Shridhar P Gejji

List of Publications by Year
in descending order

102	2,040	279798 23	289244 40
papers	citations	h-index	g-index

103	103	103	2143
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Synthesis, Electronic Structure, DNA and Protein Binding, DNA Cleavage, and Anticancer Activity of Fluorophore-Labeled Copper(II) Complexes. Inorganic Chemistry, 2011, 50, 545-558.	4.0	249
2	The imide ion: potential energy surface and geometries. Electrochimica Acta, 1998, 43, 1375-1379.	5.2	164
3	Ab Initio Structure and Vibrational Frequencies of (CF3SO2)2N-Li+Ion Pairs. Journal of Physical Chemistry A, 1999, 103, 7474-7480.	2.5	110
4	Electronic Structure, Molecular Electrostatic Potential, and NMR Chemical Shifts in Cucurbit[n]urils (n = 5â^'8), Ferrocene, and Their Complexes. Journal of Physical Chemistry A, 2008, 112, 12679-12686.	2.5	59
5	Conformational analysis of poly(ethylene oxide) oligomers: diglyme. Chemical Physics Letters, 1994, 226, 427-432.	2.6	52
6	Molecular Electrostatic Potentials and Hydrogen Bonding in Î±-, Î²-, and Î³-Cyclodextrins. Journal of Physical Chemistry A, 2006, 110, 13073-13080.	2.5	51
7	Synthesis, computational study and glycosidase inhibitory activity of polyhydroxylated conidine alkaloidsâ€"a bicyclic iminosugar. Organic and Biomolecular Chemistry, 2010, 8, 3307.	2.8	50
8	Analysis of atomic electron momentum densities: Use of information entropies in coordinate and momentum space. Chemical Physics Letters, 1985, 117, 138-142.	2.6	43
9	Density Functional Investigations on the Charge Distribution, Vibrational Spectra, and NMR Chemical Shifts in Cucurbit[n]uril (n = 5â^'12) Hosts. Journal of Physical Chemistry A, 2010, 114, 4464-4470.	2.5	41
10	Noncovalent Interactions Accompanying Encapsulation of Resorcinol within Azacalix[4]pyridine Macrocycle. Journal of Physical Chemistry A, 2017, 121, 1814-1824.	2.5	39
11	Electrostatic Potential as a Harbinger of Cation Coordination:Â CF3SO3-Ion as a Model Example. Journal of Physical Chemistry A, 1997, 101, 5678-5686.	2.5	37
12	Theoretical Studies on Hydrogen Bonding, NMR Chemical Shifts and Electron Density Topography in Î±, Î² and Î³-Cyclodextrin Conformers. Journal of Physical Chemistry A, 2007, 111, 13583-13589.	2.5	37
13	Hydrogen Bond Energies and Cooperativity in Substituted Calix[n]arenes (n = 4, 5). Journal of Physical Chemistry A, 2012, 116, 3739-3744.	2.5	37
14	Electric Field Effects on Aromatic and Aliphatic Hydrocarbons:â€‰ A Density-Functional Study. Journal of Physical Chemistry A, 2007, 111, 9111-9121.	2.5	33
15		2.5	32
16	Hartree-Fock momentum expectation values for atoms and ions. Atomic Data and Nuclear Data Tables, 1983, 28, 477-491.	2.4	30
17	Inverted Cucurbit[n]urils: Density Functional Investigations on the Electronic Structure, Electrostatic Potential, and NMR Chemical Shifts. Journal of Physical Chemistry A, 2009, 113, 1368-1376.	2.5	27
18	Cavity diameter and height of cyclodextrins and cucurbit[n]urils from the molecular electrostatic potential topography. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2010, 66, 371-380.	1.6	27

#	Article	IF	Citations
19	Deciphering Noncovalent Interactions Accompanying 7,7,8,8â€Tetracyanoquinodimethane Encapsulation within Biphene[n]arenes: Nucleusâ€Independent Chemical Shifts Approach. ChemPhysChem, 2016, 17, 2197-2209.	2.1	27
20	On the Binding of SF₆to Cucurbit[6]uril Host: Density Functional Investigations. Journal of Physical Chemistry A, 2010, 114, 2338-2343.	2.5	24
21	Understanding Binding of Cyano-Adamantyl Derivatives to Pillar[6]arene Macrocycle from Density Functional Theory. Journal of Physical Chemistry A, 2016, 120, 8738-8749.	2.5	24
22	Radiation chemical oxidation of aniline derivatives. Perkin Transactions II RSC, 2001, , 1205-1211.	1.1	23
23	Electronic Structure and Normal Vibrations in (+)-Catechin and (â^')-Epicatechin Encapsulated Î²-Cyclodextrin. Journal of Physical Chemistry A, 2010, 114, 7725-7732.	2.5	23
24	Electronic structure, molecular electrostatic potential and spectral characteristics of pillar[6]arene hosts and their complexes with n-octyltriethylammonium ions. Physical Chemistry Chemical Physics, 2012, 14, 8711.	2.8	23
25	Benzo[Î±]phenoxazines and benzo[Î±]phenothiazine from vitamin K3: synthesis, molecular structures, DFT studies and cytotoxic activity. RSC Advances, 2015, 5, 57917-57929.	3.6	23
26	Kinetics and Mechanistic Investigations of Atmospheric Oxidation of HFO-1345fz by OH Radical: Insights from Theory. Journal of Physical Chemistry A, 2017, 121, 595-607.	2.5	23
27	From molecular electron density to electron momentum density. Physical Review A, 1984, 29, 3402-3405.	2.5	22
28	CO₂ Absorption Using Fluorine Functionalized Ionic Liquids: Interplay of Hydrogen and Ïƒ-Hole Interactions. Journal of Physical Chemistry A, 2016, 120, 1243-1260.	2.5	21
29	Electronic Structure and Normal Vibrations of CH3(OCH2CH2)nOCH3â^'M+â^'CF3SO3- (n = 2â^'4, M = Li, Na,) Tj ETQq1 1 0.784314 rgB	2.5	20
30	Theoretical studies in local coordination and vibrational spectra of M+CH3O(CH2CH2O)nCH3 (n=2â€“7) complexes (M=Na, K, Mg and Ca). Chemical Physics, 2006, 323, 595-605.	1.9	19
31	Synthesis and biological evaluation of copper(<scp>ii</scp>) pyrenethiosemicarbazone. RSC Advances, 2015, 5, 47476-47487.	3.6	19
32	Cooperative Hydrogen Bonding, Molecular Electrostatic Potentials, and Spectral Characteristics of Partial Thia-Substituted Calix[4]arene Macrocycles. Journal of Physical Chemistry A, 2016, 120, 7385-7397.	2.5	19
33	Encapsulation of rhodamine-6G within p-sulfonatocalix[n]arenes: NMR, photophysical behaviour and biological activities. RSC Advances, 2016, 6, 110206-110220.	3.6	19
34	Probing Molecular Interactions in Functionalized Asymmetric Quaternary Ammonium-Based Dicationic Ionic Liquids. Journal of Physical Chemistry A, 2016, 120, 7732-7744.	2.5	18
35	Encapsulation of benzimidazole derivatives within cucurbit[7]uril: Density functional investigations. Journal of Molecular Liquids, 2016, 216, 309-317.	4.9	18
36	Electronic Structure and ¹H NMR Chemical Shifts in Host-Guest Complexes of Cucurbit[6]uril and sym-Tetramethyl Cucurbit[6]uril with Imidazole Derivatives. Journal of Physical Chemistry A, 2010, 114, 10906-10916.	2.5	17

#	Article	IF	Citations
37	Electronic Structure, Molecular Electrostatic Potentials, Vibrational Spectra in Substituted Calix[n]arenes (n= 4, 5) from Density Functional Theory. Journal of Physical Chemistry A, 2011, 115, 10624-10637.	2.5	17
38	Density functional theory investigations on binding and spectral features of complexes of ferrocenyl derivatives with cucurbit [7]uril. Journal of Molecular Liquids, 2016, 216, 298-308.	4.9	17
39	Synthesis and biological activity of imidazole based 1,4-naphthoquinones. New Journal of Chemistry, 2020, 44, 6889-6901.	2.8	17
40	Theoretical investigations on structure, electrostatic potentials and vibrational frequencies of diglyme and Li+â€“(diglyme) conformers. Chemical Physics Letters, 2001, 344, 527-535.	2.6	16
41	Hostâ€“Guest Interactions Accompanying the Encapsulation of 1,4-Diazabicyclo[2.2.2]octane within endo-Functionalized Macrocycles. Journal of Physical Chemistry A, 2017, 121, 3792-3802.	2.5	14
42	Unveiling Noncovalent Interactions in Imidazolium, Pyrrolidinium, or Quaternary Ammonium Cation and Acetate Anion Based Protic Ionic Liquids: Structure and Spectral Characteristics. Journal of Physical Chemistry A, 2018, 122, 6225-6235.	2.5	14
43	Theoretical investigations on vibrational spectra of pillar[5]arene-bis(pyridinium) complexes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 104, 368-376.	3.9	13
44	The first naphthosemiquinone complex of K+ with vitamin K3 analog: Experiment and density functional theory. Journal of Molecular Structure, 2015, 1088, 56-63.	3.6	13
45	Understanding the Atmospheric Oxidation of HFE-7500 (C₃F₇CF(OC₂H₅)CF(CF₃)₂) Initiated by Cl Atom and NO₃ Radical from Theory. Journal of Physical Chemistry A, 2018, 122, 6799-6808.	2.5	13
46	Direct and reverse transformations between electron density and electron momentum density: Connection with the locally averaged method. Physical Review A, 1983, 28, 462-463.	2.5	12
47	Theoretical and experimental investigations on the structure and vibrational spectra of 2-hydroxy-3-methyl-1,4-naphthoquinone-1-oxime. Computational and Theoretical Chemistry, 2003, 622, 211-219.	1.5	12
48	Molecular electrostatic potentials and electron densities in nitroazacubanes. Journal of Chemical Physics, 2004, 120, 749-755.	3.0	12
49	Theoretical studies on the molecular electron densities and electrostatic potentials in azacubanes. Theoretical Chemistry Accounts, 2004, 112, 27-32.	1.4	12
50	Crystal structure, NMR and theoretical investigations on 2-(o-hydroxy-anilino)-1,4-napthoquinone. Journal of Molecular Structure, 2010, 966, 144-151.	3.6	12
51	Molecular structures of 2-hydroxy-1,4-naphthoqinone derivatives and their zinc(II) complexes: Combining experiment and density functional theory. Polyhedron, 2016, 113, 61-72.	2.2	12
52	Use of energy constraint for refinement of electron momentum distributions. Journal of Chemical Physics, 1984, 80, 1175-1178.	3.0	11
53	Theoretical investigations on structure, electrostatics potentials and vibrational frequencies of Li+ - CH3- O- (CH2- CH2- O)n- CH3 (n=3-7) conformers. Theoretical Chemistry Accounts, 2006, 115, 308-321.	1.4	11
54	Synthesis and Conformational Study of Chiral Oxepines: The Baylisâ€“Hillman Reaction and RCM Approach with Sugar Aldehyde. Journal of Organic Chemistry, 2009, 74, 6486-6494.	3.2	11

#	Article	IF	Citations
55	Binding of rhodamine B and kiton red S to cucurbit[7]uril: density functional investigations. Journal of Molecular Modeling, 2012, 18, 3743-3750.	1.8	11
56	Probing molecular interactions underlying imidazolium and pyridinium based ionic liquids. Journal of Molecular Liquids, 2015, 212, 885-899.	4.9	11
57	Electronic Structure, NMR, Spinâ€“Spin Coupling, and Noncovalent Interactions in Aromatic Amino Acid Based Ionic Liquids. Journal of Physical Chemistry A, 2016, 120, 5665-5684.	2.5	11
58	Electronic structure, spectral characteristics and physicochemical properties of linear, branched and cyclic alkyl group substituted 1-alkyl-3-butylimidazolium cation based ionic liquids. Journal of Molecular Liquids, 2018, 251, 394-406.	4.9	11
59	Molecular interactions and vibrations in CH3(OCH2CH2)2OCH3â€“M+â€“Xâ^' (M=Li, Na, K and X=PF6, AsF6,) Tj ETQq1 1 0.784314 r	1.5	10
60	Alkali metals (Li, Na, and K) in methyl phosphodiester hydrolysis. Physical Chemistry Chemical Physics, 2009, 11, 5253.	2.8	10
61	Electron density to electron momentum density: The use of an energy constraint. Physical Review A, 1983, 27, 3328-3331.	2.5	9
62	Hydrogen Bonding, ¹H NMR, and Molecular Electron Density Topographical Characteristics of Ionic Liquids Based on Amino Acid Cations and Their Ester Derivatives. Journal of Physical Chemistry A, 2015, 119, 8752-8764.	2.5	9
63	Bromine substituted aminonaphthoquinones: synthesis, characterization, DFT and metal ion binding studies. RSC Advances, 2016, 6, 88010-88029.	3.6	9
64	Density Functional Investigations on the Selective Binding of an endo-Functionalized Bis-urea Macrocycle. Journal of Physical Chemistry A, 2017, 121, 288-297.	2.5	9
65	Molecular insights for the HFO-1345fz +X (X = Cl, O3 or NO3) reaction and fate of alkoxy radicals initiated by Cl: DFT investigations. Journal of Fluorine Chemistry, 2017, 204, 65-75.	1.7	9
66	Modeling protic dicationic ionic liquids based on quaternary ammonium, imidazolium or pyrrolidinium cations and bis(trifluoromethanesulfonyl)imide anion: Structure and spectral characteristics. Journal of Molecular Graphics and Modelling, 2018, 85, 304-315.	2.4	9
67	Atmospheric degradation of HCFO-1233zd(E) initiated by OH radical, Cl atom and O3 molecule: Kinetics, reaction mechanisms and implications. Journal of Fluorine Chemistry, 2018, 211, 180-193.	1.7	9
68	Reactions of 2,3-dichloro-1,4-naphthoquinone with aminophenols: evidence for hydroxy benzophenoxazine intermediate and antibacterial activity. Journal of Molecular Structure, 2019, 1176, 194-206.	3.6	9
69	Probing Binding of Ethylated Pillar[5]arene with Pentene and Chlorobutane Positional Isomers. Journal of Physical Chemistry A, 2019, 123, 8391-8396.	2.5	9
70	Tautomerism in o-hydroxyanilino-1,4-naphthoquinone derivatives: Structure, NMR, HPLC and density functional theoretic investigations. Journal of Molecular Structure, 2016, 1123, 245-260.	3.6	8
71	Binding selectivity of vitamin K3 based chemosensors towards nickel(II) and copper(II) metal ions. Journal of Molecular Structure, 2017, 1143, 495-514.	3.6	8
72	X-ray structure, spectral characteristics, thermal and redox behavior of quinoline encapsulated in sulfonatocalix[4]arene. Journal of Molecular Liquids, 2017, 246, 187-196.	4.9	8

#	Article	IF	Citations
73	Crystal structures and biological activity of homologated (N)-n-alkylammonium salts of 2-bromo-3-oxido-1,4-naphthoquinone. Structural Chemistry, 2019, 30, 2257-2270.	2.0	8
74	Molecular electrostatic potentials and electron densities in nitrotriprismanes. Computational and Theoretical Chemistry, 2005, 724, 87-93.	1.5	7
75	Structure and spectral characteristics of diquat-cucurbituril complexes from density functional theory. Journal of Molecular Modeling, 2013, 19, 5113-5127.	1.8	7
76	Targeting a chemorefractory COLO205 (BRAF V600E) cell line using substituted benzo[Î±]phenoxazines. RSC Advances, 2015, 5, 82549-82563.	3.6	7
77	Partial rotation of the isopropyl group in the solid state: single-crystal-to-single-crystal phase transformation in a carvacrol derivative. CrystEngComm, 2015, 17, 7482-7485.	2.6	7
78	A computational study on structure and bonding in ion pairs accompanying pyrrolidinium and piperidinium based ionic liquids. Journal of Molecular Liquids, 2017, 234, 227-239.	4.9	7
79	Electron momentum distributions and atomicã€ˆrnã€‰expectation values. Physical Review A, 1982, 26, 1768-1770.	2.5	6
80	CH3OHâ‹¯(H2O)n [n = 1-4] clusters in external electric fields. Journal of Chemical Physics, 2015, 142, 214309.	3.0	6
81	Encaged molecules in external electric fields: A molecular â€œtug-of-warâ€• Journal of Chemical Physics, 2016, 145, 074302.	3.0	6
82	Polymorphism in chloro derivatives of 1,4-naphthoquinone: Experiment and density functional theoretic investigations. Journal of Molecular Structure, 2016, 1120, 281-293.	3.6	6
83	Encapsulation of creatinine within aryl extended calix[4]pyrrole derivatives: Insights from theory. Journal of Molecular Liquids, 2017, 247, 456-466.	4.9	6
84	Naphthoquinone based chemosensors for transition metal ions: experiment and theory. RSC Advances, 2017, 7, 55163-55174.	3.6	6
85	Distinct photophysical behaviour and transport of cell-impermeable [Ru(bpy)₂dppz]²⁺ in live cells using cucurbit[7]uril as a delivery system. Dalton Transactions, 2018, 47, 3857-3863.	3.3	6
86	p-Sulfonatocalixarene versus p-thiasulfonatocalixarene: encapsulation of tenofovir disoproxil fumarate and implications to ESI-MS, HPLC, NMR, DFT and anti-MRSA activities. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2021, 99, 43-59.	1.6	6
87	Ab initio and density functional studies on the structure and vibrational spectra of 2-hydroxy-1,4-naphthoquinone-1-oxime derivatives. Theoretical Chemistry Accounts, 2003, 110, 322-327.	1.4	5
88	Is high electric field capable of selectively inducing a covalent-like bond between polar and non-polar molecular species?. Theoretical Chemistry Accounts, 2009, 123, 501-511.	1.4	5
89	Binding of nitrophenol isomers to calix[n]arene (n=4, 6) hosts. Computational and Theoretical Chemistry, 2012, 991, 201-211.	2.5	5
90	Regioselective synthesis of a vitamin K3 based dihydrobenzophenazine derivative: its novel crystal structure and DFT studies. RSC Advances, 2015, 5, 76419-76423.	3.6	5

#	Article	IF	Citations
91	Exploring Chimeric Calix[4]tetrolarene Molecular Scaffolds: Theoretical Investigations. Journal of Physical Chemistry A, 2018, 122, 4189-4197.	2.5	4
92	Hydrogen Bonding versus Hâˆ’H Interactions in Pillar[n]arenes. ChemistrySelect, 2019, 4, 9354-9359.	1.5	3
93	Amphiphilic polypyridyl ruthenium complexes: Synthesis, characterization and aggregation studies. Polyhedron, 2019, 164, 96-107.	2.2	3
94	Perethylated pillar[n]arenes versus pillar[n]arenes: theoretical perspectives. Journal of Molecular Modeling, 2020, 26, 3.	1.8	3
95	Molecular Recognition, Conformational Behavior, and Spectral Characteristics of Oxatub[4]arene Macrocycle. Journal of Physical Chemistry A, 2018, 122, 714-723.	2.5	2
96	Electronic structure, vibrational spectra and 1H NMR chemical shifts of the ion pair composites within imidazolium functionalized geminal dicationic ionic liquids from density functional theory. Journal of Molecular Structure, 2020, 1201, 127112.	3.6	2
97	Enlightening binding behaviour of sulfonatocalix[4]arene receptor with 2-acetoxybenzoic acid through the lens of experiments and theory. Journal of Molecular Liquids, 2020, 320, 114417.	4.9	2
98	Supramolecular Binding of bisâ€naphthalene Cleft based Molecular Tubes. ChemistrySelect, 2018, 3, 10537-10542.	1.5	1
99	Design and synthesis of piezochromic materials exploring intermolecular charge transfer: chalconoids bound to the p-sulfonatocalix[6]arene macrocycle. Physical Chemistry Chemical Physics, 0, , .	2.8	1
100	Cu(ii) conjugation along the transformation of a vitamin K3derivative to a dinaphthoquinone methide radical. New Journal of Chemistry, 2014, 38, 277-284.	2.8	0
101	Regioselectivity in nonsymmetric methyl pentyl Pillar[5]arene bound to non-symmetric axles. Journal of Molecular Graphics and Modelling, 2020, 94, 107460.	2.4	0
102	1H and 13C NMR chemical shifts of 2-n-alkylamino-naphthalene-1,4-diones. Heliyon, 2021, 7, e06044.	3.2	0