# Supporting Information

***For***

# A Nanocomposite Gel Based on 1D Coordination Polymers and Nanoclusters Reversibly Gelate Water upon Heating

*Jin-Ji Wu, Man-Li Cao, Jian-Yong Zhang* and Bao-Hui Ye**

MOE Key Laboratory of Bioinorganic and Synthetic Chemistry, School of Chemistry and Chemical Engineering, Sun Yat-Sen University, Guangzhou 510275, China; Department of Chemistry, Guangdong University of Education, Guangzhou 510303, China

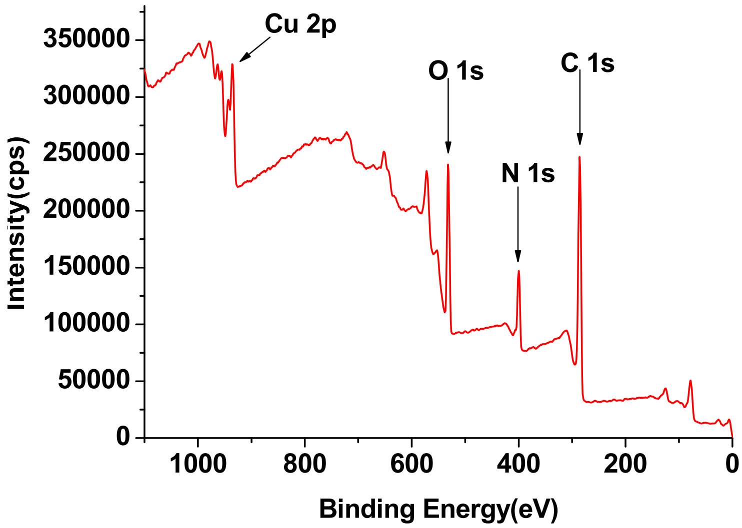


***Fig. S1.*** XPS survey of complex **3**·$NO_3$. No peak is found in the range from 770 to 800 eV indicating that all the metal ions in **3**·$NO_3$ are copper.[8]

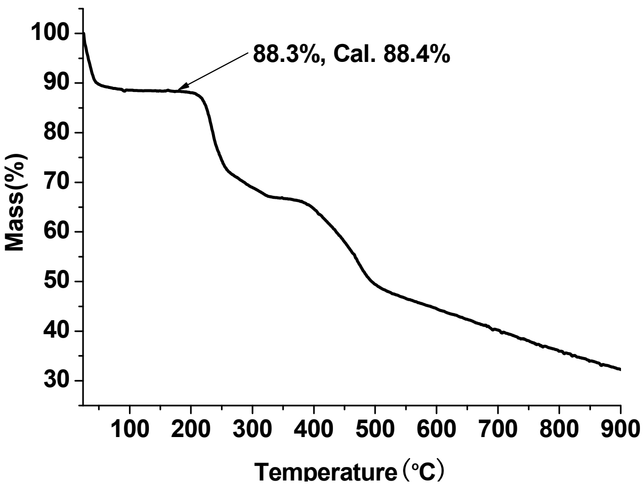


***Fig. S2.*** TGA curve of **3**·$NO_3$, revealing that there were 32 lattice water molecules in **3**·$NO_3$.

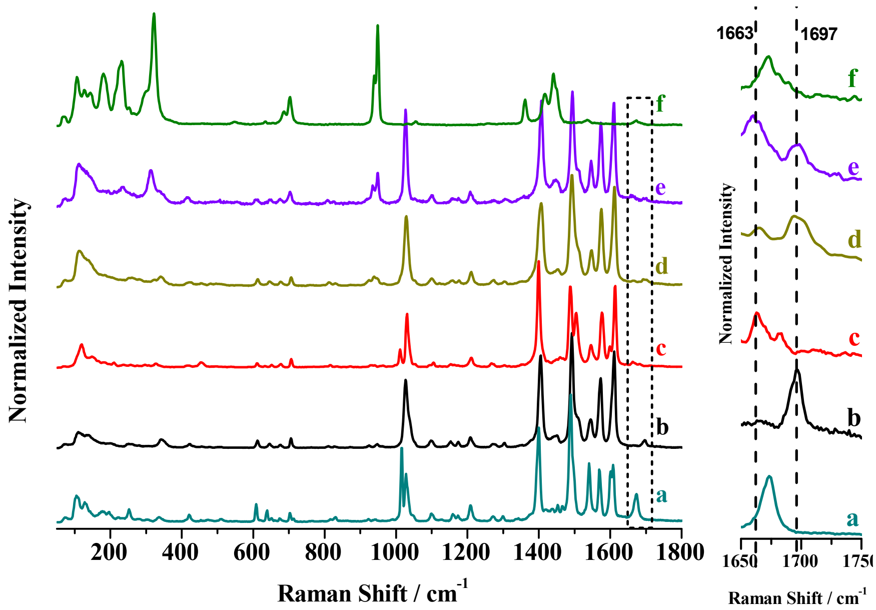


***Fig. S3.*** Comparison of Raman spectra of **2** (a), **3**·$NO_3$ (b), **1** (c), **S** (d), **G** (e), **Cu(OAc)$_2$·$H_2O$** (f); and the magnified region of 1650 – 1750 $cm^{-1}$ (right).

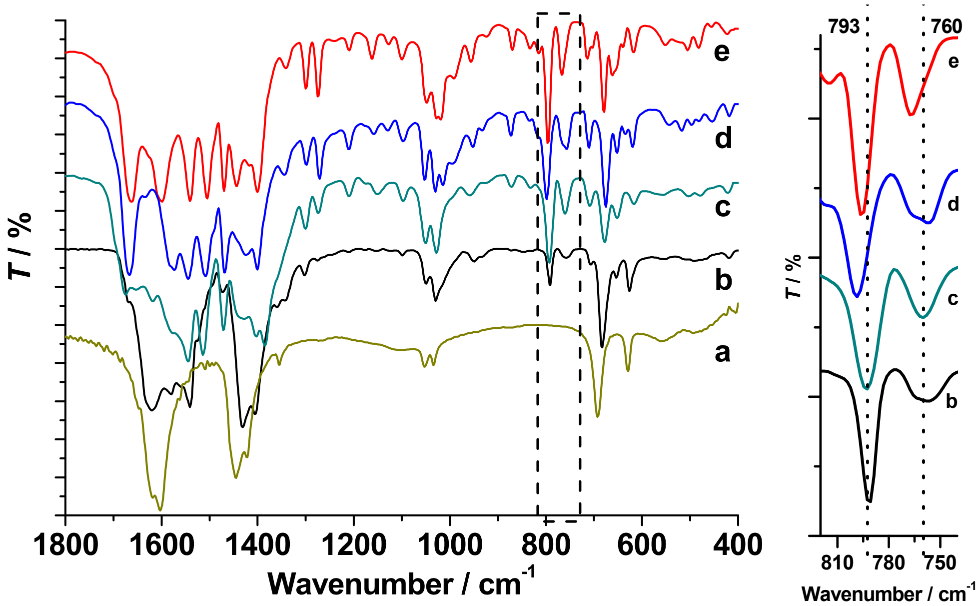


***Figure S4.*** Comparison of IR spectra of Cu(OAc)$_2$·$H_2O$ (a), filtrate (b), **3**·$NO_3$ (c), **1** (d), **2** (e); and the magnified region of 820 – 740 $cm^{-1}$ for b, c, d and e (right).

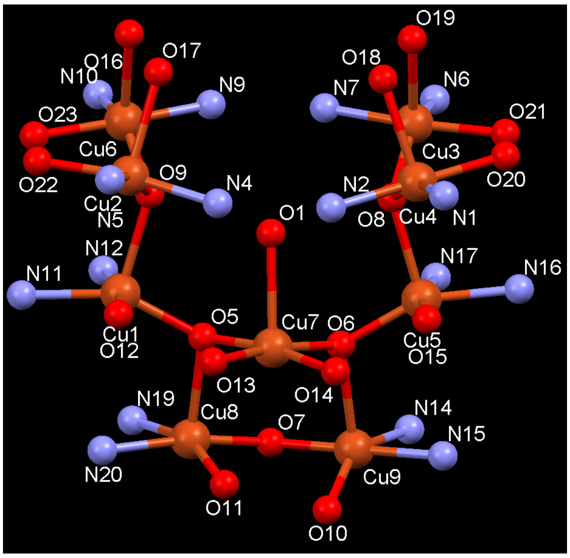


***Figure S3***. Representation of the inner coordination spheres of $Cu_9$ cluster for complex **3**·$NO_3$ (only atoms in the coordination geometries of the metal centers was present for clarity).

***Table S2.*** Selected bond lengths involving the coordination geometries of the metal centers.

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| Cu1 | O9 | 2.204(2) | Cu5 | N16 | 2.032(3) |
| Cu1 | O5 | 1.971(2) | Cu5 | N17 | 2.012(3) |
| Cu1 | O12 | 1.929(3) | Cu6 | O9 | 1.973(2) |
| Cu1 | N11 | 2.048(3) | Cu6 | O16 | 2.139(3) |
| Cu1 | N12 | 2.004(3) | Cu6 | O23 | 1.934(3) |
| Cu2 | O9 | 1.932(2) | Cu6 | N10 | 2.058(3) |
| Cu2 | O22 | 1.965(3) | Cu6 | N9 | 1.990(3) |
| Cu2 | N5 | 2.019(3) | Cu7 | O1 | 2.396(2) |
| Cu2 | N4 | 2.053(3) | Cu7 | O6 | 1.941(2) |
| Cu2 | O17 | 2.237(2) | Cu7 | O5 | 1.953(2) |
| Cu3 | O8 | 1.973(2) | Cu7 | O14 | 1.970(3) |
| Cu3 | O19 | 2.144(3) | Cu7 | O13 | 1.968(3) |
| Cu3 | O21 | 1.943(3) | Cu8 | O5 | 2.281(2) |
| Cu3 | N6 | 2.056(3) | Cu8 | N20 | 2.030(3) |
| Cu3 | N7 | 1.998(3) | Cu8 | N19 | 2.038(3) |
| Cu4 | O8 | 1.937(2) | Cu8 | O7 | 1.886(3) |
| Cu4 | O20 | 1.957(3) | Cu8 | O11 | 1.966(3) |
| Cu4 | O18 | 2.264(3) | Cu9 | O6 | 2.360(2) |
| Cu4 | N2 | 2.037(3) | Cu9 | N14 | 2.040(3) |
| Cu4 | N1 | 2.013(3) | Cu9 | O10 | 1.955(3) |
| Cu5 | O8 | 2.243(2) | Cu9 | O7 | 1.895(3) |
| Cu5 | O6 | 1.951(2) | Cu9 | N15 | 2.013(3) |
| Cu5 | O15 | 1.938(3) | | | |

***Table S3.*** Selected bond angles involving the coordination geometries of the metal centers.

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|---|---|---|
| O5 | Cu1 | O9 | 103.80(9) | O15 | Cu5 | N16 | 88.38(12) |
| O5 | Cu1 | N11 | 148.70(11) | O15 | Cu5 | N17 | 168.17(12) |
| O5 | Cu1 | N12 | 93.60(11) | N16 | Cu5 | O8 | 100.29(11) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| O12 | Cu1 | O9 | 90.32(10) | N17 | Cu5 | O8 | 92.25(10) |
| O12 | Cu1 | O5 | 96.98(11) | N17 | Cu5 | N16 | 79.81(13) |
| O12 | Cu1 | N11 | 88.77(12) | O9 | Cu6 | O16 | 109.02(10) |
| O12 | Cu1 | N12 | 168.36(12) | O9 | Cu6 | N10 | 144.56(11) |
| N11 | Cu1 | O9 | 106.93(10) | O9 | Cu6 | N9 | 97.05(11) |
| N12 | Cu1 | O9 | 91.86(10) | O23 | Cu6 | O9 | 90.79(11) |
| N12 | Cu1 | N11 | 79.65(12) | O23 | Cu6 | O16 | 93.85(11) |
| O9 | Cu2 | O22 | 93.08(10) | O23 | Cu6 | N10 | 89.00(12) |
| O9 | Cu2 | N5 | 166.11(12) | O23 | Cu6 | N9 | 168.55(12) |
| O9 | Cu2 | N4 | 95.00(11) | N10 | Cu6 | O16 | 106.35(11) |
| O9 | Cu2 | O17 | 101.01(10) | N9 | Cu6 | O16 | 91.47(11) |
| O22 | Cu2 | N5 | 90.49(12) | N9 | Cu6 | N10 | 79.76(12) |
| O22 | Cu2 | N4 | 167.78(12) | O6 | Cu7 | O1 | 93.44(9) |
| O22 | Cu2 | O17 | 97.16(10) | O6 | Cu7 | O5 | 94.58(10) |
| N5 | Cu2 | N4 | 79.56(12) | O6 | Cu7 | O14 | 90.76(11) |
| N5 | Cu2 | O17 | 91.84(11) | O6 | Cu7 | O13 | 170.42(11) |
| N4 | Cu2 | O17 | 90.29(11) | O5 | Cu7 | O1 | 87.27(9) |
| O8 | Cu3 | O19 | 107.35(10) | O5 | Cu7 | O14 | 170.63(11) |
| O8 | Cu3 | N6 | 142.24(11) | O5 | Cu7 | O13 | 92.96(11) |
| O8 | Cu3 | N7 | 97.04(11) | O14 | Cu7 | O1 | 100.12(10) |
| O21 | Cu3 | O8 | 92.35(11) | O13 | Cu7 | O1 | 92.82(10) |
| O21 | Cu3 | O19 | 89.56(11) | O13 | Cu7 | O14 | 81.00(11) |
| O21 | Cu3 | N6 | 89.05(12) | N20 | Cu8 | O5 | 93.35(10) |
| O21 | Cu3 | N7 | 168.86(12) | N20 | Cu8 | N19 | 79.60(12) |
| N6 | Cu3 | O19 | 110.39(11) | N19 | Cu8 | O5 | 99.59(10) |
| N7 | Cu3 | O19 | 93.34(11) | O7 | Cu8 | O5 | 95.98(10) |
| N7 | Cu3 | N6 | 79.86(13) | O7 | Cu8 | N20[1] | 170.67(11) |
| O8 | Cu4 | O20 | 95.01(10) | O7 | Cu8 | N19[1] | 98.79(12) |
| O8 | Cu4 | O18 | 100.09(9) | O7 | Cu8 | O11 | 92.98(12) |
| O8 | Cu4 | N2 | 95.88(11) | O11 | Cu8 | O5 | 96.80(13) |
| O8 | Cu4 | N1 | 162.13(11) | O11 | Cu8 | N20[1] | 85.91(13) |
| O20 | Cu4 | O18 | 93.06(10) | O11 | Cu8 | N19[1] | 158.66(15) |
| O20 | Cu4 | N2 | 169.05(11) | N14 | Cu9 | O6 | 101.14(10) |
| O20 | Cu4 | N1 | 89.73(11) | O10 | Cu9 | O6 | 106.58(12) |
| N2 | Cu4 | O18 | 86.11(11) | O10 | Cu9 | N14 | 148.98(13) |
| N1 | Cu4 | O18 | 96.84(10) | O10 | Cu9 | N15 | 86.06(14) |
| N1 | Cu4 | N2 | 79.54(12) | O7 | Cu9 | O6 | 88.71(10) |
| O6 | Cu5 | O8 | 104.68(9) | O7 | Cu9 | N14 | 100.44(12) |
| O6 | Cu5 | N16 | 154.72(12) | O7 | Cu9 | O10 | 93.91(12) |
| O6 | Cu5 | N17 | 95.15(11) | O7 | Cu9 | N15 | 179.74(13) |
| O15 | Cu5 | O8 | 90.53(10) | N15 | Cu9 | O6 | 91.05(11) |
| O15 | Cu5 | O6 | 95.26(11) | N15 | Cu9 | N14 | 79.71(13) |

## References:

[1] Handbook of X-ray photoelectron Specroscopy, C. D. Wagner, W. M. Riggs, L. E. Davis, J. F. Moulder, G. E. Muilenberg, Perkin-Elmer Corp. 1979, 78-83.