

Supporting Information

Size-selective catalysts in five functionalized porous coordination polymers with unsaturated zinc centers

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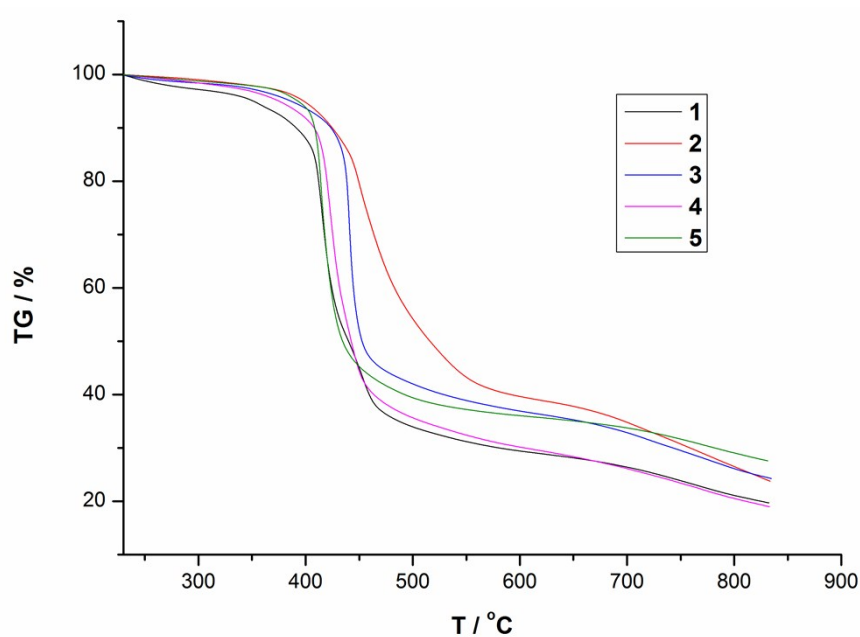


Fig. S1. TGA curves of compounds 1–5.

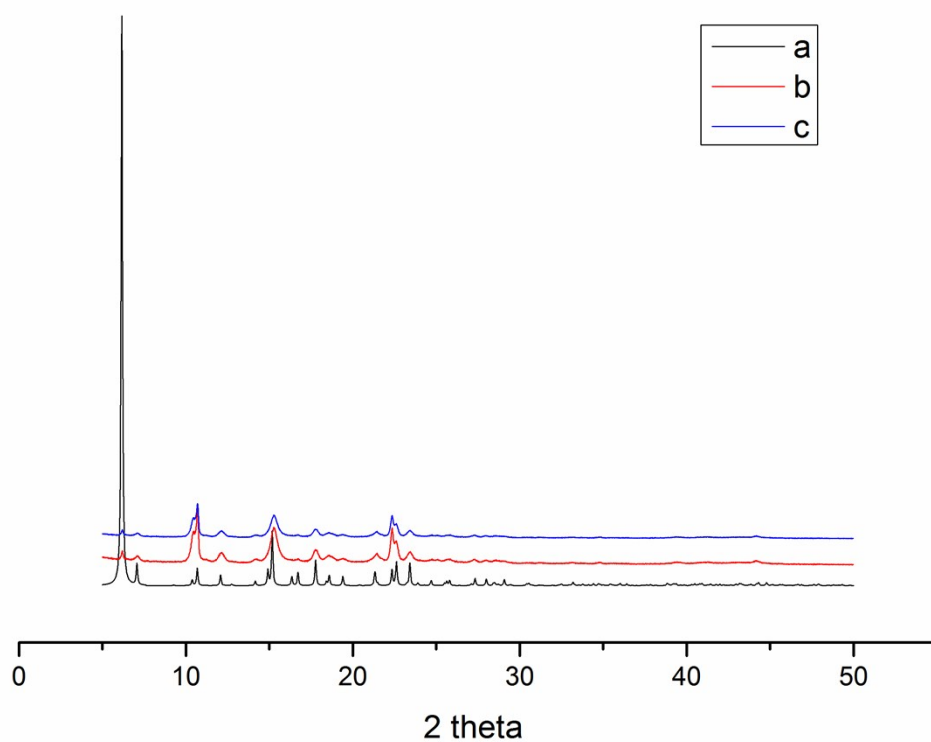


Fig. S2. XRD patterns of **1**: (a) the simulated XRD pattern, (b) the experimental one, (c) after the reaction.

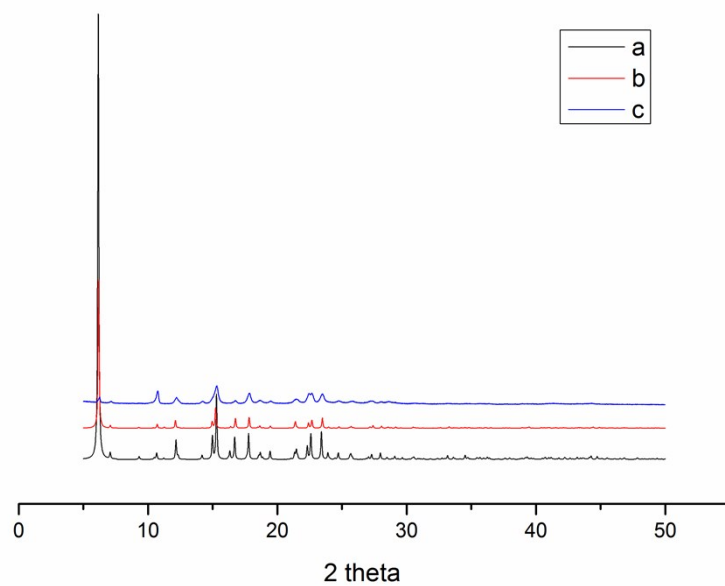


Fig. S3. XRD patterns of **3**: (a) the simulated XRD pattern, (b) the experimental one, (c) after the reaction.

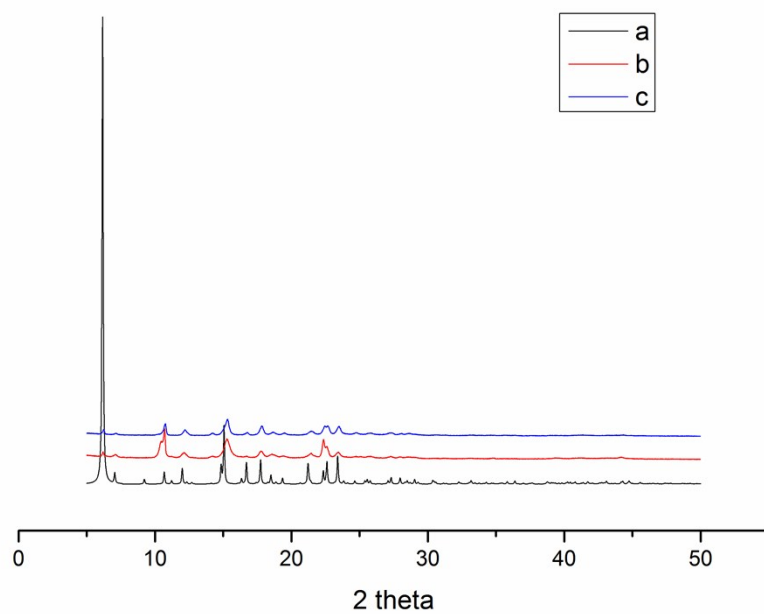


Fig. S4. XRD patterns of **4**: (a) the simulated XRD pattern, (b) the experimental one, (c) after the reaction.

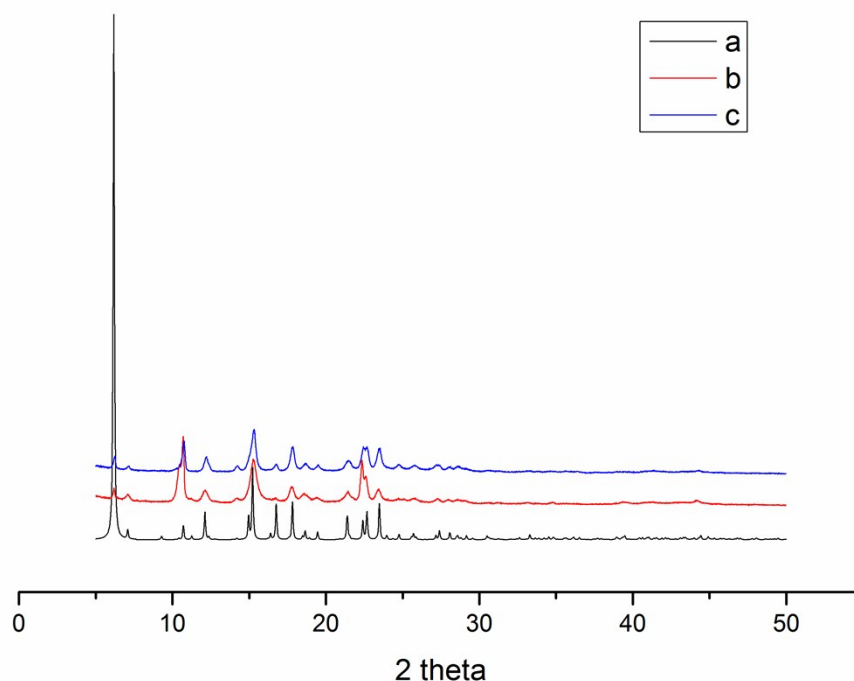


Fig. S5. XRD patterns of **5**: (a) the simulated XRD pattern, (b) the experimental one, (c) after the reaction.

NMR data of the acetylation of phenols

2.1. *p*-tolyl acetate (Table 2, entry 1)

Colorless liquid, 74.3 mg, 99% yield. $^1\text{H-NMR}$ (CDCl_3): 7.17 (d, $J = 7.6$ Hz, 2H), 6.96 (d, $J = 8.0$ Hz, 2H), 2.33 (s, 3H), 2.27 (s, 3H).

2.2. 4-*tert*-butylphenyl acetate (Table 2, entry 2)

Colorless liquid, 95.1 mg, 99% yield. $^1\text{H-NMR}$ (CDCl_3): 7.37 (d, $J = 8.0$ Hz, 2H), 6.99 (d, $J = 8.0$ Hz, 2H), 2.23 (s, 3H), 1.30 (s, 9H).

2.2. 4-chlorophenyl acetate (Table 2, entry 3)

Colorless liquid, 84.5 mg, 99% yield. $^1\text{H-NMR}$ (CDCl_3): 7.50 (d, $J = 7.6$ Hz, 2H), 7.02 (d, $J = 7.6$ Hz, 2H), 2.31 (s, 3H).

2.4. 4-bromophenyl acetate (Table 2, entry 4)

White solid, 106.4 mg, 99% yield. $^1\text{H-NMR}$ (CDCl_3): 7.43 (d, $J = 6.8$ Hz, 2H), 6.94 (d, $J = 7.2$ Hz, 2H), 2.19 (s, 3H).

2.5. 3,5-dimethylphenyl acetate (Table 2, entry 5)

Colorless liquid, 81.2 mg, 99% yield. ¹H-NMR (CDCl₃): 6.83 (s, 1H), 6.68 (s, 2H), 2.28 (s, 3H), 2.23 (s, 3H).

2.6. 3-chlorophenyl acetate (Table 2, entry 6)

Colorless liquid, 84.4 mg, 99% yield. ¹H-NMR (CDCl₃): 7.33 (s, 1H), 7.26 (d, J = 1.2 Hz, 1H), 7.03 (q, J = 1.2 Hz, 2H), 7.01 (d, J = 0.4 Hz, 2H), 2.32 (s, 3H).

2.7. 4-chloro-3-methylphenyl acetate (Table 2, entry 7)

White solid, 91.3 mg, 99% yield. ¹H-NMR (CDCl₃): 7.36 (d, J = 7.2 Hz, 1H), 7.00 (d, J = 1.6 Hz, 1H), 6.91 (s, 1H), 2.39 (s, 3H), 2.31 (s, 3H).

2.8. 4-methoxy-3-methylphenyl acetate (Table 2, entry 8)

Colorless liquid, 82.1 mg, 99% yield. ¹H-NMR (CDCl₃): 7.02 (d, J = 1.6 Hz, 2H), 6.93 (d, J = 2.0 Hz, 2H), 3.81 (s, 3H), 2.29 (s, 3H).

2.9. 4-methyl-2-nitrophenyl acetate (Table 2, entry 9)

Yellow solid, 96.5 mg, 99% yield. ¹H-NMR (CDCl₃): 7.91 (d, J = 1.2 Hz, 2H), 7.46 (q, J = 1.6 Hz, 1H), 7.13 (d, J = 6.4 Hz, 1H), 2.44 (s, 3H), 2.37 (s, 3H).

2.10. 2,4-tert-butylphenyl acetate (Table 2, entry 10)

Yellow solid, 122.9 mg, 99% yield. ¹H-NMR (CDCl₃): 7.39 (d, J = 2.0 Hz, 1H), 7.21 (q, J = 1.6 Hz, 1H), 6.92 (s, 1H), 2.31 (s, 3H), 1.35 (s, 9H), 1.31 (s, 9H).

2.11. 4-acetoxyphenyl acetate (Table 2, entry 11)

White solid, 95.2 mg, 98% yield. ¹H-NMR (CDCl₃): 7.09 (s, 4H), 2.30 (s, 6H).

2.12. o-acetoxyphenyl acetate (Table 2, entry 12)

White solid, 95 mg, 98% yield. ¹H-NMR (CDCl₃): 7.26 (m, 2H), 7.21 (m, 2H), 2.30 (s, 6H).