Malgorzata Biczysko

List of Publications by Year
in descending order

120	5,936	81434	87275
papers	citations	41 h-index	74 g-index

130	130	130	4859
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A radical approach to radicals. Acta Crystallographica Section D: Structural Biology, 2022, 78, 43-51.	1.1	0
2	Editorial: Theoretical Characterization of Astrophysical Species. Frontiers in Astronomy and Space Sciences, 2022, 9, .	1.1	0
3	Computational molecular spectroscopy. Nature Reviews Methods Primers, 2021, 1, .	11.8	73
4	Structural and Vibrational Properties of Amino Acids from Composite Schemes and Double-Hybrid DFT: Hydrogen Bonding in Serine as a Test Case. Journal of Physical Chemistry A, 2021, 125, 9099-9114.	1.1	9
5	Identification of DNA Bases and Their Cations in Astrochemical Environments: Computational Spectroscopy of Thymine as a Test Case. Frontiers in Astronomy and Space Sciences, 2021, 8, .	1.1	0
6	Structural and Energetic Properties of Amino Acids and Peptides Benchmarked by Accurate Theoretical and Experimental Data. Journal of Physical Chemistry A, 2021, 125, 9826-9837.	1.1	6
7	Toward accurate prediction of amino acid derivatives structure and energetics from DFT: glycine conformers and their interconversions. Journal of Molecular Modeling, 2020, 26, 129.	0.8	15
8	The challenging equilibrium structure of HSSH: Another success of the rotational spectroscopy / quantum chemistry synergism. Journal of Molecular Structure, 2020, 1211, 127933.	1.8	11
9	Including crystallographic symmetry in quantum-based refinement: Q | R#2. Acta Crystallographica Section D: Structural Biology, 2020, 76, 41-50.	1.1	13
10	Real-space quantum-based refinement for cryo-EM: Q | R#3. Acta Crystallographica Section D: Structural Biology, 2020, 76, 1184-1191.	1.1	7
11	UV Irradiation and Near Infrared Characterization of Laboratory Mars Soil Analog Samples. Frontiers in Astronomy and Space Sciences, 2020, 7, .	1.1	8
12	Pressure-induced reversible framework rearrangement and increased polarization in the polar [NH4][Cd(HCOO)3] hybrid perovskite. Inorganic Chemistry Frontiers, 2019, 6, 2379-2386.	3.0	9
13	The role of dispersion and anharmonic corrections in conformational analysis of flexible molecules: the allyl group rotamerization of matrix isolated safrole. Physical Chemistry Chemical Physics, 2019, 21, 8352-8364.	1.3	5
14	Internal Hydrogen Bond Influences the Formation of [2+2] Schiff Base Macrocycle: Openâ€€Chain Vs. Hemiaminal and Macrocycle Forms. European Journal of Organic Chemistry, 2019, 2019, 2243-2252.	1.2	4
15	Absorption-emission symmetry breaking and the different origins of vibrational structures of the 1Qy and 1Qx electronic transitions of pheophytin a. Journal of Chemical Physics, 2019, 151, 165102.	1.2	17
16	Conformational Equilibria and Molecular Structures of Model Sulfurâ€“Sulfur Bridge Systems: Diisopropyl Disulfide. Journal of Physical Chemistry A, 2019, 123, 10714-10720.	1.1	5
17	MAPPING THE CONFORMATION SPACE OF _-PROLINE BY MATRIX-ISOLATION IR SPECTROSCOPY COMBINED WITH NIR LASER INDUCED CONFORMATIONAL CHANGE AND STATE-OF-THE-ART AB INITIO COMPUTATIONS. , 2019, , .		0
18	Hydrogen detachment driven by a repulsive 1Ï€Ïƒ* state â€“ an electron localization function study of 3-amino-1,2,4-triazole. Physical Chemistry Chemical Physics, 2018, 20, 5210-5216.	1.3	9

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19	Accurate geometries for â€œMountain passâ€•regions of the Ramachandran plot using quantum chemical calculations. Proteins: Structure, Function and Bioinformatics, 2018, 86, 273-278.	1.5	7
20	Computational challenges in Astrochemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1349.	6.2	43
21	Cover Image, Volume 8, Issue 3. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1368.	6.2	1
22	Molecules in confinement in clusters, quantum solvents and matrices: general discussion. Faraday Discussions, 2018, 212, 569-601.	1.6	4
23	Accurate rest frequencies for propargylamine in the ground and low-lying vibrational states. Astronomy and Astrophysics, 2018, 615, A176.	2.1	10
24	Theoretical studies of atmospheric molecular complexes interacting with NIR to UV light. Faraday Discussions, 2018, 212, 421-441.	1.6	7
25	A combined theoretical and experimental study of the ionic states of iodopentafluorobenzene. Journal of Chemical Physics, 2017, 146, 084302.	1.2	3
26	Accurate Vibrationalâ€“Rotational Parameters and Infrared Intensities of 1-Bromo-1-fluoroethene: A Joint Experimental Analysis and Ab Initio Study. Journal of Physical Chemistry A, 2017, 121, 3305-3317.	1.1	18
27	A combined theoretical and experimental study of the valence and Rydberg states of iodopentafluorobenzene. Journal of Chemical Physics, 2017, 146, 174301.	1.2	6
28	Structural and Vibrational Properties of Iodopentafluorobenzene: A Combined Raman and Infrared Spectral and Theoretical Study. Journal of Physical Chemistry A, 2017, 121, 7917-7924.	1.1	3
29	The ionic states of difluoromethane: A reappraisal of the low energy photoelectron spectrum including ab initio configuration interaction computations. Journal of Chemical Physics, 2017, 147, 074305.	1.2	3
30	Accurate spectroscopic characterization of the HOC(O)O radical: A route toward its experimental identification. Journal of Chemical Physics, 2017, 147, 024302.	1.2	4
31	Challenges facing an understanding of the nature of low-energy excited states in photosynthesis. Biochimica Et Biophysica Acta - Bioenergetics, 2016, 1857, 1627-1640.	0.5	74
32	Combined theoretical and experimental study of the valence, Rydberg, and ionic states of chlorobenzene. Journal of Chemical Physics, 2016, 144, 124302.	1.2	11
33	Combined theoretical and experimental study of the valence, Rydberg and ionic states of fluorobenzene. Journal of Chemical Physics, 2016, 144, 204305.	1.2	15
34	Correction to Semi-Experimental Equilibrium Structure Determinations by Employing B3LYP/SNSD Anharmonic Force Fields: Validation and Application to Semirigid Organic Molecules. Journal of Physical Chemistry A, 2016, 120, 3754-3754.	1.1	17
35	Simulation of Vacuum UV Absorption and Electronic Circular Dichroism Spectra of Methyl Oxirane: The Role of Vibrational Effects. Journal of Chemical Theory and Computation, 2016, 12, 2820-2833.	2.3	38
36	Aiming at an accurate prediction of vibrational and electronic spectra for mediumâ€toâ€•large molecules: An overview. International Journal of Quantum Chemistry, 2016, 116, 1543-1574.	1.0	161

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37	Reliable vibrational wavenumbers for Cî€Ð and Nâ€“H stretchings of isolated and hydrogen-bonded nucleic acid bases. Physical Chemistry Chemical Physics, 2016, 18, 8479-8490.	1.3	47
38	Interpretation of the photoelectron, ultraviolet, and vacuum ultraviolet photoabsorption spectra of bromobenzene by ab initio configuration interaction and DFT computations. Journal of Chemical Physics, 2015, 143, 164303.	1.2	19
39	Interpretation of the vacuum ultraviolet photoabsorption spectrum of iodobenzene by ab initio computations. Journal of Chemical Physics, 2015, 142, 134302.	1.2	51
40	Anharmonic Effects on Vibrational Spectra Intensities: Infrared, Raman, Vibrational Circular Dichroism, and Raman Optical Activity. Journal of Physical Chemistry A, 2015, 119, 11862-11874.	1.1	101
41	Virtual eyes for technology and cultural heritage: towards computational strategy for new and old indigo-based dyes. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	5
42	Identification of Serine Conformers by Matrix-Isolation IR Spectroscopy Aided by Near-Infrared Laser-Induced Conformational Change, 2D Correlation Analysis, and Quantum Mechanical Anharmonic Computations. Journal of Physical Chemistry B, 2015, 119, 10496-10510.	1.2	38
43	Toward Feasible and Comprehensive Computational Protocol for Simulation of the Spectroscopic Properties of Large Molecular Systems: The Anharmonic Infrared Spectrum of Uracil in the Solid State by the Reduced Dimensionality/Hybrid VPT2 Approach. Journal of Physical Chemistry A, 2015, 119, 5313-5326.	1.1	28
44	Semi-Experimental Equilibrium Structure Determinations by Employing B3LYP/SNSD Anharmonic Force Fields: Validation and Application to Semirigid Organic Molecules. Journal of Physical Chemistry A, 2015, 119, 2058-2082.	1.1	155
45	Conformational Switching in Pyruvic Acid Isolated in Ar and N₂ Matrixes: Spectroscopic Analysis, Anharmonic Simulation, and Tunneling. Journal of Physical Chemistry A, 2015, 119, 2614-2627.	1.1	62
46	Microsolvation of 2-Thiouracil: Molecular Structure and Spectroscopic Parameters of the Thiouracilâ€“Water Complex. Journal of Physical Chemistry A, 2015, 119, 5386-5395.	1.1	22
47	The ionic states of iodobenzene studied by photoionization and ab initio configuration interaction and DFT computations. Journal of Chemical Physics, 2015, 142, 134301.	1.2	18
48	Quantum Chemistry Meets Spectroscopy for Astrochemistry: Increasing Complexity toward Prebiotic Molecules. Accounts of Chemical Research, 2015, 48, 1413-1422.	7.6	83
49	Hydrogen-Bonding Effects on Infrared Spectra from Anharmonic Computations: Uracilâ€“Water Complexes and Uracil Dimers. Journal of Physical Chemistry A, 2015, 119, 4224-4236.	1.1	142
50	Anharmonicity Effects in IR Spectra of [Re(X)(CO)₃(Î±-diimine)] (Î±-diimine = 2,2â€²-bipyridine or) Tj ETQq0 0 0 rgBT /Overl Journal of Physical Chemistry A, 2015, 119, 10137-10146.	1.1	19
51	CC/DFT Route toward Accurate Structures and Spectroscopic Features for Observed and Elusive Conformers of Flexible Molecules: Pyruvic Acid as a Case Study. Journal of Chemical Theory and Computation, 2015, 11, 4342-4363.	2.3	75
52	Toward the design of alkynylimidazole fluorophores: computational and experimental characterization of spectroscopic features in solution and in poly(methyl methacrylate). Physical Chemistry Chemical Physics, 2015, 17, 26710-26723.	1.3	13
53	Implementation of a graphical user interface for the virtual multifrequency spectrometer: The VMSâ€Draw tool. Journal of Computational Chemistry, 2015, 36, 321-334.	1.5	84
54	Accurate molecular structures and infrared spectra of trans-2,3-dideuterooxirane, methyloxirane, and trans-2,3-dimethyloxirane. Journal of Chemical Physics, 2014, 141, 034107.	1.2	57

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55	A Multifrequency Virtual Spectrometer for Complex Bioâ€Organic Systems: Vibronic and Environmental Effects on the UV/Vis Spectrum of Chlorophyll a. ChemPhysChem, 2014, 15, 3355-3364.	1.0	31
56	ACCURATE SPECTROSCOPIC CHARACTERIZATION OF OXIRANE: A VALUABLE ROUTE TO ITS IDENTIFICATION IN TITAN'S ATMOSPHERE AND THE ASSIGNMENT OF UNIDENTIFIED INFRARED BANDS. Astrophysical Journal, 2014, 785, 107.	1.6	47
57	Environmental and complexation effects on the structures and spectroscopic signatures of organic pigments relevant to cultural heritage: the case of alizarin and alizarinâ€“Mg(ii)/Al(iii) complexes. Physical Chemistry Chemical Physics, 2014, 16, 2897.	1.3	32
58	Computational Investigation on the Spectroscopic Properties of Thiophene Based Europium Î²-Diketonate Complexes. Journal of Chemical Theory and Computation, 2014, 10, 767-777.	2.3	20
59	Fully anharmonic IR and Raman spectra of medium-size molecular systems: accuracy and interpretation. Physical Chemistry Chemical Physics, 2014, 16, 1759-1787.	1.3	363
60	Dispersion corrected DFT approaches for anharmonic vibrational frequency calculations: nucleobases and their dimers. Physical Chemistry Chemical Physics, 2014, 16, 10112-10128.	1.3	92
61	Ultrafast resonance energy transfer in the umbelliferoneâ€“alizarin bichromophore. Physical Chemistry Chemical Physics, 2014, 16, 10059-10074.	1.3	12
62	ACCURATE SPECTROSCOPIC CHARACTERIZATION OF PROTONATED OXIRANE: A POTENTIAL PREBIOTIC SPECIES IN TITAN'S ATMOSPHERE. Astrophysical Journal, 2014, 792, 118.	1.6	15
63	Accurate Characterization of the Peptide Linkage in the Gas Phase: A Joint Quantum-Chemical and Rotational Spectroscopy Study of the Glycine Dipeptide Analogue. Journal of Physical Chemistry Letters, 2014, 5, 534-540.	2.1	87
64	Environmental and dynamical effects on the optical properties of molecular systems by time-independent and time-dependent approaches: Coumarin derivatives as test cases. Computational and Theoretical Chemistry, 2014, 1037, 35-48.	1.1	21
65	Molecular Structure and Spectroscopic Signatures of Acrolein: Theory Meets Experiment. Journal of Physical Chemistry A, 2014, 118, 6648-6656.	1.1	37
66	Reprint of â€œEnvironmental and dynamical effects on the optical properties of molecular systems by time-independent and time-dependent approaches: Coumarin derivatives as test casesâ€• Computational and Theoretical Chemistry, 2014, 1040-1041, 144-157.	1.1	1
67	ACCURATE CHARACTERIZATION OF THE PEPTIDE LINKAGE IN THE GAS PHASE: A JOINT QUANTUM-CHEMICAL AND ROTATIONAL SPECTROSCOPY STUDY OF THE GLYCINE DIPEPTIDE ANALOGUE. , 2014, , .		0
68	ACCURATE ANHARMONIC IR SPECTRA FROM INTEGRATED CC/DFT APPROACH. , 2014, , .		0
69	SIMULATION OF ACCURATE VIBRATIONALLY RESOLVED ELECTRONIC SPECTRA: THE INTEGRATED TIME-DEPENDENT AND TIME-INDEPENDENT FRAMEWORK. , 2014, , .		0
70	ANHARMONIC IR SPECTRA OF BIOMOLECULES: NUCLEOBASES AND THEIR OLIGOMERS. , 2014, , .		0
71	Accurate molecular structure and spectroscopic properties of nucleobases: a combined computationalâ€“microwave investigation of 2-thiouracil as a case study. Physical Chemistry Chemical Physics, 2013, 15, 16965.	1.3	74
72	Anharmonic theoretical simulations of infrared spectra of halogenated organic compounds. Journal of Chemical Physics, 2013, 139, 074310.	1.2	72

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73	Computational Design, Synthesis, and Mechanochromic Properties of New Thiopheneâ€Based Ï€â€Conjugated Chromophores. Chemistry - A European Journal, 2013, 19, 1996-2004.	1.7	43
74	Glycine conformers: a never-ending story?. Physical Chemistry Chemical Physics, 2013, 15, 1358-1363.	1.3	81
75	Characterization of the Elusive Conformers of Glycine from State-of-the-Art Structural, Thermodynamic, and Spectroscopic Computations: Theory Complements Experiment. Journal of Chemical Theory and Computation, 2013, 9, 1533-1547.	2.3	72
76	Including nuclear quantum effects into highly correlated electronic structure calculations of weakly bound systems. Journal of Chemical Physics, 2013, 138, 184113.	1.2	14
77	Accurate structure, thermodynamic and spectroscopic parameters from CC and CC/DFT schemes: the challenge of the conformational equilibrium in glycine. Physical Chemistry Chemical Physics, 2013, 15, 10094.	1.3	117
78	An integrated experimental and quantum-chemical investigation on the vibrational spectra of chlorofluoromethane. Journal of Chemical Physics, 2013, 139, 164302.	1.2	36
79	Accurate structure, thermodynamics, and spectroscopy of medium-sized radicals by hybrid coupled cluster/density functional theory approaches: The case of phenyl radical. Journal of Chemical Physics, 2013, 138, 234303.	1.2	28
80	Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: pyrimidine as a test case. Highlights in Theoretical Chemistry, 2013, , 319-337.	0.0	0
81	Implementation and validation of a multi-purpose virtual spectrometer for large systems in complex environments. Physical Chemistry Chemical Physics, 2012, 14, 12404.	1.3	128
82	General Perturbative Approach for Spectroscopy, Thermodynamics, and Kinetics: Methodological Background and Benchmark Studies. Journal of Chemical Theory and Computation, 2012, 8, 1015-1036.	2.3	256
83	Toward anharmonic computations of vibrational spectra for large molecular systems. International Journal of Quantum Chemistry, 2012, 112, 2185-2200.	1.0	101
84	Solvent effects on electron-driven proton-transfer processes: adenineâ€“thymine base pairs. Physical Chemistry Chemical Physics, 2012, 14, 8981.	1.3	55
85	Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: pyrimidine as a test case. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	64
86	Fully ab initio IR spectra for complex molecular systems from perturbative vibrational approaches: Glycine as a test case. Journal of Molecular Structure, 2012, 1009, 74-82.	1.8	48
87	Reliable structural, thermodynamic, and spectroscopic properties of organic molecules adsorbed on silicon surfaces from computational modeling: the case of glycine@Si(100). Physical Chemistry Chemical Physics, 2011, 13, 16713.	1.3	37
88	Noncovalent Interactions in the Gas Phase: The Anisoleâ€“Phenol Complex. Journal of Physical Chemistry A, 2011, 115, 9603-9611.	1.1	38
89	Accurate Anharmonic Vibrational Frequencies for Uracil: The Performance of Composite Schemes and Hybrid CC/DFT Model. Journal of Chemical Theory and Computation, 2011, 7, 3702-3710.	2.3	113
90	Reinvestigation of spectroscopic properties for ammoniaâ€“hydrogen halide complexes from Carâ€“Parrinello Molecular Dynamics. Chemical Physics Letters, 2011, 514, 44-48.	1.2	5

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91	Accurate Harmonic/Anharmonic Vibrational Frequencies for Open-Shell Systems: Performances of the B3LYP/N07D Model for Semirigid Free Radicals Benchmarked by CCSD(T) Computations. Journal of Chemical Theory and Computation, 2010, 6, 828-838.	2.3	120
92	Magnetic Properties of Nitroxide Spin Probes: Reliable Account of Molecular Motions and Nonspecific Solvent Effects by Time-Dependent and Time-Independent Approaches. Journal of Physical Chemistry B, 2010, 114, 11509-11514.	1.2	25
93	Environmental Effects in Computational Spectroscopy: Accuracy and Interpretation. ChemPhysChem, 2010, 11, 1812-1832.	1.0	51
94	General Approach to Compute Vibrationally Resolved One-Photon Electronic Spectra. Journal of Chemical Theory and Computation, 2010, 6, 1256-1274.	2.3	253
95	Harmonic and Anharmonic Vibrational Frequency Calculations with the Double-Hybrid B2PLYP Method: Analytic Second Derivatives and Benchmark Studies. Journal of Chemical Theory and Computation, 2010, 6, 2115-2125.	2.3	274
96	Extending the Range of Computational Spectroscopy by QM/MM Approaches: Time-Dependent and Time-Independent Routes. Advances in Quantum Chemistry, 2010, , 17-57.	0.4	27
97	Validation of the DFT/N07D computational model on the magnetic, vibrational and electronic properties of vinyl radical. Physical Chemistry Chemical Physics, 2010, 12, 1092-1101.	1.3	69
98	Integrated experimental and computational spectroscopy study on Ї€-stacking interaction: the anisole dimer. Physical Chemistry Chemical Physics, 2010, 12, 13547.	1.3	24
99	The Gas Phase Anisole Dimer: A Combined High-Resolution Spectroscopy and Computational Study of a Stacked Molecular System. Journal of Physical Chemistry A, 2009, 113, 14343-14351.	1.1	52
100	First principle simulation of vibrationally resolved <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si127.gif" display="inline" overflow="scroll"><mml:mrow><mml:msup><mml:mrow><mml:mi>A</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msup></mml:mrow></mml:math> electronic spectra: The <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si128.gif" display="inline" overflow="scroll"><mml:mover accent="true"><mml:mrow><mml:mtext>X</mml:mtext></mml:mrow><mml:mrow><mml:mo>Ëœ</mml:mo></mml:mrow></mml:mover></mml:math> Chemical Physics Letters, 2009, 471, 143-147.	1.2	27
101	Toward spectroscopic studies of biologically relevant systems: Vibrational spectrum of adenine as a test case for performances of long-range/dispersion corrected density functionals. Chemical Physics Letters, 2009, 475, 105-110.	1.2	48
102	Fully Integrated Approach to Compute Vibrationally Resolved Optical Spectra: From Small Molecules to Macrosystems. Journal of Chemical Theory and Computation, 2009, 5, 540-554.	2.3	406
103	Accurate ab initio based DMBE potential energy surface for the ground electronic state of N2H2. Journal of Chemical Physics, 2009, 131, 044309.	1.2	27
104	The role of dispersion correction to DFT for modelling weakly bound molecular complexes in the ground and excited electronic states. Chemical Physics, 2008, 346, 247-256.	0.9	77
105	Integrated computational approach to vibrationally resolved electronic spectra: Anisole as a test case. Journal of Chemical Physics, 2008, 128, 244105.	1.2	117
106	On the properties of microsolvated molecules in the ground (S) and excited (S1) states: The anisole-ammonia 1:1 complex. Journal of Chemical Physics, 2007, 127, 144303.	1.2	35
107	Isotopomeric Conformational Changes in the Anisoleâ‹¯Water Complex:Â New Insights from HR-UV Spectroscopy and Theoretical Studiesâ€. Journal of Physical Chemistry A, 2007, 111, 12363-12371.	1.1	29
108	Predicting Catalysis:Â Understanding Ammonia Synthesis from First-Principles Calculations. Journal of Physical Chemistry B, 2006, 110, 17719-17735.	1.2	192

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109	Accurate MRCI study of ground-state N2H2 potential energy surface. Chemical Physics Letters, 2006, 424, 46-53.	1.2	30
110	Rennerâ€“Teller interactions coupled to large spinâ€“orbit splittings: The BrCN+ case. Chemical Physics Letters, 2005, 415, 223-229.	1.2	9
111	Computational Study of the Adsorption Energetics and Vibrational Wavenumbers of NH3Adsorbed on the Ni(111) Surface. Journal of Physical Chemistry B, 2005, 109, 8954-8960.	1.2	22
112	Variational calculations of HBN energy levels in the Xâ€‰2Î and Aâ€‰2Î£+ states. Journal of Chemical Physics, 2003, 119, 4197-4203.	1.2	15
113	Accuracy of Theoretical Potential Energy Profiles along Proton-Transfer Coordinate for XHâ‹¯NH3 (X =) Tj ETQq1 1 0.784314 rgBT /Ov	1.1	31
114	Theoretical study of anharmonic resonances in HBS+. Molecular Physics, 2002, 100, 3667-3676.	0.8	2
115	Theoretical calculation of rovibronic energy levels and anharmonic resonances in the ground Xâ€‰2Î state of HCP+ and DCP+Electronic supplementary information (ESI) available: Expansion coefficients of the PESs (Table). See http://www.rsc.org/suppdata/cp/b1/b107282j/. Physical Chemistry Chemical Physics, 2002, 4, 708-715.	1.3	9
116	Proton transfer in strongly hydrogen-bonded molecular complexes: matrix effects. Journal of Molecular Structure, 2002, 614, 11-21.	1.8	35
117	Solvent effect on hydrogen bonded ammoniaâ€“hydrogen halide complexes: continuum medium versus cluster models. Computers & Chemistry, 2000, 24, 303-309.	1.2	22
118	The influence of water molecules on the proton position in H3Nâ€“HX (X=F, Cl, Br) complexes. Chemical Physics Letters, 1999, 313, 366-373.	1.2	39
119	Interplay of Stereoelectronic Vibrational and Environmental Effects in Tuning Physicochemical Properties of Carbon-Centered Radicals. , 0, , 105-139.		2
120	The chirality of isotopomers of glycine compared using nextâ€generation <scp>QTAIM</scp>. International Journal of Quantum Chemistry, 0, , .	1.0	3