Alexandre Giuliani

List of Publications by Year
in descending order

131	2,776	172457	233421
papers	citations	29 h-index	45 g-index

141	141	141	3162
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	UV/VUV photoprocessing of protonatedN-hetero(poly)acenes. Monthly Notices of the Royal Astronomical Society, 2022, 511, 5656-5660.	4.4	2
2	Ultraviolet Photoactivation Using Synchrotron Radiation for Tandem Mass Spectrometry of Polysiloxanes. Journal of the American Society for Mass Spectrometry, 2021, 32, 901-912.	2.8	1
3	Mammal hyaluronidase activity on chondroitin sulfate and dermatan sulfate: Mass spectrometry analysis of oligosaccharide products. Glycobiology, 2021, 31, 751-761.	2.5	8
4	UV and VUV-induced fragmentation of tin-oxo cage ions. Physical Chemistry Chemical Physics, 2021, 23, 20909-20918.	2.8	8
5	Photo-processing of astro-PAHs. Journal of Physics: Conference Series, 2020, 1412, 062002.	0.4	12
6	State-dependent fragmentation of protonated uracil and uridine. Journal of Physics: Conference Series, 2020, 1412, 212010.	0.4	0
7	Astrochemical relevance of VUV ionization of large PAH cations. Astronomy and Astrophysics, 2020, 641, A98.	5.1	25
8	New exploration of the Î³-gliadin structure through its partial hydrolysis. International Journal of Biological Macromolecules, 2020, 165, 654-664.	7.5	6
9	Oxygen K-shell spectroscopy of isolated progressively solvated peptide. Physical Chemistry Chemical Physics, 2020, 22, 12909-12917.	2.8	9
10	Synchrotron UV photoactivation of trapped sodiated ions produced from poly(ethylene glycol) by electrospray ionization. Rapid Communications in Mass Spectrometry, 2020, 34, e8773.	1.5	4
11	Photon-induced Fragmentation of Zinc-based Oxoclusters for EUV Lithography Applications. Journal of Photopolymer Science and Technology = [Fotoporima Konwakai Shi], 2020, 33, 153-158.	0.3	5
12	Time resolved transient circular dichroism spectroscopy using synchrotron natural polarization. Structural Dynamics, 2019, 6, 054307.	2.3	14
13	Role of protein conformation and weak interactions on Î³-gliadin liquid-liquid phase separation. Scientific Reports, 2019, 9, 13391.	3.3	18
14	Vacuum-UV induced DNA strand breaks â€“ influence of the radiosensitizers 5-bromouracil and 8-bromoadenine. Physical Chemistry Chemical Physics, 2019, 21, 1972-1979.	2.8	10
15	State-Dependent Fragmentation of Protonated Uracil and Uridine. Journal of Physical Chemistry A, 2019, 123, 3551-3557.	2.5	7
16	Vacuumâ€UV and Lowâ€Energy Electronâ€Induced DNA Strand Breaks â€“ Influence of the DNA Sequence and Substrate. ChemPhysChem, 2019, 20, 823-830.	2.1	15
17	Photoprocessing of large PAH cations. Proceedings of the International Astronomical Union, 2019, 15, 388-389.	0.0	0
18	Tuning photoionization mechanisms of molecular hybrid materials for EUV lithography applications. Journal of Materials Chemistry C, 2019, 7, 33-37.	5.5	18

#	Article	IF	Citations
19	Investigation of secondary structure evolution of micellar casein powder upon aging by FTIR and SRCD: consequences on solubility. Journal of the Science of Food and Agriculture, 2018, 98, 2243-2250.	3.5	21
20	Photo-induced Fragmentation of a Tin-oxo Cage Compound. Journal of Photopolymer Science and Technology = [Fotoporima Konwakai Shi], 2018, 31, 243-247.	0.3	15
21	Carotenoids: Experimental Ionization Energies and Capacity at Inhibiting Lipid Peroxidation in a Chemical Model of Dietary Oxidative Stress. Journal of Physical Chemistry B, 2018, 122, 5860-5869.	2.6	13
22	Extreme Ultraviolet Radiation: A Means of Ion Activation for Tandem Mass Spectrometry. Analytical Chemistry, 2018, 90, 7176-7180.	6.5	17
23	Radical Anions of Oxidized vs. Reduced Oxytocin: Influence of Disulfide Bridges on CID and Vacuum UV Photo-Fragmentation. Journal of the American Society for Mass Spectrometry, 2018, 29, 1826-1834.	2.8	0
24	Spectroscopy and Photodissociation of the Perfluorooctanoate Anion. Chemistry - A European Journal, 2018, 24, 15572-15576.	3.3	1
25	MS/MS-Guided Isolation of Clarinoside, a New Anti-Inflammatory Pentalogin Derivative. Molecules, 2018, 23, 1237.	3.8	7
26	Gas-Phase Structural and Optical Properties of Homo- and Heterobimetallic Rhombic Dodecahedral Nanoclusters [Ag_{14â€“n}Cu_n(Câ‰¡CtBu)₁₂X]⁺ (X = Cl, I, 2017, 121, 10719-10727.	3.1	0
27	Multiple electron capture from isolated protein poly-anions in collision with slow highly charged ions. Physical Chemistry Chemical Physics, 2017, 19, 19691-19698.	2.8	5
28	Photoionization of the Buckminsterfullerene Cation. Journal of Physical Chemistry Letters, 2017, 8, 7-12.	4.6	10
29	Structural proteomics: Topology and relative accessibility of plant lipid droplet associated proteins. Journal of Proteomics, 2017, 169, 87-98.	2.4	14
30	Polyaromatic disordered carbon grains as carriers of the UV bump: Far-UV to mid-IR spectroscopy of laboratory analogs. Astronomy and Astrophysics, 2017, 607, A73.	5.1	23
31	SOLEIL shining on the solution-state structure of biomacromolecules by synchrotron X-ray footprinting at the Metrology beamline. Journal of Synchrotron Radiation, 2017, 24, 576-585.	2.4	6
32	VUV PHOTO-PROCESSING OF PAH CATIONS: QUANTITATIVE STUDY ON THE IONIZATION VERSUS FRAGMENTATION PROCESSES. Astrophysical Journal, 2016, 822, 113.	4.5	61
33	VUV spectroscopy of carbon dust analogs: contribution to interstellar extinction. Astronomy and Astrophysics, 2016, 586, A106.	5.1	18
34	Charge Transfer Dissociation of Complex Oligosaccharides: Comparison with Collision-Induced Dissociation and Extreme Ultraviolet Dissociative Photoionization. Journal of the American Society for Mass Spectrometry, 2016, 27, 1614-1619.	2.8	29
35	Online coupling of high-resolution chromatography with extreme UV photon activation tandem mass spectrometry: Application to the structural investigation of complex glycans by dissociative photoionization. Analytica Chimica Acta, 2016, 933, 1-9.	5.4	24
36	Gas-Phase Near-Edge X-Ray Absorption Fine Structure (NEXAFS) Spectroscopy of Nanoparticles, Biopolymers, and Ionic Species. , 2016, , 451-505.		4

#	Article	IF	Citations
37	Electron impact action spectroscopy of mass/charge selected macromolecular ions: Inner-shell excitation of ubiquitin protein. Applied Physics Letters, 2016, 108, .	3.3	3
38	Design and performance of an instrument for electron impact tandem mass spectrometry and action spectroscopy of mass/charge selected macromolecular ions stored in RF ion trap*. European Physical Journal D, 2016, 70, 1.	1.3	3
39	Single-Photon, Double Photodetachment of Nickel Phthalocyanine Tetrasulfonic Acid 4- Anions. Journal of Physical Chemistry Letters, 2016, 7, 2586-2590.	4.6	0
40	Probing the solution structure of Factor H using hydroxyl radical protein footprinting and cross-linking. Biochemical Journal, 2016, 473, 1805-1819.	3.7	9
41	VUV action spectroscopy of protonated leucine-enkephalin peptide in the 6-14 eV range. Journal of Chemical Physics, 2015, 143, 244311.	3.0	10
42	Photon activation of peptides in the VUV. Journal of Physics: Conference Series, 2015, 635, 012032.	0.4	2
43	Photoinduced fragmentation of gas-phase protonated leucine- enkephalin peptide in the VUV range. Journal of Physics: Conference Series, 2015, 635, 012034.	0.4	2
44	Photodissociation of protonated Leucine-Enkephalin peptide in the VUV range. Journal of Physics: Conference Series, 2015, 635, 112030.	0.4	0
45	K-Shell Excitation and Ionization of a Gas-Phase Protein: Interplay between Electronic Structure and Protein Folding. Journal of Physical Chemistry Letters, 2015, 6, 3132-3138.	4.6	21
46	Binding site of different tannins on a human salivary proline-rich protein evidenced by dissociative photoionization tandem mass spectrometry. Tetrahedron, 2015, 71, 3039-3044.	1.9	37
47	High-Energy Photon Activation Tandem Mass Spectrometry Provides Unprecedented Insights into the Structure of Highly Sulfated Oligosaccharides Extracted from Macroalgal Cell Walls. Analytical Chemistry, 2015, 87, 1042-1049.	6.5	24
48	Exploring the peptide fragmentation mechanisms under atmospheric pressure photoionization using tunable VUV synchrotron radiation. International Journal of Mass Spectrometry, 2015, 379, 80-86.	1.5	3
49	Action spectroscopy of a protonated peptide in the ultraviolet range. Physical Chemistry Chemical Physics, 2015, 17, 25725-25733.	2.8	26
50	Gas-phase VUV photoionisation and photofragmentation of the silver deuteride nanocluster [Ag₁₀D₈L<sub>6</]²⁺ (L = bis(diphenylphosphino)methane). A joint experimental and theoretical study. Physical Chemistry Chemical Physics, 2015, 17, 25772-25777.	2.8	25
51	X-ray-induced radiophotodynamic therapy (RPDT) using lanthanide micelles: Beyond depth limitations. Nano Research, 2015, 8, 2373-2379.	10.4	77
52	Using DNA Origami Nanostructures To Determine Absolute Cross Sections for UV Photon-Induced DNA Strand Breakage. Journal of Physical Chemistry Letters, 2015, 6, 4589-4593.	4.6	30
53	Contribution of synchrotron radiation to photoactivation studies of biomolecular ions in the gas phase. Mass Spectrometry Reviews, 2014, 33, 424-441.	5.4	35
54	Synthetic oligomer analysis using atmospheric pressure photoionization mass spectrometry at different photon energies. Analytica Chimica Acta, 2014, 808, 220-230.	5.4	2

#	Article	IF	Citations
55	X-ray induced fragmentation of size-selected salt cluster-ions stored in an ion trap. RSC Advances, 2014, 4, 47743-47751.	3.6	3
56	Multiple Electron Ejection from Proteins Resulting from Single-Photon Excitation in the Valence Shell. Journal of Physical Chemistry Letters, 2014, 5, 1666-1671.	4.6	2
57	VUV photofragmentation of protonated leucine-enkephalin peptide dimer below ionization energy. European Physical Journal D, 2014, 68, 1.	1.3	7
58	Energy-Dependent UV Photodissociation of Gas-Phase Adenosine Monophosphate Nucleotide Ions: The Role of a Single Solvent Molecule. Journal of Physical Chemistry Letters, 2014, 5, 1994-1999.	4.6	14
59	Deciphering the structure of isomeric oligosaccharides in a complex mixture by tandem mass spectrometry: Photon activation with vacuum ultra-violet brings unique information and enables definitive structure assignment. Analytica Chimica Acta, 2014, 807, 84-95.	5.4	32
60	Letter: Determination of Ionization Energies of a Monoterpene Series by Atmospheric Pressure Photoionization Using Tunable Vacuum Ultraviolet Synchrotron Radiation. European Journal of Mass Spectrometry, 2014, 20, 403-407.	1.0	5
61	Vacuum Ultraviolet Action Spectroscopy of Polysaccharides. Journal of the American Society for Mass Spectrometry, 2013, 24, 1271-1279.	2.8	8
62	Fold of an oleosin targeted to cellular oil bodies. Biochimica Et Biophysica Acta - Biomembranes, 2013, 1828, 1881-1888.	2.6	19
63	Titan's atmosphere simulation experiment using continuum UVâ€VUV synchrotron radiation. Journal of Geophysical Research E: Planets, 2013, 118, 778-788.	3.6	27
64	Aggregation of the Salivary Proline-Rich Protein IB5 in the Presence of the Tannin EgCG. Langmuir, 2013, 29, 1926-1937.	3.5	96
65	Valence shell direct double photodetachment in polyanions. New Journal of Physics, 2013, 15, 063024.	2.9	4
66	Photo-induced electron detachment of protein polyanions in the VUV range. Journal of Chemical Physics, 2013, 138, 064301.	3.0	17
67	VUV photochemistry simulation of planetary upper atmosphere using synchrotron radiation. Journal of Synchrotron Radiation, 2013, 20, 587-590.	2.4	8
68	Application of VUV synchrotron radiation to proteomic and analytical mass spectrometry. Journal of Physics: Conference Series, 2013, 425, 122001.	0.4	2
69	Synchrotron infrared confocal microscope: Application to infrared 3D spectral imaging. Journal of Physics: Conference Series, 2013, 425, 142002.	0.4	9
70	Nanosolvationâ€Induced Stabilization of a Protonated Peptide Dimer Isolated in the Gas Phase. Angewandte Chemie - International Edition, 2013, 52, 7286-7290.	13.8	15
71	Photodissociation and Dissociative Photoionization Mass Spectrometry of Proteins and Noncovalent Proteinâ€“Ligand Complexes. Angewandte Chemie - International Edition, 2013, 52, 8377-8381.	13.8	45
72	DUV cleaning of aluminium optics left at the atmosphere. Journal of Physics: Conference Series, 2013, 425, 122005.	0.4	1

#	Article	IF	Citations
73	Characterization of Hydrophobic Peptides in the Presence of Detergent by Photoionization Mass Spectrometry. PLoS ONE, 2013, 8, e79033.	2.5	29
74	Photochemistry simulation of planetary atmosphere using synchrotron radiation at soleil. Application to Titanâ€™s atmosphere. EAS Publications Series, 2012, 58, 199-203.	0.3	0
75	Photoionization of atomic and molecular positively charged ions. Journal of Physics: Conference Series, 2012, 399, 012002.	0.4	2
76	DISCO synchrotron-radiation circular-dichroism endstation at SOLEIL. Journal of Synchrotron Radiation, 2012, 19, 831-835.	2.4	49
77	Atmospheric pressure photoionization study of post-translational modifications: The case of palmitoylation. International Journal of Mass Spectrometry, 2012, 328-329, 23-27.	1.5	8
78	Gas-Phase Protein Inner-Shell Spectroscopy by Coupling an Ion Trap with a Soft X-ray Beamline. Journal of Physical Chemistry Letters, 2012, 3, 1191-1196.	4.6	55
79	Atmospheric pressure photoionization mass spectrometry of guanine using tunable synchrotron VUV radiation. International Journal of Mass Spectrometry, 2012, 321-322, 14-18.	1.5	4
80	Structure and Chargeâ€State Dependence of the Gasâ€Phase Ionization Energy of Proteins. Angewandte Chemie - International Edition, 2012, 51, 9552-9556.	13.8	34
81	Mid- and far-infrared absorption spectroscopy of Titanâ€™s aerosols analogues. Icarus, 2012, 221, 320-327.	2.5	63
82	Fast in vacuo photon shutter for synchrotron radiation quadrupole ion trap tandem mass spectrometry. Nuclear Instruments & Methods in Physics Research B, 2012, 279, 34-36.	1.4	13
83	Atmospheric pressure photoionization using tunable VUV synchrotron radiation. Nuclear Instruments & Methods in Physics Research B, 2012, 279, 114-117.	1.4	14
84	VUV synchrotron radiation: a new activation technique for tandem mass spectrometry. Journal of Synchrotron Radiation, 2012, 19, 174-178.	2.4	65
85	Formation and Fragmentation of Radical Peptide Anions: Insights from Vacuum Ultra Violet Spectroscopy. Journal of the American Society for Mass Spectrometry, 2012, 23, 274-281.	2.8	24
86	Photoionization of a protein isolated in vacuo. Physical Chemistry Chemical Physics, 2011, 13, 15432.	2.8	60
87	Gas phase Photo-Formation and Vacuum UV Photofragmentation Spectroscopy of Tryptophan and Tyrosine Radical-Containing Peptides. Journal of Physical Chemistry A, 2011, 115, 8933-8939.	2.5	31
88	High water solubility and fold in amphipols of proteins with large hydrophobic regions: Oleosins and caleosin from seed lipid bodies. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 706-716.	2.6	30
89	Atmospheric pressure photoionization of peptides. International Journal of Mass Spectrometry, 2011, 299, 1-4.	1.5	11
90	A differential pumping system to deliver windowless VUV photons at atmospheric pressure. Journal of Synchrotron Radiation, 2011, 18, 546-549.	2.4	22

#	Article	IF	Citations
91	Separation of peptides from detergents using ion mobility spectrometry. Rapid Communications in Mass Spectrometry, 2011, 25, 3436-3440.	1.5	9
92	Photoionization study of Kr⁺and Xe⁺ions with the combined use of a merged-beam set-up and an ion trap. Journal of Physics B: Atomic, Molecular and Optical Physics, 2011, 44, 055205.	1.5	30
93	Performances and reliability tests of AlGaN based focal plane array for deep-UV imaging. Proceedings of SPIE, 2011, , .	0.8	2
94	Gas-phase spectroscopy of a protein. Journal of Physics: Conference Series, 2010, 257, 012006.	0.4	6
95	Performances of AlGaN-based focal plane arrays from 10nm to 200nm. Proceedings of SPIE, 2010, , .	0.8	7
96	Ability of a salivary intrinsically unstructured protein to bind different tannin targets revealed by mass spectrometry. Analytical and Bioanalytical Chemistry, 2010, 398, 815-822.	3.7	56
97	Structural study of acetogenins by tandem mass spectrometry under high and low collision energy. Rapid Communications in Mass Spectrometry, 2010, 24, 3602-3608.	1.5	27
98	Synchrotron UV Fluorescence Microscopy Uncovers New Probes in Cells and Tissues. Microscopy and Microanalysis, 2010, 16, 507-514.	0.4	78
99	Characterization, stoichiometry, and stability of salivary proteinâ€“tannin complexes by ESI-MS and ESI-MS/MS. Analytical and Bioanalytical Chemistry, 2009, 395, 2535-2545.	3.7	49
100	DISCO: a low-energy multipurpose beamline at synchrotron SOLEIL. Journal of Synchrotron Radiation, 2009, 16, 835-841.	2.4	129
101	Electronic states of neutral and ionized tetrahydrofuran studied by VUV spectroscopy and ab initio calculations. European Physical Journal D, 2009, 51, 97-108.	1.3	50
102	Chemical Characterization of Titanâ€™s Tholins: Solubility, Morphology and Molecular Structure Revisited. Journal of Physical Chemistry A, 2009, 113, 11195-11203.	2.5	81
103	Electronic excitation of gaseous acetic acid studied by K-shell electron energy loss spectroscopy and ab initio calculations. International Journal of Mass Spectrometry, 2008, 277, 70-78.	1.5	7
104	Electronic State Spectroscopy of c-C5F8 Explored by Photoabsorption, Electron Impact, Photoelectron Spectroscopies and Ab Initio Calculations. Journal of Physical Chemistry A, 2008, 112, 2782-2793.	2.5	7
105	Photoionization Cross Section of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mi>Xe</mml:mi><mml:mo>+</mml:mo></mml:msup></mml:math>Ion in the Pure<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mn>5</mml:mn><mml:msup><mml:mi>p</mml:mi><mml:mn>5</mml:mn></mml:msup></mml:math><mml:ma xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mmultiscripts><mml:mi>P</mml:mi><mml:mrow><mml:mn>3</mml:mn><mml:mo>/</mml:mo><mml:.	7.8	29
106	Atmospheric Pressure Photoionization Mass Spectrometry of Oligodeoxyribonucleotides. European Journal of Mass Spectrometry, 2008, 14, 71-80.	1.0	10
107	Perfluorocyclobutane electronic state spectroscopy by high-resolution vacuum ultraviolet photoabsorption, electron impact,Helphotoelectron spectroscopy, andab initiocalculations. Physical Review A, 2007, 76, .	2.5	5
108	C1sand N1score excitation of aniline: Experiment by electron impact andab initiocalculations. Physical Review A, 2007, 75, .	2.5	10

#	Article	IF	Citations
109	Atmospheric pressure photoionization mass spectrometry of nucleic bases, ribonucleosides and ribonucleotides. International Journal of Mass Spectrometry, 2007, 264, 1-9.	1.5	33
110	Study of a Bisquaternary Ammonium Salt by Atmospheric Pressure Photoionization Mass Spectrometry. European Journal of Mass Spectrometry, 2006, 12, 189-197.	1.0	23
111	Acetic acid electronic state spectroscopy by high-resolution vacuum ultraviolet photo-absorption, electron impact, He(I) photoelectron spectroscopy and ab initio calculations. Chemical Physics, 2006, 324, 339-349.	1.9	24
112	Electronic structure of hexafluorobenzene by high-resolution vacuum ultraviolet photo-absorption and He(I) photoelectron spectroscopy. Chemical Physics, 2006, 328, 183-189.	1.9	16
113	Fragmentation induced in atmospheric pressure photoionization of peptides. Journal of Mass Spectrometry, 2006, 41, 1554-1560.	1.6	30
114	Ab initio and experimental study of the K-shell spectra of 2,5-dihydrofuran. Chemical Physics, 2005, 310, 67-75.	1.9	6
115	Water VUV electronic state spectroscopy by synchrotron radiation. Chemical Physics Letters, 2005, 416, 152-159.	2.6	181
116	Elastic scattering of electrons from tetrahydrofuran molecule. European Physical Journal D, 2005, 35, 411-416.	1.3	56
117	$Ab~initio$ and experimental study of the K-shell spectra of s-triazine. European Physical Journal D, 2005, 35, 239-248.	1.3	7
118	On the valence shell electronic spectroscopy of 2-vinyl furan. Journal of Chemical Physics, 2004, 120, 10972-10982.	3.0	4
119	An experimental study of SF5CF3 by electron energy loss spectroscopy, VUV photo-absorption and photoelectron spectroscopy. International Journal of Mass Spectrometry, 2004, 233, 335-341.	1.5	20
120	The electronic states of isoxazole studied by VUV absorption, electron energy-loss spectroscopies and ab initio multi-reference configuration interaction calculations. Chemical Physics, 2004, 297, 289-306.	1.9	33
121	Molecular structure and vibrational analysis of 2-vinyl furan. Chemical Physics Letters, 2003, 379, 406-411.	2.6	2
122	Thiazyl chloride: an experimental and theoretical study of the valence shell HeI photoelectron spectrum. Chemical Physics, 2003, 288, 95-104.	1.9	2
123	Electron and photon induced processes in SF5CF3. Radiation Physics and Chemistry, 2003, 68, 193-197.	2.8	10
124	The electronic states of 2-furanmethanol (furfuryl alcohol) studied by photon absorption and electron impact spectroscopies. Journal of Chemical Physics, 2003, 119, 7282-7288.	3.0	8
125	Core shell excitation of furan at the O1s and C1s edges:â€,An experimental and ab initio study. Journal of Chemical Physics, 2003, 119, 8946-8955.	3.0	24
126	2-methyl furan: An experimental study of the excited electronic levels by electron energy loss spectroscopy, vacuum ultraviolet photoabsorption, and photoelectron spectroscopy. Journal of Chemical Physics, 2003, 119, 3670-3680.	3.0	25

#	Article	IF	Citations
127	Electronic excitation and optical cross sections of methylamine and ethylamine in the UVâ€“VUV spectral region. Journal of Chemical Physics, 2002, 116, 9261-9268.	3.0	36
128	Lowest energy triplet states of furan, studied by high resolution electron energy loss spectroscopy. International Journal of Mass Spectrometry, 2001, 205, 163-169.	1.5	20
129	Spectroscopic study of the lowest energy triplet states of 2-methyl furan. Chemical Physics Letters, 2001, 348, 34-38.	2.6	6
130	Electronic excitation and oscillator strength of ethyl bromide by vacuum ultraviolet photoabsorption and electron energy loss spectroscopy. Journal of Chemical Physics, 2000, 112, 6285-6292.	3.0	9
131	Electronic excitation and oscillator strength of ethyl iodide by VUV photoabsorption and electron energy loss spectroscopy. Journal of Chemical Physics, 1999, 110, 10307-10315.	3.0	8