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 \(^{a}\text{Sc}\) mediated various insertion manners of styrene. Energies are relative to the corresponding cationic species \(^{a}\text{Sc}\) 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 $\alpha$PS (Table 1, entry 4) obtained in toluene. (25°C, 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.