Craig A Bayse

List of Publications by Year
in descending order

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		186209	289141
89	2,050	28	40
papers	citations	h-index	g-index

90	90	90	2405
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular Dynamics Simulations of Reduced and Oxidized TFIIIA Zinc Fingers Free and Interacting with 5S RNA. Journal of Chemical Information and Modeling, 2022, , .	2.5	3
2	Trigger bond analysis of azoâ€based energetic materials. Journal of Physical Organic Chemistry, 2022, 35, .	0.9	0
3	In silico insights into the dimer structure and deiodinase activity of type III iodothyronine deiodinase from bioinformatics, molecular dynamics simulations, and QM/MM calculations. Journal of Biomolecular Structure and Dynamics, 2022, , 1-11.	2.0	0
4	Halogen Bonding Interactions of Polychlorinated Biphenyls and the Potential for Thyroid Disruption. Chemistry - A European Journal, 2020, 26, 5200-5207.	1.7	15
5	Zinc(II) thione and selone complexes: The effect of metal redox activity on ligand-based oxidation. Inorganica Chimica Acta, 2020, 502, 119379.	1.2	4
6	Frontispiece: Halogen Bonding Interactions of Polychlorinated Biphenyls and the Potential for Thyroid Disruption. Chemistry - A European Journal, 2020, 26, .	1.7	0
7	Thyroxine binding to type III iodothyronine deiodinase. Scientific Reports, 2020, 10, 15401.	1.6	14
8	N-substituted 2-pyridinecarbothioamides and polypyridyl mixed-ligand cobalt(III)-containing complexes for photocatalytic hydrogen generation. Inorganica Chimica Acta, 2020, 510, 119726.	1.2	4
9	A Halogen Bonding Perspective on Iodothyronine Deiodinase Activity. Molecules, 2020, 25, 1328.	1.7	17
10	Examination of the composition and mechanism of discoloration of the fugitive pigment copper resinate. Inorganica Chimica Acta, 2020, 504, 119407.	1.2	2
11	Bonding analysis of the effect of strain on trigger bonds in organic-cage energetic materials. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	9
12	The effect of nitro groups on N2 extrusion from aromatic azide-based energetic materials. New Journal of Chemistry, 2019, 43, 15326-15334.	1.4	12
13	Conformation dynamics of cyclic disulfides and selenosulfides in CXXC(U) (XÂ=ÂGly, Ala) tetrapeptide redox motifs. Journal of Peptide Science, 2019, 25, e3160.	0.8	1
14	DFT modeling of the prevention of Fe(II)-mediated redox damage by imidazole-based thiones and selones. Journal of Inorganic Biochemistry, 2019, 193, 9-14.	1.5	9
15	Trigger bond analysis of nitroaromatic energetic materials using wiberg bond indices. Journal of Computational Chemistry, 2018, 39, 1236-1248.	1.5	38
16	Halogen bonding from the bonding perspective with considerations for mechanisms of thyroid hormone activation and inhibition. New Journal of Chemistry, 2018, 42, 10623-10632.	1.4	28
17	Interpreting geometric preferences in Ï€â€stacking interactions through molecular orbital analysis. International Journal of Quantum Chemistry, 2018, 118, e25513.	1.0	6
18	Halogenâ€Bonding Interactions of Polybrominated Diphenyl Ethers and Thyroid Hormone Derivatives: A Potential Mechanism for the Inhibition of Iodothyronine Deiodinase. Chemistry - A European Journal, 2017, 23, 6625-6633.	1.7	21

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19	Enhancement of the physicochemical properties of [Pt(dien)(nucleobase)]2+ for HIVNCp7 targeting. Chemical Science, 2017, 8, 1269-1281.	3.7	15
20	Computational, electrochemical, and spectroscopic studies of two mononuclear cobaloximes: the influence of an axial pyridine and solvent on the redox behaviour and evidence for pyridine coordination to cobalt(<scp>i</scp>) and cobalt(<scp>ii</scp>) metal centres. Dalton Transactions, 2016, 45, 10326-10342.	1.6	29
21	Chalcogen bonding interactions between reducible sulfur and selenium compounds and models of zinc finger proteins. Journal of Inorganic Biochemistry, 2016, 157, 94-103.	1.5	12
22	TD-DFT and structural investigation of natural photosensitive phenanthroperylene quinone derivatives. New Journal of Chemistry, 2016, 40, 413-422.	1.4	10
23	Synthesis, characterization, DFT calculations, and electrochemical comparison of novel iron(<scp>ii</scp>) complexes with thione and selone ligands. Dalton Transactions, 2016, 45, 4697-4711.	1.6	37
24	Metal Ion Capture Mechanism of a Copper Metallochaperone. Biochemistry, 2016, 55, 501-509.	1.2	9
25	Predicting Trigger Bonds in Explosive Materials through Wiberg Bond Index Analysis. ChemPhysChem, 2015, 16, 3886-3892.	1.0	51
26	Effect of Methoxy Substituents on the Activation Barriers of the Glutathione Peroxidase-Like Mechanism of an Aromatic Cyclic Seleninate. Molecules, 2015, 20, 10244-10252.	1.7	7
27	Sulfur and selenium antioxidants: Challenging radical scavenging mechanisms and developing structureâ€“activity relationships based on metal binding. Journal of Inorganic Biochemistry, 2015, 145, 30-40.	1.5	100
28	Modeling the chelation of As(III) in lewisite by dithiols using density functional theory and solvent-assisted proton exchange. Journal of Inorganic Biochemistry, 2015, 153, 60-67.	1.5	8
29	Redox active motifs in selenoproteins. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 6976-6981.	3.3	54
30	Thiol Reduction of Arsenite and Selenite: DFT Modeling of the Pathways to an Asâ€“Se Bond. Chemical Research in Toxicology, 2014, 27, 2119-2127.	1.7	5
31	Modulation of the stacking interaction of MN4 (M=Pt, Pd, Au) complexes with tryptophan through N-heterocyclic ligands. Journal of Inorganic Biochemistry, 2014, 132, 2-5.	1.5	11
32	Theoretical insights into the effect of amine and phosphine decoration on the photoluminescence of copper(i) and silver(i) coordination polymers. Dalton Transactions, 2014, 43, 11243-11251.	1.6	2
33	Mechanistic Insights into Mg2+-Independent Prenylation by CloQ from Classical Molecular Mechanics and Hybrid Quantum Mechanics/Molecular Mechanics Molecular Dynamics Simulations. Biochemistry, 2014, 53, 5034-5041.	1.2	9
34	Ruthenium(II) Dichloride Complexes of Chiral, Tetradentate Aminosulfoxide Ligands: Stereoisomerism and Redox-Induced Linkage Isomerism. Inorganic Chemistry, 2013, 52, 1170-1172.	1.9	8
35	Oxidation of Biologically Relevant Chalcogenones and Their Cu(I) Complexes: Insight into Selenium and Sulfur Antioxidant Activity. Inorganic Chemistry, 2013, 52, 11685-11687.	1.9	28
36	Orbital-based insights into parallel-displaced and twisted conformations in Ï€â€“Ï€ interactions. Physical Chemistry Chemical Physics, 2013, 15, 9397.	1.3	19

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37	Density Functional Theory Study of the Attack of Ebselen on a Zinc-Finger Model. Inorganic Chemistry, 2013, 52, 13803-13805.	1.9	13
38	Modeling of Mechanisms of Selenium Bioactivity Using Density Functional Theory. ACS Symposium Series, 2013, , 179-200.	0.5	2
39	Modeling the Glutathione Peroxidase-Like Activity of a Cyclic Seleninate by DFT and Solvent-Assisted Proton Exchange. European Journal of Inorganic Chemistry, 2013, 2013, 3680-3688.	1.0	16
40	Oxidation of Zinc-Sulfur Centers by Reducible Organoselenium Compounds: A Review and Bonding Perspective. Current Chemical Biology, 2013, 7, 57-64.	0.2	7
41	Complementary SeleniumÂ·Â·Â·Iodine Halogen Bonding and Phenyl Embraces: Cocrystals of Triphenylphosphine Selenide with Organoiodides. Crystal Growth and Design, 2012, 12, 4315-4323.	1.4	45
42	Platinumâ€“nucleobase PtN4 complexes as chemotypes for selective peptide reactions with biomolecules. Inorganica Chimica Acta, 2012, 393, 222-229.	1.2	10
43	Network formation and photoluminescence in copper(i) halide complexes with substituted piperazine ligands. Dalton Transactions, 2012, 41, 11663.	1.6	65
44	Transition states for cysteine redox processes modeled by DFT and solvent-assisted proton exchange. Organic and Biomolecular Chemistry, 2011, 9, 4748.	1.5	36
45	Synthesis, characterization, and DFT studies of thione and selone Cu(i) complexes with variable coordination geometries. Dalton Transactions, 2011, 40, 3711.	1.6	58
46	Interactions of Cu(I) with Selenium-Containing Amino Acids Determined by NMR, XAS, and DFT Studies. Inorganic Chemistry, 2011, 50, 10893-10900.	1.9	15
47	Tuning the activity of glutathione peroxidase mimics through intramolecular Seâ‹¯N,O interactions: A DFT study incorporating solvent-assisted proton exchange (SAPE). Organic and Biomolecular Chemistry, 2011, 9, 8006.	1.5	20
48	Photoluminescence of silver(I) and gold(I) cyanide 1D coordination polymers. Inorganica Chimica Acta, 2011, 375, 47-52.	1.2	21
49	Modeling the Mechanism of the Glutathione Peroxidase Mimic Ebselen. Inorganic Chemistry, 2011, 50, 12075-12084.	1.9	81
50	Syntheses, 95Mo NMR Spectroscopy and Structures of Distorted Cubic Mo4(Î¼3-O)4(Î¼2-O2P(CH2C6H5)2)4O4 and the Open Mixed-Valent Cluster, Mo4(Î¼3-O)2(Î¼2-O2P(CH2C6H5)2)4O6. Journal of Cluster Science, 2011, 22, 193-210.	2.7	10
51	Model mechanisms of sulfhydryl oxidation by methyl- and benzeneseleninic acid, inhibitors of zinc-finger transcription factors. Journal of Inorganic Biochemistry, 2010, 104, 1-8.	1.5	12
52	Structure and luminescence of copper(I) cyanideâ€“amine and â€“sulfide networks. Inorganica Chimica Acta, 2010, 364, 102-114.	1.2	36
53	Is Halogen Bonding the Basis for Iodothyronine Deiodinase Activity?. Inorganic Chemistry, 2010, 49, 5365-5367.	1.9	76
54	Theoretical Studies of [2,3]-Sigmatropic Rearrangements of Allylic Selenoxides and Selenimides. Molecules, 2009, 14, 3229-3236.	1.7	5

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55	Theoretical Studies of Models of the Active Site of the Tungstoenzyme Acetylene Hydratase. Organometallics, 2009, 28, 4938-4944.	1.1	38
56	Photoluminescence of 1-D Copper(I) Cyanide Chains: A Theoretical Description. Inorganic Chemistry, 2009, 48, 174-182.	1.9	45
57	Modeling the Oxidation of Ebselen and Other Organoselenium Compounds Using Explicit Solvent Networks. Journal of Physical Chemistry A, 2009, 113, 5780-5785.	1.1	20
58	Density-functional theory models of xanthine oxidoreductase activity: comparison of substrate tautomerization and protonation. Dalton Transactions, 2009, , 2306.	1.6	21
59	Rational Synthesis of Molybdenum(V) Tetramers Consisting of [Mo2O4]2+ Dimers Held Together by Bridging Phosphinate Ligands and the Tungsten(VI) Dimer [(CH3O)2(O)W(Î¼-O)(Î¼-O2PPh2)2W(O)(CH3O)2]: Structural and Theoretical Considerations. Journal of Cluster Science, 2008, 19, 181-195.	1.7	15
60	The Lewis acidity of bismuth(III) halides: a DFT analysis. Tetrahedron, 2008, 64, 7685-7689.	1.0	37
61	Effects of Nucleobase Metalation on Frontier Molecular Orbitals: Potential Implications for Ï€-Stacking Interactions with Tryptophan. Inorganic Chemistry, 2008, 47, 10425-10431.	1.9	35
62	Molecular modeling of bioactive selenium compounds. Main Group Chemistry, 2007, 6, 185-200.	0.4	26
63	Experimental and Theoretical Studies of the Reactions Y (a²D) + H₂CO and Y (a²D) + CH₃CHO. Journal of Physical Chemistry A, 2007, 111, 11421-11429.	1.1	17
64	Calculation of Photoelectron Spectra of Molybdenum and Tungsten Complexes Using Green's Functions Methods. Journal of Physical Chemistry A, 2007, 111, 7841-7847.	1.1	6
65	DFT Study of the Glutathione Peroxidase-Like Activity of Phenylselenol Incorporating Solvent-Assisted Proton Exchange. Journal of Physical Chemistry A, 2007, 111, 9070-9075.	1.1	38
66	Theoretical Characterization of the â€œVery Rapidâ€•Mo(V) Species Generated in the Oxidation of Xanthine Oxidase. Inorganic Chemistry, 2006, 45, 2199-2202.	1.9	10
67	Activation energies of selenoxide elimination from Se-substituted selenocysteine. Journal of Molecular Modeling, 2006, 13, 47-53.	0.8	20
68	Relative strengths of Seâ‹¯N,O interactions: Implications for glutathione peroxidase activity. Inorganica Chimica Acta, 2005, 358, 3849-3854.	1.2	39
69	Reexamination of the structure of MoO(O2)2(H2O)(hmpa), hmpa=hexamethylphosphoramide by crystallographic and theoretical means. Journal of Molecular Structure, 2005, 754, 96-99.	1.8	4
70	Considerations for Reliable Calculation of77Se Chemical Shifts. Journal of Chemical Theory and Computation, 2005, 1, 1119-1127.	2.3	32
71	Experimental and theoretical evidence for cyclic selenurane formation during selenomethionine oxidation. Organic and Biomolecular Chemistry, 2005, 3, 4337.	1.5	37
72	The Theoretical77Se Chemical Shift as a Probe of Selenium State in Selenoproteins and Their Mimics. Inorganic Chemistry, 2004, 43, 1208-1210.	1.9	52

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73	ROOM-TEMPERATURE REDUCTIVE DIALKYLATION OF DIETHYL NAPHTHALENEDICARBOXYLATE. Synthetic Communications, 2002, 32, 2705-2709.	1.1	1
74	Theoretical Study of the Reaction of Yttrium with Formaldehyde. Journal of Physical Chemistry A, 2002, 106, 4226-4229.	1.1	27
75	Synthesis and Characterization of ReCl(H2)(AsMePh2)4, a Classical Hydride Complex; Reexamination of ReCl(H2)(PMePh2)4and Theoretical Calculations on Model Compounds. Inorganic Chemistry, 2001, 40, 3463-3467.	1.9	17
76	Interaction of Dihydrogen with Gold (I) Hydride:Â Prospects for Matrix-Isolation Studies. Journal of Physical Chemistry A, 2001, 105, 5902-5905.	1.1	20
77	meso-1,2-Bis(methylazo)-1,2-diphenylethane. Acta Crystallographica Section C: Crystal Structure Communications, 2001, 57, 1429-1430.	0.4	1
78	Determination of copper binding sites in peptides containing basic residues: a combined experimental and theoretical study. International Journal of Mass Spectrometry, 2001, 204, 31-46.	0.7	42
79	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms 13: Methane, Ethylene, and Acetylene Activation at a Cationic Iridium Center. ACS Symposium Series, 1999, , 138-150.	0.5	6
80	Prediction of the Geometries of Simple Transition Metal Polyhydride Complexes by Symmetry Analysis. Journal of the American Chemical Society, 1999, 121, 1348-1358.	6.6	79
81	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms. 14. Î²-Hydrogen Transfer and Alkene/Alkyne Insertion at a Cationic Iridium Center. Organometallics, 1998, 17, 5139-5147.	1.1	29
82	Transition Metal Polyhydride Complexes. 9. The Effect of Ligand Ïƒ- and Ï€-Bonding on the Hâˆ’Taâˆ’H Bond Angle in Six-Coordinate Tantalum(V) Dihydride Complexes. Organometallics, 1998, 17, 4861-4868.	1.1	14
83	Experimental and Theoretical Studies of Nonclassical d0Cyclopentadienyl Polyhydride Complexes of Molybdenum and Tungsten. Organometallics, 1998, 17, 4309-4315.	1.1	31
84	Synthesis, Structure, and Hydrideâˆ’Deuteride Exchange Studies of CpMoH3(PMe2Ph)2and Theoretical Studies of the CpMoH3(PMe3)2Model System. Organometallics, 1997, 16, 1179-1185.	1.1	21
85	Pseudo second-order Jahn-Teller effects and symmetry considerations in transition metal polyhydride complexes. Inorganica Chimica Acta, 1997, 259, 179-184.	1.2	15
86	Extremely localized molecular orbitals (ELMO): a non-orthogonal Hartree-Fock method. Theoretical Chemistry Accounts, 1997, 97, 96-109.	0.5	30
87	Transition Metal Polyhydride Complexes. 8. Pentahydrido(cyclopentadienyl)osmium(VI). Journal of the American Chemical Society, 1996, 118, 8916-8919.	6.6	32
88	Controversial Exothermicity of the Oxidative Addition of Methane to (Cyclopentadienyl)rhodium Carbonyl. The Journal of Physical Chemistry, 1996, 100, 13976-13978.	2.9	31
89	Toward the Generation of NO in Biological Systems Theoretical Studies of the N2O2 Grouping. Journal of Organic Chemistry, 1995, 60, 435-444.	1.7	37