Nikolas Kaltsoyannis

List of Publications by Year
in descending order

203	8,511	38660 50	58464 82
papers	citations	h-index	g-index

219	219	219	5010
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A Stable Two-Coordinate Acyclic Silylene. Journal of the American Chemical Society, 2012, 134, 6500-6503.	6.6	387
2	Does Covalency Increase or Decrease across the Actinide Series? Implications for Minor Actinide Partitioning. Inorganic Chemistry, 2013, 52, 3407-3413.	1.9	285
3	Small Molecule Activation by Uranium Tris(aryloxides): Experimental and Computational Studies of Binding of N₂, Coupling of CO, and Deoxygenation Insertion of CO₂under Ambient Conditions. Journal of the American Chemical Society, 2011, 133, 9036-9051.	6.6	218
4	Recent developments in computational actinide chemistry. Chemical Society Reviews, 2003, 32, 9-16.	18.7	209
5	Structure, Reactivity, and Density Functional Theory Analysis of the Six-Electron Reductant, [(C5Me5)2U]2(Î¼-Î·6:Î·6-C6H6), Synthesized via a New Mode of (C5Me5)3M Reactivity. Journal of the American Chemical Society, 2004, 126, 14533-14547.	6.6	206
6	Multinuclear NMR, Raman, EXAFS, and X-ray diffraction studies of uranyl carbonate complexes in near-neutral aqueous solution. X-ray structure of [C(NH2)3]6[(UO2)3(CO3)6].cntdot.6.5H2O. Inorganic Chemistry, 1995, 34, 4797-4807.	1.9	199
7	Experimental and Theoretical Comparison of Actinide and Lanthanide Bonding in M[N(EPR₂)₂]₃ Complexes (M = U, Pu, La, Ce; E = S, Se, Te; R = Ph,) Tj ETQq1 1 0.784314 rgBT /Overlock 10	1.1	174
8	Covalency in AnCp4 (An = Thâ€“Cm): a comparison of molecular orbital, natural population and atoms-in-molecules analyses. Dalton Transactions, 2010, 39, 6719.	1.6	153
9	Does covalency really increase across the 5f series? A comparison of molecular orbital, natural population, spin and electron density analyses of AnCp₃(An = Thâ€“Cm; Cp =) Tj ETQq1 1 0.784314 rgBT /Overlock 10	1.1	150
10	Uncovering f-element bonding differences and electronic structure in a series of 1â€‰:â€‰3 and 1â€‰:â€‰4 complexes with a diselenophosphinate ligand. Chemical Science, 2013, 4, 1189.	3.7	146
11	A Generic Oneâ€Pot Route to Acyclic Twoâ€Coordinate Silylenes from Silicon(IV) Precursors: Synthesis and Structural Characterization of a Silylsilylene. Angewandte Chemie - International Edition, 2013, 52, 568-571.	7.2	138
12	Covalency in Ce^{IV} and U^{IV} Halide and Nâ€Heterocyclic Carbene Bonds. Chemistry - A European Journal, 2010, 16, 9623-9629.	1.7	137
13	Relativistic effects in inorganic and organometallic chemistry. Journal of the Chemical Society Dalton Transactions, 1997, , 1-12.	1.1	129
14	Does metallophilicity increase or decrease down group 11? Computational investigations of [Clâ€“Mâ€“PH3]2(Mâ€‰=â€‰Cu, Ag, Au, [111]). Physical Chemistry Chemical Physics, 2004, 6, 680-687.	1.3	116
15	Trivalent [(C5Me5)2(THF)Ln]2(Î¼-Î·2:Î·2-N2) Complexes as Reducing Agents Including the Reductive Homologation of CO to a Ketene Carboxylate, (Î¼-Î·4-O2CCCO)2-. Journal of the American Chemical Society, 2006, 128, 14176-14184.	6.6	113
16	Synthesis, Molecular and Electronic Structure of U^V(O)[N(SiMe₃)₂]₃. Inorganic Chemistry, 2012, 51, 1625-1633.	1.9	109
17	High Uptake of ReO₄^{â^’} and CO₂ Conversion by a Radiationâ€Resistant Thoriumâ€“Nickle [Th₄₈Ni₆] Nanocageâ€Based Metalâ€“Organic Framework. Angewandte Chemie - International Edition, 2019, 58, 6022-6027.	7.2	109
18	Energy-Degeneracy-Driven Covalency in Actinide Bonding. Journal of the American Chemical Society, 2018, 140, 17977-17984.	6.6	108

#	Article	IF	Citations
19	Covalency in the f Elementâ^'Chalcogen Bond. Computational Studies of M[N(EPR₂)₂]₃ (M = La, Ce, Pr, Pm, Eu, U, Np, Pu, Am, Cm; E = O, S, Se,) Tj ETQq1 1 0.784314	1.9	104
20	Computational Study of Analogues of the Uranyl Ion Containing the â^'NUNâ^' Unit:Â Density Functional Theory Calculations on UO22+, UON+, UN2, UO(NPH3)3+, U(NPH3)24+, [UCl4{NPR3}2] (R = H, Me), and [UOCl4{NP(C6H5)3}]-. Inorganic Chemistry, 2000, 39, 6009-6017.	1.9	103
21	Group 3 and Lanthanide Boryl Compounds: Syntheses, Structures, and Bonding Analyses of Scâ^'B, Yâ^'B, and Luâ^'B Ïƒ-Coordinated NHC Analogues. Journal of the American Chemical Society, 2011, 133, 3836-3839.	6.6	102
22	Stable GaX2, InX2 and TlX2 radicals. Nature Chemistry, 2014, 6, 315-319.	6.6	101
23	Probing the Reactivity and Electronic Structure of a Uranium(V) Terminal Oxo Complex. Journal of the American Chemical Society, 2011, 133, 14224-14227.	6.6	96
24	The Oxidation State of Ce in the Sandwich Molecule Cerocene. Journal of the American Chemical Society, 1996, 118, 13115-13116.	6.6	88
25	Organometallic neptunium(III) complexes. Nature Chemistry, 2016, 8, 797-802.	6.6	88
26	On the inverse trans influence. Density functional studies of [MOX5]nâ€“ (M = Pa, n = 2; M = U, n = 1; M =) Tj ETQq0 0 0 rgBT /Overlock	2.3	86
27	The Three-Dimensional Structure of the Titanium-Centered Active Site during Steady-State Catalytic Epoxidation of Alkenes. Journal of Physical Chemistry B, 2001, 105, 9028-9030.	1.2	84
28	Synthesis and Spectroscopic and Computational Characterization of the Chalcogenido-Substituted Analogues of the Uranyl Ion, [OUE]²⁺ (E = S, Se). Journal of the American Chemical Society, 2013, 135, 5352-5355.	6.6	81
29	Do QTAIM metrics correlate with the strength of heavy elementâ€“ligand bonds?. Dalton Transactions, 2013, 42, 13477.	1.6	80
30	Quantum chemical calculations on a selection of iodine-containing species (IO, OIO, INO3, (IO)2, I2O3,) Tj ETQq0 0 0 rgBT /Overlock 10	1.3	79
31	Metalâ€“Metal Bonding in Uraniumâ€“Group 10 Complexes. Journal of the American Chemical Society, 2016, 138, 3333-3345.	6.6	79
32	Synthesis and electronic structure of permethylindenyl complexes of iron and cobalt. Organometallics, 1992, 11, 48-55.	1.1	77
33	Bonding Trends Traversing the Tetravalent Actinide Series: Synthesis, Structural, and Computational Analysis of An^{IV}(^{Ar}acnac)₄ Complexes (An = Th, U, Np, Pu;) Tj ETQq1 1 0.784314 rgBT /Overlock 8557-8566.	1.9	76
34	On the structure and coordination of the oxygen-donating species in Tiâ†'MCM-41/TBHP oxidation catalysts: a density functional theory and EXAFS study. Physical Chemistry Chemical Physics, 2002, 4, 1228-1240.	1.3	74
35	Hole localization in [AlO4]0 defects in silica materials. Journal of Chemical Physics, 2005, 122, 144704.	1.2	74
36	Is Cerocene Really a Ce(III) Compound? All-Electron Spinâ^'Orbit Coupled CASPT2 Calculations on M(Î·⁸-C₈H₈)₂ (M = Th, Pa, Ce). Journal of Physical Chemistry A, 2009, 113, 2896-2905.	1.1	72

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37	The strength of actinideâ€“element bonds from the quantum theory of atoms-in-molecules. Dalton Transactions, 2015, 44, 2554-2566.	1.6	72
38	Electronic and structural investigations of technetium compounds by x-ray absorption spectroscopy. Inorganic Chemistry, 1995, 34, 193-198.	1.9	68
39	Heterobimetallic Complexes Containing Caâ€“Fe or Ybâ€“Fe Bonds: Synthesis and Molecular and Electronic Structures of [M{CpFe(CO)₂}₂(THF)₃]₂(M) Tj ETQq1 1 0.784314 rgBT /O	6.1	68
40	Formation of a Ce(IV) Oxo Complex via Inner Sphere Nitrate Reduction. Journal of the American Chemical Society, 2016, 138, 12743-12746.	6.6	63
41	Nature of the Cycloheptatrienyl-Transition Metal Bond. A Study of Electron Distribution in the Mixed-Ring Sandwich Molecules [Ti(.eta.-C7H7)(.eta.-C5H5)], [Nb(.eta.-C7H7)(.eta.-C5H5)], [Ta(.eta.-C7H7)(.eta.-C5H4Me)], and [Mo(.eta.-C7H7)(.eta.-C5H5)] by Photoelectron Spectroscopy with Variable Photon Energy. Journal of the American Chemical Society, 1994, 116, 1994-2004.	6.6	61
42	Density functional theory investigation of the geometric and electronic structures of [UO2(H2O)m(OH)n]2â^'n(n + m = 5). Dalton Transactions, 2006, , 2403-2414.	1.6	60
43	Thallium(I) Sandwich, Multidecker, and Ether Complexes Stabilized by Weakly-Coordinating Anions:Â A Spectroscopic, Structural, and Theoretical Investigation. Journal of the American Chemical Society, 2007, 129, 881-894.	6.6	60
44	Electronic structure of f1 lanthanide and actinide complexes. Part 2. Non-relativistic and relativistic calculations of the ground state electronic structures and optical transition energies of [Ce(Î·-C5H5)3], [Th(Î·-C5H5)3] and [Pa(Î·-C8H8)2]. Journal of Organometallic Chemistry, 1997, 528, 19-33.	0.8	58
45	Back bonding without Ïƒ-bonding: a unique Ï€-complex of dinitrogen with uranium. Journal of Organometallic Chemistry, 2001, 635, 69-74.	0.8	58
46	Thoriumâ€“ligand multiple bonds via reductive deprotection of a trityl group. Chemical Science, 2015, 6, 3891-3899.	3.7	55
47	Switchable Ï€-coordination and Câ€“H metallation in small-cavity macrocyclic uranium and thorium complexes. Chemical Science, 2014, 5, 756-765.	3.7	53
48	Electronic Structure of [U2(Î¼2-N2)(Î·5-C5Me5)2(Î·8-C8H4(SiPri3)2)2]. Organometallics, 2004, 23, 832-835.	1.1	52
49	Characterizing Pressureâ€Induced Uranium Cï£¿H Agostic Bonds. Angewandte Chemie - International Edition, 2015, 54, 6735-6739.	7.2	52
50	A crystalline tri-thorium cluster with Ïƒ-aromatic metalâ€“metal bonding. Nature, 2021, 598, 72-75.	13.7	52
51	Nature of the Transition Metalâ^'Cycloheptatrienyl Bond. Computational Studies of the Electronic Structure of [M(Î·7-C7H7)(Î·5-C5H5)] (M = groups 4â^'6). Organometallics, 2005, 24, 1189-1197.	1.1	51
52	Theoretical study of the geometric and electronic structures of pseudo-octahedral d0 imido compounds of titanium: the trans influence in mer-[Ti(NR)Cl2(NH3)3] (Râ€¦=â€¦But, C6H5 or C6H4NO2-4). Journal of the Chemical Society Dalton Transactions, 1999, , 781-790.	1.1	50
53	On the Paucity of Molecular Actinide Complexes with Unsupported Metalâ^'Metal Bonds:Â A Comparative Investigation of the Electronic Structure and Metalâ^'Metal Bonding in U2X6(X = Cl, F, OH, NH2, CH3) Complexes and d-Block Analogues. Inorganic Chemistry, 2006, 45, 6828-6839.	1.9	50
54	The Kubas interaction in M(ii) (M = Ti, V, Cr) hydrazine-based hydrogen storage materials: a DFT study. Dalton Transactions, 2012, 41, 8515.	1.6	50

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55	Emergence of the structure-directing role of f-orbital overlap-driven covalency. Nature Communications, 2019, 10, 634.	5.8	50
56	Systematic Investigation of Thorium(IV)â€“ and Uranium(IV)â€“Ligand Bonding in Dithiophosphonate, Thioselenophosphinate, and Diselenophosphonate Complexes. Inorganic Chemistry, 2013, 52, 10623-10631.	1.9	49
57	Synthesis and reactions of Î²-diketiminate-supported complexes with Mgâ€“Fe or Ybâ€“Fe bonds. Chemical Communications, 2013, 49, 3315.	2.2	49
58	Water Adsorption on AnO₂ {111}, {110}, and {100} Surfaces (An = U and Pu): A Density Functional Theory + U Study. Journal of Physical Chemistry C, 2017, 121, 1675-1682.	1.5	48
59	Neptunium(vi) chain and neptunium(vi/v) mixed valence cluster complexes. Chemical Communications, 2009, , 917.	2.2	47
60	Transuranic Computational Chemistry. Chemistry - A European Journal, 2018, 24, 2815-2825.	1.7	47
61	Back-bonding between an electron-poor, high-oxidation-state metal and poor Ï€-acceptor ligand in a uranium(v)â€“dinitrogen complex. Nature Chemistry, 2019, 11, 806-811.	6.6	47
62	Electronic Structure of f1 Actinide Complexes. 1. Nonrelativistic and Relativistic Calculations of the Optical Transition Energies of AnX6q- Complexes. Inorganic Chemistry, 1995, 34, 2735-2744.	1.9	46
63	Oxygen Vacancy Formation and Water Adsorption on Reduced AnO₂{111}, {110}, and {100} Surfaces (An = U, Pu): A Computational Study. Journal of Physical Chemistry C, 2018, 122, 7149-7165.	1.5	45
64	Covalency in the f-elementâ€“chalcogen bond. Journal of Alloys and Compounds, 2007, 444-445, 369-375.	2.8	44
65	Covalency hinders AnO₂(H₂O)⁺ â†' AnO(OH)₂⁺ isomerisation (An = Paâ€“Pu). Dalton Transactions, 2016, 45, 3158-3162.	1.6	44
66	Variable photon energy photoelectron spectroscopy of osmium tetroxide and pseudopotential calculations of the valence ionization energies of OsO4 and ruthenium tetroxide. Inorganic Chemistry, 1992, 31, 1588-1594.	1.9	43
67	Molecular Structures of Two Metal Tetrakis(tetrahydroborates), Zr(BH4)4and U(BH4)4:Â Equilibrium Conformations and Barriers to Internal Rotation of the Triply Bridging BH4Groups. Inorganic Chemistry, 2002, 41, 6646-6655.	1.9	43
68	Zinc(II) Î·1- and Î·2-Toluene Complexes:Â Structure and Bonding in Zn(C6F5)2Â·(toluene) and Zn(C6F4-2-C6F5)2Â·(toluene). Organometallics, 2006, 25, 3311-3313.	1.1	43
69	Evidence for actinide metal to ligand Ï€ backbonding. Density functional investigations of the electronic structure of [{(NH2)3(NH3)U}2(Î¼2-Î·2:Î·2-N2)]. Chemical Communications, 1998, , 1665-1666.	2.2	41
70	Are the Ground States of the Later Actinocenes Multiconfigurational? All-Electron Spinâ^'Orbit Coupled CASPT2 Calculations on An(Î·⁸-C₈H₈)₂(An =) Tj ETQq1 1 0 rgBT /Overlock	1.1	41
71	A manganese hydride molecular sieve for practical hydrogen storage under ambient conditions. Energy and Environmental Science, 2019, 12, 1580-1591.	15.6	41
72	Synthesis and electronic and molecular structures of .eta.-cycloheptatrienyl .eta.-cyclopentadienyl derivatives of vanadium, niobium, and tantalum: photoelectron spectroscopic, electrochemical, and x-ray crystallographic study. Organometallics, 1992, 11, 3353-3361.	1.1	40

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73	Metalâ€“metal bonding in molecular actinide compounds: electronic structure of [M2X8]2â¯(M = U, Np,) Tj ETQq1 1 0.784314 rgBT 5476-5483.	1.6	39
74	Tetravalent Metal Complexation by Keggin and Lacunary Phosphomolybdate Anions. Inorganic Chemistry, 2008, 47, 5787-5798.	1.9	39
75	Energy Decomposition Analysis of Metalâ¯Metal Bonding in [M2X8]2- (X = Cl, Br) Complexes of 5f (U, Np,) Tj ETQq1 1 0.784314 rgBT	1.9	38
76	The first group 4 metal bis(imido) and tris(imido) complexes. Chemical Science, 2012, 3, 819-824.	3.7	37
77	Uraniumâ€“Carbeneâ€“Imido Metallaâ€Allenes: Ancillaryâ€Ligandâ€Controlled cisâ€/transâ€Isomerisation and Assessment of trans Influence in the R₂C=U^{IV}=NRâ€² Unit (R=Ph₂PNSiMe₃;) Tj ETQq1 1 0.784314 rgBT /Overlock 10	1.7	37
78	Why is the F2 bond so weak? A bond energy decomposition analysis. New Journal of Chemistry, 2003, 27, 1108.	1.4	36
79	Bond-Forming Reactions of Dications with Molecules:â€‰ A Computational and Experimental Study of the Mechanisms for the Formation of HCF2+ from CF32+ and H2. Journal of Physical Chemistry A, 2006, 110, 2898-2905.	1.1	36
80	Catalyst: Nuclear Power in the 21 st Century. CheM, 2016, 1, 659-662.	5.8	36
81	Mono(arene) Complexes of Thallium(I) Supported by a Weakly Coordinating Anion. Organometallics, 2007, 26, 1811-1815.	1.1	34
82	Reductive silylation of a uranyl dibenzoylmethanate complex: an example of controlled uranyl oxo ligand cleavage. Chemical Science, 2014, 5, 3204-3213.	3.7	34
83	Electronic structure of metal chalcogen cubane clusters: photoelectron spectroscopic, electrochemical, and theoretical studies of [(.eta.-C5H4Me)TiS]4, [(.eta.-C5H4Me)VS]4, [(.eta.-C5H5)CrO]4, [(.eta.-C5H4Me)CrO]4, [(.eta.-C5H4Me)CrS]4, [(.eta.-C5H4Me)CrSe]4, [(.eta.-C5H4-iso-Pr)MoS]4, and [(.eta.-C5H4-iso-Pr)MoSe]4. Inorganic Chemistry, 1992, 31, 3779-3791.	1.9	33
84	Uranium Metallaâ€Allenes with Carbene Imido R₂C=U^{IV}=NRâ€² Units (R=Ph₂PNSiMe₃; Râ€²=CPh₃): Alkaliâ€Metalâ€Mediated Pushâ€“Pull Effects with an Amido Auxiliary. Chemistry - A European Journal, 2016, 22, 11554-11558.	5.7	33
85	Theoretical Studies of the Electronic Structure of Compounds of the Actinide Elements. , 2008, , 1893-2012.		31
86	Electron localization in the bis-arene complexes [(Î·-C6H6)2Cr] and [(Î·-C6H5Me)2Mo]: an investigation by photoelectron spectroscopy with variable photon energy. Chemical Physics, 1992, 164, 271-281.	0.9	30
87	Synthesis and characterisation of permethylindenyl complexes of cobalt and chromium: crystal structures of [Cr(Î·5-C9Me7)2], [Co(Î·5-C9Me7)2][PF6] and [Cr(Î·5-C9Me7)2][PF6]. Journal of the Chemical Society Dalton Transactions, 1993, , 383-392.	1.1	30
88	Synthesis, NMR studies, and molecular orbital calculations on cyclohexadienyl derivatives of (Î·6-arene)tris(pyrazolyl)ruthenium(II) compounds. Journal of the Chemical Society Dalton Transactions, 1998, , 3379-3390.	1.1	30
89	Are metal alkoxides linear owing to electrostatic repulsion?. Chemical Communications, 2002, , 2458-2459.	2.2	30
90	A Structural and Theoretical Investigation of Equatorial cis and trans Uranyl Phosphinimine and Uranyl Phosphine Oxide Complexes UO2Cl2(Cy3PNH)2and UO2Cl2(Cy3PO)2. Inorganic Chemistry, 2007, 46, 4868-4875.	1.9	30

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91	Computational Study of Silica-Supported Transition Metal Fragments for Kubas-type Hydrogen Storage. Journal of the American Chemical Society, 2010, 132, 17296-17305.	6.6	30
92	Probing the Limits of Alkaline Earthâ€“Transition Metal Bonding: An Experimental and Computational Study. Journal of the American Chemical Society, 2015, 137, 12352-12368.	6.6	30
93	Electronic structure of bulk AnO 2 (AnÂ=ÂU, Np, Pu) and water adsorption on the (111) and (110) surfaces of UO 2 and PuO 2 from hybrid density functional theory within the periodic electrostatic embedded cluster method. Journal of Nuclear Materials, 2016, 482, 124-134.	1.3	30
94	The performance of density functional theory for the description of ground and excited state properties of inorganic and organometallic uranium compounds. Journal of Organometallic Chemistry, 2018, 857, 58-74.	0.8	30
95	Quantum chemical topology and natural bond orbital analysis of Mâ€“O covalency in M(OC₆H₅)₄ (M = Ti, Zr, Hf, Ce, Th, Pa, U, Np). Physical Chemistry Chemical Physics, 2020, 22, 16804-16812.	1.3	29
96	The shortest Thâ€“Th distance from a new type of quadruple bond. Physical Chemistry Chemical Physics, 2017, 19, 5070-5076.	1.3	28
97	Theoretical investigation of the effects of spin-orbit coupling on the valence photoelectron spectrum of OsO4. Inorganic Chemistry, 1994, 33, 2315-2316.	1.9	27
98	The Reaction Chemistry of Plutonyl(VI) Chloride Complexes with Triphenyl Phosphineoxide and Triphenyl Phosphinimine. Inorganic Chemistry, 2010, 49, 9554-9562.	1.9	27
99	Computational analysis of Mâ€“O covalency in M(OC₆H₅)₄ (M = Ti,) Tj ETQq1 1 0.784314 rgBT	1.6	26
100	Exceptional uranium(VI)-nitride triple bond covalency from 15N nuclear magnetic resonance spectroscopy and quantum chemical analysis. Nature Communications, 2021, 12, 5649.	5.8	26
101	Transition Metal Hydrazideâ€Based Hydrogenâ€Storage Materials: the First Atomsâ€Inâ€Molecules Analysis of the Kubas Interaction. Chemistry - A European Journal, 2012, 18, 1750-1760.	1.7	25
102	Thorium(IV) and Uranium(IV) trans-Calix[2]benzene[2]pyrrolide Alkyl and Alkynyl Complexes: Synthesis, Reactivity, and Electronic Structure. Organometallics, 2017, 36, 4669-4681.	1.1	24
103	Expanding metallaborane chemistry: an octahedral BH6moiety supported through Mâ€“Hâ€“B bridges. New Journal of Chemistry, 2004, 28, 444-446.	1.4	23
104	Density Functional Theory-Based Prediction of Some Aqueous-Phase Chemistry of Superheavy Element 111. Roentgenium(I) Is the â€˜Softest' Metal Ion. Inorganic Chemistry, 2006, 45, 10780-10785.	1.9	23
105	All-electron CASPT2 study of Ce(Î·8â€“C8H6)2. Comptes Rendus Chimie, 2010, 13, 853-859.	0.2	23
106	Crystallinity-Modulated Co_{2â€“x}V_xO₄ Nanoplates for Efficient Electrochemical Water Oxidation. ACS Catalysis, 2021, 11, 14884-14891.	5.5	23
107	Electron localization in a mixed-valence diniobium benzene complex. Chemical Science, 2015, 6, 993-1003.	3.7	22
108	A XANES and EXAFS Investigation of the Speciation of Selenite following Bacterial Metabolization. Inorganic Chemistry, 1995, 34, 1617-1619.	1.9	21

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109	Laser photofragmentation and collision-induced reactions of SiF22+ and SiF32+. Journal of Chemical Physics, 1997, 106, 7981-7994.	1.2	21
110	Time dependent DFT study of the electronic transition energies of RuO4 and OsO4. Chemical Physics Letters, 2005, 415, 64-68.	1.2	21
111	Planar Trimethylenemethane Dianion Chemistry of Lanthanide Metallocenes:Â Synthesis, Structure, Density Functional Theory Analysis, and Reactivity of [(C5Me5)2Ln]2[Î¼-Î·3:Î·3-C(CH2)3] Complexes. Journal of the American Chemical Society, 2006, 128, 16178-16189.	6.6	21
112	A mystery solved? Photoelectron spectroscopic and quantum chemical studies of the ion states of CeCp3+. Dalton Transactions, 2009, , 5943.	1.6	21
113	Are Metalâ€“Metal Interactions Involved in the Rising Enthalpies Observed in The Kubas Binding of H₂ to Hydrazine-Linked Hydrogen Storage Materials?. Journal of Physical Chemistry C, 2012, 116, 19134-19144.	1.5	20
114	Variable Photon Energy Photoelectron Spectroscopic, and Theoretical Investigations of the Electronic Structure of TiCl4. Inorganic Chemistry, 1994, 33, 5086-5093.	1.9	19
115	Theoretical investigation of the electronic structures of the mixed-ring sandwich molecules [M(Î·7-C7H7)(Î·5-C5H5)](M = Ti, V, Nb or Ta). Journal of the Chemical Society Dalton Transactions, 1995, , 3727-3730.	1.1	19
116	Molecular and electronic structures of bis[1,4-bis(trimethylsilyl)cyclooctatetraene] sandwich complexes of titanium and zirconium. Journal of the Chemical Society Dalton Transactions, 1994, , 2867.	1.1	18
117	A theoretical investigation of the electron-transfer reactions of the SiF2+3 dication with the rare gases, neon, argon, krypton and xenon. International Journal of Mass Spectrometry and Ion Processes, 1998, 172, 57-69.	1.9	18
118	Ab initio investigations of the potential energy surfaces of the XOâ€‰+â€‰HO2 reaction (Xâ€‰=â€‰chlorine or) Tj ETQq0 0 0 rgBT	1.3	18
119	The Bond-Forming Reactions of Atomic Dications with Neutral Molecules:Â Formation of ArNH+and ArN+from Collisions of Ar2+with NH3. Journal of the American Chemical Society, 2004, 126, 3658-3663.	6.6	18
120	Synthesis, structure, and reactivity of uranium(<scp>vi</scp>) nitrides. Chemical Science, 2021, 12, 8096-8104.	3.7	18
121	Electron-transfer and neutral-loss reactions in collisions of CF32+ with argon. International Journal of Mass Spectrometry, 1999, 192, 205-214.	0.7	17
122	Computational investigation of the geometric structures of [(CN)5PtTl(CN)n]nâ¯ (n=0, 1, 2 or 3). Inorganica Chimica Acta, 2001, 312, 221-225.	1.2	17
123	Quantum Chemical Studies of the Hydration of Sr²⁺ in Vacuum and Aqueous Solution. Chemistry - A European Journal, 2011, 17, 5060-5067.	1.7	17
124	Formation of a U(VI)â€“Persulfide Complex during Environmentally Relevant Sulfidation of Iron (Oxyhydr)oxides. Environmental Science & Technology, 2020, 54, 129-136.	4.6	17
125	Covalency in AnCl₃ (An = Thâ€“No). Dalton Transactions, 2021, 50, 1478-1485.	1.6	17
126	Photoelectron spectroscopy of Ce(Î·-C5H5)3 â€“ Accessing two ion states on 4f ionization. Chemical Physics Letters, 2006, 432, 17-21.	1.2	16

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127	Probing the Nature of Acetylene Bound to the Active Site of a NiNaâ^'Zeolite Y Catalyst by in situ Neutron Scattering. Journal of Physical Chemistry B, 2000, 104, 7570-7573.	1.2	15
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