Yunjie Xu

List of Publications by Year
in descending order

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113 papers	3,642 citations	101543 36 h-index	175258 52 g-index
122 all docs	122 docs citations	122 times ranked	1485 citing authors

#	Article	IF	Citations
1	Evidence for heavy atom large amplitude motions in RG-cyclopropane van der Waals complexes (RG=Ne,) Tj ETQq1 1 0.784314 rgBT /	3.0	161
2	Chirality transfer through hydrogen-bonding: Experimental and ab initio analyses of vibrational circular dichroism spectra of methyl lactate in water. Physical Chemistry Chemical Physics, 2007, 9, 3127.	2.8	133
3	Spectroscopic Studies of Quantum Solvation inHeN4â^'N2OClusters. Physical Review Letters, 2003, 91, 163401.	7.8	111
4	Lactic acid in solution: Investigations of lactic acid self-aggregation and hydrogen bonding interactions with water and methanol using vibrational absorption and vibrational circular dichroism spectroscopies. Journal of Chemical Physics, 2008, 128, 014508.	3.0	95
5	Solvation of Propylene Oxide in Water: Vibrational Circular Dichroism, Optical Rotation, and Computer Simulation Studies. Journal of Physical Chemistry A, 2008, 112, 5621-5627.	2.5	87
6	Rotational spectroscopic investigation of carbonyl sulfide solvated with helium atoms. Journal of Chemical Physics, 2003, 119, 5457-5466.	3.0	82
7	Chiral Self-Recognition:Â Direct Spectroscopic Detection of the Homochiral and Heterochiral Dimers of Propylene Oxide in the Gas Phase. Journal of the American Chemical Society, 2006, 128, 17126-17131.	13.7	81
8	Rotational spectrum, structure, and chlorine nuclear quadrupole coupling constants of the van der Waals complex Arâ€“Cl2. Journal of Chemical Physics, 1993, 98, 3726-3731.	3.0	77
9	Pure rotational spectra of the mixed rare gas van der Waals complexes Neâ€“Xe, Arâ€“Xe, and Krâ€“Xe. Journal of Chemical Physics, 1993, 99, 919-927.	3.0	69
10	Microwave spectroscopy of ternary and quaternary van der Waals clusters. International Reviews in Physical Chemistry, 2005, 24, 301-338.	2.3	65
11	Vibrational Circular Dichroism Spectroscopy of Chiral Molecules. Topics in Current Chemistry, 2010, 298, 189-236.	4.0	65
12	Solvent-induced conformational changes in cyclic peptides: a vibrational circular dichroism study. Physical Chemistry Chemical Physics, 2014, 16, 5627-5633.	2.8	62
13	Recurrences in rotational dynamics and experimental measurement of superfluidity in doped helium clusters. Journal of Chemical Physics, 2006, 124, 081101.	3.0	61
14	The Clusters-in-a-Liquid Approach for Solvation: New Insights from the Conformer Specific Gas Phase Spectroscopy and Vibrational Optical Activity Spectroscopy. Frontiers in Chemistry, 2016, 4, 9.	3.6	61
15	Probing chiral solute-water hydrogen bonding networks by chirality transfer effects: A vibrational circular dichroism study of glycidol in water. Journal of Chemical Physics, 2009, 130, 164506.	3.0	60
16	Infrared spectrum of the COâ€“N2 van der Waals complex: Assignments for CO-paraN2 and observation of a bending state for CO-orthoN2. Journal of Chemical Physics, 2000, 113, 525-533.	3.0	59
17	A Direct Link from the Gas to the Condensed Phase: A Rotational Spectroscopic Study of 2,2,2â€Trifluoroethanol Trimers. Angewandte Chemie - International Edition, 2017, 56, 6289-6293.	13.8	52
18	Conformational Stability of the Propylene Oxideâ^'Water Adduct:Â Direct Spectroscopic Detection of Oâ^'HÂ·Â·Â·O Hydrogen Bonded Conformers. Journal of the American Chemical Society, 2006, 128, 6755-6760.	13.7	51

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19	Spectroscopic Studies of OCS-Doped4He Clusters with 9â^'72 Helium Atoms:Â Observation of Broad Oscillations in the Rotational Moment of Inertiaâ€. Journal of Physical Chemistry A, 2007, 111, 7329-7337.	2.5	50
20	Chirality Transfer in a Methyl Lactateâ€“Ammonia Complex Observed by Matrixâ€Isolation Vibrational Circular Dichroism Spectroscopy. Angewandte Chemie - International Edition, 2013, 52, 2073-2076.	13.8	49
21	Direct Spectroscopic Detection of the Orientation of Free OH Groups in Methyl Lactateâ€“(Water)_{1,2} Clusters: Hydration of a Chiral Hydroxy Ester. Angewandte Chemie - International Edition, 2014, 53, 1156-1159.	13.8	49
22	Lock-and-Key Principle on a Microscopic Scale: The Case of the Propylene Oxideâ‹…â‹…â‹…Ethanol Complex. Angewandte Chemie - International Edition, 2007, 46, 2276-2279.	13.8	48
23	Discovering the Elusive Global Minimum in a Ternary Chiral Cluster: Rotational Spectra of Propylene Oxide Trimer. Angewandte Chemie - International Edition, 2020, 59, 22427-22430.	13.8	47
24	High resolution spectroscopy of Ne and Ar containing noble gas clusters. Journal of Chemical Physics, 1997, 107, 4788-4796.	3.0	46
25	Anharmonicity Effects in the Vibrational CD Spectra of Propylene Oxide. Journal of Physical Chemistry Letters, 2013, 4, 3424-3428.	4.6	46
26	Rotational spectra and theoretical study of tetramers and trimers of 2-fluoroethanol: dramatic intermolecular compensation for intramolecular instability. Physical Chemistry Chemical Physics, 2018, 20, 27630-27637.	2.8	46
27	The Chiral Trimer and a Metastable Chiral Dimer of Achiral Hexafluoroisopropanol: A Multiâ€Messenger Study. Angewandte Chemie - International Edition, 2019, 58, 5080-5084.	13.8	46
28	Microwave-submillimeter wave double-resonance spectrometer for the investigation of van der Waals complexes. Review of Scientific Instruments, 1998, 69, 4061-4067.	1.3	45
29	The rich conformational landscape of perillyl alcohol revealed by broadband rotational spectroscopy and theoretical modelling. Physical Chemistry Chemical Physics, 2019, 21, 15408-15416.	2.8	45
30	A comparative VCD study of methyl mandelate in methanol, dimethyl sulfoxide, and chloroform: explicit and implicit solvation models. Physical Chemistry Chemical Physics, 2013, 15, 1655-1665.	2.8	42
31	Rotational spectrum of a chiral Î±-hydroxyester: conformation stability and internal rotation barrier heights of methyl lactate. Physical Chemistry Chemical Physics, 2007, 9, 1324-1328.	2.8	41
32	Conformations of Serine in Aqueous Solutions as Revealed by Vibrational Circular Dichroism. ChemPhysChem, 2012, 13, 1272-1281.	2.1	41
33	Conformational Distributions of Nâ€Acetylâ€<scp>L</scp>â€cysteine in Aqueous Solutions: A Combined Implicit and Explicit Solvation Treatment of VA and VCD Spectra. ChemPhysChem, 2012, 13, 2310-2321.	2.1	41
34	Rotational spectra of the mixed rare gas dimers Neâ€“Kr and Arâ€“Kr. Journal of Chemical Physics, 1995, 103, 2827-2833.	3.0	37
35	Unusual Hâ€Bond Topology and Bifurcated Hâ€bonds in the 2â€Fluoroethanol Trimer. Angewandte Chemie - International Edition, 2015, 54, 11711-11715.	13.8	37
36	Conservation of Helicity in a Chiral Pyrrol-2-yl Schiff-Base Ligand and Its Transition Metal Complexes. Inorganic Chemistry, 2015, 54, 4539-4549.	4.0	37

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37	Chirality Synchronization in Trifluoroethanol Dimer Revisited: The Missing Heterochiral Dimer. Journal of Physical Chemistry Letters, 2014, 5, 1850-1855.	4.6	36
38	Conformational Panorama and Chirality Controlled Structureâ€"Energy Relationship in a Chiral Carboxylic Acid Dimer. Angewandte Chemie - International Edition, 2020, 59, 15703-15710.	13.8	36
39	The microwave rotational spectrum of the van der Waals complex Krâ€"N2. Journal of Chemical Physics, 1993, 99, 7510-7520.	3.0	35
40	Molecular recognition in 1 : 1 hydrogen-bonded complexes of oxirane and trans-2,3-dimethyloxirane with ethanol: a rotational spectroscopic and ab initio study. Physical Chemistry Chemical Physics, 2007, 9, 4514.	2.8	35
41	Quantitative Chiral Analysis by Molecular Rotational Spectroscopy. , 2018, , 679-729.		35
42	Two Spectroscopies in One: Interference of Circular Dichroism and Raman Optical Activity. Angewandte Chemie - International Edition, 2020, 59, 21895-21898.	13.8	35
43	Microwave spectroscopic investigation of the mixed rare gas van der Waals trimers Ne2â€"Kr and Ne2â€"Xe. Journal of Chemical Physics, 1994, 100, 4171-4180.	3.0	33
44	Vibrational absorption, vibrational circular dichroism, and theoretical studies of methyl lactate self-aggregation and methyl lactate-methanol intermolecular interactions. Journal of Chemical Physics, 2010, 132, 234513.	3.0	33
45	The dynamics of the COâ€"N2 interaction: Strong Coriolis coupling in CO-paraN2. Journal of Chemical Physics, 2000, 113, 514-524.	3.0	32
46	Hydration of a Chiral Molecule: The Propylene Oxideâ‹…â‹…â‹…(Water)₂ Cluster in the Gas Phase. Angewandte Chemie - International Edition, 2007, 46, 6163-6166.	13.8	32
47	Tailoring the Key in a Molecular Lock-and-Key Model System: The Propylene OxideÂ·Â·Â·2-Fluoroethanol Complex. Journal of the American Chemical Society, 2008, 130, 5916-5921.	13.7	32
48	IR and Vibrational Circular Dichroism Spectroscopy of Matrine- and Artemisinin-Type Herbal Products: Stereochemical Characterization and Solvent Effects. Journal of Natural Products, 2016, 79, 1012-1023.	3.0	31
49	Hydration of the simplest Î±-keto acid: a rotational spectroscopic and ab initio study of the pyruvic acidâ€"water complex. Physical Chemistry Chemical Physics, 2017, 19, 4440-4446.	2.8	31
50	A Direct Link from the Gas to the Condensed Phase: A Rotational Spectroscopic Study of 2,2,2â€Trifluoroethanol Trimers. Angewandte Chemie, 2017, 129, 6386-6390.	2.0	31
51	Conformational dynamics of 1-phenyl-2,2,2-trifluoroethanol by rotational spectroscopy and ab initio calculations. Journal of Molecular Spectroscopy, 2018, 351, 62-67.	1.2	31
52	The effects of self-aggregation on the vibrational circular dichroism and optical rotation measurements of glycidol. Physical Chemistry Chemical Physics, 2008, 10, 6787.	2.8	30
53	Vibrational absorption and vibrational circular dichroism spectra of leucine in water under different pH conditions: Hydrogen-bonding interactions with water. Journal of Chemical Physics, 2012, 137, 194308.	3.0	30
54	Chirality recognition of the protonated serine dimer and octamer by infrared multiphoton dissociation spectroscopy. Physical Chemistry Chemical Physics, 2013, 15, 1873-1886.	2.8	30

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55	Evidence of Dihydrogen Bonding of a Chiral Amineâ€“Borane Complex in Solution by VCD Spectroscopy. Angewandte Chemie - International Edition, 2014, 53, 9940-9943.	13.8	30
56	Rotational Spectra of Two Hydrogen-Bonded Methyl Salicylate Monohydrates: Relative Stability and Tunneling Motions. Journal of Physical Chemistry Letters, 2015, 6, 3126-3131.	4.6	30
57	Chirality Recognition in the Glycidolâ‹…â‹…â‹…Propylene Oxide Complex: A Rotational Spectroscopic Study. Chemistry - A European Journal, 2011, 17, 4582-4587.	3.3	29
58	Chirped-Pulse and Cavity-Based Fourier Transform Microwave Spectroscopy of a Chiral Epoxy Ester: Methyl Glycidate. Journal of Physical Chemistry A, 2013, 117, 13249-13254.	2.5	28
59	The rotational spectra of the fluorobenzeneâ‹¯water and p-difluorobenzeneâ‹¯water dimers: Structure and internal dynamics. Journal of Molecular Spectroscopy, 2011, 268, 47-52.	1.2	27
60	Transfer and Amplification of Chirality Within the â€œRing of Fireâ€•Observed in Resonance Raman Optical Activity Experiments. Angewandte Chemie - International Edition, 2019, 58, 16495-16498.	13.8	27
61	Molecular Selfâ€Recognition: Rotational Spectra of the Dimeric 2â€Fluoroethanol Conformers. Chemistry - A European Journal, 2009, 15, 270-277.	3.3	26
62	Matrix Isolationâ€Vibrational Circular Dichroism Spectroscopy of 3â€Butynâ€2â€ol and its Binary Aggregates. ChemPhysChem, 2013, 14, 213-219.	2.1	25
63	Direct observation of rotational transitions of the COâ€“CO dimer. Journal of Chemical Physics, 1999, 111, 5754-5756.	3.0	24
64	Chirality Induction and Amplification in the 2,2,2â€Trifluoroethanolâ‹…â‹…â‹…Propylene Oxide Adduct. Angewandte Chemie - International Edition, 2014, 53, 7277-7280.	13.8	22
65	Rotational spectroscopy of chiral tetrahydro-2-furoic acid: Conformational landscape, conversion, and abundances. Journal of Chemical Physics, 2018, 149, 224306.	3.0	21
66	IR, Raman, and Vibrational Optical Activity Spectra of Methyl Glycidate in Chloroform and Water: The Clustersâ€inâ€aâ€Liquid Solvation Model. ChemPhysChem, 2018, 19, 2234-2242.	2.1	21
67	The Chiral Trimer and a Metastable Chiral Dimer of Achiral Hexafluoroisopropanol: A Multiâ€Messenger Study. Angewandte Chemie, 2019, 131, 5134-5138.	2.0	20
68	Chirpedâ€Pulse and Cavityâ€Based Fourier Transform Microwave Spectra of the Methyl Lactateâ‹…â‹…â‹…Ammonia Adduct. Angewandte Chemie - International Edition, 2013, 52, 4402-4405.	13.8	19
69	Structure and tunneling dynamics in a model system of peptide co-solvents: Rotational spectroscopy of the 2,2,2-trifluoroethanolâ‹¯water complex. Journal of Chemical Physics, 2014, 140, 234307.	3.0	19
70	Competition Between Intraâ€and Intermolecular Hydrogen Bonding:oâ€Anisic Acidâ‹…â‹…â‹…Formic Acid Heterodimer. Chemistry - A European Journal, 2019, 25, 12325-12331.	3.3	19
71	Can One Measure Resonance Raman Optical Activity?. Angewandte Chemie - International Edition, 2021, 60, 22004-22009.	13.8	18
72	Tunnelling and barrier-less motions in the 2-fluoroethanolâ€“water complex: a rotational spectroscopic and ab initio study. Physical Chemistry Chemical Physics, 2017, 19, 12221-12228.	2.8	17

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73	Rotational spectroscopy of the methyl glycidateâ€“water complex: conformation and water and methyl rotor tunnelling motions. Physical Chemistry Chemical Physics, 2017, 19, 29508-29515.	2.8	17
74	Aggregation of lactic acid in cold rare-gas matrices and the link to solution: a matrix isolation-vibrational circular dichroism study. Physical Chemistry Chemical Physics, 2019, 21, 3574-3584.	2.8	17
75	Absolute Configuration and Conformation of Two FrÃ¡terâ€“Seebach Alkylation Reaction Products by Film VCD and ECD Spectroscopic Analyses. Journal of Organic Chemistry, 2015, 80, 428-437.	3.2	16
76	Perfluorobutyric Acid and Its Monohydrate: A Chirped Pulse and Cavity Based Fourier Transform Microwave Spectroscopic Study. Chemistry - A European Journal, 2014, 20, 6148-6153.	3.3	14
77	Chirality Induction and Amplification in the 2,2,2â€Trifluoroethanolâ‹…â‹…â‹…Propylene Oxide Adduct. Angewandte Chemie, 2014, 126, 7405-7408.	2.0	13
78	Transfer and Amplification of Chirality Within the â€œRing of Fireâ€•Observed in Resonance Raman Optical Activity Experiments. Angewandte Chemie, 2019, 131, 16647-16650.	2.0	11
79	Discovering the Elusive Global Minimum in a Ternary Chiral Cluster: Rotational Spectra of Propylene Oxide Trimer. Angewandte Chemie, 2020, 132, 22613-22616.	2.0	11
80	Ab initio study of chiral recognition in the propylene imineÂ·hydrogen peroxide complex. Physical Chemistry Chemical Physics, 2005, 7, 2554.	2.8	10
81	Infrared diode laser spectroscopic investigation of four Câ€“H stretching vibrational modes of propylene oxide. Chemical Physics Letters, 2010, 494, 14-20.	2.6	10
82	A spectroscopic andab initiostudy of the hydrogen peroxideâ€“formic acid complex: hindering the internal motion of H₂O₂. Physical Chemistry Chemical Physics, 2018, 20, 21345-21351.	2.8	10
83	Conformational Landscape, Chirality Recognition and Chiral Analyses: Rotational Spectroscopy of Tetrahydroâ€2â€Furoic Acidâ‹…â‹…â‹…Propylene Oxide Conformers. ChemPhysChem, 2021, 22, 455-460.	2.1	10
84	Spectroscopic study of the mixed rare-gasâ€“molecule van der Waals trimer NeArHCl. Journal of Chemical Physics, 1999, 110, 4354-4362.	3.0	9
85	Pulsed jet rotational spectra of the propylene oxideâ€“neon molecular adduct. Journal of Molecular Spectroscopy, 2005, 232, 112-114.	1.2	9
86	Two Spectroscopies in One: Interference of Circular Dichroism and Raman Optical Activity. Angewandte Chemie, 2020, 132, 22079-22082.	2.0	9
87	Conformational Panorama and Chirality Controlled Structureâ€“Energy Relationship in a Chiral Carboxylic Acid Dimer. Angewandte Chemie, 2020, 132, 15833-15840.	2.0	9
88	Electronic Circular Dichroismâ€Circularly Polarized Raman (eCPâ€Raman): A New Form of Chiral Raman Spectroscopy. Chemistry - A European Journal, 2022, 28, .	3.3	9
89	Identifying dominant conformations of N-acetyl-l-cysteine methyl ester and N-acetyl-l-cysteine in water: VCD signatures of the amide I and the CO stretching bands. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 131-140.	3.9	8
90	Rotational spectroscopic and theoretical study of the perfluorobutyric acidâ‹¯formic acid complex. Journal of Molecular Spectroscopy, 2017, 335, 88-92.	1.2	8

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91	Modifying conformational distribution of chiral tetrahydro-2-furoic acid through its interaction with water: a rotational spectroscopic and theoretical investigation. Physical Chemistry Chemical Physics, 2021, 23, 3820-3825.	2.8	8
92	Raman Optical Activity of Nâ€Acetylâ€Lâ€Cysteine in Water and in Methanol: The â€œClustersâ€inâ€aâ€Liquidâ€•Model and ab Initio Molecular Dynamics Simulations. ChemPhysChem, 2022, 23, .	2.1	8
93	Matrix Isolationâ€Vibrational Circular Dichroism Spectroscopic Study of Conformations and Nonâ€Covalent Interactions of Tetrahydroâ€2â€Furoic Acid. ChemPhysChem, 2021, 22, 1336-1343.	2.1	7
94	Vibrational Spectroscopy of Homo- and Heterochiral Amino Acid Dimers: Conformational Landscapes. Molecules, 2022, 27, 38.	3.8	7
95	Conformational Landscape of m-Anisic Acid and Its Complexes with Formic Acid. Journal of Physical Chemistry A, 2019, 123, 6772-6780.	2.5	6
96	Microwave spectrum of the complex of 3,3,3-trifluoro-2-(trifluoromethyl)propanoic acid and formic acid. Molecular Physics, 2019, 117, 1193-1199.	1.7	6
97	2,2,3,3,3-Pentafluoro-1-propanol and its dimer: structural diversity, conformational conversion, and tunnelling motion. Physical Chemistry Chemical Physics, 2022, 24, 14975-14984.	2.8	6
98	The pyrrole-water complex: Multidimensional large amplitude dynamics and rotational spectra of its 13C isotopologues. Journal of Molecular Spectroscopy, 2020, 374, 111381.	1.2	5
99	Structural and dynamical features of the 2,2,2-trifluoroethanolâ‹¯ammonia complex. Physical Chemistry Chemical Physics, 2020, 22, 23019-23027.	2.8	5
100	The ArNe-N2O van der Waals trimer: a high resolution spectroscopic study of its rotational spectrum, structure and dynamics. Molecular Physics, 2001, 99, 13-24.	1.7	4
101	Rotational spectra of two six-membered heterocyclic N-methyl-piperidinol compounds: Conformations by OH rotation, N-methyl inversion, and ring puckering. Journal of Chemical Physics, 2017, 146, 104303.	3.0	4
102	Rotational Spectrum and Molecular Structures of the Binary Aggregates of 1,1,1,3,3,3-Hexafluoro-2-propanol with Ne and Ar. Journal of Physical Chemistry A, 2021, 125, 5355-5364.	2.5	4
103	Higher-Energy HexafluoroisopropanolÂ·Â·Â·Water Isomer and Its Large Amplitude Motions: Rotational Spectra and DFT Calculations. Journal of Physical Chemistry A, 2021, 125, 10401-10409.	2.5	4
104	Conformational Landscape of the Hydrogen-Bonded 1-Phenyl-2,2,2-TrilfuoroethanolÂ·Â·Â·1,4-Dioxane Complex: Dispersion Interactions and Conformational Conversion. Journal of Physical Chemistry A, 2022, 126, 2942-2949.	2.5	4
105	Structural and energetic properties of protonated and sodiated asparagine probed by a new laboratory IRMPD spectrometer. Journal of Molecular Spectroscopy, 2018, 352, 36-44.	1.2	3
106	Conformational landscape and intricate conformational relaxation paths of 4,4,4-trifluoro-1-butanol: Rotational spectroscopy and quantum chemical calculations. Journal of Molecular Structure, 2020, 1217, 128359.	3.6	3
107	Hydrogen bonding interactions in the 1,1,1,3,3,3-hexafluoro-2-propanolâ˜™â˜™1,4-dioxane complex: Rotational spectroscopy and density functional theory calculations. Journal of Molecular Spectroscopy, 2021, 376, 111408.	1.2	2
108	Stereochemical Properties of Multidentate Nitrogen Donor Ligands and Their Copper Complexes by Electronic CD and DFT. Chirality, 2016, 28, 545-555.	2.6	1

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109	Unusual binary aggregates of perylene bisimide revealed by their electronic transitions in helium nanodroplets and DFT calculations. Physical Chemistry Chemical Physics, 2021, 23, 13862-13872.	2.8	1
110	Rotational Spectroscopy of 2â€Furoic Acid and Its Dimer: Conformational Distribution and Double Proton Tunneling. ChemPhysChem, 2022, , .	2.1	1
111	Titelbild: Two Spectroscopies in One: Interference of Circular Dichroism and Raman Optical Activity (Angew. Chem. 49/2020). Angewandte Chemie, 2020, 132, 21973-21973.	2.0	0
112	Can One Measure Resonance Raman Optical Activity?. Angewandte Chemie, 2021, 133, 22175-22180.	2.0	0
113	Frontispiece: Electronic Circular Dichroismâ€Circularly Polarized Raman (eCPâ€Raman): A New Form of Chiral Raman Spectroscopy. Chemistry - A European Journal, 2022, 28, .	3.3	0