An ultra-high H₂S-resistant gold-based imidazolium ionic liquid catalyist for acetylene hydrochlorination

Supporting Information

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<table>
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<th>Impurity</th>
<th>H₂S</th>
<th>DVS&lt;sup&gt;a&lt;/sup&gt;</th>
<th>PH₃</th>
<th>VA&lt;sup&gt;b&lt;/sup&gt;</th>
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<tr>
<td>ppm</td>
<td>250</td>
<td>700</td>
<td>400</td>
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<sup>a</sup> Divinyl Sulfide  
<sup>b</sup> Vinyl Acetyl
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<tr>
<th>Element</th>
<th>Weight %</th>
<th>Atomic %</th>
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<tbody>
<tr>
<td>C(K)</td>
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<td>99.78</td>
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<tr>
<td>S(K)</td>
<td>0.35</td>
<td>0.13</td>
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<tr>
<td>Cl(K)</td>
<td>0.07</td>
<td>0.02</td>
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<tr>
<td>Au(L)</td>
<td>0.85</td>
<td>0.05</td>
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*Table S2 EDS-mapping Quantification Results of Au/AC-S catalyst.*
**Fig. S1.** TEM images of (a) Au/AC-Used, (b) and (c) Au/AC-S.
Figure S2. EDS spectrum source data of (a) Au/AC (b) Au/AC-S (c) Au-IL/AC (d) Au-IL/AC-S.
Figure S3. (a) FT-IR spectrum of fresh and H$_2$S-treated IL and Au-IL (b) S 2p spectral line of the Au-IL/AC catalyst treated with H$_2$S at 180 °C for different time
Figure S4. Schematic diagram of the hydrochlorination reactor.
Adsorptivity of H$_2$S in the Au-IL/AC is determined by referring to the methods in the relevant literature$^{1-2}$, which was depicted in Figure S5. Figure S6 and S7 show the adsorption quantity and fit linear of H$_2$S in Au-IL/AC at 30 °C (303K) and 180 °C (453K), respectively. The relationship curve between $q$ (adsorption quantity, mg$_{H2S}$/g$_{IL}$) and $C_e$ (equilibrium concentration, mg$_{H2S}$/L$_{IL}$) conforms to Langmuir adsorption isotherm. *Langmuir* adsorption isotherm is the most commonly used equation to describe the adsorption isotherm. The commonly used linear form of *Langmuir* adsorption isotherm can be described by the following equation:

$$\frac{C_e}{q_e} = \frac{1}{K \cdot q_m} + \frac{1}{q_m} C_e$$

Where: $C_e$ is equilibrium concentration, mg$_{H2S}$/L$_{IL}$; $q_e$ is equilibrium adsorption quantity, mg$_{H2S}$/g$_{IL}$; $K$ is equilibrium constant, L/mg; $q_m$ is maximal equilibrium adsorption quantity, mg$_{H2S}$/g$_{IL}$.

It can be seen that $C_e/q_e$ has a linear relationship with $C_e$, as shown in Figure S6 and S7 (red dashed line). The adsorption equilibrium constant ($K$) at 30 °C (303K) and 160 °C (303K) calculated from the slope and intercept of the straight line is 0.83 and 0.24 L/mg, respectively.
Figure S5. Adsorption isotherm at 30 °C (303K) and 180 °C (453K).
Figure S6. Adsorption isotherm and linear fit using Langmuir model at 30 °C (303K).
Figure S7. Adsorption isotherm and linear fit using Langmuir model at 180 °C (453K).
To further investigate the influence of IL addition, we performed the Au-IL/AC catalyst at high temperature (180 °C) and high GHSV (740h⁻¹), Au/AC catalyst was used for comparison. The result was shown in Figure S8. From Figure S8b, we can see that Au-IL/AC catalyst exhibits good stability and catalytic activity in the presence of H₂S, which almost consistent with H₂S-free test. As for Au/AC catalyst, the presence of H₂S during the reaction extremely poisoning the active site, because the initial activity and catalytic stability were greatly decreased (Figure S8a). Figure S9 displays the catalytic performance of Au-IL/AC catalyst at higher reaction temperature (200 °C), we can see that the catalyst still performed a good stability with the presence of H₂S. Thus it is very clear that the addition of IL can slow down the deactivation process.
Figure S8. Catalytic performance of (a) 1% Au/AC and (b) 1% Au-20%IL/AC at 740 h$^{-1}$ and 180 °C with and without H$_2$S.
Figure S9. Catalytic performance of 1% Au-20%IL/AC at 740 h⁻¹ and 200 °C with and without H₂S.
Notes and references