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	Electronic Circular Dichroismâ€Circularly Polarized Raman (eCPâ€Raman): A New Form of Chiral Raman Spectroscopy. Chemistry - A European Journal, 2022, 28, .	3.3	9
2	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
3	Rotational Spectroscopy of 2â€Furoic Acid and Its Dimer: Conformational Distribution and Double Proton Tunneling. ChemPhysChem, 2022, , .	2.1	1
4	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
5	Vibrational Spectroscopy of Homo- and Heterochiral Amino Acid Dimers: Conformational Landscapes. Molecules, 2022, 27, 38.	3.8	7
6	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
7	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
8	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
9	Hydrogen bonding interactions in the 1,1,1,3,3,3-hexafluoro-2-propanolâ˜™â˜™â˜™1,4-dioxane complex: Rotational spectroscopy and density functional theory calculations. Journal of Molecular Spectroscopy, 2021, 376, 111408.	1.2	2
10	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
11	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
12	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
13	Can One Measure Resonance Raman Optical Activity?. Angewandte Chemie - International Edition, 2021, 60, 22004-22009.	13.8	18
14	Can One Measure Resonance Raman Optical Activity?. Angewandte Chemie, 2021, 133, 22175-22180.	2.0	0
15	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
16	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
17	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
18	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

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19	Two Spectroscopies in One: Interference of Circular Dichroism and Raman Optical Activity. Angewandte Chemie - International Edition, 2020, 59, 21895-21898.	13.8	35
20	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
21	Two Spectroscopies in One: Interference of Circular Dichroism and Raman Optical Activity. Angewandte Chemie, 2020, 132, 22079-22082.	2.0	9
22	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
23	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
24	Conformational Panorama and Chirality Controlled Structureâ€"Energy Relationship in a Chiral Carboxylic Acid Dimer. Angewandte Chemie, 2020, 132, 15833-15840.	2.0	9
25	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
26	Structural and dynamical features of the 2,2,2-trifluoroethanolâ‹¯ammonia complex. Physical Chemistry Chemical Physics, 2020, 22, 23019-23027.	2.8	5
27	Conformational Landscape of m-Anisic Acid and Its Complexes with Formic Acid. Journal of Physical Chemistry A, 2019, 123, 6772-6780.	2.5	6
28	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
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	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
31	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
32	The Chiral Trimer and a Metastable Chiral Dimer of Achiral Hexafluoroisopropanol: A Multiâ€Messenger Study. Angewandte Chemie, 2019, 131, 5134-5138.	2.0	20
33	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
34	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
35	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
36	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

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37	Quantitative Chiral Analysis by Molecular Rotational Spectroscopy. , 2018, , 679-729.		35
38	Rotational spectroscopy of chiral tetrahydro-2-furoic acid: Conformational landscape, conversion, and abundances. Journal of Chemical Physics, 2018, 149, 224306.	3.0	21
39	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
40	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
41	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
42	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
43	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
44	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
45	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
46	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
47	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
48	Rotational spectroscopic and theoretical study of the perfluorobutyric acidâ€formic acid complex. Journal of Molecular Spectroscopy, 2017, 335, 88-92.	1.2	8
49	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
50	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
51	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
52	Stereochemical Properties of Multidentate Nitrogen Donor Ligands and Their Copper Complexes by Electronic CD and DFT. Chirality, 2016, 28, 545-555.	2.6	1
53	Unusual Hâ€Bond Topology and Bifurcated Hâ€bonds in the 2â€Fluoroethanol Trimer. Angewandte Chemie - International Edition, 2015, 54, 11711-11715.	13.8	37
54	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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55	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
56	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
57	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
58	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
59	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
60	Chirality Induction and Amplification in the 2,2,2â€Trifluoroethanolâ‹…â‹…â‹…Propylene Oxide Adduct. Angewandte Chemie, 2014, 126, 7405-7408.	2.0	13
61	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
62	Solvent-induced conformational changes in cyclic peptides: a vibrational circular dichroism study. Physical Chemistry Chemical Physics, 2014, 16, 5627-5633.	2.8	62
63	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
64	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
65	Chirality Synchronization in Trifluoroethanol Dimer Revisited: The Missing Heterochiral Dimer. Journal of Physical Chemistry Letters, 2014, 5, 1850-1855.	4.6	36
66	Anharmonicity Effects in the Vibrational CD Spectra of Propylene Oxide. Journal of Physical Chemistry Letters, 2013, 4, 3424-3428.	4.6	46
67	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
68	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
69	Matrix Isolationâ€Vibrational Circular Dichroism Spectroscopy of 3â€Butynâ€2â€ol and its Binary Aggregates. ChemPhysChem, 2013, 14, 213-219.	2.1	25
70	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
71	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
72	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

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73	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
74	Conformations of Serine in Aqueous Solutions as Revealed by Vibrational Circular Dichroism. ChemPhysChem, 2012, 13, 1272-1281.	2.1	41
75	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
76	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
77	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
78	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
79	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
80	Vibrational Circular Dichroism Spectroscopy of Chiral Molecules. Topics in Current Chemistry, 2010, 298, 189-236.	4.0	65
81	Molecular Selfâ€Recognition: Rotational Spectra of the Dimeric 2â€Fluoroethanol Conformers. Chemistry - A European Journal, 2009, 15, 270-277.	3.3	26
82	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
83	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
84	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
85	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
86	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
87	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
88	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
89	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
90	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

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91	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
92	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
93	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
94	Conformational Stability of the Propylene Oxideâˆ’Water Adduct:Â Direct Spectroscopic Detection of Oâˆ’HÂ·Â·Â·O Hydrogen Bonded Conformers. Journal of the American Chemical Society, 2006, 128, 6755-6760.	13.7	51
95	Recurrences in rotational dynamics and experimental measurement of superfluidity in doped helium clusters. Journal of Chemical Physics, 2006, 124, 081101.	3.0	61
96	Pulsed jet rotational spectra of the propylene oxideâ€“neon molecular adduct. Journal of Molecular Spectroscopy, 2005, 232, 112-114.	1.2	9
97	Microwave spectroscopy of ternary and quaternary van der Waals clusters. International Reviews in Physical Chemistry, 2005, 24, 301-338.	2.3	65
98	Ab initio study of chiral recognition in the propylene imineÂ·hydrogen peroxide complex. Physical Chemistry Chemical Physics, 2005, 7, 2554.	2.8	10
99	Rotational spectroscopic investigation of carbonyl sulfide solvated with helium atoms. Journal of Chemical Physics, 2003, 119, 5457-5466.	3.0	82
100	Spectroscopic Studies of Quantum Solvation inHeN4âˆ’N2OClusters. Physical Review Letters, 2003, 91, 163401.	7.8	111
101	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
102	The dynamics of the COâ€“N2 interaction: Strong Coriolis coupling in CO-paraN2. Journal of Chemical Physics, 2000, 113, 514-524.	3.0	32
103	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
104	Spectroscopic study of the mixed rare-gasâ€“molecule van der Waals trimer NeArHCl. Journal of Chemical Physics, 1999, 110, 4354-4362.	3.0	9
105	Direct observation of rotational transitions of the COâ€“CO dimer. Journal of Chemical Physics, 1999, 111, 5754-5756.	3.0	24
106	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
107	High resolution spectroscopy of Ne and Ar containing noble gas clusters. Journal of Chemical Physics, 1997, 107, 4788-4796.	3.0	46
108	Evidence for heavy atom large amplitude motions in RG-cyclopropane van der Waals complexes (RG=Ne,) Tj ETQq0 0 0 rgBT /Overlock 1	3.0	161

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109	Rotational spectra of the mixed rare gas dimers Neâ€“Kr and Arâ€“Kr. Journal of Chemical Physics, 1995, 103, 2827-2833.	3.0	37
110	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
111	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
112	The microwave rotational spectrum of the van der Waals complex Krâ€“N2. Journal of Chemical Physics, 1993, 99, 7510-7520.	3.0	35
113	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