

## **N-Heterocyclic Carbene-Stabilized Gold-Copper Nanoclusters: Synthesis, Bonding and Mechanochromism**

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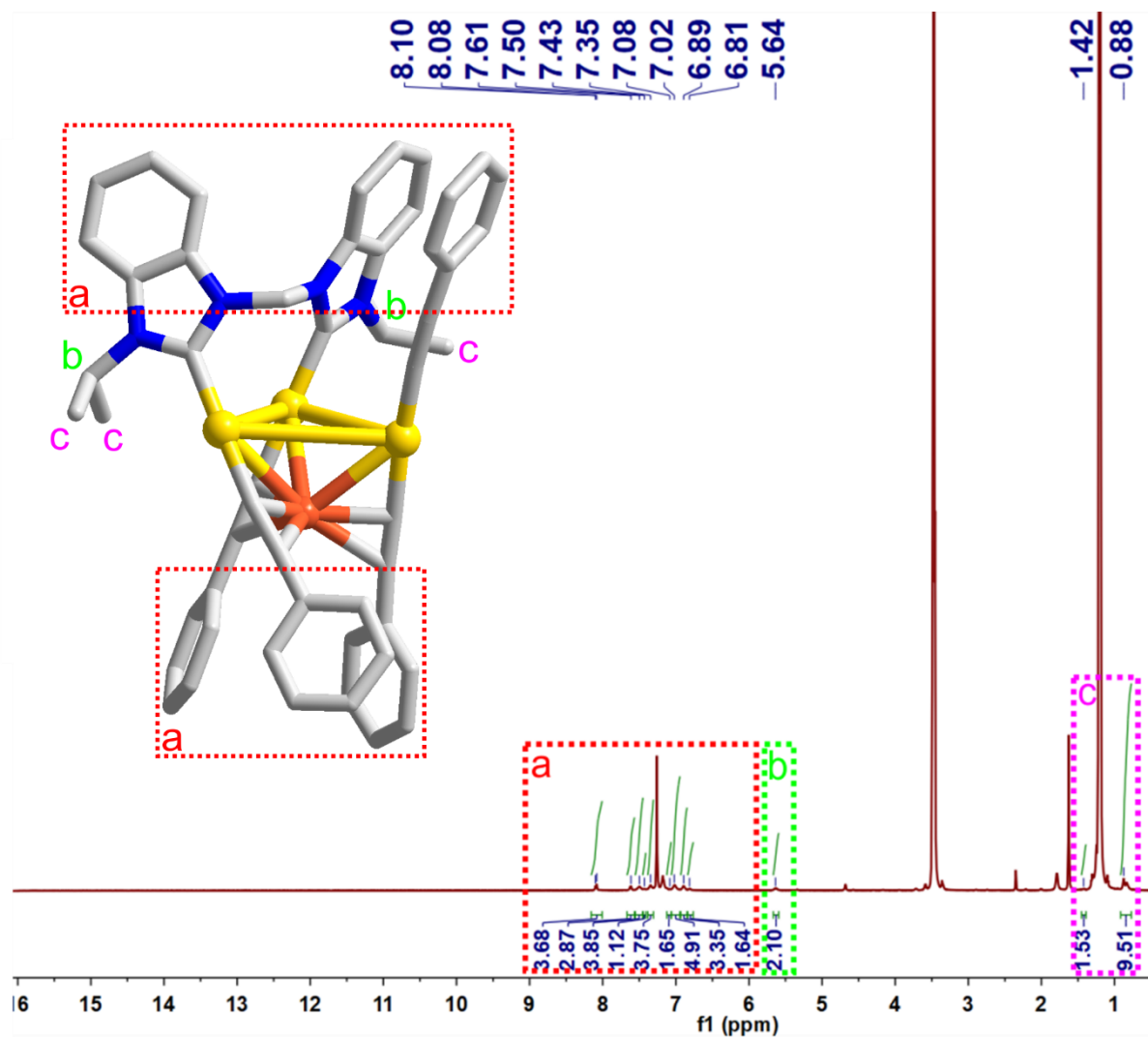
E-mail: shen@imu.edu.cn



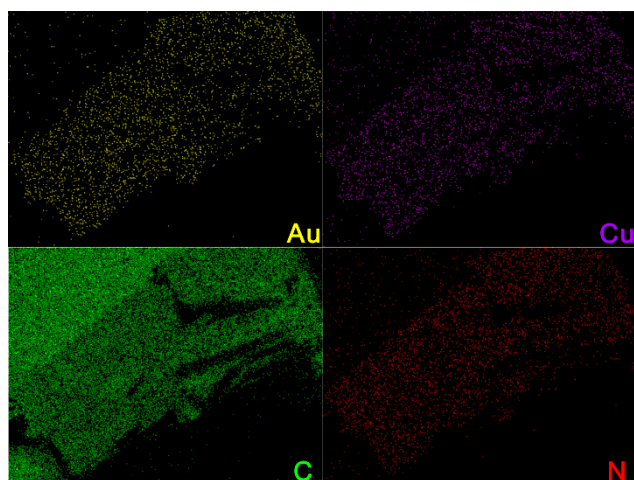
**Figure S1.** Digital photographs showing raw product in the presence (left) and absence (right) of the Cu salt in the cluster synthesis.



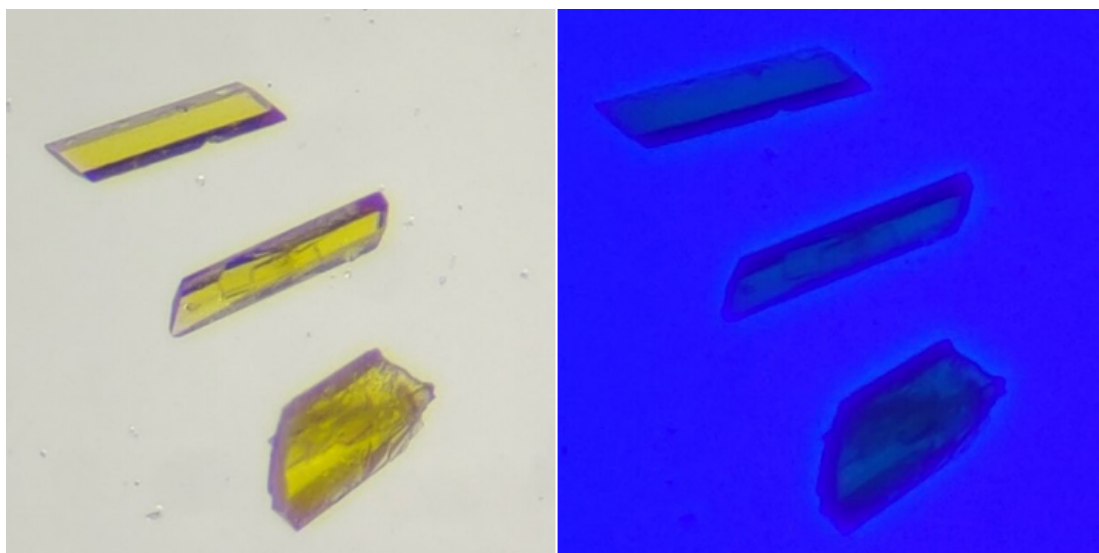
**Figure S2.** Digital photograph of Au<sub>3</sub>Cu crystals.



**Figure S3.**  $^1\text{H}$  NMR spectra (600 MHz, 298 K) of  $\text{Au}_3\text{Cu}$  in  $\text{CDCl}_3$ .



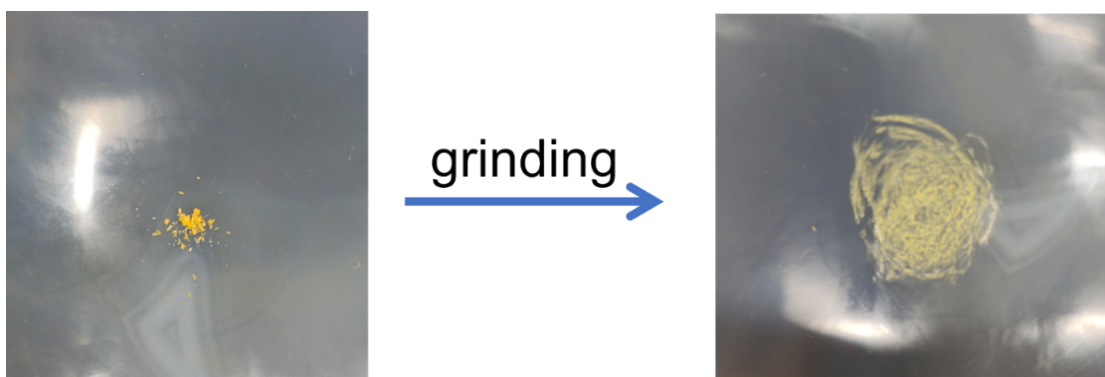
**Figure S4.** EDS image of the Au<sub>3</sub>Cu nanocluster.



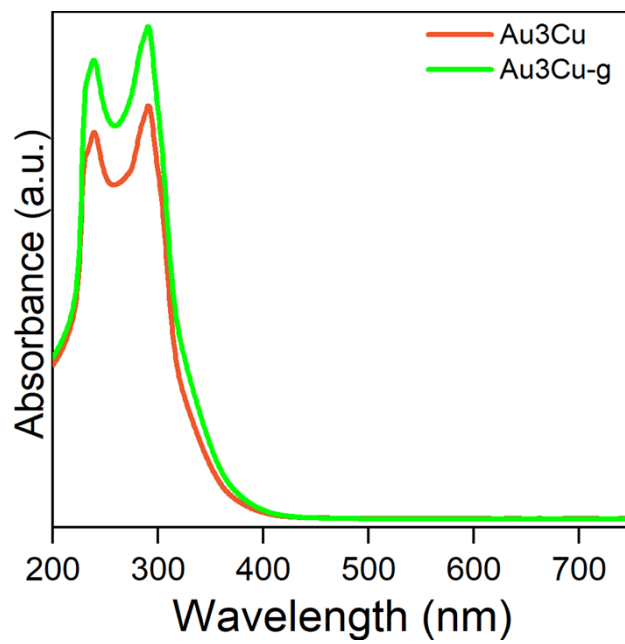
**Ambient light**

**UV light**

**Figure S5.** Luminescent phenomena of Au<sub>3</sub>Cu clusters under ambient and UV light.



**Figure S6.** Digital photographs showing the grinding process of the  $\text{Au}_3\text{Cu}$  cluster under ambient light.



**Figure S7.** The UV-Vis spectrum of Au<sub>3</sub>Cu before and after grinding.



**Table S1.** Crystallographic data of Au<sub>3</sub>Cu(iPrNHCiPr)(PA)<sub>4</sub>.

Identification code	Au <sub>3</sub> Cu(iPrNHCiPr)(PA) <sub>4</sub>
<b>Formula</b>	C <sub>53</sub> H <sub>44</sub> Au <sub>3.1</sub> Cu <sub>0.9</sub> N <sub>4</sub>
<b>Formula wight</b>	1404.70
<b>Temperature/K</b>	100.00(10)
<b>Crystal system</b>	monoclinic
<b>Space group</b>	P21/c
<b>a (Å)</b>	11.30910(10)
<b>b (Å)</b>	15.7826(2)
<b>c (Å)</b>	25.6534(2)
<b>α (°)</b>	90
<b>β (°)</b>	100.2160(10)
<b>γ (°)</b>	90
<b>V (Å<sup>3</sup>)</b>	4506.21(8)
<b>Z</b>	4
<b>D<sub>c</sub> / (g·cm<sup>-3</sup>)</b>	2.071
<b>Radiation</b>	Cu Kα (λ= 1.54184 Å)
<b>Theta (°) range</b>	6.604 to 150.066
<b>Index ranges</b>	-14 ≤ h ≤ 7, -16 ≤ k ≤ 19, -32 ≤ l ≤ 31
<b>Refls. Total</b>	29993
<b>Restraints</b>	48
<b>Parameters</b>	554
<b>R<sub>int</sub></b>	0.0371
<b>R<sub>1</sub>/wR<sub>2</sub></b>	0.0329
<b>[I&gt;2σ(I)]</b>	0.0830
<b>R<sub>1</sub>/wR<sub>2</sub></b>	0.0377
<b>(all data)</b>	0.0853
<b>Completeness</b>	0.998
<b>Goof</b>	1.036

**Table S2.** Selected bond lengths (Å) of Au<sub>3</sub>Cu.

<i>Parameter</i>	<i>Value (Å)</i>	<i>Parameter</i>	<i>Value (Å)</i>
Au01-Cu04	2.9595(9)	Au04-C012	2.436(6)
Au02-Au04	2.8737(9)	Au04-C018	2.352(7)
Au02-C00G	2.002(6)	C00F-Cu04	2.119(6)
Au02-C00H	2.023(6)	C00G-Cu04	2.149(6)
Au03-Cu04	2.8968(9)	C00K-Cu04	2.254(6)
Au04-C00F	2.119(6)	C00R-Cu04	2.091(6)
Au04-C00G	2.149(6)	C012-Cu04	2.436(6)
Au04-C00K	2.254(6)	C018-Cu04	2.352(7)
Au04-C00R	2.091(6)		