Friedrich Matthias Bickelhaupt

List of Publications by Citations

382 papers	26,133 citations	70 h-index	152 g-index
436 ext. papers	29,018 ext. citations	5.3 avg, IF	7.48 L-index

#	Paper	IF	Citations
382	Chemistry with ADF. *Journal of Computational Chemistry*, **2001**, 22, 931-967	3.5	7628
381	Voronoi deformation density (VDD) charges: Assessment of the Mulliken, Bader, Hirshfeld, Weinhold, and VDD methods for charge analysis. *Journal of Computational Chemistry*, **2004**, 25, 189-210	3.5	782
380	Analyzing Reaction Rates with the Distortion/Interaction-Activation Strain Model. *Angewandte Chemie - International Edition*, **2017**, 56, 10070-10086	16.4	649
379	The activation strain model of chemical reactivity. *Organic and Biomolecular Chemistry*, **2010**, 8, 3118-27	3.9	506
378	Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry. *Reviews in Computational Chemistry*, **2007**, 1-86		466
377	The activation strain model and molecular orbital theory: understanding and designing chemical reactions. *Chemical Society Reviews*, **2014**, 43, 4953-67	58.5	455
376	Understanding reactivity with Kohn–Sham molecular orbital theory: E2–SN2 mechanistic spectrum and other concepts. *Journal of Computational Chemistry*, **1999**, 20, 114-128	3.5	438
375	Hydrogen Bonding in DNA Base Pairs: Reconciliation of Theory and Experiment. *Journal of the American Chemical Society*, **2000**, 122, 4117-4128	16.4	379
374	Charge transport in columnar stacked triphenylenes: Effects of conformational fluctuations on charge transfer integrals and site energies. *Journal of Chemical Physics*, **2003**, 119, 9809-9817	3.9	346
373	Absolute rates of hole transfer in DNA. *Journal of the American Chemical Society*, **2005**, 127, 14894-903	16.4	303
372	The Nature of the Hydrogen Bond in DNA Base Pairs: The Role of Charge Transfer and Resonance Assistance. *Chemistry - A European Journal*, **1999**, 5, 3581-3594	4.8	303
371	Hydrogen-hydrogen bonding in planar biphenyl, predicted by atoms-in-molecules theory, does not exist. *Chemistry - A European Journal*, **2006**, 12, 2889-95	4.8	280
370	Orbital overlap and chemical bonding. *Chemistry - A European Journal*, **2006**, 12, 9196-216	4.8	254
369	The Carbon–lithium Electron Pair Bond in (CH3Li)n (n = 1, 2, 4). *Organometallics*, **1996**, 15, 2923-2931	3.8	249
368	The activation strain model and molecular orbital theory. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2015**, 5, 324-343	7.9	218
367	The Nature of the Transition Metal–Carbonyl Bond and the Question about the Valence Orbitals of Transition Metals. A Bond-Energy Decomposition Analysis of TM(CO)6q(TMq= Hf2-, Ta-, W, Re+, Os2+, Ir3+)–*Journal of the American Chemical Society*, **2000**, 122, 6449-6458	16.4	218
366	The case for steric repulsion causing the staggered conformation of ethane. *Angewandte Chemie - International Edition*, **2003**, 42, 4183-8; discussion 4188-94	16.4	204

365	A model of the chemical bond must be rooted in quantum mechanics, provide insight, and possess predictive power. *Chemistry - A European Journal*, **2006**, 12, 2902-5	4.8	191
364	Polycyclic benzenoids: why kinked is more stable than straight. *Journal of Organic Chemistry*, **2007**, 72, 1134-42	4.2	177
363	Nucleophilicity and leaving-group ability in frontside and backside S(N)2 reactions. *Journal of Organic Chemistry*, **2008**, 73, 7290-9	4.2	170
362	Alternatives to the CO Ligand: Coordination of the Isolobal Analogues BF, BNH2, BN(CH3)2, and BO□In Mono- and Binuclear First-Row Transition Metal Complexes. *Chemistry - A European Journal*, **1998**, 4, 210-221	4.8	165
361	Central bond in the three CN.cntdot.dimers NC-CN, CN-CN and CN-NC: electron pair bonding and Pauli repulsion effects. *The Journal of Physical Chemistry*, **1992**, 96, 4864-4873		165
360	The many faces of halogen bonding: a review of theoretical models and methods. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 523-540	7.9	163
359	Transition-state energy and position along the reaction coordinate in an extended activation strain model. *ChemPhysChem*, **2007**, 8, 1170-81	3.2	158
358	Halogen Bonding versus Hydrogen Bonding: A Molecular Orbital Perspective. *ChemistryOpen*, **2012**, 1, 96-105	2.3	149
357	Is CO a Special Ligand in Organometallic Chemistry? Theoretical Investigation of AB, Fe(CO)4AB, and Fe(AB)5 (AB = N2, CO, BF, SiO). *Inorganic Chemistry*, **1998**, 37, 1080-1090	5.1	149
356	Nucleophilic substitution at silicon (SN2@Si) via a central reaction barrier. *Journal of Organic Chemistry*, **2007**, 72, 2201-7	4.2	142
355	Performance of various density functionals for the hydrogen bonds in DNA base pairs. *Chemical Physics Letters*, **2006**, 426, 415-421	2.5	141
354	Multicomponent synthesis of 2-imidazolines. *Journal of Organic Chemistry*, **2005**, 70, 3542-53	4.2	141
353	The EDA Perspective of Chemical Bonding **2014**, 121-157		137
352	Das Distortion/Interaction-Activation-Strain-Modell zur Analyse von Reaktionsgeschwindigkeiten. *Angewandte Chemie*, **2017**, 129, 10204-10221	3.6	136
351	Oxidative addition of Pd to C□H, C□C and C□Cl bonds: Importance of relativistic effects in DFT calculations. *Journal of Chemical Physics*, **2001**, 115, 4030-4040	3.9	131
350	Activation of H-H, C-H, C-C and C-Cl Bonds by Pd and PdCl(-). Understanding Anion Assistance in C-X Bond Activation. *Journal of Chemical Theory and Computation*, **2005**, 1, 286-98	6.4	129
349	Nucleophilic substitution at phosphorus (S(N)2@P): disappearance and reappearance of reaction barriers. *Journal of the American Chemical Society*, **2006**, 128, 10738-44	16.4	126
348	Ab initio and DFT benchmark study for nucleophilic substitution at carbon (SN2@C) and silicon (SN2@Si). *Journal of Computational Chemistry*, **2005**, 26, 1497-504	3.5	120

347	Highly accelerated inverse electron-demand cycloaddition of electron-deficient azides with aliphatic cyclooctynes. *Nature Communications*, **2014**, 5, 5378	17.4	117
346	Bonding capabilities of imidazol-2-ylidene ligands in group-10 transition-metal chemistry. *Coordination Chemistry Reviews*, **2009**, 253, 678-686	23.2	116
345	Telomere structure and stability: covalency in hydrogen bonds, not resonance assistance, causes cooperativity in guanine quartets. *Chemistry - A European Journal*, **2011**, 17, 12612-22	4.8	114
344	QUILD: QUantum-regions interconnected by local descriptions. *Journal of Computational Chemistry*, **2008**, 29, 724-34	3.5	114
343	Pi-pi stacking tackled with density functional theory. *Journal of Molecular Modeling*, **2007**, 13, 1245-57	2	111
342	Adenine tautomers: relative stabilities, ionization energies, and mismatch with cytosine. *Journal of Physical Chemistry A*, **2006**, 110, 4012-20	2.8	111
341	Activation of H H, C H, C C, and C Cl Bonds by Pd(0). Insight from the Activation Strain Model. *Journal of Physical Chemistry A*, **2004**, 108, 8460-8466	2.8	111
340	Adenine versus guanine quartets in aqueous solution: dispersion-corrected DFT study on the differences in stacking and hydrogen-bonding behavior. *Theoretical Chemistry Accounts*, **2010**, 125, 245-252	1.9	110
339	Normal-to-abnormal rearrangement and NHC activation in three-coordinate iron(II) carbene complexes. *Journal of the American Chemical Society*, **2013**, 135, 13338-41	16.4	107
338	Contiguous metal-mediated base pairs comprising two Ag(I) ions. *Chemistry - A European Journal*, **2011**, 17, 6533-44	4.8	104
337	A new all-round density functional based on spin states and S(N)2 barriers. *Journal of Chemical Physics*, **2009**, 131, 094103	3.9	104
336	Charge Transfer and Environment Effects Responsible for Characteristics of DNA Base Pairing. *Angewandte Chemie - International Edition*, **1999**, 38, 2942-2945	16.4	103
335	Catalytic Carbon-Halogen Bond Activation: Trends in Reactivity, Selectivity, and Solvation. *Journal of Chemical Theory and Computation*, **2007**, 3, 514-29	6.4	99
334	Nature of the Three-Electron Bond in H2S?SH2+ *Journal of Physical Chemistry A*, **1998**, 102, 9549-9553	2.8	96
333	Optimization of strong and weak coordinates. *International Journal of Quantum Chemistry*, **2006**, 106, 2536-2544	2.1	92
332	Understanding chemical reactivity using the activation strain model. *Nature Protocols*, **2020**, 15, 649-667	18.8	91
331	Why do cycloaddition reactions involving C60 prefer [6,6] over [5,6] bonds?. *Chemistry - A European Journal*, **2013**, 19, 7416-22	4.8	88
330	Oxidative Insertion as Frontside SN2 Substitution: A Theoretical Study of the Model Reaction System Pd + CH3Cl. *Organometallics*, **1995**, 14, 2288-2296	3.8	88

329	Energy landscapes of nucleophilic substitution reactions: a comparison of density functional theory and coupled cluster methods. *Journal of Computational Chemistry*, **2007**, 28, 1551-1560	3.5	87
328	DFT benchmark study for the oxidative addition of CH4 to Pd. Performance of various density functionals. *Chemical Physics*, **2005**, 313, 261-270	2.3	87
327	Mapping the sites for selective oxidation of guanines in DNA. *Journal of the American Chemical Society*, **2003**, 125, 13658-9	16.4	86
326	Nucleophilic Substitution (S 2): Dependence on Nucleophile, Leaving Group, Central Atom, Substituents, and Solvent. *ChemPhysChem*, **2018**, 19, 1315-1330	3.2	85
325	Alder-ene reaction: aromaticity and activation-strain analysis. *Journal of Computational Chemistry*, **2012**, 33, 509-16	3.5	83
324	Proton Affinities in Water of Maingroup-Element Hydrides Effects of Hydration and Methyl Substitution. *European Journal of Inorganic Chemistry*, **2007**, 2007, 3646-3654	2.3	82
323	Hypervalent silicon versus carbon: ball-in-a-box model. *Chemistry - A European Journal*, **2008**, 14, 819-28	4.8	82
322	Hydrogen bonds of RNA are stronger than those of DNA, but NMR monitors only presence of methyl substituent in uracil/thymine. *Journal of the American Chemical Society*, **2004**, 126, 16718-9	16.4	81
321	Theoretical investigation on base-induced 1,2-eliminations in the model system fluoride ion + fluoroethane. The role of the base as a catalyst. *Journal of the American Chemical Society*, **1993**, 115, 9160-9173	16.4	81
320	Aromaticity and activation strain analysis of [3 + 2] cycloaddition reactions between group 14 heteroallenes and triple bonds. *Journal of Organic Chemistry*, **2011**, 76, 2310-4	4.2	80
319	Oxidative Addition of the Chloromethane C-Cl Bond to Pd, an ab Initio Benchmark and DFT Validation Study. *Journal of Chemical Theory and Computation*, **2006**, 2, 322-35	6.4	77
318	E2 and SN2 Reactions of X(-) + CH3CH2X (X = F, Cl); an ab Initio and DFT Benchmark Study. *Journal of Chemical Theory and Computation*, **2008**, 4, 929-40	6.4	76
317	Double group transfer reactions: role of activation strain and aromaticity in reaction barriers. *Chemistry - A European Journal*, **2009**, 15, 13022-32	4.8	72
316	Type-I dyotropic reactions: understanding trends in barriers. *Chemistry - A European Journal*, **2012**, 18, 12395-403	4.8	71
315	Catalyst selection based on intermediate stability measured by mass spectrometry. *Nature Chemistry*, **2010**, 2, 417-21	17.6	70
314	Aromaticity: molecular-orbital picture of an intuitive concept. *Chemistry - A European Journal*, **2007**, 13, 6321-8	4.8	70
313	Theoretical study of structure, pKa, lipophilicity, solubility, absorption, and polar surface area of some centrally acting antihypertensives. *Bioorganic and Medicinal Chemistry*, **2006**, 14, 1715-28	3.4	70
312	Orbital Interactions in Strong and Weak Hydrogen Bonds are Essential for DNA Replication. *Angewandte Chemie - International Edition*, **2002**, 41, 2092	16.4	70

311	The Effect of Microsolvation on E2 and SN2 Reactions: Theoretical Study of the Model System F⁻ + C2H5F + nHF. *Chemistry - A European Journal*, **1996**, 2, 196-207	4.8	70
310	Cyclotrimerization Reactions Catalyzed by Rhodium(I) Half-Sandwich Complexes: A Mechanistic Density Functional Study. *Organometallics*, **2007**, 26, 3816-3830	3.8	68
309	para-Selective C-H Olefination of Aniline Derivatives via Pd/S,O-Ligand Catalysis. *Journal of the American Chemical Society*, **2019**, 141, 6719-6725	16.4	67
308	Origin of the "endo rule" in Diels-Alder reactions. *Journal of Computational Chemistry*, **2014**, 35, 371-6	3.5	66
307	Ab initio benchmark study for the oxidative addition of CH4 to Pd: importance of basis-set flexibility and polarization. *Journal of Chemical Physics*, **2004**, 121, 9982-92	3.9	66
306	A ditopic ion-pair receptor based on stacked nucleobase quartets. *Angewandte Chemie - International Edition*, **2009**, 48, 3285-7	16.4	64
305	The Case for Steric Repulsion Causing the Staggered Conformation of Ethane. *Angewandte Chemie*, **2003**, 115, 4315-4320	3.6	63
304	Oxidative addition of the ethane C-C bond to Pd. An ab initio benchmark and DFT validation study. *Journal of Computational Chemistry*, **2005**, 26, 1006-20	3.5	63
303	CH3⁻ Is Planar Due to H⁻⁻H Steric Repulsion. Theoretical Study of MH3⁻ and MH3Cl (M = C, Si, Ge, Sn). *Organometallics*, **1996**, 15, 1477-1487	3.8	62
302	The donor-stabilized silylene bis[N,N'-diisopropylbenzamidinato(-)]silicon(II): synthesis, electronic structure, and reactivity. *Chemistry - A European Journal*, **2014**, 20, 9319-29	4.8	59
301	Controlling the oxidative addition of aryl halides to Au(I). *Journal of Computational Chemistry*, **2014**, 35, 2140-5	3.5	58
300	Might BF and BNR2 be alternatives to CO? A theoretical quest for new ligands in organometallic chemistry. *New Journal of Chemistry*, **1998**, 22, 1-3	3.6	58
299	Chemical basis for the recognition of trimethyllysine by epigenetic reader proteins. *Nature Communications*, **2015**, 6, 8911	17.4	57
298	Nucleophilic Substitution at C, Si and P: How Solvation Affects the Shape of Reaction Profiles. *European Journal of Organic Chemistry*, **2008**, 2008, 649-654	3.2	57
297	Oxidative addition of the fluoromethane C-F bond to Pd. An ab initio benchmark and DFT validation study. *Journal of Physical Chemistry A*, **2005**, 109, 9685-99	2.8	57
296	Silver(I)-mediated Hoogsteen-type base pairs. *Journal of Inorganic Biochemistry*, **2011**, 105, 1398-404	4.2	56
295	Nucleophilic substitution at phosphorus centers (SN2@p). *ChemPhysChem*, **2007**, 8, 2452-63	3.2	55
294	How Dihalogens Catalyze Michael Addition Reactions. *Angewandte Chemie - International Edition*, **2019**, 58, 8922-8926	16.4	54

293	How Lewis Acids Catalyze Diels-Alder Reactions. *Angewandte Chemie - International Edition*, **2020**, 59, 6201-6206	16.4	54
292	The steric nature of the bite angle. *Chemistry - A European Journal*, **2009**, 15, 6112-5	4.8	54
291	Frontside versus Backside S(N)2 substitution at group 14 atoms: origin of reaction barriers and reasons for their absence. *Chemistry - an Asian Journal*, **2008**, 3, 1783-92	4.5	52
290	B-DNA structure and stability: the role of hydrogen bonding, π-stacking interactions, twist-angle, and solvation. *Organic and Biomolecular Chemistry*, **2014**, 12, 4691-700	3.9	51
289	Bonding of Imidazol-2-ylidene Ligands in Nickel Complexes. *Organometallics*, **2008**, 27, 3410-3414	3.8	51
288	Role of Steric Attraction and Bite-Angle Flexibility in Metal-Mediated C–H Bond Activation. *ACS Catalysis*, **2015**, 5, 5766-5775	13.1	50
287	Nonlinear d(10)-ML2 Transition-Metal Complexes. *ChemistryOpen*, **2013**, 2, 106-14	2.3	50
286	Ene-ene-yne reactions: activation strain analysis and the role of aromaticity. *Chemistry - A European Journal*, **2014**, 20, 10791-801	4.8	49
285	Orbital Interactions in Hydrogen Bonds Important for Cohesion in Molecular Crystals and Mismatched Pairs of DNA Bases. *Crystal Growth and Design*, **2002**, 2, 239-245	3.5	49
284	Role of Orbital Interactions and Activation Strain (Distortion Energies) on Reactivities in the Normal and Inverse Electron-Demand Cycloadditions of Strained and Unstrained Cycloalkenes. *Journal of Organic Chemistry*, **2017**, 82, 8668-8675	4.2	48
283	Chemical shifts in nucleic acids studied by density functional theory calculations and comparison with experiment. *Chemistry - A European Journal*, **2012**, 18, 12372-87	4.8	48
282	Theoretical investigation of the relative stabilities of XSSX and X2SS isomers (X = F, Cl, H, and CH3). *Journal of Computational Chemistry*, **1995**, 16, 465-477	3.5	48
281	Selectivity in DNA replication. Interplay of steric shape, hydrogen bonds, π-stacking and solvent effects. *Chemical Communications*, **2011**, 47, 7326-8	5.8	47
280	Proton Affinities of Anionic Bases: Trends Across the Periodic Table, Structural Effects, and DFT Validation. *Journal of Chemical Theory and Computation*, **2006**, 2, 281-7	6.4	46
279	Supramolecular switches based on the guanine-cytosine (GC) Watson-Crick pair: effect of neutral and ionic substituents. *Chemistry - A European Journal*, **2006**, 12, 3032-42	4.8	45
278	Steric nature of the bite angle. A closer and a broader look. *Dalton Transactions*, **2011**, 40, 3028-38	4.3	44
277	Hypervalent carbon atom: "freezing" the S(N)2 transition state. *Angewandte Chemie - International Edition*, **2009**, 48, 6469-71	16.4	44
276	Covalency in Highly Polar Bonds. Structure and Bonding of Methylalkalimetal Oligomers (CH3M)n (M = Li-Rb; n = 1, 4). *Journal of Chemical Theory and Computation*, **2006**, 2, 965-80	6.4	43

275	The short N [bond] F bond in N(2)F(+) and how Pauli repulsion influences bond lengths. Theoretical study of N(2)X(+), NF(3)X(+), and NH(3)X(+) (X [double bond] F, H). *Journal of the American Chemical Society*, **2002**, 124, 1500-5	16.4	43
274	Unusual reactivity of small cyclophanes: nucleophilic attack on 11-chloro- and 8,11-dichloro[5]metacyclophane. *Journal of the American Chemical Society*, **1990**, 112, 6638-6646	16.4	43
273	Understanding the reactivity of endohedral metallofullerenes: C78 versus Sc3N@C78. *Chemistry - A European Journal*, **2015**, 21, 5760-8	4.8	42
272	Reactivity of the Donor-Stabilized Silylenes [iPrNC(Ph)NiPr]2 Si and [iPrNC(NiPr2)NiPr]2 Si: Activation of CO2 and CS2. *Chemistry - A European Journal*, **2015**, 21, 16665-72	4.8	42
271	Double CH Activation of a Masked Cationic Bismuth Amide. *Angewandte Chemie - International Edition*, **2018**, 57, 3825-3829	16.4	41
270	On the origin of the steric effect. *Physical Chemistry Chemical Physics*, **2012**, 14, 9846-54	3.6	41
269	Stepwise walden inversion in nucleophilic substitution at phosphorus. *Physical Chemistry Chemical Physics*, **2009**, 11, 259-67	3.6	41
268	Intercalation of daunomycin into stacked DNA base pairs. DFT study of an anticancer drug. *Journal of Biomolecular Structure and Dynamics*, **2008**, 26, 115-30	3.6	41
267	PyFrag--Streamlining your reaction path analysis. *Journal of Computational Chemistry*, **2008**, 29, 312-5	3.5	41
266	Hydrogen bonding in mimics of Watson-Crick base pairs involving C-H proton donor and F proton acceptor groups: a theoretical study. *ChemPhysChem*, **2004**, 5, 481-7	3.2	41
265	Ladungstransfer und molekulare Umgebung sind verantwortlich f□ Eigenschaften von Wasserstoffbr□ken in DNA-Basenpaaren. *Angewandte Chemie*, **1999**, 111, 3120-3122	3.6	40
264	Deeper Insight into the Diels-Alder Reaction through the Activation Strain Model. *Chemistry - an Asian Journal*, **2016**, 11, 3297-3304	4.5	39
263	Alpha-stabilization of carbanions: fluorine is more effective than the heavier halogens. *Angewandte Chemie - International Edition*, **2006**, 45, 823-6	16.4	39
262	Oxidative addition to main group versus transition metals: Insights from the Activation Strain model. *Journal of Organometallic Chemistry*, **2006**, 691, 4341-4349	2.3	39
261	Activation-strain analysis reveals unexpected origin of fast reactivity in heteroaromatic azadiene inverse-electron-demand diels-alder cycloadditions. *Journal of Organic Chemistry*, **2015**, 80, 548-58	4.2	38
260	Proton affinities of maingroup-element hydrides and noble gases: trends across the periodic table, structural effects, and DFT validation. *Journal of Computational Chemistry*, **2006**, 27, 1486-93	3.5	38
259	Theoretical and experimental study of charge transfer through DNA: impact of mercury mediated T-Hg-T base pair. *Journal of Physical Chemistry B*, **2014**, 118, 5374-81	3.4	37
258	Bonding of xenon hydrides. *Journal of Physical Chemistry A*, **2009**, 113, 9700-6	2.8	37

257	Oxidative Addition versus Dehydrogenation of Methane, Silane, and Heavier AH4 Congeners Reacting with Palladium. *Organometallics*, **2006**, 25, 4260-4268	3.8	37
256	Carbon monoxide insertion at a heavy p-block element: unprecedented formation of a cationic bismuth carbamoyl. *Chemical Science*, **2019**, 10, 4169-4176	9.4	36
255	Stereodivergent SN2@P reactions of borane oxazaphospholidines: experimental and theoretical studies. *Journal of the American Chemical Society*, **2013**, 135, 4483-91	16.4	36
254	Hypervalent versus nonhypervalent carbon in noble-gas complexes. *Chemistry - A European Journal*, **2008**, 14, 6901-11	4.8	36
253	Structure and bonding of transition metal-boryl compounds. Theoretical study of [(PH3)2(CO)ClOs-BR2] and [(PH3)2(CO)2ClOs-BR2] (BR2 = BH2, BF2, B(OH)2, B(OCH=CHO), Bcat). *Inorganic Chemistry*, **2000**, 39, 4776-85	5.1	36
252	Role of the Chalcogen (S, Se, Te) in the Oxidation Mechanism of the Glutathione Peroxidase Active Site. *ChemPhysChem*, **2017**, 18, 2990-2998	3.2	35
251	Radon hydrides: structure and bonding. *Physical Chemistry Chemical Physics*, **2011**, 13, 2222-7	3.6	35
250	Aromaticity and antiaromaticity in 4-, 6-, 8-, and 10-membered conjugated hydrocarbon rings. *Journal of Physical Chemistry A*, **2008**, 112, 12816-22	2.8	35
249	Structural Distortion of Cycloalkynes Influences Cycloaddition Rates both by Strain and Interaction Energies. *Chemistry - A European Journal*, **2019**, 25, 6342-6348	4.8	34
248	Neutral six-coordinate and cationic five-coordinate silicon(IV) complexes with two bidentate monoanionic N,S-pyridine-2-thiolato(-) ligands. *Inorganic Chemistry*, **2013**, 52, 10664-76	5.1	34
247	Reaction Coordinates and the Transition-Vector Approximation to the IRC. *Journal of Chemical Theory and Computation*, **2008**, 4, 920-8	6.4	34
246	Mechanism of thioredoxin-catalyzed disulfide reduction. Activation of the buried thiol and role of the variable active-site residues. *Journal of Physical Chemistry B*, **2008**, 112, 2511-23	3.4	34
245	Orbital interactions and charge redistribution in weak hydrogen bonds: The Watson□rick AT mimic adenine-2,4-difluorotoluene. *Journal of Chemical Physics*, **2003**, 119, 4262-4273	3.9	34
244	Nucleophilic Substitution in Solution: Activation Strain Analysis of Weak and Strong Solvent Effects. *Chemistry - A European Journal*, **2018**, 24, 5927-5938	4.8	33
243	Origin of Reactivity Trends of Noble Gas Endohedral Fullerenes Ng2@C60 (Ng = He to Xe). *Journal of Chemical Theory and Computation*, **2014**, 10, 3863-70	6.4	32
242	Inter- and intramolecular dispersion interactions. *Journal of Computational Chemistry*, **2011**, 32, 1117-27	3.5	32
241	Fragment-oriented design of catalysts based on the activation strain model. *Molecular Physics*, **2005**, 103, 995-998	1.7	32
240	Bonding in methylalkalimetals (CH(3)M)(n) (M = Li, Na, K; n = 1, 4). Agreement and divergences between AIM and ELF analyses. *Journal of Physical Chemistry B*, **2006**, 110, 7189-98	3.4	32

239	Origins of the Endo and Exo Selectivities in Cyclopropenone, Iminocyclopropene, and Triafulvene Diels-Alder Cycloadditions. *Journal of Organic Chemistry*, **2018**, 83, 3164-3170	4.2	31
238	Understanding E2 versus SN2 Competition under Acidic and Basic Conditions. *ChemistryOpen*, **2014**, 3, 29-36	2.3	31
237	Reactivity in nucleophilic vinylic substitution (S(N)V):S(N)V versus S(N)V mechanistic dichotomy. *Journal of Organic Chemistry*, **2013**, 78, 8574-84	4.2	31
236	Factors controlling elimination reactions in group 10 metal complexes. *Chemistry - A European Journal*, **2015**, 21, 14362-9	4.8	31
235	New concepts for designing d10 -M(L)n catalysts: d regime, s regime and intrinsic bite-angle flexibility. *Chemistry - A European Journal*, **2014**, 20, 11370-81	4.8	31
234	Synthesis and structural characterisation of neutral pentacoordinate silicon(IV) complexes with a tridentate dianionic N,N,S chelate ligand. *Dalton Transactions*, **2012**, 41, 2148-62	4.3	31
233	Dihydrogen bonding: donor-acceptor bonding (AH...HX) versus the H2 molecule (A-H2-X). *Chemistry - A European Journal*, **2009**, 15, 5814-22	4.8	31
232	Reactivity and Selectivity of Bowl-Shaped Polycyclic Aromatic Hydrocarbons: Relationship to C60. *Chemistry - A European Journal*, **2016**, 22, 1368-78	4.8	31
231	PyFrag 2019-Automating the exploration and analysis of reaction mechanisms. *Journal of Computational Chemistry*, **2019**, 40, 2227-2233	3.5	30
230	Didehydrophenanthrenes: structure, singlet-triplet splitting, and aromaticity. *Journal of Physical Chemistry A*, **2007**, 111, 5063-70	2.8	30
229	Chimeric GNA/DNA metal-mediated base pairs. *Chemical Communications*, **2011**, 47, 11041-3	5.8	29
228	Rare tautomers of 1-methyluracil and 1-methylthymine: tuning relative stabilities through coordination to PtII complexes. *Chemistry - A European Journal*, **2009**, 15, 209-18	4.8	29
227	Understanding the Reactivity of Ion-Encapsulated Fullerenes. *Chemistry - A European Journal*, **2017**, 23, 11030-11036	4.8	28
226	Direct detection of the mercury-nitrogen bond in the thymine-Hg(II)-thymine base-pair with (199)Hg NMR spectroscopy. *Chemical Communications*, **2015**, 51, 8488-91	5.8	28
225	3-Substituted xanthines as promising candidates for quadruplex formation: computational, synthetic and analytical studies. *New Journal of Chemistry*, **2011**, 35, 476-482	3.6	28
224	Highly Stable and Selective Tetrazines for the Coordination-Assisted Bioorthogonal Ligation with Vinylboronic Acids. *Bioconjugate Chemistry*, **2018**, 29, 3054-3059	6.3	27
223	Substituent Effects on Hydrogen Bonding in Watson Crick Base Pairs. A Theoretical Study. *Structural Chemistry*, **2005**, 16, 211-221	1.8	27
222	Addition-Elimination or Nucleophilic Substitution? Understanding the Energy Profiles for the Reaction of Chalcogenolates with Dichalcogenides. *Journal of Chemical Theory and Computation*, **2016**, 12, 2752-61	6.4	27

221	(4 + 2) and (2 + 2) Cycloadditions of Benzyne to C60 and Zig-Zag Single-Walled Carbon Nanotubes: The Effect of the Curvature. *Journal of Physical Chemistry C*, **2016**, 120, 1716-1726	3.8	26
220	Thermodynamics of the Cu(II) Ethiolate and Cu(I) disulfide equilibrium: a combined experimental and theoretical study. *Inorganic Chemistry*, **2014**, 53, 8494-504	5.1	26
219	Bis[N,N'-diisopropylbenzamidinato(-)]silicon(II): Lewis acid/base reactions with triorganylboranes. *Chemistry - A European Journal*, **2014**, 20, 12411-5	4.8	26
218	In silico design of heteroaromatic half-sandwich RhI catalysts for acetylene [2+2+2] cyclotrimerization: evidence of a reverse indenyl effect. *Chemistry - A European Journal*, **2013**, 19, 13337-47	4.8	26
217	Stable Four-Coordinate Guanidinatosilicon(IV) Complexes with SiN3El Skeletons (El = S, Se, Te) and Si=El Double Bonds. *Chemistry - A European Journal*, **2015**, 21, 14011-21	4.8	26
216	B-DNA Structure and Stability as Function of Nucleic Acid Composition: Dispersion-Corrected DFT Study of Dinucleoside Monophosphate Single and Double Strands. *ChemistryOpen*, **2013**, 2, 186-93	2.3	26
215	Methyl cation affinities of neutral and anionic maingroup-element hydrides: trends across the periodic table and correlation with proton affinities. *Journal of Physical Chemistry A*, **2010**, 114, 7604-8	2.8	26
214	Density Functional Calculations of E2 and SN2 Reactions: Effects of the Choice of Method, Algorithm, and Numerical Accuracy. *Journal of Chemical Theory and Computation*, **2010**, 6, 3145-52	6.4	26
213	Scope and limitations of an efficient four-component reaction for dihydropyridin-2-ones. *Journal of Organic Chemistry*, **2010**, 75, 1723-32	4.2	26
212	Bite-angle bending as a key for understanding group-10 metal reactivity of d-[M(NHC)] complexes with sterically modest NHC ligands. *Chemical Science*, **2015**, 6, 1426-1432	9.4	25
211	Origin of rate enhancement and asynchronicity in iminium catalyzed Diels-Alder reactions. *Chemical Science*, **2020**, 11, 8105-8112	9.4	25
210	Ion-Pair SN 2 Substitution: Activation Strain Analyses of Counter-Ion and Solvent Effects. *Chemistry - A European Journal*, **2016**, 22, 4431-9	4.8	25
209	How the electron-deficient cavity of heterocalixarenes recognizes anions: insights from computation. *Physical Chemistry Chemical Physics*, **2017**, 19, 24696-24705	3.6	25
208	Solvent effects on hydrogen bonds in WatsonCrick, mismatched, and modified DNA base pairs. *Computational and Theoretical Chemistry*, **2012**, 998, 57-63	2	25
207	Aromaticity in Heterocyclic and Inorganic Benzene Analogues. *Australian Journal of Chemistry*, **2008** , 61, 209	1.2	25
206	Gas-Phase Base-Induced 1,4-Eliminations: Occurrence of Single-, Double-, and Triple-Well E1cb Mechanisms. *Journal of the American Chemical Society*, **1995**, 117, 9889-9899	16.4	25
205	Chemoselectivity of Tertiary Azides in Strain-Promoted Alkyne-Azide Cycloadditions. *Chemistry - A European Journal*, **2019**, 25, 754-758	4.8	25
204	Indenyl effect due to metal slippage? Computational exploration of rhodium-catalyzed acetylene [2+2+2] cyclotrimerization. *ChemPhysChem*, **2014**, 15, 219-28	3.2	24

203	Rationalizing the structural variability of the exocyclic amino groups in nucleobases and their metal complexes: cytosine and adenine. *Chemistry - A European Journal*, **2014**, 20, 9494-9	4.8	24
202	Theoretical study of the structure and bonding in ThC2 and UC2. *Journal of Physical Chemistry A*, **2012**, 116, 747-55	2.8	24
201	Activation of C H, C C and C bonds by Pd and cis-Pd(CO)2I2. Catalyst ubstrate adaptation. *Journal of Organometallic Chemistry*, **2005**, 690, 2191-2199	2.3	24
200	Base-induced 1,4-elimination: insights from theory and mass spectrometry. *Mass Spectrometry Reviews*, **2001**, 20, 347-61	11	24
199	Computationally Guided Molecular Design to Minimize the LE/CT Gap in D- A Fluorinated Triarylboranes for Efficient TADF via D and Bridge Tuning. *Advanced Functional Materials*, **2020**, 30, 2002064	15.6	23
198	Oxidation of organic diselenides and ditellurides by HO for bioinspired catalyst design. *Physical Chemistry Chemical Physics*, **2018**, 20, 20874-20885	3.6	23
197	Elucidating the Trends in Reactivity of Aza-1,3-Dipolar Cycloadditions. *European Journal of Organic Chemistry*, **2019**, 2019, 378-386	3.2	23
196	Hypervalence and the delocalizing versus localizing propensities of H , Li , CH and SiH . *Structural Chemistry*, **2007**, 18, 813-819	1.8	23
195	Structure and Stability of the Li2CN Molecule. An Experimental and ab Initio Study. *The Journal of Physical Chemistry*, **1995**, 99, 6477-6482		23
194	Silicon Effect: A Systematic Experimental and Computational Study of the Hydrolysis of C and C Functionalized Alkoxytriorganylsilanes of the Formula Type ROSiMe2(CH2)nX (R = Me, Et; n = 1, 3; X = Functional Group). *Organometallics*, **2014**, 33, 2721-2737	3.8	22
193	Role of s-p orbital mixing in the bonding and properties of second-period diatomic molecules. *Journal of Physical Chemistry A*, **2008**, 112, 2437-46	2.8	22
192	1,4-Diphosphabutadiyne: A Realistic Target for Synthesis? A Theoretical Investigation of C2P2, C2N2, [Cr(CO)5PCCP], and [(CO)5Cr(PCCP)Cr(CO)5]. *Chemistry - A European Journal*, **1999**, 5, 162-174	4.8	22
191	The Pauli Repulsion-Lowering Concept in Catalysis. *Accounts of Chemical Research*, **2021**, 54, 1972-1981	24.3	22
190	How Lewis Acids Catalyze Diels Alder Reactions. *Angewandte Chemie*, **2020**, 132, 6260-6265	3.6	21
189	Deracemization of a Racemic Allylic Sulfoxide Using Viedma Ripening. *Crystal Growth and Design*, **2017**, 17, 4454-4457	3.5	20
188	Koordinationseigenschaften der isolobalen Phosphaniminatound Cyclopentadienyl-Liganden in TiCl3(NPH3), TiCl3Cp, ReO3(NPH3) und ReO3Cp. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **1999**, 625, 892-900	1.3	20
187	Anion Recognition by Organometallic Calixarenes: Analysis from Relativistic DFT Calculations. *Organometallics*, **2018**, 37, 2167-2176	3.8	20
186	Activation Strain Analysis of S2 Reactions at C, N, O, and F Centers. *Journal of Physical Chemistry A*, **2017**, 121, 885-891	2.8	19

185	Tuning Heterocalixarenes to Improve Their Anion Recognition: A Computational Approach. *Journal of Physical Chemistry A*, **2018**, 122, 3328-3336	2.8	19
184	Understanding the Oxidative Addition of □Bonds to Group 13 Compounds. *Chemistry - A European Journal*, **2016**, 22, 13669-76	4.8	19
183	A helicoid ferrocene. *Inorganic Chemistry*, **2009**, 48, 2714-6	5.1	19
182	Comment on "The interplay between steric and electronic effects in SN2 reactions". *Chemistry - A European Journal*, **2010**, 16, 5538-41; author reply 5542-3	4.8	19
181	Bifunctional Hydrogen Bond Donor-Catalyzed Diels-Alder Reactions: Origin of Stereoselectivity and Rate Enhancement. *Chemistry - A European Journal*, **2021**, 27, 5180-5190	4.8	19
180	Nature and strength of chalcogen-□bonds. *Physical Chemistry Chemical Physics*, **2018**, 20, 27592-27599	3.6	19
179	How Alkali Cations Catalyze Aromatic Diels-Alder Reactions. *Chemistry - an Asian Journal*, **2020**, 15, 1167-1174	4.5	18
178	Doppelte CH-Aktivierung eines maskierten Bismutamid-Kations. *Angewandte Chemie*, **2018**, 130, 3887-3891	3.6	18
177	Neutral Pentacoordinate Halogeno- and Pseudohalogenosilicon(IV) Complexes with a Tridentate Dianionic O,N,O or N,N,O Ligand: Synthesis and Structural Characterization in the Solid State and in Solution. *European Journal of Inorganic Chemistry*, **2012**, 2012, 3216-3228	2.3	18
176	Remote communication in a DNA-based nanoswitch. *Chemistry - A European Journal*, **2011**, 17, 8816-8	4.8	18
175	Switching between OPTX and PBE exchange functionals. *Journal of Computational Methods in Sciences and Engineering*, **2009**, 9, 69-77	0.3	18
174	Linkage Isomerism of Nitriles in Rhodium Half-Sandwich Metallacycles. *Organometallics*, **2008**, 27, 4028-4030	3.8	18
173	Nanoswitches based on DNA base pairs: why adenine-thymine is less suitable than guanine-cytosine. *ChemPhysChem*, **2006**, 7, 1971-9	3.2	18
172	Orbitalwechselwirkungen in starken und schwachen Wasserstoffbr□ken sind essentiell f□ die DNA-Replikation. *Angewandte Chemie*, **2002**, 114, 2194	3.6	18
171	Reaction Mechanism and Regioselectivity of the Bingel-Hirsch Addition of Dimethyl Bromomalonate to La@C2v -C82. *Chemistry - A European Journal*, **2016**, 22, 5953-62	4.8	18
170	B-DNA model systems in non-terran bio-solvents: implications for structure, stability and replication. *Physical Chemistry Chemical Physics*, **2017**, 19, 16969-16978	3.6	17
169	Symmetrical P4 cleavage at cobalt half sandwich complexes [(□5-C5H5)Co(L)] (L = CO, NHC)--a computational case study on the mechanism of symmetrical P4 degradation to P2 ligands. *Dalton Transactions*, **2013**, 42, 7468-81	4.3	17
168	Table salt and other alkali metal chloride oligomers: structure, stability, and bonding. *Inorganic Chemistry*, **2007**, 46, 5411-8	5.1	17

167	Chemical reactivity from an activation strain perspective. *Chemical Communications*, **2021**, 57, 5880-5896	5.8	17
166	A Quantitative Molecular Orbital Perspective of the Chalcogen Bond. *ChemistryOpen*, **2021**, 10, 391-401	2.3	17
165	Factors Controlling the Diels-Alder Reactivity of Hetero-1,3-Butadienes. *ChemistryOpen*, **2018**, 7, 995-1004	2.3	17
164	Rational design of near-infrared absorbing organic dyes: Controlling the HOMO-LUMO gap using quantitative molecular orbital theory. *Journal of Computational Chemistry*, **2018**, 39, 2690-2696	3.5	17
163	N-Heterocyclic Silylenes as Ligands in Transition Metal Carbonyl Chemistry: Nature of Their Bonding and Supposed Innocence. *Chemistry - A European Journal*, **2020**, 26, 11276-11292	4.8	16
162	Differential stabilization of adenine quartets by anions and cations. *Journal of Biological Inorganic Chemistry*, **2010**, 15, 387-97	3.7	16
161	Highly polar bonds and the meaning of covalency and ionicity--structure and bonding of alkali metal hydride oligomers. *Faraday Discussions*, **2007**, 135, 451-68; discussion 489-506	3.6	16
160	Multi-step processes in gas-phase reactions of halomethyl anions XCH2□(X = Cl,Br) with CH3X and NH3. *Journal of Physical Organic Chemistry*, **1992**, 5, 179-190	2.1	16
159	Wie Dihalogene Michael-Additionsreaktionen katalysieren. *Angewandte Chemie*, **2019**, 131, 9015-9020	3.6	15
158	How Mg ions lower the S2@P barrier in enzymatic triphosphate hydrolysis. *Chemical Communications*, **2018**, 54, 3448-3451	5.8	15
157	Stereoselective Synthesis of 1-Tuberculosinyl Adenosine; a Virulence Factor of Mycobacterium tuberculosis. *Journal of Organic Chemistry*, **2016**, 81, 6686-96	4.2	15
156	Reactions of the donor-stabilized silylene bis[N,N'-diisopropyl-benzamidinato(-)]silicon(II) with Brønsted acids. *Chemistry - A European Journal*, **2014**, 20, 16462-6	4.8	15
155	Neutral and positively charged new purine tetramer structures: a computational study of xanthine and uric acid derivatives. *New Journal of Chemistry*, **2011**, 35, 119-126	3.6	15
154	Alkali Metal Complexes of Silyl-Substituted ansa-(Tris)allyl Ligands: Metal-, Co-Ligand- and Substituent-Dependent Stereochemistry. *European Journal of Inorganic Chemistry*, **2009**, 2009, 4157-4167	2.3	15
153	Halogen versus halide electronic structure. *Science China Chemistry*, **2010**, 53, 210-215	7.9	15
152	Forbidden Four-Center Reactions: Molecular Orbital Considerations for N2 + N2 and N2 + N2+. *Journal of Physical Chemistry A*, **1997**, 101, 8255-8263	2.8	15
151	Stabilisierung von Carbanionen: Fluor übertrifft die schwereren Halogene. *Angewandte Chemie*, **2006**, 118, 838-841	3.6	15
150	8 Energy decomposition analysis in the context of quantitative molecular orbital theory **2021**, 199-212		15

149	Cesium's Off-the-Map Valence Orbital. *Angewandte Chemie - International Edition*, **2017**, 56, 9772-9776	16.4	14
148	Trifluoromethyl Vinyl Sulfide: A Building Block for the Synthesis of CFS-Containing Isoxazolidines. *Journal of Organic Chemistry*, **2018**, 83, 1779-1789	4.2	14
147	Arylic C-X Bond Activation by Palladium Catalysts: Activation Strain Analyses of Reactivity Trends. *Scientific Reports*, **2018**, 8, 10729	4.9	14
146	The substituent effect on benzene dications. *Physical Chemistry Chemical Physics*, **2014**, 16, 4752-63	3.6	14
145	Regioselectivity in Electrophilic Aromatic Substitution: Insights from Interaction Energy Decomposition Potentials. *European Journal of Organic Chemistry*, **2011**, 2011, 2958-2968	3.2	14
144	Steric effects on alkyl cation affinities of maingroup-element hydrides. *Journal of Computational Chemistry*, **2011**, 32, 681-8	3.5	14
143	Structural interpretation of J coupling constants in guanosine and deoxyguanosine: modeling the effects of sugar pucker, backbone conformation, and base pairing. *Journal of Physical Chemistry A*, **2009**, 113, 8379-86	2.8	14
142	Bond activation by group-11 transition-metal cations. *Canadian Journal of Chemistry*, **2009**, 87, 806-817	0.9	14
141	Covalent versus ionic bonding in alkalimetal fluoride oligomers. *Journal of Computational Chemistry* , **2007**, 28, 238-50	3.5	14
140	Base-induced imine-forming 1,2-elimination reactions in the gas phase. *Journal of Organic Chemistry* , **1993**, 58, 2436-2441	4.2	14
139	Asymmetric identity S N 2 transition states: Nucleophilic substitution at □substituted carbon and silicon centers. *International Journal of Mass Spectrometry*, **2017**, 413, 85-91	1.9	13
138	How the disulfide conformation determines the disulfide/thiol redox potential. *Journal of Biomolecular Structure and Dynamics*, **2015**, 33, 93-103	3.6	13
137	Performance of TDDFT Vertical Excitation Energies of Core-Substituted Naphthalene Diimides. *Journal of Computational Chemistry*, **2020**, 41, 1448-1455	3.5	13
136	Understanding the 1,3-Dipolar Cycloadditions of Allenes. *Chemistry - A European Journal*, **2020**, 26, 11529-11539	4.8	13
135	Ambident Nucleophilic Substitution: Understanding Non-HSAB Behavior through Activation Strain and Conceptual DFT Analyses. *Chemistry - A European Journal*, **2020**, 26, 3884-3893	4.8	13
134	Halogen Bonds in Ligand-Protein Systems: Molecular Orbital Theory for Drug Design. *Journal of Chemical Information and Modeling*, **2020**, 60, 1317-1328	6.1	13
133	Source of Cooperativity in Halogen-Bonded Haloamine Tetramers. *ChemPhysChem*, **2016**, 17, 474-80	3.2	13
132	A methodology for the photocatalyzed radical trifluoromethylation of indoles: A combined experimental and computational study. *Journal of Fluorine Chemistry*, **2018**, 214, 94-100	2.1	13

131	Stabilisation of 2,6-diarylpyridinium cation by through-space polar-Interactions. *Chemistry - A European Journal*, **2014**, 20, 6268-71	4.8	13
130	tert-Butyl cation affinities of maingroup-element hydrides: effect of methyl substituents at the protophilic center. *Journal of Physical Chemistry A*, **2011**, 115, 8310-5	2.8	13
129	A donor-functionalized, silyl-substituted pentadienyllithium: structural insight from experiment and theory. *Chemical Communications*, **2011**, 47, 6162-4	5.8	13
128	Homolytic versus heterolytic dissociation of alkalimetal halides: the effect of microsolvation. *ChemPhysChem*, **2009**, 10, 2955-65	3.2	13
127	Isolated excited electronic states in the unimolecular gas-phase ion dissociation processes of the radical cations of isocyanogen and cyanogen. *International Journal of Mass Spectrometry and Ion Processes*, **1991**, 103, 157-168		13
126	A Unified Framework for Understanding Nucleophilicity and Protophilicity in the S 2/E2 Competition. *Chemistry - A European Journal*, **2020**, 26, 15538-15548	4.8	13
125	Dual Activation of Aromatic Diels-Alder Reactions. *Chemistry - A European Journal*, **2019**, 25, 9902-9912	4.8	12
124	Regioselectivity of Epoxide Ring-Openings via SN2 Reactions Under Basic and Acidic Conditions. *European Journal of Organic Chemistry*, **2020**, 2020, 3822-3828	3.2	12
123	Aggregation and cooperative effects in the aldol reactions of lithium enolates. *Chemistry - A European Journal*, **2013**, 19, 13761-73	4.8	12
122	Enhanced Back-Donation as a Way to Higher Coordination Numbers in d [M(NHC)] Complexes: A DFT Study. *Chemistry - A European Journal*, **2017**, 23, 614-622	4.8	12
121	Supramolecular H-bonded porous networks at surfaces: exploiting primary and secondary interactions in a bi-component melamine-xanthine system. *Physical Chemistry Chemical Physics*, **2013**, 15, 12442-6	3.6	12
120	Organomagnesium clusters: Structure, stability, and bonding in archetypal models. *Journal of Organometallic Chemistry*, **2011**, 696, 4104-4111	2.3	12
119	Hydrogen bonding of 3- and 5-methyl-6-aminouracil with natural DNA bases. *New Journal of Chemistry*, **2008**, 32, 1981	3.6	12
118	Conformational behavior of basic monomeric building units of glycosaminoglycans: isolated systems and solvent effect. *Journal of Physical Chemistry B*, **2007**, 111, 2313-21	3.4	12
117	(Ph4P)S64 A Compound Containing the Cyclic Radical Anion S6. *Angewandte Chemie - International Edition*, **2000**, 39, 4580-4582	16.4	12
116	Bismuth Amides Mediate Facile and Highly Selective Pn-Pn Radical-Coupling Reactions (Pn=N, P, As). *Angewandte Chemie - International Edition*, **2021**, 60, 6441-6445	16.4	12
115	How Oriented External Electric Fields Modulate Reactivity. *Chemistry - A European Journal*, **2021**, 27, 5683-5693	4.8	12
114	Eight-coordinate fluoride in a silicate double-four-ring. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 828-833	11.5	11

113	Nature of the Ru-NO Coordination Bond: Kohn-Sham Molecular Orbital and Energy Decomposition Analysis. *ChemistryOpen*, **2017**, 6, 410-416	2.3	11
112	Recognition of shorter and longer trimethyllysine analogues by epigenetic reader proteins. *Chemical Communications*, **2018**, 54, 2409-2412	5.8	11
111	X2Y2 isomers: tuning structure and relative stability through electronegativity differences (X = H, Li, Na, F, Cl, Br, I; Y = O, S, Se, Te). *Inorganic Chemistry*, **2013**, 52, 2458-65	5.1	11
110	Stabilization of 2,6-Diarylanilinum Cation by Through-Space Cation-□Interactions. *Journal of Organic Chemistry*, **2017**, 82, 9418-9424	4.2	11
109	Computational (DFT) and Experimental (EXAFS) Study of the Interaction of [Ir(IMes)(H)2 (L)3] with Substrates and Co-substrates Relevant for SABRE in Dilute Systems. *Chemistry - A European Journal*, **2015**, 21, 10482-9	4.8	11
108	All-metal aromatic clusters M4(2-) (M = B, Al, and Ga). Are □electrons distortive or not?. *Physical Chemistry Chemical Physics*, **2011**, 13, 20673-81	3.6	11
107	Role of the variable active site residues in the function of thioredoxin family oxidoreductases. *Journal of Computational Chemistry*, **2009**, 30, 710-24	3.5	11
106	Lewis Acid-Catalyzed Diels-Alder Reactions: Reactivity Trends across the Periodic Table. *Chemistry - A European Journal*, **2021**, 27, 10610-10620	4.8	11
105	Substituent effects on the optical properties of naphthalenediimides: A frontier orbital analysis across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 304-13	3.5	11
104	The pnictogen bond: a quantitative molecular orbital picture. *Physical Chemistry Chemical Physics*, **2021**, 23, 13842-13852	3.6	11
103	Origin of the □Effect in S 2 Reactions. *Angewandte Chemie - International Edition*, **2021**, 60, 20840-20848	16.4	11
102	Six-coordinate Group 13 complexes: the role of d orbitals and electron-rich multi-center bonding. *Angewandte Chemie - International Edition*, **2015**, 54, 12034-8	16.4	10
101	Alkali Metal Cation Affinities of Anionic Main Group-Element Hydrides Across the Periodic Table. *Chemistry - an Asian Journal*, **2017**, 12, 2604-2611	4.5	10
100	The role of protein plasticity in computational rationalization studies on regioselectivity in testosterone hydroxylation by cytochrome P450 BM3 mutants. *Current Drug Metabolism*, **2012**, 13, 155-66	3.5	10
99	Trends and anomalies in H-AH(n) and CH(3)-AH(n) bond strengths (AH(n) = CH3, NH2, OH, F). *Physical Chemistry Chemical Physics*, **2009**, 11, 10317-22	3.6	10
98	Tricarbonylchromium complexes of [5]- and [6]metacyclophane: an experimental and theoretical study. *Tetrahedron*, **2008**, 64, 11641-11646	2.4	10
97	Ligand-Mediated Regioselective Rhodium-Catalyzed Benzotriazole-Allene Coupling: Mechanistic Exploration and Quantum Chemical Analysis. *Chemistry - A European Journal*, **2020**, 26, 2342-2348	4.8	10
96	New Insights into the Reactivity of Cisplatin with Free and Restrained Nucleophiles: Microsolvation Effects and Base Selectivity in Cisplatin-DNA Interactions. *ChemPhysChem*, **2016**, 17, 3932-3947	3.2	10

95	Proton Transfer and S 2 Reactions as Steps of Fast Selenol and Thiol Oxidation in Proteins: A Model Molecular Study Based on GPx. *ChemPlusChem*, **2021**, 86, 525-532	2.8	10
94	Understanding the differences between iron and palladium in cross-coupling reactions. *Physical Chemistry Chemical Physics*, **2019**, 21, 9651-9664	3.6	9
93	Selective C-H and C-C Bond Activation: Electronic Regimes as a Tool for Designing d(10) MLn Catalysts. *Chemistry - an Asian Journal*, **2015**, 10, 2272-82	4.5	9
92	Diastereoselective Synthesis of Lactams by Ligand-Controlled Stereodivergent Intramolecular Tsuji-Trost Allylation. *Journal of Organic Chemistry*, **2020**, 85, 9566-9584	4.2	9
91	Ion-Pair S 2 Reaction of OH and CH Cl: Activation Strain Analyses of Counterion and Solvent Effects. *Chemistry - an Asian Journal*, **2018**, 13, 1138-1147	4.5	9
90	Self-assembly of N3-substituted xanthines in the solid state and at the solid-liquid interface. *Langmuir*, **2013**, 29, 7283-90	4	9
89	Oxidative addition of hydrogen halides and dihalogens to Pd. Trends in reactivity and relativistic effects. *Journal of Physical Chemistry A*, **2006**, 110, 7943-51	2.8	9
88	Chalcogen bonds: Hierarchical ab initio benchmark and density functional theory performance study. *Journal of Computational Chemistry*, **2021**, 42, 688-698	3.5	9
87	Origin of asynchronicity in Diels-Alder reactions. *Physical Chemistry Chemical Physics*, **2021**, 23, 20095-20106	3.6	9
86	Group 9 Metallacyclopentadienes as Key Intermediates in [2+2+2] Alkyne Cyclotrimerizations. Insight from Activation Strain Analyses. *ChemPhysChem*, **2018**, 19, 1766-1773	3.2	8
85	Steric Effects Dictate the Formation of Terminal Arylborylene Complexes of Ruthenium from Dihydroboranes. *Chemistry - A European Journal*, **2019**, 25, 13566-13571	4.8	8
84	Complexes of 4-substituted phenolates with HF and HCN: energy decomposition and electronic structure analyses of hydrogen bonding. *Journal of Computational Chemistry*, **2013**, 34, 696-705	3.5	8
83	Orbital interactions and charge redistribution in weak hydrogen bonds: Watson Crick GC mimic involving C?H proton donor and F proton acceptor groups. *International Journal of Quantum Chemistry*, **2006**, 106, 2428-2443	2.1	8
82	Structure and bonding of methyl alkali metal molecules. *Journal of Molecular Modeling*, **2006**, 12, 563-8	2	8
81	High-resolution infrared spectroscopy of the charge-transfer complex [Ar-N2]+: a combined experimental/theoretical study. *Journal of Chemical Physics*, **2005**, 123, 144305	3.9	8
80	S2 versus E2 Competition of F and PH Revisited. *Journal of Organic Chemistry*, **2020**, 85, 14087-14093	4.2	8
79	Not Carbon s-p Hybridization, but Coordination Number Determines C-H and C-C Bond Length. *Chemistry - A European Journal*, **2021**, 27, 7074-7079	4.8	8
78	How metallylenes activate small molecules. *Chemical Science*, **2021**, 12, 4526-4535	9.4	8

77	The Gauche Effect in XCH CH X Revisited. *ChemPhysChem*, **2021**, 22, 641-648	3.2	8
76	Charge Transfer and Environment Effects Responsible for Characteristics of DNA Base Pairing. *Angewandte Chemie - International Edition*, **1999**, 38, 2942-2945	16.4	8
75	Orbital interactions in strong and weak hydrogen bonds are essential for DNA replication. *Angewandte Chemie - International Edition*, **2002**, 41, 2092-5	16.4	8
74	Probing Through-Space Polar-Interactions in 2,6-Diarylphenols. *Journal of Organic Chemistry*, **2019**, 84, 3632-3637	4.2	7
73	Formation of a Trifluorophosphane Platinum(II) Complex by P-F Bond Activation of Phosphorus Pentafluoride with a Pt Complex. *Chemistry - A European Journal*, **2017**, 23, 5948-5952	4.8	7
72	Alkali-metal-supported bismuth polyhedra-principles and theoretical studies. *Inorganic Chemistry*, **2011**, 50, 5755-62	5.1	7
71	Tandem mass spectrometry of silver-adducted ferrocenyl catalyst complexes. *Journal of Mass Spectrometry*, **2010**, 45, 1332-43	2.2	7
70	Half-Sandwich Metal-Catalyzed Alkyne [2+2+2] Cycloadditions and the Slippage Span Model. *ChemistryOpen*, **2019**, 8, 143-154	2.3	6
69	Regioselectivity of the Pauson-Khand reaction in single-walled carbon nanotubes. *Nanoscale*, **2018**, 10, 15078-15089	7.7	6
68	A computational study on the reactivity enhancement in the free radical polymerization of alkyl -hydroxymethacrylate and acrylate derivatives. *Journal of Polymer Science Part A*, **2013**, 51, 880-889	2.5	6
67	Watson-crick base pairs with thiocarbonyl groups: How sulfur changes the hydrogen bonds in DNA. *Open Chemistry*, **2008**, 6, 15-21	1.6	6
66	The Chemical Bond: When Atom Size Instead of Electronegativity Difference Determines Trend in Bond Strength. *Chemistry - A European Journal*, **2021**, 27, 15616-15622	4.8	6
65	The Nature of Nonclassical Carbonyl Ligands Explained by Kohn-Sham Molecular Orbital Theory. *Chemistry - A European Journal*, **2020**, 26, 15690-15699	4.8	6
64	Glucose-Nucleobase Pseudo Base Pairs: Biomolecular Interactions within DNA. *Angewandte Chemie - International Edition*, **2016**, 55, 8643-7	16.4	6
63	On the Origin of Regioselectivity in Palladium-Catalyzed Oxidation of Glucosides. *European Journal of Organic Chemistry*, **2021**, 2021, 632-636	3.2	6
62	Silylene-Induced Reduction of [Mn2(CO)10]: Formation of a Five-Coordinate Silicon(IV) Complex with an O-Bound [(OC)4Mn=Mn(CO)4]2-Ligand. *European Journal of Inorganic Chemistry*, **2017**, 2017, 186-191	2.3	5
61	Diels-Alder reactivities of cycloalkenediones with tetrazine. *Journal of Molecular Modeling*, **2019**, 25, 33	2	5
60	Racemization and Deracemization through Intermolecular Redox Behaviour. *Chemistry - A European Journal*, **2019**, 25, 9639-9642	4.8	5

59	Is There a Need to Discuss Atomic Orbital Overlap When Teaching Hydrogen–Halide Bond Strength and Acidity Trends in Organic Chemistry?. *Journal of Chemical Education*, **2015**, 92, 286-290	2.4	5
58	Through-Space Polar-π Interactions in 2,6-Diarylthiophenols. *ChemPhysChem*, **2020**, 21, 1092-1100	3.2	5
57	Toward Transition-Metal-Templated Construction of Arylated B Chains by Dihydroborane Dehydrocoupling. *Chemistry - A European Journal*, **2019**, 25, 16544	4.8	5
56	Diastereoselective one-pot synthesis of tetrafunctionalized 2-imidazolines. *Journal of Organic Chemistry*, **2014**, 79, 5219-26	4.2	5
55	Cesium's Off-the-Map Valence Orbital. *Angewandte Chemie*, **2017**, 129, 9904-9908	3.6	5
54	Macrocycles All Aflutter: Substitution at an Allylic Center Reveals the Conformational Dynamics of [13]-Macrodilactones. *Chemistry - an Asian Journal*, **2017**, 12, 2623-2633	4.5	5
53	Six-Coordinate Group 13 Complexes: The Role of d Orbitals and Electron-Rich Multi-Center Bonding. *Angewandte Chemie*, **2015**, 127, 12202-12206	3.6	5
52	C(CN)5– transition state or intermediate?. *Mendeleev Communications*, **2010**, 20, 72-73	1.9	5
51	Distortion-Controlled Redshift of Organic Dye Molecules. *Chemistry - A European Journal*, **2020**, 26, 2080-2093	4.8	5
50	Nucleophilic substitution at di- and triphosphates: leaving group ability of phosphate versus diphosphate. *Electronic Structure*, **2019**, 1, 024001	2.6	4
49	Mechanism of biomolecular recognition of trimethyllysine by the fluorinated aromatic cage of KDM5A PHD3 finger. *Communications Chemistry*, **2020**, 3,	6.3	4
48	Electronic communication through mono and multinuclear gold(I) complexes. *International Journal of Quantum Chemistry*, **2009**, 109, 2507-2519	2.1	4
47	The rotation barrier in ethane. *Nachrichten Aus Der Chemie*, **2004**, 52, 581-581	0.1	4
46	Alkali Metal Cation versus Proton and Methyl Cation Affinities: Structure and Bonding Mechanism. *ChemistryOpen*, **2016**, 5, 247-53	2.3	4
45	Designing Rh(I)-Half-Sandwich Catalysts for Alkyne [2+2+2] Cycloadditions. *Synlett*, **2021**, 32, 561-572	2.2	4
44	Regio- and Stereoselectivity in 1,3-Dipolar Cycloadditions: Activation Strain Analyses for Reactions of Hydrazoic Acid with Substituted Alkenes. *European Journal of Organic Chemistry*, **2017**, 2017, 4313-4318	3.3	3
43	Hydride affinities of cationic maingroup-element hydrides across the periodic table. *Results in Chemistry*, **2019**, 1, 100007	2.1	3
42	Comparison of Molecular Recognition of Trimethyllysine and Trimethylthialysine by Epigenetic Reader Proteins. *Molecules*, **2020**, 25,	4.8	3

41	Effects of the protonation state in the interaction of an HIV-1 reverse transcriptase (RT) amino acid, Lys101, and a non nucleoside RT inhibitor, GW420867X. *Journal of Molecular Modeling*, **2014**, 20, 2332	2	3
40	Supramolecular ring structures of 7-methylguanine: a computational study of its self-assembly and anion binding. *Molecules*, **2012**, 18, 225-35	4.8	3
39	Gas-Phase Base-Induced 1,4-Eliminations: Occurrence of Single-, Double-, and Triple-Well E1cb Mechanisms J. Am. Chem. Soc. 1995, 117, 9889 9899. *Journal of the American Chemical Society*, **1996**, 118, 1579-1579	16.4	3
38	Activation Strain Analyses of Counterion and Solvent Effects on the Ion-Pair S 2 Reaction of and CH Cl. *Journal of Computational Chemistry*, **2020**, 41, 317-327	3.5	3
37	Probing Halogen- versus CH- Interactions in Molecular Balance. *Organic Letters*, **2020**, 22, 7870-7873	6.2	3
36	The Hydrogenation Problem in Cobalt-based Catalytic Hydroaminomethylation. *ChemistrySelect*, **2020**, 5, 13981-13994	1.8	3
35	Nucleophilic Substitution (SN2): Dependence on Nucleophile, Leaving Group, Central Atom, Substituents, and Solvent. *ChemPhysChem*, **2018**, 19, 1248-1248	3.2	2
34	Integrative Theory/Experiment-Driven Exploration of a Multicomponent Reaction towards Imidazoline-2-(thi)ones. *European Journal of Organic Chemistry*, **2018**, 2018, 104-112	3.2	2
33	Synthesis and Hydrolysis of Alkoxy(aminoalkyl)diorganylsilanes of the Formula Type R2(RO)Si(CH2)nNH2 (R = Alkyl, n = 1): A Systematic Experimental and Computational Study. *European Journal of Inorganic Chemistry*, **2016**, 2016, 1641-1659	2.3	2
32	Benchmark study on the smallest bimolecular nucleophilic substitution reaction: H?+CH >CH H?. *Molecules*, **2013**, 18, 7726-38	4.8	2
31	Outer valence orbital response to proton positions in prototropic tautomers of adenine. *Journal of Computational Methods in Sciences and Engineering*, **2007**, 6, 251-267	0.3	2
30	Aromaticity: Molecular-Orbital Picture of an Intuitive Concept. *Chemistry - A European Journal*, **2007** , 13, 8371-8371	4.8	2
29	Attractive and convincing. *Angewandte Chemie - International Edition*, **2008**, 47, 7172	16.4	2
28	Watson rick hydrogen bonds: nature and role in DNA replication **2006**, 79-97		2
27	Origin of the Effect in SN2 Reactions. *Angewandte Chemie*, **2021**, 133, 21008-21016	3.6	2
26	Glucose Nucleobase Pseudo Base Pairs: Biomolecular Interactions within DNA. *Angewandte Chemie* , **2016**, 128, 8785-8789	3.6	2
25	Bismutamide als einfache Vermittler hochselektiver Pn Pn-Radikal-Kupplungsreaktionen (Pn=N, P, As). *Angewandte Chemie*, **2021**, 133, 6513-6518	3.6	2
24	Switch From Pauli-Lowering to LUMO-Lowering Catalysis in Br sted Acid-Catalyzed Aza-Diels-Alder Reactions. *ChemistryOpen*, **2021**, 10, 784-789	2.3	2

23	How Lewis Acids Catalyze Ene Reactions. *European Journal of Organic Chemistry*, **2021**, 2021, 5275	3.2	2
22	Nature of Alkali- and Coinage-Metal Bonds versus Hydrogen Bonds. *Chemistry - an Asian Journal*, **2021**, 16, 315-321	4.5	2
21	Cation affinities throughout the periodic table. *Advances in Inorganic Chemistry*, **2019**, 73, 123-158	2.1	1
20	4th International Conference on Chemical Bonding. *Journal of Physical Chemistry A*, **2016**, 120, 9353-9356	2.8	1
19	Alkali Metal Cation Affinities of Neutral Maingroup-Element Hydrides across the Periodic Table. *Journal of Physical Chemistry A*, **2019**, 123, 9137-9148	2.8	1
18	d10-ML2 Complexes: Structure, Bonding, and Catalytic Activity. *Structure and Bonding*, **2014**, 139-161	0.9	1
17	Stacked DNA-base quartets: Structure, chemistry and computational intricacies. *Procedia Computer Science*, **2010**, 1, 1147-1148	1.6	1
16	Do Sulfonamides Interact with Aromatic Rings?. *Chemistry - A European Journal*, **2021**, 27, 5721-5729	4.8	1
15	Dipolar repulsion in α-halocarbonyl compounds revisited. *Physical Chemistry Chemical Physics*, **2021**, 23, 20883-20891	3.6	1
14	Proton Transfer and S 2 Reactions as Steps of Fast Selenol and Thiol Oxidation in Proteins: A Model Molecular Study Based on GPx. *ChemPlusChem*, **2021**, 86, 524	2.8	1
13	Radical Scavenging Potential of the Phenothiazine Scaffold: A Computational Analysis. *ChemMedChem*, **2021**,	3.7	1
12	Role of the Chalcogen (S, Se, Te) in the Oxidation Mechanism of the Glutathione Peroxidase Active Site. *ChemPhysChem*, **2017**, 18, 2950-2950	3.2	0
11	A Quantitative Molecular Orbital Perspective of the Chalcogen Bond. *ChemistryOpen*, **2021**, 10, 390	2.3	0
10	Polycyclic Aromatic Hydrocarbons (PAHs) in Interstellar Ices: A Computational Study into How the Ice Matrix Influences the Ionic State of PAH Photoproducts.. *ACS Earth and Space Chemistry*, **2022**, 6, 766-774	3.2	0
9	Through-Space Polar-π Interactions in 2,6-Diarylthiophenols. *ChemPhysChem*, **2020**, 21, 1080	3.2	
8	Glucose-nucleobase pairs within DNA: impact of hydrophobicity, alternative linking unit and DNA polymerase nucleotide insertion studies. *Chemical Science*, **2018**, 9, 3544-3554	9.4	
7	Innentitelbild: Das Distortion/Interaction-Activation-Strain-Modell zur Analyse von Reaktionsgeschwindigkeiten (Angew. Chem. 34/2017). *Angewandte Chemie*, **2017**, 129, 10134-10134	3.6	
6	Buchbesprechung: Computational Chemistry. A Practical Guide for Applying Techniques to Real World Problems. Von David Young. *Angewandte Chemie*, **2002**, 114, 377-378	3.6	

List of Publications

5	B-DNA Structure and Stability: The Role of Nucleotide Composition and Order.. *ChemistryOpen*, **2022**, e202100231	2.3
4	B-DNA Structure and Stability: The Role of Nucleotide Composition and Order.. *ChemistryOpen*, **2022**, 11, e202200013	2.3
3	Structure and bonding of methyl alkali metal molecules563-568	
2	In My Element: Carbon. *Chemistry - A European Journal*, **2019**, 25, 19-19	4.8
1	Innenr□ktitelbild: Origin of the ⊟ffect in SN2 Reactions (Angew. Chem. 38/2021). *Angewandte Chemie*, **2021**, 133, 21239-21239	3.6