Imre PÃ¡pai

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	Carboxylate Catalyzed Isomerization of Î²,Î³â€Unsaturated Nâ€Acetylcysteamine Thioesters**. Chemistry - A European Journal, 2022, 28, .	3.3	3
2	Are bis(pyridine)iodine(<scp>i</scp>) complexes applicable for asymmetric halogenation?. Organic and Biomolecular Chemistry, 2021, 19, 8307-8323.	2.8	4
3	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
4	Transition Metal-Free Direct Hydrogenation of Esters via a Frustrated Lewis Pair. ACS Catalysis, 2021, 11, 9143-9150.	11.2	9
5	The Influence of Secondary Interactions on the [Nâ^'Iâ^'N]⁺ Halogen Bond. Chemistry - A European Journal, 2021, 27, 13748-13756.	3.3	14
6	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
7	Synthesis of azahelicenes through Mallory reaction of imine precursors: corannulene substrates provide an exception to the rule in oxidative photocyclizations of diarylethenes. Chemical Science, 2021, 12, 3977-3983.	7.4	14
8	Oâ€“Iâ€“O halogen bond of halonium ions. Chemical Communications, 2020, 56, 9671-9674.	4.1	7
9	Origin of Stereoselectivity in FLP-Catalyzed Asymmetric Hydrogenation of Imines. ACS Catalysis, 2020, 10, 14290-14301.	11.2	24
10	Mechanochemical Synthesis of Corannuleneâ€Based Curved Nanographenes. Angewandte Chemie - International Edition, 2020, 59, 21620-21626.	13.8	53
11	Total Synthesis of Stemoamide, 9a-epi-Stemoamide, and 9a,10-epi-Stemoamide: Divergent Stereochemistry of the Final Methylation Steps. Synlett, 2020, 31, 1581-1586.	1.8	11
12	Mechanochemical Synthesis of Corannuleneâ€Based Curved Nanographenes. Angewandte Chemie, 2020, 132, 21804-21810.	2.0	14
13	Enantioselective Acetalization by Dynamic Kinetic Resolution for the Synthesis of Î³â€Alkoxybutenolides by Thiourea/Quaternary Ammonium Salt Catalysts: Application to Strigolactones. Angewandte Chemie, 2020, 132, 13581-13585.	2.0	5
14	Metalâ€Free Câ^'H Borylation of Nâ€Heteroarenes by Boron Trifluoride. Chemistry - A European Journal, 2020, 26, 13873-13879.	3.3	21
15	Establishing the Role of Triflate Anions in H₂ Activation by a Cationic Triorganotin(IV) Lewis Acid. ACS Catalysis, 2020, 10, 7573-7583.	11.2	12
16	Catalytic Activity of trans-Bis(pyridine)gold Complexes. Journal of the American Chemical Society, 2020, 142, 6439-6446.	13.7	25
17	Conformationally Locked Pyramidality Explains the Diastereoselectivity in the Methylation of trans-Fused Butyrolactones. Organic Letters, 2020, 22, 4597-4601.	4.6	4
18	Enantioselective Acetalization by Dynamic Kinetic Resolution for the Synthesis of Î³â€Alkoxybutenolides by Thiourea/Quaternary Ammonium Salt Catalysts: Application to Strigolactones. Angewandte Chemie - International Edition, 2020, 59, 13479-13483.	13.8	24

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19	Frontispiz: Halogen Bonding Helicates Encompassing Iodonium Cations. Angewandte Chemie, 2019, 131, .	2.0	0
20	Frontispiece: Halogen Bonding Helicates Encompassing Iodonium Cations. Angewandte Chemie - International Edition, 2019, 58, .	13.8	0
21	Mechanism of Au(III)-Mediated Alkoxycyclization of a 1,6-Enyne. Journal of the American Chemical Society, 2019, 141, 18221-18229.	13.7	22
22	Dynamic Refolding of Ion-Pair Catalysts in Response to Different Anions. Journal of Organic Chemistry, 2019, 84, 15009-15019.	3.2	3
23	Mechanism of Heterolytic Hydrogen Splitting by Frustrated Lewis Pairs: Comparison of Static and Dynamic Models. ACS Catalysis, 2019, 9, 6049-6057.	11.2	30
24	Halogen Bonding Helicates Encompassing Iodonium Cations. Angewandte Chemie - International Edition, 2019, 58, 9012-9016.	13.8	66
25	Halogen Bonding Helicates Encompassing Iodonium Cations. Angewandte Chemie, 2019, 131, 9110-9114.	2.0	16
26	RuBisCOâ€inspirierte CO₂â€Aktivierung und Umwandlung durch einen Iridium(I)â€Komplex. Angewandte Chemie, 2018, 130, 2480-2483.	2.0	9
27	RuBisCOâ€Inspired CO₂ Activation and Transformation by an Iridium(I) Complex. Angewandte Chemie - International Edition, 2018, 57, 2455-2458.	13.8	16
28	Base-induced reversible H₂ addition to a single Sn(<scp>ii</scp>) centre. Chemical Science, 2018, 9, 8716-8722.	7.4	19
29	Mechanistic Insight into Asymmetric Hetero-Michael Addition of Î±,Î²-Unsaturated Carboxylic Acids Catalyzed by Multifunctional Thioureas. Journal of the American Chemical Society, 2018, 140, 12216-12225.	13.7	68
30	Replacing C₆F₅ groups with Cl and H atoms in frustrated Lewis pairs: H₂ additions and catalytic hydrogenations. Dalton Transactions, 2017, 46, 2263-2269.	3.3	25
31	Correlating electronic and catalytic properties of frustrated Lewis pairs for imine hydrogenation. Journal of Organometallic Chemistry, 2017, 847, 258-262.	1.8	18
32	Expanding the Boundaries of Waterâ€Tolerant Frustrated Lewis Pair Hydrogenation: Enhanced Back Strain in the Lewis Acid Enables the Reductive Amination of Carbonyls. Angewandte Chemie - International Edition, 2017, 56, 9512-9516.	13.8	79
33	Expanding the Boundaries of Waterâ€Tolerant Frustrated Lewis Pair Hydrogenation: Enhanced Back Strain in the Lewis Acid Enables the Reductive Amination of Carbonyls. Angewandte Chemie, 2017, 129, 9640-9644.	2.0	16
34	Organocatalysts Fold To Generate an Active Site Pocket for the Mannich Reaction. ACS Catalysis, 2017, 7, 3284-3294.	11.2	22
35	Stereocontrol in Diphenylprolinol Silyl Ether Catalyzed Michael Additions: Steric Shielding or Curtinâ€“Hammett Scenario?. Journal of the American Chemical Society, 2017, 139, 17052-17063.	13.7	29
36	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

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37	Synthesis and Characterization of Fe⁰(2,2â€²â€bipyridine) (2â€aminoethylâ€pyridine) and its Reaction with Dihydrogen. ChemSusChem, 2017, 10, 220-225.	6.8	2
38	Nuclear spin hyperpolarization with ansa-aminoboranes: a metal-free perspective for parahydrogen-induced polarization. Physical Chemistry Chemical Physics, 2016, 18, 27784-27795.	2.8	34
39	Atomâ€Efficient Synthesis of Alkynylfluoroborates Using BF₃â€Based Frustrated Lewis Pairs. Angewandte Chemie - International Edition, 2016, 55, 14146-14150.	13.8	32
40	Atomâ€Efficient Synthesis of Alkynylfluoroborates Using BF₃â€Based Frustrated Lewis Pairs. Angewandte Chemie, 2016, 128, 14352-14356.	2.0	12
41	A Catalyst Designed for the Enantioselective Construction of Methylâ€and Alkylâ€Substituted Tertiary Stereocenters. Angewandte Chemie - International Edition, 2016, 55, 669-673.	13.8	25
42	Thiourea Derivatives as BrÃ¸nsted Acid Organocatalysts. ACS Catalysis, 2016, 6, 4379-4387.	11.2	74
43	Ionizing radiation induced degradation of monuron in dilute aqueous solution. Radiation Physics and Chemistry, 2016, 124, 191-197.	2.8	16
44	Metal-Free sp²-Câ€“H Borylation as a Common Reactivity Pattern of Frustrated 2-Aminophenylboranes. Journal of the American Chemical Society, 2016, 138, 4860-4868.	13.7	115
45	Folding Patterns in a Family of Oligoamide Foldamers. Chemistry - A European Journal, 2015, 21, 9493-9504.	3.3	16
46	RÃ¼cktitelbild: Intramolecular Frustrated Lewis Pair with the Smallest Boryl Site: Reversible H2Addition and Kinetic Analysis (Angew. Chem. 6/2015). Angewandte Chemie, 2015, 127, 1998-1998.	2.0	0
47	Chiral Molecular Tweezers: Synthesis and Reactivity in Asymmetric Hydrogenation. Journal of the American Chemical Society, 2015, 137, 4038-4041.	13.7	151
48	Reaction Mechanisms in the Direct Carboxylation of Alcohols for the Synthesis of Acyclic Carbonates. Topics in Catalysis, 2015, 58, 2-14.	2.8	22
49	Moisture-Tolerant Frustrated Lewis Pair Catalyst for Hydrogenation of Aldehydes and Ketones. ACS Catalysis, 2015, 5, 5366-5372.	11.2	144
50	Intramolecular Frustrated Lewis Pair with the Smallest Boryl Site: Reversible H₂ Addition and Kinetic Analysis. Angewandte Chemie - International Edition, 2015, 54, 1749-1753.	13.8	89
51	Superstable Palladium(0) Complex as an Airâ€and Thermostable Catalyst for Suzuki Coupling Reactions. European Journal of Organic Chemistry, 2015, 2015, 60-66.	2.4	19
52	Steric Control of Geminal Lewis Pair Behavior: Frustration Induced Dyotropic Rearrangement. Synlett, 2014, 25, 1525-1528.	1.8	8
53	On the Mechanism of Bifunctional Squaramideâ€Catalyzed Organocatalytic Michael Addition: A Protonated Catalyst as an Oxyanion Hole. Chemistry - A European Journal, 2014, 20, 5631-5639.	3.3	103
54	Mukaiyamaâ€“Michael Reactions with transâ€2,5â€Diarylpyrrolidine Catalysts: Enantioselectivity Arises from Attractive Noncovalent Interactions, Not from Steric Hindrance. Chemistry - A European Journal, 2014, 20, 5983-5993.	3.3	48

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55	The reaction mechanism in the ethanolysis of urea with transition metal-based catalysts: DFT calculations and experiments. Journal of CO2 Utilization, 2014, 8, 27-33.	6.8	18
56	Cross-Dehydrogenative Couplings between Indoles and Î²-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
57	A frustrated-Lewis-pair approach to catalytic reduction of alkynes to cis-alkenes. Nature Chemistry, 2013, 5, 718-723.	13.6	343
58	Reactivity Models of Hydrogen Activation by Frustrated Lewis Pairs: Synergistic Electron Transfers or Polarization by Electric Field?. Journal of the American Chemical Society, 2013, 135, 4425-4437.	13.7	193
59	Catalytic Synthesis of Hydroxymethylâ€2â€oxazolidinones from Glycerol or Glycerol Carbonate and Urea. ChemSusChem, 2013, 6, 345-352.	6.8	25
60	Hydrogen Activation by Frustrated Lewis Pairs: Insights from Computational Studies. Topics in Current Chemistry, 2013, 332, 157-211.	4.0	47
61	Dihydrooxazine Oxides as Key Intermediates in Organocatalytic Michael Additions of Aldehydes to Nitroalkenes. Angewandte Chemie - International Edition, 2012, 51, 13144-13148.	13.8	89
62	Association of frustrated phosphineâ€“borane pairs in toluene: molecular dynamics simulations. Dalton Transactions, 2012, 41, 9023.	3.3	57
63	Cooperative Assistance in Bifunctional Organocatalysis: Enantioselective Mannich Reactions with Aliphatic and Aromatic Imines. Angewandte Chemie - International Edition, 2012, 51, 8495-8499.	13.8	78
64	Catalytic Hydrogenation with Frustrated Lewis Pairs: Selectivity Achieved by Sizeâ€Exclusion Design of Lewis Acids. Chemistry - A European Journal, 2012, 18, 574-585.	3.3	151
65	A Cyclobuteneâ€1,2â€bis(imidazolium) Salt as Preligand for Palladiumâ€Catalyzed Crossâ€Coupling Reactions: Properties and Applications. European Journal of Organic Chemistry, 2012, 2012, 754-763.	2.4	5
66	Dual Hydrogenâ€Bond/Enamine Catalysis Enables a Direct Enantioselective Threeâ€Component Domino Reaction. Angewandte Chemie - International Edition, 2011, 50, 6123-6127.	13.8	47
67	Stereoelectronic Requirements for Optimal Hydrogenâ€Bondâ€Catalyzed Enolization. Chemistry - A European Journal, 2011, 17, 2859-2866.	3.3	15
68	Influence of Al2O3 on the performance of CeO2 used as catalyst in the direct carboxylation of methanol to dimethylcarbonate and the elucidation of the reaction mechanism. Journal of Catalysis, 2010, 269, 44-52.	6.2	113
69	Rearrangements of Nâ€Heterocyclic Carbenes of Pyrazole to 4â€Aminoquinolines and Benzoquinolines. European Journal of Organic Chemistry, 2010, 2010, 4296-4305.	2.4	31
70	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
71	Expanding the Scope of Metalâ€Free Catalytic Hydrogenation through Frustrated Lewis Pair Design. Angewandte Chemie - International Edition, 2010, 49, 6559-6563.	13.8	234
72	Cover Picture: Expanding the Scope of Metalâ€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

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73	Raman, Infrared, Far-infrared and Theoretical Studies of Urea Derivatives with Biological Interest. , 2010, , .		0
74	The solid state structure and reactivity of NbCl5Â·(N,Nâ€²-dicyclohexylurea) in solution: evidence for co-ordinated urea dehydration to the relevant carbodiimide. Dalton Transactions, 2010, 39, 6985.	3.3	31
75	H₂CO₃ Forms via HCO₃^{â^'} in Water. Journal of Physical Chemistry B, 2010, 114, 16854-16859.	2.6	92
76	Vibrational Spectroscopic and Theoretical Studies of Urea Derivatives with Biochemical Interest:N,Nâ€²-Dimethylurea,N,N,Nâ€²,Nâ€²-Tetramethylurea, andN,Nâ€²-Dimethylpropyleneurea. Applied Spectroscopy Reviews, 2010, 45, 274-326.	6.7	10
77	Observation and interpretation of 157.5ÂT internal magnetic field in Fe[C(SiMe3)3]2 coordination compound. Structural Chemistry, 2009, 20, 453-460.	2.0	11
78	Mechanism of hydrogen activation by frustrated Lewis pairs: A molecular orbital approach. International Journal of Quantum Chemistry, 2009, 109, 2416-2425.	2.0	124
79	Glyphosate complexation to aluminium(III). An equilibrium and structural study in solution using potentiometry, multinuclear NMR, ATRâ€“FTIR, ESI-MS and DFT calculations. Journal of Inorganic Biochemistry, 2009, 103, 1426-1438.	3.5	27
80	Rationalizing the Reactivity of Frustrated Lewis Pairs: Thermodynamics of H₂ Activation and the Role of Acidâ^'Base Properties. Journal of the American Chemical Society, 2009, 131, 10701-10710.	13.7	303
81	On the Mechanism of B(C₆F₅)₃-Catalyzed Direct Hydrogenation of Imines: Inherent and Thermally Induced Frustration. Journal of the American Chemical Society, 2009, 131, 2029-2036.	13.7	247
82	Synthesis and X-ray characterization of [RhCl(C2H4)(PiPr3)]2. Multinuclear NMR and DFT investigation of its solid-state and solution reaction with dihydrogen. Ethene and propene hydrogenation by the solid Rh-hydrides. Dalton Transactions, 2009, , 7924.	3.3	9
83	157ÂT internal magnetic field in Fe[C(SiMe3)3]2 compound at 20ÂK. Hyperfine Interactions, 2008, 185, 185-189.	0.5	4
84	Turning Frustration into Bond Activation: A Theoretical Mechanistic Study on Heterolytic Hydrogen Splitting by Frustrated Lewis Pairs. Angewandte Chemie - International Edition, 2008, 47, 2435-2438.	13.8	364
85	Concerted attack of frustrated Lewis acidâ€“base pairs on olefinic double bonds: a theoretical study. Chemical Communications, 2008, , 3148.	4.1	106
86	Dimerization of (+)-Lysergic Acid Esters. Heterocycles, 2007, 71, 1075.	0.7	4
87	Evidence for Spontaneous Release of Acrylates from a Transitionâ€Metal Complex Upon Coupling Ethene or Propene with a Carboxylic Moiety or CO₂. Chemistry - A European Journal, 2007, 13, 9028-9034.	3.3	61
88	A novel ambident reactivity of azolylacroleins. Tetrahedron, 2007, 63, 4730-4736.	1.9	9
89	Multinuclear NMR and DFT studies of the structure and fluxionality for MIIIâ€“ethylenediamine-tetraacetate complexes (M(EDTA)â^', M=Al, Ga and In) in solution. Journal of Molecular Liquids, 2007, 131-132, 72-80.	4.9	6
90	Computing Reliable Energetics for Conjugate Addition Reactions. Organic Letters, 2007, 9, 4279-4282.	4.6	67

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91	Hydride Donor Abilities of Cationic Transition Metal Hydrides from DFT-PCM Calculations. Organometallics, 2006, 25, 820-825.	2.3	31
92	Theoretical investigation of catalytic HCO3â^' hydrogenation in aqueous solutions. Catalysis Today, 2006, 115, 53-60.	4.4	57
93	Theoretical Studies on the Bifunctionality of Chiral Thiourea-Based Organocatalysts:Â Competing Routes to Câ^'C Bond Formation. Journal of the American Chemical Society, 2006, 128, 13151-13160.	13.7	408
94	Reaction mechanism of the direct carboxylation of methanol to dimethylcarbonate: experimental and theoretical studies. Topics in Catalysis, 2006, 40, 71-81.	2.8	50
95	On the Existence of the Elusive Monomethyl Ester of Carbonic Acid [CH3OC(O)OH] at 300 K:1H- and13C NMR Measurements and DFT Calculations. European Journal of Inorganic Chemistry, 2006, 2006, 908-913.	2.0	48
96	Theoretical Mechanistic Study of Rhodium(I) Phosphine-Catalyzed H/D Exchange Processes in Aqueous Solutions. Organometallics, 2005, 24, 3059-3065.	2.3	49
97	Theoretical Investigation of the Reactivity of Copper Atoms with OCS:Â Comparison with CS2and CO2. Journal of Physical Chemistry A, 2005, 109, 7932-7937.	2.5	25
98	Mechanism of Formation of Organic Carbonates from Aliphatic Alcohols and Carbon Dioxide under Mild Conditions Promoted by Carbodiimides. DFT Calculation and Experimental Study. Journal of Organic Chemistry, 2005, 70, 6177-6186.	3.2	90
99	MÃ¶ssbauer 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
100	Behaviour of[PdH(dppe)2]X (X=CF3SO3â^', SbF6â^', BF4â^') as Proton or Hydride Donor: Relevance to Catalysis. Chemistry - A European Journal, 2004, 10, 3708-3716.	3.3	21
101	Mechanistic Details of Nickel(0)-Assisted Oxidative Coupling of CO₂ with C₂H₄. Organometallics, 2004, 23, 5252-5259.	2.3	95
102	N-benzoylimido complexes of palladium. Synthesis, structural characterisation and structureâ€"reactivity relationship. Dalton Transactions, 2004, , 2041-2050.	3.3	7
103	Rotational reorientation dynamics of nile blue A and oxazine 720 in protic solvents. Chemical Physics, 2003, 286, 81-96.	1.9	31
104	Metal Insertion Route of the Ni + CO2 â†' NiO + CO Reaction. Journal of Physical Chemistry A, 2003, 107, 6708-6713.	2.5	29
105	Structure and Properties of the [Ru(bpy)(CN)4]2- Complex and Its Solvent Environment:â€‰ X-ray Diffraction and Density Functional Study. Journal of Physical Chemistry A, 2003, 107, 9903-9909.	2.5	15
106	Acrylate Formation via Metal-Assisted Câ^'C Coupling between CO2and C2H4:Â Reaction Mechanism as Revealed from Density Functional Calculations. Journal of the American Chemical Society, 2003, 125, 14847-14858.	13.7	66
107	Theoretical Investigation of the Reactivity of Copper Atoms with Carbon Disulfide. Journal of Physical Chemistry A, 2003, 107, 2711-2715.	2.5	15
108	2Aâ€˜ and2Aâ€˜Ââ€˜ Energy Surfaces for the Sc + CO2â†' ScO + CO Reaction. Journal of Physical Chemistry A, 2002, 106, 9551-9557.	2.5	39

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109	Vanadium Insertion into CO2, CS2and OCS: A Comparative Theoretical Study. Journal of Physical Chemistry A, 2002, 106, 4181-4186.	2.5	49
110	Synthesis, Characterization, and Reactivity of Cationic Hydride [HPd(diphosphine)2]+CF3SO3-, the Missing Member of the Family [HM(dppe)2]+X-(M = Ni, Pd, Pt). DFT QM/MM Structural Predictions for the [HPd(dppe)2]+Moiety. Inorganic Chemistry, 2002, 41, 6550-6552.	4.0	17
111	Theoretical analysis of bis(ethylene) complexes of molybdenum and tungsten. Journal of Organometallic Chemistry, 2002, 663, 83-90.	1.8	8
112	Unprecedented formal â€˜2+2â€™ addition of allene to CO2 promoted by [RhCl(C2H4)(PiPr3)]2: direct synthesis of the four membered lactone Î±-methylene-Î²-oxiethanone. The intermediacy of [RhH2Cl(PiPr3)]2: theoretical aspects and experiments. Inorganica Chimica Acta, 2002, 334, 294-300.	2.4	22
113	Analysis of the vibrational spectra, force fields, and molecular structures of pentacarbonyl(methyl)manganese(I) and pentacarbonyl(methyl)rhenium(I). Journal of Organometallic Chemistry, 2000, 616, 1-9.	1.8	15
114	The Ti 2 H 2 molecule: terminal or bridging hydrogens ?. Theoretical Chemistry Accounts, 2000, 104, 131-139.	1.4	10
115	Identification of Cu2(N2) and Cu2(N2)2Complexes:Â Matrix Isolation and Density Functional Studiesâ€. Journal of Physical Chemistry A, 2000, 104, 3572-3578.	2.5	16
116	Hydrogen Bonding in Methyl-Substituted Pyridineâ‹¯Water Complexes:â€‰ A Theoretical Study. Journal of Physical Chemistry A, 2000, 104, 2132-2137.	2.5	100
117	Spectroscopic and theoretical study of [PdCl3(C2H4)]â‹¯ and [PdCl3(C2D4)]â‹¯ complexes. Journal of Organometallic Chemistry, 1999, 584, 118-121.	1.8	20
118	Carbon dioxide interaction with metal atoms: matrix isolation spectroscopic study and DFT calculations. Coordination Chemistry Reviews, 1999, 190-192, 557-576.	18.8	54
119	Can the FeCO bending be higher than the FeC stretching frequency in CO adducts of heme proteins?. Chemical Physics Letters, 1998, 287, 531-534.	2.6	11
120	CO2Coordination to Nickel Atoms:Â Matrix Isolation and Density Functional Studies. Journal of Physical Chemistry A, 1997, 101, 2626-2633.	2.5	64
121	An IR Matrix Isolation and DFT Theoretical Study of the First Steps of the Ti(0) Ethylene Reaction: Vinyl Titanium Hydride and Titanacyclopropene. Journal of Physical Chemistry A, 1997, 101, 9650-9659.	2.5	53
122	Theoretical Study of the Interaction of the Ti Atom with CO2:â€‰ Cleavage of the Câ‹¯O Bond. Journal of Physical Chemistry A, 1997, 101, 4465-4471.	2.5	71
123	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
124	A density functional study of Sc2 and Sc3. Chemical Physics Letters, 1997, 267, 551-556.	2.6	32
125	The covalently bound N3O2 molecule: Two possible isomers. Chemical Physics Letters, 1996, 253, 196-200.	2.6	11
126	Modeling of adsorption properties of zeolites. Studies in Surface Science and Catalysis, 1995, , 109-116.	1.5	5

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127	Theoretical study of the Cu(H2O) and Cu(NH3) complexes and their photolysis products. Journal of Chemical Physics, 1995, 103, 1860-1870.	3.0	36
128	Modeling of N2 and O2 Adsorption in Zeolites. The Journal of Physical Chemistry, 1995, 99, 12925-12932.	2.9	54
129	Density Functional Calculations on Model Clusters of Zeolite-.beta.. The Journal of Physical Chemistry, 1994, 98, 4654-4659.	2.9	55
130	Numerical grids for density functional calculations of molecular properties. International Journal of Quantum Chemistry, 1994, 52, 799-807.	2.0	30
131	First principles molecular dynamics calculation of the structure and acidity of a bulk zeolite. Chemical Physics Letters, 1994, 226, 245-250.	2.6	44
132	Density functional study of nitrogen oxides. Journal of Chemical Physics, 1994, 100, 2910-2923.	3.0	196
133	Chemisorption of formate and acetate on cluster models of Rh and bimetallic RhSn clusters. Surface Science, 1993, 282, 262-272.	1.9	19
134	Singlet- and triplet-state (ethene)nickel: a density functional study. The Journal of Physical Chemistry, 1993, 97, 9986-9991.	2.9	39
135	Theoretical Study of CO Chemisorption on Rh and Pd Clusters. Studies in Surface Science and Catalysis, 1993, 75, 1547-1550.	1.5	2
136	Gaussian density functional calculations on hydrogen-bonded systems. Journal of the American Chemical Society, 1992, 114, 4391-4400.	13.7	462
137	Vibrational analysis of formate adsorbed on Ni(110): LCGTO-MCP-LSD study. Surface Science, 1992, 262, L134-L138.	1.9	25
138	Density functional study of carbon monoxide chemisorption on model clusters of rhodium and palladium: a comparative analysis of the site selection. Journal of the American Chemical Society, 1992, 114, 7452-7458.	13.7	81
139	Molecular structure of mono- and dicarbonyls of rhodium and palladium. Theoretica Chimica Acta, 1992, 84, 217-235.	0.8	37
140	Calculation of equilibrium geometries and harmonic frequencies by theLCGTO-MCP-local spin density method. International Journal of Quantum Chemistry, 1990, 38, 29-39.	2.0	42
141	An LCGTO-MCP-LSD study of the (2 Ã— 1) H-covered Pd(110) surface. Surface Science, 1990, 236, 241-249.	1.9	21
142	Calculation of normal frequencies of adsorbed molecules by the LCGTO-MCP-LSD method. Surface Science, 1990, 240, L604-L608.	1.9	11
143	Recent developments of FT-IR and Raman spectroscopy in coordination chemistry. Pure and Applied Chemistry, 1989, 61, 973-978.	1.9	10