Josep M Luis

List of Publications by Year
in descending order

150 papers	5,622 citations	61687 45 h-index	116156 66 g-index
157 all docs	157 docs citations	157 times ranked	4637 citing authors

#	Article	IF	Citations
1	How Reliable Are Modern Density Functional Approximations to Simulate Vibrational Spectroscopies?. Journal of Physical Chemistry Letters, 2022, 13, 5963-5968.	2.1	12
2	Origin-Independent Decomposition of the Static Polarizability. Journal of Chemical Theory and Computation, 2021, 17, 1098-1105.	2.3	6
3	Well-Defined Aryl-FeII Complexes in Cross-Coupling and Câ€“H Activation Processes. Organometallics, 2021, 40, 1195-1200.	1.1	2
4	How Many Electrons Does a Molecular Electride Hold?. Journal of Physical Chemistry A, 2021, 125, 4819-4835.	1.1	7
5	Tailoring the nonlinear absorption of fluorescent dyes by substitution at a boron center. Journal of Materials Chemistry C, 2021, 9, 6225-6233.	2.7	6
6	Evaluation of charge-transfer rates in fullerene-based donorâ€“acceptor dyads with different density functional approximations. Physical Chemistry Chemical Physics, 2021, 23, 5376-5384.	1.3	18
7	Fast and Simple Evaluation of the Catalysis and Selectivity Induced by External Electric Fields. ACS Catalysis, 2021, 11, 14467-14479.	5.5	14
8	Infrared Spectra of Hydrogen-Bonded Molecular Complexes Under Spatial Confinement. Frontiers in Chemistry, 2021, 9, 801426.	1.8	2
9	A Unified Electro- and Photocatalytic CO₂ to CO Reduction Mechanism with Aminopyridine Cobalt Complexes. Journal of the American Chemical Society, 2020, 142, 120-133.	6.6	75
10	Bingelâ€“Hirsch Addition of Diethyl Bromomalonate to Ionâ€Encapsulated Fullerenes M@C 60 (M=Ã˜, Li + ,) Tj ETQq0 0 0 rgBT /Overloc	1.7	6
11	Mechanistic Insights into the ortho-Defluorination-Hydroxylation of 2-Halophenolates Promoted by a Bis(Î¼-oxo)dicopper(III) Complex. Inorganic Chemistry, 2020, 59, 17018-17027.	1.9	8
12	A new tuned range-separated density functional for the accurate calculation of second hyperpolarizabilities. Physical Chemistry Chemical Physics, 2020, 22, 11871-11880.	1.3	28
13	Controlling Two-Photon Action Cross Section by Changing a Single Heteroatom Position in Fluorescent Dyes. Journal of Physical Chemistry Letters, 2020, 11, 5920-5925.	2.1	14
14	Partitioning of interaction-induced nonlinear optical properties of molecular complexes. II. Halogen-bonded systems. Physical Chemistry Chemical Physics, 2020, 22, 4225-4234.	1.3	8
15	Chemodivergent Nickel(0)-Catalyzed Arene Câ€“F Activation with Alkynes: Unprecedented Câ€“F/Câ€“H Double Insertion. ACS Catalysis, 2019, 9, 11074-11081.	5.5	32
16	Nonlinear optical response of endohedral all-metal electride cages 2eâ¯Mg2+(M@E12)2â¯Ca2+ (M = Ni,) Tj ETQq0 0 0 rgBT /Overlock 1	2.7	16
17	Partition of optical properties into orbital contributions. Physical Chemistry Chemical Physics, 2019, 21, 15380-15391.	1.3	5
18	Can Density Functional Theory Be Trusted for High-Order Electric Properties? The Case of Hydrogen-Bonded Complexes. Journal of Chemical Theory and Computation, 2019, 15, 3570-3579.	2.3	21

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19	Design of Iron Coordination Complexes as Highly Active Homogenous Water Oxidation Catalysts by Deuteration of Oxidation-Sensitive Sites. Journal of the American Chemical Society, 2019, 141, 323-333.	6.6	55
20	Metal Cluster Electrides: A New Type of Molecular Electride with Delocalised Polyattractor Character. Chemistry - A European Journal, 2018, 24, 9853-9859.	1.7	28
21	Understanding light-driven H₂ evolution through the electronic tuning of aminopyridine cobalt complexes. Chemical Science, 2018, 9, 2609-2619.	3.7	31
22	Mechanism of the Selective Fe-Catalyzed Arene Carbonâ€“Hydrogen Bond Functionalization. ACS Catalysis, 2018, 8, 4313-4322.	5.5	32
23	Acidâ€Triggered Oâ”O Bond Heterolysis of a Nonheme Fe^{III}(OOH) Species for the Stereospecific Hydroxylation of Strong Câ”H Bonds. Chemistry - A European Journal, 2018, 24, 5331-5340.	1.7	43
24	Vibrational Linear and Nonlinear Optical Properties: Theory, Methods, and Application. , 2018, , 401-429.		2
25	Mechanistic insights into the SN2-type reactivity of aryl-Co(iii) masked-carbenes for Câ€“C bond forming transformations. Chemical Science, 2018, 9, 5736-5746.	3.7	14
26	An Objective Alternative to IUPAC's Approach To Assign Oxidation States. Angewandte Chemie - International Edition, 2018, 57, 10525-10529.	7.2	43
27	An Objective Alternative to IUPAC's Approach To Assign Oxidation States. Angewandte Chemie, 2018, 130, 10685-10689.	1.6	23
28	Partitioning of interaction-induced nonlinear optical properties of molecular complexes. I. Hydrogen-bonded systems. Physical Chemistry Chemical Physics, 2018, 20, 19841-19849.	1.3	12
29	Quantum Mechanics/Molecular Mechanics Studies on the Relative Reactivities of Compound I and II in Cytochrome P450 Enzymes. International Journal of Molecular Sciences, 2018, 19, 1974.	1.8	14
30	Rationalizing the relative abundances of trimetallic nitride template-based endohedral metallofullerenes from aromaticity measures. Chemical Communications, 2017, 53, 4140-4143.	2.2	5
31	Efficient External Electric Field Manipulated Nonlinear Optical Switches of All-Metal Electride Molecules with Infrared Transparency: Nonbonding Electron Transfer Forms an Excess Electron Lone Pair. Journal of Physical Chemistry C, 2017, 121, 958-968.	1.5	53
32	Relevance of the DFT method to study expanded porphyrins with different topologies. Journal of Computational Chemistry, 2017, 38, 2819-2828.	1.5	64
33	Carboxylate-Assisted Formation of Aryl-Co(III) Masked-Carbenes in Cobalt-Catalyzed Câ€“H Functionalization with Diazo Esters. Journal of the American Chemical Society, 2017, 139, 14649-14655.	6.6	36
34	Trifluoromethylation of a Wellâ€Defined Squareâ€Planar Arylâ€Ni^{II} Complex involving Ni^{III}/CF₃[.] and Ni^{IV}â”CF₃ Intermediate Species. Chemistry - A European Journal, 2017, 23, 11662-11668.	1.7	23
35	The key role of aromaticity in the structure and reactivity of C60 and endohedral metallofullerenes. Inorganica Chimica Acta, 2017, 468, 38-48.	1.2	8
36	Design of HÃ¼ckelâ€“MÃ¶bius Topological Switches with High Nonlinear Optical Properties. Journal of Physical Chemistry C, 2017, 121, 19348-19357.	1.5	34

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37	Vibrational nonlinear optical properties of spatially confined weakly bound complexes. Physical Chemistry Chemical Physics, 2017, 19, 24276-24283.	1.3	8
38	A Cu^I/Cu^{III} prototypical organometallic mechanism for the deactivation of an active pincer-like Cu^I catalyst in Ullmann-type couplings. Chemical Communications, 2017, 53, 8786-8789.	2.2	36
39	Iron and Manganese Catalysts for the Selective Functionalization of Arene C(sp²)â^'H Bonds by Carbene Insertion. Angewandte Chemie - International Edition, 2016, 55, 6530-6534.	7.2	77
40	The Regioselectivity of Bingelâ€“Hirsch Cycloadditions on Isolated Pentagon Rule Endohedral Metallofullerenes. Angewandte Chemie, 2016, 128, 2420-2423.	1.6	9
41	Iron and Manganese Catalysts for the Selective Functionalization of Arene C(sp²)â^'H Bonds by Carbene Insertion. Angewandte Chemie, 2016, 128, 6640-6644.	1.6	29
42	Numerical and exact kinetic energy operator using Eckart conditions with one or several reference geometries: Application to HONO. Journal of Chemical Physics, 2016, 144, 084116.	1.2	21
43	Isolation of Key Organometallic Aryl-Co(III) Intermediates in Cobalt-Catalyzed C(sp²)â€“H Functionalizations and New Insights into Alkyne Annulation Reaction Mechanisms. Journal of the American Chemical Society, 2016, 138, 14388-14397.	6.6	60
44	On the physical origins of interaction-induced vibrational (hyper)polarizabilities. Physical Chemistry Chemical Physics, 2016, 18, 22467-22477.	1.3	16
45	The Regioselectivity of Bingelâ€“Hirsch Cycloadditions on Isolated Pentagon Rule Endohedral Metallofullerenes. Angewandte Chemie - International Edition, 2016, 55, 2374-2377.	7.2	37
46	On the existence and characterization of molecular electrides. Chemical Communications, 2015, 51, 4865-4868.	2.2	68
47	Comparison of Property-Oriented Basis Sets for the Computation of Electronic and Nuclear Relaxation Hyperpolarizabilities. Journal of Chemical Theory and Computation, 2015, 11, 4119-4128.	2.3	14
48	On the particular importance of vibrational contributions to the static electrical properties of model linear molecules under spatial confinement. Physical Chemistry Chemical Physics, 2015, 17, 21782-21786.	1.3	17
49	Oxidant-Free Au(I)-Catalyzed Halide Exchange and C_{sp2}â€“O Bond Forming Reactions. Journal of the American Chemical Society, 2015, 137, 13389-13397.	6.6	59
50	H₂ oxidation versus organic substrate oxidation in non-heme iron mediated reactions with H₂O₂. Chemical Communications, 2015, 51, 14992-14995.	2.2	4
51	Computational Insight into the Mechanism of Alkane Hydroxylation by Non-heme Fe(PyTACN) Iron Complexes. Effects of the Substrate and Solvent. Inorganic Chemistry, 2015, 54, 8223-8236.	1.9	24
52	Understanding the Exohedral Functionalization of Endohedral Metallofullerenes Metallofullerenes. Carbon Materials, 2015, , 67-99.	0.2	0
53	Computational insight into Wilkinson's complex catalyzed [2Â+Â2Â+Â2] cycloaddition mechanism leading to pyridine formation. Journal of Organometallic Chemistry, 2014, 768, 15-22.	0.8	15
54	Computation of Nonlinear Optical Properties of Molecules with Large Amplitude Anharmonic Motions. III. Arbitrary Double-Well Potentials. Journal of Chemical Theory and Computation, 2014, 10, 236-242.	2.3	5

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55	Arylâ€Copper(III)â€Acetylides as Key Intermediates in Cï£¿C_{sp} Model Couplings under Mild Conditions. Chemistry - A European Journal, 2014, 20, 10005-10010.	1.7	30
56	The role of aromaticity in determining the molecular structure and reactivity of (endohedral) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 702 T	18.7	97
57	Direct observation of two-electron Ag(I)/Ag(III) redox cycles in coupling catalysis. Nature Communications, 2014, 5, 4373.	5.8	65
58	Theoretical Study of the Water Oxidation Mechanism with Non-heme Fe(Pytacn) Iron Complexes. Evidence That the Fe^{IV}(O)(Pytacn) Species Cannot React with the Water Molecule To Form the Oâ€“O Bond. Inorganic Chemistry, 2014, 53, 5474-5485.	1.9	40
59	Unraveling the Mechanism of Water Oxidation Catalyzed by Nonheme Iron Complexes. Chemistry - A European Journal, 2014, 20, 5696-5707.	1.7	75
60	Aromaticity as the driving force for the stability of non-IPR endohedral metallofullerene Bingelâ€“Hirsch adducts. Chemical Communications, 2013, 49, 8767.	2.2	21
61	Maximum Aromaticity as a Guiding Principle for the Most Suitable Hosting Cages in Endohedral Metallofullerenes. Angewandte Chemie - International Edition, 2013, 52, 9275-9278.	7.2	55
62	A Complete Guide on the Influence of Metal Clusters in the Dielsâ€“Alder Regioselectivity of I_hâ€C₈₀ Endohedral Metallofullerenes. Chemistry - A European Journal, 2013, 19, 14931-14940.	1.7	37
63	Electrochemical control of the regioselectivity in the exohedral functionalization of C60: the role of aromaticity. Chemical Communications, 2013, 49, 1220.	2.2	44
64	Selfâ€Assembled Tetragonal Prismatic Molecular Cage Highly Selective for Anionic Ï€ Guests. Chemistry - A European Journal, 2013, 19, 1445-1456.	1.7	38
65	Dielsâ€“Alder and Retroâ€Dielsâ€“Alder Cycloadditions of (1,2,3,4,5â€Pentamethyl)cyclopentadiene to La@C₂v</sub>â€C₈₂: Regioselectivity and Product Stability. Chemistry - A European Journal, 2013, 19, 4468-4479.	1.7	27
66	The Mechanism of Stereospecific Cï£¿H Oxidation by Fe(Pytacn) Complexes: Bioinspired Nonâ€Heme Iron Catalysts Containing cisâ€Labile Exchangeable Sites. Chemistry - A European Journal, 2013, 19, 6724-6738.	1.7	88
67	On the vibrational linear and nonlinear optical properties of compounds involving noble gas atoms: HXeOXeH, HXeOXeF, and FXeOXeF. Journal of Computational Chemistry, 2013, 34, 1446-1455.	1.5	6
68	Electronic Effects on Singleâ€Site Iron Catalysts for Water Oxidation. Chemistry - A European Journal, 2013, 19, 8042-8047.	1.7	118
69	Performance of density functional theory in computing nonresonant vibrational (hyper)polarizabilities. Journal of Computational Chemistry, 2013, 34, 1775-1784.	1.5	46
70	A Full Dimensionality Approach to Evaluate the Nonlinear Optical Properties of Molecules with Large Amplitude Anharmonic Tunneling Motions. Journal of Chemical Theory and Computation, 2013, 9, 520-532.	2.3	9
71	Resonant and Nonresonant Hyperpolarizabilities of Spatially Confined Molecules: A Case Study of Cyanoacetylene. Journal of Chemical Theory and Computation, 2013, 9, 3463-3472.	2.3	27
72	L'Oeuvre of Bernie Kirtman. , 2012, , .		0

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73	L'Oeuvre of Bernie Kirtman. , 2012, , .		0
74	Prediction of the linear and nonlinear electric susceptibilities of 3-methyl-4-nitropyridine-N-oxyde (POM) and meta-nitroaniline (mNA) crystals with account of electronic and molecular vibrational contributions. , 2012, , .		0
75	Nonlinear optical properties and large amplitude anharmonic vibrational motions. , 2012, , .		0
76	Electronic contributions to linear and nonlinear electric properties in fullerene-based molecular systems. , 2012, , .		0
77	Critical assessment of density functional theory for computing vibrational (hyper)polarizabilities. , 2012, , .		3
78	Evaluation of the nonlinear optical properties for an expanded porphyrin HÃ¼ckel-MÃ¶bius aromaticity switch. Journal of Chemical Physics, 2012, 137, 184306.	1.2	35
79	The Frozen Cage Model: A Computationally Low-Cost Tool for Predicting the Exohedral Regioselectivity of Cycloaddition Reactions Involving Endohedral Metallofullerenes. Journal of Chemical Theory and Computation, 2012, 8, 1671-1683.	2.3	18
80	Electronic and Vibrational Nonlinear Optical Properties of Five Representative Electrides. Journal of Chemical Theory and Computation, 2012, 8, 2688-2697.	2.3	78
81	On the reliability of the maximum hardness and minimum polarizability principles in nontotally symmetric vibrations. , 2012, , .		1
82	The Exohedral Dielsâ€“Alder Reactivity of the Titanium Carbide Endohedral Metallofullerene Ti₂C₂@D₃h</sub>â€C₇₈: Comparison with D₃h</sub>â€C₇₈ and M₃N@D₃h</sub>â€C₇₈ (M=Sc and Y) Reactivity. Chemistry - A European Journal, 2012, 18, 7141-7154.	1.7	54
83	Oï£¿O Bond Formation Mediated by a Hexanuclear Iron Complex Supported on a Stannoxane Core. Chemistry - A European Journal, 2012, 18, 2787-2791.	1.7	44
84	Electronic Structure, Bonding, Spectra, and Linear and Nonlinear Electric Properties of Ti@C₂₈. Journal of Physical Chemistry A, 2011, 115, 10370-10381.	1.1	33
85	Evaluation of the Nonlinear Optical Properties for Annulenes with HÃ¼ckel and MÃ¶bius Topologies. Journal of Chemical Theory and Computation, 2011, 7, 3935-3943.	2.3	86
86	Observation of Fe(V)=O using variable-temperature mass spectrometry and its enzyme-like Câ€“H and C=C oxidation reactions. Nature Chemistry, 2011, 3, 788-793.	6.6	264
87	On the contribution of mixed terms in response function treatment of vibrational nonlinear optical properties. International Journal of Quantum Chemistry, 2011, 111, 839-847.	1.0	15
88	Electronic and vibrational linear and nonlinear polarizabilities of Li@C₆₀ and [Li@C₆₀]⁺. Journal of Computational Chemistry, 2011, 32, 908-914.	1.5	26
89	Modeling the cisâ€Oxoâ€Labile Binding Site Motif of Nonâ€Heme Iron Oxygenases: Water Exchange and Oxidation Reactivity of a Nonâ€Heme Iron(IV)â€Oxo Compound Bearing a Tripodal Tetradentate Ligand. Chemistry - A European Journal, 2011, 17, 1622-1634.	1.7	105
90	O₂â€...Activation and Selective Phenolate orthoâ€...Hydroxylation by an Unsymmetric Dicopper Î¼â€Î·¹:Î·¹â€Peroxido Complex. Angewandte Chemie - International Edition, 2010, 49, 2406-2409.	7.2	104

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91	Spin-State-Corrected Gaussian-Type Orbital Basis Sets. Journal of Physical Chemistry A, 2010, 114, 7191-7197.	1.1	47
92	Electronic and vibrational contributions to first hyperpolarizability of donorâ€“acceptor-substituted azobenzene. Journal of Chemical Physics, 2010, 133, 244308.	1.2	51
93	Accurate Evaluation of Vibrational Nonlinear Optical Properties. , 2009, , .		0
94	Olefinâ€Đependent Discrimination between Two Nonheme HOï£¿Fe^Vï£¾O Tautomeric Species in Catalytic H₂O₂ Epoxidations. Chemistry - A European Journal, 2009, 15, 3359-3362.	1.7	77
95	Theoretical study of the hydroxylation of phenolates by the Cu2O2(N,Nâ€²-dimethylethylenediamine)2 2+ complex. Journal of Biological Inorganic Chemistry, 2009, 14, 229-242.	1.1	17
96	Theoretical study of the hydroxylation of phenols mediated by an end-on bound superoxoâ€“copper(II) complex. Journal of Biological Inorganic Chemistry, 2009, 14, 273-285.	1.1	12
97	The vibrational auto-adjusting perturbation theory. Theoretical Chemistry Accounts, 2009, 123, 41-49.	0.5	8
98	Structure, Bonding, and Relative Stability of the Ground and Low-Lying Electronic States of CuO2. The Role of Exact Exchange. Journal of Physical Chemistry A, 2009, 113, 1308-1317.	1.1	19
99	Linear and Nonlinear Optical Properties of [60]Fullerene Derivatives. Journal of Physical Chemistry A, 2009, 113, 1159-1170.	1.1	102
100	Treatment of nonlinear optical properties due to large amplitude anharmonic vibrational motions: Umbrella motion in NH3. Journal of Chemical Physics, 2009, 131, 034116.	1.2	37
101	Role of vibrational anharmonicity in atmospheric radical hydrogen-bonded complexes. Physical Chemistry Chemical Physics, 2009, 11, 6377.	1.3	12
102	Nanosized trigonal prismatic and antiprismatic CuII coordination cages based on tricarboxylate linkers. Dalton Transactions, 2008, , 1679.	1.6	15
103	Importance of the Basis Set for the Spin-State Energetics of Iron Complexes. Journal of Physical Chemistry A, 2008, 112, 6384-6391.	1.1	131
104	Simple finite field nuclear relaxation method for calculating vibrational contribution to degenerate four-wave mixing. Journal of Chemical Physics, 2008, 128, 114101.	1.2	13
105	Chapter 3 The breakdown of the maximum hardness and minimum polarizability principles for nontotally symmetric vibrations. Theoretical and Computational Chemistry, 2007, , 31-45.	0.2	2
106	Variational calculation of static and dynamic vibrational nonlinear optical properties. Journal of Chemical Physics, 2007, 127, 084118.	1.2	29
107	Treatment of Vibronic Interactions Using Variational Methods for Nuclear Motion. AIP Conference Proceedings, 2007, , .	0.3	0
108	Alkane Hydroxylation by a Nonheme Iron Catalyst that Challenges the Heme Paradigm for Oxygenase Action. Journal of the American Chemical Society, 2007, 129, 15766-15767.	6.6	195

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109	Imaginary Vibrational Modes in Polycyclic Aromatic Hydrocarbons: A Challenging Test for the Hardness Profiles. ChemPhysChem, 2007, 8, 1065-1070.	1.0	11
110	Redox-Controlled Molecular Flipper Based on a Chiral Cu Complex. Inorganic Chemistry, 2006, 45, 9643-9645.	1.9	10
111	Analysis of Electron Delocalization in Aromatic Systems:â€‰ Individual Molecular Orbital Contributions to Para-Delocalization Indexes (PDI). Journal of Physical Chemistry A, 2006, 110, 11569-11574.	1.1	28
112	Simulation of photoelectron spectra with anharmonicity fully included: Application to the XÌƒA22â†XÌƒA11 band of furan. Journal of Chemical Physics, 2006, 125, 014311.	1.2	17
113	A variational approach for calculating Franck-Condon factors including mode-mode anharmonic coupling. Journal of Chemical Physics, 2006, 125, 154114.	1.2	36
114	Linear response functions for a vibrational configuration interaction state. Journal of Chemical Physics, 2006, 125, 214309.	1.2	51
115	Determination of Vibrational Contributions to Linear and Nonlinear Optical Properties. Challenges and Advances in Computational Chemistry and Physics, 2006, , 101-128.	0.6	5
116	Aromaticity Analysis of Lithium Cation/ Ï€ Complexes of Aromatic Systems. ChemPhysChem, 2005, 6, 2552-2561.	1.0	46
117	The Breakdown of the Minimum Polarizability Principle in Vibrational Motions as an Indicator of the Most Aromatic Center. Chemistry - A European Journal, 2005, 11, 6024-6031.	1.7	15
118	Basis set effects on the energy and hardness profiles of the hydrogen fluoride dimer. Journal of Chemical Sciences, 2005, 117, 549-554.	0.7	4
119	Beyond vibrational self-consistent-field methods: Benchmark calculations for the fundamental vibrations of ethylene. International Journal of Quantum Chemistry, 2005, 104, 667-680.	1.0	62
120	Calculation of Franckâ€“Condon factors including anharmonicity: Simulation of the C2H4+XÌƒB3u2â†C2H4XÌƒAg1 band in the photoelectron spectrum of ethylene. Journal of Chemical Physics, 2005, 122, 184104.	1.2	25
121	An assessment of a simple hardness kernel approximation for the calculation of the global hardness in a series of Lewis acids and bases. Computational and Theoretical Chemistry, 2005, 727, 139-148.	1.5	31
122	Generalizing the Breakdown of the Maximum Hardness and Minimum Polarizabilities Principles for Nontotally Symmetric Vibrations to Non-Ï€-Conjugated Organic Molecules. Journal of Physical Chemistry A, 2005, 109, 615-621.	1.1	26
123	Variational calculation of vibrational linear and nonlinear optical properties. Journal of Chemical Physics, 2005, 122, 204108.	1.2	53
124	The hardness profile as a tool to detect spurious stationary points in the potential energy surface. Journal of Chemical Physics, 2004, 120, 10914-10924.	1.2	32
125	Basis set and electron correlation effects on initial convergence for vibrational nonlinear optical properties of conjugated organic molecules. Journal of Chemical Physics, 2004, 120, 6346-6355.	1.2	60
126	A different approach for calculating Franckâ€“Condon factors including anharmonicity. Journal of Chemical Physics, 2004, 120, 813-822.	1.2	62

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127	Nonadiabatic and Bornâ€“Oppenheimer calculations of the polarizabilites of LiH and LiD. Computational and Theoretical Chemistry, 2003, 633, 113-122.	1.5	22
128	Evaluation of the Analogy between Exceptions to the Generalized Maximum Hardness Principle for Non-Totally-Symmetric Vibrations and the Pseudo-Jahnâ^'Teller Effect. Journal of Physical Chemistry A, 2003, 107, 7337-7339.	1.1	18
129	Basis set and electron correlation effects on ab initio electronic and vibrational nonlinear optical properties of conjugated organic molecules. Journal of Chemical Physics, 2003, 118, 711-718.	1.2	105
130	Relations among several nuclear and electronic density functional reactivity indexes. Journal of Chemical Physics, 2003, 119, 9393-9400.	1.2	22
131	Vibration and two-photon absorption. Journal of Chemical Physics, 2002, 116, 9729-9739.	1.2	71
132	Are the maximum hardness and minimum polarizability principles always obeyed in nontotally symmetric vibrations?. Journal of Chemical Physics, 2002, 117, 10561-10570.	1.2	77
133	Initial convergence of the perturbation series expansion for vibrational nonlinear optical properties. Journal of Chemical Physics, 2002, 116, 5363-5373.	1.2	43
134	On the Validity of the Maximum Hardness and Minimum Polarizability Principles for Nontotally Symmetric Vibrations. Journal of the American Chemical Society, 2001, 123, 7951-7952.	6.6	112
135	Second-Order ab Initio MÃ¸llerâ^'Plesset Study of Optimum Chain Length for Total (Electronic Plus) Tj ETQq1 1 0.784314 rgBT /Overlo 9748-9755.	1.1	50
136	Field-induced coordinates for the determination of dynamic vibrational nonlinear optical properties. Journal of Chemical Physics, 2001, 115, 4473-4483.	1.2	41
137	Efficient treatment of the effect of vibrations on electrical, magnetic, and spectroscopic properties. Journal of Computational Chemistry, 2000, 21, 1572-1588.	1.5	48
138	Calculation of static zero-point vibrational averaging corrections and other vibrational curvature contributions to polarizabilities and hyperpolarizabilities using field-induced coordinates. International Journal of Quantum Chemistry, 2000, 80, 471-479.	1.0	37
139	Determination of vibrational polarizabilities and hyperpolarizabilities using field-induced coordinates. Journal of Chemical Physics, 2000, 113, 5203.	1.2	72
140	Theoretical study of the second-order vibrational Stark effect. Molecular Physics, 2000, 98, 513-520.	0.8	4
141	Anharmonicity contributions to the vibrational second hyperpolarizability of conjugated oligomers. Journal of Chemical Physics, 2000, 112, 1011-1019.	1.2	54
142	Finite field treatment of vibrational polarizabilities and hyperpolarizabilities: On the role of the Eckart conditions, their implementation, and their use in characterizing key vibrations. Journal of Chemical Physics, 1999, 111, 875-884.	1.2	82
143	Simple finite field method for calculation of static and dynamic vibrational hyperpolarizabilities: Curvature contributions. Journal of Chemical Physics, 1998, 108, 10008-10012.	1.2	80
144	Additional compact formulas for vibrational dynamic dipole polarizabilities and hyperpolarizabilities. Journal of Chemical Physics, 1998, 108, 10013-10017.	1.2	129

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145	Nuclear relaxation contribution to static and dynamic (infinite frequency approximation) nonlinear optical properties by means of electrical property expansions: Application to HF, CH4, CF4, and SF6. Journal of Chemical Physics, 1998, 108, 4123-4130.	1.2	63
146	A systematic and feasible method for computing nuclear contributions to electrical properties of polyatomic molecules. Journal of Chemical Physics, 1997, 107, 1501-1512.	1.2	67
147	Nuclear relaxation and vibrational contributions to the static electrical properties of polyatomic molecules: beyond the Hartree-Fock approximation. Chemical Physics, 1997, 217, 29-42.	0.9	30
148	Analysis of the changes on the potential energy surface of Menshutkin reactions induced by external perturbations. Computational and Theoretical Chemistry, 1996, 371, 171-183.	1.5	26
149	Systematic study of the static electrical properties of the CO molecule: Influence of the basis set size and correlation energy. Journal of Chemical Physics, 1995, 102, 7573-7583.	1.2	24
150	The Dual Effect of Coordinating â^'NH Groups and Light in the Electrochemical CO 2 Reduction with Pyridylamino Co Complexes. ChemElectroChem, 0, , .	1.7	5