

Electronic Supplementary Information

Self-Assembly and Alterable Relxivity of an Organic Cation- Encapsulated Gadolinium-Containing Polyoxometalate

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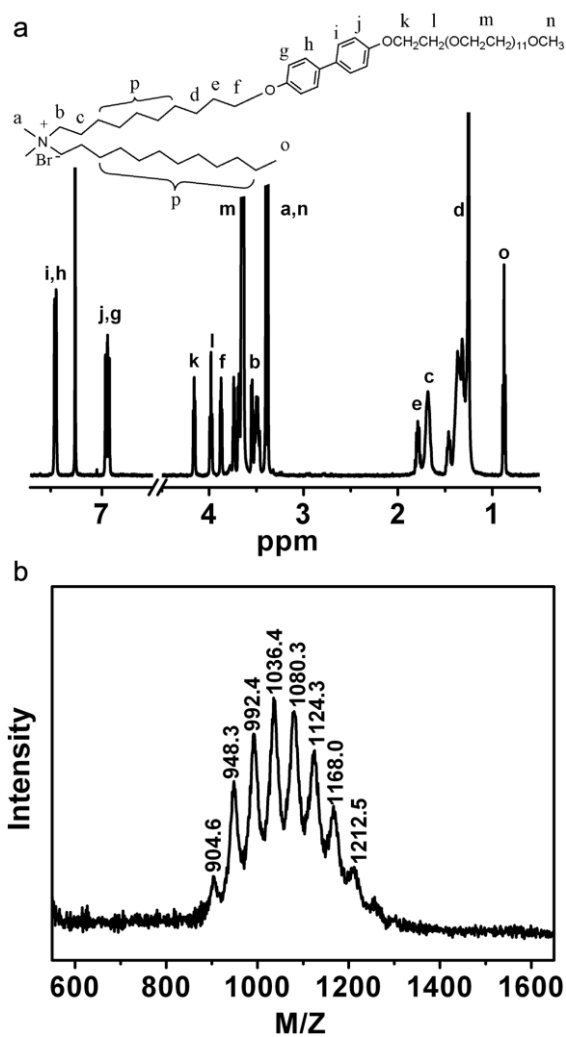


Figure S1. (a) ^1H NMR and (b) MALDI-TOF mass spectra of $\text{EO}_{12}\text{BphC}_{10}\text{NC}_{12}$. The increments of m/z values of adjacent peaks in MS spectrum are about 44, corresponding to the molecular weight of the repeat unit of PEO chain.

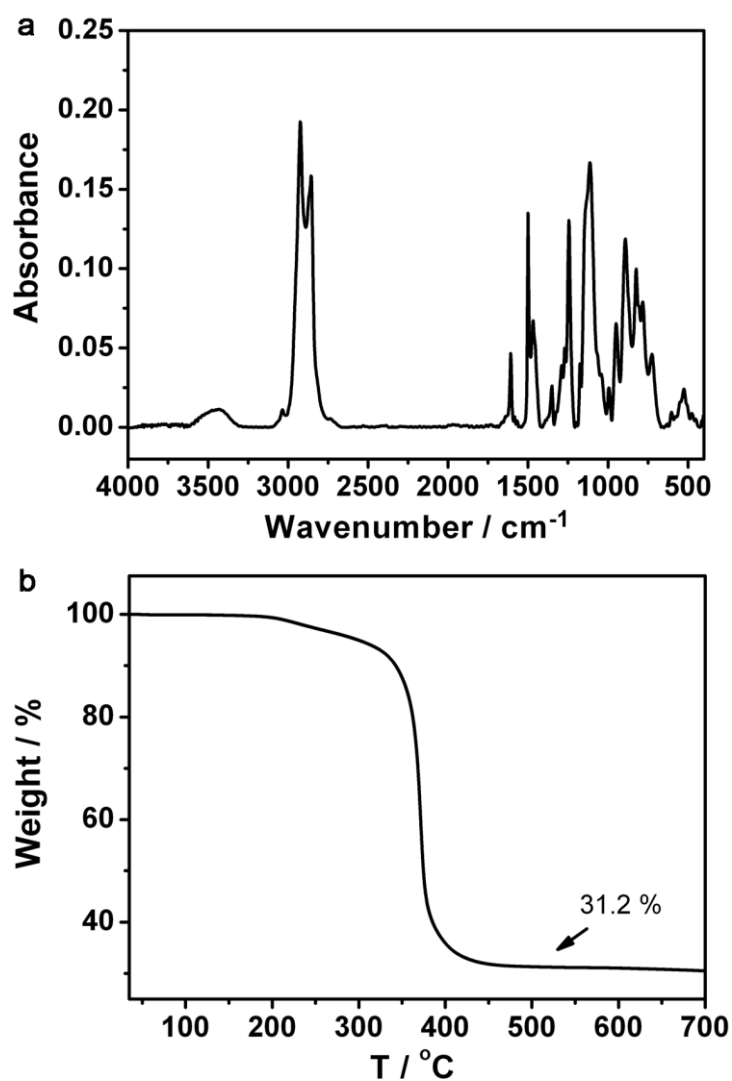


Figure S2. (a) The FT-IR and TGA results of OCEP-Gd.

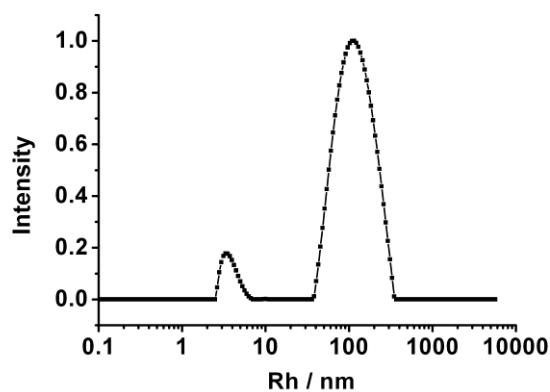


Figure S3. DLS curve of 1 mg ml^{-1} OCEP-Gd aqueous solution.

The calculation of OCEP-Gd lay distance:

The Length of EO₁₂BphC₁₀NC₁₂ except PEO parts is measured to be 2.1 nm.

We assumed the density of PEO is the same with the bulk sample, 1.061 g cm⁻³, and the volume of amorphous PEO layer can be evaluated as:

$$V_{PEO} = \frac{M_{PEO}}{\rho_{PEO}} \quad (1)$$

where M_{PEO} is molecular weight of PEO, 518.4 cm³ mol⁻¹.

Because the volume of different layer is based on the height of layer, the ratio of H_{PEO}/H_{POM} is equal to the ratio of V_{PEO}/V_{POM} , which is expressed in equation (2)

$$\frac{H_{PEO}}{H_{POM}} = \frac{V_{PEO}}{V_{POM}} \quad (2)$$

The height of POM layer is equal to the diameter of lacunary Keggin-type POMs, 1.04 nm. So the height of PEO layers is

$$H_{PEO} = \frac{H_{POM} V_{PEO}}{V_{POM}} = \frac{1.04 \text{ nm} \times 518.4 \text{ cm}^3 / \text{mol}}{6.02 \times 10^{23} \times \left(\frac{4}{3} \times \pi \times 0.5 \text{ nm} \times 0.5 \text{ nm} \times 1 \text{ nm}\right)} = 0.86 \text{ nm} \quad (3)$$

Then, we can calculate the layer distance of phase-separated OCEP-Gd from Equation (4):

$$D_{\text{OCEP-Gd}} = H_{POM} + 2(H_{PEO} + H_{\text{BphC}_{10}\text{NC}_{12}}) = 1.04 + 2(0.55 + 2.1) = 6.9 \text{ nm} \quad (4)$$