Yaoming Xie

List of Publications by Year
in descending order

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128	2,702	201575	214721
papers	citations	27 h-index	47 g-index

132	132	132	2298
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A Viable Anionic N-Heterocyclic Dicarbene. Journal of the American Chemical Society, 2010, 132, 14370-14372.	6.6	206
2	The protonated water dimer: Extensive theoretical studies of H5O+2. Journal of Chemical Physics, 1994, 101, 4878-4884.	1.2	174
3	Mechanism of the C2H5+O2 reaction. Journal of Chemical Physics, 1997, 107, 141-155.	1.2	142
4	The Nature of the Galliumâ^'Gallium Triple Bond. Journal of the American Chemical Society, 1998, 120, 3773-3780.	6.6	124
5	Stabilization of elusive silicon oxides. Nature Chemistry, 2015, 7, 509-513.	6.6	104
6	Hydrogen bonding between the water molecule and the hydroxyl radical (H2Oâ‹...HO): The global minimum. Journal of Chemical Physics, 1993, 98, 8829-8834.	1.2	89
7	Stabilization of Siliconâ€“Carbon Mixed Oxides. Journal of the American Chemical Society, 2015, 137, 8396-8399.	6.6	71
8	Hydrogen bonding between the water molecule and the hydroxyl radical (H2Oâ‹...OH): The 2Aâ€˜ and 2Aâ€™ minima. Journal of Chemical Physics, 1991, 94, 2057-2062.	1.2	63
9	The entrance complex, transition state, and exit complex for the F + H2O â†' HF + OH reaction. Definitive predictions. Comparison with popular density functional methods. Physical Chemistry Chemical Physics, 2012, 14, 10891.	1.3	63
10	Theory and applications of spin-restricted open-shell MÃ¸ller-Plesset theory. Molecular Physics, 1993, 79, 777-793.	0.8	55
11	The alkaline earth dimer cations (Be₂ ⁺, Mg₂ ⁺,) Tj ETQq1 1 0.784314 rgBT /Over Coupled cluster and full configuration interaction studies^{â€}. Molecular Physics, 2013, 111, 2292-2298.	0.8	54
12	Hexalithiobenzene: a D6h equilibrium geometry with six lithium atoms in bridging positions. Chemical Physics Letters, 1991, 179, 563-567.	1.2	53
13	Is the oxywater radical cation more stable than neutral oxywater?. Journal of Chemical Physics, 1996, 104, 7615-7623.	1.2	53
14	Binuclear Homoleptic Manganese Carbonyls:â€‰ Mn2(CO)x (x = 10, 9, 8, 7). Inorganic Chemistry, 2003, 42, 5219-5230.	1.9	51
15	Why does Togni's reagent I exist in the high-energy hypervalent iodine form? Re-evaluation of benziodoxole based hypervalent iodine reagents. Chemical Communications, 2016, 52, 5371-5374.	2.2	50
16	A Stable Anionic Dithiolene Radical. Journal of the American Chemical Society, 2017, 139, 6859-6862.	6.6	49
17	The radical anions and the electron affinities of perfluorinated benzene, naphthalene and anthraceneElectronic supplementary information (ESI) available: calculated energies and electron affinities for perfluorinated benzene, naphthalene and anthracene and their anions. Calculated structures for perfluorinated naphthalene and anthracene and their anions. See http://www.rsc.org/suppdata/cc/b2/b208831m/. Chemical Communications, 2003, , 102-103.	2.2	47
18	Structures, thermochemistry, and electron affinities of the germanium fluorides, GeFn/GeFnâ^'(n=1â€“5). Journal of Chemical Physics, 1999, 111, 7945-7953.	1.2	45

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19	Can Oxywater Be Made?. The Journal of Physical Chemistry, 1996, 100, 6076-6080.	2.9	43
20	Ammonia alane. Journal of Chemical Physics, 1992, 96, 5310-5317.	1.2	40
21	Flat Potential Energy Surface of the Saturated Binuclear Homoleptic Chromium Carbonyl Cr2(CO)11 with One, Two, and Three Bridging Carbonyls:â€‰ Comparison with the Well-Known [HCr2(CO)10]- Anion and the Related [(Î¼-H)2Cr2(CO)9]2- and [(Î¼-H)2Cr2(CO)8]2- Dianions. Journal of Physical Chemistry A, 2001, 105, 11134-11143.	1.1	37
22	A Twist of the Twist Mechanism, 2-Iodoxybenzoic Acid (IBX)-Mediated Oxidation of Alcohol Revisited: Theory and Experiment. Organic Letters, 2017, 19, 6502-6505.	2.4	35
23	Reduction of Dinitrogen via 2,3â€²-Bipyridine-Mediated Tetraboration. Journal of the American Chemical Society, 2020, 142, 6244-6250.	6.6	35
24	The germanium clusters Gen(n= 1â€“6) and their anions: structures, thermochemistry and electron affinities. Molecular Physics, 2004, 102, 579-598.	0.8	33
25	Metalâ^'Metal Quintuple and Sextuple Bonding in Bent Dimetallocenes of the Third Row Transition Metals. Journal of Chemical Theory and Computation, 2010, 6, 735-746.	2.3	30
26	Communication: Some critical features of the potential energy surface for the Cl + H2O â†' HCl + OH forward and reverse reactions. Journal of Chemical Physics, 2013, 139, 041101.	1.2	29
27	Acetylene: Synergy between theory and experiment. Journal of Chemical Physics, 1993, 98, 8384-8391.	1.2	28
28	Naked organosulfur clusters: The infrared spectrum of the C2S molecule. Journal of Chemical Physics, 1992, 96, 3714-3717.	1.2	26
29	Pushâ€“Pull Stabilization of Parent Monochlorosilylenes. Journal of the American Chemical Society, 2016, 138, 9799-9802.	6.6	26
30	Stabilizing a different cyclooctatetraene stereoisomer. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 9803-9808.	3.3	26
31	Metalâ€“Substrate Cooperation Mechanism for Dehydrogenative Amidation Catalyzed by a PNN-Ru Catalyst. Inorganic Chemistry, 2018, 57, 8778-8787.	1.9	24
32	What is the lowest energy structure of the NS2molecule?. Journal of Chemical Physics, 1990, 92, 3683-3687.	1.2	23
33	Sulfur clusters: structure, infrared, and Raman spectra of cyclo-S6and comparison with the hypothetical cyclo-O6molecule. Molecular Physics, 1992, 76, 537-546.	0.8	23
34	The Symmetric Exchange Reaction OH + H2O â†' H2O + OH: Convergent Quantum Mechanical Predictions. Journal of Physical Chemistry A, 2016, 120, 10223-10230.	1.1	23
35	Stable Boron Dithiolene Radicals. Angewandte Chemie - International Edition, 2018, 57, 7865-7868.	7.2	23
36	F + (H2O)2 Reaction: The Second Water Removes the Barrier. Journal of Physical Chemistry A, 2013, 117, 11979-11982.	1.1	20

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37	Transitionâ€Metalâ€Mediated Cleavage of a Sï¿¾Si Double Bond. Angewandte Chemie - International Edition, 2015, 54, 10267-10270.	7.2	20
38	The barrier height for decomposition of HN2. Journal of Chemical Physics, 1998, 108, 8029-8030.	1.2	19
39	Binuclear Alkaline Earth Metal Compounds (Be, Mg, Ca, Sr, Ba) with Î±-Diimine Ligands: A Computational Study. Organometallics, 2011, 30, 3113-3118.	1.1	18
40	Benchmarking the Electron Affinity of Uracil. Journal of Chemical Theory and Computation, 2014, 10, 609-612.	2.3	18
41	Synthesis and molecular structure of an unusual â€“Gaâ€“Gaâ€“Gaâ€“ linked organometallic. Chemical Communications, 2000, , 453-454.	2.2	17
42	The puzzling infrared spectra of the nitric oxide dimer radical cation: a systematic application of Brueckner methods. Molecular Physics, 2000, 98, 955-959.	0.8	17
43	Facile Conversion of Bis-Silylene to Cyclic Silylene Isomers: Unexpected Câ€“N and Câ€“H Bond Cleavage. Journal of the American Chemical Society, 2017, 139, 16109-16112.	6.6	17
44	Carbeneâ€Stabilized Disilicon as a Siliconâ€Transfer Agent: Synthesis of a Dianionic Silicon Tris(dithiolene) Complex. Angewandte Chemie - International Edition, 2020, 59, 8864-8867.	7.2	16
45	The silaformyl radical HSiO and its SiOH isomer. Journal of Chemical Physics, 1990, 93, 1196-1199.	1.2	15
46	The infrared spectrum of trimethylenemethane. Predictions of inâ€plane vibrational frequencies from correlated wave functions. Journal of Chemical Physics, 1990, 92, 1174-1179.	1.2	15
47	The description of elementary organoaluminum fragments: AlCHx (x=1,2,3). Journal of Chemical Physics, 1991, 95, 1834-1837.	1.2	14
48	The SiOHâ€“HSiO system: A high level quantum mechanical study. Journal of Chemical Physics, 1996, 105, 1951-1958.	1.2	14
49	Structures, thermochemistry, and electron affinities of the disilicon fluorides, Si2Fn/Si2Fâ^'n(n= 1â€“6). Molecular Physics, 2001, 99, 1053-1074.	0.8	14
50	Protonation of carbene-stabilized diphosphorus: complexation of HP₂⁺. Chemical Communications, 2016, 52, 5746-5748.	2.2	14
51	Acceleration Effect of Bases on Mn Pincer Complex-Catalyzed CO₂ Hydroboration. Inorganic Chemistry, 2022, 61, 3970-3980.	1.9	14
52	The electron affinity of CF. Journal of Chemical Physics, 1994, 101, 10191-10192.	1.2	13
53	Conformational Preferences of Gas-Phase Helices: Experiment and Theory Struggle to Agree: The Seven-Residue Peptide Ac-Phe-(Ala)5-Lys-H+. Chemistry - A European Journal, 2012, 18, 12941-12944.	1.7	13
54	Electron affinities, molecular structures, and thermochemistry of the fluorine, chlorine and bromine substituted methyl radicals. Molecular Physics, 2002, 100, 3615-3648.	0.8	12

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55	Molecular structures, thermochemistry, and electron affinities for the dichlorine oxides: Cl2On/Cl2Oâ€‰â^'n (n= 1-4). International Journal of Quantum Chemistry, 2003, 95, 731-757.	1.0	12
56	Designing new Togni reagents by computation. Chemical Communications, 2019, 55, 5667-5670.	2.2	12
57	Redox chemistry of an anionic dithiolene radical. Dalton Transactions, 2019, 48, 3543-3546.	1.6	12
58	III: PROPERTIES OF COMPLEX SYSTEMS. Molecular Physics, 2003, 101, 211-225.	0.8	11
59	(Acetylene)dicobalt Carbonyl Derivatives: Decarbonylation of the H₂C₂Co₂(CO)₆Tetrahedrane. Organometallics, 2009, 28, 3390-3394.	1.1	11
60	Does the metalâ€“metal sextuple bond exist in the bimetallic sandwich compounds Cr₂(C₆H₆)₂, Mo₂(C₆H₆)₂, and W₂(C₆H₆)₂?^{â€}. Molecular Physics, 2013, 111, 2523-2535.	0.8	11
61	From Gasâ€Phase to Liquidâ€Water Chemical Reactions: The Fluorine Atom Plus Water Trimer System. Angewandte Chemie - International Edition, 2015, 54, 11223-11226.	7.2	11
62	The Hydrogen Abstraction Reaction H₂S + OH â†' H₂O + SH: Convergent Quantum Mechanical Predictions. Journal of Physical Chemistry A, 2017, 121, 9136-9145.	1.1	11
63	A Stable Naked Dithiolene Radical Anion and Synergic THF Ring-Opening. Journal of the American Chemical Society, 2020, 142, 17301-17305.	6.6	11
64	Anchoring the potential energy surface for the BrÂ+ÂH2OÂ†'ÂHBrÂ+ÂOH reaction. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	10
65	Conformers, properties, and docking mechanism of the anticancer drug docetaxel: DFT and molecular dynamics studies. Journal of Computational Chemistry, 2018, 39, 889-900.	1.5	10
66	The Recently Synthesized Dimagnesiabutadiene and the Analogous Dimetallaâ€Beryllium, â€Calcium, â€Strontium, and â€Barium Compounds. Chemistry - A European Journal, 2016, 22, 15019-15026.	1.7	9
67	Lewis base-complexed magnesium dithiolenes. Chemical Communications, 2019, 55, 8087-8089.	2.2	9
68	The HO2 + ion. Molecular Physics, 1989, 68, 1095-1109.	0.8	8
69	The silyl anion (SiHâ^'3): Harmonic vibrational frequencies and infrared intensities predicted at the SCF, CISD, and CCSD levels of theory with substantial basis sets. Journal of Chemical Physics, 1990, 93, 8098-8104.	1.2	8
70	Ring structure of the NO dimer radical cation: A possible new assignment of the mysterious IR absorption at 1424 cmâ^'1. Journal of Chemical Physics, 2002, 117, 9727-9732.	1.2	8
71	Hypervalent molecules, sulfuranes, and persulfuranes: review and studies related to the recent synthesis of the first persulfurane with all substituents carbon-linked. Theoretical Chemistry Accounts, 2009, 124, 151-159.	0.5	8
72	The exothermic HCl + OHÂ·(H2O) reaction: Removal of the HCl + OH barrier by a single water molecule. Journal of Chemical Physics, 2014, 140, 124316.	1.2	8

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73	The electronic spectra of SNS. Lowâ€lying doublet states. Journal of Chemical Physics, 1990, 93, 5053-5061.	1.2	7
74	The silyl anion (SiHâ¯3): Cubic/quartic force field and anharmonic contributions to the fundamental vibrational frequencies. Journal of Chemical Physics, 1991, 94, 8112-8121.	1.2	7
75	Features of the potential energy surface for the SiO + OH â† SiO2+ H reaction: relationship to oxygen isotopic partitioning during gas phase SiO2formation. RSC Advances, 2014, 4, 47163-47168.	1.7	7
76	The electronic spectrum of NS2: Lowâ€lying quartet states. Journal of Chemical Physics, 1991, 94, 1277-1287.	1.2	6
77	Novel bromine oxyfluorides: structures, thermochemistry and electron affinities of BrOFn/BrO (nâ€‰=â€‰1â€“5). Molecular Physics, 2005, 103, 1995-2008.	0.8	6
78	Binuclear hexafluorocyclopentadiene iron carbonyls: bis(dihapto) versus trihaptoâ€“monohapto bonding in ironâ€“iron bonded structures. New Journal of Chemistry, 2013, 37, 2902.	1.4	6
79	Ligand conformations and spin states in open metallocenes of the first row transition metals having U-shaped 2,4-dimethylpentadienyl ligands. New Journal of Chemistry, 2016, 40, 8511-8521.	1.4	6
80	From gas-phase to liquid water chemical reactions: The F + (H2O) , n= 1â€“4 systems. Chemical Physics Letters, 2016, 648, 1-7.	1.2	6
81	Stable Boron Dithiolene Radicals. Angewandte Chemie, 2018, 130, 7991-7994.	1.6	6
82	Unusual Î·¹â€Coordinated Alkyne and Alkene Complexes. Chemistry - A European Journal, 2019, 25, 15628-15633.	1.7	6
83	Binding modes of cabazitaxel with the different human Î²-tubulin isotypes: DFT and MD studies. Journal of Molecular Modeling, 2020, 26, 162.	0.8	6
84	Carbonylic-Carbon-Centered Mechanism for Catalytic Î±-Methylation. Organometallics, 2021, 40, 2420-2429.	1.1	6
85	Carbeneâ€Stabilized Dithiolene (L⁰) Zwitterions. Angewandte Chemie - International Edition, 2021, 60, 22706-22710.	7.2	6
86	The lowest triplet electronic states of polyacenes and perfluoropolyacenes. Molecular Physics, 2007, 105, 2743-2752.	0.8	5
87	Binuclear Cyclopentadienylmolybdenum Carbonyl Derivatives: Where is the Missing Moâ•Mo Double-Bonded Species Cp₂Mo₂(CO)₅?. Organometallics, 2009, 28, 2818-2829.	1.1	5
88	Iron carbonyl thioboronyls: effect of substitution of sulfur for oxygen in the viability of binuclear complexes toward dissociation reactions. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	4
89	How Small Can a Catenane Be?. Journal of Chemical Theory and Computation, 2014, 10, 1511-1517.	2.3	4
90	Tris(butadiene) Metal Complexes of the First-Row Transition Metals versus Coupling of Butadiene to Eight- and Twelve-Carbon Hydrocarbon Chains. Journal of Physical Chemistry A, 2019, 123, 5542-5554.	1.1	4

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91	Labile Imidazolium Cyclopentadienides. Organometallics, 2019, 38, 4578-4584.	1.1	4
92	Carbeneâ€Stabilized Disilicon as a Siliconâ€Transfer Agent: Synthesis of a Dianionic Silicon Tris(dithiolene) Complex. Angewandte Chemie, 2020, 132, 8949-8952.	1.6	4
93	Heteroatom (N, P, As, Sb, Bi) Effects on the Resonance-Stabilized 2-, 3-, and 4-Picolyl Radicals. Inorganic Chemistry, 2021, 60, 5860-5867.	1.9	4
94	Protonated Digermane, Distannane, and Diplumbane: Can They Be Made in the Laboratory?. European Journal of Inorganic Chemistry, 2014, 2014, 5015-5020.	1.0	3
95	The LiÂ·Â·Â·HF van der Waals minimum and the barrier to the deep HFâ€“Li potential well. Molecular Physics, 2014, 112, 770-773.	0.8	3
96	From spiropentane to butterfly and tetrahedral structures in tetranuclear iron carbonyl carbide chemistry. New Journal of Chemistry, 2014, 38, 3762-3769.	1.4	3
97	I + (H₂O)₂ â†' HI + (H₂O)OH Forward and Reverse Reactions. CCSD(T) Studies Including Spinâ€“Orbit Coupling. Journal of Physical Chemistry B, 2016, 120, 1743-1748.	1.2	3
98	The Reaction between Bromine and the Water Dimer and the Highly Exothermic Reverse Reaction. Journal of Computational Chemistry, 2016, 37, 177-182.	1.5	3
99	Noncovalent Interactions between Molecular Hydrogen and the Alkali Fluorides: Hâ€“HÂ·Â·Â·Fâ€“M (M = Li,) Tj ETQq1 1 0.784314 rgBT Computation, 2018, 14, 5118-5127.	2.3	3
100	Quantitative Theoretical Predictions and Qualitative Bonding Analysis of the Divinylborinium System and Its Al, Ga, In, and Tl Congeners. Inorganic Chemistry, 2018, 57, 7851-7859.	1.9	3
101	Dibridged, Monobridged, Vinylidene-Like, and Linear Structures for the Alkaline Earth Dihydrides Be₂H₂, Mg₂H₂, Ca₂H₂, Sr₂H₂, and Ba₂H₂. Proposals for Observations. Inorganic Chemistry, 2020, 59, 10404-10408.	1.9	3
102	Carbene-mediated synthesis of a germanium tris(dithiolene)dianion. Chemical Communications, 2021, 57, 2543-2546.	2.2	3
103	The Energy Difference between the Triply-Bridged and All-Terminal Structures of Co₄(CO)₁₂, Rh₄(CO)₁₂, and Ir₄(CO)₁₂: A Difficult Test for Conventional Density Functional Methods. Journal of Chemical Theory and Computation, 2015, 11, 940-949.	2.3	2
104	New Titanium Carbonyls: Ti2(CO)10, Ti2(CO)11, and Ti2(CO)12. Journal of Physical Chemistry A, 2015, 119, 5224-5232.	1.1	2
105	1,1â€Dilithioethylene: Toward Spectroscopic Identification of the Definitive Singlet Ground Electronic State of a Peculiar Structure. ChemPhysChem, 2016, 17, 1623-1629.	1.0	2
106	Alternative modes of bonding of C4F8 units in mononuclear and binuclear iron carbonyl complexes. New Journal of Chemistry, 2019, 43, 6932-6942.	1.4	2
107	Stabilizing Borinium Cations [Xâ€“Bâ€“X]⁺ through Conjugation and Hyperconjugation Effects. Inorganic Chemistry, 2019, 58, 243-249.	1.9	2
108	Hydrogen Abstraction Reaction H2Se + OH â†' H2O + SeH: Comparison with the Analogous Hydrogen Sulfide and Water Reactions. Inorganic Chemistry, 2019, 58, 2069-2079.	1.9	2

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109	C5 Metalation of Imidazole-Based Monothiolates en Route to Selenothiolates. Organometallics, 2020, 39, 4178-4182.	1.1	2
110	Unusual Structures of the Parent Molecules Diarsene, Distibene, and Dibismuthene: Toward Their Observation. Chemistry - A European Journal, 2020, 26, 14159-14166.	1.7	2
111	Fluorine Migration from Carbon to Iron and Fluorineâ€“Iron Dative Bonds in Octafluorocyclohexadiene Iron Carbonyl Chemistry. Organometallics, 2021, 40, 397-407.	1.1	2
112	Synthesis of Methanesulfonic Acid Directly from Methane: The Cation Mechanism or the Radical Mechanism?. Journal of Physical Chemistry Letters, 2021, 12, 6486-6491.	2.1	2
113	Potential energy profile for the Cl + (H2O)3 â†' HCl + (H2O)2OH reaction. A CCSD(T) study. Physical Chemistry Chemical Physics, 2021, 23, 26837-26842.	1.3	2
114	¹³C NMR relaxation and computational study of anisole and derivatives in the solution state. Journal of Physical Organic Chemistry, 2012, 25, 1374-1379.	0.9	1
115	Molecular orbital interpretation of the metalâ€“metal multiple bonding in coaxial dibenzene dimetal compounds of iron, manganese, and chromium. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	1
116	The Nature of Lithium Bonding in C₂H₂Li₂, C₆Li₆, and Lithium Halide Dimers. Organometallics, 2019, 38, 4708-4716.	1.1	1
117	Phosphine-Mediated Cleavage of Sulfurâ€“Sulfur Bonds. Organometallics, 2022, 41, 3099-3103.	1.1	1
118	Some â€œremarkably stableâ€•chalcogen(ii) dications, including comparisons with their structurally distinct monocations and neutrals. New Journal of Chemistry, 2012, 36, 2000.	1.4	0
119	Prototypical metalâ€“oxo bonds: the reactions of Cr(PF3)6, Fe(PF3)5, and Ni(PF3)4 with oxygen. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	0
120	Effect of metal complexation on the equilibrium between methylphosphepine and methylphosphanorcaradiene and their benzo analogues. New Journal of Chemistry, 2016, 40, 7804-7813.	1.4	0
121	Metalâ€“metal bonding in biscycloheptatrienyl dimetal compounds of the secondâ€row transition metals. International Journal of Quantum Chemistry, 2017, 117, e25374.	1.0	0
122	Tetranuclear iron carbonyl complexes with a central tin atom: relationship to iron carbonyl carbides. New Journal of Chemistry, 2018, 42, 10898-10905.	1.4	0
123	Increasing the Ligand Field Strength in Butadiene Open Sandwich Compounds from the First to the Second Row Transition Metals. ChemistrySelect, 2020, 5, 6350-6359.	0.7	0
124	Tris(Butadiene) Compounds versus Butadiene Oligomerization in Second-Row Transition Metal Chemistry: Effects of Increased Ligand Fields. Molecules, 2021, 26, 2220.	1.7	0
125	Carbeneâ€Stabilized Dithiolene (L 0) Zwitterions. Angewandte Chemie, 2021, 133, 22888.	1.6	0
126	The role of the phosphorus lone pair in the low-energy binuclear phospholyl vanadium carbonyl structures: comparison with cyclopentadienyl analogues. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	0

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127	Carbon-hydrogen bond activation in bridging cyclobutadiene ligands in unsaturated binuclear vanadium carbonyl derivatives. Journal of Molecular Modeling, 2022, 28, 39.	0.8	0
128	A Cationic Magnesium-Based Dithiolene Radical. Organometallics, 2022, 41, 527-531.	1.1	0