Spectroscopic determination of site symmetry and space group in lanthanide-doped crystals: resolving intricate symmetry aspects for β-$NaLnF_4$.

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Rok wydania

2016

Czasopismo

Polyhedron

Numer woluminu

105

Strony

42-48

DOI

10.1016/j.poly.2015.11.044

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

There exists a controversy in the hitherto reported studies concerning the actual space group that accounts for spectroscopic results observed for the trivalent lanthanide (Ln3+) ions doped into b-NaLnF4 hosts. The two competing assignments of the space group: P6 or P63/m, bear on the associated point symmetry groups, which describe the local site symmetry of the dopant Ln ions. This paper aims at resolving this controversy. For this purpose two approaches are utilized. First, several new samples were synthesized and characterized by photoluminescence (PL) spectroscopy. Both the emission and excitation PL spectra have been measured. The analysis of the present experimental data indicates unequivocally that the dopant Ln3+ ions enter the crystal lattice b-NaGF4 and b-NaYF4 at two crystallographically distinct sites. Hence, the correct space group for these hosts is P6 and not P63/m. The intricacies arising from the sample preparation methods, which bear on the interpretation of the results, are also clarified. Second, the theoretical modeling of the crystal-field parameters (CFPs) is carried out based on superposition model to correlate the available crystallographic and spectroscopic data. The crystal-field analysis enables to ascribe unambiguously the spectroscopically determined sites to the crystallographic sites 1a and 1f. In this way an interpretation of photoluminescence spectra is achieved that fully corroborates the available crystallographic data. The influence of structural disorder occurring in b-NaLnF4 family of compounds on the 5D0?7F1 photoluminescence spectra of dopant Eu3+ ion and its role in interpretation of experimental data is also discussed.

Słowa kluczowe

lanthanides, photoluminescence, structure elucidation, symmetry

Adres publiczny

http://dx.doi.org/10.1016/j.poly.2015.11.044

Strona internetowa wydawcy

http://www.elsevier.com