

# Michael BÃ¼hl

## List of Publications by Year in descending order

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136  
papers

4,767  
citations

109321

35  
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114465

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139  
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139  
docs citations

139  
times ranked

4182  
citing authors

#	ARTICLE	IF	CITATIONS
1	Geometries of Transition-Metal Complexes from Density-Functional Theory. Journal of Chemical Theory and Computation, 2006, 2, 1282-1290.	5.3	557
2	Geometries of Third-Row Transition-Metal Complexes from Density-Functional Theory. Journal of Chemical Theory and Computation, 2008, 4, 1449-1459.	5.3	421
3	The DFT route to NMR chemical shifts. Journal of Computational Chemistry, 1999, 20, 91-105.	3.3	274
4	Hydrogen Generation from Alcohols Catalyzed by Ruthenium <sup>II</sup> -Triphenylphosphine Complexes: Multiple Reaction Pathways. Journal of the American Chemical Society, 2010, 132, 8056-8070.	13.7	215
5	Geometries of Second-Row Transition-Metal Complexes from Density-Functional Theory. Journal of Chemical Theory and Computation, 2007, 3, 2234-2242.	5.3	154
6	Density functional computations of transition metal NMR chemical shifts: dramatic effects of Hartree-Fock exchange. Chemical Physics Letters, 1997, 267, 251-257.	2.6	143
7	Noncovalent Interactions in a Transition-Metal Triphenylphosphine Complex: a Density Functional Case Study. Inorganic Chemistry, 2009, 48, 4622-4624.	4.0	136
8	Medium Effects on <sup>51</sup> V NMR Chemical Shifts: A Density Functional Study. Chemistry - A European Journal, 2001, 7, 4487-4494.	3.3	108
9	Mechanism of Alkyne Alkoxy carbonylation at a Pd Catalyst with P,N Hemilabile Ligands: A Density Functional Study. Chemistry - A European Journal, 2014, 20, 13923-13926.	3.3	79
10	NMR spectroscopy: quantum <sup>2</sup> chemical calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 634-647.	14.6	76
11	Simulation of <sup>59</sup> Co NMR Chemical Shifts in Aqueous Solution. Chemistry - A European Journal, 2006, 12, 477-488.	3.3	63
12	Understanding a Hydroformylation Catalyst that Produces Branched Aldehydes from Alkyl Alkenes. Journal of the American Chemical Society, 2017, 139, 15921-15932.	13.7	63
13	Uncovering the Mechanism of Homogeneous Methyl Methacrylate Formation with P,N Chelating Ligands and Palladium: Favored Reaction Channels and Selectivities. Organometallics, 2015, 34, 438-449.	2.3	57
14	Molecular mechanism of activation of human musk receptors OR5AN1 and OR1A1 by ( <i>i&gt;R&lt;/i&gt; ) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 2 Sciences of the United States of America, 2018, 115, E3950-E3958.</i>	7.1	57
15	Mechanism of Water Exchange in Aqueous Uranyl(VI) Ion. A Density Functional Molecular Dynamics Study. Inorganic Chemistry, 2006, 45, 3834-3836.	4.0	56
16	Insights into Uranyl Chemistry from Molecular Dynamics Simulations. ChemPhysChem, 2011, 12, 3095-3105.	2.1	54
17	First-Principles Calculations of Paramagnetic NMR Shifts. , 2004, , 325-338.		52
18	Theoretical investigations of NMR chemical shifts and reactivities of oxovanadium(v) compounds. Journal of Computational Chemistry, 1998, 19, 113-122.	3.3	51

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19	Liquid Methanol from DFT and DFT/MM Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 106-118.	5.3	51
20	Thermal and solvent effects on <sup>57</sup> Fe NMR chemical shifts. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 5508-5514.	2.8	50
21	Density Functional Theory Study of Uranium(VI) Aquo Chloro Complexes in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2008, 112, 2428-2436.	2.5	50
22	Oxygen Exchange in Uranyl Hydroxide via Two "Nonclassical" Ions. <i>Inorganic Chemistry</i> , 2010, 49, 3821-3827.	4.0	48
23	Water versus Acetonitrile Coordination to Uranyl. Density Functional Study of Cooperative Polarization Effects in Solution. <i>Inorganic Chemistry</i> , 2011, 50, 299-308.	4.0	48
24	X-ray Structures and DFT Calculations on Rhodium <sup>+</sup> Olefin Complexes: Comments on the <sup>103</sup> Rh NMR Shift-Stability Correlation. <i>Organometallics</i> , 2000, 19, 5589-5596.	2.3	47
25	Calculations of One-Electron Redox Potentials of Oxoiron(IV) Porphyrin Complexes. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 243-251.	5.3	47
26	Remarkably Large Geometry Dependence of <sup>57</sup> Fe NMR Chemical Shifts. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 2312-2315.	13.8	46
27	Chapter 3 DFT Computations of Transition-Metal Chemical Shifts. <i>Annual Reports on NMR Spectroscopy</i> , 2008, , 77-126.	1.5	43
28	Geometrically Enforced Donor-Facilitated Dehydrocoupling Leading to an Isolable Arsanylidine-Phosphorane. <i>Journal of the American Chemical Society</i> , 2014, 136, 6247-6250.	13.7	41
29	Hyperconjugation Is the Source of Helicity in Perfluorinated <i>n</i> -Alkanes. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 7867-7870.	13.8	41
30	Modeling Molecular Crystals by QM/MM: Self-Consistent Electrostatic Embedding for Geometry Optimizations and Molecular Property Calculations in the Solid. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 498-508.	5.3	39
31	The Role of Metal Hydroxide Complexes in Late Transition Metal-Mediated Transmetalation Reaction: The Case of Gold. <i>Advanced Synthesis and Catalysis</i> , 2012, 354, 2380-2386.	4.3	39
32	On the Importance of Decarbonylation as a Side- <i>Reaction</i> in the Ruthenium-Catalysed Dehydrogenation of Alcohols: A Combined Experimental and Density Functional Study. <i>Chemistry - A European Journal</i> , 2014, 20, 4141-4155.	3.3	39
33	Density-Functional Computation of <sup>99</sup> Ru NMR Parameters. <i>Chemistry - A European Journal</i> , 2000, 6, 3272-3280.	3.3	37
34	On the rate-determining step and the ligand electronic effects in rhodium catalysed hydrogenation of enamines and the hydroaminomethylation of alkenes. <i>Catalysis Science and Technology</i> , 2011, 1, 431.	4.1	36
35	Analysis of C-F...FC Interactions on Cyclohexane and Naphthalene Frameworks. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7901-7910.	2.5	36
36	Bicarbonate and Alkyl Carbonate Radicals: Structural Integrity and Reactions with Lipid Components. <i>Journal of the American Chemical Society</i> , 2015, 137, 16153-16162.	13.7	36

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37	Density Functional Calculations of <sup>95</sup> Mo NMR Chemical Shifts: Applications to Model Catalysts for Imine Metathesis. <i>Chemistry - A European Journal</i> , 1999, 5, 3514-3522.	3.3	35
38	Weak Te,Te Interactions through the Looking Glass of NMR Spin-Spin Coupling. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 2495-2498.	13.8	34
39	Structural, Spectroscopic and Computational Examination of the Dative Interaction in Constrained Phosphine-Sbines and Phosphine-Sboranes. <i>Chemistry - A European Journal</i> , 2015, 21, 7520-7531.	3.3	33
40	Density functional computation of <sup>55</sup> Mn NMR parameters. <i>Theoretical Chemistry Accounts</i> , 2002, 107, 336-342.	1.4	31
41	Computational <sup>59</sup> Co NMR Spectroscopy: Beyond Static Molecules. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 181-193.	5.3	30
42	The X-ray Structures of Sulfones. <i>Journal of Chemical Crystallography</i> , 2010, 40, 253-265.	1.1	29
43	Acidity of Uranyl(VI) Hydrate Studied with First-Principles Molecular Dynamics Simulations. <i>ChemPhysChem</i> , 2006, 7, 2290-2293.	2.1	27
44	Stereoelectronic Interactions and the One-Bond C-F Coupling Constant in Sevoflurane. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1677-1682.	2.5	26
45	Structure-directing effects in (110)-layered hybrid perovskites containing two distinct organic moieties. <i>Chemical Communications</i> , 2019, 55, 9935-9938.	4.1	26
46	Density functional computation of <sup>49</sup> Ti NMR chemical shifts. <i>Magnetic Resonance in Chemistry</i> , 2004, 42, 737-744.	1.9	25
47	Density functional study of aqueous uranyl(VI) fluoride complexes. <i>Chemical Physics Letters</i> , 2009, 467, 287-293.	2.6	25
48	Effect of Counterions on the Structure and Stability of Aqueous Uranyl(VI) Complexes. A First-Principles Molecular Dynamics Study. <i>Inorganic Chemistry</i> , 2009, 48, 9977-9979.	4.0	25
49	Selenation/Thionation of $\alpha$ -Amino Acids: Formation and X-ray Structures of Diselenopiperazine and Dithiopiperazine and Related Compounds. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 3067-3073.	2.4	25
50	Water versus Acetonitrile Coordination to Uranyl. Effect of Chloride Ligands. <i>Inorganic Chemistry</i> , 2012, 51, 1943-1952.	4.0	24
51	Structure and Dynamics of Iron Pentacarbonyl. <i>Organometallics</i> , 2019, 38, 4288-4297.	2.3	24
52	1,2-Difluoroethane: the angular dependence on <sup>1</sup> JCF coupling constants is independent of hyperconjugation. <i>Chemical Communications</i> , 2012, 48, 2433.	4.1	23
53	Geminally Substituted Tris(acenaphthyl) and Bis(acenaphthyl) Arsines, Stibines, and Bismuthine: A Structural and Nuclear Magnetic Resonance Investigation. <i>Inorganic Chemistry</i> , 2016, 55, 7117-7125.	4.0	23
54	Density-functional computation of <sup>53</sup> Cr NMR chemical shifts. <i>Magnetic Resonance in Chemistry</i> , 2006, 44, 661-668.	1.9	22

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55	Density-functional computation of <sup>99</sup> Tc NMR chemical shifts. <i>Magnetic Resonance in Chemistry</i> , 2008, 46, S36-S44.	1.9	22
56	An efficient route for the synthesis of phosphorus-selenium macro-heterocycles. <i>Chemical Communications</i> , 2013, 49, 2619-2621.	4.1	22
57	Particularly strong C-H interactions between benzene and all-cis 1,2,3,4,5,6-hexafluorocyclohexane. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 29475-29478.	2.8	22
58	Paramagnetic NMR of Phenolic Oxime Copper Complexes: A Joint Experimental and Density Functional Study. <i>Chemistry - A European Journal</i> , 2016, 22, 15328-15339.	3.3	22
59	Prediction of a New Delocalised Bonding Motif between Group 15 or Group 16 Atoms. <i>ChemPhysChem</i> , 2011, 12, 2405-2408.	2.1	21
60	Artificial Metalloenzymes as Catalysts for Oxidative Lignin Degradation. <i>ACS Sustainable Chemistry and Engineering</i> , 2018, 6, 15100-15107.	6.7	21
61	Ligand electronic fine-tuning and its repercussion on the photocatalytic activity and mechanistic pathways of the copper-photocatalysed aza-Henry reaction. <i>Catalysis Science and Technology</i> , 2020, 10, 7745-7756.	4.1	21
62	A Density Functional Study of the Rotational Barrier of Tricarbonyl(1,4-norbornadiene)iron. Effect of the Torsional Angle on the Carbonyl Stretching Spectra. <i>Inorganic Chemistry</i> , 1997, 36, 2922-2924.	4.0	20
63	Isomerisation versus carbonylative pathways in the hydroxy-carbonylation, methoxy-carbonylation, and amino-carbonylation of N-tosyl-3-pyrroline. <i>Catalysis Science and Technology</i> , 2016, 6, 7477-7485.	4.1	20
64	On the Origin of <sup>35/37</sup> Cl Isotope Effects on <sup>195</sup> Pt NMR Chemical Shifts. A Density Functional Study. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1344-1350.	5.3	19
65	Hydricity of 3d Transition Metal Complexes from Density Functional Theory: A Benchmarking Study. <i>Molecules</i> , 2021, 26, 4072.	3.8	19
66	peri-Substituted Phosphino-Phosphonium Salts: Synthesis and Reactivity. <i>Organometallics</i> , 2013, 32, 3481-3492.	2.3	18
67	Sterically Restricted Tin Phosphines, Stabilized by Weak Intramolecular Donor-Acceptor Interactions. <i>Organometallics</i> , 2014, 33, 2424-2433.	2.3	18
68	Insights into structure and redox potential of lignin peroxidase from QM/MM calculations. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 2385-2389.	2.8	18
69	Density-functional computation of <sup>93</sup> Nb NMR chemical shifts. <i>Magnetic Resonance in Chemistry</i> , 2010, 48, S61-S68.	1.9	17
70	Inter- and intramolecular C-F...O interactions on aliphatic and cyclohexane carbonyl derivatives. <i>Journal of Computational Chemistry</i> , 2016, 37, 25-33.	3.3	17
71	Dealkenative Main Group Couplings across the peri-Gap. <i>Journal of the American Chemical Society</i> , 2017, 139, 18545-18551.	13.7	17
72	NMR chemical shifts of urea loaded copper benzoate. A joint solid-state NMR and DFT study. <i>Solid State Nuclear Magnetic Resonance</i> , 2019, 101, 31-37.	2.3	17

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73	First experimental evidence for a bis-ethene chromium(I) complex forming from an activated ethene oligomerization catalyst. <i>Science Advances</i> , 2020, 6, .	10.3	17
74	Understanding Catalyst Structure–Selectivity Relationships in Pd-Catalyzed Enantioselective Methoxycarbonylation of Styrene. <i>Organometallics</i> , 2020, 39, 4544-4556.	2.3	17
75	Manganese-Catalyzed Dehydrogenative Synthesis of Urea Derivatives and Polyureas. <i>ACS Catalysis</i> , 2022, 12, 6923-6933.	11.2	17
76	A Study of Through-Space and Through-Bond JPP Coupling in a Rigid Nonsymmetrical Bis(phosphine) and Its Metal Complexes. <i>Inorganic Chemistry</i> , 2018, 57, 3387-3398.	4.0	16
77	Computational NMR Spectroscopy of Transition-Metal/Nitroimidazole Complexes: Theoretical Investigation of Potential Radiosensitizers. <i>Helvetica Chimica Acta</i> , 2005, 88, 2705-2721.	1.6	15
78	Bridging the Gap: Attractive 3c-4e Interactions in peri-Substituted Acenaphthylenes. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 1512-1523.	2.0	15
79	NMR Chemical Shifts of Zr@C28. How Shielded Can 91Zr Get?. <i>Journal of Physical Chemistry A</i> , 1997, 101, 2514-2517.	2.5	14
80	Sterically Crowded Tin Acenaphthenes. <i>Organometallics</i> , 2012, 31, 2922-2930.	2.3	14
81	Hyperconjugation Is the Source of Helicity in Perfluorinated <i>n</i> -Alkanes. <i>Angewandte Chemie</i> , 2017, 129, 7975-7978.	2.0	14
82	Benzylic Functionalisation of Phenyl all-cis-2,3,5,6-Tetrafluorocyclohexane Provides Access to New Organofluorine Building Blocks. <i>Chemistry - A European Journal</i> , 2018, 24, 13290-13296.	3.3	14
83	Palladium-catalysed alkyne alkoxy carbonylation with P,N-chelating ligands revisited: a density functional theory study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8543-8552.	2.8	14
84	Phosphorus–Bismuth <i>peri</i> -Substituted Acenaphthenes: A Synthetic, Structural, and Computational Study. <i>Inorganic Chemistry</i> , 2020, 59, 5616-5625.	4.0	13
85	Effect of Ligand Backbone on the Selectivity and Stability of Rhodium Hydroformylation Catalysts Derived from Phospholane-Phosphites. <i>Organometallics</i> , 2021, 40, 3966-3978.	2.3	13
86	Hydride Abstraction and Deprotonation - an Efficient Route to Low Coordinate Phosphorus and Arsenic Species. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 659-666.	2.0	12
87	Laccase Redox Potentials: pH Dependence and Mutants, a QM/MM Study. <i>Journal of Physical Chemistry B</i> , 2016, 120, 9265-9276.	2.6	12
88	Substituent effects on 61Ni NMR chemical shifts. <i>Dalton Transactions</i> , 2009, , 6037.	3.3	11
89	Binding modes of oxalate in UO2(oxalate) in aqueous solution studied with first-principles molecular dynamics simulations. Implications for the chelate effect. <i>Dalton Transactions</i> , 2011, 40, 11192.	3.3	11
90	Speciation of La(III) Chloride Complexes in Water and Acetonitrile: A Density Functional Study. <i>Inorganic Chemistry</i> , 2012, 51, 13396-13407.	4.0	11

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91	Modelling Zwitterions in Solution: 3-Fluoro- $\beta$ -aminobutyric Acid (3FGABA). Chemistry - A European Journal, 2012, 18, 184-195.	3.3	11
92	Calculation and experimental measurement of paramagnetic NMR parameters of phenolic oximate Cu(II) complexes. Chemical Communications, 2017, 53, 10512-10515.	4.1	11
93	Mechanism of the Catalytic Carboxylation of Alkylboronates with CO <sub>2</sub> Using Ni <sup>II</sup> -NHC Complexes: A DFT Study. Chemistry - A European Journal, 2017, 23, 14954-14961.	3.3	11
94	Design of a Highly Active Pd Catalyst with P,N Hemilabile Ligands for Alkoxy carbonylation of Alkynes and Allenes: A Density Functional Theory Study. Chemistry - A European Journal, 2019, 25, 11625-11629.	3.3	11
95	Palladium-catalysed methoxycarbonylation of ethene with bidentate diphosphine ligands: a density functional theory study. Physical Chemistry Chemical Physics, 2020, 22, 24330-24336.	2.8	11
96	Janus Face All-cis-1,2,4,5-tetrakis(trifluoromethyl)- and All-cis-1,2,3,4,5,6-hexakis(trifluoromethyl)-Cyclohexanes. Angewandte Chemie - International Edition, 2020, 59, 19905-19909.	13.8	11
97	Systematic Evaluation of Modern Density Functional Methods for the Computation of NMR Shifts of 3d Transition-Metal Nuclei. Journal of Chemical Theory and Computation, 2022, 18, 273-292.	5.3	11
98	Conformational preferences of Ac-Gly-NHMe in solution. RSC Advances, 2015, 5, 13052-13060.	3.6	10
99	Nuclear Magnetic Shielding of Monoboranes: Calculation and Assessment of <sup>11</sup> B NMR Chemical Shifts in Planar BX <sub>3</sub> and in Tetrahedral [BX <sub>4</sub> ] <sup>+</sup> Systems. Journal of Physical Chemistry A, 2017, 121, 9631-9637.	2.5	10
100	Isothiourea-Catalyzed Enantioselective Michael Addition of Malonates to $\hat{1},\hat{1}^2$ -Unsaturated Aryl Esters. Organic Letters, 2022, 24, 4040-4045.	4.6	9
101	Computational Insight into <sup>103</sup> Rh Chemical Shifts: Structure Correlations in Rhodium Bis(phosphine) Complexes. Organometallics, 2013, 32, 6437-6444.	2.3	8
102	[UO <sub>2</sub> (NH <sub>3</sub> ) <sub>5</sub> ]Br <sub>2</sub> ·NH <sub>3</sub> : synthesis, crystal structure, and speciation in liquid ammonia solution by first-principles molecular dynamics simulations. Dalton Transactions, 2015, 44, 7332-7337.	3.3	8
103	Dodeka(ethylene)octamine. Chemistry - A European Journal, 2011, 17, 3575-3578.	3.3	7
104	The Synthesis and Evaluation of Fluoro-, Trifluoromethyl-, and Iodomuscimols as GABA Agonists. Chemistry - A European Journal, 2017, 23, 10848-10852.	3.3	7
105	Computational modelling of Pd-catalysed alkoxy carbonylation of alkenes and alkynes. Physical Chemistry Chemical Physics, 2021, 23, 15869-15880.	2.8	7
106	Ab Initio Molecular Dynamics Investigation of Beryllium Complexes. Inorganic Chemistry, 2020, 59, 2413-2425.	4.0	7
107	Expanding the structural chemistry of the weakly coordinating closo-carborane CB <sub>11</sub> H <sub>12</sub> <sup>+</sup> : its monoiodo derivatives with and without C <sub>5v</sub> symmetry. Structural Chemistry, 2013, 24, 927-932.	2.0	6
108	Accommodation of Lattice Mismatch in a Thiol Self-Assembled Monolayer. Journal of Physical Chemistry C, 2013, 117, 4647-4656.	3.1	6

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109	Structure of a uranyl peroxy complex in aqueous solution from first-principles molecular dynamics simulations. Dalton Transactions, 2014, 43, 11129-11137.	3.3	6
110	± and ± Lapachone Isomerization in Acidic Media: Insights from Experimental and Implicit/Explicit Solvation Approaches. ChemPlusChem, 2019, 84, 52-61.	2.8	6
111	Density functional study of the one-bond C F coupling constant in ±-fluorocarbonyl and ±-fluorosulfonyl compounds. Journal of Fluorine Chemistry, 2012, 140, 82-87.	1.7	5
112	Janus Face All-cis-1,2,4,5-tetrakis(trifluoromethyl)- and All-cis-1,2,3,4,5,6-hexakis(trifluoromethyl)-Cyclohexanes. Angewandte Chemie, 2020, 132, 20077-20081.	2.0	5
113	Density Functional Study of Interactions between Fluorinated Cyclohexanes and Arenes. Helvetica Chimica Acta, 2014, 97, 797-807.	1.6	4
114	Acetyl Coenzyme A Analogues as Rationally Designed Inhibitors of Citrate Synthase. ChemBioChem, 2019, 20, 1174-1182.	2.6	4
115	Probing the helical integrity of multivincinal all-syn-fluoro alkanes. Organic and Biomolecular Chemistry, 2020, 18, 878-887.	2.8	4
116	On the Catalytic Activity of [RuH <sub>2</sub> (PPh <sub>3</sub> ) <sub>3</sub> (CO)] (PPh <sub>3</sub> =triphenylphosphine) in Ruthenium-Catalysed Generation of Hydrogen from Alcohols: a Combined Experimental and DFT study. ChemCatChem, 2020, 12, 2995-3009.	3.7	4
117	Unveiling the mechanism of N-methylation of indole with dimethylcarbonate using either DABCO or DBU as catalyst. Journal of Mass Spectrometry, 2021, 56, e4707.	1.6	4
118	Synthetic and Structural Study of peri-Substituted Phosphine-Arsines. Molecules, 2021, 26, 7222.	3.8	4
119	Carbene-like reactivity of methoxy groups in a single crystal SAPO-34 MTO catalyst. Catalysis Science and Technology, 2022, 12, 2289-2305.	4.1	4
120	The Preparation and Structure of [Pt(S <sub>2</sub> N <sub>2</sub> ) <sub>2</sub> ]{P(OR) <sub>n</sub> } <sup>2+</sup> and [Pt(SeSN <sub>2</sub> ) <sub>2</sub> ]{P(OMe) <sub>n</sub> Ph <sub>3</sub> } <sup>+</sup> (n = 0-3). European Journal of Inorganic Chemistry, 2010, 2010, 3185-3194.	2.0	3
121	Computational thermochemistry of iron-platinum carbonyl clusters. Chemical Physics Letters, 2011, 509, 158-161.	2.6	3
122	Infrared Dynamics of Iron Carbonyl Diene Complexes. Journal of Physical Chemistry A, 2018, 122, 3497-3505.	2.5	3
123	SERS of Trititanate Nanotubes: Selective Enhancement of Catechol Compounds. ChemistrySelect, 2018, 3, 8338-8343.	1.5	3
124	Organofluorine chemistry: Difluoromethylene motifs spaced 1,3 to each other imparts facial polarity to a cyclohexane ring. Beilstein Journal of Organic Chemistry, 2016, 12, 2823-2827.	2.2	2
125	Thionylimido Complexes. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2020, 646, 1795-1798.	1.2	2
126	Computational Screening of Anode Coatings for Garnet-type Solid-State Batteries. Batteries and Supercaps, 0, , .	4.7	2



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127	Sulfur and Phosphorus Oxyacid Radicals. Journal of Physical Chemistry A, 2022, 126, 760-771.	2.5	2
128	Origin of the temperature dependence of <sup>13</sup> C pNMR shifts for copper paddlewheel MOFs. Chemical Science, 2022, 13, 2674-2685.	7.4	2
129	Formation of metallacarboxylic acids through Hieber base reaction. A density functional theory study. Journal of Molecular Modeling, 2019, 25, 45.	1.8	1
130	Density Functional Theory Study of Pd Aggregation on a Pyridine-Terminated Self-Assembled Monolayer. Chemistry - A European Journal, 2020, 26, 10555-10563.	3.3	1
131	Inside Cover: Conformational Dependence of Through-Space Tellurium-Tellurium Spin-Spin Coupling in <i>Peri</i> -Substituted Bis(Tellurides) (Chem. Eur. J. 9/2015). Chemistry - A European Journal, 2015, 21, 3506-3506.	3.3	0
132	Modelling uranyl chemistry in liquid ammonia from density functional theory. Chemical Communications, 2018, 54, 10431-10434.	4.1	0
133	Origin of the Diastereoselectivity of the Heterogeneous Hydrogenation of a Substituted Indolizine. Journal of Organic Chemistry, 2020, 85, 11541-11548.	3.2	0
134	Bridging (Thionylimido)metal Complexes. Inorganic Chemistry, 2021, 60, 8423-8427.	4.0	0
135	Electrochemical Generation of Metal Nanostructures Using Self-Assembled Monolayers As Templates. ECS Meeting Abstracts, 2019, , .	0.0	0
136	(Invited) Templated Electrodeposition By Molecular Assemblies: Exploring Limits. ECS Meeting Abstracts, 2020, MA2020-01, 1134-1134.	0.0	0