

Helene F Gerard

List of Publications by Year in descending order

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71
papers

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236925

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times ranked

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#	ARTICLE	IF	CITATIONS
1	Coordinated carbenes from electron-rich olefins on RuHCl(PPr3i)2. <i>New Journal of Chemistry</i> , 2000, 24, 9-26.	2.8	87
2	Sulfonyl vs. carbonyl group: which is the more electron-withdrawing?. <i>Chemical Communications</i> , 2007, , 3288.	4.1	84
3	Stereoselective and Catalytic Access to \hat{I}^2 -Enaminones: An Entry to Pyrimidines. <i>Journal of Organic Chemistry</i> , 2012, 77, 9205-9220.	3.2	65
4	What can be learnt on biologically relevant systems from the topological analysis of the electron localization function?. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1951-1969.	2.0	59
5	Geminal dehydrogenation of ether and amine C(sp ³)H ₂ groups by electron-rich Ru(II) and Os. Electronic supplementary information (ESI) available: crystallographic data, fractional coordinates and isotropic thermal parameters, anisotropic thermal parameters, and bond distances and angles. See http://www.rsc.org/suppdata/ni/b2/b200168n/ . <i>New Journal of Chemistry</i> , 2002, 26, 687-700.	2.8	57
6	A comprehensive view of M ⁺ -H addition across the RC \equiv CH bond: frustration culminating in ultimate union. <i>New Journal of Chemistry</i> , 2001, 25, 1244-1255.	2.8	56
7	Experimental and Theoretical Study of the Regiospecific Coordination of Rulland OsII Fragments on the Lacunary Polyoxometalate [PW ₁₁ O ₃₉] ⁷⁻ . <i>Journal of Physical Chemistry A</i> , 2006, 110, 6345-6355.	2.5	52
8	Carbene Complexes from Olefins, Using RuHCl(PiPr ₃) ₂ . Influence of the Olefin Substituent. <i>Journal of the American Chemical Society</i> , 1998, 120, 9388-9389.	13.7	49
9	Ph ₂ P(BH ₃) ₃ Li: From Ditopicity to Dual Reactivity. <i>Journal of the American Chemical Society</i> , 2011, 133, 6472-6480.	13.7	48
10	Benzofurans as Efficient Dienophiles in Normal Electron Demand [4 + 2] Cycloadditions. <i>Journal of Organic Chemistry</i> , 2009, 74, 1237-1246.	3.2	45
11	Vinyl C ⁺ F Cleavage by Os(H)3Cl(PiPr ₃) ₂ . <i>Inorganic Chemistry</i> , 2002, 41, 6440-6449.	4.0	43
12	Exploring the Hydration of Pb ²⁺ : Ab Initio Studies and First-Principles Molecular Dynamics. <i>Chemistry - A European Journal</i> , 2006, 12, 5024-5032.	3.3	42
13	MeLi + LiCl in THF: One Heterodimer and No Tetramers. <i>Journal of Organic Chemistry</i> , 2010, 75, 5976-5983.	3.2	42
14	Theoretical Exploration of the Oxidative Properties of a [(tren ^{Me})CuO ₂] ⁺ Adduct Relevant to Copper Monooxygenase Enzymes: Insights into Competitive Dehydrogenation versus Hydroxylation Reaction Pathways. <i>Chemistry - A European Journal</i> , 2008, 14, 6465-6473.	3.3	40
15	Understanding Lead Chemistry from Topological Insights: The Transition between Holo \hat{C} and Hemidirected Structures within the [Pb(CO) _n] ²⁺ Model Series. <i>Chemistry - A European Journal</i> , 2008, 14, 2730-2743.	3.3	38
16	A comparative study of olefin or acetylene insertion into Ru \hat{C} - \hat{C} H or Os \hat{C} - \hat{C} H of MHCl(CO)(phosphine) ₂ . <i>New Journal of Chemistry</i> , 2001, 25, 1382-1388.	2.8	35
17	Theoretical modelling of tripodal CuN ₃ and CuN ₄ cuprous complexes interacting with O ₂ , CO or CH ₃ CN. <i>Journal of Biological Inorganic Chemistry</i> , 2006, 11, 593-608.	2.6	35
18	Hcp cobalt nanocrystals with high magnetic anisotropy prepared by easy one-pot synthesis. <i>Nanoscale</i> , 2016, 8, 18640-18645.	5.6	35

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19	Double Silyl Migration Converting $\text{ORe}[\text{N}(\text{SiMe}_2\text{CH}_2\text{PCy}_2)_2]$ to $\text{NRe}[\text{O}(\text{SiMe}_2\text{CH}_2\text{PCy}_2)_2]$ Substructures. <i>Inorganic Chemistry</i> , 2002, 41, 5615-5625.	4.0	29
20	Copper-Catalyzed Asymmetric Conjugate Addition of Dimethylzinc to Acyl-N-methylimidazole Michael Acceptors: Scope, Limitations and Iterative Reactions. <i>Advanced Synthesis and Catalysis</i> , 2016, 358, 2519-2540.	4.3	29
21	Isomerization of a Peptidic Fragment Studied Theoretically in Vacuum and in Explicit Water Solvent at Finite Temperature. <i>Journal of the American Chemical Society</i> , 2004, 126, 4080-4081.	13.7	28
22	Dearomatization of 3-Nitroindoles with Highly Functionalized Allenolates in Formal (3+2) Cycloadditions. <i>Chemistry - A European Journal</i> , 2019, 25, 13688-13693.	3.3	28
23	Addition of Hetero Allenyl Copper Reagents to Aldehydes: Scope and Behavior. <i>Journal of Organic Chemistry</i> , 2007, 72, 1770-1779.	3.2	26
24	Revisiting the holo- and hemidirected structural transition within the $[\text{Pb}(\text{CO})_n]^{2+}$ model series using first-principles Molecular Dynamics. <i>Dalton Transactions</i> , 2011, 40, 11282.	3.3	26
25	Unifying the mechanisms for alkane dehydrogenation and alkene H/D exchange with $[\text{IrH}_2(\text{O}_2\text{CCF}_3)(\text{PAr}_3)_2]$: the key role of CF_3CO_2 in the 'sticky' alkane route. <i>New Journal of Chemistry</i> , 2001, 25, 1121-1131.	2.8	25
26	A Combined Experimental-Theoretical Study on the Lithiation/Electrophilic Quench Sequence of $(\eta^5\text{-Cyclohexadienyl})\text{Mn}(\text{CO})_3$ Complexes. <i>Organometallics</i> , 2008, 27, 626-636.	2.3	25
27	Facile $\text{C}(\text{sp}^2)/\text{OR}$ Bond Cleavage by Ru or Os. <i>Inorganic Chemistry</i> , 2001, 40, 6610-6621.	4.0	23
28	Selectivities of Multicomponent $[4 + 2]/[3 + 2]$ Cycloadditions of 3-Nitroindole with Substituted Alkenes: A DFT Analysis. <i>Journal of Organic Chemistry</i> , 2013, 78, 9233-9242.	3.2	23
29	Facile $\text{C}(\text{sp}^2)/\text{O}_2\text{CR}$ bond cleavage by Ru or Os. <i>New Journal of Chemistry</i> , 2003, 27, 1451-1462.	2.8	22
30	Comparison of $\eta^5\text{-CH}$ and CF activation in alkyl transition metal complexes: a DFT and CASSCF study. <i>Molecular Physics</i> , 2002, 100, 533-540.	1.7	21
31	Quantum chemistry insight into Mg-substitution in chlorophyll by toxic heavy metals: Cd, Hg and Pb. <i>Chemical Physics Letters</i> , 2016, 663, 27-32.	2.6	21
32	Role of Oleylamine Revisited: An Original Disproportionation Route to Monodispersed Cobalt and Nickel Nanocrystals. <i>Chemistry of Materials</i> , 2019, 31, 960-968.	6.7	21
33	Solution and Solid-State Structure of $\text{Ru}(\text{CO})_2(\text{Bu}_2\text{PtC}_2\text{H}_4\text{PtBu}_2)$: Square Planar and Monomeric?. <i>Journal of the American Chemical Society</i> , 1999, 121, 3242-3243.	13.7	20
34	Unprecedented $(\eta^5\text{-Formylcyclohexadienyl})\text{Mn}(\text{CO})_3$ Complexes: Synthesis, Structural and Theoretical Characterizations, and Resolution of the Planar Chirality. <i>Organometallics</i> , 2008, 27, 2505-2517.	2.3	20
35	How to optimize a $\text{C}\ddot{\text{C}}\text{H}$ cleavage with a mononuclear copper-dioxygen adduct?. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1898-1904.	2.0	19
36	Ab Initio and Empirical Model MD Simulation Studies of Solvent Effects on the Properties of N-Methylacetamide along a cis-trans Isomerization Pathway. <i>Journal of Physical Chemistry B</i> , 2006, 110, 13523-13538.	2.6	18

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37	Fate of CH ₂ CH(E) in the Presence of Unsaturated Ru(X)(H)L ₂ q+(X = Cl,q= 0; X = CO,q= 1): [^] Highly Sensitive to X and E. <i>Organometallics</i> , 2000, 19, 2291-2298.	2.3	17
38	Unsaturated Ru(0) Species with a Constrained Bis-Phosphine Ligand: [Ru(CO) ₂ (tBu ₂ PCH ₂ CH ₂ PtBu ₂)] ₂ . Comparison to [Ru(CO) ₂ (PtBu ₂ Me) ₂]. <i>Inorganic Chemistry</i> , 2000, 39, 3957-3962.	4.0	17
39	Revisiting the Structure of (LiCH ₃) _n Aggregates Using Car [^] Parrinello Molecular Dynamics. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4787-4794.	2.5	17
40	First-Principles Molecular Dynamics Evaluation of Thermal Effects on the NMR Li, C Spin [^] Spin Coupling. <i>Chemistry - A European Journal</i> , 2007, 13, 3459-3469.	3.3	17
41	Theoretical Study of the Relative Stabilities of the $\text{Li}^{\pm} \text{Li}^{\pm} \text{Li}^{\pm} \text{O} \text{O} \text{O}$ Lacunary Polyoxometalates (X) $\text{Li}^{\pm} \text{Li}^{\pm} \text{Li}^{\pm} \text{O} \text{O} \text{O}$	17.7843	14
42	Diastereodivergent Behavior of Alkyl versus Cyano Allenylcuprates toward Aldehydes: A Key Role for Lithium. <i>Journal of the American Chemical Society</i> , 2011, 133, 10790-10802.	13.7	17
43	A Simple Route to Keto-Substituted (1 [^] -Cyclohexadienyl)Mn(CO) ₃ Complexes Using Organomanganese Transmetalation: Structural and Theoretical Characterizations. <i>Organometallics</i> , 2009, 28, 925-928.	2.3	16
44	Interactions of copper(II) and zinc(II) with chlorophyll: insights from density functional theory studies. <i>New Journal of Chemistry</i> , 2016, 40, 4543-4549.	2.8	15
45	1,3 [^] Li/H Shift of 1 [^] -Aryl-2 [^] -Cyclohexadienyl Reagents: An Experimental and Theoretical Study. <i>Chemistry - A European Journal</i> , 2009, 15, 45-48.	3.3	14
46	Spin [^] -Driven activation of dioxygen in various metalloenzymes and their inspired models. <i>Journal of Computational Chemistry</i> , 2011, 32, 1178-1182.	3.3	14
47	L [^] = CO vs Cl- Transposition: Remarkable Consequences for the Product of (L [^]) [^] Ru(L) ₂ (H) and Vinyl Ether. <i>Organometallics</i> , 1999, 18, 5441-5443.	2.3	13
48	How the topological analysis of the electron localization function accounts for the inductive effect. <i>Computational and Theoretical Chemistry</i> , 2007, 811, 69-76.	1.5	13
49	Catalytic enantioselective nucleophilic addition of organolithium derivatives: pitfalls and opportunities. <i>New Journal of Chemistry</i> , 2012, 36, 2441.	2.8	13
50	Asymmetric Sequential Cu [^] Catalyzed 1,6/1,4 [^] Conjugate Additions of Hard Nucleophiles to Cyclic Dienones: Determination of Absolute Configurations and Origins of Enantioselectivity. <i>Chemistry - A European Journal</i> , 2017, 23, 7515-7525.	3.3	13
51	A computational study of the effects of ancillary ligands on copper(II) ethylene interaction. <i>New Journal of Chemistry</i> , 2015, 39, 5410-5419.	2.8	12
52	Dioxygen Activation by Mononuclear Copper Enzymes: Insights from a Tripodal Ligand Mimicking Their CuM Coordination Sphere. <i>Inorganic Chemistry</i> , 2009, 48, 7003-7005.	4.0	11
53	Diversity in Synthesis of N-Heterocycles from Simple Propargylic Alcohols. <i>Synlett</i> , 2015, 26, 2336-2350.	1.8	10
54	Mechanism of Enolate Transfer between Si and Cu. <i>Chemistry - A European Journal</i> , 2018, 24, 6617-6624.	3.3	10

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55	Direct Synthesis of Nitriles from Carboxylic Acids Using Indium-Catalyzed Transnitration: Mechanistic and Kinetic Study. <i>ACS Catalysis</i> , 2019, 9, 9705-9714.	11.2	10
56	Shuffling lithiated mixed aggregates: NMR and Carâ€Parrinello molecular dynamics reveal an unexpected associative pathway. <i>Chemical Communications</i> , 2009, , 319-321.	4.1	9
57	Development of a Radical Silylzincation of (Het)Arylâ€Substituted Alkynes and Computational Insights into the Origin of the <i>trans</i>-stereoselectivity. <i>Advanced Synthesis and Catalysis</i> , 2021, 363, 2634-2647.	4.3	9
58	Olefin insertion in the Ruâ€H and Ruâ€F bonds of pentacoordinated d6 Ru(ii) species: a DFT study. <i>Dalton Transactions</i> , 2003, , 839.	3.3	8
59	Competitive ligand/chelate binding in [Cu(TMPA)]+ and [Cu(tren)]+ based complexes. <i>Catalysis Today</i> , 2011, 177, 79-86.	4.4	7
60	DFT and TD-DFT Studies of Mg-Substitution in Chlorophyll by Cr(II), Fe(II) and Ni(II). <i>Chemistry Africa</i> , 2018, 1, 79-86.	2.4	7
61	Vinyl (Thio)Ethers versus Enamines: A DFT Insight into Their Divergent Reactivities toward Nitroalkenes. <i>Chemistry - A European Journal</i> , 2017, 23, 13711-13717.	3.3	6
62	Catalytically Active Species in Copper/DiPPAMâ€Catalyzed 1,6â€Asymmetric Conjugate Addition of Dialkylzinc to Dienones: A Computational Overview. <i>ChemCatChem</i> , 2019, 11, 4108-4115.	3.7	6
63	Dynamic Kinetic Resolution Processes Based on the Switchable Configurational Instability of Allenyl Copper Reagents. <i>Organic Letters</i> , 2021, 23, 6305-6310.	4.6	4
64	A combined experimentalâ€theoretical study on the lithiation/electrophilic quench reaction of benzylic position of (Î-5-tetramethylcyclohexadienyl)-Mn(CO)3. <i>New Journal of Chemistry</i> , 2011, 35, 2375.	2.8	3
65	Intertwined Analytical, Experimental and Theoretical Studies on the Formation and Structure of a Copper Dienolate. <i>Chemistry - A European Journal</i> , 2021, 27, 7942-7950.	3.3	3
66	Li+-Controlled Diastereoselectivity of the Addition of Allenyl Cuprate Reagents to Aldehydes. <i>Synthesis</i> , 2017, 49, 526-531.	2.3	1
67	Selective Formation of Epoxylimonene Catalyzed by Phosphonyl/Arsonyl Derivatives of Trivalent Polyoxotungstates at Low Temperature. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 605-612.	2.0	1
68	Ligand effects on coordination properties of organolithium compounds: insights from computational experiments on a â€weakenedâ€Li+. <i>Journal of Molecular Modeling</i> , 2020, 26, 59.	1.8	1
69	Triggering Electron Transfer in Co(I) Dimers: Computational Evidences for a Reversible Disproportionation Mechanism. <i>ChemPhysChem</i> , 2021, 22, 788-795.	2.1	1
70	Cu(I)-Assisted Addition of Li- or Zn-Organometallics to Carbonyl Compounds: Learning from Analogies and Differences Between Intermediates and Transition States. <i>Topics in Catalysis</i> , 2022, 65, 481-492.	2.8	1
71	Selective Formation of Epoxylimonene Catalyzed by Phosphonyl/Arsonyl Derivatives of Trivalent Polyoxotungstates at Low Temperature. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 596-596.	2.0	0