

Supplementary Material for

New catalysts for carboxylation of propylene glycol to propylene carbonate via high-throughput screening

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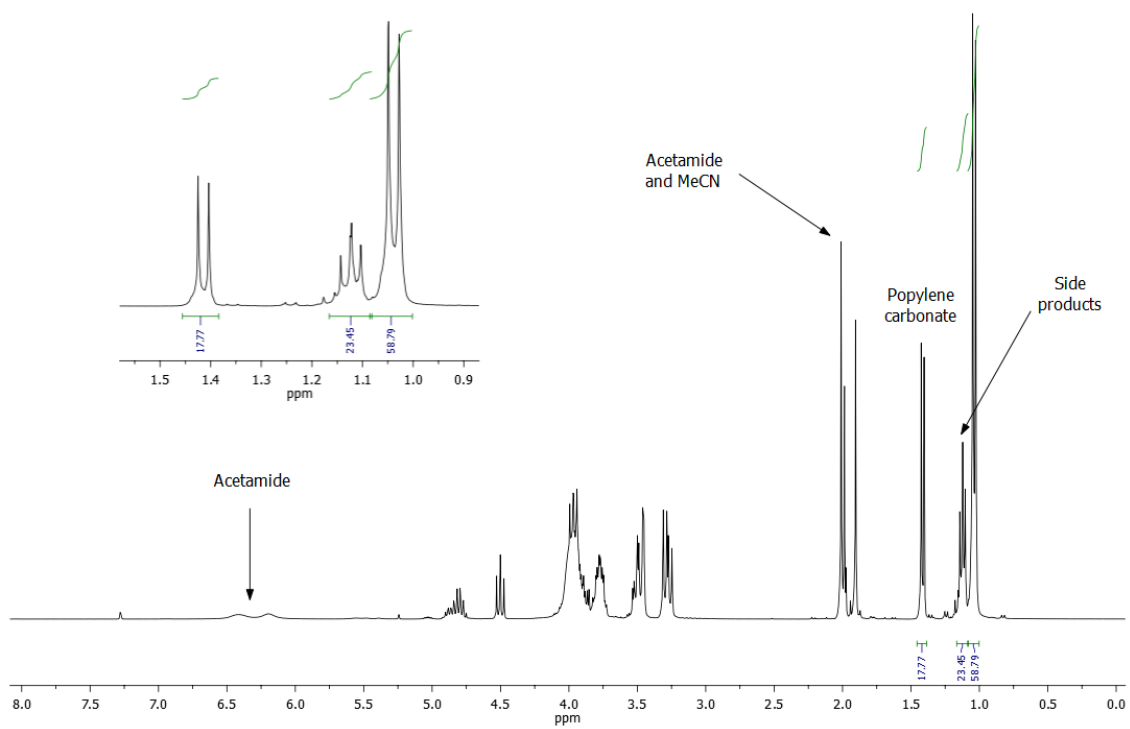


Figure S1. ^1H NMR spectrum of a PG to PC reaction mixture showing side product formation.

Table S1. List of all new catalyst formulations tested in the high throughput screening experiments.

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|---|--|---|
| Zn(OAc) ₂ + p-CBSA; 10 mol % | ZnI ₂ + p-CBSA | Cu(OAc) ₂ + p-TSA |
| Zn(OAc) ₂ + p-TSA; 10 mol % | ZnI ₂ + p-TSA | Cu(acac) ₂ |
| Zn(OAc) ₂ + 10 mol % p-CBSA | Zn(F ₆ -acac) ₂ | Cu(acac) ₂ + p-CBSA |
| Zn(OAc) ₂ + KI | Zn(F ₆ -acac) ₂ + p-CBSA | Cu(acac) ₂ + p-TSA |
| Zn(OAc) ₂ + p-CBSA + KI | Zn(acac) ₂ + p-CBSA | Cu(OTf) ₂ |
| Zn(OAc) ₂ + NEt ₄ Br | Zn(TFA) ₂ | Cu(OTf) ₂ + p-CBSA |
| Zn(OAc) ₂ + p-CBSA + NEt ₄ Br | Zn(TFA) ₂ + p-CBSA | Zn(OTf) ₂ |
| Zn(OAc) ₂ + KOH | ZnSO ₄ | Zn(OTf) ₂ + p-CBSA |
| Zn(OAc) ₂ + K ₂ CO ₃ | ZnSO ₄ + p-CBSA | Zn(OTf) ₂ + p-TSA |
| Zn(OAc) ₂ + DBSI | Zn(BF ₄) ₂ | Zn(OTf) ₂ + DBSI |
| Zn(OAc) ₂ + p-NBSA | Zn(BF ₄) ₂ + p-CBSA | Zn(OTf) ₂ + p-NBSA |
| Zn(OAc) ₂ + bipy | Fe(OTf) ₃ | Zn(Tos) ₂ |
| Zn(OAc) ₂ + p-CBSA + bipy | Fe(OTf) ₃ + p-CBSA | Zn(Tos) ₂ + p-CBSA |
| Zn(OAc) ₂ + p-TSA + bipy | Co(OAc) ₂ + p-CBSA | Zn(Tos) ₂ + p-TSA |
| Zn(OAc) ₂ + Li(OTf) | CoCO ₃ | Zn(Tos) ₂ + DBSI |
| Zn(OAc) ₂ + Mg(OTf) ₂ | CoCO ₃ + p-CBSA | Zn(Tos) ₂ + p-NBSA |
| Zn(OAc) ₂ + Ca(OTf) ₂ | (dppe)NiCl ₂ | Zn(Tos) ₂ + KOH |
| Zn(OAc) ₂ + Al(OTf) ₃ | Ni(OAc) ₂ + p-CBSA | Zn(Tos) ₂ + K ₂ CO ₃ |
| Zn(OAc) ₂ + Sc(OTf) ₃ | Ni(OAc) ₂ + p-TSA | LiOTf |
| Zn(OAc) ₂ + Y(OTf) ₃ | NiBr ₂ | Mg(OTf) ₂ |
| Zn(OAc) ₂ + La(OTf) ₃ | NiBr ₂ + CBSA | Ca(OTf) ₂ |
| Zn(OAc) ₂ + Sm(OTf) ₃ | NiBr ₂ + p-TSA | Al(OTf) ₃ |
| Zn(OAc) ₂ + Yb(OTf) ₃ | Ni(OTf) ₂ | Sc(OTf) ₃ |
| ZnCl ₂ + p-CBSA | Ni(OTf) ₂ + p-CBSA | Y(OTf) ₃ |
| ZnCl ₂ + p-TSA | Pd(OAc) ₂ | La(OTf) ₃ |
| ZnBr ₂ + p-CBSA | Pd(OAc) ₂ + p-CBSA | Yb(OTf) ₃ |
| ZnBr ₂ + p-TSA | Cu(OAc) ₂ + p-CBSA | Sm(OTf) ₃ |

All compounds added at the 5 mol % level (with respect to propylene glycol), unless otherwise indicated. Abbreviations: p-CBSA, p-chlorobenzenesulfonic acid; p-TSA, p-toluenesulfonic acid; DBSI, dibenzenesulfonimide; p-NBSA, p-nitrobenzenesulfonic acid; bipy, 2,2'-bipyridine; OTf, trifluoromethanesulfonate; F₆-acac, hexafluoroacetylacetonate; acac, acetylacetonate; TFA, trifluoroacetate; dppe, 1,2-(diphenylphosphino)ethane; Tos, p-toluenesulfonate;

All materials were anhydrous apart from the following compounds: p-toluenesulfonic acid hydrate, 4-nitrobenzenesulfonic acid hydrate, copper acetate monohydrate, nickel acetate tetrahydrate, cobalt carbonate hydrate, cobalt acetate tetrahydrate, zinc tetraborate hydrate, zinc trifluoroacetate hydrate, zinc p-toluenesulfonate hydrate, zinc hexafluoroacetylacetonate dihydrate, zinc sulfate monohydrate, zinc acetylacetonate hydrate and yttrium trifluoromethanesulfonate hydrate.