Rui Zheng

List of Publications by Year
in descending order

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42	317	840776 11	996975 15
papers	citations	h-index	g-index

42	42	42	242
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A theoretical study of the intermolecular interactions of H2â€“CuF complex: Intermolecular vibrations, isotope effects, and rotational structure. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 274, 121134.	3.9	1
2	An efficient error-correction model to investigate the rotational structure and microwave spectrum of Arâ€“AgF complex. Chemical Physics, 2022, , 111545.	1.9	3
3	Theoretical and experimental studies of the isotope effects for Heâ€“CO2 and Neâ€“CO2 complexes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 250, 119391.	3.9	1
4	Theoretical investigation of potential energy surface and bound states for the N2â€“OCS van der Waals complex. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 228, 117768.	3.9	1
5	Investigating the spectroscopic characteristics of twelve isotopologues for the Arâ€“CO2 complex. Journal of Quantitative Spectroscopy and Radiative Transfer, 2020, 242, 106778.	2.3	4
6	Structural characterization of the NO(X2Î)â€“N2O complex with mid-infrared laser absorption spectroscopy and quantum chemical calculations. Journal of Chemical Physics, 2020, 152, 154303.	3.0	1
7	Investigating the influence of intramolecular bond lengths on the intermolecular interaction of H2â€“AgCl complex: Binding energy, intermolecular vibrations, and isotope effects. Journal of Chemical Physics, 2019, 150, 164301.	3.0	2
8	Theoretical study of infrared spectra for the Arâ€“N2O complex: Fundamental and combination bands. Journal of Molecular Spectroscopy, 2019, 357, 24-31.	1.2	4
9	Theoretical studies of infrared spectra for the N2â€“N2O complex: The tunneling effects of fundamental and combination bands. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 221, 117199.	3.9	1
10	New potential energy surfaces for the complexes Arâ€“CuX (Xâ€¯=â€¯F, Cl, Br, and I). Journal of Quantitative Spectroscopy and Radiative Transfer, 2019, 231, 79-87.	2.3	2
11	Mode-specific quantum dynamics and kinetics of the hydrogen abstraction reaction OH + H₂O â†’ H₂O + OH. Physical Chemistry Chemical Physics, 2019, 21, 24054-24060.	2.8	6
12	Solvent controlling excited state proton transfer reaction in quinoline/isoquinolineâ€pyrazole isomer QPâ€I: A theoretical study. Journal of Physical Organic Chemistry, 2018, 31, e3729.	1.9	11
13	Theoretical studies of Arâ€“AgX (Xâ€¯=â€¯F, Cl, Br, I) complexes: Potential energy surfaces, intermolecualr vibrations and microwave spectra. Journal of Molecular Spectroscopy, 2018, 353, 28-39.	1.2	4
14	Mode specific dynamics in bond selective reaction Oâ€²(3P) + HOD â†’ Oâ€²H + OD/Oâ€²D + OH. Journal of Chemical Physics, 2018, 149, 054304.	3.0	8
15	Theoretical studies for the infrared spectra of Arâ€“CO2 complex: Fundamental and combination bands. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 204, 308-316.	3.9	10
16	A competitive excited state dynamical process for the 2,2â€²-((1E,1â€²E)-((3,3â€²-dimethyl-[1,1â€²-biphenyl]-4,4â€²-diyl)-bis(azanylylidene))bis(methanylylidene))-diphenol system RSC Advances, 2017, 7, 1299-1304.	3.6	20
17	Improving analysis of infrared spectrum of van der Waals complex with theoretical calculation: Applied to Xeâ€“N2O complex. Journal of Molecular Spectroscopy, 2017, 333, 12-18.	1.2	6
18	A theoretical assignment on excitedâ€state intramolecular proton transfer mechanism for quercetin. Journal of Physical Organic Chemistry, 2017, 30, e3684.	1.9	8

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19	Elaborating the excited-state proton transfer behaviors for novel 3H-MC and P2H-CH. Organic Chemistry Frontiers, 2017, 4, 1935-1942.	4.5	31
20	A DFT/TDDFT Study on Excited State Process of a Novel Probe 4â€²-Fluoroflavonol. Journal of Cluster Science, 2017, 28, 2449-2460.	3.3	9
21	An accurate prediction of the infrared spectra for Rgâ€“CS2 (Rg = He, Ne, Ar) complexes in the Î½1 + Î½3 region of CS2 monomer. Chemical Physics Letters, 2017, 687, 31-37.	2.6	3
22	A Theoretical Investigation on Intramolecular Hydrogen Bond: The ESIPT Mechanism of dmahf Sensor. Journal of Cluster Science, 2017, 28, 937-947.	3.3	10
23	Investigations of the Rg-BrCl (Rg = He, Ne, Ar, Kr, Xe) binary van der Waals complexes: ab initio intermolecular potential energy surfaces, vibrational states and predicted pure rotational transition frequencies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 174, 105-117.	3.9	6
24	Hydrogen bonding and excited state properties of the photoexcited hydrogenâ€bonded (E)â€Sâ€(2â€aminopropyl) 3â€(4â€hydroxyphenyl)propâ€2â€enethioate complexes. Journal of Physical Organic Chemistry, 2017, 30, e3634.	1.9	3
25	The ESIPT mechanism of dibenzimidazolo diimine sensor: a detailed TDDFT study. Journal of Physical Organic Chemistry, 2016, 29, 161-165.	1.9	11
26	Time-dependent density functional theory study on excited-state spectral and dynamic properties of hydrogen-bonded complexes formed by DMACA and water. RSC Advances, 2016, 6, 79196-79203.	3.6	2
27	A research on excited-state intramolecular proton-transfer mechanism of a new chemosensor. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	13
28	Theoretical investigation on ESIPT mechanism of a new fluorescent sensor in different solvents. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 159, 30-34.	3.9	13
29	Theoretical studies of three-dimensional potential energy surfaces using neural networks and rotational spectra of the Arâ€“N₂complex. Molecular Physics, 2016, 114, 72-82.	1.7	2
30	Theoretical studies for the N2â€“N2O van der Waals complex: The potential energy surface, intermolecular vibrations, and rotational transition frequencies. Journal of Chemical Physics, 2015, 143, 154304.	3.0	11
31	Some new studies on intermolecular interaction of C3-Ar complex. Open Chemistry, 2015, 13, .	1.9	0
32	Rovibrational Spectra of the Polar and Nonpolar Nitrous Oxide Dimers. Spectroscopy Letters, 2015, 48, 198-212.	1.0	1
33	A DFT/TDDFT investigation of the excited state proton transfer reaction of fisetin chromophore. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 151, 368-374.	3.9	32
34	Theoretical study of LiClâ¯and LiBrâ¯molecular ions. Molecular Physics, 2015, 113, 1433-1441.	1.7	8
35	A detailed theoretical investigation on the excited-state intramolecular proton-transfer mechanism of 3-BTHPB chemosensor. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	14
36	Theoretical study on the ground electronic state of FO+ and FOâ¯. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 133, 735-740.	3.9	7

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37	Infrared diode laser spectroscopy of the trimers Rg2N2O (Rg=Ne, Ar, and Kr): The Î½1 symmetric stretch region of N2O. Journal of Molecular Spectroscopy, 2013, 284-285, 1-7.	1.2	1
38	Infrared diode laser spectroscopy of the Krâ€“N₂O van der Waals complex: thev₁symmetric stretch region of N₂O. Molecular Physics, 2011, 109, 823-830.	1.7	14
39	Rovibrational spectrum and potential energy surface of the N2â€“N2O van der Waals complex. Journal of Molecular Spectroscopy, 2011, 265, 102-105.	1.2	7
40	Rovibrational spectrum of the Neâ€“N2O van der Waals complex in the 1285cmâ^'1 region. Journal of Molecular Spectroscopy, 2010, 263, 174-177.	1.2	12
41	Infrared diode laser spectroscopy of the Heâ€“N2O van der Waals complex in the 1285cmâ^'1 region. Journal of Molecular Spectroscopy, 2009, 253, 88-91.	1.2	13
42	The regulation mechanism of the excited-state behaviour of 3-Hydroxy-2-(1-ethyl-1H-pyrazol-3-yl)-4H-chromen-4-one fluorophore by solvent polarity: a computational study. Molecular Physics, 0, , .	1.7	1