G Naresh Patwari

List of Publications by Year
in descending order

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83	1,432	304743	414414
papers	citations	22 h-index	32 g-index

96	96	96	1290
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Vibrational Stark Fields in Carboxylic Acid Dimers. Physical Chemistry Chemical Physics, 2022, , .	2.8	3
2	Ultrafast Proton-Transfer Reaction in Phenolâ€“(Ammonia)_n Clusters: An Ab Initio Molecular Dynamics Investigation. Journal of Physical Chemistry B, 2022, 126, 1590-1597.	2.6	3
3	Binary Matrix Method to Enumerate, Hierarchically Order, and Structurally Classify Peptide Aggregation. Journal of Chemical Information and Modeling, 2022, 62, 1585-1594.	5.4	0
4	Dynamics of Methyl Radical Formation Following 266 nm Dissociative Photoionization of Xylenes and Mesitylene. Journal of Physical Chemistry A, 2022, 126, 1960-1965.	2.5	3
5	Identification of allosteric hotspots regulating the ribosomal RNA binding by antibiotic resistance-conferring Erm methyltransferases. Journal of Biological Chemistry, 2022, 298, 102208.	3.4	4
6	Hierarchy of Ï€-stacking determines the conformational preferences of bis-squaramates. CrystEngComm, 2021, 23, 5331-5336.	2.6	2
7	Dipole moment enhanced Ï€â€“Ï€ stacking in fluorophenylacetylenes is carried over from gas-phase dimers to crystal structures propagated through liquid like clusters. Physical Chemistry Chemical Physics, 2021, 23, 9938-9947.	2.8	5
8	Isolation of a telluroxane cluster [(R2TeO)(Î¼-TeO2)(OTeR2)][TeO(OH)2] (RÂ=ÂC6H5NNC6H4) stabilized by intra- and intermolecular secondary bonding interactions: Molecular and electronic structure analysis. Polyhedron, 2021, 198, 115037.	2.2	1
9	Î-Stacking in Heterodimers of Propargylbenzene with (Fluoro)phenylacetylenes. ACS Omega, 2021, 6, 17720-17725.	3.5	1
10	Understanding Fermi resonances in the complex vibrational spectra of the methyl groups in methylamines. Physical Chemistry Chemical Physics, 2021, 23, 3739-3747.	2.8	13
11	Is Dissociation of HCl in DMSO Clusters Bistable?. Journal of Physical Chemistry A, 2021, 125, 10351-10358.	2.5	5
12	Photodissociation of o-xylene at 266 nm: imaging the CH3 dissociation channel. Journal of Chemical Sciences, 2021, 133, 1.	1.5	7
13	Hydration of Fluorobenzenes: A Molecular Dynamics Simulation Investigation. Journal of the Indian Institute of Science, 2020, 100, 221-230.	1.9	1
14	Probing the interaction between human serum albumin and the sodium dodecyl sulphate with fluorescence correlation spectroscopy. Journal of Chemical Sciences, 2020, 132, 1.	1.5	0
15	Dipole Moment Propels Ï€-Stacking of Heterodimers of Fluorophenylacetylenes. Journal of Physical Chemistry A, 2020, 124, 7470-7477.	2.5	4
16	Unraveling the Origin of Differentiable â€˜Turnâ€Onâ€™ Fluorescence Sensing of Zn²⁺ and Cd²⁺ Ions with Squaramides. ChemPhysChem, 2020, 21, 1564-1570.	2.1	14
17	Hydrogenâ€Bonded Complexes of Fluorophenylacetylenes: To Fluoresce or Not?. ChemPhysChem, 2020, 21, 1711-1717.	2.1	1
18	Ï€-Stacking Driven Aggregation and Folding of Squaramides. Journal of Physical Chemistry A, 2020, 124, 5832-5839.	2.5	6

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19	Bend-to-Break: Curvilinear Proton Transfer in Phenol-Ammonia Clusters. Journal of Physical Chemistry A, 2020, 124, 3101-3108.	2.5	9
20	Internal electric fields in methanol [MeOH]_{2â€“6} clusters. Physical Chemistry Chemical Physics, 2020, 22, 10917-10923.	2.8	4
21	Vibrational spectroscopic signatures of hydrogen bond induced NH stretchâ€“bend Fermi-resonance in amines: The methylamine clusters and other Nâ€“Hâ‹¯N hydrogen-bonded complexes. Journal of Chemical Physics, 2020, 153, 194301.	3.0	15
22	Probing the role of dispersion energy on structural transformation of double-stranded xylo- and ribo-nucleic acids. Physical Chemistry Chemical Physics, 2019, 21, 3842-3848.	2.8	6
23	A liquid crucible model for aggregation of phenylacetylene in the gas phase. Physical Chemistry Chemical Physics, 2019, 21, 13623-13632.	2.8	11
24	Progressive Hydrophobicity of Fluorobenzenes. Journal of Physical Chemistry B, 2019, 123, 10083-10088.	2.6	6
25	Electrostatics and Dispersion in Xâ€“HÂ·Â·Y (X = C, N, O; Y = N, O) Hydrogen Bonds and Their Role in Xâ€“H Vibrational Frequency Shifts. ACS Omega, 2018, 3, 18518-18527.	3.5	17
26	Synthesis and structure of arylselenium(ii) and aryltellurium(ii) cations based on rigid 5-tert-butyl-1,3-bis-(N-pentylbenzimidazol-2â€²-yl)benzenes. Dalton Transactions, 2018, 47, 9114-9127.	3.3	9
27	Hydrogen bond induced enhancement of Fermi resonances in Nâ€“Hâ‹¯N hydrogen bonded complexes of anilines. Physical Chemistry Chemical Physics, 2018, 20, 21557-21566.	2.8	16
28	The role of electronegativity on the extent of nitridation of group 5 metals as revealed by reactions of tantalum cluster cations with ammonia molecules. Physical Chemistry Chemical Physics, 2018, 20, 13974-13982.	2.8	15
29	Insights into acid dissociation of HCl and HBr with internal electric fields. Physical Chemistry Chemical Physics, 2017, 19, 7461-7464.	2.8	23
30	Ï€-Stacked Dimers of Fluorophenylacetylenes: Role of Dipole Moment. Journal of Physical Chemistry A, 2017, 121, 3383-3391.	2.5	17
31	Elusive Double-Eight-Ring Zeolitic Secondary Building Unit. Journal of the American Chemical Society, 2017, 139, 59-62.	13.7	26
32	Probing the role of electrostatics of polypeptide main-chain in protein folding by perturbing N-terminal residue stereochemistry: DFT study with oligoalanine models. RSC Advances, 2016, 6, 113611-113619.	3.6	2
33	Internal electric fields in small water clusters [(H₂O)_n; n = 2â€“6]. Physical Chemistry Chemical Physics, 2016, 18, 16730-16737.	2.8	20
34	Three-Fold C 3-Symmetric Off-On Fluorescent Chemo-Sensors for Fluoride. Journal of Fluorescence, 2016, 26, 997-1005.	2.5	7
35	Spectroscopic and Abâ€…Initio Investigation of Câˆ’Hâ‹…â‹…â‹…Nâ€…Hydrogenâ€Bonded Complexes of Fluorophenylacetylenes: Frequency Shifts and Correlations. ChemPhysChem, 2016, 17, 2509-2515.	2.1	8
36	The propargylbenzene dimer: Câ€“Hâ‹¯Ï€ assisted Ï€â€“Ï€ stacking. Physical Chemistry Chemical Physics, 2015, 17, 9090-9097.	2.8	15

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37	Octanuclear Zinc Phosphates with Hitherto Unknown Cluster Architectures: Ancillary Ligand and Solvent Assisted Structural Transformations Thereof. Inorganic Chemistry, 2015, 54, 9458-9469.	4.0	29
38	Spectroscopic and ab initio investigation of 2,6-difluorophenylacetyleneâ€“amine complexes: coexistence of Câ€“Hâ‹¯N and lone-pairâ‹¯Ï€ complexes and intermolecular coulombic decay. Physical Chemistry Chemical Physics, 2015, 17, 434-443.	2.8	14
39	Charge transfer aided selective sensing and capture of picric acid by triphenylbenzenes. New Journal of Chemistry, 2015, 39, 886-892.	2.8	59
40	Electrostatics determine vibrational frequency shifts in hydrogen bonded complexes. Physical Chemistry Chemical Physics, 2014, 16, 25247-25250.	2.8	26
41	Selective fluorescence sensing of polynitroaromatic explosives using triaminophenylbenzene scaffolds. Physical Chemistry Chemical Physics, 2014, 16, 10651-10658.	2.8	64
42	Fluorescence Quenching Studies of Î³-Butyrolactone Binding Protein (CprB) from Streptomyces coelicolor A3(2). Journal of Physical Chemistry B, 2014, 118, 10035-10042.	2.6	18
43	Studies of Structural Isomers o-, m-, and p-Fluorophenylacetylene by Two-Color Resonant Two-Photon Mass-Analyzed Threshold Ionization Spectroscopy. Journal of Physical Chemistry A, 2014, 118, 8277-8286.	2.5	16
44	Water-Induced Adsorption of Carbon Monoxide and Oxygen on the Gold Dimer Cation. Journal of Physical Chemistry A, 2014, 118, 8293-8297.	2.5	9
45	Phenylacetylene dimer: Ab initio and DFT study. Chemical Physics, 2013, 415, 150-155.	1.9	14
46	Binary Complexes of Ammonia with Phenylacetylenes: A Combined Experimental and Computational Approach to Explore Multiple Minima on Intermolecular Potentials. ChemPhysChem, 2013, 14, 746-753.	2.1	7
47	Infrared-Optical Double Resonance Spectroscopic Investigation of Trifluoromethylphenols and Their Water Complexes. Journal of Physical Chemistry A, 2012, 116, 6996-7003.	2.5	2
48	Intermolecular structure on binary complexes of water with phenylacetylene and its substituted analogs: a combined spectroscopic and ab initio investigation. Indian Journal of Physics, 2012, 86, 173-179.	1.8	3
49	Interaction of Alcohols with 2-Fluoro- and 4-Fluorophenylacetylenes: Infrared-Optical Double Resonance Spectroscopic and Computational Investigation. Journal of Physical Chemistry A, 2011, 115, 11229-11237.	2.5	6
50	A Ï€-stacked phenylacetylene dimer. Physical Chemistry Chemical Physics, 2011, 13, 16706.	2.8	33
51	Do N-heterocyclic aromatic rings prefer Ï€-stacking?. Physical Chemistry Chemical Physics, 2011, 13, 5514.	2.8	35
52	Estimation of interfacial acidity of sodium dodecyl sulfate micelles. Journal of Chemical Sciences, 2011, 123, 909-918.	1.5	12
53	Phenylacetylene: A Hydrogen Bonding Chameleon. ChemPhysChem, 2011, 12, 26-46.	2.1	29
54	A Combined Spectroscopic and ab Initio Investigation of Phenylacetyleneâ‹¯Methylamine Complex. Observation of Ïƒ and Ï€ Type Hydrogen-Bonded Configurations and Fluorescence Quenching by Weak Câ‹¯HÂ·Â·Â·N Hydrogen Bondingâ€. Journal of Physical Chemistry A, 2010, 114, 11347-11352.	2.5	18

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55	Hydrogen Bonding to Multifunctional Molecules: Spectroscopic and ab Initio Investigation of 4-Ethynylbenzonitrileâˆ'(Water)_{1âˆ'3} Complexes. Journal of Physical Chemistry A, 2010, 114, 8337-8344.	2.5	8
56	Infrared-Optical Double Resonance Spectroscopic Measurements on 2-(2â€²-Pyridyl)benzimidazole and its Hydrogen Bonded Complexes with Water and Methanol. Journal of Physical Chemistry A, 2010, 114, 8323-8330.	2.5	10
57	Binary complexes of tertiary amines with phenylacetylene. Dispersion wins over electrostatics. Physical Chemistry Chemical Physics, 2010, 12, 6150.	2.8	23
58	Hydrogen Bonding to Multifunctional Molecules: Spectroscopic and ab Initio Investigation of Water Complexes of Fluorophenylacetylenes. Journal of Physical Chemistry A, 2009, 113, 1760-1769.	2.5	23
59	Infraredâ€“optical double resonance spectroscopic measurements and high level ab initio calculations on a binary complex between phenylacetylene and borane-trimethylamine. Understanding the role of Câ€“Hâ‹Ï€ interactions. Physical Chemistry Chemical Physics, 2009, 11, 9738.	2.8	29
60	Hydrogen-Bonded Complexes of Phenylacetylene with Water, Methanol, Ammonia, and Methylamine. The Origin of Methyl Group-Induced Hydrogen Bond Switching. Journal of Physical Chemistry A, 2009, 113, 6620-6625.	2.5	38
61	A Ï€-stacked phenylacetylene and 1,3,5-triazine heterodimer: a combined spectroscopic and ab initio investigation. Physical Chemistry Chemical Physics, 2009, 11, 11207.	2.8	20
62	Structure of the Phenylacetyleneâˆ'Water Complex as Revealed by Infrared-Ultraviolet Double Resonance Spectroscopy. Journal of Physical Chemistry A, 2008, 112, 3360-3363.	2.5	39
63	Electronic and Vibrational Spectroscopic Investigation of Phenylacetyleneâˆ'Amine Complexes. Evidence for the Diversity in the Intermolecular Structures. Journal of Physical Chemistry A, 2008, 112, 4426-4431.	2.5	20
64	IRâˆ'UV Double Resonance Spectroscopic Investigation of Phenylacetyleneâˆ'Alcohol Complexes. Alkyl Group Induced Hydrogen Bond Switching. Journal of Physical Chemistry A, 2008, 112, 5121-5125.	2.5	29
65	Infrared-Optical Double-Resonance Measurements on Oâˆ'HÂ·Â·Â·Hâˆ'Ge Dihydrogen-Bonded Phenolâˆ'Triethylgermanium Hydride Complex in the Gas Phase. Journal of Physical Chemistry A, 2008, 112, 5930-5934.	2.5	10
66	Water Complexes of Styrene and 4-Fluorostyrene: A Combined Electronic, Vibrational Spectroscopic and Ab-Initio Investigation. Journal of Physical Chemistry A, 2008, 112, 9702-9707.	2.5	10
67	Photoelectron spectroscopy of hydrated hexafluorobenzene anions. Journal of Chemical Physics, 2007, 127, 114312.	3.0	18
68	Proton Affinity Correlations between Hydrogen and Dihydrogen Bond Acceptors. Journal of Physical Chemistry A, 2007, 111, 3178-3183.	2.5	37
69	Cyclohexane as a Li+Selective Ionophoreâ€. Journal of Physical Chemistry A, 2007, 111, 7585-7588.	2.5	22
70	Theoretical Investigation of In-Plane Hydrogen-Bonded Complexes of Ammonia with Partially Substituted Fluorobenzenes. Journal of Physical Chemistry A, 2007, 111, 2772-2777.	2.5	7
71	Theoretical investigation of Câ€“Hâ‹¯Hâ€“B dihydrogen bonded complexes of acetylenes with borane-trimethylamine. Chemical Physics Letters, 2006, 419, 5-9.	2.6	26
72	The Câ€“Hâ‹¯Hâ€“B dihydrogen bonded borane-trimethylamine dimer: A computational study. Chemical Physics Letters, 2006, 419, 265-268.	2.6	42

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73	Complete infrared spectroscopic characterization of phenol-borane-trimethylamine dihydrogen-bonded complex in the gas phase. Journal of Chemical Physics, 2006, 124, 241103.	3.0	20
74	Proton Affinities of Boraneâ^'Amines:Â Consequences on Dihydrogen Bonding. Journal of Physical Chemistry A, 2005, 109, 2035-2038.	2.5	42
75	IR Photodissociation Spectroscopy of Na+[H2O]m[C6F6]n Clusters:â€‰ Evidence for Separation of Aqueous and Nonaqueous Phases. Journal of Physical Chemistry A, 2003, 107, 9495-9498.	2.5	19
76	Mimicking the solvation of aqueous Na+ in the gas phase. Journal of Chemical Physics, 2003, 118, 8555-8558.	3.0	75
77	Dihydrogen bonded phenolâ€“borane-dimethylamine complex: An experimental and theoretical study. Journal of Chemical Physics, 2002, 116, 6056-6063.	3.0	31
78	Fluorescence enhancement detected IR (FEDIR) spectroscopy: a new background free IR spectroscopic technique for highly fluorescent molecules. Chemical Physics Letters, 2002, 361, 453-456.	2.6	5
79	Dehydrogenation Reaction from a Dihydrogen Bonded Precursor Complex in the Gas Phase. Journal of Physical Chemistry A, 2001, 105, 10753-10758.	2.5	20
80	Electronic and Vibrational Spectroscopy of Dihydrogen Bonded 2-Pyridoneâ^'Boraneâ^'Trimethylamine Complex in Supersonic Jets. Journal of Physical Chemistry A, 2001, 105, 8642-8645.	2.5	19
81	Spectroscopic investigation of tetrahydroisoquinoline in supersonic jet. Journal of Chemical Physics, 2001, 115, 5184-5191.	3.0	17
82	Gas phase dihydrogen bonded phenolâ€“boraneâ€“trimethylamine complex. Journal of Chemical Physics, 2001, 114, 8877-8879.	3.0	33
83	Evidence of a dihydrogen bond in gas phase: Phenolâ€“borane-dimethylamine complex. Journal of Chemical Physics, 2000, 113, 9885-9888.	3.0	45