

Teobald Kupka

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/5388056/publications.pdf>

Version: 2024-02-01

109
papers

2,417
citations

186209

28
h-index

254106

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 \hat{I}^2 -carotenoids. The case of butadiene and isoprene. <i>Food Chemistry</i> , 2022, 369, 130880.	4.2	1
2	Simple Rules for Complex Near-Glass-Transition Phenomena in Medium-Sized Schiff Bases. <i>International Journal of Molecular Sciences</i> , 2022, 23, 5185.	1.8	3
3	On the aromaticity of uracil and its 5-halogeno derivatives as revealed by theoretically derived geometric and magnetic indexes. <i>Structural Chemistry</i> , 2021, 32, 275-283.	1.0	4
4	Interaction of 5-Fluorouracil with \hat{I}^2 -Cyclodextrin: A density functional theory study with dispersion correction. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26487.	1.0	9
5	Anharmonicity modeling in hydrogen bonded solvent dimers. <i>Journal of Molecular Liquids</i> , 2021, 339, 116735.	2.3	1
6	Liposomes as nonspecific nanocarriers for 5-Fluorouracil in the presence of cyclodextrins. <i>Journal of Molecular Liquids</i> , 2021, 343, 117623.	2.3	2
7	What is the form of muscimol from fly agaric mushroom (<i>Amanita muscaria</i>) in water? An insight from NMR experiment supported by molecular modeling. <i>Magnetic Resonance in Chemistry</i> , 2020, 58, 584-593.	1.1	9
8	Local aromaticity in polyacenes manifested by individual proton and carbon shieldings: DFT mapping of aromaticity. <i>Magnetic Resonance in Chemistry</i> , 2020, 58, 145-153.	1.1	2
9	Factors Governing the Chemical Stability and NMR Parameters of Uracil Tautomers and Its 5-Halogen Derivatives. <i>Molecules</i> , 2020, 25, 3931.	1.7	8
10	On Complex Formation between 5-Fluorouracil and \hat{I}^2 -Cyclodextrin in Solution and in the Solid State: IR Markers and Detection of Short-Lived Complexes by Diffusion NMR. <i>Molecules</i> , 2020, 25, 5706.	1.7	13
11	One-bond $\langle \sup{1} \rangle \langle i \rangle \langle \sup{15} \rangle \langle N,H \rangle$ coupling constants at sp^2 -hybridized nitrogen of Schiff bases, enamines and similar compounds: A theoretical study. <i>Magnetic Resonance in Chemistry</i> , 2020, 58, 750-762.	1.1	4
12	Impact of the \hat{I}^m Phe configuration on the Boc-Gly- \hat{I}^m Phe-NHMe conformation: experiment and theory. <i>Structural Chemistry</i> , 2019, 30, 1685-1697.	1.0	5
13	Dynamic Polarizability and Higher-Order Electric Properties of Fluorene, Carbazole, and Dibenzofuran. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9753-9762.	1.1	5
14	Phosphorus mononitride: A difficult case for theory. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e26032.	1.0	10
15	Performance of polarization-consistent vs. correlation-consistent basis sets for CCSD(T) prediction of water dimer interaction energy. <i>Journal of Molecular Modeling</i> , 2019, 25, 313.	0.8	3
16	Performance of revised STO(1M)-3G basis set for prediction of 5-Fluorocytosine chemical shifts. <i>Magnetic Resonance in Chemistry</i> , 2019, 57, 489-498.	1.1	4
17	Local aromaticity mapping in the vicinity of planar and nonplanar molecules. <i>Magnetic Resonance in Chemistry</i> , 2019, 57, 359-372.	1.1	7
18	Spectroscopic characterization of non-covalent CuPc-GO system. Experiment and theory. <i>Materials Chemistry and Physics</i> , 2019, 231, 301-310.	2.0	4

#	ARTICLE	IF	CITATIONS
19	Convergence of nuclear magnetic shieldings and one-bond $\langle \sigma_{11}^B \rangle$ indirect spin-spin coupling constants in small boron molecules. <i>Magnetic Resonance in Chemistry</i> , 2018, 56, 338-351.	1.1	4
20	Solvent impact on the planarity and aromaticity of free and monohydrated zinc phthalocyanine: a theoretical study. <i>Structural Chemistry</i> , 2018, 29, 667-679.	1.0	15
21	Method and basis set dependence of the NICS indexes of aromaticity for benzene. <i>Magnetic Resonance in Chemistry</i> , 2018, 56, 265-275.	1.1	23
22	Computational modeling of molecularly imprinted polymers as a green approach to the development of novel analytical sorbents. <i>TrAC - Trends in Analytical Chemistry</i> , 2018, 98, 64-78.	5.8	73
23	On the convergence of zero-point vibrational corrections to nuclear shieldings and shielding anisotropies towards the complete basis set limit in water. <i>Molecular Physics</i> , 2017, 115, 144-160.	0.8	19
24	DFT study of zigzag (n, 0) single-walled carbon nanotubes: ^{13}C NMR chemical shifts. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 67, 14-19.	1.3	16
25	DFT studies on the structural and vibrational properties of polyenes. <i>Journal of Molecular Modeling</i> , 2016, 22, 101.	0.8	21
26	Calculation of Raman parameters of real-size zigzag (n, 0) single-walled carbon nanotubes using finite-size models. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 25058-25069.	1.3	13
27	Spin-orbit ZORA and four-component D-iracoulomb estimation of relativistic corrections to isotropic nuclear shieldings and chemical shifts of noble gas dimers. <i>Journal of Computational Chemistry</i> , 2016, 37, 395-403.	1.5	14
28	Modeling red coral (<i>Corallium rubrum</i>) and African snail (<i>Helix aspersa</i>) shell pigments: Raman spectroscopy versus DFT studies. <i>Journal of Raman Spectroscopy</i> , 2016, 47, 908-916.	1.2	10
29	DFT and experimental studies on structure and spectroscopic parameters of 3,6-diiodo-9-ethyl-9H-carbazole. <i>Structural Chemistry</i> , 2016, 27, 199-207.	1.0	12
30	Predicting the structure and vibrational frequencies of ethylene using harmonic and anharmonic approaches at the Kohn-Sham complete basis set limit. <i>Journal of Molecular Modeling</i> , 2016, 22, 42.	0.8	21
31	Theoretical and experimental NMR studies on muscimol from fly agaric mushroom (<i>Amanita muscaria</i>). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 153, 216-225.	2.0	8
32	The Impact of Model Peptides on Structural and Dynamic Properties of Egg Yolk Lecithin Liposomes - Experimental and DFT Studies. <i>Chemistry and Biodiversity</i> , 2015, 12, 1007-1024.	1.0	8
33	Molecular modeling and experimental studies on structure and NMR parameters of 9-benzyl-3,6-diiodo-9H-carbazole. <i>Structural Chemistry</i> , 2015, 26, 997-1006.	1.0	18
34	^1H and ^{13}C shielding measurements in comparison with DFT calculations performed for two 2-(acetylamino)-N,N-dimethyl-3-phenylacrylamide isomers. <i>Chemical Physics Letters</i> , 2015, 627, 1-6.	1.2	7
35	Density functional theory (DFT) prediction of structural and spectroscopic parameters of cytosine using harmonic and anharmonic approximations. <i>Structural Chemistry</i> , 2015, 26, 1083-1093.	1.0	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. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 62, 26-37.	1.3	8

#	ARTICLE	IF	CITATIONS
37	³ He NMR studies on helium-pyrrole, helium-indole, and helium-carbazole systems: a new tool for following chemistry of heterocyclic compounds. <i>Magnetic Resonance in Chemistry</i> , 2015, 53, 103-109.	1.1	9
38	DFT studies on armchair (5, 5) SWCNT functionalization. Modification of selected structural and spectroscopic parameters upon two-atom molecule attachment. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 55, 105-114.	1.3	12
39	From small to medium and beyond: a pragmatic approach in predicting properties of Ne containing structures. <i>Molecular Physics</i> , 2014, 112, 645-653.	0.8	6
40	Nano, Ceramic, and Metallic Materials for Energy Application. <i>Advances in Materials Science and Engineering</i> , 2014, 2014, 1-2.	1.0	1
41	Theoretical prediction of nuclear magnetic shieldings and indirect spin-spin coupling constants in 1,1-, cis-, and trans-1,2-difluoroethylenes. <i>Journal of Chemical Physics</i> , 2014, 140, 144303.	1.2	21
42	Substituent Effect of Nitro Group on Aromaticity of Carbazole Rings. <i>Chemistry of Heterocyclic Compounds</i> , 2014, 50, 1244-1251.	0.6	5
43	Toward engineering efficient peptidomimetics. Screening conformational landscape of two modified dehydroaminoacids. <i>Biopolymers</i> , 2014, 101, 28-40.	1.2	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. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 52, 36-45.	1.3	5
45	Sensitivity of Noble Gas NMR Parameters to the Heterocyclic Ring Proximity. Density Functional Theory Studies of Ne-Furan and Ar-Furan Complexes. <i>Chemistry of Heterocyclic Compounds</i> , 2014, 50, 429-437.	0.6	4
46	Experimental and theoretical NMR studies of interaction between phenylalanine derivative and egg yolk lecithin. <i>Magnetic Resonance in Chemistry</i> , 2014, 52, 298-305.	1.1	8
47	Efficient Modeling of NMR Parameters in Carbon Nanosystems. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4275-4286.	2.3	33
48	Halogen effect on structure and ¹³ C NMR chemical shift of 3,6-disubstituted N-alkyl carbazoles. <i>Magnetic Resonance in Chemistry</i> , 2013, 51, 630-635.	1.1	27
49	Modeling ²¹ Ne NMR parameters for carbon nanosystems. <i>Magnetic Resonance in Chemistry</i> , 2013, 51, 676-681.	1.1	8
50	³ He NMR: from free gas to its encapsulation in fullerene. <i>Magnetic Resonance in Chemistry</i> , 2013, 51, 463-468.	1.1	23
51	Estimation of isotropic nuclear magnetic shieldings in the CCSD(T) and MP2 complete basis set limit using affordable correlation calculations. <i>Magnetic Resonance in Chemistry</i> , 2013, 51, 482-489.	1.1	24
52	Anharmonic vibrational frequency calculations for solvated molecules in the B3LYP Kohn-Sham basis set limit. <i>Vibrational Spectroscopy</i> , 2012, 63, 432-439.	1.2	25
53	DFT calculations of structures, ¹³ C NMR chemical shifts and Raman RBM mode of simple models of ultra small diameter (4,0) zigzag hydroxylated single wall carbon nanotubes. <i>Synthetic Metals</i> , 2012, 162, 573-583.	2.1	13
54	Basis Set Convergence of Indirect Spin-Spin Coupling Constants in the Kohn-Sham Limit for Several Small Molecules. <i>Journal of Physical Chemistry A</i> , 2012, 116, 3728-3738.	1.1	61

#	ARTICLE	IF	CITATIONS
55	DFT calculations of structures, ¹³ C NMR chemical shifts, and Raman RBM mode of simple models of small-diameter zigzag (4,0) carboxylated single-walled carbon nanotubes. <i>Magnetic Resonance in Chemistry</i> , 2012, 50, 142-151.	1.1	14
56	OH-functionalized open-ended armchair single-wall carbon nanotubes (SWCNT) studied by density functional theory. <i>Journal of Molecular Modeling</i> , 2012, 18, 1463-1472.	0.8	31
57	DFT studies of COOH tip-functionalized zigzag and armchair single wall carbon nanotubes. <i>Journal of Molecular Modeling</i> , 2012, 18, 2241-2246.	0.8	37
58	Estimating the carbonyl anharmonic vibrational frequency from affordable harmonic frequency calculations. <i>Journal of Molecular Modeling</i> , 2012, 18, 2471-2478.	0.8	10
59	Extrapolation of water and formaldehyde harmonic and anharmonic frequencies to the B3LYP/CBS limit using polarization consistent basis sets. <i>Journal of Molecular Modeling</i> , 2011, 17, 2029-2040.	0.8	30
60	Estimation of formamide harmonic and anharmonic modes in the Kohn-Sham limit using the polarization consistent basis sets. <i>Journal of Molecular Modeling</i> , 2011, 17, 2265-2274.	0.8	28
61	DFT studies of OH-functionalized open-ended zigzag, armchair, and chiral single wall carbon nanotubes. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2011, 208, 1774-1777.	0.8	8
62	From CCSD(T)/aug-cc-pVTZ to CCSD(T) complete basis set limit isotropic nuclear magnetic shieldings via affordable DFT/CBS calculations. <i>Magnetic Resonance in Chemistry</i> , 2011, 49, 231-236.	1.1	50
63	Experimental and theoretical NMR and IR studies of the side-chain orientation effects on the backbone conformation of dehydrophenylalanine residue. <i>Magnetic Resonance in Chemistry</i> , 2011, 49, 343-349.	1.1	16
64	DFT calculation of structures and NMR chemical shifts of simple models of small diameter zigzag single wall carbon nanotubes (SWCNTs). <i>Magnetic Resonance in Chemistry</i> , 2011, 49, 549-557.	1.1	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. <i>Journal of Raman Spectroscopy</i> , 2010, 41, 651-658.	1.2	34
66	Density functional theory studies of OH-modified open-ended single-wall zigzag carbon nanotubes (SWCNTs). <i>Computational and Theoretical Chemistry</i> , 2010, 948, 93-98.	1.5	23
67	Convergence of Nuclear Magnetic Shieldings in the Kohn-Sham Limit for Several Small Molecules. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1580-1589.	2.3	108
68	Prediction of water's isotropic nuclear shieldings and indirect nuclear spin-spin coupling constants (SSCCs) using correlation-consistent and polarization-consistent basis sets in the Kohn-Sham basis set limit. <i>Magnetic Resonance in Chemistry</i> , 2009, 47, 210-221.	1.1	37
69	Complete basis set prediction of methanol isotropic nuclear magnetic shieldings and indirect nuclear spin-spin coupling constants (SSCC) using polarization-consistent and XZP basis sets and B3LYP and BHandH density functionals. <i>Magnetic Resonance in Chemistry</i> , 2009, 47, 674-683.	1.1	28
70	H ₂ O, H ₂ , HF, F ₂ and F ₂ O nuclear magnetic shielding constants and indirect nuclear spin-spin coupling constants (SSCCs) in the BHandH/pc- <i>n</i> and BHandH/XZP Kohn-Sham limits. <i>Magnetic Resonance in Chemistry</i> , 2009, 47, 959-970.	1.1	36
71	Complete basis set B3LYP NMR calculations of CDCl ₃ solvent's water fine spectral details. <i>Magnetic Resonance in Chemistry</i> , 2008, 46, 851-858.	1.1	31
72	From correlation-consistent to polarization-consistent basis sets estimation of NMR spin-spin coupling constant in the B3LYP Kohn-Sham basis set limit. <i>Chemical Physics Letters</i> , 2008, 461, 33-37.	1.2	25

#	ARTICLE	IF	CITATIONS
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.	0.3	4
75	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
76	Cross-relaxation bottleneck in water ¹⁵ O-lysozyme proton magnetization exchange. Biopolymers, 2006, 83, 11-19.	1.2	3
77	Spectroscopic characterization of natural corals. Analytical and Bioanalytical Chemistry, 2003, 377, 1032-1037.	1.9	39
78	Hartree-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
79	Propagation of light in metallic nanowire arrays: Finite-difference time-domain studies of silver cylinders. Physical Review B, 2003, 68, .	1.1	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.	1.1	17
81	Toward Hartree-Fock- and Density Functional Complete Basis-Set-Predicted NMR Parameters. Journal of Physical Chemistry A, 2002, 106, 10396-10407.	1.1	68
82	Theoretical DFT and experimental NMR studies on uracil and 5-fluorouracil. Journal of Molecular Structure, 2002, 613, 153-166.	1.8	59
83	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
84	Theoretical and experimental vibrational studies on liquid thiophene and its acetonitrile solution. Journal of Molecular Structure, 2002, 614, 297-304.	1.8	23
85	GIAO NMR calculations for carbazole and its N-methyl and N-ethyl derivatives. Comparison of theoretical and experimental ¹³ C chemical shifts. Magnetic Resonance in Chemistry, 2000, 38, 149-155.	1.1	31
86	Density functional study of a model amide. Prediction of formamide geometry, dipole moment, IR harmonic vibration $\hat{1}/2$ 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.	0.2	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.	1.8	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

#	ARTICLE	IF	CITATIONS
91	GIAO-DFT prediction of accurate NMR parameters in selected glucose derivatives. <i>Magnetic Resonance in Chemistry</i> , 1999, 37, 421-426.	1.1	33
92	A Regioselective Route to New Polytopic Receptors by Diaminolysis of Chlorocyclophosphazatriene-Containing Crown Ethers. <i>Journal of Organic Chemistry</i> , 1999, 64, 7299-7304.	1.7	44
93	Application of Optical Nuclear Polarization Enhanced ¹³ C NMR. <i>Journal of Physical Chemistry A</i> , 1998, 102, 5794-5801.	1.1	24
94	Thermodynamic vs Supramolecular Effects in the Regiocontrol of the Formation of New Cyclophosphazene-Containing Chiral Ligands with 1,1'-Binaphthyl Units: Spiro vs Ansa Substitution at the N3P3 Ring. <i>Journal of the American Chemical Society</i> , 1997, 119, 12432-12440.	6.6	54
95	Host-Guest Complex Dependent Regioselectivity in Substitution Reactions of Chlorocyclophosphazene-Containing PNP-Crowns with Alkylenediamines. <i>Journal of the American Chemical Society</i> , 1997, 119, 1143-1144.	6.6	36
96	¹⁵ N-Lactam antibiotics. Spectroscopy and molecular orbital (MO) calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1997, 53, 2649-2658.	2.0	32
97	New dioxytetraethyleneoxy macrocyclic cyclophosphazene derivatives. <i>Inorganica Chimica Acta</i> , 1995, 228, 187-192.	1.2	64
98	New Lariat Ether-Type Macrocycles with Cyclophosphazene Subunits. <i>Journal of Organic Chemistry</i> , 1995, 60, 7433-7438.	1.7	38
99	Histamine H ₂ antagonists: powerful ligands for copper(II). Reinterpretation of the famotidine-copper(II) system. <i>Journal of the Chemical Society Dalton Transactions</i> , 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. <i>Macromolecular Chemistry and Physics</i> , 1994, 195, 1843-1850.	1.1	27
103	New Heterofunctional Cyclophosphazenes with Carbonyl and Double Bond Functions. <i>Inorganic Chemistry</i> , 1994, 33, 3602-3604.	1.9	2
104	NMR studies on penicillins: Hydrogen bonding, self-association and micellar solutions of cloxacillin Na-salt in D ₂ O. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1993, 11, 103-116.	1.4	20
105	Determination of penicillin complexation sites in the presence of Zn(II) ions by AM1 and PM3 methods. <i>Computational and Theoretical Chemistry</i> , 1993, 283, 213-226.	1.5	10
106	Copper-d-penicillamine complex as potential contrast agent for MRI. <i>Magnetic Resonance Imaging</i> , 1992, 10, 855-858.	1.0	10
107	Simple, rapid and non-destructive detection and determination of phosphines and phosphine oxides in solution by ¹ H and ³¹ P NMR. <i>Fresenius' Journal of Analytical Chemistry</i> , 1991, 339, 253-257.	1.5	4
108	Application of data processing for sensitivity and resolution enhancement of ³¹ P and ¹³ C NMR spectra of humic substances. <i>Magnetic Resonance in Chemistry</i> , 1989, 27, 21-26.	1.1	8

#	ARTICLE	IF	CITATIONS
109	Improvement in the evaluation of quantitative data in FT NMR spectroscopy by the convolution difference resolution enhancement (CDRE) technique. <i>Magnetic Resonance in Chemistry</i> , 1988, 26, 353-357.	1.1	12