Computer Applications in Chemistry: Visualisation of Chemical Reactions and Generation of QSAR Models

Within the scope of this work methods and computer programs for visualising chemical reactions and a software tool for the generation of quantitative structure activity relationships (QSAR) were developed.

The visualisation of chemical reactions by means of computer animations shall serve a better understanding of underlying reaction mechanisms. To this end, a system of programs (*CAVOC*) was developed that allows the user to follow animations of precalculated organic reaction mechanisms in a three dimensional ball&stick representation via the internet. By adding isosurfaces mapped with certain physical properties (orbitals, electron and spin densities, electrostatic potentials) the user is given the ability to rate the effect of these properties in terms of the process of the reaction.
This work describes the implementation of *CAVOC*'s components, the Java 3D based applet and the server responsible for the calculation of the isosurfaces. In addition, a brief introduction to the underlying calculations of the reactions is given.

QSAR (Quantitative Structure Activity Relationship) models play a major role in modern drug design. Therefore a modular system was developed that allows modeling of such relationships by means of correlating activities of chemical compounds with so called molecular descriptors. Mathematical methods used within this program are PLS (Partial Least Squares) and KNN (K Nearest Neighbours). In order to obtain a highly predictive, accurate model, redundant descriptors are eliminated under the control of the leave one out method with help of either genetic algorithms or simulated annealing.
Satisfying results were obtained by testing the final program with a know dataset from the literature. A new variant of the KNN method (KNN with weighted distances) showed slightly better predictive character than the original implementation.