

Magdalena Pecul-Kudelska

List of Publications by Year in descending order

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83
papers

2,983
citations

117453

34
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182168

51
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89
all docs

89
docs citations

89
times ranked

2214
citing authors

#	ARTICLE	IF	CITATIONS
1	The quantum-chemical calculation of NMR indirect spin-spin coupling constants. Progress in Nuclear Magnetic Resonance Spectroscopy, 2008, 53, 249-268.	3.9	252
2	Density functional theory calculation of electronic circular dichroism using London orbitals. Chemical Physics Letters, 2004, 388, 110-119.	1.2	123
3	The Ab Initio Calculation of Optical Rotation and Electronic Circular Dichroism. Advances in Quantum Chemistry, 2005, 50, 185-212.	0.4	109
4	Conformational Effects on the Optical Rotation of Alanine and Proline. Journal of Physical Chemistry A, 2004, 108, 4269-4276.	1.1	103
5	Vibrational Raman and Raman Optical Activity Spectra of d-Lactic Acid, d-Lactate, and d-Glyceraldehyde: Ab Initio Calculations. Journal of Physical Chemistry A, 2002, 106, 11008-11016.	1.1	94
6	Explicit versus Implicit Solvent Modeling of Raman Optical Activity Spectra. Journal of Physical Chemistry B, 2011, 115, 4128-4137.	1.2	92
7	The selectivity of diglycolamide (TODGA) and bis-triazine-bipyridine (BTBP) ligands in actinide/lanthanide complexation and solvent extraction separation - a theoretical approach. Dalton Transactions, 2015, 44, 2657-2666.	1.6	91
8	Chiral bias of amyloid fibrils revealed by the twisted conformation of Thioflavin T: An induced circular dichroism/DFT study. FEBS Letters, 2005, 579, 6601-6603.	1.3	83
9	A simple scheme for magnetic balance in four-component relativistic Kohn-Sham calculations of nuclear magnetic resonance shielding constants in a Gaussian basis. Journal of Chemical Physics, 2012, 136, 014108.	1.2	80
10	Nuclear Magnetic Shielding and Spin-Spin Coupling of 1,2- ¹³ C-Enriched Acetylene in Gaseous Mixtures with Xenon and Carbon Dioxide. Journal of Physical Chemistry A, 2000, 104, 5955-5958.	1.1	70
11	Conformational structures and optical rotation of serine and cysteine. Chemical Physics Letters, 2006, 418, 1-10.	1.2	68
12	Ab initio calculation of vibrational Raman optical activity. International Journal of Quantum Chemistry, 2005, 104, 816-829.	1.0	67
13	Characterization of dihydrogen-bonded D ₂ H ₂ complexes on the basis of infrared and magnetic resonance spectroscopic parameters. Journal of Chemical Physics, 2003, 119, 5094-5104.	1.2	66
14	The Shielding Constants and Scalar Couplings in N ⁺ H ⁻ OC and N ⁺ H ⁻ NC Hydrogen Bonded Systems: An ab Initio MO Study. Journal of Physical Chemistry A, 2000, 104, 8105-8113.	1.1	59
15	Solvent Effects on Raman Optical Activity Spectra Calculated Using the Polarizable Continuum Model. Journal of Physical Chemistry A, 2006, 110, 2807-2815.	1.1	59
16	Polarizable continuum model study of solvent effects on electronic circular dichroism parameters. Journal of Chemical Physics, 2005, 122, 024106.	1.2	58
17	Ab initio study of magnetochiral birefringence. Journal of Chemical Physics, 2002, 117, 6417-6428.	1.2	51
18	Solvent effects on NMR spectrum of acetylene calculated by ab initio methods. Chemical Physics, 1998, 234, 111-119.	0.9	49

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19	Comprehensive ab initio studies of nuclear magnetic resonance shielding and coupling constants in XHâ€O hydrogen-bonded complexes of simple organic molecules. <i>Journal of Chemical Physics</i> , 2000, 112, 7930-7938.	1.2	49
20	High-order correlation effects on dynamic hyperpolarizabilities and their geometric derivatives: A comparison with density functional results. <i>Journal of Chemical Physics</i> , 2006, 124, 114101.	1.2	46
21	The optical activity of \hat{I}^2, \hat{I}^3 -enones in ground and excited states using circular dichroism and circularly polarized luminescence. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 643-650.	1.3	45
22	The ^{19}F - ^1H coupling constants transmitted through covalent, hydrogen bond, and van der Waals interactions. <i>Journal of Chemical Physics</i> , 2001, 115, 5498-5506.	1.2	43
23	Vibrational Optical Activity of Cysteine in Aqueous Solution: A Comparison of Theoretical and Experimental Spectra. <i>Journal of Physical Chemistry B</i> , 2012, 116, 4976-4990.	1.2	42
24	Electric field effects on the shielding constants of noble gases: A four-component relativistic Hartree-Fock study. <i>Journal of Chemical Physics</i> , 2004, 121, 3051-3057.	1.2	40
25	The Spinâ€Spin Coupling Constants in Ethane, Methanol and Methylamine: A Comparison of DFT, MCSCF and CCSD Results. <i>International Journal of Molecular Sciences</i> , 2003, 4, 143-157.	1.8	39
26	New applications and challenges for computational ROA spectroscopy. <i>Chirality</i> , 2009, 21, E98-104.	1.3	39
27	The nuclear spinâ€spin coupling constants in the water dimer. <i>Chemical Physics Letters</i> , 1999, 308, 486-494.	1.2	37
28	Relativistic calculation of NMR properties of XeF ₂ , XeF ₄ and XeF ₆ . <i>Chemical Physics Letters</i> , 2006, 427, 281-288.	1.2	37
29	Ab initio calculations of the NMR spectra of [1.1.1]propellane and bicyclo[1.1.1]pentane. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 1986-1991.	1.3	36
30	Raman optical activity spectra: basis set and electron correlation effects. <i>Molecular Physics</i> , 2003, 101, 2073-2081.	0.8	36
31	Density functional and coupled cluster calculations of dynamic hyperpolarizabilities and their geometry derivatives. <i>Chemical Physics Letters</i> , 2005, 404, 217-226.	1.2	36
32	Circularly polarized component in surface-enhanced Raman spectra. <i>Chemical Physics Letters</i> , 2010, 496, 86-90.	1.2	35
33	Singlet excited states of Be ₂ . <i>Journal of Chemical Physics</i> , 2000, 112, 3671-3679.	1.2	34
34	A comparison of two-component and four-component approaches for calculations of spin-spin coupling constants and NMR shielding constants of transition metal cyanides. <i>Journal of Chemical Physics</i> , 2012, 137, 014311.	1.2	34
35	Thioflavinâ€T: Electronic Circular Dichroism and Circularly Polarized Luminescence Induced by Amyloid Fibrils. <i>ChemPhysChem</i> , 2016, 17, 2931-2937.	1.0	33
36	Full configuration-interaction and coupled-cluster calculations of the indirect spinâ€spin coupling constant of BH. <i>Chemical Physics Letters</i> , 2003, 368, 172-176.	1.2	32

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37	The nuclear spin-spin coupling constant in He ₂ . Journal of Chemical Physics, 2000, 113, 10835-10836.	1.2	31
38	Linear response coupled cluster calculation of Raman scattering cross sections. Journal of Chemical Physics, 2002, 116, 1259-1268.	1.2	28
39	A Chiral "Frozen" Hydrogen Bonding in C ₄ -Symmetric Inherently Chiral Resorcin[4]arenes: NMR, X-ray, Circular Dichroism, and Theoretical Study. European Journal of Organic Chemistry, 2008, 2008, 3069-3078.	1.2	28
40	Interaction of 2-mercaptoethanesulfonate monolayers on silver with sodium cations. Journal of Raman Spectroscopy, 2002, 33, 796-800.	1.2	27
41	Calculations of hydrogen-bond-transmitted indirect nuclear spin-spin couplings: a comparison of density-functional and ab initio methods. Chemical Physics Letters, 2003, 372, 476-484.	1.2	27
42	Solvent effects on the spin-spin coupling constants of acetylene revisited: supermolecular and polarizable continuum model calculations. Magnetic Resonance in Chemistry, 2004, 42, S128-S137.	1.1	26
43	Theoretical investigation on the linear and nonlinear susceptibilities of urea crystal. Journal of Chemical Physics, 2008, 128, 244713.	1.2	26
44	The geometry dependence of the spin-spin coupling constants in ethane: a theoretical study. Chemical Physics Letters, 1999, 305, 139-146.	1.2	25
45	Spin-Spin Coupling Constants with HF and DFT Methods. , 2004, , 101-121.		25
46	The Influence of a Presence of a Heavy Atom on ¹³ C Shielding Constants in Organomercury Compounds and Halogen Derivatives. Journal of Chemical Theory and Computation, 2013, 9, 1909-1917.	2.3	24
47	Benchmark calculations of the shielding constants in the water dimer. Chemical Physics Letters, 2001, 333, 139-145.	1.2	23
48	Theoretical Studies of Nuclear Magnetic Resonance Parameters for the Proton-Exchange Pathways in Porphyrin and Porphycene. Journal of Physical Chemistry A, 2005, 109, 4162-4171.	1.1	22
49	The effect of triple excitations in coupled cluster calculations of Raman scattering cross-sections. Chemical Physics Letters, 2002, 355, 327-338.	1.2	21
50	Theoretical simulation of the ROA spectra of neutral cysteine and serine. Chemical Physics Letters, 2006, 427, 166-176.	1.2	21
51	DFT calculations of ³¹ P spin-spin coupling constants and chemical shift in dioxaphosphorinanes. Magnetic Resonance in Chemistry, 2011, 49, 399-404.	1.1	19
52	Improper Hydrogen C-H...O Bonds Cause Self-Association of α,β -Enaminoketones Containing Fluorosubstituted Alkyl Groups. ChemPhysChem, 2004, 5, 209-215.	1.0	18
53	Potential Energy and Spin-Spin Coupling Constants Surface of Glycolaldehyde. Journal of Physical Chemistry A, 2004, 108, 2758-2769.	1.1	18
54	On the calculations of the nuclear spin-spin coupling constants in small water clusters. Chemical Physics, 2006, 326, 431-444.	0.9	18

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55	Electronic circular dichroism of disulphide bridge: Ab initio quantum-chemical calculations. Journal of Chemical Physics, 2007, 127, 085102.	1.2	18
56	Relativistic effects on the electric polarizabilities and their geometric derivatives for hydrogen halides and dihalogens – a Dirac–Hartree–Fock study. Chemical Physics Letters, 2003, 370, 578-588.	1.2	17
57	Ab initio calculation of and NMR shielding constants in solid acetylene. Solid State Nuclear Magnetic Resonance, 1997, 8, 139-145.	1.5	16
58	The aqueous Raman optical activity spectra of 4-hydroxyproline: theory and experiment. Journal of Raman Spectroscopy, 2010, 41, 1200-1210.	1.2	16
59	Circular Dichroism and Optical Rotation of Lactamide and 2-Aminopropanol in Aqueous Solution. Journal of Physical Chemistry B, 2013, 117, 5136-5147.	1.2	16
60	The nuclear spin–spin coupling constants in methanol and methylamine: geometry and solvent effects. Chemical Physics, 2000, 255, 137-148.	0.9	15
61	The spin–spin coupling constants in the ammonia dimer. Chemical Physics Letters, 2002, 360, 272-282.	1.2	15
62	Spin–Spin Coupling Constants Transmitted through Ir–H...N Dihydrogen Bonds. ChemPhysChem, 2009, 10, 1247-1259.	1.0	15
63	A computational protocol for the study of circularly polarized phosphorescence and circular dichroism in spin-forbidden absorption. Physical Chemistry Chemical Physics, 2015, 17, 19079-19086.	1.3	15
64	The influence of electrostatic and dispersion interactions on the NMR parameters of acetylene. Chemical Physics, 1999, 248, 27-40.	0.9	13
65	Electronic Circular Dichroism of Fluorescent Proteins: A Computational Study. Journal of Physical Chemistry B, 2015, 119, 3377-3386.	1.2	13
66	Singlet excitations and dipole polarizabilities of Li ₂ , Li ₄ and Li ₈ clusters. Molecular Physics, 2000, 98, 1455-1465.	0.8	11
67	A protein backbone γ and β angle dependence of $2J_{N(i),C(i-1)}$: The new NMR experiment and quantum chemical calculations. Journal of Biomolecular NMR, 2005, 31, 87-95.	1.6	10
68	What Factors Influence the Metal–Proton Spin–Spin Coupling Constants in Mercury- and Cadmium-Substituted Rubredoxin?. Journal of Physical Chemistry A, 2014, 118, 4471-4479.	1.1	10
69	The Relativistic Effects on the Carbon–Carbon Coupling Constants Mediated by a Heavy Atom. Journal of Physical Chemistry A, 2016, 120, 5624-5634.	1.1	10
70	A full configuration interaction calculation of the density dependence of the ³ He shielding constant. Molecular Physics, 2002, 100, 447-451.	0.8	9
71	The nature of the rotational barriers in simple carbonyl compounds. Tetrahedron, 2004, 60, 179-185.	1.0	8
72	Spin–Spin Artificial DNA Intercalated with Silver Cations: Theoretical Prediction. ChemPhysChem, 2012, 13, 1332-1338.	1.0	8

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73	The influence of a presence of a heavy atom on the spin-spin coupling constants between two light nuclei in organometallic compounds and halogen derivatives. <i>Journal of Chemical Physics</i> , 2014, 140, 024319.	1.2	8
74	Spin-spin coupling constants in $\text{HC}\equiv\text{CXH}_3$ molecules; $\text{X}=\text{F}$. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	7
75	Theoretical Prediction of the Spin-Spin Coupling Constants between an Axis and Macrocycle of a Rotaxane. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10795-10800.	1.1	6
76	Nuclear Magnetic Resonance parameters of mercury atom and water molecule complex: Relativistic calculations. <i>Chemical Physics Letters</i> , 2019, 736, 136775.	1.2	4
77	Nuclear magnetic resonance parameters in Zn_2 , Cd_2 and Hg_2 dimers: relativistic calculations. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	4
78	Ab Initio Calculations of the Intermolecular Nuclear Spin-Spin Coupling Constants. <i>Computational Chemistry - Reviews of Current Trends</i> , 2003, , 131-160.	0.4	4
79	Properties and Spectroscopies. , 0, , 125-312.		3
80	Relativistic Four-Component DFT Calculations of Vibrational Frequencies. <i>Journal of Physical Chemistry A</i> , 2021, 125, 10315-10320.	1.1	2
81	Induced circular dichroism of thioflavin T interacting with acetylcholinesterase: A computational study. <i>Chemical Physics</i> , 2015, 463, 82-87.	0.9	1
82	Electronic Circular Dichroism Spectroscopy in Structural Analysis of Biomolecular Systems. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2014, , 161-177.	0.6	1
83	Linear and nonlinear second order susceptibilities of molecular crystals. , 2012, , .		0