

- Next week (38) the lectures will be on Monday and Tuesday. On Tuesday Martin Hanczyc from FKF will introduce us to HCN chemistry.  
<http://flint.sdu.dk/index.php?page=martin-hanczyc>  
[http://www.ted.com/talks/martin\\_hanczyc\\_the\\_line\\_between\\_life\\_and\\_not\\_life.html](http://www.ted.com/talks/martin_hanczyc_the_line_between_life_and_not_life.html)
- This weeks (37) topics: More on graph isomorphism, McKay's Canonical Graph Labeling Algorithm, Ring Perception, Hanser Algorithm.

- Mandatory Reading:

- Section 2.5 of the book by Gasteiger et al.
- S. G. Hartke and A. Radcliffe. *McKay's canonical graph labeling algorithm*. In Communicating Mathematics, volume 479 of Contemporary Mathematics, pages 99-111. American Mathematical Society, (2009).
- 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)
- 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)