

K V Jovan Jose

List of Publications by Year in descending order

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26
papers

989
citations

516710

16
h-index

580821

25
g-index

27
all docs

27
docs citations

27
times ranked

1221
citing authors

#	ARTICLE	IF	CITATIONS
1	Towards crystal structure prediction of complex organic compounds – a report on the fifth blind test. <i>Acta Crystallographica Section B: Structural Science</i> , 2011, 67, 535-551.	1.8	358
2	Construction of high-dimensional neural network potentials using environment-dependent atom pairs. <i>Journal of Chemical Physics</i> , 2012, 136, 194111.	3.0	107
3	Is there a hydrogen bond radius? Evidence from microwave spectroscopy, neutron scattering and X-ray diffraction results. <i>New Journal of Chemistry</i> , 2005, 29, 371.	2.8	50
4	Effect of matrix on IR frequencies of acetylene and acetylene-methanol complex: Infrared matrix isolation and <i>ab initio</i> study. <i>Journal of Chemical Physics</i> , 2007, 127, 104501.	3.0	46
5	Vibrational Circular Dichroism Spectra for Large Molecules through Molecules-in-Molecules Fragment-Based Approach. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4238-4247.	5.3	40
6	Fragment-Based Approach for the Evaluation of NMR Chemical Shifts for Large Biomolecules Incorporating the Effects of the Solvent Environment. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1147-1158.	5.3	40
7	Evaluation of Energy Gradients and Infrared Vibrational Spectra through Molecules-in-Molecules Fragment-Based Approach. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 950-961.	5.3	39
8	An <i>ab initio</i> investigation on (CO ₂) _n and CO ₂ (Ar) _m clusters: Geometries and IR spectra. <i>Journal of Chemical Physics</i> , 2008, 128, 124310.	3.0	33
9	Raman Optical Activity Spectra for Large Molecules through Molecules-in-Molecules Fragment-Based Approach. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 585-594.	5.3	32
10	Molecular tailoring approach for exploring structures, energetics and properties of clusters. <i>Journal of Chemical Sciences</i> , 2010, 122, 47-56.	1.5	30
11	Iodo-Cycloisomerization of Aryl(indol-3-yl)methane-Tethered Propargyl Alcohols to 3-Iodocarbazoles via Selective 1,2-Alkyl Migration. <i>ACS Omega</i> , 2018, 3, 15024-15034.	3.5	30
12	Assessment of Fragmentation Strategies for Large Proteins Using the Multilayer Molecules-in-Molecules Approach. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1383-1394.	5.3	29
13	Electrostatic guidelines and molecular tailoring for density functional investigation of structures and energetics of (Li) _n clusters. <i>Journal of Chemical Physics</i> , 2008, 129, 164314.	3.0	23
14	Molecules-in-molecules fragment-based method for the evaluation of Raman spectra of large molecules. <i>Molecular Physics</i> , 2015, 113, 3057-3066.	1.7	22
15	<i>Ab initio</i> study on (CO ₂) _n clusters via electrostatics and molecular tailoring-based algorithm. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2238-2247.	2.0	19
16	Carbazole-based π -conjugated 2,2'-Bipyridines, a new class of organic chromophores: Photophysical, ultrafast nonlinear optical and computational studies. <i>Dyes and Pigments</i> , 2021, 185, 108932.	3.7	17
17	Molecules-in-molecules fragment-based method for the calculation of chiroptical spectra of large molecules: Vibrational circular dichroism and Raman optical activity spectra of alanine polypeptides. <i>Chirality</i> , 2016, 28, 755-768.	2.6	15
18	Fragment-Based Approaches for Supramolecular Interaction Energies: Applications to Foldamers and Their Complexes with Anions. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 6226-6239.	5.3	12

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19	Synthetic access to calix[3]pyrroles <i>via meso</i> -expansion: hosts with diverse guest chemistry. <i>Chemical Communications</i> , 2020, 56, 5637-5640.	4.1	9
20	Electrostatic Potential-Based Method of Balancing Charge Transfer Across ONIOM QM:QM Boundaries. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4351-4359.	5.3	8
21	<i>Meso</i> -Free Boron(III)subchlorin and Its 1/4-Oxo Dimer with Interacting Chromophores. <i>Organic Letters</i> , 2020, 22, 9735-9739.	4.6	8
22	A ² - and A ³ -Type Boron(III)Subchlorins Derived from <i>meso</i> -Diethoxycarbonyltripyrrane: Synthesis and Photophysical Exploration. <i>Journal of Organic Chemistry</i> , 2021, 86, 10280-10287.	3.2	6
23	1,2-Phenylene-Incorporated Smallest Expanded Calix[4]pyrrole via One-Step Synthesis of Tetrapyrrene: A Fluorescent Host for Fluoride Ion. <i>Journal of Organic Chemistry</i> , 2021, 86, 10536-10543.	3.2	6
24	Cooperative Formation of Icosahedral Proline Clusters from Dimers. <i>Journal of the American Society for Mass Spectrometry</i> , 2018, 29, 95-102.	2.8	3
25	Experimental and theoretical investigation of intramolecular cooperativity in cyclic benzene trimer motif. <i>RSC Advances</i> , 2019, 9, 753-760.	3.6	1
26	Bronsted Acid Promoted Thermal Ring-Rearrangement of Fluorenoxyprans to 2-(1 <i>H</i> -inden-3-yl)-9 <i>H</i> -fluoren-3-ols Bearing Two All-Quaternary Centres. <i>European Journal of Organic Chemistry</i> , 2020, 2020, 2199-2209.	3.6	1