Novel AuCl₃-thiourea catalyst with a low Au content and an excellent

catalytic performance for acetylene hydrochlorination

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Catalyst characterization

For the TEM experiment, a JEM-2010 electron microscope with an accelerating voltage of 200 kV, a line resolution of 0.14 nm, and a point-to-point resolution of 0.23 nm was used. XRD data were collected on a Bruker Advance D8 X-ray diffractometer using Cu-K α irradiation ($\lambda = 1.5406$ Å) as a source at 40 kV and 40 mA in the scanning range of 20 between 20° and 90°. XPS data were recorded on a Thermo ESCALAB 250XI experiment with a monochromatized Al, Ka X-ray source (225 W), minimum energy resolution of 0.45 eV (Ag 3d_{5/2}), and minimum XPS analysis area of 3 µm. The obtained spectra were analyzed using XPS peak software. A TPR experiment was carried out on an Auto Chem 2720 instrument. The catalysts were pretreated by passing through high-purity N₂ (50 mL/min) at 100 °C for 30 min and then heated at a rate of 10 K/min from 50 °C to 600 °C. TPD was also analyzed using an Auto Chem 2720 instrument. The samples were pretreated under hydrogen chloride atmosphere at a reactive temperature of 170 °C for 4 h, and then high-purity N₂ (50 mL/min) was passed through the sample at 100 °C for 30 min. The sample was heated at a rate of 10 °C/min from 100 °C to 600 °C to collect the data. TGA of the samples was conducted in a TGDSC simultaneous thermal analyzer (NETZSCH STA 449F3 Jupiter1, Germany). A 7 mg sample was used and heated to 900 °C in oxygen atmosphere at a flow rate of 30 mL/min and a heating rate of 10 °C/min.

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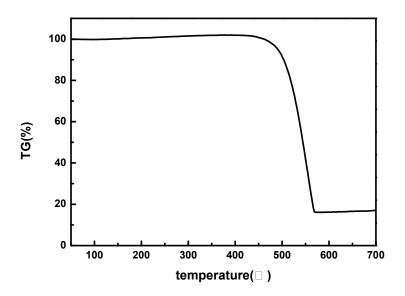


Fig. S1. TGA curves of the 0.4%AuCl₃-0.75%T/AC complex at a heating rate of 20 K/min under in O₂ atmosphere.

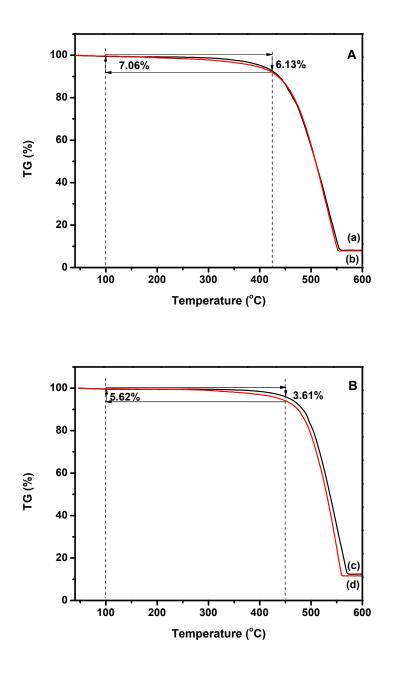


Fig. S2. TGA curves of (a) fresh 0.4%AuCl₃/AC, (b) used 0.4%AuCl₃/AC, (c) fresh 0.4%AuCl₃-0.75%T/AC and (d) used 0.4%AuCl₃-0.75%T/AC catalysts in oxygen atmosphere.

Catalyst	$S_{BET} (m^2/g)$	Pore volume (cm^{3}/g)
	Fresh	Fresh
0.4%AuCl ₃ /AC	961	0.56
0.4%AuCl ₃ -0.75%T/AC	973	0.55

Table S1. Pore structure parameters of the 0.4% AuCl_3-0.75% T/AC and

0.4%AuCl₃/AC catalysts.

Table S2. Screening of initial catalytic conversion and selectivity of acetylene in 1 h.

Catalyst	Conversion (%)	Selectivity (%)
0.4%AuCl ₃ /AC	33.26	99.87
0.4%AuCl ₃ -0.375%T/AC	73.16	99.94
0.4%AuCl ₃ -0.75%T/AC	77.45	99.95
0.4%AuCl ₃ -1.5%T/AC	70.81	99.96