Kim Baldridge

List of Publications by Year in Descending Order

241 papers	25,604 citations	49 h-index	159 g-index
276 ext. papers	27,003 ext. citations	7.7 avg, IF	6.2 L-index

#	Paper	IF	Citations
241	Cooperative Weak Dispersive Interactions Actuate Catalysis in a Shape-Selective Abiological Racemase.. *Journal of the American Chemical Society*, **2022**,	16.4	3
240	Synthesis and Acidity of 5-(-Terphenyl-2'-yl)-1-tetrazoles: Evidence for an Enhanced Polar-Effect Compared to Carboxylic Acids. *Journal of Medicinal Chemistry*, **2021**, 64, 3197-3203	8.3	0
239	The Unusual Photochromic and Hydrochromic Switching Behavior of Cellulose-Embedded 1,8-Naphthalimide-Viologen Derivatives in the Solid-State. *Chemistry - A European Journal*, **2021**, 27, 9360-9371	4.8	3
238	The chemistry of branched condensed phosphates. *Nature Communications*, **2021**, 12, 5368	17.4	4
237	Enantiopure C Pentaindenocorannulenes: Chiral Graphenoid Materials. *Angewandte Chemie - International Edition*, **2021**, 60, 25809-25814	16.4	2
236	Spontaneous and induced chiral symmetry breaking of stereolabile pillar[5]arene derivatives upon crystallisation. *Chemical Science*, **2021**, 12, 10985-10989	9.4	2
235	Thiophene fused indenocorannulenes: synthesis, variable emission, and exceptional chiral configurational stability. *Organic Chemistry Frontiers*, **2021**, 8, 3653-3658	5.2	0
234	Classical and non-classical melatonin receptor agonist-directed micellization of bipyridinium-based supramolecular amphiphiles in water. *Soft Matter*, **2020**, 16, 4788-4799	3.6	2
233	An -Symmetric 5-Fold Interlocked [2]Catenane. *Journal of the American Chemical Society*, **2020**, 142, 10267-10272	16.4	27
232	Transition-Metal Catalysis of Triene 6-Electrocyclization: The -Complexation Strategy Realized. *Angewandte Chemie - International Edition*, **2020**, 59, 17958-17965	16.4	7
231	Generalized Analytic Approach for Determination of Multidimensional Franck-Condon Factors: Simulated Photoelectron Spectra of Polynuclear Aromatic Hydrocarbons. *Journal of Chemical Theory and Computation*, **2020**, 16, 4521-4532	6.4	0
230	Transition-Metal Catalysis of Triene 6-Electrocyclization: The -Complexation Strategy Realized. *Angewandte Chemie*, **2020**, 132, 18114-18121	3.6	
229	X-ray Crystallography and Unexpected Chiroptical Properties Reassign the Configuration of Haliclonadiamine. *Journal of the American Chemical Society*, **2020**, 142, 2755-2759	16.4	3
228	Fluorous Corannulenes: Ab initio Predictions and the Synthesis of sym-Pentafluorocorannulene. *Angewandte Chemie - International Edition*, **2020**, 59, 1460-1464	16.4	4
227	Innentitelbild: Fluorous Corannulenes: Ab initio Predictions and the Synthesis of sym-Pentafluorocorannulene (Angew. Chem. 4/2020). *Angewandte Chemie*, **2020**, 132, 1374-1374	3.6	
226	Fluorous Corannulenes: Ab initio Predictions and the Synthesis of sym-Pentafluorocorannulene. *Angewandte Chemie*, **2020**, 132, 1476-1480	3.6	2
225	Involvement of aryl hydrocarbon receptor in the cytotoxicity of corannulene and its derivatives. *Toxicology Letters*, **2020**, 321, 114-121	4.4	2

224	Diastereoselective Monofluorocyclopropanation Using Fluoromethylsulfonium Salts. *Organic Letters*, **2019**, 21, 7174-7178	6.2	13
223	Synthesis of Modified Nucleoside Oligophosphates Simplified: Fast, Pure, and Protecting Group Free. *Journal of the American Chemical Society*, **2019**, 141, 15013-15017	16.4	14
222	Acid-Induced Liberation of Polysubstituted Cyclopentadiene Ligands from Cyclopentadienyl Cobalt: A [2 + 2 + 1] Cycloaddition Route toward 1,2,4-Trisubstituted Cyclopentadienes. *Journal of Organic Chemistry*, **2019**, 84, 13992-14004	4.2	0
221	Peraryl-X-onium ions of nitrogen and oxygen. *Organic Chemistry Frontiers*, **2019**, 6, 2640-2646	5.2	6
220	Versatile hydrochromic fluorescent materials based on a 1,8-naphthalimide integrated fluorophore-receptor system. *Journal of Materials Chemistry C*, **2019**, 7, 7399-7410	7.1	15
219	Azaindenocorannulenes: Synthesis, Properties, and Chirality. *Organic Letters*, **2019**, 21, 3510-3513	6.2	9
218	Corannurylene Pentapetalae. *Journal of the American Chemical Society*, **2019**, 141, 5402-5408	16.4	63
217	Pathways towards true catalysts: computational modelling and structural transformations of Zn-polyoxotungstates. *Dalton Transactions*, **2019**, 48, 13293-13304	4.3	3
216	Fivefold Symmetry and 2D Crystallization: Self-Assembly of the Buckybowl Pentaindenocorannulene on a Cu(100) Surface. *Chemistry - A European Journal*, **2019**, 25, 11555-11559	4.8	3
215	Triple carbon–fluorine bond activation for modification of metal ligands: Synthesis of the first η5-C5Me4(CHPh2) transition metal complex. *Polyhedron*, **2019**, 157, 406-409	2.7	0
214	Systems with Extensive Delocalization **2018**, 227-272		
213	Chiral Atropisomeric Indenocorannulene Bowls: Critique of the Cahn-Ingold-Prelog Conception of Molecular Chirality. *Angewandte Chemie - International Edition*, **2018**, 57, 6470-6474	16.4	13
212	1,2,3- versus 1,2-Indeno Ring Fusions Influence Structure Property and Chirality of Corannulene Bowls. *Journal of Organic Chemistry*, **2018**, 83, 3979-3986	4.2	8
211	Melatonin-directed micellization: a case for tryptophan metabolites and their classical bioisosteres as templates for the self-assembly of bipyridinium-based supramolecular amphiphiles in water. *Soft Matter*, **2018**, 14, 2893-2905	3.6	7
210	Performance analysis of open-source distributed file systems for practical large-scale molecular ab initio, density functional theory, and GW + BSE calculations. *International Journal of Quantum Chemistry*, **2018**, 118, e25392	2.1	0
209	From charge-transfer excitations to charge-transport phenomena in organic molecular crystals. *International Journal of Quantum Chemistry*, **2018**, 118, e25413	2.1	1
208	Pauli Repulsion Versus van der Waals: Interaction of Indenocorannulene with a Cu(111) Surface. *Journal of Physical Chemistry B*, **2018**, 122, 871-877	3.4	5
207	Chiral Atropisomeric Indenocorannulene Bowls: Critique of the Cahn–Ingold–Prelog Conception of Molecular Chirality. *Angewandte Chemie*, **2018**, 130, 6580-6584	3.6	2

206	Indenocorannulene-Based Materials: Effect of Solid-State Packing and Intermolecular Interactions on Optoelectronic Properties. *Journal of Physical Chemistry C*, **2017**, 121, 1220-1234	3.8	14
205	[3+3] Cyclocondensation of Disubstituted Biphenyl Dialdehydes: Access to Inherently Luminescent and Optically Active Hexa-substituted C-Symmetric and Asymmetric Trianglimine Macrocycles. *Journal of Organic Chemistry*, **2017**, 82, 2472-2480	4.2	13
204	An Efficient Analytic Approach for Calculation of Multi-Dimensional Franck-Condon Factors and Associated Photoelectron Spectra. *Journal of Chemical Theory and Computation*, **2017**, 13, 2147-2158	6.4	7
203	Diindenocorannulenes: Curved Aromatics Blending Bowl-in-Bowl Assembly and Nanocarbon Material Properties. *European Journal of Organic Chemistry*, **2017**, 2017, 2801-2805	3.2	11
202	Dispersion-Corrected Spin-Component-Scaled Double-Hybrid Density Functional Theory: Implementation and Performance for Non-covalent Interactions. *Journal of Chemical Theory and Computation*, **2017**, 13, 2650-2666	6.4	8
201	Stereoselective Formation of η6-Arene Ruthenium(II) Complexes via Metal-Triggered Bergman and Hopf Cycloaromatizations. *Organometallics*, **2017**, 36, 4256-4267	3.8	3
200	Photoactivated Transition-Metal Triggers for Ambient Temperature Enediyne and Dienyne Cyclization: Ruthenium-η6-Naphthalene Complexes. *Organometallics*, **2017**, 36, 3967-3973	3.8	6
199	Evidence of enhanced photocurrent response in corannulene films. *RSC Advances*, **2017**, 7, 45601-45606	3.7	3
198	General optimization procedure towards the design of a new family of minimal parameter spin-component-scaled double-hybrid density functional theory. *Physical Chemistry Chemical Physics*, **2017**, 19, 26191-26200	3.6	12
197	Transition Metal Complexes of a Monocarba-closo-dodecaborate Ligand via B–H Activation. *European Journal of Inorganic Chemistry*, **2017**, 2017, 4420-4424	2.3	17
196	Decakis(arylthio)corannulenes: Transferable Photochemical and Redox Parameters and Photovoltaic Device Performance. *European Journal of Organic Chemistry*, **2017**, 2017, 4338-4342	3.2	13
195	Trifluoromethyl/Perfluoroalkyl Corannulenes: Directed Synthesis and Photophysical Characterization. *European Journal of Organic Chemistry*, **2017**, 2017, 875-879	3.2	15
194	Synthesis and full characterization of an iridium B-H activation intermediate of the monocarba-closo-dodecaborate anion. *Chemical Communications*, **2016**, 53, 176-179	5.8	33
193	On the Origins of Nonradiative Excited State Relaxation in Aryl Sulfoxides Relevant to Fluorescent Chemosensing. *Journal of the American Chemical Society*, **2016**, 138, 15889-15895	16.4	15
192	Cobalt complexes of tetradentate, bipyridine-based macrocycles: their structures, properties and photocatalytic proton reduction. *Dalton Transactions*, **2016**, 45, 1737-45	4.3	37
191	Tunable Photochemical/Redox Properties of (Phenylthio)ncorannulenes: Application to a Photovoltaic Device. *Journal of the Brazilian Chemical Society*, **2016**,	1.5	2
190	Pentaindenocorannulene: Properties, Assemblies, and C Complex. *Angewandte Chemie - International Edition*, **2016**, 55, 14648-14652	16.4	39
189	Pentaindenocorannulene: Properties, Assemblies, and C60 Complex. *Angewandte Chemie*, **2016**, 128, 14868-14872	3.6	24

188	Intramolecular C–H insertion vs. Friedel–Crafts coupling induced by silyl cation-promoted C–F activation. *Organic Chemistry Frontiers*, **2015**, 2, 1018-1021	5.2	28
187	Structure and dynamics in unsymmetrically substituted five-coordinate iridacyclopentadiene complexes. *Journal of Physical Organic Chemistry*, **2015**, 28, 199-202	2.1	3
186	Molecular compression chambers: exceeding the Euler modulus. *Journal of Physical Organic Chemistry*, **2015**, 28, 223-225	2.1	5
185	DFT-based Green's function pathways model for prediction of bridge-mediated electronic coupling. *Physical Chemistry Chemical Physics*, **2015**, 17, 30842-53	3.6	10
184	Stereospecific Oxidative Demetallation of Highly Functionalized CpCo(1,3-Diene) Complexes: An Experimental and Computational Study. *Synlett*, **2015**, 26, 2243-2246	2.2	2
183	Tuning electron transport through functionalized C20H10 molecular junctions. *Journal of Chemical Theory and Computation*, **2015**, 11, 4900-10	6.4	6
182	Mechanism of photocatalytic hydrogen generation by a polypyridyl-based cobalt catalyst in aqueous solution. *Inorganic Chemistry*, **2015**, 54, 646-57	5.1	94
181	Thiophene-fused bowl-shaped polycyclic aromatics with a dibenzo[a,g]corannulene core for organic field-effect transistors. *Chemical Communications*, **2015**, 51, 1681-4	5.8	63
180	Extended Corannulenes: Aromatic Bowl/Sheet Hybridization. *Angewandte Chemie*, **2015**, 127, 10942-10946	5.8	26
179	Extended Corannulenes: Aromatic Bowl/Sheet Hybridization. *Angewandte Chemie - International Edition*, **2015**, 54, 10792-6	16.4	44
178	Boronic esters of corannulene: potential building blocks toward icosahedral supramolecules. *Organic Chemistry Frontiers*, **2015**, 2, 626-633	5.2	27
177	Buckybowl superatom states: a unique route for electron transport?. *Physical Chemistry Chemical Physics*, **2015**, 17, 6114-21	3.6	20
176	Through-space interactions in enshrouded m-terphenylsilanes. *Journal of Physical Organic Chemistry*, **2014**, 27, 277-283	2.1	3
175	Induced-fit catalysis of corannulene bowl-to-bowl inversion. *Nature Chemistry*, **2014**, 6, 222-8	17.6	122
174	Cu(I) and Ag(I) complexes of 7,10-bis-N-heterocycle-diazafluoranthenes: programmed molecular grids?. *Dalton Transactions*, **2014**, 43, 11027-38	4.3	7
173	Corannulene derivatives as non-fullerene acceptors in solution-processed bulk heterojunction solar cells. *Journal of Materials Chemistry A*, **2014**, 2, 20515-20519	13	56
172	Close covalent contacts: gauging molecular compression in a molecular compression chamber. *Physical Chemistry Chemical Physics*, **2014**, 16, 1379-84	3.6	6
171	Synthesis of Bioconjugated sym-pentasubstituted corannulenes: experimental and theoretical investigations of supramolecular architectures. *Bioconjugate Chemistry*, **2014**, 25, 115-28	6.3	26

170	Structure-property relationships of curved aromatic materials from first principles. *Accounts of Chemical Research*, **2014**, 47, 3310-20	24.3	19
169	Code interoperability and standard data formats in quantum chemistry and quantum dynamics: The Q5/D5Cost data model. *Journal of Computational Chemistry*, **2014**, 35, 611-21	3.5	17
168	Electron transport and optical properties of curved aromatics. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 1-12	7.9	18
167	Quadruple anionic buckybowls by solid-state chemistry of corannulene and cesium. *Journal of the American Chemical Society*, **2013**, 135, 12857-60	16.4	24
166	Tunable star-shaped triphenylamine fluorophores for fluorescence quenching detection and identification of nitro-aromatic explosives. *Chemical Communications*, **2013**, 49, 780-2	5.8	78
165	Static and Field-Oriented Properties of Bowl-Shaped Polynuclear Aromatic Hydrocarbon Fragments. *Journal of Chemical Theory and Computation*, **2013**, 9, 4797-804	6.4	11
164	Defined-Sector Explicit Solvent in Continuum Cluster Model for Computational Prediction of pKa: Consideration of Secondary Functionality and Higher Degree of Solvation. *Journal of Chemical Theory and Computation*, **2013**, 9, 1027-35	6.4	10
163	Of graphs and graphenes: molecular design and chemical studies of aromatic compounds. *Angewandte Chemie - International Edition*, **2013**, 52, 5436-8	16.4	25
162	Von Graphen und Graphenen: molekulares Design und chemische Studien aromatischer Verbindungen. *Angewandte Chemie*, **2013**, 125, 5546-5548	3.6	12
161	Chemistry at the alkyne-carbene intersection: a metallacyclobutene-□-vinylcarbene equilibration. *Journal of the American Chemical Society*, **2013**, 135, 8826-9	16.4	15
160	Structural Characterization of (C5H5)Co(PPh3)(□-alkyne) and (C5H5)Co(□-alkyne) Complexes of Highly Polarized Alkynes. *Organometallics*, **2013**, 32, 5473-5480	3.8	9
159	Molecular spur gears comprising triptycene rotators and bibenzimidazole-based stators. *Journal of the American Chemical Society*, **2012**, 134, 1528-35	16.4	101
158	Structural, optical, and electrochemical properties of three-dimensional push-pull corannulenes. *Journal of Organic Chemistry*, **2012**, 77, 11014-26	4.2	60
157	Defined-sector explicit solvent in the continuum model approach for computational prediction of pK a. *Molecular Physics*, **2012**, 110, 2401-2412	1.7	5
156	Molecular nesting in co-crystals of tetrabenzoquadrannulene and C60: application of the sphere in a cone model. *Chemical Communications*, **2012**, 48, 9882-4	5.8	22
155	New perspectives on polyoxometalate catalysts: alcohol oxidation with Zn/Sb-polyoxotungstates. *Chemistry - A European Journal*, **2012**, 18, 13293-8	4.8	40
154	Pentagonal tiling with buckybowls: pentamethylcorannulene on Cu(111). *Physical Chemistry Chemical Physics*, **2012**, 14, 13365-9	3.6	15
153	Synthesis and characterization of open and sandwich-type polyoxometalates reveals visible-light-driven water oxidation via POM-photosensitizer complexes. *Green Chemistry*, **2012**, 14, 1680	10	114

152	Basicity of (2,6-Pyridino)paracyclophanes: Lone Pair–Cation–and Solvation Effects. *Angewandte Chemie*, **2012**, 124, 2957-2960	3.6	2
151	Basicity of (2,6-pyridino)paracyclophanes: lone pair-–cation-–and solvation effects. *Angewandte Chemie - International Edition*, **2012**, 51, 2903-6	16.4	11
150	Competition between π-arene and lone-pair halogen coordination of silylium ions?. *Journal of the American Chemical Society*, **2011**, 133, 11844-6	16.4	37
149	Effect of molecular packing on corannulene-based materials electroluminescence. *Journal of the American Chemical Society*, **2011**, 133, 14002-9	16.4	74
148	Proton-catalyzed, silane-fueled Friedel-Crafts coupling of fluoroarenes. *Science*, **2011**, 332, 574-7	33.3	248
147	Stereoselective Coordination of C5-Symmetric Corannulene Derivatives with an Enantiomerically Pure [RhI(nbd*)] Metal Complex. *Angewandte Chemie*, **2011**, 123, 895-897	3.6	10
146	Stereoselective coordination of C5-symmetric corannulene derivatives with an enantiomerically pure [Rh(I)(nbd*)] metal complex. *Angewandte Chemie - International Edition*, **2011**, 50, 865-7	16.4	45
145	Back Cover: Stereoselective Coordination of C5-Symmetric Corannulene Derivatives with an Enantiomerically Pure [RhI(nbd*)] Metal Complex (Angew. Chem. Int. Ed. 4/2011). *Angewandte Chemie - International Edition*, **2011**, 50, 966-966	16.4	
144	Surface-assisted bowl-in-bowl stacking of nonplanar aromatic hydrocarbons. *Chemical Communications*, **2011**, 47, 7995-7	5.8	28
143	Large Induced Interface Dipole Moments without Charge Transfer: Buckybowls on Metal Surfaces. *Journal of Physical Chemistry Letters*, **2011**, 2, 2805-2809	6.4	39
142	Implementation and Performance of DFT-D with Respect to Basis Set and Functional for Study of Dispersion Interactions in Nanoscale Aromatic Hydrocarbons. *Journal of Chemical Theory and Computation*, **2010**, 6, 1924	6.4	4
141	Assessment of DFT and DFT-D for Potential Energy Surfaces of Rare Gas Trimers-Implementation and Analysis of Functionals and Extrapolation Procedures. *Journal of Chemical Theory and Computation*, **2010**, 6, 1951-65	6.4	7
140	Theoretical investigation of the binding process of corannulene on a Cu(111) surface. *Journal of Physical Chemistry A*, **2010**, 114, 8864-72	2.8	21
139	A photochemical metallocene route to anionic enediynes: synthesis, solid-state structures, and ab initio computations on cyclopentadienidoenediynes. *Journal of the American Chemical Society*, **2010**, 132, 11030-2	16.4	2
138	Intramolecular halogen stabilization of silylium ions directs gearing dynamics. *Journal of the American Chemical Society*, **2010**, 132, 7828-9	16.4	50
137	Efficient discovery of fluorescent chemosensors based on a biarylpyridine scaffold. *Organic Letters*, **2010**, 12, 940-3	6.2	18
136	Synthesis, structure and properties of decakis(phenylthio)corannulene. *Organic and Biomolecular Chemistry*, **2010**, 8, 53-5	3.9	39
135	Symmetry and polar-π effects on the dynamics of enshrouded aryl-alkyne molecular rotors. *Chemical Science*, **2010**, 1, 102	9.4	34

134	C?F Activation of Fluorobenzene by Silylium Carboranes: Evidence for Incipient Phenyl Cation Reactivity. *Angewandte Chemie*, **2010**, 122, 7681-7684	3.6	41
133	C-F activation of fluorobenzene by silylium carboranes: evidence for incipient phenyl cation reactivity. *Angewandte Chemie - International Edition*, **2010**, 49, 7519-22	16.4	86
132	Thermodynamic and computational studies on the binding of p53-derived peptides and peptidomimetic inhibitors to HDM2. *ChemBioChem*, **2009**, 10, 1360-8	3.8	14
131	Reversible phase transitions in a buckybowl monolayer. *Angewandte Chemie - International Edition*, **2009**, 48, 1966-9	16.4	64
130	Synthesis and crystal structure of a silyl-stabilized allyl cation formed by disruption of an arene by a protonation-hydrosilylation sequence. *Angewandte Chemie - International Edition*, **2009**, 48, 3787-90	16.4	28
129	ERI sorting for emerging processor architectures. *Computer Physics Communications*, **2009**, 180, 1221-1229	4.2	5
128	Implementation and Optimization of DFT-D/COSab with Respect to Basis Set and Functional: Application to Polar Processes of Furfural Derivatives in Solution. *Journal of Chemical Theory and Computation*, **2009**, 5, 2772-86	6.4	8
127	Photophysics of manisyl-substituted 2-pyridin-2-yl-1,10-phenanthrolines. Dual emission dependent on structure and solvent. *Physical Chemistry Chemical Physics*, **2009**, 11, 5408-15	3.6	6
126	Ab initio quantum chemical computations of substituent effects on triaziridine strain energy and heat of formation. *Physical Chemistry Chemical Physics*, **2009**, 11, 2387-95	3.6	10
125	Diels-Alder reactions of 3,6-disubstituted 1,2,4,5-tetrazines. Synthesis and X-ray crystal structures of diazafluoranthene derivatives. *Organic and Biomolecular Chemistry*, **2009**, 7, 2082-92	3.9	13
124	Synthesis, X-ray crystal structures, and computational studies of 1,1'-bridged 4,4'-diaryl-2,2'-bibenzimidazoles: building blocks for supramolecular structures. *Organic and Biomolecular Chemistry*, **2009**, 7, 2347-52	3.9	9
123	1,3,4,6,7,9-Hexamethylbenzo[1,2-c:3,4-c':5,6-c'']trithiophene: a twisted heteroarene. *Organic and Biomolecular Chemistry*, **2009**, 7, 2748-55	3.9	5
122	Application of Structural Principles to the Design of Triptycene-Based Molecular Gears with Parallel Axes. *Chimia*, **2009**, 63, 201-204	1.3	13
121	UNICORE **2009**, 615-643		3
120	Multiethynyl corannulenes: synthesis, structure, and properties. *Journal of the American Chemical Society*, **2008**, 130, 10729-39	16.4	118
119	Through-space interactions between parallel-offset arenes at the van der Waals distance: 1,8-diarylbiphenylene syntheses, structure and QM computations. *Physical Chemistry Chemical Physics*, **2008**, 10, 2686-94	3.6	81
118	Steric isotope effects gauged by the bowl-inversion barrier in selectively deuterated pentaarylcorannulenes. *Journal of the American Chemical Society*, **2008**, 130, 1583-91	16.4	46
117	Reactions of a metallacyclobutene complex with alkenes. *Journal of the American Chemical Society*, **2008**, 130, 10093-5	16.4	17

116	Quantum tunneling in biological reactions: the interplay between theory and experiments. *Journal of the Brazilian Chemical Society*, **2008**, 19, 206-210	1.5	11
115	Uniting extrinsic vectorization and shell structure for efficient SIMD evaluation of electron repulsion integrals. *Chemical Physics*, **2008**, 349, 147-157	2.3	4
114	Quantum chemical prediction of the 13C NMR shifts in alkyl and chlorocorannulenes: correction of chlorine effects. *Theoretical Chemistry Accounts*, **2008**, 120, 95-106	1.9	12
113	Towards a special-purpose computer for Hartree–Fock computations. *Theoretical Chemistry Accounts*, **2008**, 120, 133-153	1.9	8
112	Mark S. Gordon. *Theoretical Chemistry Accounts*, **2008**, 120, 1-4	1.9	5
111	Synthesis of 2,6-diarylphenyldimethylsilyl cations: polar-pi distribution of cation character. *Angewandte Chemie - International Edition*, **2008**, 47, 1719-22	16.4	69
110	Modulating the Lewis acidity of boron using a photoswitch. *Angewandte Chemie - International Edition*, **2008**, 47, 5034-7	16.4	82
109	On ERI sorting for SIMD execution of large-scale Hartree–Fock SCF. *Computer Physics Communications*, **2008**, 178, 817-834	4.2	8
108	Implementation and Performance of DFT-D with Respect to Basis Set and Functional for Study of Dispersion Interactions in Nanoscale Aromatic Hydrocarbons. *Journal of Chemical Theory and Computation*, **2008**, 4, 2030-48	6.4	149
107	Chemomentum - UNICORE 6 Based Infrastructure for Complex Applications in Science and Technology. *Lecture Notes in Computer Science*, **2008**, 82-93	0.9	19
106	Synthesis, structure, and isomerization of decapentynylcorannulene: enediyne cyclization/interconversion of C(40)R(10) isomers. *Journal of the American Chemical Society*, **2007**, 129, 12612-3	16.4	26
105	A simple model system for the study of carbohydrate--aromatic interactions. *Journal of the American Chemical Society*, **2007**, 129, 2890-900	16.4	94
104	Rearrangement of Iridabenzvalenes to Iridabenzenes and/or η5-Cyclopentadienyliridium(I) Complexes: Experimental and Computational Analysis of the Influence of Silyl Ring Substituents and Phosphine Ligands§. *Organometallics*, **2007**, 26, 3957-3968	3.8	50
103	Optical Properties of Phthalocyanine and Naphthalocyanine Compounds. *Journal of Chemical Theory and Computation*, **2007**, 3, 870-7	6.4	32
102	Converting massive TLP to DLP **2007**,		2
101	Stereoselectivity and expanded substrate scope of an engineered PLP-dependent aldolase. *Angewandte Chemie - International Edition*, **2006**, 45, 6824-6	16.4	32
100	Exploring biomolecular machines: energy landscape control of biological reactions. *Philosophical Transactions of the Royal Society B: Biological Sciences*, **2006**, 361, 1439-43	5.8	24
99	Dodecamethoxy- and hexaoxotricyclobutabenzene: synthesis and characterization. *Journal of the American Chemical Society*, **2006**, 128, 10032-3	16.4	65

98	Stereoselectivity and Expanded Substrate Scope of an Engineered PLP-Dependent Aldolase. *Angewandte Chemie*, **2006**, 118, 6978-6980	3.6	12
97	Synthesis of fluoranthenes and indenocorannulenes: elucidation of chiral stereoisomers on the basis of static molecular bowls. *Journal of the American Chemical Society*, **2006**, 128, 6870-84	16.4	117
96	Modulation of fragmental charge transfer via hydrogen bonds. Direct measurement of electronic contributions. *Journal of Physical Chemistry A*, **2006**, 110, 412-21	2.8	12
95	d8 rhodium and iridium complexes of corannulene. *Journal of the American Chemical Society*, **2006**, 128, 10644-5	16.4	64
94	Opal: SimpleWeb Services Wrappers for Scientific Applications **2006**,		19
93	Experimental and computational investigation of the uncatalyzed rearrangement and elimination reactions of isochorismate. *Journal of the American Chemical Society*, **2006**, 128, 2043-51	16.4	27
92	GEMSTONE: GRID ENABLED MOLECULAR SCIENCE THROUGH ONLINE NETWORKED ENVIRONMENTS **2006**,		7
91	Scientific Workflow Infrastructure for Computational Chemistry on the Grid. *Lecture Notes in Computer Science*, **2006**, 69-76	0.9	7
90	Isochorismate pyruvate lyase: a pericyclic reaction mechanism?. *Journal of the American Chemical Society*, **2005**, 127, 15002-3	16.4	65
89	Application of grid computing to parameter sweeps and optimizations in molecular modeling. *Future Generation Computer Systems*, **2005**, 21, 27-35	7.5	27
88	Incorporation of middleware and grid technologies to enhance usability in Computational Chemistry applications. *Future Generation Computer Systems*, **2005**, 21, 3-10	7.5	9
87	A Framework for the Design and Reuse of Grid Workflows. *Lecture Notes in Computer Science*, **2005**, 120-133	0.9	40
86	Cluster and Grid Infrastructure for Computational Chemistry and Biochemistry **2005**, 531-550		1
85	A Dynamic Data Driven Grid System for Intra-operative Image Guided Neurosurgery. *Lecture Notes in Computer Science*, **2005**, 672-679	0.9	5
84	Incorporation of Middleware and Grid Technologies to Enhance Usability in Computational Chemistry Applications. *Lecture Notes in Computer Science*, **2004**, 75-82	0.9	
83	Applying Grid Computing to the Parameter Sweep of a Group Difference Pseudopotential. *Lecture Notes in Computer Science*, **2004**, 148-155	0.9	5
82	Parameter scan of an effective group difference pseudopotential using grid computing. *New Generation Computing*, **2004**, 22, 137-146	0.9	19
81	Stabilization of benzene versus oligoacetylenes: not another scale for aromaticity. *Journal of Physical Organic Chemistry*, **2004**, 17, 740-742	2.1	12

80	Ring selectivity and migratory aptitude of Cp*Ru+ complexation to acecorannulene. *Chemical Communications*, **2004**, 950-1	5.8	34
79	Direct experimental evaluation of charge scheme performance by a molecular charge-meter. *Journal of the American Chemical Society*, **2004**, 126, 5897-905	16.4	30
78	Structural Effects of Group VI Metal Tricarbonyl Binding to Benzenoid Rings: Interruption of Conjugation or Enhanced Aromaticity?. *Helvetica Chimica Acta*, **2003**, 86, 1587-1597	2	5
77	Outlying Charge, Stability, Efficiency, and Algorithmic Enhancements in the Quantum-Mechanical Solvation Method, COSab-GAMESS. *Helvetica Chimica Acta*, **2003**, 86, 4112-4132	2	7
76	Ab Initio Structure/Reactivity Investigations of Illudin-Based Antitumor Agents: A Model for Reaction in vivo. *Helvetica Chimica Acta*, **2003**, 86, 4133-4151	2	7
75	Synthesis and properties of sym-pentasubstituted derivatives of corannulene. *Organic Letters*, **2003**, 5, 713-6	6.2	77
74	An experimental look into subelectron charge flow. *Journal of the American Chemical Society*, **2003**, 125, 12706-7	16.4	7
73	Through-space interactions between face-to-face, center-to-edge oriented arenes: importance of polar-pi effects. *Organic and Biomolecular Chemistry*, **2003**, 1, 157-62	3.9	106
72	Ring-strain effects on the oxidation potential of enediynes and enediyne complexes. *Organic and Biomolecular Chemistry*, **2003**, 1, 763-6	3.9	9
71	Flexibility and molecular recognition in the immune system. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 92-7	11.5	101
70	Multiple versus single pathways in electron transfer in proteins: Influence of protein dynamics and hydrogen bonds. *Journal of Chemical Physics*, **2003**, 119, 3550-3558	3.9	26
69	Management of Web and Associated Grid Technologies for Quantum Chemistry Computation. *Lecture Notes in Computer Science*, **2003**, 111-121	0.9	4
68	Controlled Alcohol–Ketone Interconversion by Dihydrogen Transfer: An ab Initio Study of the Methanol–Formaldehyde Complex. *Journal of Physical Chemistry A*, **2002**, 106, 9512-9519	2.8	8
67	Mutual control of axial and equatorial ligands: model studies with [Ni]-bacteriochlorophyll-a. *Journal of the American Chemical Society*, **2002**, 124, 8406-15	16.4	19
66	Directing power of cyclobutenoid annelations on the double bonds of planar cyclooctatetraenes. *Journal of the American Chemical Society*, **2002**, 124, 5514-7	16.4	21
65	Baskets, covered baskets, and basket balls: corannulene based cyclophanes as fullerene mimics. *Tetrahedron*, **2001**, 57, 3737-3742	2.4	25
64	Quantum mechanical designs toward planar delocalized cyclooctatetraene: a new target for synthesis. *Journal of the American Chemical Society*, **2001**, 123, 1755-9	16.4	45
63	Structure/energy correlation of bowl depth and inversion barrier in corannulene derivatives: combined experimental and quantum mechanical analysis. *Journal of the American Chemical Society*, **2001**, 123, 517-25	16.4	246

62	Synthesis and Properties of 2,3-Dihydro-1H-corannuleno[2,3-cd]pyridine (=2,3-Dihydro-1H-dibenzo[1,10 : 6,7]fluoranthenо[3,4-cd]pyridine) Derivatives: Heterocyclic peri-Anellated Corannulenes. *Helvetica Chimica Acta*, **2000**, 83, 2644-2654	2	9
61	Multithreaded shared memory parallel implementation of the electronic structure code GAMESS. *Computer Physics Communications*, **2000**, 128, 55-66	4.2	12
60	Ionization of corannulene and 1,6-dimethylcorannulene: photoelectron spectra, electrochemistry, charge transfer bands and ab initio computations. *Tetrahedron Letters*, **2000**, 41, 4519-4522	2	45
59	The structure of the chromophore within DsRed, a red fluorescent protein from coral. *Proceedings of the National Academy of Sciences of the United States of America*, **2000**, 97, 11990-5	11.5	509
58	The Silabenzenes: Structure, Properties, and Aromaticity. *Organometallics*, **2000**, 19, 1477-1487	3.8	105
57	Ab Initio Computational Study of Environmentally Harmful Gasoline Additives: Methyl tert-Butyl Ether and Analogues. *Journal of Physical Chemistry A*, **2000**, 104, 11106-11110	2.8	11
56	Ground state gas and solution phase conformational dynamics of polar processes: Furfural systems. *Journal of Chemical Physics*, **2000**, 113, 7519-7529	3.9	29
55	Optical Absorption and Computational Studies of [Ni]-Bacteriochlorophyll-a. New Insight into Charge Distribution between Metal and Ligands. *Journal of the American Chemical Society*, **2000**, 122, 3937-3944	16.4	37
54	Implementation and refinement of the modified-conductorlike screening quantum mechanical solvation model at the MP2 level. *Journal of Chemical Physics*, **2000**, 113, 7511-7518	3.9	12
53	Reinvestigation of □allyl cations: High level Ab initio quantum mechanical predictions. *Tetrahedron Letters*, **1999**, 40, 3503-3506	2	5
52	Accurate ab initio anharmonic force field and heat of formation for silane. *Molecular Physics*, **1999**, 97, 945-953	1.7	29
51	Interconversion and Reactions ofIn- andOut-Isomers of a Triarylphosphine-Containing Cyclophane. *Journal of the American Chemical Society*, **1999**, 121, 12082-12087	16.4	20
50	The Structure of Hexabenzotriphenylene and the Problem of Overcrowded □3h□Polycyclic Aromatic Compounds. *Journal of the American Chemical Society*, **1999**, 121, 727-733	16.4	73
49	Canastanes: Ab Initio Quantum Mechanical Prediction of New Curved Polynuclear Aromatic Hydrocarbon Motif. *Journal of the American Chemical Society*, **1999**, 121, 5332-5333	16.4	20
48	Correlation of Empirical (□TMS) and Absolute NMR Chemical Shifts Predicted by ab Initio Computations. *Journal of Physical Chemistry A*, **1999**, 103, 4038-4042	2.8	83
47	Synthesis and Quantum Mechanical Structure of sym-Pentamethylcorannulene and Decamethylcorannulene. *Journal of the American Chemical Society*, **1999**, 121, 7439-7440	16.4	79
46	Envelope-Flip Dynamics in CpCo(Diene) Complexes: an ab Initio Quantum Mechanical Study. *Journal of Physical Chemistry A*, **1999**, 103, 10126-10131	2.8	7
45	X-Ray crystal and ab initio structure of 3-ethynylcyclopropene: a curiously short carbon□arbon double bond. *Chemical Communications*, **1998**, 1137-1138	5.8	10

44	The Nature of the Long Bond in 3,8-Dichloro-1,1,2,2-tetraphenylcyclobuta[b]naphthene. *Journal of the American Chemical Society*, **1998**, 120, 6167-6168	16.4	40
43	Hexahapto Metal Coordination to Curved Polyaromatic Hydrocarbon Surfaces: The First Transition Metal Corannulene Complex. *Journal of the American Chemical Society*, **1997**, 119, 4781-4782	16.4	114
42	First principles implementation of solvent effects without outlying charge error. *Journal of Chemical Physics*, **1997**, 106, 6622-6633	3.9	177
41	Glycolonitrile oligomerization: structure of isolated oxazolines, potential heterocycles on the early earth. *Journal of Organic Chemistry*, **1997**, 62, 5522-5	4.2	11
40	Corannulene-based fullerene fragments C20H10-C50H10: when does a buckybowl become a buckytube?. *Theoretical Chemistry Accounts*, **1997**, 97, 67-71	1.9	66
39	Ab Initio Density Funtional vs Hartree Fock Predictions for the Structure of [18]Annulene: Evidence for Bond Localization and Diminished Ring Currents in Bicycloannelated [18]Annulenes. *Angewandte Chemie International Edition in English*, **1997**, 36, 745-748		37
38	Voraussagen zur Struktur von [18]Annulenen mit ab-initio-Dichtefunktional- und Hartree-Fock-Rechnungen im Vergleich: Belege f Bindungslokalisierung und verringerte Ringstr he in bicycloanellierten [18]Annulenen. *Angewandte Chemie*, **1997**, 109, 765-768	3.6	1
37	Structure and Dynamics of the Cr(CO)3 Complexes of Triquinacene and Dimethylenecyclobutene by Hartree ock and Density Functional Methods. *The Journal of Physical Chemistry*, **1996**, 100, 6111-6115		8
36	Synthesis and Characterization of the First Corannulene Cyclophane. *Journal of the American Chemical Society*, **1996**, 118, 2754-2755	16.4	118
35	Bond Fixation in a [14]Annulene: Synthesis, Characterization, and ab Initio Computations of Furan Adducts of Dimethyldihydropyrene. *Journal of the American Chemical Society*, **1996**, 118, 2907-2911	16.4	27
34	Parallel implementation of semiempirical quantum methods for the Intel platforms. *Journal of Mathematical Chemistry*, **1996**, 19, 87-109	2.1	5
33	QMView: a computational chemistry three-dimensional visualization tool at the interface between molecules and mankind. *Journal of Molecular Graphics*, **1995**, 13, 63-6, 61		49
32	Long C?C single bonds in anthracene dimers: The structure of bi(anthracene-9,10-dimethylene) photodimer is redetermined. *Tetrahedron Letters*, **1995**, 36, 845-848	2	36
31	The crystal structure of a heptiptycene-chlorobenzene clathrate. *Tetrahedron Letters*, **1995**, 36, 2419-2422	2	26
30	Partial bond localization in the crystal structure of trisbicyclo[2.2.1]heptabenzene and its effect on Cr-arene dynamics. *Tetrahedron Letters*, **1995**, 36, 4389-4392	2	36
29	Promises and Perils of Parallel Semiempirical Quantum Methods. *ACS Symposium Series*, **1995**, 97-113	0.4	
28	Applications of Parallel GAMESS. *ACS Symposium Series*, **1995**, 29-46	0.4	2
27	Solvent, Isotope, and Substituent Effects on the Bimolecular Electron Transfer Reaction between Chlorine Oxide and Benzenes. *The Journal of Physical Chemistry*, **1995**, 99, 13938-13947		14

26	Synthesis and Characterization of Trisbicyclo[2.1.1]hexabenzene, a Highly Strained Bicycloannelated Benzene. *Journal of the American Chemical Society*, **1995**, 117, 2102-2103	16.4	84
25	The Central Bond Length in 1,2-Diarylethanes. *Journal of the American Chemical Society*, **1995**, 117, 4479-4482	16.4	22
24	Kristallographischer Nachweis der Cyclohexatrien-Struktur von Tris(bicyclo[2.1.1]hexeno)benzol: Bindungslängenalternanz nach Widerlegung der Mills-Nixon-Theorie. *Angewandte Chemie*, **1995**, 107, 1575-1577	3.6	33
23	X-Ray Diffraction Evidence for a Cyclohexatriene Motif in the Molecular Structure of Tris(bicyclo[2.1.1]hexeno)benzene: Bond Alternation after the Refutation of the Mills-Nixon Theory. *Angewandte Chemie International Edition in English*, **1995**, 34, 1454-1456		106
22	QMVIEW: As a Supramolecular Visualization Tool **1995**, 169-177		3
21	The effects of solvent screening in quantum mechanical calculations in protein systems. *Journal of Computational Chemistry*, **1994**, 15, 1217-1227	3.5	11
20	Balancing steric and electronic factors in push-pull benzenes: an ab initio study on the molecular structure of 1,3,5-triamino-2,4,6-trinitrobenzene and related compounds. *Journal of the American Chemical Society*, **1993**, 115, 10782-10785	16.4	40
19	Synthesis, structure, and dynamics of endo-(starphenylene)chromium tricarbonyl derivatives: observation of metal-arene migration and hindered metal-tripod rotation. *Journal of the American Chemical Society*, **1993**, 115, 6138-6142	16.4	38
18	Molecular design, chemical synthesis, kinetic studies, calculations, and biological studies of novel enediynes equipped with triggering, detection, and deactivating devices. Model dynemicin A epoxide and cis-diol systems. *Journal of the American Chemical Society*, **1993**, 115, 7944-7953	16.4	78
17	General atomic and molecular electronic structure system. *Journal of Computational Chemistry*, **1993**, 14, 1347-1363	3.5	17180
16	Uncatalyzed peptide bond formation in the gas phase. *The Journal of Physical Chemistry*, **1992**, 96, 8340-8351		85
15	Synthesis of trioxatricornan and derivatives. Useful keystones for the construction of rigid molecular cavities. *Journal of Organic Chemistry*, **1992**, 57, 61-69	4.2	47
14	Bond alternation in triannelated benzenes: dissection of cyclic .pi. from Mills-Nixon effects. *Journal of the American Chemical Society*, **1992**, 114, 9583-9587	16.4	116
13	Structure of centrally bound angular-(terphenylene)chromium tricarbonyl. *Journal of the American Chemical Society*, **1992**, 114, 369-371	16.4	16
12	Synthesis and dynamics of the corannulene nucleus. *Journal of the American Chemical Society*, **1992**, 114, 1921-1923	16.4	213
11	Transition state structure, barrier height, and vibrational frequencies for the reaction Cl+CH4-ĠCH3+HCl. *Journal of Chemical Physics*, **1989**, 90, 7137-7142	3.9	93
10	The transition state and barrier heights for the reaction O(3P) +HCl-ĠOH+Cl. *Chemical Physics Letters*, **1989**, 158, 189-192	2.5	15
9	Ab initio reaction paths and direct dynamics calculations. *The Journal of Physical Chemistry*, **1989**, 93, 5107-5119		309

8	Algorithms and accuracy requirements for computing reaction paths by the method of steepest descent. *The Journal of Physical Chemistry*, **1988**, 92, 1476-1488		182
7	Potentially aromatic metallocycles. *Journal of the American Chemical Society*, **1988**, 110, 4204-4208	16.4	136
6	Substituted silabenzenes. *Organometallics*, **1988**, 7, 144-155	3.8	21
5	Thermal decomposition of methanethiol and ethanethiol. *The Journal of Physical Chemistry*, **1987**, 91, 4145-4155		14
4	Theoretical Studies of Silicon Chemistry. *Annual Review of Physical Chemistry*, **1987**, 38, 211-252	15.7	44
3	A theoretical study of fluorine atom and fluoride ion attack on methane and silane. *Journal of the American Chemical Society*, **1985**, 107, 4415-4419	16.4	35
2	Theoretical studies of disilabenzenes. *Journal of Organometallic Chemistry*, **1984**, 271, 369-379	2.3	23
1	The New Biology and the Grid907-922		3