Supporting Information

Control of Aurophilic Interaction: Conformations and Electron Structures of One-Dimensional Supramolecular Architectures

Hiroaki Imoto,[a] Shintaro Nishiyama,[a] Takashi Yumura,[b] Seiji Watase,[c] Kimihiro Matsukawa,[a,c] Kensuke Naka[a]*

[a] Faculty of Molecular Chemistry and Engineering, Graduate School of Science and Technology, Kyoto Institute of Technology, Goshokaido-cho, Matsugasaki, Sakyo-ku, Kyoto 606-8585, Japan.
[b] Faculty of Materials Science and Engineering, Graduate School of Science and Technology, Kyoto Institute of Tech-nology, Goshokaido-cho, Matsugasaki, Sakyo-ku, Kyoto 606-8585, Japan.
[c] Osaka Municipal Technical Research Institute, 1-6-50 Morinomiya, Joto-ku, Osaka 536-8553, Japan.

Contents:

1. NMR spectra

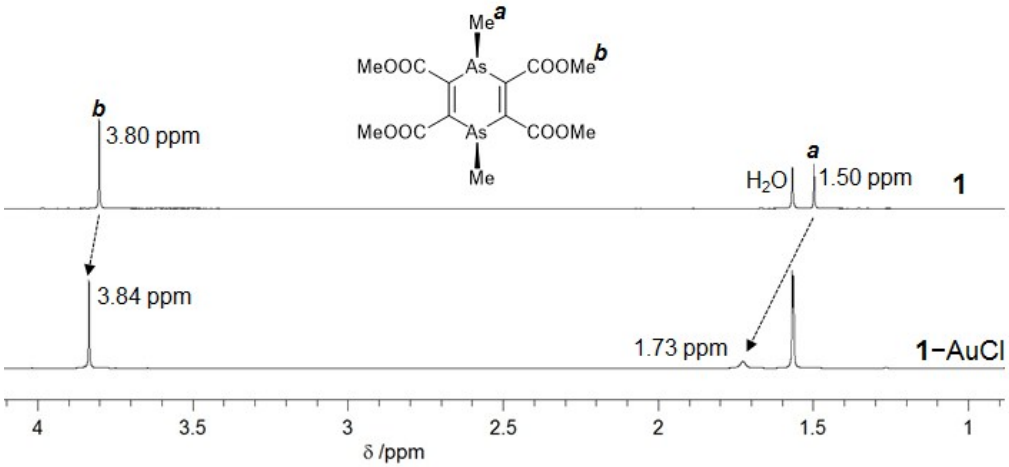

Figure S1. ^{1}H-NMR spectra (400 MHz) of **1** and **1**−AuCl in $CDCl_3$.

2. Crystallographic data

Table S1. Crystallographic Data.

	1−AuCl
Crystal data	
Empirical Formula	$C_{14}H_{18}As_2Au_2Cl_2O_8$
Formula Weight	928.97
Crystal Dimension, mm^3	0.150 × 0.100 × 0.100
Crystal System	triclinic
Space Group	P-1
a, Å	9.7958(3)
b, Å	10.6346(4)
c, Å	13.0215(4)
α, deg	79.1560(12)
β, deg	74.7870(9)
γ, deg	60.7176(10)
Volume, $Å^3$	1138.83(7)
D_{calcd}, g cm^{-3}	2.709
Z	2
F(000)	848.00
Data Collection	
Temperature, deg	23.0
2θmax, deg	54.9
Tmin/Tmax	0.082 / 0.201
Refinement	
No. of Observed Data	5167
No. of Parameters	253
R1[a], wR2[b]	0.0349, 0.0826
Goodness of Fit Indictor	1.073

[a]$R1 = \Sigma \, | |Fo| - |Fc| | / \Sigma \, |Fo|$ [b]$wR2 = [\Sigma \, w ((Fo^2-Fc^2)^2 / \Sigma \, w (Fo^2)^2]^{1/2}$ $w = [\sigma^2(Fo^2)]^{-1}$

CCDC # 1527551 (**1**−AuCl)

3. Absorption spectra

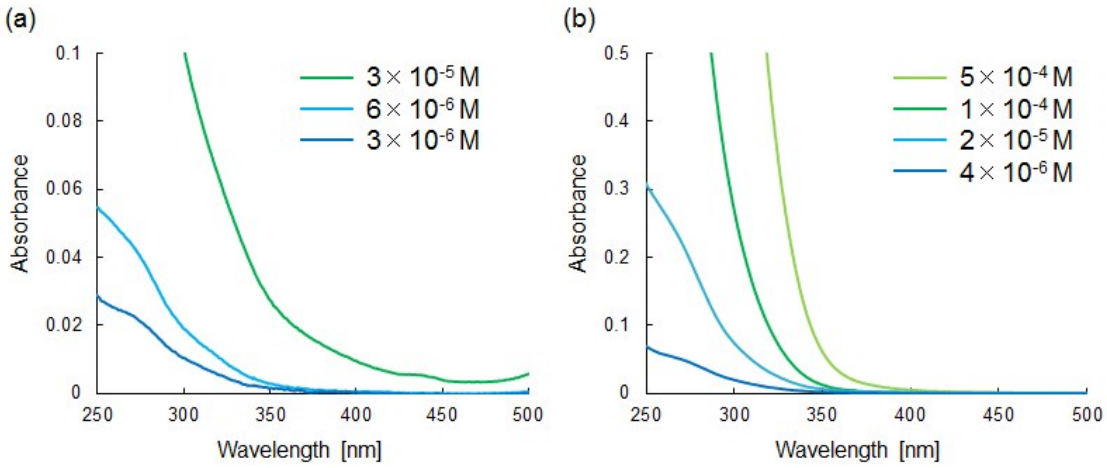

Figure S2. UV-vis absorption spectra of (a) **1**−AuCl and (b) **2**−AuCl with changing the concentration. The offsets of the spectra were red-shifted under concentrated conditions (**1**−AuCl: 3×10^{-5} M, **2**−AuCl: 5×10^{-4} M).

3. DFT calculation

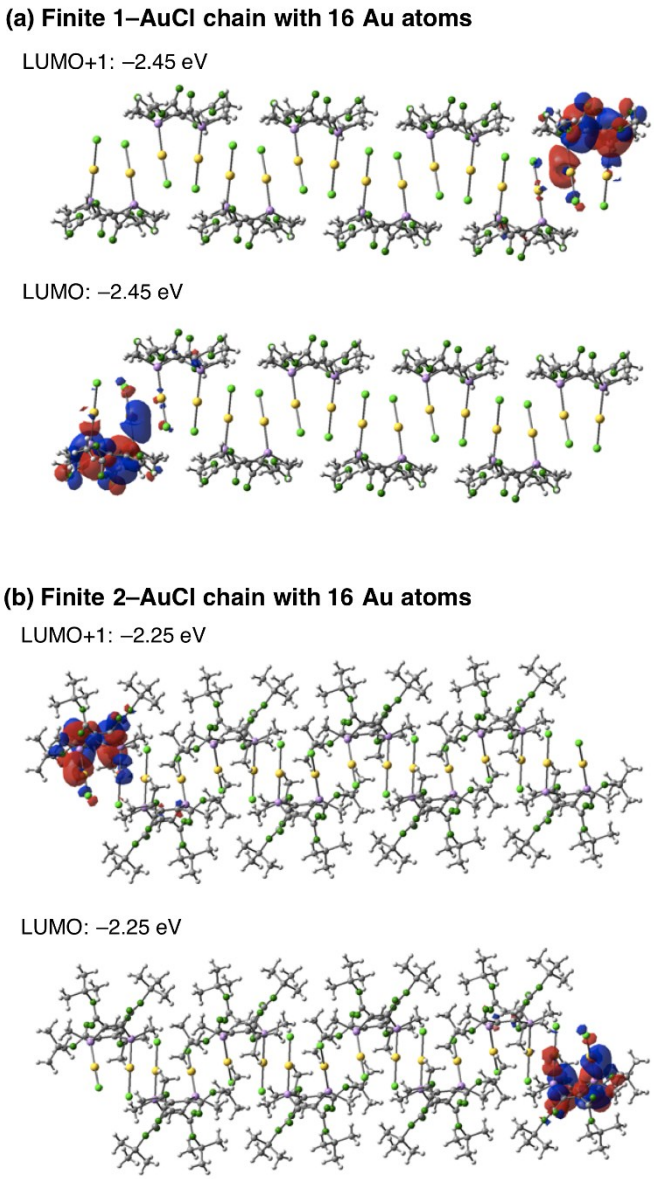

Figure S3. Unoccupied orbitals in the frontier orbitals regions finite (a) **1**−AuCl and (b) **2**−AuCl chains containing 16 Au atoms.

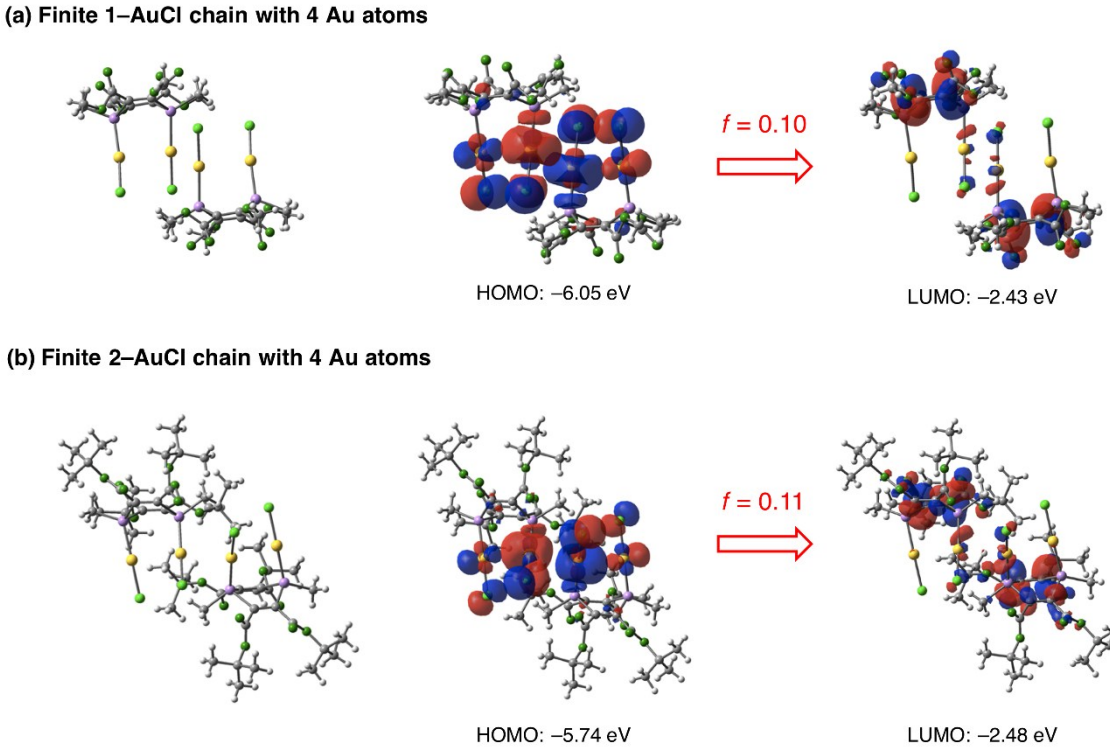

Figure S4. Frontier orbitals of finite (a) **1**−AuCl and (b) **2**−AuCl chains containing 4 Au atoms that are responsible for electronic transition with substantial oscillator strength (*f*), obtained from TD-DFT calculations with B3LYP functional.