Electronic Supplementary Material (ESI) for New Journal of Chemistry.

DFT Studies on the Effect of Additives on Stereoselectivity in the Polymerization of Styrene Catalyzed by Rare Earth Metal Complexes

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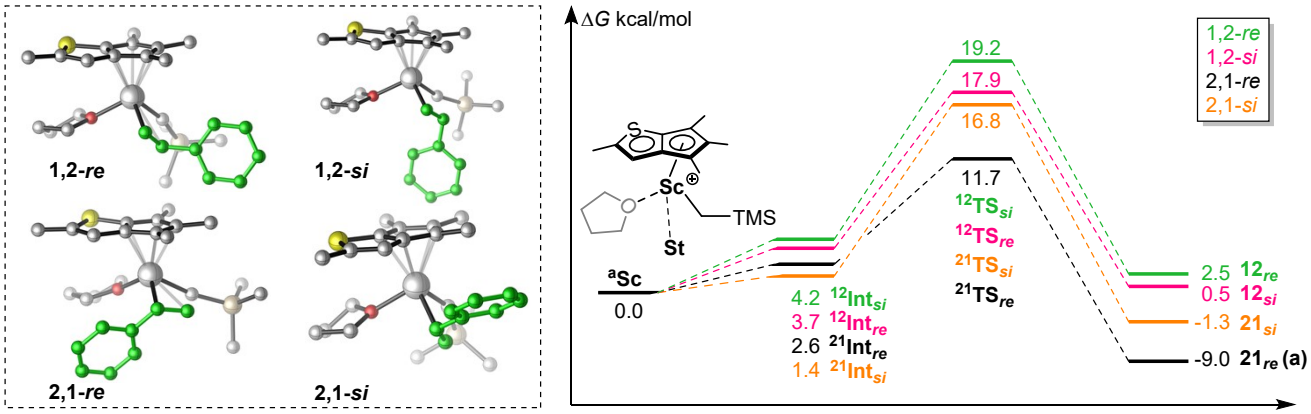

Fig. S1. Computed energy profiles for **[a]Sc** mediated various insertion manners of styrene. Energies are relative to the corresponding cationic species **[a]Sc** and styrene.

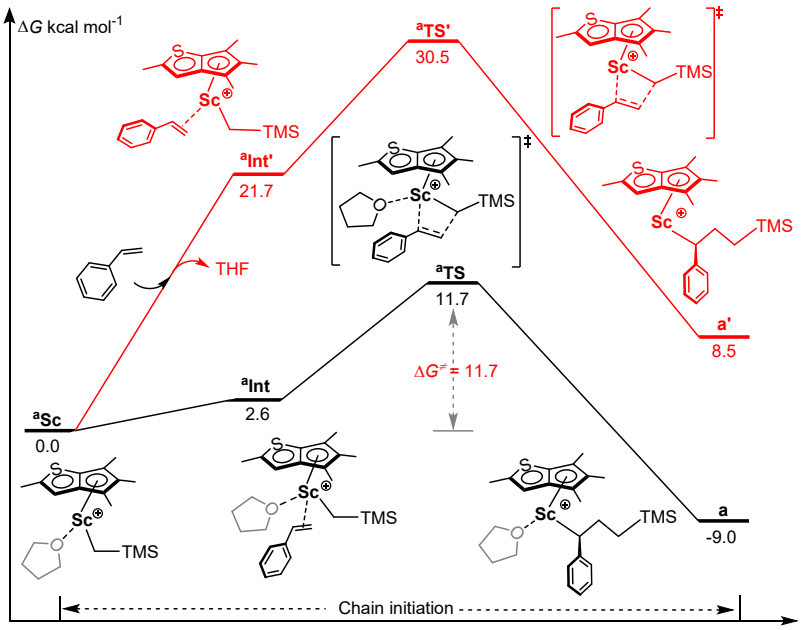

Fig. S2. Calculated energy profiles for styrene insertion into **[a]Sc** with THF (black curve) and without THF (red curve) of the first molecule. Energies are relative to the corresponding cationic species **[a]Sc** and styrene.

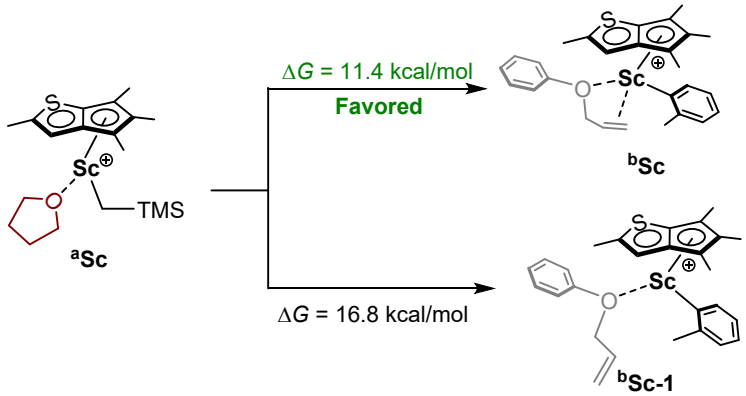

Fig. S3 Computed energy difference between **[a]Sc** and **[b]Sc** or **[b]Sc-1**.

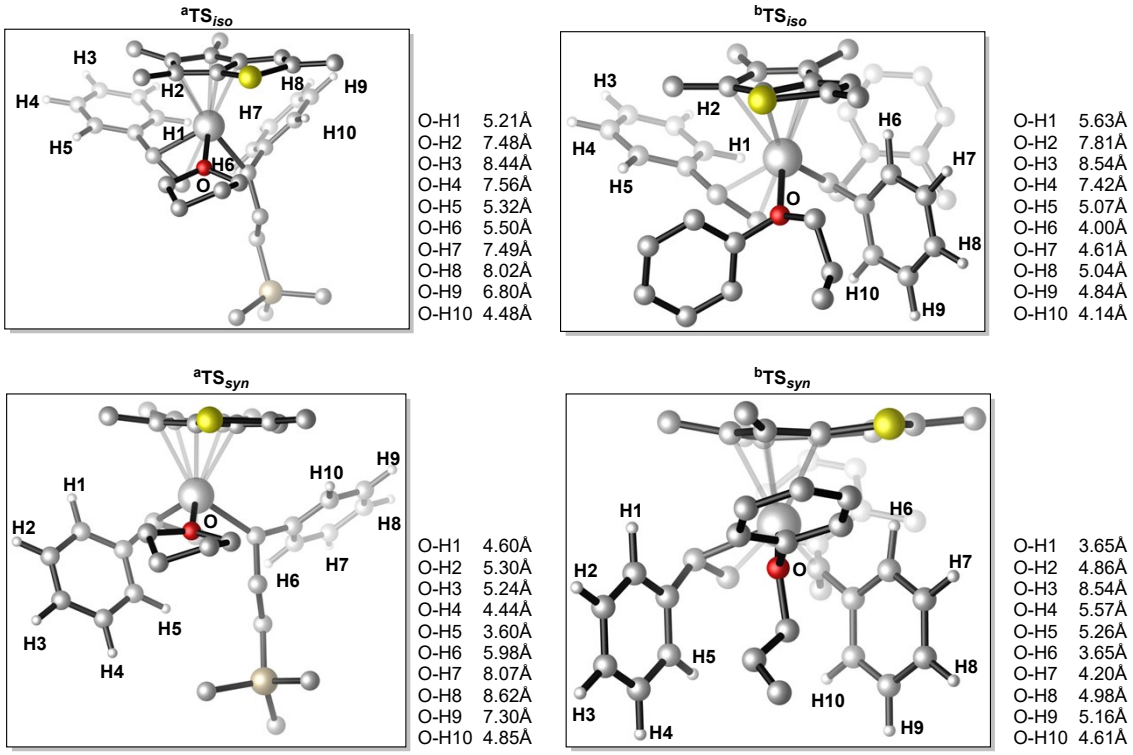

Fig. S4 Geometric structure analysis of ^{a}**TS**$_{iso}$, ^{a}**TS**$_{syn}$, ^{b}**TS**$_{iso}$ and ^{b}**TS**$_{syn}$.

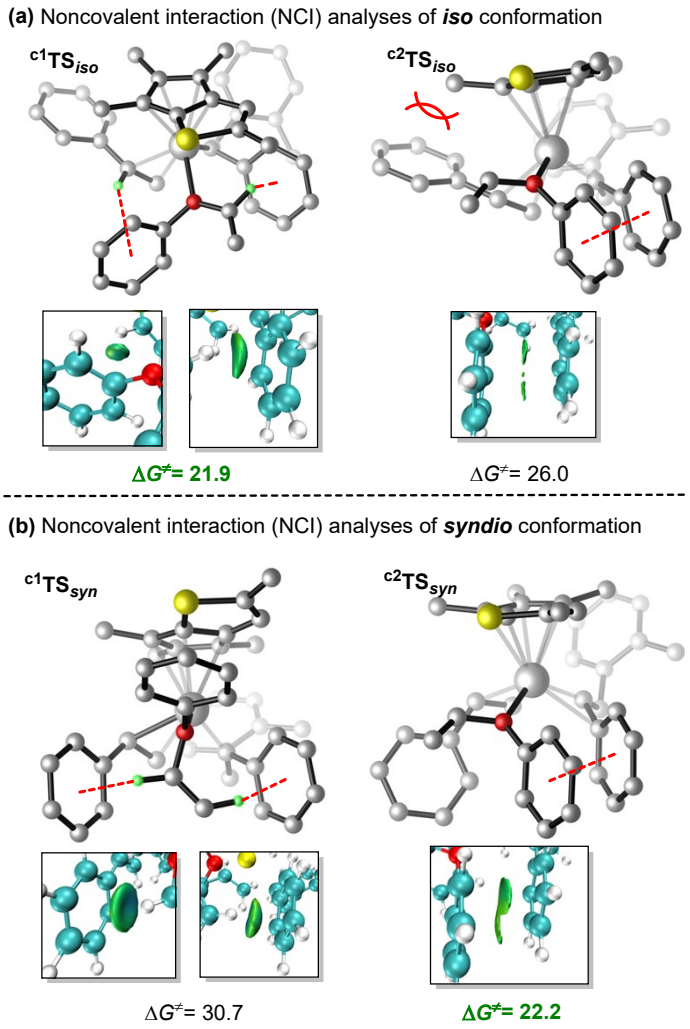

Fig. S5 Noncovalent interaction (NCI) analyses of different conformations in the presence of VOB.

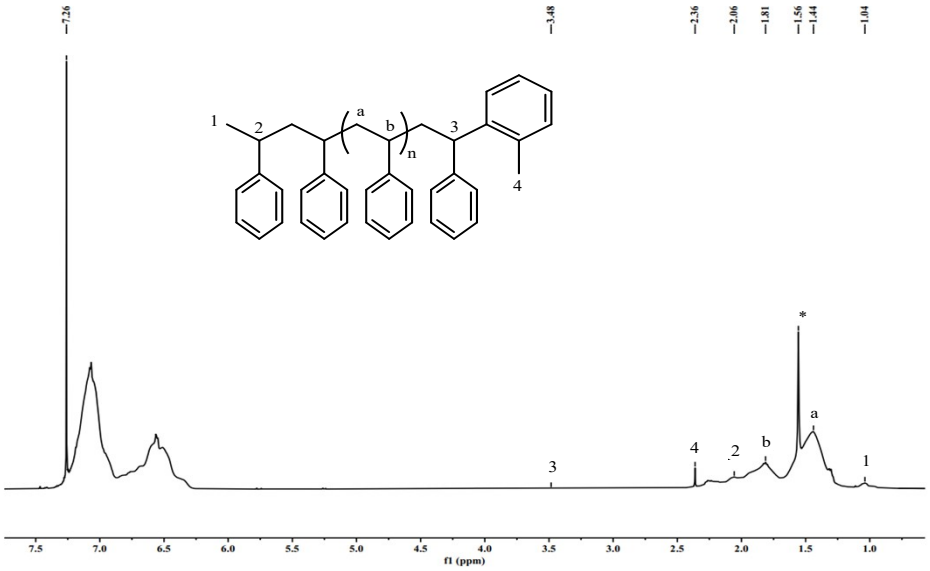

Fig. S6. ^{1}H NMR spectrum of *a*PS (Table 1, entry 4) obtained in toluene. (25℃, CDCl3, *H2O).

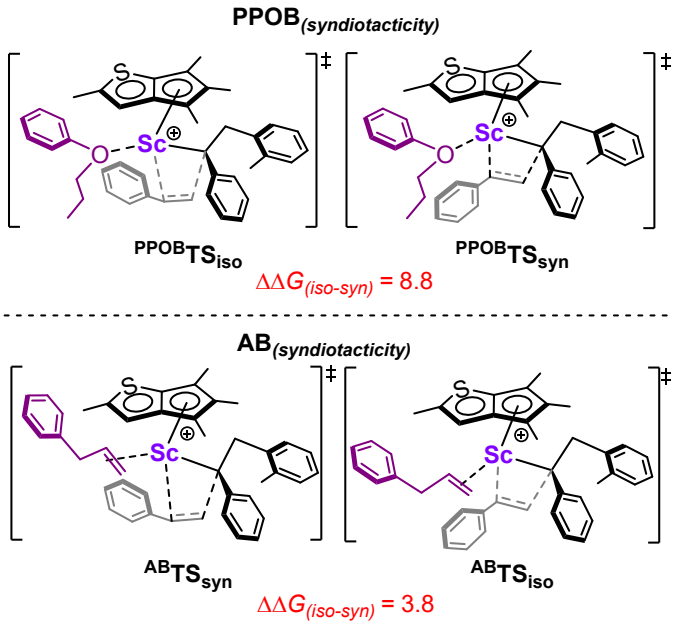

Fig. S7 The energy barrier difference between the isotactic TS and the syndiotactic TS at the chain propagation stage when the additives are PPOB and AB.