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Exploitation of solar energy

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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.

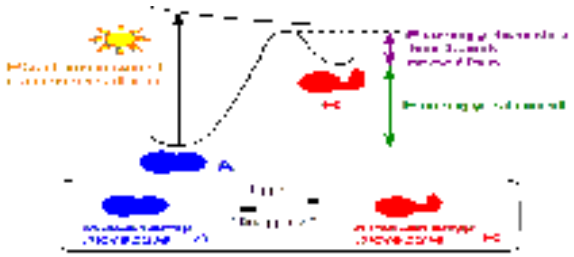

Fig. 2: DHA-VHF couple and numbering.

Recent publications

1. S Gertsen, S T Olsen, S L Broman, M B Nielsen and K V Mikkelsen (2017) 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.
2. M D Kilde, M H Hansen, S L Broman, Kurt V Mikkelsen and M B Nielsen (2017) Expanding the hammett correlations for the vinylheptafulvene ring-closure reaction. European Journal of Organic Chemistry 2017:1052-1062.
3. A B Skov, S L Broman, A S Gertsen, J Elm, M Jevric, et al. (2016) Aromaticity-controlled energy storage capacity of the dihydroazulene-vinylheptafulvene photochromic system. Chemistry-A European Journal, 22:14567-14575.
4. F E Storm, S T Olsen, T Hansen, L De Vico, N E Jackson, et al. (2016) Boron subphthalocyanine based molecular triad systems for the capture of solar energy. The Journal of Physical Chemistry A 120:7694-7703.
5. M H Hansen, J Elm, S T Olsen, A N Gejl, F E Storm, at el. (2016) Theoretical investigation of substituent effects on the dihydroazulene/vinylheptafulvene photoswitch: increasing the energy storage capacity. The Journal of Physical Chemistry A 120: 9782-9793.

Biography

Mikkelsen Kurt V and his group use scientific computing methods to investigate the dynamics and control of molecular perturbations, solvent effects, chemical reactions in homogeneous and heterogeneous environments. Presently, he is focused on areas such as biophotonics (design of optimal two-photon sensitizers), photonics (structure-property relationships for potential optical data and computer components), nanoscience (linear and nonlinear optical properties of carbon nanotubes), development of new models for homogeneous and heterogeneous solvation along with the calculation of linear and non-linear molecular properties of solutes and development of new models to describe interactions between nanosized particles and organic molecules along with the calculation of kinetic parameters used in macroscopic modelling in nanoscience and atmospheric chemistry. In the last four years he has investigated and developed methods for the capture and storage of solar energy.

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