Optical Materials 163 (2025) 116963

Contents lists available at ScienceDirect



# **Optical Materials**



journal homepage: www.elsevier.com/locate/optmat

# Research Article Deep dive into structural and optical study of stuffed-tridymite rare earth $(Sm^{3+}, Eu^{3+})$ doped CsZnPO<sub>4</sub>

Haqnawaz Rafiq, Mudasir Farooq, Mir Hashim Rasool <sup>\*</sup><sup>®</sup>, Aadil Bashir Wani, Younus Hameed <sup>®</sup>

Department of Physics, Islamic University of Science and Technology, Awantipora, Kashmir, 192122, India

#### ARTICLE INFO

## ABSTRACT

Keywords: Orthophosphate phosphors Rietveld refinement Stuffed-tridymite ABPO4 Rare-earth Dipole-quadruple mechanism Configurational coordinate model

This work used the most popular solid-state method to generate stuffed-tridymite CsZnPO4 doped with rare-earth ions (Eu<sup>3+</sup>, Sm<sup>3+</sup>). The XRD analysis performed at room temperature and Rietveld refinement using the FullProf suit package has revealed that the combination CsZnPO4 has crystallized into a monoclinic crystal structure with space group P121/a1. Crystallite size is determined using the Scherrer, modified Scherrer, and Williamson Hall procedures; a comparison study between the approaches was also conducted. In this work, the atomic positions (x, y, z) of Cs, Zn, P, and O in the unit cell, as well as the occupancy, have been estimated, and potential structural parameters such as a, b, c,  $\alpha,\beta,$  and  $\gamma$  have been calculated. A comparative FTIR analysis was carried out between orthorhombic CsMnPO<sub>4</sub> with space group Pn a 21 and monoclinic CsZnPO<sub>4</sub> with space group P121/a1. The band gap for the synthesized material CsZnPO4 was then determined using the P. Kubelka and Munk technique, and the estimated band gap energy for the compound was roughly 3.9 electron volts, which is very close to the actual band gap of the material. The PL spectra of CsZnPO4:xSm<sup>3+</sup> and CsZnPO4:xEu<sup>3+</sup> were recorded at the exact stimulation wavelengths of 401 nm and 396 nm, respectively. It is discovered that as the doping concentration rises, so does the emission intensity, and at a specific concentration of doping, it peaks, after which it begins to decline monotonically at greater concentrations. It is demonstrated that the concentration quenching process is caused by dipole-quadrupole interaction rather than the non-radiative cross-relaxation process in both the phosphor materials. The orange-red area (0.573, 0.423) and red region (0.624, 0.376) are where the chromaticity coordinates of the produced luminous material CsZnPO4:xSm<sup>3+</sup> and CsZnPO4:xEu<sup>3+</sup>, respectively, are located. As the temperature increased, the relative PL intensities decreased by a negligible amount, but their peak locations did not alter. The remarkable thermal stability of the produced material is demonstrated by the emission behavior at increasing temperatures, and to explain this behavior, the configurational coordinate model is employed. The phosphor  $CsZnPO_4$  doped with  $Eu^{3+}$  and  $Sm^{3+}$  shows excellent promise for usage as a redemitting and orange-red-emitting phosphor in a range of applications, including white LEDs and displays, based on the study conducted in the present work.

### 1. Introduction

All recognized XYPO<sub>4</sub> compounds with known structures can be grouped into three series according to the coordination number, size of X, and size of Y. Type one structure: the tetrahedral site (PO<sub>4</sub>) has a single cation. All compounds in this series have coordination numbers greater than four for both X and Y. When cations X and Y are roughly the same size but smaller and both are hexacoordinated, the structural type adopted is olivine. When X and Y are roughly the same size but bigger and have coordination number greater than 6, the structural type adopted is arcanite. Finally, when there is large size difference between X and Y but coordination number is till greater than 6, the structural type adopted is glaserite. Type two structure: beryllonite and stuffed tridymite are the two subtypes that make up this kind. The Y cations in the compounds that produce the type 2 structure have a relatively short ionic radius. The size of cation X determines which structure the compound adopts—the beryllonite or stuffed tridymite structure. The compound takes on the form of a stuffed tridymite when the cationic radius of X is reasonably large and the beryllonite structure when the ionic radius of X is small. Additionally, this structure type exhibits some

\* Corresponding author. *E-mail address:* hrasool23@gmail.com (M.H. Rasool).

https://doi.org/10.1016/j.optmat.2025.116963

Received 15 January 2025; Received in revised form 4 March 2025; Accepted 19 March 2025 Available online 20 March 2025

0925-3467/© 2025 Elsevier B.V. All rights are reserved, including those for text and data mining, AI training, and similar technologies.