

Supporting Information for

A novel aggregation-induced emission poly(phosphoramidate): fluorescence properties and visual detection for Cu²⁺

Liulong Guo, Hongxia Yan,* Lianlian Wang, Pengfei Yang, Lirong Yan and Yan Zhao*

Key Laboratory of Polymer Science and Technology of Shaanxi Province, School of Chemistry and Chemical Engineering, Northwestern Polytechnical University, Xi'an 710072, China.

E-mail: hongxiayan@nwpu.edu.cn; zhaoyan@nwpu.edu.cn.

Table S1 The specific data during P1–P4 synthesis.

	P1	P2	P3	P4
Reactant A	TEP	TEP	TEP	TEP
Reactant B	DEM	DEM	DEM	DAH
A/B(mol/mol)	1:1.6	1:1.4	1:1.8	1:1.6
m _A /g (n _A /mol)	27.32 (0.15)	27.32 (0.15)	27.32 (0.15)	27.32 (0.15)
m _B /g (n _B /mol)	14.42 (0.24)	12.60 (0.21)	16.20 (0.27)	24.89 (0.24)
-OCH ₂ CH ₃ /- NH ₂ (mol/mol)	3:3.2	3:2.8	3:3.6	3:3.2

Where m_A: the mass of reactant A

n_A: the amount of substance of reactant A

m_B: the mass of reactant B

n_B: the amount of substance of reactant B

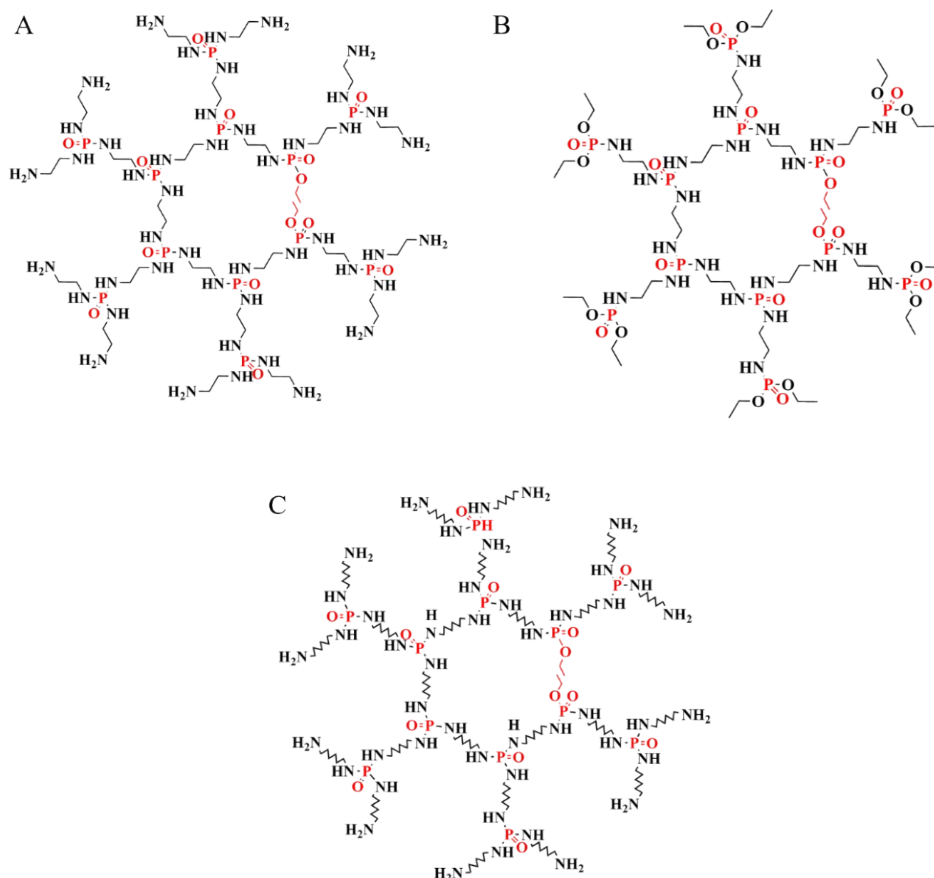
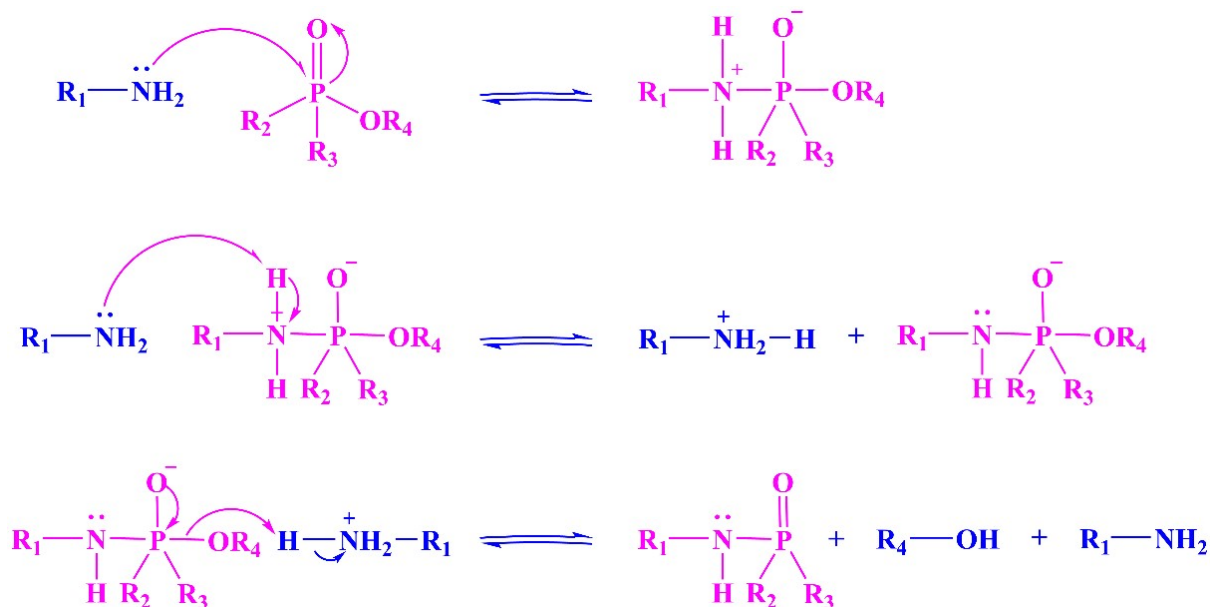


Fig. S1. Schematic structure of (A) P1 and P3, (B) P2, (C) P4



Scheme S1 The aminolysis reaction mechanism of phosphate and polyamines.

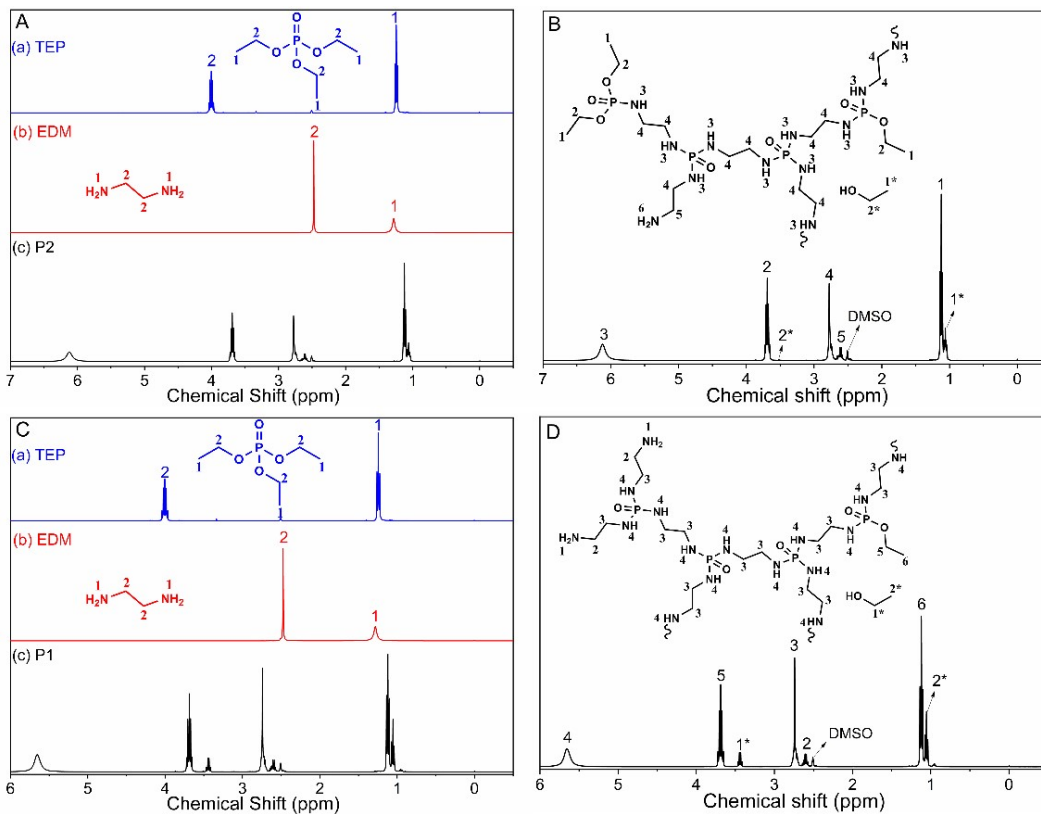


Fig. S2 The ^1H NMR spectra of reactants and P2-P3

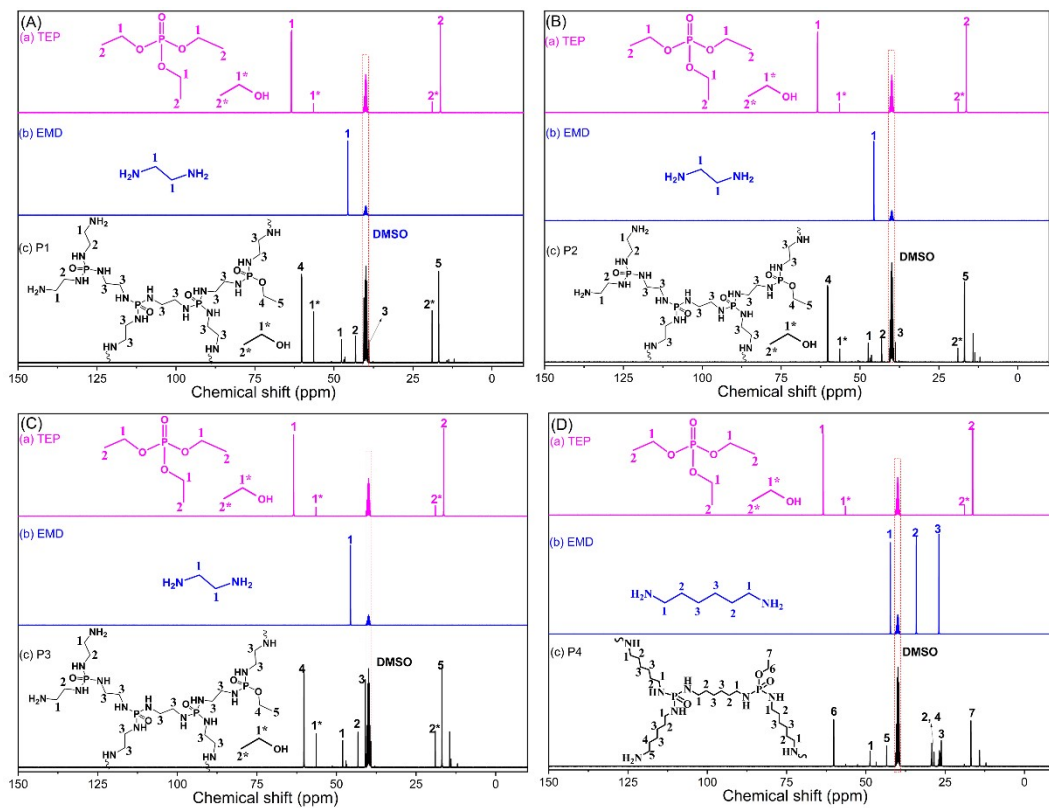


Fig. S3 The ^{13}C NMR spectra of reactants and P1-P4

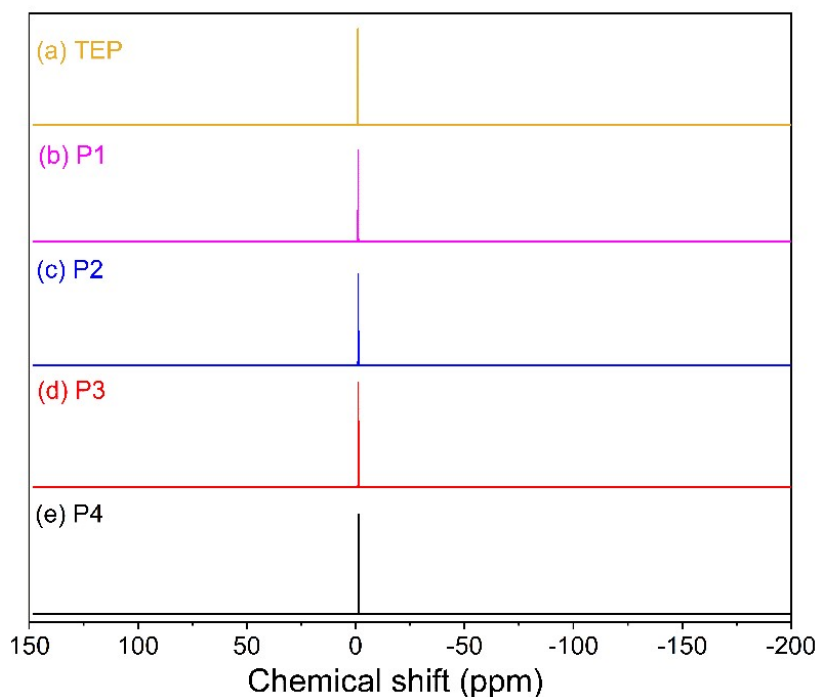


Fig. S4 ^{31}P NMR spectra of TEP and P1-P4

Table S2 The degree of branching (DB) of P1-P4 .

	P1	P2	P3	P4
DB	0.50	0.43	0.19	0.19

As for P1, the molar ratio of triethyl phosphate (TEP) and ethanediamine (EDM) is 1:1.6, therefore the TEP can be incorporated as dendritic (D), linear (L) and terminal (T) unit, and we can identify the amount of L units by the proton signal marked with H5 and H6. At the same time, we can confirm the total number of TEP (T+D+L) through the proton signal marked with H4 (according to Fig.2B). The DB was calculated using equation (1), which is feasible for the polymerization of A_2 and B_3 monomer.

$$\text{DB} = \frac{T + D}{T + D + L} \quad (1)$$

The calculated DB values of P1-P4 are summarized in Table S2.

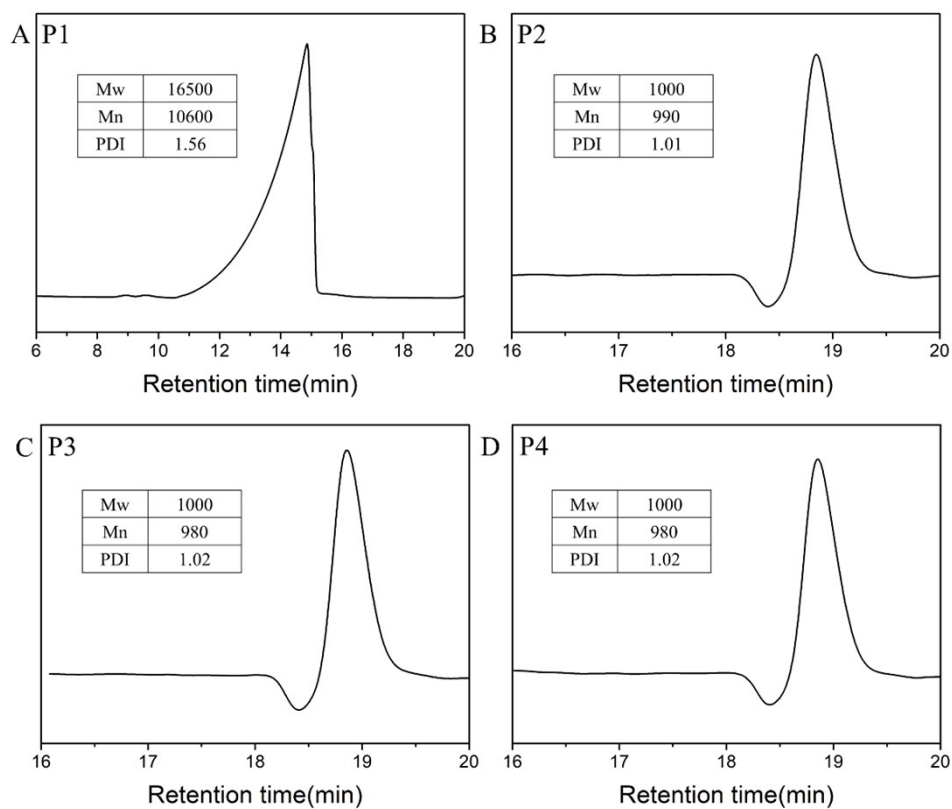


Fig. S5. GPC curve of P1-P4 (eluent: 0.1M NaNO₃ aqueous solution, narrow standard)

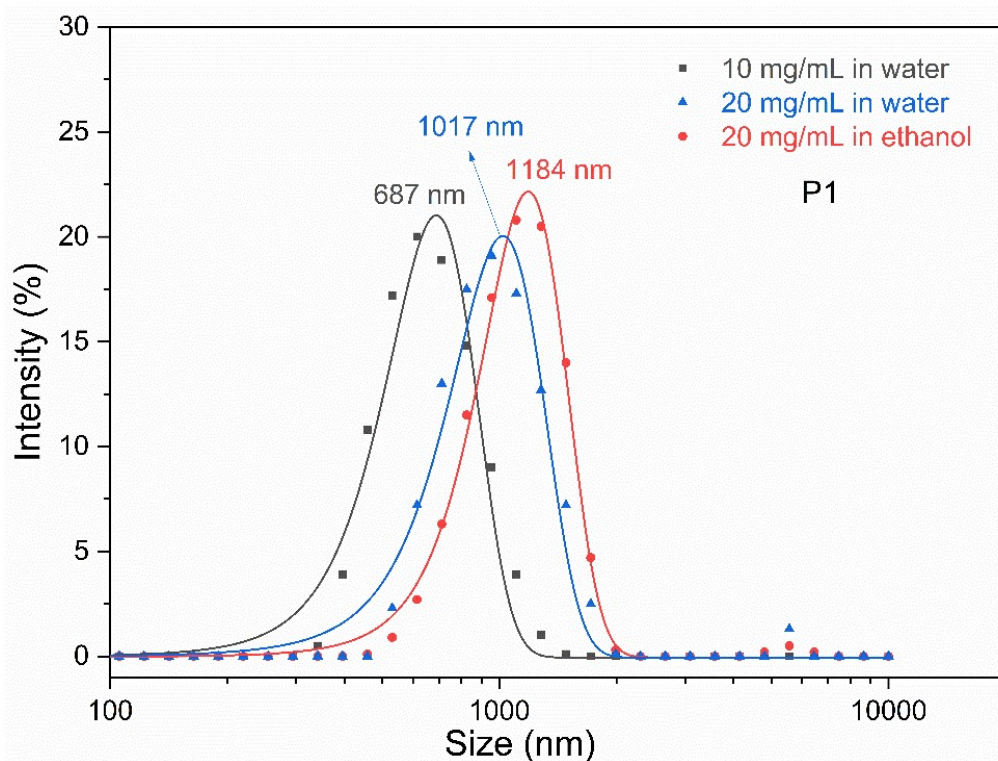


Fig. S6 The aggregated size of P1 in different solvents

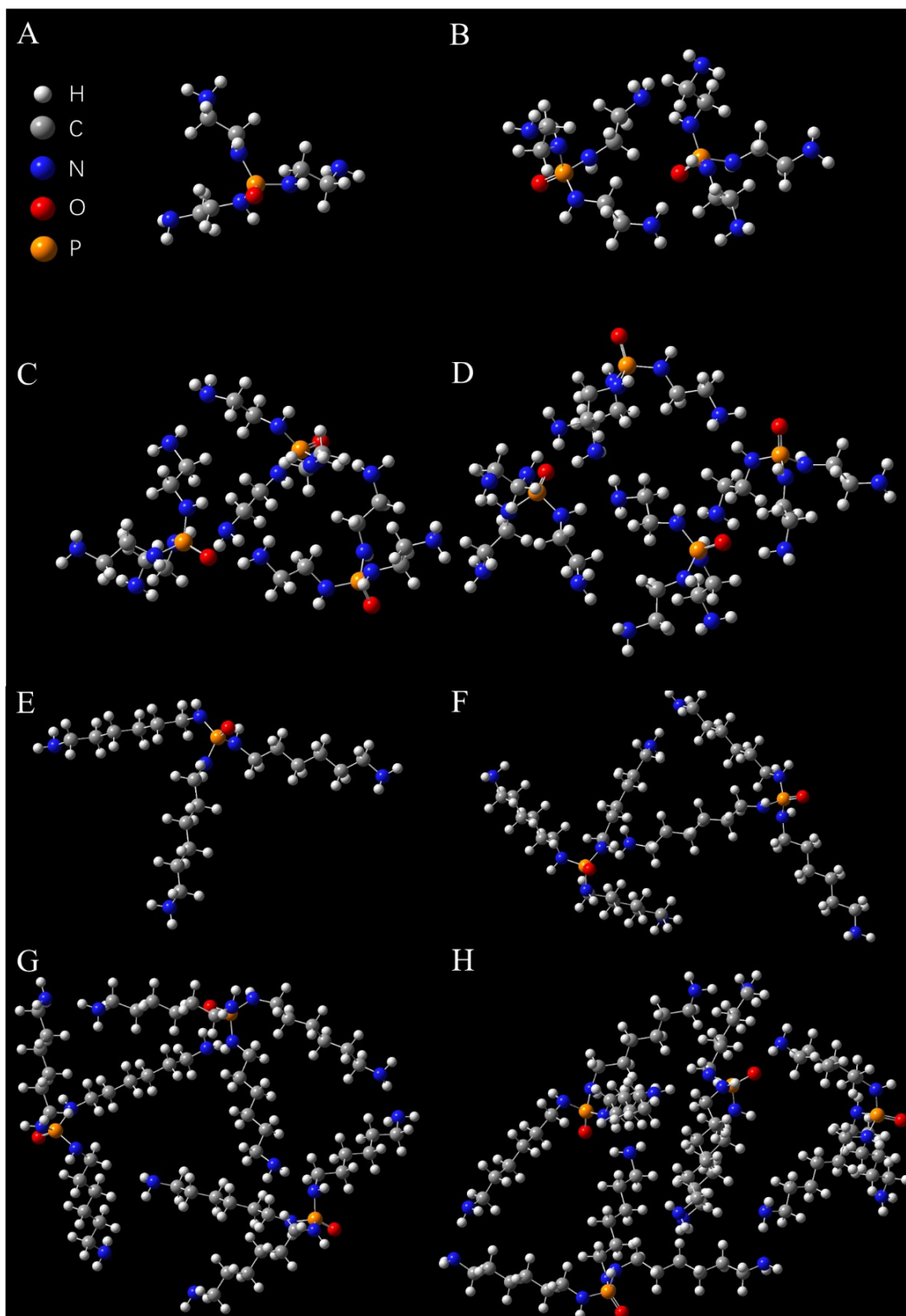
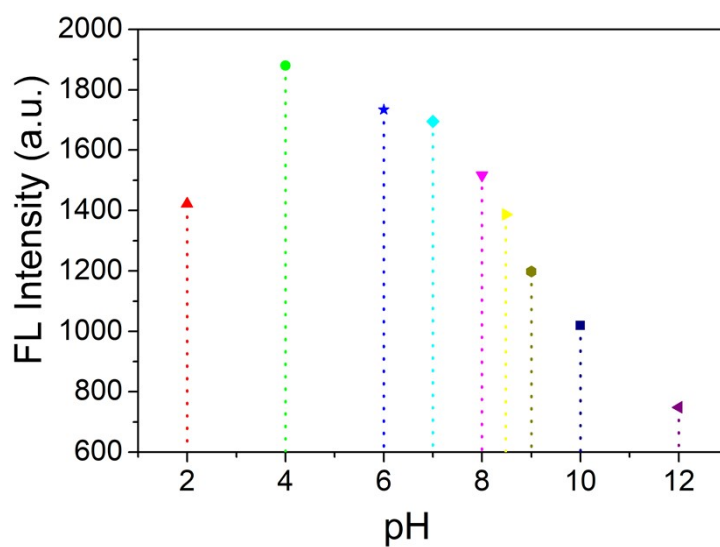
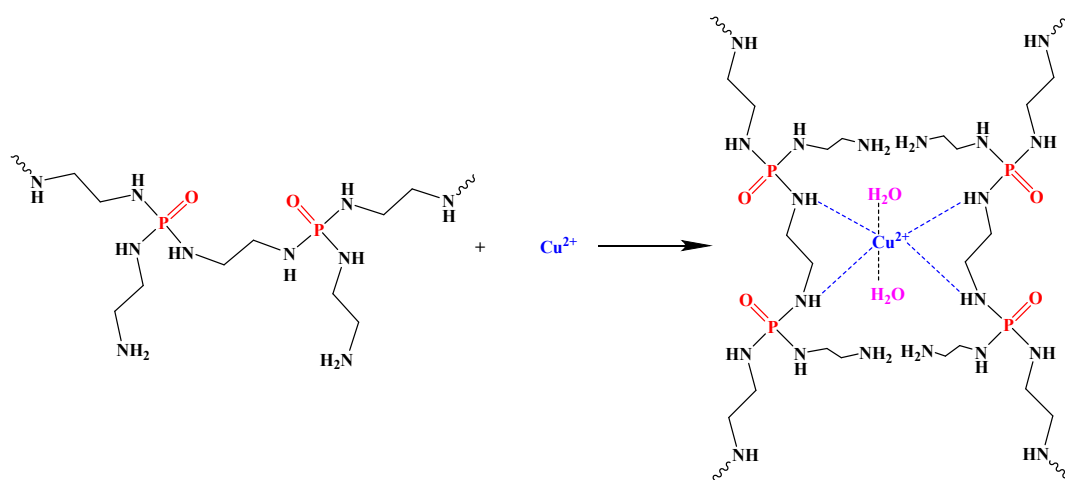


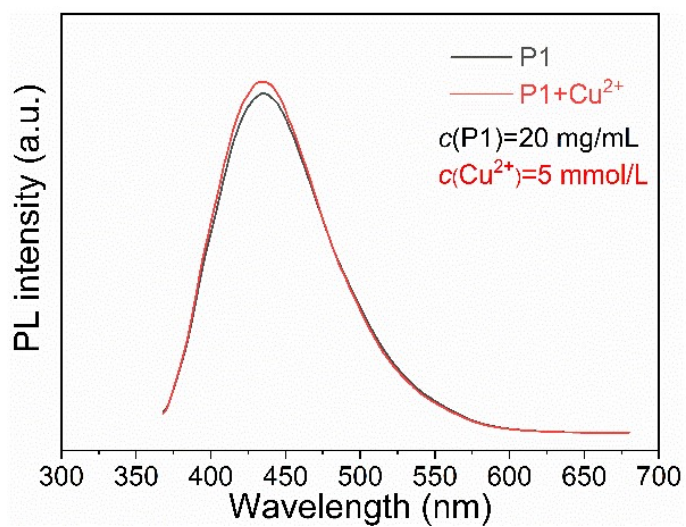
Fig. S7 Optimized conformations of the first generation P1 with molecules increase from 1 to 4 (A~D) and P4 molecules increase from 1 to 4 (E~H)



Scheme S2. The mechanism of copper ion discoloration by PPA

Fig. S8. The emission spectra of P1 in water solution (5 mg/mL) at different pH

Fig.S9 Fluorescence intensity of P1 aqueous solution (20 mg/mL) with/without the copper ions (5 mmol/L)



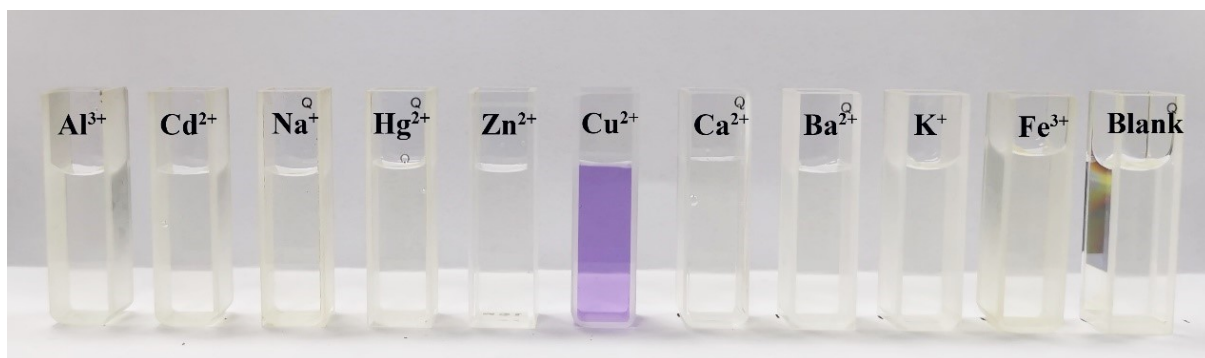


Fig.S10 Color change of P1 aqueous solution (10 mg/mL) with different metal ions (5 mmol/L)

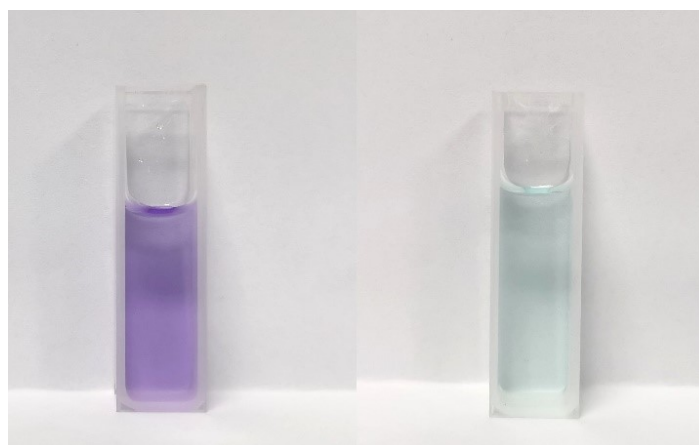


Fig. S11 The color change of PPA-Cu²⁺ solution by adding equivalent EDTA-2Na

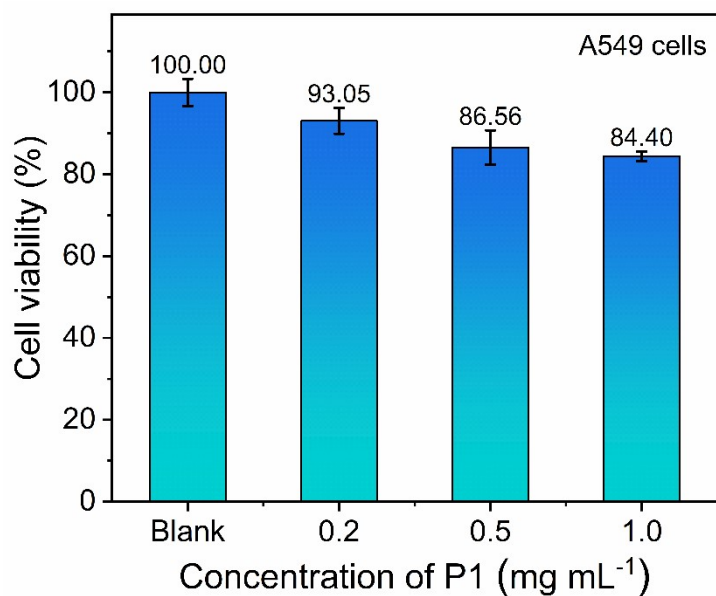


Fig. S12 The cell biocompatibility assays of PPA at different concentrations (0.2, 0.5 and 1.0 mg mL⁻¹)

References:

- 1 D. Tomalia, B. Klajnert-Maculewicz, K. Johnson, H. Brinkman, A. Janaszewska, D. Hedstrand, *Prog. Polym. Sci.*, 2019, **90**, 35-117.
- 2 Y. Feng, T. Bai, H. Yan, F. Ding, L. Bai, W. Feng, *Macromolecules*, 2019, **52**, 3075-3082.
- 3 L. Bai, H. Yan, Y. Feng, W. Feng, L Yuan, *Chem. Eng. J.*, 2019, **373**, 963-972.