Christopher M Hadad

List of Publications by Citations

255 papers	8,027 citations	50 h-index	72 g-index
271 ext. papers	8,656 ext. citations	7.2 avg, IF	5.79 L-index

#	Paper	IF	Citations
255	The interplay of theory and experiment in the study of phenylnitrene. *Accounts of Chemical Research*, **2000**, 33, 765-71	24.3	200
254	Analysis of the effect of electron correlation on charge density distributions. *The Journal of Physical Chemistry*, **1992**, 96, 671-679		188
253	Comparison of different atomic charge schemes for predicting pKa variations in substituted anilines and phenols*. *International Journal of Quantum Chemistry*, **2002**, 90, 445-458	2.1	159
252	CH and NH Bond Dissociation Energies of Small Aromatic Hydrocarbons. *Journal of the American Chemical Society*, **1999**, 121, 491-500	16.4	145
251	Electronically excited states of ethylene. *The Journal of Physical Chemistry*, **1992**, 96, 10756-10768		139
250	Electrode-assisted catalytic water oxidation by a flavin derivative. *Nature Chemistry*, **2012**, 4, 794-801	17.6	130
249	Excited states of carbonyl compounds. 1. Formaldehyde and acetaldehyde. *The Journal of Physical Chemistry*, **1993**, 97, 4293-4312		130
248	Dimeric [Mo2 S12](2-) Cluster: A Molecular Analogue of MoS2 Edges for Superior Hydrogen-Evolution Electrocatalysis. *Angewandte Chemie - International Edition*, **2015**, 54, 15181-5	16.4	128
247	Computational analysis of the potential energy surfaces of glycerol in the gas and aqueous phases: effects of level of theory, basis set, and solvation on strongly intramolecularly hydrogen-bonded systems. *Journal of the American Chemical Society*, **2001**, 123, 11743-54	16.4	118
246	Substituent effects. 4. Nature of substituent effects at carbonyl groups. *Journal of the American Chemical Society*, **1992**, 114, 8644-8654	16.4	118
245	Substituent effects on the electronic structure and pKa of benzoic acid. *International Journal of Quantum Chemistry*, **2002**, 90, 1396-1403	2.1	117
244	Early events in the photochemistry of aryl azides from femtosecond UV/Vis spectroscopy and quantum chemical calculations. *Journal of the American Chemical Society*, **2006**, 128, 13402-11	16.4	115
243	Photochemical fate of sulfadimethoxine in aquaculture waters. *Environmental Science & Technology*, **2009**, 43, 8587-92	10.3	112
242	Laser Flash Photolysis and Computational Study of Singlet Phenylnitrene. *Journal of the American Chemical Society*, **1999**, 121, 1202-1207	16.4	109
241	Assignment of the ~A state in bicyclobutane. The multiphoton ionization spectrum and calculations of transition energies. *Journal of the American Chemical Society*, **1991**, 113, 4782-4791	16.4	101
240	The reaction of triplet flavin with indole. A study of the cascade of reactive intermediates using density functional theory and time resolved infrared spectroscopy. *Journal of the American Chemical Society*, **2002**, 124, 7226-34	16.4	98
239	The final catalytic step of cytochrome p450 aromatase: a density functional theory study. *Journal of the American Chemical Society*, **2005**, 127, 5224-37	16.4	97

238	Insights into the structure of cutin and cutan from Agave americana leaf cuticle using HRMAS NMR spectroscopy. *Organic Geochemistry*, **2005**, 36, 1072-1085	3.1	92
237	Hydrogen Migration vs Carbon Migration in Dialkylcarbenes. A Study of the Preferred Product in the Carbene Rearrangements of Ethylmethylcarbene, Cyclobutylidene, 2-Norbornylidene, and 2-Bicyclo[2.1.1]hexylidene. *Journal of the American Chemical Society*, **1997**, 119, 5682-5689	16.4	90
236	Large-scale synthesis of a persistent trityl radical for use in biomedical EPR applications and imaging. *Bioorganic and Medicinal Chemistry Letters*, **2007**, 17, 6801-5	2.9	81
235	On the electrophilicity of hydroxyl radical: a laser flash photolysis and computational study. *Journal of the American Chemical Society*, **2005**, 127, 7094-109	16.4	81
234	A comparison of acetyl- and methoxycarbonylnitrenes by computational methods and a laser flash photolysis study of benzoylnitrene. *Journal of Organic Chemistry*, **2004**, 69, 8583-93	4.2	80
233	Kinetic Study and Theoretical Analysis of Hydroxyl Radical Trapping and Spin Adduct Decay of Alkoxycarbonyl and Dialkoxyphosphoryl Nitrones in Aqueous Media. *Journal of Physical Chemistry A* , **2003**, 107, 4407-4414	2.8	74
232	Electronic properties of 4-substituted naphthalimides. *Journal of Physical Chemistry A*, **2009**, 113, 6453-61	2.8	72
231	Oxalate-bridged complexes of dimolybdenum and ditungsten supported by pivalate ligands: ((t)BuCO(2))(3)M(2)(mu-O(2)CCO(2))M(2)(O(2)C(t)Bu)(3). Correlation of the solid-state, molecular, and electronic structures with Raman, resonance Raman, and electronic spectral data. *Journal of the American Chemical Society*, **2002**, 124, 3050-63	16.4	69
230	Computational study of the electronic structure of substituted phenylcarbene in the gas phase. *Journal of Organic Chemistry*, **2000**, 65, 8348-56	4.2	69
229	Reactivity of superoxide radical anion with cyclic nitrones: role of intramolecular H-bond and electrostatic effects. *Journal of the American Chemical Society*, **2007**, 129, 8177-91	16.4	68
228	A laser flash photolysis and quantum chemical study of the fluorinated derivatives of singlet phenylnitrene. *Journal of the American Chemical Society*, **2001**, 123, 1951-62	16.4	68
227	Gated molecular baskets. *Chemical Society Reviews*, **2015**, 44, 500-14	58.5	66
226	A Mechanistic Study of the Reactions of H, O (3P), and OH with Monocyclic Aromatic Hydrocarbons by Density Functional Theory. *Journal of Physical Chemistry A*, **2001**, 105, 140-152	2.8	65
225	Theoretical and experimental studies of the spin trapping of inorganic radicals by 5,5-dimethyl-1-pyrroline N-oxide (DMPO). 1. Carbon dioxide radical anion. *Journal of Physical Chemistry A*, **2006**, 110, 13253-8	2.8	64
224	Theoretical and experimental studies of the spin trapping of inorganic radicals by 5,5-dimethyl-1-pyrroline N-oxide (DMPO). 2. Carbonate radical anion. *Journal of Physical Chemistry A*, **2007**, 111, 384-91	2.8	63
223	Design, synthesis, and conformational dynamics of a gated molecular basket. *Journal of the American Chemical Society*, **2006**, 128, 5887-94	16.4	62
222	Adsorption/Desorption Behavior of Ethanol Steam Reforming Reactants and Intermediates over Supported Cobalt Catalysts. *Catalysis Letters*, **2011**, 141, 43-54	2.8	60
221	Computational Study of the Unimolecular Decomposition Pathways of Phenylperoxy Radical. *Journal of Physical Chemistry A*, **2000**, 104, 3004-3011	2.8	59

220	Computational Study of the Mechanisms for the Reaction of O2(3Σg) with Aromatic Radicals. *Journal of Physical Chemistry A*, **1999**, 103, 8108-8117	2.8	57
219	Assembly of amphiphilic baskets into stimuli-responsive vesicles. Developing a strategy for the detection of organophosphorus chemical nerve agents. *Journal of the American Chemical Society*, **2013**, 135, 14964-7	16.4	55
218	The fragmentation pathways of protonated glycine: a computational study. *Journal of the American Society for Mass Spectrometry*, **2000**, 11, 687-96	3.5	55
217	Photoaffinity labeling via nitrenium ion chemistry: protonation of the nitrene derived from 4-amino-3-nitrophenyl azide to afford reactive nitrenium ion pairs. *Journal of the American Chemical Society*, **2009**, 131, 11535-47	16.4	54
216	Synthesis and characterization of amino derivatives of persistent trityl radicals as dual function pH and oxygen paramagnetic probes. *Journal of the American Chemical Society*, **2008**, 130, 10780-7	16.4	53
215	Superoxide radical anion adduct of 5,5-dimethyl-1-pyrroline N-oxide (DMPO). 2. The thermodynamics of decay and EPR spectral properties. *Journal of Physical Chemistry A*, **2005**, 109, 6089-98	2.8	53
214	Surface complexes of phthalic acid at the hematite/water interface. *Journal of Colloid and Interface Science*, **2007**, 307, 124-34	9.3	52
213	Spin trapping by 5-carbamoyl-5-methyl-1-pyrroline N-oxide (AMPO): theoretical and experimental studies. *Journal of Organic Chemistry*, **2004**, 69, 7994-8004	4.2	52
212	The Photochemistry of Riboflavin Tetraacetate and Nucleosides. A Study Using Density Functional Theory, Laser Flash Photolysis, Fluorescence, UV−Vis, and Time Resolved Infrared Spectroscopy. *Journal of Physical Chemistry B*, **2002**, 106, 10263-10271	3.4	52
211	Butadiene. 3. Charge distribution in electronically excited states. *The Journal of Physical Chemistry*, **1993**, 97, 13586-13597		52
210	A First-Principles Study of the Role of Quaternary-N Doping on the Oxygen Reduction Reaction Activity and Selectivity of Graphene Edge Sites. *Topics in Catalysis*, **2013**, 56, 1623-1633	2.3	51
209	A double-acceptor as a superior organic dye design for p-type DSSCs: high photocurrents and the observed light soaking effect. *Physical Chemistry Chemical Physics*, **2014**, 16, 26103-11	3.6	50
208	Septanose carbohydrates: synthesis and conformational studies of methyl alpha-D-glycero-D-idoseptanoside and methyl beta-D-glycero-D-guloseptanoside. *Journal of Organic Chemistry*, **2005**, 70, 24-38	4.2	50
207	Theoretical study of the spin trapping of hydroxyl radical by cyclic nitrones: a density functional theory approach. *Journal of the American Chemical Society*, **2004**, 126, 1816-29	16.4	50
206	Perfluoroterephthalate bridged complexes with M-M quadruple bonds: ((t)BuCO(2))(3)M(2)(mu-O(2)CC(6)F(4)CO(2))M(2)(O(2)C(t)Bu)(3), where M = Mo or W. Studies of solid-state, molecular, and electronic structure and correlations with electronic and Raman spectral data. *Journal of the American Chemical Society*, **2002**, 124, 12244-54	16.4	50
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203	Photoelectron spectroscopy of HCCN− and HCNC− reveals the quasilinear triplet carbenes, HCCN and HCNC. *Journal of Chemical Physics*, **2002**, 117, 4323-4339	3.9	49

202	Photomodulated chiral induction in helical azobenzene oligomers. *Organic Letters*, **2008**, 10, 1671-4	6.2	48
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199	A computational study of the ground and excited state structure and absorption spectra of free-base N-confused porphine and free-base N-confused tetraphenylporphyrin. *Journal of Physical Chemistry A*, **2008**, 112, 6533-49	2.8	44
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193	Synthesis of L-daunosamine and L-ristosamine glycosides via photoinduced aziridination. Conversion to thioglycosides for use in glycosylation reactions. *Journal of Organic Chemistry*, **2006**, 71, 8059-70	4.2	40
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190	Spectroscopic and computational studies of aqueous ethylene glycol solution surfaces. *Journal of Physical Chemistry B*, **2005**, 109, 811-8	3.4	39
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187	Gated molecular recognition and dynamic discrimination of guests. *Journal of the American Chemical Society*, **2010**, 132, 773-6	16.4	37
186	Competition between alpha-cleavage and energy transfer in alpha-azidoacetophenones. *Journal of Organic Chemistry*, **2007**, 72, 2757-68	4.2	37
185	A 3-fold "butterfly valve" in command of the encapsulation's kinetic stability. Molecular baskets at work. *Journal of the American Chemical Society*, **2008**, 130, 15127-33	16.4	36

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176	The reaction of triplet nitrenes with oxygen: a computational study. *Organic Letters*, **2005**, 7, 549-52	6.2	34
175	Reactivity of molecular oxygen with ethoxycarbonyl derivatives of tetrathiatriarylmethyl radicals. *Journal of Organic Chemistry*, **2006**, 71, 7268-79	4.2	34
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171	Observation of the A-X electronic transition of the 1-C3H7O2 and 2-C3H7O2 radicals using cavity ringdown spectroscopy. *Journal of Physical Chemistry A*, **2005**, 109, 1308-15	2.8	33
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162	Structures and energies of ions derived from bicyclo[1.1.1]pentane. *Journal of the American Chemical Society*, **1992**, 114, 5820-5828	16.4	31
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151	Rate constants of hydroperoxyl radical addition to cyclic nitrones: a DFT study. *Journal of Physical Chemistry A*, **2007**, 111, 9995-10001	2.8	29
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148	Ultrafast spectroscopy and computational study of the photochemistry of diphenylphosphoryl azide: direct spectroscopic observation of a singlet phosphorylnitrene. *Journal of the American Chemical Society*, **2010**, 132, 16796-804	16.4	27
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