Peter Hrobarik

List of Publications by Year
in descending order

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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	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
2	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
3	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
4	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
5	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 1 1 0.784314 rg BT 138, 814-825.	13.7	104
6	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
7	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
8	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
9	Mechanism of the cooperative Siâ€“H bond activation at Ruâ€“S bonds. Chemical Science, 2015, 6, 4324-4334.	7.4	76
10	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
11	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
12	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
13	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
14	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
15	Synthesis, Thermochemistry, Bonding, and¹³C NMR Chemical Shift Analysis of a Phosphorano-Stabilized Carbene of Thorium. Organometallics, 2017, 36, 4519-4524.	2.3	54
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	Quadrupolar Benzobisthiazole-Cored Arylamines as Highly Efficient Two-Photon Absorbing Fluorophores. Organic Letters, 2014, 16, 6358-6361.	4.6	52
18	Computational design of benzothiazole-derived pushâ€“pull dyes with high molecular quadratic hyperpolarizabilities. Physical Chemistry Chemical Physics, 2004, 6, 495-502.	2.8	51

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19	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
20	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
21	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
22	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
23	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
24	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
25	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
26	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
27	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
28	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
29	Synthesis, structure and bonding of hexaphenyl thorium(iv): observation of a non-octahedral structure. Chemical Communications, 2016, 52, 689-692.	4.1	30
30	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
31	A time resolved fluorescence and quantum chemical study of the solar cell sensitizer D149. Dyes and Pigments, 2013, 96, 304-312.	3.7	27
32	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
33	Diselenadiphosphetandiselenide und Triselenadiphospholandiselenide - Synthese und Charakterisierung mittels31P- und77Se-FestkÃ¶rper-NMRSpektroskopie. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2001, 627, 1269-1278.	1.2	25
34	A Ketimide-Stabilized Palladium Nanocluster with a Hexagonal Aromatic Pd₇ Core. Inorganic Chemistry, 2020, 59, 1471-1480.	4.0	24
35	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
36	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

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37	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
38	A free boratriptycene-type Lewis superacid. Chemical Science, 2022, 13, 1608-1617.	7.4	20
39	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
40	Is Allred's [Hg(cyclam)]³⁺ a True Mercury(III) Complex?. Angewandte Chemie - International Edition, 2008, 47, 8631-8633.	13.8	18
41	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
42	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
43	Computational study of bonding trends in the metalloactinyl series EThM and MThMâ€² (E=Nâˆ’, O, F+; M,) Tj ETQq1 1 0.784314 rgBT	2.6	16
44	Stable Actinide Ï€ Complexes of a Neutral 1,4â€Diborabenzene. Angewandte Chemie - International Edition, 2020, 59, 13109-13115.	13.8	15
45	[TeX₃]⁺ Cations Stabilized by the Weakly Coordinating [Al(OR^F)₄]^{âˆ’} 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
46	Molecular Thorium Compounds with Dichalcogenide Ligands: Synthesis, Structure, ⁷⁷Se NMR Study, and Thermolysis. Inorganic Chemistry, 2018, 57, 14821-14833.	4.0	14
47	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
48	Synthesis and Characterization of a Linear, Two-Coordinate Pt(II) Ketimide Complex. Inorganic Chemistry, 2019, 58, 15927-15935.	4.0	11
49	Thorium Cubanesâ€“Synthesis, Solid-State and Solution Structures, Thermolysis, and Chalcogen Exchange Reactions. Inorganic Chemistry, 2018, 57, 7129-7141.	4.0	10
50	Hydride Transfer to Gold: Yes or No? Exploring the Unexpected Versatility of Auâ‹…â‹…â‹…Hâˆ’M Bonding in Heterobimetallic Dihydrides. Chemistry - A European Journal, 2020, 26, 8267-8280.	3.3	10
51	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
52	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
53	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
54	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

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55	Ein neutrales 1,4â€Diborabenzol als Ï€â€Ligand in Actinoidkomplexen. Angewandte Chemie, 2020, 132, 13209-13216.	2.0	5
56	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
57	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
58	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