

Figure S1. The comparison of reaction rate vs time plots of (a) native $\text{g-C}_3\text{N}_4$ with self-methanolysis, (b) native $\text{g-C}_3\text{N}_4$ with $\text{H@g-C}_3\text{N}_4$ (H: B, P or S) on dehydrogenation reaction of NaBH_4 in methanol [Reaction condition: 50 mg catalyst, 20 mL methanol, 0.0965 g NaBH_4 , 25 $^\circ\text{C}$, 1000 rpm].

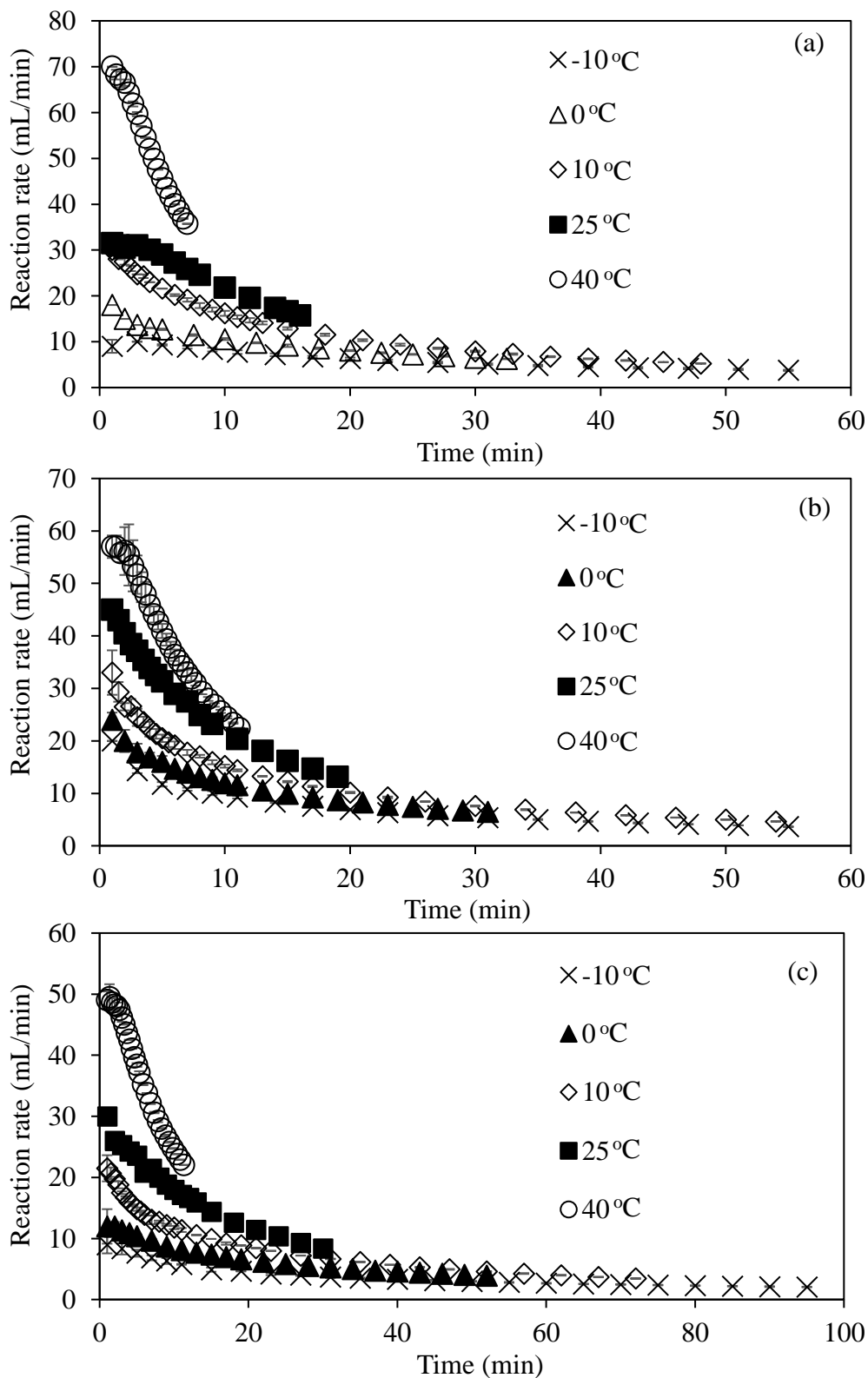


Figure S2. The comparison of calculated reaction values for (a) B@g-C₃N₄, (b) P@g-C₃N₄, and (c) S@g-C₃N₄ catalyzed dehydrogenation reaction of NaBH₄ in methanol.

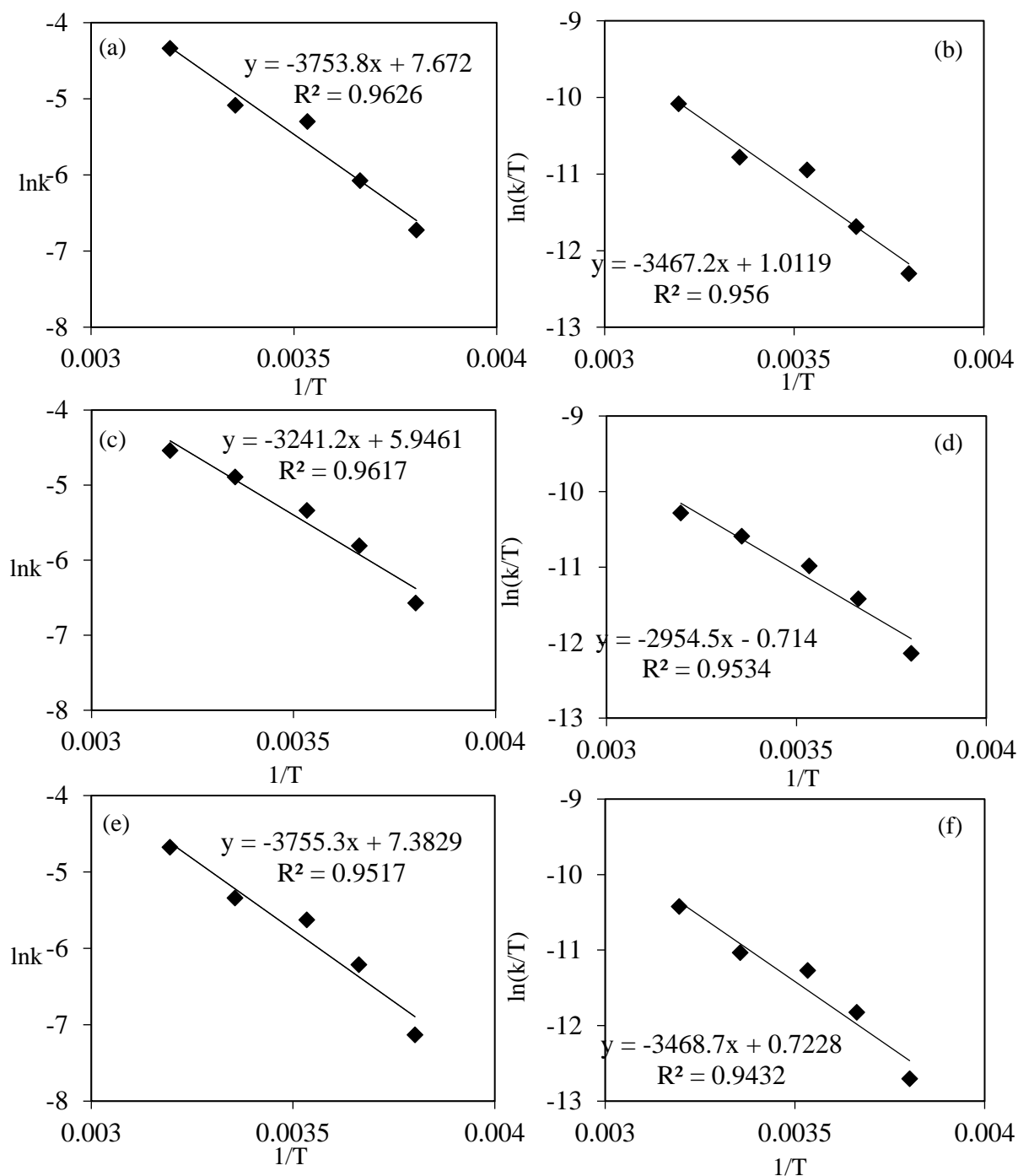


Figure S3. The plotted (a) Arrhenius, and (b) Eyring graph for B@g-C₃N₄ catalyzed reaction, (c) Arrhenius, and (d) Eyring graph for P@g-C₃N₄ catalyzed reaction, and (e) Arrhenius, and (f) Eyring graph for S@g-C₃N₄ catalyzed reaction.