

SUPPLEMENTARY INFORMATION

A NEW APPROACH IN THE MECHANISM FOR THE ACETALIZATION OF BENZALDEHYDE OVER MOFs CATALYSTS

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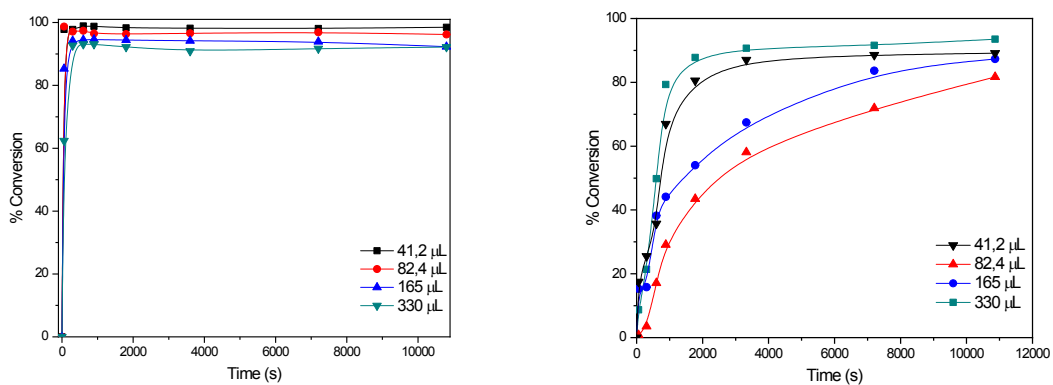


Fig. S.1 Conversion in function of time for UiO-66F (left) and UiO-66 (right)

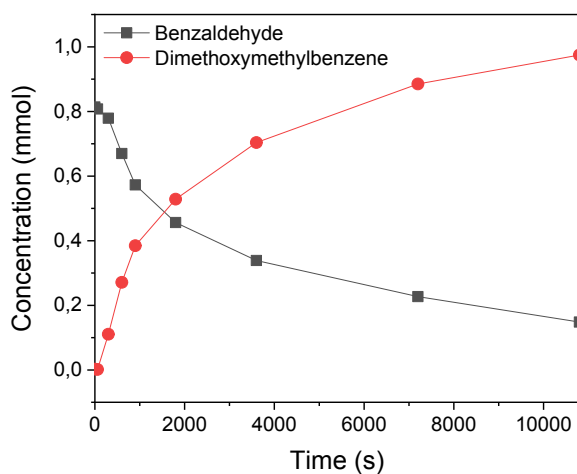


Fig. S.2 Concentrations of the reactant and detected products from the benzaldehyde acetalization over UiO-66 catalyst.

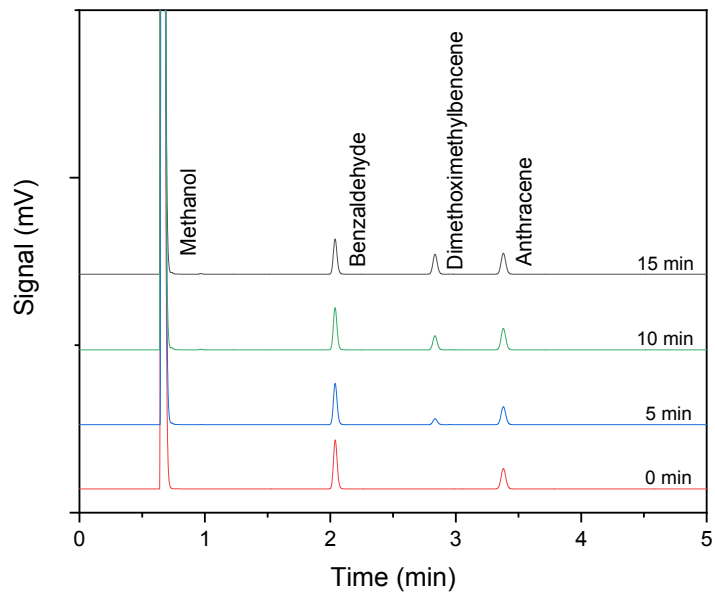
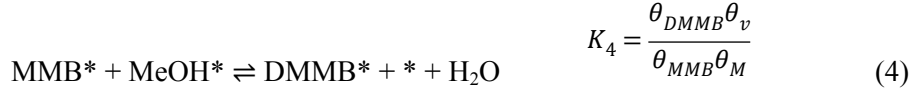
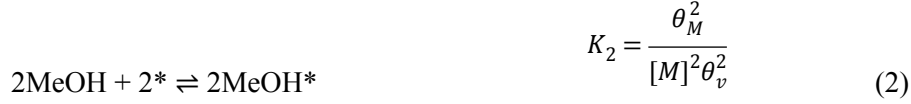


Fig. S.3 Reactants and products identified at different times for benzaldehyde acetalization over UiO-66 catalyst.

L-H model



$$\theta_{\text{Bz}} = K_1[\text{Bz}]\theta_v$$

$$\theta_M = \sqrt{K_2}[M]\theta_v$$

$$\theta_{\text{MMB}} = \frac{[\text{DMMB}]\theta_v}{K_4 K_5 \sqrt{K_2}[M]}$$

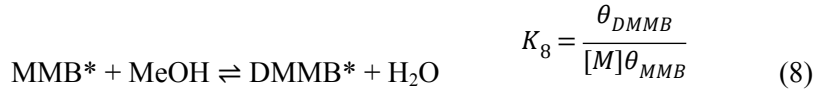
$$\theta_{\text{DMMB}} = \frac{[\text{DMMB}]\theta_v}{K_5}$$

$$r = (k_3\theta_{\text{Bz}}\theta_M - k_{-3}\theta_{\text{MMB}}\theta_v)$$

$$r = \left(k_3 K_1 \sqrt{K_2} [\text{Bz}][M] - \frac{k_{-3}[\text{DMMB}]}{\sqrt{K_2} K_4 K_5 [M]} \right) \theta_v^2$$

$$\theta_v = \frac{1}{\left(1 + K_1[\text{Bz}] + \sqrt{K_2}[M] + \frac{[\text{DMMB}]}{\sqrt{K_2} K_4 K_5 [M]} + \frac{[\text{DMMB}]}{K_5} \right)}$$

E-R model



$$\theta_{\text{Bz}} = K_6[\text{Bz}]\theta_v$$

$$\theta_{\text{MMB}} = \frac{[\text{DMMB}]\theta_v}{K_8 K_9 [\text{M}]}$$

$$\theta_{\text{DMMB}} = \frac{[\text{DMMB}]\theta_v}{K_9}$$

$$r = (k_7 \theta_{\text{Bz}} [\text{M}] - k_{-7} \theta_{\text{MMB}})$$

$$r = \left(k_7 K_6 [\text{Bz}] [\text{M}] - \frac{k_{-7} [\text{DMMB}]}{K_8 K_9 [\text{M}]} \right) \theta_v$$

$$\theta_v = \frac{1}{\left(1 + K_6 [\text{Bz}] + \frac{[\text{DMMB}]}{K_8 K_9 [\text{M}]} + \frac{[\text{DMMB}]}{K_9} \right)}$$