Michael BÃ¼hl

List of Publications by Year
in descending order

136 papers	4,767 citations	109321 35 h-index	114465 63 g-index
139 all docs	139 docs citations	139 times ranked	4182 citing authors

#	Article	IF	Citations
1	Sulfur and Phosphorus Oxyacid Radicals. Journal of Physical Chemistry A, 2022, 126, 760-771.	2.5	2
2	Origin of the temperature dependence of ¹³C pNMR shifts for copper paddlewheel MOFs. Chemical Science, 2022, 13, 2674-2685.	7.4	2
3	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
4	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
5	Manganese-Catalyzed Dehydrogenative Synthesis of Urea Derivatives and Polyureas. ACS Catalysis, 2022, 12, 6923-6933.	11.2	17
6	Isothiourea-Catalyzed Enantioselective Michael Addition of Malonates to Î±,Î²-Unsaturated Aryl Esters. Organic Letters, 2022, 24, 4040-4045.	4.6	9
7	Unveiling the mechanism of Nâ€methylation of indole with dimethylcarbonate using either DABCO or DBU as catalyst. Journal of Mass Spectrometry, 2021, 56, e4707.	1.6	4
8	Bridging (Thionylimido)metal Complexes. Inorganic Chemistry, 2021, 60, 8423-8427.	4.0	0
9	Hydricity of 3d Transition Metal Complexes from Density Functional Theory: A Benchmarking Study. Molecules, 2021, 26, 4072.	3.8	19
10	Computational modelling of Pd-catalysed alkoxycarbonylation of alkenes and alkynes. Physical Chemistry Chemical Physics, 2021, 23, 15869-15880.	2.8	7
11	Effect of Ligand Backbone on the Selectivity and Stability of Rhodium Hydroformylation Catalysts Derived from Phospholane-Phosphites. Organometallics, 2021, 40, 3966-3978.	2.3	13
12	Synthetic and Structural Study of peri-Substituted Phosphine-Arsines. Molecules, 2021, 26, 7222.	3.8	4
13	Probing the helical integrity of multivicinal all-syn-fluoro alkanes. Organic and Biomolecular Chemistry, 2020, 18, 878-887.	2.8	4
14	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
15	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
16	Origin of the Diastereoselectivity of the Heterogeneous Hydrogenation of a Substituted Indolizine. Journal of Organic Chemistry, 2020, 85, 11541-11548.	3.2	0
17	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
18	Thionylimido Complexes. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2020, 646, 1795-1798.	1.2	2

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19	Ligand electronic fine-tuning and its repercussion on the photocatalytic activity and mechanistic pathways of the copper-photocatalysed aza-Henry reaction. Catalysis Science and Technology, 2020, 10, 7745-7756.	4.1	21
20	First experimental evidence for a bis-ethene chromium(I) complex forming from an activated ethene oligomerization catalyst. Science Advances, 2020, 6, .	10.3	17
21	Understanding Catalyst Structureâ€“Selectivity Relationships in Pd-Catalyzed Enantioselective Methoxycarbonylation of Styrene. Organometallics, 2020, 39, 4544-4556.	2.3	17
22	Density Functional Theory Study of Pd Aggregation on a Pyridineâ€Terminated Selfâ€Assembled Monolayer. Chemistry - A European Journal, 2020, 26, 10555-10563.	3.3	1
23	On the Catalytic Activity of [RuH₂(PPh₃)₃(CO)] (PPh₃=triphenylphosphine) in Rutheniumâ€Catalysed Generation of Hydrogen from Alcohols: a Combined Experimental and DFT study. ChemCatChem, 2020, 12, 2995-3009.	3.7	4
24	Phosphorusâ€“Bismuth Peri-Substituted Acenaphthenes: A Synthetic, Structural, and Computational Study. Inorganic Chemistry, 2020, 59, 5616-5625.	4.0	13
25	Ab Initio Molecular Dynamics Investigation of Beryllium Complexes. Inorganic Chemistry, 2020, 59, 2413-2425.	4.0	7
26	(Invited) Templated Electrodeposition By Molecular Assemblies: Exploring Limits. ECS Meeting Abstracts, 2020, MA2020-01, 1134-1134.	0.0	0
27	Î±â€•and Î²â€Lapachone Isomerization in Acidic Media: Insights from Experimental and Implicit/Explicit Solvation Approaches. ChemPlusChem, 2019, 84, 52-61.	2.8	6
28	Structure-directing effects in (110)-layered hybrid perovskites containing two distinct organic moieties. Chemical Communications, 2019, 55, 9935-9938.	4.1	26
29	Design of a Highly Active Pd Catalyst with P,N Hemilabile Ligands for Alkoxycarbonylation of Alkynes and Allenes: A Density Functional Theory Study. Chemistry - A European Journal, 2019, 25, 11625-11629.	3.3	11
30	Structure and Dynamics of Iron Pentacarbonyl. Organometallics, 2019, 38, 4288-4297.	2.3	24
31	Formation of metallacarboxylic acids through Hieber base reaction. A density functional theory study. Journal of Molecular Modeling, 2019, 25, 45.	1.8	1
32	NMR chemical shifts of urea loaded copper benzoate. A joint solid-state NMR and DFT study. Solid State Nuclear Magnetic Resonance, 2019, 101, 31-37.	2.3	17
33	Palladium-catalysed alkyne alkoxycarbonylation with P,N-chelating ligands revisited: a density functional theory study. Physical Chemistry Chemical Physics, 2019, 21, 8543-8552.	2.8	14
34	Acetyl Coenzymeâ€…A Analogues as Rationally Designed Inhibitors of Citrate Synthase. ChemBioChem, 2019, 20, 1174-1182.	2.6	4
35	Electrochemical Generation of Metal Nanostructures Using Self-Assembled Monolayers As Templates. ECS Meeting Abstracts, 2019, , .	0.0	0
36	A Study of Through-Space and Through-Bond JPP Coupling in a Rigid Nonsymmetrical Bis(phosphine) and Its Metal Complexes. Inorganic Chemistry, 2018, 57, 3387-3398.	4.0	16

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37	Molecular mechanism of activation of human musk receptors OR5AN1 and OR1A1 by (R) Tj ETQq1 1 0.784314 rgBT /Overlock Sciences of the United States of America, 2018, 115, E3950-E3958.	7.1	57
38	Infrared Dynamics of Iron Carbonyl Diene Complexes. Journal of Physical Chemistry A, 2018, 122, 3497-3505.	2.5	3
39	Artificial Metalloenzymes as Catalysts for Oxidative Lignin Degradation. ACS Sustainable Chemistry and Engineering, 2018, 6, 15100-15107.	6.7	21
40	SERS of Trititanate Nanotubes: Selective Enhancement of Catechol Compounds. ChemistrySelect, 2018, 3, 8338-8343.	1.5	3
41	Modelling uranyl chemistry in liquid ammonia from density functional theory. Chemical Communications, 2018, 54, 10431-10434.	4.1	0
42	Benzylic Functionalisation of Phenyl allâ€cisâ€2,3,5,6â€Tetrafluorocyclohexane Provides Access to New Organofluorine Building Blocks. Chemistry - A European Journal, 2018, 24, 13290-13296.	3.3	14
43	The Synthesis and Evaluation of Fluoroâ€, Trifluoromethylâ€, and Iodomuscimols as GABA Agonists. Chemistry - A European Journal, 2017, 23, 10848-10852.	3.3	7
44	Hyperconjugation Is the Source of Helicity in Perfluorinated nâ€Alkanes. Angewandte Chemie, 2017, 129, 7975-7978.	2.0	14
45	Hyperconjugation Is the Source of Helicity in Perfluorinated nâ€Alkanes. Angewandte Chemie - International Edition, 2017, 56, 7867-7870.	13.8	41
46	Understanding a Hydroformylation Catalyst that Produces Branched Aldehydes from Alkyl Alkenes. Journal of the American Chemical Society, 2017, 139, 15921-15932.	13.7	63
47	Calculation and experimental measurement of paramagnetic NMR parameters of phenolic oximate Cu(<scp>ii</scp>) complexes. Chemical Communications, 2017, 53, 10512-10515.	4.1	11
48	Mechanism of the Catalytic Carboxylation of Alkylboronates with CO₂ Using Niâ^'NHC Complexes: A DFT Study. Chemistry - A European Journal, 2017, 23, 14954-14961.	3.3	11
49	Dealkanative Main Group Couplings across the peri-Gap. Journal of the American Chemical Society, 2017, 139, 18545-18551.	13.7	17
50	Nuclear Magnetic Shielding of Monoboranes: Calculation and Assessment of ¹¹B NMR Chemical Shifts in Planar BX₃ and in Tetrahedral [BX₄]^{â^'} Systems. Journal of Physical Chemistry A, 2017, 121, 9631-9637.	2.5	10
51	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
52	Hydride Abstraction and Deprotonation - an Efficient Route to Low Coordinate Phosphorus and Arsenic Species. European Journal of Inorganic Chemistry, 2016, 2016, 659-666.	2.0	12
53	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
54	Isomerisation versus carbonylative pathways in the hydroxy-carbonylation, methoxy-carbonylation, and amino-carbonylation of N-tosyl-3-pyrroline. Catalysis Science and Technology, 2016, 6, 7477-7485.	4.1	20

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55	Laccase Redox Potentials: pH Dependence and Mutants, a QM/MM Study. Journal of Physical Chemistry B, 2016, 120, 9265-9276.	2.6	12
56	Geminally Substituted Tris(acenaphthyl) and Bis(acenaphthyl) Arsines, Stibines, and Bismuthine: A Structural and Nuclear Magnetic Resonance Investigation. Inorganic Chemistry, 2016, 55, 7117-7125.	4.0	23
57	Insights into structure and redox potential of lignin peroxidase from QM/MM calculations. Organic and Biomolecular Chemistry, 2016, 14, 2385-2389.	2.8	18
58	Interâ€•and intramolecular CFÂ·Â·Â·cï£¾o interactions on aliphatic and cyclohexane carbonyl derivatives. Journal of Computational Chemistry, 2016, 37, 25-33.	3.3	17
59	Inside Cover: Conformational Dependence of Throughâ€Space Telluriumâ€“Tellurium Spinâ€“Spin Coupling in Periâ€Substituted Bis(Tellurides) (Chem. Eur. J. 9/2015). Chemistry - A European Journal, 2015, 21, 3506-3506.	3.3	0
60	Structural, Spectroscopic and Computational Examination of the Dative Interaction in Constrained Phosphineâ€“Stibines and Phosphineâ€“Stiboranes. Chemistry - A European Journal, 2015, 21, 7520-7531.	3.3	33
61	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
62	Conformational preferences of Ac-Gly-NHMe in solution. RSC Advances, 2015, 5, 13052-13060.	3.6	10
63	[UO₂(NH₃)₅]Br₂·NH₃: synthesis, crystal structure, and speciation in liquid ammonia solution by first-principles molecular dynamics simulations. Dalton Transactions, 2015, 44, 7332-7337.	3.3	8
64	Bicarbonate and Alkyl Carbonate Radicals: Structural Integrity and Reactions with Lipid Components. Journal of the American Chemical Society, 2015, 137, 16153-16162.	13.7	36
65	Particularly strong Câ€“Hâ‹¯Ï€ interactions between benzene and all-cis 1,2,3,4,5,6-hexafluorocyclohexane. Physical Chemistry Chemical Physics, 2015, 17, 29475-29478.	2.8	22
66	Bridging the Gap: Attractive 3c-4e Interactions inperi-Substituted Acenaphthylenes. European Journal of Inorganic Chemistry, 2014, 2014, 1512-1523.	2.0	15
67	Sterically Restricted Tin Phosphines, Stabilized by Weak Intramolecular Donorâ€“Acceptor Interactions. Organometallics, 2014, 33, 2424-2433.	2.3	18
68	On the Importance of Decarbonylation as a Sideâ€Reaction in the Rutheniumâ€Catalysed Dehydrogenation of Alcohols: A Combined Experimental and Density Functional Study. Chemistry - A European Journal, 2014, 20, 4141-4155.	3.3	39
69	Calculations of One-Electron Redox Potentials of Oxoiron(IV) Porphyrin Complexes. Journal of Chemical Theory and Computation, 2014, 10, 243-251.	5.3	47
70	Mechanism of Alkyne Alkoxycarbonylation at a Pd Catalyst with P,N Hemilabile Ligands: A Density Functional Study. Chemistry - A European Journal, 2014, 20, 13923-13926.	3.3	79
71	Structure of a uranyl peroxo complex in aqueous solution from first-principles molecular dynamics simulations. Dalton Transactions, 2014, 43, 11129-11137.	3.3	6
72	Analysis of CFÂ·Â·Â·FC Interactions on Cyclohexane and Naphthalene Frameworks. Journal of Physical Chemistry A, 2014, 118, 7901-7910.	2.5	36

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73	Geometrically Enforced Donor-Facilitated Dehydrocoupling Leading to an Isolable Arsanylidine-Phosphorane. Journal of the American Chemical Society, 2014, 136, 6247-6250.	13.7	41
74	Density Functional Study of Interactions between Fluorinated Cyclohexanes and Arenes. Helvetica Chimica Acta, 2014, 97, 797-807.	1.6	4
75	Expanding the structural chemistry of the weakly coordinating closo-carborane CB11H12 â¯: its monoiodo derivatives with and without C 5v symmetry. Structural Chemistry, 2013, 24, 927-932.	2.0	6
76	Computational Insight into ¹⁰³Rh Chemical Shiftâ€“Structure Correlations in Rhodium Bis(phosphine) Complexes. Organometallics, 2013, 32, 6437-6444.	2.3	8
77	Liquid Methanol from DFT and DFT/MM Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 106-118.	5.3	51
78	An efficient route for the synthesis of phosphorusâ€“selenium macro-heterocycles. Chemical Communications, 2013, 49, 2619-2621.	4.1	22
79	Accommodation of Lattice Mismatch in a Thiol Self-Assembled Monolayer. Journal of Physical Chemistry C, 2013, 117, 4647-4656.	3.1	6
80	peri-Substituted Phosphino-Phosphonium Salts: Synthesis and Reactivity. Organometallics, 2013, 32, 3481-3492.	2.3	18
81	Weak Te,Te Interactions through the Looking Glass of NMR Spinâ€“Spin Coupling. Angewandte Chemie - International Edition, 2013, 52, 2495-2498.	13.8	34
82	Sterically Crowded Tin Acenaphthenes. Organometallics, 2012, 31, 2922-2930.	2.3	14
83	Modeling Molecular Crystals by QM/MM: Self-Consistent Electrostatic Embedding for Geometry Optimizations and Molecular Property Calculations in the Solid. Journal of Chemical Theory and Computation, 2012, 8, 498-508.	5.3	39
84	Stereoelectronic Interactions and the One-Bond Câ€“F Coupling Constant in Sevoflurane. Journal of Physical Chemistry A, 2012, 116, 1677-1682.	2.5	26
85	Water versus Acetonitrile Coordination to Uranyl. Effect of Chloride Ligands. Inorganic Chemistry, 2012, 51, 1943-1952.	4.0	24
86	1,2-Difluoroethane: the angular dependance on 1JCF coupling constants is independent of hyperconjugation. Chemical Communications, 2012, 48, 2433.	4.1	23
87	The Role of Metal Hydroxide Complexes in Late Transition Metalâ€Mediated Transmetalation Reaction: The Case of Gold. Advanced Synthesis and Catalysis, 2012, 354, 2380-2386.	4.3	39
88	Speciation of La(III) Chloride Complexes in Water and Acetonitrile: A Density Functional Study. Inorganic Chemistry, 2012, 51, 13396-13407.	4.0	11
89	On the Origin of ^{35/37}Cl Isotope Effects on ¹⁹⁵Pt NMR Chemical Shifts. A Density Functional Study. Journal of Chemical Theory and Computation, 2012, 8, 1344-1350.	5.3	19
90	Density functional study of the one-bond C F coupling constant in Î±-fluorocarbonyl and Î±-fluorosulfonyl compounds. Journal of Fluorine Chemistry, 2012, 140, 82-87.	1.7	5

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91	Modelling Zwitterions in Solution: 3â€Fluoroâ€Î³â€aminobutyric Acid (3Fâ€GABA). Chemistry - A European Journal, 2012, 18, 184-195.	3.3	11
92	Binding modes of oxalate in UO2(oxalate) in aqueous solution studied with first-principles molecular dynamics simulations. Implications for the chelate effect. Dalton Transactions, 2011, 40, 11192.	3.3	11
93	On the rate-determining step and the ligand electronic effects in rhodium catalysed hydrogenation of enamines and the hydroaminomethylation of alkenes. Catalysis Science and Technology, 2011, 1, 431.	4.1	36
94	Water versus Acetonitrile Coordination to Uranyl. Density Functional Study of Cooperative Polarization Effects in Solution. Inorganic Chemistry, 2011, 50, 299-308.	4.0	48
95	NMR spectroscopy: quantumâ€chemical calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 634-647.	14.6	76
96	Selenation/Thionation of Î±â€Amino Acids: Formation and Xâ€ray Structures of Diselenopiperazine and Dithiopiperazine and Related Compounds. European Journal of Organic Chemistry, 2011, 2011, 3067-3073.	2.4	25
97	Prediction of a New Delocalised Bonding Motif between Group 15 or Group 16 Atoms. ChemPhysChem, 2011, 12, 2405-2408.	2.1	21
98	Insights into Uranyl Chemistry from Molecular Dynamics Simulations. ChemPhysChem, 2011, 12, 3095-3105.	2.1	54
99	Dodeka(ethylene)octamine. Chemistry - A European Journal, 2011, 17, 3575-3578.	3.3	7
100	Computational thermochemistry of ironâ€“platinum carbonyl clusters. Chemical Physics Letters, 2011, 509, 158-161.	2.6	3
101	The X-ray Structures of Sulfones. Journal of Chemical Crystallography, 2010, 40, 253-265.	1.1	29
102	The Preparation and Structure of [Pt(S₂N₂){P(OR)_nRâ€²_{3â€“n}}₂] and [Pt(SeSN₂)Â{P(OMe)_nPh_{3â€“n}}₂] (n = 0â€“3). European Journal of Inorganic Chemistry, 2010, 2010, 3185-3194.	2.0	3
103	Density-functional computation of 93Nb NMR chemical shifts. Magnetic Resonance in Chemistry, 2010, 48, S61-S68.	1.9	17
104	Oxygen Exchange in Uranyl Hydroxide via Two â€œNonclassicalâ€•Ions. Inorganic Chemistry, 2010, 49, 3821-3827.	4.0	48
105	Hydrogen Generation from Alcohols Catalyzed by Rutheniumâ^'Triphenylphosphine Complexes: Multiple Reaction Pathways. Journal of the American Chemical Society, 2010, 132, 8056-8070.	13.7	215
106	Density functional study of aqueous uranyl(VI) fluoride complexes. Chemical Physics Letters, 2009, 467, 287-293.	2.6	25
107	Effect of Counterions on the Structure and Stability of Aqueous Uranyl(VI) Complexes. A First-Principles Molecular Dynamics Study. Inorganic Chemistry, 2009, 48, 9977-9979.	4.0	25
108	Noncovalent Interactions in a Transition-Metal Triphenylphosphine Complex: a Density Functional Case Study. Inorganic Chemistry, 2009, 48, 4622-4624.	4.0	136

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109	Substituent effects on 61Ni NMR chemical shifts. Dalton Transactions, 2009, , 6037.	3.3	11
110	Density-functional computation of 99Tc NMR chemical shifts. Magnetic Resonance in Chemistry, 2008, 46, S36-S44.	1.9	22
111	Geometries of Third-Row Transition-Metal Complexes from Density-Functional Theory. Journal of Chemical Theory and Computation, 2008, 4, 1449-1459.	5.3	421
112	Density Functional Theory Study of Uranium(VI) Aquo Chloro Complexes in Aqueous Solution. Journal of Physical Chemistry A, 2008, 112, 2428-2436.	2.5	50
113	Chapter 3 DFT Computations of Transition-Metal Chemical Shifts. Annual Reports on NMR Spectroscopy, 2008, , 77-126.	1.5	43
114	Geometries of Second-Row Transition-Metal Complexes from Density-Functional Theory. Journal of Chemical Theory and Computation, 2007, 3, 2234-2242.	5.3	154
115	Geometries of Transition-Metal Complexes from Density-Functional Theory. Journal of Chemical Theory and Computation, 2006, 2, 1282-1290.	5.3	557
116	Mechanism of Water Exchange in Aqueous Uranyl(VI) Ion. A Density Functional Molecular Dynamics Study. Inorganic Chemistry, 2006, 45, 3834-3836.	4.0	56
117	Simulation of59Co NMR Chemical Shifts in Aqueous Solution. Chemistry - A European Journal, 2006, 12, 477-488.	3.3	63
118	Acidity of Uranyl(VI) Hydrate Studied with First-Principles Molecular Dynamics Simulations. ChemPhysChem, 2006, 7, 2290-2293.	2.1	27
119	Density-functional computation of53Cr NMR chemical shifts. Magnetic Resonance in Chemistry, 2006, 44, 661-668.	1.9	22
120	Computational NMR Spectroscopy of Transition-Metal/Nitroimidazole Complexes: Theoretical Investigation of Potential Radiosensitizers. Helvetica Chimica Acta, 2005, 88, 2705-2721.	1.6	15
121	Computational59Co NMR Spectroscopy:Â Beyond Static Moleculesâ€. Journal of Chemical Theory and Computation, 2005, 1, 181-193.	5.3	30
122	First-Principles Calculations of Paramagnetic NMR Shifts. , 2004, , 325-338.		52
123	Density functional computation of49Ti NMR chemical shifts. Magnetic Resonance in Chemistry, 2004, 42, 737-744.	1.9	25
124	Thermal and solvent effects on57Fe NMR chemical shifts. Physical Chemistry Chemical Physics, 2002, 4, 5508-5514.	2.8	50
125	Remarkably Large Geometry Dependence of57Fe NMR Chemical Shifts. Angewandte Chemie - International Edition, 2002, 41, 2312-2315.	13.8	46
126	Density functional computation of 55 Mn NMR parameters. Theoretical Chemistry Accounts, 2002, 107, 336-342.	1.4	31

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127	Medium Effects on51V NMR Chemical Shifts: A Density Functional Study. Chemistry - A European Journal, 2001, 7, 4487-4494.	3.3	108
128	Density-Functional Computation of99Ru NMR Parameters. Chemistry - A European Journal, 2000, 6, 3272-3280.	3.3	37
129	X-ray Structures and DFT Calculations on Rhodiumâ˜Olefin Complexes:Â Comments on the103Rh NMR Shiftâ˜Stability Correlation. Organometallics, 2000, 19, 5589-5596.	2.3	47
130	The DFT route to NMR chemical shifts. Journal of Computational Chemistry, 1999, 20, 91-105.	3.3	274
131	Density Functional Calculations of95Mo NMR Chemical Shifts: Applications to Model Catalysts for Imine Metathesis. Chemistry - A European Journal, 1999, 5, 3514-3522.	3.3	35
132	Theoretical investigations of NMR chemical shifts and reactivities of oxovanadium(v) compounds. Journal of Computational Chemistry, 1998, 19, 113-122.	3.3	51
133	NMR Chemical Shifts of Zr@C28. How Shielded Can 91Zr Get?. Journal of Physical Chemistry A, 1997, 101, 2514-2517.	2.5	14
134	A Density Functional Study of the Rotational Barrier of Tricarbonyl(Î·4-norbornadiene)iron. Effect of the Torsional Angle on the Carbonyl Stretching Spectra. Inorganic Chemistry, 1997, 36, 2922-2924.	4.0	20
135	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
136	Computational Screening of Anode Coatings for Garnetâ€type Solidâ€State Batteries. Batteries and Supercaps, 0, , .	4.7	2