Electronic Supplementary Material (ESI) for Dalton Transactions.
This journal is © The Royal Society of Chemistry 2020

Supplementary material of :

Structure, Polymorphism and Luminescence of Cyanate Iodides MI(OCN) (M = Ba, Eu, Sr)

Amira Siai,[a*] Luzian Hämmerle,[a] David Enseling,[b] Markus Ströbele,[a] Thomas Jüstel,[b] and Hans-Jürgen Meyer[a]

[a] Section for Solid State and Theoretical Inorganic Chemistry, Institute of Inorganic Chemistry, University of Tübingen, Auf der Morgenstelle 18, 72076 Tübingen, Germany.

[b] Münster University of Applied Sciences, Department Chemical Engineering, Stegerwaldstrasse 39, 48565 Steinfurt, Germany.

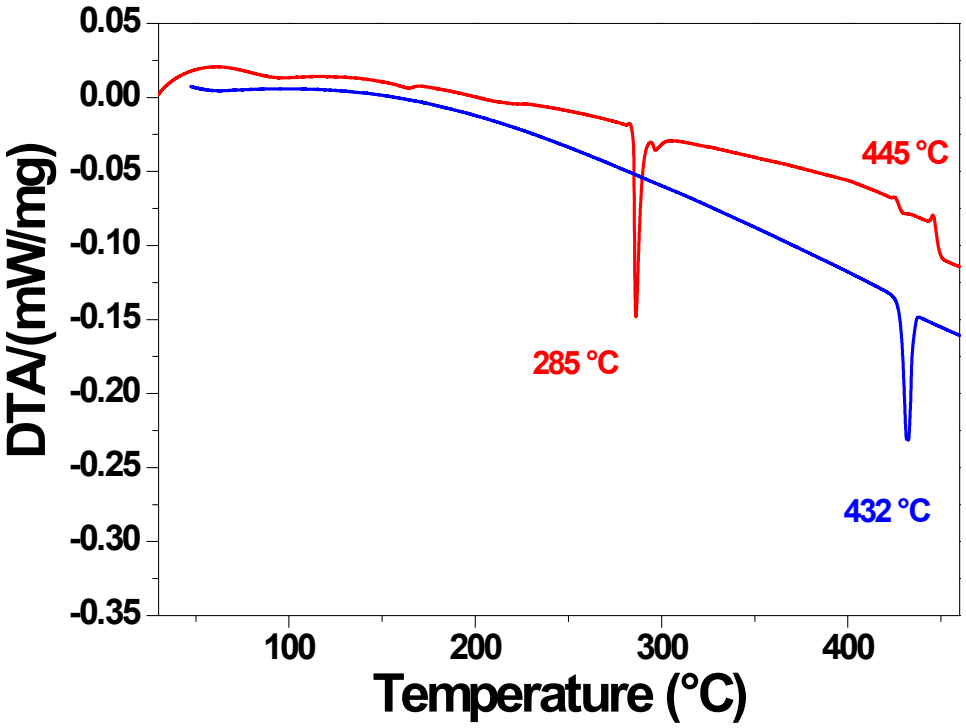

Figure S1. Differential thermal analysis (DTA) of the reaction SrI_2 and KOCN (1:1) in silica ampoule.

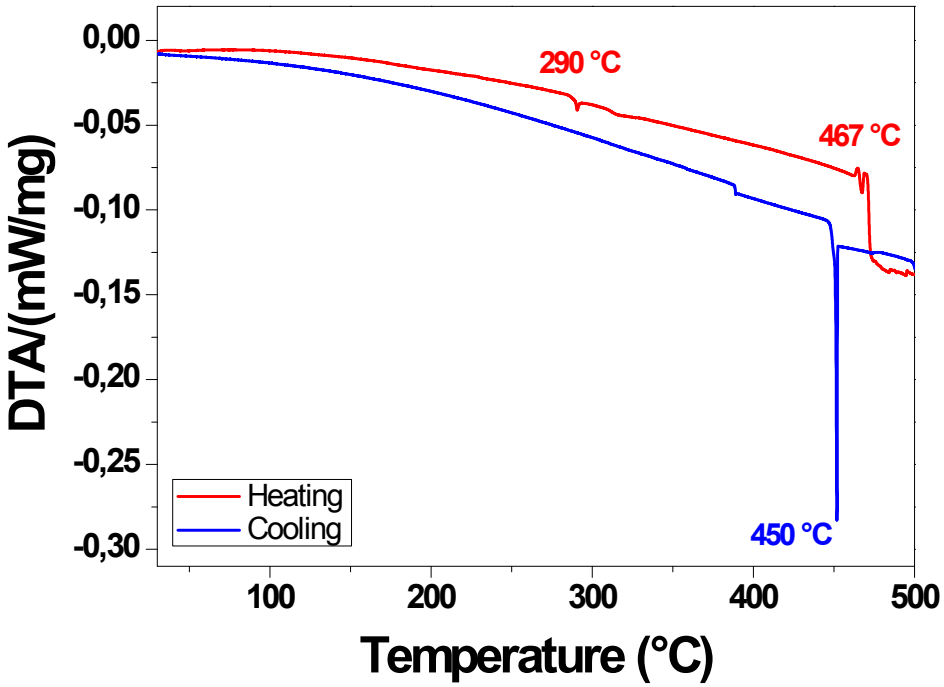

Figure S2. Differential thermal analysis (DTA) of the reaction BaI_2 and KOCN (1:1) in silica ampoule. Heating and cooling cycles are represented in red and blue respectively.

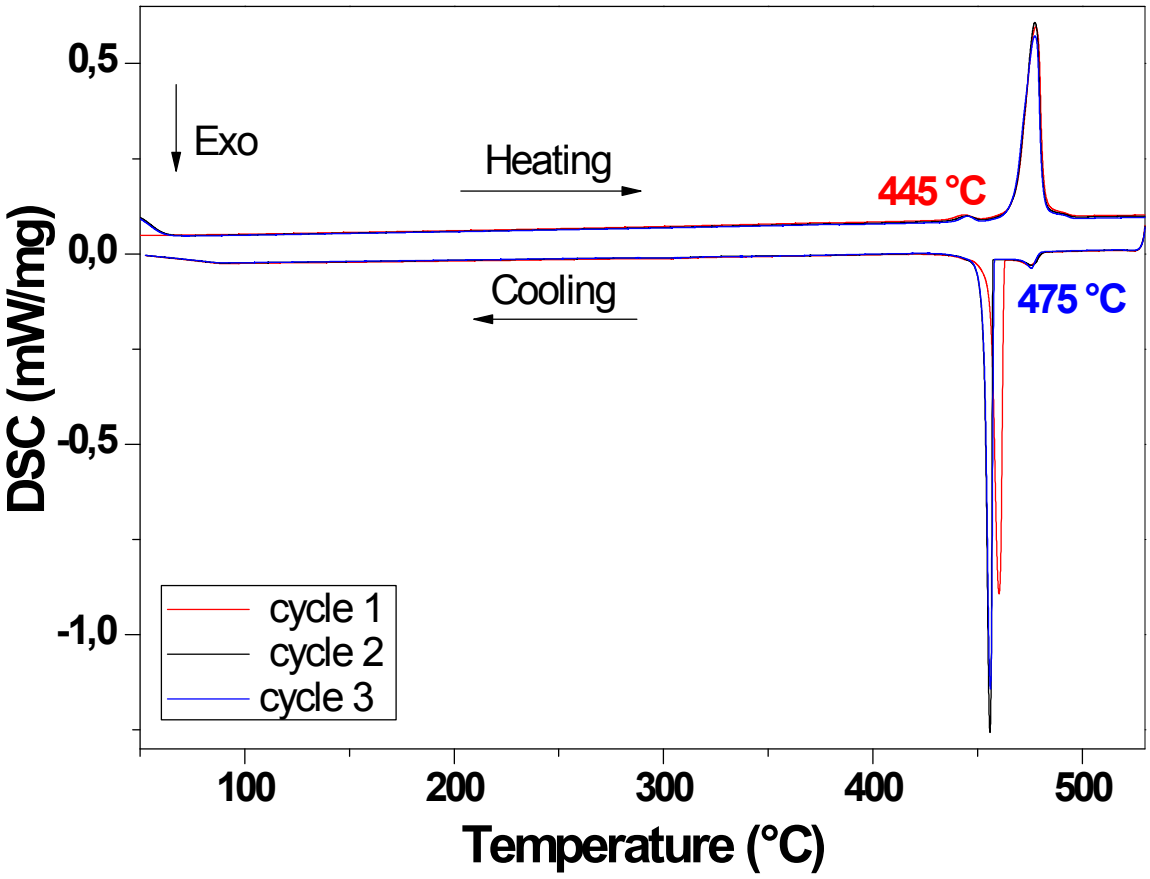

Figure S3. Differential scanning calorimetry (DSC) of α-BaI(OCN) phase.

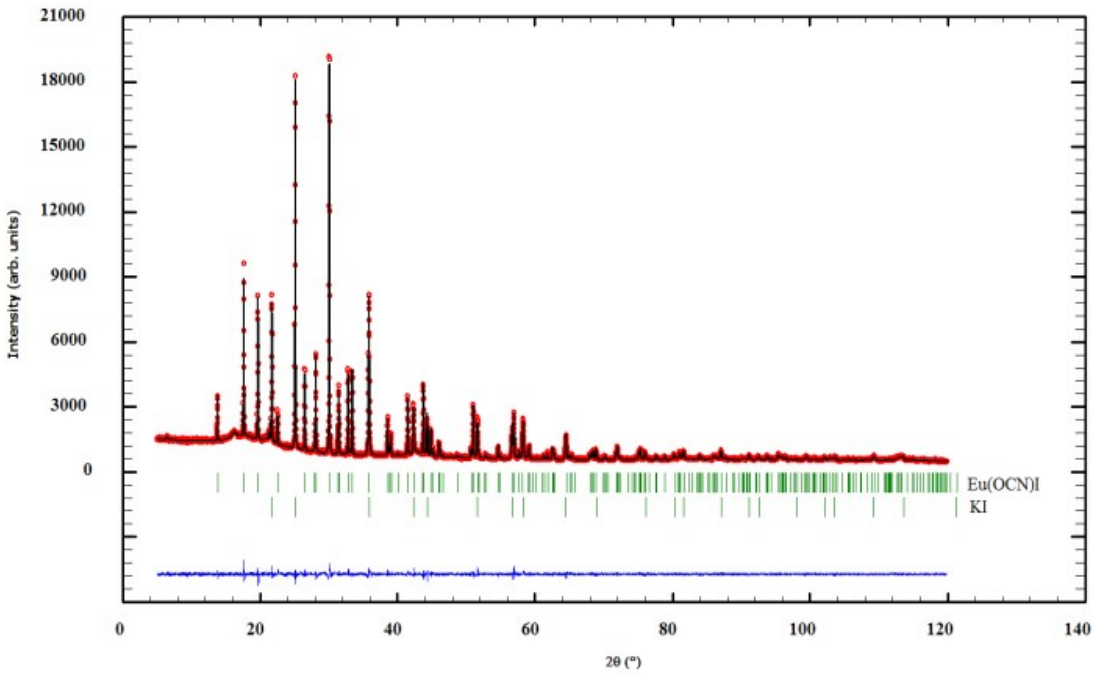

Figure S4. Crystal structure refinement plot of EuI(OCN) based on X-ray powder pattern data. Green ticks mark Bragg reflections relative to EuI(OCN) and KI phase. The difference curve (blue) highlights the difference between observed (red) and calculated pattern (black).

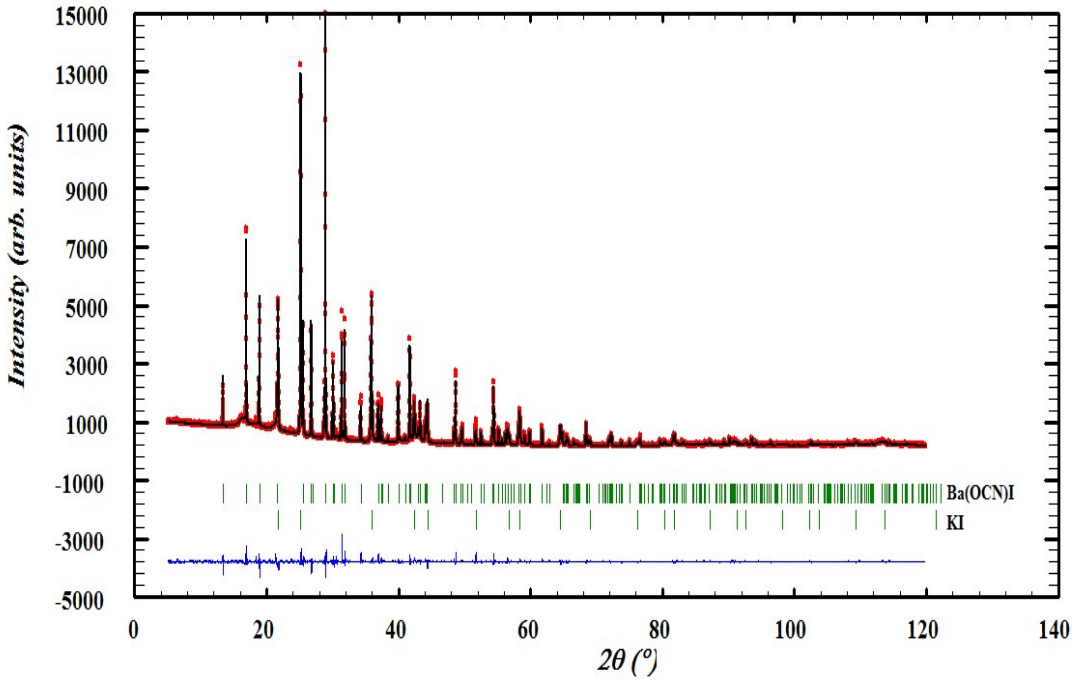

Figure S5. Crystal structure refinement plot of BaI(OCN) based on X-ray powder pattern data. Green ticks mark Bragg reflections relative to BaI(OCN) and KI phase. The difference curve (blue) highlights the difference between observed (red) and calculated pattern (black).

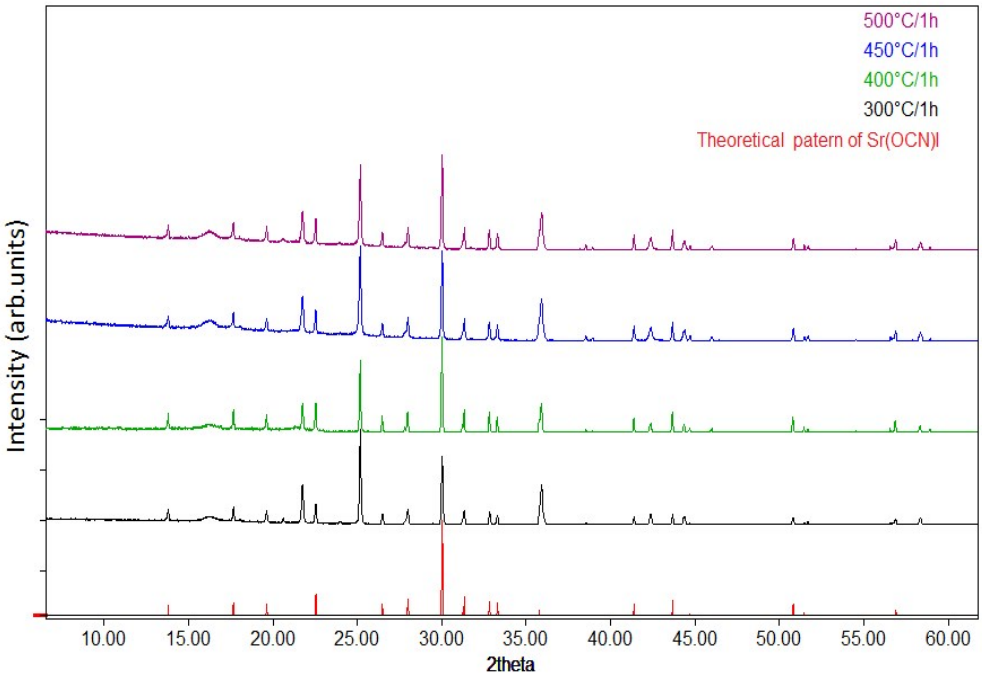

Figure S6. Powder X-ray patterns of the products obtained at different temperatures of solid-state reaction of SrI_2 with KOCN (1:1).

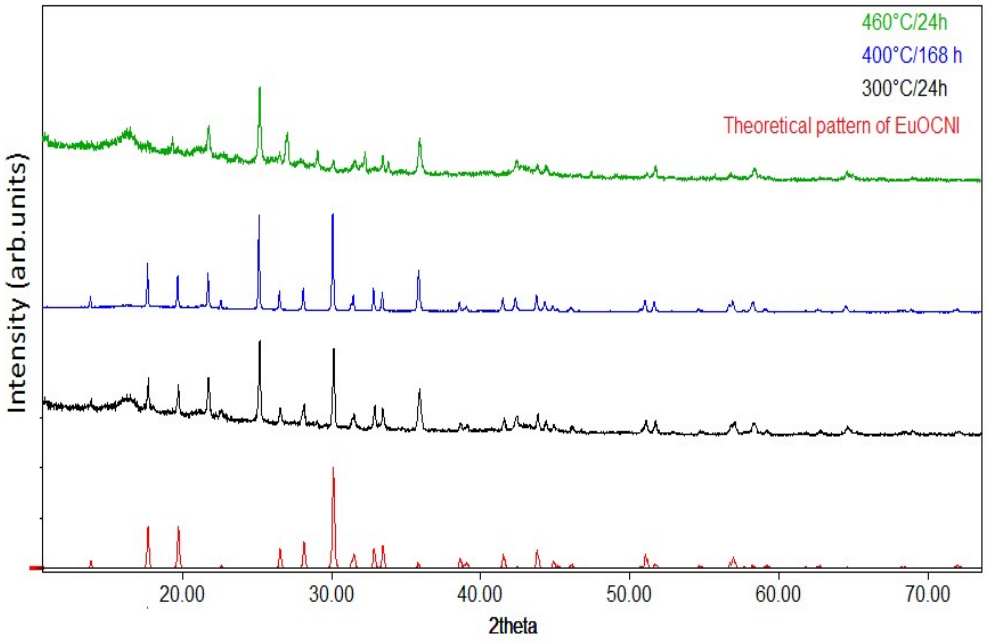

Figure S7. Powder X-ray patterns of the products obtained at different temperatures of solid-state reaction of EuI_2 with KOCN (1:1).

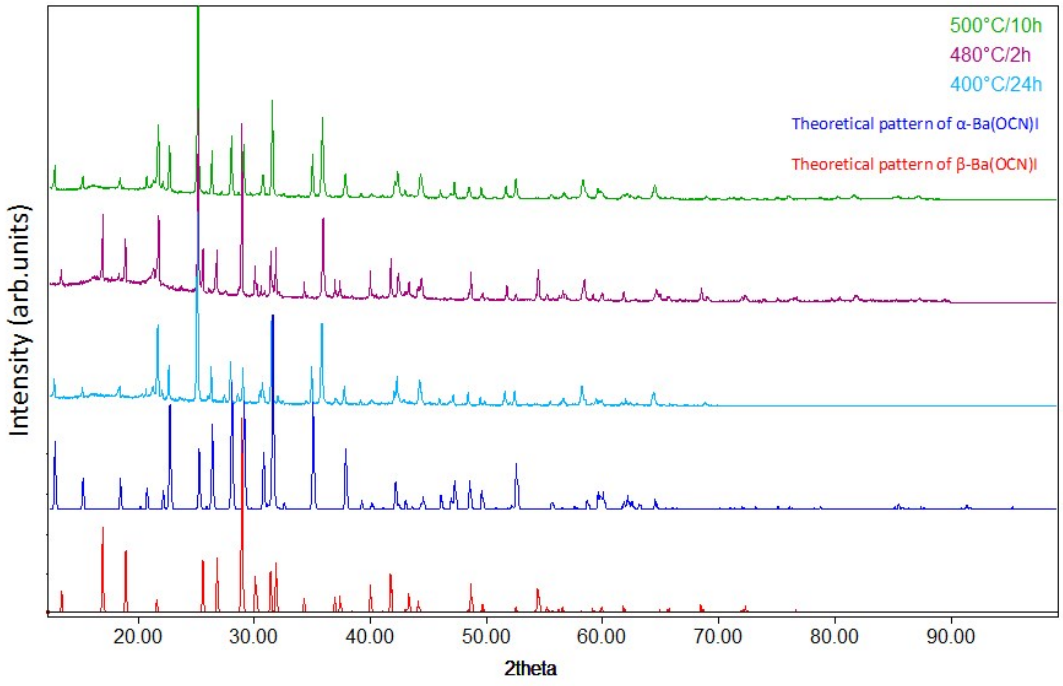

Figure S8. Powder X-ray patterns of the products obtained at different temperatures of solid-state reaction of BaI_2 with KOCN (1:1).

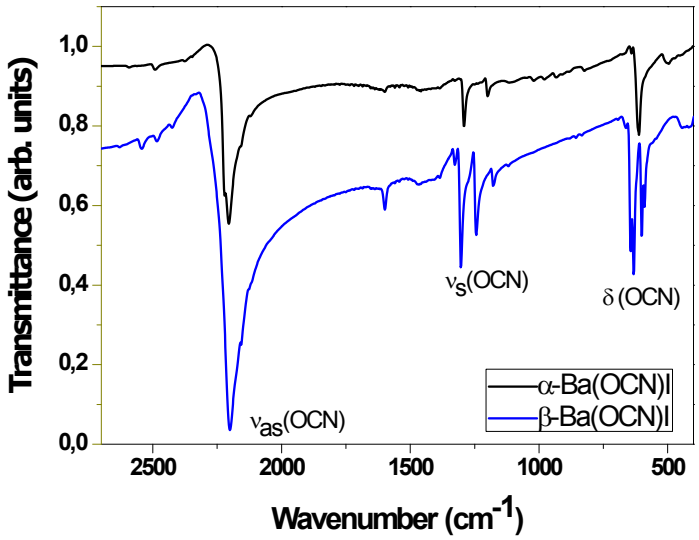

Figure S9. FTIR spectra of α-BaI(OCN) (SG: *Pnma*) and β-BaI(OCN) (SG: *Cmcm*) compounds.

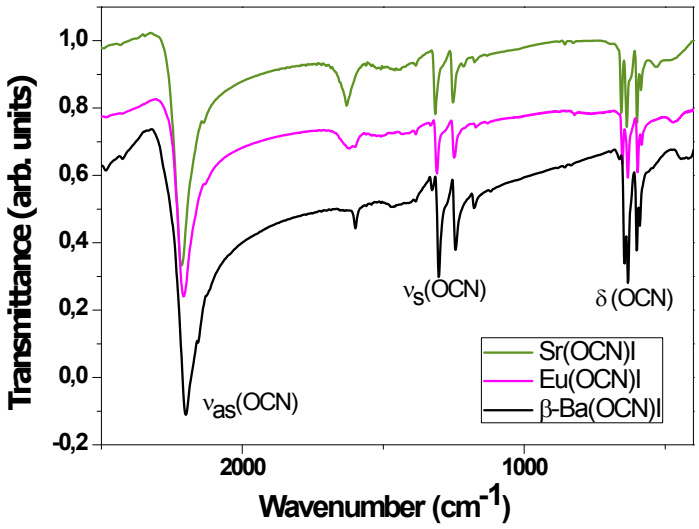

Figure S10. Fourier transform infrared spectrum of MI(OCN) compounds.

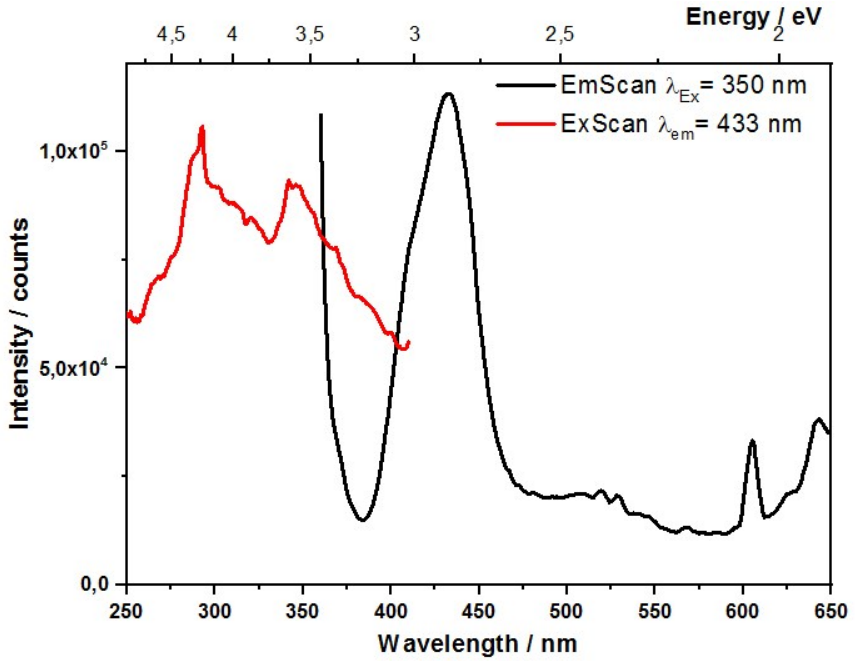

Figure S11. Excitation (red) and emission spectra (black) of Eu^{2+} (2%)-doped β-BaI(OCN) compound.

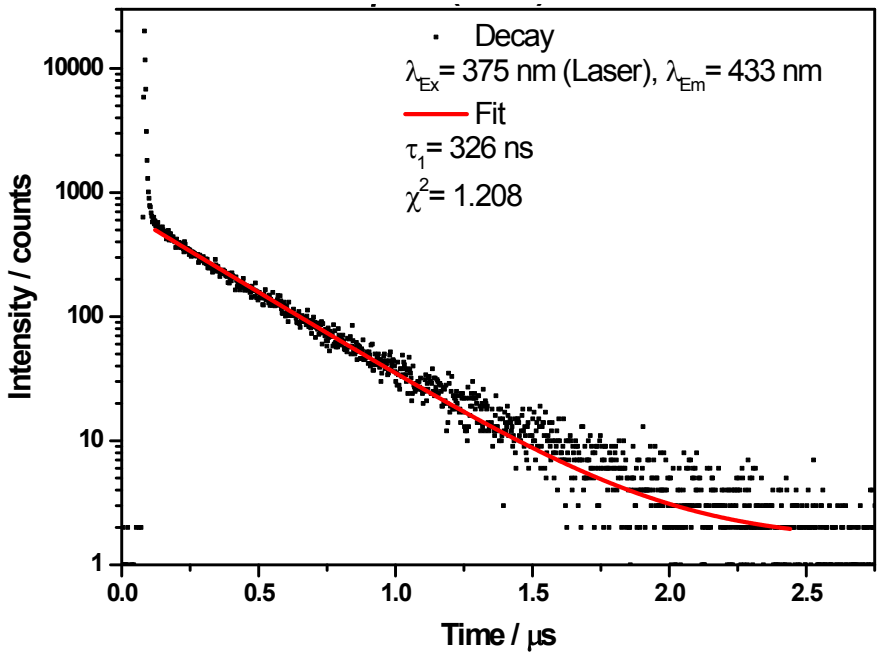

Figure S12. Decay curve of β-BaI(OCN): Eu^{2+}recorded for the europium blue transition at 431 nm.