Gregory A Chass

List of Publications by Year
in descending order

94 papers	2,845 citations	304743 22 h-index	182427 51 g-index
94 all docs	94 docs citations	94 times ranked	2669 citing authors

#	Article	IF	Citations
1	Easily Prepared Air- and Moisture-Stable Pdâ€“NHC (NHC=N-Heterocyclic Carbene) Complexes: A Reliable, User-Friendly, Highly Active Palladium Precatalyst for the Suzukiâ€“Miyaura Reaction. Chemistry - A European Journal, 2006, 12, 4743-4748.	3.3	734
2	Recycling the Waste: The Development of a Catalytic Wittig Reaction. Angewandte Chemie - International Edition, 2009, 48, 6836-6839.	13.8	272
3	Pd-NHC (PEPPSI) Complexes: Synthetic Utility and Computational Studies into Their Reactivity. Synthesis, 2008, 2008, 2776-2797.	2.3	199
4	Towards the rational design of palladium-N-heterocyclic carbene catalysts by a combined experimental and computational approach. Tetrahedron, 2005, 61, 9723-9735.	1.9	116
5	Density Functional Theory Investigation of the Alkylâ€“Alkyl Negishi Crossâ€Coupling Reaction Catalyzed by Nâ€Heterocyclic Carbene (NHC)â€“Pd Complexes. Chemistry - A European Journal, 2009, 15, 4281-4288.	3.3	91
6	Persistently Folded Circular Aromatic Amide Pentamers Containing Modularly Tunable Cation-Binding Cavities with High Ion Selectivity. Journal of the American Chemical Society, 2010, 132, 9564-9566.	13.7	86
7	An ab initio computational study on selected lycopene isomers. Computational and Theoretical Chemistry, 2001, 571, 27-37.	1.5	82
8	The Gas-Phase Dipeptide Analogue Acetyl-phenylalanyl-amide:Â A Model for the Study of Side Chain/Backbone Interactions in Proteins. Journal of Physical Chemistry A, 2005, 109, 5281-5288.	2.5	60
9	A Quantitative Scale for the Extent of Conjugation of the Amide Bond. Amidity Percentage as a Chemical Driving Force. Journal of Physical Chemistry A, 2007, 111, 13245-13254.	2.5	55
10	Atomic and vibrational origins of mechanical toughness in bioactive cement during setting. Nature Communications, 2015, 6, 8631.	12.8	55
11	Toward a computed peptide structure database: The role of a universal atomic numbering system of amino acids in peptides and internal hierarchy of database. International Journal of Quantum Chemistry, 2002, 90, 933-968.	2.0	54
12	Balancing the atomic waistline: Isodensityâ€based scrf radii for mainâ€group elements and transition metals. International Journal of Quantum Chemistry, 2013, 113, 975-984.	2.0	53
13	Amidicity Change as a Significant Driving Force and Thermodynamic Selection Rule of Transamidation Reactions. A Synergy between Experiment and Theory. Journal of Physical Chemistry B, 2008, 112, 7885-7893.	2.6	51
14	Peptide and protein folding. Computational and Theoretical Chemistry, 2001, 537, 319-361.	1.5	43
15	Pd(OAc)₂-Catalyzed Câ€“H Activation/Câ€“O Cyclization: Mechanism, Role of Oxidantâ€”Probed by Density Functional Theory. Journal of Organic Chemistry, 2013, 78, 8376-8385.	3.2	35
16	Characterization of the Conformational Probability of N-Acetyl-Phenylalanyl-NH2by RHF, DFT, and MP2 Computation and AIM Analyses, Confirmed by Jet-Cooled Infrared Data. Journal of Physical Chemistry A, 2005, 109, 5289-5302.	2.5	32
17	Prospects in computational molecular medicine: a millennial mega-project on peptide folding. Computational and Theoretical Chemistry, 2000, 500, 5-58.	1.5	29
18	First Principle Computational Study on the Full Conformational Space ofl-Proline Diamides. Journal of Physical Chemistry A, 2005, 109, 2660-2679.	2.5	29

#	Article	IF	Citations
19	How the Surface Structure Determines the Properties of CuH. Inorganic Chemistry, 2015, 54, 2213-2220.	4.0	27
20	The role of enhanced aromatic -electron donating aptitude of the tyrosyl sidechain with respect to that of phenylalanyl in intramolecular interactions. European Physical Journal D, 2002, 20, 481-497.	1.3	25
21	Quantitative Scale for the Extent of Conjugation of Carbonyl Groups: â€œCarbonylicityâ€•Percentage as a Chemical Driving Force. Journal of Physical Chemistry A, 2008, 112, 9153-9165.	2.5	25
22	Penicillin's catalytic mechanism revealed by inelastic neutrons and quantum chemical theory. Physical Chemistry Chemical Physics, 2013, 15, 20447-20455.	2.8	24
23	An ab initio exploratory study of side chain conformations for selected backbone conformations of N -acetyl- l -glutamine- N -methylamide. Computational and Theoretical Chemistry, 2001, 545, 29-47.	1.5	22
24	Ab initio and DFT conformational analysis of selected flavones: 5,7-dihydroxyflavone (chrysin) and 7,8-dihydroxyflavone. Canadian Journal of Chemistry, 2002, 80, 845-855.	1.1	22
25	Geometric, electronic and elastic properties of dental silver amalgam Î³-(Ag3Sn), Î³1-(Ag2Hg3), Î³2-(Sn8Hg) phases, comparison of experiment and theory. Intermetallics, 2010, 18, 756-760.	3.9	21
26	The fine balance between one cross-coupling and two Î²-hydride elimination pathways: a DFT mechanistic study of Ni(Ï€-allyl)2-catalyzed cross-coupling of alkyl halides and alkyl Grignard reagents. Chemical Communications, 2010, 46, 2727-2729.	4.1	21
27	Periodic vs. molecular cluster approaches to resolving glass structure and properties: Anorthite a case study. Journal of Non-Crystalline Solids, 2016, 451, 138-145.	3.1	20
28	Between a reactant rock and a solvent hard place â€“ molecular corrals guide aromatic substitutions. Physical Chemistry Chemical Physics, 2014, 16, 1078-1083.	2.8	19
29	Phase separation in an ionomer glass: Insight from calorimetry and phase transitions. Journal of Non-Crystalline Solids, 2015, 415, 24-29.	3.1	19
30	Density functional molecular computations on protonated serotonin in the gas phase and various solvent media. Chemical Physics Letters, 2002, 365, 542-551.	2.6	18
31	A Hartreeâ€“Fock, MP2 and DFT computational study of the structures and energies of â€³b2 ions derived from deprotonated peptides. A comparison of method and basis set used on relative product stabilities. Computational and Theoretical Chemistry, 2004, 675, 149-162.	1.5	18
32	Qualitative assessment of microstructure and Hertzian indentation failure in biocompatible glass ionomer cements. Journal of Materials Science: Materials in Medicine, 2012, 23, 677-685.	3.6	18
33	New insights into the role of solution additive anions in Mg²⁺ dehydration: implications for mineral carbonation. CrystEngComm, 2021, 23, 4896-4900.	2.6	18
34	Resolving nanoscopic structuring and interfacial THz dynamics in setting cements. Materials Advances, 2022, 3, 4982-4990.	5.4	18
35	Systemic Energy Management by Strategically Located Functional Components within Molecular Frameworks, Determined by Systems Chemistry. Journal of Physical Chemistry B, 2009, 113, 10308-10314.	2.6	17
36	Vitamin E models. Conformational analysis and stereochemistry of tetralin, chroman, thiochroman and selenochroman. Computational and Theoretical Chemistry, 2002, 594, 161-172.	1.5	16

#	Article	IF	Citations
37	Excitonic Character in Optical Properties of Tetrahedral CdX (X = S, Se, Te) Clusters. Journal of Physical Chemistry C, 2015, 119, 29171-29177.	3.1	16
38	Competing Mechanisms, Substituent Effects, and Regioselectivities of Nickel-Catalyzed [2 + 2 + 2] Cycloaddition between Carboryne and Alkynes: A DFT Study. Journal of Organic Chemistry, 2015, 80, 9108-9117.	3.2	16
39	Vitamin E models. Shortened sidechain models of Î±, Î², Î³ and Î´ tocopherol and tocotrienolâ€"a density functional study. Computational and Theoretical Chemistry, 2003, 637, 11-26.	1.5	15
40	An exploratory study of side-chainâ€"backbone interaction in selected conformations of N -acetyl- l -glutamate- N -methylamide. An ab initio study. Computational and Theoretical Chemistry, 2001, 543, 203-222.	1.5	14
41	Fragmentation Reactions of a2Ions Derived From Deprotonated DipeptidesA Synergy Between Experiment and Theoryâ€. Journal of Physical Chemistry A, 2002, 106, 9695-9704.	2.5	14
42	Conformational effects of one glycine residue on the other glycine residues in the Ac-Gly-Gly-Gly-NHMe tripeptide motif: an ab initio exploratory study. Computational and Theoretical Chemistry, 2002, 588, 187-200.	1.5	14
43	Simulations reveal the role of composition into the atomic-level flexibility of bioactive glass cements. Physical Chemistry Chemical Physics, 2016, 18, 837-845.	2.8	14
44	Conformational potential energy surfaces of a Lycopene model. Computational and Theoretical Chemistry, 2001, 571, 7-26.	1.5	13
45	Exploration of the Four-Dimensional-Conformational Potential Energy Hypersurface ofN-Acetyl-l-aspartic AcidNâ€˜-Methylamide with Its Internally Hydrogen Bonded Side-Chain Orientation. Journal of Physical Chemistry A, 2002, 106, 6999-7009.	2.5	13
46	Flexibility of â€œPolyunsaturated Fatty Acid Chainsâ€•and Peptide Backbones:â€‰ A Comparative ab Initio Study. Journal of Physical Chemistry A, 2005, 109, 520-533.	2.5	13
47	Density Functional Molecular Study on the Full Conformational Space of the S-4-(2-Hydroxypropoxy)carbazol Fragment of Carvedilol (1-(9Hâ^Carbazol-4-yloxy)-3-) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 342 Physical Chemistry A, 2002, 106, 10423-10436.	2.5	11
48	A modular numbering system of selected oligopeptides for molecular computations: using pre-computed amino acid building blocks. Computational and Theoretical Chemistry, 2003, 666-667, 169-218.	1.5	11
49	A comparative conformational analysis of selected central nervous system stimulants. Computational and Theoretical Chemistry, 2003, 623, 51-62.	1.5	11
50	Generation and analysis of the conformational potential energy surfaces of N-acetyl-N-methyl-l-alanine-Nâ€²-methylamide. An exploratory ab initio study. Computational and Theoretical Chemistry, 2003, 625, 121-136.	1.5	11
51	Structure and spectroscopy of CuH preparedviaborohydride reduction. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2015, 71, 608-612.	1.1	11
52	Systematic characterisation of the structure and radical scavenging potency of Pu'Er tea () polyphenol theaflavin. Organic and Biomolecular Chemistry, 2019, 17, 9942-9950.	2.8	11
53	An assessment of the chiral environment created by adjacent d- and l-alanyl residues on a glycine unit within the tripeptide N-Ac-Ala-Gly-Ala-NHMe: an ab initio exploratory study. Computational and Theoretical Chemistry, 2003, 621, 163-187.	1.5	10
54	Vitamin E models. Can the anti-oxidant and pro-oxidant dichotomy of Î±-tocopherol be related to ionic ring closing and radical ring opening redox reactions?. Computational and Theoretical Chemistry, 2003, 620, 93-106.	1.5	10

#	Article	IF	Citations
55	Simplification through complexity: the role of Ni-complexes in catalysed diyneâ€“cyclobutanone [4+2+2] cycloadditions, a comparative DFT study. Physical Chemistry Chemical Physics, 2012, 14, 6937.	2.8	10
56	Cationic intermediates in trans- to cis- isomerization reactions of allylic systems. An exploratory ab initio study. Computational and Theoretical Chemistry, 2001, 546, 143-162.	1.5	9
57	How reliable could economic Hartreeâ€“Fock computations be in studying large, folded peptides? A comparative HF and DFT case study on N- and C-protected aspartic acid. Computational and Theoretical Chemistry, 2002, 619, 143-194.	1.5	9
58	Asparagineâ€”ab initio structural analyses. Computational and Theoretical Chemistry, 2003, 666-667, 273-278.	1.5	9
59	A Quantitative Scale for the Extent of Conjugation of Substituted Olefines. Journal of Physical Chemistry A, 2009, 113, 7953-7962.	2.5	9
60	The fitting and functional analysis of a double rotor potential energy surface for the R and S enantiomers of 1-chloro-3-fluoro-isobutane. Computational and Theoretical Chemistry, 2003, 666-667, 79-87.	1.5	8
61	An ab initio exploratory study on the conformational features of the dipeptide MeCO-Ala-Ala-NH-Me in its four different configurations: determination of the behaviour of d-enantiomer amino acids within a peptide chain. Computational and Theoretical Chemistry, 2003, 666-667, 291-301.	1.5	8
62	An ab initio exploratory study of the full conformational space of MeCO-l-threonine-NH-Me. Computational and Theoretical Chemistry, 2003, 666-667, 251-267.	1.5	7
63	An ab initio conformational study on 2,3-dihydrobilin-1,19(21H,24H)-dione, a model compound for open-chain tetrapyrroles. Computational and Theoretical Chemistry, 2004, 680, 219-225.	1.5	7
64	Ab initio conformational analysis of N- and C-terminally-protected valyl-alanine dipeptide model. Computational and Theoretical Chemistry, 2005, 729, 177-184.	1.5	7
65	Multidimensional conformational analysis of the sidechain conformers of the fully extended backbone (Î²L) of N-Ac-Homocysteine-NHMe; an ab initio exploratory study. Computational and Theoretical Chemistry, 2002, 619, 21-35.	1.5	6
66	Multiâ€Pathway Consequent Chemoselectivities of CpRuCl(PPh₃)₂/Melâ€Catalysed Norbornadiene Alkyne Cycloadditions. Chemistry - A European Journal, 2016, 22, 15396-15403.	3.3	6
67	Dynamic chirality in selected diaryl methane containing drugs. An exploratory ab initio conformational study. Computational and Theoretical Chemistry, 2001, 549, 217-228.	1.5	5
68	N-acetyl-L-aspartic acid-N'-methylamide with side-chain orientation capable of external hydrogen bonding. European Physical Journal D, 2002, 20, 499-511.	1.3	5
69	A model study of the IgA hinge region: an exploratory study of selected backbone conformations of MeCO-l-Pro-l-Thr-NH-Me. Computational and Theoretical Chemistry, 2003, 666-667, 311-319.	1.5	5
70	Exploratory study on the full conformation space of Î±-tocopherol and its selected congeners. Computational and Theoretical Chemistry, 2003, 666-667, 439-443.	1.5	5
71	Conformational dependence of the intrinsic acidity of the aspartic acid residue sidechain in N-acetyl-l-aspartic acid-Nâ€²-methylamide. Computational and Theoretical Chemistry, 2003, 620, 231-255.	1.5	5
72	Molecular orbital computations on lipids: an ab initio exploratory study on the conformations of glycerol and its fluorine congeners. Computational and Theoretical Chemistry, 2005, 722, 79-96.	1.5	5

#	Article	IF	Citations
73	Vitamin E models. European Physical Journal D, 2002, 20, 609-618.	1.3	4
74	Molecular orbital analysis of the effect of d- and l-alanyl residues on the glycine chirality within the tripeptide N-Ac-Ala-Gly[Î²]-Ala-NH-Me. An ab initio and DFT study. Computational and Theoretical Chemistry, 2003, 666-667, 321-326.	1.5	4
75	An ab initio exploratory study on selected conformational features of MeCO-l-Ala-l-Ala-l-Ala-NH-Me as a XxxYyyZzz tripeptide motif within a protein structure. Computational and Theoretical Chemistry, 2003, 666-667, 327-336.	1.5	4
76	Ramachandran backbone potential energy surfaces of aspartic acid and aspartate residues: implications on allosteric sites in receptorâ€“ligand complexations. Computational and Theoretical Chemistry, 2003, 666-667, 279-284.	1.5	4
77	Bridging the gap between pure science and the general public: comparison of the informational exchange for these extremities in scientific awareness. Computational and Theoretical Chemistry, 2003, 666-667, 699-706.	1.5	4
78	The pivotal role of electronics in preferred alkene over alkyne Niâ€“carboryne insertions and absolute regioselectivities. Dalton Transactions, 2018, 47, 6494-6498.	3.3	4
79	Molecular computations on lipids: a numbering system for phospholipids and triglyceride. Computational and Theoretical Chemistry, 2002, 619, 1-20.	1.5	3
80	Toward a computed structure database: methodology for effective molecular orbital computations. Computational and Theoretical Chemistry, 2003, 666-667, 61-67.	1.5	3
81	The benefits of a pre-computed amino acid structure database in quantum chemical geometry optimizations of Î²-turns of peptides. Computational and Theoretical Chemistry, 2003, 666-667, 355-359.	1.5	3
82	The multidimensional conformational analysis for the backbone across the disrotatory axis at selected side-chain conformers of N-Ac-homocysteine-NHMeâ€”an ab initio exploratory study. Computational and Theoretical Chemistry, 2003, 666-667, 243-249.	1.5	3
83	Discussion: Nuclear Quantum Dynamics - Protons and Beyond. Journal of Physics: Conference Series, 2014, 571, 012004.	0.4	3
84	Quantum topological resolution of catalyst proficiency. International Journal of Quantum Chemistry, 2015, 115, 875-883.	2.0	3
85	An exploratory ab initio conformational analysis of selected fragments of nicotinamide adenine dinucleotide (NAD+). Part II: adenosine. Computational and Theoretical Chemistry, 2003, 666-667, 431-437.	1.5	2
86	Stereoelectronic effects and dynamic chirality in ethyl nitrite (Et-ONO) computed at the HF and DFT levels of theory. Computational and Theoretical Chemistry, 2001, 548, 39-46.	1.5	1
87	An exploratory conformational analysis of d and l Î²-6-deoxyglucose. An ab initio and DFT approach. Computational and Theoretical Chemistry, 2003, 666-667, 393-396.	1.5	1
88	An isodesmic comparison of the C1 modified reduced pteridine ring as a folic acid model. Computational and Theoretical Chemistry, 2003, 666-667, 409-414.	1.5	1
89	An exploratory ab initio conformational analysis of selected fragments of nicotinamide adenine dinucleotide (NAD+). Part I: 5-deoxyribose nicotinamide N-glycoside. Computational and Theoretical Chemistry, 2003, 666-667, 415-429.	1.5	1
90	Chemical structure of the chlorination product of tribromoethylene. Computational and Theoretical Chemistry, 2002, 583, 145-151.	1.5	0

#	Article	IF	Citations
91	Intermolecular interactions of small biologically active molecules: acetone, methylamine and water; methyl phosphate, water and divalent ions; phenol and water; N-Ac-l-Gly-NH-Me and water. Computational and Theoretical Chemistry, 2003, 666-667, 99-107.	1.5	0
92	Molecular orbital computations on lipids: modular numbering. Computational and Theoretical Chemistry, 2003, 666-667, 445-449.	1.5	0
93	The power of VNA-driven quasi-optics to sense group molecular action in condensed phase systems. , 2014, , .		0
94	Reply to the â€˜Comment on â€œPenicillin's catalytic mechanism revealed by inelastic neutrons and quantum chemical theoryâ€â€™ by S. A. Glover, Phys. Chem. Chem. Phys., 2019, 21, 18012. Physical Chemistry Chemical Physics, 2019, 21, 25513-25517.	2.8	0