

# Paul G Mezey

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

152  
papers

4,237  
citations

31  
h-index

61  
g-index

155  
ext. papers

4,490  
ext. citations

2.7  
avg, IF

5.62  
L-index

#	Paper	IF	Citations
152	From quantum similarity measures to quantum analogy functors: tools for QShAR, quantitative shape-activity relations. <i>Theoretical Chemistry Accounts</i> , <b>2021</b> , 140, 1	1.9	1
151	A functorial approach to analogous molecular systems <b>2019</b> ,		3
150	On the dimension dependence of the level of optimality of certain multidimensional sampling strategies. <i>Journal of Computational Methods in Sciences and Engineering</i> , <b>2017</b> , 16, 713-717	0.3	
149	An alternative to the "Star Path" enhancement of the ADMA linear scaling method for protein modeling. <i>Journal of Computational Chemistry</i> , <b>2017</b> , 38, 1774-1779	3.5	2
148	The Holographic Electron Density Theorem, de-quantization, re-quantization, and nuclear charge space extrapolations of the Universal Molecule Model <b>2017</b> ,		3
147	Iterated similarity sequences and factorial level similarities in databases. <i>Journal of Computational Methods in Sciences and Engineering</i> , <b>2017</b> , 16, 719-727	0.3	
146	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> , <b>2017</b> , 16, 729-732	0.3	2
145	Compensation effects in molecular interactions and the quantum chemical le Chatelier principle. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 5305-12	2.8	8
144	Relations between real molecules through abstract molecules: the reference cluster approach. <i>Theoretical Chemistry Accounts</i> , <b>2015</b> , 134, 1	1.9	4
143	Fuzzy electron density fragments in macromolecular quantum chemistry, combinatorial quantum chemistry, functional group analysis, and shape-activity relations. <i>Accounts of Chemical Research</i> , <b>2014</b> , 47, 2821-7	24.3	27
142	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> , <b>2012</b> , 131, 1	1.9	5
141	Natural molecular fragments, functional groups, and holographic constraints on electron densities. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 8516-22	3.6	20
140	Fuzzy Electron-Density Fragments as Building Blocks in Crystal-Engineering Design <b>2012</b> , 233-241		6
139	Discrete skeletons of continua in the universal molecule model <b>2012</b> ,		6
138	Unexpected expectation values for latent molecular properties. <i>Journal of Mathematical Chemistry</i> , <b>2012</b> , 50, 843-849	2.1	
137	Molecular fragment shape variation index for functional groups and the holographic properties of electron density. <i>Journal of Mathematical Chemistry</i> , <b>2012</b> , 50, 926-933	2.1	5
136	Fragment shape variation index for periodicity deficiency and gradual changes of internal coordinates along linear polymers. <i>Journal of Mathematical Chemistry</i> , <b>2012</b> , 50, 934-941	2.1	3

135	Molecular fragment shape variation index applied to intramolecular interaction studies. <i>Journal of Mathematical Chemistry</i> , <b>2012</b> , 50, 942-948	2.1	2
134	Some dimension problems in molecular databases. <i>Journal of Mathematical Chemistry</i> , <b>2009</b> , 45, 1-6	2.1	13
133	QSAR and the ultimate molecular descriptor: the shape of electron density clouds. <i>Journal of Mathematical Chemistry</i> , <b>2009</b> , 45, 544-549	2.1	5
132	Energy relations between small and large unit cell boron-nitrogen polymer analogues of spiral graphite and nanoneedle structures. <i>Journal of Mathematical Chemistry</i> , <b>2009</b> , 45, 550-556	2.1	3
131	The isoelectronic and isoprotonic energy hypersurface and the topology of the nuclear charge space. <i>International Journal of Quantum Chemistry</i> , <b>2009</b> , 20, 279-285	2.1	3
130	An approach to conformation analysis on multidimensional potential surfaces. <i>International Journal of Quantum Chemistry</i> , <b>2009</b> , 24, 153-160	2.1	
129	The differentiable manifold model of quantum-chemical reaction networks. <i>International Journal of Quantum Chemistry</i> , <b>2009</b> , 24, 137-152	2.1	1
128	Inequalities and homotopy relations in reaction topology. <i>International Journal of Quantum Chemistry</i> , <b>2009</b> , 24, 453-460	2.1	
127	Group theory of electrostatic potentials: A tool for quantum chemical drug design. <i>International Journal of Quantum Chemistry</i> , <b>2009</b> , 28, 113-122	2.1	2
126	The reaction polyhedron and group theory of reaction mechanisms. <i>International Journal of Quantum Chemistry</i> , <b>2009</b> , 28, 93-105	2.1	
125	Two approaches to the concept of chemical species: Relations between potential energy and molecular shape. <i>International Journal of Quantum Chemistry</i> , <b>2009</b> , 36, 305-320	2.1	
124	On the Balance of Simplification and Reality in Molecular Modeling of the Electron Density. <i>Journal of Chemical Theory and Computation</i> , <b>2008</b> , 4, 1627-36	6.4	7
123	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> , <b>2008</b> , 44, 981-987	2.1	2
122	Charge-conserving electron density averaging for a set of nuclear configurations. <i>Journal of Mathematical Chemistry</i> , <b>2008</b> , 44, 1023-1032	2.1	2
121	Large-Scale Chirality Measures and General Symmetry Deficiency Measures for Functional Group Polyhedra of Proteins. <i>Journal of Mathematical Chemistry</i> , <b>2006</b> , 40, 145-153	2.1	5
120	Evaluation of the field-adapted ADMA approach: absolute and relative energies of crambin and derivatives. <i>Physical Chemistry Chemical Physics</i> , <b>2005</b> , 7, 4061-9	3.6	40
119	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> , <b>2005</b> , 104, 847-860	2.1	38
118	Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution VII. <i>International Journal of Quantum Chemistry</i> , <b>2004</b> , 97, 765-775	2.1	9

117	The Field-Adapted ADMA Approach: Introducing Point Charges. <i>Journal of Physical Chemistry A</i> , <b>2004</b> , 108, 4301-4309	2.8	86
116	Ab initio quality properties for macromolecules using the ADMA approach. <i>Journal of Computational Chemistry</i> , <b>2003</b> , 24, 1980-6	3.5	95
115	Possible Reaction Pathway of HN <sub>3</sub> + N <sub>5</sub> <sup>+</sup> and Stability of the Products' Isomers. <i>Journal of Physical Chemistry A</i> , <b>2002</b> , 106, 1872-1876	2.8	19
114	Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution. VI*. <i>International Journal of Quantum Chemistry</i> , <b>2001</b> , 84, 389-400	2.1	14
113	Dimension Concepts and Reduced Dimensions in Toxicological QShAR Databases as Tools for Data Quality Assessment. <i>Journal of Mathematical Chemistry</i> , <b>2001</b> , 30, 375-387	2.1	7
112	Treatment of small deformations of polyhedral shapes of functional group distributions in biomolecules. <i>International Journal of Quantum Chemistry</i> , <b>2000</b> , 76, 756-761	2.1	7
111	Fractional simplex designs for interaction screening in complex mixtures. <i>Biometrics</i> , <b>2000</b> , 56, 824-32	1.8	9
110	Computer Aided Drug Design: Some Fundamental Aspects. <i>Journal of Molecular Modeling</i> , <b>2000</b> , 6, 150-157		6
109	A fuzzy-set approach to functional-group comparisons based on an asymmetric similarity measure. <i>International Journal of Quantum Chemistry</i> , <b>1999</b> , 74, 503-514	2.1	7
108	The topology of catchment regions of potential energy hypersurfaces. <i>Theoretical Chemistry Accounts</i> , <b>1999</b> , 102, 279-284	1.9	6
107	Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution. V. <i>International Journal of Quantum Chemistry</i> , <b>1999</b> , 74, 633-644	2.1	14
106	The holographic electron density theorem and quantum similarity measures. <i>Molecular Physics</i> , <b>1999</b> , 96, 169-178	1.7	142
105	Holographic electron density shape theorem and its role in drug design and toxicological risk assessment. <i>Journal of Chemical Information and Computer Sciences</i> , <b>1999</b> , 39, 224-30		40
104	Heuristic lipophilicity potential for computer-aided rational drug design: optimizations of screening functions and parameters. <i>Journal of Computer-Aided Molecular Design</i> , <b>1998</b> , 12, 451-70	4.2	9
103	A Functional Group Database: A Charge Density IDARC Approach. <i>Molecular Engineering</i> , <b>1998</b> , 8, 251-265		3
102	Generalized chirality and symmetry deficiency. <i>Journal of Mathematical Chemistry</i> , <b>1998</b> , 23, 65-84	2.1	29
101	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> , <b>1998</b> , 17, 1207-1215	3.8	21
100	Averaged electron densities for averaged conformations. <i>Journal of Computational Chemistry</i> , <b>1998</b> , 19, 1337-1344	3.5	15

99	Polyhedral shapes of functional group distributions in biomolecules and related similarity measures. <i>International Journal of Quantum Chemistry</i> , <b>1998</b> , 66, 99-105	2.1	16
98	Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution. IV. <i>International Journal of Quantum Chemistry</i> , <b>1998</b> , 67, 57-69	2.1	9
97	Mislow's label paradox, chirality-preserving conformational changes, and related chirality measures. <i>Chirality</i> , <b>1998</b> , 10, 173-179	2.1	9
96	Heuristic lipophilicity potential for computer-aided rational drug design. <i>Journal of Computer-Aided Molecular Design</i> , <b>1997</b> , 11, 503-15	4.2	20
95	Cell-shedding transformations, equivalence relations, and similarity measures for square-cell configurations. <i>International Journal of Quantum Chemistry</i> , <b>1997</b> , 62, 353-361	2.1	20
94	A proof of the metric properties of the symmetric scaling-nesting dissimilarity measure and related symmetry deficiency measures. <i>International Journal of Quantum Chemistry</i> , <b>1997</b> , 63, 105-109	2.1	11
93	Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution. III. <i>International Journal of Quantum Chemistry</i> , <b>1997</b> , 63, 149-163	2.1	9
92	Quantum similarity measures and Löwdin's transform for approximate density matrices and macromolecular forces. <i>International Journal of Quantum Chemistry</i> , <b>1997</b> , 63, 39-48	2.1	72
91	Molecular geometry and symmetry from a differential geometry viewpoint. <i>International Journal of Quantum Chemistry</i> , <b>1997</b> , 64, 669-678	2.1	6
90	Functional Groups in Quantum Chemistry. <i>Advances in Quantum Chemistry</i> , <b>1996</b> , 163-222	1.4	51
89	T-hull relations for shape envelopes of molecular contours. <i>Theoretica Chimica Acta</i> , <b>1996</b> , 94, 177-182		1
88	A topological analysis of molecular shape and structure. <i>International Journal of Quantum Chemistry</i> , <b>1996</b> , 59, 379-390	2.1	14
87	The diet transform of lattice patterns, equivalence relations, and similarity measures. <i>Molecular Engineering</i> , <b>1996</b> , 6, 415-426		6
86	Local-Shape Analysis of Macromolecular Electron Densities. <i>Computational Chemistry - Reviews of Current Trends</i> , <b>1996</b> , 109-137		15
85	Shape analysis of macromolecular electron densities. <i>Structural Chemistry</i> , <b>1995</b> , 6, 261-270	1.8	34
84	Macromolecular density matrices and electron densities with adjustable nuclear geometries. <i>Journal of Mathematical Chemistry</i> , <b>1995</b> , 18, 141-168	2.1	93
83	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> , <b>1995</b> , 17, 203-234	2.1	60
82	Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution. I. <i>International Journal of Quantum Chemistry</i> , <b>1995</b> , 53, 375-386	2.1	14

81	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> , <b>1995</b> , 53, 387-406	2.1	11
80	Three properties of relative shape envelopes of molecular electron density contours. <i>Theoretica Chimica Acta</i> , <b>1995</b> , 92, 333-338		10
79	The T-hull approach to shape analysis. <i>Theoretica Chimica Acta</i> , <b>1995</b> , 91, 67-71		1
78	Toward similarity measures for macromolecular bodies: Medla test calculations for substituted benzene systems. <i>Journal of Computational Chemistry</i> , <b>1995</b> , 16, 1238-1249	3.5	48
77	Application of the shape group method to conformational processes: Shape and conjugation changes in the conformers of 2-phenyl pyrimidine. <i>Journal of Computational Chemistry</i> , <b>1995</b> , 16, 1474-1482	2.5	18
76	Semisimilarity of molecular bodies: Scaling besting similarity measures. <i>International Journal of Quantum Chemistry</i> , <b>1994</b> , 51, 255-264	2.1	19
75	Shape groups of the electronic isodensity surfaces for small molecules: Shapes of 10-electron hydrides. <i>Journal of Computational Chemistry</i> , <b>1993</b> , 14, 1172-1183	3.5	10
74	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> , <b>1993</b> , 45, 177-187	2.1	23
73	Shape-similarity measures for molecular bodies: A 3D topological approach to quantitative shape-activity relations. <i>Journal of Chemical Information and Computer Sciences</i> , <b>1992</b> , 32, 650-656		64
72	A global characterization and similarity analysis of two-dimensional potential energy surfaces. <i>International Journal of Quantum Chemistry</i> , <b>1992</b> , 41, 557-579	2.1	4
71	Shape similarity and shape stability along reaction paths: The case of the PPO $\rightarrow$ OPP isomerization. <i>International Journal of Quantum Chemistry</i> , <b>1992</b> , 42, 459-474	2.1	11
70	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> , <b>1992</b> , 43, 375-392	2.1	12
69	Relations among functional groups within a stoichiometry: A nuclear configuration space approach. <i>International Journal of Quantum Chemistry</i> , <b>1992</b> , 43, 647-658	2.1	9
68	Similarity analysis in two and three dimensions using lattice animals and polycubes. <i>Journal of Mathematical Chemistry</i> , <b>1992</b> , 11, 27-45	2.1	49
67	The shapes of backbones of chain molecules: Three-dimensional characterization by spherical shape maps. <i>Biopolymers</i> , <b>1992</b> , 32, 1609-1621	2.2	39
66	A complete shape characterization for molecular charge densities represented by Gaussian-type functions. <i>Journal of Computational Chemistry</i> , <b>1991</b> , 12, 220-230	3.5	33
65	A topological analysis of molecular electrostatic potential on van der Waals surfaces for histamine and 4-substituted derivatives as H <sub>2</sub> -receptor agonists. <i>Journal of Computational Chemistry</i> , <b>1991</b> , 12, 705-716	3.5	21
64	Variable atomic radii based on some approximate configurational invariance and transferability properties of the electron density. <i>Journal of Computational Chemistry</i> , <b>1991</b> , 12, 1198-1210	3.5	21

63	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> , <b>1991</b> , 40, 269-288	2.1	8
62	Shape analysis along reaction paths of ring opening reactions. <i>International Journal of Quantum Chemistry</i> , <b>1991</b> , 40, 335-345	2.1	4
61	A measure of roughness of cross sections of molecular surfaces. <i>Theoretica Chimica Acta</i> , <b>1991</b> , 81, 79-93		2
60	Similarity and complexity of the shapes of square-cell configurations. <i>Theoretica Chimica Acta</i> , <b>1991</b> , 79, 379-387		17
59	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> , <b>1990</b> , 38, 699-711	2.1	8
58	Analysis of molecular shape changes along reaction paths. <i>International Journal of Quantum Chemistry</i> , <b>1990</b> , 38, 713-726	2.1	8
57	A quantitative approach to structural similarity from molecular topology of reaction paths. <i>International Journal of Quantum Chemistry</i> , <b>1990</b> , 38, 1-13	2.1	10
56	The concept of Eynotyπ <i>Molecular Physics</i> , <b>1990</b> , 69, 97-113	1.7	42
55	Shape group theory of van der Waals surfaces. <i>Journal of Mathematical Chemistry</i> , <b>1989</b> , 3, 43-71	2.1	17
54	A fast intrinsic localization procedure applicable for ab initio and semiempirical linear combination of atomic orbital wave functions. <i>Journal of Chemical Physics</i> , <b>1989</b> , 90, 4916-4926	3.9	1337
53	Shape characterization of some molecular model surfaces. <i>Journal of Computational Chemistry</i> , <b>1988</b> , 9, 554-563	3.5	51
52	Shape group studies of molecular similarity and regioselectivity in chemical reactions. <i>Journal of Computational Chemistry</i> , <b>1988</b> , 9, 608-619	3.5	35
51	Validity of the Hammond postulate and constraints on general one-dimensional reaction barriers. <i>Journal of Computational Chemistry</i> , <b>1988</b> , 9, 728-744	3.5	30
50	Shape group studies of molecular similarity: Shape groups and shape graphs of molecular contour surfaces. <i>Journal of Mathematical Chemistry</i> , <b>1988</b> , 2, 299-323	2.1	67
49	Global and local relative convexity and oriented relative convexity; application to molecular shapes in external fields. <i>Journal of Mathematical Chemistry</i> , <b>1988</b> , 2, 325-346	2.1	50
48	Symmetry and periodicity of potential surfaces: a test for multicenter interactions. <i>Theoretica Chimica Acta</i> , <b>1988</b> , 73, 221-228		11
47	Molecular conformations and molecular shape: A discrete characterization of continua of van der Waals surfaces. <i>International Journal of Quantum Chemistry</i> , <b>1988</b> , 34, 517-526	2.1	19
46	Shape description of conformationally flexible molecules: Application to two-dimensional conformational problems. <i>International Journal of Quantum Chemistry</i> , <b>1988</b> , 34, 33-54	2.1	18

45	Dependence of MO shapes on a continuous measure of delocalization. <i>International Journal of Quantum Chemistry</i> , <b>1988</b> , 34, 1-13	2.1	22
44	Approximate eigenvalues of parameter-dependent systems from boundaries of level sets. <i>Journal of Mathematical Physics</i> , <b>1988</b> , 29, 119-127	1.2	2
43	Constant electronic energy trajectories in abstract nuclear charge space and level set topology. <i>Journal of Chemical Physics</i> , <b>1987</b> , 87, 5882-5891	3.9	10
42	Reflection properties of reaction paths in the reduced nuclear configuration space. <i>International Journal of Quantum Chemistry</i> , <b>1987</b> , 32, 191-198	2.1	1
41	Group theory of shapes of asymmetric biomolecules. <i>International Journal of Quantum Chemistry</i> , <b>1987</b> , 32, 127-132	2.1	51
40	A method for the characterization of molecular conformations. <i>International Journal of Quantum Chemistry</i> , <b>1987</b> , 32, 133-147	2.1	43
39	The shape of molecular charge distributions: Group theory without symmetry. <i>Journal of Computational Chemistry</i> , <b>1987</b> , 8, 462-469	3.5	115
38	New global constraints on electronic energy hypersurfaces. <i>International Journal of Quantum Chemistry</i> , <b>1986</b> , 29, 85-99	2.1	13
37	Nuclear charges and molecular total energies: A rule on nested reaction globes. <i>International Journal of Quantum Chemistry</i> , <b>1986</b> , 29, 333-343	2.1	8
36	A comparison of two group theoretical models of reaction mechanisms on potential surfaces. <i>International Journal of Quantum Chemistry</i> , <b>1985</b> , 28, 387-398	2.1	1
35	Ab initioSCF MO calculations on the reactions of hydroxyl radical with imidazole and monoprotonated imidazole. <i>Journal of Computational Chemistry</i> , <b>1985</b> , 6, 68-75	3.5	
34	A simple relation between nuclear charges and potential surfaces. <i>Journal of the American Chemical Society</i> , <b>1985</b> , 107, 3100-3105	16.4	31
33	The Future and Impact of Quantum Mechanical Calculations in the Description and Characterization of Zeolites. <i>ACS Symposium Series</i> , <b>1984</b> , 145-156	0.4	1
32	Constraints on electronic energy hypersurfaces of higher multiplicities. <i>Journal of Chemical Physics</i> , <b>1984</b> , 80, 5055-5057	3.9	17
31	A theoretical study on the protonation of cycloalkanes C <sub>n</sub> H <sub>2n</sub> (n = 3 to 6). <i>Journal of Computational Chemistry</i> , <b>1984</b> , 5, 190-196	3.5	3
30	A general formulation of the "quantum chemical Le Chatelier principle" <i>International Journal of Quantum Chemistry</i> , <b>1984</b> , 25, 853-861	2.1	7
29	The metric properties of the reduced nuclear configuration space. <i>International Journal of Quantum Chemistry</i> , <b>1984</b> , 26, 983-985	2.1	23
28	Hyperspherical coordinate representation of potential surfaces of large molecules. <i>International Journal of Quantum Chemistry</i> , <b>1984</b> , 26, 267-272	2.1	1



27	The algebraic structure of quantum-chemical reaction mechanisms. <i>International Journal of Quantum Chemistry</i> , <b>1984</b> , 26, 77-85	2.1	10
26	Network relations on potential surfaces as aids to computer-based quantum-chemical synthesis planning. <i>International Journal of Quantum Chemistry</i> , <b>1984</b> , 26, 675-681	2.1	6
25	A molecular geometry invariant property of energy level set boundaries in z space. <i>International Journal of Quantum Chemistry</i> , <b>1983</b> , 24, 523-526	2.1	12
24	The thioketone $\rightleftharpoons$ thiol tautomerism of aliphatic thiocarbonyls: An ab initio study. <i>Journal of Computational Chemistry</i> , <b>1983</b> , 4, 104-109	3.5	5
23	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> , <b>1983</b> , 4, 482-487	3.5	11
22	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> , <b>1983</b> , 78, 6182-6186	3.9	34
21	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> , <b>1982</b> , 77, 870-876	3.9	52
20	The symmetry of electronic energy level sets and total energy relations in the abstract nuclear charge space. <i>Molecular Physics</i> , <b>1982</b> , 47, 121-126	1.7	29
19	Theoretical studies on $\beta$ cetylenic zipper $\rightarrow$ reaction intermediates. <i>Journal of Computational Chemistry</i> , <b>1982</b> , 3, 185-190	3.5	3
18	Topology of energy hypersurfaces. <i>Theoretica Chimica Acta</i> , <b>1982</b> , 62, 133-161		55
17	Quantum chemical reaction networks, reaction graphs and the structure of potential energy hypersurfaces. <i>Theoretica Chimica Acta</i> , <b>1982</b> , 60, 409-428		40
16	Level set topology of the nuclear charge space and the electronic energy functional. <i>International Journal of Quantum Chemistry</i> , <b>1982</b> , 22, 101-114	2.1	40
15	Electronic energy inequalities for isoelectronic molecular systems. <i>Theoretica Chimica Acta</i> , <b>1981</b> , 59, 321-332		31
14	Manifold theory of multidimensional potential surfaces. <i>International Journal of Quantum Chemistry</i> , <b>1981</b> , 20, 185-196	2.1	29
13	Reactive domains of energy hypersurfaces and the stability of minimum energy reaction paths. <i>Theoretica Chimica Acta</i> , <b>1980</b> , 54, 95-111		92
12	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> , <b>1980</b> , 1, 134-140	3.5	5
11	Two large-amplitude motions in triatomic molecules. Force field of the 1B <sub>2</sub> (1A <sub>2</sub> ) state of SO <sub>2</sub> . <i>Journal of Chemical Physics</i> , <b>1980</b> , 72, 121-125	3.9	11
10	Electronic energy inequalities for isoelectronic molecular systems <b>1980</b> , 59, 321		3

9	A study on universal Gaussian basis sets for first-row atoms. <i>Theoretica Chimica Acta</i> , <b>1979</b> , 53, 183-192		23
8	Non-empirical SCF MO studies on the protonation of biopolymer constituents. <i>Theoretica Chimica Acta</i> , <b>1979</b> , 51, 323-329		16
7	Dependence of approximate ab initio molecular loge sizes on the quality of basis functions. <i>International Journal of Quantum Chemistry</i> , <b>1979</b> , 16, 1009-1019	2.1	4
6	A THEORETICAL STUDY ON THE CONFORMATIONAL PROPERTIES AND GEOMETRICAL DEFORMATIONS OF DIMETHYL SULFOXIDE. <i>Phosphorous and Sulfur and the Related Elements</i> , <b>1979</b> , 6, 199-199		
5	A NON-EMPIRICAL SCF MO STUDY ON THE GROUND STATE AND FIRST TRIPLET STATE POTENTIAL ENERGY SURFACES OF SIMPLE THIOCARBONYLS. <i>Phosphorous and Sulfur and the Related Elements</i> , <b>1979</b> , 6, 201-202		
4	The holographic electron density theorem and quantum similarity measures		9
3	A wavefunction model to chemical bonding. <i>International Journal of Quantum Chemistry</i> , e26686	2.1	
2	Quantum similarity measures and Löwdin's transform for approximate density matrices and macromolecular forces		1
1	Molecular Surfaces. <i>Reviews in Computational Chemistry</i> , 265-294		14