# Riccardo Zanasi

List of Publications by Year
in descending order

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|---|---|---|---|
| 209 papers | 6,669 citations | 53660 45 h-index | 91712 69 g-index |
| 224 all docs | 224 docs citations | 224 times ranked | 2310 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Dynamic toroidizability as ubiquitous property of atoms and molecules in optical electric fields. Journal of Chemical Physics, 2022, 156, 054106. | 1.2 | 6 |
| 2 | Origin independent current density vector fields induced by time-dependent magnetic field. I. The LiH molecule. Journal of Chemical Physics, 2022, 156, 154105. | 1.2 | 6 |
| 3 | Magnetic Characterization of the Infinitene Molecule. Journal of Physical Chemistry A, 2022, 126, 3717-3723. | 1.1 | 14 |
| 4 | Program Package for the Calculation of Origin-Independent Electron Current Density and Derived Magnetic Properties in Molecular Systems. Journal of Chemical Information and Modeling, 2021, 61, 270-283. | 2.5 | 47 |
| 5 | Assessment of the performance of DFT functionals in the fulfillment of off-diagonal hypervirial relationships. Physical Chemistry Chemical Physics, 2021, 23, 15268-15274. | 1.3 | 13 |
| 6 | Electronic Currents Induced by Optical Fields and Rotatory Power Density in Chiral Molecules. Molecules, 2021, 26, 4195. | 1.7 | 8 |
| 7 | Origin-Independent Densities of Static and Dynamic Molecular Polarizabilities. Journal of Physical Chemistry Letters, 2021, 12, 8855-8864. | 2.1 | 5 |
| 8 | Decomposition of Molecular Integrals into Atomic Contributions via Becke Partitioning Scheme: a Caveat. Croatica Chemica Acta, 2021, 94, . | 0.1 | 2 |
| 9 | NICSâ€‹XYâ€‹Scan Predictions of Local, Semiâ€‹Global, and Global Ring Currents in Annulated Pentalene and sâ€‹ndacene Cores Compared to Firstâ€‹Principles Current Density Maps. ChemPhysChem, 2020, 21, 65-82. | 1.0 | 26 |
| 10 | The molecular electronic structure revealed by the magnetically induced Lorentz force density. Journal of Chemical Physics, 2020, 153, 104114. | 1.2 | 2 |
| 11 | Disentangling the Contributions to the Proton Magnetic Shielding in Carbon Nanohoops and Nanobelts: Evidence for a Paratropic Belt-Current. Journal of Physical Chemistry Letters, 2020, 11, 7489-7494. | 2.1 | 7 |
| 12 | On the topology of total and diamagnetic induced electronic currents in molecules. Journal of Chemical Physics, 2020, 152, 194101. | 1.2 | 8 |
| 13 | Reversal of Clar's Aromaticâ€‹extet Rule in Ultrashort Singleâ€‹ndâ€‹Capped [5,5] Carbon Nanotubes. ChemistryOpen, 2020, 9, 616-622. | 0.9 | 4 |
| 14 | Design of annulene-within-an-annulene systems by the altanisation approach. A study of altan-[n]annulenes. Physical Chemistry Chemical Physics, 2020, 22, 5476-5486. | 1.3 | 4 |
| 15 | Atomic size adjusted calculation of the magnetically induced current density. Chemical Physics Letters, 2020, 745, 137281. | 1.2 | 10 |
| 16 | Magnetically Induced Current Density Spatial Domains. Journal of Physical Chemistry A, 2019, 123, 1558-1569. | 1.1 | 13 |
| 17 | Delocalization energy retrieved from the current density tensor. Physical Chemistry Chemical Physics, 2019, 21, 11564-11568. | 1.3 | 10 |
| 18 | AACID: Anisotropy of the Asymmetric Magnetically Induced Current Density Tensor. Journal of Physical Chemistry A, 2018, 122, 4681-4686. | 1.1 | 12 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Field-independent current strength. Theoretical Chemistry Accounts, 2018, 137, 1. | 0.5 | 2 |
| 20 | Absolute Configuration Assignment of Chiral Resorcin[4]arenes from ECD Spectra. Journal of Organic Chemistry, 2017, 82, 202-210. | 1.7 | 5 |
| 21 | Model-averaging of ab initio spectra for the absolute configuration assignment via vibrational circular dichroism. Physical Chemistry Chemical Physics, 2017, 19, 28028-28036. | 1.3 | 10 |
| 22 | Analysis of the Nucleus-Independent Chemical Shifts of [10]Cyclophenacene: Is It an Aromatic or Antiaromatic Molecule?. Journal of Physical Chemistry Letters, 2017, 8, 4673-4678. | 2.1 | 23 |
| 23 | Determination of the absolute configuration of a novel tetrasubstituted isoindolinone by vibrational circular dichroism. Journal of Pharmaceutical and Biomedical Analysis, 2017, 144, 52-58. | 1.4 | 5 |
| 24 | The intriguing class of altanâ€molecules. Journal of Physical Organic Chemistry, 2016, 29, 793-798. | 0.9 | 7 |
| 25 | Absolute Configuration Assignment of a Paraconic Acid Derivative via Vibrational Circular Dichroism Spectroscopy and Density Functional Theory Calculation. Chirality, 2016, 28, 110-115. | 1.3 | 4 |
| 26 | The making of ring currents. Physical Chemistry Chemical Physics, 2016, 18, 11800-11812. | 1.3 | 19 |
| 27 | Stoppedâ€Flow Enantioselective HPLCâ€CD Analysis and TDâ€DFT Stereochemical Characterization of Methyl Transâ€3â€(3,4â€Dimethoxyphenyl)Glycidate. Chirality, 2015, 27, 914-918. | 1.3 | 6 |
| 28 | Hydrogenâ€“hydrogen bonding: The current density perspective. Journal of Computational Chemistry, 2015, 36, 707-716. | 1.5 | 19 |
| 29 | Topology of the magnetically induced current density and proton magnetic shielding in hydrogen bonded systems. Physical Chemistry Chemical Physics, 2015, 17, 5966-5972. | 1.3 | 19 |
| 30 | Characterization of the species-dependent ketoprofen/albumin binding modes by induced CD spectroscopy and TD-DFT calculations. Journal of Pharmaceutical and Biomedical Analysis, 2015, 112, 176-180. | 1.4 | 11 |
| 31 | Short-Range Solvation Effects on Chiroptical Properties: A Time-Dependent Density Functional Theory and ab Initio Molecular Dynamics Computational Case Study on Austdiol. Journal of Physical Chemistry A, 2014, 118, 11751-11757. | 1.1 | 7 |
| 32 | Stereochemical and conformational study on fenoterol by ECD spectroscopy and TD-DFT calculations. Journal of Pharmaceutical and Biomedical Analysis, 2014, 91, 92-96. | 1.4 | 4 |
| 33 | Cationic half-sandwich quinolinophaneoxazoline-based (Î·<sup>6</sup>-p-cymene)ruthenium(<scp>ii</scp>) complexes exhibiting different chirality types: synthesis and structural determination by complementary spectroscopic methods. Dalton Transactions, 2014, 43, 1636-1650. | 1.6 | 6 |
| 34 | Delocalized Currents without a Ring of Bonded Atoms: Strong Delocalized Electron Currents Induced by Magnetic Fields in Noncyclic Molecules. Journal of Physical Chemistry A, 2014, 118, 3367-3375. | 1.1 | 14 |
| 35 | Assessment of Ring Current Models for Monocycles. Journal of Physical Chemistry A, 2014, 118, 1673-1683. | 1.1 | 46 |
| 36 | Mycoleptones Aâ€“C and Polyketides from the Endophyte Mycoleptodiscus indicus. Journal of Natural Products, 2014, 77, 70-78. | 1.5 | 30 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | Additivity of current density patterns in altanâ€molecules. Journal of Physical Organic Chemistry, 2013, 26, 109-114. | 0.9 | 16 |
| 38 | Investigation of the p-coronene series in the context of the â€˜annulene-within-an-annuleneâ€™ model by means of ipso-centric ab initio calculations of Ï€-electron currents. Physical Chemistry Chemical Physics, 2013, 15, 17654. | 1.3 | 12 |
| 39 | Absolute configuration assignment made easier by the VCD of coupled oscillating carbonyls: the case 2013, 54, 6242-6246. | 0.7 | 23 |
| 40 | Chiral Triazole Fungicide Difenoconazole: Absolute Stereochemistry, Stereoselective Bioactivity, Aquatic Toxicity, and Environmental Behavior in Vegetables and Soil. Environmental Science & Technology, 2013, 47, 3386-3394. | 4.6 | 218 |
| 41 | Linearized ring current models for the retrieval of Ï€ ring current strength in monocycles. Chemical Physics Letters, 2013, 588, 247-252. | 1.2 | 7 |
| 42 | Anionic derivatives of altanâ€corannulene. Journal of Physical Organic Chemistry, 2013, 26, 730-736. | 0.9 | 15 |
| 43 | Beyond NICS. AIP Conference Proceedings, 2012, , . | 0.3 | 11 |
| 44 | Three Contra-Rotating Currents from a Rational Design of Polycyclic Aromatic Hydrocarbons: altan-Corannulene and altan-Coronene. Journal of Physical Chemistry A, 2012, 116, 9020-9026. | 1.1 | 24 |
| 45 | Conformational Flexibility and Absolute Stereochemistry of (3R)â€3â€hydroxyâ€4â€arylâ€Î²â€lactams Investigated by Chiroptical Properties and TDâ€DFT Calculations. Chirality, 2012, 24, 741-750. | 1.3 | 6 |
| 46 | Stereochemical characterization of fluorinated 2-(phenanthren-1-yl)propionic acids by enantioselective high performance liquid chromatography analysis and electronic circular dichroism detection. Journal of Chromatography A, 2012, 1232, 128-133. | 1.8 | 4 |
| 47 | Beyond NICS: estimation of the magnetotropicity of inorganic unsaturated planar rings. Physical Chemistry Chemical Physics, 2011, 13, 20666. | 1.3 | 58 |
| 48 | Magnetic-field induced electronic anapoles in small molecules. Rendiconti Lincei, 2011, 22, 105-112. | 1.0 | 24 |
| 49 | Searching for a good candidate to perform a chiral nuclear magnetic resonance experiment in disordered phase: A study of 8,9â€difluoroâ€Pâ€hexahelicene. Chirality, 2011, 23, 752-755. | 1.3 | 11 |
| 50 | Absolute configuration assignment of (3â€phenyloxiraneâ€2,2â€diyl)bis(phenylmethanone) via density functional calculations of optical rotation and vibrational circular dichroism. Chirality, 2010, 22, E130-5. | 1.3 | 5 |
| 51 | Absolute Configuration Assignment of Norcamphor-Derived Furyl Hydroperoxide Using Density Functional Theory Calculations of Optical Rotation and Vibrational Circular Dichroism. Journal of Organic Chemistry, 2010, 75, 2179-2188. | 1.7 | 13 |
| 52 | Absolute Configuration through the DFT Simulation of the Optical Rotation. Importance of the Correct Selection of the Input Geometry: A Caveat. Journal of Organic Chemistry, 2010, 75, 4600-4603. | 1.7 | 28 |
| 53 | Relative Weights of Ïƒ and Ï€ Ring Currents in a Few Simple Monocycles. Journal of Chemical Theory and Computation, 2010, 6, 3343-3351. | 2.3 | 82 |
| 54 | Ring Current Model and Anisotropic Magnetic Response of Cyclopropane. Journal of Chemical Theory and Computation, 2010, 6, 2002-2018. | 2.3 | 62 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | Absolute Configuration Assignment of Inherently Chiral Calix[4]arenes using DFT Calculations of Chiroptical Properties. Organic Letters, 2010, 12, 2912-2915. | 2.4 | 33 |
| 56 | On the additivity of current density in polycyclic aromatic hydrocarbons. Journal of Chemical Physics, 2009, 131, 044126. | 1.2 | 31 |
| 57 | Topological models of magnetic field induced current density field in small molecules. Theoretical Chemistry Accounts, 2009, 123, 353-364. | 0.5 | 29 |
| 58 | On the analysis of some orbital contributions to the current density in circulenes. International Journal of Quantum Chemistry, 2009, 109, 243-249. | 1.0 | 11 |
| 59 | Induced Orbital Paramagnetism and Paratropism in Closed-Shell Molecules. Journal of Physical Chemistry A, 2009, 113, 14465-14479. | 1.1 | 20 |
| 60 | Quantitative Indicators of Bond Current Susceptibility. , 2009, , . | | 16 |
| 61 | Response tensors for chiral discrimination in NMR spectroscopy. Theoretical Chemistry Accounts, 2008, 119, 99-106. | 0.5 | 22 |
| 62 | Magnetic Euripi in Corannulene. Journal of Physical Chemistry A, 2008, 112, 8136-8147. | 1.1 | 34 |
| 63 | Assessment of Ïƒ-Diatropicity of the Cyclopropane Molecule. Journal of Physical Chemistry A, 2007, 111, 8163-8169. | 1.1 | 67 |
| 64 | Spatial Ring Current Model of the [2.2]Paracyclophane Molecule. Journal of Physical Chemistry A, 2007, 111, 3110-3123. | 1.1 | 25 |
| 65 | Nuclear Magnetoelectric Shieldings for Chiral Discrimination in NMR Spectroscopy. Theoretical Study of (R<sub>a</sub>)-1,3-Dimethylallene, (2R)-2-Methyloxirane, and (2R)-N-Methyloxaziridine Molecules. Journal of Chemical Theory and Computation, 2007, 3, 1691-1698. | 2.3 | 14 |
| 66 | Analysis of Some Orbital Contributions to the Current Density in Circulenes. AIP Conference Proceedings, 2007, , . | 0.3 | 5 |
| 67 | Designing Paramagnetic Circulenes. Angewandte Chemie - International Edition, 2007, 46, 1889-1892. | 7.2 | 36 |
| 68 | Chiral discrimination via nuclear magnetic shielding polarisabilities from NMR spectroscopy: Theoretical study of (Ra)-1,3-dimethylallene, (2R)-2-methyloxirane, and (2R)-N-methyloxaziridine. Journal of Computational Chemistry, 2007, 28, 2159-2163. | 1.5 | 22 |
| 69 | Designing Ring-Current Patterns:Â [10,5]-Coronene, a Circulene with Inverted Rim and Hub Currents. Journal of Physical Chemistry A, 2006, 110, 7447-7452. | 1.1 | 45 |
| 70 | Determination of 13C/12C Carbon Isotope Ratio. Analytical Chemistry, 2006, 78, 3080-3083. | 3.2 | 19 |
| 71 | Invariance of magnetic-field induced current density to a continuous transformation of the origin of the coordinate system. Chemical Physics Letters, 2006, 421, 21-26. | 1.2 | 19 |
| 72 | Efficient mapping ofÂring currents inÂfullerenes andÂother curved carbon networks. Comptes Rendus Chimie, 2006, 9, 1085-1093. | 0.2 | 17 |

| # | Article | IF | Citations |
|---|---|---|---|
| 73 | Topology of magnetic-field-induced current-density field in diatropic monocyclic molecules. Physical Review A, 2006, 74, . | 1.0 | 59 |
| 74 | Ring-current signatures in shielding-density maps. Chemical Physics Letters, 2005, 401, 164-169. | 1.2 | 58 |
| 75 | The Importance of Molecular Vibrations: The Sign Change of the Optical Rotation of Methyloxirane. Angewandte Chemie - International Edition, 2005, 44, 3594-3596. | 7.2 | 98 |
| 76 | Why Downfield Proton Chemical Shifts Are Not Reliable Aromaticity Indicators. Organic Letters, 2005, 7, 3457-3460. | 2.4 | 78 |
| 77 | Ab Initio Calculation of Optical Rotatory Dispersion (ORD) Curves:Â A Simple and Reliable Approach to the Assignment of the Molecular Absolute Configuration. Journal of the American Chemical Society, 2004, 126, 12968-12976. | 6.6 | 118 |
| 78 | Ring Currents and Magnetic Properties of C48N12 Dodecaaza[60-S6]fullerenes. ChemInform, 2004, 35, no. | 0.1 | 0 |
| 79 | Understanding proton magnetic shielding in the benzene molecule. Chemical Physics Letters, 2004, 390, 268-271. | 1.2 | 38 |
| 80 | Ring currents and magnetic properties of C48N12dodecaaza[60-S6]fullerenes. Physical Chemistry Chemical Physics, 2004, 6, 295-302. | 1.3 | 7 |
| 81 | Local Aromaticity of the Six-Membered Rings in Pyracylene. A Difficult Case for the NICS Indicator of Aromaticity. Journal of Organic Chemistry, 2004, 69, 7537-7542. | 1.7 | 113 |
| 82 | Time Dependent Density Functional Response Theory Calculation of Optical Rotation as a Method for the Assignment of Absolute Configuration of Camphor-Derived Furyl Hydroperoxide and Alcohol. Journal of Physical Chemistry A, 2004, 108, 10749-10753. | 1.1 | 19 |
| 83 | Are Ring Currents Still Useful to Rationalize the Benzene Proton Magnetic Shielding?. Organic Letters, 2004, 6, 2265-2267. | 2.4 | 87 |
| 84 | Calculation of the gas phase specific rotation of (S)-propylene oxide at 355 nm. Chemical Physics Letters, 2003, 376, 452-456. | 1.2 | 45 |
| 85 | Assignment of the Molecular Absolute Configuration through the ab Initio Hartreeâ˜Fock Calculation of the Optical Rotation:Â Can the Circular Dichroism Data Help in Reducing Basis Set Requirements?â€. Journal of Organic Chemistry, 2003, 68, 5186-5192. | 1.7 | 49 |
| 86 | Structure, ring currents and magnetic properties of 12b,12d,12f-triaza-12c,12e,12g-tribora-coronene. Chemical Physics Letters, 2002, 355, 471-477. | 1.2 | 17 |
| 87 | Parity-violating effects in asymmetric chemical reactions:â€, A theoretical study on the CHFClBr molecule. Physical Review E, 2000, 62, 8395-8399. | 0.8 | 19 |
| 88 | Theoretical determination of parity-violating vibrational frequency differences between the enantiomers of the CHFClBr molecule. Physical Review A, 2000, 62, . | 1.0 | 33 |
| 89 | Energetic stabilization ofd-camphor via weak neutral currents. Physical Review E, 1999, 60, 871-874. | 0.8 | 18 |
| 90 | Resolution of molecular electric hyperpolarizabilities into atomic terms. Chemical Physics Letters, 1999, 315, 217-223. | 1.2 | 4 |

| # | Article | IF | Citations |
|---|---|---|---|
| 91 | Current Density Maps, Magnetizability, and Nuclear Magnetic Shielding Tensors for Anthracene, Phenanthrene, and Triphenylene. Journal of the American Chemical Society, 1999, 121, 5513-5518. | 6.6 | 78 |
| 92 | Theoretical results which strengthen the hypothesis of electroweak bioenantioselection. Physical Review E, 1999, 59, 3382-3385. | 0.8 | 45 |
| 93 | On the Stabilization of Natural l-Î±-Amino Acids and d-Sugars via Parity-Violating Effects. , 1999, , 377-385. | | 10 |
| 94 | Electric and magnetic properties of hexaethynylbenzene. Molecular Physics, 1999, 96, 1099-1108. | 0.8 | 54 |
| 95 | On the stabilization of natural L-enantiomers of Î±-amino acids via parity-violating effects. Chemical Physics Letters, 1998, 286, 240-242. | 1.2 | 49 |
| 96 | Distributed-Gauge Calculations of Current Density Maps, Magnetizabilities, and Shieldings for a Series of Neutral and Dianionic Fused Tetracycles:â€‰ Pyracylene (C14H8), Acepleiadylene (C16H10), and Dipleiadiene (C18H12). Journal of Physical Chemistry A, 1998, 102, 7297-7302. | 1.1 | 34 |
| 97 | Ring current model of the naphthalene molecule. Molecular Physics, 1997, 92, 609-618. | 0.8 | 11 |
| 98 | Magnetic properties of C60 calculated by continuous transformation of the origin of the current density. Chemical Physics Letters, 1997, 278, 251-255. | 1.2 | 24 |
| 99 | On the calculation of parity-violating energies in hydrogen peroxide and hydrogen disulphide molecules within the random-phase approximation. Chemical Physics Letters, 1997, 279, 349-354. | 1.2 | 87 |
| 100 | Ring current model of the naphthalene molecule. Molecular Physics, 1997, 92, 609-617. | 0.8 | 28 |
| 101 | Molecular magnetic properties via formal annihilation of paramagnetic contribution to electronic current density. International Journal of Quantum Chemistry, 1996, 60, 249-259. | 1.0 | 42 |
| 102 | Ring currents and magnetic properties of pyracylene. Chemical Physics Letters, 1996, 251, 132-140. | 1.2 | 52 |
| 103 | Coupled Hartreeâ€“Fock calculations of molecular magnetic properties annihilating the transverse paramagnetic current density. Journal of Chemical Physics, 1996, 105, 1460-1469. | 1.2 | 172 |
| 104 | Effects of a static electric field on molecular magnetic properties: an approach using continuous transformation of origin of current density. Molecular Physics, 1996, 89, 157-170. | 0.8 | 23 |
| 105 | Coupled Hartree-Fock Approach to Electric Hyperpolarizability Tensors in Benzene. Topics in Molecular Organization and Engineering, 1996, , 279-296. | 0.1 | 0 |
| 106 | Ring currents and magnetisability in C60. Chemical Physics Letters, 1995, 238, 270-280. | 1.2 | 67 |
| 107 | Coupled Hartree-Fock electric polarizabilities of second-row fluorides. AIP Conference Proceedings, 1995, , . | 0.3 | 1 |
| 108 | Molecular magnetic properties within continuous transformations of origin of the current density. Journal of Chemical Physics, 1995, 102, 7150-7157. | 1.2 | 136 |

| # | Article | IF | Citations |
|---|---|---|---|
| 109 | Coupled Hartreeâ€“Fock calculations of originâ€independent magnetic properties of benzene molecule. Journal of Chemical Physics, 1995, 102, 9619-9625. | 1.2 | 55 |
| 110 | Conditions for invariance of molecular magnetic properties in Landau gauge transformations. Journal of Chemical Physics, 1995, 103, 1852-1859. | 1.2 | 9 |
| 111 | Ab initio and experimental study of NMR coupling constants in bicyclo[1.1.1]pentane. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 4031-4035. | 1.7 | 25 |
| 112 | Proximity Effects on Nuclear Spin-Spin Coupling Constants. 1. J(CH) Couplings in the Vicinity of an Atom Bearing Lone Pairs. The Journal of Physical Chemistry, 1994, 98, 8858-8861. | 2.9 | 78 |
| 113 | Vicinal proton-proton coupling constants. Molecular Physics, 1994, 82, 913-928. | 0.8 | 30 |
| 114 | Theoretical study of the magnetic properties of a methane molecule in a nonuniform magnetic field. Physical Review A, 1994, 49, 3445-3449. | 1.0 | 16 |
| 115 | On CHF calculations of second-order magnetic properties using the method of continuous transformation of origin of the current density. Theoretica Chimica Acta, 1994, 89, 181-192. | 0.9 | 206 |
| 116 | Computational approach to molecular magnetic properties by continuous transformation of the origin of the current density. Chemical Physics Letters, 1994, 220, 299-304. | 1.2 | 288 |
| 117 | Random phase approximation calculations of K-edge rotational strengths of chiral molecules: propylene oxide. Chemical Physics Letters, 1994, 223, 402-410. | 1.2 | 25 |
| 118 | Theoretical study of the magnetic properties of water molecules in non-uniform magnetic fields. Computational and Theoretical Chemistry, 1994, 305, 89-99. | 1.5 | 15 |
| 119 | Electronic current density induced by nuclear magnetic dipoles. Computational and Theoretical Chemistry, 1994, 313, 299-304. | 1.5 | 19 |
| 120 | Vicinal protonâ€”proton coupling constants. Basis set dependence in SCF ab initio calculations. Chemical Physics Letters, 1993, 206, 253-259. | 1.2 | 18 |
| 121 | Theoretical determination of electric polarizability and hyperpolarizabilities of pyridine N-oxide and 4-nitropyridine N-oxide. Computational and Theoretical Chemistry, 1993, 288, 255-259. | 1.5 | 5 |
| 122 | Calculation of molecular magnetic properties in the isoelectronic series PH2â^', PH3 and PH4+. Computational and Theoretical Chemistry, 1993, 287, 77-88. | 1.5 | 2 |
| 123 | Electronic Current Density Induced by Magnetic Fields and Magnetic Moments in Molecules. , 1993, , 163-190. | | 11 |
| 124 | Calculation of infrared and vibrational circular dichroism intensities via nuclear electromagnetic shieldings. The Journal of Physical Chemistry, 1993, 97, 2535-2542. | 2.9 | 16 |
| 125 | Calculation of molecular magnetic properties within the Landau gauge in hydrogen fluoride, ammonia, and methane molecules. Journal of Chemical Physics, 1993, 98, 4030-4040. | 1.2 | 23 |
| 126 | Calculation of dynamic electric dipole polarizability, nuclear electric shieldings, and their Cauchy moments in benzene. Journal of Chemical Physics, 1993, 99, 6027-6030. | 1.2 | 8 |

| # | Article | IF | Citations |
|---|---|---|---|
| 127 | Use of Symmetry in Coupled Hartree-Fock Calculations of Non-linear Response Tensors in Molecules. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1993, 48, 141-144. | 0.7 | 6 |
| 128 | Calculation of molecular magnetic properties within the Landau gauge. Physical Review A, 1992, 45, 6272-6281. | 1.0 | 20 |
| 129 | THEORETICAL DETERMINATION OF THE ELECTRIC DIPOLE AND QUADRUPOLE RESPONSE PROPERTIES OF C60. International Journal of Modern Physics B, 1992, 06, 3903-3907. | 1.0 | 6 |
| 130 | Dipole moments and polarizabilities of some substituted pyridine-1-oxides for optoelectronics. Computational and Theoretical Chemistry, 1992, 254, 205-218. | 1.5 | 19 |
| 131 | Coupled Hartree-Fock calculations of magnetic properties of the benzene molecule: estimate of the hartree-fock limit for magnetic susceptibilities and. Computational and Theoretical Chemistry, 1991, 234, 127-145. | 1.5 | 54 |
| 132 | Magnetic properties of C60 and C70. Chemical Physics Letters, 1991, 179, 174-180. | 1.2 | 71 |
| 133 | Theoretical determination of paramagnetic susceptibilities from nuclear electromagnetic shieldings. Chemical Physics, 1991, 150, 173-185. | 0.9 | 32 |
| 134 | Electromagnetic moments and fields induced by nuclear vibrational motion in molecules. Chemical Physics Letters, 1991, 179, 297-302. | 1.2 | 5 |
| 135 | Structure and properties of C70. Chemical Physics Letters, 1991, 184, 182-186. | 1.2 | 133 |
| 136 | Virial sum rules for nuclear electric shieldings and geometrical derivatives of dipole and quadrupole molecular moments. Journal of Chemical Physics, 1991, 94, 448-453. | 1.2 | 8 |
| 137 | Anisotropic nuclear magnetic shielding in footballene (C60). The Journal of Physical Chemistry, 1991, 95, 6404-6405. | 2.9 | 20 |
| 138 | Coupled Hartree-Fock calculations of atomic polar tensors and the dipole polarisability of the benzene molecule. Chemical Physics Letters, 1990, 167, 101-104. | 1.2 | 21 |
| 139 | Electric and magnetic properties of the aromatic sixty-carbon cage. Chemical Physics Letters, 1990, 165, 79-86. | 1.2 | 180 |
| 140 | Ab initio calculations of atomic polar and axial tensors for hydrogen fluoride, water, ammonia, and methane. The Journal of Physical Chemistry, 1990, 94, 1811-1830. | 2.9 | 62 |
| 141 | Nuclear shielding tensors, atomic polar and axial tensors, and vibrational dipole and rotational strengths of NHDT. Journal of Chemical Physics, 1989, 90, 3204-3213. | 1.2 | 21 |
| 142 | Anisotropic dispersion forces in methane mixtures. Molecular Physics, 1989, 68, 853-865. | 0.8 | 30 |
| 143 | Random phase approximation calculations of vibrational circular dichroism: trans-2,3-dideuteriooxirane. The Journal of Physical Chemistry, 1989, 93, 6583-6584. | 2.9 | 11 |
| 144 | The theory of sternheimer shielding in molecules in external fields. Chemical Physics, 1989, 133, 221-235. | 0.9 | 32 |

| # | Article | IF | Citations |
|---|---|---|---|
| 145 | Calculation of paramagnetic susceptibilities using electronic atomic axial tensors (or nuclear) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 509-519. | 1.2 | 24 |
| 146 | The electrostatic model of field gradients at nuclei. An application to hydrogen-bonded complexes of HCl. Journal of the Chemical Society, Faraday Transactions 2, 1989, 85, 901. | 1.1 | 42 |
| 147 | Carbon-proton and proton-proton spin-spin coupling surfaces for the methane molecule. Molecular Physics, 1989, 66, 831-846. | 0.8 | 12 |
| 148 | The nuclear electromagnetic shielding approach to IR and VCD intensities: A theoretical study of ethylene oxide and cyclopropane. Chemical Physics Letters, 1988, 150, 515-521. | 1.2 | 16 |
| 149 | Ab initio study of a 32-boron cluster: B32H322-. Inorganic Chemistry, 1988, 27, 1298-1300. | 1.9 | 8 |
| 150 | The effects of rotation and vibration on the carbon-13 shielding, magnetizabilities and geometrical parameters of some methane isotopomers. Molecular Physics, 1988, 64, 143-162. | 0.8 | 59 |
| 151 | Two methods of computing molecular dipole and quadrupole derivatives. Journal of Chemical Physics, 1988, 88, 272-276. | 1.2 | 10 |
| 152 | Electromagnetic nuclear shielding tensors and their relation to other secondâ€order properties: A study of the ammonia molecule. Journal of Chemical Physics, 1988, 89, 987-997. | 1.2 | 21 |
| 153 | Vibration-rotation effects on the polarizabilities of CH4and CD4calculated from anab initiopolarizability surface. Molecular Physics, 1988, 64, 1061-1071. | 0.8 | 28 |
| 154 | Calculations of the force field of the methane molecule. Molecular Physics, 1987, 60, 509-525. | 0.8 | 56 |
| 155 | Magnetizability and carbon-13 shielding surfaces for the methane molecule. Molecular Physics, 1987, 62, 605-616. | 0.8 | 35 |
| 156 | Electromagnetic nuclear shielding tensors and their relation to other secondâ€order properties. A study of the methane molecule. Journal of Chemical Physics, 1987, 87, 472-480. | 1.2 | 45 |
| 157 | Theory of the carbon-13 proton spin-spin coupling and the proton shielding surfaces of the methane molecule. Molecular Physics, 1987, 61, 1415-1421. | 0.8 | 12 |
| 158 | On the CH bond dipole moment in alkanes. Journal of Chemical Physics, 1987, 87, 1681-1684. | 1.2 | 21 |
| 159 | Analytic geometrical derivatives of second-order molecular properties from perturbation theory. Chemical Physics Letters, 1987, 135, 571-575. | 1.2 | 5 |
| 160 | The zero point vibrational contribution to the13Câ€“H spinâ€“spin coupling constant in methane. An ab initio result. Journal of the Chemical Society Chemical Communications, 1986, , 57-58. | 2.0 | 6 |
| 161 | Magnetic dipole transition moments and rotational strengths of vibrational transitions: an alternative formalism. The Journal of Physical Chemistry, 1986, 90, 6761-6763. | 2.9 | 30 |
| 162 | Theory of the proton-proton spin-spin coupling surface of the methane molecule. Chemical Physics Letters, 1986, 132, 173-180. | 1.2 | 10 |

| # | Article | IF | Citations |
|---|---|---|---|
| 163 | Analytic dipole moment geometric derivatives from nuclear electric shielding in molecules. II. Application to twoâ€heavy atom molecules. Journal of Chemical Physics, 1986, 85, 5932-5935. | 1.2 | 25 |
| 164 | Electric and magnetic nuclear shielding tensors: A study of the water molecule. Physical Review A, 1986, 33, 3727-3741. | 1.0 | 61 |
| 165 | Analytic dipole moment geometric derivatives from nuclear electric shielding in molecules. Journal of Chemical Physics, 1986, 84, 3916-3920. | 1.2 | 39 |
| 166 | Theory of magnetic susceptibility in terms of atomic quantities. Journal of Chemical Physics, 1986, 85, 5924-5931. | 1.2 | 15 |
| 167 | Resolution of molecular magnetic susceptibility into atomic terms. Chemical Physics Letters, 1985, 114, 79-81. | 1.2 | 7 |
| 168 | The gradient of a molecular wavefunction and its relation to the nuclear electric shielding. Chemical Physics Letters, 1985, 118, 217-220. | 1.2 | 16 |
| 169 | Quantum mechanical approach to IR intensities via nuclear electric shielding tensors. I. Water. Journal of Chemical Physics, 1985, 83, 1218-1222. | 1.2 | 37 |
| 170 | Quantum-mechanical sum rules and gauge invariance: A study of the HF molecule. Physical Review A, 1985, 32, 2607-2614. | 1.0 | 67 |
| 171 | The proton spinâ€“spin coupling surface in methane. A test of the J(H,H)=(Î³H/Î³D)J(H,D) rule for geminal protons. Journal of the Chemical Society Chemical Communications, 1985, , 1538-1540. | 2.0 | 8 |
| 172 | Nuclear electric shielding and its connections with other second-order properties. Computational and Theoretical Chemistry, 1985, 120, 265-275. | 1.5 | 0 |
| 173 | Firstâ€order polarization propagator approach to nuclear spinâ€“spin coupling tensors in SiH4 and AlHâ‚„. Journal of Chemical Physics, 1984, 80, 315-318. | 1.2 | 9 |
| 174 | Connection between the nuclear electric shielding tensor and the infrared intensity. Chemical Physics Letters, 1984, 112, 103-105. | 1.2 | 54 |
| 175 | Resolution of molecular polarizability into atomic terms. Chemical Physics Letters, 1984, 109, 89-91. | 1.2 | 17 |
| 176 | Singularities of magnetic-field induced electron current density: A study of the ethylene molecule. International Journal of Quantum Chemistry, 1984, 25, 929-940. | 1.0 | 19 |
| 177 | Magnetic properties and induced current density in acetylene. International Journal of Quantum Chemistry, 1984, 25, 1123-1134. | 1.0 | 18 |
| 178 | Localized second-order electric properties in water, ammonia and methane. Journal of the Chemical Society, Faraday Transactions 2, 1984, 80, 235. | 1.1 | 5 |
| 179 | The validity of Musher's model for the magnetic properties of aromatic molecules. Chemical Physics Letters, 1983, 100, 67-69. | 1.2 | 18 |
| 180 | Frequency-dependence of the nuclear electric shielding in the HF molecule via equation-of-motion-approaches. Journal of Molecular Structure, 1983, 93, 207-212. | 1.8 | 0 |

| # | Article | IF | Citations |
|---|---|---|---|
| 181 | Frequency-dependence of the nuclear electric shielding in the HF molecule via equation-of-motion-approaches. Computational and Theoretical Chemistry, 1983, 93, 207-212. | 1.5 | 1 |
| 182 | Nuclear magnetic shielding in cyclopropane and cyclopropenyl cation. Journal of the American Chemical Society, 1983, 105, 12-15. | 6.6 | 27 |
| 183 | Polarization propagator approach to the dynamic nuclear electric shielding in LiH molecule. Journal of Chemical Physics, 1983, 79, 889-893. | 1.2 | 24 |
| 184 | Equation-of-motion approach to frequency-dependent nuclear electric shielding tensors in the HF molecule. Physical Review A, 1983, 27, 1301-1309. | 1.0 | 38 |
| 185 | Coupled Hartreeâ€“Fock study of nuclear electric shielding in SF6 molecule. Journal of Chemical Physics, 1983, 79, 4085-4086. | 1.2 | 10 |
| 186 | Calculation of the diamagnetic spinâ€orbit contribution to the nuclear spinâ€“spin coupling tensors in the water molecule. Journal of Chemical Physics, 1983, 79, 1554-1556. | 1.2 | 16 |
| 187 | Theoretical determination of the nuclear spinâ€“spin coupling tensors in NHâ^'2, NH+4, BHâ^'4molecular ions. Journal of Chemical Physics, 1982, 77, 2023-2027. | 1.2 | 10 |
| 188 | Bond length dependence of the electric properties of lithium hydride. Journal of Physics B: Atomic and Molecular Physics, 1982, 15, 521-526. | 1.6 | 21 |
| 189 | Theoretical studies on the benzene molecule. II. Criticism of the ring current model. Journal of Chemical Physics, 1982, 77, 3129-3139. | 1.2 | 50 |
| 190 | Anisotropy of the nuclear spin coupling in PHâ^'2, PH3, and PH+4molecules. Journal of Chemical Physics, 1982, 77, 408-414. | 1.2 | 20 |
| 191 | Anisotropy of the nuclear spinâ€“spin coupling tensor in water, ammonia, and methane molecules. Journal of Chemical Physics, 1982, 77, 2448-2453. | 1.2 | 46 |
| 192 | Paramagnetic vortices and proton magnetic shielding in aromatic molecules. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1982, 1, 70-80. | 0.4 | 13 |
| 193 | Theoretical studies of the benzene molecule: Magnetic susceptibility and nuclear shielding constants. Journal of Chemical Physics, 1981, 75, 5019-5027. | 1.2 | 62 |
| 194 | Inconsistency of the ring-current model for the cyclopropenyl cation. Chemical Physics Letters, 1981, 80, 533-536. | 1.2 | 48 |
| 195 | Theory of nuclear electric shielding in molecules. Physical Review A, 1981, 24, 1696-1704. | 1.0 | 33 |
| 196 | On the theoretical determination of molecular first hyperpolarizability. Journal of Chemical Physics, 1981, 74, 5216-5224. | 1.2 | 75 |
| 197 | Bond length dependence of first hyperpolarisabilities in HF and HCl molecules. Journal of Physics B: Atomic and Molecular Physics, 1981, 14, L269-L274. | 1.6 | 25 |
| 198 | A proof of pitzer's theorem for abelian groups and its application to two-electron integral transformation. Chemical Physics Letters, 1980, 75, 392-394. | 1.2 | 12 |

| # | Article | IF | Citations |
|---|---|---|---|
| 199 | Calculations of nuclear electric shielding in molecules. Chemical Physics Letters, 1980, 71, 529-533. | 1.2 | 24 |
| 200 | Theoretical determination of the magnetic properties of HCl, H2S, PH3, and SiH4 molecules. Journal of Chemical Physics, 1980, 72, 6768-6776. | 1.2 | 106 |
| 201 | On the use of symmetry in first-order perturbedHF theory. II. International Journal of Quantum Chemistry, 1979, 15, 645-653. | 1.0 | 16 |
| 202 | Conformations of ten-membered-ring sesquiterpenes. Crystal and molecular structures of agerol diepoxide and ageratriol. Journal of the Chemical Society Perkin Transactions II, 1978, , 217. | 0.9 | 12 |
| 203 | Calculations of proton magnetic shielding constants in polyatomic molecules. Journal of Chemical Physics, 1978, 68, 832-839. | 1.2 | 37 |
| 204 | Perturbed Hartreeâ€“Fock calculations: Electric and magnetic properties of water in static fields. Journal of Chemical Physics, 1978, 68, 1523-1530. | 1.2 | 55 |
| 205 | Calculations of magnetic susceptibility of polyatomic molecules. Journal of Chemical Physics, 1977, 67, 382-388. | 1.2 | 46 |
| 206 | Calculations of the magnetic shielding constants of heavy nuclei in polyatomic molecules. International Journal of Quantum Chemistry, 1977, 12, 93-103. | 1.0 | 36 |
| 207 | Coupled Hartree-Fock calculations of nuclear magnetic resonance carbon-carbon coupling constants in substituted benzenes. Journal of the American Chemical Society, 1976, 98, 7989-7993. | 6.6 | 25 |
| 208 | Calculations of electric dipole hyperpolarizability of polyatomic molecules. Chemical Physics Letters, 1976, 39, 323-327. | 1.2 | 15 |
| 209 | Calculations of vertical ionization potentials of CF4 and SiF4 by the green-function method. Chemical Physics Letters, 1976, 42, 411-414. | 1.2 | 11 |