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	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
2	Modeling the Mechanism of the Glutathione Peroxidase Mimic Ebselen. Inorganic Chemistry, 2011, 50, 12075-12084.	1.9	81
3	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
4	Is Halogen Bonding the Basis for Iodothyronine Deiodinase Activity?. Inorganic Chemistry, 2010, 49, 5365-5367.	1.9	76
5	Network formation and photoluminescence in copper(i) halide complexes with substituted piperazine ligands. Dalton Transactions, 2012, 41, 11663.	1.6	65
6	Synthesis, characterization, and DFT studies of thione and selone Cu(i) complexes with variable coordination geometries. Dalton Transactions, 2011, 40, 3711.	1.6	58
7	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
8	The Theoretical77Se Chemical Shift as a Probe of Selenium State in Selenoproteins and Their Mimics. Inorganic Chemistry, 2004, 43, 1208-1210.	1.9	52
9	Predicting Trigger Bonds in Explosive Materials through Wiberg Bond Index Analysis. ChemPhysChem, 2015, 16, 3886-3892.	1.0	51
10	Photoluminescence of 1-D Copper(I) Cyanide Chains: A Theoretical Description. Inorganic Chemistry, 2009, 48, 174-182.	1.9	45
11	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
12	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
13	Relative strengths of Seâ‹¯N,O interactions: Implications for glutathione peroxidase activity. Inorganica Chimica Acta, 2005, 358, 3849-3854.	1.2	39
14	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
15	Theoretical Studies of Models of the Active Site of the Tungstoenzyme Acetylene Hydratase. Organometallics, 2009, 28, 4938-4944.	1.1	38
16	Trigger bond analysis of nitroaromatic energetic materials using wiberg bond indices. Journal of Computational Chemistry, 2018, 39, 1236-1248.	1.5	38
17	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
18	Experimental and theoretical evidence for cyclic selenurane formation during selenomethionine oxidation. Organic and Biomolecular Chemistry, 2005, 3, 4337.	1.5	37

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19	The Lewis acidity of bismuth(III) halides: a DFT analysis. Tetrahedron, 2008, 64, 7685-7689.	1.0	37
20	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
21	Structure and luminescence of copper(I) cyanideâ€“amine and â€“sulfide networks. Inorganica Chimica Acta, 2010, 364, 102-114.	1.2	36
22	Transition states for cysteine redox processes modeled by DFT and solvent-assisted proton exchange. Organic and Biomolecular Chemistry, 2011, 9, 4748.	1.5	36
23	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
24	Transition Metal Polyhydride Complexes. 8. Pentahydrido(cyclopentadienyl)osmium(VI). Journal of the American Chemical Society, 1996, 118, 8916-8919.	6.6	32
25	Considerations for Reliable Calculation of77Se Chemical Shifts. Journal of Chemical Theory and Computation, 2005, 1, 1119-1127.	2.3	32
26	Controversial Exothermicity of the Oxidative Addition of Methane to (Cyclopentadienyl)rhodium Carbonyl. The Journal of Physical Chemistry, 1996, 100, 13976-13978.	2.9	31
27	Experimental and Theoretical Studies of Nonclassical d0Cyclopentadienyl Polyhydride Complexes of Molybdenum and Tungsten. Organometallics, 1998, 17, 4309-4315.	1.1	31
28	Extremely localized molecular orbitals (ELMO): a non-orthogonal Hartree-Fock method. Theoretical Chemistry Accounts, 1997, 97, 96-109.	0.5	30
29	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
30	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
31	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
32	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
33	Theoretical Study of the Reaction of Yttrium with Formaldehyde. Journal of Physical Chemistry A, 2002, 106, 4226-4229.	1.1	27
34	Molecular modeling of bioactive selenium compounds. Main Group Chemistry, 2007, 6, 185-200.	0.4	26
35	Synthesis, Structure, and Hydrideâ^'Deuteride Exchange Studies of CpMoH3(PMe2Ph)2and Theoretical Studies of the CpMoH3(PMe3)2Model System. Organometallics, 1997, 16, 1179-1185.	1.1	21
36	Density-functional theory models of xanthine oxidoreductase activity: comparison of substrate tautomerization and protonation. Dalton Transactions, 2009, , 2306.	1.6	21

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37	Photoluminescence of silver(I) and gold(I) cyanide 1D coordination polymers. Inorganica Chimica Acta, 2011, 375, 47-52.	1.2	21
38	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
39	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
40	Activation energies of selenoxide elimination from Se-substituted selenocysteine. Journal of Molecular Modeling, 2006, 13, 47-53.	0.8	20
41	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
42	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
43	Orbital-based insights into parallel-displaced and twisted conformations in Ï€â€“Ï€ interactions. Physical Chemistry Chemical Physics, 2013, 15, 9397.	1.3	19
44	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
45	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
46	A Halogen Bonding Perspective on Iodothyronine Deiodinase Activity. Molecules, 2020, 25, 1328.	1.7	17
47	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
48	Pseudo second-order Jahn-Teller effects and symmetry considerations in transition metal polyhydride complexes. Inorganica Chimica Acta, 1997, 259, 179-184.	1.2	15
49	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
50	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
51	Enhancement of the physicochemical properties of [Pt(dien)(nucleobase)]2+ for HIVNCp7 targeting. Chemical Science, 2017, 8, 1269-1281.	3.7	15
52	Halogen Bonding Interactions of Polychlorinated Biphenyls and the Potential for Thyroid Disruption. Chemistry - A European Journal, 2020, 26, 5200-5207.	1.7	15
53	Transition Metal Polyhydride Complexes. 9. The Effect of Ligand Ïƒ- and Ï€-Bonding on the Hâ^'Taâ^'H Bond Angle in Six-Coordinate Tantalum(V) Dihydride Complexes. Organometallics, 1998, 17, 4861-4868.	1.1	14
54	Thyroxine binding to type III iodothyronine deiodinase. Scientific Reports, 2020, 10, 15401.	1.6	14

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55	Density Functional Theory Study of the Attack of Ebselen on a Zinc-Finger Model. Inorganic Chemistry, 2013, 52, 13803-13805.	1.9	13
56	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
57	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
58	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
59	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
60	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
61	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.	1.2	10
62	Platinumâ€“nucleobase PtN4 complexes as chemotypes for selective peptide reactions with biomolecules. Inorganica Chimica Acta, 2012, 393, 222-229.	1.2	10
63	TD-DFT and structural investigation of natural photosensitive phenanthroperylene quinone derivatives. New Journal of Chemistry, 2016, 40, 413-422.	1.4	10
64	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
65	Metal Ion Capture Mechanism of a Copper Metallochaperone. Biochemistry, 2016, 55, 501-509.	1.2	9
66	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
67	Bonding analysis of the effect of strain on trigger bonds in organic-cage energetic materials. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	9
68	Ruthenium(II) Dichloride Complexes of Chiral, Tetradentate Aminosulfoxide Ligands: Stereoisomerism and Redox-Induced Linkage Isomerism. Inorganic Chemistry, 2013, 52, 1170-1172.	1.9	8
69	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
70	Oxidation of Zinc-Sulfur Centers by Reducible Organoselenium Compounds: A Review and Bonding Perspective. Current Chemical Biology, 2013, 7, 57-64.	0.2	7
71	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
72	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

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73	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
74	Interpreting geometric preferences in Ï€â€¢stacking interactions through molecular orbital analysis. International Journal of Quantum Chemistry, 2018, 118, e25513.	1.0	6
75	Theoretical Studies of [2,3]-Sigmatropic Rearrangements of Allylic Selenoxides and Selenimides. Molecules, 2009, 14, 3229-3236.	1.7	5
76	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
77	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
78	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
79	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
80	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
81	Modeling of Mechanisms of Selenium Bioactivity Using Density Functional Theory. ACS Symposium Series, 2013, , 179-200.	0.5	2
82	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
83	Examination of the composition and mechanism of discoloration of the fugitive pigment copper resinate. Inorganica Chimica Acta, 2020, 504, 119407.	1.2	2
84	meso-1,2-Bis(methylazo)-1,2-diphenylethane. Acta Crystallographica Section C: Crystal Structure Communications, 2001, 57, 1429-1430.	0.4	1
85	ROOM-TEMPERATURE REDUCTIVE DIALKYLATION OF DIETHYL NAPHTHALENEDICARBOXYLATE. Synthetic Communications, 2002, 32, 2705-2709.	1.1	1
86	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
87	Frontispiece: Halogen Bonding Interactions of Polychlorinated Biphenyls and the Potential for Thyroid Disruption. Chemistry - A European Journal, 2020, 26, .	1.7	0
88	Trigger bond analysis of azoâ€based energetic materials. Journal of Physical Organic Chemistry, 2022, 35, .	0.9	0
89	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