Supporting Information

Magnetic and thermal properties of three ionothermally synthesized metal-carboxylate frameworks of $[M_3(ip)_4][EMIm]_2$ (M = Co, Ni, Mn, ip = isophthalic acid, EMIm = 1-ethyl-3-methyl imidazolium)

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***XMMAG* Simulation Program**

This program was written based on following algorithm: For N nuclear metal clusters, all spin wave functions can be derived from base sets $\Psi_i = |Ms_{i1}, Ms_{i2}, Ms_{i3}, \ldots Ms_{ij}, \ldots, Ms_{iN}\rangle$, where M_{sij} is the j th microstate corresponding to the i th magnetic ion[1]. Each microstate Ms_{ij} can take a set of values: $-S_i, -S_i+1, -S_i+2, \ldots, S_i-1, S_i$, where S_i is the spin quantum number of the i th magnetic ion. The total M_{sT} value of the i base set, corresponding to total spin S_T, is $M_{sT} = \sum Ms_{ij}$.

The spin Hamiltonian of N nuclear metal clusters based on Heisengerg theory[2] is $H = -2\sum J_{mn} S_m S_n$. Base on the ladder operator of spin angular momentum, the spin Hamiltonian can be reduced to be following formula: $H = -2\sum J_{mn}\{S_{mz}S_{nz} + (S_m^+ + S_n^-)/2\}$. Moreover, the eigenvalue of the S_{mz}, S_m^+, S_n^- operator on the base set Ψ_i is $S_{mz}\Psi_i = Ms_{im}\Psi_i, S_m^+\Psi_i = \sqrt{(S_m - Ms_{im})(S_m + Ms_{im}+1)}, S_n^-\Psi_i = \sqrt{(S_n + Ms_{in})(S_n - Ms_{in}+1)}$. Thus the matrix corresponding to Hamiltonian with matrix element $\langle\Psi_i|H|\Psi_j\rangle$ can be constructed. Given a set of J_{mn} value, the matrix can be diagonalized with the help of *LAPACK* package and generates a set of energy E_i corresponding to specific total spin number M_{sT}. Consequently, the molar magnetic susceptibility is derived from the Van Vleck equation[2], as shown in

$$\chi_M = \frac{N\mu_\beta^2 g^2}{3kT} \frac{\sum M_{sT}(M_{sT}+1)(2M_{sT}+1)e^{-E_i/kT}}{\sum (2M_{sT}+1)e^{-E_i/kT}}$$

Additionally, the inter-unit interaction zJ was taken into account based on the formula[2]

$$\chi_M^{mf} = \frac{\chi_M}{1 - 2z_J\chi_M/(Ng^2\mu_\beta^2)}$$

And the reliability factor of R is obtained by use of the formula[2]

$$R = \sum[(\chi_M T)_{obs} - (\chi_M^{mf} T)]^2 / \sum[(\chi_M T)_{obs}]^2$$

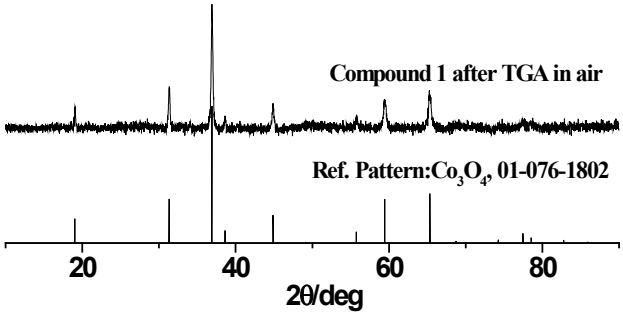

Fig. S1. X-ray powder diffraction for the residual product of **1** after TGA and the ref. pattern:Co_3O_4, 01-076-1802.

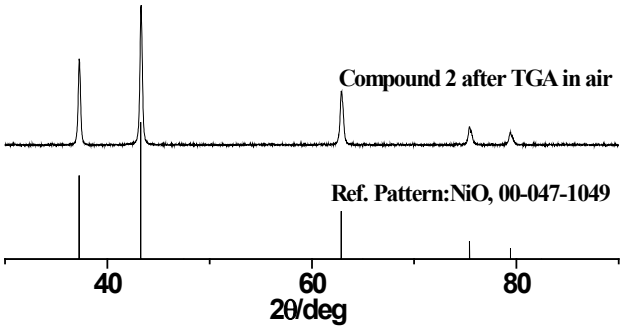

Fig. S2. X-ray powder diffraction for the residual product of **2** after TGA and the ref. pattern:NiO, 00-047-1049.

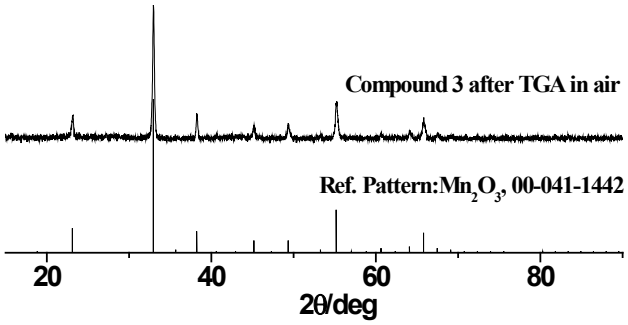

Fig. S3. X-ray powder diffraction for the residual product of **3** after TGA and the ref. pattern:Mn_2O_3, 00-041-1442.

1. N. S. Dalal, L. Nadjo, A. G. Marshall, et al. *Inorg. Chem.*, **2005**, 44, 9795.
2. O. Kahn, Molecular Magnetism; VCH: New York, **1993**; S. G. Vulfson, Molecular Magnetochemistry; Gordon and Breach Science: Newark, NJ, **1998**.