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Supporting Information

Syntheses, Structures and Photocatalytic Properties of Five New Praseodymium–Antimony Oxochlorides: From Discrete Cluster to 3D Inorganic–Organic Hybrid Racemic Compound

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Fig. S1 The two possible structural types with equal probability in 2 shown schematically.



Fig. S2 (a) The zigzag-like chain in **2**; (b) the 1D nanotubular structure along the *a*-axis in **2**. All of the Sb, O, and Cl atoms (except for O atoms from the COO⁻ groups and the central Cl atoms) in the clusters are omitted for clarity.



Fig. S3 TGA-MS curves: (a) for compound 3 and (b) for compound 4.

As shown in Fig. S3a, TGA-MS analysis shows two obvious peaks at around 463 K and 573 K, respectively, which respectively respresent the neutral and protonated 3-Mepy escaping from compound **3**. Moreover, the relative intensities of both peaks are similar, revealing that the ratio of neutral and protonated 3-Mepy is 1:1.

As shown in Fig. S3b, different from that of compound **3**, TGA-MS analysis of the crystals of **4** shows that only the single molecular ion peaks of 3-Mepy was detected; and it was removed at about 450 K, which is close to the first peak at around 463 K on the TGA-MS curve of compound **3**. Therefore, we presume all three 3-Mepy in compound **4** are neutral.



Fig. S4 The connecting modes of the six crystallographically independent H_3 bpdc ligands in compound 5 (including five Hpdc²⁻ and one pdc³⁻ ligands). Color codes: N atoms (blue), H atoms (green). All of the Sb, O, Cl and H atoms (except for O atoms from the COO⁻ groups, the central Cl atoms and the H atoms bonded to N atoms) in the clusters are omitted for clarity.



Fig. S5 Prospective view of the two-fold interpenetrating anionic network of 5 along the *c*-axis, with the $[Fe(1,10-phen)_3]^{2+}$ complexes labeled.



Fig. S6 χ_{m}^{-1} vs *T* plots for compounds **1** and **5**, respectively. The solid red line for compound **1** and blue line for compound **5** indicate fit to the Curie–Weiss law (for χ_{m}^{-1}).



Fig. S8 PXRD patterns of compound 2.



Fig. S9 PXRD patterns of compound 3.



Fig. S10 PXRD patterns of compound 4.



Fig. S11 PXRD patterns of compound 5.



Fig. S12 TGA curve of compound 1.



Fig. S13 TGA curve of compound 2.



Fig. S14 TGA curve of compound 5.