Roberto Cammi

List of Publications by Year
in descending order

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148 papers	28,956 citations	36303 51 h-index	10158 140 g-index
156 all docs	156 docs citations	156 times ranked	23488 citing authors

#	Article	IF	Citations
1	Highâ€Pressure Reaction Profiles and Activation Volumes of 1,3â€Cyclohexadiene Dimerizations Computed by the Extreme Pressureâ€Polarizable Continuum Model (XPâ€PCM). Chemistry - A European Journal, 2022, 28, .	3.3	6
2	The second derivative of the electronic energy with respect to the compression scaling factor in the <scp>XPâ€PCM</scp> model: Theory and applications to compression response functions of atoms. Journal of Computational Chemistry, 2022, 43, 1176-1185.	3.3	2
3	Relating atomic energy, radius and electronegativity through compression. Chemical Science, 2021, 12, 2397-2403.	7.4	23
4	Toward an Understanding of the Pressure Effect on the Intramolecular Vibrational Frequencies of Sulfur Hexafluoride. Journal of Physical Chemistry A, 2021, 125, 6362-6373.	2.5	6
5	On the analytical evaluation of the pressure for the extreme-pressure polarizable continuum model (XP-PCM), with application to atoms. Annual Reports in Computational Chemistry, 2021, 17, 3-22.	1.7	2
6	Nonâ€Bonded Radii of the Atoms Under Compression. ChemPhysChem, 2020, 21, 2441-2453.	2.1	24
7	High-Pressure-Promoted and Facially Selective Dielsâ€“Alder Reactions of Enzymatically Derived cis-1,2-Dihydrocatechols and Their Acetonide Derivatives: Enantiodivergent Routes to Homochiral and Polyfunctionalized Bicyclo[2.2.2]octenes. Journal of Organic Chemistry, 2020, 85, 13080-13095.	3.2	7
8	An open quantum system theory for polarizable continuum models. Journal of Chemical Physics, 2020, 152, 174114.	3.0	14
9	Varying Electronic Configurations in Compressed Atoms: From the Role of the Spatial Extension of Atomic Orbitals to the Change of Electronic Configuration as an Isobaric Transformation. Journal of Chemical Theory and Computation, 2020, 16, 5047-5056.	5.3	14
10	Linear chains of hydrogen molecules under pressure: An extreme-pressure continuum model study. Journal of Chemical Physics, 2019, 150, 164122.	3.0	4
11	The Role of Computational Chemistry in the Experimental Determination of the Dipole Moment of Molecules in Solution. Journal of Computational Chemistry, 2019, 40, 2309-2317.	3.3	2
12	Squeezing All Elements in the Periodic Table: Electron Configuration and Electronegativity of the Atoms under Compression. Journal of the American Chemical Society, 2019, 141, 10253-10271.	13.7	138
13	Quantum optimal control theory for solvated systems. Journal of Chemical Physics, 2019, 151, 194109.	3.0	8
14	Quantum Chemistry at the High Pressures: The eXtreme Pressure Polarizable Continuum Model (XP-PCM). , 2018, , 273-287.		10
15	Analytical calculation of pressure for confined atomic and molecular systems using the eXtremeâ€Pressure Polarizable Continuum Model. Journal of Computational Chemistry, 2018, 39, 2243-2250.	3.3	19
16	Quantum Cluster Theory for the Polarizable Continuum Model (PCM). , 2017, , 1517-1556.		1
17	Equation of motion for the solvent polarization apparent charges in the polarizable continuum model: Application to time-dependent CI. Journal of Chemical Physics, 2017, 146, 064116.	3.0	14
18	Dielsâ€“Alder Cycloaddition of Cyclopentadiene and C₆₀ at the Extreme High Pressure. Journal of Physical Chemistry A, 2017, 121, 4363-4371.	2.5	18

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19	Insights on the Realgar Crystal Under Pressure from XP-PCM and Periodic Model Calculations. Journal of Physical Chemistry A, 2017, 121, 8825-8834.	2.5	14
20	Druckeffekte auf organische Reaktionen in Fluiden â€“ eine neue theoretische Perspektive. Angewandte Chemie, 2017, 129, 11278-11295.	2.0	10
21	The Effect of Pressure on Organic Reactions in Fluidsâ€”a New Theoretical Perspective. Angewandte Chemie - International Edition, 2017, 56, 11126-11142.	13.8	89
22	The Quantum Chemical Study of Chemical Reactions at Extreme High Pressure by Means of the Extreme-Pressure Polarizable Continuum Model. Annual Reports in Computational Chemistry, 2017, 13, 117-135.	1.7	11
23	XP-PCM Calculations of High Pressure Structural and Vibrational Properties of P₄S₃. Journal of Physical Chemistry A, 2016, 120, 5136-5144.	2.5	14
24	A new extension of the polarizable continuum model: Toward a quantum chemical description of chemical reactions at extreme high pressure. Journal of Computational Chemistry, 2015, 36, 2246-2259.	3.3	51
25	Equation of Motion for the Solvent Polarization Apparent Charges in the Polarizable Continuum Model: Application to Real-Time TDDFT. Journal of Physical Chemistry A, 2015, 119, 5405-5416.	2.5	43
26	Modeling Molecular Systems at Extreme Pressure by an Extension of the Polarizable Continuum Model (PCM) Based on the Symmetry-Adapted Cluster-Configuration Interaction (SACâ€“CI) Method: Confined Electronic Excited States of Furan as a Test Case. Journal of Chemical Theory and Computation, 2015, 11, 2063-2076.	5.3	31
27	Quantum Cluster Theory for the Polarizable Continuum Model (PCM). , 2015, , 1-40.		1
28	Electronic excitation spectra of molecules in solution calculated using the symmetry-adapted cluster-configuration interaction method in the polarizable continuum model with perturbative approach. Journal of Chemical Physics, 2014, 140, 064114.	3.0	10
29	The virial theorem for the polarizable continuum model. Journal of Chemical Physics, 2014, 140, 084112.	3.0	7
30	Vibrational Frequencies of Fullerenes C₆₀ and C₇₀ under Pressure Studied with a Quantum Chemical Model Including Spatial Confinement Effects. Journal of Physical Chemistry A, 2014, 118, 5098-5111.	2.5	45
31	The cavity electromagnetic field within the polarizable continuum model of solvation: An application to the real-time time dependent density functional theory. Computational and Theoretical Chemistry, 2014, 1040-1041, 112-119.	2.5	19
32	The cavity electromagnetic field within the polarizable continuum model of solvation. Journal of Chemical Physics, 2014, 140, 164114.	3.0	23
33	Molecular Response Functions for the Polarizable Continuum Model. Springer Briefs in Molecular Science, 2013, , .	0.1	28
34	Modelling vibrational coupling in DNA oligomers: a computational strategy combining QM and continuum solvation models. Highlights in Theoretical Chemistry, 2013, , 143-152.	0.0	0
35	The PCM Model. Springer Briefs in Molecular Science, 2013, , 1-11.	0.1	0
36	Analytical Derivatives Theory for Molecular Solutes. Springer Briefs in Molecular Science, 2013, , 13-22.	0.1	0

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37	Calculation and analysis of the harmonic vibrational frequencies in molecules at extreme pressure: Methodology and diborane as a test case. Journal of Chemical Physics, 2012, 137, 154112.	3.0	64
38	Optical absorption and fluorescence of PRODAN in solution: Quantum chemical study based on the symmetry-adapted cluster-configuration interaction method. Chemical Physics Letters, 2012, 552, 53-57.	2.6	16
39	Recent Advances in the Coupled-Cluster Analytical Derivatives Theory for Molecules in Solution Described With the Polarizable Continuum Model (PCM). Advances in Quantum Chemistry, 2012, , 1-29.	0.8	4
40	Coupledâ€cluster theory for the polarizable continuum model. III. A response theory for molecules in solution. International Journal of Quantum Chemistry, 2012, 112, 2547-2560.	2.0	30
41	Quantum Cluster Theory for the Polarizable Continuum Model (PCM). , 2012, , 1043-1066.		1
42	Modelling vibrational coupling in DNA oligomers: a computational strategy combining QM and continuum solvation models. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	13
43	Absolute stereochemistry and preferred conformations of urate degradation intermediates from computed and experimental circular dichroism spectra. Organic and Biomolecular Chemistry, 2011, 9, 5149-5155.	2.8	10
44	Cavity field effects within a polarizable continuum model of solvation: Application to the calculation of electronic circular dichroism spectra of Râ€(+)â€3â€methylâ€cyclopentanone. International Journal of Quantum Chemistry, 2011, 111, 826-838.	2.0	20
45	Modeling solvent effects on chiroptical properties. Chirality, 2011, 23, 717-729.	2.6	106
46	Nonequilibrium solvation for vertical photoemission and photoabsorption processes using the symmetry-adapted clusterâ€“configuration interaction method in the polarizable continuum model. Journal of Chemical Physics, 2011, 134, 104109.	3.0	51
47	Coupledâ€cluster theories for the polarizable continuum model. II. Analytical gradients for excited states of molecular solutes by the equation of motion coupledâ€cluster method. International Journal of Quantum Chemistry, 2010, 110, 3040-3052.	2.0	43
48	Symmetry-adapted cluster and symmetry-adapted cluster-configuration interaction method in the polarizable continuum model: Theory of the solvent effect on the electronic excitation of molecules in solution. Journal of Chemical Physics, 2010, 133, 024104.	3.0	71
49	Toward a Quantum-Mechanical Description of 2D-IR Spectra of Solvated Systems: The Vibrational Mode Coupling within A Polarizable Continuum Model. Journal of Physical Chemistry B, 2010, 114, 4924-4930.	2.6	7
50	Structure versus Solvent Effects on Nonlinear Optical Properties of Pushâ^'Pull Systems: A Quantum-Mechanical Study Based on a Polarizable Continuum Model. Journal of Physical Chemistry A, 2009, 113, 14774-14784.	2.5	31
51	Quantum cluster theory for the polarizable continuum model. I. The CCSD level with analytical first and second derivatives. Journal of Chemical Physics, 2009, 131, 164104.	3.0	79
52	Properties of Excited States of Molecules in Solution Described with Continuum Solvation Models. , 2009, , 19-36.		1
53	Structures and Properties of Electronically Excited Chromophores in Solution from the Polarizable Continuum Model Coupled to the Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2009, 113, 3009-3020.	2.5	173
54	Mechanistic Insights into Acetophenone Transfer Hydrogenation Catalyzed by Halfâ€Sandwich Ruthenium(II) Complexes Containing 2â€(Diphenylphosphanyl)aniline â€“ A Combined Experimental and Theoretical Study. European Journal of Inorganic Chemistry, 2008, 2008, 4462-4473.	2.0	45

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55	Towards the elaboration of a QM method to describe molecular solutes under the effect of a very high pressure. Chemical Physics, 2008, 344, 135-141.	1.9	59
56	Calculation of pK_a Values of Nucleobases and the Guanine Oxidation Products Guanidinohydantoin and Spiroiminodihydantoin using Density Functional Theory and a Polarizable Continuum Model. Journal of Physical Chemistry B, 2008, 112, 16860-16873.	2.6	179
57	How the Environment Controls Absorption and Fluorescence Spectra of PRODAN:â€‰ A Quantum-Mechanical Study in Homogeneous and Heterogeneous Media. Journal of Physical Chemistry B, 2008, 112, 414-423.	2.6	65
58	Structure and Properties of Molecular Solutes in Electronic Excited States: a Polarizable Continuum Model approach based on the Time-Dependent Density Functional Theory. Challenges and Advances in Computational Chemistry and Physics, 2008, , 179-208.	0.6	4
59	How the Molecular Environment Controls Excitation Energy Transfer and Light Harvesting: a Quantum Mechanical Model. AIP Conference Proceedings, 2007, , .	0.4	1
60	How Solvent Controls Electronic Energy Transfer and Light Harvesting:â€‰ Toward a Quantum-Mechanical Description of Reaction Field and Screening Effects. Journal of Physical Chemistry B, 2007, 111, 13253-13265.	2.6	117
61	How Solvent Controls Electronic Energy Transfer and Light Harvesting. Journal of Physical Chemistry B, 2007, 111, 6978-6982.	2.6	167
62	Mononuclear and Polynuclear Copper(I) Complexes with a New N,Nâ€˜,S-Donor Ligand and with Structural Analogies to the Copper Thionein Core. Inorganic Chemistry, 2007, 46, 10143-10152.	4.0	14
63	Ultrafast light harvesting dynamics in the cryptophyte phycocyanin 645. Photochemical and Photobiological Sciences, 2007, 6, 964-975.	2.9	62
64	A quantum mechanical polarizable continuum model for the calculation of resonance Raman spectra in condensed phase. Theoretical Chemistry Accounts, 2007, 117, 1029-1039.	1.4	46
65	Formation and relaxation of excited states in solution: A new time dependent polarizable continuum model based on time dependent density functional theory. Journal of Chemical Physics, 2006, 124, 124520.	3.0	484
66	Geometries and properties of excited states in the gas phase and in solution: Theory and application of a time-dependent density functional theory polarizable continuum model. Journal of Chemical Physics, 2006, 124, 094107.	3.0	1,143
67	Cu(I) Dinuclear Complexes with Tripodal Ligands vs Monodentate Donors:â€‰ Triphenylphosphine, Thiourea, and Pyridine. A 1H NMR Titration Study. Inorganic Chemistry, 2006, 45, 3456-3466.	4.0	10
68	Self-consistent quantum mechanical model for the description of excitation energy transfers in molecules at interfaces. Journal of Chemical Physics, 2006, 125, 054710.	3.0	14
69	On the Reaction of Ph2PNHPPh2 with RNCS (R=Et, Ph,p-NO2C6H4): Preparation of the Zwitterionic Ligand EtNHC(S)Ph2Pï£¾NPPh2C(S)NEt (HSNS) and the Zwitterionic Metalate [(SNS)Rh(CO)]. Chemistry - A European Journal, 2005, 11, 3413-3419.	3.3	10
70	Quantum Mechanical Continuum Solvation Models. ChemInform, 2005, 36, no.	0.0	24
71	Infrared linear dichroism in stretched films: Quantum mechanical approach within the polarizable continuum model. International Journal of Quantum Chemistry, 2005, 104, 716-726.	2.0	9
72	Electronic excitation energies of molecules in solution within continuum solvation models: Investigating the discrepancy between state-specific and linear-response methods. Journal of Chemical Physics, 2005, 123, 134512.	3.0	187

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73	Electronic excitation energies of molecules in solution: State specific and linear response methods for nonequilibrium continuum solvation models. Journal of Chemical Physics, 2005, 122, 104513.	3.0	271
74	Quantum Mechanical Polarizable Continuum Model Approach to the Kerr Effect of Pure Liquids. Journal of Physical Chemistry B, 2005, 109, 18706-18714.	2.6	29
75	Quantum Mechanical Continuum Solvation Models. Chemical Reviews, 2005, 105, 2999-3094.	47.7	14,149
76	Synthesis, Structure, and Electrochemical Properties of Copper(I) Complexes with S/N Homoscorpionate and Heteroscorpionate Ligands. Inorganic Chemistry, 2005, 44, 4333-4345.	4.0	28
77	A polarizable continuum model for molecules at diffuse interfaces. Journal of Chemical Physics, 2004, 120, 3893-3907.	3.0	66
78	Excitation energy transfer (EET) between molecules in condensed matter: A novel application of the polarizable continuum model (PCM). Journal of Chemical Physics, 2004, 120, 7029-7040.	3.0	184
79	Excitonic splitting in conjugated molecular materials:â€ƒA quantum mechanical model including interchain interactions and dielectric effects. Physical Review B, 2004, 70, .	3.2	10
80	Quantum-Mechanical Continuum Solvation Study of the Polarizability of Halides at the Water/Air Interface. Journal of Physical Chemistry B, 2004, 108, 13796-13806.	2.6	37
81	Second-order MÃ¸llerâ€“Plesset second derivatives for the polarizable continuum model: theoretical bases and application to solvent effects in electrophilic bromination of ethylene. Theoretical Chemistry Accounts, 2004, 111, 66-77.	1.4	13
82	New developments in the symmetry-adapted algorithm of the Polarizable Continuum Model. Journal of Computational Chemistry, 2004, 25, 375-385.	3.3	14
83	A density functional theory study of structural and NMR properties of SNN thiosemicarbazone ligands and their Pd(II) chlorocomplexes. Computational and Theoretical Chemistry, 2003, 623, 105-119.	1.5	6
84	Calculation of nonlinear optical susceptibilities of pure liquids within the Polarizable Continuum Model: the effect of the macroscopic nonlinear polarization at the output frequency. Computational and Theoretical Chemistry, 2003, 633, 209-216.	1.5	11
85	Ab initio model to predict NMR shielding tensors for solutes in liquid crystals. International Journal of Quantum Chemistry, 2003, 93, 121-130.	2.0	20
86	Synthesis and Molecular Structure of the Dihydrobis(thioxotriazolinyl)borato Complexes of Zinc(II), Bismuth(III), and Nickel(II). MÂ·Â·Â·Hâ¯B Interaction Studied by Ab Initio Calculations. Inorganic Chemistry, 2003, 42, 1769-1778.	4.0	27
87	Solvent Effects on the Indirect Spinâ€“Spin Coupling Constants of Benzene: The DFT-PCM Approach. International Journal of Molecular Sciences, 2003, 4, 119-134.	4.1	68
88	The Cottonâ€“Mouton effect of furan and its homologues in the gas phase, for the pure liquids and in solution. Journal of Chemical Physics, 2003, 118, 10712-10724.	3.0	37
89	Multiconfigurational self-consistent field linear response for the polarizable continuum model: Theory and application to ground and excited-state polarizabilities of para-nitroaniline in solution. Journal of Chemical Physics, 2003, 119, 5818-5827.	3.0	113
90	Vibrational Circular Dichroism within the Polarizable Continuum Model:Â A Theoretical Evidence of Conformation Effects and Hydrogen Bonding for (S)-(â¯)-3-Butyn-2-ol in CCl4Solution. Journal of Physical Chemistry A, 2002, 106, 12331-12339.	2.5	83

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91	Polarizable Continuum Model (PCM) Calculations of Solvent Effects on Optical Rotations of Chiral Molecules. Journal of Physical Chemistry A, 2002, 106, 6102-6113.	2.5	607
92	Molecular properties in solution described with a continuum solvation model. Physical Chemistry Chemical Physics, 2002, 4, 5697-5712.	2.8	277
93	A second-order, quadratically convergent multiconfigurational self-consistent field polarizable continuum model for equilibrium and nonequilibrium solvation. Journal of Chemical Physics, 2002, 117, 13-26.	3.0	71
94	Theoretical Approach to the Calculation of Vibrational Raman Spectra in Solution within the Polarizable Continuum Model. Journal of Physical Chemistry A, 2001, 105, 8310-8316.	2.5	53
95	A Symmetry adapted tessellation of the GEPOL surface: applications to molecular properties in solution. Journal of Computational Chemistry, 2001, 22, 1262-1272.	3.3	24
96	The Cottonâ€“Mouton effect of gaseous N2, CO, CO2, N2O, OCS and CS2: a density functional approach to high-order mixed electric and magnetic properties. Chemical Physics Letters, 2001, 346, 251-258.	2.6	16
97	Nonequilibrium formulation of infrared frequencies and intensities in solution: Analytical evaluation within the polarizable continuum model. Journal of Chemical Physics, 2000, 113, 11270-11279.	3.0	69
98	An Attempt To Bridge the Gap between Computation and Experiment for Nonlinear Optical Properties:Â Macroscopic Susceptibilities in Solutionâ€. Journal of Physical Chemistry A, 2000, 104, 4690-4698.	2.5	118
99	On the Calculation of Infrared Intensities in Solution within the Polarizable Continuum Model. Journal of Physical Chemistry A, 2000, 104, 9874-9879.	2.5	81
100	Fast Evaluation of Geometries and Properties of Excited Molecules in Solution:Â A Tamm-Dancoff Model with Application to 4-Dimethylaminobenzonitrile. Journal of Physical Chemistry A, 2000, 104, 5631-5637.	2.5	541
101	Solvent Effects on 15N NMR Shielding of 1,2,4,5-Tetrazine and Isomeric Tetrazoles:â€‰ Continuous Set Gauge Transformation Calculation Using the Polarizable Continuum Model. Journal of Physical Chemistry A, 2000, 104, 9600-9604.	2.5	28
102	Linear response theory for the polarizable continuum model. Journal of Chemical Physics, 1999, 110, 9877-9886.	3.0	313
103	Nuclear magnetic shieldings in solution: Gauge invariant atomic orbital calculation using the polarizable continuum model. Journal of Chemical Physics, 1999, 110, 7627-7638.	3.0	106
104	Analytical free energy second derivatives with respect to nuclear coordinates: Complete formulation for electrostatic continuum solvation models. Journal of Chemical Physics, 1999, 110, 6858-6870.	3.0	115
105	Medium effects on the properties of chemical systems: An overview of recent formulations in the polarizable continuum model (PCM). International Journal of Quantum Chemistry, 1999, 75, 783-803.	2.0	108
106	Second-Order MÃ¸llerâ^'Plesset Analytical Derivatives for the Polarizable Continuum Model Using the Relaxed Density Approach. Journal of Physical Chemistry A, 1999, 103, 9100-9108.	2.5	230
107	Solvent and vibrational effects on molecular electric properties. Static and dynamic polarizability and hyperpolarizabilities of urea in water. Computational and Theoretical Chemistry, 1998, 426, 191-198.	1.5	22
108	An ab initio time-dependent Hartreeâ€“Fock study of solvent effects on the polarizability and second hyperpolarizability of polyacetylene chains within the polarizable continuum model. Chemical Physics, 1998, 238, 153-163.	1.9	28

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109	Recent Advances in the Description of Solvent Effects with the Polarizable Continuum Model. Advances in Quantum Chemistry, 1998, 32, 227-261.	0.8	411
110	On the Calculation of Local Field Factors for Microscopic Static Hyperpolarizabilities of Molecules in Solution with the Aid of Quantum-Mechanical Methods. Journal of Physical Chemistry A, 1998, 102, 870-875.	2.5	114
111	Solvent Effects on Linear and Nonlinear Optical Properties of Donorâ"Acceptor Polyenes:â€‰Investigation of Electronic and Vibrational Components in Terms of Structure and Charge Distribution Changes. Journal of the American Chemical Society, 1998, 120, 8834-8847.	13.7	101
112	Excited states and solvatochromic shifts within a nonequilibrium solvation approach: A new formulation of the integral equation formalism method at the self-consistent field, configuration interaction, and multiconfiguration self-consistent field level. Journal of Chemical Physics, 1998, 109, 2798-2807.	3.0	366
113	The Hartreeâ€"Fock calculation of the magnetic properties of molecular solutes. Journal of Chemical Physics, 1998, 109, 3185-3196.	3.0	77
114	Solvent effects on static and dynamic polarizability and hyperpolarizabilities of acetonitrile. Journal of Molecular Structure, 1997, 436-437, 567-575.	3.6	19
115	Analytical first derivatives of molecular surfaces with respect to nuclear coordinates. Journal of Computational Chemistry, 1996, 17, 57-73.	3.3	102
116	Time-dependent variational principle for nonlinear Hamiltonians and its application to molecules in the liquid phase. International Journal of Quantum Chemistry, 1996, 60, 297-306.	2.0	24
117	Energy and energy derivatives for molecular solutes: Perspectives of application to hybrid quantum and molecular methods. International Journal of Quantum Chemistry, 1996, 60, 1165-1178.	2.0	13
118	Ab initio study of solvated molecules: a new implementation of the polarizable continuum model. Chemical Physics Letters, 1996, 255, 327-335.	2.6	3,086
119	Analytical derivatives for molecular solutes. III. Hartreeâ€"Fock static polarizability and hyperpolarizabilities in the polarizable continuum model. Journal of Chemical Physics, 1996, 104, 4611-4620.	3.0	148
120	Analytical Hartreeâ€"Fock calculation of the dynamical polarizabilities Î±, Î², and Î³ of molecules in solution. Journal of Chemical Physics, 1996, 105, 10556-10564.	3.0	149
121	On the evaluation of the solvent polarization apparent charges in the polarizable continuum model: A new formulation. Journal of Computational Chemistry, 1995, 16, 20-30.	3.3	47
122	Remarks on the use of the apparent surface charges (ASC) methods in solvation problems: Iterative versus matrix-inversion procedures and the renormalization of the apparent charges. Journal of Computational Chemistry, 1995, 16, 1449-1458.	3.3	1,211
123	Nonequilibrium solvation theory for the polarizable continuum model: A new formulation at theSCF level with application to the case of the frequency-dependent linear electric response function. International Journal of Quantum Chemistry, 1995, 56, 465-474.	2.0	104
124	Analytical expressions of the free energy derivatives for molecules in solution. Application to the geometry optimization. International Journal of Quantum Chemistry, 1995, 56, 695-702.	2.0	27
125	Analytical derivatives for molecular solutes. II. Hartreeâ€"Fock energy first and second derivatives with respect to nuclear coordinates. Journal of Chemical Physics, 1994, 101, 3888-3897.	3.0	94
126	Analytical derivatives for molecular solutes. I. Hartreeâ€"Fock energy first derivatives with respect to external parameters in the polarizable continuum model. Journal of Chemical Physics, 1994, 100, 7495-7502.	3.0	127

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127	SYMMETRY: A computer program for the analysis of the distortions of the MX6(Oh) and MX4(Td) complexes in crystalline environments. Computers & Chemistry, 1994, 18, 405-411.	1.2	8
128	Molecular interactions in a homogeneous electric field: the (HF)2 complex. Theoretica Chimica Acta, 1993, 85, 167-187.	0.8	8
129	Analysis of the interaction energy in the Cu+-H2O and Cl?-H2O systems, with CP corrections to the BSSE of the separate terms, and MC simulations of the aqueous systems with and without CP corrections. Theoretica Chimica Acta, 1992, 82, 165-187.	0.8	9
130	Electron correlation and solvation effects. Computational and Theoretical Chemistry, 1991, 230, 295-312.	1.5	32
131	Theoretical chemistry in solution. Some results and perspectives of the continuum methods and in particular of the polarizable continuum model. Computational and Theoretical Chemistry, 1991, 234, 401-424.	1.5	183
132	On theab initio geometry optimization of molecular solutes. Journal of Computational Chemistry, 1991, 12, 301-309.	3.3	28
133	Low Temperature Absorption Spectrum of LiNiPO₄. Physica Status Solidi (B): Basic Research, 1991, 163, 281-292.	1.5	8
134	The Extramolecular Electrostatic Potential. An Indicator of the Chemical Reactivity. , 1991, , 229-268.		13
135	Proton and lithium cation interactions with hydrogen sulfide and hydrogen persulfide. Chemical Physics, 1989, 136, 399-404.	1.9	7
136	Decomposition of the interaction energy between metal cations and water or ammonia with inclusion of counterpoise corrections to the interaction energy terms. Theoretica Chimica Acta, 1989, 76, 297-313.	0.8	30
137	Noncovalent interactions of medium strength. A revised interpretation and examples of its applications. International Journal of Quantum Chemistry, 1989, 35, 223-239.	2.0	17
138	Decomposition of the interaction energy with counterpoise corrections to the basis set superposition error for dimers in solution. Method and application to the hydrogen fluoride dimer. Chemical Physics, 1988, 122, 63-74.	1.9	29
139	A Reappraisal of the Hydrogen Bonding Interaction Obtained by Combining Energy Decomposition Analyses and Counterpoise Corrections. Topics in Molecular Organization and Engineering, 1988, , 507-559.	0.1	15
140	The effect of ?full? and ?limited? counterpoise corrections with different basis sets on the energy and the equilibrium distance of hydrogen bonded dimers. International Journal of Quantum Chemistry, 1987, 32, 207-226.	2.0	44
141	The decomposition of the SCF interaction energy in hydrogen bonded dimers corrected for basis set superposition errors: An examination of the basis set dependence. International Journal of Quantum Chemistry, 1987, 32, 227-248.	2.0	31
142	Counterpoise corrections to the evaluation of the bimolecular interaction energy components. Theoretica Chimica Acta, 1986, 69, 11-22.	0.8	33
143	Counterpoise corrections to the components of bimolecular energy interactions: An examination of three methods of decomposition. International Journal of Quantum Chemistry, 1986, 29, 373-378.	2.0	24
144	Neutral organic lewis acids of ? type. International Journal of Quantum Chemistry, 1986, 29, 527-539.	2.0	14

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145	Symmetry descent in molecular systems. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1986, 8, 1-18.	0.4	5
146	Counterpoise corrections to the interaction energy components in bimolecular complexes. Theoretica Chimica Acta, 1985, 68, 271-283.	0.8	93
147	Properties and Spectroscopies. , 0, , 125-312.		3
148	Beyond the Continuum Approach. , 0, , 499-605.		6