

## Contents

### Editorial foreword

1.	Maximum Entropy charge density studies: Bayesian viewpoint and test applications Pietro Roversi, John J. Irwin, Gérard Bricogne	1
2.	Reliability of charge density distributions derived by the Maximum Entropy method Bo Brummerstedt Iversen	27
3.	Maximum entropy reconstruction of spin densities involving non-uniform prior J. Schweizer, R.J. Papoulier, E. Ressouche, F. Tasset and A.I. Zheludev	37
4.	Transferability, adjustability, and additivity of fuzzy electron density fragments Paul G. Mezey	45
5.	Beyond the local-density approximation in calculations of Compton profiles Yasunori Kubo	71
6.	Interaction energy and density in the water dimer. A quantum theory of atoms in molecules: insight on the effect of basis set superposition error removal Carlo Gatti and Antonino Famulari	93
7.	Topological analysis of X-ray protein relative density maps utilizing the eigenvector following method Kenneth E. Edgecombe, Alan Ableson, Kim Baxter, Antony Chiverton, Janice Glasgow and Suzanne Fortier	115
8.	The number of independent parameters defining a projector: proof in matrix representation and resolution of previously conflicting arguments Arnaud J.A. Soirat and Lou Massa	127
9.	Kinetic equation, optical potential, tensor theory and structure factor refinement in high-energy electron diffraction Lian-Mao Peng	147

vi *Contents*

10.	'Compton microscope effect'? : image of intra-unit-cell atom theoretically observed in Compton $B(\mathbf{r})$ -function Teiji Kobayashi	169
11.	New light on electron correlation in simple metals: inelastic X-ray scattering results vs. current theoretical treatment A. Kaprolat, K. Höppner, Ch. Sternemann and W. Schülke	179
12.	The measurement of spectral momentum densities of solids by electron momentum spectroscopy Maarten Vos and Erich Weigold	195
13.	Accurate structure factor determination using 100 keV synchrotron radiation T. Lippmann, D. Waasmeier, A. Kirfel and J.R. Schneider	209
14.	Charge density data from CCD detectors A. Alan Pinkerton	213
15.	Recent studies in magnetisation densities E. Lelièvre-Berna	225
16.	Magnetisation densities and polarised neutron diffraction: optimised flipping ratio measurements E. Lelièvre-Berna, M. Portes de Albuquerque, F. Tasset and P.J. Brown	235
17.	Concerning the magnetisation density in magnetic neutron scattering experiments Dylan Jayatilaka	245
18.	A wave function for beryllium from X-ray diffraction data Dylan Jayatilaka	253
19.	Spin density in interacting nitronyl nitroxide radicals Y. Pontillon, A. Caneschi, D. Gatteschi, E. Ressouche, F. Romero, J. Schweizer, R. Sessoli and R. Ziessel	265
20.	Electrostatic potential of a new angiotensin II receptor antagonist from X-ray diffraction and <i>ab initio</i> calculations Raffaella Soave, Riccardo Destro, Laura Belvisi and Carlo Scolastico	275
21.	Hat matrix and leverages in charge density refinements: example of atomic net charges determination in a natural zeolite, the scolecite Sandrine Kuntzinger, Nour Eddine Ghermani, Claude Lecomte and Yves Dusausoy	285

22.	The $\beta$ decay in anapole crystal Liu Xiaodong	301
23.	Three-dimensional reconstruction of electron momentum densities and occupation number densities of Cu and CuAl alloys G. Döring, K. Höppner, A. Kaprolat and W. Schülke	303
24.	X-ray and neutron studies of <i>cis</i> -enol systems at liquid helium temperatures Georg K.H. Madsen and Claire Wilson	313
25.	Effect of pressure on the Compton scattering of metallic Li Gendo Oomi, Fuminori Honda, Tomoko Kagayama, Fumitake Itoh, Hiroshi Sakurai, Hiroshi Kawata and Osamu Shimomura	323
26.	Magnetic Compton profile in uranium chalcogenide compounds UX (X = Se, Te) F. Itoh, H. Hashimoto, H. Sakurai, A. Ochiai, H. Aoki and T. Suzuki	327