Helene F Gerard

List of Publications by Year
in descending order

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71	1,670	236925	330143
papers	citations	25 h-index	37 g-index

79	79	79	1778
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Cu(I)-Assisted Addition of Li- or Zn-Organometallics to Carbonyl Compounds: Learning from Analogies and Differences Between Intermediates and Transition States. Topics in Catalysis, 2022, 65, 481-492.	2.8	1
2	Development of a Radical Silylzincation of (Het)Arylâ€Substituted Alkynes and Computational Insights into the Origin of the transâ€Stereoselectivity. Advanced Synthesis and Catalysis, 2021, 363, 2634-2647.	4.3	9
3	Triggering Electron Transfer in Co(I) Dimers: Computational Evidences for a Reversible Disproportionation Mechanism. ChemPhysChem, 2021, 22, 788-795.	2.1	1
4	Intertwined Analytical, Experimental and Theoretical Studies on the Formation and Structure of a Copper Dienolate. Chemistry - A European Journal, 2021, 27, 7942-7950.	3.3	3
5	Dynamic Kinetic Resolution Processes Based on the Switchable Configurational Instability of Allenyl Copper Reagents. Organic Letters, 2021, 23, 6305-6310.	4.6	4
6	Selective Formation of Epoxylimonene Catalyzed by Phosphonyl/Arsonyl Derivatives of Trivacant Polyoxotungstates at Low Temperature. European Journal of Inorganic Chemistry, 2020, 2020, 605-612.	2.0	1
7	Selective Formation of Epoxylimonene Catalyzed by Phosphonyl/ArsonÃyl Derivatives of Trivacant Polyoxotungstates at Low Temperature. European Journal of Inorganic Chemistry, 2020, 2020, 596-596.	2.0	0
8	Ligand effects on coordination properties of organolithium compounds: insights from computational experiments on a â€œweakenedâ€•Li+. Journal of Molecular Modeling, 2020, 26, 59.	1.8	1
9	Dearomatization of 3â€Nitroindoles with Highly Î³â€Functionalized Allenoates in Formal (3+2) Cycloadditions. Chemistry - A European Journal, 2019, 25, 13688-13693.	3.3	28
10	Direct Synthesis of Nitriles from Carboxylic Acids Using Indium-Catalyzed Transnitrilation: Mechanistic and Kinetic Study. ACS Catalysis, 2019, 9, 9705-9714.	11.2	10
11	Catalytically Active Species in Copper/DiPPAMâ€Catalyzed 1,6â€Asymmetric Conjugate Addition of Dialkylzinc to Dienones: A Computational Overview. ChemCatChem, 2019, 11, 4108-4115.	3.7	6
12	Role of Oleylamine Revisited: An Original Disproportionation Route to Monodispersed Cobalt and Nickel Nanocrystals. Chemistry of Materials, 2019, 31, 960-968.	6.7	21
13	Mechanism of Enolate Transfer between Si and Cu. Chemistry - A European Journal, 2018, 24, 6617-6624.	3.3	10
14	DFT and TD-DFT Studies of Mg-Substitution in Chlorophyll by Cr(II), Fe(II) and Ni(II). Chemistry Africa, 2018, 1, 79-86.	2.4	7
15	Asymmetric Sequential Cuâ€Catalyzed 1,6/1,4â€Conjugate Additions of Hard Nucleophiles to Cyclic Dienones: Determination of Absolute Configurations and Origins of Enantioselectivity. Chemistry - A European Journal, 2017, 23, 7515-7525.	3.3	13
16	Vinyl (Thio)Ethers versus Enamines: A DFT Insight into Their Divergent Reactivities toward Nitroalkenes. Chemistry - A European Journal, 2017, 23, 13711-13717.	3.3	6
17	Li+-Controlled Diastereoselectivity of the Addition of Allenyl Cuprate Reagents to Aldehydes. Synthesis, 2017, 49, 526-531.	2.3	1
18	Copperâ€Catalyzed Asymmetric Conjugate Addition of Dimethylzinc to Acylâ€Nâ€•methylimidazole Michael Acceptors: Scope, Limitations and Iterative Reactions. Advanced Synthesis and Catalysis, 2016, 358, 2519-2540.	4.3	29

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19	Quantum chemistry insight into Mg-substitution in chlorophyll by toxic heavy metals: Cd, Hg and Pb. Chemical Physics Letters, 2016, 663, 27-32.	2.6	21
20	Hcp cobalt nanocrystals with high magnetic anisotropy prepared by easy one-pot synthesis. Nanoscale, 2016, 8, 18640-18645.	5.6	35
21	Interactions of copper(<scp>ii</scp>) and zinc(<scp>ii</scp>) with chlorophyll: insights from density functional theory studies. New Journal of Chemistry, 2016, 40, 4543-4549.	2.8	15
22	A computational study of the effects of ancillary ligands on copper(<scp>i</scp>)â€“ethylene interaction. New Journal of Chemistry, 2015, 39, 5410-5419.	2.8	12
23	Diversity in Synthesis of N-Heterocycles from Simple Propargylic Alcohols. Synlett, 2015, 26, 2336-2350.	1.8	10
24	Selectivities of Multicomponent [4 + 2]/[3 + 2] Cycloadditions of 3-Nitroindole with Substituted Alkenes: A DFT Analysis. Journal of Organic Chemistry, 2013, 78, 9233-9242.	3.2	23
25	Catalytic enantioselective nucleophilic addition of organolithium derivatives: pitfalls and opportunities. New Journal of Chemistry, 2012, 36, 2441.	2.8	13
26	Stereoselective and Catalytic Access to Î²-Enaminones: An Entry to Pyrimidines. Journal of Organic Chemistry, 2012, 77, 9205-9220.	3.2	65
27	Revisiting the holo- and hemidirected structural transition within the [Pb(CO)n]2+ model series using first-principles Molecular Dynamics. Dalton Transactions, 2011, 40, 11282.	3.3	26
28	A combined experimentalâ€“theoretical study on the lithiation/electrophilic quench reaction of benzylic position of (Î·5-tetramethylcyclohexadienyl)-Mn(CO)3. New Journal of Chemistry, 2011, 35, 2375.	2.8	3
29	Diastereodivergent Behavior of Alkyl versus Cyano Allenylcuprates toward Aldehydes: A Key Role for Lithium. Journal of the American Chemical Society, 2011, 133, 10790-10802.	13.7	17
30	Ph₂P(BH₃)Li: From Ditopicity to Dual Reactivity. Journal of the American Chemical Society, 2011, 133, 6472-6480.	13.7	48
31	Competitive ligand/chelate binding in [Cu(TMPA)]+ and [Cu(tren)]+ based complexes. Catalysis Today, 2011, 177, 79-86.	4.4	7
32	Spinâ€driven activation of dioxygen in various metalloenzymes and their inspired models. Journal of Computational Chemistry, 2011, 32, 1178-1182.	3.3	14
33	MeLi + LiCl in THF: One Heterodimer and No Tetramers. Journal of Organic Chemistry, 2010, 75, 5976-5983.	3.2	42
34	1,3â€Li/H Shift of 1â€Arylâ€1,2â€alkadienyl Reagents: An Experimental and Theoretical Study. Chemistry - A European Journal, 2009, 15, 45-48.	3.3	14
35	Benzofurans as Efficient Dienophiles in Normal Electron Demand [4 + 2] Cycloadditions. Journal of Organic Chemistry, 2009, 74, 1237-1246.	3.2	45
36	Dioxygen Activation by Mononuclear Copper Enzymes: Insights from a Tripodal Ligand Mimicking Their CuM Coordination Sphere. Inorganic Chemistry, 2009, 48, 7003-7005.	4.0	11

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37	A Simple Route to Keto-Substituted (Î·⁵-Cyclohexadienyl)Mn(CO)₃ Complexes Using Organomanganese Transmetalation: Structural and Theoretical Characterizations. Organometallics, 2009, 28, 925-928.	2.3	16
38	Shuffling lithiated mixed aggregates: NMR and Carâ€“Parrinello molecular dynamics reveal an unexpected associative pathway. Chemical Communications, 2009, , 319-321.	4.1	9
39	How to optimize a Cï£¿H cleavage with a mononuclear copperâ€“dioxygen adduct?. International Journal of Quantum Chemistry, 2008, 108, 1898-1904.	2.0	19
40	What can be learnt on biologically relevant systems from the topological analysis of the electron localization function?. International Journal of Quantum Chemistry, 2008, 108, 1951-1969.	2.0	59
41	Understanding Lead Chemistry from Topological Insights: The Transition between Holoâ€•and Hemidirected Structures within the [Pb(CO)_n]²⁺ Model Series. Chemistry - A European Journal, 2008, 14, 2730-2743.	3.3	38
42	Theoretical Exploration of the Oxidative Properties of a [(tren^{Me1})CuO₂]⁺ Adduct Relevant to Copper Monooxygenase Enzymes: Insights into Competitive Dehydrogenation versus Hydroxylation Reaction Pathways. Chemistry - A European Journal, 2008, 14, 6465-6473.	3.3	40
43	Theoretical Study of the Relative Stabilities of the Î±-Î²₃-[XW₁₁O₃₉]^{mâ^’} Lacunary Polyoxometalates (X) 4jdETQq1 1 0.784314	1	0
44	A Combined Experimentalâ^’Theoretical Study on the Lithiation/Electrophilic Quench Sequence of (Î·⁵-Cyclohexadienyl)Mn(CO)₃ Complexes. Organometallics, 2008, 27, 626-636.	2.3	25
45	Unprecedented (Î·⁵-Formylcyclohexadienyl)Mn(CO)₃ Complexes: Synthesis, Structural and Theoretical Characterizations, and Resolution of the Planar Chirality. Organometallics, 2008, 27, 2505-2517.	2.3	20
46	Sulfonyl vs. carbonyl group: which is the more electron-withdrawing?. Chemical Communications, 2007, , 3288.	4.1	84
47	Addition of Hetero Allenyl Copper Reagents to Aldehydes: Scope and Behavior. Journal of Organic Chemistry, 2007, 72, 1770-1779.	3.2	26
48	First-Principles Molecular Dynamics Evaluation of Thermal Effects on the NMR1JLi,C Spinâ€“Spin Coupling. Chemistry - A European Journal, 2007, 13, 3459-3469.	3.3	17
49	How the topological analysis of the electron localization function accounts for the inductive effect. Computational and Theoretical Chemistry, 2007, 811, 69-76.	1.5	13
50	Experimental and Theoretical Study of the Regiospecific Coordination of RuIland OsIIFragments on the Lacunary Polyoxometalate [Î±-PW11O39]7-. Journal of Physical Chemistry A, 2006, 110, 6345-6355.	2.5	52
51	Ab Initio and Empirical Model MD Simulation Studies of Solvent Effects on the Properties of N-Methylacetamide along a cisâ^’trans Isomerization Pathway. Journal of Physical Chemistry B, 2006, 110, 13523-13538.	2.6	18
52	Revisiting the Structure of (LiCH3)nAggregates Using Carâ^’Parrinello Molecular Dynamics. Journal of Physical Chemistry A, 2006, 110, 4787-4794.	2.5	17
53	Theoretical modelling of tripodal CuN3 and CuN4 cuprous complexes interacting with O2, CO or CH3CN. Journal of Biological Inorganic Chemistry, 2006, 11, 593-608.	2.6	35
54	Exploring the Hydration of Pb2+: Ab Initio Studies and First-Principles Molecular Dynamics. Chemistry - A European Journal, 2006, 12, 5024-5032.	3.3	42

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55	Isomerization of a Peptidic Fragment Studied Theoretically in Vacuum and in Explicit Water Solvent at Finite Temperature. Journal of the American Chemical Society, 2004, 126, 4080-4081.	13.7	28
56	Olefin insertion in the Ruâ€“H and Ruâ€“F bonds of pentacoordinated d6 Ru(ii) species: a DFT study. Dalton Transactions, 2003, , 839.	3.3	8
57	Facile C(sp2)/O2CR bond cleavage by Ru or Os. New Journal of Chemistry, 2003, 27, 1451-1462.	2.8	22
58	Vinyl Câ^'F Cleavage by Os(H)3Cl(PiPr3)2. Inorganic Chemistry, 2002, 41, 6440-6449.	4.0	43
59	Comparison of Î± CH and CF activation in alkyl transition metal complexes: a DFT and CASSCF study. Molecular Physics, 2002, 100, 533-540.	1.7	21
60	Geminal dehydrogenation of ether and amine C(sp3)H2 groups by electron-rich Ru(ii) and OsElectronic 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/nj/b2/b200168n/. New Journal of Chemistry, 2002, 26, 687-700.	2.8	57
61	Double Silyl Migration Converting ORe[N(SiMe2CH2PCy2)2] to NRe[O(SiMe2CH2PCy2)2] Substructures. Inorganic Chemistry, 2002, 41, 5615-5625.	4.0	29
62	Unifying the mechanisms for alkane dehydrogenation and alkene H/D exchange with [IrH2(O2CCF3)(PAr3)2]: the key role of CF3CO2 in the â€œstickyâ€™ alkane route. New Journal of Chemistry, 2001, 25, 1121-1131.	2.8	25
63	A comprehensive view of Mâ€“H addition across the RCî€,CH bond: frustration culminating in ultimate union. New Journal of Chemistry, 2001, 25, 1244-1255.	2.8	56
64	A comparative study of olefin or acetylene insertion into RuÃ¢â‚¬â€œH or OsÃ¢â‚¬â€œH of MHCl(CO)(phosphine)2. New Journal of Chemistry, 2001, 25, 1382-1388.	2.8	35
65	Facile C(sp2)/OR Bond Cleavage by Ru or Os. Inorganic Chemistry, 2001, 40, 6610-6621.	4.0	23
66	Coordinated carbenes from electron-rich olefins on RuHCl(PPr3i)2. New Journal of Chemistry, 2000, 24, 9-26.	2.8	87
67	Fate of CH2CHE (E = H, OMe) in the Presence of Unsaturated Ru(X)(H)L2q+(X = Cl,q= 0; X = CO,q= 1):Â Highly Sensitive to X and E. Organometallics, 2000, 19, 2291-2298.	2.3	17
68	Unsaturated Ru(0) Species with a Constrained Bis-Phosphine Ligand:â€‰ [Ru(CO)2(tBu2PCH2CH2PtBu2)]2. Comparison to [Ru(CO)2(PtBu2Me)2]. Inorganic Chemistry, 2000, 39, 3957-3962.	4.0	17
69	Lâ€˜ = CO vs Cl- Transposition:â€‰ Remarkable Consequences for the Product of (Lâ€˜)â^'Ru(L)2â^'(H) and Vinyl Ether. Organometallics, 1999, 18, 5441-5443.	2.3	13
70	Solution and Solid-State Structure of Ru(CO)2(Bu2PtC2H4PtBu2):Â Square Planar and Monomeric?. Journal of the American Chemical Society, 1999, 121, 3242-3243.	13.7	20
71	Carbene Complexes from Olefins, Using RuHCl(PiPr3)2. Influence of the Olefin Substituent. Journal of the American Chemical Society, 1998, 120, 9388-9389.	13.7	49