

# Krzysztof B BeÄ

## List of Publications by Year in descending order

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Version: 2024-02-01

82  
papers

2,177  
citations

218677

26  
h-index

254184

43  
g-index

88  
all docs

88  
docs citations

88  
times ranked

1045  
citing authors

#	ARTICLE	IF	CITATIONS
1	Rapid discrimination of <i>Curcuma longa</i> and <i>Curcuma xanthorrhiza</i> using Direct Analysis in Real Time Mass Spectrometry and Near Infrared Spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 265, 120347.	3.9	14
2	Quantification of Silymarin in <i>Silybi mariani fructus</i> : Challenging the Analytical Performance of Benchtop vs. Handheld NIR Spectrometers on Whole Seeds. <i>Planta Medica</i> , 2022, 88, 20-32.	1.3	6
3	Physical principles of infrared spectroscopy. <i>Comprehensive Analytical Chemistry</i> , 2022, , 1-43.	1.3	9
4	Miniaturized NIR Spectroscopy in Food Analysis and Quality Control: Promises, Challenges, and Perspectives. <i>Foods</i> , 2022, 11, 1465.	4.3	64
5	In silico NIR spectroscopy – A review. Molecular fingerprint, interpretation of calibration models, understanding of matrix effects and instrumental difference. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 279, 121438.	3.9	13
6	Infrared and near-infrared spectroscopic techniques for the quality control of herbal medicines. , 2022, , 603-627.		1
7	<i>Theae nigrae folium</i> : Comparing the analytical performance of benchtop and handheld near-infrared spectrometers. <i>Talanta</i> , 2021, 221, 121165.	5.5	39
8	Near-infrared spectroscopy in quality control of <i>Piper nigrum</i> : A comparison of performance of benchtop and handheld spectrometers. <i>Talanta</i> , 2021, 223, 121809.	5.5	36
9	Issues in Hyperspectral Traceability of Foods. , 2021, , 258-289.		2
10	Challenging handheld NIR spectrometers with moisture analysis in plant matrices: Performance of PLSR vs. GPR vs. ANN modelling. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 249, 119342.	3.9	29
11	NIR spectroscopy of natural medicines supported by novel instrumentation and methods for data analysis and interpretation. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2021, 193, 113686.	2.8	43
12	Principles and Applications of Miniaturized Near-Infrared (NIR) Spectrometers. <i>Chemistry - A European Journal</i> , 2021, 27, 1514-1532.	3.3	169
13	Advances, challenges and perspectives of quantum chemical approaches in molecular spectroscopy of the condensed phase. <i>Chemical Society Reviews</i> , 2021, 50, 10917-10954.	38.1	34
14	The comprehensive sourcebook for modern NIR spectroscopy: A commentary on “Near-Infrared Spectroscopy Theory, Spectral Analysis, Instrumentation, and Applications” NIR News, 2021, 32, 5-10.	0.3	1
15	Novel near-infrared and Raman spectroscopic technologies for print and photography identification, classification, and authentication. <i>NIR News</i> , 2021, 32, 11-16.	0.3	2
16	ATR-far-ultraviolet spectroscopy in the condensed phase – The present status and future perspectives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 253, 119549.	3.9	14
17	Current and future research directions in computer-aided near-infrared spectroscopy: A perspective. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 254, 119625.	3.9	26
18	Theoretical Simulation of Near-Infrared Spectrum of Piperine: Insight into Band Origins and the Features of Regression Models. <i>Applied Spectroscopy</i> , 2021, 75, 1022-1032.	2.2	20

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19	Anharmonic DFT Study of Near-Infrared Spectra of Caffeine: Vibrational Analysis of the Second Overtones and Ternary Combinations. <i>Molecules</i> , 2021, 26, 5212.	3.8	12
20	Spectra-structure correlations in NIR region of polymers from quantum chemical calculations. The cases of aromatic ring, C=O, C=N and C-Cl functionalities. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 262, 120085.	3.9	26
21	Insect Protein Content Analysis in Handcrafted Fitness Bars by NIR Spectroscopy. Gaussian Process Regression and Data Fusion for Performance Enhancement of Miniaturized Cost-Effective Consumer-Grade Sensors. <i>Molecules</i> , 2021, 26, 6390.	3.8	25
22	A Simple guide to complex world of overtone and combination bands: Theoretical simulation and interpretation of NIR spectra – summary of the workshop at NIR-2021 Beijing Conference. <i>NIR News</i> , 2021, 32, 15-18.	0.3	2
23	Anharmonicity and Spectra-Structure Correlations in MIR and NIR Spectra of Crystalline Menadione (Vitamin K3). <i>Molecules</i> , 2021, 26, 6779.	3.8	5
24	Near-Infrared (NIR) Sensors in Environmental Analysis. , 2021, , .		2
25	Scald-Cold: Joint Austrian-Italian consortium in the Euregio project for the comprehensive dissection of the superficial scald in apples. <i>NIR News</i> , 2020, 31, 5-9.	0.3	1
26	Principles and Applications of Vibrational Spectroscopic Imaging in Plant Science: A Review. <i>Frontiers in Plant Science</i> , 2020, 11, 1226.	3.6	35
27	Near-Infrared Spectroscopy as a Rapid Screening Method for the Determination of Total Anthocyanin Content in <i>Sambucus Fructus</i> . <i>Sensors</i> , 2020, 20, 4983.	3.8	29
28	Effect of conformational isomerism on NIR spectra of ethanol isotopologues. Spectroscopic and anharmonic DFT study. <i>Journal of Molecular Liquids</i> , 2020, 310, 113271.	4.9	14
29	Vibrational coupling to hydration shell – Mechanism to performance enhancement of qualitative analysis in NIR spectroscopy of carbohydrates in aqueous environment. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 237, 118359.	3.9	17
30	Near-Infrared Spectroscopy in Bio-Applications. <i>Molecules</i> , 2020, 25, 2948.	3.8	185
31	Biomolecular and bioanalytical applications of infrared spectroscopy – A review. <i>Analytica Chimica Acta</i> , 2020, 1133, 150-177.	5.4	107
32	Handheld near-infrared spectrometers: Where are we heading?. <i>NIR News</i> , 2020, 31, 28-35.	0.3	96
33	Comparative studies of vibrational properties and phase transitions in perovskite-like frameworks of $[(C_3H_7)_4N][M(N(CN)_2)_3]$ with $M = \frac{3}{4}Mn, Co, Ni$ . <i>Journal of Raman Spectroscopy</i> , 2019, 50, 1561-1571.	2.5	6
34	IR Spectra of Crystalline Nucleobases: Combination of Periodic Harmonic Calculations with Anharmonic Corrections Based on Finite Models. <i>Journal of Physical Chemistry B</i> , 2019, 123, 10001-10013.	2.6	18
35	The essential role of omni-capable research laboratories in advancing analytical spectroscopy. <i>NIR News</i> , 2019, 30, 30-34.	0.3	0
36	Spectra-Structure Correlations in Isotopomers of Ethanol (CX <sub>3</sub> CX <sub>2</sub> OX; X = H, D): Combined Near-Infrared and Anharmonic Computational Study. <i>Molecules</i> , 2019, 24, 2189.	3.8	19

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37	Overtone of $1\frac{1}{2}C\alpha\%N$ Vibration as a Probe of Structure of Liquid $CH_3CN$ , $CD_3CN$ , and $CCl_3CN$ : Combined Infrared, Near-Infrared, and Raman Spectroscopic Studies with Anharmonic Density Functional Theory Calculations. <i>Journal of Physical Chemistry A</i> , 2019, 123, 4431-4442.	2.5	27
38	Recent advances in modeling vibrational spectra of food adulterants – Theoretical simulation of IR and NIR bands of melamine. <i>NIR News</i> , 2019, 30, 5-10.	0.3	2
39	The fundamental handbook for analytical spectroscopy. Release of the second edition of –Chemometrics in spectroscopy–™ by Howard Mark and Jerry Workman, Jr. and its impact on the spectroscopic community. <i>NIR News</i> , 2019, 30, 11-13.	0.3	0
40	Distinct Difference in Sensitivity of NIR vs. IR Bands of Melamine to Inter-Molecular Interactions with Impact on Analytical Spectroscopy Explained by Anharmonic Quantum Mechanical Study. <i>Molecules</i> , 2019, 24, 1402.	3.8	38
41	Simulated NIR spectra as sensitive markers of the structure and interactions in nucleobases. <i>Scientific Reports</i> , 2019, 9, 17398.	3.3	20
42	Advances in Near-Infrared Spectroscopy and Related Computational Methods. <i>Molecules</i> , 2019, 24, 4370.	3.8	13
43	The use of vibrational spectroscopy in medicinal plant analysis: current and future directions. <i>Planta Medica</i> , 2019, 85, .	1.3	2
44	Breakthrough Potential in Near-Infrared Spectroscopy: Spectra Simulation. A Review of Recent Developments. <i>Frontiers in Chemistry</i> , 2019, 7, 48.	3.6	170
45	NIR spectroscopy in simulation – a new way for augmenting near-infrared phytoanalysis. , 2019, 85, .		0
46	Quantum mechanical modeling of NIR spectra of thymol. , 2019, 85, .		0
47	Handling of uncertainty due to interference fringe in FT-NIR transmittance spectroscopy – Performance comparison of interference elimination techniques using glucose-water system. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 197, 208-215.	3.9	7
48	Spectra-structure correlations in NIR region: Spectroscopic and anharmonic DFT study of n-hexanol, cyclohexanol and phenol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 197, 176-184.	3.9	33
49	Rydberg transitions as a probe for structural changes and phase transition at polymer surfaces: an ATR-FUV-DUV and quantum chemical study of poly(3-hydroxybutyrate) and its nanocomposite with graphene. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 8859-8873.	2.8	20
50	Advances in Anharmonic Methods and Their Applications to Vibrational Spectroscopies. , 2018, , 483-512.		9
51	Electronic Spectra of Graphene in Far- and Deep-Ultraviolet Region: Attenuated Total Reflection Spectroscopy and Quantum Chemical Calculation Study. <i>Journal of Physical Chemistry C</i> , 2018, 122, 28998-29008.	3.1	9
52	Computer simulations of NIR spectra of thymol – Towards linking basic and analytical NIRS. <i>NIR News</i> , 2018, 29, 13-16.	0.3	3
53	Near-IR Spectroscopy and Its Applications. , 2018, , 11-38.		24
54	Quantum mechanical simulations of near-infrared spectra of biomolecules – Long-chain fatty acids. <i>NIR News</i> , 2018, 29, 13-19.	0.3	3

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55	NIR spectra simulation of thymol for better understanding of the spectra forming factors, phase and concentration effects and PLS regression features. <i>Journal of Molecular Liquids</i> , 2018, 268, 895-902.	4.9	42
56	NIR Spectra Simulations by Anharmonic DFT-Saturated and Unsaturated Long-Chain Fatty Acids. <i>Journal of Physical Chemistry B</i> , 2018, 122, 6931-6944.	2.6	39
57	Influence of Non-fundamental Modes on Mid-infrared Spectra: Anharmonic DFT Study of Aliphatic Ethers. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1412-1424.	2.5	27
58	Correlations between Structure and Near-Infrared Spectra of Saturated and Unsaturated Carboxylic Acids. Insight from Anharmonic Density Functional Theory Calculations. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3437-3451.	2.5	64
59	Spectra-structure correlations of saturated and unsaturated medium-chain fatty acids. Near-infrared and anharmonic DFT study of hexanoic acid and sorbic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 185, 35-44.	3.9	38
60	Critical Evaluation of NIR and ATR-IR Spectroscopic Quantifications of Rosmarinic Acid in <i>Rosmarini folium</i> Supported by Quantum Chemical Calculations. <i>Planta Medica</i> , 2017, 83, 1076-1084.	1.3	25
61	Temperature Drift of Conformational Equilibria of Butyl Alcohols Studied by Near-Infrared Spectroscopy and Fully Anharmonic DFT. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1950-1961.	2.5	48
62	Critical evaluation of spectral information of benchtop vs. portable near-infrared spectrometers: quantum chemistry and two-dimensional correlation spectroscopy for a better understanding of PLS regression models of the rosmarinic acid content in <i>Rosmarini folium</i> . <i>Analyst</i> , 2017, 142, 455-464.	3.5	94
63	Spectroscopic and Quantum Mechanical Calculation Study of the Effect of Isotopic Substitution on NIR Spectra of Methanol. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7925-7936.	2.5	29
64	Interpretation of the $\tilde{\nu}_f$ transition of hydrated protons in aqueous solutions observed in the far-UV region with quantum chemical calculations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 21490-21499.	2.8	6
65	Quantum chemical calculation of NIR spectra of practical materials. <i>NIR News</i> , 2017, 28, 13-20.	0.3	12
66	FUV-DUV spectra of graphene, carbon nanotubes, and polymer nanocomposites (Conference) Tj ETQq0 0 0 rgBT /Overlock 1Q Tf 50 302		
67	Quantum Chemical Calculations of Basic Molecules: Alcohols and Carboxylic Acids. <i>NIR News</i> , 2016, 27, 15-21.	0.3	14
68	A spectroscopic and theoretical study in the near-infrared region of low concentration aliphatic alcohols. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 13666-13682.	2.8	72
69	Spectroscopic and Computational Study of Acetic Acid and Its Cyclic Dimer in the Near-Infrared Region. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6170-6183.	2.5	44
70	Computational and quantum chemical study on high-frequency dielectric function of tert-butylmethyl ether in mid-infrared and near-infrared regions. <i>Journal of Molecular Liquids</i> , 2016, 224, 1189-1198.	4.9	9
71	On optimization of absorption dispersion spectra. <i>Journal of Molecular Structure</i> , 2016, 1126, 11-18.	3.6	1
72	Dielectric functions of iso-propanol and di-iso-propylether in the infrared. <i>Journal of Molecular Liquids</i> , 2015, 203, 143-152.	4.9	3

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73	Vibrational analysis of neat liquid tert-butylmethylether. Journal of Molecular Liquids, 2014, 196, 26-31.	4.9	14
74	Vibrational analysis of liquid n-butylmethylether. Vibrational Spectroscopy, 2013, 64, 164-171.	2.2	13
75	Infrared dispersion of liquid di-n-propylether. Journal of Molecular Liquids, 2013, 181, 127-132.	4.9	6
76	Infrared Optical Constants and Computational Studies of Neat Liquid -Butylethylether. Journal of Spectroscopy, 2013, 2013, 1-8.	1.3	3
77	Analysis of Infrared Spectra of Neat Liquid N-Methylpyrrole. Acta Physica Polonica A, 2013, 124, 115-121.	0.5	6
78	Optical constants of liquid pyrrole in the infrared. Journal of Molecular Liquids, 2012, 172, 34-40.	4.9	18
79	Thin film IR and computational studies of liquid di-n-butylether. Journal of Molecular Structure, 2012, 1026, 51-58.	3.6	4
80	Vibrational spectra of liquid di-iso-propylether. Vibrational Spectroscopy, 2011, 55, 44-48.	2.2	10
81	Vibrational spectra of liquid di-n-propylether. Journal of Molecular Structure, 2010, 975, 205-210.	3.6	8
82	SciX 2021 summary including NIR spectroscopy session. NIR News, 0, , 096033602210763.	0.3	0