Paul G Mezey

List of Publications by Citations

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	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	3.9	1337
151	The holographic electron density theorem and quantum similarity measures. *Molecular Physics*, **1999**, 96, 169-178	1.7	142
150	The shape of molecular charge distributions: Group theory without symmetry. *Journal of Computational Chemistry*, **1987**, 8, 462-469	3.5	115
149	Ab initio quality properties for macromolecules using the ADMA approach. *Journal of Computational Chemistry*, **2003**, 24, 1980-6	3.5	95
148	Macromolecular density matrices and electron densities with adjustable nuclear geometries. *Journal of Mathematical Chemistry*, **1995**, 18, 141-168	2.1	93
147	Reactive domains of energy hypersurfaces and the stability of minimum energy reaction paths. *Theoretica Chimica Acta*, **1980**, 54, 95-111		92
146	The Field-Adapted ADMA Approach: Introducing Point Charges. *Journal of Physical Chemistry A*, **2004**, 108, 4301-4309	2.8	86
145	Quantum similarity measures and Löwdin's transform for approximate density matrices and macromolecular forces. *International Journal of Quantum Chemistry*, **1997**, 63, 39-48	2.1	72
144	Shape group studies of molecular similarity: Shape groups and shape graphs of molecular contour surfaces. *Journal of Mathematical Chemistry*, **1988**, 2, 299-323	2.1	67
143	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		64
142	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	2.1	60
141	Topology of energy hypersurfaces. *Theoretica Chimica Acta*, **1982**, 62, 133-161		55
140	The propagation of basis set error and geometry optimization in ab initio calculations. A statistical analysis of the sulfur d-orbital problem. *Journal of Chemical Physics*, **1982**, 77, 870-876	3.9	52
139	Functional Groups in Quantum Chemistry. *Advances in Quantum Chemistry*, **1996**, 163-222	1.4	51
138	Group theory of shapes of asymmetric biomolecules. *International Journal of Quantum Chemistry*, **1987**, 32, 127-132	2.1	51
137	Shape characterization of some molecular model surfaces. *Journal of Computational Chemistry*, **1988**, 9, 554-563	3.5	51
136	Global and local relative convexity and oriented relative convexity; application to molecular shapes in external fields. *Journal of Mathematical Chemistry*, **1988**, 2, 325-346	2.1	50

135	Similarity analysis in two and three dimensions using lattice animals and polycubes. *Journal of Mathematical Chemistry*, **1992**, 11, 27-45	2.1	49
134	Toward similarity measures for macromolecular bodies: Medla test calculations for substituted benzene systems. *Journal of Computational Chemistry*, **1995**, 16, 1238-1249	3.5	48
133	A method for the characterization of molecular conformations. *International Journal of Quantum Chemistry*, **1987**, 32, 133-147	2.1	43
132	The concept of Synтopy *Molecular Physics*, **1990**, 69, 97-113	1.7	42
131	Evaluation of the field-adapted ADMA approach: absolute and relative energies of crambin and derivatives. *Physical Chemistry Chemical Physics*, **2005**, 7, 4061-9	3.6	40
130	Holographic electron density shape theorem and its role in drug design and toxicological risk assessment. *Journal of Chemical Information and Computer Sciences*, **1999**, 39, 224-30		40
129	Quantum chemical reaction networks, reaction graphs and the structure of potential energy hypersurfaces. *Theoretica Chimica Acta*, **1982**, 60, 409-428		40
128	Level set topology of the nuclear charge space and the electronic energy functional. *International Journal of Quantum Chemistry*, **1982**, 22, 101-114	2.1	40
127	The shapes of backbones of chain molecules: Three-dimensional characterization by spherical shape maps. *Biopolymers*, **1992**, 32, 1609-1621	2.2	39
126	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	2.1	38
125	Shape group studies of molecular similarity and regioselectivity in chemical reactions. *Journal of Computational Chemistry*, **1988**, 9, 608-619	3.5	35
124	Shape analysis of macromolecular electron densities. *Structural Chemistry*, **1995**, 6, 261-270	1.8	34
123	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	3.9	34
122	A complete shape characterization for molecular charge densities represented by Gaussian-type functions. *Journal of Computational Chemistry*, **1991**, 12, 220-230	3.5	33
121	A simple relation between nuclear charges and potential surfaces. *Journal of the American Chemical Society*, **1985**, 107, 3100-3105	16.4	31
120	Electronic energy inequalities for isoelectronic molecular systems. *Theoretica Chimica Acta*, **1981**, 59, 321-332		31
119	Validity of the Hammond postulate and constraints on general one-dimensional reaction barriers. *Journal of Computational Chemistry*, **1988**, 9, 728-744	3.5	30
118	Generalized chirality and symmetry deficiency. *Journal of Mathematical Chemistry*, **1998**, 23, 65-84	2.1	29

117	Manifold theory of multidimensional potential surfaces. *International Journal of Quantum Chemistry* , **1981**, 20, 185-196	2.1	29
116	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	29
115	Fuzzy electron density fragments in macromolecular quantum chemistry, combinatorial quantum chemistry, functional group analysis, and shape-activity relations. *Accounts of Chemical Research*, **2014**, 47, 2821-7	24.3	27
114	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	2.1	23
113	The metric properties of the reduced nuclear configuration space. *International Journal of Quantum Chemistry*, **1984**, 26, 983-985	2.1	23
112	A study on universal Gaussian basis sets for first-row atoms. *Theoretica Chimica Acta*, **1979**, 53, 183-192		23
111	Dependence of MO shapes on a continuous measure of delocalization. *International Journal of Quantum Chemistry*, **1988**, 34, 1-13	2.1	22
110	Use of quantitative shape-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	3.8	21
109	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	3.5	21
108	Variable atomic radii based on some approximate configurational invariance and transferability properties of the electron density. *Journal of Computational Chemistry*, **1991**, 12, 1198-1210	3.5	21
107	Natural molecular fragments, functional groups, and holographic constraints on electron densities. *Physical Chemistry Chemical Physics*, **2012**, 14, 8516-22	3.6	20
106	Heuristic lipophilicity potential for computer-aided rational drug design. *Journal of Computer-Aided Molecular Design*, **1997**, 11, 503-15	4.2	20
105	Cell-shedding transformations, equivalence relations, and similarity measures for square-cell configurations. *International Journal of Quantum Chemistry*, **1997**, 62, 353-361	2.1	20
104	Possible Reaction Pathway of HN3 + N5+ and Stability of the Products' Isomers. *Journal of Physical Chemistry A*, **2002**, 106, 1872-1876	2.8	19
103	Semisimilarity of molecular bodies: Scaling□esting similarity measures. *International Journal of Quantum Chemistry*, **1994**, 51, 255-264	2.1	19
102	Molecular conformations and molecular shape: A discrete characterization of continua of van der Waals surfaces. *International Journal of Quantum Chemistry*, **1988**, 34, 517-526	2.1	19
101	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	3.5	18
100	Shape description of conformationally flexible molecules: Application to two-dimensional conformational problems. *International Journal of Quantum Chemistry*, **1988**, 34, 33-54	2.1	18

99	Similarity and complexity of the shapes of square-cell configurations. *Theoretica Chimica Acta*, **1991**, 79, 379-387		17
98	Shape group theory of van der Waals surfaces. *Journal of Mathematical Chemistry*, **1989**, 3, 43-71	2.1	17
97	Constraints on electronic energy hypersurfaces of higher multiplicities. *Journal of Chemical Physics*, **1984**, 80, 5055-5057	3.9	17
96	Polyhedral shapes of functional group distributions in biomolecules and related similarity measures. *International Journal of Quantum Chemistry*, **1998**, 66, 99-105	2.1	16
95	Non-empirical SCF MO studies on the protonation of biopolymer constituents. *Theoretica Chimica Acta*, **1979**, 51, 323-329		16
94	Averaged electron densities for averaged conformations. *Journal of Computational Chemistry*, **1998**, 19, 1337-1344	3.5	15
93	Local-Shape Analysis of Macromolecular Electron Densities. *Computational Chemistry - Reviews of Current Trends*, **1996**, 109-137		15
92	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	2.1	14
91	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	2.1	14
90	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	2.1	14
89	A topological analysis of molecular shape and structure. *International Journal of Quantum Chemistry*, **1996**, 59, 379-390	2.1	14
88	Molecular Surfaces. *Reviews in Computational Chemistry*,265-294		14
87	Some dimension problems in molecular databases. *Journal of Mathematical Chemistry*, **2009**, 45, 1-6	2.1	13
86	New global constraints on electronic energy hypersurfaces. *International Journal of Quantum Chemistry*, **1986**, 29, 85-99	2.1	13
85	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	2.1	12
84	A molecular geometry invariant property of energy level set boundaries in z space. *International Journal of Quantum Chemistry*, **1983**, 24, 523-526	2.1	12
83	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	2.1	11
82	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	2.1	11

81	Shape similarity and shape stability along reaction paths: The case of the PPO -nOPP isomerization. *International Journal of Quantum Chemistry*, **1992**, 42, 459-474	2.1	11
80	Symmetry and periodicity of potential surfaces: a test for multicenter interactions. *Theoretica Chimica Acta*, **1988**, 73, 221-228		11
79	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. *Journal of Computational Chemistry*, **1983**, 4, 482-487	3.5	11
78	Two large-amplitude motions in triatomic molecules. Force field of the 1B2 (1A?) state of SO2. *Journal of Chemical Physics*, **1980**, 72, 121-125	3.9	11
77	Three properties of relative shape envelopes of molecular electron density contours. *Theoretica Chimica Acta*, **1995**, 92, 333-338		10
76	Shape groups of the electronic isodensity surfaces for small molecules: Shapes of 10-electron hydrides. *Journal of Computational Chemistry*, **1993**, 14, 1172-1183	3.5	10
75	A quantitative approach to structural similarity from molecular topology of reaction paths. *International Journal of Quantum Chemistry*, **1990**, 38, 1-13	2.1	10
74	Constant electronic energy trajectories in abstract nuclear charge space and level set topology. *Journal of Chemical Physics*, **1987**, 87, 5882-5891	3.9	10
73	The algebraic structure of quantum-chemical reaction mechanisms. *International Journal of Quantum Chemistry*, **1984**, 26, 77-85	2.1	10
72	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	2.1	9
71	Heuristic lipophilicity potential for computer-aided rational drug design: optimizations of screening functions and parameters. *Journal of Computer-Aided Molecular Design*, **1998**, 12, 451-70	4.2	9
70	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	2.1	9
69	Mislow's label paradox, chirality-preserving conformational changes, and related chirality measures. *Chirality*, **1998**, 10, 173-179	2.1	9
68	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	2.1	9
67	Fractional simplex designs for interaction screening in complex mixtures. *Biometrics*, **2000**, 56, 824-32	1.8	9
66	Relations among functional groups within a stoichiometry: A nuclear configuration space approach. *International Journal of Quantum Chemistry*, **1992**, 43, 647-658	2.1	9
65	The holographic electron density theorem and quantum similarity measures		9
64	Compensation effects in molecular interactions and the quantum chemical le Chatelier principle. *Journal of Physical Chemistry A*, **2015**, 119, 5305-12	2.8	8

63	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	2.1	8
62	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	2.1	8
61	Analysis of molecular shape changes along reaction paths. *International Journal of Quantum Chemistry*, **1990**, 38, 713-726	2.1	8
60	Nuclear charges and molecular total energies: A rule on nested reaction globes. *International Journal of Quantum Chemistry*, **1986**, 29, 333-343	2.1	8
59	On the Balance of Simplification and Reality in Molecular Modeling of the Electron Density. *Journal of Chemical Theory and Computation*, **2008**, 4, 1627-36	6.4	7
58	Dimension Concepts and Reduced Dimensions in Toxicological QShAR Databases as Tools for Data Quality Assessment. *Journal of Mathematical Chemistry*, **2001**, 30, 375-387	2.1	7
57	Treatment of small deformations of polyhedral shapes of functional group distributions in biomolecules. *International Journal of Quantum Chemistry*, **2000**, 76, 756-761	2.1	7
56	A fuzzy-set approach to functional-group comparisons based on an asymmetric similarity measure. *International Journal of Quantum Chemistry*, **1999**, 74, 503-514	2.1	7
55	A general formulation of the quantum chemical le Chatelier principle *International Journal of Quantum Chemistry*, **1984**, 25, 853-861	2.1	7
54	Fuzzy Electron-Density Fragments as Building Blocks in Crystal-Engineering Design **2012**, 233-241		6
53	Discrete skeletons of continua in the universal molecule model **2012**,		6
52	Molecular geometry and symmetry from a differential geometry viewpoint. *International Journal of Quantum Chemistry*, **1997**, 64, 669-678	2.1	6
51	Computer Aided Drug Design: Some Fundamental Aspects. *Journal of Molecular Modeling*, **2000**, 6, 150-157		6
50	The topology of catchment regions of potential energy hypersurfaces. *Theoretical Chemistry Accounts*, **1999**, 102, 279-284	1.9	6
49	The diet transform of lattice patterns, equivalence relations, and similarity measures. *Molecular Engineering*, **1996**, 6, 415-426		6
48	Network relations on potential surfaces as aids to computer-based quantum-chemical synthesis planning. *International Journal of Quantum Chemistry*, **1984**, 26, 675-681	2.1	6
47	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	1.9	5
46	Molecular fragment shape variation index for functional groups and the holographic properties of electron density. *Journal of Mathematical Chemistry*, **2012**, 50, 926-933	2.1	5

45	QSAR and the ultimate molecular descriptor: the shape of electron density clouds. *Journal of Mathematical Chemistry*, **2009**, 45, 544-549	2.1	5
44	Large-Scale Chirality Measures and General Symmetry Deficiency Measures for Functional Group Polyhedra of Proteins. *Journal of Mathematical Chemistry*, **2006**, 40, 145-153	2.1	5
43	The thioketone–enethiol tautomerism of aliphatic thiocarbonyls: An ab initio study. *Journal of Computational Chemistry*, **1983**, 4, 104-109	3.5	5
42	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	3.5	5
41	Relations between real molecules through abstract molecules: the reference cluster approach. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	4
40	Shape analysis along reaction paths of ring opening reactions. *International Journal of Quantum Chemistry*, **1991**, 40, 335-345	2.1	4
39	A global characterization and similarity analysis of two-dimensional potential energy surfaces. *International Journal of Quantum Chemistry*, **1992**, 41, 557-579	2.1	4
38	Dependence of approximate ab initio molecular loge sizes on the quality of basis functions. *International Journal of Quantum Chemistry*, **1979**, 16, 1009-1019	2.1	4
37	The Holographic Electron Density Theorem, de-quantization, re-quantization, and nuclear charge space extrapolations of the Universal Molecule Model **2017**,		3
36	Fragment shape variation index for periodicity deficiency and gradual changes of internal coordinates along linear polymers. *Journal of Mathematical Chemistry*, **2012**, 50, 934-941	2.1	3
35	Energy relations between small and large unit cell boron–nitrogen polymer analogues of spiral graphite and nanoneedle structures. *Journal of Mathematical Chemistry*, **2009**, 45, 550-556	2.1	3
34	The isoelectronic and isoprotonic energy hypersurface and the topology of the nuclear charge space. *International Journal of Quantum Chemistry*, **2009**, 20, 279-285	2.1	3
33	A Functional Group Database: A Charge Density–DARC Approach. *Molecular Engineering*, **1998**, 8, 251-265		3
32	A theoretical study on the protonation of cycloalkanes CnH2n (n = 3 to 6). *Journal of Computational Chemistry*, **1984**, 5, 190-196	3.5	3
31	Theoretical studies on acetylenic zipper–reaction intermediates. *Journal of Computational Chemistry*, **1982**, 3, 185-190	3.5	3
30	Electronic energy inequalities for isoelectronic molecular systems **1980**, 59, 321		3
29	A functorial approach to analogous molecular systems **2019**,		3
28	An alternative to the "Star Path" enhancement of the ADMA linear scaling method for protein modeling. *Journal of Computational Chemistry*, **2017**, 38, 1774-1779	3.5	2

27	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	0.3	2
26	Molecular fragment shape variation index applied to intramolecular interaction studies. *Journal of Mathematical Chemistry*, **2012**, 50, 942-948	2.1	2
25	Group theory of electrostatic potentials: A tool for quantum chemical drug design. *International Journal of Quantum Chemistry*, **2009**, 28, 113-122	2.1	2
24	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	2.1	2
23	Charge-conserving electron density averaging for a set of nuclear configurations. *Journal of Mathematical Chemistry*, **2008**, 44, 1023-1032	2.1	2
22	A measure of roughness of cross sections of molecular surfaces. *Theoretica Chimica Acta*, **1991**, 81, 79-93		2
21	Approximate eigenvalues of parameter-dependent systems from boundaries of level sets. *Journal of Mathematical Physics*, **1988**, 29, 119-127	1.2	2
20	The differentiable manifold model of quantum-chemical reaction networks. *International Journal of Quantum Chemistry*, **2009**, 24, 137-152	2.1	1
19	TheT-hull approach to shape analysis. *Theoretica Chimica Acta*, **1995**, 91, 67-71		1
18	T-hull relations for shape envelopes of molecular contours. *Theoretica Chimica Acta*, **1996**, 94, 177-182		1
17	Reflection properties of reaction paths in the reduced nuclear configuration space. *International Journal of Quantum Chemistry*, **1987**, 32, 191-198	2.1	1
16	The Future and Impact of Quantum Mechanical Calculations in the Description and Characterization of Zeolites. *ACS Symposium Series*, **1984**, 145-156	0.4	1
15	Hyperspherical coordinate representation of potential surfaces of large molecules. *International Journal of Quantum Chemistry*, **1984**, 26, 267-272	2.1	1
14	A comparison of two group theoretical models of reaction mechanisms on potential surfaces. *International Journal of Quantum Chemistry*, **1985**, 28, 387-398	2.1	1
13	From quantum similarity measures to quantum analogy functors: tools for QShAR, quantitative shape-activity relations. *Theoretical Chemistry Accounts*, **2021**, 140, 1	1.9	1
12	Quantum similarity measures and L□wdin's transform for approximate density matrices and macromolecular forces		1
11	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	0.3	
10	Iterated similarity sequences and factorial level similarities in databases. *Journal of Computational Methods in Sciences and Engineering*, **2017**, 16, 719-727	0.3	

9	Unexpected expectation values for latent molecular properties. *Journal of Mathematical Chemistry*, **2012**, 50, 843-849	2.1
8	An approach to conformation analysis on multidimensional potential surfaces. *International Journal of Quantum Chemistry*, **2009**, 24, 153-160	2.1
7	Inequalities and homotopy relations in reaction topology. *International Journal of Quantum Chemistry*, **2009**, 24, 453-460	2.1
6	The reaction polyhedron and group theory of reaction mechanisms. *International Journal of Quantum Chemistry*, **2009**, 28, 93-105	2.1
5	Two approaches to the concept of chemical species: Relations between potential energy and molecular shape. *International Journal of Quantum Chemistry*, **2009**, 36, 305-320	2.1
4	Ab initioSCF MO calculations on the reactions of hydroxyl radical with imidazole and monoprotonated imidazole. *Journal of Computational Chemistry*, **1985**, 6, 68-75	3.5
3	A THEORETICAL STUDY ON THE CONFORMATIONAL PROPERTIES AND GEOMETRICAL DEFORMATIONS OF DIMETHYL SULFOXIDE. *Phosphorous and Sulfur and the Related Elements*, **1979** , 6, 199-199	
2	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	
1	A wavefunction model to chemical bonding. *International Journal of Quantum Chemistry*,e26686	2.1