

Poster session I

1. **A. Antušek**, M. Jaszunski: Coupled cluster studies of NMR shielding constants and spin-rotation constants in SiH₄, PH₃ and H₂S molecules
2. **J. Brabec**: The state specific multireference Brillouin-Wigner coupled cluster method: The singlet-triplet gap of trimethylenemethane; The ring-opening of methylenecyclopropane
3. **A. Bronowska**, C. A. Laughton, S. H. Homans: Estimation of entropy of D-galactose in complex with L-arabinose binding protein from MD simulation
4. **H. Cybulski**, J. Sadlej: On the calculations of the nuclear shielding constants in small water cluster
5. **A. Hamza**, I. Papi: Revealing the mechanism of asymmetric organocatalytic reactions
6. **D. Hrivňák**, L. Mlejnecká, I. Janeček, R. Kalus: Dynamics of excited rare gas cluster cations
7. **M. Ilčin**, V. Lukeš, D. Vegh, V. Laurinc: Theoretical characterisation of thiophene-anthrone π -conjugated derivatives
8. **A. Jurkiewicz**: Interaction of thymidylate synthase with dUMP and its C(5)-OH, C(5)-CH₂OH and C(5)-OCH₃ analogues - molecular dynamics study
9. **J. Kaminski**, R. W. Gora, J. Leszczynski: From van der Waals interactions to a chemical bond. An ab initio study of the nature of interactions between the methyl cation and the rare gas atoms
10. **F. Karlický**, R. Kalus: Accurate ab initio three-body potential for argon
11. **S. Kedžuch**: Alternative formulation of the matrix elements in R12 theory
12. **A. M. Kelterer, V. Lukeš**, T. Palszegi: Time-dependant Density Functional Method versus CEO Method: a comparison for the optical excitation in dicyano-p-phenylenediamine
13. **K. Kowalska**, M. Musial, S. A. Kucharski: Harmonic and anharmonic frequencies in the excited states with EOM-CC method
14. **I. Paidarová**, S. P. A. Sauer: MCSCF calculations of C6 coefficients of hydrogenhalides
15. **J. J. Szymczak**, Jan Urban, S. Roszak, J. Leszczynski: The influence of the micro-solvation on the proton affinity of ammonia