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Absorption spectra and activity of s-tetrazine derivatives on [4+2] Diels-Alder cycloaddition reaction

Derivatives of s-tetrazine (R-T-R') are theoretical studied to examine the effect of the connected groups (R and R') to their absorption spectra and their reactivities on Diels-Alder cycloaddition. In case of absorption spectra, all s-tetrazine derivatives have absorption spectrum about 550nm which cause by n⟶π*transition in the tetrazine ring. Another absorption peak around 300-450nm can only be observed when electron donating groups OH, NH2 and phenyl were added to the tetrazine ring which correspond to the* π⟶π transition and their aptitudes follow their strengths of the electron donating groups (except OH-T-H, OH-T-COOH and NH2-T-COOH). In case of electron withdrawing groups attached to the tetrazine ring, it does not change a peak at 550 nm but cause the red shift and reduce adsorption strength of 300-450 nm region. For reaction activities of s-tetrazine derivatives when reacted with ethylene. The molecular electronic structures state that the reaction follows the inverse electron demand Diels-Alder addition fashion. The activation energies for this reaction increase when an electron donating groups is added but decrease when an electron withdrawing group is attached to the tetrazine ring.

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