# Coumarin based Gold(I)-Alkynyl Complex: A new class of Supramolecular Hydrogelator

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# Supporting Information

**Figure S1.** Hydrogel formation with complex **1** checked by the inverted tube method.

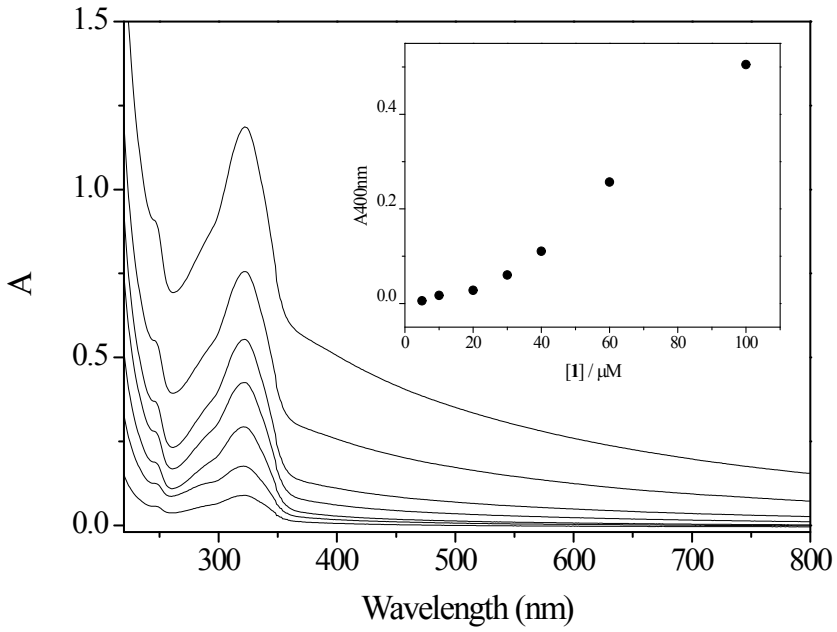


**Figure S2.** Absorption spectra of **1** between 5 to 100 μM in water. Inset: Plot of the absorption at 400 nm *vs*. concentration.

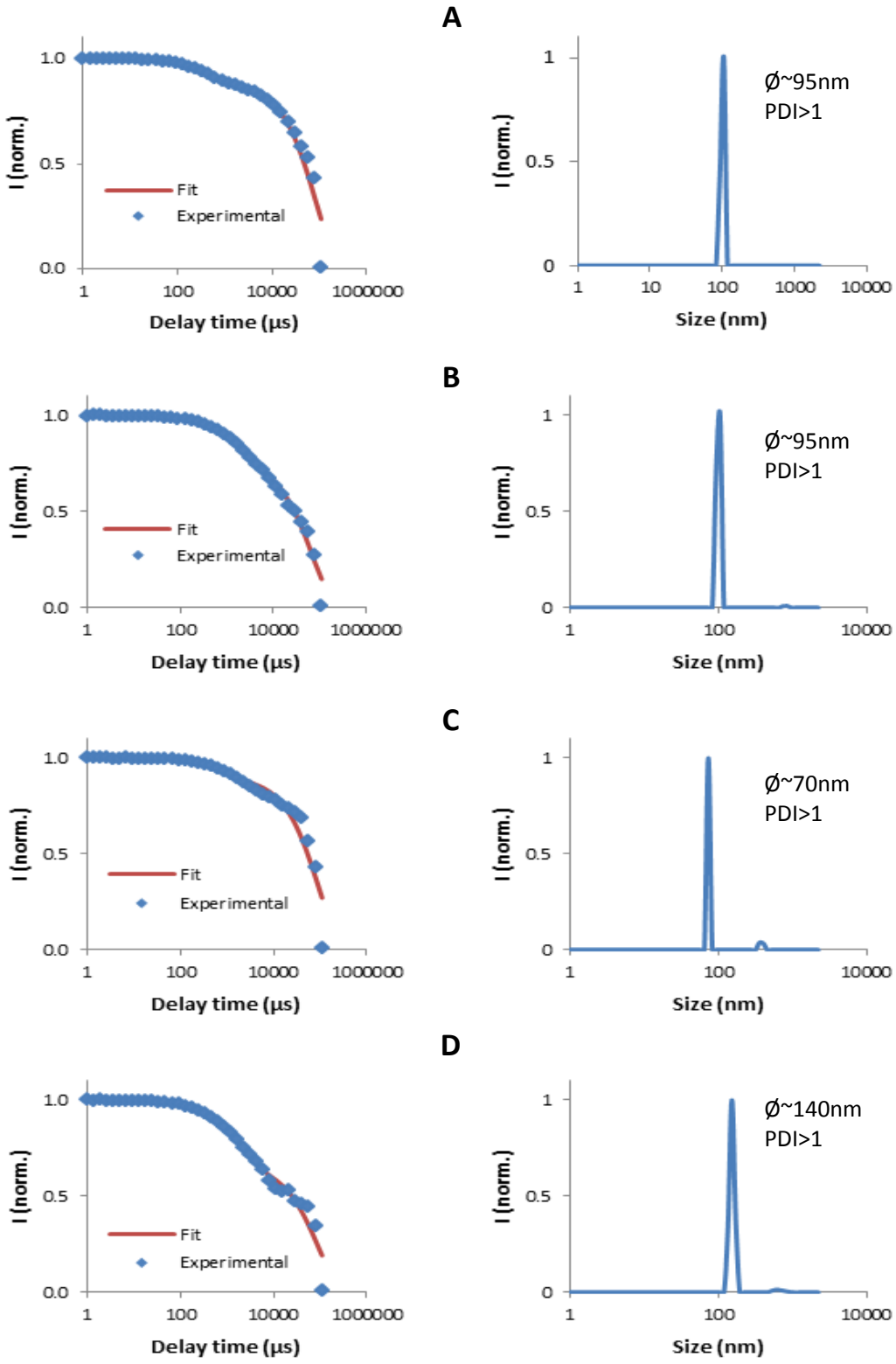


**Figure S3.** DLS auto-correlation data (left) and resulting size distributions (right) of aqueous solutions of **1** at different concentrations in water: (A) $1x10^{-4}$M, (B) $1x10^{-5}$M, (C) $1x10^{-6}$M and (D) $1x10^{-7}$M.

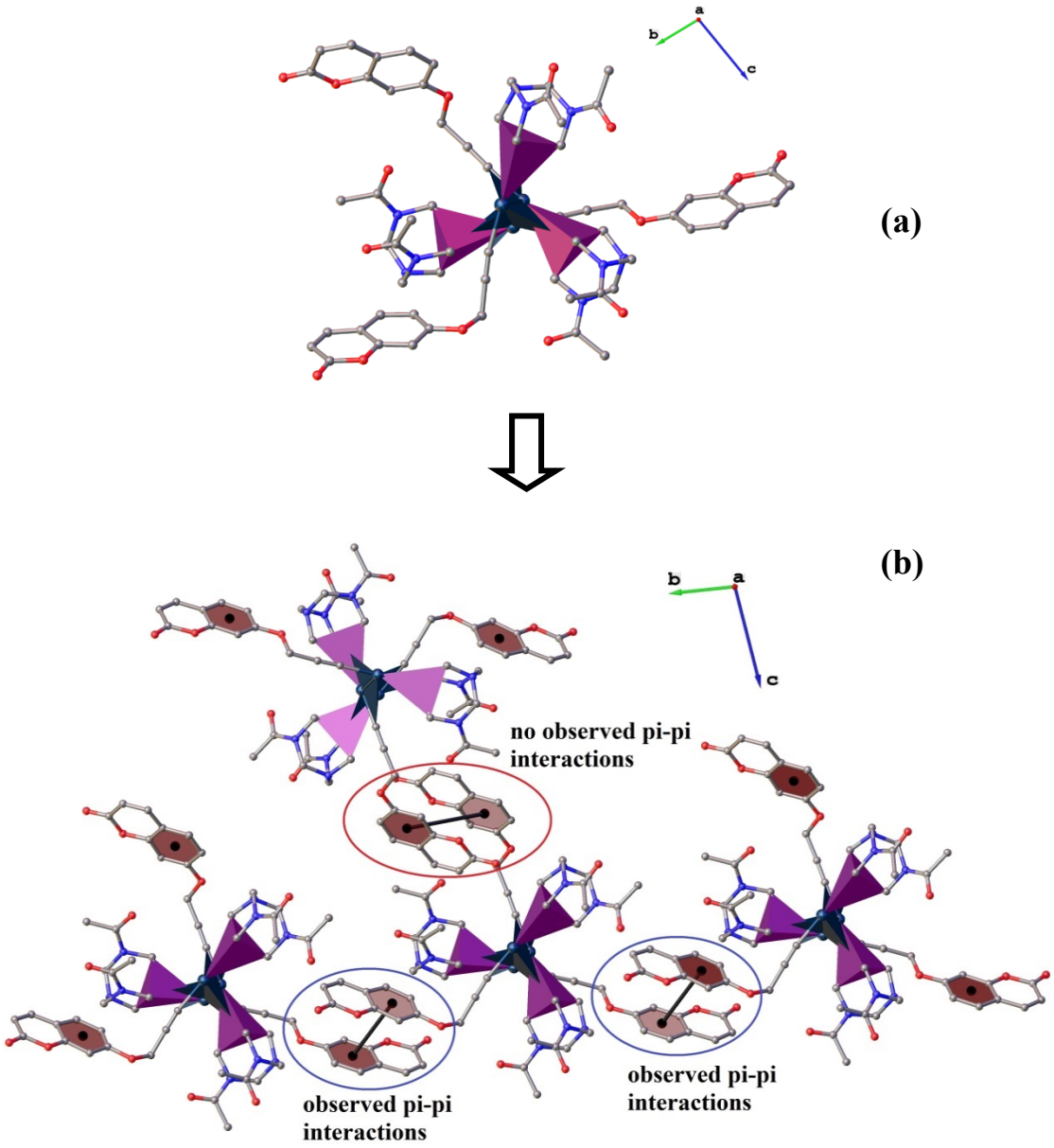


**Figure S4.** Schematic representation of (a) star-shaped 1-D polymeric structure of **1** and (b) observed π–π interactions. Hydrogen atoms and dichloromethane molecules are omitted for clarity.

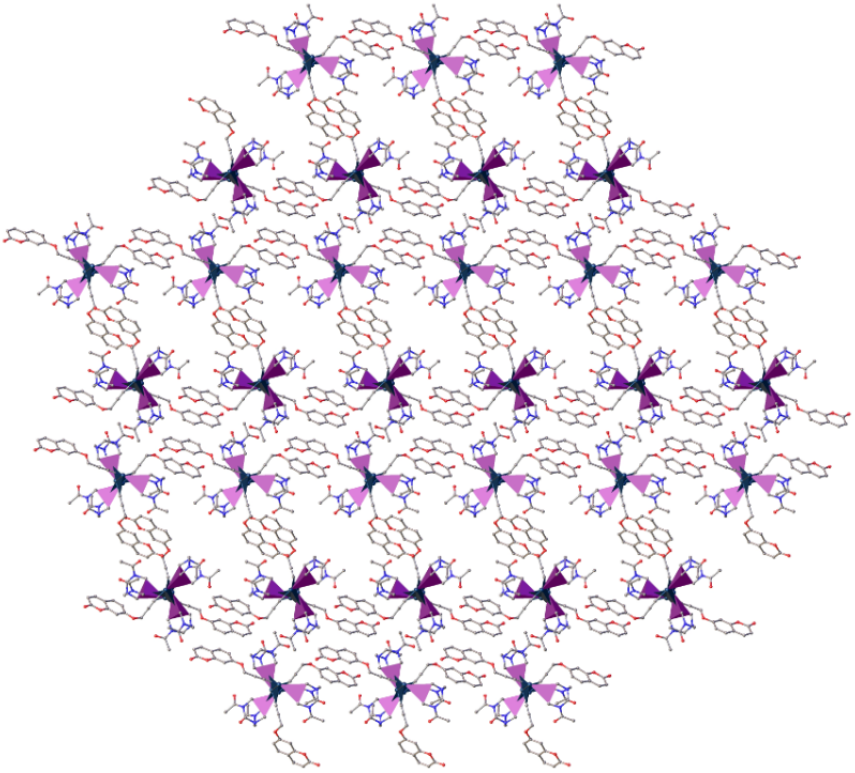

**Figure S5.** 3-D crystal packing of **1** viewed down the *a*-axis. Hydrogen atoms and dichloromethane molecules are omitted for clarity.

**Table S1.** X-ray crystallographic data for **1**.

| | **1** |
|---|---|
| Empirical Formula | $C_{21}H_{23}AuN_3O_5P$ |
| Molecular Weight (g/mol) | 625.36 |
| Temperature (K) | 123 |
| Wavelength (Å) | 1.54184 |
| Crystal System, space group | Triclínic, *P-1* |
| a (Å) | 8.8818(3) |
| b (Å) | 16.2625(6) |
| c (Å) | 26.4923(9) |
| α (º) | 97.863(3) |
| β (º) | 90.585(3) |
| γ (º) | 105.420(3) |
| V (Å$^3$) | 3649.8(2) |
| Z, $D_{calcld}$ (g cm$^{-3}$) | 2, 1.7844(1) |
| Absorption coefficient (mm$^{-1}$) | 12.973 |
| *F*(000) | 1908.0 |
| Crystal size (mm) | 0.13×0.04×0.04 |
| $\vartheta$ range for data collection [°] | 3.1 to 66.7 |
| Index ranges | -9 ≤ h ≤ 10 |
| | -18 ≤ k ≤ 19 |
| | -31 ≤ l ≤ 30 |
| Collected reflections No. | 19902 |
| Independent reflections No. / $R_{Int.}$ | 12079 / 0.0342 |
| Reflections No. $I \geq 2\sigma(I)$ | 10358 |

| | |
|---|---|
| Refinement method | full-matrix least-squares on $F^2$ |
| Data/restraints/parameters | 12079 / 24 / 865 |
| Goodness-of-fit on $F^2$ | 1.036 |
| Final *R* indices [$I > 2\sigma(I)$] | R1 = 0.0415, wR2 = 0.1100 |
| *R* indices (all data) | R1 = 0.0492, wR2 = 0.1140 |
| Largest diff. peak and hole ($e Å^{-3}$) | $1.81 < \Delta\rho < -1.61$ |