Teobald Kupka

List of Publications by Year
in descending order

109 papers	2,417 citations	186265 28 h-index	254184 43 g-index
113 all docs	113 docs citations	113 times ranked	1883 citing authors

#	Article	IF	Citations
1	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.	8.2	1
2	Simple Rules for Complex Near-Glass-Transition Phenomena in Medium-Sized Schiff Bases. International Journal of Molecular Sciences, 2022, 23, 5185.	4.1	3
3	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.	2.0	4
4	Interaction of 5â€fluorouracil with Î²â€cyclodextrin: A density functional theory study with dispersion correction. International Journal of Quantum Chemistry, 2021, 121, e26487.	2.0	9
5	Anharmonicity modeling in hydrogen bonded solvent dimers. Journal of Molecular Liquids, 2021, 339, 116735.	4.9	1
6	Liposomes as nonspecific nanocarriers for 5-Fluorouracil in the presence of cyclodextrins. Journal of Molecular Liquids, 2021, 343, 117623.	4.9	2
7	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.	1.9	9
8	Local aromaticity in polyacenes manifested by individual proton and carbon shieldings: DFT mapping of aromaticity. Magnetic Resonance in Chemistry, 2020, 58, 145-153.	1.9	2
9	Factors Governing the Chemical Stability and NMR Parameters of Uracil Tautomers and Its 5-Halogen Derivatives. Molecules, 2020, 25, 3931.	3.8	8
10	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.	3.8	13
11	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.	1.9	4
12	Impact of the Î”Phe configuration on the Boc-Gly-Î”Phe-NHMe conformation: experiment and theory. Structural Chemistry, 2019, 30, 1685-1697.	2.0	5
13	Dynamic Polarizability and Higher-Order Electric Properties of Fluorene, Carbazole, and Dibenzofuran. Journal of Physical Chemistry A, 2019, 123, 9753-9762.	2.5	5
14	Phosphorus mononitride: A difficult case for theory. International Journal of Quantum Chemistry, 2019, 119, e26032.	2.0	10
15	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.	1.8	3
16	Performance of revised STO(1M)â€3G basis set for prediction of 5â€fluorocytosine chemical shifts. Magnetic Resonance in Chemistry, 2019, 57, 489-498.	1.9	4
17	Local aromaticity mapping in the vicinity of planar and nonplanar molecules. Magnetic Resonance in Chemistry, 2019, 57, 359-372.	1.9	7
18	Spectroscopic characterization of non-covalent CuPc-GO system. Experiment and theory. Materials Chemistry and Physics, 2019, 231, 301-310.	4.0	4

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19	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.	1.9	4
20	Solvent impact on the planarity and aromaticity of free and monohydrated zinc phthalocyanine: a theoretical study. Structural Chemistry, 2018, 29, 667-679.	2.0	15
21	Method and basis set dependence of the NICS indexes of aromaticity for benzene. Magnetic Resonance in Chemistry, 2018, 56, 265-275.	1.9	23
22	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.	11.4	73
23	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.	1.7	19
24	DFT study of zigzag (n, 0) single-walled carbon nanotubes: 13C NMR chemical shifts. Journal of Molecular Graphics and Modelling, 2016, 67, 14-19.	2.4	16
25	DFT studies on the structural and vibrational properties of polyenes. Journal of Molecular Modeling, 2016, 22, 101.	1.8	21
26	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.	2.8	13
27	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.	3.3	14
28	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.	2.5	10
29	DFT and experimental studies on structure and spectroscopic parameters of 3,6-diiodo-9-ethyl-9H-carbazole. Structural Chemistry, 2016, 27, 199-207.	2.0	12
30	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.	1.8	21
31	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.	3.9	8
32	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.	2.1	8
33	Molecular modeling and experimental studies on structure and NMR parameters of 9-benzyl-3,6-diiodo-9H-carbazole. Structural Chemistry, 2015, 26, 997-1006.	2.0	18
34	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.	2.6	7
35	Density functional theory (DFT) prediction of structural and spectroscopic parameters of cytosine using harmonic and anharmonic approximations. Structural Chemistry, 2015, 26, 1083-1093.	2.0	33
36	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.	2.4	8

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37	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.	1.9	9
38	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.	2.4	12
39	From small to medium and beyond: a pragmatic approach in predicting properties of Ne containing structures. Molecular Physics, 2014, 112, 645-653.	1.7	6
40	Nano, Ceramic, and Metallic Materials for Energy Application. Advances in Materials Science and Engineering, 2014, 2014, 1-2.	1.8	1
41	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.	3.0	21
42	Substituent Effect of Nitro Group on Aromaticity of Carbazole Rings. Chemistry of Heterocyclic Compounds, 2014, 50, 1244-1251.	1.2	5
43	Toward engineering efficient peptidomimetics. Screening conformational landscape of two modified dehydroaminoacids. Biopolymers, 2014, 101, 28-40.	2.4	21
44	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.	2.4	5
45	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.	1.2	4
46	Experimental and theoretical NMR studies of interaction between phenylalanine derivative and egg yolk lecithin. Magnetic Resonance in Chemistry, 2014, 52, 298-305.	1.9	8
47	Efficient Modeling of NMR Parameters in Carbon Nanosystems. Journal of Chemical Theory and Computation, 2013, 9, 4275-4286.	5.3	33
48	Halogen effect on structure and ¹³C NMR chemical shift of 3,6â€disubstitutedâ€Nâ€alkyl carbazoles. Magnetic Resonance in Chemistry, 2013, 51, 630-635.	1.9	27
49	Modeling ²¹Ne NMR parameters for carbon nanosystems. Magnetic Resonance in Chemistry, 2013, 51, 676-681.	1.9	8
50	³He NMR: from free gas to its encapsulation in fullerene. Magnetic Resonance in Chemistry, 2013, 51, 463-468.	1.9	23
51	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.	1.9	24
52	Anharmonic vibrational frequency calculations for solvated molecules in the B3LYP Kohnâ€“Sham basis set limit. Vibrational Spectroscopy, 2012, 63, 432-439.	2.2	25
53	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.	3.9	13
54	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.	2.5	61

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55	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.	1.9	14
56	OH-functionalized open-ended armchair single-wall carbon nanotubes (SWCNT) studied by density functional theory. Journal of Molecular Modeling, 2012, 18, 1463-1472.	1.8	31
57	DFT studies of COOH tip-functionalized zigzag and armchair single wall carbon nanotubes. Journal of Molecular Modeling, 2012, 18, 2241-2246.	1.8	37
58	Estimating the carbonyl anharmonic vibrational frequency from affordable harmonic frequency calculations. Journal of Molecular Modeling, 2012, 18, 2471-2478.	1.8	10
59	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.	1.8	30
60	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.	1.8	28
61	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.	1.8	8
62	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.	1.9	50
63	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.	1.9	16
64	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.	1.9	21
65	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.	2.5	34
66	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
67	Convergence of Nuclear Magnetic Shieldings in the Kohnâ^'Sham Limit for Several Small Molecules. Journal of Chemical Theory and Computation, 2010, 6, 1580-1589.	5.3	108
68	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.	1.9	37
69	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.	1.9	28
70	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.	1.9	36
71	Complete basis set B3LYP NMR calculations of CDCl₃ solvent's water fine spectral details. Magnetic Resonance in Chemistry, 2008, 46, 851-858.	1.9	31
72	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.	2.6	25

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73	From planar to nonplanar cyclotriphosphazenes. Computational and Theoretical Chemistry, 2008, 866, 21-26.	1.5	7
74	Quantum Chemical Studies of Li Ion Hopping Mechanism in Polymer Electrolytes. ECS Transactions, 2007, 3, 163-167.	0.5	4
75	Polarization-Consistent versus Correlation-Consistent Basis Sets in Predicting Molecular and Spectroscopic Properties. Journal of Physical Chemistry A, 2007, 111, 1927-1932.	2.5	62
76	Cross-relaxation bottleneck in waterâ€“lysozyme proton magnetization exchange. Biopolymers, 2006, 83, 11-19.	2.4	3
77	Spectroscopic characterization of natural corals. Analytical and Bioanalytical Chemistry, 2003, 377, 1032-1037.	3.7	39
78	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.	2.3	25
79	Propagation of light in metallic nanowire arrays:â€ƒFinite-difference time-domain studies of silver cylinders. Physical Review B, 2003, 68, .	3.2	205
80	Nuclear magnetic resonance monitoring of capillary imbibition and diffusion of water into hardened white cement paste. Journal of Applied Physics, 2002, 91, 6588.	2.5	17
81	Toward Hartreeâ^'Fock- and Density Functional Complete Basis-Set-Predicted NMR Parameters. Journal of Physical Chemistry A, 2002, 106, 10396-10407.	2.5	68
82	Theoretical DFT and experimental NMR studies on uracil and 5-fluorouracil. Journal of Molecular Structure, 2002, 613, 153-166.	3.6	59
83	Theoretical DFT and experimental Raman and NMR studies on thiophene, 3-methylthiophene and selenophene. Journal of Molecular Structure, 2002, 616, 17-32.	3.6	60
84	Theoretical and experimental vibrational studies on liquid thiophene and its acetonitrile solution. Journal of Molecular Structure, 2002, 614, 297-304.	3.6	23
85	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.	1.9	31
86	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
87	Experimental and Theoretical Spectroscopic Studies on Selected Igepals. Acta Physica Polonica A, 2000, 98, 651-654.	0.5	0
88	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.	3.6	14
89	Title is missing!. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 1999, 35, 281-289.	1.6	15
90	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

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91	GIAO-DFT prediction of accurate NMR parameters in selected glucose derivatives. Magnetic Resonance in Chemistry, 1999, 37, 421-426.	1.9	33
92	A Regioselective Route to New Polytopic Receptors by Diaminolysis of Chlorocyclotriphosphazatriene-Containing Crown Ethers. Journal of Organic Chemistry, 1999, 64, 7299-7304.	3.2	44
93	Application of Optical Nuclear Polarization Enhanced13C NMR. Journal of Physical Chemistry A, 1998, 102, 5794-5801.	2.5	24
94	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.	13.7	54
95	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.	13.7	36
96	Î²-Lactam antibiotics. Spectroscopy and molecular orbital (MO) calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1997, 53, 2649-2658.	3.9	32
97	New dioxytetraethyleneoxy macrocyclic cyclophosphazene derivatives. Inorganica Chimica Acta, 1995, 228, 187-192.	2.4	64
98	New Lariat Ether-Type Macrocycles with Cyclophosphazene Subunits. Journal of Organic Chemistry, 1995, 60, 7433-7438.	3.2	38
99	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
100	Penicillin Action and Metal Ions. IR Studies and Model Semi Empirical Calculations. , 1995, , 559-560.		0
101	Use of HR NMR to Tissue Characterisation. Data Processing of Noisy Phosphorus Spectra. , 1995, , 503-504.		0
102	Optically active polymers, 2. Copolymerization of limonene with maleic anhydride. Macromolecular Chemistry and Physics, 1994, 195, 1843-1850.	2.2	27
103	New Heterofunctional Cyclophosphazenes with Carbonyl and Double Bond Functions. Inorganic Chemistry, 1994, 33, 3602-3604.	4.0	2
104	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.	2.8	20
105	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
106	Copper-d-penicillamine complex as potential contrast agent for MRI. Magnetic Resonance Imaging, 1992, 10, 855-858.	1.8	10
107	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
108	Application of data processing for sensitivity and resolution enhancement of31P and13C NMR spectra of humic substances. Magnetic Resonance in Chemistry, 1989, 27, 21-26.	1.9	8

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109	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.	1.9	12