

Edith Botek

List of Publications by Year in descending order

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91
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citations

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#	ARTICLE	IF	CITATIONS
1	Observations of Electron Fluxes in the Radiation Belts with PROBA-V/EPT at Polar Low Earth Orbit and Van Allen Probes/MagEIS at Near Equatorial Elliptical Orbit. , 2022, , .		0
2	Improving Predictions of the 3D Dynamic Model of the Plasmasphere. <i>Frontiers in Astronomy and Space Sciences</i> , 2021, 8, .	2.8	10
3	Observations and Simulations of Dropout Events and Flux Decays in October 2013: Comparing MEO Equatorial With LEO Polar Orbit. <i>Journal of Geophysical Research: Space Physics</i> , 2021, 126, e2020JA028850.	2.4	21
4	Links of the Plasmopause With Other Boundary Layers of the Magnetosphere: Ionospheric Convection, Radiation Belt Boundaries, Auroral Oval. <i>Frontiers in Astronomy and Space Sciences</i> , 2021, 8, .	2.8	7
5	Assessment of the Earth's Cold Plasmatrough Modeling by Using Van Allen Probes/EMFISIS and Arase/PWE Electron Density Data. <i>Journal of Geophysical Research: Space Physics</i> , 2021, 126, e2021JA029737.	2.4	6
6	Observation of High-Energy Electrons Precipitated by NWC Transmitter From PROBA-V Low-Earth Orbit Satellite. <i>Geophysical Research Letters</i> , 2020, 47, e2020GL089077.	4.0	12
7	Electron Dropout Events and Flux Enhancements Associated With Geomagnetic Storms Observed by PROBA-V/Energetic Particle Telescope From 2013 to 2019. <i>Journal of Geophysical Research: Space Physics</i> , 2020, 125, e2020JA028487.	2.4	13
8	Dynamics of Megaelectron Volt Electrons Observed in the Inner Belt by PROBA-V/EPT. <i>Journal of Geophysical Research: Space Physics</i> , 2019, 124, 1651-1659.	2.4	10
9	Mixed Electric-Magnetic Second Order Response of Helicenes. , 2019, , 769-770.		0
10	Evaluation of Second-Order Susceptibilities of 2-methyl-4-nitroaniline (MNA) and 3-methyl-4-nitropyridine-l-oxyde (POM) Crystals. , 2019, , 783-786.		0
11	ONIOM Investigation of the Second-Order Nonlinear Optical Responses of Fluorescent Proteins. <i>Journal of Physical Chemistry B</i> , 2018, 122, 4993-5005.	2.6	18
12	Modeling the space environment and its effects on spacecraft and astronauts using SPENVIS. , 2018, , .		1
13	Approximate spin projected spin-unrestricted density functional theory method: Application to diradical character dependences of second hyperpolarizabilities. , 2015, , .		1
14	Prediction of first hyperpolarizability of fluorescent proteins. <i>AIP Conference Proceedings</i> , 2015, , .	0.4	3
15	Relationship between second hyperpolarizability and diradical character in open-shell singlet metal-metal multiply bonded systems. , 2015, , .		0
16	Validation of reactive gases and aerosols in the MACC global analysis and forecast system. <i>Geoscientific Model Development</i> , 2015, 8, 3523-3543.	3.6	49
17	Static electric field effect on third-order nonlinear optical (NLO) properties of singlet diradical molecules: Toward the realization of an electric field induced open-shell NLO switch. , 2015, , .		0
18	In situ nitroxide-mediated polymerization of styrene promoted by the tert-butyl- α -cyclopropylnitron/bpo pair: ESR investigations. <i>Journal of Polymer Science Part A</i> , 2013, 51, 1786-1795.	2.3	2

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19	Electron donor solvent effects on the (Hyper) polarizabilities of a solute presenting singlet diradical character. AIP Conference Proceedings, 2012, , .	0.4	2
20	Spin polarization and third-order nonlinear optical properties of open-shell singlet graphene nanoflakes. , 2012, , .		0
21	Electron spin resonance spectra of nitroxyl radicals. , 2012, , .		0
22	Second hyperpolarizabilities of singlet diradical compounds and their radical ions. , 2012, , .		0
23	Long-range-corrected UDFT study on second hyperpolarizabilities of open-shell singlet systems. , 2012, , .		0
24	Theoretical consideration of singlet open-shell character of polyperiacenes using Clar's aromatic sextet valence bond model and quantum chemical calculations. AIP Conference Proceedings, 2012, , .	0.4	54
25	One- and two-photon absorptions in open-shell singlet systems. AIP Conference Proceedings, 2012, , .	0.4	13
26	Theoretical aspects on the evaluation and interpretation of the third-order nonlinear optical properties of diradical compounds. , 2012, , .		0
27	Linear and nonlinear second order susceptibilities of molecular crystals. , 2012, , .		0
28	Second-order nonlinear optical responses of flexible pyridine-pyrimidine foldamers. , 2012, , .		0
29	Combined experimentalâ€”theoretical NMR study on 2,5â€”bis(5â€”arylâ€”hexylthiophenâ€”2â€”yl)â€”thiazolo[5,4â€”d</i>]thiazole derivatives for printable electronics. Magnetic Resonance in Chemistry, 2012, 50, 379-387.	3.9	6
30	Functionalized Dithienylthiazolo[5,4â€”d</i>]thiazoles For Solutionâ€”Processable Organic Fieldâ€”Effect Transistors. ChemPlusChem, 2012, 77, 923-930.	2.8	12
31	Enhancement of Second Hyperpolarizabilities in Open-Shell Singlet Slipped-Stack Dimers Composed of Square Planar Nickel Complexes Involving <i>o</i>-Semiquinonato Type Ligands. Journal of Physical Chemistry A, 2011, 115, 1117-1124.	2.5	21
32	Amyloseâ€”Vanillin Complexation Assessed by a Joint Experimental and Theoretical Analysis. Journal of Physical Chemistry C, 2011, 115, 23315-23322.	3.1	19
33	Fingerprints for Structural Defects in Poly(thienylene vinylene) (PTV): A Joint Theoreticalâ€”Experimental NMR Study on Model Molecules. Journal of Physical Chemistry B, 2011, 115, 12040-12050.	2.6	8
34	(Hyper)polarizability density analysis for open-shell molecular systems based on natural orbitals and occupation numbers. Theoretical Chemistry Accounts, 2011, 130, 711-724.	1.4	125
35	Openâ€”Shell Characters and Second Hyperpolarizabilities of Oneâ€”Dimensional Graphene Nanoflakes Composed of Trigonal Graphene Units. ChemPhysChem, 2011, 12, 1697-1707.	2.1	46
36	From Molecular to Macroscopic Engineering: Shaping Hydrogenâ€”Bonded Organic Nanomaterials. Chemistry - A European Journal, 2011, 17, 3262-3273.	3.3	29

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37	Synthesis and Characterization of Teranthene: A Singlet Biradical Polycyclic Aromatic Hydrocarbon Having Kekulé Structures. <i>Journal of the American Chemical Society</i> , 2010, 132, 11021-11023.	13.7	285
38	A joint theoretical and experimental investigation on the ¹³ C and ¹ H NMR chemical shifts of coumarin derivatives. <i>Theoretical Chemistry Accounts</i> , 2010, 125, 461-470.	1.4	6
39	Electrostatic modeling of the linear optical susceptibilities of 2-methyl-4-nitroaniline, m-nitroaniline, 3-methyl-4-nitropyridine N-oxide and 2-carboxylic acid-4-nitropyridine-1-oxide crystals. <i>Chemical Physics Letters</i> , 2010, 487, 256-262.	2.6	23
40	Signature of multiradical character in second hyperpolarizabilities of rectangular graphene nanoflakes. <i>Chemical Physics Letters</i> , 2010, 489, 212-218.	2.6	90
41	Approximate spin-projected spin-unrestricted density functional theory method: Application to the diradical character dependences of the (hyper)polarizabilities in p-quinodimethane models. <i>Chemical Physics Letters</i> , 2010, 501, 140-145.	2.6	32
42	Theoretical investigation on the second hyperpolarizabilities of open-shell singlet systems by spin-unrestricted density functional theory with long-range correction: Range separating parameter dependence. <i>Chemical Physics Letters</i> , 2010, 493, 195-199.	2.6	59
43	NONLINEAR OPTICAL PROPERTIES OF mSTRAWBERRY AND mCHERRY FOR SECOND HARMONIC IMAGING. <i>Journal of Nonlinear Optical Physics and Materials</i> , 2010, 19, 1-13.	1.8	10
44	A Singlet Biradical Polycyclic Aromatic Hydrocarbon. <i>Synfacts</i> , 2010, 2010, 1238-1238.	0.0	0
45	Long-range corrected density functional theory study on static second hyperpolarizabilities of singlet diradical systems. <i>Journal of Chemical Physics</i> , 2010, 132, 094107.	3.0	82
46	A Three-Step Synthetic Approach to Asymmetrically Functionalized 4-H-Cyclopenta[2,1-b:3,4-b ²]dithiophenes. <i>Journal of Organic Chemistry</i> , 2010, 75, 7202-7209.	3.2	24
47	Singlet Diradical Character from Experiment. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 937-940.	4.6	181
48	Giant electric field effect on the second hyperpolarizability of symmetric singlet diradical molecules. <i>Journal of Chemical Physics</i> , 2010, 133, 154302.	3.0	38
49	Theoretical and experimental investigation of the structural and spectroscopic properties of coumarin 343 fluoroionophores. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 14172.	2.8	23
50	Nonlinear and Chiro-Optical Properties of Aromatic Foldamers. , 2009, , .		0
51	Third-Order Nonlinear Optical Properties of Open-Shell Systems: Diradical Character and Spin State Dependences. , 2009, , .		0
52	Study of Structural Effects in Poly(vinyl Chloride) by Theoretical Simulation and Interpretation of NMR Spectra. , 2009, , .		0
53	Third-order nonlinear optical properties of trigonal, rhombic and bow-tie graphene nanoflakes with strong structural dependence of diradical character. <i>Chemical Physics Letters</i> , 2009, 480, 278-283.	2.6	49
54	Electron donor solvent effects on the (hyper)polarizabilities of a singlet diradical molecule involving a boron atom. <i>Chemical Physics Letters</i> , 2009, 477, 309-314.	2.6	9

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55	Theoretical study on third-order nonlinear optical properties in hexagonal graphene nanoflakes: Edge shape effect. <i>Chemical Physics Letters</i> , 2009, 477, 355-359.	2.6	74
56	Effect of the Dynamical Disorder on the Second-Order Nonlinear Optical Responses of Helicity-Encoded Polymer Strands. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6552-6554.	2.5	25
57	Second-order nonlinear optical properties of fluorescent proteins for second-harmonic imaging. <i>Journal of Materials Chemistry</i> , 2009, 19, 7514.	6.7	42
58	Remarkable two-photon absorption in open-shell singlet systems. <i>Journal of Chemical Physics</i> , 2009, 131, 114316.	3.0	54
59	Theoretical study on the second hyperpolarizability of open-shell singlet one-dimensional systems with a charged defect. <i>Chemical Physics Letters</i> , 2008, 451, 111-115.	2.6	13
60	Intermolecular interaction effects on the second hyperpolarizability of open-shell singlet diphenalenyl radical dimer. <i>Chemical Physics Letters</i> , 2008, 454, 97-104.	2.6	36
61	Theoretical study of third-order nonlinear optical properties in square nanographenes with open-shell singlet ground states. <i>Chemical Physics Letters</i> , 2008, 467, 120-125.	2.6	96
62	A Joined Theoretical~Experimental Investigation on the 1H and 13C NMR Signatures of Defects in Poly(vinyl chloride). <i>Journal of Physical Chemistry B</i> , 2008, 112, 14804-14818.	2.6	33
63	Theoretical and Experimental Investigation of Electric Field Induced Second Harmonic Generation in Tetrathia[7]helicenes. <i>Journal of Physical Chemistry C</i> , 2008, 112, 7900-7907.	3.1	104
64	Joint Theoretical Experimental Investigation of the Electron Spin Resonance Spectra of Nitroxyl Radicals: Application to Intermediates in in Situ Nitroxide Mediated Polymerization (in Situ NMP) of Vinyl Monomers. <i>Journal of Physical Chemistry B</i> , 2008, 112, 10432-10442.	2.6	9
65	Theoretical investigation on the linear and nonlinear susceptibilities of urea crystal. <i>Journal of Chemical Physics</i> , 2008, 128, 244713.	3.0	26
66	Evaluation of the Molecular Polarizability Using the IPPP~CLOPPA~INDO/S Method. Application to Molecules of Biological Interest. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6992-6998.	2.5	11
67	Theoretical Study on Second Hyperpolarizabilities of Singlet Diradical Square Planar Nickel Complexes Involving σ -Semiquinonato Type Ligands. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8423-8429.	2.5	49
68	Second-Harmonic Generation in GFP-like Proteins. <i>Journal of the American Chemical Society</i> , 2008, 130, 15713-15719.	13.7	66
69	Spin State Dependence of Second Hyperpolarizabilities of Zethrenes. <i>AIP Conference Proceedings</i> , 2008, , .	0.4	0
70	Theoretical Evaluation of the Faraday Effect in Organic Compounds. <i>Computing Letters</i> , 2007, 3, 193-200.	0.5	3
71	Second Hyperpolarizability of Zethrenes. <i>Computing Letters</i> , 2007, 3, 333-338.	0.5	60
72	Relationship between Third-Order Nonlinear Optical Properties and Magnetic Interactions in Open-Shell Systems: A New Paradigm for Nonlinear Optics. <i>Physical Review Letters</i> , 2007, 99, 033001.	7.8	258

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73	Circular dichroism of helical structures using semiempirical methods. <i>Journal of Chemical Physics</i> , 2007, 127, 204101.	3.0	34
74	Finite-Field Spin-Flip Configuration Interaction Calculation of the Second Hyperpolarizabilities of Singlet Diradical Systems. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1699-1707.	5.3	41
75	Theoretical Study on the Second Hyperpolarizabilities of Phenalenyl Radical Systems Involving Acetylene and Vinylene Linkers: A Diradical Character and Spin Multiplicity Dependences. <i>Journal of Physical Chemistry A</i> , 2007, 111, 3633-3641.	2.5	84
76	Second Hyperpolarizabilities of Singlet Polycyclic Diphenalenyl Radicals: Effects of the Nature of the Central Heterocyclic Ring and Substitution to Diphenalenyl Rings. <i>Journal of Physical Chemistry A</i> , 2007, 111, 9102-9110.	2.5	25
77	Second Hyperpolarizabilities ($\hat{\beta}^3$) of 1,3-Dipole Systems: Diradical Character Dependence of $\hat{\beta}^3$. AIP Conference Proceedings, 2007, . .	0.4	0
78	A joined theoretical/experimental investigation on the ^1H and ^{13}C NMR chemical shifts of chloro-alkenes. <i>Chemical Physics Letters</i> , 2007, 436, 388-393.	2.6	20
79	Theoretical investigation on bridged triarylamine helicenes: UV/visible and circular dichroism spectra. <i>Chemical Physics Letters</i> , 2007, 439, 213-218.	2.6	29
80	First and second hyperpolarizabilities of donor/acceptor disubstituted diphenalenyl radical systems. <i>Chemical Physics Letters</i> , 2007, 443, 95-101.	2.6	43
81	Theoretical investigation on ^1H and ^{13}C NMR chemical shifts of small alkanes and chloroalkanes. <i>Journal of Chemical Physics</i> , 2006, 125, 144309.	3.0	37
82	Second Hyperpolarizabilities ($\hat{\beta}^3$) of Bisimidazole and Bistriazole Benzenes: A Diradical Character, Charged State, and Spin State Dependences. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4238-4243.	2.5	100
83	Elongation method and supermolecule approach for the calculation of nonlinear susceptibilities. Application to the 3-Methyl-4-Nitropyridine 1-Oxide and 2-Methyl-4-Nitroaniline crystals. <i>Journal of Computational Methods in Sciences and Engineering</i> , 2006, 6, 171-188.	0.2	9
84	Theoretical investigation of the chain length effects on the NMR chemical shifts of oligomers. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 3113-3121.	2.0	5
85	Second hyperpolarizability of phenalenyl radical system involving acetylene π -conjugated bridge. <i>Chemical Physics Letters</i> , 2006, 420, 432-437.	2.6	33
86	Second hyperpolarizabilities of polycyclic diphenalenyl radicals: Effects of para/ortho-quinoid structures and central ring modification. <i>Chemical Physics Letters</i> , 2006, 429, 174-179.	2.6	20
87	Second hyperpolarizabilities ($\hat{\beta}^3$) of open-shell singlet one-dimensional systems: Intersite interaction effects on the average diradical character and size dependences of $\hat{\beta}^3$. <i>Chemical Physics Letters</i> , 2006, 432, 473-479.	2.6	34
88	Theoretical Investigation of the Second-Order Nonlinear Optical Properties of Helical Pyridine/Pyrimidine Oligomers. <i>Chemistry - A European Journal</i> , 2006, 12, 8687-8695.	3.3	38
89	A Joint Theoretical/Experimental Investigation of the Faraday Effect in Benzene, Toluene, and p-Xylene. <i>ChemPhysChem</i> , 2006, 7, 1654-1656.	2.1	22
90	Origin of the enhancement of the second hyperpolarizability of singlet diradical systems with intermediate diradical character. <i>Journal of Chemical Physics</i> , 2006, 125, 074113.	3.0	88

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91	Theoretical Study on the Second Hyperpolarizabilities of Diphenalenyl Radical Systems. , 2006, , 231-240.		0