC-1583

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Department of Chemistry, Georgetown University, Washington DC 20057

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Inorg. Chim. Acta **12** (1975) L16

BCC-1585

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BCC-1586

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Laboratory of Inorganic Chemistry, Faculty of Technology, University of Zagreb, POB 179, 41001 Zagreb, Croatia, Yugoslavia

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Institute of Organic Chemistry and Biochemistry, University of Zagreb, Strossmayerov trg 14, 41000 Zagreb, Croatia, Yugoslavia

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Tetrahedron Lett. (1975) 799.

BCC-1590

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

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BCC-1591

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Max-Planck-Institut für Metallforschung, Stuttgart (Bundesrepublik Deutschland)

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Faculty of Technology and Metallurgy, University of Skopje, Skopje, Yugoslavia and Research and Development Institute INA, Zagreb, Yugoslavia

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BCC-1593

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Department of Chemistry, Tufts University, Medford, Massachusetts 02155

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BCC-1594

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Department of Chemistry, Harvard University, Cambridge, MA. 02138, U.S.A.

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BCC-1595

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Center for Marine Research, »Ruđer Bošković«, Institute, Zagreb, Croatia, (Yugoslavia)

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»Ruđer Bošković« Institute, Center for Marine Research, Zagreb, Croatia, Yugoslavia

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

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CRC, Compagnia di Ricerca Chimica, 6830 Chiasso, Switzerland and Institute of Organic Chemistry and Biochemistry, University of Zagreb, Zagreb, Yugoslavia

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Acta Pharm. Jugoslav. **25** (1975) 135.

BCC-1601

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University of Zagreb, Faculty of Science, Zagreb, Jugoslavia and Istituto di Chimica delle Macromolecole, CNR, Milan, Italy

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Istituto di Chimica delle Macromolecole, CNR, Via Alfonso Corti 12, Milan, Italy

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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.)

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Department of Chemistry, Northwestern University, Evanston, Ill. 60201

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Institut »Ruđer Bošković«, Zagreb, Jugoslawien

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Institute of Colloid and Surface Science and Department of Chemistry, Clarkson College of Technology, Potsdam, New York 13676

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Department of Chemistry, University of Texas at El Paso, El Paso, Texas 79968 and Institute »Ruđer Bošković«, P. O. Box 1016, Zagreb, Croatia, Yugoslavia

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Laboratory of Analytical Chemistry, Faculty of Science, The University of Zagreb, ((Yugoslavia)

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BCC-1612

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

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Institut für Medizinforschung und Arbeitsmedizin. Jugoslawische Akademie der Wissenschaften und Künste, Zagreb, Kroatien, Jugoslawien

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Zavod za farmakognoziju, Farmaceutsko-biokemijski fakultet, Zagreb

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Laboratory of Analytical Chemistry, Faculty of Science and Institute of Inorganic and Analytical Chemistry University of Zagreb, Yugoslavia

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BCC-1617

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J. Colloid Interface Sci. **50** (1975) 451.

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Cornell University, Department of Chemistry, Ithaca, N. Y., 14850, U.S.A. and Institute »Ruđer Bošković«, P.O.B. 1016, 41001 Zagreb, and Chemistry Department, Faculty of Science and Mathematics, University of Zagreb, Zagreb, Croatia, Yugoslavia

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Institute of Medicinal Biochemistry, Faculty of Pharmacy and Biochemistry, University of Zagreb

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