Paul G Mezey

List of Publications by Year
in descending order

152 papers	4,936 citations	117625 34 h-index	102487 66 g-index
155 all docs	155 docs citations	155 times ranked	2491 citing authors

#	Article	IF	Citations
1	From quantum similarity measures to quantum analogy functors: tools for QShAR, quantitative shape-activity relations. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	3
2	A functorial approach to analogous molecular systems. AIP Conference Proceedings, 2019, , .	0.4	4
3	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
4	An alternative to the â€œStar Pathâ€•enhancement of the ADMA linear scaling method for protein modeling. Journal of Computational Chemistry, 2017, 38, 1774-1779.	3.3	4
5	The Holographic Electron Density Theorem, de-quantization, re-quantization, and nuclear charge space extrapolations of the Universal Molecule Model. AIP Conference Proceedings, 2017, , .	0.4	3
6	Iterated similarity sequences and factorial level similarities in databases. Journal of Computational Methods in Sciences and Engineering, 2017, 16, 719-727.	0.2	0
7	A trigonometrically scaled multiple tiling approach for error reduction of models built from fuzzy fragments. Journal of Computational Methods in Sciences and Engineering, 2017, 16, 729-732.	0.2	2
8	Alternative algebraic approaches in quantum chemistry. , 2015, , .		0
9	Compensation Effects in Molecular Interactions and the Quantum Chemical le Chatelier Principle. Journal of Physical Chemistry A, 2015, 119, 5305-5312.	2.5	10
10	Relations between real molecules through abstract molecules: the reference cluster approach. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	4
11	Fuzzy Electron Density Fragments in Macromolecular Quantum Chemistry, Combinatorial Quantum Chemistry, Functional Group Analysis, and Shapeâ€“Activity Relations. Accounts of Chemical Research, 2014, 47, 2821-2827.	15.6	38
12	Natural molecular fragments, functional groups, and holographic constraints on electron densities. Physical Chemistry Chemical Physics, 2012, 14, 8516.	2.8	24
13	Discrete skeletons of continua in the universal molecule model. , 2012, , .		7
14	Unexpected expectation values for latent molecular properties. Journal of Mathematical Chemistry, 2012, 50, 843-849.	1.5	0
15	Molecular fragment shape variation index for functional groups and the holographic properties of electron density. Journal of Mathematical Chemistry, 2012, 50, 926-933.	1.5	5
16	Fragment shape variation index for periodicity deficiency and gradual changes of internal coordinates along linear polymers. Journal of Mathematical Chemistry, 2012, 50, 934-941.	1.5	3
17	Molecular fragment shape variation index applied to intramolecular interaction studies. Journal of Mathematical Chemistry, 2012, 50, 942-948.	1.5	2
18	Imperfect periodicity and systematic changes of some structural features along linear polymers: the case of rod-like boron/nitrogen nanostructures. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	6

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19	Some dimension problems in molecular databases. Journal of Mathematical Chemistry, 2009, 45, 1-6.	1.5	17
20	QSAR and the ultimate molecular descriptor: the shape of electron density clouds. Journal of Mathematical Chemistry, 2009, 45, 544-549.	1.5	7
21	Energy relations between small and large unit cell boronâ€“nitrogen polymer analogues of spiral graphite and nanoneedle structures. Journal of Mathematical Chemistry, 2009, 45, 550-556.	1.5	4
22	The isoelectronic and isoprotonic energy hypersurface and the topology of the nuclear charge space. International Journal of Quantum Chemistry, 2009, 20, 279-285.	2.0	4
23	The differentiable manifold model of quantum-chemical reaction networks. International Journal of Quantum Chemistry, 2009, 24, 137-152.	2.0	2
24	Group theory of electrostatic potentials: A tool for quantum chemical drug design. International Journal of Quantum Chemistry, 2009, 28, 113-122.	2.0	7
25	The reaction polyhedron and group theory of reaction mechanisms. International Journal of Quantum Chemistry, 2009, 28, 93-105.	2.0	2
26	Generalisation of a property of Hamiltonians depending linearly upon a parameter: application to a model of inert gas matrix effect on vibrational spectra. Journal of Mathematical Chemistry, 2008, 44, 981-987.	1.5	3
27	Charge-conserving electron density averaging for a set of nuclear configurations. Journal of Mathematical Chemistry, 2008, 44, 1023-1032.	1.5	2
28	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
29	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
30	Fuzzy fragment selection strategies, basis set dependence and HF-DFT comparisons in the applications of the ADMA method of macromolecular quantum chemistry. International Journal of Quantum Chemistry, 2005, 104, 847-860.	2.0	46
31	Evaluation of the field-adapted ADMA approach: absolute and relative energies of crambin and derivatives. Physical Chemistry Chemical Physics, 2005, 7, 4061.	2.8	45
32	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
33	The Field-Adapted ADMA Approach:â€‰ Introducing Point Charges. Journal of Physical Chemistry A, 2004, 108, 4301-4309.	2.5	94
34	Ab initioquality properties for macromolecules using the ADMA approach. Journal of Computational Chemistry, 2003, 24, 1980-1986.	3.3	105
35	Possible Reaction Pathway of HN3+ N5+and Stability of the Products' Isomers. Journal of Physical Chemistry A, 2002, 106, 1872-1876.	2.5	19
36	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

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37	Title is missing!. Journal of Mathematical Chemistry, 2001, 30, 375-387.	1.5	9
38	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
39	Fractional Simplex Designs for Interaction Screening in Complex Mixtures. Biometrics, 2000, 56, 824-832.	1.4	11
40	Computer Aided Drug Design: Some Fundamental Aspects. Journal of Molecular Modeling, 2000, 6, 150-157.	1.8	9
41	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
42	The topology of catchment regions of potential energy hypersurfaces. Theoretical Chemistry Accounts, 1999, 102, 279-284.	1.4	8
43	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
44	The holographic electron density theorem and quantum similarity measures. Molecular Physics, 1999, 96, 169-178.	1.7	161
45	Holographic Electron Density Shape Theorem and Its Role in Drug Design and Toxicological Risk Assessment. Journal of Chemical Information and Computer Sciences, 1999, 39, 224-230.	2.8	52
46	The holographic electron density theorem and quantum similarity measures. Molecular Physics, 1999, 96, 169-178.	1.7	107
47	Heuristic lipophilicity potential for computer-aided rational drug design: optimizations of screening functions and parameters. , 1998, 12, 451-470.		10
48	A Functional Group Database: A Charge Density â€“ DARC Approach. Molecular Engineering, 1998, 8, 251-265.	0.2	4
49	Generalized chirality and symmetry deficiency. Journal of Mathematical Chemistry, 1998, 23, 65-84.	1.5	40
50	Use of quantitative shapeâ€activity relationships to model the photoinduced toxicity of polycyclic aromatic hydrocarbons: Electron density shape features accurately predict toxicity. Environmental Toxicology and Chemistry, 1998, 17, 1207-1215.	4.3	21
51	Averaged electron densities for averaged conformations. Journal of Computational Chemistry, 1998, 19, 1337-1344.	3.3	16
52	Polyhedral shapes of functional group distributions in biomolecules and related similarity measures. International Journal of Quantum Chemistry, 1998, 66, 99-105.	2.0	20
53	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
54	Mislow's label paradox, chirality-preserving conformational changes, and related chirality measures. Chirality, 1998, 10, 173-179.	2.6	12

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55	Heuristic lipophilicity potential for computer-aided rational drug design. Journal of Computer-Aided Molecular Design, 1997, 11, 503-515.	2.9	27
56	Cell-shedding transformations, equivalence relations, and similarity measures for square-cell configurations. International Journal of Quantum Chemistry, 1997, 62, 353-361.	2.0	21
57	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
58	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
59	Quantum similarity measures and Lï¿½wdin's transform for approximate density matrices and macromolecular forces. International Journal of Quantum Chemistry, 1997, 63, 39-48.	2.0	81
60	Molecular geometry and symmetry from a differential geometry viewpoint. International Journal of Quantum Chemistry, 1997, 64, 669-678.	2.0	8
61	T-hull relations for shape envelopes of molecular contours. Theoretica Chimica Acta, 1996, 94, 177-182.	0.8	2
62	A topological analysis of molecular shape and structure. International Journal of Quantum Chemistry, 1996, 59, 379-390.	2.0	15
63	The diet transform of lattice patterns, equivalence relations, and similarity measures. Molecular Engineering, 1996, 6, 415-426.	0.2	6
64	Local-Shape Analysis of Macromolecular Electron Densities. Computational Chemistry - Reviews of Current Trends, 1996, , 109-137.	0.4	24
65	Functional Groups in Quantum Chemistry. Advances in Quantum Chemistry, 1996, , 163-222.	0.8	64
66	Toward similarity measures for macromolecular bodies: Medla test calculations for substituted benzene systems. Journal of Computational Chemistry, 1995, 16, 1238-1249.	3.3	53
67	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
68	Shape analysis of macromolecular electron densities. Structural Chemistry, 1995, 6, 261-270.	2.0	42
69	Macromolecular density matrices and electron densities with adjustable nuclear geometries. Journal of Mathematical Chemistry, 1995, 18, 141-168.	1.5	106
70	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. Journal of Mathematical Chemistry, 1995, 17, 203-234.	1.5	64
71	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
72	Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution. II. International Journal of Quantum Chemistry, 1995, 53, 387-406.	2.0	11

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73	Three properties of relative shape envelopes of molecular electron density contours. Theoretica Chimica Acta, 1995, 92, 333-338.	0.8	12
74	TheT-hull approach to shape analysis. Theoretica Chimica Acta, 1995, 91, 67-71.	0.8	3
75	Semisimilarity of molecular bodies: Scaling-nesting similarity measures. International Journal of Quantum Chemistry, 1994, 51, 255-264.	2.0	20
76	Shape groups of the electronic isodensity surfaces for small molecules: Shapes of 10-electron hydrides. Journal of Computational Chemistry, 1993, 14, 1172-1183.	3.3	10
77	The fundamental syntopy of quasi-symmetric systems: Geometric criteria and the underlying syntopy of a nuclear configuration space. International Journal of Quantum Chemistry, 1993, 45, 177-187.	2.0	25
78	Shape-similarity measures for molecular bodies: A 3D topological approach to quantitative shape-activity relations. Journal of Chemical Information and Computer Sciences, 1992, 32, 650-656.	2.8	75
79	A global characterization and similarity analysis of two-dimensional potential energy surfaces. International Journal of Quantum Chemistry, 1992, 41, 557-579.	2.0	6
80	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
81	Representation of square-cell configurations in the complex plane: Tools for the characterization of molecular monolayers and cross sections of molecular surfaces. International Journal of Quantum Chemistry, 1992, 43, 375-392.	2.0	12
82	Relations among functional groups within a stoichiometry: A nuclear configuration space approach. International Journal of Quantum Chemistry, 1992, 43, 647-658.	2.0	10
83	Similarity analysis in two and three dimensions using lattice animals and polycubes. Journal of Mathematical Chemistry, 1992, 11, 27-45.	1.5	57
84	The shapes of backbones of chain molecules: Three-dimensional characterization by spherical shape maps. Biopolymers, 1992, 32, 1609-1621.	2.4	40
85	Oxidation properties of mesophase pitch prepared by a heterogeneous nucleation method. Journal of Materials Science, 1992, 27, 5199-5202.	3.7	4
86	A complete shape characterization for molecular charge densities represented by Gaussian-type functions. Journal of Computational Chemistry, 1991, 12, 220-230.	3.3	37
87	A topological analysis of molecular electrostatic potential on van der Waals surfaces for histamine and 4-substituted derivatives as H2-receptor agonists. Journal of Computational Chemistry, 1991, 12, 705-716.	3.3	24
88	Variable atomic radii based on some approximate configurational invariance and transferability properties of the electron density. Journal of Computational Chemistry, 1991, 12, 1198-1210.	3.3	24
89	On the inhibition of alcohol dehydrogenase: Shape group analysis of molecular electrostatic potential on van der Waals surfaces for some pyrazole derivatives. International Journal of Quantum Chemistry, 1991, 40, 269-288.	2.0	10
90	Shape analysis along reaction paths of ring opening reactions. International Journal of Quantum Chemistry, 1991, 40, 335-345.	2.0	7

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91	A measure of roughness of cross sections of molecular surfaces. Theoretica Chimica Acta, 1991, 81, 79-93.	0.8	4
92	Similarity and complexity of the shapes of square-cell configurations. Theoretica Chimica Acta, 1991, 79, 379-387.	0.8	19
93	Molecular point symmetry and the phase of the electronic wave function: Tools for the prediction of critical points of potential energy surfaces. International Journal of Quantum Chemistry, 1990, 38, 699-711.	2.0	12
94	Analysis of molecular shape changes along reaction paths. International Journal of Quantum Chemistry, 1990, 38, 713-726.	2.0	12
95	A quantitative approach to structural similarity from molecular topology of reaction paths. International Journal of Quantum Chemistry, 1990, 38, 1-13.	2.0	13
96	The concept of â€˜syntopyâ€™. Molecular Physics, 1990, 69, 97-113.	1.7	49
97	Shape group theory of van der Waals surfaces. Journal of Mathematical Chemistry, 1989, 3, 43-71.	1.5	20
98	A fast intrinsic localization procedure applicable for ab initio and semiempirical linear combination of atomic orbital wave functions. Journal of Chemical Physics, 1989, 90, 4916-4926.	3.0	1,517
99	Two approaches to the concept of chemical species: Relations between potential energy and molecular shape. International Journal of Quantum Chemistry, 1989, 36, 305-320.	2.0	2
100	Shape characterization of some molecular model surfaces. Journal of Computational Chemistry, 1988, 9, 554-563.	3.3	58
101	Shape group studies of molecular similarity and regioselectivity in chemical reactions. Journal of Computational Chemistry, 1988, 9, 608-619.	3.3	39
102	Validity of the Hammond postulate and constraints on general one-dimensional reaction barriers. Journal of Computational Chemistry, 1988, 9, 728-744.	3.3	32
103	Shape group studies of molecular similarity: Shape groups and shape graphs of molecular contour surfaces. Journal of Mathematical Chemistry, 1988, 2, 299-323.	1.5	73
104	Global and local relative convexity and oriented relative convexity; application to molecular shapes in external fields. Journal of Mathematical Chemistry, 1988, 2, 325-346.	1.5	59
105	Symmetry and periodicity of potential surfaces: a test for multicenter interactions. Theoretica Chimica Acta, 1988, 73, 221-228.	0.8	11
106	Molecular conformations and molecular shape: A discrete characterization of continua of van der Waals surfaces. International Journal of Quantum Chemistry, 1988, 34, 517-526.	2.0	24
107	Shape description of conformationally flexible molecules: Application to two-dimensional conformational problems. International Journal of Quantum Chemistry, 1988, 34, 33-54.	2.0	22
108	Dependence ofMO shapes on a continuous measure of delocalization. International Journal of Quantum Chemistry, 1988, 34, 1-13.	2.0	25

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109	Approximate eigenvalues of parameterâ€dependent systems from boundaries of level sets. Journal of Mathematical Physics, 1988, 29, 119-127.	1.1	2
110	Constant electronic energy trajectories in abstract nuclear charge space and level set topology. Journal of Chemical Physics, 1987, 87, 5882-5891.	3.0	10
111	Reflection properties of reaction paths in the reduced nuclear configuration space. International Journal of Quantum Chemistry, 1987, 32, 191-198.	2.0	2
112	Group theory of shapes of asymmetric biomolecules. International Journal of Quantum Chemistry, 1987, 32, 127-132.	2.0	57
113	A method for the characterization of molecular conformations. International Journal of Quantum Chemistry, 1987, 32, 133-147.	2.0	49
114	The shape of molecular charge distributions: Group theory without symmetry. Journal of Computational Chemistry, 1987, 8, 462-469.	3.3	125
115	New global constraints on electronic energy hypersurfaces. International Journal of Quantum Chemistry, 1986, 29, 85-99.	2.0	15
116	Nuclear charges and molecular total energies: A rule on nested reaction globes. International Journal of Quantum Chemistry, 1986, 29, 333-343.	2.0	10
117	A comparison of two group theoretical models of reaction mechanisms on potential surfaces. International Journal of Quantum Chemistry, 1985, 28, 387-398.	2.0	2
118	Ab initioSCF MO calculations on the reactions of hydroxyl radical with imidazole and monoprotonated imidazole. Journal of Computational Chemistry, 1985, 6, 68-75.	3.3	1
119	A simple relation between nuclear charges and potential surfaces. Journal of the American Chemical Society, 1985, 107, 3100-3105.	13.7	33
120	The Future and Impact of Quantum Mechanical Calculations in the Description and Characterization of Zeolites. ACS Symposium Series, 1984, , 145-156.	0.5	2
121	Constraints on electronic energy hypersurfaces of higher multiplicities. Journal of Chemical Physics, 1984, 80, 5055-5057.	3.0	18
122	A theoretical study on the protonation of cycloalkanes CnH2n (n = 3 to 6). Journal of Computational Chemistry, 1984, 5, 190-196.	3.3	3
123	A general formulation of the ?quantum chemical le Chatelier principle?. International Journal of Quantum Chemistry, 1984, 25, 853-861.	2.0	10
124	The metric properties of the reduced nuclear configuration space. International Journal of Quantum Chemistry, 1984, 26, 983-985.	2.0	25
125	Hyperspherical coordinate representation of potential surfaces of large molecules. International Journal of Quantum Chemistry, 1984, 26, 267-272.	2.0	2
126	The algebraic structure of quantum-chemical reaction mechanisms. International Journal of Quantum Chemistry, 1984, 26, 77-85.	2.0	12

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127	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
128	A molecular geometry invariant property of energy level set boundaries inz space. International Journal of Quantum Chemistry, 1983, 24, 523-526.	2.0	14
129	The thioketone-enethiol tautomerism of aliphatic thiocarbonyls: Anab initio study. Journal of Computational Chemistry, 1983, 4, 104-109.	3.3	7
130	The propagation of basis-set error and geometry optimization inab initio calculations. II. Correlation between the balance of Gaussian basis sets and calculated molecular properties. Journal of Computational Chemistry, 1983, 4, 482-487.	3.3	11
131	Classification schemes of nuclear geometries and the concept of chemical structure. Metric spaces of chemical structure sets over potential energy hypersurfaces. Journal of Chemical Physics, 1983, 78, 6182-6186.	3.0	36
132	An approach to conformation analysis on multidimensional potential surfaces. International Journal of Quantum Chemistry, 1983, 24, 153-160.	2.0	1
133	Inequalities and homotopy relations in reaction topology. International Journal of Quantum Chemistry, 1983, 24, 453-460.	2.0	2
134	The propagation of basis set error and geometry optimization in ab initio calculations. A statistical analysis of the sulfur dâ€orbital problem. Journal of Chemical Physics, 1982, 77, 870-876.	3.0	55
135	The symmetry of electronic energy level sets and total energy relations in the abstract nuclear charge space. Molecular Physics, 1982, 47, 121-126.	1.7	30
136	Theoretical studies on ?acetylenic zipper? reaction intermediates. Journal of Computational Chemistry, 1982, 3, 185-190.	3.3	4
137	Topology of energy hypersurfaces. Theoretica Chimica Acta, 1982, 62, 133-161.	0.8	59
138	Quantum chemical reaction networks, reaction graphs and the structure of potential energy hypersurfaces. Theoretica Chimica Acta, 1982, 60, 409-428.	0.8	41
139	Level set topology of the nuclear charge space and the electronic energy functional. International Journal of Quantum Chemistry, 1982, 22, 101-114.	2.0	42
140	Electronic energy inequalities for isoelectronic molecular systems. Theoretica Chimica Acta, 1981, 59, 321-332.	0.8	33
141	Manifold theory of multidimensional potential surfaces. International Journal of Quantum Chemistry, 1981, 20, 185-196.	2.0	31
142	Reactive domains of energy hypersurfaces and the stability of minimum energy reaction paths. Theoretica Chimica Acta, 1980, 54, 95-111.	0.8	94
143	On the relative importance of core and valence shell representations in the calculation of conformational energies using small Gaussian basis sets. Journal of Computational Chemistry, 1980, 1, 134-140.	3.3	5
144	Two largeâ€amplitude motions in triatomic molecules. Force field of the1B2â€‰(1Aâ€²) state of SO2. Journal of Chemical Physics, 1980, 72, 121-125.	3.0	12

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145	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
146	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
147	A study on universal Gaussian basis sets for first-row atoms. Theoretica Chimica Acta, 1979, 53, 183-192.	0.8	24
148	Non-empirical SCF MO studies on the protonation of biopolymer constituents. Theoretica Chimica Acta, 1979, 51, 323-329.	0.8	17
149	Dependence of approximateab initio molecular loge sizes on the quality of basis functions. International Journal of Quantum Chemistry, 1979, 16, 1009-1019.	2.0	4
150	A wavefunction model to chemical bonding. International Journal of Quantum Chemistry, 0, , e26686.	2.0	1
151	Quantum similarity measures and LÃ¶wdin's transform for approximate density matrices and macromolecular forces. , 0, .		1
152	Molecular Surfaces. Reviews in Computational Chemistry, 0, , 265-294.	1.5	26