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	Amide I Two-Dimensional Infrared Spectroscopy of Proteins. Accounts of Chemical Research, 2008, 41, 432-441.	7.6	427
2	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
3	Characterization of spectral diffusion from two-dimensional line shapes. Journal of Chemical Physics, 2006, 125, 084502.	1.2	270
4	Two-Dimensional Infrared Spectroscopy of Antiparallel Î²-Sheet Secondary Structure. Journal of the American Chemical Society, 2004, 126, 7981-7990.	6.6	267
5	Ultrafast 2D IR spectroscopy of the excess proton in liquid water. Science, 2015, 350, 78-82.	6.0	264
6	Water vibrations have strongly mixed intra- and intermolecular character. Nature Chemistry, 2013, 5, 935-940.	6.6	236
7	Vibrational Spectroscopic Map, Vibrational Spectroscopy, and Intermolecular Interaction. Chemical Reviews, 2020, 120, 7152-7218.	23.0	205
8	Two-dimensional Fourier transform spectroscopy in the pump-probe geometry. Optics Letters, 2007, 32, 2966.	1.7	191
9	Multidimensional infrared spectroscopy of water. I. Vibrational dynamics in two-dimensional IR line shapes. Journal of Chemical Physics, 2006, 125, 194521.	1.2	180
10	Structural Rearrangements in Water Viewed Through Two-Dimensional Infrared Spectroscopy. Accounts of Chemical Research, 2009, 42, 1239-1249.	7.6	177
11	Multidimensional infrared spectroscopy of water. II. Hydrogen bond switching dynamics. Journal of Chemical Physics, 2006, 125, 194522.	1.2	175
12	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
13	Source for ultrafast continuum infrared and terahertz radiation. Optics Letters, 2010, 35, 1962.	1.7	158
14	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
15	Electric Field Fluctuations Drive Vibrational Dephasing in Water. Journal of Physical Chemistry A, 2005, 109, 9424-9436.	1.1	150
16	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
17	Signatures of Î²-sheet secondary structures in linear and two-dimensional infrared spectroscopy. Journal of Chemical Physics, 2004, 120, 8201-8215.	1.2	139
18	Two-Dimensional Line Shapes Derived from Coherent Third-Order Nonlinear Spectroscopy. Journal of Physical Chemistry A, 2000, 104, 4247-4255.	1.1	134

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19	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
20	Crossover from hydrogen to chemical bonding. Science, 2021, 371, 160-164.	6.0	123
21	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
22	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
23	Broadband 2D IR spectroscopy reveals dominant asymmetric H5O2+ proton hydration structures in acid solutions. Nature Chemistry, 2018, 10, 932-937.	6.6	105
24	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
25	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
26	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
27	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
28	Spectral Signatures of Heterogeneous Protein Ensembles Revealed by MD Simulations of 2DIR Spectra. Biophysical Journal, 2006, 91, 2636-2646.	0.2	91
29	Hydrogen Bond Rearrangements in Water Probed with Temperature-Dependent 2D IR. Journal of Physical Chemistry Letters, 2010, 1, 1068-1072.	2.1	89
30	Electrostatic frequency shifts in amide I vibrational spectra: Direct parameterization against experiment. Journal of Chemical Physics, 2013, 138, 134116.	1.2	87
31	Nonlinear Infrared Spectroscopy of Protein Conformational Change during Thermal Unfolding. Journal of Physical Chemistry B, 2004, 108, 15332-15342.	1.2	83
32	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
33	Structural information from two-dimensional fifth-order Raman spectroscopy. Journal of Chemical Physics, 1999, 111, 492-503.	1.2	73
34	Insulin dimer dissociation and unfolding revealed by amide I two-dimensional infrared spectroscopy. Physical Chemistry Chemical Physics, 2010, 12, 3579-3588.	1.3	71
35	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
36	Variation of the transition dipole moment across the OH stretching band of water. Chemical Physics, 2007, 341, 218-229.	0.9	70

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37	Ultrafast 2D IR microscopy. Optics Express, 2014, 22, 18724.	1.7	69
38	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
39	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
40	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
41	Transient two-dimensional IR spectrometer for probing nanosecond temperature-jump kinetics. Review of Scientific Instruments, 2007, 78, 063101.	0.6	66
42	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
43	Sequence-Dependent Mechanism of DNA Oligonucleotide Dehybridization Resolved through Infrared Spectroscopy. Journal of the American Chemical Society, 2016, 138, 11792-11801.	6.6	66
44	Coherent two-dimensional infrared spectroscopy: Quantitative analysis of protein secondary structure in solution. Analyst, The, 2012, 137, 1793.	1.7	65
45	IR spectral assignments for the hydrated excess proton in liquid water. Journal of Chemical Physics, 2017, 146, 154507.	1.2	61
46	Residual Native Structure in a Thermally Denatured Î²-Hairpin. Journal of Physical Chemistry B, 2005, 109, 17025-17027.	1.2	60
47	Intrinsic optical heterodyne detection of a two-dimensional fifth order Raman response. Chemical Physics Letters, 1997, 272, 48-54.	1.2	58
48	Solvent and conformation dependence of amide I vibrations in peptides and proteins containing proline. Journal of Chemical Physics, 2011, 135, 234507.	1.2	58
49	Shining Light on the Rapidly Evolving Structure of Water. Science, 2007, 317, 54-55.	6.0	57
50	Two-dimensional line-shape analysis of photon-echo signal. Chemical Physics Letters, 1999, 314, 488-495.	1.2	56
51	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
52	Probing Local Structural Events in Î²â€Hairpin Unfolding with Transient Nonlinear Infrared Spectroscopy. Angewandte Chemie - International Edition, 2007, 46, 7984-7987.	7.2	53
53	Collective vibrations of water-solvated hydroxide ions investigated with broadband 2DIR spectroscopy. Journal of Chemical Physics, 2014, 140, 204508.	1.2	53
54	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

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55	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
56	Anharmonic exciton dynamics and energy dissipation in liquid water from two-dimensional infrared spectroscopy. Journal of Chemical Physics, 2016, 145, 094501.	1.2	51
57	Delocalization and stretch-bend mixing of the HOH bend in liquid water. Journal of Chemical Physics, 2017, 147, 084503.	1.2	51
58	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
59	Direct observation of intermolecular interactions mediated by hydrogen bonding. Journal of Chemical Physics, 2014, 141, 034502.	1.2	50
60	Visualization and Characterization of the Infrared Active Amide I Vibrations of Proteins. Journal of Physical Chemistry B, 2006, 110, 2888-2898.	1.2	49
61	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
62	A Molecular Interpretation of 2D IR Protein Folding Experiments with Markov State Models. Biophysical Journal, 2014, 106, 1359-1370.	0.2	48
63	Polarization-selective femtosecond Raman spectroscopy of low-frequency motions in hydrated protein films. Chemical Physics Letters, 2003, 376, 20-25.	1.2	46
64	Proton Transfer in Concentrated Aqueous Hydroxide Visualized Using Ultrafast Infrared Spectroscopy. Journal of Physical Chemistry A, 2011, 115, 3957-3972.	1.1	45
65	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
66	Picosecond Proton Transfer Kinetics in Water Revealed with Ultrafast IR Spectroscopy. Journal of Physical Chemistry B, 2018, 122, 2792-2802.	1.2	44
67	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
68	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
69	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
70	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
71	Direct Observation of Activated Kinetics and Downhill Dynamics in DNA Dehybridization. Journal of Physical Chemistry B, 2018, 122, 3088-3100.	1.2	40
72	Ultrafast Nâˆ’H Vibrational Dynamics of Cyclic Doubly Hydrogen-Bonded Homo- and Heterodimers. Journal of Physical Chemistry B, 2008, 112, 13167-13171.	1.2	36

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73	Heterodyne-Detected Dispersed Vibrational Echo Spectroscopy. Journal of Physical Chemistry A, 2009, 113, 14060-14066.	1.1	35
74	Insulin Dissociates by Diverse Mechanisms of Coupled Unfolding and Unbinding. Journal of Physical Chemistry B, 2020, 124, 5571-5587.	1.2	35
75	Structural Characterization of Protonated Water Clusters Confined in HZSM-5 Zeolites. Journal of the American Chemical Society, 2021, 143, 10203-10213.	6.6	35
76	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
77	Single-stage MHz mid-IR OPA using LiGaS₂and a fiber laser pump source. Optics Letters, 2018, 43, 1363.	1.7	34
78	Single-shot two-dimensional infrared spectroscopy. Optics Express, 2007, 15, 233.	1.7	33
79	Upconversion multichannel infrared spectrometer. Optics Letters, 2005, 30, 1818.	1.7	32
80	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
81	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
82	Ultrafast Fluctuations of High Amplitude Electric Fields in Lipid Membranes. Journal of the American Chemical Society, 2017, 139, 4743-4752.	6.6	30
83	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
84	Dynamic and Programmable Cellular-Scale Granules Enable Tissue-like Materials. Matter, 2020, 2, 948-964.	5.0	30
85	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
86	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
87	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
88	Communication: Quantitative multi-site frequency maps for amide I vibrational spectroscopy. Journal of Chemical Physics, 2015, 143, 061102.	1.2	27
89	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
90	Vibrational dynamics of aqueous hydroxide solutions probed using broadband 2DIR spectroscopy. Journal of Chemical Physics, 2015, 143, 194501.	1.2	26

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91	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
92	DNA minor-groove binder Hoechst 33258 destabilizes base-pairing adjacent to its binding site. Communications Biology, 2020, 3, 525.	2.0	25
93	Fluorescence-Encoded Infrared Vibrational Spectroscopy with Single-Molecule Sensitivity. Journal of the American Chemical Society, 2021, 143, 3060-3064.	6.6	25
94	Preface: Special Topic on Biological Water. Journal of Chemical Physics, 2014, 141, 22D101.	1.2	24
95	Structural Disorder of Folded Proteins: Isotope-Edited 2D IR Spectroscopy and Markov State Modeling. Biophysical Journal, 2015, 108, 1747-1757.	0.2	23
96	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
97	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
98	A fast-scanning Fourier transform 2D IR interferometer. Optics Communications, 2011, 284, 1062-1066.	1.0	21
99	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
100	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
101	Efficient Total Chemical Synthesis of ¹³C=¹⁸O Isotopomers of Human Insulin for Isotopeâ€Edited FTIR. ChemBioChem, 2016, 17, 415-420.	1.3	19
102	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
103	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
104	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
105	Temperatureâ€dependent downhill unfolding of ubiquitin. II. Modeling the free energy surface. Proteins: Structure, Function and Bioinformatics, 2008, 72, 488-497.	1.5	18
106	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
107	Exchange-Mediated Transport in Battery Electrolytes: Ultrafast or Ultraslow?. Journal of the American Chemical Society, 2022, 144, 8591-8604.	6.6	18
108	Isotope-enriched protein standards for computational amide I spectroscopy. Journal of Chemical Physics, 2015, 142, 125104.	1.2	17

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109	Two-Photon-Excited Fluorescence-Encoded Infrared Spectroscopy. Journal of Physical Chemistry A, 2016, 120, 9178-9187.	1.1	17
110	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
111	Fourier Transform Fluorescence-Encoded Infrared Spectroscopy. Journal of Physical Chemistry A, 2018, 122, 554-562.	1.1	16
112	Refinement of Peptide Conformational Ensembles by 2D IR Spectroscopy: Application to Alaâ€'Alaâ€'Ala. Biophysical Journal, 2018, 114, 2820-2832.	0.2	16
113	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
114	Single-shot two-dimensional spectrometer. Optics Letters, 2006, 31, 113.	1.7	15
115	Characterization of Acetonitrile Isotopologues as Vibrational Probes of Electrolytes. Journal of Physical Chemistry B, 2022, 126, 278-291.	1.2	15
116	Computational IR Spectroscopy of Insulin Dimer Structure and Conformational Heterogeneity. Journal of Physical Chemistry B, 2021, 125, 4620-4633.	1.2	14
117	Entropic barriers in the kinetics of aqueous proton transfer. Journal of Chemical Physics, 2019, 151, 034501.	1.2	13
118	Vibrational Probe of Aqueous Electrolytes: The Field Is Not Enough. Journal of Physical Chemistry B, 2020, 124, 7013-7026.	1.2	13
119	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
120	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
121	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
122	Temperature-Jump 2D IR Spectroscopy with Intensity-Modulated CW Optical Heating. Journal of Physical Chemistry B, 2020, 124, 8665-8677.	1.2	11
123	Distinguishing gramicidin D conformers through two-dimensional infrared spectroscopy of vibrational excitons. Journal of Chemical Physics, 2015, 142, 212424.	1.2	10
124	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
125	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
126	Resonance conditions, detection quality, and single-molecule sensitivity in fluorescence-encoded infrared vibrational spectroscopy. Journal of Chemical Physics, 2022, 156, 174202.	1.2	8

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127	Infrared spectroscopy of tritiated water. Chemical Physics Letters, 2007, 449, 130-134.	1.2	7
128	A lattice model for the interpretation of oligonucleotide hybridization experiments. Journal of Chemical Physics, 2019, 150, 185104.	1.2	6
129	A phenomenological approach to modeling chemical dynamics in nonlinear and two-dimensional spectroscopy. Journal of Chemical Physics, 2012, 136, 134507.	1.2	5
130	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
131	Structural Ensemble of the Insulin Monomer. Biochemistry, 2021, 60, 3125-3136.	1.2	5
132	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
133	Information from two-dimensional fifth-order Raman spectroscopy: Anharmonicity, nonlinearity, mode coupling, and molecular structure. AIP Conference Proceedings, 2000, , .	0.3	0