

Marek Freindorf

List of Publications by Year in descending order

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papers

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citations

394286

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32
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times ranked

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citing authors

#	ARTICLE	IF	CITATIONS
1	A comprehensive analysis of hydrogen bond interactions based on local vibrational modes. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3174-3187.	1.0	121
2	Lennard-Jones parameters for the combined QM/MM method using the B3LYP/6-31G*/AMBER potential. <i>Journal of Computational Chemistry</i> , 2005, 26, 1270-1278.	1.5	82
3	A New Method for Describing the Mechanism of a Chemical Reaction Based on the Unified Reaction Valley Approach. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 650-663.	2.3	41
4	New insights into Fe-H ₂ and Fe-H bonding of a [NiFe] hydrogenase mimic: a local vibrational mode study. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	34
5	Combined QM/MM Study of Thyroid and Steroid Hormone Analogue Interactions with Integrin. <i>Journal of Biomedicine and Biotechnology</i> , 2012, 2012, 1-12.	3.0	32
6	Interplay of Ring Puckering and Hydrogen Bonding in Deoxyribonucleosides. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7087-7103.	1.1	32
7	Energetics and Mechanism of the Hydrogenation of XH _n for Group IV to Group VII Elements X. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4931-4943.	2.3	30
8	Solving the Pericyclic-Pseudopericyclic Puzzle in the Ring-Closure Reactions of 1,2,4,6-Heptatetraene Derivatives. <i>Journal of Organic Chemistry</i> , 2016, 81, 404-414.	1.7	29
9	A Critical Evaluation of Vibrational Stark Effect (VSE) Probes with the Local Vibrational Mode Theory. <i>Sensors</i> , 2020, 20, 2358.	2.1	29
10	Local vibrational force constants – From the assessment of empirical force constants to the description of bonding in large systems. <i>Chemical Physics Letters</i> , 2020, 748, 137337.	1.2	27
11	Exceptionally Long Covalent CC Bonds – A Local Vibrational Mode Study. <i>Molecules</i> , 2021, 26, 950.	1.7	26
12	Hydrogen Bonding in Natural and Unnatural Base Pairs – A Local Vibrational Mode Study. <i>Molecules</i> , 2021, 26, 2268.	1.7	26
13	Chiral Discrimination by Vibrational Spectroscopy Utilizing Local Modes. <i>Chirality</i> , 2013, 25, 185-196.	1.3	25
14	Critical assessment of the FeC and CO bond strength in carboxymyoglobin: a QM/MM local vibrational mode study. <i>Journal of Molecular Modeling</i> , 2020, 26, 281.	0.8	24
15	The mechanism of the cycloaddition reaction of 1,3-dipole molecules with acetylene: an investigation with the unified reaction valley approach. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	23
16	New mechanistic insights into the Claisen rearrangement of chorismate – a Unified Reaction Valley Approach study. <i>Molecular Physics</i> , 2019, 117, 1172-1192.	0.8	22
17	Local Vibrational Mode Analysis of π-Hole Interactions between Aryl Donors and Small Molecule Acceptors. <i>Crystals</i> , 2020, 10, 556.	1.0	22
18	A Reaction Valley Investigation of the Cycloaddition of 1,3-Dipoles with the Dipolarophiles Ethene and Acetylene: Solution of a Mechanistic Puzzle. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8400-8418.	1.1	21

#	ARTICLE	IF	CITATIONS
19	Generative adversarial networks for transition state geometry prediction. <i>Journal of Chemical Physics</i> , 2021, 155, 024116.	1.2	21
20	Exploring the Mechanism of Catalysis with the Unified Reaction Valley Approach (URVA) – A Review. <i>Catalysts</i> , 2020, 10, 691.	1.6	20
21	Gold(I)-assisted catalysis – a comprehensive view on the [3,3]-sigmatropic rearrangement of allyl acetate. <i>Molecular Physics</i> , 2018, 116, 611-630.	0.8	18
22	Halogen Bonding Involving I ₂ and d ⁸ Transition-Metal Pincer Complexes. <i>Crystals</i> , 2021, 11, 373.	1.0	14
23	Metal–ring interactions in actinide sandwich compounds: A combined normalized elimination of the small component and local vibrational mode study. <i>Molecular Physics</i> , 2020, 118, e1768314.	0.8	14
24	Modeling Hydrogen Release from Water with Borane and Alane Catalysts: A Unified Reaction Valley Approach. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8978-8993.	1.1	12
25	Theoretical Insights into [NHC]Au(I) Catalyzed Hydroalkoxylation of Allenes: A Unified Reaction Valley Approach Study. <i>Journal of Organic Chemistry</i> , 2021, 86, 5714-5726.	1.7	11
26	A revised formulation of the generalized subsystem vibrational analysis (GSVA). <i>Theoretical Chemistry Accounts</i> , 2021, 140, 31.	0.5	6
27	Vibrational Analysis of Benziodoxoles and Benziodazolotetrazaoles. <i>Physchem</i> , 2021, 1, 45-68.	0.5	5
28	Characterizing the Metal–Ligand Bond Strength via Vibrational Spectroscopy: The Metal–Ligand Electronic Parameter (MLEP). <i>Topics in Organometallic Chemistry</i> , 2020, , 227-269.	0.7	3
29	BF ₃ –Catalyzed Diels–Alder Reaction between Butadiene and Methyl Acrylate in Aqueous Solution – An URVA and Local Vibrational Mode Study. <i>Catalysts</i> , 2022, 12, 415.	1.6	3
30	On the formation of CN bonds in Titan–™s atmosphere – a unified reaction valley approach study. <i>Journal of Molecular Modeling</i> , 2021, 27, 320.	0.8	2
31	A Closer Look at the Isomerization of 5-androstene-3,17-dione to 4-androstene-3,17-dione in Ketosteroid Isomerase. <i>Journal of Computational Biophysics and Chemistry</i> , 0, , 1-21.	1.0	2
32	Chemical Bonding in Homogenous Catalysis – Seen Through the Eyes of Vibrational Spectroscopy. , 2024, , 622-648.		0