Electronic Supplementary Information

Unprecedented 3-D SHG MOF Material of Silver (I) Induced by Chiral Triple helices

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General Information

Commercially available reagents were used as received without further purification. Elemental analyses (C, H, N) were performed with a vario MICRO elemental analyzer. Thermal gravimetric analysis was performed under N_2 on a STA449C-QMS403C instrument. The measurements of SHG were carried out on the sieved powder samples by using the Kurtz and Perry method with a 2.05 μm Q-switch laser. The SHG intensity has been shown to depend strongly on particle size, thus the sample of Ag-AMIDN was grounded and sieved into several distinct particle size ranges (25-45, 45-53, 53-75, 75-105, 105-150, 150-210 and 210-300μm).

Experimental Section

Synthesis of 1: A mixture of $AgNO_3$, HAMIDN and H_2O was sealed into a glassed plate and heated at 90°C for 3 days and then cooled to room temperature for 1 day. Colorless prism crystals were obtained in 55% yield (based on $AgNO_3$). Anal. Calcd for $C_5H_2AgN_5$: C, 25.03; H, 0.84; N, 29.18; Found: C,25.37; H,0.89; N 29.76.

Crystallographic Analyses

The intensity data were collected on a Saturn 724 CCD diffractometer for 1, with graphite-monochromated $Mo_{K\alpha}$ radiation (λ = 0.71073 Å) at room temperature. The structure was solved by direct methods and refined by full-matrix least squares on F^2 with the SHELXTL-97 program. CCDC-880870 contain the supplementary crystallographic data for this paper, these data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

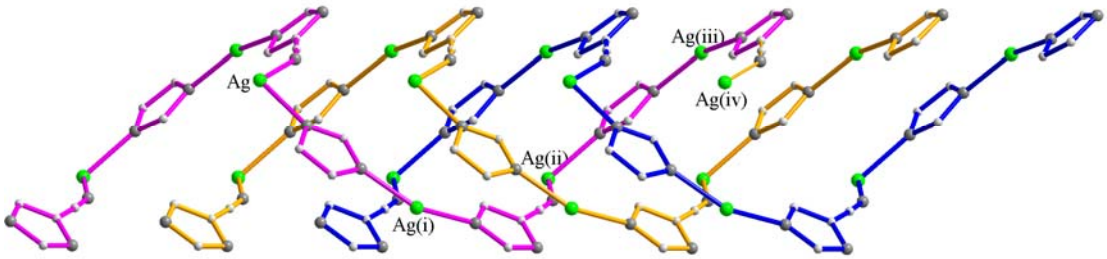

Fig. S1 Triple right-handed (T-R) helices showing symmetry operations from Ag (x, y, z), Ag(i) (-0.5+x, 2.5-y, 1+z), Ag(ii) (1-x, 2-y, 1.5 +z), Ag(iii) (1.5-x, -0.5+y, 2.5+z) to Ag(iv)(x, y, 3+z).

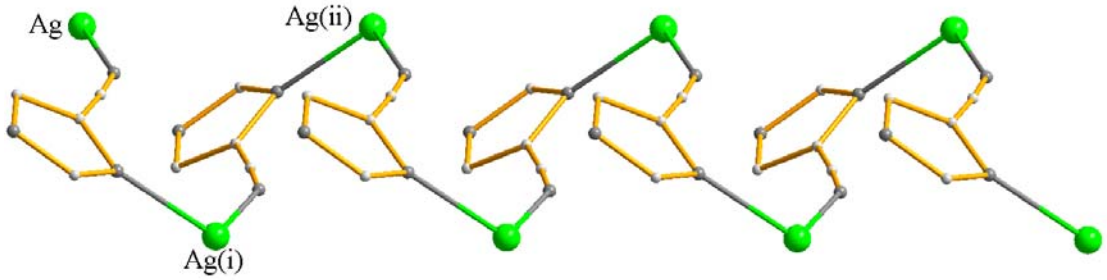

Fig. S2 Single right-handed (S-R) helix. **Ag, x, y, z; Ag(i), 2-x, 2-y, 0.5+z; Ag(ii), x, y, 1+z.**

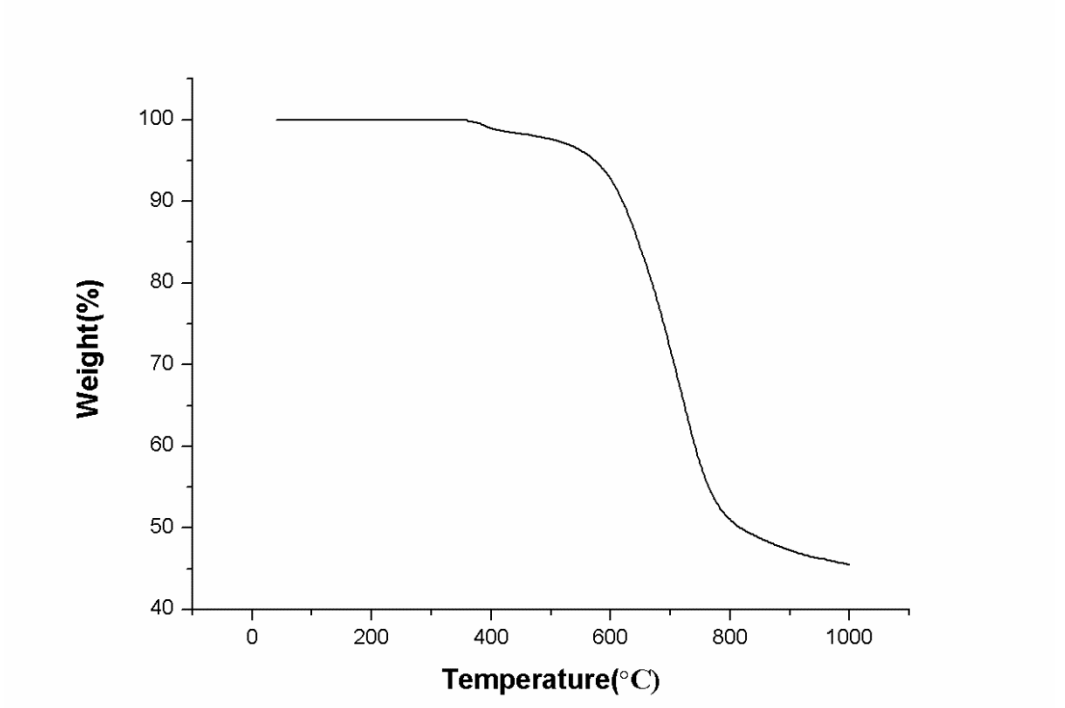

Fig. S3. TGA for Ag-Amidn (**1**)