reaction clips

High-quality visualisation of chemical reactions

A joint project of the University of Applied Arts Vienna and the University of Vienna

Background

Teaching Organic Chemistry or Medicinal Chemistry requires a lot imagination by students in order to fully understand what actually happens during a chemical reaction. The usual ways of 2-dimensional depiction is fine for quickly capturing the reaction type and the nature of reactants and products. However, a better understanding of mechanistic aspects would definitely benefit from a good animated visualisation of the entire reaction process. For this purpose, various cartoon-like animations have been utilised in chemical education in the past, but these approaches usually represent (more or less coarse) approximations and abstractions of reality. In the present project, we aim at a novel way of high-quality visualisation of a selected set of chemical reactions in combination with a highly accurate description of these reactions by state-of-the-art quantum chemistry calculations. The results are available in different formats:

a) high-definition video clips for lecture-hall projection

b) interactive 3D Flash animations for incorporation in web pages and for download

Calculations

All reaction paths were obtained by ab-initio quantum chemistry calculations, using the Gaussian 09 software package at the Schrödinger III cluster (University of Vienna) and at the Vienna Scientific Cluster.

Example clips

These video clips can be best viewed with a dedicated video player software like VLC.
SN1 reaction (monomolecular nucleophilic substitution)
SN2 reaction (bimolecular nucleophilic substitution)
bromination of benzene (electrophilic aromatic substitution)

Example 3D animations

bromination of benzene (electrophilic aromatic substitution)

Auxiliary material

For special didactic purposes, Flash animations are perfectly suited to complement the video clips, e.g. for depiction of resonance structures of pi-electron systems.
resonance structures of aniline
resonance structures of phenolate
resonance structures of 4-nitrophenolate

Project partners

Visualisation (video, 3D animations):

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Institute of Technical Chemistry
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Quantum-chemical calculations:

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Institute of Theoretical Chemistry
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Didactic concept, 2D animations:

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