Non-linear optical properties of magnetic fluorescent ytterbium(III) complexes

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Preparing materials with many functionalities have been investigated by the material scientist all over the worlds. We have reported several compounds exhibiting spin-crossover, non-linear optical properties within cyanido-bridged molecular assemblies.[1,2] Learning from these works, we have prepared two complexes $Yb^{III}(NCS)_3(TPPO)_3$ (**Yb-S**) and $Yb^{III}(NCSe)_3(TPPO)_3$ (**Yb-Se**) (Triphenylphosphine oxide = TPPO). They crystallize into *R*3 non-centrosymmetric space group due to the presence of bulkier TPPO organic ligand (**Figure 1a**). Each compound has two right-handed and left-handed phases giving rise to four different crystal structures.

We measured second harmonic generation (SHG) properties for the powdered sample. Both compounds have SHG signal as high as potassium diphosphate (KDP) originating due to the non-centrosymmetric nature of compounds (**Figure 1b**). Apart from non-linear optical behavior these complexes also exhibit a decrease of near-infrared emission intensity upon cooling in the temperature range of 350-85 K acting like a thermometer (**Figure 1c**). In the lower temperature range emission peak around 978 nm splits into five components revealing the constituents of the electronic ground state of Yb(III) ions. Upon substitution by **Se**, the absorption properties of the compound change significantly in the UV-region. Measurement of ac magnetic properties revealed weaker single-molecule magnet behavior originating from the anisotropic Yb(III) ion.

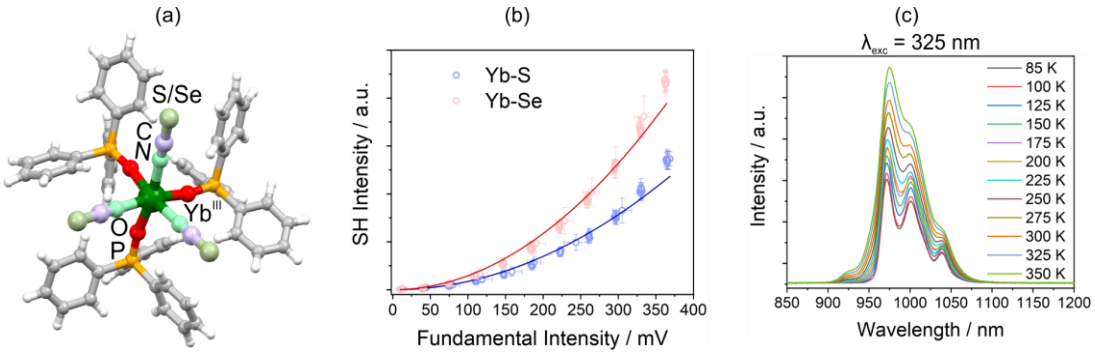

Figure 1. Representative crystal structure of **Yb-S** and **Yb-Se** (a), second-harmonic generation signal (b) and temperature dependent-near infrared properties of **Yb-S** (c).

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