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List of Publications by Year in descending order

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114 papers	5,669 citations	147801 31 h-index	76900 74 g-index
123 all docs	123 docs citations	123 times ranked	5388 citing authors

#	Article	IF	Citations
1	Definition of the hydrogen bond (IUPAC Recommendations 2011). Pure and Applied Chemistry, 2011, 83, 1637-1641.	1.9	1,449
2	Defining the hydrogen bond: An account (IUPAC Technical Report). Pure and Applied Chemistry, 2011, 83, 1619-1636.	1.9	856
3	Structure and Spectra of Three-Dimensional(H2O)nClusters,n=8,9,10. Physical Review Letters, 1998, 80, 2578-2581.	7.8	309
4	Intermolecular potential of carbon dioxide dimer from symmetry-adapted perturbation theory. Journal of Chemical Physics, 1999, 110, 3785-3803.	3.0	279
5	Theoretical Study of Structure and Spectra of Cage Clusters (H2O)n,n= 7â^'10. Journal of Physical Chemistry A, 1999, 103, 4933-4947.	2.5	163
6	Infrared Spectra of Large H2O Clusters:â€‰ New Understanding of the Elusive Bending Mode of Ice. Journal of Physical Chemistry A, 2001, 105, 974-983.	2.5	146
7	Solvation and Ionization Stages of HCl on Ice Nanocrystals. Journal of Physical Chemistry A, 2002, 106, 9374-9389.	2.5	127
8	VCD spectroscopy as a novel probe for chirality transfer in molecular interactions. Chemical Society Reviews, 2010, 39, 1478-1488.	38.1	118
9	The asymmetric cage structure of (H2O)7 from a combined spectroscopic and computational study. Journal of Chemical Physics, 1999, 110, 10649-10652.	3.0	113
10	Abinitiostudy of van der Waals interaction of CO2with Ar. Journal of Chemical Physics, 1996, 104, 6569-6576.	3.0	70
11	Nuclear Magnetic Shielding and Spinâ^'Spin Coupling of 1,2-13C-Enriched Acetylene in Gaseous Mixtures with Xenon and Carbon Dioxide. Journal of Physical Chemistry A, 2000, 104, 5955-5958.	2.5	70
12	Characterization of dihydrogen-bonded Dâ€“Hâ‹¯Hâ€“A complexes on the basis of infrared and magnetic resonance spectroscopic parameters. Journal of Chemical Physics, 2003, 119, 5094-5104.	3.0	66
13	Cysteine conformations revisited. Computational and Theoretical Chemistry, 2007, 810, 129-134.	1.5	65
14	Theoretical Prediction and the First IR Matrix Observation of SeveralL-Cysteine Molecule Conformers. ChemPhysChem, 2007, 8, 1085-1094.	2.1	61
15	The importance of high-order correlation effects for the COâ€“CO interaction potential. Chemical Physics Letters, 1999, 314, 326-332.	2.6	60
16	The Shielding Constants and Scalar Couplings in Nâ^'HÂ·Â·Â·OC and Nâ^'HÂ·Â·Â·NC Hydrogen Bonded Systems:Â An ab Initio MO Study. Journal of Physical Chemistry A, 2000, 104, 8105-8113.	2.5	59
17	DFT study of vibrational circular dichroismspectra ofd-lactic acidâ€“water complexes. Physical Chemistry Chemical Physics, 2006, 8, 101-113.	2.8	55
18	Ab initio study of energy, structure and dynamics of the waterâ€“carbon dioxide complex. Journal of Chemical Physics, 1998, 109, 3919-3927.	3.0	51

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19	Symmetry-Adapted Perturbation-Theory Interaction-Energy Decomposition for Hydrogen-Bonded and Stacking Structures. Journal of Chemical Theory and Computation, 2008, 4, 892-897.	5.3	50
20	Solvent effects on NMR spectrum of acetylene calculated by ab initio methods. Chemical Physics, 1998, 234, 111-119.	1.9	49
21	Comprehensive ab initio studies of nuclear magnetic resonance shielding and coupling constants in XHâ‹¯O hydrogen-bonded complexes of simple organic molecules. Journal of Chemical Physics, 2000, 112, 7930-7938.	3.0	49
22	Excitedâ€State Intramolecular Proton Transfer: Photoswitching in Salicylidene Methylamine Derivatives. ChemPhysChem, 2014, 15, 1643-1652.	2.1	49
23	Photophysics of Schiff Bases: Theoretical Study of Salicylidene Methylamine. ChemPhysChem, 2012, 13, 4287-4294.	2.1	45
24	The 19Fâ€“1H coupling constants transmitted through covalent, hydrogen bond, and van der Waals interactions. Journal of Chemical Physics, 2001, 115, 5498-5506.	3.0	43
25	Fentanyl Family at the Mu-Opioid Receptor: Uniform Assessment of Binding and Computational Analysis. Molecules, 2019, 24, 740.	3.8	39
26	The nuclear spinâ€“spin coupling constants in the water dimer. Chemical Physics Letters, 1999, 308, 486-494.	2.6	37
27	Relativistic calculation of NMR properties of XeF2, XeF4 and XeF6. Chemical Physics Letters, 2006, 427, 281-288.	2.6	37
28	A quantum chemical study of the hydrogen bonding in the CO2?HF and N2O?HF complexes. Theoretica Chimica Acta, 1989, 76, 173-185.	0.8	36
29	Ab initiostudy of He(1S)+Cl2(Xâ€‰1Î£g,3Îu) potential energy surfaces. Journal of Chemical Physics, 1994, 101, 6800-6809.	3.0	36
30	Cooperative and anticooperative mixed trimers of HCl and methanol. Journal of Molecular Structure, 2006, 790, 18-26.	3.6	35
31	The Properties of Weak and Strong Dihydrogen-Bonded Dï£¿Hâ‹…â‹…â‹…Hï£¿A Complexes. ChemPhysChem, 2006, 7, 629-639.	2.1	34
32	IR Lowâ€Temperature Matrix and ab Initio Study on Î²â€Alanine Conformers. ChemPhysChem, 2008, 9, 2042-2051.	2.1	32
33	Symmetry-adapted perturbation theory interaction energy decomposition for some noble gas complexes. Chemical Physics Letters, 2008, 459, 44-48.	2.6	30
34	Tailoring the Schiff base photoswitching â€“ a non-adiabatic molecular dynamics study of substituent effect on excited state proton transfer. Physical Chemistry Chemical Physics, 2017, 19, 5318-5325.	2.8	30
35	Calculations of hydrogen-bond-transmitted indirect nuclear spinâ€“spin couplings: a comparison of density-functional and ab initio methods. Chemical Physics Letters, 2003, 372, 476-484.	2.6	27
36	On the nature of the interaction energy in the Ar-Cl2 complex. Computational and Theoretical Chemistry, 1994, 307, 187-199.	1.5	26

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37	On the calculations of the vibrational Raman spectra of small water clusters. Chemical Physics, 2007, 342, 163-172.	1.9	26
38	The geometry dependence of the spinâ€“spin coupling constants in ethane: a theoretical study. Chemical Physics Letters, 1999, 305, 139-146.	2.6	25
39	Ab initio study for the intermolecular potential of the waterâ€“nitric oxide complex. Chemical Physics Letters, 2000, 318, 232-239.	2.6	25
40	On the nature of the interaction energy in the Arâ€“ClF complex. Journal of Chemical Physics, 1993, 99, 3700-3706.	3.0	24
41	Benchmark calculations of the shielding constants in the water dimer. Chemical Physics Letters, 2001, 333, 139-145.	2.6	23
42	Theoretical infrared and Raman spectroscopic parameters for H2O and the H2O ? Li+ system. Faraday Discussions of the Chemical Society, 1977, 64, 112.	2.2	22
43	Reply to the Comment on â€œThe importance of high-order correlation effects for the COâ€“CO interaction potentialâ€•[Chem. Phys. Lett. 314 (1999) 326]. Chemical Physics Letters, 2001, 334, 424-425.	2.6	22
44	Structure and energetics of weakly bound waterâ€“sulfur dioxide complexes. Computational and Theoretical Chemistry, 2007, 819, 41-51.	1.5	22
45	The water-nitric oxide intermolecular potential-energy surface revisited. Journal of Chemical Physics, 2009, 130, 104303.	3.0	22
46	IR low-temperature matrix, X-ray and ab initio study on l-isoserine conformations. Physical Chemistry Chemical Physics, 2010, 12, 10818.	2.8	22
47	Ab initio study of the ground and first excited state of LiAr. International Journal of Quantum Chemistry, 1995, 53, 607-615.	2.0	21
48	HCl Solvation at the Surface and within Methanol Clusters/Nanoparticles II:Â Evidence for Molecular Wires. Journal of Physical Chemistry B, 2006, 110, 21751-21763.	2.6	21
49	Density Functional Theory Study on Vibrational Circular Dichroism as a Tool for Analysis of Intermolecular Systems:â€‰(1:1) Cysteineâ€™Water Complex Conformations. Journal of Physical Chemistry A, 2007, 111, 10703-10711.	2.5	21
50	Investigations of the anaesthetic activity of nitrous oxide by quantum-chemical calculations. Computational and Theoretical Chemistry, 1990, 204, 1-14.	1.5	20
51	Solvation Stages of HCl and HBr in Crystalline Phases with Methanol and Small Ethers:Â Acidâ€™Ether Cluster Complexes in Amorphous and Crystal Phases. Journal of Physical Chemistry A, 2004, 108, 2030-2043.	2.5	20
52	Nuclear Magnetic Resonance Parameters for Methane Molecule Trapped in Clathrate Hydrates. Journal of Physical Chemistry A, 2011, 115, 612-619.	2.5	20
53	On the calculations of the nuclear shielding constants in small water clusters. Chemical Physics, 2006, 323, 218-230.	1.9	19
54	HCl solvation in methanol clusters and nanoparticles: Evidence for proton-wires. Chemical Physics Letters, 2006, 422, 179-183.	2.6	19

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55	Prediction ofl-Methionine VCD Spectra in the Gas Phase and Water Solution. Journal of Physical Chemistry B, 2013, 117, 14202-14214.	2.6	19
56	A study of the weak interaction in SCO/He and SCO/N2 systems. International Journal of Quantum Chemistry, 1993, 46, 623-634.	2.0	18
57	Potential Energy and Spinâ˜Spin Coupling Constants Surface of Glycolaldehyde. Journal of Physical Chemistry A, 2004, 108, 2758-2769.	2.5	18
58	On the calculations of the nuclear spinâ€“spin coupling constants in small water clusters. Chemical Physics, 2006, 326, 431-444.	1.9	18
59	Ab initio calculation of and NMR shielding constants in solid acetylene. Solid State Nuclear Magnetic Resonance, 1997, 8, 139-145.	2.3	16
60	Ab initio study of bending modes in water cage clusters, (H2O)n, nï£¾6-10. International Journal of Quantum Chemistry, 2002, 90, 1191-1205.	2.0	16
61	The nuclear spinâ€“spin coupling constants in methanol and methylamine: geometry and solvent effects. Chemical Physics, 2000, 255, 137-148.	1.9	15
62	The spinâ€“spin coupling constants in the ammonia dimer. Chemical Physics Letters, 2002, 360, 272-282.	2.6	15
63	The (H2O)2CO ternary complex: cyclic or linear?. Chemical Physics Letters, 2001, 342, 220-230.	2.6	14
64	Ammonia dimer, linear or cyclic?. Computational and Theoretical Chemistry, 1986, 139, 233-240.	1.5	13
65	The influence of electrostatic and dispersion interactions on the NMR parameters of acetylene. Chemical Physics, 1999, 248, 27-40.	1.9	13
66	Ab initio study on mixed methanolâ€“hydrogen chloride dimer and trimers. Chemical Physics Letters, 2004, 393, 228-235.	2.6	13
67	Theoretical predictions of the spectroscopic parameters in noble-gas molecules: HXeOH and its complex with water. Physical Chemistry Chemical Physics, 2011, 13, 15455.	2.8	13
68	On Vibrational Circular Dichroism Chirality Transfer in Electron Donorâ€“Acceptor Complexes: A Prediction for the QuinineÂ·Â·Â·BF‹sub›3‹/sub› System. Journal of Physical Chemistry A, 2012, 116, 7916-7926.	2.5	13
69	A computational study of the nuclear magnetic resonance parameters for double proton exchange pathways in the formamideâ€“formic acid and formamideâ€“formamidine complexes. Physical Chemistry Chemical Physics, 2009, 11, 11232.	2.8	12
70	Predicted NMR properties of noble gas hydride cations RgH+. Chemical Physics Letters, 2008, 467, 18-22.	2.6	11
71	Spectroscopic parameters in noble gas molecule: HXeF and its complex with HF. Chemical Physics Letters, 2011, 517, 155-161.	2.6	11
72	Abinitiostudy of the H2COâ€“Ar complex. Journal of Chemical Physics, 1993, 99, 5211-5218.	3.0	10

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73	Ab initio calculations of nonadditive effects in the trimers (H2O)2â‹¯XY,XY=N2, BF, CS. Chemical Physics Letters, 2002, 358, 237-249.	2.6	10
74	Inverse hydrogen bond: theoretical investigation on the nature of interaction and spectroscopic properties. Structural Chemistry, 2012, 23, 1323-1332.	2.0	10
75	Calculations of NMR properties for sI and sII clathrate hydrates of carbon dioxide. Chemical Physics, 2014, 433, 31-41.	1.9	10
76	Affinity of fentanyl and its derivatives for the Ïƒ1-receptor. MedChemComm, 2019, 10, 1187-1191.	3.4	10
77	Spectroscopic parameters of interacting systems. Computational and Theoretical Chemistry, 1982, 88, 71-78.	1.5	9
78	The nonadditive effects in the mixed trimers composed of the water dimer and diatomics H2, HF, HCl, HBr, and ClF. Chemical Physics Letters, 2003, 368, 754-768.	2.6	9
79	Phenylisoserine in the gas-phase and water: Ab initio studies on neutral and zwitterion conformers. Journal of Molecular Modeling, 2011, 17, 961-970.	1.8	9
80	Ab initio simulations of the NMR spectra of Î²-alanine conformers. Computational and Theoretical Chemistry, 2011, 964, 148-154.	2.5	9
81	Correlatedab initio geometry and vibrational spectra of imidazole and its different forms. International Journal of Quantum Chemistry, 1992, 44, 409-420.	2.0	7
82	Calculations of NMR properties for sI and sII clathrate hydrates of methane, ethane and propane. Journal of Molecular Modeling, 2014, 20, 2511.	1.8	7
83	The FMO analysis of the molecular interaction of fentanyl derivatives with the Î¼-opioid receptor. Chemical Papers, 2017, 71, 1429-1443.	2.2	7
84	The influence of the dispersion corrections on the performance of DFT method in modeling HNgY noble gas molecules and their complexes. Chemical Physics Letters, 2018, 691, 319-324.	2.6	7
85	Molecular dynamics simulations suggest why the A2058G mutation in 23S RNA results in bacterial resistance against clindamycin. Journal of Molecular Modeling, 2018, 24, 191.	1.8	7
86	Spectroscopic parameters of interacting systems. IV.Ab initio study of vibrational band intensity changÃ©s due to ion-molecule interaction in HOHâ€¦Fâ¯. Advances in Molecular Relaxation and Interaction Processes, 1979, 15, 163-172.	0.5	6
87	Static electric polarizabilities and first hyperpolarizabilities of molecular ions RgH+ (Rg=He, Ne, Ar,) Tj ETQq1 1 0.784314 rgBT /Overlo	2.6	6
88	Quantum mechanical studies of lincosamides. Journal of Molecular Modeling, 2012, 18, 2727-2740.	1.8	6
89	Ab initio study of the ground and excited states of LiNe. International Journal of Quantum Chemistry, 1993, 48, 731-741.	2.0	5
90	Theoretical study of the hydrogen chloride trihydrate. International Journal of Quantum Chemistry, 2002, 90, 1151-1162.	2.0	5

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91	Modified CNDO [complete neglect of differential overlap] method. IV. Ion-molecule interactions in the acetone solutions of electrolytes. The Journal of Physical Chemistry, 1971, 75, 3581-3585.	2.9	4
92	Spectroscopic parameters of interacting systems. V. Ab initio study of vibrational band intensity changes due to hydrogen bonding of the hcnâ€¦hf complex. Advances in Molecular Relaxation and Interaction Processes, 1979, 15, 173-180.	0.5	4
93	Ab initio molecular orbital calculations of the IR spectra of hydrogen bonded and lithium bonded complexes of ammonia. Computational and Theoretical Chemistry, 1988, 180, 65-77.	1.5	4
94	Theoretical Study of the Lactic Acidâ^'Water System: Importance of Two- and Three-Body Interactions. Journal of Physical Chemistry A, 2010, 114, 4427-4436.	2.5	4
95	VCD Chirality Transfer: A New Insight into the Intermolecular Interactions. , 2011, , 451-478.		4
96	Computational study on interaction energy changes during double proton transfer process. Computational and Theoretical Chemistry, 2012, 998, 120-128.	2.5	4
97	Thermal Fluctuations and Infrared Spectra of the Formamideâ€“Formamidine Complex. Journal of Physical Chemistry A, 2012, 116, 10412-10419.	2.5	4
98	Ab Initio Calculations of the Intermolecular Nuclear Spin-Spin Coupling Constants. Computational Chemistry - Reviews of Current Trends, 2003, , 131-160.	0.4	4
99	Ab initio calculations of the vibrational force field and IR intensities of the ammonia dimers. Computational and Theoretical Chemistry, 1987, 150, 223-233.	1.5	3
100	A quantum chemical study of the hydrogen bonding in a weakly bound SCO-HF complex. Computational and Theoretical Chemistry, 1992, 253, 187-197.	1.5	3
101	Ab Initio SCF Calculations Relating to the Cls Chemical Shifts for Some Alkanes. Spectroscopy Letters, 1995, 28, 275-290.	1.0	3
102	Properties and Spectroscopies. , 0, , 125-312.		3
103	Interaction in the Ternary Complexes of HClâ^'Methanolâ^'X, X = H₂O or NH₃:â€‰ Ab Initio Calculations and On-the-Fly Molecular Dynamics. Journal of Physical Chemistry A, 2008, 112, 3870-3878.	2.5	3
104	Structural Insights into Ïƒ1 Receptor Interactions with Opioid Ligands by Molecular Dynamics Simulations. Molecules, 2018, 23, 456.	3.8	3
105	Towards Quantum-Chemical Modeling of the Activity of Anesthetic Compounds. International Journal of Molecular Sciences, 2021, 22, 9272.	4.1	3
106	The applicability of the CNDO treatment to the interpretation of the infrared spectra of electrolyte solutions in acetone. Human Development, 1973, 5, 253-259.	0.8	2
107	An attempt to evaluate the vibrational intensity changes due to long-range interactions. Advances in Molecular Relaxation and Interaction Processes, 1980, 16, 149-154.	0.5	2
108	Ab initio calculations of the vibrational spectra of the ammonia and fluoramide complexes with HF. Computational and Theoretical Chemistry, 1991, 236, 427-441.	1.5	2

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109	Microsolvation of HCl within Cold NH₃ Clusters. Journal of Physical Chemistry A, 2008, 112, 11423-11430.	2.5	2
110	Calculated Nuclear Magnetic Resonance Parameters for Multiproton-Exchange and Nonbonded-Hydrogen Rotation Processes in Cyclic Water Clusters. Journal of Physical Chemistry A, 2011, 115, 5774-5784.	2.5	2
111	Î±-Amino Acids In Water: A Review Of VCD And ROA Spectra. Challenges and Advances in Computational Chemistry and Physics, 2014, , 83-160.	0.6	2
112	Conformational space of clindamycin studied by ab initio and full-atom molecular dynamics. Journal of Molecular Modeling, 2016, 22, 20.	1.8	2
113	Recent Advances in Spectroscopy of Hydrogen-Bonded Systems. Journal of Atomic, Molecular, and Optical Physics, 2012, 2012, 1-1.	0.5	1
114	An excursion into secondary pharmacology of fentanyls with potential implications for drug design: Ïƒ1 receptor. , 2022, , 89-100.		0