List of Publications by Year in descending order

267 papers	16,672 citations	17405 63 h-index	17546 121 g-index
272 all docs	272 docs citations	272 times ranked	13928 citing authors

#	Article	IF	Citations
1	Catalysis Research of Relevance to Carbon Management:â€‰ Progress, Challenges, and Opportunities. Chemical Reviews, 2001, 101, 953-996.	23.0	1,311
2	Ionization Potential, Electron Affinity, Electronegativity, Hardness, and Electron Excitation Energy:â€‰ Molecular Properties from Density Functional Theory Orbital Energies. Journal of Physical Chemistry A, 2003, 107, 4184-4195.	1.1	1,134
3	A local density functional study of the structure and vibrational frequencies of molecular transition-metal compounds. The Journal of Physical Chemistry, 1992, 96, 6630-6636.	2.9	711
4	Hydrogen Bond Energy of the Water Dimer. The Journal of Physical Chemistry, 1996, 100, 2993-2997.	2.9	469
5	On the Enthalpy of Formation of Hydroxyl Radical and Gas-Phase Bond Dissociation Energies of Water and Hydroxyl. Journal of Physical Chemistry A, 2002, 106, 2727-2747.	1.1	466
6	Chemical accuracy in ab initio thermochemistry and spectroscopy: current strategies and future challenges. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	381
7	On a quantitative scale for Lewis acidity and recent progress in polynitrogen chemistry. Journal of Fluorine Chemistry, 2000, 101, 151-153.	0.9	372
8	A survey of factors contributing to accurate theoretical predictions of atomization energies and molecular structures. Journal of Chemical Physics, 2008, 129, 204105.	1.2	345
9	Photoelectron Spectroscopy of a Carbene/Silylene/Germylene Series. Journal of the American Chemical Society, 1994, 116, 6641-6649.	6.6	330
10	Absolute Hydration Free Energy of the Proton from First-Principles Electronic Structure Calculations. Journal of Physical Chemistry A, 2001, 105, 11534-11540.	1.1	277
11	Extended benchmark studies of coupled cluster theory through triple excitations. Journal of Chemical Physics, 2001, 115, 3484-3496.	1.2	266
12	A Hybrid Organic/Inorganic Benzene. Angewandte Chemie - International Edition, 2009, 48, 973-977.	7.2	258
13	Atomically dispersed supported metal catalysts: perspectives and suggestions for future research. Catalysis Science and Technology, 2017, 7, 4259-4275.	2.1	221
14	Electronic structure of a stable nucleophilic carbene. The Journal of Physical Chemistry, 1991, 95, 4180-4182.	2.9	217
15	Electron Distribution in a Stable Carbene. Journal of the American Chemical Society, 1994, 116, 6812-6822.	6.6	204
16	Performance of coupled cluster theory in thermochemical calculations of small halogenated compounds. Journal of Chemical Physics, 2003, 118, 3510-3522.	1.2	195
17	Further benchmarks of a composite, convergent, statistically calibrated coupled-cluster-based approach for thermochemical and spectroscopic studies. Molecular Physics, 2012, 110, 2381-2399.	0.8	170
18	Predicting the Energy of the Water Exchange Reaction and Free Energy of Solvation for the Uranyl Ion in Aqueous Solution. Journal of Physical Chemistry A, 2006, 110, 8840-8856.	1.1	167

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19	Hydration of the Fluoride Anion:Â Structures and Absolute Hydration Free Energy from First-Principles Electronic Structure Calculations. Journal of Physical Chemistry A, 2004, 108, 2020-2029.	1.1	166
20	Molecular Mechanism for H2Release from BH3NH3, Including the Catalytic Role of the Lewis Acid BH3. Journal of Physical Chemistry A, 2007, 111, 679-690.	1.1	161
21	Molecular Structures and Energetics of the (TiO₂)_n (n = 1â^'4) Clusters and Their Anions. Journal of Physical Chemistry A, 2008, 112, 6646-6666.	1.1	161
22	Accurate Thermochemistry for Transition Metal Oxide Clusters. Journal of Physical Chemistry A, 2009, 113, 7861-7877.	1.1	156
23	Hydrogen Storage by Boronâ^'Nitrogen Heterocycles: A Simple Route for Spent Fuel Regeneration. Journal of the American Chemical Society, 2010, 132, 3289-3291.	6.6	152
24	Predicting the Heats of Formation of Model Hydrocarbons up to Benzene. Journal of Physical Chemistry A, 2000, 104, 3048-3056.	1.1	146
25	Chemical Shielding Tensor of a Carbene. Journal of the American Chemical Society, 1994, 116, 6361-6367.	6.6	134
26	Heats of Formation of Simple Perfluorinated Carbon Compounds. Journal of Physical Chemistry A, 1999, 103, 4744-4751.	1.1	130
27	Thorium(IV) Molecular Clusters with a Hexanuclear Th Core. Inorganic Chemistry, 2011, 50, 9696-9704.	1.9	127
28	Reliable Predictions of the Thermochemistry of Boronâ^'Nitrogen Hydrogen Storage Compounds:â€‰ BxNxHy, x = 2, 3. Journal of Physical Chemistry A, 2007, 111, 4411-4421.	1.1	124
29	Computational Study of the Release of H2from Ammonia Borane Dimer (BH3NH3)2and Its Ion Pair Isomers. Journal of Physical Chemistry A, 2007, 111, 8844-8856.	1.1	124
30	Theoretical Study of the Heats of Formation of Small Silicon-Containing Compounds. Journal of Physical Chemistry A, 1999, 103, 6413-6419.	1.1	122
31	Molecular and Electronic Structures, BrÃ¶nsted Basicities, and Lewis Acidities of Group VIB Transition Metal Oxide Clusters. Journal of Physical Chemistry A, 2006, 110, 6231-6244.	1.1	121
32	Predicting the Proton Affinities of H2O and NH3. Journal of Physical Chemistry A, 1998, 102, 2449-2454.	1.1	116
33	Prediction of Structures and Atomization Energies of Small Silver Clusters, (Ag)_n, n < 100. Journal of Physical Chemistry A, 2013, 117, 8298-8313.	1.1	112
34	Unusual structure, bonding and properties in a californium borate. Nature Chemistry, 2014, 6, 387-392.	6.6	110
35	Third Row Transition Metal Hexafluorides, Extraordinary Oxidizers, and Lewis Acids: Electron Affinities, Fluoride Affinities, and Heats of Formation of WF₆, ReF₆, OsF₆, IrF₆, PtF₆, and AuF₆. Inorganic Chemistry, 2010, 49, 1056-1070.	1.9	109
36	Mechanism of the Hydration of Carbon Dioxide: Direct Participation of H₂O versus Microsolvation. Journal of Physical Chemistry A, 2008, 112, 10386-10398.	1.1	108

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37	The Nature and Absolute Hydration Free Energy of the Solvated Electron in Water. Journal of Physical Chemistry B, 2003, 107, 4403-4417.	1.2	107
38	A New, Self-Contained Asymptotic Correction Scheme To Exchange-Correlation Potentials for Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2003, 107, 10154-10158.	1.1	106
39	First-Principles Determination of the Absolute Hydration Free Energy of the Hydroxide Ionâ€. Journal of Physical Chemistry A, 2002, 106, 9737-9744.	1.1	105
40	Ab Initio Prediction of the Gas- and Solution-Phase Acidities of Strong BrÃ¸nsted Acids:â€‰ The Calculation of pKa Values Less Than â^'10. Journal of Physical Chemistry A, 2006, 110, 12044-12054.	1.1	101
41	Complexation of the Carbonate, Nitrate, and Acetate Anions with the Uranyl Dication:Â Density Functional Studies with Relativistic Effective Core Potentialsâ€. Journal of Physical Chemistry A, 2005, 109, 11568-11577.	1.1	100
42	The Least Stable Isomer of BN Naphthalene: Toward Predictive Trends for the Optoelectronic Properties of BN Acenes. Journal of the American Chemical Society, 2017, 139, 6082-6085.	6.6	100
43	A new inversion process at Group VA (Group 15) elements. Edge inversion through a planar T-shaped structure. Journal of the American Chemical Society, 1986, 108, 2461-2462.	6.6	99
44	Dehydration, dehydrogenation, and condensation of alcohols on supported oxide catalysts based on cyclic (WO₃)₃ and (MoO₃)₃ clusters. Chemical Society Reviews, 2014, 43, 7664-7680.	18.7	99
45	Mechanism by which Tungsten Oxide Promotes the Activity of Supported V₂O₅/TiO₂ Catalysts for NO_X Abatement: Structural Effects Revealed by ⁵¹V MAS NMR Spectroscopy. Angewandte Chemie - International Edition, 2019, 58, 12609-12616.	7.2	96
46	Coupled Cluster Theory Determination of the Heats of Formation of Combustion-Related Compounds:Â CO, HCO, CO2, HCO2, HOCO, HC(O)OH, and HC(O)OOH. Journal of Physical Chemistry A, 2003, 107, 1604-1617.	1.1	94
47	Bulky Alkylphosphines with Neopentyl Substituents as Ligands in the Amination of Aryl Bromides and Chlorides. Journal of Organic Chemistry, 2006, 71, 5117-5125.	1.7	94
48	Quantum-Chemical Calculations of Carbon-Isotope Fractionation in CO₂(g), Aqueous Carbonate Species, and Carbonate Minerals. Journal of Physical Chemistry A, 2008, 112, 542-555.	1.1	94
49	A Practical Guide to Reliable First Principles Computational Thermochemistry Predictions Across the Periodic Table. Annual Reports in Computational Chemistry, 2012, , 1-28.	0.9	94
50	Prediction of Bond Dissociation Energies/Heats of Formation for Diatomic Transition Metal Compounds: CCSD(T) Works. Journal of Chemical Theory and Computation, 2017, 13, 1057-1066.	2.3	92
51	Resonance Stabilization Energy of 1,2-Azaborines: A Quantitative Experimental Study by Reaction Calorimetry. Journal of the American Chemical Society, 2010, 132, 18048-18050.	6.6	85
52	Late-Stage Functionalization of 1,2-Dihydro-1,2-azaborines via Regioselective Iridium-Catalyzed Câ€“H Borylation: The Development of a New N,N-Bidentate Ligand Scaffold. Journal of the American Chemical Society, 2015, 137, 5536-5541.	6.6	80
53	Sterically Demanding, Sulfonated, Triarylphosphines: Application to Palladium-Catalyzed Cross-Coupling, Steric and Electronic Properties, and Coordination Chemistry. Organometallics, 2008, 27, 576-593.	1.1	79
54	Molecular Structures and Energetics of the (ZrO₂)_n and (HfO₂)_n (n = 1â^'4) Clusters and Their Anions. Journal of Physical Chemistry A, 2010, 114, 2665-2683.	1.1	77

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55	Structures and Stabilities of (MgO)_n Nanoclusters. Journal of Physical Chemistry A, 2014, 118, 3136-3146.	1.1	76
56	Interactions of 1-Methylimidazole with UO2(CH3CO2)2and UO2(NO3)2:Â Structural, Spectroscopic, and Theoretical Evidence for Imidazole Binding to the Uranyl Ion. Journal of the American Chemical Society, 2007, 129, 526-536.	6.6	75
57	A quantitative scale for the oxidizing strength of oxidative fluorinators. Journal of the American Chemical Society, 1992, 114, 2978-2985.	6.6	71
58	Nucleophilic Aromatic Substitution Reactions of 1,2â€Dihydroâ€1,2â€Azaborine. Angewandte Chemie - International Edition, 2011, 50, 8157-8160.	7.2	71
59	Tree Growthâ€"Hybrid Genetic Algorithm for Predicting the Structure of Small (TiO₂)_n, n = 2â€"13, Nanoclusters. Journal of Chemical Theory and Computation, 2013, 9, 3189-3200.	2.3	71
60	Benchmark Calculations on the Electron Detachment Energies of MO₃⁻ and M₂O₆⁻ (M = Cr, Mo, W). Journal of Physical Chemistry A, 2007, 111, 11908-11921.	1.1	67
61	Prediction of the pK_aâ€™s of Aqueous Metal Ion +2 Complexes. Journal of Physical Chemistry A, 2015, 119, 2926-2939.	1.1	67
62	Bond Dissociation Energies in Second-Row Compounds. Journal of Physical Chemistry A, 2008, 112, 3145-3156.	1.1	66
63	BN-substituted diphenylacetylene: a basic model for conjugated Ï€-systems containing the BN bond pair. Chemical Science, 2012, 3, 825-829.	3.7	66
64	Gold Nanorod-Enhanced Light Absorption and Photoelectrochemical Performance of Î±-Fe₂O₃ Thin-Film Electrode for Solar Water Splitting. Journal of Physical Chemistry C, 2013, 117, 22060-22068.	1.5	65
65	Boronâ€Substituted 1,3â€Dihydroâ€1,3â€azaborines: Synthesis, Structure, and Evaluation of Aromaticity. Angewandte Chemie - International Edition, 2013, 52, 7527-7531.	7.2	65
66	Beating Heterogeneity of Single-Site Catalysts: MgO-Supported Iridium Complexes. ACS Catalysis, 2018, 8, 3489-3498.	5.5	64
67	Lewis Acidities and Hydride, Fluoride, and Xâ¯ Affinities of the BH3â¯nXn Compounds for (X = F, Cl, Br, I,) Tj ETQq1 1 0.784314 rgBT	1.9	63
68	Thorium(IV)â€"Selenate Clusters Containing an Octanuclear Th(IV) Hydroxide/Oxide Core. Inorganic Chemistry, 2012, 51, 4239-4249.	1.9	63
69	Molecular Heterogeneous Catalysis: A Singleâ€Site Zeoliteâ€Supported Rhodium Complex for Acetylene Cyclotrimerization. Chemistry - A European Journal, 2007, 13, 7294-7304.	1.7	62
70	Ethanol Conversion on Cyclic (MO3)3 (M = Mo, W) Clusters. Journal of Physical Chemistry C, 2014, 118, 4869-4877.	1.5	62
71	Bis-BN Cyclohexane: A Remarkably Kinetically Stable Chemical Hydrogen Storage Material. Journal of the American Chemical Society, 2015, 137, 134-137.	6.6	62
72	Computational Study of the Hydrolysis Reactions of the Ground and First Excited Triplet States of Small TiO₂ Nanoclusters. Journal of Physical Chemistry C, 2011, 115, 9344-9360.	1.5	61

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73	Neopentylphosphines as effective ligands in palladium-catalyzed cross-couplings of aryl bromides and chlorides. Tetrahedron, 2008, 64, 6920-6934.	1.0	58
74	Substituent Effects on the Properties of Borafluorenes. Organometallics, 2016, 35, 3182-3191.	1.1	58
75	Energetics of the protonation of CO: Implications for the observation of HOC+ in dense interstellar clouds. Journal of Chemical Physics, 1984, 81, 3603-3611.	1.2	57
76	Thermochemistry for the Dehydrogenation of Methyl-Substituted Ammonia Borane Compounds. Journal of Physical Chemistry A, 2009, 113, 6121-6132.	1.1	56
77	Zeolite-Supported Organorhodium Fragments: Essentially Molecular Surface Chemistry Elucidated with Spectroscopy and Theory. Journal of the American Chemical Society, 2009, 131, 8460-8473.	6.6	56
78	Gas-phase acidities of aspartic acid, glutamic acid, and their amino acid amides. International Journal of Mass Spectrometry, 2007, 265, 213-223.	0.7	55
79	Reliable Potential Energy Surfaces for the Reactions of H₂O with ThO₂, PaO₂⁺, UO₂²⁺, and UO₂⁺. Journal of Physical Chemistry A, 2015, 119, 11422-11431.	1.1	55
80	Molecular Structures, Acidâ^'Base Properties, and Formation of Group 6 Transition Metal Hydroxides. Journal of Physical Chemistry C, 2011, 115, 8072-8103.	1.5	54
81	Trivalent Ion Hydrolysis Reactions:Â A Linear Free-Energy Relationship Based on Density Functional Electronic Structure Calculations. Journal of the American Chemical Society, 1999, 121, 3234-3235.	6.6	53
82	Structure and Heats of Formation of Iodine Fluorides and the Respective Closed-Shell Ions from CCSD(T) Electronic Structure Calculations and Reliable Prediction of the Steric Activity of the Free-Valence Electron Pair in ClF₆^{â^'}, BrF₆^{â^'}, and IF₆^{â^'}. Inorganic Chemistry, 2008, 47, 5485-5494.	1.9	53
83	Prototype Supported Metal Cluster Catalysts: Ir₄ and Ir₆. ChemCatChem, 2011, 3, 95-107.	1.8	53
84	Selective molecular recognition by nanoscale environments in a supported iridium cluster catalyst. Nature Nanotechnology, 2014, 9, 459-465.	15.6	53
85	Structural and Electronic Property Study of (ZnO)_n, n â‰ 168: Transition from Zinc Oxide Molecular Clusters to Ultrasmall Nanoparticles. Journal of Physical Chemistry C, 2016, 120, 20400-20418.	1.5	53
86	Accurate heats of formation and acidities for H3PO4, H2SO4, and H2CO3 from ab initio electronic structure calculations. International Journal of Quantum Chemistry, 2005, 102, 775-784.	1.0	52
87	Fundamental Thermochemical Properties of Amino Acids: Gas-Phase and Aqueous Acidities and Gas-Phase Heats of Formation. Journal of Physical Chemistry B, 2012, 116, 2905-2916.	1.2	52
88	Investigation of the Structure and Active Sites of TiO₂ Nanorod Supported VO_x Catalysts by High-Field and Fast-Spinning ⁵¹V MAS NMR. ACS Catalysis, 2015, 5, 3945-3952.	5.5	51
89	A Modular Synthetic Approach to Monocyclic 1,4â€Azaborines. Angewandte Chemie - International Edition, 2016, 55, 8333-8337.	7.2	50
90	Dielsâ€“Alder Reactions of 1,2â€Azaborines. Angewandte Chemie - International Edition, 2015, 54, 7823-7827.	7.2	49

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91	Accurate Heats of Formation of the â€œArduengo-Typeâ€•Carbene and Various Adducts Including H2 from ab Initio Molecular Orbital Theory. Journal of Physical Chemistry A, 2006, 110, 1968-1974.	1.1	48
92	Low-Lying Electronic States of M₃O₉⁻ and M₃O₉²⁻ (M = Mo, W). Journal of Physical Chemistry A, 2007, 111, 11093-11099.	1.1	47
93	Matrix Infrared Spectra and Theoretical Studies of Thorium Oxide Species: ThOxand Th2Oy. Journal of Physical Chemistry A, 2011, 115, 14407-14416.	1.1	47
94	Rhodium-Catalyzed Bâ€“H Activation of 1,2-Azaborines: Synthesis and Characterization of BN Isosteres of Stilbenes. Organic Letters, 2014, 16, 3340-3343.	2.4	46
95	Prediction of Vibrational Frequencies of UO22+ at the CCSD(T) Level. Journal of Physical Chemistry A, 2008, 112, 4095-4099.	1.1	45
96	Computational Study of H2 and O2 Production from Water Splitting by Small (MO2)n Clusters (M = Ti,) Tj ETQq0 0 0 rgBT /Overlock 10	1.1	45
97	Mechanism by which Tungsten Oxide Promotes the Activity of Supported V₂O₅/TiO₂ Catalysts for NO_X Abatement: Structural Effects Revealed by ⁵¹V MAS NMR Spectroscopy. Angewandte Chemie, 2019, 131, 12739-12746.	1.6	45
98	Degradation of Î³-irradiated linear perfluoroalkanes at high dosage. Journal of Fluorine Chemistry, 2007, 128, 575-586.	0.9	44
99	Structures and Heats of Formation of Simple Alkaline Earth Metal Compounds: Fluorides, Chlorides, Oxides, and Hydroxides for Be, Mg, and Ca. Journal of Physical Chemistry A, 2010, 114, 9349-9358.	1.1	43
100	Spectroscopic and Energetic Properties of Thorium(IV) Molecular Clusters with a Hexanuclear Core. Journal of Physical Chemistry A, 2012, 116, 6917-6926.	1.1	43
101	Gas Phase Properties of MX₂ and MX₄ (X = F, Cl) for M = Group 4, Group 14, Cerium, and Thorium. Journal of Physical Chemistry A, 2015, 119, 5790-5803.	1.1	43
102	Use of Improved Orbitals for CCSD(T) Calculations for Predicting Heats of Formation of Group IV and Group VI Metal Oxide Monomers and Dimers and UCl₆. Journal of Chemical Theory and Computation, 2016, 12, 3583-3592.	2.3	43
103	Boranes with Ultra-High Stokes Shift Fluorescence. Organometallics, 2018, 37, 3732-3741.	1.1	40
104	Molecular and Dissociative Adsorption of Water on (TiO₂)_n Clusters, n = 1â€“4. Journal of Physical Chemistry A, 2015, 119, 11406-11421.	1.1	39
105	Investigation of Silica-Supported Vanadium Oxide Catalysts by High-Field ⁵¹V Magic-Angle Spinning NMR. Journal of Physical Chemistry C, 2017, 121, 6246-6254.	1.5	39
106	The gas and solution phase acidities of HNO, HOONO, HONO, and HONO2. International Journal of Mass Spectrometry, 2003, 227, 421-438.	0.7	38
107	Heats of Formation of Triplet Ethylene, Ethylidene, and Acetylene. Journal of Physical Chemistry A, 2008, 112, 2082-2087.	1.1	38
108	Thermodynamic Properties of the XO₂, X₂O, XYO, X₂O₂, and XYO₂ (X, Y = Cl, Br, and I) Isomers. Journal of Physical Chemistry A, 2010, 114, 4254-4265.	1.1	38

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110	Tipping Point for Expansion of Layered Aluminosilicates in Weakly Polar Solvents: Supercritical CO₂. ACS Applied Materials & Interfaces, 2017, 9, 36783-36791.	4.0	38
111	Structures and Heats of Formation of Simple Alkali Metal Compounds: Hydrides, Chlorides, Fluorides, Hydroxides, and Oxides for Li, Na, and K. Journal of Physical Chemistry A, 2010, 114, 4272-4281.	1.1	37
112	Oxidation, Reduction, and Condensation of Alcohols over (MO3)3 (M = Mo, W) Nanoclusters. Journal of Physical Chemistry C, 2014, 118, 22620-22634.	1.5	37
113	Computational Study of the Hydrolysis Reactions of Small MO₂ (M = Zr and Hf) Nanoclusters with Water. Journal of Physical Chemistry C, 2012, 116, 8475-8492.	1.5	35
114	Highâ€Energyâ€Resolution Xâ€ray Absorption Spectroscopy for Identification of Reactive Surface Species on Supported Singleâ€Site Iridium Catalysts. Chemistry - A European Journal, 2017, 23, 14760-14768.	1.7	35
115	Electronic structure of phosphine. Effect of basic set and correlation on the inversion barrier. The Journal of Physical Chemistry, 1982, 86, 914-917.	2.9	34
116	Dehydrogenation Reactions of Cyclic C2B2N2H12 and C4BNH12 Isomers. Journal of Physical Chemistry A, 2010, 114, 2644-2654.	1.1	34
117	Benchmark Calculations of Energetic Properties of Groups 4 and 6 Transition Metal Oxide Nanoclusters Including Comparison to Density Functional Theory. Journal of Chemical Theory and Computation, 2016, 12, 3689-3710.	2.3	32
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120	Heptacoordination: pentagonal bipyramidal heptafluoroxenon(1+) XeF7+ and heptafluorotellurate(1-) TeF7- ions. Journal of the American Chemical Society, 1993, 115, 9461-9467.	6.6	30
121	Structural and Electronic Near Degeneracy of M3O9â€“ (M = Cr, Mo, W). Journal of Physical Chemistry C, 2011, 115, 19190-19196.	1.5	29
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123	Thermochemical Properties of HxNO Molecules and Ions from ab Initio Electronic Structure Theory. Journal of Physical Chemistry A, 2006, 110, 185-191.	1.1	28
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128	Infrared Spectra of H2ThS and H2US in Noble Gas Matrixes: Enhanced H-An-S Covalent Bonding. Inorganic Chemistry, 2013, 52, 10275-10285.	1.9	25
129	Reactions of Lanthanide Atoms with Oxygen Difluoride and the Role of the Ln Oxidation State. Inorganic Chemistry, 2014, 53, 446-456.	1.9	25
130	Singleâ€Site Zeoliteâ€Anchored Organoiridium Carbonyl Complexes: Characterization of Structure and Reactivity by Spectroscopy and Computational Chemistry. Chemistry - A European Journal, 2015, 21, 11825-11835.	1.7	25
131	MgO-Supported Iridium Metal Pair-Site Catalysts Are More Active and Resistant to CO Poisoning than Analogous Single-Site Catalysts for Ethylene Hydrogenation and Hydrogenâ€“Deuterium Exchange. ACS Catalysis, 2019, 9, 9545-9553.	5.5	25
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133	Infrared spectroscopic and theoretical studies of the OTiF2, OZrF2 and OHfF2 molecules with terminal oxo ligands. Dalton Transactions, 2012, 41, 11706.	1.6	24
134	Acid Gas Adsorption on Metalâ€“Organic Framework Nanosheets as a Model of an â€œAll-Surfaceâ€• Material. Journal of Chemical Theory and Computation, 2017, 13, 1341-1350.	2.3	23
135	Infrared Spectra and Quantum Chemical Calculations of the Bridge-Bonded HC(F)LnF₂ (Ln) Tj ETQq1 1 0.784314 rgBT /O	1.1	22
136	Density Functional Theory Study of the Complexation of the Uranyl Dication with Anionic Phosphate Ligands with and without Water Molecules. Journal of Physical Chemistry A, 2013, 117, 8939-8957.	1.1	22
137	The Synthesis, Characterization and Dehydrogenation of Sigmaâ€Complexes of BNâ€Cyclohexanes. Chemistry - A European Journal, 2016, 22, 310-322.	1.7	22
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139	Prediction of Reliable Metalâ^PH₃ Bond Energies for Ni, Pd, and Pt in the 0 and +2 Oxidation States. Inorganic Chemistry, 2010, 49, 5546-5553.	1.9	21
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141	Uranium(IV) Chloride Complexes: UCl₆^{2â€“} and an Unprecedented U(H₂O)₄Cl₄ Structural Unit. Inorganic Chemistry, 2017, 56, 9772-9780.	1.9	21
142	Surface-Catalyzed Oxygen Exchange during Mineral Carbonation in Nanoscale Water Films. Journal of Physical Chemistry C, 2019, 123, 12871-12885.	1.5	21
143	Formation of Surface Impurities on Lithiumâ€“Nickelâ€“Manganeseâ€“Cobalt Oxides in the Presence of CO₂ and H₂O. Journal of the American Chemical Society, 2021, 143, 10261-10274.	6.6	21
144	Thorium Fluorides ThF, ThF₂, ThF₃, ThF₄, ThF₃(F₂), and ThF₅^{â€“} Characterized by Infrared Spectra in Solid Argon and Electronic Structure and Vibrational Frequency Calculations. Inorganic Chemistry, 2013, 52, 8228-8233.	1.9	20

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