

Paul G Mezey

List of Publications by Year in descending order

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152
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34
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102487

66
g-index

155
all docs

155
docs citations

155
times ranked

2491
citing authors

#	ARTICLE	IF	CITATIONS
1	A fast intrinsic localization procedure applicable for ab initio and semiempirical linear combination of atomic orbital wave functions. <i>Journal of Chemical Physics</i> , 1989, 90, 4916-4926.	3.0	1,517
2	The holographic electron density theorem and quantum similarity measures. <i>Molecular Physics</i> , 1999, 96, 169-178.	1.7	161
3	The shape of molecular charge distributions: Group theory without symmetry. <i>Journal of Computational Chemistry</i> , 1987, 8, 462-469.	3.3	125
4	The holographic electron density theorem and quantum similarity measures. <i>Molecular Physics</i> , 1999, 96, 169-178.	1.7	107
5	Macromolecular density matrices and electron densities with adjustable nuclear geometries. <i>Journal of Mathematical Chemistry</i> , 1995, 18, 141-168.	1.5	106
6	Ab initio quality properties for macromolecules using the ADMA approach. <i>Journal of Computational Chemistry</i> , 2003, 24, 1980-1986.	3.3	105
7	Reactive domains of energy hypersurfaces and the stability of minimum energy reaction paths. <i>Theoretica Chimica Acta</i> , 1980, 54, 95-111.	0.8	94
8	The Field-Adapted ADMA Approach: Introducing Point Charges. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4301-4309.	2.5	94
9	Quantum similarity measures and Li ₂ wdin's transform for approximate density matrices and macromolecular forces. <i>International Journal of Quantum Chemistry</i> , 1997, 63, 39-48.	2.0	81
10	Shape-similarity measures for molecular bodies: A 3D topological approach to quantitative shape-activity relations. <i>Journal of Chemical Information and Computer Sciences</i> , 1992, 32, 650-656.	2.8	75
11	Shape group studies of molecular similarity: Shape groups and shape graphs of molecular contour surfaces. <i>Journal of Mathematical Chemistry</i> , 1988, 2, 299-323.	1.5	73
12	A new computational microscope for molecules: High resolution MEDLA images of taxol and HIV-1 protease, using additive electron density fragmentation principles and fuzzy set methods. <i>Journal of Mathematical Chemistry</i> , 1995, 17, 203-234.	1.5	64
13	Functional Groups in Quantum Chemistry. <i>Advances in Quantum Chemistry</i> , 1996, , 163-222.	0.8	64
14	Topology of energy hypersurfaces. <i>Theoretica Chimica Acta</i> , 1982, 62, 133-161.	0.8	59
15	Global and local relative convexity and oriented relative convexity; application to molecular shapes in external fields. <i>Journal of Mathematical Chemistry</i> , 1988, 2, 325-346.	1.5	59
16	Shape characterization of some molecular model surfaces. <i>Journal of Computational Chemistry</i> , 1988, 9, 554-563.	3.3	58
17	Group theory of shapes of asymmetric biomolecules. <i>International Journal of Quantum Chemistry</i> , 1987, 32, 127-132.	2.0	57
18	Similarity analysis in two and three dimensions using lattice animals and polycubes. <i>Journal of Mathematical Chemistry</i> , 1992, 11, 27-45.	1.5	57

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19	The propagation of basis set error and geometry optimization in ab initio calculations. A statistical analysis of the sulfur d-orbital problem. <i>Journal of Chemical Physics</i> , 1982, 77, 870-876.	3.0	55
20	Toward similarity measures for macromolecular bodies: Medla test calculations for substituted benzene systems. <i>Journal of Computational Chemistry</i> , 1995, 16, 1238-1249.	3.3	53
21	Holographic Electron Density Shape Theorem and Its Role in Drug Design and Toxicological Risk Assessment. <i>Journal of Chemical Information and Computer Sciences</i> , 1999, 39, 224-230.	2.8	52
22	A method for the characterization of molecular conformations. <i>International Journal of Quantum Chemistry</i> , 1987, 32, 133-147.	2.0	49
23	The concept of "syntopy". <i>Molecular Physics</i> , 1990, 69, 97-113.	1.7	49
24	Fuzzy fragment selection strategies, basis set dependence and HF-DFT comparisons in the applications of the ADMA method of macromolecular quantum chemistry. <i>International Journal of Quantum Chemistry</i> , 2005, 104, 847-860.	2.0	46
25	Evaluation of the field-adapted ADMA approach: absolute and relative energies of crambin and derivatives. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 4061.	2.8	45
26	Level set topology of the nuclear charge space and the electronic energy functional. <i>International Journal of Quantum Chemistry</i> , 1982, 22, 101-114.	2.0	42
27	Shape analysis of macromolecular electron densities. <i>Structural Chemistry</i> , 1995, 6, 261-270.	2.0	42
28	Quantum chemical reaction networks, reaction graphs and the structure of potential energy hypersurfaces. <i>Theoretica Chimica Acta</i> , 1982, 60, 409-428.	0.8	41
29	The shapes of backbones of chain molecules: Three-dimensional characterization by spherical shape maps. <i>Biopolymers</i> , 1992, 32, 1609-1621.	2.4	40
30	Generalized chirality and symmetry deficiency. <i>Journal of Mathematical Chemistry</i> , 1998, 23, 65-84.	1.5	40
31	Shape group studies of molecular similarity and regioselectivity in chemical reactions. <i>Journal of Computational Chemistry</i> , 1988, 9, 608-619.	3.3	39
32	Fuzzy Electron Density Fragments in Macromolecular Quantum Chemistry, Combinatorial Quantum Chemistry, Functional Group Analysis, and Shape-Activity Relations. <i>Accounts of Chemical Research</i> , 2014, 47, 2821-2827.	15.6	38
33	A complete shape characterization for molecular charge densities represented by Gaussian-type functions. <i>Journal of Computational Chemistry</i> , 1991, 12, 220-230.	3.3	37
34	Classification schemes of nuclear geometries and the concept of chemical structure. Metric spaces of chemical structure sets over potential energy hypersurfaces. <i>Journal of Chemical Physics</i> , 1983, 78, 6182-6186.	3.0	36
35	Electronic energy inequalities for isoelectronic molecular systems. <i>Theoretica Chimica Acta</i> , 1981, 59, 321-332.	0.8	33
36	A simple relation between nuclear charges and potential surfaces. <i>Journal of the American Chemical Society</i> , 1985, 107, 3100-3105.	13.7	33

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37	Validity of the Hammond postulate and constraints on general one-dimensional reaction barriers. <i>Journal of Computational Chemistry</i> , 1988, 9, 728-744.	3.3	32
38	Manifold theory of multidimensional potential surfaces. <i>International Journal of Quantum Chemistry</i> , 1981, 20, 185-196.	2.0	31
39	The symmetry of electronic energy level sets and total energy relations in the abstract nuclear charge space. <i>Molecular Physics</i> , 1982, 47, 121-126.	1.7	30
40	Heuristic lipophilicity potential for computer-aided rational drug design. <i>Journal of Computer-Aided Molecular Design</i> , 1997, 11, 503-515.	2.9	27
41	Molecular Surfaces. <i>Reviews in Computational Chemistry</i> , 0, , 265-294.	1.5	26
42	The metric properties of the reduced nuclear configuration space. <i>International Journal of Quantum Chemistry</i> , 1984, 26, 983-985.	2.0	25
43	Dependence of MO shapes on a continuous measure of delocalization. <i>International Journal of Quantum Chemistry</i> , 1988, 34, 1-13.	2.0	25
44	The fundamental syntopy of quasi-symmetric systems: Geometric criteria and the underlying syntopy of a nuclear configuration space. <i>International Journal of Quantum Chemistry</i> , 1993, 45, 177-187.	2.0	25
45	A study on universal Gaussian basis sets for first-row atoms. <i>Theoretica Chimica Acta</i> , 1979, 53, 183-192.	0.8	24
46	Molecular conformations and molecular shape: A discrete characterization of continua of van der Waals surfaces. <i>International Journal of Quantum Chemistry</i> , 1988, 34, 517-526.	2.0	24
47	A topological analysis of molecular electrostatic potential on van der Waals surfaces for histamine and 4-substituted derivatives as H ₂ -receptor agonists. <i>Journal of Computational Chemistry</i> , 1991, 12, 705-716.	3.3	24
48	Variable atomic radii based on some approximate configurational invariance and transferability properties of the electron density. <i>Journal of Computational Chemistry</i> , 1991, 12, 1198-1210.	3.3	24
49	Local-Shape Analysis of Macromolecular Electron Densities. <i>Computational Chemistry - Reviews of Current Trends</i> , 1996, , 109-137.	0.4	24
50	Natural molecular fragments, functional groups, and holographic constraints on electron densities. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 8516.	2.8	24
51	Shape description of conformationally flexible molecules: Application to two-dimensional conformational problems. <i>International Journal of Quantum Chemistry</i> , 1988, 34, 33-54.	2.0	22
52	Cell-shedding transformations, equivalence relations, and similarity measures for square-cell configurations. <i>International Journal of Quantum Chemistry</i> , 1997, 62, 353-361.	2.0	21
53	Use of quantitative shape-activity relationships to model the photoinduced toxicity of polycyclic aromatic hydrocarbons: Electron density shape features accurately predict toxicity. <i>Environmental Toxicology and Chemistry</i> , 1998, 17, 1207-1215.	4.3	21
54	Shape group theory of van der Waals surfaces. <i>Journal of Mathematical Chemistry</i> , 1989, 3, 43-71.	1.5	20

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55	Semisimilarity of molecular bodies: Scaling-nesting similarity measures. International Journal of Quantum Chemistry, 1994, 51, 255-264.	2.0	20
56	Polyhedral shapes of functional group distributions in biomolecules and related similarity measures. International Journal of Quantum Chemistry, 1998, 66, 99-105.	2.0	20
57	Similarity and complexity of the shapes of square-cell configurations. Theoretica Chimica Acta, 1991, 79, 379-387.	0.8	19
58	Application of the shape group method to conformational processes: Shape and conjugation changes in the conformers of 2-phenyl pyrimidine. Journal of Computational Chemistry, 1995, 16, 1474-1482.	3.3	19
59	Possible Reaction Pathway of HN ₃ ⁺ N ₅ ⁺ and Stability of the Products' Isomers. Journal of Physical Chemistry A, 2002, 106, 1872-1876.	2.5	19
60	Constraints on electronic energy hypersurfaces of higher multiplicities. Journal of Chemical Physics, 1984, 80, 5055-5057.	3.0	18
61	Non-empirical SCF MO studies on the protonation of biopolymer constituents. Theoretica Chimica Acta, 1979, 51, 323-329.	0.8	17
62	Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution. I. International Journal of Quantum Chemistry, 1995, 53, 375-386.	2.0	17
63	Some dimension problems in molecular databases. Journal of Mathematical Chemistry, 2009, 45, 1-6.	1.5	17
64	Averaged electron densities for averaged conformations. Journal of Computational Chemistry, 1998, 19, 1337-1344.	3.3	16
65	New global constraints on electronic energy hypersurfaces. International Journal of Quantum Chemistry, 1986, 29, 85-99.	2.0	15
66	A topological analysis of molecular shape and structure. International Journal of Quantum Chemistry, 1996, 59, 379-390.	2.0	15
67	Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution. VI. International Journal of Quantum Chemistry, 2001, 84, 389-400.	2.0	15
68	A molecular geometry invariant property of energy level set boundaries in space. International Journal of Quantum Chemistry, 1983, 24, 523-526.	2.0	14
69	Shape similarity and shape stability along reaction paths: The case of the PPO ? OPP isomerization. International Journal of Quantum Chemistry, 1992, 42, 459-474.	2.0	14
70	A proof of the metric properties of the symmetric scaling-nesting dissimilarity measure and related symmetry deficiency measures. International Journal of Quantum Chemistry, 1997, 63, 105-109.	2.0	14
71	Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution. V. International Journal of Quantum Chemistry, 1999, 74, 633-644.	2.0	14
72	A quantitative approach to structural similarity from molecular topology of reaction paths. International Journal of Quantum Chemistry, 1990, 38, 1-13.	2.0	13

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73	Two large-amplitude motions in triatomic molecules. Force field of the $1B_2(1A^2)$ state of SO_2 . <i>Journal of Chemical Physics</i> , 1980, 72, 121-125.	3.0	12
74	The algebraic structure of quantum-chemical reaction mechanisms. <i>International Journal of Quantum Chemistry</i> , 1984, 26, 77-85.	2.0	12
75	Molecular point symmetry and the phase of the electronic wave function: Tools for the prediction of critical points of potential energy surfaces. <i>International Journal of Quantum Chemistry</i> , 1990, 38, 699-711.	2.0	12
76	Analysis of molecular shape changes along reaction paths. <i>International Journal of Quantum Chemistry</i> , 1990, 38, 713-726.	2.0	12
77	Representation of square-cell configurations in the complex plane: Tools for the characterization of molecular monolayers and cross sections of molecular surfaces. <i>International Journal of Quantum Chemistry</i> , 1992, 43, 375-392.	2.0	12
78	Three properties of relative shape envelopes of molecular electron density contours. <i>Theoretica Chimica Acta</i> , 1995, 92, 333-338.	0.8	12
79	Mislow's label paradox, chirality-preserving conformational changes, and related chirality measures. <i>Chirality</i> , 1998, 10, 173-179.	2.6	12
80	The propagation of basis-set error and geometry optimization in ab initio calculations. II. Correlation between the balance of Gaussian basis sets and calculated molecular properties. <i>Journal of Computational Chemistry</i> , 1983, 4, 482-487.	3.3	11
81	Symmetry and periodicity of potential surfaces: a test for multicenter interactions. <i>Theoretica Chimica Acta</i> , 1988, 73, 221-228.	0.8	11
82	Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution. II. <i>International Journal of Quantum Chemistry</i> , 1995, 53, 387-406.	2.0	11
83	Fractional Simplex Designs for Interaction Screening in Complex Mixtures. <i>Biometrics</i> , 2000, 56, 824-832.	1.4	11
84	A general formulation of the "quantum chemical Le Chatelier principle". <i>International Journal of Quantum Chemistry</i> , 1984, 25, 853-861.	2.0	10
85	Nuclear charges and molecular total energies: A rule on nested reaction globes. <i>International Journal of Quantum Chemistry</i> , 1986, 29, 333-343.	2.0	10
86	Constant electronic energy trajectories in abstract nuclear charge space and level set topology. <i>Journal of Chemical Physics</i> , 1987, 87, 5882-5891.	3.0	10
87	On the inhibition of alcohol dehydrogenase: Shape group analysis of molecular electrostatic potential on van der Waals surfaces for some pyrazole derivatives. <i>International Journal of Quantum Chemistry</i> , 1991, 40, 269-288.	2.0	10
88	Relations among functional groups within a stoichiometry: A nuclear configuration space approach. <i>International Journal of Quantum Chemistry</i> , 1992, 43, 647-658.	2.0	10
89	Shape groups of the electronic isodensity surfaces for small molecules: Shapes of 10-electron hydrides. <i>Journal of Computational Chemistry</i> , 1993, 14, 1172-1183.	3.3	10
90	Heuristic lipophilicity potential for computer-aided rational drug design: optimizations of screening functions and parameters. , 1998, 12, 451-470.		10

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91	Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution VII. International Journal of Quantum Chemistry, 2004, 97, 765-775.	2.0	10
92	Compensation Effects in Molecular Interactions and the Quantum Chemical le Chatelier Principle. Journal of Physical Chemistry A, 2015, 119, 5305-5312.	2.5	10
93	Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution. III. International Journal of Quantum Chemistry, 1997, 63, 149-163.	2.0	9
94	Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution. IV. International Journal of Quantum Chemistry, 1998, 67, 57-69.	2.0	9
95	Computer Aided Drug Design: Some Fundamental Aspects. Journal of Molecular Modeling, 2000, 6, 150-157.	1.8	9
96	Title is missing!. Journal of Mathematical Chemistry, 2001, 30, 375-387.	1.5	9
97	Molecular geometry and symmetry from a differential geometry viewpoint. International Journal of Quantum Chemistry, 1997, 64, 669-678.	2.0	8
98	A fuzzy-set approach to functional-group comparisons based on an asymmetric similarity measure. International Journal of Quantum Chemistry, 1999, 74, 503-514.	2.0	8
99	The topology of catchment regions of potential energy hypersurfaces. Theoretical Chemistry Accounts, 1999, 102, 279-284.	1.4	8
100	Treatment of small deformations of polyhedral shapes of functional group distributions in biomolecules. International Journal of Quantum Chemistry, 2000, 76, 756-761.	2.0	8
101	The thioketone-enethiol tautomerism of aliphatic thiocarbonyls: Anab initio study. Journal of Computational Chemistry, 1983, 4, 104-109.	3.3	7
102	Network relations on potential surfaces as aids to computer-based quantum-chemical synthesis planning. International Journal of Quantum Chemistry, 1984, 26, 675-681.	2.0	7
103	Shape analysis along reaction paths of ring opening reactions. International Journal of Quantum Chemistry, 1991, 40, 335-345.	2.0	7
104	Large-Scale Chirality Measures and General Symmetry Deficiency Measures for Functional Group Polyhedra of Proteins. Journal of Mathematical Chemistry, 2006, 40, 145-153.	1.5	7
105	On the Balance of Simplification and Reality in Molecular Modeling of the Electron Density. Journal of Chemical Theory and Computation, 2008, 4, 1627-1636.	5.3	7
106	QSAR and the ultimate molecular descriptor: the shape of electron density clouds. Journal of Mathematical Chemistry, 2009, 45, 544-549.	1.5	7
107	Group theory of electrostatic potentials: A tool for quantum chemical drug design. International Journal of Quantum Chemistry, 2009, 28, 113-122.	2.0	7
108	Discrete skeletons of continua in the universal molecule model. , 2012, , .		7

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109	A global characterization and similarity analysis of two-dimensional potential energy surfaces. <i>International Journal of Quantum Chemistry</i> , 1992, 41, 557-579.	2.0	6
110	The diet transform of lattice patterns, equivalence relations, and similarity measures. <i>Molecular Engineering</i> , 1996, 6, 415-426.	0.2	6
111	Imperfect periodicity and systematic changes of some structural features along linear polymers: the case of rod-like boron/nitrogen nanostructures. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	6
112	On the relative importance of core and valence shell representations in the calculation of conformational energies using small Gaussian basis sets. <i>Journal of Computational Chemistry</i> , 1980, 1, 134-140.	3.3	5
113	Molecular fragment shape variation index for functional groups and the holographic properties of electron density. <i>Journal of Mathematical Chemistry</i> , 2012, 50, 926-933.	1.5	5
114	Dependence of approximate ab initio molecular loge sizes on the quality of basis functions. <i>International Journal of Quantum Chemistry</i> , 1979, 16, 1009-1019.	2.0	4
115	Theoretical studies on "acetylenic zipper" reaction intermediates. <i>Journal of Computational Chemistry</i> , 1982, 3, 185-190.	3.3	4
116	A measure of roughness of cross sections of molecular surfaces. <i>Theoretica Chimica Acta</i> , 1991, 81, 79-93.	0.8	4
117	A Functional Group Database: A Charge Density "DARC Approach. <i>Molecular Engineering</i> , 1998, 8, 251-265.	0.2	4
118	Energy relations between small and large unit cell boron-nitrogen polymer analogues of spiral graphite and nanoneedle structures. <i>Journal of Mathematical Chemistry</i> , 2009, 45, 550-556.	1.5	4
119	The isoelectronic and isoprotonic energy hypersurface and the topology of the nuclear charge space. <i>International Journal of Quantum Chemistry</i> , 2009, 20, 279-285.	2.0	4
120	Relations between real molecules through abstract molecules: the reference cluster approach. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	1.4	4
121	An alternative to the "Star Path" enhancement of the ADMA linear scaling method for protein modeling. <i>Journal of Computational Chemistry</i> , 2017, 38, 1774-1779.	3.3	4
122	A functorial approach to analogous molecular systems. <i>AIP Conference Proceedings</i> , 2019, , .	0.4	4
123	Oxidation properties of mesophase pitch prepared by a heterogeneous nucleation method. <i>Journal of Materials Science</i> , 1992, 27, 5199-5202.	3.7	4
124	A theoretical study on the protonation of cycloalkanes C _n H _{2n} (n = 3 to 6). <i>Journal of Computational Chemistry</i> , 1984, 5, 190-196.	3.3	3
125	The T-hull approach to shape analysis. <i>Theoretica Chimica Acta</i> , 1995, 91, 67-71.	0.8	3
126	Generalisation of a property of Hamiltonians depending linearly upon a parameter: application to a model of inert gas matrix effect on vibrational spectra. <i>Journal of Mathematical Chemistry</i> , 2008, 44, 981-987.	1.5	3

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127	Fragment shape variation index for periodicity deficiency and gradual changes of internal coordinates along linear polymers. <i>Journal of Mathematical Chemistry</i> , 2012, 50, 934-941.	1.5	3
128	The Holographic Electron Density Theorem, de-quantization, re-quantization, and nuclear charge space extrapolations of the Universal Molecule Model. <i>AIP Conference Proceedings</i> , 2017, , .	0.4	3
129	From quantum similarity measures to quantum analogy functors: tools for QShAR, quantitative shape-activity relations. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	1.4	3
130	The Future and Impact of Quantum Mechanical Calculations in the Description and Characterization of Zeolites. <i>ACS Symposium Series</i> , 1984, , 145-156.	0.5	2
131	Hyperspherical coordinate representation of potential surfaces of large molecules. <i>International Journal of Quantum Chemistry</i> , 1984, 26, 267-272.	2.0	2
132	A comparison of two group theoretical models of reaction mechanisms on potential surfaces. <i>International Journal of Quantum Chemistry</i> , 1985, 28, 387-398.	2.0	2
133	Reflection properties of reaction paths in the reduced nuclear configuration space. <i>International Journal of Quantum Chemistry</i> , 1987, 32, 191-198.	2.0	2
134	Approximate eigenvalues of parameter ϵ -dependent systems from boundaries of level sets. <i>Journal of Mathematical Physics</i> , 1988, 29, 119-127.	1.1	2
135	T-hull relations for shape envelopes of molecular contours. <i>Theoretica Chimica Acta</i> , 1996, 94, 177-182.	0.8	2
136	Charge-conserving electron density averaging for a set of nuclear configurations. <i>Journal of Mathematical Chemistry</i> , 2008, 44, 1023-1032.	1.5	2
137	The differentiable manifold model of quantum-chemical reaction networks. <i>International Journal of Quantum Chemistry</i> , 2009, 24, 137-152.	2.0	2
138	Inequalities and homotopy relations in reaction topology. <i>International Journal of Quantum Chemistry</i> , 1983, 24, 453-460.	2.0	2
139	The reaction polyhedron and group theory of reaction mechanisms. <i>International Journal of Quantum Chemistry</i> , 2009, 28, 93-105.	2.0	2
140	Two approaches to the concept of chemical species: Relations between potential energy and molecular shape. <i>International Journal of Quantum Chemistry</i> , 1989, 36, 305-320.	2.0	2
141	Molecular fragment shape variation index applied to intramolecular interaction studies. <i>Journal of Mathematical Chemistry</i> , 2012, 50, 942-948.	1.5	2
142	A trigonometrically scaled multiple tiling approach for error reduction of models built from fuzzy fragments. <i>Journal of Computational Methods in Sciences and Engineering</i> , 2017, 16, 729-732.	0.2	2
143	Ab initioSCF MO calculations on the reactions of hydroxyl radical with imidazole and monoprotonated imidazole. <i>Journal of Computational Chemistry</i> , 1985, 6, 68-75.	3.3	1
144	An approach to conformation analysis on multidimensional potential surfaces. <i>International Journal of Quantum Chemistry</i> , 1983, 24, 153-160.	2.0	1

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145	A wavefunction model to chemical bonding. International Journal of Quantum Chemistry, 0, , e26686.	2.0	1
146	Quantum similarity measures and Löwdin's transform for approximate density matrices and macromolecular forces. , 0, .		1
147	A THEORETICAL STUDY ON THE CONFORMATIONAL PROPERTIES AND GEOMETRICAL DEFORMATIONS OF DIMETHYL SULFOXIDE. Phosphorous and Sulfur and the Related Elements, 1979, 6, 199-199.	0.2	0
148	A NON-EMPIRICAL SCF MO STUDY ON THE GROUND STATE AND FIRST TRIPLET STATE POTENTIAL ENERGY SURFACES OF SIMPLE THIOCARBONYLS. Phosphorous and Sulfur and the Related Elements, 1979, 6, 201-202.	0.2	0
149	Unexpected expectation values for latent molecular properties. Journal of Mathematical Chemistry, 2012, 50, 843-849.	1.5	0
150	Alternative algebraic approaches in quantum chemistry. , 2015, , .		0
151	On the dimension dependence of the level of optimality of certain multidimensional sampling strategies. Journal of Computational Methods in Sciences and Engineering, 2017, 16, 713-717.	0.2	0
152	Iterated similarity sequences and factorial level similarities in databases. Journal of Computational Methods in Sciences and Engineering, 2017, 16, 719-727.	0.2	0