Supporting information

Self-assembly and ion-trapping properties of inorganic nanocapsule-

surfactant hybrid spheres

Haolong Li,^a Yang Yang,^a Yizhan Wang,^a Chunyu Wang,^a Wen Li,^a Lixin Wu*^{ab}

^aState Key Laboratory of Supramolecular Structure and Materials, College of Chemistry, Jilin University, Changchun 130012, China.

^bKey Laboratory of Natural Resources of Changbai Mountain & Functional Molecules of Ministry of Education, Yanbian University, Yanji 133002, P. R. China *Corresponding author. E-mail address: <u>wulx@jlu.edu.cn</u>

Table S1 Elemental analysis of SEC-1.

	C (%)	H (%)	N (%)
Experimental results of SEC-1	35.47	7.41	1.94
Calculated values of			
$(C_{38}H_{80}N)_{33}(NH_4)_{39}Mo_{132}O_{372}(SO_4)_{30}(H_2O)_{72}(H_2O)_{50}$	35.37	7.20	2.37
Molecular weight: 42583			



Fig. S1 TGA curves of Mo_{132} (black) and SEC-1 (red). Assuming that the organic component of SEC-1 decomposes completely at 650 °C and all the inorganic residues

are MoO_3 , the observed residual mass percentage should be 44.05 %, according to the chemical formula $(DODA)_{33}(NH_4)_{39}Mo_{132}$. This value is in agreement with the experimental value of 44.66 % and thus confirms the elemental analysis results in Table S1.



Fig. S2 DLS diagram of SEC-1 in the mixed solvent of chloroform and methanol (3:1 in volume ratio)



Fig. S3 Normalized IR spectra of SEC-1 (black curve) and SEC-1-Li (red curve). After normalization, the vibration bands of Mo_{132} part (1000 to 700 cm⁻¹) and the

vibration bands of DODA part (around 2920 and 2851 com⁻¹) have the same intensity. However, the intensity of the water band (around 3450 cm⁻¹) of SEC-1-Li is a little higher than SEC-1, which means SEC-1-Li system has more water.



Fig. S4 ⁷Li NMR spectrum of 50 mM LiCl in the mixed solvent of CDCl₃ and CD₃OD (3:1 in volume ratio). We found that the relative water content (the ratio of water to Li⁺ ions) can affect the ⁷Li signal of LiCl solution. For a 0.5 mM LiCl solution, its signal is at 2.8 ppm; but for a 50 mM LiCl solution, its signal is at 3.6 ppm. Because the relative water content of 50 mM LiCl solution is lower than that of 0.5 mM LiCl, it seems that the lower relative water content causes the ⁷Li signal shifting to high frequency.