

A Nanoscale Cobalt Functionalized Strandberg-Type Phosphomolybdate with β -Sheet Conformation Modulation Ability in Anti-Amyloid Protein Misfolding

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Table S1. Selected bond lengths (Å) for CoPM.

Mo(1)-O(1)	1.705(3)	Mo(1)-O(11)	1.936(3)
Mo(1)-O(16)	1.720(3)	Mo(1)-O(16)	2.326(3)
Mo(1)-O(15)	1.904(3)	Mo(1)-O(21)	2.371(3)
Mo(2)-O(2)	1.697(3)	Mo(2)-O(11)	1.935(3)
Mo(2)-O(7)	1.716(3)	Mo(2)-O(19)	2.168(3)
Mo(2)-O(12)	1.932(3)	Mo(2)-O(16)	2.496(3)
Mo(3)-O(8)	1.709(3)	Mo(3)-O(12)	1.938(3)
Mo(3)-O(3)	1.714(3)	Mo(3)-O(19)	2.329(3)
Mo(3)-O(13)	1.899(3)	Mo(3)-O(17)	2.362(3)
Mo(4)-O(4)	1.704(3)	Mo(4)-O(14)	1.948(3)
Mo(4)-O(9)	1.714(3)	Mo(4)-O(20)	2.260(3)
Mo(4)-O(13)	1.916(3)	Mo(4)-O(18)	2.384(3)
Mo(5)-O(5)	1.711(3)	Mo(5)-O(15)	1.953(3)
Mo(5)-O(10)	1.719(3)	Mo(5)-O(18)	2.240(3)
Mo(5)-O(14)	1.905(3)	Mo(5)-O(21)	2.312(3)
Co(1)-O(23)	2.035(3)	Co(1)-O(1W)#5	2.141(3)
Co(1)-O(23)#5	2.035(3)	Co(1)-O(2W)#5	2.179(3)
Co(1)-O(1W)	2.141(3)	Co(1)-O(2W)	2.179(3)
P(1)-O(17)	1.517(3)	P(1)-O(18)	1.541(3)
P(1)-O(16)	1.528(3)	P(1)-O(22)	1.586(3)
P(2)-O(23)	1.510(3)	P(2)-O(21)	1.566(3)
P(2)-O(20)	1.519(3)	P(1)-O(19)	1.568(3)

Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y+1, -z+1; #2 x, y, z-1; #3 x+1, -y+1/2, z+1/2.

CoPM was incubated with CuCl₂ and ZnCl₂ at 37 °C for 24h, respectively, with a molar ratio of 1:2. After incubation, the crystals were recrystallized. Those samples were then washed with purified water and filtered. Then, the residual samples were examined by IR spectra. As shown in Figure S1, there was no significant difference between the IR spectra of CoPM and CoPM +Cu²⁺/ CoPM +Zn²⁺ groups, which indicated that CuCl₂ and ZnCl₂ can not affect the skeleton structure of CoPM under such incubation conditions.

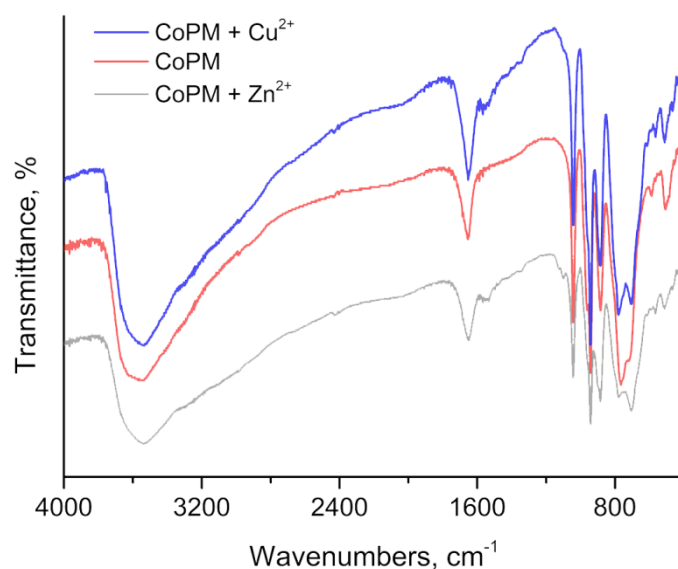


Figure S1. IR spectra for CoPM before and after incubation with Cu²⁺ and Zn²⁺ (with a molar ratio of 1:2).

Further, the stability of CoPM in Tris-buffer with DMSO was tested according to the above method. CoPM was firstly dissolved in Tris buffer solution (20 mM Tris-HCl/150 mM NaCl, with 5% DMSO), and then incubated at 37 °C for 24 h. After incubation, the pink crystals were recrystallized and examined by IR spectra. As shown in Figure S2a, compared with the non-incubation group, the most obvious difference in the incubation group was that there were some new peaks. The change in peak shape and new peaks may be due to the introduction of some organic molecules during recrystallization, in which it is not excluded that organic ligands coordinate with metal ions on the CoPM skeleton leading to changes in IR peaks. However, the location and intensity of main peaks in the incubated group of CoPM remained, as shown in Figure S2b and c, including $\nu(\text{P}-\text{O}_{\mu 4})$ (1046~1035 cm⁻¹), $\nu(\text{Mo}-\text{O}_t)$ (933~944 cm⁻¹) and $\nu(\text{Mo}-\text{O}_{\mu 2})$ (~885 cm⁻¹), which is suggesting most CoPM skeleton structure were maintained. Therefore, the conclusion can be summarized as follows although organic groups may enter the crystal through the recrystallization process or directly coordinate with CoPM during incubation, resulting in the change of IR peak shape and the appearance of new peaks, most of the CoPM skeleton structure were not affected by these incubation conditions.

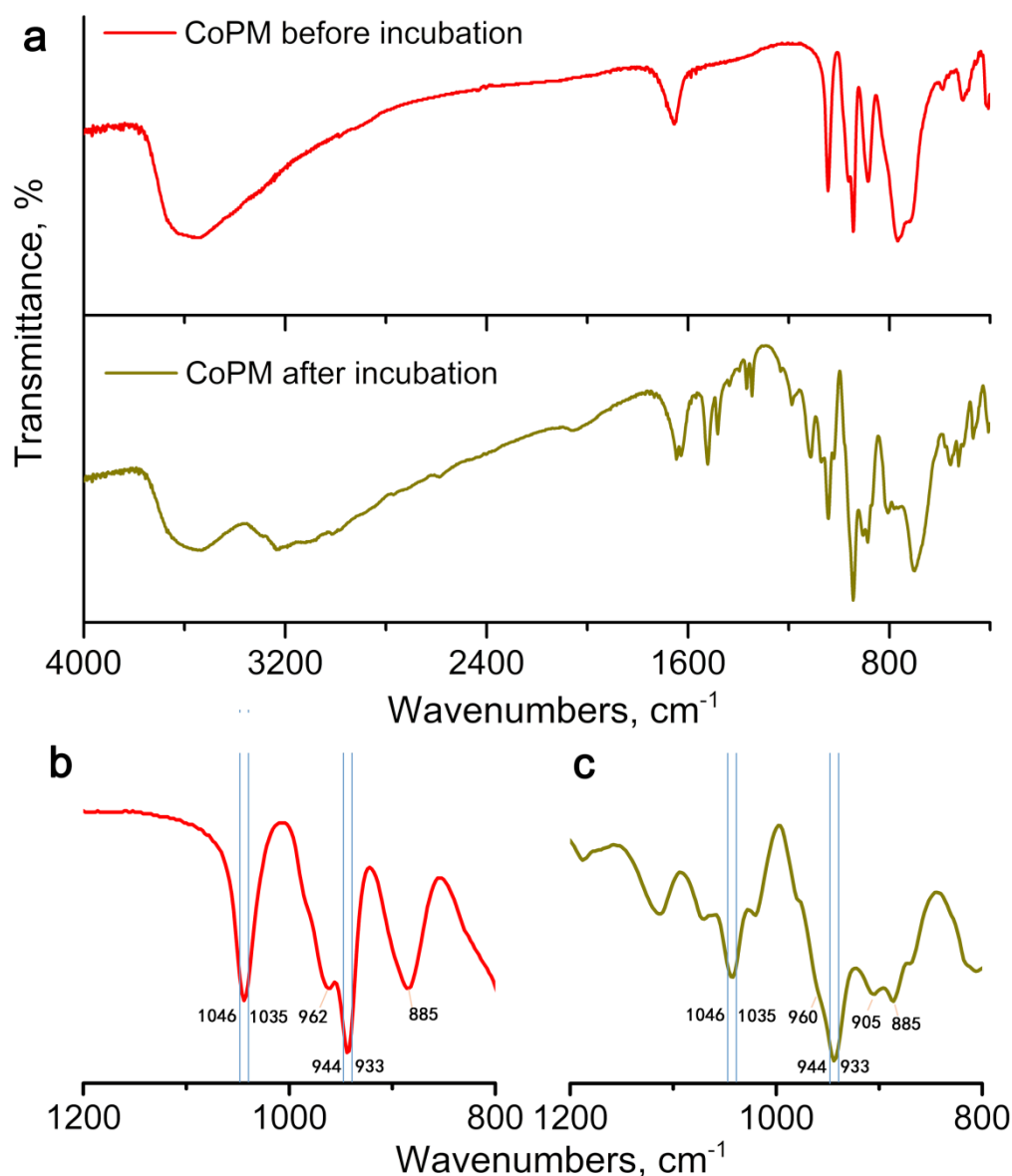


Figure S2. (a) IR spectra for CoPM before and after incubation with Tris buffer solution (20 mM Tris-HCl/150 mM NaCl, with 5% DMSO); (b) and (c) partial magnification of CoPM's IR spectra before and after incubation.

We conducted a Raman spectroscopy analysis on CoPM before and after incubation with Tris buffer solution (20 mM Tris-HCl/150 mM NaCl, with 5% DMSO). As shown in Figure S3, the peak located at 1040 cm⁻¹ may be attributed to the bond of P-O, and the peaks located at 930 and 880 cm⁻¹ may be attributed to bonds of different Mo-O, respectively. Before and after incubation, no significant alterations were detected in the Raman spectra of CoPM. With the combination of the results of IR spectra, it can be inferred that the structure of CoPM remains relatively stable under these conditions.

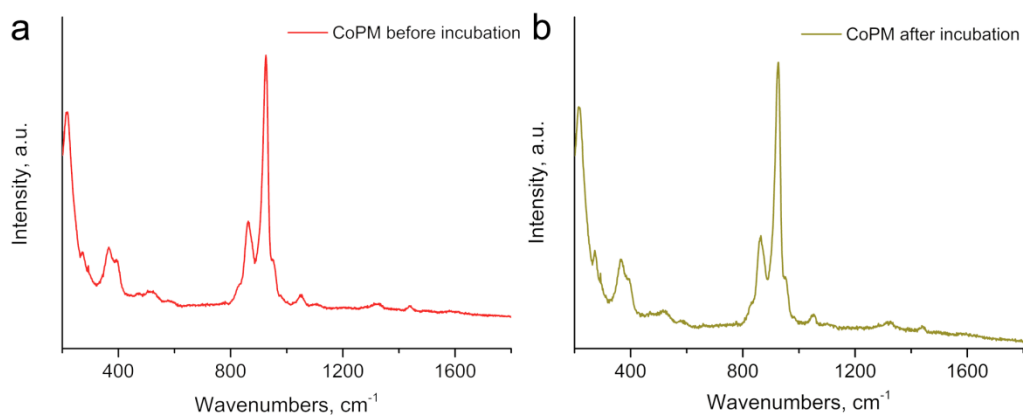


Figure. S3. Raman spectra for CoPM before (a) and after incubation (b) with Tris buffer solution (20 mM Tris-HCl/150 mM NaCl, with 5% DMSO).

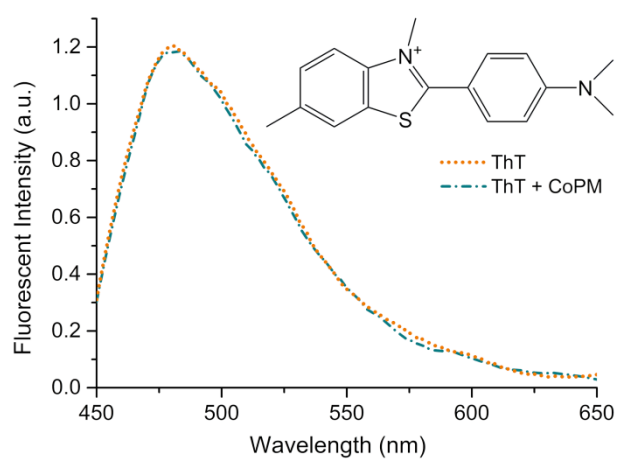


Figure. S4 The fluorescence spectra ($\lambda_{\text{ex}} = 415 \text{ nm}$) of Thioflavin T (ThT) with or without CoPM. (inset: the structural diagram of ThT)