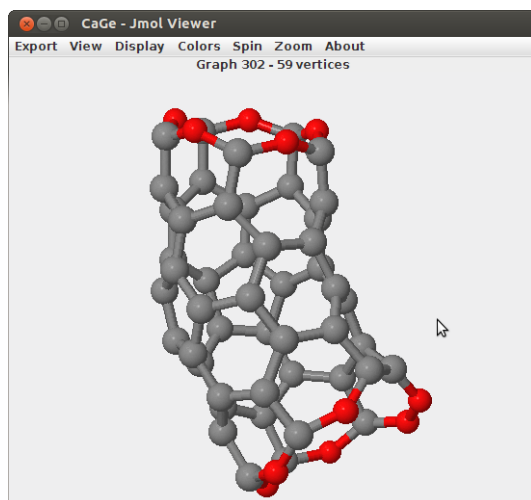# Structure Generation: Applications, Methods, Problems and Solutions.

Gunnar Brinkmann
Gunnar.Brinkmann@UGent.be
Applied Mathematics, Computer Science and Statistics
Ghent University

The intention of this talk is to present structure generation to a public that has not yet worked in this field. First some applications of structure generation will be presented to motivate its usefulness. We will present applications from chemistry and mathematics. Then examples of generation problems related to chemistry will be given. The problems to be solved in order to get an efficient algorithm differ a lot in these cases: for polycyclic hydrocarbons with a given number of rings, isomorphism rejection is the main problem to be solved. For other classes of molecules – e.g. fullerenes, nanotubes and nanojoins – the main problem is how to obtain valid structures. The key idea that allowed to develop efficient algorithms for the last 3 classes is by Andreas Dress who proposed to use a Petri-path decomposition for the decomposition of fullerenes.