

Photoswitching of Redox Potentials and Spectroscopic Properties in the UV/vis Region

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The photoswitching of optical and electrochemical properties of di-donor, di-acceptor and donor-acceptor substituted photochromic tetrahydropyrene – [2,2]metacyclophanene and dihydropyrene – [2,2]metacyclophanediene systems has been studied theoretically. A switching of the half-wave oxidation and reduction potentials should be possible in the case of bis(pyridinium) and bis(hydroxyphenyl) substituted systems. Because of the relatively great perturbation of the planarity of the π -electron systems by large torsion of the substituents out of the π -electron structure of the photochromic system and the stair-like structure of the ring-opened isomer, relatively large excitation energies for CT transitions have been calculated with the AM1-CI procedure. The ring-closed structures should absorb in the visible spectral region, and the open-ring isomers should have a longest-wavelength absorption in the UV region.

Key words: Photoswitching, Redox Properties, Absorption spectra in UV/vis