Electronic Supplementary Information

Indium Triflate-Catalysed Diels-Alder Reactions of Isochromenylium Cations with Enones

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Copies of $^1$H and $^{13}$C NMR spectra for compounds 3a-n and 5a-c and computation details and optimized geometries of transition states TS-1 and TS-2
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Computation details and optimised geometries of transition states TS-1 and TS-2:

The Density Functional Theory (DFT) calculation was performed using the Gaussian 03 package. The level of approximation used was B3LYP with a basis set LanL2DZ in dichloroethane medium. The electronic energy of TS-1 is \(-3026.85489823\) a.u. and that of TS-2 is \(-3026.79516153\) a.u. This implies that TS-1 is 37.4856 kcal mol\(^{-1}\) more stable than TS-2.

![Figure 1. The optimised geometry of TS-1](image1)

![Figure 2. The optimised geometry of TS-2](image2)