Andrei Tokmakoff

List of Publications by Year
in descending order

133 papers	8,516 citations	34016 52 h-index	49773 87 g-index
139 all docs	139 docs citations	139 times ranked	5495 citing authors

#	Article	IF	Citations
1	Characterization of Acetonitrile Isotopologues as Vibrational Probes of Electrolytes. Journal of Physical Chemistry B, 2022, 126, 278-291.	1.2	15
2	Resonance conditions, detection quality, and single-molecule sensitivity in fluorescence-encoded infrared vibrational spectroscopy. Journal of Chemical Physics, 2022, 156, 174202.	1.2	8
3	Exchange-Mediated Transport in Battery Electrolytes: Ultrafast or Ultraslow?. Journal of the American Chemical Society, 2022, 144, 8591-8604.	6.6	18
4	From Networked to Isolated: Observing Water Hydrogen Bonds in Concentrated Electrolytes with Two-Dimensional Infrared Spectroscopy. Journal of Physical Chemistry B, 2022, 126, 5305-5319.	1.2	9
5	Investigation into the mechanism and dynamics of DNA association and dissociation utilizing kinetic Monte Carlo simulations. Journal of Chemical Physics, 2021, 154, 045101.	1.2	9
6	Fluorescence-Encoded Infrared Vibrational Spectroscopy with Single-Molecule Sensitivity. Journal of the American Chemical Society, 2021, 143, 3060-3064.	6.6	25
7	Water-in-Salt LiTFSI Aqueous Electrolytes. 1. Liquid Structure from Combined Molecular Dynamics Simulation and Experimental Studies. Journal of Physical Chemistry B, 2021, 125, 4501-4513.	1.2	52
8	Computational IR Spectroscopy of Insulin Dimer Structure and Conformational Heterogeneity. Journal of Physical Chemistry B, 2021, 125, 4620-4633.	1.2	14
9	Structural Characterization of Protonated Water Clusters Confined in HZSM-5 Zeolites. Journal of the American Chemical Society, 2021, 143, 10203-10213.	6.6	35
10	Advanced Materials for Energy-Water Systems: The Central Role of Water/Solid Interfaces in Adsorption, Reactivity, and Transport. Chemical Reviews, 2021, 121, 9450-9501.	23.0	43
11	Water or Anion? Uncovering the Zn²⁺ Solvation Environment in Mixed Zn(TFSI)₂ and LiTFSI Water-in-Salt Electrolytes. ACS Energy Letters, 2021, 6, 3458-3463.	8.8	45
12	Crossover from hydrogen to chemical bonding. Science, 2021, 371, 160-164.	6.0	123
13	Structural Ensemble of the Insulin Monomer. Biochemistry, 2021, 60, 3125-3136.	1.2	5
14	Determining Sequence-Dependent DNA Oligonucleotide Hybridization and Dehybridization Mechanisms Using Coarse-Grained Molecular Simulation, Markov State Models, and Infrared Spectroscopy. Journal of the American Chemical Society, 2021, 143, 17395-17411.	6.6	30
15	Lineshape Distortions in Internal Reflection Two-Dimensional Infrared Spectroscopy: Tuning across the Critical Angle. Journal of Physical Chemistry Letters, 2021, 12, 11843-11849.	2.1	4
16	5-Carboxylcytosine and Cytosine Protonation Distinctly Alter the Stability and Dehybridization Dynamics of the DNA Duplex. Journal of Physical Chemistry B, 2020, 124, 627-640.	1.2	11
17	Temperature-Jump 2D IR Spectroscopy with Intensity-Modulated CW Optical Heating. Journal of Physical Chemistry B, 2020, 124, 8665-8677.	1.2	11
18	Vibrational Probe of Aqueous Electrolytes: The Field Is Not Enough. Journal of Physical Chemistry B, 2020, 124, 7013-7026.	1.2	13

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19	DNA minor-groove binder Hoechst 33258 destabilizes base-pairing adjacent to its binding site. Communications Biology, 2020, 3, 525.	2.0	25
20	Decoding the 2D IR spectrum of the aqueous proton with high-level VSCF/VCI calculations. Journal of Chemical Physics, 2020, 153, 124506.	1.2	20
21	Revealing the Dynamical Role of Co-solvents in the Coupled Folding and Dimerization of Insulin. Journal of Physical Chemistry Letters, 2020, 11, 4353-4358.	2.1	5
22	Insulin Dissociates by Diverse Mechanisms of Coupled Unfolding and Unbinding. Journal of Physical Chemistry B, 2020, 124, 5571-5587.	1.2	35
23	Vibrational Spectroscopic Map, Vibrational Spectroscopy, and Intermolecular Interaction. Chemical Reviews, 2020, 120, 7152-7218.	23.0	205
24	Signatures of Ion Pairing and Aggregation in the Vibrational Spectroscopy of Super-Concentrated Aqueous Lithium Bistriflimide Solutions. Journal of Physical Chemistry C, 2020, 124, 3470-3481.	1.5	44
25	Oxidized Derivatives of 5-Methylcytosine Alter the Stability and Dehybridization Dynamics of Duplex DNA. Journal of Physical Chemistry B, 2020, 124, 1160-1174.	1.2	16
26	Dynamic and Programmable Cellular-Scale Granules Enable Tissue-like Materials. Matter, 2020, 2, 948-964.	5.0	30
27	High-Level VSCF/VCI Calculations Decode the Vibrational Spectrum of the Aqueous Proton. Journal of Physical Chemistry B, 2019, 123, 7214-7224.	1.2	23
28	Entropic barriers in the kinetics of aqueous proton transfer. Journal of Chemical Physics, 2019, 151, 034501.	1.2	13
29	Fluorescence-Encoded Infrared Spectroscopy: Ultrafast Vibrational Spectroscopy on Small Ensembles of Molecules in Solution. Journal of Physical Chemistry Letters, 2019, 10, 1967-1972.	2.1	19
30	Length-Dependent Melting Kinetics of Short DNA Oligonucleotides Using Temperature-Jump IR Spectroscopy. Journal of Physical Chemistry B, 2019, 123, 756-767.	1.2	30
31	Direct Observation of Ion Pairing in Aqueous Nitric Acid Using 2D Infrared Spectroscopy. Journal of Physical Chemistry B, 2019, 123, 225-238.	1.2	12
32	A lattice model for the interpretation of oligonucleotide hybridization experiments. Journal of Chemical Physics, 2019, 150, 185104.	1.2	6
33	Direct Observation of Activated Kinetics and Downhill Dynamics in DNA Dehybridization. Journal of Physical Chemistry B, 2018, 122, 3088-3100.	1.2	40
34	Picosecond Proton Transfer Kinetics in Water Revealed with Ultrafast IR Spectroscopy. Journal of Physical Chemistry B, 2018, 122, 2792-2802.	1.2	44
35	Fourier Transform Fluorescence-Encoded Infrared Spectroscopy. Journal of Physical Chemistry A, 2018, 122, 554-562.	1.1	16
36	Broadband 2D IR spectroscopy reveals dominant asymmetric H5O2+ proton hydration structures in acid solutions. Nature Chemistry, 2018, 10, 932-937.	6.6	105

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37	Single-stage MHz mid-IR OPA using LiGaS₂and a fiber laser pump source. Optics Letters, 2018, 43, 1363.	1.7	34
38	Refinement of Peptide Conformational Ensembles by 2D IR Spectroscopy: Application to Alaâ€'Alaâ€'Ala. Biophysical Journal, 2018, 114, 2820-2832.	0.2	16
39	Ultrafast Fluctuations of High Amplitude Electric Fields in Lipid Membranes. Journal of the American Chemical Society, 2017, 139, 4743-4752.	6.6	30
40	IR spectral assignments for the hydrated excess proton in liquid water. Journal of Chemical Physics, 2017, 146, 154507.	1.2	61
41	Time-resolved measurements of an ion channel conformational change driven by a membrane phase transition. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 10840-10845.	3.3	21
42	Delocalization and stretch-bend mixing of the HOH bend in liquid water. Journal of Chemical Physics, 2017, 147, 084503.	1.2	51
43	The dynamics of peptide-water interactions in dialanine: An ultrafast amide I 2D IR and computational spectroscopy study. Journal of Chemical Physics, 2017, 147, 085101.	1.2	22
44	Crystallization of Enantiomerically Pure Proteins from Quasiâ€Racemic Mixtures: Structure Determination by Xâ€Ray Diffraction of Isotopeâ€Labeled Ester Insulin and Human Insulin. ChemBioChem, 2016, 17, 421-425.	1.3	18
45	Efficient Total Chemical Synthesis of ¹³C=¹⁸O Isotopomers of Human Insulin for Isotopeâ€Edited FTIR. ChemBioChem, 2016, 17, 415-420.	1.3	19
46	Molecular modeling and assignment of IR spectra of the hydrated excess proton in isotopically dilute water. Journal of Chemical Physics, 2016, 145, 154504.	1.2	19
47	Anharmonic exciton dynamics and energy dissipation in liquid water from two-dimensional infrared spectroscopy. Journal of Chemical Physics, 2016, 145, 094501.	1.2	51
48	Computational Amide I 2D IR Spectroscopy as a Probe of Protein Structure and Dynamics. Annual Review of Physical Chemistry, 2016, 67, 359-386.	4.8	93
49	Differences in the Vibrational Dynamics of H₂O and D₂O: Observation of Symmetric and Antisymmetric Stretching Vibrations in Heavy Water. Journal of Physical Chemistry Letters, 2016, 7, 1769-1774.	2.1	68
50	Sequence-Dependent Mechanism of DNA Oligonucleotide Dehybridization Resolved through Infrared Spectroscopy. Journal of the American Chemical Society, 2016, 138, 11792-11801.	6.6	66
51	Interplay of Ionâ€"Water and Waterâ€"Water Interactions within the Hydration Shells of Nitrate and Carbonate Directly Probed with 2D IR Spectroscopy. Journal of the American Chemical Society, 2016, 138, 9634-9645.	6.6	67
52	Refining Disordered Peptide Ensembles with Computational Amide I Spectroscopy: Application to Elastin-Like Peptides. Journal of Physical Chemistry B, 2016, 120, 11395-11404.	1.2	19
53	Two-Photon-Excited Fluorescence-Encoded Infrared Spectroscopy. Journal of Physical Chemistry A, 2016, 120, 9178-9187.	1.1	17
54	Role of Presolvation and Anharmonicity in Aqueous Phase Hydrated Proton Solvation and Transport. Journal of Physical Chemistry B, 2016, 120, 1793-1804.	1.2	68

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55	Studying Proteinâ€“Protein Binding through T-Jump Induced Dissociation: Transient 2D IR Spectroscopy of Insulin Dimer. Journal of Physical Chemistry B, 2016, 120, 5134-5145.	1.2	42
56	Weakened N3 Hydrogen Bonding by 5-Formylcytosine and 5-Carboxylcytosine Reduces Their Base-Pairing Stability. ACS Chemical Biology, 2016, 11, 470-477.	1.6	56
57	Isotope-enriched protein standards for computational amide I spectroscopy. Journal of Chemical Physics, 2015, 142, 125104.	1.2	17
58	Communication: Quantitative multi-site frequency maps for amide I vibrational spectroscopy. Journal of Chemical Physics, 2015, 143, 061102.	1.2	27
59	Vibrational dynamics of aqueous hydroxide solutions probed using broadband 2DIR spectroscopy. Journal of Chemical Physics, 2015, 143, 194501.	1.2	26
60	Distinguishing gramicidin D conformers through two-dimensional infrared spectroscopy of vibrational excitons. Journal of Chemical Physics, 2015, 142, 212424.	1.2	10
61	Two-dimensional IR spectroscopy of the anti-HIV agent KP1212 reveals protonated and neutral tautomers that influence pH-dependent mutagenicity. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 3229-3234.	3.3	16
62	Structural Disorder of Folded Proteins: Isotope-Edited 2D IR Spectroscopy and Markov State Modeling. Biophysical Journal, 2015, 108, 1747-1757.	0.2	23
63	Visualizing KcsA Conformational Changes upon Ion Binding by Infrared Spectroscopy and Atomistic Modeling. Journal of Physical Chemistry B, 2015, 119, 5824-5831.	1.2	25
64	Ultrafast 2D IR spectroscopy of the excess proton in liquid water. Science, 2015, 350, 78-82.	6.0	264
65	Preface: Special Topic on Biological Water. Journal of Chemical Physics, 2014, 141, 22D101.	1.2	24
66	Ultrafast 2D IR microscopy. Optics Express, 2014, 22, 18724.	1.7	69
67	Collective vibrations of water-solvated hydroxide ions investigated with broadband 2DIR spectroscopy. Journal of Chemical Physics, 2014, 140, 204508.	1.2	53
68	A Molecular Interpretation of 2D IR Protein Folding Experiments with Markov State Models. Biophysical Journal, 2014, 106, 1359-1370.	0.2	48
69	Direct Observation of Multiple Tautomers of Oxythiamine and their Recognition by the Thiamine Pyrophosphate Riboswitch. ACS Chemical Biology, 2014, 9, 227-236.	1.6	27
70	Direct observation of intermolecular interactions mediated by hydrogen bonding. Journal of Chemical Physics, 2014, 141, 034502.	1.2	50
71	Local and Collective Reaction Coordinates in the Transport of the Aqueous Hydroxide Ion. Journal of Physical Chemistry B, 2014, 118, 8062-8069.	1.2	12
72	Tautomerism provides a molecular explanation for the mutagenic properties of the anti-HIV nucleoside 5-aza-5,6-dihydro-2'-deoxycytidine. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E3252-E3259.	3.3	43

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73	Robust excitons inhabit soft supramolecular nanotubes. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E3367-75.	3.3	100
74	Amide I Two-Dimensional Infrared Spectroscopy: Methods for Visualizing the Vibrational Structure of Large Proteins. Journal of Physical Chemistry A, 2013, 117, 5955-5961.	1.1	29
75	Water vibrations have strongly mixed intra- and intermolecular character. Nature Chemistry, 2013, 5, 935-940.	6.6	236
76	Electrostatic frequency shifts in amide I vibrational spectra: Direct parameterization against experiment. Journal of Chemical Physics, 2013, 138, 134116.	1.2	87
77	Experimental Evidence of Fermi Resonances in Isotopically Dilute Water from Ultrafast Broadband IR Spectroscopy. Journal of Physical Chemistry B, 2013, 117, 15319-15327.	1.2	66
78	Folding of a heterogeneous Î²-hairpin peptide from temperature-jump 2D IR spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 2828-2833.	3.3	71
79	Direct observation of ground-state lactamâ€“lactim tautomerization using temperature-jump transient 2D IR spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 9243-9248.	3.3	50
80	Transient two-dimensional spectroscopy with linear absorption corrections applied to temperature-jump two-dimensional infrared. Journal of the Optical Society of America B: Optical Physics, 2012, 29, 118.	0.9	26
81	A phenomenological approach to modeling chemical dynamics in nonlinear and two-dimensional spectroscopy. Journal of Chemical Physics, 2012, 136, 134507.	1.2	5
82	Identifying Residual Structure in Intrinsically Disordered Systems: A 2D IR Spectroscopic Study of the GVGXPGVG Peptide. Journal of the American Chemical Society, 2012, 134, 5032-5035.	6.6	48
83	Coherent two-dimensional infrared spectroscopy: Quantitative analysis of protein secondary structure in solution. Analyst, The, 2012, 137, 1793.	1.7	65
84	Identification of Lactamâ€“Lactim Tautomers of Aromatic Heterocycles in Aqueous Solution Using 2D IR Spectroscopy. Journal of Physical Chemistry Letters, 2012, 3, 3302-3306.	2.1	34
85	Proton Transfer in Concentrated Aqueous Hydroxide Visualized Using Ultrafast Infrared Spectroscopy. Journal of Physical Chemistry A, 2011, 115, 3957-3972.	1.1	45
86	Collective Hydrogen Bond Reorganization in Water Studied with Temperature-Dependent Ultrafast Infrared Spectroscopy. Journal of Physical Chemistry B, 2011, 115, 5604-5616.	1.2	92
87	Anharmonic Vibrational Modes of Nucleic Acid Bases Revealed by 2D IR Spectroscopy. Journal of the American Chemical Society, 2011, 133, 15650-15660.	6.6	108
88	A fast-scanning Fourier transform 2D IR interferometer. Optics Communications, 2011, 284, 1062-1066.	1.0	21
89	Vibrational excitons in ionophores: experimental probes for quantum coherence-assisted ion transport and selectivity in ion channels. New Journal of Physics, 2011, 13, 113030.	1.2	32
90	Solvent and conformation dependence of amide I vibrations in peptides and proteins containing proline. Journal of Chemical Physics, 2011, 135, 234507.	1.2	58

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91	Melting of a Î²-Hairpin Peptide Using Isotope-Edited 2D IR Spectroscopy and Simulations. Journal of Physical Chemistry B, 2010, 114, 10913-10924.	1.2	97
92	Hydrogen Bond Rearrangements in Water Probed with Temperature-Dependent 2D IR. Journal of Physical Chemistry Letters, 2010, 1, 1068-1072.	2.1	89
93	Source for ultrafast continuum infrared and terahertz radiation. Optics Letters, 2010, 35, 1962.	1.7	158
94	Insulin dimer dissociation and unfolding revealed by amide I two-dimensional infrared spectroscopy. Physical Chemistry Chemical Physics, 2010, 12, 3579-3588.	1.3	71
95	Observation of a Zundel-like transition state during proton transfer in aqueous hydroxide solutions. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 15154-15159.	3.3	111
96	Structural Rearrangements in Water Viewed Through Two-Dimensional Infrared Spectroscopy. Accounts of Chemical Research, 2009, 42, 1239-1249.	7.6	177
97	Amide Iâ€²â^'IIâ€² 2D IR Spectroscopy Provides Enhanced Protein Secondary Structural Sensitivity. Journal of the American Chemical Society, 2009, 131, 3385-3391.	6.6	141
98	Heterodyne-Detected Dispersed Vibrational Echo Spectroscopy. Journal of Physical Chemistry A, 2009, 113, 14060-14066.	1.1	35
99	Temperatureâ€dependent downhill unfolding of ubiquitin. II. Modeling the free energy surface. Proteins: Structure, Function and Bioinformatics, 2008, 72, 488-497.	1.5	18
100	Temperatureâ€dependent downhill unfolding of ubiquitin. I. Nanosecondâ€toâ€millisecond resolved nonlinear infrared spectroscopy. Proteins: Structure, Function and Bioinformatics, 2008, 72, 474-487.	1.5	32
101	Amide I Two-Dimensional Infrared Spectroscopy of Proteins. Accounts of Chemical Research, 2008, 41, 432-441.	7.6	427
102	Ultrafast Nâ^'H Vibrational Dynamics of Cyclic Doubly Hydrogen-Bonded Homo- and Heterodimers. Journal of Physical Chemistry B, 2008, 112, 13167-13171.	1.2	36
103	Transient 2D IR spectroscopy of ubiquitin unfolding dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 14237-14242.	3.3	164
104	Transient two-dimensional IR spectrometer for probing nanosecond temperature-jump kinetics. Review of Scientific Instruments, 2007, 78, 063101.	0.6	66
105	Shining Light on the Rapidly Evolving Structure of Water. Science, 2007, 317, 54-55.	6.0	57
106	Two-dimensional Fourier transform spectroscopy in the pump-probe geometry. Optics Letters, 2007, 32, 2966.	1.7	191
107	Single-shot two-dimensional infrared spectroscopy. Optics Express, 2007, 15, 233.	1.7	33
108	Probing Local Structural Events in Î²â€Hairpin Unfolding with Transient Nonlinear Infrared Spectroscopy. Angewandte Chemie - International Edition, 2007, 46, 7984-7987.	7.2	53

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109	Infrared spectroscopy of tritiated water. Chemical Physics Letters, 2007, 449, 130-134.	1.2	7
110	Variation of the transition dipole moment across the OH stretching band of water. Chemical Physics, 2007, 341, 218-229.	0.9	70
111	Visualization and Characterization of the Infrared Active Amide I Vibrations of Proteins. Journal of Physical Chemistry B, 2006, 110, 2888-2898.	1.2	49
112	Water Penetration into Protein Secondary Structure Revealed by Hydrogenâ^'Deuterium Exchange Two-Dimensional Infrared Spectroscopy. Journal of the American Chemical Society, 2006, 128, 16520-16521.	6.6	52
113	Characterization of spectral diffusion from two-dimensional line shapes. Journal of Chemical Physics, 2006, 125, 084502.	1.2	270
114	Spectral Signatures of Heterogeneous Protein Ensembles Revealed by MD Simulations of 2DIR Spectra. Biophysical Journal, 2006, 91, 2636-2646.	0.2	91
115	Multidimensional infrared spectroscopy of water. I. Vibrational dynamics in two-dimensional IR line shapes. Journal of Chemical Physics, 2006, 125, 194521.	1.2	180
116	Multidimensional infrared spectroscopy of water. II. Hydrogen bond switching dynamics. Journal of Chemical Physics, 2006, 125, 194522.	1.2	175
117	The Anharmonic Vibrational Potential and Relaxation Pathways of the Amide I and II Modes ofN-Methylacetamideâ€. Journal of Physical Chemistry B, 2006, 110, 18973-18980.	1.2	123
118	Single-shot two-dimensional spectrometer. Optics Letters, 2006, 31, 113.	1.7	15
119	From The Cover: Conformational changes during the nanosecond-to-millisecond unfolding of ubiquitin. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 612-617.	3.3	150
120	Polarizable molecules in the vibrational spectroscopy of water. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 11611-11616.	3.3	77
121	Residual Native Structure in a Thermally Denatured Î²-Hairpin. Journal of Physical Chemistry B, 2005, 109, 17025-17027.	1.2	60
122	Electric Field Fluctuations Drive Vibrational Dephasing in Water. Journal of Physical Chemistry A, 2005, 109, 9424-9436.	1.1	150
123	Upconversion multichannel infrared spectrometer. Optics Letters, 2005, 30, 1818.	1.7	32
124	Local hydrogen bonding dynamics and collective reorganization in water: Ultrafast infrared spectroscopy of HOD/D2O. Journal of Chemical Physics, 2005, 122, 054506.	1.2	295
125	Nonlinear Infrared Spectroscopy of Protein Conformational Change during Thermal Unfolding. Journal of Physical Chemistry B, 2004, 108, 15332-15342.	1.2	83
126	Two-Dimensional Infrared Spectroscopy of Antiparallel Î²-Sheet Secondary Structure. Journal of the American Chemical Society, 2004, 126, 7981-7990.	6.6	267

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127	Signatures of Î²-sheet secondary structures in linear and two-dimensional infrared spectroscopy. Journal of Chemical Physics, 2004, 120, 8201-8215.	1.2	139
128	Polarization-selective femtosecond Raman spectroscopy of low-frequency motions in hydrated protein films. Chemical Physics Letters, 2003, 376, 20-25.	1.2	46
129	Information from two-dimensional fifth-order Raman spectroscopy: Anharmonicity, nonlinearity, mode coupling, and molecular structure. AIP Conference Proceedings, 2000, , .	0.3	0
130	Two-Dimensional Line Shapes Derived from Coherent Third-Order Nonlinear Spectroscopy. Journal of Physical Chemistry A, 2000, 104, 4247-4255.	1.1	134
131	Structural information from two-dimensional fifth-order Raman spectroscopy. Journal of Chemical Physics, 1999, 111, 492-503.	1.2	73
132	Two-dimensional line-shape analysis of photon-echo signal. Chemical Physics Letters, 1999, 314, 488-495.	1.2	56
133	Intrinsic optical heterodyne detection of a two-dimensional fifth order Raman response. Chemical Physics Letters, 1997, 272, 48-54.	1.2	58