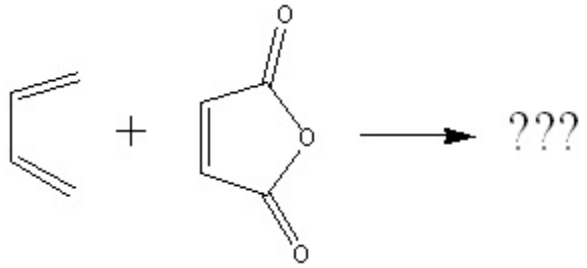
9 Transition States

The Diels-Alder Reaction

α,β-unsaturated carbonyl compounds undergo an exceedingly useful reaction with conjugated dienes known as the Diels-Alder reaction. In this *cycloaddition* reaction, C-1 and C-4 of the conjugated diene become attached to the doubly-bonded carbons of the unsaturated carbonyl compound to form a six-membered ring. The reaction involves systems with 4π electrons (diene) and 2π electrons (dienophile), and is therefore a [4+2] cycloaddition.

We will look at a simple Diels-Alder reaction involving butadiene and maleic anhydride:



Click Templates / Transition States / Diels-Alder. A template representing the transition structure is drawn where atoms 1, 2, 3 and 4 are the four C atoms from the *cis*-butadiene and atoms 5 and 6 are from the C=C maleic anhydride.
Click the add H tool to remove the H atoms from the structure.
Use the draw, periodic table, and add bonds tools to construct the rest of the maleic anhydride. Click the add H tool and Save as dielsts.pcm.
Minimize and record $\Delta_f H$ = _____ kcal mol^{-1}.
Draw a molecule of *cis*-butadiene. Save as cisbut.pcm. Minimize and record $\Delta_f H$ = _____ kcal mol^{-1}.
Draw a molecule of maleic anhydride. Save as maleic.pcm. Minimize and record $\Delta_f H$ = _____ kcal mol^{-1}.
Calculate $\Delta H^{\ddagger} = \Delta_f H(\ddagger) - \Delta_f H(\text{maleic}) - \Delta_f H(cis)$ = _____ kcal mol^{-1}.
Save and Close.