Peter Hrobarik

List of Publications by Year
in descending order

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Version: 2024-02-01

58 papers	2,384 citations	186265 28 h-index	214800 47 g-index
66 all docs	66 docs citations	66 times ranked	2715 citing authors

#	Article	IF	Citations
1	A free boratriptycene-type Lewis superacid. Chemical Science, 2022, 13, 1608-1617.	7.4	20
2	Investigations on the Spin States of Two Mononuclear Iron(II) Complexes Based on N-Donor Tridentate Schiff Base Ligands Derived from Pyridine-2,6-Dicarboxaldehyde. Inorganics, 2022, 10, 98.	2.7	1
3	Direct Iodination of Electron-Deficient Benzothiazoles: Rapid Access to Two-Photon Absorbing Fluorophores with Quadrupolar D-Ï€-A-Ï€-D Architecture and Tunable Heteroaromatic Core. Organic Letters, 2021, 23, 3460-3465.	4.6	19
4	Oxidative Câ€“H Homocoupling of Pushâ€“Pull Benzothiazoles: An Atom-Economical Route to Highly Emissive Quadrupolar Arylamine-Functionalized 2,2â€²-Bibenzothiazoles with Enhanced Two-Photon Absorption. Organic Letters, 2021, 23, 5512-5517.	4.6	17
5	Nicotinamide-based supergelator self-assembling via asymmetric hydrogen bonding NHâ‹¯OC and Hâ‹¯Brâ‹¯ pattern for reusable, moldable and self-healable nontoxic fuel gels. Journal of Colloid and Interface Science, 2021, 603, 182-190.	9.4	3
6	A Ketimide-Stabilized Palladium Nanocluster with a Hexagonal Aromatic Pd₇ Core. Inorganic Chemistry, 2020, 59, 1471-1480.	4.0	24
7	Hydride Transfer to Gold: Yes or No? Exploring the Unexpected Versatility of Auâ‹…â‹…â‹…Hâ‹¯M Bonding in Heterobimetallic Dihydrides. Chemistry - A European Journal, 2020, 26, 8267-8280.	3.3	10
8	Ein neutrales 1,4â€Diborabenzol als Ï€â€Ligand in Actinoidkomplexen. Angewandte Chemie, 2020, 132, 13209-13216.	2.0	5
9	Stable Actinide Ï€ Complexes of a Neutral 1,4â€Diborabenzene. Angewandte Chemie - International Edition, 2020, 59, 13109-13115.	13.8	15
10	Synthesis and Characterization of a Linear, Two-Coordinate Pt(II) Ketimide Complex. Inorganic Chemistry, 2019, 58, 15927-15935.	4.0	11
11	Siâ€“H Bond Activation with Bullockâ€™s Cationic Tungsten(II) Catalyst: CO as Cooperating Ligand. Journal of the American Chemical Society, 2019, 141, 18845-18850.	13.7	17
12	13C NMR Shifts as an Indicator of Uâ€“C Bond Covalency in Uranium(VI) Acetylide Complexes: An Experimental and Computational Study. Inorganic Chemistry, 2019, 58, 4152-4163.	4.0	34
13	Molecular Thorium Compounds with Dichalcogenide Ligands: Synthesis, Structure, ⁷⁷Se NMR Study, and Thermolysis. Inorganic Chemistry, 2018, 57, 14821-14833.	4.0	14
14	Thorium Cubanesâ€“Synthesis, Solid-State and Solution Structures, Thermolysis, and Chalcogen Exchange Reactions. Inorganic Chemistry, 2018, 57, 7129-7141.	4.0	10
15	Solvent-Acidity-Driven Change in Photophysics and Significant Efficiency Improvement in Dye-Sensitized Solar Cells of a Benzothiazole-Derived Organic Sensitizer. Journal of Physical Chemistry C, 2018, 122, 20122-20134.	3.1	9
16	Unlocking Structural Diversity in Gold(III) Hydrides: Unexpected Interplay of cis/trans-Influence on Stability, Insertion Chemistry, and NMR Chemical Shifts. Journal of the American Chemical Society, 2018, 140, 8287-8302.	13.7	53
17	Synthesis, Thermochemistry, Bonding, and¹³C NMR Chemical Shift Analysis of a Phosphorano-Stabilized Carbene of Thorium. Organometallics, 2017, 36, 4519-4524.	2.3	54
18	Insights into transâ€Ligand and Spinâ€Orbit Effects on Electronic Structure and Ligand NMR Shifts in Transitionâ€Metal Complexes. Chemistry - A European Journal, 2017, 23, 9790-9803.	3.3	42

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19	Cooperative Alâ€“H Bond Activation in DIBAL-H: Catalytic Generation of an Alumenium-Ion-Like Lewis Acid for Hydrodefluorinative Friedelâ€“Crafts Alkylation. Journal of the American Chemical Society, 2017, 139, 16334-16342.	13.7	39
20	Insights into trans -Ligand and Spin-Orbit Effects on Electronic Structure and Ligand NMR Shifts in Transition-Metal Complexes. Chemistry - A European Journal, 2017, 23, 9702-9702.	3.3	5
21	Four-Component Relativistic Density Functional Calculations of EPR Parameters for Model Complexes of Tungstoenzymes. Journal of Physical Chemistry A, 2017, 121, 9106-9117.	2.5	5
22	Four-component relativistic density functional theory with the polarisable continuum model: application to EPR parameters and paramagnetic NMR shifts. Molecular Physics, 2017, 115, 214-227.	1.7	21
23	Completing the Heterocubane Family [Cp*AlE]₄ (E = O, S, Se, and Te) by Selective Oxygenation and Sulfuration of [Cp*Al]₄: Density Functional Theory Calculations of [Cp*AlE]₄ and Reactivity of [Cp*AlO]₄ toward Hydrolysis. Inorganic Chemistry, 2016, 55, 4915-4923.	4.0	38
24	Paramagnetic NMR of Phenolic Oxime Copper Complexes: A Joint Experimental and Density Functional Study. Chemistry - A European Journal, 2016, 22, 15328-15339.	3.3	22
25	Giant spinâ€“orbit effects on ¹H and ¹³C NMR shifts for uranium(<scp>vi</scp>) complexes revisited: role of the exchangeâ€“correlation response kernel, bonding analyses, and new predictions. Physical Chemistry Chemical Physics, 2016, 18, 30462-30474.	2.8	42
26	Use of ⁷⁷Se and ¹²⁵Te NMR Spectroscopy to Probe Covalency of the Actinide-Chalcogen Bonding in [Th(E_n){N(SiMe₃)₂}₃]^{â¯} (E = Se, Te;) Tj ET Q q 0 0 0 rg BT /Overlo 138, 814-825.	13.7	98
27	Synthesis, structure and bonding of hexaphenyl thorium(iv): observation of a non-octahedral structure. Chemical Communications, 2016, 52, 689-692.	4.1	30
28	Four-Component Relativistic Density Functional Theory Calculations of EPRg- and Hyperfine-Coupling Tensors Using Hybrid Functionals: Validation on Transition-Metal Complexes with Large Tensor Anisotropies and Higher-Order Spinâ€“Orbit Effects. Journal of Physical Chemistry A, 2015, 119, 12892-12905.	2.5	49
29	A Relativistic Quantum-Chemical Analysis of the trans Influence on ¹H NMR Hydride Shifts in Square-Planar Platinum(II) Complexes. Inorganic Chemistry, 2015, 54, 7199-7208.	4.0	60
30	Mechanism of the cooperative Siâ€“H bond activation at Ruâ€“S bonds. Chemical Science, 2015, 6, 4324-4334.	7.4	76
31	Quadrupolar Benzobisthiazole-Cored Arylamines as Highly Efficient Two-Photon Absorbing Fluorophores. Organic Letters, 2014, 16, 6358-6361.	4.6	52
32	Excited State and Injection Dynamics of Triphenylamine Sensitizers Containing a Benzothiazole Electron-Accepting Group on TiO₂ and Al₂O₃ Thin Films. Journal of Physical Chemistry C, 2014, 118, 28509-28519.	3.1	41
33	Insight into the Mechanism of Carbonyl Hydrosilylation Catalyzed by Brookhartâ€™s Cationic Iridium(III) Pincer Complex. Journal of the American Chemical Society, 2014, 136, 6912-6915.	13.7	93
34	A Heterobimetallic Approach To Stabilize the Elusive Disulfur Radical Trianion (â€œSubsulfideâ€) ${{m S}{{{{ullet}}3- hfill atop 2hfill}}}$. Chemistry - A European Journal, 2013, 19, 1246-1253.	3.3	9
35	A time resolved fluorescence and quantum chemical study of the solar cell sensitizer D149. Dyes and Pigments, 2013, 96, 304-312.	3.7	27
36	A Rare Uranyl(VI)â€“Alkyl Ate Complex [Li(DME)_{1.5}]₂[UO₂(CH₂SiMe₃)₄] and Its Comparison with a Homoleptic Uranium(VI)â€“Hexaalkyl. Angewandte Chemie - International Edition, 2013, 52, 3259-3263.	13.8	67

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37	The Family of Ferroceneâ€Stabilized Silylium Ions: Synthesis,29Siâ€…NMR Characterization, Lewis Acidity, Substituent Scrambling, and Quantumâ€Chemical Analyses. Chemistry - A European Journal, 2013, 19, 16579-16594.	3.3	69
38	Innentitelbild: Gigantische Spin-Bahn-Effekte auf NMR-Verschiebungen in diamagnetischen Actinoid-Komplexen: Richtlinien fÃ¼r die Suche nach Uran(VI)-Hydridkomplexen (Angew. Chem. 43/2012). Angewandte Chemie, 2012, 124, 10830-10830.	2.0	0
39	Giant Spinâ€Orbit Effects on NMR Shifts in Diamagnetic Actinide Complexes: Guiding the Search of Uranium(VI) Hydride Complexes in the Correct Spectral Range. Angewandte Chemie - International Edition, 2012, 51, 10884-10888.	13.8	81
40	[TeX₃]⁺ Cations Stabilized by the Weakly Coordinating [Al(OR^F)₄]^{â^'} Anion: FIR Spectra, Raman Spectra, and Evaluation of an Abnormal Halogen Dependence of the ¹²⁵Teâ€…NMR Chemical Shifts. ChemPlusChem, 2012, 77, 643-651.	2.8	14
41	Relativistic Four-Component DFT Calculations of ¹H NMR Chemical Shifts in Transition-Metal Hydride Complexes: Unusual High-Field Shifts Beyond the Buckinghamâ€“Stephens Model. Journal of Physical Chemistry A, 2011, 115, 5654-5659.	2.5	120
42	Benzothiazoles with Tunable Electron-Withdrawing Strength and Reverse Polarity: A Route to Triphenylamine-Based Chromophores with Enhanced Two-Photon Absorption. Journal of Organic Chemistry, 2011, 76, 8726-8736.	3.2	138
43	Assessment of higher-order spinâ€“orbit effects on electronic g-tensors of d 1 transition-metal complexes by relativistic two- and four-component methods. Theoretical Chemistry Accounts, 2011, 129, 715-725.	1.4	39
44	Molecular Engineering of Benzothiazolium Salts with Large Quadratic Hyperpolarizabilities: Can Auxiliary Electron-Withdrawing Groups Enhance Nonlinear Optical Responses?. Journal of Physical Chemistry C, 2010, 114, 22289-22302.	3.1	111
45	Benzothiazole-Based Fluorophores of Donorâ^'Ï€-Acceptorâ^'Ï€-Donor Type Displaying High Two-Photon Absorption. Journal of Organic Chemistry, 2010, 75, 3053-3068.	3.2	135
46	Relativistic two-component calculations of electronic g-tensor for oxo-molybdenum(V) and oxo-tungsten(V) complexes: The important role of higher-order spin-orbit contributions. Chemical Physics, 2009, 356, 229-235.	1.9	23
47	Jacobsenâ€™s Catalyst for Hydrolytic Kinetic Resolution: Structure Elucidation of Paramagnetic Co(III) Salen Complexes in Solution via Combined NMR and Quantum Chemical Studies. Journal of the American Chemical Society, 2009, 131, 4172-4173.	13.7	54
48	Is Allred's [Hg(cyclam)]³⁺ a True Mercury(III) Complex?. Angewandte Chemie - International Edition, 2008, 47, 8631-8633.	13.8	18
49	Donorâ€“Ï€-acceptor benzothiazole-derived dyes with an extended heteroaryl-containing conjugated system: synthesis, DFT study and antimicrobial activity. Tetrahedron, 2008, 64, 10605-10618.	1.9	71
50	Density functional calculations of NMR shielding tensors for paramagnetic systems with arbitrary spin multiplicity: Validation on 3d metallocenes. Journal of Chemical Physics, 2007, 126, 024107.	3.0	98
51	Computational Studies of Electron Paramagnetic Resonance Parameters for Paramagnetic Molybdenum Complexes. 1. Method Validation on Small and Medium-Sized Systems. Journal of Physical Chemistry B, 2007, 111, 4616-4629.	2.6	34
52	Computational Studies of EPR Parameters for Paramagnetic Molybdenum Complexes. II. Larger MoVSystems Relevant to Molybdenum Enzymes. Inorganic Chemistry, 2007, 46, 8146-8161.	4.0	27
53	The impact of the Ï€â€electron conjugation on ¹⁵N, ¹³C and ¹H NMR chemical shifts in pushâ€“pull benzothiazolium salts. Experimental and theoretical study. Magnetic Resonance in Chemistry, 2007, 45, 942-953.	1.9	12
54	Computational study of bonding trends in the metalloactinyl series EThM and MThMâ€² (E=Nâ^', O, F+; M,) Tj ETQq0 0 0 rgBT /Overlock	2.6	16

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55	Preparation of Novel Push-Pull Benzothiazole Derivatives with Reverse Polarity: Compounds with Potential Non-Linear Optic Application. Synthesis, 2005, 2005, 600-604.	2.3	26
56	Understanding Structure and Bonding in Early Actinide 6d05f0MX6q(M = Thâ˜Np; X = H, F) Complexes in Comparison with Their Transition Metal 5d0Analogues. Journal of the American Chemical Society, 2005, 127, 2591-2599.	13.7	49
57	Computational design of benzothiazole-derived pushâ€“pull dyes with high molecular quadratic hyperpolarizabilities. Physical Chemistry Chemical Physics, 2004, 6, 495-502.	2.8	51
58	Diselenadiphosphetandiselenide und Triselenadiphospholandiselenide - Synthese und Charakterisierung mittels31P- und77Se-FestkÃ¶rper-NMRSpektroskopie. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2001, 627, 1269-1278.	1.2	25