

- This weeks (40) topics: Graph isomorphism (traces), Ring Perception, Hanser Algorithm.

- Mandatory Reading:

- McKay, B.D. and Piperno, A., Practical Graph Isomorphism, II, Journal of Symbolic Computation, 60 (2014), pp.94-112. (understand the core difference between traces and nauty)
- Franziska Berger, Christoph Flamm, Petra M. Gleiss, Josef Leydold, Peter F. Stadler: *Counterexamples in Chemical Ring Perception*. Journal of Chemical Information and Modeling 44(2): 323-331 (2004)
- Section 2.5 of the book by Gasteiger et al. (for an easy introduction)
- Hanser T, Jauffret P, Kaufmann G, (1996), *A New Algorithm for Exhaustive Ring Perception in a Molecular Graph*. J Chem Inf Comput Sci, 36(6):1146-1152. DOI:10.1021/ci960322f

- Recommended Reading:

- Downs, G.M., Gillet, V.J., Holliday, J.D., Lynch, M.F.: *Theoretical aspects of ring perception and development of the extended set of smallest rings concept*. Journal of Chemical Information and Computer Sciences, 187-206 (1989)