Martin Breza

List of Publications by Year
in descending order

181	1,869	331670 21	434195 31
papers	citations	h-index	g-index

191	191	191	2018
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantumâ€chemical studies of the antioxidant effectiveness of paraâ€phenylene diamines. Journal of Vinyl and Additive Technology, 2022, 28, 352-366.	3.4	3
2	DFT studies of camptothecins cytotoxicity II. Protonated lactone forms of camptothecin. Computational and Theoretical Chemistry, 2022, 1211, 113677.	2.5	5
3	Structural and Biofunctional Insights into the Cyclo(Pro-Pro-Phe-Phe-) Scaffold from Experimental and In Silico Studies: Melanoma and Beyond. International Journal of Molecular Sciences, 2022, 23, 7173.	4.1	5
4	Comparative DFT study of the effectiveness of p-phenylenediamine antioxidants through their coordination ability towards the late 1st row transition metals. Polymer Degradation and Stability, 2021, 183, 109438.	5.8	15
5	Dimethyl amino phenyl substituted silver phthalocyanine as a UV- and visible-light absorbing photoinitiator: in situ preparation of silver/polymer nanocomposites. Polymer Chemistry, 2021, 12, 1273-1285.	3.9	10
6	Electronic structure of Schiff-base peroxo{2,2â€²-[1,2-phenylenebis(nitrilomethanylylidene)]bis(6-methoxyphenolato)}titanium(IV) monohydrate: a possible model structure of the reaction center for the theoretical study of hemoglobin. IUCrJ, 2021, 8, 295-304.	2.2	2
7	The First Insight Into the Supramolecular System of D,L-Î±-Difluoromethylornithine: A New Antiviral Perspective. Frontiers in Chemistry, 2021, 9, 679776.	3.6	7
8	On the relation between oxidation states and d-electron populations of the 1st row transition metal complexes I. Tetrachloro complexes. Polyhedron, 2021, 201, 115172.	2.2	4
9	Lawsone Derivatives as Efficient Photopolymerizable Initiators for Free-Radical, Cationic Photopolymerizations, and Thiolâ€"Ene Reactions. Polymers, 2021, 13, 2015.	4.5	10
10	Triapine Analogues and Their Copper(II) Complexes: Synthesis, Characterization, Solution Speciation, Redox Activity, Cytotoxicity, and mR2 RNR Inhibition. Inorganic Chemistry, 2021, 60, 11297-11319.	4.0	10
11	DFT Studies of Substituted Phenols Cytotoxicity I. Para â€substituted Phenols. ChemistrySelect, 2021, 6, 7049-7055.	1.5	12
12	DFT studies of the toxicity of alkylphenols to Tetrahymena pyriformis. Polyhedron, 2021, 207, 115360.	2.2	12
13	DFT studies of camptothecins cytotoxicity I. Active and inactive forms of camptothecin. Computational and Theoretical Chemistry, 2021, 1206, 113461.	2.5	9
14	Quantum-chemical studies of rutile nanoparticles toxicity II. Comparison of B3LYP and PM6 data. Acta Chimica Slovaca, 2021, 14, 38-50.	0.8	15
15	Quantumâ€chemical study of octafluoroâ€spirobi[triphosphazene]. International Journal of Quantum Chemistry, 2021, 121, e26613.	2.0	0
16	DFT studies of the toxicity of 4-substituted 1,2-benzoquinones. Polyhedron, 2021, 210, 115532.	2.2	9
17	Electronic structure of (MePh₃P)₂[Ni^{II}(bdtCl₂)₂]Â·2(CH₃)₂SO and (MePh₃P)[Ni^{III}(bdtCl₂)₂] (bdtCl₂ =) Tj ETQq1 1 0.784314 rgBT /O Engineering and Materials, 2021, 77, 919-929.	1.1	3
18	Nickel(II), Copper(II) and Palladium(II) Complexes with Bis-Semicarbazide Hexaazamacrocycles: Redox-Noninnocent Behavior and Catalytic Activity in Oxidation and Câ€"C Coupling Reactions. Inorganic Chemistry, 2020, 59, 10650-10664.	4.0	5

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19	A Proline-Based Tectons and Supramolecular Synthons for Drug Design 2.0: A Case Study of ACEI. Pharmaceuticals, 2020, 13, 338.	3.8	10
20	Mass spectrometrical and quantumâ€chemical study of pentafluorophenylhydrazones. Journal of Mass Spectrometry, 2020, 55, e4540.	1.6	1
21	Comparative study of p-phenylenediamine antioxidant effectiveness in styrene-butadiene and polyisoprene rubber through NMR calculations. Polymer Degradation and Stability, 2020, 177, 109196.	5.8	4
22	A Supramolecular Approach to Structure-Based Design with A Focus on Synthons Hierarchy in Ornithine-Derived Ligands: Review, Synthesis, Experimental and in Silico Studies. Molecules, 2020, 25, 1135.	3.8	45
23	On shape dependence of the toxicity of rutile nanoparticles. Journal of Nanoparticle Research, 2020, 22, 1.	1.9	19
24	Unexpected Cleavage of Nâ€N Bonds of Pentafluorophenylhydrazones â€“ Formation of Nitriles by a Radical Fragmentation Reaction. ChemistrySelect, 2020, 5, 3929-3933.	1.5	1
25	QTAIM study of Al Al bonding in [LiAl2H4]â^' complex anions. Polyhedron, 2019, 165, 17-21.	2.2	1
26	High-Frequency and -Field EPR (HFEPR) Investigation of a Pseudotetrahedral Cr^{IV} Siloxide Complex and Computational Studies of Related Cr^{IV}L₄ Systems. Inorganic Chemistry, 2019, 58, 4907-4920.	4.0	11
27	Quantum-chemical studies of rutile nanoparticles toxicity I. Defect-free rod-like model clusters. Acta Chimica Slovaca, 2019, 12, 168-174.	0.8	15
28	Synthesis of Branchedâ€Chain Sugars with a DHAPâ€Dependent Aldolase: Ketones are Electrophile Substrates of Rhamnuloseâ€1â€phosphate Aldolases. Angewandte Chemie, 2018, 130, 5565-5569.	2.0	7
29	Synthesis of Branchedâ€Chain Sugars with a DHAPâ€Dependent Aldolase: Ketones are Electrophile Substrates of Rhamnuloseâ€1â€phosphate Aldolases. Angewandte Chemie - International Edition, 2018, 57, 5467-5471.	13.8	23
30	Synthesis and isomerization of acridine substituted 1,3-thiazolidin-4-ones and 4-oxo-1,3-thiazolidin-5-ylidene acetates. An experimental and computational study. Journal of Molecular Structure, 2018, 1154, 152-164.	3.6	12
31	The design and NMR structure determination of yttrium-oligopeptide tags for recombinant proteins and antibodies. Acta Chimica Slovaca, 2018, 11, 120-133.	0.8	0
32	DFT studies of camptothecin aggregation in solutions. Computational and Theoretical Chemistry, 2018, 1143, 1-8.	2.5	6
33	Electronic structure of two isostructural `paddle-wheel' complexes: a comparative study. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2018, 74, 681-692.	1.1	14
34	Quantum-chemical study of the active sites of camptothecin through their Cu(II) coordination ability. Acta Chimica Slovaca, 2018, 11, 6-10.	0.8	11
35	DFT studies of the effectiveness of p-substituted diphenyl amine antioxidants in styrene-butadiene rubber through their Cu(II) coordination ability. Chemical Physics Letters, 2017, 680, 78-82.	2.6	18
36	Spectroscopic and Computational Studies of Spin States of Iron(IV) Nitrido and Imido Complexes. Inorganic Chemistry, 2017, 56, 4751-4768.	4.0	41

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37	On NMR prediction of the antioxidant effectiveness of heterocyclic nitrogen compounds and substituted amines in styrene-butadiene rubber. Polymer Degradation and Stability, 2017, 144, 1-6.	5.8	4
38	A five-coordinate manganese(<scp>iii</scp>) complex of a salen type ligand with a positive axial anisotropy parameter D. Dalton Transactions, 2017, 46, 11817-11829.	3.3	20
39	Ligand Substituent Effects in Manganese Pyridinophane Complexes: Implications for Oxygen-Evolving Catalysis. Inorganic Chemistry, 2017, 56, 14315-14325.	4.0	22
40	Antioxidant effectiveness of dehydrogenated p-phenylene diamines through NMR calculations. Acta Chimica Slovaca, 2016, 9, 100-103.	0.8	5
41	DFT studies of the effectiveness of p-phenylenediamine antioxidants through their Cu(II) coordination ability. Polymer Degradation and Stability, 2016, 128, 15-21.	5.8	30
42	HFEPR and Computational Studies on the Electronic Structure of a High-Spin Oxidoiron(IV) Complex in Solution. Inorganic Chemistry, 2016, 55, 3933-3945.	4.0	11
43	Vanadium(V) Complexes with Substituted 1,5-bis(2-hydroxybenzaldehyde)carbohydrazones and Their Use As Catalyst Precursors in Oxidation of Cyclohexane. Inorganic Chemistry, 2016, 55, 9187-9203.	4.0	49
44	On NMR prediction of the antioxidant effectiveness of p-substituted diphenyl amines. Polymer Degradation and Stability, 2016, 130, 189-193.	5.8	5
45	QTAIM studies of [Li(DMSO)n]+ and [Al(DMSO)n]3+. AIP Conference Proceedings, 2015, , .	0.4	2
46	Charge and Spin States in Schiff Base Metal Complexes with a Disiloxane Unit Exhibiting a Strong Noninnocent Ligand Character: Synthesis, Structure, Spectroelectrochemistry, and Theoretical Calculations. Inorganic Chemistry, 2015, 54, 5691-5706.	4.0	29
47	Hemidirected [M(II)L4]q structures and Jahnâ€“Teller effect. Chemical Physics, 2015, 460, 56-63.	1.9	2
48	On molecular and electron structures of neutral and charged forms of a dinuclear zinc(II) complex with diphenylamine ligands. Chemical Physics Letters, 2015, 639, 211-216.	2.6	1
49	On NMR prediction of the effectiveness of p-phenylenediamine antioxidants. Chemical Physics Letters, 2015, 639, 78-82.	2.6	11
50	Use of activated enol ethers in the synthesis of pyrazoles: reactions with hydrazine and a study of pyrazole tautomerism. Beilstein Journal of Organic Chemistry, 2014, 10, 752-760.	2.2	16
51	Structural, magnetic and quantum-chemical study of dinuclear copper(II) thiophenecarboxylate and furancarboxylate complexes. Polyhedron, 2014, 81, 216-226.	2.2	20
52	Copper(II) complexes with 1,5-bis(2-hydroxybenzaldehyde)carbohydrazone. Polyhedron, 2014, 80, 180-192.	2.2	9
53	Structural analysis of an impurity of the drug landiolol. Magnetic Resonance in Chemistry, 2014, 52, 122-127.	1.9	0
54	Structure and vibrational spectra of copper(II) 2-pyridylmethanolate tetrahydrate. Chemical Papers, 2014, 68, .	2.2	2

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55	Redox Reactions of Nickel, Copper, and Cobalt Complexes with â€œNoninnocentâ€•Dithiolate Ligands: Combined in Situ Spectroelectrochemical and Theoretical Study. Organometallics, 2014, 33, 4846-4859.	2.3	29
56	On UVâ€“Vis spectra and structure of the anticancer drug camptothecin in solutions. Chemical Physics Letters, 2013, 580, 141-144.	2.6	15
57	Copper(II) Complexes with Schiff Bases Containing a Disiloxane Unit: Synthesis, Structure, Bonding Features and Catalytic Activity for Aerobic Oxidation of Benzyl Alcohol. European Journal of Inorganic Chemistry, 2013, 2013, 1458-1474.	2.0	58
58	On the Electronic Structure of mer,transâ€[RuCl₃(1Hâ€indazole)₂(NO)], a Hypothetical Metabolite of the Antitumor Drug Candidate KP1019: An Experimental and DFT Study. European Journal of Inorganic Chemistry, 2013, 2013, 2505-2519.	2.0	18
59	Marked Stabilization of Redox States and Enhanced Catalytic Activity in Galactose Oxidase Models Based on Transition Metal S-Methylisothiosemicarbazonates with â^’SR Group in Ortho Position to the Phenolic Oxygen. Inorganic Chemistry, 2013, 52, 7524-7540.	4.0	22
60	Preparation and Spectroscopic, Magnetic, and Electrochemical Studies of Mono-/Biradical TEMPO Derivatives. Journal of Organic Chemistry, 2013, 78, 6558-6569.	3.2	17
61	QTAIM study of transition metal complexes with cyclophosphazene-based multisite ligands II. Cobalt(II) complexes. Polyhedron, 2012, 31, 570-574.	2.2	4
62	Syntheses, Electronic Structures, and EPR/UVâ^’Visâ^’NIR Spectroelectrochemistry of Nickel(II), Copper(II), and Zinc(II) Complexes with a Tetradentate Ligand Based on S-Methylisothiosemicarbazide. Inorganic Chemistry, 2011, 50, 2918-2931.	4.0	43
63	DFT study of magnetic coupling in bis(pyridine-2-carboxylate)-copper(II) polymorphs. Solid State Communications, 2011, 151, 1920-1923.	1.9	0
64	Theoretical study of structural and optical properties of lithium cation complexes with dimethyl sulfoxide. Computational and Theoretical Chemistry, 2011, 963, 503-509.	2.5	10
65	Quantum-chemical study of transition metal complexes with benzene-1,2-dithiolate. Polyhedron, 2011, 30, 307-314.	2.2	7
66	On the origin of the hemidirected geometry of tetracoordinated lead(II) compounds. Chemical Physics, 2010, 368, 14-19.	1.9	14
67	Application of the Gouldâ€“Jacobs reaction to 4-amino-2,1,3-benzoselenadiazole. Tetrahedron, 2010, 66, 8169-8174.	1.9	22
68	Why is monoalkylation versus bis-alkylation of the Ni(II) complex of the Schiff base of (S)-N-(2-benzoylphenyl)-1-benzylpyrrolidine-2-carboxamide and glycine so selective? MP2 modelling and topological QTAIM analysis of chiral metallocomplex synthons of Î±-amino acids used for the preparation of radiopharmaceuticals for positron emission tomography. Journal of Radioanalytical and Nuclear Chemistry, 2010, 286, 829-833.	1.5	3
69	DFT study of bis(picolinato-N,O)-copper(II) complex. Polyhedron, 2010, 29, 2440-2444.	2.2	6
70	On electronic structure of tris(dimethylamino)sulphonium heptafluoro-oxocyclotetraphosphazenate. Computational and Theoretical Chemistry, 2009, 894, 32-35.	1.5	4
71	QTAIM study of transition metal complexes with cyclophosphazene-based multisite ligands I: Zinc(II) and nickel(II) complexes. Polyhedron, 2009, 28, 521-524.	2.2	27
72	A variety of oxidation products of antioxidants based on N,Nâ€²-substituted p-phenylenediamines. Polymer Degradation and Stability, 2009, 94, 1457-1466.	5.8	40

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73	Conformational and isomerizational studies of 3-N,N-dimethylhydrazino-2-acetyl propenenitrile using X-ray analysis, NMR and vibrational spectra, and ab initio calculations. Journal of Molecular Structure, 2009, 938, 97-110.	3.6	9
74	Group-Theoretical Analysis of Jahnâ€“Teller Systems. Springer Series in Chemical Physics, 2009, , 51-76.	0.2	1
75	On the structure of hexahydroxocyclotriphosphazene. Computational and Theoretical Chemistry, 2008, 861, 33-38.	1.5	4
76	On electronic structure of neutral and monocharged 9,9â€²-spirobifluorene. Computational and Theoretical Chemistry, 2008, 851, 277-283.	1.5	9
77	Conformational and isomerizational studies of 3-N,N-dimethylhydrazino-2-methylsulfonyl propenenitrile using NMR and vibrational spectra, X-ray analysis and ab initio calculations. Journal of Molecular Structure, 2008, 891, 192-204.	3.6	3
78	On the Structure of Tri- and Tetrahydroxolead(II) Complex Anions. Collection of Czechoslovak Chemical Communications, 2008, 73, 59-72.	1.0	5
79	On the dehydrogenation of N,Nâ€²-substituted p-phenylenediamine antioxidants. Vibrational Spectroscopy, 2007, 44, 1-8.	2.2	20
80	Thermochromism of bithiophenes and internal aromatic chain rotation. Computational and Theoretical Chemistry, 2007, 820, 35-39.	1.5	7
81	DFT studies of copper complexes with biphenyldiimino dithioether. Part III: AIM analysis. Polyhedron, 2007, 26, 4156-4160.	2.2	2
82	Photochemical Properties of Camptothecin in the Presence of Copper(II) Ions: The Role of Radicals as Prospective Species in Photodynamic Therapy. Molecular Biotechnology, 2007, 37, 48-51.	2.4	6
83	On SOCl2 hydrolysis at carbon nanotubes. Chemical Physics, 2006, 330, 224-230.	1.9	10
84	DFT studies of copper complexes with biphenyldiimino dithioether II. Mechanical strain. Polyhedron, 2006, 25, 2559-2564.	2.2	3
85	On the dehydrogenation of N,Nâ€²-substituted p-phenylenediamine antioxidants. I. N-Phenyl-Nâ€²-isopropyl-p-phenylenediamine (IPPD). Polymer Degradation and Stability, 2006, 91, 1775-1780.	5.8	20
86	DFT study of the reaction sites of N,Nâ€²-substituted p-phenylenediamine antioxidants. Polymer Degradation and Stability, 2006, 91, 2848-2852.	5.8	14
87	N-Salicylideneaminoacidato copper(II) complexes as galactose oxidase model compounds. Computational and Theoretical Chemistry, 2006, 760, 141-145.	1.5	1
88	On the bridging mode in tetrahedral tetralead(II) hydroxocomplexes. Computational and Theoretical Chemistry, 2006, 765, 121-126.	1.5	7
89	On the reduced form of (imidazole-N3)(N-salicylidene-alaninato-O,N,Oâ€²) copper(II). Computational and Theoretical Chemistry, 2006, 770, 139-144.	1.5	2
90	Model studies of SOCl2 adsorption on carbon nanotubes. Computational and Theoretical Chemistry, 2006, 767, 159-163.	1.5	14

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91	Conformational Influence on Deprotonation of Bis(methoxycarbimido)amine Ligand. Collection of Czechoslovak Chemical Communications, 2005, 70, 313-326.	1.0	0
92	DFT studies of copper complexes with biphenyldiimino dithioether. Computational and Theoretical Chemistry, 2005, 718, 175-181.	1.5	3
93	Torsional dependence of the reactivity of diphenylamine-type antioxidants. Computational and Theoretical Chemistry, 2005, 723, 23-28.	1.5	16
94	Quantum-chemical studies of benzazoles nitration. Arkivoc, 2005, 2005, 80-89.	0.5	7
95	On the Structure of Boat-Shaped Hexalead(II) Cations with OH Bridges. Collection of Czechoslovak Chemical Communications, 2004, 69, 2055-2067.	1.0	3
96	Electronic structure of the nickel(II) complex of the Schiff base of (S)-N-(2-benzoylphenyl)-1-benzylprolinamide and glycine. Acta Crystallographica Section A: Foundations and Advances, 2004, 60, 510-516.	0.3	19
97	The Stability of Hydroxoâ€"Dilead(II) Complex Cations. ChemInform, 2004, 35, no.	0.0	0
98	On the geometry, electrical properties and optical spectra of spirobifluorene type molecules. Journal of Molecular Structure, 2004, 699, 93-99.	3.6	7
99	Comparative study of non-planar cyclotetraphosphazenes and their isostructural hydrocarbon analogues. Computational and Theoretical Chemistry, 2004, 679, 131-136.	1.5	8
100	Quantum chemical study of the preferential ortho-addition of phenoxyl radicals to nitroso spin-traps II. AIM analysis. Computational and Theoretical Chemistry, 2004, 683, 167-169.	1.5	3
101	MP2 studies of copper complexes with bis(methoxycarbimido)amine and its anion. Computational and Theoretical Chemistry, 2004, 711, 115-121.	1.5	2
102	ESR/UVâ€"Visâ€"NIR cyclovoltammetry of macrocyclic complex [CuI(bite)]BF4 at different temperatures. Journal of Electroanalytical Chemistry, 2004, 566, 123-129.	3.8	6
103	MP2 studies of the bis(methoxycarbimido)amine ligand and its anion. Polyhedron, 2004, 23, 2235-2242.	2.2	4
104	On the Structure of Tetralead(II) Complexes with OH Bridges. Collection of Czechoslovak Chemical Communications, 2004, 69, 2045-2054.	1.0	4
105	Quantum chemical study of the preferential ortho-addition of phenoxyl radicals to nitroso spin-traps. Computational and Theoretical Chemistry, 2003, 624, 251-255.	1.5	6
106	On the structure of lead(II) complexes in aqueous solutions.. Polyhedron, 2003, 22, 2863-2867.	2.2	9
107	On non-planarity of cyclotetraphosphazenes. Polyhedron, 2003, 22, 3243-3248.	2.2	6
108	Some comments on â€œJahnâ€"Teller effect in coronene monoanion: a comparative study with corannulene monoanionâ€•[Chem. Phys. 287 (2003) 91]. Chemical Physics, 2003, 291, 207-212.	1.9	7

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109	New NIR dyes for ammonia sensing. Sensors and Actuators B: Chemical, 2003, 90, 9-14.	7.8	8
110	Role of Radicals and Singlet Oxygen in Photoactivated DNA Cleavage by the Anticancer Drug Camptothecin:Â An Electron Paramagnetic Resonance Study. Journal of Physical Chemistry B, 2003, 107, 2415-2425.	2.6	70
111	Optical properties of furanic and thiophenic ethane-1,2-diones. Synthetic Metals, 2003, 138, 399-408.	3.9	17
112	On the Stability of Hydroxo-Dilead(II) Complex Cations. Collection of Czechoslovak Chemical Communications, 2003, 68, 2377-2385.	1.0	7
113	On the Structure of Lead(II) Complexes in Aqueous Solutions. III. Hexanuclear Clusters. Collection of Czechoslovak Chemical Communications, 2002, 67, 219-227.	1.0	12
114	Optical properties of 2,3-diaza-1,3-butadiene bridged oligothiophenes. Synthetic Metals, 2002, 129, 85-94.	3.9	11
115	Structure dependence of optical properties of bridged bis-thienyls. I. Simple five-membered aromatic bridges. Computational and Theoretical Chemistry, 2002, 582, 213-224.	1.5	11
116	Structure and electronic properties of bithiophenes. I. Torsional dependence. Computational and Theoretical Chemistry, 2002, 618, 93-100.	1.5	11
117	Some comments on â€œAb initio study of the Jahnâ€“Teller distortions in the B4+â€•[J. Mol. Struct. (Theochem) 583 (2002) 63]. Computational and Theoretical Chemistry, 2002, 618, 165-169.	1.5	6
118	The spectroscopic and structural properties of copper(II) complexes of the novel tridentate (ONO) pyridine N-oxide ligand Hpoxap. Polyhedron, 2002, 21, 1561-1571.	2.2	38
119	Non-linear optical properties of new bridged bis-thienyls. Synthetic Metals, 2001, 124, 279-286.	3.9	15
120	On the Relation Between Conformational Changes and Optical Properties in Oligothiophenes, 2. Linear and Nonlinear Optical Properties. Macromolecular Theory and Simulations, 2001, 10, 592-599.	1.4	9
121	On the dependence of optical properties on conformational changes in oligothiophenes I. Electron absorption spectra. Computational and Theoretical Chemistry, 2001, 572, 151-160.	1.5	32
122	The electronic structure of planar phosphazene rings. Polyhedron, 2000, 19, 389-397.	2.2	39
123	On bonding in cyclic triphosphazenes. Computational and Theoretical Chemistry, 2000, 505, 169-177.	1.5	22
124	Dichotomy in the Ring Opening Reaction of 5-[(2-Furyl)methylidene]-2,2-dimethyl-1,3-dioxane-4,6-dione with Cyclic Secondary Amines. Collection of Czechoslovak Chemical Communications, 2000, 65, 1911-1938.	1.0	19
125	Synthesis and spectra of tetrakis (4-dimethylaminophenyl) hexadienes. Dyes and Pigments, 1999, 43, 227-233.	3.7	6
126	On the structure of lead(II) complexes in aqueous solutions. II. Polyhedron, 1999, 18, 2085-2090.	2.2	14

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127	Synthesis and spectra of tris(4-dimethylaminophenyl)divinylenes. Dyes and Pigments, 1999, 40, 43-51.	3.7	4
128	On the structure of polyphosphazenes. European Polymer Journal, 1999, 35, 581-586.	5.4	4
129	Interaction energy anisotropy of the pyrrole dimer: ab initio theoretical study. Theoretical Chemistry Accounts, 1999, 101, 319-324.	1.4	16
130	On the Reliability of the Structures of Lead(II) Hydroxo Complexes Obtained by MNDO Method. Collection of Czechoslovak Chemical Communications, 1999, 64, 1269-1273.	1.0	11
131	On dehydrochlorination of crosslinked poly(vinyl chloride). European Polymer Journal, 1998, 34, 1505-1509.	5.4	2
132	Rennerâ€“Teller vibronic potential constants for HCO. Computational and Theoretical Chemistry, 1998, 423, 245-250.	1.5	0
133	On bond alternation in simple short-chain phosphazenes. Computational and Theoretical Chemistry, 1998, 429, 111-120.	1.5	2
134	AM1 studies of hexasubstituted benzenes I. Pyrrolyl-, imidazolyl- and pyrazolyl-derivatives. Computational and Theoretical Chemistry, 1998, 453, 153-161.	1.5	1
135	On non-planarity and bond alternation of a simple short-chain phosphazene. Computational and Theoretical Chemistry, 1998, 454, 77-81.	1.5	6
136	On the structure of hexaaquacopper(II) complexes. Computational and Theoretical Chemistry, 1997, 397, 121-128.	1.5	10
137	Shape memory effect of dehydrochlorinated crosslinked poly(vinyl chloride). Macromolecular Chemistry and Physics, 1997, 198, 3161-3172.	2.2	28
138	Electronic structure of high-temperature superconductors II. La-Ba-Cu-O systems. European Physical Journal D, 1996, 46, 503-507.	0.4	1
139	CNDO studies of Y-Ba-Cu-O superconductors V. Co/Cu substitution. European Physical Journal D, 1996, 46, 873-880.	0.4	1
140	On the relation between conformational changes and electronic structure defects in polypyrrole. Macromolecular Theory and Simulations, 1996, 5, 107-120.	1.4	5
141	Ab initio study of simple short-chain phosphazenes. Computational and Theoretical Chemistry, 1995, 332, 277-281.	1.5	9
142	On the Structure of Lead(II) Complexes in Aqueous Solutions. I. Trinuclear Clusters. Collection of Czechoslovak Chemical Communications, 1995, 60, 527-536.	1.0	10
143	AM1 Calculations of Spin Distribution in Hydroxyanthrasemiquinones. Collection of Czechoslovak Chemical Communications, 1995, 60, 1081-1093.	1.0	1
144	Jahn-Teller Effect in Hexahydroxocuprate(II) Complexes. Collection of Czechoslovak Chemical Communications, 1995, 60, 1429-1434.	1.0	0

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145	Quantum-chemical studies of triangulo cluster molecules of cobalt(0) with trimethylphosphine and carbonyl ligands and of their halogen derivatives. Polyhedron, 1994, 13, 103-107.	2.2	1
146	Charge fluctuations influence on the axial oxygen position in Yî—¸Baî—¸Cuî—¸O superconductors. Solid State Communications, 1994, 89, 65-67.	1.9	0
147	Ab initio study of cyclic hexahalotriphosphazenes. Computational and Theoretical Chemistry, 1994, 309, 305-308.	1.5	13
148	CNDO studies of Y-Ba-Cu-O superconductors IV. The oxygen content effect. European Physical Journal D, 1994, 44, 695-701.	0.4	2
149	Quantum-chemical studies of triangulo cluster molecules of cobalt(0) and Nickel(0) with trimethylphosphine and carbonyl ligands. Polyhedron, 1994, 13, 723-725.	2.2	1
150	On the axial oxygen position in Yî—¸Baî—¸Cuî—¸O superconductors. Solid State Communications, 1993, 85, 713-716.	1.9	3
151	Oxygen photosensitization in the presence of sodium anthracene-1-sulphonate. Journal of Photochemistry and Photobiology A: Chemistry, 1993, 76, 159-165.	3.9	4
152	CNDO studies of Y-Ba-Cu-O superconductors III. The axial oxygen position. European Physical Journal D, 1993, 43, 569-574.	0.4	1
153	Triangulo cluster molecules of cobalt(0) and nickel(0) containing trimethylphosphine and carbonyl ligands: syntheses, properties, and x-ray structures. Organometallics, 1992, 11, 2912-2916.	2.3	11
154	Electronic structure of Biî—¸Srî—¸(Ca)î—¸Cuî—¸O systems. Solid State Communications, 1992, 83, 995-998.	1.9	0
155	On electronic structure of lanthanide analogs of Yî—¸Baî—¸Cu superconductors. Solid State Communications, 1992, 81, 673-675.	1.9	1
156	On electronic structure of H2 in palladium. European Physical Journal D, 1992, 42, 439-446.	0.4	0
157	CNDO studies of Y-Ba-Cu-O superconductors I. Comparative study of CuO n polyhedra. European Physical Journal D, 1992, 42, 191-200.	0.4	3
158	CNDO studies of Y-Ba-Cu-O superconductors II. Simple models of YBa2Cu3Ox. European Physical Journal D, 1992, 42, 201-207.	0.4	2
159	Photocatalytic hydroxylation of benzoic acid in aqueous titanium dioxide suspension. Journal of Photochemistry and Photobiology A: Chemistry, 1991, 59, 385-391.	3.9	40
160	Jahn-teller effect for eight-atom clusters. European Physical Journal D, 1991, 41, 593-598.	0.4	3
161	The environmental symmetry influence on molecular nitrogen activation. Computational and Theoretical Chemistry, 1991, 227, 213-218.	1.5	0
162	Jahnâ€“Teller phase transitions. Acta Crystallographica Section B: Structural Science, 1990, 46, 573-575.	1.8	11

#	Article	IF	Citations
163	Jahn-Teller distortions of icosahedral complexes. European Physical Journal D, 1990, 40, 1177-1184.	0.4	2
164	Electronic structure of high-temperature superconductors I. Y-Ba-Cu-O systems. European Physical Journal D, 1990, 40, 778-789.	0.4	1
165	Electronic structure of YBa2Cu3Oy. Solid State Communications, 1990, 73, 783-785.	1.9	4
166	Electronic structure of Tlî—¸Baî—¸Caî—¸Cuî—¸O systems. Solid State Communications, 1990, 74, 801-804.	1.9	2
167	Excited states of ZnS:Mn and ZnSe:Mn stabilized by the Jahnâ€“Teller active E mode: Calculations by semiempirical selfâ€consistent field methods. Journal of Chemical Physics, 1990, 92, 3018-3020.	3.0	4
168	A complete classification of stable symmetries of the Jahn-Teller systems. Collection of Czechoslovak Chemical Communications, 1990, 55, 2119-2130.	1.0	7
169	Vibronic constants for tetrahedral complexes with triple degenerate electron terms. Collection of Czechoslovak Chemical Communications, 1990, 55, 1416-1426.	1.0	0
170	Vibronic interactions in the stereochemistry of metal complexes. Structure and Bonding, 1989, , 57-97.	1.0	21
171	Models of solid-state influences in systems with Jahn-Teller distortions. European Physical Journal D, 1988, 38, 1230-1233.	0.4	0
172	An alternative model of the vibronic coupling in octahedral complexes. Collection of Czechoslovak Chemical Communications, 1988, 53, 1134-1140.	1.0	0
173	Theoretical study of the static Jahn-Teller effectâ€"II three-mode vibronic coupling in octahedral halocomplexes with triply degenerate electronic states. Polyhedron, 1986, 5, 753-760.	2.2	5
174	Theoretical study of the static Jahn-Teller effectâ€"III. Type of vibronic coupling in hexahalo complexes. Polyhedron, 1986, 5, 1607-1613.	2.2	5
175	Theoretical study of the static Jahn-Teller effectâ€"I. Two-mode vibronic coupling in octahedral halocomplexes with doubly degenerate electronic states. Polyhedron, 1985, 4, 1543-1551.	2.2	13
176	Group-theoretical analysis of the possible symmetries of the Jahn-Teller systems. Computational and Theoretical Chemistry, 1985, 124, 231-237.	1.5	17
177	Tetragonal distortions and vibronic coupling in hexaflouro nickel(II) and copper (II) complexes. Polyhedron, 1983, 2, 921-928.	2.2	12
178	The Eî—¸e vibronic interaction in octahedral complexes. Inorganica Chimica Acta, 1980, 45, L1-L3.	2.4	8
179	MO study of molecular nitrogen fixation I. Model systems: [N2 + H]., [N2 + H]+, [N2 + H]â^'. Journal of Molecular Catalysis, 1979, 5, 349-362.	1.2	8
180	Mo study of molecular nitrogen fixation II. Model systems: [N2 + H2], [N2 + H2]+, [N2 + H2]â^'. Journal of Molecular Catalysis, 1979, 6, 269-288.	1.2	5

#	Article	IF	Citations
181	Molecular orbital study of molecular nitrogen fixation. International Journal of Quantum Chemistry, 1979, 16, 485-500.	2.0	5