Roberto Cammi

List of Publications by Year in Descending Order

150 papers	24,802 citations	50 h-index	156 g-index
156 ext. papers	26,971 ext. citations	3.9 avg, IF	7.06 L-index

#	Paper	IF	Citations
150	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	1.8	0
149	Toward an Understanding of the Pressure Effect on the Intramolecular Vibrational Frequencies of Sulfur Hexafluoride. *Journal of Physical Chemistry A*, **2021**, 125, 6362-6373	2.8	1
148	Relating atomic energy, radius and electronegativity through compression. *Chemical Science*, **2021**, 12, 2397-2403	9.4	7
147	An open quantum system theory for polarizable continuum models. *Journal of Chemical Physics*, **2020**, 152, 174114	3.9	5
146	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	6.4	5
145	Non-Bonded Radii of the Atoms Under Compression. *ChemPhysChem*, **2020**, 21, 2441-2453	3.2	10
144	High-Pressure-Promoted and Facially Selective Diels-Alder Reactions of Enzymatically Derived -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	4.2	2
143	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	3.5	1
142	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	16.4	76
141	Linear chains of hydrogen molecules under pressure: An extreme-pressure continuum model study. *Journal of Chemical Physics*, **2019**, 150, 164122	3.9	1
140	Quantum optimal control theory for solvated systems. *Journal of Chemical Physics*, **2019**, 151, 194109	3.9	5
139	Quantum Chemistry at the High Pressures: The eXtreme Pressure Polarizable Continuum Model (XP-PCM) **2018**, 273-287		8
138	Analytical calculation of pressure for confined atomic and molecular systems using the eXtreme-Pressure Polarizable Continuum Model. *Journal of Computational Chemistry*, **2018**, 39, 2243-2250	3.5	9
137	Quantum Cluster Theory for the Polarizable Continuum Model (PCM) **2017**, 1517-1556		1
136	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	3.9	10
135	Diels-Alder Cycloaddition of Cyclopentadiene and C at the Extreme High Pressure. *Journal of Physical Chemistry A*, **2017**, 121, 4363-4371	2.8	12
134	Insights on the Realgar Crystal Under Pressure from XP-PCM and Periodic Model Calculations. *Journal of Physical Chemistry A*, **2017**, 121, 8825-8834	2.8	9

133	Druckeffekte auf organische Reaktionen in Fluiden Eine neue theoretische Perspektive. *Angewandte Chemie*, **2017**, 129, 11278-11295	3.6	5
132	The Effect of Pressure on Organic Reactions in Fluids-a New Theoretical Perspective. *Angewandte Chemie - International Edition*, **2017**, 56, 11126-11142	16.4	55
131	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	1.8	6
130	XP-PCM Calculations of High Pressure Structural and Vibrational Properties of P4S3. *Journal of Physical Chemistry A*, **2016**, 120, 5136-44	2.8	9
129	Modeling Molecular Systems at Extreme Pressure by an Extension of the Polarizable Continuum Model (PCM) Based on the Symmetry-Adapted Cluster-Configuration Interaction (SAC-CI) Method: Confined Electronic Excited States of Furan as a Test Case. *Journal of Chemical Theory and Computation*, **2015**, 11, 2063-76	6.4	26
128	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, 2246-59	3.5	32
127	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, 5405-16	2.8	30
126	Quantum Cluster Theory for the Polarizable Continuum Model (PCM) **2015**, 1-40		
125	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, 5098-111	2.8	35
124	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	16
123	The cavity electromagnetic field within the polarizable continuum model of solvation. *Journal of Chemical Physics*, **2014**, 140, 164114	3.9	21
122	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	3.9	10
121	The virial theorem for the Polarizable Continuum Model. *Journal of Chemical Physics*, **2014**, 140, 084112	3.9	6
120	Molecular Response Functions for the Polarizable Continuum Model. *Springer Briefs in Molecular Science*, **2013**,	0.6	25
119	General Response Theory for the Polarizable Continuum Model. *Springer Briefs in Molecular Science*, **2013**, 23-36	0.6	3
118	Modelling vibrational coupling in DNA oligomers: a computational strategy combining QM and continuum solvation models. *Highlights in Theoretical Chemistry*, **2013**, 143-152		
117	Excitation Energies and Transition Moments from the PCM Linear Response Functions. *Springer Briefs in Molecular Science*, **2013**, 37-45	0.6	
116	The PCM Model. *Springer Briefs in Molecular Science*, **2013**, 1-11	0.6	

115	Analytical Derivatives Theory for Molecular Solutes. *Springer Briefs in Molecular Science*, **2013**, 13-22	0.6	
114	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	2.5	15
113	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	1.4	4
112	Coupled-cluster theory for the polarizable continuum model. III. A response theory for molecules in solution. *International Journal of Quantum Chemistry*, **2012**, 112, 2547-2560	2.1	28
111	Quantum Cluster Theory for the Polarizable Continuum Model (PCM) **2012**, 1043-1066		1
110	Modelling vibrational coupling in DNA oligomers: a computational strategy combining QM and continuum solvation models. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	12
109	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	3.9	54
108	Absolute stereochemistry and preferred conformations of urate degradation intermediates from computed and experimental circular dichroism spectra. *Organic and Biomolecular Chemistry*, **2011**, 9, 5149-55	3.9	10
107	Cavity field effects within a polarizable continuum model of solvation: Application to the calculation of electronic circular dichroism spectra of R-(+)-3-methyl-cyclopentanone. *International Journal of Quantum Chemistry*, **2011**, 111, 826-838	2.1	18
106	Modeling solvent effects on chiroptical properties. *Chirality*, **2011**, 23, 717-29	2.1	90
105	Nonequilibrium solvation for vertical photoemission and photoabsorption processes using the symmetry-adapted cluster-configuration interaction method in the polarizable continuum model. *Journal of Chemical Physics*, **2011**, 134, 104109	3.9	50
104	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	3.9	70
103	From Molecular Electrostatic Potentials to Solvation Models and Ending with Biomolecular Photophysical Processes **2010**, 131-170		8
102	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	3.4	7
101	Coupled-cluster theories for the polarizable continuum model. II. Analytical gradients for excited states of molecular solutes by the equation of motion coupled-cluster method. *International Journal of Quantum Chemistry*, **2010**, 110, 3040-3052	2.1	39
100	Structure versus solvent effects on nonlinear optical properties of push-pull systems: a quantum-mechanical study based on a polarizable continuum model. *Journal of Physical Chemistry A* , **2009**, 113, 14774-84	2.8	28
99	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	3.9	69
98	Properties of Excited States of Molecules in Solution Described with Continuum Solvation Models **2009**, 19-36		

97	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, 3009-20	2.8	158
96	Calculation of pKa 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, 16860-73	3.4	157
95	How the environment controls absorption and fluorescence spectra of PRODAN: a quantum-mechanical study in homogeneous and heterogeneous media. *Journal of Physical Chemistry B*, **2008**, 112, 414-23	3.4	63
94	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	0.7	3
93	Mechanistic Insights into Acetophenone Transfer Hydrogenation Catalyzed by Half-Sandwich Ruthenium(II) Complexes Containing 2-(Diphenylphosphanyl)aniline □A Combined Experimental and Theoretical Study. *European Journal of Inorganic Chemistry*, **2008**, 2008, 4462-4473	2.3	44
92	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	2.3	50
91	How solvent controls electronic energy transfer and light harvesting: toward a quantum-mechanical description of reaction field and screening effects. *Journal of Physical Chemistry B*, **2007**, 111, 13253-65	3.4	102
90	How solvent controls electronic energy transfer and light harvesting. *Journal of Physical Chemistry B*, **2007**, 111, 6978-82	3.4	150
89	Mononuclear and polynuclear copper(I) complexes with a new N,N',S-donor ligand and with structural analogies to the copper thionein core. *Inorganic Chemistry*, **2007**, 46, 10143-52	5.1	14
88	Ultrafast light harvesting dynamics in the cryptophyte phycocyanin 645. *Photochemical and Photobiological Sciences*, **2007**, 6, 964-75	4.2	51
87	A quantum mechanical polarizable continuum model for the calculation of resonance Raman spectra in condensed phase. *Theoretical Chemistry Accounts*, **2007**, 117, 1029-1039	1.9	41
86	How the Molecular Environment Controls Excitation Energy Transfer and Light Harvesting: a Quantum Mechanical Model. *AIP Conference Proceedings*, **2007**,	0	1
85	Self-consistent quantum mechanical model for the description of excitation energy transfers in molecules at interfaces. *Journal of Chemical Physics*, **2006**, 125, 054710	3.9	14
84	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	3.9	407
83	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, 94107	3.9	989
82	Cu(I) dinuclear complexes with tripodal ligands vs monodentate donors: triphenylphosphine, thiourea, and pyridine. A 1H NMR titration study. *Inorganic Chemistry*, **2006**, 45, 3456-66	5.1	9
81	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	3.9	172
80	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	3.9	240

79	Quantum mechanical polarizable continuum model approach to the Kerr effect of pure liquids. *Journal of Physical Chemistry B*, **2005**, 109, 18706-14	3.4	29
78	Quantum mechanical continuum solvation models. *Chemical Reviews*, **2005**, 105, 2999-3093	68.1	11786
77	Synthesis, structure, and electrochemical properties of copper(I) complexes with S/N homoscorpionate and heteroscorpionate ligands. *Inorganic Chemistry*, **2005**, 44, 4333-45	5.1	28
76	On the reaction of Ph2PNHPPh2 with RNCS (R=Et, Ph, p-NO2C6H4): preparation of the zwitterionic ligand EtNHC(S)Ph2P==NPPh2C(S)NEt (HSNS) and the zwitterionic metalate [(SNS)Rh(CO)]. *Chemistry - A European Journal*, **2005**, 11, 3413-9	4.8	10
75	Quantum Mechanical Continuum Solvation Models. *ChemInform*, **2005**, 36, no		19
74	Infrared linear dichroism in stretched films: Quantum mechanical approach within the polarizable continuum model. *International Journal of Quantum Chemistry*, **2005**, 104, 716-726	2.1	9
73	A polarizable continuum model for molecules at diffuse interfaces. *Journal of Chemical Physics*, **2004**, 120, 3893-907	3.9	62
72	Excitation energy transfer (EET) between molecules in condensed matter: a novel application of the polarizable continuum model (PCM). *Journal of Chemical Physics*, **2004**, 120, 7029-40	3.9	155
71	Excitonic splitting in conjugated molecular materials: A quantum mechanical model including interchain interactions and dielectric effects. *Physical Review B*, **2004**, 70,	3.3	10
70	Quantum-Mechanical Continuum Solvation Study of the Polarizability of Halides at the Water/Air Interface. *Journal of Physical Chemistry B*, **2004**, 108, 13796-13806	3.4	34
69	Second-order Møller–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	1.9	13
68	New developments in the symmetry-adapted algorithm of the Polarizable Continuum Model. *Journal of Computational Chemistry*, **2004**, 25, 375-85	3.5	13
67	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		5
66	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		11
65	Ab initio model to predict NMR shielding tensors for solutes in liquid crystals. *International Journal of Quantum Chemistry*, **2003**, 93, 121-130	2.1	20
64	Synthesis and molecular structure of the dihydrobis(thioxotriazolinyl)borato complexes of zinc(II), bismuth(III), and nickel(II). M...H-B interaction studied by Ab initio calculations. *Inorganic Chemistry*, **2003**, 42, 1769-78	5.1	26
63	Solvent Effects on the Indirect Spin–Spin Coupling Constants of Benzene: The DFT-PCM Approach. *International Journal of Molecular Sciences*, **2003**, 4, 119-134	6.3	63
62	The Cotton–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	3.9	36

61	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	3.9	104
60	Vibrational Circular Dichroism within the Polarizable Continuum Model: A Theoretical Evidence of Conformation Effects and Hydrogen Bonding for (S)-(+)-3-Butyn-2-ol in CCl4 Solution. *Journal of Physical Chemistry A*, **2002**, 106, 12331-12339	2.8	79
59	Polarizable Continuum Model (PCM) Calculations of Solvent Effects on Optical Rotations of Chiral Molecules. *Journal of Physical Chemistry A*, **2002**, 106, 6102-6113	2.8	494
58	Molecular properties in solution described with a continuum solvation model. *Physical Chemistry Chemical Physics*, **2002**, 4, 5697-5712	3.6	261
57	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	3.9	65
56	A Symmetry adapted tessellation of the GEPOL surface: applications to molecular properties in solution. *Journal of Computational Chemistry*, **2001**, 22, 1262-1272	3.5	22
55	The Cotton–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	2.5	14
54	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	2.8	49
53	Nonequilibrium formulation of infrared frequencies and intensities in solution: Analytical evaluation within the polarizable continuum model. *Journal of Chemical Physics*, **2000**, 113, 11270-11279	3.9	63
52	An Attempt To Bridge the Gap between Computation and Experiment for Nonlinear Optical Properties: Macroscopic Susceptibilities in Solution *Journal of Physical Chemistry A*, **2000**, 104, 4690-4698	2.8	114
51	On the Calculation of Infrared Intensities in Solution within the Polarizable Continuum Model. *Journal of Physical Chemistry A*, **2000**, 104, 9874-9879	2.8	77
50	Fast Evaluation of Geometries and Properties of Excited Molecules in Solution: A Tamm-Dancoff Model with Application to 4-Dimethylaminobenzonitrile. *Journal of Physical Chemistry A*, **2000**, 104, 5631-5637	2.8	484
49	Solvent Effects on 15N NMR Shielding of 1,2,4,5-Tetrazine and Isomeric Tetrazoles: Continuous Set Gauge Transformation Calculation Using the Polarizable Continuum Model. *Journal of Physical Chemistry A*, **2000**, 104, 9600-9604	2.8	24
48	Linear response theory for the polarizable continuum model. *Journal of Chemical Physics*, **1999**, 110, 9877-9886	3.9	262
47	Nuclear magnetic shieldings in solution: Gauge invariant atomic orbital calculation using the polarizable continuum model. *Journal of Chemical Physics*, **1999**, 110, 7627-7638	3.9	97
46	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	3.9	107
45	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	2.1	99
44	Second-Order Møller–Plesset Analytical Derivatives for the Polarizable Continuum Model Using the Relaxed Density Approach. *Journal of Physical Chemistry A*, **1999**, 103, 9100-9108	2.8	215

43	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		22
42	An ab initio time-dependent Hartree–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	2.3	26
41	Recent Advances in the Description of Solvent Effects with the Polarizable Continuum Model. *Advances in Quantum Chemistry*, **1998**, 32, 227-261	1.4	373
40	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	2.8	107
39	Solvent Effects on Linear and Nonlinear Optical Properties of Donor–Acceptor Polyenes: Investigation of Electronic and Vibrational Components in Terms of Structure and Charge Distribution Changes. *Journal of the American Chemical Society*, **1998**, 120, 8834-8847	16.4	90
38	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, 2799-2807	3.9	326
37	The Hartree–Fock calculation of the magnetic properties of molecular solutes. *Journal of Chemical Physics*, **1998**, 109, 3185-3196	3.9	73
36	Solvent effects on static and dynamic polarizability and hyperpolarizabilities of acetonitrile. *Journal of Molecular Structure*, **1997**, 436-437, 567-575	3.4	18
35	Analytical first derivatives of molecular surfaces with respect to nuclear coordinates. *Journal of Computational Chemistry*, **1996**, 17, 57-73	3.5	98
34	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	2.1	22
33	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	2.1	13
32	Ab initio study of solvated molecules: a new implementation of the polarizable continuum model. *Chemical Physics Letters*, **1996**, 255, 327-335	2.5	2731
31	Analytical derivatives for molecular solutes. III. Hartree–Fock static polarizability and hyperpolarizabilities in the polarizable continuum model. *Journal of Chemical Physics*, **1996**, 104, 4611-4620	3.9	140
30	Analytical Hartree–Fock calculation of the dynamical polarizabilities □ and □ of molecules in solution. *Journal of Chemical Physics*, **1996**, 105, 10556-10564	3.9	142
29	Nonequilibrium solvation theory for the polarizable continuum model: A new formulation at the SCF level with application to the case of the frequency-dependent linear electric response function. *International Journal of Quantum Chemistry*, **1995**, 56, 465-474	2.1	94
28	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	2.1	27
27	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	3.5	40
26	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	3.5	1044

25	Analytical derivatives for molecular solutes. II. Hartree–Fock energy first and second derivatives with respect to nuclear coordinates. *Journal of Chemical Physics*, **1994**, 101, 3888-3897	3.9	88
24	Analytical derivatives for molecular solutes. I. Hartree–Fock energy first derivatives with respect to external parameters in the polarizable continuum model. *Journal of Chemical Physics*, **1994**, 100, 7495-7502	3.9	117
23	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		6
22	Molecular interactions in a homogeneous electric field: the (HF)2 complex. *Theoretica Chimica Acta*, **1993**, 85, 167-187		7
21	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		8
20	Electron correlation and solvation effects. *Computational and Theoretical Chemistry*, **1991**, 230, 295-312		31
19	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		169
18	On the ab initio geometry optimization of molecular solutes. *Journal of Computational Chemistry*, **1991**, 12, 301-309	3.5	25
17	Low Temperature Absorption Spectrum of LiNiPO4. *Physica Status Solidi (B): Basic Research*, **1991**, 163, 281-292	1.3	7
16	The Extramolecular Electrostatic Potential. An Indicator of the Chemical Reactivity **1991**, 229-268		13
15	Proton and lithium cation interactions with hydrogen sulfide and hydrogen persulfide. *Chemical Physics*, **1989**, 136, 399-404	2.3	6
14	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		29
13	Noncovalent interactions of medium strength. A revised interpretation and examples of its applications. *International Journal of Quantum Chemistry*, **1989**, 35, 223-239	2.1	16
12	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	2.3	27
11	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		14
10	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	2.1	44
9	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	2.1	30
8	Counterpoise corrections to the evaluation of the bimolecular interaction energy components. *Theoretica Chimica Acta*, **1986**, 69, 11-22		33

7	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	2.1	24
6	Neutral organic lewis acids of type. *International Journal of Quantum Chemistry*, **1986**, 29, 527-539	2.1	14
5	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		5
4	Counterpoise corrections to the interaction energy components in bimolecular complexes. *Theoretica Chimica Acta*, **1985**, 68, 271-283		91
3	Properties and Spectroscopies125-312		3
2	Beyond the Continuum Approach499-605		3
1	Modern Theories of Continuum Models1-123		35