• This week's (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.


  – Section 2.5 of the book by Gasteiger et al. (for an easy introduction)


• Recommended Reading: