

Supporting information for

Factors Influencing the Photocatalytic

Hydroamination of Alkynes with Anilines Catalyzed

by Supported Gold Nanoparticles under Visible

Light Irradiation

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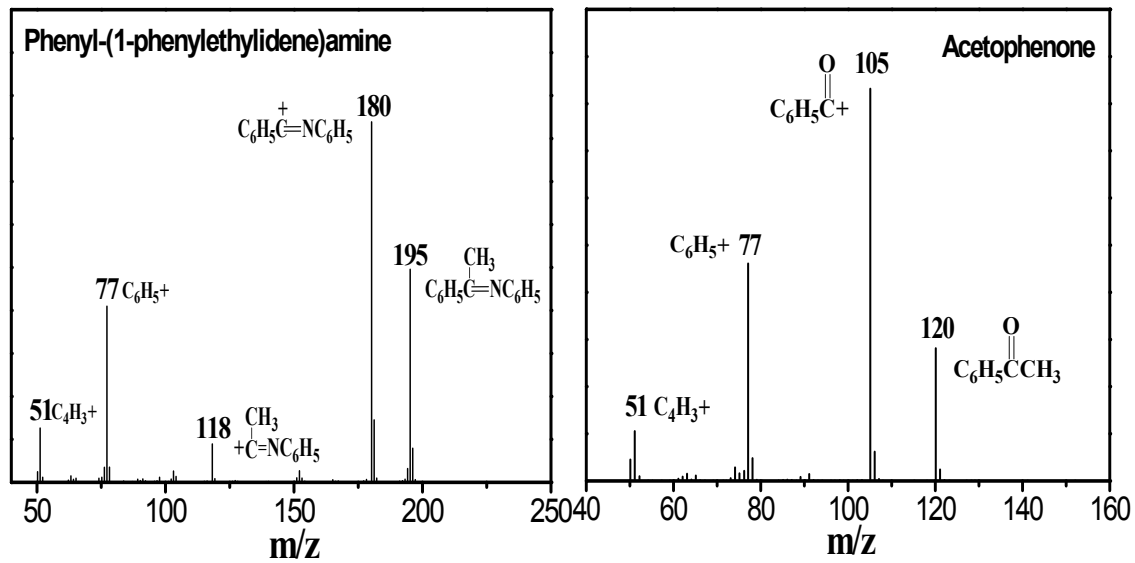


Figure S1(a). GC-MS of hydroamination products of phenylacetylene with aniline as example.

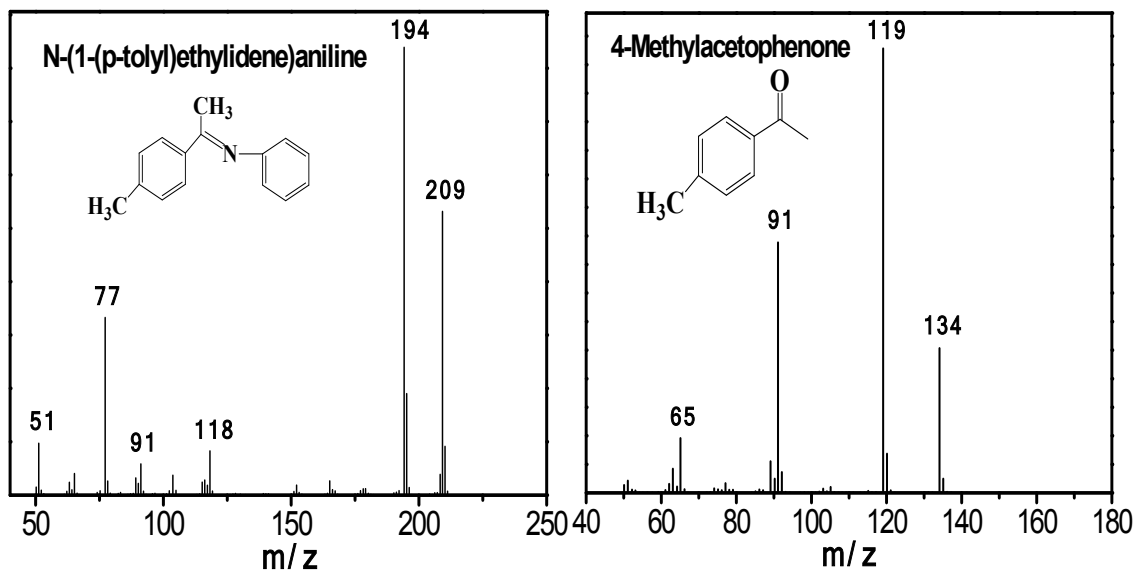


Figure S1(b). GC-MS of hydroamination products of 4-ethynyltoluene with aniline as example.

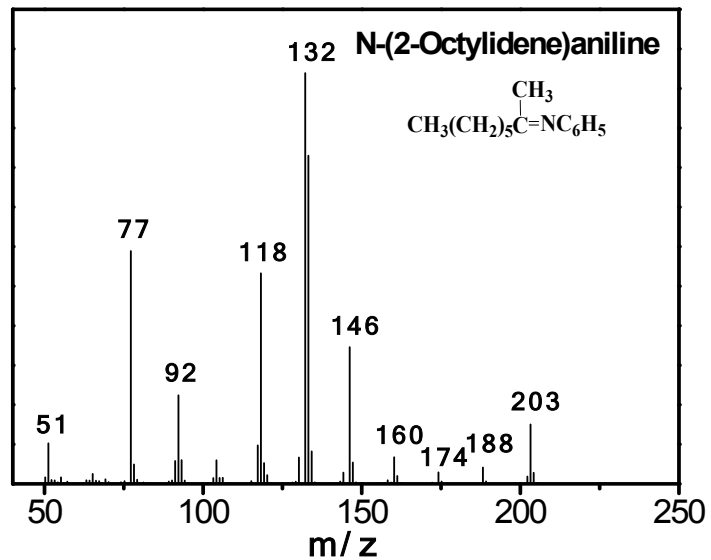


Figure S1(c). GC-MS of main product of 1-Octyne with aniline as example.

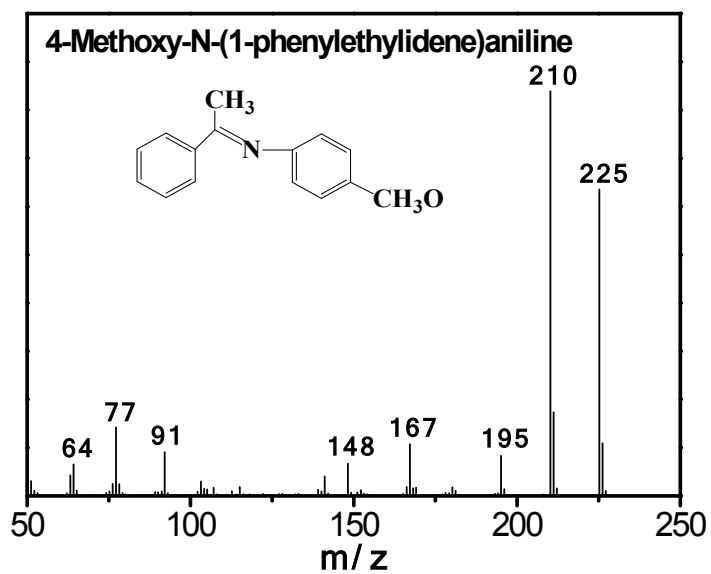


Figure S1(d). GC-MS of main product of phenylacetylene with 4-methoxyaniline as example.

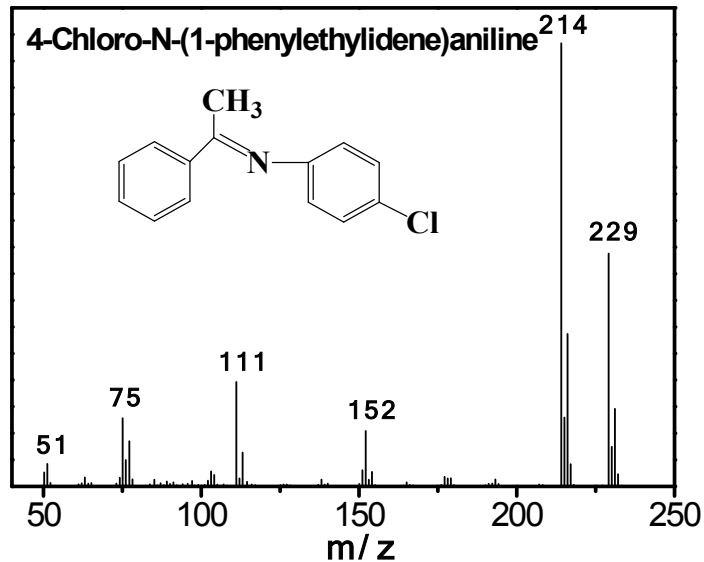


Figure S1(e). GC-MS of main product of phenylacetylene with 4-chloroaniline as example

The specific surface area of AuNPs is calculated according to $S_{Au} \text{ (m}^2\text{/g)} = C_1S_1 + C_2S_2 + \dots + C_nS_n$. S_n was obtained from following equation:¹

$$S_n = \frac{A_n}{m_n} = \frac{4\pi\left(\frac{d_n}{2}\right)^2}{\rho V_n} = \frac{\pi d_n^2}{\rho \cdot \frac{4}{3}\pi\left(\frac{d_n}{2}\right)^3} = \frac{6}{\rho d_n}$$

where C_n is the ratio of AuNPs with the diameter of d_n , ρ is the density of gold, $19.30 \text{ g}\cdot\text{cm}^{-3}$, d_n is the diameter of AuNPs in certain range, μm .

Reference

1. Janz, A., Köockritz, A., Yao, L. & Martin, A. Fundamental calculations on the surface area determination of supported gold nanoparticles by alkanethiol adsorption. *Langmuir* 26, 6783-6789 (2010).

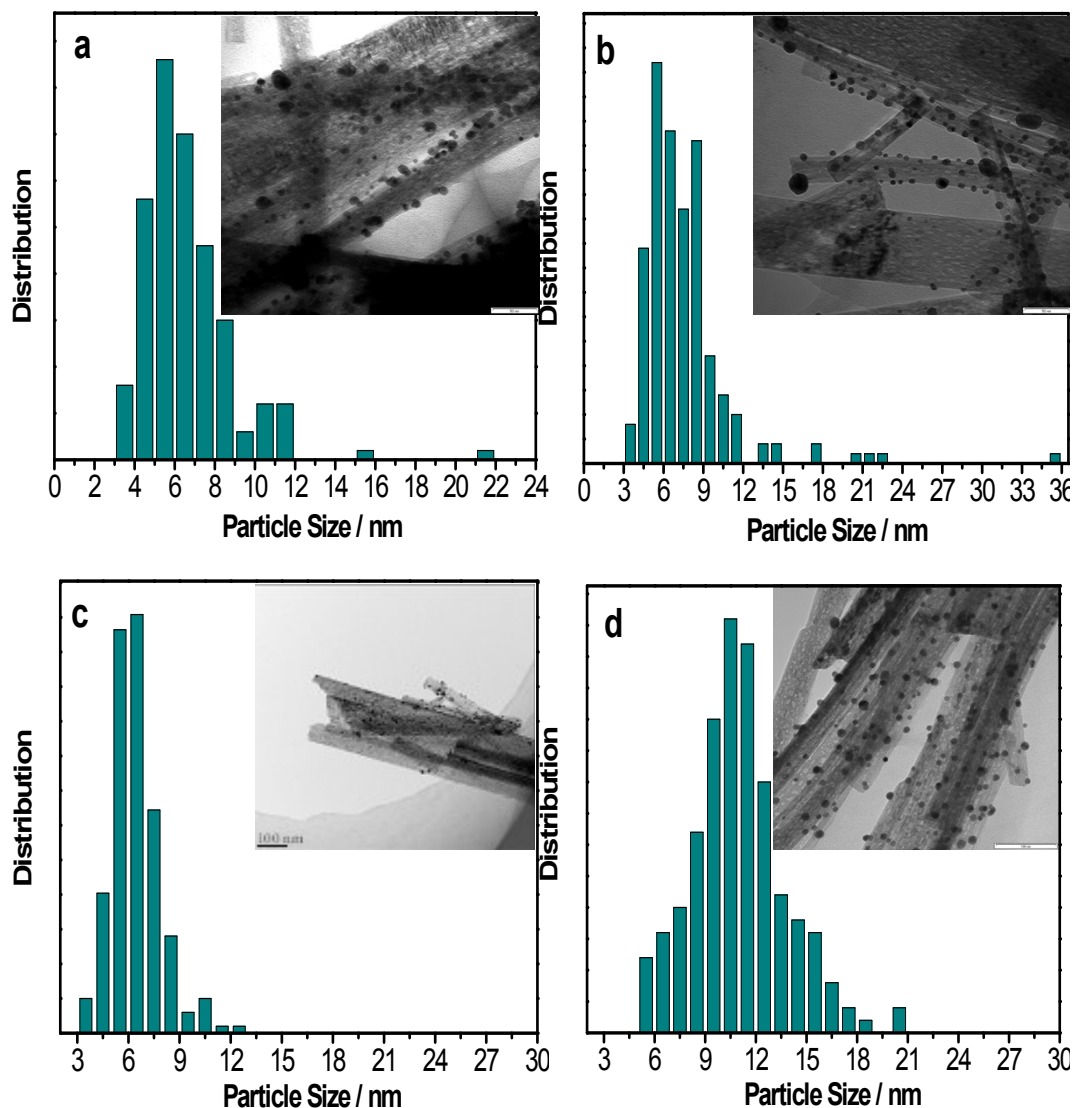


Figure S2. The size distribution of AuNPs on $\text{TiO}_2(\text{B})$ according to TEM analysis. [a] 2wt% Au/ $\text{TiO}_2(\text{B})$, 50 nm scale; [b] 2wt% Au/ $\text{TiO}_2(\text{B})$ calcined at 300 °C for 3 h, 50 nm scale; [c] 3wt% Au/ $\text{TiO}_2(\text{B})$, 100 nm scale; [d] 3wt% Au/ $\text{TiO}_2(\text{B})$ calcined at 400 °C for 12 h, 100 nm scale.

Conversion difference is only 3% for [a] 2wt% Au/ $\text{TiO}_2(\text{B})$ and [b] 2wt% Au/ $\text{TiO}_2(\text{B})$ calcined at 300 °C (size difference of AuNPs 1-2 nm), while 20% for Au/ $\text{TiO}_2(\text{B})$ and Au/ $\text{TiO}_2(\text{B})$ calcined at 400 °C (size difference of AuNPs ≥ 5 nm).

Table S1. Photocatalytic Hydroamination of 4-phenyl-1-butyne with Aniline by AuNPs on Different Supports^a.

Entry	Photocatalysts	Conv. (%) ^b	S _I (%) ^c	S _K (%) ^d
1	Au/TiO ₂ (B)	76	94	2
2	Au/TiO ₂ (B).N	90	91	1
3	Au/TiO ₂ (anatase)	59	90	5
4	Au/P25	70	95	4
5	Au/ZrO ₂	35	95	2
6	Au/CeO ₂	0.4	100	-
7	Au/Al ₂ O ₃	42	95	1
8	Au/Zeolite Y	10	85	3

^a Reaction conditions: 0.015 mmol of AuNPs, 4-phenyl-1-butyne (2 mmol), aniline (2 mmol), 2 ml of toluene as solvent, reacted under visible light at 40 °C for 25 h, argon atmosphere. ^b Determined by GC analysis, the mole of imine and ketone/mole of left alkyne and imine. ^c S_I = Selectivity for the imine. ^d S_K = Selectivity for the ketone.