

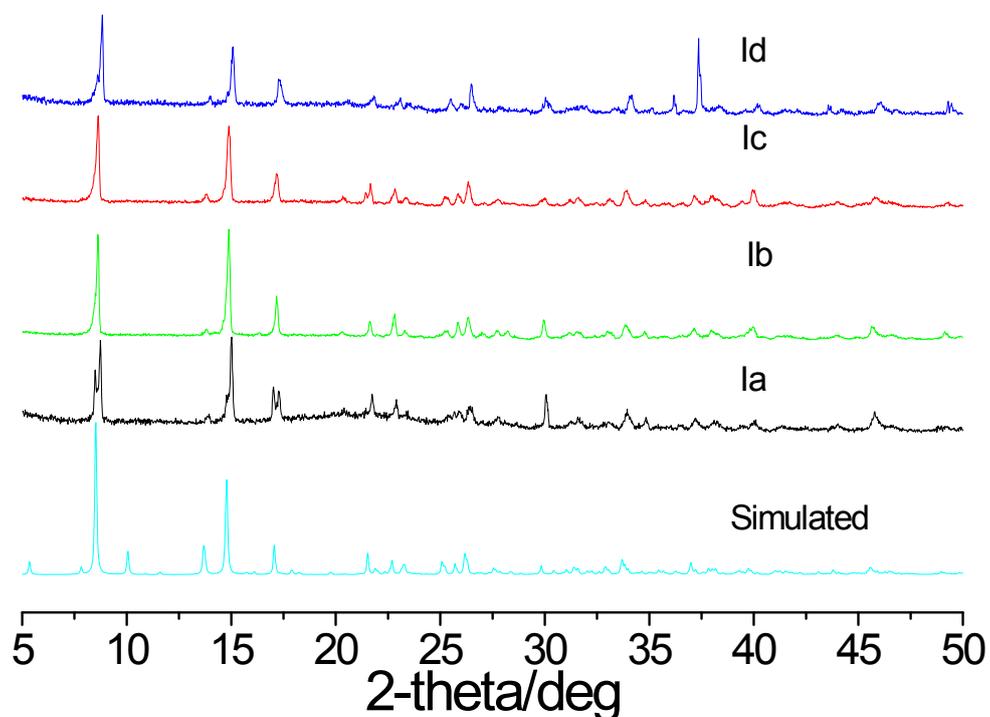
Supporting Information for

The first examples of 1-D organic hybrid lanthanoid thioarsenates based on two [As^VS₄]³⁻ linkage modes

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Computational descriptions

The band structures and density of states (DOS) of **Ia** were theoretically calculated by using the computer code CASTEP. The total energy is calculated with the density functional theory (DFT) using the Perdew–Burke–Ernzerhof generalized gradient approximation (GGA). The following orbital electrons are treated as valence electrons: H 1s¹, N 2s²2p³, C 2s²2p², S 3s²3p⁴, As 4s²3d³, and Ce 5s²5p⁶4f¹5d¹s². The number of plane waves included in the basis is determined by a cutoff energy of 330 eV (**Ia**), and the numerical integration of the Brillouin zone is performed using a Monkhorst-Pack k point sampling: 1×1×1 for **Ia**. The Fermi level ($E_f = 0$ eV) was selected as the reference of the energy.



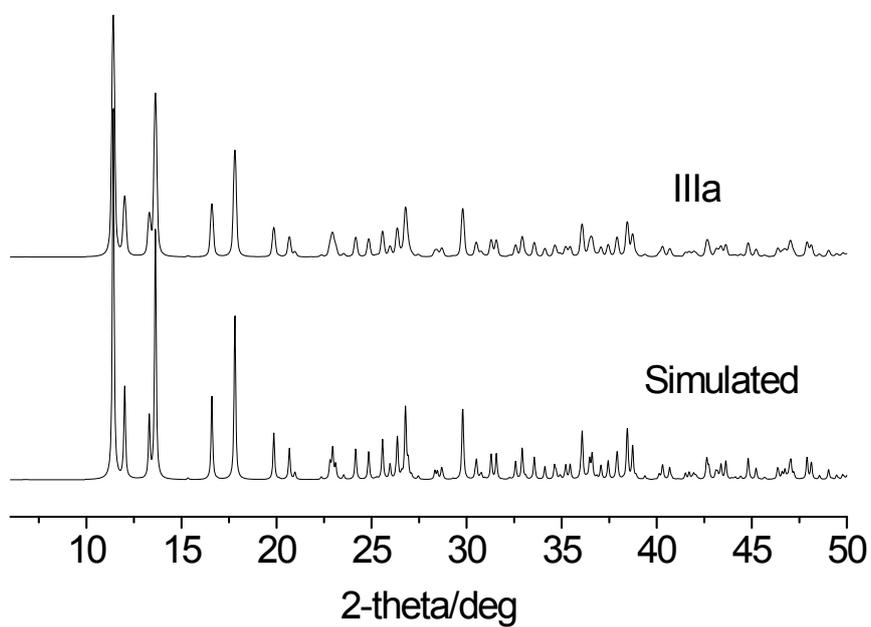
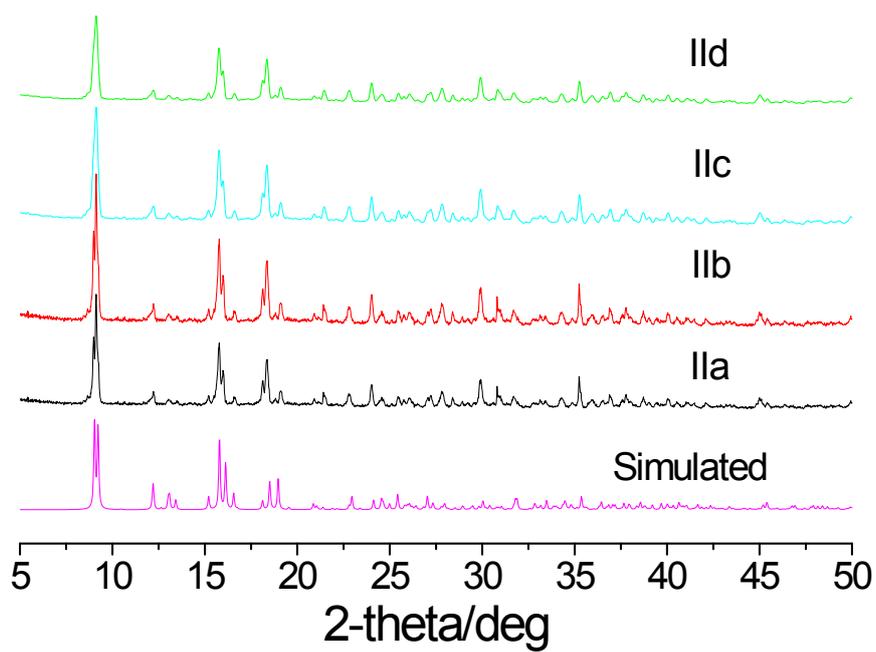


Figure S1 Simulated and experimental powder XRD patterns of all compounds.

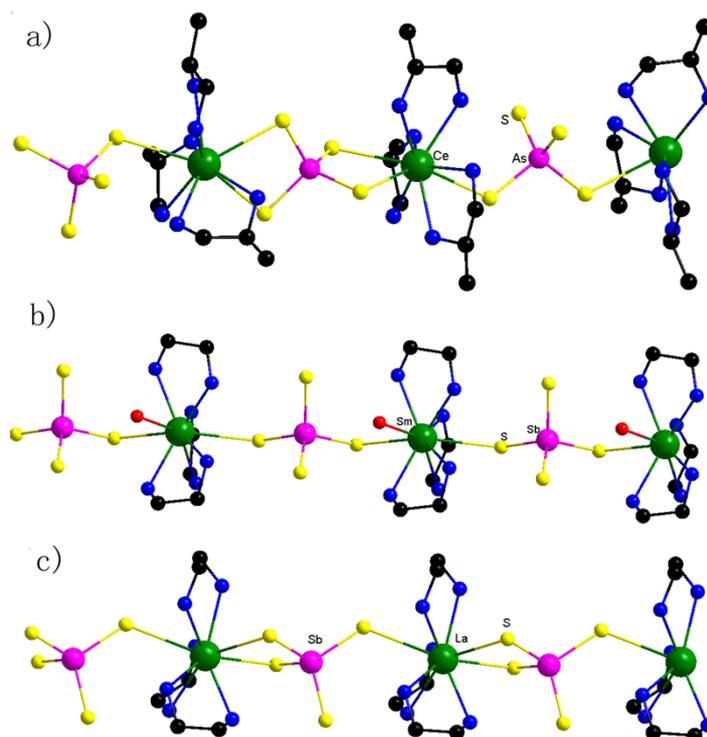


Figure S2 the tetradentate $[MS_4]$ linkage modes (H atoms bonded to C and N atoms have been omitted for clarity).

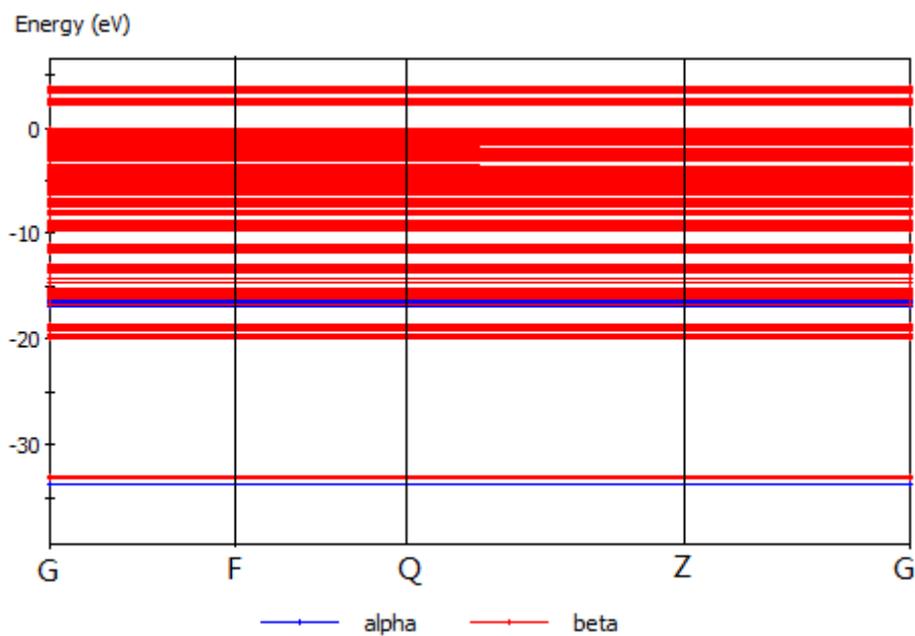


Figure S3 The calculated band structure of **Ia**.

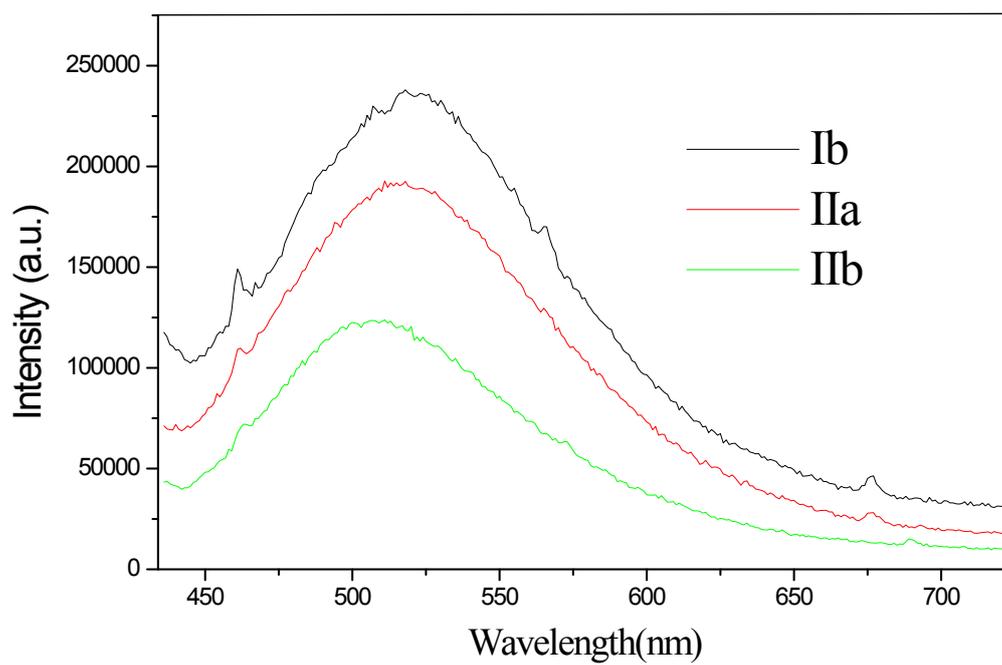


Fig. S4 Emission spectra of **Ib**, **IIa** and **IIb**.

Compounds **Ib**, **IIa** and **IIb** display the strong and broad emission band at about 490 nm upon photo-excitation at 380 nm (Fig. S4), which are probably originated from the dap ligands.

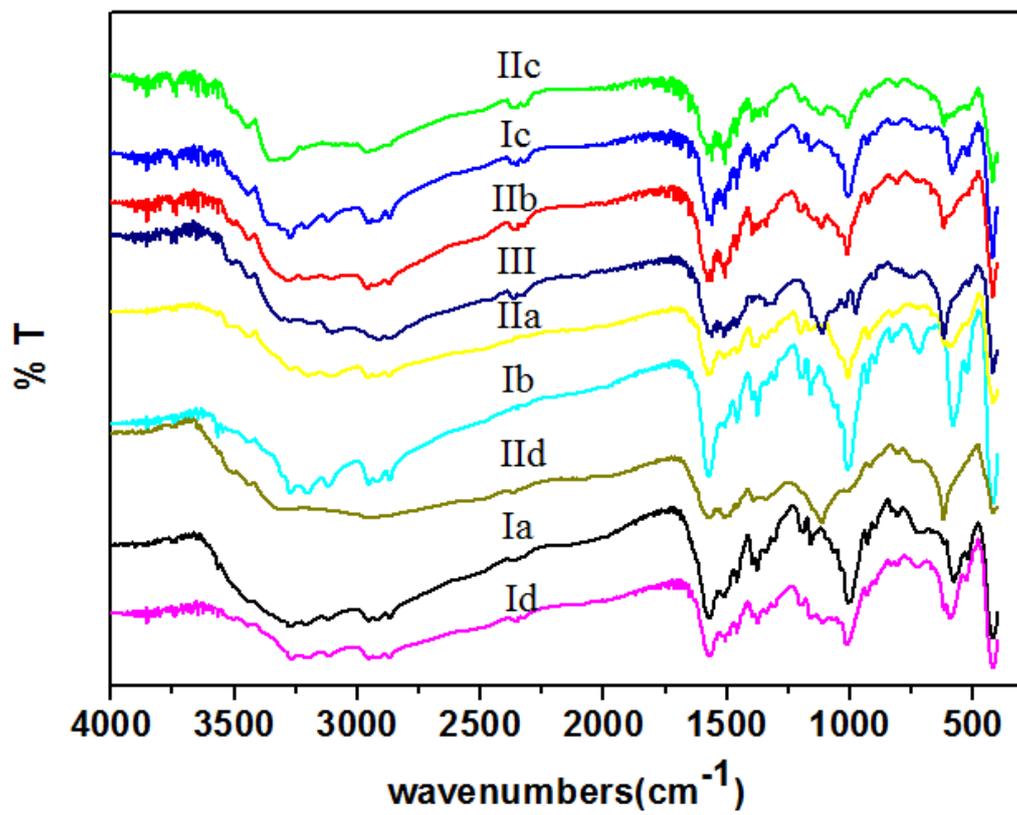


Fig. S5 IR spectra of all compounds.