

Toomas Tamm

List of Publications by Year in descending order

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40
papers

1,006
citations

471509

17
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414414

32
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42
docs citations

42
times ranked

1214
citing authors

#	ARTICLE	IF	CITATIONS
1	Density-Functional Theory Calculations of Aqueous Redox Potentials of Fourth-Period Transition Metals. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9997-10003.	2.5	141
2	Theory of the d ¹⁰ -d ¹⁰ Closed-Shell Attraction. 4. X(AuL) _n -Centered Systems. <i>Organometallics</i> , 1998, 17, 4842-4852.	2.3	82
3	Multicavity reaction field method for the solvent effect description in flexible molecular systems. <i>The Journal of Physical Chemistry</i> , 1993, 97, 11901-11907.	2.9	67
4	About the mutagenicity of chlorine-substituted furanones and halopropenals. A QSAR study using molecular orbital indices. <i>Mutation Research - Fundamental and Molecular Mechanisms of Mutagenesis</i> , 1991, 247, 97-102.	1.0	63
5	Enantioselective Organocatalytic Michael Addition of Aldehydes to β -Nitrostyrenes. <i>Journal of Organic Chemistry</i> , 2009, 74, 3772-3775.	3.2	57
6	M. O. calculations applicable to condensed phases: The combination of self-consistent reaction field theory with semi-empirical quantum-chemical methods. <i>Tetrahedron Computer Methodology</i> , 1989, 2, 295-304.	0.2	55
7	Reaction field effects on the electronic structure of carbon radical and ionic centers. <i>International Journal of Quantum Chemistry</i> , 1990, 37, 1-13.	2.0	53
8	Computational study of cation substitutions in apatites. <i>Journal of Solid State Chemistry</i> , 2006, 179, 1581-1587.	2.9	49
9	Calculations on indium and thallium cyclopentadienyls. Metal-metal interactions and possible new species. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 3441-3444.	2.8	41
10	Template-controlled synthesis of chiral cyclohexylhemicucurbit[8]uril. <i>Chemical Communications</i> , 2015, 51, 10921-10924.	4.1	38
11	Theoretical Investigation of a Parallel Catalytic Cycle in CO ₂ Hydrogenation by (PNP)IrH ₃ . <i>Organometallics</i> , 2015, 34, 4932-4940.	2.3	38
12	Calculation of hydration enthalpies of aqueous transition metal cations using two coordination shells and central ion substitution. <i>Chemical Physics Letters</i> , 2004, 400, 54-58.	2.6	36
13	Calculated Structures of MO ₂ ²⁺ , MN ₂ , and MP ₂ (M = Mo, W). <i>Journal of Physical Chemistry A</i> , 1997, 101, 8107-8114.	2.5	27
14	Identification and Structural Characterization of the Predominant Species Present in Alkaline Hydroxyberyllate Solutions. <i>Journal of the American Chemical Society</i> , 1998, 120, 2967-2968.	13.7	24
15	Reduced State of Iridium PCP Pincer Complexes in Electrochemical CO ₂ Hydrogenation. <i>ACS Catalysis</i> , 2016, 6, 3834-3839.	11.2	23
16	Calculations of hydrated titanium ion complexes: structure and influence of the first two coordination spheres. <i>Chemical Physics Letters</i> , 2001, 342, 667-672.	2.6	21
17	pK _a calculation for monoprotonated biperidine, bismorpholine and their derivatives in H ₂ O and MeCN. <i>Chemical Physics Letters</i> , 2010, 485, 83-86.	2.6	19
18	Computational and ion mobility MS study of (all-S)-cyclohexylhemicucurbit[6]uril structure and complexes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 19198-19205.	2.8	17

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19	UV-visible spectra of some nitro-substituted porphyrins. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 1995, 85, 119-126.	3.9	14
20	Synthesis, EPR and DFT calculations of rare Ag(II)porphyrins and the crystal structure of [Zn(II)tetrakis(4-bromo-2-thiophene)porphyrin]. <i>Inorganic Chemistry Communication</i> , 2008, 11, 1019-1022.	3.9	14
21	MulticavitySCRF calculation of ion hydration energies. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 339-348.	2.0	13
22	Can triple bonds exist between gold and main-group elements?. <i>Theoretical Chemistry Accounts</i> , 1998, 99, 113-115.	1.4	13
23	Calculations for XeO _n (n= 2-4): Could the Xenon Dioxide Molecule Exist?. <i>Journal of Physical Chemistry A</i> , 2000, 104, 3826-3828.	2.5	13
24	Organocatalytic asymmetric addition of malonates to unsaturated 1,4-diketones. <i>Beilstein Journal of Organic Chemistry</i> , 2012, 8, 1452-1457.	2.2	12
25	Comparison of theoretical models of solvation. <i>International Journal of Quantum Chemistry</i> , 1996, 60, 1585-1594.	2.0	10
26	Stability and Conformation of Polycopper ^{II} Thiolate Clusters Studied by Density Functional Approach. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9157-9164.	2.5	10
27	Study of Radical Merostabilization by Electrospray FTICR/MS. <i>Journal of the American Chemical Society</i> , 1996, 118, 11905-11911.	13.7	8
28	2-Substituted agelasine analogs: Synthesis and biological activity, and structure and reactivity of synthetic intermediates. <i>Pure and Applied Chemistry</i> , 2011, 83, 645-653.	1.9	8
29	Formation and trapping of the thermodynamically unfavoured inverted-hemicucurbit[6]uril. <i>Chemical Communications</i> , 2019, 55, 9307-9310.	4.1	7
30	Using theoretical descriptors to model solvent effects in the isomerization of cis-stilbene. <i>International Journal of Quantum Chemistry</i> , 1996, 60, 1595-1606.	2.0	5
31	Structure and stability of gold-substituted diborane, boranes, and borohydride ions. <i>Theoretical Chemistry Accounts</i> , 2000, 103, 399-408.	1.4	5
32	Possible high-pressure structures of sulfur trioxide Electronic supplementary information (ESI) available: technical details for calculations. See http://www.rsc.org/suppdata/cc/b1/b107778c/ . <i>Chemical Communications</i> , 2002, , 336-337.	4.1	5
33	Theoretical prediction and assignment of vicinal ¹ H- ¹ H coupling constants of diastereomeric 3-alkoxy-6,7-epoxy-2-oxabicyclo[3.3.0]octanes. <i>Magnetic Resonance in Chemistry</i> , 2011, 9, 49, 76-82.		5
34	Linearization of moment tensor potentials for multicomponent systems with a preliminary assessment for short-range interaction energy in water dimer and trimer. <i>Journal of Chemical Physics</i> , 2020, 152, 164115.	3.0	5
35	Influence of protonation upon the conformations of biperidine, bismorpholine, and their derivatives. <i>Chemical Physics Letters</i> , 2009, 471, 92-96.	2.6	4
36	Calculated tautomeric equilibria and X-ray structures of 2-substituted N-methoxy-9-methyl-9H-purin-6-amines. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 349-358.	1.4	2

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37	Effect of New Superhard Phases Formation on Properties of Composite Processed by SHS. Key Engineering Materials, 0, 527, 137-142.	0.4	1
38	Synthesis of Superhard Lightweight Composites and Improvement of Their Properties via Chemical Processing. , 2018, , 53-61.		1
39	Inclusion of Additional Coordination Sphere into Cluster-Model Redox Potential Calculations. AIP Conference Proceedings, 2007, , .	0.4	0
40	Isomers and conformers of complexes of $Ti(OiPr)_4$ with cyclopentane-1,2-dione: NMR study and DFT calculations. International Journal of Quantum Chemistry, 2014, 114, 1012-1018.	2.0	0