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Correlated calculations for the nuclear magnetic shieldings of CO and HCN

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#	Paper	IF	Citations
49	Nitrogen NMR chemical shifts in mesoionic compounds: a comparison of theory and experiment. <i>Chemical Physics Letters</i> , 1991 , 186, 313-318	2.5	19
48	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	2.6	10
47	Calculation of nuclear magnetic shieldings. VIII. Gauge invariant many-body perturbation method. <i>Journal of Chemical Physics</i> , 1992 , 96, 2039-2043	3.9	21
46	Effects of molecular association on the NMR shielding constants in acetonitrile. <i>Chemical Physics Letters</i> , 1992 , 194, 167-171	2.5	25
45	NMR shielding calculations including electron correlation: benzene, pyridine and the n-azines. <i>Chemical Physics Letters</i> , 1992 , 197, 59-66	2.5	21
44	The MC-IGLO method. <i>Chemical Physics Letters</i> , 1993 , 205, 563-571	2.5	113
43	Ab initio calculations of the oxygen atom NMR shielding in the carbonyl group. <i>Chemical Physics Letters</i> , 1993 , 203, 404-408	2.5	28
42	On the uncorrelated reference for calculation of properties. <i>Theoretica Chimica Acta</i> , 1993 , 86, 167-179		4
41	References. <i>Annual Reports on NMR Spectroscopy</i> , 1993 , 25, 431-468	1.7	
40	Effects of electron correlation in the calculation of nuclear magnetic resonance chemical shifts. <i>Journal of Chemical Physics</i> , 1993 , 99, 3629-3643	3.9	597
39	Calculations of magnetic properties. II. Electron-correlated nuclear shielding constants for nine small molecules. <i>Journal of Chemical Physics</i> , 1993 , 98, 8057-8064	3.9	51
38	Calculation of nuclear magnetic shieldings. IX. Electron correlation effects. <i>Journal of Chemical Physics</i> , 1994 , 100, 6608-6613	3.9	25
37	Correlated dipole oscillator sum rules. <i>Journal of Chemical Physics</i> , 1994 , 100, 8969-8975	3.9	30
36	The vibrational and temperature dependence of the magnetic properties of the oxonium ion (H ₃ O ⁺). <i>Chemical Physics</i> , 1994 , 184, 1-11	2.3	25
35	Correlated polarization propagator calculations of static polarizabilities. <i>International Journal of Quantum Chemistry</i> , 1994 , 50, 317-332	2.1	38
34	Nuclear spin-spin coupling and nuclear motion. <i>International Journal of Quantum Chemistry</i> , 1994 , 52, 153-163	2.1	19
33	Correlated and gauge origin independent calculations of magnetic properties. <i>Theoretica Chimica Acta</i> , 1994 , 88, 351-361		43

32	Nitrogen-15 nuclear magnetic shielding tensors in nitrite and nitrate ion. Experimental and theoretical determinations. <i>Chemical Physics Letters</i> , 1994 , 219, 491-496	2.5	15
31	GIAO-MBPT(3) and GIAO-SDQ-MBPT(4) calculations of nuclear magnetic shielding constants. <i>Chemical Physics Letters</i> , 1994 , 229, 198-203	2.5	104
30	The NMR Chemical Shift: Insight into Structure and Environment. <i>Annual Reports on NMR Spectroscopy</i> , 1994 , 29, 1-69	1.7	41
29	Correlated and gauge origin independent calculations of magnetic properties. <i>Molecular Physics</i> , 1994 , 81, 87-118	1.7	56
28	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	3.9	9
27	An approximate infinite order perturbation theory prescription for isotropic NMR chemical shieldings. <i>Chemical Physics Letters</i> , 1995 , 246, 235-238	2.5	36
26	Coupled-cluster calculations of nuclear magnetic resonance chemical shifts. <i>Journal of Chemical Physics</i> , 1995 , 103, 3561-3577	3.9	233
25	UNDERSTANDING NMR CHEMICAL SHIFTS. <i>Annual Review of Physical Chemistry</i> , 1996 , 47, 135-169	15.7	88
24	Calculation of ¹³ C shielding of the isotopomers CH ₃ Cl, CH ₂ DCl, CHD ₂ Cl, and CD ₃ Cl. <i>International Journal of Quantum Chemistry</i> , 1996 , 60, 529-534	2.1	11
23	Rovibrationally averaged nuclear magnetic shielding tensors calculated at the coupled-cluster level. <i>Journal of Chemical Physics</i> , 1996 , 105, 11051-11059	3.9	153
22	Perturbative treatment of triple excitations in coupled-cluster calculations of nuclear magnetic shielding constants. <i>Journal of Chemical Physics</i> , 1996 , 104, 2574-2583	3.9	323
21	MCSCF calculations of hypermagnetizabilities and nuclear shielding polarizabilities of CO and CH ₄ . <i>Molecular Physics</i> , 1996 , 88, 931-947	1.7	39
20	Vibrational and thermal averaging of the indirect nuclear spin-spin coupling constants of CH ₄ , SiH ₄ , GeH ₄ and SnH ₄ . <i>Molecular Physics</i> , 1997 , 91, 897-908	1.7	25
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18	A theoretical study using ab initio triple-zeta basis sets of some mesoionic compounds. 1997 , 2, 71-84		8
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13	Toward Hartree-Fock- and Density Functional Complete Basis-Set-Predicted NMR Parameters. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 10396-10407	2.8	61
12	Structure and protonation of some indolizine derivatives studied by ab initio MO calculations. <i>Journal of Molecular Structure</i> , 2002 , 605, 33-39	3.4	12
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9	Gauge invariant calculations of nuclear magnetic shielding constants using the continuous transformation of the origin of the current density approach. II. Density functional and coupled cluster theory. <i>Journal of Chemical Physics</i> , 2007 , 126, 154111	3.9	32
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7	Systematic investigation on the geometric dependence of the calculated nuclear magnetic shielding constants. <i>Journal of Computational Chemistry</i> , 2008 , 29, 1798-807	3.5	8
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4	Recent advances in wave function-based methods of molecular-property calculations. <i>Chemical Reviews</i> , 2012 , 112, 543-631	68.1	453
3	Correlated and Gauge Invariant Calculations of Nuclear Shielding Constants. 1993 , 351-365		9
2	Effects of Isotopic Substitution and Temperature on Nuclear Magnetic Shielding. 1993 , 401-420		5
1	Ab-Initio Calculation and Analysis of Nuclear Magnetic Shielding Tensors: the LORG and SOLO Approaches. 1993 , 117-140		6