A computational study of the Diels-Alder reactions between 2,3-dibromo-1,3-butadiene and maleic anhydride

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The neutral and cationic Diels-Alder-type reactions between 2,3-dibromo-1,3-butadiene and maleic anhydride have been computationally explored as the first step of a combined experimental and theoretical study. Density functional theory calculations show that the neutral reaction is concerted while the cationic reaction can be either concerted or stepwise. Further isomerizations of the Diels-Alder products have been studied in order to predict possible fragmentation pathways in gas-phase experiments. Rice-Ramsperger-Kassel-Marcus (RRKM) calculations suggest that under single-collision experimental conditions the neutral product may reform the reactants and the cationic product will most likely eliminate CO2.
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