

# Imre Pápai

## List of Publications by Year in descending order

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143  
papers

7,815  
citations

47006

47  
h-index

54911

84  
g-index

165  
all docs

165  
docs citations

165  
times ranked

5576  
citing authors

#	ARTICLE	IF	CITATIONS
1	Gaussian density functional calculations on hydrogen-bonded systems. <i>Journal of the American Chemical Society</i> , 1992, 114, 4391-4400.	13.7	462
2	Theoretical Studies on the Bifunctionality of Chiral Thiourea-Based Organocatalysts: A Competing Routes to C-C Bond Formation. <i>Journal of the American Chemical Society</i> , 2006, 128, 13151-13160.	13.7	408
3	Turning Frustration into Bond Activation: A Theoretical Mechanistic Study on Heterolytic Hydrogen Splitting by Frustrated Lewis Pairs. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 2435-2438.	13.8	364
4	A frustrated-Lewis-pair approach to catalytic reduction of alkynes to cis-alkenes. <i>Nature Chemistry</i> , 2013, 5, 718-723.	13.6	343
5	Rationalizing the Reactivity of Frustrated Lewis Pairs: Thermodynamics of H <sub>2</sub> Activation and the Role of Acid-Base Properties. <i>Journal of the American Chemical Society</i> , 2009, 131, 10701-10710.	13.7	303
6	On the Mechanism of B(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> -Catalyzed Direct Hydrogenation of Imines: Inherent and Thermally Induced Frustration. <i>Journal of the American Chemical Society</i> , 2009, 131, 2029-2036.	13.7	247
7	Expanding the Scope of Metal-Free Catalytic Hydrogenation through Frustrated Lewis Pair Design. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 6559-6563.	13.8	234
8	Density functional study of nitrogen oxides. <i>Journal of Chemical Physics</i> , 1994, 100, 2910-2923.	3.0	196
9	Reactivity Models of Hydrogen Activation by Frustrated Lewis Pairs: Synergistic Electron Transfers or Polarization by Electric Field?. <i>Journal of the American Chemical Society</i> , 2013, 135, 4425-4437.	13.7	193
10	Catalytic Hydrogenation with Frustrated Lewis Pairs: Selectivity Achieved by Size-Exclusion Design of Lewis Acids. <i>Chemistry - A European Journal</i> , 2012, 18, 574-585.	3.3	151
11	Chiral Molecular Tweezers: Synthesis and Reactivity in Asymmetric Hydrogenation. <i>Journal of the American Chemical Society</i> , 2015, 137, 4038-4041.	13.7	151
12	Moisture-Tolerant Frustrated Lewis Pair Catalyst for Hydrogenation of Aldehydes and Ketones. <i>ACS Catalysis</i> , 2015, 5, 5366-5372.	11.2	144
13	Mechanism of hydrogen activation by frustrated Lewis pairs: A molecular orbital approach. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2416-2425.	2.0	124
14	Metal-Free sp <sup>2</sup> -C-H Borylation as a Common Reactivity Pattern of Frustrated 2-Aminophenylboranes. <i>Journal of the American Chemical Society</i> , 2016, 138, 4860-4868.	13.7	115
15	Influence of Al <sub>2</sub> O <sub>3</sub> on the performance of CeO <sub>2</sub> used as catalyst in the direct carboxylation of methanol to dimethylcarbonate and the elucidation of the reaction mechanism. <i>Journal of Catalysis</i> , 2010, 269, 44-52.	6.2	113
16	Concerted attack of frustrated Lewis acid-base pairs on olefinic double bonds: a theoretical study. <i>Chemical Communications</i> , 2008, , 3148.	4.1	106
17	On the Mechanism of Bifunctional Squaramide-Catalyzed Organocatalytic Michael Addition: A Protonated Catalyst as an Oxyanion Hole. <i>Chemistry - A European Journal</i> , 2014, 20, 5631-5639.	3.3	103
18	Hydrogen Bonding in Methyl-Substituted Pyridine-Water Complexes: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2132-2137.	2.5	100

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19	Mechanistic Details of Nickel(0)-Assisted Oxidative Coupling of CO <sub>2</sub> with C <sub>2</sub> H <sub>4</sub> . <i>Organometallics</i> , 2004, 23, 5252-5259.	2.3	95
20	H <sub>2</sub> CO <sub>3</sub> Forms via HCO <sub>3</sub> <sup>•</sup> in Water. <i>Journal of Physical Chemistry B</i> , 2010, 114, 16854-16859.	2.6	92
21	Mechanism of Formation of Organic Carbonates from Aliphatic Alcohols and Carbon Dioxide under Mild Conditions Promoted by Carbodiimides. DFT Calculation and Experimental Study. <i>Journal of Organic Chemistry</i> , 2005, 70, 6177-6186.	3.2	90
22	Dihydrooxazine Oxides as Key Intermediates in Organocatalytic Michael Additions of Aldehydes to Nitroalkenes. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 13144-13148.	13.8	89
23	Intramolecular Frustrated Lewis Pair with the Smallest Boryl Site: Reversible H <sub>2</sub> Addition and Kinetic Analysis. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 1749-1753.	13.8	89
24	Density functional study of carbon monoxide chemisorption on model clusters of rhodium and palladium: a comparative analysis of the site selection. <i>Journal of the American Chemical Society</i> , 1992, 114, 7452-7458.	13.7	81
25	Expanding the Boundaries of Water-Tolerant Frustrated Lewis Pair Hydrogenation: Enhanced Back Strain in the Lewis Acid Enables the Reductive Amination of Carbonyls. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 9512-9516.	13.8	79
26	Cooperative Assistance in Bifunctional Organocatalysis: Enantioselective Mannich Reactions with Aliphatic and Aromatic Imines. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 8495-8499.	13.8	78
27	Thiourea Derivatives as Brønsted Acid Organocatalysts. <i>ACS Catalysis</i> , 2016, 6, 4379-4387.	11.2	74
28	Theoretical Study of the Interaction of the Ti Atom with CO <sub>2</sub> : Cleavage of the C=O Bond. <i>Journal of Physical Chemistry A</i> , 1997, 101, 4465-4471.	2.5	71
29	Mechanistic Insight into Asymmetric Hetero-Michael Addition of $\alpha,\beta$ -Unsaturated Carboxylic Acids Catalyzed by Multifunctional Thioureas. <i>Journal of the American Chemical Society</i> , 2018, 140, 12216-12225.	13.7	68
30	Computing Reliable Energetics for Conjugate Addition Reactions. <i>Organic Letters</i> , 2007, 9, 4279-4282.	4.6	67
31	Acrylate Formation via Metal-Assisted C=C Coupling between CO <sub>2</sub> and C <sub>2</sub> H <sub>4</sub> : Reaction Mechanism as Revealed from Density Functional Calculations. <i>Journal of the American Chemical Society</i> , 2003, 125, 14847-14858.	13.7	66
32	Halogen Bonding Helicates Encompassing Iodonium Cations. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 9012-9016.	13.8	66
33	CO <sub>2</sub> Coordination to Nickel Atoms: Matrix Isolation and Density Functional Studies. <i>Journal of Physical Chemistry A</i> , 1997, 101, 2626-2633.	2.5	64
34	Evidence for Spontaneous Release of Acrylates from a Transition-Metal Complex Upon Coupling Ethene or Propene with a Carboxylic Moiety or CO <sub>2</sub> . <i>Chemistry - A European Journal</i> , 2007, 13, 9028-9034.	3.3	61
35	Theoretical investigation of catalytic HCO <sub>3</sub> <sup>•</sup> hydrogenation in aqueous solutions. <i>Catalysis Today</i> , 2006, 115, 53-60.	4.4	57
36	Association of frustrated phosphine-borane pairs in toluene: molecular dynamics simulations. <i>Dalton Transactions</i> , 2012, 41, 9023.	3.3	57

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37	Density Functional Calculations on Model Clusters of Zeolite- $\beta$ . The Journal of Physical Chemistry, 1994, 98, 4654-4659.	2.9	55
38	Modeling of N <sub>2</sub> and O <sub>2</sub> Adsorption in Zeolites. The Journal of Physical Chemistry, 1995, 99, 12925-12932.	2.9	54
39	Carbon dioxide interaction with metal atoms: matrix isolation spectroscopic study and DFT calculations. Coordination Chemistry Reviews, 1999, 190-192, 557-576.	18.8	54
40	An IR Matrix Isolation and DFT Theoretical Study of the First Steps of the Ti(0) Ethylene Reaction: Vinyl Titanium Hydride and Titanacyclopentene. Journal of Physical Chemistry A, 1997, 101, 9650-9659.	2.5	53
41	Vibrational spectroscopic and force field studies of N,N-dimethylthioformamide, N,N-dimethylformamide, their deuterated analogues and bis(N,N-dimethylthioformamide)mercury(II) perchlorate. Vibrational Spectroscopy, 1997, 14, 207-227.	2.2	53
42	Mechanochemical Synthesis of Corannulene-Based Curved Nanographenes. Angewandte Chemie - International Edition, 2020, 59, 21620-21626.	13.8	53
43	Cross-Dehydrogenative Couplings between Indoles and $\alpha$ -Keto Esters: Ligand-Assisted Ligand Tautomerization and Dehydrogenation via a Proton-Assisted Electron Transfer to Pd(II). Journal of the American Chemical Society, 2014, 136, 6453-6462.	13.7	52
44	Reaction mechanism of the direct carboxylation of methanol to dimethylcarbonate: experimental and theoretical studies. Topics in Catalysis, 2006, 40, 71-81.	2.8	50
45	Vanadium Insertion into CO <sub>2</sub> , CS <sub>2</sub> and OCS: A Comparative Theoretical Study. Journal of Physical Chemistry A, 2002, 106, 4181-4186.	2.5	49
46	Theoretical Mechanistic Study of Rhodium(I) Phosphine-Catalyzed H/D Exchange Processes in Aqueous Solutions. Organometallics, 2005, 24, 3059-3065.	2.3	49
47	On the Existence of the Elusive Monomethyl Ester of Carbonic Acid [CH <sub>3</sub> OC(O)OH] at 300 K: <sup>1</sup> H- and <sup>13</sup> C NMR Measurements and DFT Calculations. European Journal of Inorganic Chemistry, 2006, 2006, 908-913.	2.0	48
48	Mukaiyama-Michael Reactions with <i>trans</i> -2,5-Diarylpiperidine Catalysts: Enantioselectivity Arises from Attractive Noncovalent Interactions, Not from Steric Hindrance. Chemistry - A European Journal, 2014, 20, 5983-5993.	3.3	48
49	Dual Hydrogen-Bond/Enamine Catalysis Enables a Direct Enantioselective Three-Component Domino Reaction. Angewandte Chemie - International Edition, 2011, 50, 6123-6127.	13.8	47
50	Hydrogen Activation by Frustrated Lewis Pairs: Insights from Computational Studies. Topics in Current Chemistry, 2013, 332, 157-211.	4.0	47
51	First principles molecular dynamics calculation of the structure and acidity of a bulk zeolite. Chemical Physics Letters, 1994, 226, 245-250.	2.6	44
52	Calculation of equilibrium geometries and harmonic frequencies by the LCGTO-MCP-local spin density method. International Journal of Quantum Chemistry, 1990, 38, 29-39.	2.0	42
53	Singlet- and triplet-state (ethene)nickel: a density functional study. The Journal of Physical Chemistry, 1993, 97, 9986-9991.	2.9	39
54	2A $\tilde{\Sigma}$ and 2A $\tilde{\Sigma}^+$ Energy Surfaces for the Sc + CO <sub>2</sub> $\rightarrow$ ScO + CO Reaction. Journal of Physical Chemistry A, 2002, 106, 9551-9557.	2.5	39

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55	Molecular structure of mono- and dicarbonyls of rhodium and palladium. <i>Theoretica Chimica Acta</i> , 1992, 84, 217-235.	0.8	37
56	Theoretical study of the Cu(H <sub>2</sub> O) and Cu(NH <sub>3</sub> ) complexes and their photolysis products. <i>Journal of Chemical Physics</i> , 1995, 103, 1860-1870.	3.0	36
57	Nuclear spin hyperpolarization with ansa-aminoboranes: a metal-free perspective for parahydrogen-induced polarization. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27784-27795.	2.8	34
58	A density functional study of Sc <sub>2</sub> and Sc <sub>3</sub> . <i>Chemical Physics Letters</i> , 1997, 267, 551-556.	2.6	32
59	Atom-efficient Synthesis of Alkynylfluoroborates Using BF <sub>3</sub> -Based Frustrated Lewis Pairs. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 14146-14150.	13.8	32
60	Rotational reorientation dynamics of Nile blue A and Oxazine 720 in protic solvents. <i>Chemical Physics</i> , 2003, 286, 81-96.	1.9	31
61	Hydride Donor Abilities of Cationic Transition Metal Hydrides from DFT-PCM Calculations. <i>Organometallics</i> , 2006, 25, 820-825.	2.3	31
62	Rearrangements of N-heterocyclic Carbenes of Pyrazole to 4-aminopyridines and Benzoquinolines. <i>European Journal of Organic Chemistry</i> , 2010, 2010, 4296-4305.	2.4	31
63	The solid state structure and reactivity of NbCl <sub>5</sub> ·(N,N'-dicyclohexylurea) in solution: evidence for co-ordinated urea dehydration to the relevant carbodiimide. <i>Dalton Transactions</i> , 2010, 39, 6985.	3.3	31
64	Numerical grids for density functional calculations of molecular properties. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 799-807.	2.0	30
65	Mechanism of Heterolytic Hydrogen Splitting by Frustrated Lewis Pairs: Comparison of Static and Dynamic Models. <i>ACS Catalysis</i> , 2019, 9, 6049-6057.	11.2	30
66	Metal Insertion Route of the Ni + CO <sub>2</sub> → NiO + CO Reaction. <i>Journal of Physical Chemistry A</i> , 2003, 107, 6708-6713.	2.5	29
67	Stereocontrol in Diphenylprolinol Silyl Ether Catalyzed Michael Additions: Steric Shielding or Curtin-Hammett Scenario?. <i>Journal of the American Chemical Society</i> , 2017, 139, 17052-17063.	13.7	29
68	Glyphosate complexation to aluminium(III). An equilibrium and structural study in solution using potentiometry, multinuclear NMR, ATR-FTIR, ESI-MS and DFT calculations. <i>Journal of Inorganic Biochemistry</i> , 2009, 103, 1426-1438.	3.5	27
69	Vibrational analysis of formate adsorbed on Ni(110): LCGTO-MCP-LSD study. <i>Surface Science</i> , 1992, 262, L134-L138.	1.9	25
70	Theoretical Investigation of the Reactivity of Copper Atoms with OCS: A Comparison with CS <sub>2</sub> and CO <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , 2005, 109, 7932-7937.	2.5	25
71	Catalytic Synthesis of Hydroxymethyl-oxazolidinones from Glycerol or Glycerol Carbonate and Urea. <i>ChemSusChem</i> , 2013, 6, 345-352.	6.8	25
72	A Catalyst Designed for the Enantioselective Construction of Methyl- and Alkyl-Substituted Tertiary Stereocenters. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 669-673.	13.8	25

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73	Replacing C <sub>6</sub> F <sub>5</sub> groups with Cl and H atoms in frustrated Lewis pairs: H <sub>2</sub> additions and catalytic hydrogenations. Dalton Transactions, 2017, 46, 2263-2269.	3.3	25
74	Catalytic Activity of <i>trans</i> -Bis(pyridine)gold Complexes. Journal of the American Chemical Society, 2020, 142, 6439-6446.	13.7	25
75	Origin of Stereoselectivity in FLP-Catalyzed Asymmetric Hydrogenation of Imines. ACS Catalysis, 2020, 10, 14290-14301.	11.2	24
76	Enantioselective Acetalization by Dynamic Kinetic Resolution for the Synthesis of <sup>13</sup> C-Alkoxybutenolides by Thiourea/Quaternary Ammonium Salt Catalysts: Application to Strigolactones. Angewandte Chemie - International Edition, 2020, 59, 13479-13483.	13.8	24
77	Unprecedented formal $\eta^2+\eta^2$ addition of allene to CO <sub>2</sub> promoted by [RhCl(C <sub>2</sub> H <sub>4</sub> )(P <sup>i</sup> Pr <sub>3</sub> ) <sub>2</sub> ]: direct synthesis of the four membered lactone $\pm$ -methylene- $\beta$ -oxiethanone. The intermediacy of [RhH <sub>2</sub> Cl(P <sup>i</sup> Pr <sub>3</sub> ) <sub>2</sub> ]: theoretical aspects and experiments. Inorganica Chimica Acta, 2002, 334, 294-300.	2.4	22
78	Reaction Mechanisms in the Direct Carboxylation of Alcohols for the Synthesis of Acyclic Carbonates. Topics in Catalysis, 2015, 58, 2-14.	2.8	22
79	Organocatalysts Fold To Generate an Active Site Pocket for the Mannich Reaction. ACS Catalysis, 2017, 7, 3284-3294.	11.2	22
80	Mechanism of Au(III)-Mediated Alkoxy cyclization of a 1,6-Enyne. Journal of the American Chemical Society, 2019, 141, 18221-18229.	13.7	22
81	An LCGTO-MCP-LSD study of the (2 Å <sup>-1</sup> ) H-covered Pd(110) surface. Surface Science, 1990, 236, 241-249.	1.9	21
82	Behaviour of [PdH(dppe) <sub>2</sub> ]X (X=CF <sub>3</sub> SO <sub>3</sub> <sup>-</sup> , SbF <sub>6</sub> <sup>-</sup> , BF <sub>4</sub> <sup>-</sup> ) as Proton or Hydride Donor: Relevance to Catalysis. Chemistry - A European Journal, 2004, 10, 3708-3716.	3.3	21
83	Conceptual Problem with Calculating Electron Densities in Finite Basis Density Functional Theory. Journal of Chemical Theory and Computation, 2017, 13, 3961-3963.	5.3	21
84	Metal-Free C <sup>1</sup> H Borylation of N-Heteroarenes by Boron Trifluoride. Chemistry - A European Journal, 2020, 26, 13873-13879.	3.3	21
85	Spectroscopic and theoretical study of [PdCl <sub>3</sub> (C <sub>2</sub> H <sub>4</sub> )] <sup>-</sup> and [PdCl <sub>3</sub> (C <sub>2</sub> D <sub>4</sub> )] <sup>-</sup> complexes. Journal of Organometallic Chemistry, 1999, 584, 118-121.	1.8	20
86	Chemisorption of formate and acetate on cluster models of Rh and bimetallic RhSn clusters. Surface Science, 1993, 282, 262-272.	1.9	19
87	Superstable Palladium(0) Complex as an Air- and Thermostable Catalyst for Suzuki Coupling Reactions. European Journal of Organic Chemistry, 2015, 2015, 60-66.	2.4	19
88	Base-induced reversible H <sub>2</sub> addition to a single Sn( <i>sc</i> ) centre. Chemical Science, 2018, 9, 8716-8722.	7.4	19
89	The reaction mechanism in the ethanolysis of urea with transition metal-based catalysts: DFT calculations and experiments. Journal of CO <sub>2</sub> Utilization, 2014, 8, 27-33.	6.8	18
90	Correlating electronic and catalytic properties of frustrated Lewis pairs for imine hydrogenation. Journal of Organometallic Chemistry, 2017, 847, 258-262.	1.8	18

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91	Synthesis, Characterization, and Reactivity of Cationic Hydride [HPd(diphosphine) <sub>2</sub> ]+CF <sub>3</sub> SO <sub>3</sub> <sup>-</sup> , the Missing Member of the Family [HM(dppe) <sub>2</sub> ]+X <sup>-</sup> (M = Ni, Pd, Pt). DFT QM/MM Structural Predictions for the [HPd(dppe) <sub>2</sub> ]+Moiety. <i>Inorganic Chemistry</i> , 2002, 41, 6550-6552.	4.0	17
92	Identification of Cu <sub>2</sub> (N <sub>2</sub> ) and Cu <sub>2</sub> (N <sub>2</sub> ) <sub>2</sub> Complexes: A Matrix Isolation and Density Functional Studies. <i>Journal of Physical Chemistry A</i> , 2000, 104, 3572-3578.	2.5	16
93	Folding Patterns in a Family of Oligoamide Foldamers. <i>Chemistry - A European Journal</i> , 2015, 21, 9493-9504.	3.3	16
94	Ionizing radiation induced degradation of monuron in dilute aqueous solution. <i>Radiation Physics and Chemistry</i> , 2016, 124, 191-197.	2.8	16
95	Expanding the Boundaries of Water-Tolerant Frustrated Lewis Pair Hydrogenation: Enhanced Back Strain in the Lewis Acid Enables the Reductive Amination of Carbonyls. <i>Angewandte Chemie</i> , 2017, 129, 9640-9644.	2.0	16
96	RuBisCO-Inspired CO <sub>2</sub> Activation and Transformation by an Iridium(I) Complex. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 2455-2458.	13.8	16
97	Halogen Bonding Helicates Encompassing Iodonium Cations. <i>Angewandte Chemie</i> , 2019, 131, 9110-9114.	2.0	16
98	Analysis of the vibrational spectra, force fields, and molecular structures of pentacarbonyl(methyl)manganese(I) and pentacarbonyl(methyl)rhenium(I). <i>Journal of Organometallic Chemistry</i> , 2000, 616, 1-9.	1.8	15
99	Structure and Properties of the [Ru(bpy)(CN) <sub>4</sub> ] <sup>2-</sup> Complex and Its Solvent Environment: An X-ray Diffraction and Density Functional Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9903-9909.	2.5	15
100	Theoretical Investigation of the Reactivity of Copper Atoms with Carbon Disulfide. <i>Journal of Physical Chemistry A</i> , 2003, 107, 2711-2715.	2.5	15
101	Stereoelectronic Requirements for Optimal Hydrogen-Bond-Catalyzed Enolization. <i>Chemistry - A European Journal</i> , 2011, 17, 2859-2866.	3.3	15
102	Mechanochemical Synthesis of Corannulene-Based Curved Nanographenes. <i>Angewandte Chemie</i> , 2020, 132, 21804-21810.	2.0	14
103	The Influence of Secondary Interactions on the [N <sup>+</sup> ...N <sup>-</sup> ] <sup>+</sup> Halogen Bond. <i>Chemistry - A European Journal</i> , 2021, 27, 13748-13756.	3.3	14
104	Synthesis of azahelicenes through Mallory reaction of imine precursors: corannulene substrates provide an exception to the rule in oxidative photocyclizations of diarylethenes. <i>Chemical Science</i> , 2021, 12, 3977-3983.	7.4	14
105	Atom-Efficient Synthesis of Alkynylfluoroborates Using BF <sub>3</sub> -Based Frustrated Lewis Pairs. <i>Angewandte Chemie</i> , 2016, 128, 14352-14356.	2.0	12
106	Establishing the Role of Triflate Anions in H <sub>2</sub> Activation by a Cationic Triorganotin(IV) Lewis Acid. <i>ACS Catalysis</i> , 2020, 10, 7573-7583.	11.2	12
107	Calculation of normal frequencies of adsorbed molecules by the LCGTO-MCP-LSD method. <i>Surface Science</i> , 1990, 240, L604-L608.	1.9	11
108	The covalently bound N <sub>3</sub> O <sub>2</sub> molecule: Two possible isomers. <i>Chemical Physics Letters</i> , 1996, 253, 196-200.	2.6	11

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109	Can the FeCO bending be higher than the FeC stretching frequency in CO adducts of heme proteins?. <i>Chemical Physics Letters</i> , 1998, 287, 531-534.	2.6	11
110	Observation and interpretation of 157.5 Å internal magnetic field in Fe[C(SiMe <sub>3</sub> ) <sub>3</sub> ] <sub>2</sub> coordination compound. <i>Structural Chemistry</i> , 2009, 20, 453-460.	2.0	11
111	Total Synthesis of Stemoamide, 9a-epi-Stemoamide, and 9a,10-epi-Stemoamide: Divergent Stereochemistry of the Final Methylation Steps. <i>Synlett</i> , 2020, 31, 1581-1586.	1.8	11
112	Recent developments of FT-IR and Raman spectroscopy in coordination chemistry. <i>Pure and Applied Chemistry</i> , 1989, 61, 973-978.	1.9	10
113	The Ti <sub>2</sub> H <sub>2</sub> molecule: terminal or bridging hydrogens?. <i>Theoretical Chemistry Accounts</i> , 2000, 104, 131-139.	1.4	10
114	Vibrational Spectroscopic and Theoretical Studies of Urea Derivatives with Biochemical Interest: N,N-Dimethylurea, N,N,N',N'-Tetramethylurea, and N,N'-Dimethylpropyleneurea. <i>Applied Spectroscopy Reviews</i> , 2010, 45, 274-326.	6.7	10
115	A novel ambident reactivity of azolyacroleins. <i>Tetrahedron</i> , 2007, 63, 4730-4736.	1.9	9
116	Synthesis and X-ray characterization of [RhCl(C <sub>2</sub> H <sub>4</sub> )(P <sub>i</sub> Pr <sub>3</sub> ) <sub>2</sub> ]. Multinuclear NMR and DFT investigation of its solid-state and solution reaction with dihydrogen. Ethene and propene hydrogenation by the solid Rh-hydrides. <i>Dalton Transactions</i> , 2009, , 7924.	3.3	9
117	RuBisCO-inspirierte CO <sub>2</sub> -Aktivierung und Umwandlung durch einen Iridium(I)-Komplex. <i>Angewandte Chemie</i> , 2018, 130, 2480-2483.	2.0	9
118	Transition Metal-Free Direct Hydrogenation of Esters via a Frustrated Lewis Pair. <i>ACS Catalysis</i> , 2021, 11, 9143-9150.	11.2	9
119	Theoretical analysis of bis(ethylene) complexes of molybdenum and tungsten. <i>Journal of Organometallic Chemistry</i> , 2002, 663, 83-90.	1.8	8
120	Steric Control of Geminal Lewis Pair Behavior: Frustration Induced Dyotropic Rearrangement. <i>Synlett</i> , 2014, 25, 1525-1528.	1.8	8
121	N-benzoylimido complexes of palladium. Synthesis, structural characterisation and structure-reactivity relationship. <i>Dalton Transactions</i> , 2004, , 2041-2050.	3.3	7
122	O=C=O halogen bond of halonium ions. <i>Chemical Communications</i> , 2020, 56, 9671-9674.	4.1	7
123	Multinuclear NMR and DFT studies of the structure and fluxionality for M(EDTA) <sup>4-</sup> ethylenediamine-tetraacetate complexes (M(EDTA) <sup>4-</sup> , M=Al, Ga and In) in solution. <i>Journal of Molecular Liquids</i> , 2007, 131-132, 72-80.	4.9	6
124	Modeling of adsorption properties of zeolites. <i>Studies in Surface Science and Catalysis</i> , 1995, , 109-116.	1.5	5
125	A Cyclobutene-1,2-bis(imidazolium) Salt as Preligand for Palladium-Catalyzed Cross-Coupling Reactions: Properties and Applications. <i>European Journal of Organic Chemistry</i> , 2012, 2012, 754-763.	2.4	5
126	Enantioselective Acetalization by Dynamic Kinetic Resolution for the Synthesis of $\beta$ -Alkoxybutenolides by Thiourea/Quaternary Ammonium Salt Catalysts: Application to Strigolactones. <i>Angewandte Chemie</i> , 2020, 132, 13581-13585.	2.0	5

#	ARTICLE	IF	CITATIONS
127	Halogen Bonds of Iodonium Ions: A World Dissimilar to Silver Coordination. Bulletin of the Chemical Society of Japan, 2021, 94, 191-196.	3.2	5
128	Mössbauer magnetization and nuclear magnetic resonance measurements on some iridium(I) complexes with fullerene ligands. Journal of Radioanalytical and Nuclear Chemistry, 2004, 260, 133-142.	1.5	4
129	Dimerization of (+)-Lysergic Acid Esters. Heterocycles, 2007, 71, 1075.	0.7	4
130	157Å internal magnetic field in Fe[C(SiMe <sub>3</sub> ) <sub>3</sub> ] <sub>2</sub> compound at 20Å. Hyperfine Interactions, 2008, 185, 185-189.	0.5	4
131	Conformationally Locked Pyramidity Explains the Diastereoselectivity in the Methylation of <i>trans</i> -Fused Butyrolactones. Organic Letters, 2020, 22, 4597-4601.	4.6	4
132	Are bis(pyridine)iodine complexes applicable for asymmetric halogenation?. Organic and Biomolecular Chemistry, 2021, 19, 8307-8323.	2.8	4
133	Dynamic Refolding of Ion-Pair Catalysts in Response to Different Anions. Journal of Organic Chemistry, 2019, 84, 15009-15019.	3.2	3
134	Air-stable 18-electron adducts of Schrock catalysts with tuned stability constants for spontaneous release of the active species. Communications Chemistry, 2021, 4, .	4.5	3
135	Carboxylate Catalyzed Isomerization of <sup>12</sup> C, <sup>13</sup> C-Unsaturated <i>N</i> -Acetylcysteamine Thioesters**. Chemistry - A European Journal, 2022, 28, .	3.3	3
136	Theoretical Study of CO Chemisorption on Rh and Pd Clusters. Studies in Surface Science and Catalysis, 1993, 75, 1547-1550.	1.5	2
137	Cover Picture: Expanding the Scope of Metal-Free Catalytic Hydrogenation through Frustrated Lewis Pair Design (Angew. Chem. Int. Ed. 37/2010). Angewandte Chemie - International Edition, 2010, 49, 6459-6459.	13.8	2
138	Synthesis and Characterization of Fe <sup>0</sup> (2,2'-bipyridine)(2-aminoethylpyridine) and its Reaction with Dihydrogen. ChemSusChem, 2017, 10, 220-225.	6.8	2
139	Titelbild: Expanding the Scope of Metal-Free Catalytic Hydrogenation through Frustrated Lewis Pair Design (Angew. Chem. 37/2010). Angewandte Chemie, 2010, 122, 6605-6605.	2.0	0
140	Raman, Infrared, Far-infrared and Theoretical Studies of Urea Derivatives with Biological Interest. , 2010, , .		0
141	Titelbild: Intramolecular Frustrated Lewis Pair with the Smallest Boryl Site: Reversible H <sub>2</sub> Addition and Kinetic Analysis (Angew. Chem. 6/2015). Angewandte Chemie, 2015, 127, 1998-1998.	2.0	0
142	Frontispiz: Halogen Bonding Helicates Encompassing Iodonium Cations. Angewandte Chemie, 2019, 131, .	2.0	0
143	Frontispiece: Halogen Bonding Helicates Encompassing Iodonium Cations. Angewandte Chemie - International Edition, 2019, 58, .	13.8	0