Aneta Buczek

List of Publications by Year
in descending order

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26 papers	293 citations	933264 10 h-index	940416 16 g-index
26 all docs	26 docs citations	26 times ranked	308 citing authors

#	Article	IF	Citations
1	Extrapolation of water and formaldehyde harmonic and anharmonic frequencies to the B3LYP/CBS limit using polarization consistent basis sets. Journal of Molecular Modeling, 2011, 17, 2029-2040.	0.8	30
2	Estimation of formamide harmonic and anharmonic modes in the Kohn-Sham limit using the polarization consistent basis sets. Journal of Molecular Modeling, 2011, 17, 2265-2274.	0.8	28
3	Anharmonic vibrational frequency calculations for solvated molecules in the B3LYP Kohnâ€“Sham basis set limit. Vibrational Spectroscopy, 2012, 63, 432-439.	1.2	25
4	Toward engineering efficient peptidomimetics. Screening conformational landscape of two modified dehydroaminoacids. Biopolymers, 2014, 101, 28-40.	1.2	21
5	DFT studies on the structural and vibrational properties of polyenes. Journal of Molecular Modeling, 2016, 22, 101.	0.8	21
6	Predicting the structure and vibrational frequencies of ethylene using harmonic and anharmonic approaches at the Kohnâ€“Sham complete basis set limit. Journal of Molecular Modeling, 2016, 22, 42.	0.8	21
7	On the convergence of zero-point vibrational corrections to nuclear shieldings and shielding anisotropies towards the complete basis set limit in water. Molecular Physics, 2017, 115, 144-160.	0.8	19
8	Effects of Side-Chain Orientation on the Backbone Conformation of the Dehydrophenylalanine Residue. Theoretical and X-ray Study. Journal of Physical Chemistry B, 2011, 115, 4295-4306.	1.2	15
9	On Complex Formation between 5-Fluorouracil and Î²-Cyclodextrin in Solution and in the Solid State: IR Markers and Detection of Short-Lived Complexes by Diffusion NMR. Molecules, 2020, 25, 5706.	1.7	13
10	Î²â€turn tendency in Nâ€methylated peptides with dehydrophenylalanine residue: DFT study. Biopolymers, 2012, 97, 518-528.	1.2	11
11	Estimating the carbonyl anharmonic vibrational frequency from affordable harmonic frequency calculations. Journal of Molecular Modeling, 2012, 18, 2471-2478.	0.8	10
12	Modeling red coral (Corallium rubrum) and African snail (Helixia aspersa) shell pigments: Raman spectroscopy versus DFT studies. Journal of Raman Spectroscopy, 2016, 47, 908-916.	1.2	10
13	Interaction of 5â€fluorouracil with Î²â€cyclodextrin: A density functional theory study with dispersion correction. International Journal of Quantum Chemistry, 2021, 121, e26487.	1.0	9
14	The effect of Î²â€methylation on the conformation of Î±, Î²â€dehydrophenylalanine: a DFT study. Journal of Peptide Science, 2009, 15, 465-473.	0.8	8
15	Factors Governing the Chemical Stability and NMR Parameters of Uracil Tautomers and Its 5-Halogen Derivatives. Molecules, 2020, 25, 3931.	1.7	8
16	1H and 13C shielding measurements in comparison with DFT calculations performed for two 2-(acetyloamino)-N,N-dimethyl-3-phenylacrylamide isomers. Chemical Physics Letters, 2015, 627, 1-6.	1.2	7
17	Local aromaticity mapping in the vicinity of planar and nonplanar molecules. Magnetic Resonance in Chemistry, 2019, 57, 359-372.	1.1	7
18	DFT study of Nâ€“HÂ·Â·Â·O hydrogen bond between model dehydropeptides and water molecule. Molecular Physics, 2014, 112, 639-644.	0.8	6

#	Article	IF	Citations
19	Impact of the Î”Phe configuration on the Boc-Gly-Î”Phe-NHMe conformation: experiment and theory. Structural Chemistry, 2019, 30, 1685-1697.	1.0	5
20	Convergence of nuclear magnetic shieldings and oneâ€bond ¹J(¹¹B¹H) indirect spinâ€“spin coupling constants in small boron molecules. Magnetic Resonance in Chemistry, 2018, 56, 338-351.	1.1	4
21	Spectroscopic characterization of non-covalent CuPc-GO system. Experiment and theory. Materials Chemistry and Physics, 2019, 231, 301-310.	2.0	4
22	On the aromaticity of uracil and its 5-halogeno derivatives as revealed by theoretically derived geometric and magnetic indexes. Structural Chemistry, 2021, 32, 275-283.	1.0	4
23	Performance of polarization-consistent vs. correlation-consistent basis sets for CCSD(T) prediction of water dimer interaction energy. Journal of Molecular Modeling, 2019, 25, 313.	0.8	3
24	Liposomes as nonspecific nanocarriers for 5-Fluorouracil in the presence of cyclodextrins. Journal of Molecular Liquids, 2021, 343, 117623.	2.3	2
25	Anharmonicity modeling in hydrogen bonded solvent dimers. Journal of Molecular Liquids, 2021, 339, 116735.	2.3	1
26	On the impact of side methyl groups on the structure and vibrational properties of Î²-carotenoids. The case of butadiene and isoprene. Food Chemistry, 2022, 369, 130880.	4.2	1