Teobald Kupka

List of Publications by Year
in descending order

109	2,417	212478 28	286692 43
papers	citations	h-index	g-index

113	113	113	2073
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Propagation of light in metallic nanowire arrays:â€ƒFinite-difference time-domain studies of silver cylinders. Physical Review B, 2003, 68, .	1.1	205
2	Convergence of Nuclear Magnetic Shieldings in the Kohnâ^'Sham Limit for Several Small Molecules. Journal of Chemical Theory and Computation, 2010, 6, 1580-1589.	2.3	108
3	Computational modeling of molecularly imprinted polymers as a green approach to the development of novel analytical sorbents. TrAC - Trends in Analytical Chemistry, 2018, 98, 64-78.	5.8	73
4	Toward Hartreeâ^'Fock- and Density Functional Complete Basis-Set-Predicted NMR Parameters. Journal of Physical Chemistry A, 2002, 106, 10396-10407.	1.1	68
5	New dioxytetraethyleneoxy macrocyclic cyclophosphazene derivatives. Inorganica Chimica Acta, 1995, 228, 187-192.	1.2	64
6	Polarization-Consistent versus Correlation-Consistent Basis Sets in Predicting Molecular and Spectroscopic Properties. Journal of Physical Chemistry A, 2007, 111, 1927-1932.	1.1	62
7	Basis Set Convergence of Indirect Spinâ€“Spin Coupling Constants in the Kohnâ€“Sham Limit for Several Small Molecules. Journal of Physical Chemistry A, 2012, 116, 3728-3738.	1.1	61
8	Theoretical DFT and experimental Raman and NMR studies on thiophene, 3-methylthiophene and selenophene. Journal of Molecular Structure, 2002, 616, 17-32.	1.8	60
9	Theoretical DFT and experimental NMR studies on uracil and 5-fluorouracil. Journal of Molecular Structure, 2002, 613, 153-166.	1.8	59
10	ThermodynamicvsSupramolecular Effects in the Regiocontrol of the Formation of New Cyclotriphosphazene-Containing Chiral Ligands with 1,1â€˜-Binaphthyl Units:Â SpirovsAnsa Substitution at the N3P3Ring. Journal of the American Chemical Society, 1997, 119, 12432-12440.	6.6	54
11	From CCSD(T)/augâ€ccâ€pVTZâ€¦ to CCSD(T) complete basis set limit isotropic nuclear magnetic shieldings via affordable DFT/CBS calculations. Magnetic Resonance in Chemistry, 2011, 49, 231-236.	1.1	50
12	A Regioselective Route to New Polytopic Receptors by Diaminolysis of Chlorocyclotriphosphazatriene-Containing Crown Ethers. Journal of Organic Chemistry, 1999, 64, 7299-7304.	1.7	44
13	Spectroscopic characterization of natural corals. Analytical and Bioanalytical Chemistry, 2003, 377, 1032-1037.	1.9	39
14	New Lariat Ether-Type Macrocycles with Cyclophosphazene Subunits. Journal of Organic Chemistry, 1995, 60, 7433-7438.	1.7	38
15	Prediction of water's isotropic nuclear shieldings and indirect nuclear spinâ€“spin coupling constants (SSCCs) using correlationâ€consistent and polarizationâ€consistent basis sets in the Kohnâ€“Sham basis set limit. Magnetic Resonance in Chemistry, 2009, 47, 210-221.	1.1	37
16	DFT studies of COOH tip-functionalized zigzag and armchair single wall carbon nanotubes. Journal of Molecular Modeling, 2012, 18, 2241-2246.	0.8	37
17	Hostâ^'Guest Complex Dependent Regioselectivity in Substitution Reactions of Chlorocyclotriphosphazene-Containing PNP-Crowns with Alkylenediamines. Journal of the American Chemical Society, 1997, 119, 1143-1144.	6.6	36
18	H₂O, H₂, HF, F₂ and F₂O nuclear magnetic shielding constants and indirect nuclear spinâ€“spin coupling constants (SSCCs) in the BHandH/pcJâ€n and BHandH/XZP Kohnâ€“Sham limits. Magnetic Resonance in Chemistry, 2009, 47, 959-970.	1.1	36

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19	Experimental and theoretical studies on corals. I. Toward understanding the origin of color in precious red corals from Raman and IR spectroscopies and DFT calculations. Journal of Raman Spectroscopy, 2010, 41, 651-658.	1.2	34
20	GIAO-DFT prediction of accurate NMR parameters in selected glucose derivatives. Magnetic Resonance in Chemistry, 1999, 37, 421-426.	1.1	33
21	Efficient Modeling of NMR Parameters in Carbon Nanosystems. Journal of Chemical Theory and Computation, 2013, 9, 4275-4286.	2.3	33
22	Density functional theory (DFT) prediction of structural and spectroscopic parameters of cytosine using harmonic and anharmonic approximations. Structural Chemistry, 2015, 26, 1083-1093.	1.0	33
23	Î²-Lactam antibiotics. Spectroscopy and molecular orbital (MO) calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1997, 53, 2649-2658.	2.0	32
24	GIAO NMR calculations for carbazole and itsN-methyl andN-ethyl derivatives. Comparison of theoretical and experimental13C chemical shifts. Magnetic Resonance in Chemistry, 2000, 38, 149-155.	1.1	31
25	Complete basis set B3LYP NMR calculations of CDCl₃ solvent's water fine spectral details. Magnetic Resonance in Chemistry, 2008, 46, 851-858.	1.1	31
26	OH-functionalized open-ended armchair single-wall carbon nanotubes (SWCNT) studied by density functional theory. Journal of Molecular Modeling, 2012, 18, 1463-1472.	0.8	31
27	Extrapolation of water and formaldehyde harmonic and anharmonic frequencies to the B3LYP/CBS limit using polarization consistent basis sets. Journal of Molecular Modeling, 2011, 17, 2029-2040.	0.8	30
28	Density functional study of a model amide. Prediction of formamide geometry, dipole moment, IR harmonic vibration Î½ CO and GIAO NMR shieldings. Computational and Theoretical Chemistry, 2000, 531, 143-157.	1.5	29
29	Complete basis set prediction of methanol isotropic nuclear magnetic shieldings and indirect nuclear spinâ€“spin coupling constants (SSCC) using polarizationâ€consistent and XZP basis sets and B3LYP and BHandH density functionals. Magnetic Resonance in Chemistry, 2009, 47, 674-683.	1.1	28
30	Estimation of formamide harmonic and anharmonic modes in the Kohn-Sham limit using the polarization consistent basis sets. Journal of Molecular Modeling, 2011, 17, 2265-2274.	0.8	28
31	Optically active polymers, 2. Copolymerization of limonene with maleic anhydride. Macromolecular Chemistry and Physics, 1994, 195, 1843-1850.	1.1	27
32	Halogen effect on structure and ¹³C NMR chemical shift of 3,6â€disubstitutedâ€Nâ€alkyl carbazoles. Magnetic Resonance in Chemistry, 2013, 51, 630-635.	1.1	27
33	Hartreeâ€“Fock and density functional complete basis-set (CBS) predicted nuclear shielding anisotropy and shielding tensor components. Solid State Nuclear Magnetic Resonance, 2003, 23, 145-167.	1.5	25
34	From correlation-consistent to polarization-consistent basis sets estimation of NMR spinâ€“spin coupling constant in the B3LYP Kohnâ€“Sham basis set limit. Chemical Physics Letters, 2008, 461, 33-37.	1.2	25
35	Anharmonic vibrational frequency calculations for solvated molecules in the B3LYP Kohnâ€“Sham basis set limit. Vibrational Spectroscopy, 2012, 63, 432-439.	1.2	25
36	Application of Optical Nuclear Polarization Enhanced13C NMR. Journal of Physical Chemistry A, 1998, 102, 5794-5801.	1.1	24

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37	Estimation of isotropic nuclear magnetic shieldings in the CCSD(T) and MP2 complete basis set limit using affordable correlation calculations. Magnetic Resonance in Chemistry, 2013, 51, 482-489.	1.1	24
38	Theoretical and experimental vibrational studies on liquid thiophene and its acetonitrile solution. Journal of Molecular Structure, 2002, 614, 297-304.	1.8	23
39	Density functional theory studies of OH-modified open-ended single-wall zigzag carbon nanotubes (SWCNTs). Computational and Theoretical Chemistry, 2010, 948, 93-98.	1.5	23
40	³He NMR: from free gas to its encapsulation in fullerene. Magnetic Resonance in Chemistry, 2013, 51, 463-468.	1.1	23
41	Method and basis set dependence of the NICS indexes of aromaticity for benzene. Magnetic Resonance in Chemistry, 2018, 56, 265-275.	1.1	23
42	Towards more reliable prediction of formaldehyde multinuclear NMR parameters and harmonic vibrations in the gas phase and solution. Computational and Theoretical Chemistry, 1999, 467, 63-78.	1.5	22
43	DFT calculation of structures and NMR chemical shifts of simple models of small diameter zigzag single wall carbon nanotubes (SWCNTs). Magnetic Resonance in Chemistry, 2011, 49, 549-557.	1.1	21
44	Theoretical prediction of nuclear magnetic shieldings and indirect spin-spin coupling constants in 1,1-, cis-, and trans-1,2-difluoroethylenes. Journal of Chemical Physics, 2014, 140, 144303.	1.2	21
45	Toward engineering efficient peptidomimetics. Screening conformational landscape of two modified dehydroaminoacids. Biopolymers, 2014, 101, 28-40.	1.2	21
46	DFT studies on the structural and vibrational properties of polyenes. Journal of Molecular Modeling, 2016, 22, 101.	0.8	21
47	Predicting the structure and vibrational frequencies of ethylene using harmonic and anharmonic approaches at the Kohnâ€“Sham complete basis set limit. Journal of Molecular Modeling, 2016, 22, 42.	0.8	21
48	NMR studies on penicillins: Hydrogen bonding, self-association and micellar solutions of cloxacillin Na-salt in D2O. Journal of Pharmaceutical and Biomedical Analysis, 1993, 11, 103-116.	1.4	20
49	On the convergence of zero-point vibrational corrections to nuclear shieldings and shielding anisotropies towards the complete basis set limit in water. Molecular Physics, 2017, 115, 144-160.	0.8	19
50	Molecular modeling and experimental studies on structure and NMR parameters of 9-benzyl-3,6-diiodo-9H-carbazole. Structural Chemistry, 2015, 26, 997-1006.	1.0	18
51	Nuclear magnetic resonance monitoring of capillary imbibition and diffusion of water into hardened white cement paste. Journal of Applied Physics, 2002, 91, 6588.	1.1	17
52	Experimental and theoretical NMR and IR studies of the sideâ€chain orientation effects on the backbone conformation of dehydrophenylalanine residue. Magnetic Resonance in Chemistry, 2011, 49, 343-349.	1.1	16
53	DFT study of zigzag (n, 0) single-walled carbon nanotubes: 13C NMR chemical shifts. Journal of Molecular Graphics and Modelling, 2016, 67, 14-19.	1.3	16
54	Histamine H2antagonists: powerful ligands for copper(II). Reinterpretation of the famotidineâ€“copper(II) system. Journal of the Chemical Society Dalton Transactions, 1995, , 2909-2913.	1.1	15

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55	Title is missing!. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 1999, 35, 281-289.	1.6	15
56	Solvent impact on the planarity and aromaticity of free and monohydrated zinc phthalocyanine: a theoretical study. Structural Chemistry, 2018, 29, 667-679.	1.0	15
57	Molecular orbital studies of harmonic vibrations of nitrobenzene in the gas phase and solution using semi-empirical, ab initio and density functional theory calculations. Journal of Molecular Structure, 1999, 482-483, 409-414.	1.8	14
58	DFT calculations of structures, ¹³C NMR chemical shifts, and Raman RBM mode of simple models of smallâ€diameter zigzag (4,0) carboxylated singleâ€walled carbon nanotubes. Magnetic Resonance in Chemistry, 2012, 50, 142-151.	1.1	14
59	Spinâ€orbit <scp>ZORA</scp> and fourâ€component <scp>D</scp>iracâ€“<scp>C</scp>oulomb estimation of relativistic corrections to isotropic nuclear shieldings and chemical shifts of noble gas dimers. Journal of Computational Chemistry, 2016, 37, 395-403.	1.5	14
60	DFT calculations of structures, 13C NMR chemical shifts and Raman RBM mode of simple models of ultra small diameter (4,0) zigzag hydroxylated single wall carbon nanotubes. Synthetic Metals, 2012, 162, 573-583.	2.1	13
61	Calculation of Raman parameters of real-size zigzag (n, 0) single-walled carbon nanotubes using finite-size models. Physical Chemistry Chemical Physics, 2016, 18, 25058-25069.	1.3	13
62	On Complex Formation between 5-Fluorouracil and Î²-Cyclodextrin in Solution and in the Solid State: IR Markers and Detection of Short-Lived Complexes by Diffusion NMR. Molecules, 2020, 25, 5706.	1.7	13
63	Improvement in the evaluation of quantitative data in FT NMR spectroscopy by the convolution difference resolution enhancement (CDRE) technique. Magnetic Resonance in Chemistry, 1988, 26, 353-357.	1.1	12
64	DFT studies on armchair (5, 5) SWCNT functionalization. Modification of selected structural and spectroscopic parameters upon two-atom molecule attachment. Journal of Molecular Graphics and Modelling, 2015, 55, 105-114.	1.3	12
65	DFT and experimental studies on structure and spectroscopic parameters of 3,6-diiodo-9-ethyl-9H-carbazole. Structural Chemistry, 2016, 27, 199-207.	1.0	12
66	Copper-d-penicillamine complex as potential contrast agent for MRI. Magnetic Resonance Imaging, 1992, 10, 855-858.	1.0	10
67	Determination of penicillin complexation sites in the presence of Zn(II) ions by AM1 and PM3 methods. Computational and Theoretical Chemistry, 1993, 283, 213-226.	1.5	10
68	Estimating the carbonyl anharmonic vibrational frequency from affordable harmonic frequency calculations. Journal of Molecular Modeling, 2012, 18, 2471-2478.	0.8	10
69	Modeling red coral (Corallium rubrum) and African snail (Helixia aspersa) shell pigments: Raman spectroscopy versus DFT studies. Journal of Raman Spectroscopy, 2016, 47, 908-916.	1.2	10
70	Phosphorus mononitride: A difficult case for theory. International Journal of Quantum Chemistry, 2019, 119, e26032.	1.0	10
71	³He NMR studies on heliumâ€“pyrrole, heliumâ€“indole, and heliumâ€“carbazole systems: a new tool for following chemistry of heterocyclic compounds. Magnetic Resonance in Chemistry, 2015, 53, 103-109.	1.1	9
72	What is the form of muscimol from fly agaric mushroom (Amanita muscaria) in water? An insight from NMR experiment supported by molecular modeling. Magnetic Resonance in Chemistry, 2020, 58, 584-593.	1.1	9

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73	Interaction of 5â€fluorouracil with Î²â€cyclodextrin: A density functional theory study with dispersion correction. International Journal of Quantum Chemistry, 2021, 121, e26487.	1.0	9
74	Application of data processing for sensitivity and resolution enhancement of31P and13C NMR spectra of humic substances. Magnetic Resonance in Chemistry, 1989, 27, 21-26.	1.1	8
75	DFT studies of OHâ€functionalized openâ€ended zigzag, armchair, and chiral single wall carbon nanotubes. Physica Status Solidi (A) Applications and Materials Science, 2011, 208, 1774-1777.	0.8	8
76	Modeling ²¹Ne NMR parameters for carbon nanosystems. Magnetic Resonance in Chemistry, 2013, 51, 676-681.	1.1	8
77	Experimental and theoretical NMR studies of interaction between phenylalanine derivative and egg yolk lecithin. Magnetic Resonance in Chemistry, 2014, 52, 298-305.	1.1	8
78	The Impact of Model Peptides on Structural and Dynamic Properties of Egg Yolk Lecithin Liposomes â€“ Experimental and DFT Studies. Chemistry and Biodiversity, 2015, 12, 1007-1024.	1.0	8
79	On novel magnetic probe for fullerene characterization: Theoretical studies on NMR parameters of free and confined in fullerenes HD and H 2 molecules. Journal of Molecular Graphics and Modelling, 2015, 62, 26-37.	1.3	8
80	Theoretical and experimental NMR studies on muscimol from fly agaric mushroom (Amanita muscaria). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 153, 216-225.	2.0	8
81	Factors Governing the Chemical Stability and NMR Parameters of Uracil Tautomers and Its 5-Halogen Derivatives. Molecules, 2020, 25, 3931.	1.7	8
82	From planar to nonplanar cyclotriphosphazenes. Computational and Theoretical Chemistry, 2008, 866, 21-26.	1.5	7
83	1H and 13C shielding measurements in comparison with DFT calculations performed for two 2-(acetyloamino)-N,N-dimethyl-3-phenylacrylamide isomers. Chemical Physics Letters, 2015, 627, 1-6.	1.2	7
84	Local aromaticity mapping in the vicinity of planar and nonplanar molecules. Magnetic Resonance in Chemistry, 2019, 57, 359-372.	1.1	7
85	From small to medium and beyond: a pragmatic approach in predicting properties of Ne containing structures. Molecular Physics, 2014, 112, 645-653.	0.8	6
86	Substituent Effect of Nitro Group on Aromaticity of Carbazole Rings. Chemistry of Heterocyclic Compounds, 2014, 50, 1244-1251.	0.6	5
87	Theoretical prediction of structural, vibrational and NMR parameters of plastic optical fiber (POF) material precursors. Cis and trans perhydro- and perfluoro-2-methylene-4,5-dimethyl-1,3-dioxolanes. Journal of Molecular Graphics and Modelling, 2014, 52, 36-45.	1.3	5
88	Impact of the Î”Phe configuration on the Boc-Gly-Î”Phe-NHMe conformation: experiment and theory. Structural Chemistry, 2019, 30, 1685-1697.	1.0	5
89	Dynamic Polarizability and Higher-Order Electric Properties of Fluorene, Carbazole, and Dibenzofuran. Journal of Physical Chemistry A, 2019, 123, 9753-9762.	1.1	5
90	Simple, rapid and non-destructive detection and determination of phosphines and phosphine oxides in solution by 1H and 31P NMR. Fresenius' Journal of Analytical Chemistry, 1991, 339, 253-257.	1.5	4

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91	Quantum Chemical Studies of Li Ion Hopping Mechanism in Polymer Electrolytes. ECS Transactions, 2007, 3, 163-167.	0.3	4
92	Sensitivity of Noble Gas NMR Parameters to the Heterocyclic Ring Proximity. Density Functional Theory Studies of Neâ€“Furan and Arâ€“Furan Complexes. Chemistry of Heterocyclic Compounds, 2014, 50, 429-437.	0.6	4
93	Convergence of nuclear magnetic shieldings and oneâ€bond ¹J(¹¹B¹H) indirect spinâ€“spin coupling constants in small boron molecules. Magnetic Resonance in Chemistry, 2018, 56, 338-351.	1.1	4
94	Performance of revised STO(1M)â€3G basis set for prediction of 5â€fluorocytosine chemical shifts. Magnetic Resonance in Chemistry, 2019, 57, 489-498.	1.1	4
95	Spectroscopic characterization of non-covalent CuPc-GO system. Experiment and theory. Materials Chemistry and Physics, 2019, 231, 301-310.	2.0	4
96	Oneâ€bond ¹J(¹⁵N,H) coupling constants at sp²â€hybridized nitrogen of Schiff bases, enaminones and similar compounds: A theoretical study. Magnetic Resonance in Chemistry, 2020, 58, 750-762.	1.1	4
97	On the aromaticity of uracil and its 5-halogeno derivatives as revealed by theoretically derived geometric and magnetic indexes. Structural Chemistry, 2021, 32, 275-283.	1.0	4
98	Cross-relaxation bottleneck in waterâ€“lysozyme proton magnetization exchange. Biopolymers, 2006, 83, 11-19.	1.2	3
99	Performance of polarization-consistent vs. correlation-consistent basis sets for CCSD(T) prediction of water dimer interaction energy. Journal of Molecular Modeling, 2019, 25, 313.	0.8	3
100	Simple Rules for Complex Near-Glass-Transition Phenomena in Medium-Sized Schiff Bases. International Journal of Molecular Sciences, 2022, 23, 5185.	1.8	3
101	New Heterofunctional Cyclophosphazenes with Carbonyl and Double Bond Functions. Inorganic Chemistry, 1994, 33, 3602-3604.	1.9	2
102	Local aromaticity in polyacenes manifested by individual proton and carbon shieldings: DFT mapping of aromaticity. Magnetic Resonance in Chemistry, 2020, 58, 145-153.	1.1	2
103	Liposomes as nonspecific nanocarriers for 5-Fluorouracil in the presence of cyclodextrins. Journal of Molecular Liquids, 2021, 343, 117623.	2.3	2
104	Nano, Ceramic, and Metallic Materials for Energy Application. Advances in Materials Science and Engineering, 2014, 2014, 1-2.	1.0	1
105	Anharmonicity modeling in hydrogen bonded solvent dimers. Journal of Molecular Liquids, 2021, 339, 116735.	2.3	1
106	On the impact of side methyl groups on the structure and vibrational properties of Î²-carotenoids. The case of butadiene and isoprene. Food Chemistry, 2022, 369, 130880.	4.2	1
107	Experimental and Theoretical Spectroscopic Studies on Selected Igepals. Acta Physica Polonica A, 2000, 98, 651-654.	0.2	0
108	Penicillin Action and Metal Ions. IR Studies and Model Semi Empirical Calculations. , 1995, , 559-560.		0

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109	Use of HR NMR to Tissue Characterisation. Data Processing of Noisy Phosphorus Spectra. , 1995, , 503-504.		0