

### Calculated tautomeric equilibria and X-ray structures of 2-substituted N-methoxy-9-methyl-9H-purin-6-amines

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### Calculation of hydration enthalpies of aqueous transition metal cations using two coordination shells and central ion substitution

**Uudsemaa, Merle**; **Tamm, Toomas** Chemical physics letters 2004 / 1/3, lk. 54-58 : ill  
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### Controlling chirogenic effects in porphyrin based supramolecular systems: theoretical analysis versus experimental observations

**Osadchuk, Irina**; **Luts, Hanna-Eliisa**; **Zahharova, Aleksandra**; **Tamm, Toomas**; **Borovkov, Victor** ChemPhysChem 2024 / art. e202400104 <https://doi.org/10.1002/cphc.202400104> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

### A DFT study of an organocatalytic enantioselective Mannich reaction under the sway of noncovalent interactions

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### Efficient defect-driven cation exchange beyond the nanoscale semiconductors toward antibacterial functionalization

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### Investigation of the solar cell materials Cu(In,Ga)Se<sub>2</sub> and Cu<sub>2</sub>ZnSnS<sub>4</sub> with muon spin spectroscopy and density-functional calculations

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### Isomers and conformers of complexes of Ti(OiPr)<sub>4</sub> with cuclopentane-1,2-dione : NMR study and DFT calculations

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### Redox potentials from DFT calculations

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### Shortfall of B3LYP in reproducing NMR JCH couplings in some isomeric epoxy structures with strong stereoelectronic effects : a benchmark study on DFT functionals

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### Solution-mediated inversion of SnSe to Sb<sub>2</sub>Se<sub>3</sub> thin-films

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### Supramolecular chirogenesis in a sterically hindered Porphyrin : a critical theoretical analysis

**Osadchuk, Irina**; **Luts, Hanna-Eliisa**; **Norvaiša, Karolis**; **Borovkov, Victor**; **Senge, Mathias O.** Chemistry : a European journal 2023 / art. e202301408 <https://doi.org/10.1002/chem.202301408>

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**Synthesis, EPR and DFT calculations of rare Ag(II)porphyrins and the crystal structure of [Zn(II)tetrakis(4-bromo-2-thiophene)porphyrin]**

Ghazzali, Mohamed; Abu-Youssef, Morsy; Larsson, Krister; Hansson, Örjan; Amer, Adel; **Tamm, Toomas**; Öhström, Lars Inorganic chemistry communications 2008 / 9, p. 1019-1022 : ill <https://www.sciencedirect.com/science/article/pii/S1387700308002281>

**2-Substituted agelasine analogs : Synthesis and biological activity, and structure and reactivity of synthetic intermediates**

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