Rita Kakkar

List of Publications by Year
in descending order

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132 papers	3,066 citations	257101 24 h-index	197535 49 g-index
133 all docs	133 docs citations	133 times ranked	4446 citing authors

#	Article	IF	Citations
1	A combination strategy of structure-based virtual screening, MM-GBSA, cross docking, molecular dynamics and metadynamics simulations used to investigate natural compounds as potent and specific inhibitors of tumor linked human carbonic anhydrase IX. Journal of Biomolecular Structure and Dynamics, 2023, 41, 5465-5480.	2.0	8
2	A comparative study of different docking methodologies to assess the proteinâ€“ligand interaction for the E. coli MurB enzyme. Journal of Biomolecular Structure and Dynamics, 2022, 40, 11229-11238.	2.0	2
3	Identification of potent human carbonic anhydrase IX inhibitors: a combination of pharmacophore modeling, 3D-QSAR, virtual screening and molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2022, 40, 4516-4531.	2.0	8
4	II-VI core/shell quantum dots and doping with transition metal ions as a means of tuning the magnetoelectronic properties of CdS/ZnS core/shell QDs: A DFT study. Journal of Molecular Graphics and Modelling, 2022, 111, 108099.	1.3	12
5	Size-dependent structural and electronic properties of stoichiometric IIâ€“VI quantum dots and gas sensing ability of CdSe quantum dots: a DFT study. Journal of Nanoparticle Research, 2022, 24, .	0.8	2
6	The selective removal of Congo red using dumbbell-shaped hierarchically porous Ca-Mg mixed oxide. Applied Surface Science Advances, 2022, 8, 100221.	2.9	2
7	Exploring structural requirements of isoform selective histone deacetylase inhibitors: a comparative in silico study. Journal of Biomolecular Structure and Dynamics, 2021, 39, 502-517.	2.0	11
8	Structure-based virtual screening, free energy of binding and molecular dynamics simulations to propose novel inhibitors of Mtb-MurB oxidoreductase enzyme. Journal of Biomolecular Structure and Dynamics, 2021, 39, 656-671.	2.0	11
9	Chem-bioinformatic approach for drug discovery. , 2021, , 207-243.		1
10	DFT study of carbaryl pesticide adsorption on vacancy and nitrogen-doped graphene decorated with platinum clusters. Structural Chemistry, 2021, 32, 1541-1551.	1.0	5
11	Decontamination of chloropicrin (PS) and its analogues using graphene and modified graphene surfaces: a computational study. Structural Chemistry, 2021, 32, 1883-1892.	1.0	1
12	Theoretical investigation of the structural and electronic features of SLC-0111, a novel inhibitor of human carbonic anhydrase IX, and its anion. Structural Chemistry, 2021, 32, 1843-1856.	1.0	3
13	Computational Studies on Reactions of Some Organic Azides with Cî”H Bonds. ChemistrySelect, 2021, 6, 4368-4381.	0.7	2
14	In silico study of the synergistic anti-tumor effect of hybrid topoisomerase-HDAC inhibitors. Pure and Applied Chemistry, 2021, 93, 1213-1228.	0.9	1
15	A theoretical assessment of the structural and electronic features of some retrochalcones. International Journal of Quantum Chemistry, 2021, 121, e26797.	1.0	7
16	The antioxidant potential of retrochalcones isolated from liquorice root: A comparative DFT study. Phytochemistry, 2021, 192, 112964.	1.4	14
17	Synthetic methods and biological applications of retrochalcones isolated from the root of Glycyrrhiza species: A review. Results in Chemistry, 2021, 3, 100216.	0.9	5
18	An insight into selective and potent inhibition of histone deacetylase 8 through induced-fit docking, pharmacophore modeling and QSAR studies. Journal of Biomolecular Structure and Dynamics, 2020, 38, 48-65.	2.0	15

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19	Graphene-based adsorbents for water remediation by removal of organic pollutants: Theoretical and experimental insights. Chemical Engineering Research and Design, 2020, 153, 21-36.	2.7	48
20	Peanut shell biotemplate to fabricate porous magnetic Co3O4 coral reef and its catalytic properties for p-nitrophenol reduction and oxidative dye degradation. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2020, 604, 125328.	2.3	18
21	A DFT-D2 study on the adsorption of phosgene derivatives and chloromethyl chloroformate on pristine and Fe4-decorated graphene. Journal of Molecular Graphics and Modelling, 2020, 101, 107754.	1.3	12
22	The effect of solvent polarity on the antioxidant potential of echinatin, a retrochalcone, towards various ROS: a DFT thermodynamic study. Free Radical Research, 2020, 54, 777-786.	1.5	17
23	A comparative study of the binding modes of SLC-0111 and its analogues in the hCA II and hCA IX active sites using QM/MM, molecular docking, MM-GBSA and MD approaches. Biophysical Chemistry, 2020, 265, 106439.	1.5	9
24	A DFT-D2 study on Mo4-xCox (x = 0â€“3) cluster-decorated graphene and the adsorption of SO2F2 and SOF2 on Mo4-decorated graphene. Journal of Nanoparticle Research, 2020, 22, 1.	0.8	2
25	Recent Advances on Graphene-Based Gas Sensors. Russian Journal of Physical Chemistry A, 2020, 94, 2115-2120.	0.1	9
26	A DFT study of the conformational and electronic properties of echinatin, a retrochalcone, and its anion in the gas phase and aqueous solution. Structural Chemistry, 2020, 31, 2513-2524.	1.0	12
27	Selective adsorption and separation of toxic cationic dyes using hierarchically porous SDBS modified vaterite microspheres (Hr-SMV). Journal of Physics and Chemistry of Solids, 2020, 146, 109598.	1.9	20
28	Pharmacophore-enabled virtual screening, molecular docking and molecular dynamics studies for identification of potent and selective histone deacetylase 8 inhibitors. Computers in Biology and Medicine, 2020, 123, 103850.	3.9	9
29	Facile synthesis of mesoporous magnesium oxideâ€“graphene oxide composite for efficient and highly selective adsorption of hazardous anionic dyes. Research on Chemical Intermediates, 2020, 46, 2497-2521.	1.3	15
30	DFT study of adsorption of glyphosate pesticide on Pt-Cu decorated pyridine-like nitrogen-doped graphene. Journal of Nanoparticle Research, 2020, 22, 1.	0.8	17
31	Adsorptive Degradation of Phosmet Using Hierarchically Porous Calcium Oxide : An Experimental and Theoretical Study. ChemistrySelect, 2020, 5, 1235-1246.	0.7	7
32	Theoretical study of the structural features and antioxidant potential of 4-thiazolidinones. Structural Chemistry, 2020, 31, 1599-1608.	1.0	8
33	Adsorption of methyl isocyanate on M4 (M=Fe, Ni, and Cu) cluster-decorated graphene and vacancy graphene: a DFT-D2 study. Structural Chemistry, 2020, 31, 1983-1997.	1.0	16
34	Mesoporous rGO@ZnO composite: Facile synthesis and excellent water treatment performance by pesticide adsorption and catalytic oxidative dye degradation. Chemical Engineering Research and Design, 2020, 160, 254-263.	2.7	21
35	Combined approach of homology modeling, molecular dynamics, and docking: computer-aided drug discovery. Physical Sciences Reviews, 2019, 4, .	0.8	2
36	Isatin and its derivatives: a survey of recent syntheses, reactions, and applications. MedChemComm, 2019, 10, 351-368.	3.5	202

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37	Arousing the Reactive Fe Sites in Pyrite (FeS₂) via Integration of Electronic Structure Reconfiguration and in Situ Electrochemical Topotactic Transformation for Highly Efficient Oxygen Evolution Reaction. Inorganic Chemistry, 2019, 58, 7615-7627.	1.9	53
38	Synthesis and Reactions of Diazoketones. Organic Preparations and Procedures International, 2019, 51, 103-146.	0.6	11
39	Adsorption of Bromonitromethane over Grapheneâ€Based Substrates: A Density Functional Theory Analysis. ChemistrySelect, 2019, 4, 4967-4974.	0.7	8
40	Multifunctional mesoporous curcumin encapsulated iron-phenanthroline nanocluster: A new Anti-HIV agent. Colloids and Surfaces B: Biointerfaces, 2019, 180, 289-297.	2.5	24
41	Thiazolidinones: Synthesis, Reactivity, and Their Biological Applications. Journal of Heterocyclic Chemistry, 2019, 56, 1239-1253.	1.4	54
42	Hostâ€“guest complexation studies of p-tertbutylcalix[4]arene against ions of interest for radiological decontamination. Inorganica Chimica Acta, 2019, 484, 111-124.	1.2	11
43	Identification of novel urease inhibitors: pharmacophore modeling, virtual screening and molecular docking studies. Journal of Biomolecular Structure and Dynamics, 2019, 37, 4312-4326.	2.0	9
44	Pharmacophore modeling, 3D-QSAR and molecular docking studies of quinazolines and aminopyridines as selective inhibitors of inducible nitric oxide synthase. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950002.	1.8	1
45	Combined pharmacophore-guided 3D-QSAR, molecular docking, and virtual screening on bis-benzimidazoles and ter-benzimidazoles as DNAâ€“topoisomerase I poisons. Structural Chemistry, 2019, 30, 1185-1201.	1.0	8
46	Use of metal oxides for the adsorptive removal of toxic organic pollutants. Separation and Purification Technology, 2019, 211, 522-539.	3.9	92
47	Recent advances in nano-photocatalysts for organic synthesis. Arabian Journal of Chemistry, 2019, 12, 4550-4578.	2.3	49
48	Effects of increasing number of rings on the ion sensing ability of CdSe quantum dots: a theoretical study. Journal of Nanoparticle Research, 2018, 20, 1.	0.8	2
49	Nanocrystalline Hierarchical ZSM-5: An Efficient Catalyst for the Alkylation of Phenol with Cyclohexene. Journal of Nanoscience and Nanotechnology, 2018, 18, 5404-5413.	0.9	6
50	Structural, electronic, and reactivity parameters of some triorganotin(IV) carboxylates: a DFT analysis. Structural Chemistry, 2018, 29, 753-763.	1.0	9
51	Rearrangements in radical cations of diazoketones: A DFT mechanistic study. Computational and Theoretical Chemistry, 2018, 1134, 30-36.	1.1	1
52	In Silico study of the active site of Helicobacter pylori urease and its inhibition by hydroxamic acids. Journal of Molecular Graphics and Modelling, 2018, 83, 64-73.	1.3	20
53	Tertiary Butylation of Aniline Over Nanosized Zeolite Beta Catalyst. Journal of Nanoscience and Nanotechnology, 2018, 18, 7960-7968.	0.9	0
54	6. DFT studies on storage and adsorption capacities of gases on MOFs. , 2018, , 83-112.		0

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55	Magnetically retrievable one-pot fabrication of mesoporous magnesium ferrite (MgFe2O4) for the remediation of chlorpyrifos and real pesticide wastewater. Journal of Environmental Chemical Engineering, 2018, 6, 6891-6903.	3.3	38
56	DFT study on the adsorption of p-nitrophenol over vacancy and Pt-doped graphene sheets. Computational and Theoretical Chemistry, 2018, 1142, 88-96.	1.1	26
57	An evolving energy solution: Intermediate hydrogen storage. International Journal of Hydrogen Energy, 2018, 43, 12168-12188.	3.8	72
58	Design, Synthesis and Evaluation of 1Hâ€1,2,3â€Triazolâ€4â€ylâ€methyl Tethered 3â€Pyrrolylisatins as Potent Antiâ€Breast Cancer Agents. ChemistrySelect, 2018, 3, 5263-5268.	0.7	17
59	DFT studies on storage and adsorption capacities of gases on MOFs. Physical Sciences Reviews, 2018, 3, .	0.8	2
60	Influence of intrinsic and extrinsic factors on the antiradical activity of Gallic acid: a theoretical study. Structural Chemistry, 2018, 29, 359-373.	1.0	12
61	Theoretical investigation of organotin(IV) complexes of substituted benzohydroxamic acids. Computational and Theoretical Chemistry, 2018, 1138, 57-65.	1.1	2
62	Negative ion Wolff rearrangement of some diazoketones: A theoretical mechanistic study. Computational and Theoretical Chemistry, 2017, 1106, 50-57.	1.1	3
63	Theoretical study of the molecular structure and intramolecular proton transfer in benzohydroxamic acid. Computational and Theoretical Chemistry, 2017, 1105, 18-26.	1.1	13
64	Conformational properties of DNA minor groove binder Hoechst 33258 in gas phase and in aqueous solution. Computational and Theoretical Chemistry, 2017, 1113, 32-41.	1.1	9
65	Synthesis, pharmacological evaluation and molecular docking of pyranopyrazole-linked 1,4-dihydropyridines as potent positive inotropes. Molecular Diversity, 2017, 21, 533-546.	2.1	9
66	DFT study of structural and electronic properties of gallic acid and its anions in gas phase and in aqueous solution. Structural Chemistry, 2017, 28, 1789-1802.	1.0	31
67	Hierarchical Porous Magnesium Oxide (Hr-MgO) Microspheres for Adsorption of an Organophosphate Pesticide: Kinetics, Isotherm, Thermodynamics, and DFT Studies. ACS Applied Materials & Interfaces, 2017, 9, 38629-38642.	4.0	66
68	Bis-triazolylated-1,4-dihydropyridine - Highly selective hydrophilic fluorescent probe for detection of Fe3+. Dyes and Pigments, 2017, 147, 420-428.	2.0	29
69	Hierarchically structured magnesium based oxides: synthesis strategies and applications in organic pollutant remediation. CrystEngComm, 2017, 19, 6913-6926.	1.3	16
70	DFT studies on the acid-catalyzed Curtius reaction: the Schmidt reaction. Structural Chemistry, 2017, 28, 1743-1756.	1.0	8
71	In silico studies on potential MCF-7 inhibitors: a combination of pharmacophore and 3D-QSAR modeling, virtual screening, molecular docking, and pharmacokinetic analysis. Journal of Biomolecular Structure and Dynamics, 2017, 35, 1950-1967.	2.0	26
72	Design, synthesis and biological evaluation of antimalarial activity of new derivatives of 2,4,6-s-triazine. Chemistry Central Journal, 2017, 11, 132.	2.6	24

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73	Spectroscopic and molecular modelling studies of binding mechanism of metformin with bovine serum albumin. Journal of Molecular Structure, 2016, 1118, 267-274.	1.8	47
74	Theoretical study of the mechanism of the Wolff rearrangement of some diazocarbonyl compounds. Computational and Theoretical Chemistry, 2016, 1094, 32-41.	1.1	6
75	Docking Modes of BB-3497 into the PDF Active Site â€“ A Comparison of the Pure MM and QM/MM Based Docking Strategies. Current Computer-Aided Drug Design, 2015, 10, 315-326.	0.8	11
76	Adsorption of sarin on MgO nanotubes: Role of doped and defect sites. Journal of Computational Science, 2015, 10, 225-236.	1.5	26
77	Gallic acid: a versatile antioxidant with promising therapeutic and industrial applications. RSC Advances, 2015, 5, 27540-27557.	1.7	691
78	Assessment of molecular binding of Hoechst 33258 analogues into DNA using docking and MM/GBSA approach. Journal of Computational Science, 2015, 10, 166-177.	1.5	11
79	An insight into pyruvate dehydrogenase kinase (PDHK) inhibition through pharmacophore modeling and QSAR studies. Journal of Computational Science, 2014, 5, 558-567.	1.5	7
80	A Chloro-Bridged Heterobimetallic (Î·⁶-Arene)rutheniumâ€“Organotin Complex as an Efficient Topoisomerase IÎ± Inhibitor. Organometallics, 2013, 32, 2546-2551.	1.1	41
81	Theoretical investigation of the alloxan-dialuric acid redox cycle. International Journal of Quantum Chemistry, 2013, 113, 2060-2069.	1.0	14
82	Assessment of theoretical methods for the study of hydrogen abstraction kinetics of global warming gas species during their degradation and byproduct formation (IUPAC Technical Report). Pure and Applied Chemistry, 2013, 85, 1901-1918.	0.9	6
83	DFT STUDY OF SOME TRIVALENT d- AND f-BLOCK METAL ION COMPLEXES OF ALLOXAN. Journal of Theoretical and Computational Chemistry, 2013, 12, 1350052.	1.8	1
84	Structures and Stabilities of Alkaline Earth Metal Oxide Nanoclusters: A DFT Study. Journal of Theoretical Chemistry, 2013, 2013, 1-14.	1.5	21
85	Metal Ion Selectivity of Kojate Complexes: A Theoretical Study. Journal of Theoretical Chemistry, 2013, 2013, 1-9.	1.5	5
86	Theoretical Studies on Hydroxamic Acids. , 2013, , 19-53.		9
87	Quantum Dots For Diagnosis Of Cancers. Advanced Materials Letters, 2013, 4, 811-822.	0.3	12
88	Tautomeric transformations and reactivity of alloxan. Computational and Theoretical Chemistry, 2012, 986, 14-24.	1.1	23
89	Quantitative Structure Activity Relationship Study of 2,4,6â€Trisubstitutedâ€sâ€triazine Derivatives as Antimalarial Inhibitors of Plasmodium Falciparum Dihydrofolate Reductase. Chemical Biology and Drug Design, 2011, 77, 57-62.	1.5	22
90	Theoretical study of the kojic acid structure in gas phase and aqueous solution. International Journal of Quantum Chemistry, 2011, 111, 4318-4329.	1.0	13

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91	Role of surface modification of colloidal CdSe quantum dots on the properties of hybrid organicâ€“inorganic nanocomposites. Colloid and Polymer Science, 2010, 288, 841-849.	1.0	18
92	Controlling the assembly of hydrophobized gold nanoparticles at the airâ€“water interface by varying the interfacial tension. Thin Solid Films, 2010, 519, 1072-1077.	0.8	17
93	Surface modification of CdSe quantum dots for biosensing applications: Role of ligands. Thin Solid Films, 2010, 519, 1202-1212.	0.8	14
94	Size- and shape-controlled synthesis and properties of colloidal PbSe nanocrystals. Materials Chemistry and Physics, 2009, 113, 107-114.	2.0	24
95	Formation of water-soluble and biocompatible TOPO-capped CdSe quantum dots with efficient photoluminescence. Journal of Materials Science: Materials in Medicine, 2009, 20, 123-130.	1.7	11
96	The Curtius rearrangement of some organic azides: A DFT mechanistic study. International Journal of Quantum Chemistry, 2009, 109, 1058-1069.	1.0	30
97	Effect of aqueous solvation on the structures of pyruvic acid isomers and their reactions in solution: a computational study. Journal of Physical Organic Chemistry, 2008, 21, 23-29.	0.9	18
98	Structural aspects of the anti-cancer drug oxaliplatin: A combined theoretical and experimental study. Polyhedron, 2008, 27, 3567-3574.	1.0	33
99	Effect of surface passivating ligand on structural and optoelectronic properties of polymerâ€‰:â€‰CdSe quantum dot composites. Journal Physics D: Applied Physics, 2008, 41, 235409.	1.3	44
100	Density functional study of the conformations and intramolecular proton transfer in thiohydroxamic acids. Organic and Biomolecular Chemistry, 2007, 5, 547-557.	1.5	13
101	A novel non-TOPO route for the synthesis of colloidal CdSe quantum dots with high luminescence and stability. , 2007, , .		1
102	Metal ion complexes of thioformin: A density functional study. Polyhedron, 2007, 26, 5301-5308.	1.0	8
103	Preparation, properties and infrared spectral studies of N-(p-ethylphenyl)thiobenzohydroxamic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 68, 1362-1369.	2.0	3
104	A DFT study of the structures of pyruvic acid isomers and their decarboxylation. Organic and Biomolecular Chemistry, 2006, 4, 886.	1.5	28
105	First Principles Density Functional Study of the Adsorption and Dissociation of Carbonyl Compounds on Magnesium Oxide Nanosurfaces. Journal of Physical Chemistry B, 2006, 110, 25941-25949.	1.2	37
106	Density functional study of the properties of isomeric aminophenylhydroxamic acids and their copper (II) complexes. Polyhedron, 2006, 25, 759-766.	1.0	32
107	Metal ion selectivity of hydroxamates: A density functional study. Computational and Theoretical Chemistry, 2006, 767, 175-184.	1.5	17
108	Partial molar volumes and adiabatic compressibilities at infinite dilution of aminocarboxylic acids and glycylglycine in water and aqueous solutions of sodium sulphate at (288.15, 298.15 and 308.15)K. Journal of Chemical Thermodynamics, 2006, 38, 1385-1395.	1.0	44

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109	Spectral and theoretical studies of N-p-(ethylbenzene)thiobenzohydroxamic acid metal chelates. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 62, 819-825.	2.0	1
110	QSAR studies on the mechanism of radioprotection by Hoechst 33258 analogues. Computational and Theoretical Chemistry, 2005, 714, 35-42.	1.5	4
111	Theoretical study of unimolecular rearrangements of vinylidenes to acetylenes. International Journal of Quantum Chemistry, 2005, 102, 189-199.	1.0	6
112	Theoretical Study of Molecular Recognition by Hoechst 33258 Derivatives. Journal of Biomolecular Structure and Dynamics, 2005, 23, 37-47.	2.0	15
113	Theoretical studies on the mechanism of radioprotection by Hoechst 33258 derivatives. Computational and Theoretical Chemistry, 2004, 668, 243-248.	1.5	5
114	Trans and cis influence in square planar Pt(II) complexes: a density functional study of [PtClX(dms)2] and related complexes. Computational and Theoretical Chemistry, 2004, 679, 149-156.	1.5	19
115	Theoretical Study of the Adsorption of Formaldehyde on Magnesium Oxide Nanosurfaces:Â Size Effects and the Role of Low-Coordinated and Defect Sites. Journal of Physical Chemistry B, 2004, 108, 18140-18148.	1.2	67
116	Theoretical study of the effect of radiation on thymine. Computational and Theoretical Chemistry, 2003, 620, 139-147.	1.5	16
117	Density functional (DFT) study of acyloxy carbeneâ€“carbene rearrangements. Computational and Theoretical Chemistry, 2003, 626, 187-194.	1.5	1
118	C3H4: Density functional study of interconversion of isomers. International Journal of Quantum Chemistry, 2003, 94, 93-104.	1.0	14
119	Conformational behavior of some hydroxamic acids. Organic and Biomolecular Chemistry, 2003, 1, 2200.	1.5	50
120	Theoretical study of the excited state intramolecular proton transfer in barbituric acid. Computational and Theoretical Chemistry, 2002, 578, 169-175.	1.5	20
121	Theoretical study of tautomeric structures and fluorescence spectra of Hoechst 33258. Computational and Theoretical Chemistry, 2002, 579, 109-113.	1.5	80
122	Towards understanding the molecular recognition process in Hoechstâ€“DNA complexes. Computational and Theoretical Chemistry, 2002, 584, 37-44.	1.5	19
123	C3H4: density functional (DFT) study of structures and stabilities of isomers. Computational and Theoretical Chemistry, 2002, 617, 141-147.	1.5	13
124	Theoretical study of the excited singlet and triplet states of alloxan. International Journal of Quantum Chemistry, 2002, 86, 502-509.	1.0	2
125	Theoretical study of the mechanism of proton transfer in tautomeric systems: Alloxan. Journal of Chemical Sciences, 2001, 113, 297-306.	0.7	5
126	AM1 study of proton-transfer reactions of barbituric acid. International Journal of Quantum Chemistry, 1999, 74, 327-336.	1.0	9

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127	C3H4: Theoretical study of structures and stabilities of isomers. International Journal of Quantum Chemistry, 1998, 58, 389-398.	1.0	9
128	A semiempirical MO study of tautomerism and the electronic structure of barbituric acid. Journal of Chemical Sciences, 1998, 110, 535.	0.7	12
129	C3H4: Theoretical study of structures and stabilities of isomers. , 1996, 58, 389.		2
130	Theoretical study of the thermal unimolecular rearrangement of fluoroethylidenes. International Journal of Quantum Chemistry, 1992, 44, 363-377.	1.0	3
131	Unimolecular rearrangements of ethylnitrene: An exploratory theoretical study. Journal of Computational Chemistry, 1991, 12, 1211-1216.	1.5	0
132	Theoretical Study of the Stability of Tautomers and Conformers of Isatin-3-Thiosemicarbazone (IBT). Canadian Chemical Transactions, 0, , 327-342.	0.2	11