

# Abdo-Reza Nekoei

## List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Structural, electronic, vibrational and optical properties of all 23 isolated-pentagon rule isomers of C <sub>58</sub> N <sub>2</sub> azafullerene; a DFT study. Computational and Theoretical Chemistry, 2021, 1196, 113123.	2.5	3
2	Metal oxide adsorption on fullerene C <sub>60</sub> and its potential for adsorption of pollutant gases; density functional theory studies. RSC Advances, 2021, 11, 17377-17390.	3.6	15
3	Electronic transport behavior of 2-amino-4,5-bis(2,5-dimethylthiophen-3-yl)furan-3-carbonitrile (a) Tj ETQq1 1 0.784314 rgBT /Overlo Accounts, 2021, 140, 1.	1.4	2
4	DFT investigation on electrophilic and nucleophilic activities of some nitrogen-doped fullerenes, in comparison to C <sub>60</sub> . Structural Chemistry, 2020, 31, 385-397.	2.0	3
5	Nanoencapsulation of quercetin and curcumin in casein-based delivery systems. Food Hydrocolloids, 2019, 87, 394-403.	10.7	141
6	π-Hydrogen bonding and aromaticity: a systematic interplay study. Physical Chemistry Chemical Physics, 2019, 21, 623-630.	2.8	29
7	Development of casein-based nanoencapsulation systems for delivery of epigallocatechin gallate and folic acid. Food Science and Nutrition, 2019, 7, 519-527.	3.4	37
8	DFT investigation on some nitrogen-doped fullerenes with more antiradical and antioxidant activities than C <sub>60</sub> . Structural Chemistry, 2019, 30, 1737-1748.	2.0	6
9	Normal coordinate analysis of pyridine and its C <sub>2v</sub> 2 H-isotopomers. A new approach. Journal of Molecular Structure, 2018, 1151, 236-244.	3.6	4
10	Structure, isomerism, and vibrational assignment of aluminumtrifluoroacetylacetonate. An experimental and theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 190, 15-22.	3.9	6
11	Vibrational spectra, normal coordinate analysis, and hydrogen bond investigation of pyridinium perchlorate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 191, 558-565.	3.9	7
12	Efficient delivery of quercetin after binding to beta-lactoglobulin followed by formation soft-condensed core-shell nanostructures. Food Chemistry, 2017, 233, 282-289.	8.2	50
13	Theoretical study on azafullerene structures with many N-N connections, having an opening cavity. Computational and Theoretical Chemistry, 2017, 1121, 35-43.	2.5	3
14	Tautomerism, molecular structure, intramolecular hydrogen bond, and enol-enol equilibrium of para halo substituted 4,4,4-trifluoro-1-phenyl-1,3-butanedione; Experimental and theoretical studies. Journal of Molecular Structure, 2017, 1150, 427-437.	3.6	9
15	RAHB concept and π-skeleton in some oximes of 3-hydroxy fulvene; DFT, AIM, ELF and NBO studies. Structural Chemistry, 2015, 26, 1039-1048.	2.0	16
16	Introduction and theoretical investigation of new azafullerene structures with nitrogen belts. Computational and Theoretical Chemistry, 2015, 1067, 148-157.	2.5	8
17	Highly Efficient One-Pot Synthesis of N-Alkyl Sulfonamides from Alcohols Using N-(p-Toluenesulfonyl) Imidazole (Tsim). Phosphorus, Sulfur and Silicon and the Related Elements, 2014, 189, 465-476.	1.6	2
18	Blue to red electroluminescence emission from organic light-emitting diodes based on π-conjugated organic semiconductor materials. Journal of Photonics for Energy, 2014, 4, 043599.	1.3	11

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19	Conformational analysis, intramolecular hydrogen bonding, and vibrational assignment of 4,4-dimethyl-1-phenylpentane-1,3-dione. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 117, 284-298.	3.9	17
20	Theoretical study, and infrared and Raman spectra of copper(II) chelated complex with dibenzoylmethane. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 128, 272-279.	3.9	21
21	Generalized anomeric effect of $\beta$ -chloro-O-oxime ethers; influence of various substitutions by DFT, NBO and AIM studies. <i>Computational and Theoretical Chemistry</i> , 2014, 1029, 13-20.	2.5	1
22	Structure and vibrational assignment of bis(benzoylacetato)copper(II). <i>Journal of Molecular Structure</i> , 2014, 1058, 308-317.	3.6	28
23	Intramolecular hydrogen bonding and vibrational assignment of 1,1,1-trifluoro-5,5-dimethyl-2,4-hexanedione. <i>Journal of Molecular Structure</i> , 2014, 1076, 262-271.	3.6	17
24	An intramolecular hydrogen bond study in some Schiff bases of fulvene: a challenge between the RAHB concept and the $\beta$ -skeleton influence. <i>New Journal of Chemistry</i> , 2014, 38, 5886-5891.	2.8	20
25	Very strong intramolecular hydrogen bonding of 1,2-dithenoylcyclopentadiene; DFT and spectroscopic studies. <i>Journal of Molecular Structure</i> , 2014, 1075, 85-95.	3.6	4
26	8-Bromocaffeine (8-BC): A New Versatile Reagent for Conversion of $\alpha$ -Aldoximes into Nitriles. <i>Synlett</i> , 2012, 23, 1191-1198.	1.8	18
27	Conformation, molecular structure, and intramolecular hydrogen bonding of 1,1,1-trifluoro-5,5-dimethyl-2,4-hexanedione. <i>Journal of Molecular Structure</i> , 2012, 1021, 102-111.	3.6	17
28	Sensitive Ion-Flotation Separation of Ag(I) Traces Using 2-(2-Methoxyphenyl)benzimidazole before Flame Atomic Absorption Spectrometric Determination in Water. <i>Clean - Soil, Air, Water</i> , 2012, 40, 640-647.	1.1	0
29	Fabrication and electrical characterization of red organic light emitting diode using an isatin derivative as an organic chromophore. <i>Optical Engineering</i> , 2011, 50, 044002.	1.0	3
30	Ion-Flotation Separation of Cd(II), Co(II) and Pb(II) Traces Using a New Ligand before Their Flame Atomic Absorption Spectrometric Determinations in Colored Hair and Dryer Agents of Paint. <i>Journal of the Chinese Chemical Society</i> , 2011, 58, 199-206.	1.4	12
31	Conformational stability, molecular structure, intramolecular hydrogen bonding, and vibrational spectra of 5,5-dimethylhexane-2,4-dione. <i>Journal of Molecular Structure</i> , 2011, 998, 99-109.	3.6	17
32	Three-Component Synthesis of Some Novel N-Heterocycle Methyl-O-oxime Ethers. <i>Synthesis</i> , 2011, 2011, 4068-4076.	2.3	10
33	Structure, intramolecular hydrogen bonding, and vibrational spectra of 2,2,6,6-tetramethyl-3,5-heptanedione. <i>Journal of Molecular Structure</i> , 2010, 970, 160-170.	3.6	19
34	Conformation and vibrational spectra and assignment of 2-thenoyltrifluoroacetone. <i>Journal of Molecular Structure</i> , 2009, 932, 112-122.	3.6	31
35	Conformation, structure, intramolecular hydrogen bonding, and vibrational assignment of 4,4,4-trifluoro-1-(2-furyl)-1,3-butanedione. <i>Journal of Molecular Structure</i> , 2008, 882, 153-167.	3.6	12
36	Vibrational assignment and structure of dibenzoylmethane. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007, 66, 394-404.	3.9	57

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37	Vibrational assignment and structure of trifluorobenzoylacetone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007, 66, 626-636.	3.9	34
38	Vibrational assignment and structure of benzoylacetone: A density functional theoretical study. <i>Journal of Molecular Structure</i> , 2006, 794, 204-214.	3.6	33
39	CONFORMATIONAL STABILITY, MOLECULAR STRUCTURE, AND INTRAMOLECULAR HYDROGEN BONDING OF THENOYLTRIFLUOROACETONE. <i>Journal of Theoretical and Computational Chemistry</i> , 2006, 05, 647-664.	1.8	11