Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.


# Chiral Biomolecule Based Dodecanuclear Dysprosium(III)-Copper(II) Clusters: Structural Analyses and Magnetic Properties

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## Experimental Section

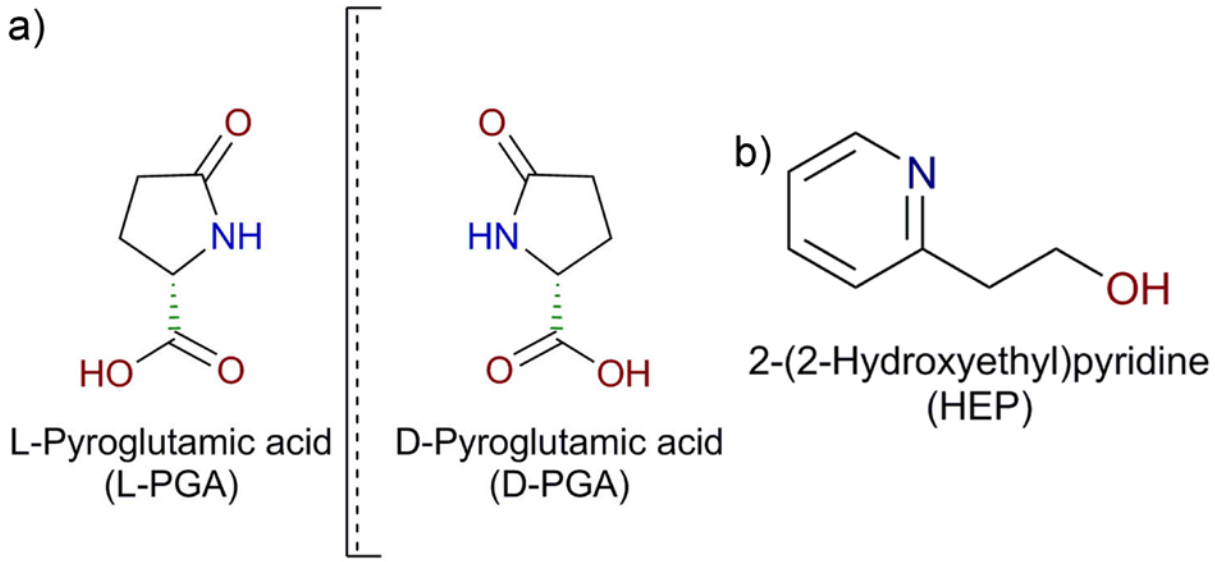


**Fig. S1: a)** Pyroglutamic acid (PGA) ligands of unlike chirality; b) ancillary ligand 2-(2-Hydroxyethyl)pyridine (HEP) employed in the formation of the synthesized $M_4Cu_8$ complexes.

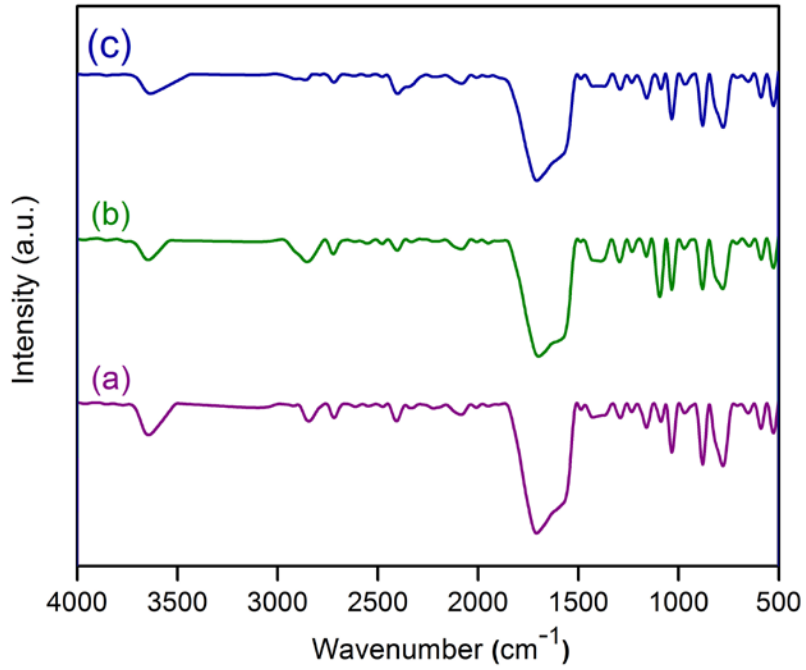


**Fig. S2:** IR spectra for compounds a) **1L**, b) **1D**, c) **2L**.

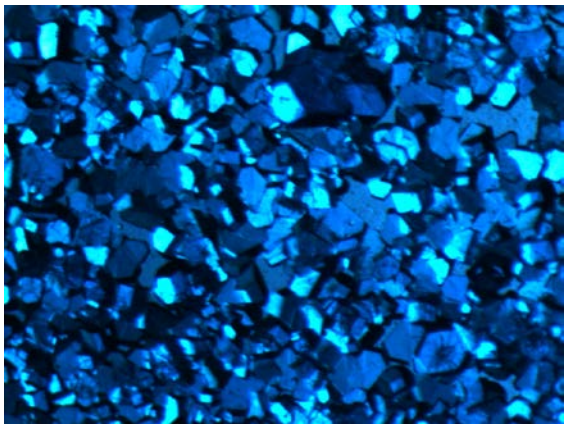

**Fig. S2:** Shiny square-shaped blue single crystals of compound **1L**, when viewed under microscope.

**Table S1**. Crystal data and structure refinement for compound **1L**.

| | | |
|---|---|---|
| Identification code | Compound **1L** | |
| Empirical formula | $C_{96}H_{112}Cu_8Dy_4N_{16}O_{40}$ | |
| Formula weight | 3,288.33 | |
| Temperature | 200(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Tetragonal | |
| Space group | *P 4 2 2* | |
| Unit cell dimensions | *a* = 16.9996(10) Å | $\alpha$= 90°. |
| | *b* = 16.9996(10) Å | $\beta$= 90°. |
| | *c* = 13.1497(8) Å | $\gamma$ = 90°. |
| Volume | 3800.1(5) $Å^3$ | |
| Z | 1 | |
| Density (calculated) | 1.437 $Mg/m^3$ | |
| Absorption coefficient | 3.101 $mm^{-1}$ | |
| F(000) | 1616 | |
| Crystal size | 0.120 x 0.100 x 0.090 $mm^3$ | |
| Theta range for data collection | 1.198 to 24.995°. | |
| Index ranges | -20<=h<=16, -8<=k<=20, -13<=l<=15 | |
| Reflections collected | 14822 | |
| Independent reflections | 3375 [R(int) = 0.0493] | |
| Completeness to theta = 25.242° | 97.4 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.7468 and 0.7267 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 3375 / 60 / 158 | |
| Goodness-of-fit on $F^2$ | 1.636 | |
| Final R indices [I>2sigma(I)] | $R_1$ = 0.1045, $wR_2$ = 0.3538 | |
| R indices (all data) | $R_1$ = 0.1087, $wR_2$ = 0.3586 | |
| Absolute structure parameter | 0.128(16) | |
| Extinction coefficient | 0.009(3) | |
| Largest diff. peak and hole | 2.938 and -1.429 e.$Å^{-3}$ | |

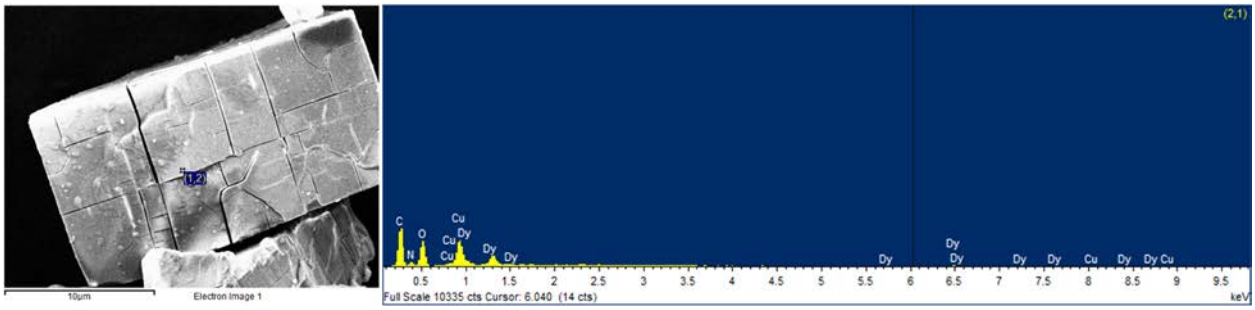


**Fig. S3:** EDX spectra of the crystals of compound **1L**, revealing the metal analysis data.

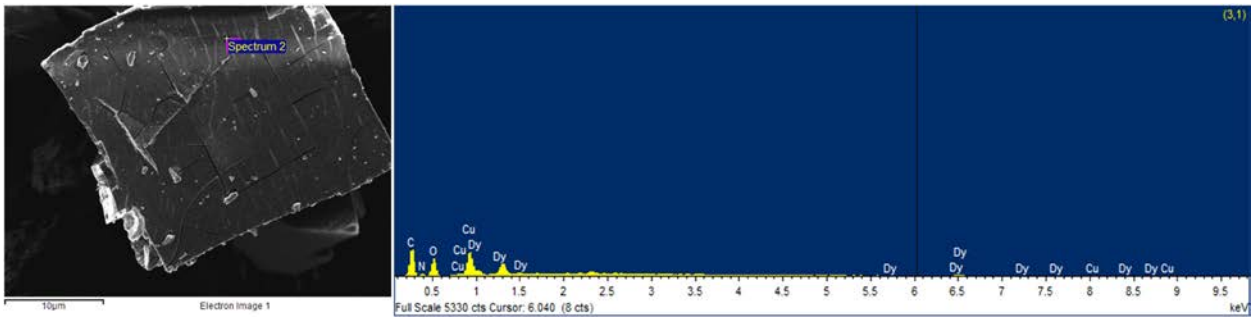


**Fig. S4:** EDX spectra of the crystals of compound **1D**, revealing the metal analysis data.

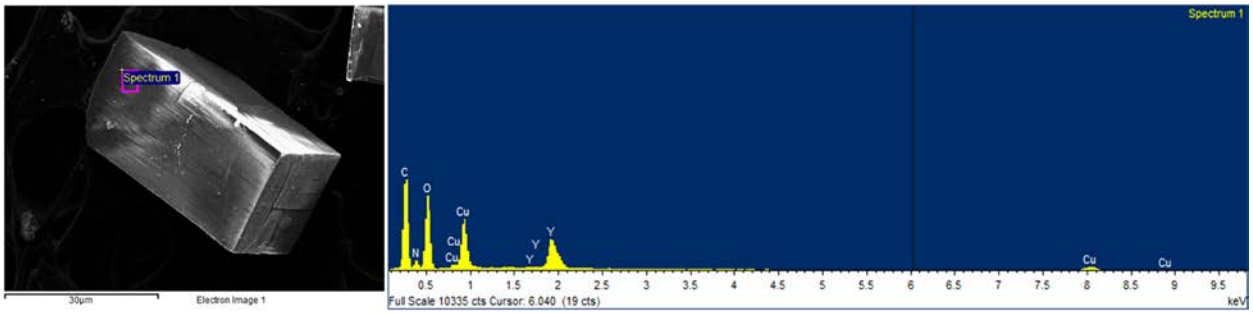


**Fig. S5:** EDX spectra of the crystals of compound **2L**, revealing the metal analysis data.