



Supplementary Fig. S1. Bond scan to ensure the correct transition state.

Supplementary Fig. S1 illustrates a relaxed potential energy surface (PES) scan along the C1-C2 bond in CS5, with a total of 20 steps and an interval of 0.1 Å, aimed at identifying the transition state connecting CS5 to the product P14. The results indicate that direct methyl (CH₃) elimination from CS5 is unfavorable. Specifically, when the C1-C2 bond length reaches approximately 2.0 Å, the methyl radical preferentially migrates to the para site of the C₆H₅O group due to stronger radical stabilization, leading to the formation of reaction intermediate CS10. Upon further elongation of the distance between C1 and C2 atoms, the CH₃ group fully dissociates from the C₆H₅O moiety, forming isolated CH₃ and C₆H₅O radicals without encountering a significant energy barrier. This suggests a barrierless CH₃ elimination from CS10. Therefore, the bond scan efficiently excludes the existence of a distinct transition state between CS5 and P14, and clarifies the preferred reaction pathway.