Supporting Information

Kinetics and Mechanistic Insight into Efficient Fixation of CO_2 to Epoxides over *N*-heterocyclic Compound/$ZnBr_2$ Catalysts

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The Formula Deduction Procedures of Reaction Rate for PC Formation[1,2]

The rate of PC formation was described as Eq. (S1)

$$\frac{d[P]}{dt} = k_2[CO_2][SIZ^{\xi}] \quad \text{(S1)}$$

Where, $d[P]$ was PC concentration at a particular reaction time. The different rate expression describing the formation of SIZ^{ξ} was described as Eq. (S2)

$$\frac{d[SIZ^{\xi}]}{dt} = k_1[S][IZ] - k_{-1}[SIZ^{\xi}] - k_2[CO_2][SIZ^{\xi}] \quad \text{(S2)}$$

To simplify, assuming the reaction at pseudo-steady state, we obtained the following Eq. (S3) and Eq. (S4),

$$\frac{d[SIZ^{\xi}]}{dt} = k_1[S][IZ] - k_{-1}[SIZ^{\xi}] - k_2[CO_2][SIZ^{\xi}] = 0 \quad \text{(S3)}$$

$$[SIZ^{\xi}] = \frac{k_1[S][IZ]}{k_{-1} + k_2[CO_2]} \quad \text{(S4)}$$

Substituting $[SIZ^{\xi}]$ into Eq. (S1) gave Eq. (S5).

$$\frac{d[P]}{dt} = \frac{k_1 k_2[S][IZ][CO_2]}{k_{-1} + k_2[CO_2]} \quad \text{(S5)}$$

As the reaction carried out in a constant volume reactor, and CO_2 was excessively used, the concentrations of CO_2 and catalyst could be assumed constant, and Eq. (S5) could be shorten to the following Eq.:

$$\frac{d[P]}{dt} = -\frac{\mathrm{d}[S]}{\mathrm{d}t} = k[PO]$$

Table S1. Kinetic Equations and Kinetic Parameters at Different Temperature

T/(°C)	Kinetic equation	R′	*k* (min^{-1})	1/T (K^{-1})	ln*k*
130	$y = 0.02593x$-0.08567	0.9883	0.02593	0.00248	-3.652
140	$y = 0.03798x$-0.24142	0.9961	0.03798	0.00242	-3.271
150	$y = 0.04988x$-0.38295	0.9969	0.04988	0.00236	-2.998
160	$y = 0.06073x$-0.39659	0.9973	0.06073	0.00231	-2.801

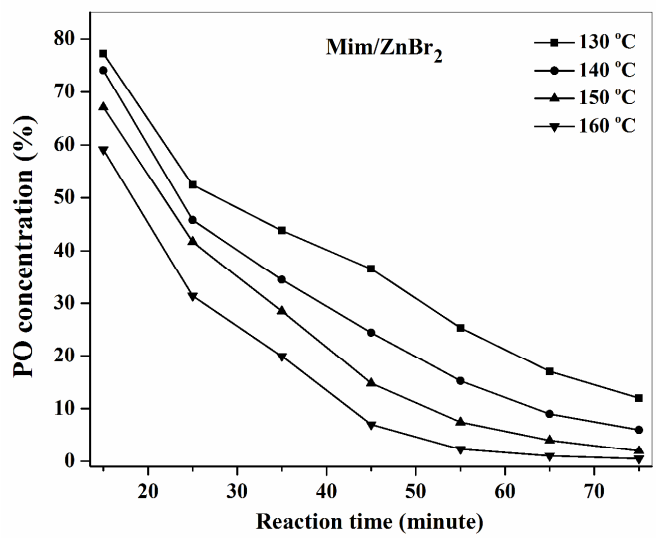

Figure S1. The remaining PO concentration-time profile at different temperatures over Mim/$ZnBr_2$ catalysts. Reaction conditions: PO 34.5 mmol, P (CO_2) = 2.5 MPa, $ZnBr_2$ 0.09 mmol, Mim 0.36 mmol.

References

(1) Yu, J. I.; Choi, H. J.; Selvaraj, M.; Park, D. W. Catalytic performance of polymer-supported ionic liquids in the cycloaddition of carbon dioxide to allyl glycidyl ether. *Reac. Kinet. Mech. Cat*. **2011**, *102*, 353–365.

(2) Chatelet, B.; Joucla, L.; Dutasta, J.; Martinez, A.; Szeto, K.; Dufaud, V. Azaphosphatranes as structurally tunable organocatalysts for carbonate synthesis from CO_2 and epoxides. *J. Am. Chem. Soc*., **2013**, *135*, 5348–5351.