

Editorial

Current Density and Spectroscopy—A Themed Issue in Honor of Professor Riccardo Zanasi on the Occasion of His 70th Birthday

 Andrea Peluso * and Guglielmo Monaco * 

Dipartimento di Chimica e Biologia Adolfo Zambelli, Università di Salerno, Via Giovanni Paolo II, 132, I-84084 Fisciano, SA, Italy

* Correspondence: apeluso@unisa.it (A.P.); gmonaco@unisa.it (G.M.)

It is our great pleasure to introduce the *Festschrift* of *Chemistry* to honor Professor Riccardo Zanasi (Figure 1) on the occasion of his 70th birthday and to recognize his important contributions to quantum chemistry, particularly in the field of magnetic response and chiroptical spectroscopies.



Figure 1. Professor Riccardo Zanasi.

Riccardo was born in Vignola, Italy, in 1951. He graduated in Chemistry with honors at the University of Modena and Reggio Emilia in 1975, under the supervision of Prof. Paolo Lazzeretti, with whom he acknowledges a lifelong collaboration. Assistant Professor in Physical Chemistry in Modena since 1981, he then became Associate Professor in Salerno in 1998, where he became full Professor in 2002.

He has worked with many distinguished theoretical chemists (Amos, Buckingham, Sadlej, Stephens, to cite a few, and a special mention should be given to the many collaborations with Prof. PW Fowler), but he has also collaborated with experimentalists, especially in the field of chiroptical spectroscopies. His most known contributions are related to the development and the implementation of methods to compute, visualize, and manipulate the magnetically induced current density, which ended up in the SYSMO [1] and SYSMOIC [2] packages. The former is widely used in literature in the field of magnetic aromaticity, and the latter has recently been recognized as a useful tool to develop new methods [3].

This issue is composed of seventeen papers authored by scholars from twelve countries.

The topic common to most of the papers is the discussion of aromaticity, especially from the magnetic point of view, of well-known and novel molecules, either in their ground state (coronene and corannulene [4], metallacyclopentadienes [5], cycloporphyrin nanorings [6], Li_3B_2^- and Li_4B_2 clusters enclosing a B2 unit [7], pentagonal-pyramidal hexamethylbenzene dication [8], heterocirculenes [9], starphenes [10], and Si_3C_5 and Si_4C_8 clusters [11]) or in their excited triplet state [12].



Citation: Peluso, A.; Monaco, G. Current Density and Spectroscopy—A Themed Issue in Honor of Professor Riccardo Zanasi on the Occasion of His 70th Birthday. *Chemistry* **2022**, *4*, 118–120. <https://doi.org/10.3390/chemistry4010010>

Received: 22 February 2022

Accepted: 22 February 2022

Published: 23 February 2022

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



Copyright: © 2022 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

Other papers present theoretical and methodological advances in the calculation of the magnetic response: a topological analysis of the magnetically induced current density in strong magnetic fields [13], the partitioning of Hückel–London currents into cycle contributions [14], and decomposition in spatial contributions to ^1H NMR chemical shifts [15].

A third set of papers is connected with chiroptical spectroscopies, either experimentally or theoretically: a report of a chirality transfer in a calixarene-based pseudorotaxane [16], a test of photoelectron circular dichroism as a probe for chirality [17], and a theoretical scrutiny of the electronic currents and anapolar response induced in molecules by monochromatic light [18].

Two more papers, one on the role of spin density in the nitration of aromatic compounds [19], the other on the absorption and isomerization of azobenzene in polymeric nanoporous crystalline phases [20], have been contributed by the Department of Chemistry, where Riccardo's good mood helped in pursuing collaborations and promoting new fields of research [21].

For us, having known him in Salerno for a couple of decades, Riccardo has been a source of cheerfulness and enthusiasm in approaching research and many aspects of life. We recall him playing the guitar in classroom to introduce the wave equation, organizing small mountaineering excursions, commenting on sports, music, and politics, and sharing good occasions for a glass of wine or good cuisine. As his retirement from the department has concerned only the teaching and the administrative part, Riccardo is actively pursuing his research, and we wish him a long continuation of his activity.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Lazzeretti, P.; Malagoli, M.; Zanasi, R. *SYSMO Package; Research Report 1/67 on Project "Sistemi Informatici e Calcolo Parallelo"*; CNR: Rome, Italy, 1991.
2. Monaco, G.; Summa, F.F.; Zanasi, R. Program Package for the Calculation of Origin-Independent Electron Current Density and Derived Magnetic Properties in Molecular Systems. *J. Chem. Inf. Model.* **2021**, *61*, 270–283. [[CrossRef](#)] [[PubMed](#)]
3. Gershoni-Poranne, R.; Stanger, A. Magnetic Criteria of Aromaticity. *Chem. Soc. Rev.* **2015**, *44*, 6597–6615. [[CrossRef](#)] [[PubMed](#)]
4. Karadakov, P.B. Magnetic Shielding Study of Bonding and Aromaticity in Corannulene and Coronene. *Chemistry* **2021**, *3*, 861–872. [[CrossRef](#)]
5. Casiano-González, R.; Barquera-Lozada, J.E. Are Metallacyclopentadienes Always Non-Aromatic? *Chemistry* **2021**, *3*, 1302–1313. [[CrossRef](#)]
6. Landi, A.; Summa, F.F.; Monaco, G. Magnetic Aromaticity of Cycloporphyrin Nanorings. *Chemistry* **2021**, *3*, 991–1004. [[CrossRef](#)]
7. Đorđević, S.; Radenković, S. The B2 Structural Motif as a Tool for Modulating Ring Currents in Monocyclic Li Clusters. *Chemistry* **2021**, *3*, 1063–1073. [[CrossRef](#)]
8. MacLeod-Carey, D.; Muñoz-Castro, A. On the Aromaticity and ^{13}C -NMR Pattern of Pentagonal-Pyramidal Hexamethylbenzene Dication $[\text{C}_6(\text{CH}_3)_6]^{2+}$: A $[\text{C}_5(\text{CH}_3)_5]^-$ - $[\text{CCH}_3]^{3+}$ Aggregate. *Chemistry* **2021**, *3*, 1363–1370. [[CrossRef](#)]
9. Karaush-Karmazin, N.N.; Baryshnikov, G.V.; Minaev, B.F. Aromaticity of Heterocirculenes. *Chemistry* **2021**, *3*, 1411–1436. [[CrossRef](#)]
10. Orozco-Ic, M.; Merino, G. The Magnetic Response of Starphenes. *Chemistry* **2021**, *3*, 1381–1391. [[CrossRef](#)]
11. Torres-Vega, J.J.; Alcoba, D.R.; Oña, O.B.; Vásquez-Espinal, A.; Báez-Grez, R.; Lain, L.; Torre, A.; García, V.; Tiznado, W. Analysis of Local and Global Aromaticity in Si_3C_5 and Si_4C_8 Clusters. Aromatic Species Containing Planar Tetracoordinate Carbon. *Chemistry* **2021**, *3*, 1101–1112. [[CrossRef](#)]
12. Stojanović, M.; Aleksić, J.; Baranac-Stojanović, M. Singlet/Triplet State Anti/Aromaticity of Cyclopentadienyl Cation: Sensitivity to Substituent Effect. *Chemistry* **2021**, *3*, 765–782. [[CrossRef](#)]
13. Irons, T.J.P.; Garner, A.; Teale, A.M. Topological Analysis of Magnetically Induced Current Densities in Strong Magnetic Fields Using Stagnation Graphs. *Chemistry* **2021**, *3*, 916–934. [[CrossRef](#)]
14. Myrvold, W.; Fowler, P.W.; Clarke, J. Partitioning Hückel–London Currents into Cycle Contributions. *Chemistry* **2021**, *3*, 1138–1156. [[CrossRef](#)]
15. Fliegl, H.; Dimitrova, M.; Berger, R.J.F.; Sundholm, D. Spatial Contributions to ^1H NMR Chemical Shifts of Free-Base Porphyrinoids. *Chemistry* **2021**, *3*, 1005–1021. [[CrossRef](#)]
16. Concilio, G.; Gaeta, C.; Della Sala, P.D.; Iuliano, V.; Talotta, C.; Monaco, G.; Superchi, S.; Belviso, S.; Neri, P. Chirality Transfer in a Calixarene-Based Directional Pseudorotaxane Complex. *Chemistry* **2021**, *3*, 1089–1100. [[CrossRef](#)]
17. Declava, P. Photoelectron Circular Dichroism as a Probe of Chiral Hydrocarbons. *Chemistry* **2022**, *4*, 31–41. [[CrossRef](#)]

18. Summa, F.F.; Lazzeretti, P. Electronic Currents and Anapolar Response Induced in Molecules by Monochromatic Light. *Chemistry* **2021**, *3*, 1022–1036. [[CrossRef](#)]
19. Capobianco, A.; Landi, A.; Peluso, A. Is Aromatic Nitration Spin Density Driven? *Chemistry* **2021**, *3*, 1286–1301. [[CrossRef](#)]
20. Coscia, N.; Cozzolino, A.; Golla, M.; Rizzo, P. Absorption and Isomerization of Azobenzene Guest Molecules in Polymeric Nanoporous Crystalline Phases. *Chemistry* **2021**, *3*, 1074–1088. [[CrossRef](#)]
21. Pironti, C.; Ricciardi, M.; Motta, O.; Camin, F.; Bontempo, L.; Proto, A. Application of ¹³C Quantitative NMR Spectroscopy to Isotopic Analyses for Vanillin Authentication Source. *Foods* **2021**, *10*, 2635. [[CrossRef](#)] [[PubMed](#)]