Paolo Lazzeretti

List of Publications by Year
in descending order

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279	8,087	53794	76900
papers	citations	45 h-index	74 g-index

282	282	282	2427
all docs	docs citations	times ranked	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.	3.0	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.	3.0	6
3	Assessment of the performance of DFT functionals in the fulfillment of off-diagonal hypervirial relationships. Physical Chemistry Chemical Physics, 2021, 23, 15268-15274.	2.8	13
4	Physical achirality in geometrically chiral rotamers of hydrazine and boranylborane molecules. Journal of Computational Chemistry, 2021, 42, 1772-1782.	3.3	2
5	Electronic Currents Induced by Optical Fields and Rotatory Power Density in Chiral Molecules. Molecules, 2021, 26, 4195.	3.8	8
6	Origin-Independent Densities of Static and Dynamic Molecular Polarizabilities. Journal of Physical Chemistry Letters, 2021, 12, 8855-8864.	4.6	5
7	Electronic Currents and Anapolar Response Induced in Molecules by Monochromatic Light. Chemistry, 2021, 3, 1022-1036.	2.2	4
8	Anisotropy of the vorticity tensor as a magnetic indicator of aromaticity. Physical Chemistry Chemical Physics, 2020, 22, 1299-1305.	2.8	2
9	Static and optical anapole magnetizabilities and polarizabilities. Journal of Chemical Physics, 2020, 153, 074102.	3.0	4
10	Cubic magnetic response of diamagnetic molecules via third-order electronic current density. Journal of Chemical Physics, 2020, 153, 234112.	3.0	1
11	Tests of accuracy for computed magnetic properties via off-diagonal hypervirial relations. Journal of Chemical Physics, 2020, 153, 214108.	3.0	1
12	Continuity equations for electron charge densities and current densities induced in molecules by electric and magnetic fields. Journal of Chemical Physics, 2019, 151, 114108.	3.0	9
13	Stagnation graphs and separatrices of local bifurcations in velocity and current density planar vector fields. Rendiconti Lincei, 2019, 30, 515-535.	2.2	5
14	Frequency-dependent current density tensors as density functions of dynamic polarizabilities. Journal of Chemical Physics, 2019, 150, 184117.	3.0	13
15	Could Electronic Anapolar Interactions Drive Enantioselective Syntheses in Strongly Nonuniform Magnetic Fields? A Computational Study. Journal of Chemical Theory and Computation, 2019, 15, 961-971.	5.3	5
16	Anapolar interaction of aminoacids and sugars in nonuniform magnetic fields. Rendiconti Lincei, 2018, 29, 199-207.	2.2	2
17	Current density tensors. Journal of Chemical Physics, 2018, 148, 134109.	3.0	40
18	Polygonal current models for polycyclic aromatic hydrocarbons and graphene sheets of various shapes. Journal of Computational Chemistry, 2018, 39, 21-34.	3.3	11

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19	Gauge invariance and origin independence of electronic charge density and current density induced by optical fields. Journal of Chemical Physics, 2018, 149, 154106.	3.0	18
20	The abstract <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si264.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mi>G</mml:mi></mml:mrow><mml:mrow><mml:mi mathvariant="italic">PT</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si137.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mi>G</mml:mi></mml:mrow><mml:mrow><mml:mi mathvariant="italic">CPT</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math. Journal of Mo	1.2	11
21	Chiral discrimination in nuclear magnetic resonance spectroscopy. Journal of Physics Condensed Matter, 2017, 29, 443001.	1.8	18
22	Electric Dipoleâ€“Magnetic Dipole Polarizability and Anapole Magnetizability of Hydrogen Peroxide as Functions of the HOOH Dihedral Angle. Journal of Physical Chemistry A, 2017, 121, 9369-9376.	2.5	8
23	Computational study of basis set and electron correlation effects on anapole magnetizabilities of chiral molecules. Journal of Computational Chemistry, 2016, 37, 1552-1558.	3.3	16
24	Topological definition of ring currents. Physical Chemistry Chemical Physics, 2016, 18, 11765-11771.	2.8	17
25	On the definition of molecular dynamic magnetizability. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	4
26	Theoretical prediction of the optical rotation of chiral molecules in ordered media: A computational study of (R_a)â€1,3â€dimethylallene, (2R)â€2â€methyloxirane, and (2R)â€Nâ€methyloxaziridine. International Journal of Quantum Chemistry, 2015, 115, 900-906.	2.0	3
27	Chiral discrimination in NMR spectroscopy: computation of the relevant molecular pseudoscalars. Molecular Physics, 2015, 113, 1780-1785.	1.7	18
28	Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16.	2.5	99
29	Theoretical estimates of the anapole magnetizabilities of C4H4X2 cyclic molecules for X=O, S, Se, and Te. Journal of Chemical Physics, 2014, 141, 094305.	3.0	15
30	Invariance of molecular response properties under a coordinate translation. International Journal of Quantum Chemistry, 2014, 114, 1364-1392.	2.0	15
31	On the determination of the diagonal components of the optical activity tensor in chiral molecules. Journal of Chemical Physics, 2014, 140, 074105.	3.0	19
32	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.	2.5	14
33	Magnetizabilities of Diatomic and Linear Triatomic Molecules in a Time-Independent Nonuniform Magnetic Field. Journal of Physical Chemistry A, 2014, 118, 6333-6342.	2.5	19
34	Polygonal Current Model: An Effective Quantifier of Aromaticity on the Magnetic Criterion. Journal of Physical Chemistry A, 2013, 117, 9083-9092.	2.5	39
35	Chiral discrimination via nuclear magnetic resonance spectroscopy. Rendiconti Lincei, 2013, 24, 283-289.	2.2	13
36	On the origin independence of the Verdet tensor^{â€}. Molecular Physics, 2013, 111, 1405-1413.	1.7	5

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37	Parity violation energies of C₄H₄X₂molecules for X = O, S, Se, Te and Po^{â€}. Molecular Physics, 2013, 111, 2387-2391.	1.7	12
38	Gauge invariance of the nuclear spin/electron orbit interaction and NMR spectral parameters. Journal of Chemical Physics, 2012, 137, 074108.	3.0	14
39	Beyond NICS. AIP Conference Proceedings, 2012, , .	0.4	11
40	On the Chan-Das gauge for the calculation of molecular magnetizabilities. Journal of Chemical Physics, 2012, 137, 154105.	3.0	1
41	On the existence of a natural common gauge-origin for the calculation of magnetic properties of atoms and molecules via gaugeless basis sets. Journal of Chemical Physics, 2012, 136, 164110.	3.0	18
42	Methods of continuous translation of the origin of the current density revisited. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	23
43	Nuclear magnetic resonance J coupling constant polarizabilities of hydrogen peroxide: A basis set and correlation study. Journal of Computational Chemistry, 2012, 33, 1845-1853.	3.3	13
44	Correlation between the out-of-Plane Components of Magnetizability and Central Magnetic Shielding in Unsaturated Cyclic Molecules. Journal of Physical Chemistry A, 2011, 115, 4553-4557.	2.5	38
45	Beyond NICS: estimation of the magnetotropicity of inorganic unsaturated planar rings. Physical Chemistry Chemical Physics, 2011, 13, 20666.	2.8	58
46	Electric field effects on nuclear spinâ€“spin coupling tensors and chiral discrimination via NMR spectroscopy. Theoretical Chemistry Accounts, 2011, 129, 359-366.	1.4	18
47	Magnetic-field induced electronic anapoles in small molecules. Rendiconti Lincei, 2011, 22, 105-112.	2.2	24
48	Stagnation graphs and topological models of magneticâ€field induced electron current density for some small molecules in connection with their magnetic symmetry. International Journal of Quantum Chemistry, 2011, 111, 356-367.	2.0	22
49	Geometry distortion of the benzene molecule in a strong magnetic field. International Journal of Quantum Chemistry, 2011, 111, 772-779.	2.0	5
50	The ring current model of the pentaprismane molecule. Journal of Computational Chemistry, 2011, 32, 1599-1611.	3.3	11
51	Magnetic Field-Induced Alignment of Molecular Rotor-Shaped Cyclophanes. Journal of Physical Chemistry Letters, 2010, 1, 1463-1467.	4.6	3
52	Relative Weights of Ïƒ and Ï€ Ring Currents in a Few Simple Monocycles. Journal of Chemical Theory and Computation, 2010, 6, 3343-3351.	5.3	82
53	Ring Current Model and Anisotropic Magnetic Response of Cyclopropane. Journal of Chemical Theory and Computation, 2010, 6, 2002-2018.	5.3	62
54	On the Aromatic Character of 1,2-Dihydro-1,2-azaborine According to Magnetic Criteria. Journal of Physical Chemistry Letters, 2010, 1, 1563-1568.	4.6	51

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55	Assessment of the CTOCD-DZ method in a hierarchy of coupled cluster methods. Physical Chemistry Chemical Physics, 2010, 12, 6163.	2.8	8
56	Understanding the ring current effects on magnetic shielding of hydrogen and carbon nuclei in naphthalene and anthracene. Journal of Computational Chemistry, 2009, 30, 551-564.	3.3	32
57	Ring current models for acetylene and ethylene molecules. Chemical Physics, 2009, 356, 153-163.	1.9	26
58	Topological models of magnetic field induced current density field in small molecules. Theoretical Chemistry Accounts, 2009, 123, 353-364.	1.4	29
59	Calculation of Hypershielding Contribution to Isotropic Nitrogen Shielding in Strong Magnetic Fields. Journal of Chemical Theory and Computation, 2009, 5, 1343-1349.	5.3	8
60	Can Induced Orbital Paramagnetism Be Controlled by Strong Magnetic Fields?. Journal of Chemical Theory and Computation, 2009, 5, 3049-3059.	5.3	5
61	Aromaticity of Î±-Oligothiophenes and Equivalent Oligothienoacenes. Journal of Chemical Theory and Computation, 2009, 5, 1767-1775.	5.3	6
62	Induced Orbital Paramagnetism and Paratropism in Closed-Shell Molecules. Journal of Physical Chemistry A, 2009, 113, 14465-14479.	2.5	20
63	Response tensors for chiral discrimination in NMR spectroscopy. Theoretical Chemistry Accounts, 2008, 119, 99-106.	1.4	22
64	Electronic Structure of the Ground and Excited States of Î²â€Carboline. ChemPhysChem, 2008, 9, 896-901.	2.1	2
65	Relation between Ï€-Electron Localization/Delocalization and H-Bond Strength in Derivatives ofo-Hydroxy-Schiff Bases. Journal of Organic Chemistry, 2008, 73, 2138-2145.	3.2	44
66	Spatial Ring Current Model for the Prismane Molecule. Journal of Physical Chemistry A, 2008, 112, 5175-5186.	2.5	14
67	Rototranslational sum rules for electromagnetic hypershielding at the nuclei and related atomic Cartesian derivatives of the optical rotatory power. Journal of Chemical Physics, 2008, 128, 244107.	3.0	2
68	Topology of magnetic-field induced electron current density in the cubane molecule. Journal of Chemical Physics, 2008, 128, 194305.	3.0	21
69	Calculation of the electric hypershielding at the nuclei of molecules in a strong magnetic field. Journal of Chemical Physics, 2007, 126, 154103.	3.0	10
70	General Connections Among Nuclear Electromagnetic Shieldings and Polarizabilities. Advances in Chemical Physics, 2007, , 507-549.	0.3	65
71	Assessment of Ïƒ-Diatropicity of the Cyclopropane Molecule. Journal of Physical Chemistry A, 2007, 111, 8163-8169.	2.5	67
72	Spatial Ring Current Model of the [2.2]Paracyclophane Molecule. Journal of Physical Chemistry A, 2007, 111, 3110-3123.	2.5	25

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73	Nuclear Magnetoelectric Shieldings for Chiral Discrimination in NMR Spectroscopy. Theoretical Study of (R_a)-1,3-Dimethylallene, (2R)-2-Methyloxirane, and (2R)-N-Methyloxaziridine Molecules. Journal of Chemical Theory and Computation, 2007, 3, 1691-1698.	5.3	14
74	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.	3.3	22
75	Parity violation energy of 5-pyrimidyl alkanol, a chiral autocatalytic molecule. Chemical Physics Letters, 2007, 435, 346-349.	2.6	11
76	Magnetotropicity of five-membered heterocyclic molecules. Theoretical Chemistry Accounts, 2007, 117, 903-913.	1.4	16
77	Magnetotropicity of phosphole and its arsenic analogue. Theoretical Chemistry Accounts, 2007, 118, 89-97.	1.4	16
78	Invariance of multipole polarisabilities of nuclear magnetic shielding within the approach of continuous transformation of the origin of the current density. Theoretical Chemistry Accounts, 2007, 118, 863-868.	1.4	3
79	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.	2.6	19
80	Parity violation energy of biomolecules â€“ III: RNA. Chemical Physics Letters, 2006, 432, 263-268.	2.6	10
81	Forces on the Nuclei of a Molecule in Optical Fields. Theoretical Chemistry Accounts, 2006, 116, 420-426.	1.4	6
82	Structure, magnetizability, and nuclear magnetic shielding tensors of bis-heteropentalenes. IV. Dihydrophospholophosphole isomers. Journal of Computational Chemistry, 2006, 27, 344-351.	3.3	8
83	Diatropicity of tetraazanaphthalenes. Journal of Computational Chemistry, 2006, 27, 1980-1989.	3.3	9
84	From Pentalene to Dicyclopenta[b,g]naphthalene, or the Change towards Delocalized Structures. ChemPhysChem, 2006, 7, 240-244.	2.1	19
85	Critique of the Multipath Model for 1J(C,C) Nuclear Spin-Spin Coupling via Electron Current Induced by 13C Nuclear Magnetic Dipoles. ChemPhysChem, 2006, 7, 679-684.	2.1	16
86	Calculation of the fourth-rank nuclear magnetic hypershielding of some small molecules. Physical Review A, 2006, 74, .	2.5	11
87	Topology of magnetic-field-induced current-density field in diatropic monocyclic molecules. Physical Review A, 2006, 74, .	2.5	59
88	Rototranslational sum rules for static and dynamic polarisabilities. Computer Physics Communications, 2005, 173, 131-139.	7.5	1
89	Ring-current signatures in shielding-density maps. Chemical Physics Letters, 2005, 401, 164-169.	2.6	58
90	The ring-current model of the paratropic pentalene molecule. Chemical Physics Letters, 2005, 401, 282-287.	2.6	16

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91	Parity violation energy of biomolecules â€“ II: DNA. Chemical Physics Letters, 2005, 407, 522-526.	2.6	19
92	Sum rules for invariance of the fourth-rank hypermagnetisability in a gauge translation. Chemical Physics Letters, 2005, 408, 403-408.	2.6	9
93	Interpretation of vicinal spinâ€“spin coupling constants in ethane via the current-density induced by nuclear magnetic dipoles. Chemical Physics Letters, 2005, 409, 177-186.	2.6	18
94	Ring current effects on nuclear magnetic shielding of carbon in the benzene molecule. Magnetic Resonance in Chemistry, 2005, 43, 316-320.	1.9	30
95	Fourth-rank hypermagnetizability of medium-size planar conjugated molecules and fullerene. Physical Review A, 2005, 72, .	2.5	12
96	Nonlinear response of the benzene molecule to strong magnetic fields. Journal of Chemical Physics, 2005, 122, 074318.	3.0	12
97	Current density maps, magnetizability, and nuclear magnetic shielding tensors of bis-heteropentalenes. III. Thieno-thiophene isomers. Molecular Physics, 2005, 103, 789-801.	1.7	10
98	Why Downfield Proton Chemical Shifts Are Not Reliable Aromaticity Indicators. Organic Letters, 2005, 7, 3457-3460.	4.6	78
99	Can aromaticity be connected with molecular polarizability? A theoretical study of benzene isomers and five-membered heterocyclic molecules. Journal of Computational Methods in Sciences and Engineering, 2004, 4, 665-676.	0.2	0
100	Current density maps, magnetizability, and nuclear magnetic shielding tensors of bis-heteropentalenes. II. Furo-furan Isomers. Journal of Chemical Physics, 2004, 120, 6542-6550.	3.0	12
101	Calculation of electric dipole hypershieldings at the nuclei in the Hellmannâ€“Feynman approximation. Journal of Chemical Physics, 2004, 120, 3142-3151.	3.0	11
102	Electric Field Gradient Effects on Magnetic Susceptibility. Advances in Quantum Chemistry, 2004, 47, 177-191.	0.8	3
103	Molecular response to a time-independent non-uniform magnetic-field. Chemical Physics, 2004, 304, 289-299.	1.9	33
104	The vibrational spectrum of camphor from ab initio and density functional theory and parity violation in the Câ€“C*â€“CO bending mode. Chemical Physics Letters, 2004, 383, 496-501.	2.6	18
105	Understanding proton magnetic shielding in the benzene molecule. Chemical Physics Letters, 2004, 390, 268-271.	2.6	38
106	Effects of strong magnetic fields on the electron distribution and magnetisability of rare gas atoms. Chemical Physics Letters, 2004, 400, 133-138.	2.6	13
107	Localisation and reversal of paratropic ring currents in molecules with formal anti-aromatic electron counts. Physical Chemistry Chemical Physics, 2004, 6, 289-294.	2.8	35
108	Calculation of the fourth-rank molecular hypermagnetizability of some small molecules. Journal of Chemical Physics, 2004, 120, 9556-9560.	3.0	19

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109	Are Ring Currents Still Useful to Rationalize the Benzene Proton Magnetic Shielding?. Organic Letters, 2004, 6, 2265-2267.	4.6	87
110	Assessment of aromaticity via molecular response properties. Physical Chemistry Chemical Physics, 2004, 6, 217-223.	2.8	415
111	Ring-Current Models from the Differential Biot-Savart Law. Organic Letters, 2004, 6, 4451-4454.	4.6	54
112	Calculation of Dipole-Shielding Polarizabilities (Ìƒ Î±Î²Î³):â€‰ The Influence of Uniform Electric Field Effects on the Shielding of Backbone Nuclei in Proteins. Journal of the American Chemical Society, 2003, 125, 9556-9557.	13.7	16
113	Magnetic response of dithiin molecules: is there anti-aromaticity in nature?. Chemical Physics Letters, 2003, 375, 583-590.	2.6	27
114	Electric field gradient effects on nuclear magnetic shieldings. Computational and Theoretical Chemistry, 2003, 633, 105-111.	1.5	7
115	Sum rules related to third-order properties: a numerical check. Chemical Physics, 2003, 288, 281-289.	1.9	8
116	Correlated and gauge invariant calculations of nuclear magnetic shielding constants using the continuous transformation of the origin of the current density approach. Journal of Chemical Physics, 2003, 118, 6830-6845.	3.0	46
117	Nuclear spin-spin coupling density in molecules. Journal of Chemical Physics, 2003, 118, 7165.	3.0	43
118	Parity-violating contributions to nuclear magnetic shielding. Physical Review A, 2003, 68, .	2.5	47
119	Theoretical determination of the magnetic properties of 2-pyrone and 4-pyrone, ando-benzoquinone andp-benzoquinone. Molecular Physics, 2003, 101, 2497-2509.	1.7	5
120	Current density maps, magnetizability, and nuclear magnetic shielding tensors of bis-heteropentalenes. I. Di-hydro-pyrroloâ€“pyrrole isomers. Journal of Chemical Physics, 2003, 119, 5518-5526.	3.0	18
121	Nuclear spinâ€“spin coupling density functions and the Fermi hole. Journal of Chemical Physics, 2003, 119, 1343-1349.	3.0	44
122	Calculation of third-rank molecular hypermagnetizabilities by continuous transformation of the origin of the current density. Journal of Chemical Physics, 2002, 116, 9611-9615.	3.0	4
123	Ring Currents and Magnetic Properties of s-Indacene, an Archetypal Paratropic, Non-Antiaromatic Molecule. Journal of Physical Chemistry A, 2002, 106, 11806-11814.	2.5	38
124	The Leap-Frog Effect of Ring Currents in Benzene. Journal of the American Chemical Society, 2002, 124, 2008-2014.	13.7	37
125	Theoretical determination of magnetic properties of planar benzene isomers. Journal of Chemical Physics, 2002, 116, 964-973.	3.0	14
126	On the resolution of the optical rotatory power of chiral molecules into atomic terms. A study of hydrogen peroxide. Journal of Chemical Physics, 2002, 116, 6427-6434.	3.0	22

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127	Calculation of electric dipole hypershieldings at the nuclei in diatomic molecules. Chemical Physics, 2002, 284, 601-606.	1.9	6
128	Nuclear electromagnetic shieldings via charge and current density functions. International Journal of Quantum Chemistry, 2002, 90, 464-471.	2.0	1
129	An efficient coupled Hartreeâ€“Fock computational scheme for parity-violating energy differences in enantiomeric molecules. Computer Physics Communications, 2002, 144, 130-140.	7.5	2
130	Understanding parity violation in molecular systems. Physical Review E, 2001, 65, 011904.	2.1	35
131	Resolution of molecular polarizabilities of CH3â€“X and CH3â€“CH2â€“X derivatives into atomic terms. Journal of Chemical Physics, 2001, 114, 4053-4057.	3.0	12
132	Some mathematical properties of gauge transformations with respect to the Coulomb gauge: Variational analysis of an energy functional. International Journal of Quantum Chemistry, 2000, 77, 599-606.	2.0	2
133	Thomasâ€“Reicheâ€“Khun populations in Xâ€“CH3 and Xâ€“C2H5 series of molecules. Chemical Physics, 2000, 259, 1-9.	1.9	6
134	Ring currents. Progress in Nuclear Magnetic Resonance Spectroscopy, 2000, 36, 1-88.	7.5	437
135	Parity-violating effects in asymmetric chemical reactions:â€, A theoretical study on the CHFClBr molecule. Physical Review E, 2000, 62, 8395-8399.	2.1	19
136	Shielding polarizabilities via continuous transformation of the origin of the current density in the set of small molecules: H2O2, F2, H2C2, H2CO, NH3, HCN, and HNC. Journal of Chemical Physics, 2000, 112, 6141-6151.	3.0	12
137	Energetic stabilization ofd-camphor via weak neutral currents. Physical Review E, 1999, 60, 871-874.	2.1	18
138	Thomasâ€“Reicheâ€“Kuhn populations in alkanes. Chemical Physics, 1999, 246, 75-85.	1.9	7
139	Current Density Maps, Magnetizability, and Nuclear Magnetic Shielding Tensors for Anthracene, Phenanthrene, and Triphenylene. Journal of the American Chemical Society, 1999, 121, 5513-5518.	13.7	78
140	Theoretical results which strengthen the hypothesis of electroweak bioenantioselection. Physical Review E, 1999, 59, 3382-3385.	2.1	45
141	On the stabilization of natural L-enantiomers of Î±-amino acids via parity-violating effects. Chemical Physics Letters, 1998, 286, 240-242.	2.6	49
142	Calculation of magnetic properties of HF, H2O, NH3, and CH4 molecules using a longitudinal gauge for the vector potential. International Journal of Quantum Chemistry, 1998, 66, 31-45.	2.0	2
143	Resolution of alkane molecular polarizabilities into atomic terms. Journal of Chemical Physics, 1998, 109, 2987-2993.	3.0	19
144	Forces at the nuclei of a molecule in the presence of non-uniform electric field. Computational and Theoretical Chemistry, 1997, 390, 57-60.	1.5	1

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145	Dependence of geminal1Hâ˜1H and31Pâ˜1H spin-spin coupling constants on the specific intramolecular Câ˜H...X interaction. Russian Chemical Bulletin, 1997, 46, 292-296.	1.5	4
146	Magnetic properties of C60 calculated by continuous transformation of the origin of the current density. Chemical Physics Letters, 1997, 278, 251-255.	2.6	24
147	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.	2.6	87
148	Ring current model of the naphthalene molecule. Molecular Physics, 1997, 92, 609-617.	1.7	28
149	Molecular magnetic properties via formal annihilation of paramagnetic contribution to electronic current density. International Journal of Quantum Chemistry, 1996, 60, 249-259.	2.0	42
150	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.	1.7	23
151	Theoretical study of magnetic properties of ammonia molecule in nonuniform magnetic field. Theoretica Chimica Acta, 1996, 94, 155.	0.8	2
152	Longitudinal vector potentials for molecular magnetic properties. Computational and Theoretical Chemistry, 1995, 336, 1-5.	1.5	6
153	Molecular magnetic properties within continuous transformations of origin of the current density. Journal of Chemical Physics, 1995, 102, 7150-7157.	3.0	136
154	Coupled Hartreeâ€“Fock calculations of originâ€independent magnetic properties of benzene molecule. Journal of Chemical Physics, 1995, 102, 9619-9625.	3.0	55
155	Conditions for invariance of molecular magnetic properties in Landau gauge transformations. Journal of Chemical Physics, 1995, 103, 1852-1859.	3.0	9
156	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
157	Vicinal proton-proton coupling constants. Molecular Physics, 1994, 82, 913-928.	1.7	30
158	Theoretical study of the magnetic properties of a methane molecule in a nonuniform magnetic field. Physical Review A, 1994, 49, 3445-3449.	2.5	16
159	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.	0.8	206
160	Computational approach to molecular magnetic properties by continuous transformation of the origin of the current density. Chemical Physics Letters, 1994, 220, 299-304.	2.6	288
161	Random phase approximation calculations of K-edge rotational strengths of chiral molecules: propylene oxide. Chemical Physics Letters, 1994, 223, 402-410.	2.6	25
162	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

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163	Electronic current density induced by nuclear magnetic dipoles. Computational and Theoretical Chemistry, 1994, 313, 299-304.	1.5	19
164	IGLO Study of Benzene and Some of Its Isomers and Related Molecules. Search for Evidence of the Ring Current Model. Journal of the American Chemical Society, 1994, 116, 5298-5306.	13.7	252
165	Vicinal protonâ€"proton coupling constants. Basis set dependence in SCF ab initio calculations. Chemical Physics Letters, 1993, 206, 253-259.	2.6	18
166	Magnetic properties of a molecule in non-uniform magnetic field. Theoretica Chimica Acta, 1993, 87, 59-73.	0.8	35
167	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
168	Calculation of molecular magnetic properties in the isoelectronic series PH2â^', PH3 and PH4+. Computational and Theoretical Chemistry, 1993, 287, 77-88.	1.5	2
169	Calculation of molecular magnetic properties within the Landau gauge in hydrogen fluoride, ammonia, and methane molecules. Journal of Chemical Physics, 1993, 98, 4030-4040.	3.0	23
170	Calculation of dynamic electric dipole polarizability, nuclear electric shieldings, and their Cauchy moments in benzene. Journal of Chemical Physics, 1993, 99, 6027-6030.	3.0	8
171	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.	1.5	6
172	Calculation of molecular magnetic properties within the Landau gauge. Physical Review A, 1992, 45, 6272-6281.	2.5	20
173	Dipole moments and polarizabilities of some substituted pyridine-1-oxides for optoelectronics. Computational and Theoretical Chemistry, 1992, 254, 205-218.	1.5	19
174	Coupled Hartree-Fock calculations of the electric dipole polarizability and first hyperpolarizability of some â€œinorganic benzenesâ€• Computational and Theoretical Chemistry, 1991, 236, 403-410.	1.5	36
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