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.

<table>
<thead>
<tr>
<th>Identification code</th>
<th>URJC-1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Empirical formula</td>
<td>C₆₅H₅₅CuN₁₀₅O₁.₂₅</td>
</tr>
<tr>
<td>Formula weight</td>
<td>314.25</td>
</tr>
<tr>
<td>Temperature/K</td>
<td>100.0</td>
</tr>
<tr>
<td>Crystal system</td>
<td>orthorhombic</td>
</tr>
<tr>
<td>Space group</td>
<td>Pn2₁a</td>
</tr>
<tr>
<td>a/Å</td>
<td>8.6577(6)</td>
</tr>
<tr>
<td>b/Å</td>
<td>9.0478(9)</td>
</tr>
<tr>
<td>c/Å</td>
<td>14.9973(11)</td>
</tr>
<tr>
<td>α/°</td>
<td>90</td>
</tr>
<tr>
<td>β/°</td>
<td>90</td>
</tr>
<tr>
<td>γ/°</td>
<td>90</td>
</tr>
<tr>
<td>Volume/Å³</td>
<td>1,174.79(17)</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
</tr>
<tr>
<td>ρcalcg/cm³</td>
<td>1.777</td>
</tr>
<tr>
<td>μ/mm⁻¹</td>
<td>2.811</td>
</tr>
<tr>
<td>F(000)</td>
<td>628.0</td>
</tr>
<tr>
<td>Crystal size/mm³</td>
<td>0.02 × 0.02 × 0.02</td>
</tr>
<tr>
<td>Radiation</td>
<td>CuKα (λ = 1.54178)</td>
</tr>
<tr>
<td>2θ range for data collection/°</td>
<td>11.802 to 136.714</td>
</tr>
<tr>
<td>Index ranges</td>
<td>−10 ≤ h ≤ 9, −10 ≤ k ≤ 10, −17 ≤ l ≤ 17</td>
</tr>
<tr>
<td>Reflections collected</td>
<td>7090</td>
</tr>
<tr>
<td>Independent reflections</td>
<td>1999 [Rint = 0.1146, Rσ = 0.0795]</td>
</tr>
<tr>
<td>Goodness-of-fit on F²</td>
<td>1.127</td>
</tr>
<tr>
<td>Final R indexes [I&gt;2σ (I)]</td>
<td>R₁ = 0.0619, wR₁ = 0.1311</td>
</tr>
<tr>
<td>Final R indexes [all data]</td>
<td>R₁ = 0.0801, wR₁ = 0.1399</td>
</tr>
<tr>
<td>Largest diff. peak/hole/e Å⁻³</td>
<td>0.39/−0.46</td>
</tr>
<tr>
<td>Flack parameter</td>
<td>0.20(7)</td>
</tr>
</tbody>
</table>
S2. Structural Details of URJC-1 Structure

![Diagram showing structural details of URJC-1's pore system.]

**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.

<table>
<thead>
<tr>
<th>Catalyst</th>
<th>TOF (h⁻¹)</th>
<th>Active sites a (mmol/mg)</th>
<th>Si/Al</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>URJC-1</td>
<td>47</td>
<td>0.0038</td>
<td>-</td>
<td>This work</td>
</tr>
<tr>
<td>HKUST-1 b</td>
<td>24</td>
<td>0.0050</td>
<td>-</td>
<td>This work</td>
</tr>
<tr>
<td>ZSM-5 b</td>
<td>76</td>
<td>0.00053</td>
<td>30</td>
<td>This work</td>
</tr>
<tr>
<td>BEA ZEOLITEb</td>
<td>110</td>
<td>0.00083</td>
<td>19</td>
<td>This work</td>
</tr>
<tr>
<td>ZSM-5c</td>
<td>26</td>
<td>0.00053</td>
<td>31</td>
<td>[30]</td>
</tr>
</tbody>
</table>

* 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.

<table>
<thead>
<tr>
<th>Catalyst</th>
<th>TOF (h⁻¹)</th>
<th>Active sites a (mmol/mg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>URJC-1</td>
<td>4</td>
<td>0.0038</td>
</tr>
<tr>
<td>HKUST-1</td>
<td>19</td>
<td>0.0099</td>
</tr>
<tr>
<td>UiO-66-NH₂</td>
<td>83</td>
<td>0.00061</td>
</tr>
</tbody>
</table>

* 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-NH₂.

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