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Electronic Supplementary Information

# Synthesis, structure and properties of an octahedral dinuclear-based $Cu_{12}$ nanocage of trimesoyltri(*L*-alanine)

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**Table S1** Crystallographic data of **1**

| | **1** |
|---|---|
| Empirical formula | $C_{160}H_{296}Cu_{12}N_{24}O_{132}$ |
| Formula weight | 5430.69 |
| Temperature / K | 103(2) |
| Wavelength / Å | 0.71073 |
| Crystal system | Tetragonal |
| Space group | $P4_22_12$ |
| $a$ / Å | 33.227(2) |
| $b$ / Å | 33.227(2) |
| $c$ / Å | 24.546(2) |
| $\alpha$ / º | 90 |
| $\beta$ / º | 90 |
| $\gamma$ / º | 90 |
| $V$ / Å$^3$ | 27100(4) |
| $Z$ | 4 |
| $D_c$ / g cm$^{-3}$ | 1.331 |
| $\mu$ / mm$^{-1}$ | 1.018 |
| F(000) | 11312 |
| Crystal size / mm | 0.27 × 0.27 × 0.27 |
| $\theta$ range for data / ° | 3.02 to 25.01 |
| Reflections collected | 181177 |
| Unique reflections | 23864 |
| $R_{int}$ | 0.0927 |
| Goodness-of-fit on $F^2$ | 0.999 |
| Final $R$ indices ($I > 2\sigma(I)$) | $R_1 = 0.0707$, $wR_2 = 0.1849$ |
| $R$ indices (all data) | $R_1 = 0.0912$, $wR_2 = 0.2030$ |
| Largest diff. peak and hole | 0.776 and -0.404 |
| Flack | 0.066(13) |

**Table S2** Selected bond lengths [Å] and angles [°] for **1**

| | | | |
|---|---|---|---|
| Cu1-O34 | 1.969(4) | Cu4-O32A | 1.952(5) |
| Cu1-O10 | 1.971(5) | Cu4-O17 | 1.956(5) |
| Cu1-O1 | 1.973(5) | Cu4-O20 | 1.962(5) |
| Cu1-O13A | 1.989(5) | Cu4-O5 | 1.986(5) |
| Cu1-O37 | 2.131(5) | Cu4-O40 | 2.361(5) |
| Cu2-O14A | 1.968(6) | Cu5-O22A | 1.964(5) |
| Cu2-O11 | 1.973(5) | Cu5-O7 | 1.967(5) |
| Cu2-O35 | 1.974(5) | Cu5-O25 | 1.967(5) |
| Cu2-O2 | 1.988(6) | Cu5-O28 | 1.983(5) |
| Cu2-O38 | 2.379(5) | Cu5-O41 | 2.144(4) |
| Cu3-O16 | 1.944(5) | Cu6-O29 | 1.956(6) |
| Cu3-O19 | 1.965(5) | Cu6-O26 | 1.960(5) |
| Cu3-O31A | 1.975(5) | Cu6-O8 | 1.966(5) |
| Cu3-O4 | 1.999(5) | Cu6-O23A | 1.996(5) |
| Cu3-O39 | 2.222(5) | Cu6-O42 | 2.410(5) |
| O34-Cu1-O10 | 169.47(19) | O32A-Cu4-O17 | 89.8(2) |
| O34-Cu1-O1 | 88.6(2) | O32A-Cu4-O20 | 89.8(2) |
| O10-Cu1-O1 | 88.6(2) | O17-Cu4-O20 | 166.1(2) |
| O34-Cu1-O13A | 90.7(2) | O32A-Cu4-O5 | 167.56(19) |
| O10-Cu1-O13A | 89.9(2) | O17-Cu4-O5 | 89.1(2) |
| O1-Cu1-O13A | 167.7(2) | O20-Cu4-O5 | 88.3(2) |
| O34-Cu1-O37 | 97.98(18) | O32A-Cu4-O40 | 94.5(2) |
| O10-Cu1-O37 | 92.41(19) | O17-Cu4-O40 | 97.9(2) |
| O1-Cu1-O37 | 96.0(2) | O20-Cu4-O40 | 96.0(2) |
| O13A-Cu1-O37 | 96.3(2) | O5-Cu4-O40 | 97.9(2) |
| O14A-Cu2-O11 | 89.0(2) | O22A-Cu5-O7 | 169.8(2) |
| O14A-Cu2-O35 | 90.0(2) | O22A-Cu5-O25 | 88.3(2) |
| O11-Cu2-O35 | 165.8(2) | O7-Cu5-O25 | 89.8(2) |
| O14A-Cu2-O2 | 166.9(2) | O22A-Cu5-O28 | 90.9(2) |
| O11-Cu2-O2 | 89.5(2) | O7-Cu5-O28 | 89.2(2) |
| O35-Cu2-O2 | 88.2(2) | O25-Cu5-O28 | 169.6(2) |
| O14A-Cu2-O38 | 95.5(3) | O22A-Cu5-O41 | 95.76(19) |
| O11-Cu2-O38 | 96.0(2) | O7-Cu5-O41 | 94.37(19) |
| O35-Cu2-O38 | 98.2(2) | O25-Cu5-O41 | 93.5(2) |
| O2-Cu2-O38 | 97.6(3) | O28-Cu5-O41 | 96.9(2) |
| O16-Cu3-O19 | 167.9(2) | O29-Cu6-O26 | 166.0(2) |
| O16-Cu3-O31A | 89.7(2) | O29-Cu6-O8 | 90.3(2) |
| O19-Cu3-O31A | 90.1(2) | O26-Cu6-O8 | 89.4(2) |
| O16-Cu3-O4 | 89.2(2) | O29-Cu6-O23A | 89.1(2) |
| O19-Cu3-O4 | 88.5(2) | O26-Cu6-O23A | 88.0(2) |
| O31A-Cu3-O4 | 168.1(2) | O8-Cu6-O23A | 167.0(2) |
| O16-Cu3-O39 | 93.2(2) | O29-Cu6-O42 | 93.8(3) |
| O19-Cu3-O39 | 98.9(2) | O26-Cu6-O42 | 100.1(3) |
| O31A-Cu3-O39 | 96.7(2) | O8-Cu6-O42 | 96.2(2) |
| O4-Cu3-O39 | 95.2(2) | O23A-Cu6-O42 | 96.8(2) |

Symmetry code: A) $-y + 1, -x + 1, -z$

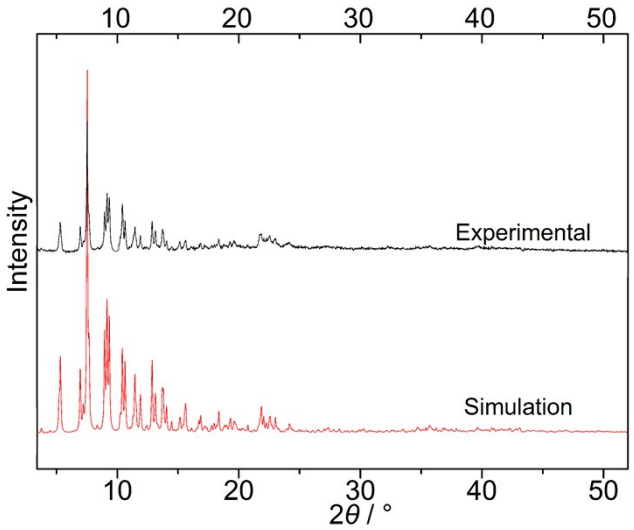


**Fig. S1** PXRD patterns of **1**.

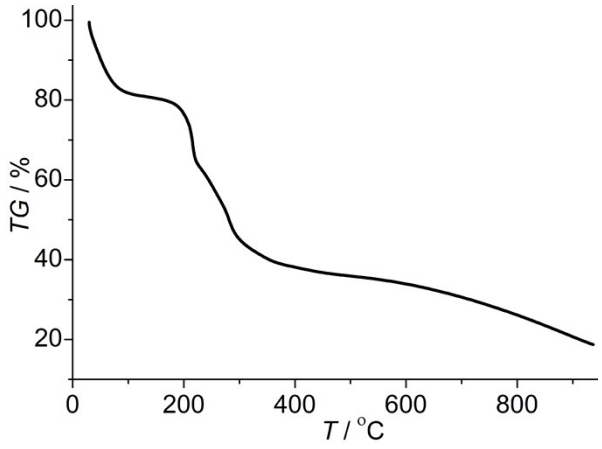


**Fig. S2** TG curve of **1**.

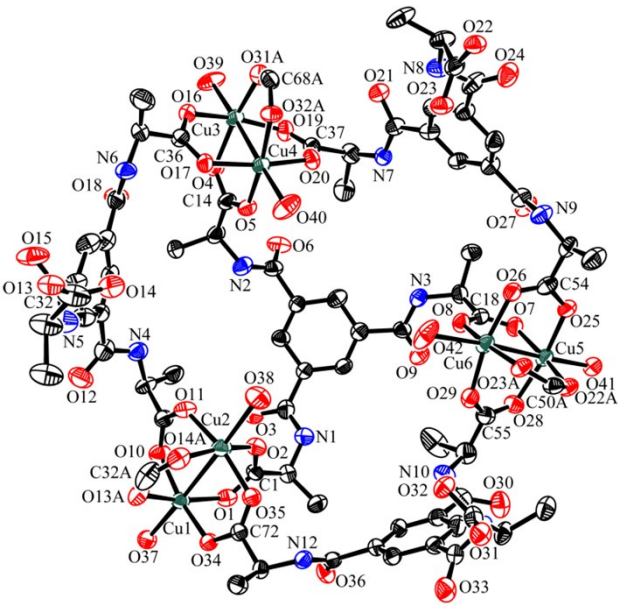


**Fig. S3** ORTEP view of the structure of **1** showing the atom-labeling scheme and 30% thermal ellipsoids. Hydrogen atoms are omitted for clarity. Symmetry codes: A) $-y + 1, -x + 1, -z$.

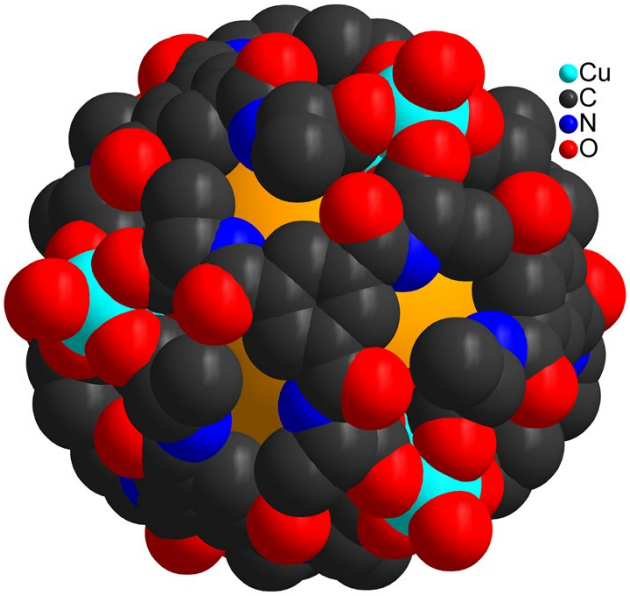


**Fig. S4** TG curve of complex 1a and 1b.

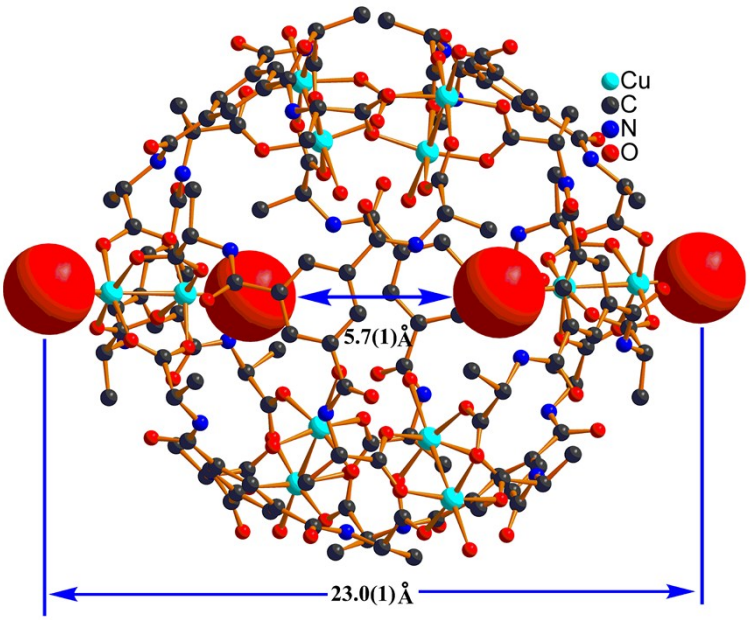


**Fig. S5** A show of the size of the nanoball and its pore.

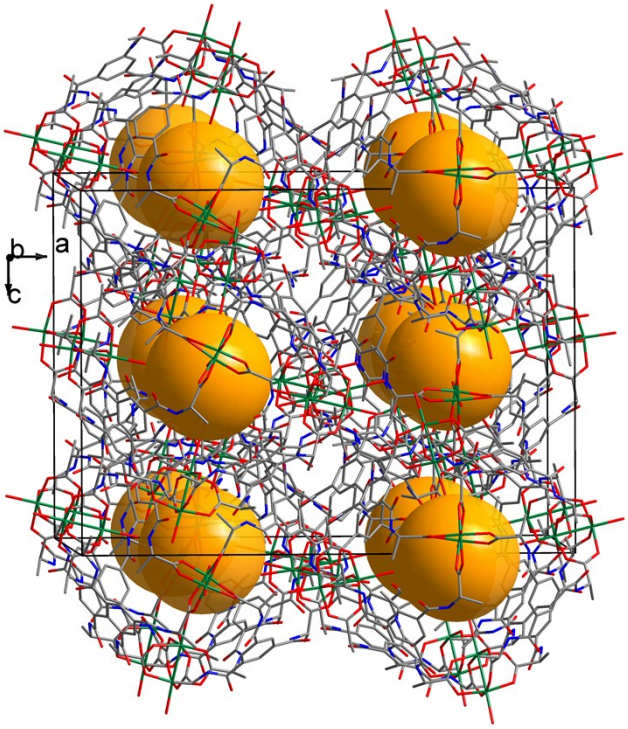


**Fig. S6** Packing diagram of the nanocages of **1** in a ball-and-stick model, with a yellow dummy ball showing the solvent-accessible cavity in the nanocage.