Supplementary Materials: The ZSM-5-Catalyzed Oxidation of Benzene to Phenol with N₂O: Effect of Lewis Acid Sites

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Figure. S1. XRD patterns of (a) H-ZSM-5-773, (b) H-ZSM-5-873, (c) H-ZSM-5-973 and (d) H-ZSM-5-1073.

Figure. S2. Pyridine FT-IR spectra on (a) H-ZSM-5-773, (b) H-ZSM-5-873, (c) H-ZSM-5-973 and (d) H-ZSM-5-1073.
Table S1. Acidity properties from Py-IR analysis for catalysts H-ZSM-5-773, H-ZSM-5-873, H-ZSM-5-973 and H-ZSM-5-1073.

<table>
<thead>
<tr>
<th>Samples</th>
<th>423 K(total) (mmol g⁻¹)</th>
<th>B/L</th>
<th>573 K(strong) (mmol g⁻¹)</th>
<th>B/L</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Brønsted⁺</td>
<td>Lewis⁺</td>
<td>Brønsted⁺</td>
<td>Lewis⁺</td>
</tr>
<tr>
<td>H-ZSM-5-773</td>
<td>0.17</td>
<td>0.06</td>
<td>2.83</td>
<td>0.12</td>
</tr>
<tr>
<td>H-ZSM-5-873</td>
<td>0.14</td>
<td>0.07</td>
<td>2.00</td>
<td>0.12</td>
</tr>
<tr>
<td>H-ZSM-5-973</td>
<td>0.11</td>
<td>0.09</td>
<td>1.22</td>
<td>0.08</td>
</tr>
<tr>
<td>H-ZSM-5-1073</td>
<td>0.08</td>
<td>0.09</td>
<td>0.89</td>
<td>0.04</td>
</tr>
</tbody>
</table>

⁺ Determined by FTIR spectra of absorbed pyridine.

Table S2. Benzene oxidation to phenol with N₂O after 20min of the reaction.

<table>
<thead>
<tr>
<th>Samples</th>
<th>N₂O selectivity to phenol (%)</th>
<th>LAS</th>
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<tbody>
<tr>
<td>H-ZSM-5-773</td>
<td>74.2</td>
<td>0.056</td>
</tr>
<tr>
<td>H-ZSM-5-873</td>
<td>70.3</td>
<td>0.067</td>
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<tr>
<td>H-ZSM-5-973</td>
<td>60.8</td>
<td>0.088</td>
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<tr>
<td>H-ZSM-5-1073</td>
<td>58.9</td>
<td>0.092</td>
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</table>

Table S3. Carbon calculation in the outlet flow after 3 h reaction time for samples.

<table>
<thead>
<tr>
<th>sample</th>
<th>The ratio between the carbon in the outlet flow to the inlet flow⁺ / %</th>
<th>Cokeᵇ / %</th>
</tr>
</thead>
<tbody>
<tr>
<td>H-ZSM-5</td>
<td>78</td>
<td>22</td>
</tr>
<tr>
<td>Fe-ZSM-5</td>
<td>74</td>
<td>26</td>
</tr>
<tr>
<td>H-ZSM-5-ST</td>
<td>82</td>
<td>18</td>
</tr>
<tr>
<td>Fe-ZSM-5-ST</td>
<td>87</td>
<td>13</td>
</tr>
<tr>
<td>H-ZSM-5-773</td>
<td>74</td>
<td>26</td>
</tr>
<tr>
<td>H-ZSM-5-873</td>
<td>74</td>
<td>26</td>
</tr>
<tr>
<td>H-ZSM-5-973</td>
<td>72</td>
<td>28</td>
</tr>
<tr>
<td>H-ZSM-5-1073</td>
<td>72</td>
<td>28</td>
</tr>
</tbody>
</table>

⁺ the amount of products such as CO and CO₂ were ignored as their marginally moles

ᵇ coke = (1-the ratio between the carbon in the outlet flow to the inlet flow)100%