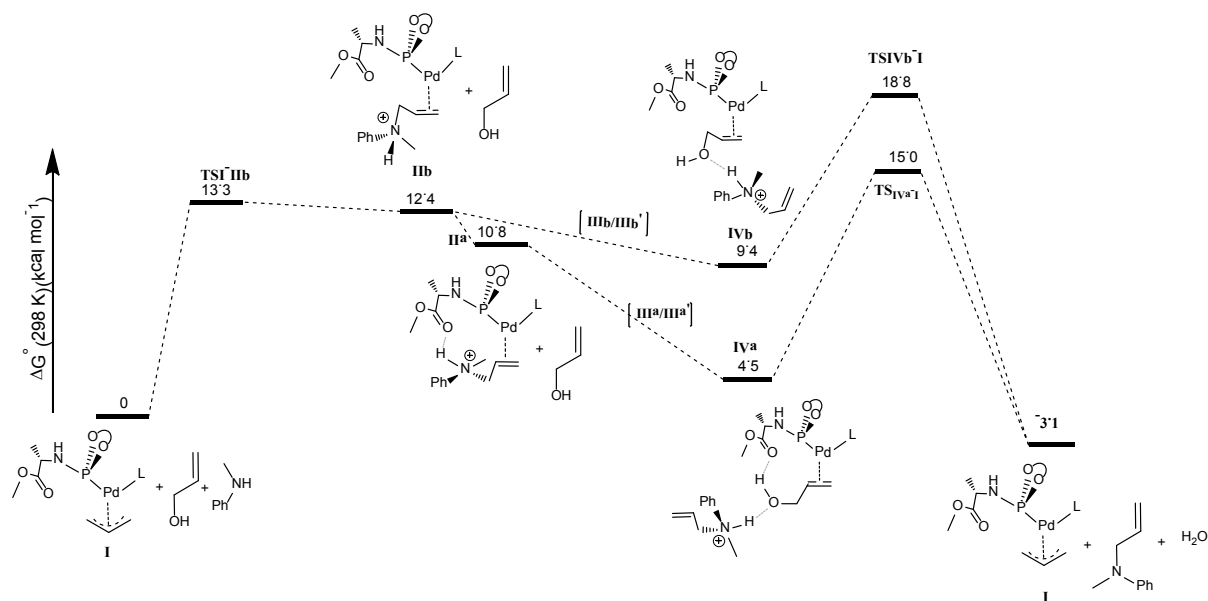
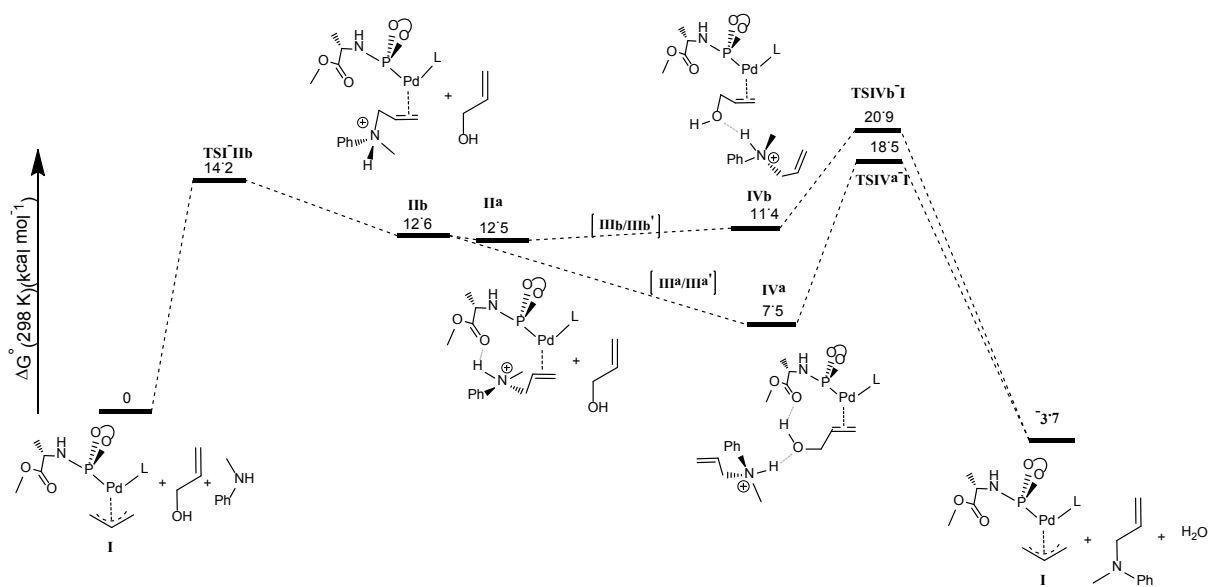


Supplementary Information



(a)



(b)

Figure 1S. Cont.

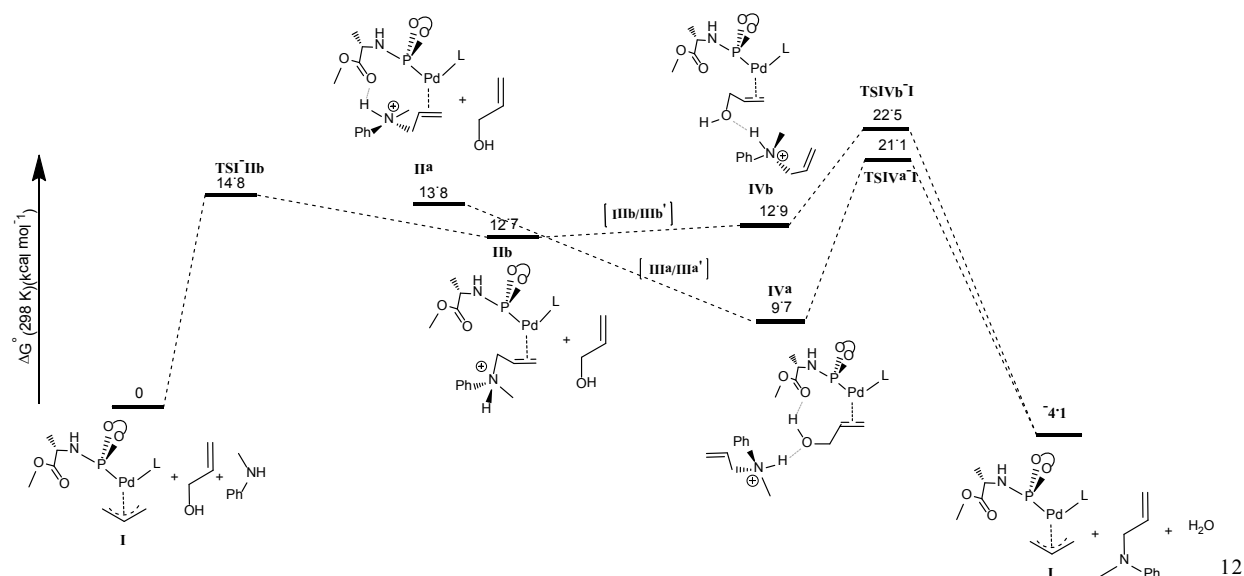


Figure S1. Solvents effect with COSMO dielectric constant corrections. (a) For toluene; (b) For ethyl acetate; (c) For water.

Table S1. COSMO (toluene) Corrected Free energies.

Species	Cosmo corrected Free Energies (toluene)		
	Energy at 298K	ΔG _{298K} –kcal/mol	ΔG _{298K} –entropy corrected–kcal/mol
water	–76.46996	-	-
allyl alcohol	–193.15806	-	-
N-methylaniline	–326.95034	-	-
product	–443.64338	–3.1	-
I	–2268.77379	0.0	-
IVb	–2788.8481	21.4	9.4
IVa	–2788.85591	16.5	4.5
IIb	–2595.69483	18.4	12.4
IIa	–2595.69728	16.8	10.8
TSIVb–I	–2788.83311	30.8	18.8
TSIVa–I	–2788.83915	27.0	15
TSI–IIb	–2595.6933	19.3	13.3

Table S2. COSMO (EtOAc) Corrected Free energies.

Species	Cosmo corrected Energies for EtOAc		
	Energy at 298K	ΔG_{298K} —kcal/mol	ΔG_{298K} —entropy corrected—kcal/mol
water	−76.47365	-	-
allyl alcohol	−193.16063	-	-
<i>N</i> -methylaniline	−326.95311	-	-
product	−443.64593	−3.7	-
I	−2268.79319	0.0	-
IVb	−2788.86964	23.4	11.4
IVa	−2788.87590	19.5	7.5
IIb	−2595.71661	18.6	12.6
IIa	−2595.71676	18.5	12.5
TSIVb—I	−2788.85445	32.9	20.9
TSIVa—I	−2788.85832	30.5	18.5
TSI—IIb	−2595.7141	20.2	14.2

Table S3. COSMO (water) Corrected Free energies.

Species	Cosmo corrected Energies for water		
	Energy at 298K	ΔG_{298K} —kcal/mol	ΔG_{298K} —entropy corrected—kcal/mol
water	−76.476530	-	-
allyl alcohol	−193.162620	-	-
<i>N</i> -methylaniline	−326.955310	-	-
product	−443.647940	−4.1	-
I	−2268.807460	0.0	-
IVb	−2788.885770	24.9	12.9
IVa	−2788.890880	21.7	9.7
IIb	−2595.732940	18.7	12.7
IIa	−2595.731230	19.8	13.8
TSIVb—I	−2788.870440	34.5	22.5
TSIVa—I	−2788.872600	33.1	21.1
TSI—IIb	−2595.72963	20.8	14.8