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	Ring currents. Progress in Nuclear Magnetic Resonance Spectroscopy, 2000, 36, 1-88.	7.5	437
2	Assessment of aromaticity via molecular response properties. Physical Chemistry Chemical Physics, 2004, 6, 217-223.	2.8	415
3	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
4	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
5	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
6	Electric and magnetic properties of the aromatic sixty-carbon cage. Chemical Physics Letters, 1990, 165, 79-86.	2.6	180
7	Molecular magnetic properties within continuous transformations of origin of the current density. Journal of Chemical Physics, 1995, 102, 7150-7157.	3.0	136
8	Structure and properties of C70. Chemical Physics Letters, 1991, 184, 182-186.	2.6	133
9	Theoretical determination of the magnetic properties of HCl, H2S, PH3, and SiH4 molecules. Journal of Chemical Physics, 1980, 72, 6768-6776.	3.0	106
10	Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16.	2.5	99
11	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
12	Are Ring Currents Still Useful to Rationalize the Benzene Proton Magnetic Shielding?. Organic Letters, 2004, 6, 2265-2267.	4.6	87
13	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
14	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
15	Why Downfield Proton Chemical Shifts Are Not Reliable Aromaticity Indicators. Organic Letters, 2005, 7, 3457-3460.	4.6	78
16	On the theoretical determination of molecular first hyperpolarizability. Journal of Chemical Physics, 1981, 74, 5216-5224.	3.0	75
17	Magnetic properties of C60 and C70. Chemical Physics Letters, 1991, 179, 174-180.	2.6	71
18	Quantum-mechanical sum rules and gauge invariance: A study of the HF molecule. Physical Review A, 1985, 32, 2607-2614.	2.5	67

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19	Assessment of Ïƒ-Diatropicity of the Cyclopropane Molecule. Journal of Physical Chemistry A, 2007, 111, 8163-8169.	2.5	67
20	General Connections Among Nuclear Electromagnetic Shieldings and Polarizabilities. Advances in Chemical Physics, 2007, , 507-549.	0.3	65
21	Theoretical studies of the benzene molecule: Magnetic susceptibility and nuclear shielding constants. Journal of Chemical Physics, 1981, 75, 5019-5027.	3.0	62
22	Ring Current Model and Anisotropic Magnetic Response of Cyclopropane. Journal of Chemical Theory and Computation, 2010, 6, 2002-2018.	5.3	62
23	Electric and magnetic nuclear shielding tensors: A study of the water molecule. Physical Review A, 1986, 33, 3727-3741.	2.5	61
24	Calculation of NMR parameters for bridging oxygens in H3T?O?T?H3 linkages (T, T?=Al, Si, P), for oxygen in SiH3O?, SiH3OH and SiH3OMg+ and for bridging fluorine in H3SiFSiH 3 +. Physics and Chemistry of Minerals, 1988, 15, 564-569.	0.8	60
25	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.	1.7	59
26	Topology of magnetic-field-induced current-density field in diatropic monocyclic molecules. Physical Review A, 2006, 74, .	2.5	59
27	Ring-current signatures in shielding-density maps. Chemical Physics Letters, 2005, 401, 164-169.	2.6	58
28	Beyond NICS: estimation of the magnetotropicity of inorganic unsaturated planar rings. Physical Chemistry Chemical Physics, 2011, 13, 20666.	2.8	58
29	Calculations of the force field of the methane molecule. Molecular Physics, 1987, 60, 509-525.	1.7	56
30	Perturbed Hartreeâ€“Fock calculations: Electric and magnetic properties of water in static fields. Journal of Chemical Physics, 1978, 68, 1523-1530.	3.0	55
31	Ab initio calculations of 29Si NMR chemical shifts for some gas phase and solid state silicon fluorides and oxides. Journal of Chemical Physics, 1986, 84, 369-374.	3.0	55
32	Coupled Hartreeâ€“Fock calculations of originâ€independent magnetic properties of benzene molecule. Journal of Chemical Physics, 1995, 102, 9619-9625.	3.0	55
33	Connection between the nuclear electric shielding tensor and the infrared intensity. Chemical Physics Letters, 1984, 112, 103-105.	2.6	54
34	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
35	Ring-Current Models from the Differential Biot-Savart Law. Organic Letters, 2004, 6, 4451-4454.	4.6	54
36	Calculation of nuclear spinâ€“spin coupling constants in methanol molecule. Journal of Chemical Physics, 1979, 71, 2514-2521.	3.0	53

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37	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
38	Theoretical studies on the benzene molecule. II. Criticism of the ring current model. Journal of Chemical Physics, 1982, 77, 3129-3139.	3.0	50
39	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
40	Inconsistency of the ring-current model for the cyclopropenyl cation. Chemical Physics Letters, 1981, 80, 533-536.	2.6	48
41	Parity-violating contributions to nuclear magnetic shielding. Physical Review A, 2003, 68, .	2.5	47
42	An interpretation of1H and13C chemical shifts in substituted benzenes on the basis of M.O. charge densities. Magnetic Resonance in Chemistry, 1971, 3, 283-291.	0.7	46
43	Calculations of magnetic susceptibility of polyatomic molecules. Journal of Chemical Physics, 1977, 67, 382-388.	3.0	46
44	Anisotropy of the nuclear spinâ€“spin coupling tensor in water, ammonia, and methane molecules. Journal of Chemical Physics, 1982, 77, 2448-2453.	3.0	46
45	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
46	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.	3.0	45
47	Theoretical results which strengthen the hypothesis of electroweak bioenantioselection. Physical Review E, 1999, 59, 3382-3385.	2.1	45
48	Nuclear spinâ€“spin coupling density functions and the Fermi hole. Journal of Chemical Physics, 2003, 119, 1343-1349.	3.0	44
49	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
50	Nuclear spin-spin coupling density in molecules. Journal of Chemical Physics, 2003, 118, 7165.	3.0	43
51	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
52	Current density tensors. Journal of Chemical Physics, 2018, 148, 134109.	3.0	40
53	Analytic dipole moment geometric derivatives from nuclear electric shielding in molecules. Journal of Chemical Physics, 1986, 84, 3916-3920.	3.0	39
54	Polygonal Current Model: An Effective Quantifier of Aromaticity on the Magnetic Criterion. Journal of Physical Chemistry A, 2013, 117, 9083-9092.	2.5	39

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55	Equation-of-motion approach to frequency-dependent nuclear electric shielding tensors in the HF molecule. Physical Review A, 1983, 27, 1301-1309.	2.5	38
56	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
57	Understanding proton magnetic shielding in the benzene molecule. Chemical Physics Letters, 2004, 390, 268-271.	2.6	38
58	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
59	Calculations of proton magnetic shielding constants in polyatomic molecules. Journal of Chemical Physics, 1978, 68, 832-839.	3.0	37
60	Quantum mechanical approach to IR intensities via nuclear electric shielding tensors. I. Water. Journal of Chemical Physics, 1985, 83, 1218-1222.	3.0	37
61	The Leap-Frog Effect of Ring Currents in Benzene. Journal of the American Chemical Society, 2002, 124, 2008-2014.	13.7	37
62	Calculations of the magnetic shielding constants of heavy nuclei in polyatomic molecules. International Journal of Quantum Chemistry, 1977, 12, 93-103.	2.0	36
63	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
64	Magnetizability and carbon-13 shielding surfaces for the methane molecule. Molecular Physics, 1987, 62, 605-616.	1.7	35
65	Magnetic properties of a molecule in non-uniform magnetic field. Theoretica Chimica Acta, 1993, 87, 59-73.	0.8	35
66	Understanding parity violation in molecular systems. Physical Review E, 2001, 65, 011904.	2.1	35
67	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
68	Theory of nuclear electric shielding in molecules. Physical Review A, 1981, 24, 1696-1704.	2.5	33
69	Ab initio calculations of oxygen nuclear quadrupole coupling constants and oxygen and silicon NMR shielding constants in molecules containing Siî—‚O bonds. Chemical Physics, 1987, 112, 205-212.	1.9	33
70	Molecular response to a time-independent non-uniform magnetic-field. Chemical Physics, 2004, 304, 289-299.	1.9	33
71	NMR chemical shifts of CX and XCY molecules (X, Y = O, S, Se, Te): A comparison of coupled Hartree-Fock, semi-empirical rex and experimental results. Chemical Physics, 1988, 123, 339-350.	1.9	32
72	The theory of sternheimer shielding in molecules in external fields. Chemical Physics, 1989, 133, 221-235.	1.9	32

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73	Theoretical determination of paramagnetic susceptibilities from nuclear electromagnetic shieldings. Chemical Physics, 1991, 150, 173-185.	1.9	32
74	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
75	Geometric approximation to nuclear spin-spin coupling constants in the water molecule. International Journal of Quantum Chemistry, 1979, 15, 181-196.	2.0	30
76	Anisotropic dispersion forces in methane mixtures. Molecular Physics, 1989, 68, 853-865.	1.7	30
77	Vicinal proton-proton coupling constants. Molecular Physics, 1994, 82, 913-928.	1.7	30
78	Ring current effects on nuclear magnetic shielding of carbon in the benzene molecule. Magnetic Resonance in Chemistry, 2005, 43, 316-320.	1.9	30
79	Coupled and uncoupled Hartree-Fock calculations of ring currents and proton chemical shifts: the aromatic character of five-membered heterocycles. Molecular Physics, 1973, 26, 41-47.	1.7	29
80	Topological models of magnetic field induced current density field in small molecules. Theoretical Chemistry Accounts, 2009, 123, 353-364.	1.4	29
81	Calculations of electric dipole polarizabilities of polyatomic molecules. International Journal of Quantum Chemistry, 1976, 10, 771-780.	2.0	28
82	Vibration-rotation effects on the polarizabilities of CH4and CD4calculated from anab initiopolarizability surface. Molecular Physics, 1988, 64, 1061-1071.	1.7	28
83	Ring current model of the naphthalene molecule. Molecular Physics, 1997, 92, 609-617.	1.7	28
84	Charge density and NMR parameters. Aliphatic derivatives. Magnetic Resonance in Chemistry, 1971, 3, 113-125.	0.7	27
85	Nuclear magnetic shielding in cyclopropane and cyclopropenyl cation. Journal of the American Chemical Society, 1983, 105, 12-15.	13.7	27
86	Magnetic response of dithiin molecules: is there anti-aromaticity in nature?. Chemical Physics Letters, 2003, 375, 583-590.	2.6	27
87	The1H NMR spectra of quinoline, quinolineN-oxide, the quinolinium ion and of their monomethyl derivatives. Magnetic Resonance in Chemistry, 1975, 7, 451-454.	0.7	26
88	Ring current models for acetylene and ethylene molecules. Chemical Physics, 2009, 356, 153-163.	1.9	26
89	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.	13.7	25
90	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.	3.0	25

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91	Random phase approximation calculations of K-edge rotational strengths of chiral molecules: propylene oxide. Chemical Physics Letters, 1994, 223, 402-410.	2.6	25
92	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
93	Spatial Ring Current Model of the [2.2]Paracyclophane Molecule. Journal of Physical Chemistry A, 2007, 111, 3110-3123.	2.5	25
94	Calculations of nuclear electric shielding in molecules. Chemical Physics Letters, 1980, 71, 529-533.	2.6	24
95	Polarization propagator approach to the dynamic nuclear electric shielding in LiH molecule. Journal of Chemical Physics, 1983, 79, 889-893.	3.0	24
96	Calculation of paramagnetic susceptibilities using electronic atomic axial tensors (or nuclear) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 547 509-519.	2.6	24
97	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
98	Magnetic-field induced electronic anapoles in small molecules. Rendiconti Lincei, 2011, 22, 105-112.	2.2	24
99	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
100	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
101	Methods of continuous translation of the origin of the current density revisited. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	23
102	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
103	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
104	Response tensors for chiral discrimination in NMR spectroscopy. Theoretical Chemistry Accounts, 2008, 119, 99-106.	1.4	22
105	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
106	On the CH bond dipole moment in alkanes. Journal of Chemical Physics, 1987, 87, 1681-1684.	3.0	21
107	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.	3.0	21
108	Nuclear shielding tensors, atomic polar and axial tensors, and vibrational dipole and rotational strengths of NHDT. Journal of Chemical Physics, 1989, 90, 3204-3213.	3.0	21

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109	Coupled Hartree-Fock calculations of atomic polar tensors and the dipole polarisability of the benzene molecule. Chemical Physics Letters, 1990, 167, 101-104.	2.6	21
110	Topology of magnetic-field induced electron current density in the cubane molecule. Journal of Chemical Physics, 2008, 128, 194305.	3.0	21
111	Uncoupled Hartree-Fock calculation of ring currents in substituted benzenes. Molecular Physics, 1971, 22, 941-943.	1.7	20
112	Anisotropy of the nuclear spin coupling in PHâ˜2, PH3, and PH+4molecules. Journal of Chemical Physics, 1982, 77, 408-414.	3.0	20
113	Calculation of molecular magnetic properties within the Landau gauge. Physical Review A, 1992, 45, 6272-6281.	2.5	20
114	Induced Orbital Paramagnetism and Paratropism in Closed-Shell Molecules. Journal of Physical Chemistry A, 2009, 113, 14465-14479.	2.5	20
115	Singularities of magnetic-field induced electron current density: A study of the ethylene molecule. International Journal of Quantum Chemistry, 1984, 25, 929-940.	2.0	19
116	Dipole moments and polarizabilities of some substituted pyridine-1-oxides for optoelectronics. Computational and Theoretical Chemistry, 1992, 254, 205-218.	1.5	19
117	Electronic current density induced by nuclear magnetic dipoles. Computational and Theoretical Chemistry, 1994, 313, 299-304.	1.5	19
118	Resolution of alkane molecular polarizabilities into atomic terms. Journal of Chemical Physics, 1998, 109, 2987-2993.	3.0	19
119	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
120	Calculation of the fourth-rank molecular hypermagnetizability of some small molecules. Journal of Chemical Physics, 2004, 120, 9556-9560.	3.0	19
121	Parity violation energy of biomolecules â€“ II: DNA. Chemical Physics Letters, 2005, 407, 522-526.	2.6	19
122	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
123	From Pentalene to Dicyclopenta[b,g]naphthalene, or the Change towards Delocalized Structures. ChemPhysChem, 2006, 7, 240-244.	2.1	19
124	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
125	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
126	Uncoupled Hartree-Fock perturbation theory for the density matrix: the second-order properties of conjugated molecules. Molecular Physics, 1974, 28, 1389-1395.	1.7	18

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127	The validity of Musher's model for the magnetic properties of aromatic molecules. Chemical Physics Letters, 1983, 100, 67-69.	2.6	18
128	Magnetic properties and induced current density in acetylene. International Journal of Quantum Chemistry, 1984, 25, 1123-1134.	2.0	18
129	On the â€œsagging patternâ€•of29 Si NMR shieldings in the series SiHaFb, a+b = 4. Chemical Physics Letters, 1986, 132, 464-466.	2.6	18
130	Electromagnetic moments and fields induced by nuclear spin, vibrational electric and magnetic field at the nuclei, and nuclear electromagnetic couplings in molecules. Chemical Physics, 1989, 134, 269-278.	1.9	18
131	Vicinal protonâ€”proton coupling constants. Basis set dependence in SCF ab initio calculations. Chemical Physics Letters, 1993, 206, 253-259.	2.6	18
132	Energetic stabilization ofd-camphor via weak neutral currents. Physical Review E, 1999, 60, 871-874.	2.1	18
133	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
134	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
135	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
136	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
137	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
138	Chiral discrimination in NMR spectroscopy: computation of the relevant molecular pseudoscalars. Molecular Physics, 2015, 113, 1780-1785.	1.7	18
139	Chiral discrimination in nuclear magnetic resonance spectroscopy. Journal of Physics Condensed Matter, 2017, 29, 443001.	1.8	18
140	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
141	Resolution of molecular polarizability into atomic terms. Chemical Physics Letters, 1984, 109, 89-91.	2.6	17
142	Topological definition of ring currents. Physical Chemistry Chemical Physics, 2016, 18, 11765-11771.	2.8	17
143	On the use of symmetry in first-order perturbedHF theory. II. International Journal of Quantum Chemistry, 1979, 15, 645-653.	2.0	16
144	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.	3.0	16

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145	The gradient of a molecular wavefunction and its relation to the nuclear electric shielding. Chemical Physics Letters, 1985, 118, 217-220.	2.6	16
146	Coupled Hartreeâ€“Fock calculations of31P NMR shieldings in phosphorous fluorides and PO3â^'4. Journal of Chemical Physics, 1987, 86, 4066-4069.	3.0	16
147	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.	2.6	16
148	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
149	Calculation of Dipole-Shielding Polarizabilities (Ïƒ(1)Î²(3)):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
150	The ring-current model of the paratropic pentalene molecule. Chemical Physics Letters, 2005, 401, 282-287.	2.6	16
151	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
152	Magnetotropicity of five-membered heterocyclic molecules. Theoretical Chemistry Accounts, 2007, 117, 903-913.	1.4	16
153	Magnetotropicity of phosphole and its arsenic analogue. Theoretical Chemistry Accounts, 2007, 118, 89-97.	1.4	16
154	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
155	Calculations of electric dipole hyperpolarizability of polyatomic molecules. Chemical Physics Letters, 1976, 39, 323-327.	2.6	15
156	Ab initio coupled Hartree-Fock calculation of the 29Si NMR shielding constants in SiH4, Si2H6, Si2H4 and H2SiO. Chemical Physics Letters, 1986, 128, 420-424.	2.6	15
157	Theory of magnetic susceptibility in terms of atomic quantities. Journal of Chemical Physics, 1986, 85, 5924-5931.	3.0	15
158	Ab initio calculation of the 31P NMR shielding tensor for the series POaFbâ^'(2a+bâ^'5), a+b=4 and for HPO42â^'. Chemical Physics Letters, 1987, 140, 37-40.	2.6	15
159	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
160	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
161	Invariance of molecular response properties under a coordinate translation. International Journal of Quantum Chemistry, 2014, 114, 1364-1392.	2.0	15
162	Critical examination of the1H NMR spectra of aryl epoxides. Magnetic Resonance in Chemistry, 1973, 5, 385-389.	0.7	14

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163	Theoretical determination of magnetic properties of planar benzene isomers. Journal of Chemical Physics, 2002, 116, 964-973.	3.0	14
164	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
165	Spatial Ring Current Model for the Prismane Molecule. Journal of Physical Chemistry A, 2008, 112, 5175-5186.	2.5	14
166	Gauge invariance of the nuclear spin/electron orbit interaction and NMR spectral parameters. Journal of Chemical Physics, 2012, 137, 074108.	3.0	14
167	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
168	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
169	Ab initio calculation of B and O nuclear quadrupole coupling constants and NMR shielding constants in molecular models for B2O3 glass. Journal of Non-Crystalline Solids, 1988, 99, 267-275.	3.1	13
170	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
171	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
172	Chiral discrimination via nuclear magnetic resonance spectroscopy. Rendiconti Lincei, 2013, 24, 283-289.	2.2	13
173	Frequency-dependent current density tensors as density functions of dynamic polarizabilities. Journal of Chemical Physics, 2019, 150, 184117.	3.0	13
174	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
175	Variable temperature n.m.r. behaviour of 1,5-benzodiazepinones and 1,5-benzodiazepinthiones. Magnetic Resonance in Chemistry, 1976, 8, 387-388.	0.7	12
176	A proof of pitzer's theorem for abelian groups and its application to two-electron integral transformation. Chemical Physics Letters, 1980, 75, 392-394.	2.6	12
177	Theory of the carbon-13 proton spin-spin coupling and the proton shielding surfaces of the methane molecule. Molecular Physics, 1987, 61, 1415-1421.	1.7	12
178	Carbon-proton and proton-proton spin-spin coupling surfaces for the methane molecule. Molecular Physics, 1989, 66, 831-846.	1.7	12
179	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
180	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

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