Toomas Tamm

List of Publications by Year
in descending order

40 papers	1,006 citations	471509 17 h-index	414414 32 g-index
42 all docs	42 docs citations	42 times ranked	1214 citing authors

#	Article	IF	Citations
1	Linearization of moment tensor potentials for multicomponent systems with a preliminary assessment for short-range interaction energy in water dimer and trimer. Journal of Chemical Physics, 2020, 152, 164115.	3.0	5
2	Formation and trapping of the thermodynamically unfavoured inverted-hemicucurbit[6]uril. Chemical Communications, 2019, 55, 9307-9310.	4.1	7
3	Synthesis of Superhard Lightweight Composites and Improvement of Their Properties via Chemical Processing. , 2018, , 53-61.		1
4	Reduced State of Iridium PCP Pincer Complexes in Electrochemical CO₂ Hydrogenation. ACS Catalysis, 2016, 6, 3834-3839.	11.2	23
5	Template-controlled synthesis of chiral cyclohexylhemicucurbit[8]uril. Chemical Communications, 2015, 51, 10921-10924.	4.1	38
6	Theoretical Investigation of a Parallel Catalytic Cycle in CO₂ Hydrogenation by (PNP)IrH₃. Organometallics, 2015, 34, 4932-4940.	2.3	38
7	Isomers and conformers of complexes of Ti(OiPr)₄ with cyclopentaneâ€1,2â€dione: NMR study and DFT calculations. International Journal of Quantum Chemistry, 2014, 114, 1012-1018.	2.0	0
8	Computational and ion mobility MS study of (all-S)-cyclohexylhemicucurbit[6]uril structure and complexes. Physical Chemistry Chemical Physics, 2014, 16, 19198-19205.	2.8	17
9	Organocatalytic asymmetric addition of malonates to unsaturated 1,4-diketones. Beilstein Journal of Organic Chemistry, 2012, 8, 1452-1457.	2.2	12
10	Calculated tautomeric equilibria and X-ray structures of 2-substituted N-methoxy-9-methyl-9H-purin-6-amines. Theoretical Chemistry Accounts, 2011, 129, 349-358.	1.4	2
11	Theoretical prediction and assignment of vicinal ¹Hâ€“¹H coupling constants of diastereomeric 3â€alkoxyâ€6,7â€epoxyâ€2â€oxabicyclo[3.3.0]octanes. Magnetic Resonance in Chemistry, 2011, 49, 76-82.	1.9	5
12	2-Substituted agelasine analogs: Synthesis and biological activity, and structure and reactivity of synthetic intermediates. Pure and Applied Chemistry, 2011, 83, 645-653.	1.9	8
13	pKa calculation for monoprotonated bipiperidine, bimorpholine and their derivatives in H2O and MeCN. Chemical Physics Letters, 2010, 485, 83-86.	2.6	19
14	Influence of protonation upon the conformations of bipiperidine, bimorpholine, and their derivatives. Chemical Physics Letters, 2009, 471, 92-96.	2.6	4
15	Stability and Conformation of Polycopperâ^'Thiolate Clusters Studied by Density Functional Approach. Journal of Physical Chemistry A, 2009, 113, 9157-9164.	2.5	10
16	Enantioselective Organocatalytic Michael Addition of Aldehydes to Î²-Nitrostyrenes. Journal of Organic Chemistry, 2009, 74, 3772-3775.	3.2	57
17	Synthesis, EPR and DFT calculations of rare Ag(II)porphyrins and the crystal structure of [Zn(II)tetrakis(4-bromo-2-thiophene)porphyrin]. Inorganic Chemistry Communication, 2008, 11, 1019-1022.	3.9	14
18	Inclusion of Additional Coordination Sphere into Cluster-Model Redox Potential Calculations. AIP Conference Proceedings, 2007, , .	0.4	0

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19	Computational study of cation substitutions in apatites. Journal of Solid State Chemistry, 2006, 179, 1581-1587.	2.9	49
20	Calculation of hydration enthalpies of aqueous transition metal cations using two coordination shells and central ion substitution. Chemical Physics Letters, 2004, 400, 54-58.	2.6	36
21	Density-Functional Theory Calculations of Aqueous Redox Potentials of Fourth-Period Transition Metals. Journal of Physical Chemistry A, 2003, 107, 9997-10003.	2.5	141
22	Possible high-pressure structures of sulfur trioxideElectronic supplementary information (ESI) available: technical details for calculations. See http://www.rsc.org/suppdata/cc/b1/b107778c/. Chemical Communications, 2002, , 336-337.	4.1	5
23	Calculations of hydrated titanium ion complexes: structure and influence of the first two coordination spheres. Chemical Physics Letters, 2001, 342, 667-672.	2.6	21
24	Structure and stability of gold-substituted diborane, boranes, and borohydride ions. Theoretical Chemistry Accounts, 2000, 103, 399-408.	1.4	5
25	Calculations for XeOn(n= 2â^'4):Â Could the Xenon Dioxide Molecule Exist?â€. Journal of Physical Chemistry A, 2000, 104, 3826-3828.	2.5	13
26	Calculations on indium and thallium cyclopentadienyls. Metalâ€“metal interactions and possible new species. Physical Chemistry Chemical Physics, 1999, 1, 3441-3444.	2.8	41
27	Can triple bonds exist between gold and main-group elements?. Theoretical Chemistry Accounts, 1998, 99, 113-115.	1.4	13
28	Theory of the d10â^'d10Closed-Shell Attraction. 4. X(AuL)nm+Centered Systems. Organometallics, 1998, 17, 4842-4852.	2.3	82
29	Identification and Structural Characterization of the Predominant Species Present in Alkaline Hydroxyberyllate Solutions. Journal of the American Chemical Society, 1998, 120, 2967-2968.	13.7	24
30	Calculated Structures of MO22+, MN2, and MP2 (M = Mo, W). Journal of Physical Chemistry A, 1997, 101, 8107-8114.	2.5	27
31	Study of Radical Merostabilization by Electrospray FTICR/MS. Journal of the American Chemical Society, 1996, 118, 11905-11911.	13.7	8
32	Comparison of theoretical models of solvation. International Journal of Quantum Chemistry, 1996, 60, 1585-1594.	2.0	10
33	Using theoretical descriptors to model solvent effects in the isomerization ofcis-stilbene. International Journal of Quantum Chemistry, 1996, 60, 1595-1606.	2.0	5
34	UV-visible spectra of some nitro-substituted porphyrins. Journal of Photochemistry and Photobiology A: Chemistry, 1995, 85, 119-126.	3.9	14
35	MulticavitySCRF calculation of ion hydration energies. International Journal of Quantum Chemistry, 1994, 52, 339-348.	2.0	13
36	Multicavity reaction field method for the solvent effect description in flexible molecular systems. The Journal of Physical Chemistry, 1993, 97, 11901-11907.	2.9	67

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37	About the mutagenicity of chlorine-substituted furanones and halopropenals. A QSAR study using molecular orbital indices. Mutation Research - Fundamental and Molecular Mechanisms of Mutagenesis, 1991, 247, 97-102.	1.0	63
38	Reaction field effects on the electronic structure of carbon radical and ionic centers. International Journal of Quantum Chemistry, 1990, 37, 1-13.	2.0	53
39	M. O. calculations applicable to condensed phases: The combination of self-consistent reaction field theory with semi-empirical quantum-chemical methods. Tetrahedron Computer Methodology, 1989, 2, 295-304.	0.2	55
40	Effect of New Superhard Phases Formation on Properties of Composite Processed by SHS. Key Engineering Materials, 0, 527, 137-142.	0.4	1