Supporting Information

A theoretical study of DABCO and PPh_3 catalyzed annulations of allenoates with azodicarboxylate

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Fig 1. Free energy profile of the reaction channels proceeded via 1 (down attack mode). The solvation-corrected relative free energies at SMD(1,4-dioxane)/M06-2X/6-311++G(d,p) level are given in kcal/mol.

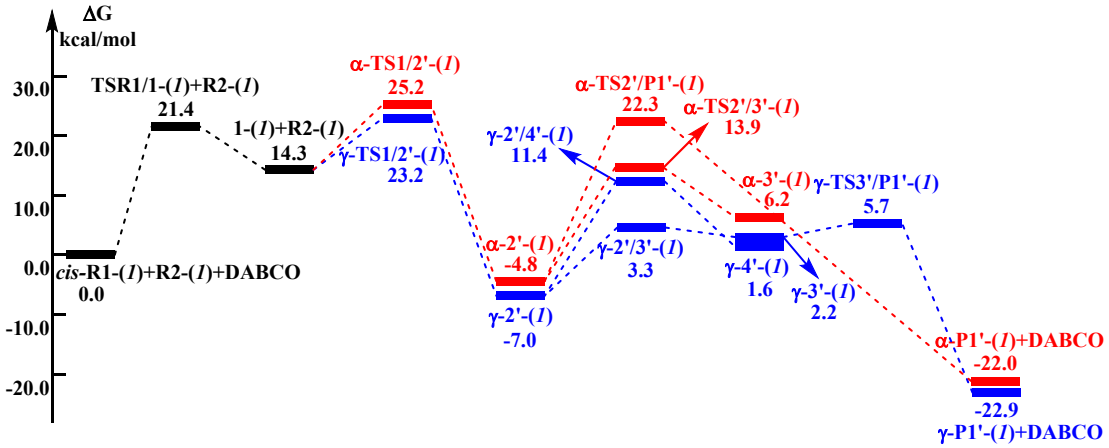

Fig 2. Free energy profile of the reaction channels proceeded via 1a (up attack mode). The solvation-corrected relative free energies at SMD(1,4-dioxane)/M06-2X/6-311++G(d,p) level are given in kcal/mol.