Supplementary Material (ESI) for Chemical Communications

<Supporting Information>

A Palladium(II) triangle as Building Blocks of Microporous Molecular Materials: Structures and Catalytic Performance

Yang Liu, Rong Zhang, Cheng He, Dongbin Dang and Chunying Duan

State Key Laboratory of Fine Chemicals, Dalian University of Technology, Dalian 116012, China. E-mail: cyduan@dlut.edu.cn

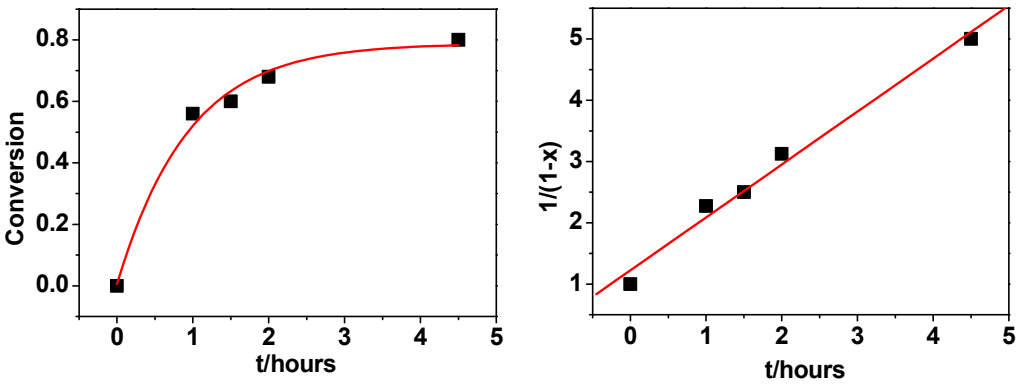
Contents:

Experimental Section

All chemicals were of reagent grade quality obtained from commercial sources and the solvents used were purification by standard procedure. The elemental analyses of C, H and N were performed on a Vario EL III elemental analyzer. ^{1}H NMR and ^{13}C NMR spectra were measured on a Varian INOVA 400M spectrometer.

Preparation of L: 3,3´,5,5´-Tetracarboxydiphenylmethane tetrachloride[S1] (4.18g, 10mmol) in THF solution was added dropwise to a mixture of 4-Aminomethylpyridine (5.45g, 50mmol) and triethylamine (11.2ml, 80mmol) in dry THF and stirred for 48h at room temperature. Yellow solid was collected by filtration, washed with 10% NaOH aqueous solution, water and dried under vacuum. Yield: 49%. ^{1}H NMR (400 MHz, DMSO-d6, ppm): δ = 4.21 (s, 2H), 4.50 (s, 8H), 7.31 (d, 8H), 7.99 (s, 4H), 8.31 (s, 2H), 8.50 (d, 8H), 9.26 (m, 4H). ^{13}C-NMR (100 MHz, DMSO-d6): δ= 40.58, 42.30, 122.65, 124.82, 131.14, 135.09, 141.69, 148.86, 149.98, 166.53. Anal. Calcd. for $C_{41}H_{36}N_8O_4 \cdot 4H_2O$: C, 63.39; H, 5.71; N, 14.42 %. Found: C, 63.25; H, 5.73; N, 14.38 %.

Calculation of the second grade reaction rate constant



Conversion (%) *vs* time (left) and linear fit according to the second grade reaction, x is the conversion (right).

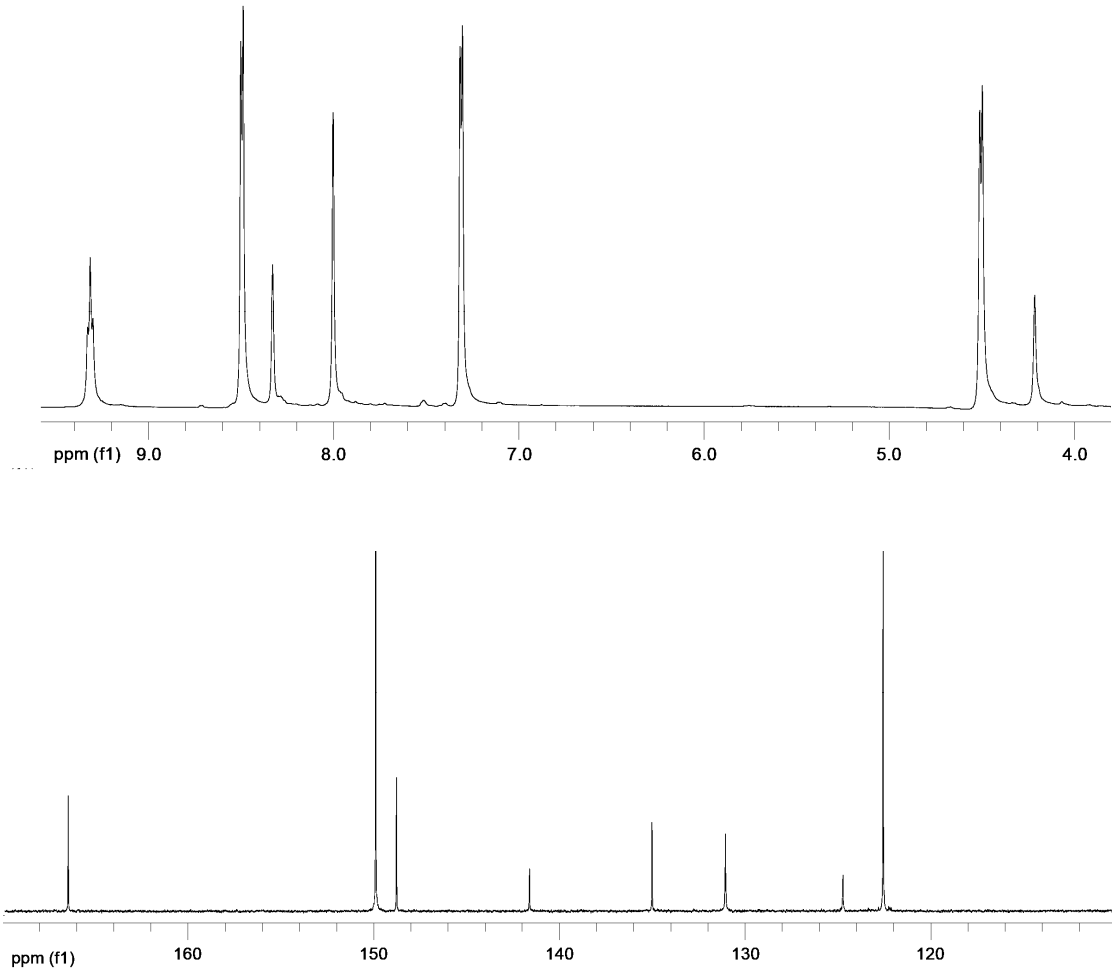


Figure S1. ^{1}H-NMR (top picture) and ^{13}C-NMR (bottom one) spectra of the ligand in d_6-DMSO

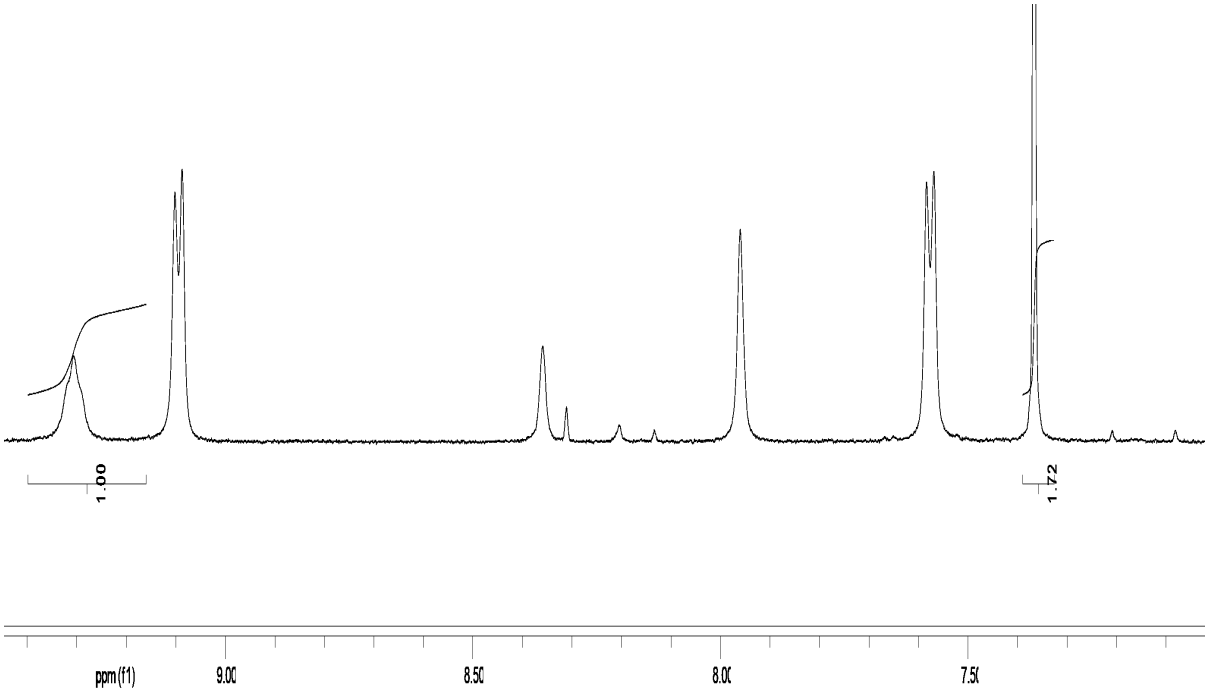


Figure S2. ^{1}H-NMR (d_6-DMSO) spectra of compound **1** immersed in benzene for 24 hours.

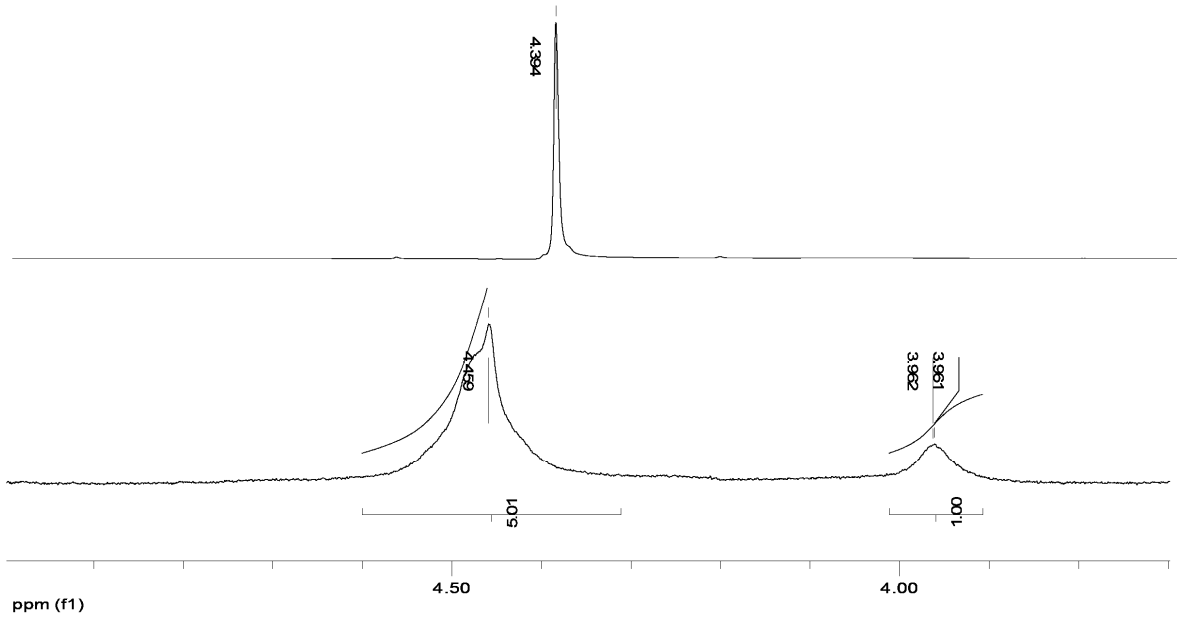


Figure S3. ^{1}H-NMR spectra (d_6-DMSO) of malononitrile (top) and compound **1** adsorbed malononitrile (bottom).

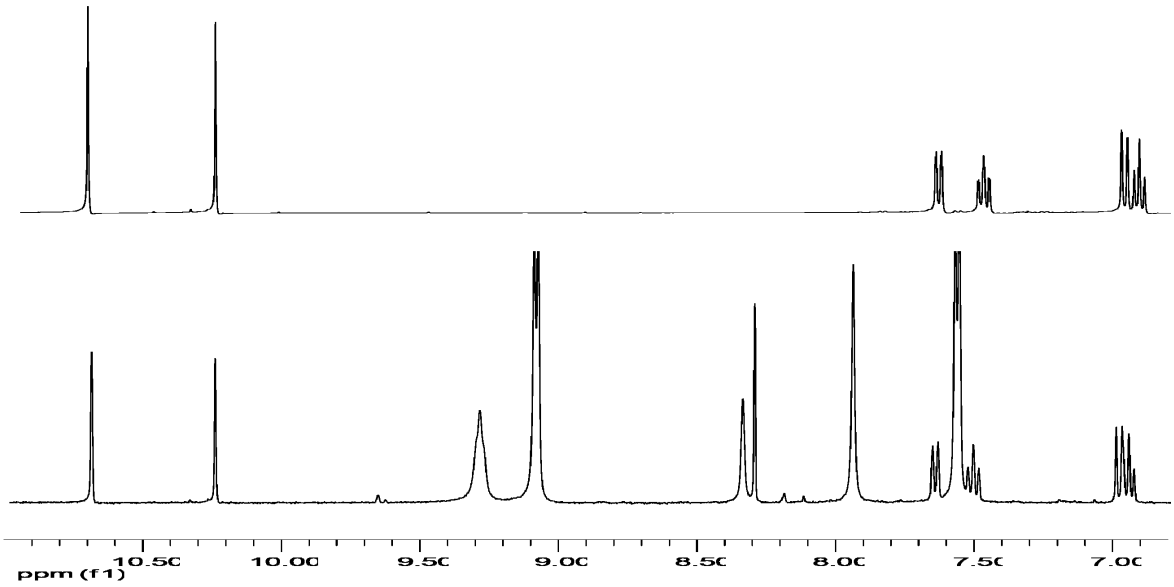


Figure S4. ^{1}H-NMR spectra (d_6-DMSO) of salicylaldehyde(top picture) and compound **1** triangle adsorbed salicylaldehyde (bottom)

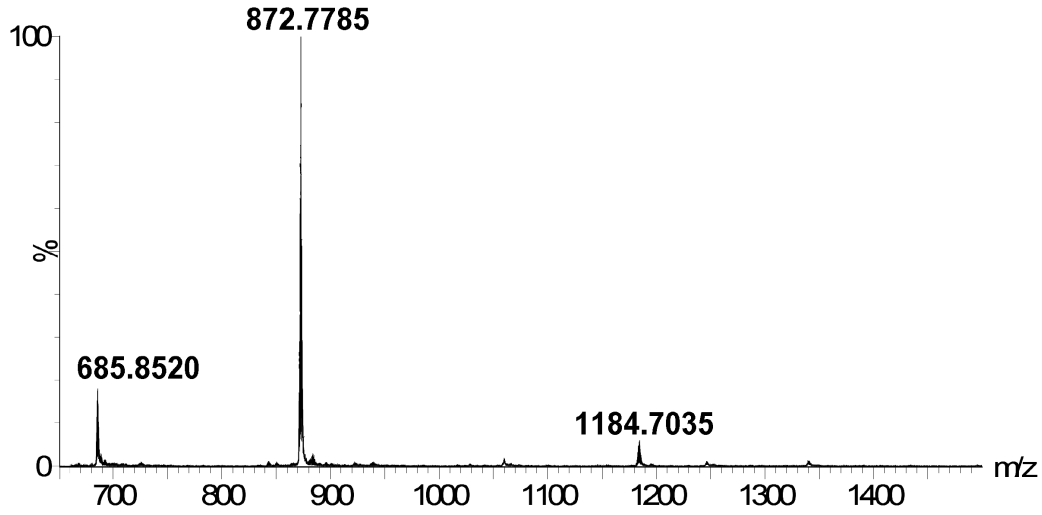


Figure S5 ESI-TOF spectra of the Pd(II)-based triangles formed in DMSO solution

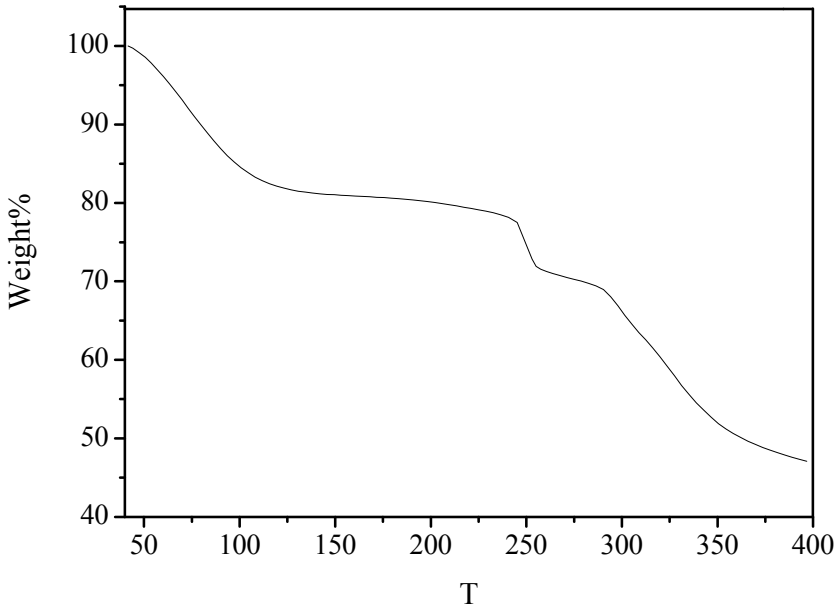


Figure S6. TGA curve of deslovent compound **1** immersed in methanol for 4 hours (bottom one).

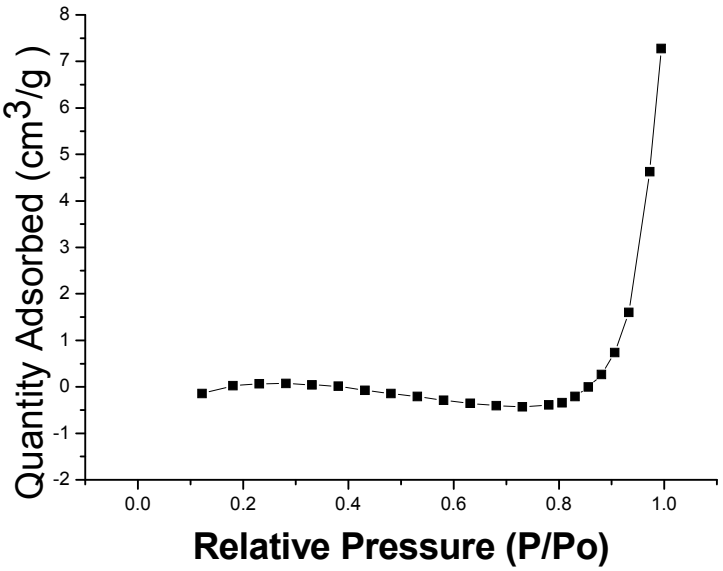


Figure S7. Gas adsorption isotherms for the uptake of N_2 (77 K) of the crystalline powder of the as-synthesized compound **1**

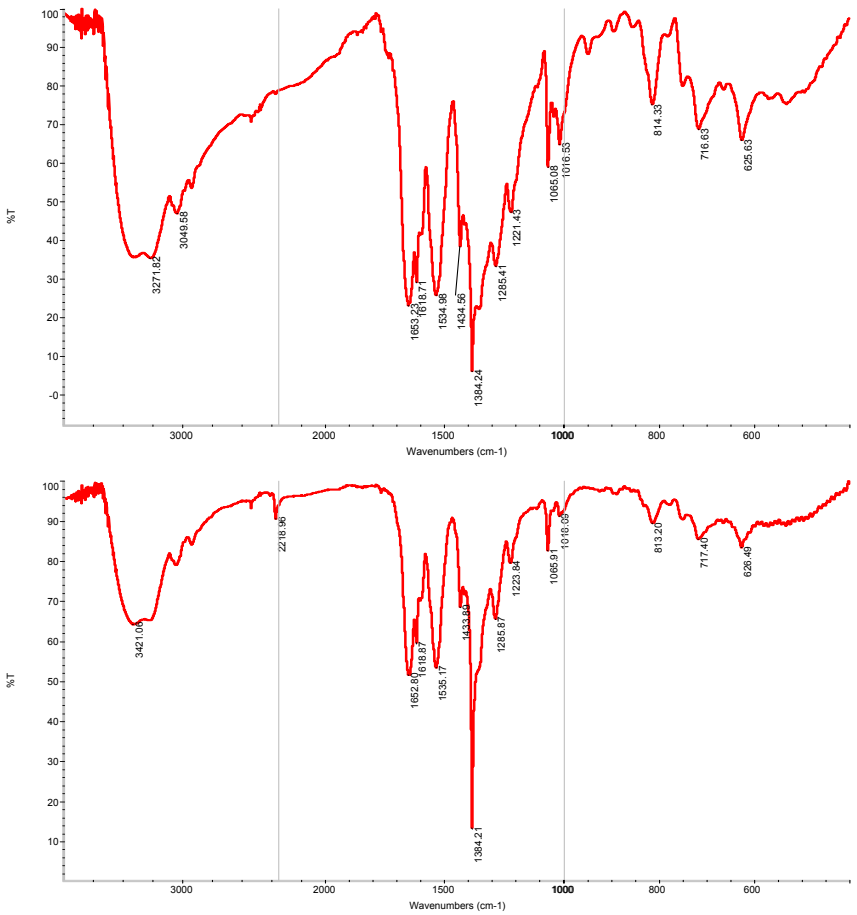


Figure S8. IR spectra of compound **1** and of compound **1** after immersing in benzene containing malononitrile (bottom)

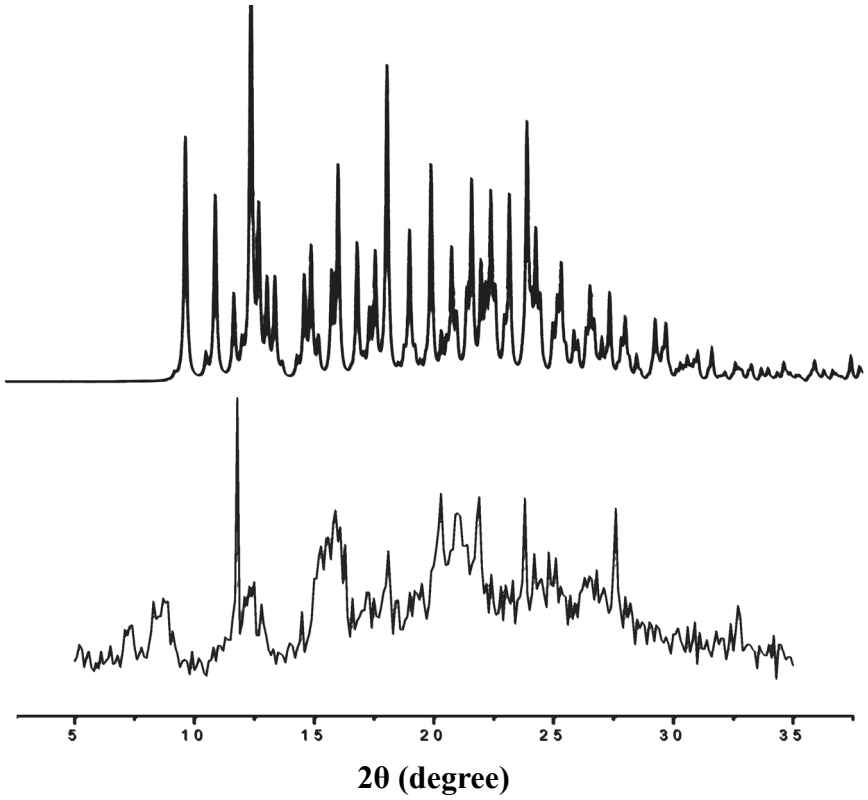


Figure S9. XRD pattern of compound **1** data after the reabsorb of methanol (bottom) and simulation of the XRD according to single crystal diffraction of compound **1** (top).

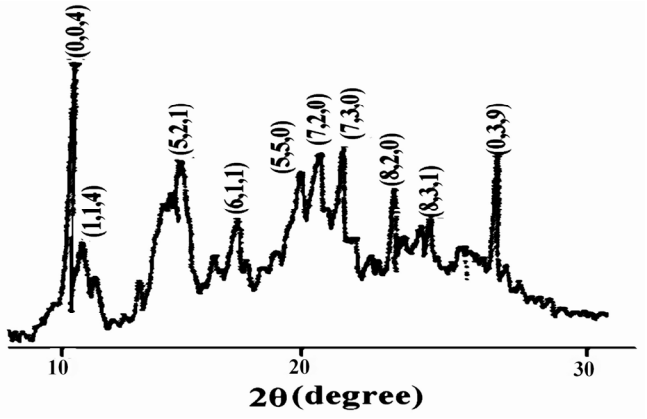


Figure S10. XRD pattern of compound **1** after the catalysis reaction with the indexes of some selected diffractions (the crystallographic index of the polycrystals was based on the least-square fitting of the cell parameters and the 2θ of these diffractions).

Reference:

S1. M. Mazik and A. König, *Eur. J. Org. Chem.* 2007, 3271–3276