# **Supplementary Information**

# A binuclear copper substituted phosphormolybdates with ROS-

# catalytic ability and anti-microbial activity †

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### 1. Supplementary Figures and Tables

Empirical formula	$C_6H_{45}Cu_2Mo_5N_6O_{32.5}P_2$
Formula weight	1390.20
Crystal system	Monoclinic
Space group	12/a
a / Å	18.240(8)
<i>b</i> / Å	18.298(8)
c / Å	24.280(15)
$\alpha$ / deg	90
<i>β</i> / deg	96.445(6)
γ/deg	90
V / Å <sup>3</sup>	8053(7)
Ζ	8
$D_{\rm c}$ / g cm <sup>-3</sup>	2.293
μ / mm⁻¹	2.727
Т/К	296.15
Limiting indices	$-21 \le h \le 21$
	$-21 \le k \le 21$
	$-16 \le l \le 28$
Measured reflections	20518
Independent reflections	7152
R <sub>int</sub>	0.0331
Data / restrains / parameters	7152 / 2 / 457
GOF on F <sup>2</sup>	1.086
Final <i>R</i> indices $[l > 2\sigma(l)]$	$R_1 = 0.0418,$
	$wR_2 = 0.1164$
R indices (all data)	$R_1 = 0.0442$
	$wR_2 = 0.1181$
Completeness	99.60 %

### Table S1 Crystallographic data and structural refinements for CPM

## Table S2 Selected bond length (Å) for CPM

Mo(1)-O(5)	1.937(4)	Mo(2)-O(19)	1.706(5)	Mo(4)-O(9)	1.719(4)
Mo(1)-O(6)	2.299(4)	Mo(2)-O(20)	1.702(5)	Mo(4)-O(15)	2.211(4)
Mo(1)-O(12)	1.923(4)	Mo(3)-O(2)	2.236(4)	Mo(4)-O(18)	1.723(4)
Mo(1)-O(14)	2.307(4)	Mo(3)-O(3)	1.914(4)	Mo(4)-O(21)	1.896(4)
Mo(1)-O(20)	1.707(4)	Mo(3)-O(13)	1.724(4)	Mo(5)-O(4)	2.232(4)
Mo(1)-O(23)	1.714(4)	Mo(3)-O(17)	1.703(4)	Mo(5)-O(8)	1.949(4)
Mo(2)-O(1)	2.229(4)	Mo(3)-O(21)	1.907(4)	Mo(5)-O(10)	1.708(5)
Mo(2)-O(3)	1.954(4)	Mo(3)-O(1)	2.458(4)	Mo(5)-O(12)	1.929(4)
Mo(2)-O(5)	1.940(4)	Mo(4)-O(4)	2.352(4)	Mo(5)-O(14)	2.350(4)
Mo(2)-O(6)	2.352(4)	Mo(4)-O(8)	1.922(4)	Mo(5)-O(16)	1.715(5)
Cu(1)-O(7)	1.995(4)	Cu(1)-O(11)	1.980(4)	Cu(1)-O(5W)	2.700(5)
Cu(1)-N(1)	2.006(5)	Cu(1)-N(2)	2.002(5)	Cu(2)-O(1W)	1.979(5)
Cu(2)-O(2W)	1.965(5)	Cu(2)-O(3W)	2.574(9)	Cu(2)-O(5W)	2.596(5)
Cu(2)-N(3)	2.002(6)	Cu(2)-N(4)	2.000(6)	P(1)-O(11)	1.524(4)
P(1)-O(2)	1.527(4)	P(1)-O(4)	1.560(4)	P(1)-O(6)	1.549(4)
P(2)-O(1)	1.552(4)	P(2)-O(7)	1.538(4)	P(2)-O(14)	1.549(4)
P(2)-O(15)	1.527(4)				

## Table S3 Selected angles (°) for CPM

P(1)-O(11) -Cu(1)	129.0(3)
P(2)-O(7) -Cu(1)	123.4(2)
Cu(1)-O(5W)-Cu(2)	120.5(1)

## Table S4 Crystallographic data and structural refinements for C1

Empirical formula	$C_{6}H_{35}Cu_{1}Mo_{5}N_{6}O_{28.5}P_{2}$
Formula weight	1252.58
Crystal system	Monoclinic
Space group	Cc
a / Å	14.8162(9)
b / Å	14.5193(9)
c / Å	16.0799(10)
$\alpha$ / deg	90
<i>β</i> / deg	109.2660(10)
γ/deg	90
V / Å <sup>3</sup>	3265.4(3)
Ζ	4
$D_{\rm c}$ / g cm <sup>-3</sup>	2.548
μ / mm⁻¹	2.711
Т/К	296.15
Limiting indices	$-17 \le h \le 17$
	–17≤ <i>k</i> ≤ 15

	$-19 \leq l \leq 10$
Measured reflections	8239
Independent reflections	4932
R <sub>int</sub>	0.0331
Data / restrains / parameters	4932 / 2 / 443
GOF on F <sup>2</sup>	1.040
Final <i>R</i> indices $[l > 2\sigma(l)]$	$R_1 = 0.0182,$
	$wR_2 = 0.0479$
R indices (all data)	$R_1 = 0.0183$
	$wR_2 = 0.0480$
Completeness	99.50 %

## Table S5 Selected bond length (Å) for C1

Mo(1)-O(1)	1.687(4)	Mo(2)-O(17)	2.376(4)	Mo(4)-O(13)	1.946(4)
Mo(1)-O(6)	1.741(4)	Mo(2)-O(20)	2.183(4)	Mo(4)-O(14)	1.919(4)
Mo(1)-O(11)	1.927(4)	Mo(3)-O(3)	1.704(4)	Mo(4)-O(18)	2.183(4)
Mo(1)-O(15)	1.902(4)	Mo(3)-O(8)	1.707(4)	Mo(4)-O(21)	2.396(4)
Mo(1)-O(16)	2.206(4)	Mo(3)-O(12)	1.915(4)	Mo(5)-O(5)	1.697(4)
Mo(1)-O(20)	2.379(4)	Mo(3)-O(13)	1.909(4)	Mo(5)-O(10)	1.724(4)
Mo(2)-O(2)	1.692(4)	Mo(3)-O(17)	2.304(4)	Mo(5)-O(14)	1.942(4)
Mo(2)-O(7)	1.717(4)	Mo(3)-O(21)	2.366(4)	Mo(5)-O(15)	1.904(4)
Mo(2)-O(11)	1.907(4)	Mo(4)-O(4)	1.722(4)	Mo(5)-O(18)	2.393(4)
Mo(2)-O(12)	1.940(4)	Mo(4)-O(9)	1.704(5)	Mo(5)-O(22)	2.213(4)
Cu(1)-O(19)	2.012(4)	Cu(1)-O(23)	1.939(4)	Cu(1)-O(1W)	2.443(5)
Cu(1)-N(1)	2.005(5)	Cu(1)-N(2)	1.985(5)	Cu(1)-O(2W)	2.799(5)
P(1)-O(16)	1.516(4)	P(1)-O(17)	1.547(4)	P(1)-O(18)	1.554(4)
P(1)-O(19)	1.531(4)	P(2)-O(20)	1.547(4)	P(2)-O(21)	1.547(4)
P(2)-O(22)	1.532(4)	P(2)-O(23)	1.524(4)		

## Table S6 Selected angles (°) for C1

P(1)-O(19) -Cu(1)	124.0(0)
P(2)-O(23) -Cu(1)	141.5(2)



**Fig. S1** View of the effective coordination site of the oxygen atoms in our reported POM building blocks. Color code: MoO<sub>6</sub>: green octahedrons; PO<sub>4</sub>: purple tetrahedrons; Oxygen atoms: red (The big red balls represent the effective coordination site). (A) Strandberg-type fragment; (B)  $[B-\beta-AsW_8O_{31}]^{9-}$  fragment;<sup>1</sup> (C)  $[P_4Mo_6O_{34}]^{12-}$  fragment;<sup>2</sup> (D)  $[B-\alpha-AsW_9O_{34}]^{9-}$  fragment.<sup>3</sup>



**Fig. S2** (A) Combined polyhedral/ball-and-stick view of the 1-D linear structure of  $[H_2en]_2[{Cu(en)(OH_2)}]$ Mo<sub>5</sub>P<sub>2</sub>O<sub>23</sub>]·4H<sub>2</sub>O. (B) Combined polyhedral/ball-and-stick representation of one  $[{Cu(en)(OH_2)}]$  Mo<sub>5</sub>P<sub>2</sub>O<sub>23</sub>]<sup>4+</sup> subunit in the crystal. (C) Polyhedral view of the coordination mode of Cu ions in  $[H_2en]_2[{Cu(en)(OH_2)}]$  Mo<sub>5</sub>P<sub>2</sub>O<sub>23</sub>]·4H<sub>2</sub>O. (lattice water molecules and protonated en molecules are omitted)



Fig. S3 Comparison of the simulated and experimental XRPD patterns of CPM.



Fig. S4 SEM images of CPM crystal surface.



Fig. S5 SEM images of C1 crystal surface.



Fig. S6 EDX spectrum of CPM (Corresponding to Fig. S3).



Fig. S7 EDX spectrum of C1 (Corresponding to Fig. S4).





Temperature(°C)

Fig. S9 TG curve of CPM.



Fig. S10 The location and numbering of Cu, N, O in di-nuclear Cu cluster of CPM.

Bond	Valence	Bond	Valence	Bond	Valence	Atom	Σs
Cu(1)-O(7)	0.4256	Cu(1)-O(11)	0.4432	Cu(1)-O(5W)	0.0633		
Cu(1)-N(1)	0.3429	Cu(1)-N(2)	0.3466			Cu(1)	1.6216
Cu(2)-O(1W)	0.4445	Cu(2)-O(2W)	0.4616	Cu(2)-O(3W)	0.0890		
Cu(2)-O(5W)	0.0838	Cu(2)-N(3)	0.3466	Cu(2)-N(4)	0.3485	Cu(2)	1.7740
Mo(1)-O(5)	0.9221	Mo(1)-O(6)	0.3466	Mo(1)-O(12)	0.9576		
Mo(1)-O(14)	0.3392	Mo(1)-O(20)	1.7169	Mo(1)-O(23)	1.6847	Mo(1)	5.9673
Mo(2)-O(1)	0.4188	Mo(2)-O(3)	0.8807	Mo(2)-O(5)	0.9146		
Mo(2)-O(6)	0.3003	Mo(2)-O(19)	1.7215	Mo(2)-O(20)	1.7402	Mo(2)	5.9764
Mo(3)-O(2)	0.4109	Mo(3)-O(3)	0.9812	Mo(3)-O(13)	1.6398		
Mo(3)-O(17)	1.7355	Mo(3)-O(21)	1.0000	Mo(3)-O(1)	0.2255	Mo(3)	5.9932
Mo(4)-O(21)	1.0301	Mo(4)-O(4)	0.3003	Mo(4)-O(8)	0.9602		
Mo(4)-O(9)	1.6621	Mo(4)-O(15)	0.4397	Mo(4)-O(18)	1.6442	Mo(4)	6.0369
Mo(5)-O(4)	0.4154	Mo(5)-O(8)	0.8926	Mo(5)-O(10)	1.7123		
Mo(5)-O(12)	0.9422	Mo(5)-O(14)	0.3020	Mo(5)-O(16)	1.6802	Mo(5)	5.9449
P(1)-O(2)	1.2753	P(1)-O(4)	1.1665	P(1)-O(6)	1.2017		
P(1)-O(11)	1.2857					P(1)	4.9295
P(2)-O(1)	1.1920	P(2)-O(7)	1.2380	P(2)-O(14)	1.2017		
P(2)-O(15)	1.2753					P(2)	4.9072

## Table S7 Bond valence and $\boldsymbol{\Sigma}s$ of Cu, Mo, P in CPM



Fig. S11 The location and numbering of Cu, N, O in di-nuclear Cu cluster of C1.

Bond	Valence	Bond	Valence	Bond	Valence	Atom	Σs
Cu(1)-O(19)	0.4065	Cu(1)-O(23)	0.4952	Cu(1)-O(1W)	0.1268		
Cu(1)-O(2W)	0.0484	Cu(1)-N(1)	0.2419	Cu(1)-N(2)	0.2554	Cu(1)	1.5742
Mo(1)-O(1)	1.8122	Mo(1)-O(6)	1.5661	Mo(1)-O(11)	0.9473		
Mo(1)-O(15)	1.0136	Mo(1)-O(16)	0.4457	Mo(1)-O(20)	0.2792	Mo(1)	6.0644
Mo(2)-O(2)	1.7879	Mo(2)-O(7)	1.6711	Mo(2)-O(11)	1.0000		
Mo(2)-O(12)	0.9146	Mo(2)-O(17)	0.2815	Mo(2)-O(20)	0.4742	Mo(2)	6.1295
Mo(3)-O(3)	1.7309	Mo(3)-O(8)	1.7169	Mo(3)-O(12)	0.9786		
Mo(3)-O(13)	0.9946	Mo(3)-O(17)	0.3419	Mo(3)-O(21)	0.2892	Mo(3)	6.0522
Mo(4)-O(4)	1.6487	Mo(4)-O(9)	1.7309	Mo(4)-O(13)	0.8999		
Mo(4)-O(14)	0.9680	Mo(4)-O(18)	0.4742	Mo(4)-O(21)	0.2667	Mo(4)	5.9886
Mo(5)-O(5)	1.7639	Mo(5)-O(10)	1.6398	Mo(5)-O(14)	0.9097		
Mo(5)-O(15)	1.0081	Mo(5)-O(18)	0.2688	Mo(5)-O(22)	0.4373	Mo(5)	6.0279
P(1)-O(16)	1.3138	P(1)-O(17)	1.2082	P(1)-O(18)	1.1856		
P(1)-O(19)	1.2616					P(1)	4.9694
P(2)-O(20)	1.2082	P(2)-O(21)	1.2083	P(2)-O(22)	1.2582		
P(2)-O(23)	1.2857					P(2)	4.9605

## Table S8 Bond valence and $\Sigma s$ of Cu, Mo, P in C1



**Fig. S12** XPS spectra of Mo and P. (A) Mo<sup>6+</sup>  $3d_{5/2}$  (231.7 eV) and Mo<sup>6+</sup>  $3d_{3/2}$  (234.8 eV); (B) Mo<sup>6+</sup>  $3d_{5/2}$  (231.9 eV) and Mo<sup>6+</sup>  $3d_{3/2}$  (234.9 eV);<sup>4</sup> (C) P<sup>5+</sup> 2p (132.4 eV); (D) P<sup>5+</sup> 2p (132.5 eV).<sup>5</sup>



**Fig. S13** Temperature dependence of the molar magnetic susceptibility  $\chi_M$  (**a**) and the  $\chi_M$ T(O) product for the new preparation crystals of CPM between 2 and 300 K.



Fig. S14 Temperature evolution of the inverse magnetic susceptibility  $\chi_M$  for CPM between 2 K and 300 K.



**Fig. S15** Temperature dependence of the molar magnetic susceptibility  $\chi_M$  (**■**) and the  $\chi_M T(\circ)$  product for C1 between 2 and 300 K.

### 2. Experimental Section

#### 2.1 Materials and methods

Reagents used in this study were all of analytical grade, purchased from commercial suppliers and used as received unless otherwise stated. 2',7'-dichlorofluorescin diacetate (DCFH-DA) was purchased from Sigma-Aldrich. CuCl<sub>2</sub>·4H<sub>2</sub>O, NaMoO<sub>4</sub>·2H<sub>2</sub>O, Na<sub>2</sub>HPO<sub>4</sub>·12H<sub>2</sub>O and ethanediamine were purchased from J & K. All the solutions were prepared with Milli-Q water and filtered through a 0.22  $\mu$ m filter (Millipore). *E. coli* DH5 and puc57 plasmid were purchased from Sangon Biotech, Shanghai in China.

The single crystal data of CPM and C1 were collected on a Bruker CCD, Apex-II diffractometer with graphite monochromated Mo K $\alpha$  ( $\lambda$  = 0.71073 Å) radiation at room temperature. Routine Lorentz and polarization corrections were applied and an absorption correction was performed using the SADABS program. The structure was solved by direct methods and refined using full-matrix least squares on  $F^2$ . All calculations were performed using the SHELXL-97 program package. Turbidity and DCF fluorescence were conducted on a Thermo Scientific Varioskan Flash microplate reader. Elemental analysis was performed on a PQEXCe II ICP-MS. IR/UV spectra were recorded on a NICOLET iS10 and UV-3600 spectrometer respectively. XPS spectra were scanned by PHI 5000 VersaProbe (ULVAC-PHI).

#### 2.2 Synthesis of CPM

Two solutions were prepared separately. Solution A:  $Na_2MoO_4 \cdot 2H_2O$  (2.416 g, 10.00 mmol) and  $Na_2HPO_4 \cdot 12H_2O$  (2.399 g, 6.70 mmol) were dissolved in water (30 mL) under stirring. Solution B:  $CuCl_2 \cdot 4H_2O$  (1.705 g, 10.00 mmol) and en (0.10 mL, 1.49 mmol) were added to water (30 mL) under stirring. The resulting mixture of B is added to solution A. The mixture was stirred for 10 min at room temperature and then the pH value was adjusted to 5.0 by adding 4 mol·L<sup>-1</sup> HCl dropwise. The solution was kept at 85 °C for 1h and filtered when it was still hot. The filtrate was allowed to evaporate in an open beaker at room temperature. About 3 weeks, navy blue rhombus crystals CPM formed. (Yield: ca 33% based on  $Na_2MoO_4 \cdot 2H_2O$ ). Elemental analysis (%) calcd for  $(H_2en)[Cu(en)(H_2O)Cu(en)(H_2O)_3][P_2Mo_5O_{23}] \cdot 5.5H_2O$ : H 2.82, C 5.20, N 6.07, P 4.48, Cu 9.18, Mo 34.65; found: H 3.10, C 5.13, N 5.98, P 4.41, Cu 9.14, Mo 34.56.

The results showed that CPM was generated from 4.5 to 6.7, and the crystal morphology was best when the initial pH was 5.0. The CPM yield was the highest when the initial pH was 5.5-6.0. When pH was 7.0 and above, no CPM crystals were obtained.

#### 2.3 Synthesis of C1

Two solutions were prepared separately. Solution A:  $Na_2MoO_4 \cdot 2H_2O$  (2.416 g, 10.00 mmol) and  $Na_2HPO_4 \cdot 12H_2O$  (2.399 g, 6.70 mmol) were dissolved in water (30 mL) under stirring. Solution B:  $CuCl_2 \cdot 4H_2O$  (1.705 g, 10.00 mmol) and en (0.20 mL, 2.98 mmol) were added to water (30 mL) under stirring. The resulting mixture of B is added to solution A. The mixture was stirred for 10 min at room temperature and then the pH value was adjusted to 6.0 by adding 4 mol·L<sup>-1</sup> HCl dropwise. The solution was kept at 85 °C for 1h and filtered when it was still hot. The filtrate was allowed to evaporate in an open beaker at room temperature. The filtrate was allowed to evaporate in an open beaker at room temperature. After two weeks wathet blue acicular crystals C1 suitable for X-ray crystallography were isolated. (Yield: ca 21% based on  $Na_2MoO_4$ ·2H<sub>2</sub>O).

### 2.4 EDX-SEM

The SEM images of CPM and C1 as well as the corresponding EDX spectra were detected according to the reported method.<sup>6</sup>

### 2.5 IR spectra

The IR spectra of CPM and C1 were recorded on a NICOLET iS10 spectrometer in the range of 400–4000 cm<sup>-1</sup>.

#### 2.6 XRPD spectrum

The XRPD spectrum of CPM was recorded on a D8 ADVANCE X-Ray Powder Diffractometer from 5 to 45°.

### 2.7 TG analysis

The TG was tested on a STA449F3 TG-DSC from 25-600 °C.

#### 2.8 XPS spectra

The XPS spectra of CPM and C1 were detected according to the reported method.<sup>7</sup>

#### 2.9 Calculation of bond valance sum $(\Sigma s)^8$

Using the formula S1, we can calculate the oxidation states of the elements constructing the POMs. As we introduced in the paper, we can figure out the average valence of Cu, Mo and P after we calculated oxidation states of O atoms. Then, we can use the results to estimate the probabilities that Cu<sup>+</sup> and Cu<sup>2+</sup> exist in each position of CPM and C1.

$$V_i = \sum_j s_{ij} = \sum_j \exp\left(\frac{r_0 - r_{ij}}{B}\right)$$
(formula S1)

In formula S1, the  $r_0$  represents the theoretical value of bond distance between two atoms. And the  $r_{ij}$  represents the observed value of bond distance. The value of B has been set to 0.37.

According to the results of XPS shown in Fig. 3 and Fig. S10, we can reach a conclusion that the oxidation states of Mo, P in CPM and C1 are all +6, +5, repectively. While, the oxidation states of Cu in CPM and C1 are mixture valence of +1 and +2. Based on the oxidation states of Mo, P and Cu, we can get the theoretical value of Mo–O, P–O and Cu–O from literatures, which the  $r_0$  (Mo<sup>6+</sup>–O) is 1.907 Å,  $r_0$  (P<sup>5+</sup>–O) is 1.617 Å,  $r_0$  (Cu<sup>2+</sup>–O) is 1.679 Å and  $r_0$  (Cu<sup>+</sup>–O) is 1.610 Å.

The observed value of bond distance of CPM and C1 are listed in Table S2 and Table S4.

The oxidation states of O atoms building the POMs can be calculated and the results are shown in Table S7 for CPM and Table S8 for C1.

#### 2.10 Magnetic property

The magnetic property of CPM was detected according to the literaure.9

The solid state direct-current magnetic susceptibility of CPM was measured on polycrystalline samples from 2K to 300K in the 1 kOe field. As shown in Fig. S13, the magnetic data for CPM are plotted as  $\chi_M$  and  $\chi_M T$  versus T. The temperature dependence of  $\chi_M$  shows a slight increase from 0.002 to 0.042 emu mol<sup>-1</sup> in the range of 300–36 K, and then exponentially reaches the maximum value of 0.450 emu mol<sup>-1</sup> at 2 K. With decreasing temperature, the value of  $\chi_M T$  continuously increases and reaches to the maximum of 1.535 emu K mol<sup>-1</sup> at 23 K. Those

results indicated that a characteristic ferromagnetic coupling magnetic behavior is in the dinuclear Cu clusters of fresh CPM samples. As shown in Fig. S14, the dependence of the reciprocal susceptibility data is well fitted by Curie–Weiss expression [ $\chi_M = C/(T - \theta)$  with C = 1.375 emu K mol<sup>-1</sup>,  $\theta = 6.083$  K].

It is interesting to note that further decreasing the temperature results in a sudden decrease of the  $\chi_M T$  product, which takes the value of 1.138 emu K mol<sup>-1</sup> at 2 K. The sharp drop in the  $\chi_M T$  value below the apex temperature may be attributed to the presence of significant zero-field splitting effects in the ground state or molecular interactions.<sup>10</sup> Such ferromagnetic coupling in the Cu<sup>2+</sup>-cluster have been observed in [(CuCl)<sub>6</sub>(AsW<sub>9</sub>O<sub>33</sub>)<sub>2</sub>] and [Cu(deta)(H<sub>2</sub>O)]<sub>2</sub> [Cu<sub>6</sub>(en)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>(B- $\alpha$ -GeW<sub>9</sub>O<sub>34</sub>)<sub>2</sub>]·GH<sub>2</sub>O already.<sup>11,12</sup> Also the predominant ferromagnetic exchange interactions in the octa-Cu<sup>2+</sup> substituted POMs [Cu(H<sub>2</sub>O)<sub>2</sub>]H<sub>2</sub>[Cu<sub>8</sub>(dap)<sub>4</sub>(H<sub>2</sub>O)<sub>2</sub>(B- $\alpha$ -XW<sub>9</sub>O<sub>34</sub>)<sub>2</sub>] (X = Si<sup>IV</sup>, Ge<sup>IV</sup>) and H<sub>4</sub>[Cu<sub>8</sub>(dap)<sub>4</sub>(H<sub>2</sub>O)<sub>2</sub>(B- $\alpha$ -GeW<sub>9</sub>O<sub>34</sub>)<sub>2</sub>]·13H<sub>2</sub>O have also been reported.<sup>13,14</sup>

The magnetization of C1 was further performed on polycrystalline samples from 2K to 300K in the 1 kOe field. As shown in Fig. S15, at room temperature the  $\chi_M T$  values is 0.25, which are a little lower than expected for the spin-only value for one isolated Cu<sup>2+</sup> with S = 1/2 and g = 2.00. The  $\chi_M T$  value of C1 decreased with the temperature going down gradually, which indicated the presence of antiferromagnetic interactions in mononuclear entities.<sup>15</sup>

#### 2.11 Catalytic ROS production of CPM and C1

DCFH stock solution (1 mM) was prepared with a buffer (20 mM Tris-HCl/150 mM NaCl, pH 7.4) according to the reported procedures.<sup>16</sup> Horseradish peroxidase (HRP) stock solution (4  $\mu$ M) was prepared with the same buffer. Ascorbate (10  $\mu$ M) without or with CPM or C1 (10 mg) were added to each sample and incubated at 37 °C. The sample (200  $\mu$ L) was transferred to the wells of a flat-bottomed 96-well black plate. HRP (0.04  $\mu$ M) and DCFH (100  $\mu$ M) were added to each solution and incubated in the dark at 37 °C for 1 h. Fluorescence spectra ( $\lambda_{ex}$  = 485 nm) at  $\lambda_{em}$  = 525 nm were measured by a Varioskan Flash microplate reader (Thermo Scientific) every 10 min for 60 h.

#### 2.12 Inhibition of E. coli DH5 growth

Inhibition of *E. coli* DH5 growth was studied according to the reported procedures.<sup>17</sup> *E. coli* DH5 cells transformed with the puc57 plasmid were cultivated in the LB medium (10 g/L tryptone, 5 g/L yeast extract, 10 g/L NaCl) supplemented with 50 g/ml of ampicillin. The cells were cultivated at 37°C with constantly shaking at 250 rpm following a 1:100 inoculation from an overnight culture. The solubility of CPM or C1 is about 100 mg L<sup>-1</sup>. The antibacterial activity was carried out in a saturated solution of CPM or C1. Turbidity of the solution was measured using the absorbance at 600 nm by a Varioskan Flash microplate reader (Thermo Scientific) every 30 min. After inoculation for 1.5 h, we divided the LB medium into two parts to insure the same concentration from the beginning. Then, CPM or C1 (50 mg in 25 ml solution) was added, and the turbidity was measured every 15-30 min until the growth rate slowed down.

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