Electronic Supplementary Material (ESI) for Soft Matter.

Electronic Supplementary Information

Hedgehog-shaped {Mo_{368}} cluster: unique electronic/structural properties, surfactant encapsulation and related self-assembly into vesicles and films †

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1. Vibrational characterization of 1 and hybrids 2 and 3 by IR, Raman and SERS spectroscopy

The IR spectra of **1** (a), **2** (b) and **3** (c) (Fig. S1) show the characteristic vibrational modes of the cluster anion **1a** (including the three-component ν_3 mode of bridging bidentate sulfate ligands) between 1200 and 500 cm^{-1}. In addition, the spectra of **2** and **3** show respectively the characteristic absorptions of the DODA and guanidinium cations.

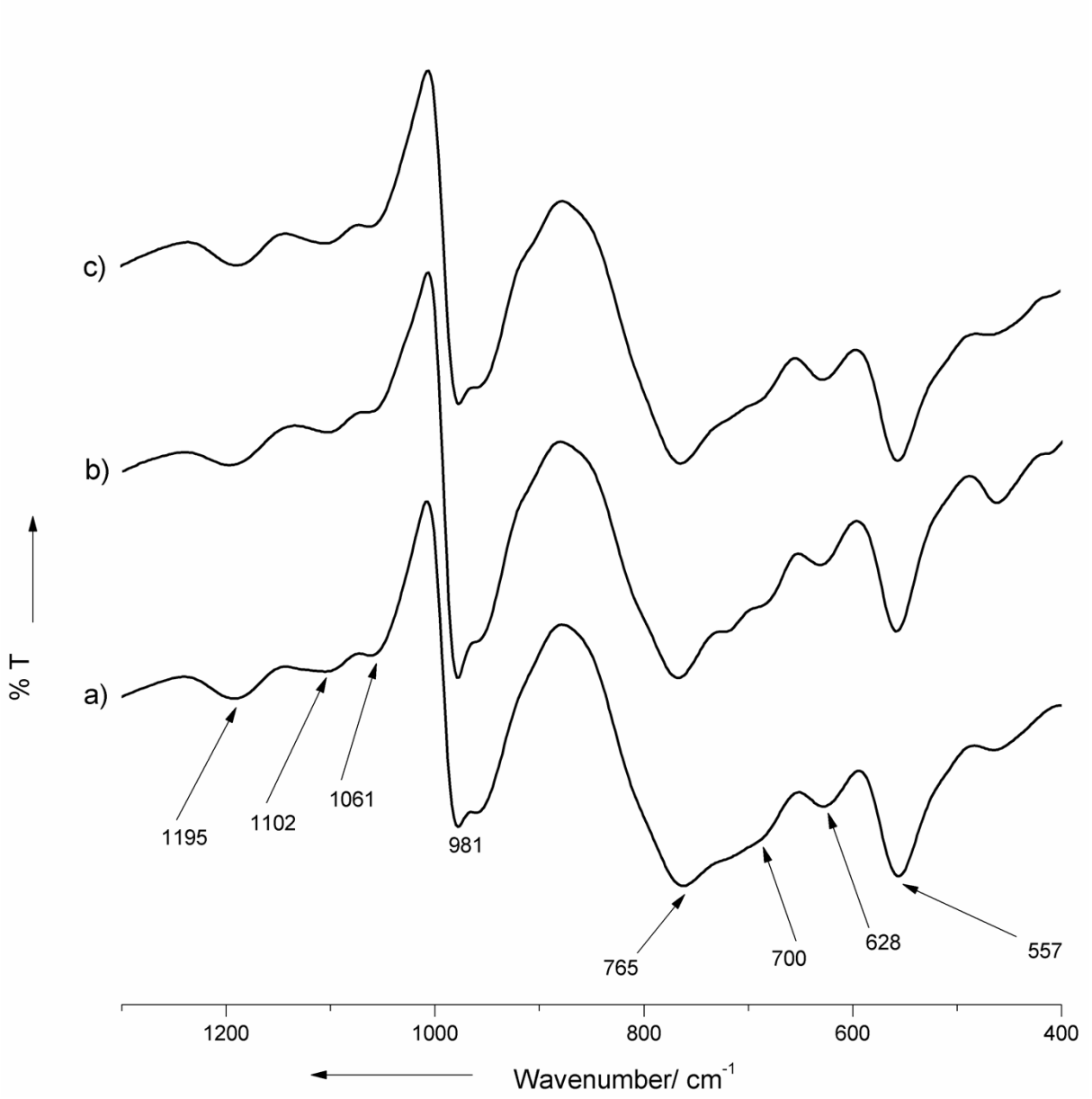

Fig. S1 IR spectra of **1** (a),[1] **2** (b) and **3** (c) (KBr disk).

The SERS spectrum of **3** (Fig. S2) is similar to that of **1** (see Fig. 3), though less well-resolved.

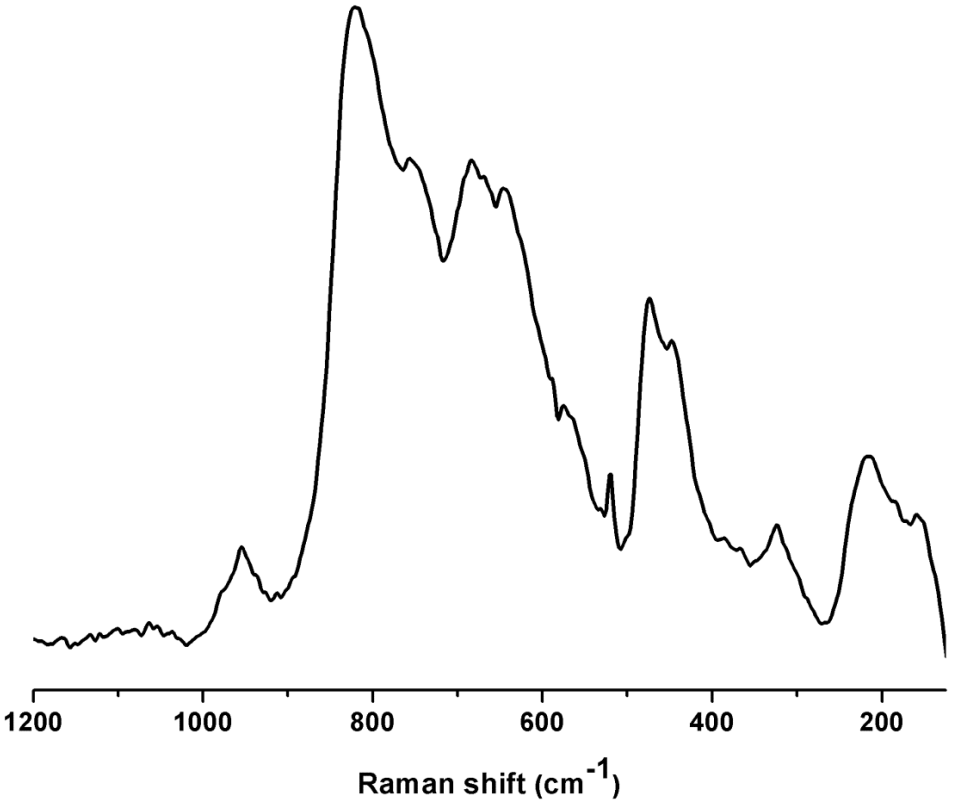

Fig. S2 SERS spectrum obtained by depositing an aqueous solution of **3** onto a gold substrate; λ_{exc} = 1064 nm.

2. Characterization of 2 and 3 by electronic spectroscopy

The electronic absorption spectrum of a solution of **2** in a mixture of $CHCl_3$ and acetone shows a quite intense and broad band from the visible to the near-infrared. The spectrum of a fresh solution of **3** in ethanol-water (not shown) is similar but the absorbance decreases fairly quickly.

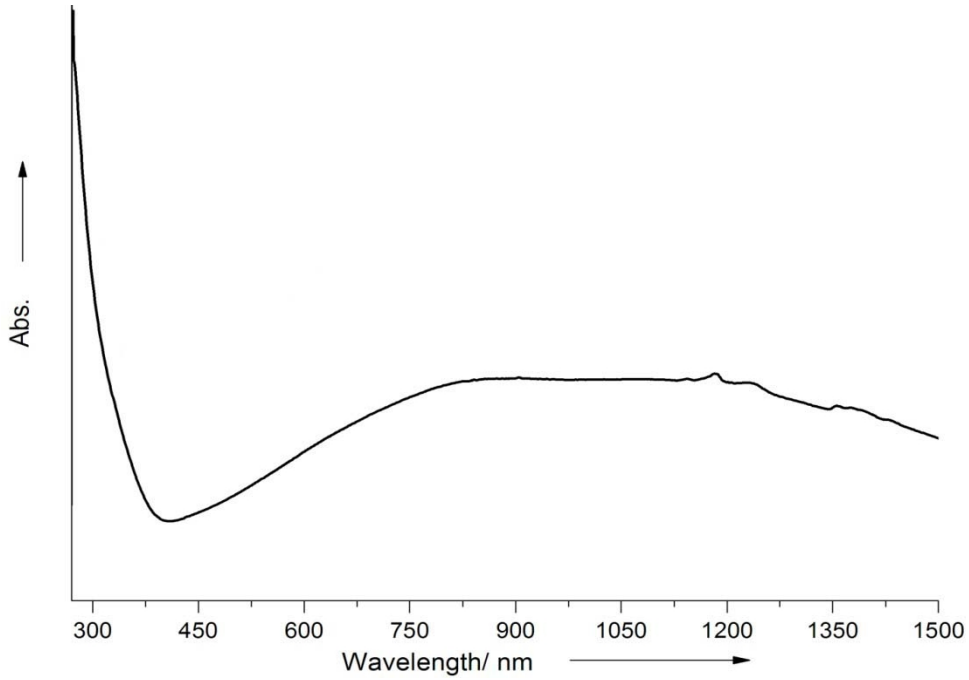

Fig. S3 Electronic absorption spectra of **2** ($CHCl_3$/acetone solution, $\varepsilon \approx 5.6 \times 10^5$ M^{-1} cm^{-1}).

3. AFM characterization of a cast film of 2

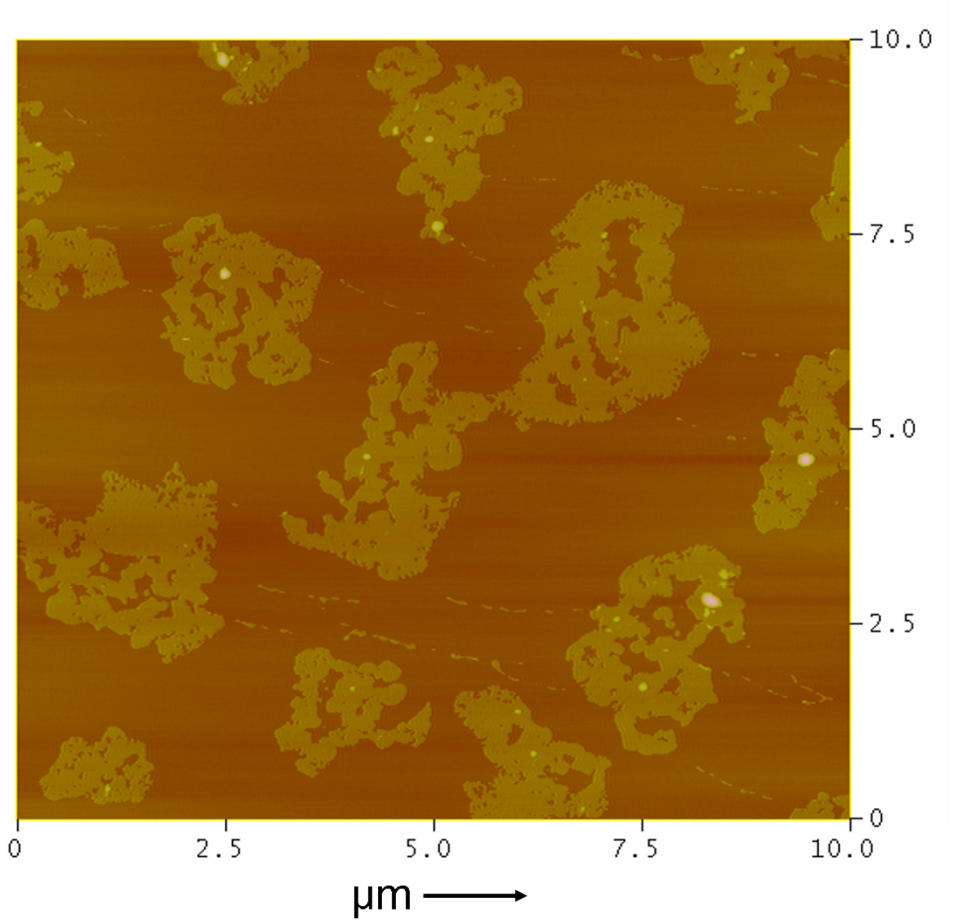

Fig. S4 AFM image of a cast film of **2** at 10 × 10 mm^2 scanning area revealing an irregular pattern (the patterned Langmuir monolayer was formed at a surface pressure of 35 mN m^{-1}). The height of the surface features is about 3.2 nm and their surface is very flat, which might indicate a single layer of **2**. The vertical height of **1a** is about 2 nm according to the single-crystal X-ray analysis.[1a]

References

1 (*a*) A. Müller, E. Beckmann, H. Bögge, M. Schmidtmann and A. Dress, *Angew. Chem. Int. Ed.,* 2002, **41**, 1162–1167; (*b*) A. Müller, B. Botar, S. K. Das, H. Bögge, M. Schmidtmann and A. Merca, *Polyhedron*, 2004, **23**, 2381-2385.