

Gyula Tasi

List of Publications by Year in descending order

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52
papers

838
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516215

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all docs

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54
times ranked

773
citing authors

#	ARTICLE	IF	CITATIONS
1	Generation, Characterization, and Transformations of Unsaturated Carbenium Ions in Zeolites. <i>Chemical Reviews</i> , 1999, 99, 2085-2114.	23.0	131
2	Enumeration of the Conformers of Unbranched Aliphatic Alkanes. <i>Journal of Physical Chemistry A</i> , 1998, 102, 7698-7703.	1.1	45
3	The Origin of Systematic Error in the Standard Enthalpies of Formation of Hydrocarbons Computed via Atomization Schemes. <i>ChemPhysChem</i> , 2006, 7, 1664-1667.	1.0	45
4	Catalytic detoxification of C2-chlorohydrocarbons over iron-containing oxide and zeolite catalysts. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2005, 265, 171-177.	2.3	41
5	High-Accuracy Theoretical Thermochemistry of Atmospherically Important Sulfur-Containing Molecules. <i>Journal of Physical Chemistry A</i> , 2011, 115, 7823-7833.	1.1	36
6	Proton affinity and enthalpy of formation of formaldehyde. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2393-2409.	1.0	33
7	Hartreeâ€Fock-limit energies and structures with a few dozen distributed Gaussians. <i>Chemical Physics Letters</i> , 2007, 438, 139-143.	1.2	32
8	Calculation of electrostatic potential maps and atomic charges for large molecules. <i>Journal of Chemical Information and Computer Sciences</i> , 1993, 33, 296-299.	2.8	28
9	Positional Isomerization of Dialkyl-naphthalenes: A Comprehensive Interpretation of the Selective Formation of 2,6-DIPN over HM Zeolite. <i>Journal of Physical Chemistry A</i> , 2001, 105, 6513-6518.	1.1	27
10	Using molecular electrostatic potential maps for similarity studies. <i>Topics in Current Chemistry</i> , 1995, , 45-71.	4.0	25
11	Quantum algebraicâ€combinatoric study of the conformational properties of n-alkanes. II. <i>Journal of Mathematical Chemistry</i> , 2000, 27, 191-199.	0.7	21
12	Hydrogen bonding interactions of $\hat{\pm}$ -phenylcinnamic acid isomers in the liquid phase studied by IR and NMR spectroscopies and computational methods. <i>Journal of Molecular Structure</i> , 1995, 348, 57-60.	1.8	20
13	Scaled Effective One-Electron Method Based on G2 Theory: Results for Aliphatic Alkane Molecules. <i>Journal of Chemical Information and Computer Sciences</i> , 1998, 38, 632-638.	2.8	20
14	Investigation of the surface reactions of CCl ₄ on zeolites studied by IR and MAS NMR spectroscopy. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 1995, 101, 199-206.	2.3	19
15	High-Accuracy Theoretical Study on the Thermochemistry of Several Formaldehyde Derivatives. <i>Journal of Physical Chemistry A</i> , 2010, 114, 13213-13221.	1.1	19
16	Quantum algebraicâ€combinatoric study of the conformational properties of (n)-alkanes. I. <i>Journal of Mathematical Chemistry</i> , 1999, 25, 55-64.	0.7	17
17	Molecular shape, dimensions, and shape selective catalysis. <i>Computational and Theoretical Chemistry</i> , 2003, 666-667, 69-77.	1.5	16
18	Analysis of permanent electric dipole moments of aliphatic hydrocarbon molecules. <i>Computational and Theoretical Chemistry</i> , 1997, 401, 21-27.	1.5	15

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19	Preparation of monodispersed Pt nanoparticles in MCM-41, catalytic applications. <i>Catalysis Communications</i> , 2008, 9, 762-768.	1.6	15
20	Adiabatic Jacobi corrections on the vibrational energy levels of H ₂ ⁺ isotopologues. <i>Journal of Chemical Physics</i> , 2009, 130, 134314.	1.2	14
21	Representation of molecules by atomic charges: A new population analysis. <i>Journal of Computational Chemistry</i> , 1992, 13, 371-379.	1.5	13
22	Molecular Electrostatics, Energetics, and Dynamics of the Alkylation of Naphthalene: Positional Isomerization of Monoalkylnaphthalenes at Hartree-Fock and Correlated Levels with BSSE Corrections. <i>Journal of Physical Chemistry A</i> , 2000, 104, 1337-1345.	1.1	13
23	Conformational analysis of melatonin at Hartree-Fock ab initio level. <i>Computational and Theoretical Chemistry</i> , 2003, 640, 69-77.	1.5	13
24	Infrared spectroscopy studies of cyclohexene hydrogenation and dehydrogenation catalyzed by platinum nanoparticles supported on mesoporous silicate (SBA-15). Part 1: The role of particle size of Pt nanocrystals supported on SBA-15 silicate. <i>Catalysis Letters</i> , 2005, 101, 159-167.	1.4	13
25	Benchmarking Experimental and Computational Thermochemical Data: A Case Study of the Butane Conformers. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 479-486.	2.3	13
26	Formation of Carbocations from C ₆ Compounds in Zeolites. <i>Studies in Surface Science and Catalysis</i> , 1989, , 355-364.	1.5	12
27	1,5-Hydride shift in Wolff-Kishner reduction of (20R)-3 ¹ ,20, 26-trihydroxy-27-norcholest-5-en-22-one: synthetic, quantum chemical, and NMR studies. <i>Steroids</i> , 2002, 67, 31-38.	0.8	12
28	Shape-Selective Alkylation of Isopropylnaphthalene over HM Zeolite. A Theoretical Study. <i>Reaction Kinetics and Catalysis Letters</i> , 2001, 74, 317-322.	0.6	11
29	SYVA: A program to analyze symmetry of molecules based on vector algebra. <i>Computer Physics Communications</i> , 2017, 215, 156-164.	3.0	10
30	Generation Characterization, and Transformations of Unsaturated Carbenium Ions in Zeolites. (Chem.) Tj ETQq0 0 0 regBT /Overlock 10 T	2.3	9
31	Similarity analysis of the conformational potential energy surface of n-pentane. <i>Computational and Theoretical Chemistry</i> , 2011, 963, 378-383.	1.1	9
32	Enthalpy Differences of then-Pentane Conformers. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2679-2688.	2.3	9
33	Simple algebraic solutions to the kinetic problems of triangle, quadrangle and pentangle reactions. <i>Journal of Mathematical Chemistry</i> , 2016, 54, 85-99.	0.7	9
34	Adsorption-induced Fermi resonance among the vibrations of intermediates formed on Brønsted acidic zeolites. Spectroscopic and theoretical description. <i>Journal of Molecular Structure</i> , 1995, 351, 1-5.	1.8	7
35	A new program for effective one-electron (EHMO-ASED) calculations. <i>Computers & Chemistry</i> , 1997, 21, 319-325.	1.2	6
36	Analysis of Permanent Electric Dipole Moments of Aliphatic Hydrocarbon Molecules. 2. DFT Results. <i>Journal of Chemical Information and Computer Sciences</i> , 1998, 38, 313-316.	2.8	6

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37	The effect of electron correlation on the conformational space of melatonin. Journal of Computational Chemistry, 2008, 29, 1466-1471.	1.5	6
38	MEP maps as useful tools for prediction of selectivity of alkylations of fused N-heteroaromatics. Computational and Theoretical Chemistry, 1998, 455, 191-198.	1.5	5
39	The stereochemistry of the chemical expression of darkness. Computational and Theoretical Chemistry, 2003, 666-667, 515-520.	1.5	5
40	First-order chemical reaction networks I: theoretical considerations. Journal of Mathematical Chemistry, 2016, 54, 1863-1878.	0.7	5
41	Spectra of carbanions formed from allyl cyanide during isomerization in zeolite NaY-FAU with strong basic sites. Journal of Molecular Structure, 1995, 348, 345-348.	1.8	4
42	Semispectroscopic and Quantitative Structure-Property Relationship Estimates of the Equilibrium and Vibrationally Averaged Structure and Dipole Moment of 1-Buten-3-yne. Journal of Physical Chemistry A, 2005, 109, 4824-4828.	1.1	4
43	Energy decomposition based on the extended virial theorem: Hartree-Fock and second-order Møller-Plesset results. International Journal of Quantum Chemistry, 2009, 109, 2599-2605.	1.0	4
44	Comment on "Enthalpy Difference between Conformations of Normal Alkanes: Raman Spectroscopy Study of n-Pentane and n-Butane". Journal of Physical Chemistry A, 2010, 114, 6728-6728.	1.1	4
45	Analytical and numerical computation of error propagation of model parameters. Journal of Mathematical Chemistry, 2011, 49, 1322-1329.	0.7	4
46	An extension of the virial theorem for general wave functions. Chemical Physics Letters, 2007, 449, 221-226.	1.2	3
47	Comment on "Causation or only correlation? Application of causal inference graphs for evaluating causality in nano-QSAR models" by N. Sizochenko, A. Gajewicz, J. Leszczynski and T. Puzyn, <i>Nanoscale</i>, 2016, 8, 7203. <i>Nanoscale</i>, 2018, 10, 20863-20866.	2.8	3
48	Vector algebra and molecular symmetry: a tribute to Professor Josiah Willard Gibbs. Journal of Mathematical Chemistry, 2013, 51, 2187-2195.	0.7	2
49	Definitive thermochemistry and kinetics of the interconversions among conformers of <i>n</i>-butane and <i>n</i>-pentane. Journal of Computational Chemistry, 2018, 39, 424-437.	1.5	2
50	Conformational analysis of substituted (E)-4-phenylbut-3-en-2-ones. Computational and Theoretical Chemistry, 2003, 666-667, 131-134.	1.5	1
51	Comments on "Shape-selective diisopropylation of naphthalene in H-mordenite: Myth or reality?". Journal of Catalysis, 2011, 279, 229-230.	3.1	1
52	Molecular Shape, Dimensions, and Shape Selective Catalysis. ChemInform, 2004, 35, no.	0.1	0