# Supplementary Materials: New URJC-1 Material with Remarkable Stability and Acid-Base Catalytic Properties

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## S1. Crystallographic Data of URJC-1 Material

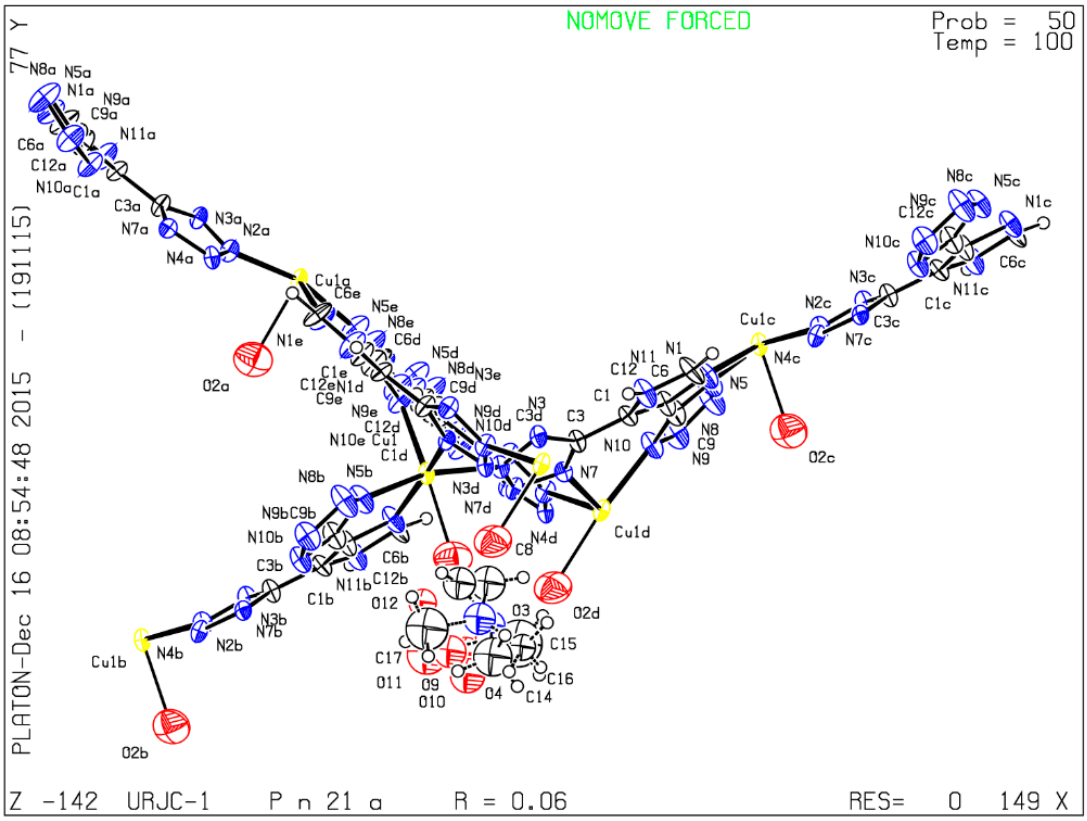


**Figure S1.** URJC-1 structure from checkcif file.

**Table S1.** Crystal data and structure refinement for compound URJC-1.

| Identification code | URJC-1 |
|---|---|
| Empirical formula | $C_{6.5}H_{5.5}CuN_{10.5}O_{1.25}$ |
| Formula weight | 314.25 |
| Temperature/K | 100.0 |
| Crystal system | orthorhombic |
| Space group | $Pn2_1a$ |
| *a*/Å | 8.6577(6) |
| *b*/Å | 9.0478(9) |
| *c*/Å | 14.9973(11) |
| $\alpha$/° | 90 |
| $\beta$/° | 90 |
| $\gamma$/° | 90 |
| Volume/Å$^3$ | 1,174.79(17) |
| Z | 4 |
| $\varrho_{calc}$g/cm$^3$ | 1.777 |
| $\mu$/mm$^{-1}$ | 2.811 |
| F(000) | 628.0 |
| Crystal size/mm$^3$ | 0.02 × 0.02 × 0.02 |
| Radiation | CuK$\alpha$ ($\lambda$ = 1.54178) |
| 2$\theta$ range for data collection/° | 11.802 to 136.714 |
| Index ranges | $-10 \le h \le 9$, $-10 \le k \le 10$, $-17 \le l \le 17$ |
| Reflections collected | 7090 |
| Independent reflections | 1999 [$R_{int}$ = 0.1146, $R_{sigma}$ = 0.0795] |
| Data/restraints/parameters | 1,999/101/210 |
| Goodness-of-fit on $F^2$ | 1.127 |
| Final R indexes [$I$>=2$\sigma$ (I)] | $R_1$ = 0.0619, $wR_2$ = 0.1311 |
| Final R indexes [all data] | $R_1$ = 0.0801, $wR_2$ = 0.1399 |
| Largest diff. peak/hole/e Å$^{-3}$ | 0.39/−0.46 |
| Flack parameter | 0.20(7) |

## S2. Structural Details of URJC-1 Structure

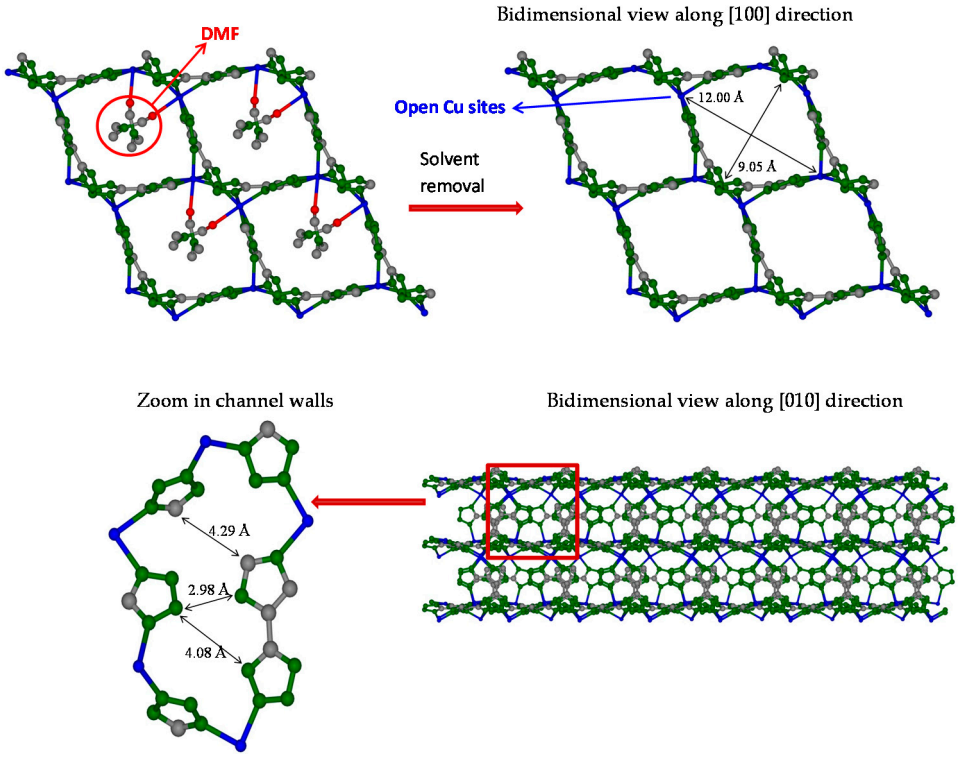


**Figure S2.** Structural details of URJC-1's pore system.

## S3. Reaction Turnover Frequency Parameters (TOF)

**Table S2.** TOF parameter of different catalysts after 1 h of anisole acylation reaction.

| Catalyst | TOF ($h^{-1}$) | Active sites [a] (mmol/mg) | Si/Al | Reference |
|---|---|---|---|---|
| URJC-1 | 47 | 0.0038 | - | This work |
| HKUST-1 [b] | 24 | 0.0050 | - | This work |
| ZSM-5 [b] | 76 | 0.00053 | 30 | This work |
| BEA ZEOLITE[b] | 110 | 0.00083 | 19 | This work |
| ZSM-5[c] | 26 | 0.00053 | 31 | [30] |

[a] Aluminum atoms in the case of zeolites, and copper atoms in the case of URJC-1 and HKUST-1 MOF materials; [b] HKUST-1, ZSM-5, and BETA were purchased to Sigma–Aldrich Química S.L., Sud Chemie Iberia S.L. and Zeolyst International, respectively; [c]: Synthesized by the authors of reference [30].

**Table S3.** TOF parameter of different catalysts after 1 h of Knoevenagel reaction.

| Catalyst | TOF ($h^{-1}$) | Active sites [a] (mmol/mg) |
|---|---|---|
| URJC-1 | 4 | 0.0038 |
| HKUST-1 | 19 | 0.0099 |
| UiO-66-$NH_2$ | 83 | 0.00061 |

[a] Basic non-coordinated nitrogen atoms from tetrazole rings for URJC-1; basic oxygen atoms from the carboxylate ligand for HKUST-1; basic amino groups for UiO-66-$NH_2$.