

## Supporting Information for

### Syntheses, structures and properties of three new lanthanoid thioarsenates: the only example of thioarsenate acting as a ligand to a lanthanide complex

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Table S1. Hydrogen bonds for **1** [Å and deg].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N1-H1A...S3	0.90	2.96	3.821(6)	161.4
N1-H1B...S3#1	0.90	2.98	3.876(6)	172.3
N2-H2A...S3#2	0.90	2.89	3.751(5)	160.7
N2-H2B...S2#3	0.90	2.86	3.740(6)	166.1
N3-H3B...S4#2	0.90	2.73	3.590(5)	159.3
N4-H4A...S3#4	0.90	2.86	3.656(6)	148.8
N5-H5A...S4#2	0.90	2.52	3.334(5)	151.0
N5-H5B...S3#2	0.90	2.66	3.471(6)	150.1
N6-H6A...S3#1	0.90	2.74	3.479(5)	139.9
N6-H6B...S1#4	0.90	2.46	3.334(5)	164.8

Symmetry transformations used to generate equivalent atoms: (#1)  $-x+1, -y+1, -z$ ; (#2)  $x-1, y, z$ ; (#3)  $-x+1, y+1/2, -z+1/2$ ; (#4)  $-x+1, y-1/2, -z+1/2$ .

Table S2. Hydrogen bonds for **3** [Å and deg].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N1-H1A...S2#2	0.90	2.83	3.523(3)	134.5
N1-H1B...S3#1	0.90	2.59	3.457(3)	162.1
N2-H2C...S1#3	0.91	2.67	3.494(3)	151.9
N5-H5A...S1#2	0.90	2.55	3.448(3)	172.4
N3-H3C...S2#1	0.91	3.05	3.436(3)	107.2
N4-H4C...S1	0.91	2.83	3.343(3)	117.3

Symmetry transformations used to generate equivalent atoms: (#1)  $-x, -y+1, -z+1$ ; (#2)  $-x, y, -z+1/2$ ; (#3)  $x+1/2, -y+1/2, z+1/2$ .

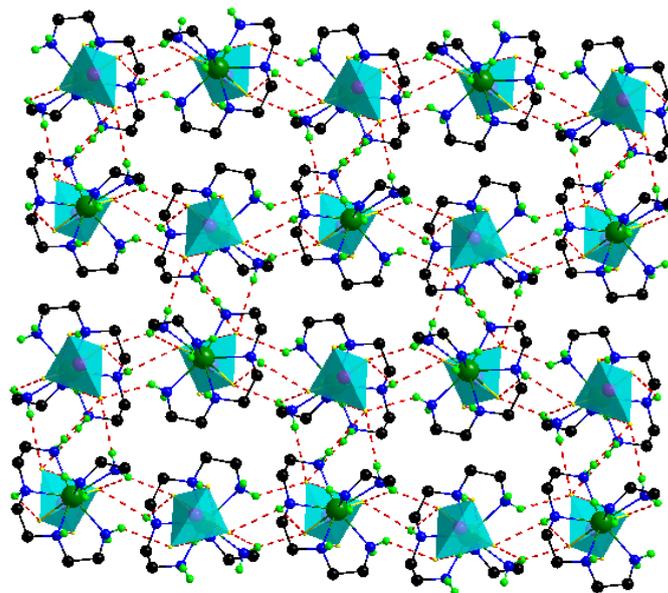


Figure S1 Crystal packing of **2**, showing the 3-D H-bonding network. Blue tetrahedra: [AsS<sub>4</sub>]. H atoms bonded to C atoms have been omitted for clarity.

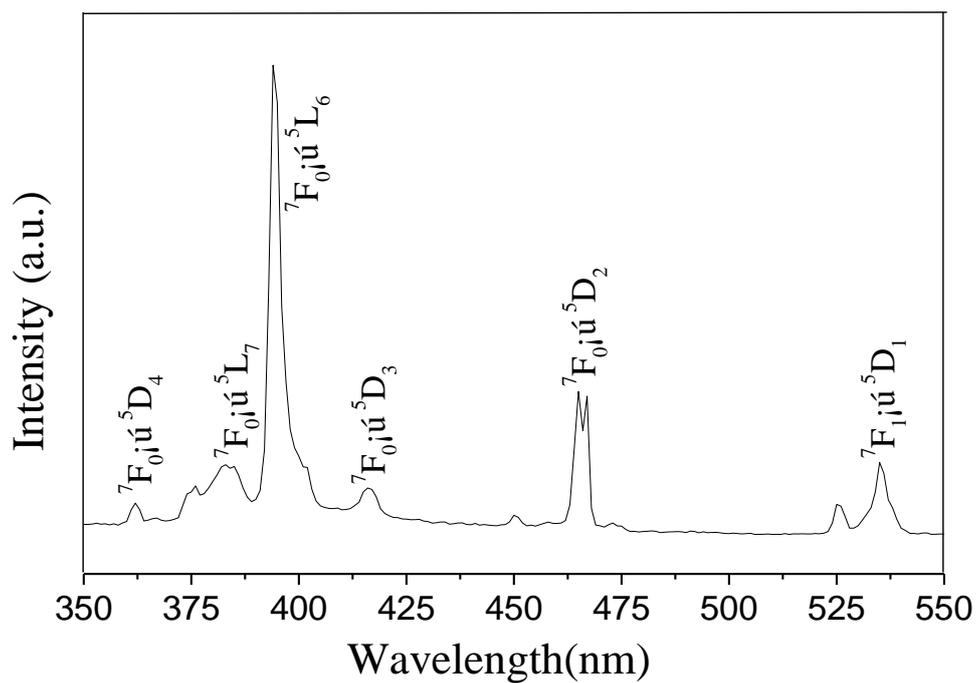


Fig. S2 Absorption spectrum of **1**.

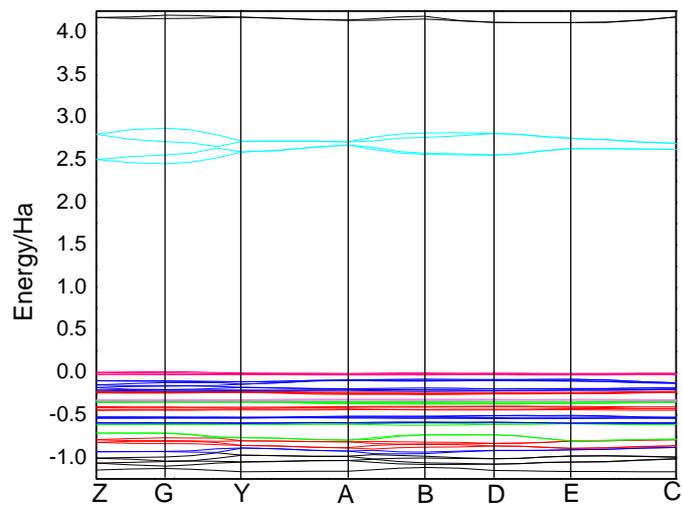


Figure S3 Band structure for **2**. The Fermi level is set at 0 eV.

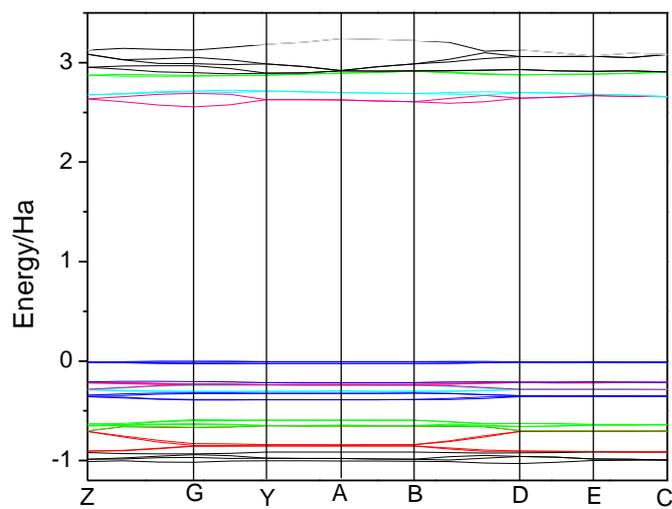


Figure S4 Band structure for **3**. The Fermi level is set at 0 eV.