Exploitation of Solar Energy

Mikkelsen, Kurt V.

Department of Chemistry, University of Copenhagen, Copenhagen, Denmark
Contact: kmi@chem.ku.dk

Purpose of the Project

The Sun delivers within an hour to Earth an amount of energy similar to that consumed by all humans in one year. One major challenge for society is to be able to store solar energy. Our fundamental hypothesis is that we can store energy in chemical bonds via light-induced isomerization reactions of photoactive molecules as illustrated in Fig. 1. Upon irradiation, molecule A is converted to the high-energy photo-isomer B, which upon a certain trigger will return to A and release the absorbed energy as heat. This corresponds to a closed-energy cycle of light-harvesting, energy storage and release, with no emission of CO_2. The overall purpose of this project is to develop suitable organic molecules for such cycles based on fundamental structure-property relationships (SPRs).

We will focus on the dihydroazulene (DHA) – vinylheptafulvene (VHF) couple (Fig. 2), being attractive as only the DHA to VHF reaction is photoinduced.

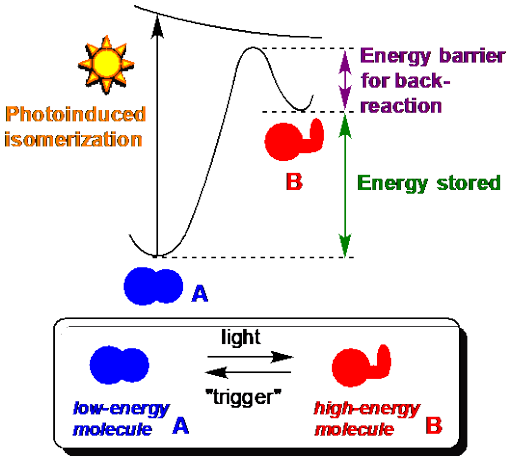

Fig. 1: *Energy storage using photoswitch.*

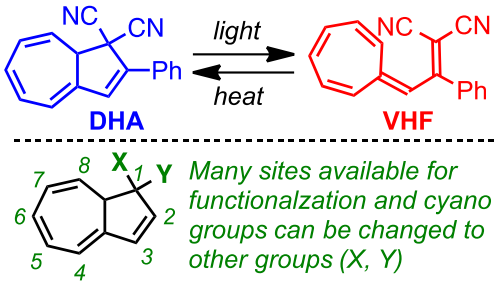

Fig. 2: *DHA-VHF couple and numbering.*

Recent Publications

A.B. Skov, S.L. Broman, A.S. Gertsen, J. Elm, M. Jevric, M. Cacciarini, A. Kadziola, K. V. Mikkelsen, M. B. Nielsen:"Aromaticity-Controlled Energy Storage Capacity of the Dihydroazulene-Vinylheptafulvene Photochromic System" Chemistry-A European Journal, 22, 14567-14575 (2016)

F.E. Storm, S.T. Olsen, T. Hansen, L. De Vico, N.E. Jackson, M.A. Ratner, K.V.Mikkelsen: "Boron Subphthalocyanine Based Molecular Triad Systems for the Capture of Solar Energy" The Journal of Physical Chemistry A, 120, 7694-7703 (2016)

M. H. Hansen, J. Elm, S. T. Olsen, A. N. Gejl, F. E. Storm, B. N. Frandsen, Anders B Skov, M. B. Nielsen, H. G. Kjaergaard, Kurt V Mikkelsen:"Theoretical Investigation of Substituent Effects on the Dihydroazulene/Vinylheptafulvene Photoswitch: Increasing the Energy Storage Capacity" The Journal of Physical Chemistry A, 120, 9782-9793 (2016)

A. S. Gertsen, S. T. Olsen, S. L. Broman, M. B. Nielsen, K. V. Mikkelsen:"A DFT Study of Multimode Switching in a Combined DHA/VHF-DTE/DHB System for Use in Solar Heat Batteries" The Journal of Physical Chemistry C, 121, 195-201 (2017)

M. D. Kilde, M. H. Hansen, S. L. Broman, Kurt V. Mikkelsen, M. B. Nielsen: "Expanding the Hammett Correlations for the Vinylheptafulvene Ring-Closure Reaction", European Journal of Organic Chemistry, 2017, 1052-1062 (2017)