- This weeks (10) topics (Ring perception also next week): Graph isomorphism (traces), SMILES, Ring Perception, Hanser Algorithm.

- We are currently working on a C++ implementation for graph canonicalisation. The source code, developed by Jakob L Andersen, can be found in the dm840 directory in the terminal room.

- Mandatory Reading:

  - Mandatory Reading: Articles by Weininger (SMILES1 and SMILES2, see blackboard). Please note again, that the graph canonicalisation described in these articles is not correct.

  - 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)