Regioselectivity in the Diels-Alder reaction of 8,8-dimethylnaphthalene-1,4,5(8H)-trione with 2,4-hexadien-1-ol

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The Diels-Alder reactions of 8,8-dimethylnaphtalene-1,4,5(8H)-trione with 2,4-hexadien-1-ol and its O-acetyl derivative were investigated in different solvents. The regiochemistry of the cycloaddition of the hexadienol was determined through chemical correlation of one of the products. The solvent effect on the regioselectivity and endo/exo selectivity of this reaction is attributed to intermolecular hydrogen bonding between the hydroxyl group of the diene and the carbonyl oxygen atoms at C-4 and C-5 of the quinone in the transition state. The possible transition states have been modelled by AMI calculations in order to better interpret these experimental results.