

A solution of the gauge-origin problem for the magnetic

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Configuration-interaction and Hylleraas configuration-interaction methods in valence-bond theory: Calculation of the nuclear shielding constant for the ground state of the hydrogen molecule. <i>Physical Review A</i> , 1992, 46, 2351-2355.	1.0	11
2	Theoretical calculations of the nuclear magnetic shielding tensors for the ethylenic carbon atoms in cyclopropenes. <i>Molecular Physics</i> , 1992, 77, 381-396.	0.8	26
3	Chapter 2. NMR spectroscopy. <i>Annual Reports on the Progress of Chemistry Section C</i> , 1992, 89, 3.	4.4	1
4	A comparison of dipole polarizability obtained from linear and quadratic response functions. <i>International Journal of Quantum Chemistry</i> , 1992, 44, 487-495.	1.0	0
5	The MC-IGLO method. <i>Chemical Physics Letters</i> , 1993, 205, 563-571.	1.2	129
6	Effects of electron correlation in the calculation of nuclear magnetic resonance chemical shifts. <i>Journal of Chemical Physics</i> , 1993, 99, 3629-3643.	1.2	671
7	Calculations of magnetic properties. II. Electron-correlated nuclear shielding constants for nine small molecules. <i>Journal of Chemical Physics</i> , 1993, 98, 8057-8064.	1.2	54
8	A sum-over-states formulation of the diamagnetic contribution to the indirect nuclear spin-spin coupling constant. <i>Journal of Chemical Physics</i> , 1993, 98, 9220-9221.	1.2	29
9	The vibrational and temperature dependence of the magnetic properties of the oxonium ion (H <sub>3</sub> O <sup>+</sup> ). <i>Chemical Physics</i> , 1994, 184, 1-11.	0.9	26
10	Computational approach to molecular magnetic properties by continuous transformation of the origin of the current density. <i>Chemical Physics Letters</i> , 1994, 220, 299-304.	1.2	288
11	Effects of the order of the energy asymptotes on the calculations of nuclear magnetic shieldings and static polarizabilities. <i>Journal of Chemical Physics</i> , 1994, 101, 10775-10782.	1.2	10
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13	Ab initio calculations of magnetic susceptibilities on HF, H <sub>2</sub> O, CH <sub>4</sub> and NH <sub>3</sub> compounds employing the Geertsen's gauge independent method. <i>Computational and Theoretical Chemistry</i> , 1995, 335, 69-76.	1.5	6
14	<sup>19</sup> F nuclear magnetic shielding tensor of CH <sub>3</sub> F. <i>Molecular Physics</i> , 1995, 86, 235-249.	0.8	13
15	Description of the gauge invariance of molecular magnetic properties of the SF <sub>6</sub> molecule. <i>Computational and Theoretical Chemistry</i> , 1996, 364, 69-77.	1.5	0
16	Molecular magnetic properties via formal annihilation of paramagnetic contribution to electronic current density. <i>International Journal of Quantum Chemistry</i> , 1996, 60, 249-259.	1.0	42
17	Ring currents and magnetic properties of pyracylene. <i>Chemical Physics Letters</i> , 1996, 251, 132-140.	1.2	52
18	Coupled Hartree-Fock calculations of molecular magnetic properties annihilating the transverse paramagnetic current density. <i>Journal of Chemical Physics</i> , 1996, 105, 1460-1469.	1.2	172

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19	Effects of a static electric field on molecular magnetic properties: an approach using continuous transformation of origin of current density. <i>Molecular Physics</i> , 1996, 89, 157-170.	0.8	23
20	The vibrational dependence of the hydrogen and oxygen nuclear magnetic shielding constants in OH <sup>+</sup> and OH <sup>-</sup> . <i>Chemical Physics</i> , 1997, 214, 91-101.	0.9	19
21	Theory and calculation of nuclear shielding constants. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 1997, 31, 317-342.	3.9	59
22	Calculation of magnetic properties of HF, H <sub>2</sub> O, NH <sub>3</sub> , and CH <sub>4</sub> molecules using a longitudinal gauge for the vector potential. <i>International Journal of Quantum Chemistry</i> , 1998, 66, 31-45.	1.0	2
23	Application of Optical Nuclear Polarization Enhanced <sup>13</sup> C NMR. <i>Journal of Physical Chemistry A</i> , 1998, 102, 5794-5801.	1.1	24
24	Pauli principle and hyperfine tensors in molecules with identical nuclei. <i>Europhysics Letters</i> , 1998, 41, 377-382.	0.7	0
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29	CTOCD-DZ shielding polarizabilities in a set of small molecules: N <sub>2</sub> , H <sub>2</sub> , HF, HCl, HCN and SH <sub>2</sub> . <i>Computational and Theoretical Chemistry</i> , 2000, 501-502, 407-418.	1.5	1
30	Shielding polarizabilities via continuous transformation of the origin of the current density in the set of small molecules: H <sub>2</sub> O <sub>2</sub> , F <sub>2</sub> , H <sub>2</sub> C <sub>2</sub> , H <sub>2</sub> CO, NH <sub>3</sub> , HCN, and HNC. <i>Journal of Chemical Physics</i> , 2000, 112, 6141-6151.	1.2	12
31	Aromaticity and Ring Currents. <i>Chemical Reviews</i> , 2001, 101, 1349-1384.	23.0	554
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33	Electric field gradient effects on nuclear magnetic shieldings. <i>Computational and Theoretical Chemistry</i> , 2003, 633, 105-111.	1.5	7
34	Electric Field Gradient Effects on Magnetic Susceptibility. <i>Advances in Quantum Chemistry</i> , 2004, 47, 177-191.	0.4	3
35	Calculations of chemical shieldings: Theory and applications. <i>Concepts in Magnetic Resonance</i> , 2004, 20A, 42-69.	1.3	94
36	Molecular response to a time-independent non-uniform magnetic-field. <i>Chemical Physics</i> , 2004, 304, 289-299.	0.9	33
37	The Rotational g Tensor of HF, H <sub>2</sub> O, NH <sub>3</sub> , and CH <sub>4</sub> : A Comparison of Correlated Ab Initio Methods. <i>Advances in Quantum Chemistry</i> , 2005, 48, 469-490.	0.4	5

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40	Invariance of multipole polarisabilities of nuclear magnetic shielding within the approach of continuous transformation of the origin of the current density. <i>Theoretical Chemistry Accounts</i> , 2007, 118, 863-868.	0.5	3
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44	Qualitative Study of Substituent Effects on NMR <sup>15</sup> N and <sup>17</sup> O Chemical Shifts. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9874-9880.	1.1	11
45	The ab initio calculation of molecular electric, magnetic and geometric properties. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 2627-2651.	1.3	58
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47	Gauge invariance of the nuclear spin/electron orbit interaction and NMR spectral parameters. <i>Journal of Chemical Physics</i> , 2012, 137, 074108.	1.2	14
48	Methods of continuous translation of the origin of the current density revisited. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	23
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51	An Origin-Independent Theory for Calculation of NMR Shielding Constants. , 1993, , 335-349.		2
53	Ab-Initio Calculation and Analysis of Nuclear Magnetic Shielding Tensors: the LORG and SOLO Approaches. , 1993, , 117-140.		8