

## Exploring Ln(III)-Ion-Based Luminescent Species as Down-Shifters for Photovoltaic Solar Cells

Gabriela Brito-Santos <sup>1</sup>, Cecilio Hernández-Rodríguez <sup>2,\*</sup>, Beatriz Gil-Hernández <sup>3</sup>,  
Joaquín Sanchiz <sup>3</sup>, Inocencio R. Martín <sup>2</sup>, Benjamín González-Díaz <sup>4</sup>  
and Ricardo Guerrero-Lemus <sup>2</sup>

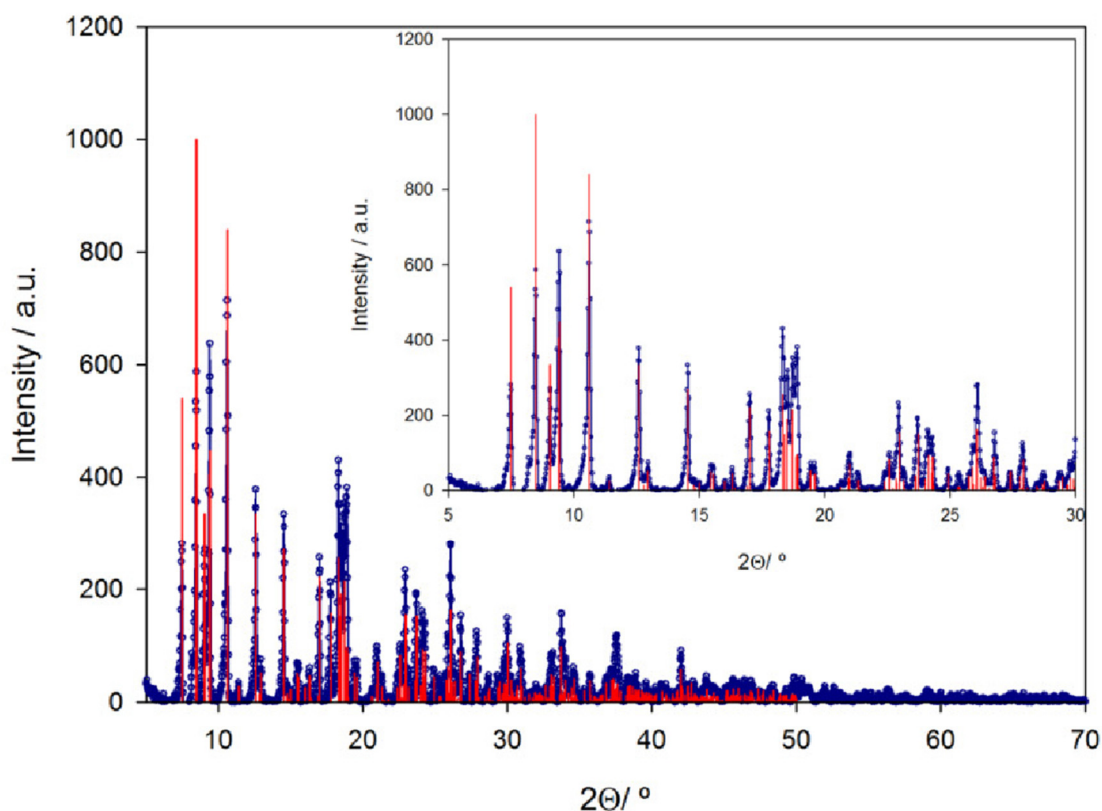
<sup>1</sup> Departamento de Química, Facultad de Ciencias, Universidad de La Laguna (ULL), Avenida Astrofísico Francisco Sánchez S/N, 38206 La Laguna, Tenerife, Spain; gbritosa@ull.edu.es

<sup>2</sup> Departamento de Física, Facultad de Ciencias, Instituto Universitario de Materiales y Nanotecnología, Universidad de La Laguna (ULL), Avenida Astrofísico Francisco Sánchez S/N, 38206 La Laguna, Tenerife, Spain; imartin@ull.edu.es (I.R.M.); rglemus@ull.edu.es (R.G.-L.)

<sup>3</sup> Departamento de Química, Facultad de Ciencias, Instituto Universitario de Materiales y Nanotecnología, Universidad de La Laguna (ULL), Avenida Astrofísico Francisco Sánchez S/N, 38206 La Laguna, Tenerife, Spain; beagher@ull.edu.es (B.G.-H.); jsanchiz@ull.edu.es (J.S.)

<sup>4</sup> Departamento de Ingeniería Industrial, Escuela Superior de Ingeniería y Tecnología, Universidad de La Laguna, Camino San Francisco de Paula S/N, 38206 La Laguna, Tenerife, Spain; bgdiaz@ull.edu.es

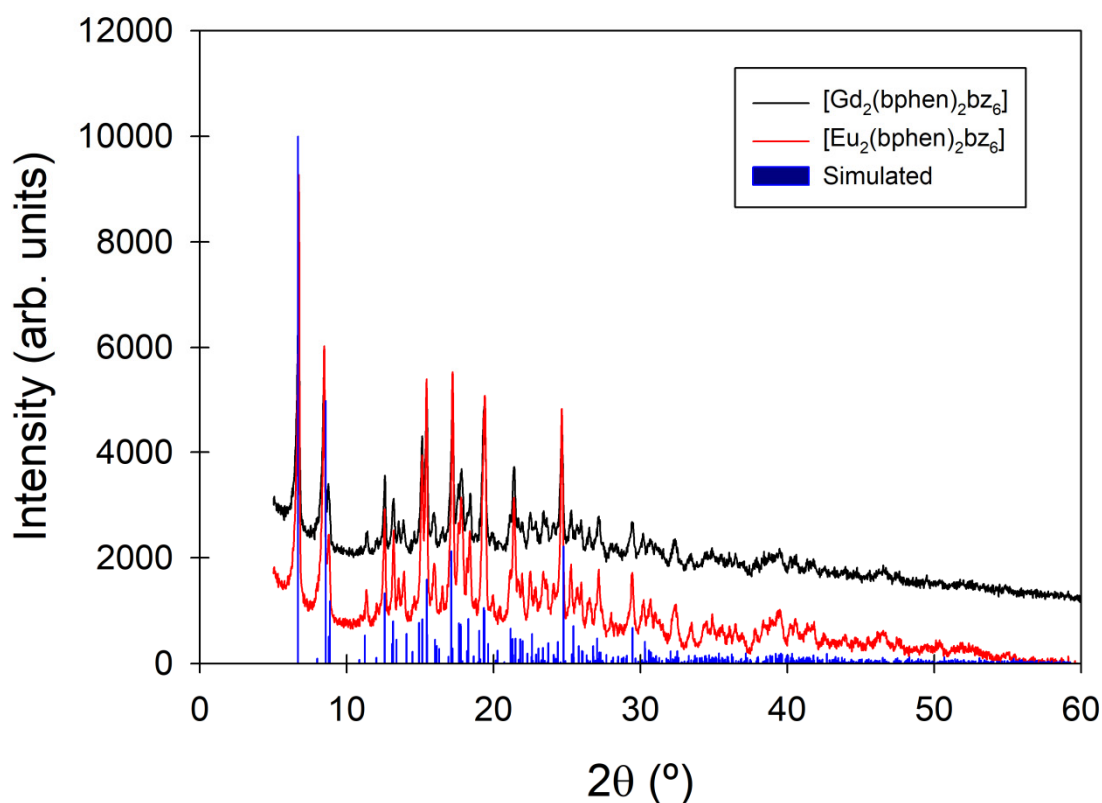
\* Correspondence: chdezr@ull.edu.es; Tel.: +34-922318243



**Figure S1.** Simulated (red bars) and experimental (blue dots) X-Ray powder diffraction patterns for  $[\text{Eu}_2(\text{phen})_2(\text{bz})_6]$ .

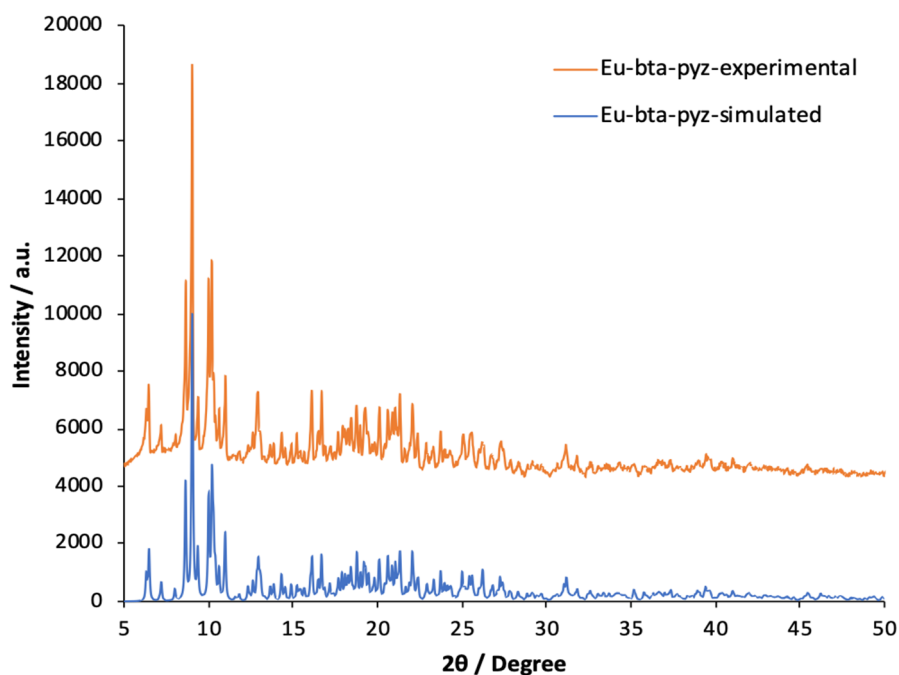
Niu, S. Y.; Yang, B.; Cao, J. Q.; Yang, G. D.; Bu, W. M., Synthesis, characterization and structure of tetrabenzoyloxy bridged binuclear Eu(III) complex. Kao Teng Hsueh Hsiao Hua Heush Hsueh Pao/ *Chemical Journal of Chinese Universities* **1997**; 18, 1917-1920.

Ooi, P. H.; Teoh, S. G.; Yeap, C. S.; Fun, H. K. Tetra- $\mu$ -benzoato- $\kappa$ 4O: O';  $\kappa$ 3O: O, O';  $\kappa$ 3O, O': O'-bis [(benzoato- $\kappa$ 2O, O')(1, 10-phenanthroline- $\kappa$ 2N, N') europium (III)] benzoic acid disolvate. *Acta Crystallographica Section E: Structure Reports Online* **2010**, 66(5), m597-m598. doi: 10.1107/S1600536810015229. CCDC: 1258413.



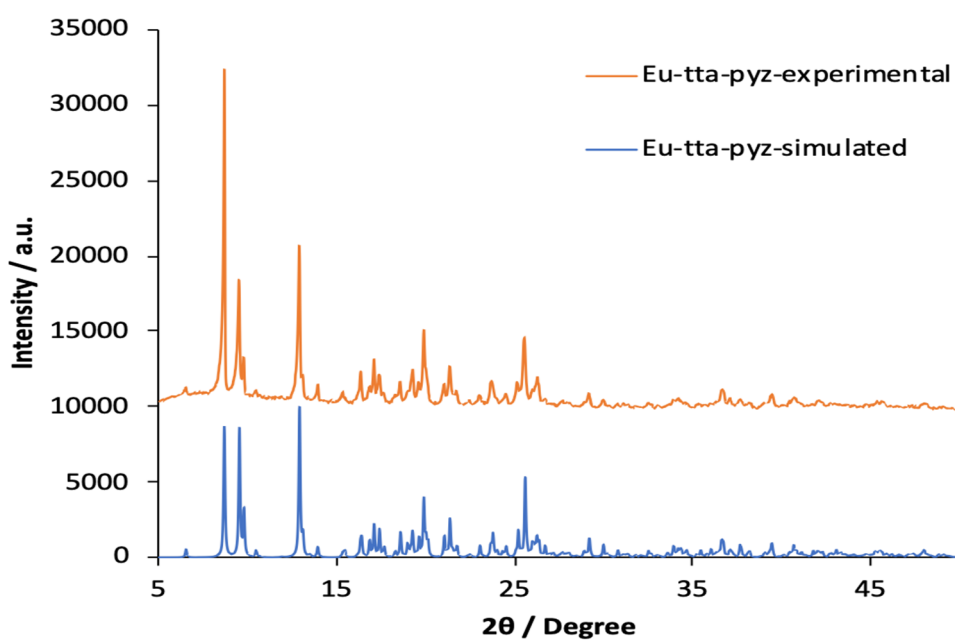
**Figure S2.** Experimental X-Ray powder diffraction patterns for compounds [Eu<sub>2</sub>(bphen)<sub>2</sub>(bz)<sub>6</sub>] (red) and [Gd<sub>2</sub>(bphen)<sub>2</sub>(bz)<sub>6</sub>] (black). There is an almost perfect overlap between both patterns which means both compounds display the same structure. The simulated spectrum from the single-crystal structure of [Eu<sub>2</sub>(bphen)<sub>2</sub>(bz)<sub>6</sub>] is also showed (blue).

[25] González-Pérez, S.; Sanchiz, J.; Rodríguez, V. D.; Cañadillas-Ramallo, D.; González-Platas, J.; Borchert, D.; González-Díaz, B.; Hernández-Rodríguez, C.; Guerrero-Lemus, R. Highly luminescent film as enhancer of photovoltaic devices. *J. Lumin.* **2018**, 201, 148–155. doi: 10.1016/j.jlumin.2018.04.038. CCDC: 1494543.



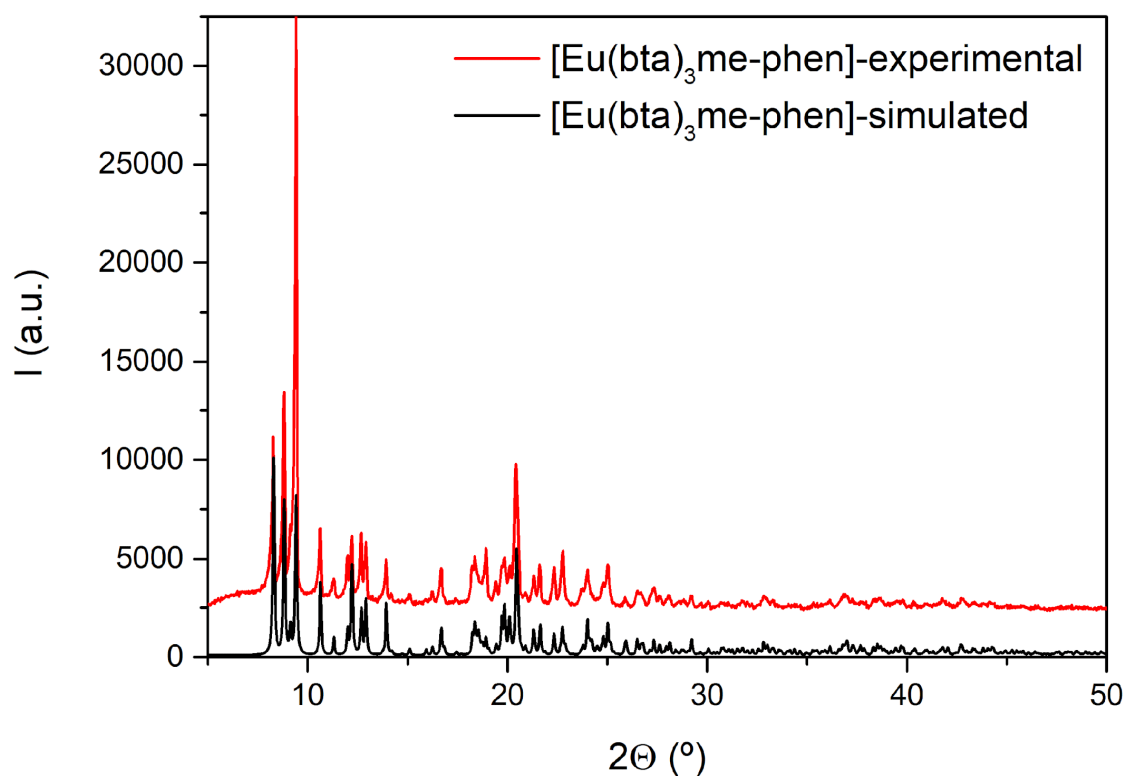
**Figure S3.** Simulated and experimental PXRD patterns (blue and orange lines, respectively for [Eu(bta)<sub>3</sub>pyz-phen] complex.

Zhang, C.; Ma, X.; Cen, P.; Yang, H.; He, Z.; Guo, Y.; Liu, X. Dual-sensitized Eu (III)/Tb (III) complexes exhibiting tunable luminescence emission and their application in cellular-imaging. *Dalton Transactions* **2022**, 51(8), 3180-3187. doi: 10.1039/D2DT00051B. CCDC: 2030986.



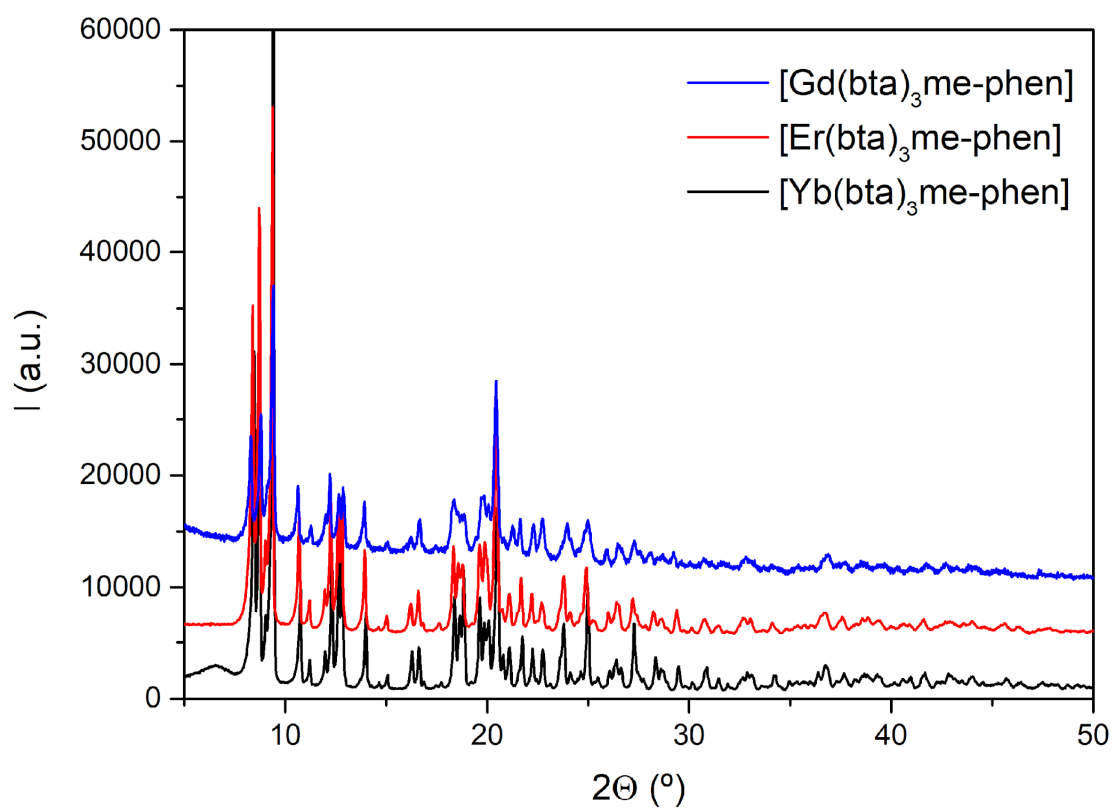
**Figure S4.** Simulated and experimental PXRD patterns (blue and orange lines, respectively for [Eu(tta)<sub>3</sub>pyz-phen] complex.

Cabral, F. M.; Gállico, D. A.; Mazali, I. O.; Sigoli, F. A. Crystal structure and temperature dependence of the photophysical properties of the [Eu (tta) 3 (pyphen)] complex. *Inorganic Chemistry Communications* **2018**, 98, 29-33. doi: 10.1016/j.inoche.2018.09.041. CCDC: 1839940.



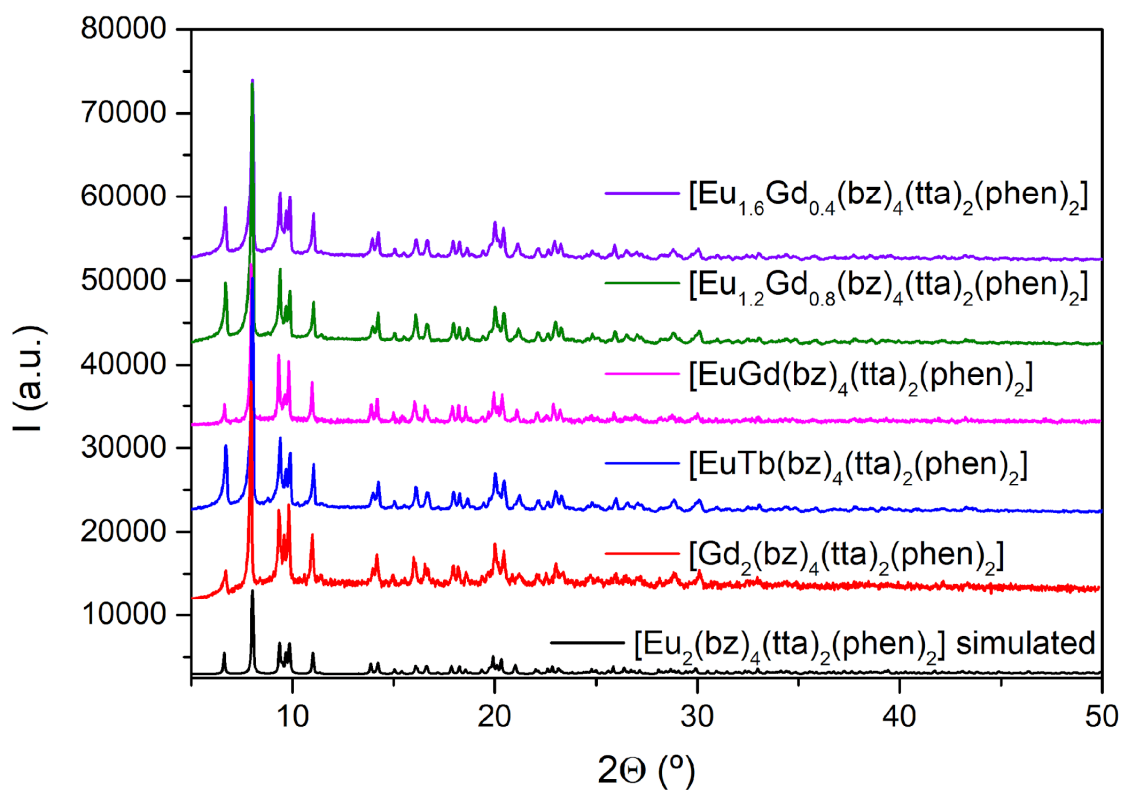
**Figure S5.** Simulated and experimental PXRD patterns (black and red lines, respectively for [Eu(bta)<sub>3</sub>me-phen] complex.

[30] Brito-Santos, G.; Gil-Hernández, B.; Hernández-Rodríguez, C.; González-Díaz, B.; Guerrero-Lemus, R.; Sanchiz, J. Degradation analysis of highly UV-resistant down-shifting layers for silicon-based PV module applications. *Mater. Sci. Eng. B.* **2023**, 288, 116207. doi: 10.1016/j.mseb.2022.116207. CCDC: 2169076.



**Figure S6.** Experimental PXRD patterns of [Yb(bta)<sub>3</sub>me-phen], [Er(bta)<sub>3</sub>me-phen] and [Gd(bta)<sub>3</sub>me-phen].

[30] Brito-Santos, G.; Gil-Hernández, B.; Hernández-Rodríguez, C.; González-Díaz, B.; Guerrero-Lemus, R.; Sanchiz, J. Degradation analysis of highly UV-resistant down-shifting layers for silicon-based PV module applications. *Mater. Sci. Eng. B.* **2023**, 288, 116207. doi: 10.1016/j.mseb.2022.116207. CCDC: 2169076.



**Figure S7.** Experimental PXRD patterns of  $[M_1M_2(bz)_4(tta)_2(phen)_2]$ .

[33] Brito-Santos, G.; Hernández-Rodríguez, C.; Gil-Hernández, B.; González-Díaz, B.; Martín, I. R.; Guerrero-Lemus, R.; Sanchiz, J. Highly luminescent mixed-ligand bimetallic lanthanoid (III) complexes for photovoltaic applications. *Dalton Trans.* **2022**, 51(8), 3146–3158. doi: 10.1039/d1dt04248c. CCDC: 2110403.