K V Jovan Jose

List of Publications by Year
in descending order

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26	989	516710	580821
papers	citations	16	25
		h-index	g-index

27	27	27	1221
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Carbazole-based Ï€-conjugated 2,2â€²-Bipyridines, a new class of organic chromophores: Photophysical, ultrafast nonlinear optical and computational studies. Dyes and Pigments, 2021, 185, 108932.	3.7	17
2	A₂B- and A₃-Type Boron(III)Subchlorins Derived from meso-Diethoxycarbonyltripyrrane: Synthesis and Photophysical Exploration. Journal of Organic Chemistry, 2021, 86, 10280-10287.	3.2	6
3	1,2-Phenylene-Incorporated Smallest Expanded Calix[4]pyrrole via One-Step Synthesis of Tetrapyrrane: A Fluorescent Host for Fluoride Ion. Journal of Organic Chemistry, 2021, 86, 10536-10543.	3.2	6
4	Meso-Free Boron(III)subchlorin and Its Î¼-Oxo Dimer with Interacting Chromophores. Organic Letters, 2020, 22, 9735-9739.	4.6	8
5	BrÃ¸nsted Acid Promoted Thermalâ€Ringâ€Rearrangement of Fluorenopyrans to 2â€(1Hâ€Indenâ€3â€yl)â€9Hâ€fluorenâ€3â€ols Bearing Two Allâ€Carbonâ€Quaternary Centres. European Journal of Organic Chemistry, 2020, 2020, 2199-2209.	2.9	1
6	Synthetic access to calix[3]pyrroles via meso-expansion: hosts with diverse guest chemistry. Chemical Communications, 2020, 56, 5637-5640.	4.1	9
7	Experimental and theoretical investigation of intramolecular cooperativity in cyclic benzene trimer motif. RSC Advances, 2019, 9, 753-760.	3.6	1
8	Assessment of Fragmentation Strategies for Large Proteins Using the Multilayer Molecules-in-Molecules Approach. Journal of Chemical Theory and Computation, 2018, 14, 1383-1394.	5.3	29
9	Cooperative Formation of Icosahedral Proline Clusters from Dimers. Journal of the American Society for Mass Spectrometry, 2018, 29, 95-102.	2.8	3
10	Iodo-Cycloisomerization of Aryl(indol-3-yl)methane-Tethered Propargyl Alcohols to 3-Iodocarbazoles via Selective 1,2-Alkyl Migration. ACS Omega, 2018, 3, 15024-15034.	3.5	30
11	Fragment-Based Approaches for Supramolecular Interaction Energies: Applications to Foldamers and Their Complexes with Anions. Journal of Chemical Theory and Computation, 2018, 14, 6226-6239.	5.3	12
12	Fragment-Based Approach for the Evaluation of NMR Chemical Shifts for Large Biomolecules Incorporating the Effects of the Solvent Environment. Journal of Chemical Theory and Computation, 2017, 13, 1147-1158.	5.3	40
13	Moleculesâ€inâ€molecules fragmentâ€based method for the calculation of chiroptical spectra of large molecules: Vibrational circular dichroism and Raman optical activity spectra of alanine polypeptides. Chirality, 2016, 28, 755-768.	2.6	15
14	Raman Optical Activity Spectra for Large Molecules through Molecules-in-Molecules Fragment-Based Approach. Journal of Chemical Theory and Computation, 2016, 12, 585-594.	5.3	32
15	Molecules-in-molecules fragment-based method for the evaluation of Raman spectra of large molecules. Molecular Physics, 2015, 113, 3057-3066.	1.7	22
16	Evaluation of Energy Gradients and Infrared Vibrational Spectra through Molecules-in-Molecules Fragment-Based Approach. Journal of Chemical Theory and Computation, 2015, 11, 950-961.	5.3	39
17	Vibrational Circular Dichroism Spectra for Large Molecules through Molecules-in-Molecules Fragment-Based Approach. Journal of Chemical Theory and Computation, 2015, 11, 4238-4247.	5.3	40
18	Electrostatic Potential-Based Method of Balancing Charge Transfer Across ONIOM QM:QM Boundaries. Journal of Chemical Theory and Computation, 2014, 10, 4351-4359.	5.3	8

#	Article	IF	Citations
19	Construction of high-dimensional neural network potentials using environment-dependent atom pairs. Journal of Chemical Physics, 2012, 136, 194111.	3.0	107
20	Towards crystal structure prediction of complex organic compounds â€“ a report on the fifth blind test. Acta Crystallographica Section B: Structural Science, 2011, 67, 535-551.	1.8	358
21	Molecular tailoring approach for exploring structures, energetics and properties of clusters. Journal of Chemical Sciences, 2010, 122, 47-56.	1.5	30
22	Ab initio study on (CO₂)_nclusters via electrostaticsâ€•and molecular tailoringâ€based algorithm. International Journal of Quantum Chemistry, 2009, 109, 2238-2247.	2.0	19
23	An ab initio investigation on (CO2)n and CO2(Ar)m clusters: Geometries and IR spectra. Journal of Chemical Physics, 2008, 128, 124310.	3.0	33
24	Electrostatic guidelines and molecular tailoring for density functional investigation of structures and energetics of (Li)n clusters. Journal of Chemical Physics, 2008, 129, 164314.	3.0	23
25	Effect of matrix on IR frequencies of acetylene and acetylene-methanol complex: Infrared matrix isolation and ab initio study. Journal of Chemical Physics, 2007, 127, 104501.	3.0	46
26	Is there a hydrogen bond radius? Evidence from microwave spectroscopy, neutron scattering and X-ray diffraction results. New Journal of Chemistry, 2005, 29, 371.	2.8	50