

## Semiempirical and DFT computations of the influence of Tb(III) dopant on unit cell dimensions of cerium(III) fluoride.

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### Streszczenie

Several computational methods, both semiempirical and *ab initio*, were used to study the influence of the amount of dopant on crystal cell dimensions of  $\text{CeF}_3$  doped with  $\text{Tb}^{3+}$  ions ( $\text{CeF}_3:\text{Tb}^{3+}$ ). AM1, RM1, PM3, PM6, and PM7 semiempirical parameterization models were used, while the Sparkle model was used to represent the lanthanide cations in all cases. *Ab initio* calculations were performed by means of GGA+U/PBE projector augmented wave density functional theory. The computational results agree well with the experimental data. According to both computation and experiment, the crystal cell parameters undergo a linear decrease with increasing amount of the dopant. The computations performed using Sparkle/PM3 and DFT methods resulted in the best agreement with the experiment with the average deviation of about 1% in both cases. Typical Sparkle/PM3 computation on a  $2 \times 2 \times 2$  supercell of  $\text{CeF}_3:\text{Tb}^{3+}$  lasted about two orders of magnitude shorter than the DFT computation concerning a unit cell of this material.

### Słowa kluczowe

cerium fluoride, lanthanides, semiempirical, density functional theory, modelling, computations

### Adres publiczny

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### Strona internetowa wydawcy

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