Natalie Fey

List of Publications by Year
in descending order

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Version: 2024-02-01

77	3,653	94433 37	138484 58
papers	citations	h-index	g-index

90	90	90	3907
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computational Mapping of Dirhodium(II) Catalysts. Chemistry - A European Journal, 2021, 27, 2402-2409.	3.3	10
2	Catalytic mechanism of the colistin resistance protein MCR-1. Organic and Biomolecular Chemistry, 2021, 19, 3813-3819.	2.8	11
3	Building a Toolbox for the Analysis and Prediction of Ligand and Catalyst Effects in Organometallic Catalysis. Accounts of Chemical Research, 2021, 54, 837-848.	15.6	41
4	Iron Catalyzed Double Bond Isomerization: Evidence for an Fe^I/Fe^{III} Catalytic Cycle. Chemistry - A European Journal, 2021, 27, 5972-5977.	3.3	12
5	3Ã— Axial vs 3Ã— Equatorial: The Î”G_{GA} Value Is a Robust Computational Measure of Substituent Steric Effects. Journal of the American Chemical Society, 2021, 143, 13573-13578.	13.7	6
6	Visibleâ€Lightâ€Driven Strainâ€Increase Ring Contraction Allows the Synthesis of Cyclobutyl Boronic Esters. Angewandte Chemie - International Edition, 2020, 59, 6525-6528.	13.8	46
7	Visibleâ€Lightâ€Driven Strainâ€Increase Ring Contraction Allows the Synthesis of Cyclobutyl Boronic Esters. Angewandte Chemie, 2020, 132, 6587-6590.	2.0	18
8	How Big is the Pinacol Boronic Ester as a Substituent?. Angewandte Chemie, 2020, 132, 22589-22593.	2.0	7
9	How Big is the Pinacol Boronic Ester as a Substituent?. Angewandte Chemie - International Edition, 2020, 59, 22403-22407.	13.8	32
10	Resistance to the â€œlast resortâ€•antibiotic colistin: a single-zinc mechanism for phosphointermediate formation in MCR enzymes. Chemical Communications, 2020, 56, 6874-6877.	4.1	10
11	Mapping the properties of bidentate ligands with calculated descriptors (LKB-bid). Dalton Transactions, 2020, 49, 8169-8178.	3.3	18
12	RÃ¼cktitelbild: Visibleâ€Lightâ€Driven Strainâ€Increase Ring Contraction Allows the Synthesis of Cyclobutyl Boronic Esters (Angew. Chem. 16/2020). Angewandte Chemie, 2020, 132, 6694-6694.	2.0	0
13	On the Basicity of Carboranylphosphines. Inorganic Chemistry, 2019, 58, 14818-14829.	4.0	12
14	Tipping the polaronâ€“bipolaron balance: concentration and spin effects in doped oligo(aniline)s observed by UV-vis-NIR and TD-DFT. Molecular Systems Design and Engineering, 2019, 4, 103-109.	3.4	6
15	Computational mapping of redox-switchable metal complexes based on ferrocene derivatives. Chemical Communications, 2019, 55, 7021-7024.	4.1	20
16	Computational Ligand Descriptors for Catalyst Design. Chemical Reviews, 2019, 119, 6561-6594.	47.7	254
17	Understanding unusual element-element bond formation and activation: general discussion. Faraday Discussions, 2019, 220, 376-385.	3.2	0
18	Physical methods for mechanistic understanding: general discussion. Faraday Discussions, 2019, 220, 144-178.	3.2	0

#	Article	IF	Citations
19	Computational and theoretical approaches for mechanistic understanding: general discussion. Faraday Discussions, 2019, 220, 464-488.	3.2	3
20	Biocatalytic Routes to Lactone Monomers for Polymer Production. Biochemistry, 2018, 57, 1997-2008.	2.5	33
21	Accessing Alkyl- and Alkenylcyclopentanes from Cr-Catalyzed Ethylene Oligomerization Using 2-Phosphinophosphinine Ligands. Organometallics, 2018, 37, 1062-1073.	2.3	32
22	Inorganic Triphenylphosphine. Angewandte Chemie - International Edition, 2018, 57, 15802-15806.	13.8	9
23	Inorganic Triphenylphosphine. Angewandte Chemie, 2018, 130, 16028-16032.	2.0	2
24	Insights into the Mechanistic Basis of Plasmid-Mediated Colistin Resistance from Crystal Structures of the Catalytic Domain of MCR-1. Scientific Reports, 2017, 7, 39392.	3.3	107
25	A Simple and Broadly Applicable Câ^'N Bond Forming Dearomatization Protocol Enabled by Bifunctional Amino Reagents. Angewandte Chemie, 2017, 129, 14723-14727.	2.0	20
26	A Simple and Broadly Applicable Câ^'N Bond Forming Dearomatization Protocol Enabled by Bifunctional Amino Reagents. Angewandte Chemie - International Edition, 2017, 56, 14531-14535.	13.8	70
27	Heavily Substituted Atropisomeric Diarylamines by Unactivated Smiles Rearrangement of N â€Aryl Anthranilamides. Angewandte Chemie, 2017, 129, 12707-12711.	2.0	20
28	Heavily Substituted Atropisomeric Diarylamines by Unactivated Smiles Rearrangement of Nâ€Aryl Anthranilamides. Angewandte Chemie - International Edition, 2017, 56, 12533-12537.	13.8	57
29	Exploring Redox States, Doping and Ordering of Electroactive Starâ€Shaped Oligo(aniline)s. Chemistry - A European Journal, 2016, 22, 16950-16956.	3.3	15
30	Spectroscopic, structural and computational analysis of [Re(CO)₃(dippM)Br]ⁿ⁺ (dippM = 1,1â€²-bis(diiso-propylphosphino)metallocene, M =) Tj ET Q q 0 0 0 rgBT /Ove	3	
31	Setting P-Donor Ligands into Context: An Application of the Ligand Knowledge Base (LKB) Approach. Phosphorus, Sulfur and Silicon and the Related Elements, 2015, 190, 706-714.	1.6	8
32	Dispersion, solvent and metal effects in the binding of gold cations to alkynyl ligands: implications for Au(<scp>i</scp>) catalysis. Chemical Communications, 2015, 51, 9702-9705.	4.1	18
33	Self-Assembly of a Functional Oligo(Aniline)-Based Amphiphile into Helical Conductive Nanowires. Journal of the American Chemical Society, 2015, 137, 14288-14294.	13.7	57
34	Lost in chemical space? Maps to support organometallic catalysis. Chemistry Central Journal, 2015, 9, 38.	2.6	39
35	Cooperative Lewis Pairs Based on Late Transition Metals: Activation of Small Molecules by Platinum(0) and B(C₆F₅)₃. Angewandte Chemie - International Edition, 2015, 54, 2223-2227.	13.8	49
36	The Computational Road to Better Catalysts. Chemistry - an Asian Journal, 2014, 9, 1714-1723.	3.3	57

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37	Computational Discovery of Stable Transition-Metal Vinylidene Complexes. Organometallics, 2014, 33, 1751-1761.	2.3	51
38	Computed ligand effects on the oxidative addition of phenyl halides to phosphine supported palladium(0) catalysts. Dalton Transactions, 2014, 43, 13545-13556.	3.3	100
39	Screening substituent and backbone effects on the properties of bidentate P,P-donor ligands (LKB-PP_{screen}). Dalton Transactions, 2013, 42, 172-181.	3.3	30
40	Expansion of the Ligand Knowledge Base for Chelating P,P-Donor Ligands (LKB-PP). Organometallics, 2012, 31, 5302-5306.	2.3	69
41	Synthesis and spectroelectrochemistry of transition metal carbonyls with 1,1â€²-bis(phosphino)metallocene ligands. Journal of Organometallic Chemistry, 2012, 712, 37-45.	1.8	14
42	Regioselective B-Cyclometalation of a Bulky o-Carboranyl Phosphine and the Unexpected Formation of a Dirhodium(II) Complex. Organometallics, 2012, 31, 2907-2913.	2.3	55
43	Stable Fluorophosphines: Predicted and Realized Ligands for Catalysis. Angewandte Chemie - International Edition, 2012, 51, 118-122.	13.8	46
44	Remarkably reactive dihydroindoloindoles via palladium-catalysed dearomatisation. Chemical Communications, 2011, 47, 3649.	4.1	74
45	Organometallic reactivity: the role of metalâ€“ligand bond energies from a computational perspective. Dalton Transactions, 2011, 40, 11184.	3.3	57
46	Functional block-like structures from electroactive tetra(aniline) oligomers. Journal of Materials Chemistry, 2011, 21, 18137.	6.7	67
47	Delineating Poly(Aniline) Redox Chemistry by Using Tailored Oligo(Aryleneamine)s: Towards Oligo(Aniline)â€Based Organic Semiconductors with Tunable Optoelectronic Properties. Chemistry - A European Journal, 2011, 17, 12512-12521.	3.3	45
48	A computational study of phosphine ligand effects in Suzukiâ€“Miyaura couplingâ˜†. Journal of Molecular Catalysis A, 2010, 324, 39-47.	4.8	144
49	Computational study of PtBu3 as ligand in the palladium-catalysed amination of phenylbromide with morpholineâ˜†. Journal of Molecular Catalysis A, 2010, 324, 48-55.	4.8	26
50	The contribution of computational studies to organometallic catalysis: descriptors, mechanisms and models. Dalton Transactions, 2010, 39, 296-310.	3.3	109
51	Accurate modelling of Pd(0) + PhX oxidative addition kinetics. Dalton Transactions, 2010, 39, 10833.	3.3	179
52	Structural Fluctuations in Enzyme-Catalyzed Reactions: Determinants of Reactivity in Fatty Acid Amide Hydrolase from Multivariate Statistical Analysis of Quantum Mechanics/Molecular Mechanics Paths. Journal of Chemical Theory and Computation, 2010, 6, 2948-2960.	5.3	61
53	Palladium Complexes of the Heterodiphosphine o-C₆H₄(CH₂P^tBu₂)(CH₂PPh₂) Are Highly Selective and Robust Catalysts for the Hydromethoxycarbonylation of Ethene. Organometallics, 2010, 29, 2292-2305.	2.3	49
54	Expansion of the Ligand Knowledge Base for Monodentate P-Donor Ligands (LKB-P). Organometallics, 2010, 29, 6245-6258.	2.3	117

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55	Cryptocatalytic 1,2â€Alkene Migration in a Ïƒâ€Alkyl Palladium Diene Complex. Angewandte Chemie - International Edition, 2009, 48, 6262-6265.	13.8	27
56	Building ligand knowledge bases for organometallic chemistry: Computational description of phosphorus(III)-donor ligands and the metalâ€“phosphorus bond. Coordination Chemistry Reviews, 2009, 253, 704-722.	18.8	180
57	A ligand knowledge base for carbenes (LKB-C): maps of ligand space. Dalton Transactions, 2009, , 8183.	3.3	59
58	Anatomy of Phobanes. Diastereoselective Synthesis of the Three Isomers ofn-Butylphobane and a Comparison of their Donor Properties. Journal of the American Chemical Society, 2009, 131, 3078-3092.	13.7	38
59	Computational Descriptors for Chelating P,P- and P,N-Donor Ligands¹. Organometallics, 2008, 27, 1372-1383.	2.3	96
60	Counterintuitive Kinetics in Tsuji-Trost Allylation: Ion-Pair Partitioning and Implications for Asymmetric Catalysis. Journal of the American Chemical Society, 2008, 130, 14471-14473.	13.7	97
61	Photophysical Properties of Platinum(II)â^'Acetylide Complexes: the Effect of a Strongly Electron-Accepting Diimine Ligand on Excited-State Structure. Inorganic Chemistry, 2008, 47, 8242-8257.	4.0	65
62	Synthesis, structures and properties of a new series of platinumâ€“diimineâ€“dithiolate complexes. Dalton Transactions, 2007, , 4446.	3.3	42
63	Near-Infrared Luminescence from Platinum(II) Diimine Compounds. Inorganic Chemistry, 2006, 45, 6105-6107.	4.0	50
64	Adding Value to Crystallographically-Derived Knowledge Basesâ€. Journal of Chemical Information and Modeling, 2006, 46, 912-929.	5.4	18
65	Statistical Modeling of a Ligand Knowledge Base. Journal of Chemical Information and Modeling, 2006, 46, 2591-2600.	5.4	27
66	A molecular mechanics approach to mapping the conformational space of diaryl and triarylphosphines. Dalton Transactions, 2006, , 5464.	3.3	19
67	Development of a Ligand Knowledge Base, Part 1: Computational Descriptors for Phosphorus Donor Ligands. Chemistry - A European Journal, 2006, 12, 291-302.	3.3	110
68	DommiMOE: An implementation of ligand field molecular mechanics in the molecular operating environment. Journal of Computational Chemistry, 2005, 26, 123-130.	3.3	76
69	Inclusion of the ligand field contribution in a polarizable molecular mechanics: SIBFA-LF. Journal of Computational Chemistry, 2004, 25, 308-308.	3.3	1
70	The performance of nonhybrid density functionals for calculating the structures and spin states of Fe(II) and Fe(III) complexes. Journal of Computational Chemistry, 2004, 25, 1840-1848.	3.3	86
71	A Molecular Mechanics Study of Copper(II)-Catalyzed Asymmetric Dielsâ^'Alder Reactions. Organometallics, 2004, 23, 1042-1054.	2.3	19
72	Inclusion of the ligand field contribution in a polarizable molecular mechanics: SIBFA-LF. Journal of Computational Chemistry, 2003, 24, 1963-1970.	3.3	65

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73	Molecular Mechanics Analysis of Structure and Diastereoselectivity toward Lithiation in Amido- and Î±-Aminoferrocene Complexes. Organometallics, 2002, 21, 5272-5286.	2.3	14
74	Conformational Properties of Substituted Ferrocenes:Â Experimental and Theoretical Studies of the Molecular Structures of 1,1â€˜-Di-tert-butylferrocene and Isopropylferrocene. Organometallics, 2001, 20, 2309-2320.	2.3	26
75	Organometallic molecular modelling - the computational chemistry of metallocenes: a review. , 1999, 74, 852-862.		36
76	Effect of fluorine and trifluoromethyl substitution on the donor properties and stereodynamical behaviour of triarylphosphines. Journal of the Chemical Society Dalton Transactions, 1999, , 3015-3028.	1.1	48
77	Computational mechanistic study in organometallic catalysis: Why prediction is still a challenge. Wiley Interdisciplinary Reviews: Computational Molecular Science, 0, , e1590.	14.6	8