Supporting Information for The first examples of thiogermanate anion [GeS₃(SH)]³⁻ as a bridging ligand to a lanthanide complex

Jian Zhou,* Rong Li, Xing Ling,* Rong Chen, Filong Hu and Yefan Zeng

Table S1 Some important bond lengths (Å) and angles (°) for 1 and 2.			
		1	
La1-N	2.712(3)-2.758(3)	La1-S	2.9955(10)- 3.0381(9)
Ge1-S	2.1701(10)-2.3214(10)		
N-La1-N	61.84(9)-145.46(10)	N-La1-S	69.44(6)-139.16(7)
S-La1-S	72.50(2)-143.83(2)	S-Ge1-S	103.59(4)-114.92(4)
		2	
Nd1-N	2.651(3)-2.690(3)	Nd1-S	2.9491(10)-3.0207(11)
Ge1-S	2.1687(10)-2.3227(11)		
N-Nd1-N	62.52(10)-144.34(11)	N-Nd1-S	69.02(7)-139.47(7)
S-Nd1-S	73.30(3)-143.19(3)	S-Ge1-S	103.95(5)-115.47(4)



Fig. S1. The solid state UV–vis absorption spectra of 1–2.



Fig. S2 Band structure for 1. The Fermi level is set at 0 eV



Fig. S3 Calculated electronic band structure and the HOMO and LUMO population of the $[Ln(\text{dien})_2(\mu_3-\eta^1,\eta^2-\text{GeS}_3(\text{SH}))]$ species.

Density functional theory calculations were performed by using Gaussian03 suite of programs. Single point energy calculations were carried out with B3LYP hybrid functional, 6-31G(d) basis set for C, N and H, and the Stuttgart–Dresden–Dunning (SDD) relativistic effective core potential (RECP) for S, Ge and La). The calculation gap from HOMO to LUMO is 2.20 eV which is very close to 2.11 eV obtained in the experiment, hence the calculation on the $[Ln(\text{dien})_2(\mu_3-\eta^1,\eta^2-\text{GeS}_3(\text{SH}))]$ species supports the fact that the transition of **1** is related to a result of charge transfer from the S²⁻-dominated valence band to the Ge⁴⁺ and La³⁺-dominated conduction band.



Fig. S4 IR spectra of 1 and 2.