

## Implications of invalid conversions between crystal-field parameters and zero-field splitting ones used in superposition model.

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The methodology used in recent study of the zero-field splitting parameters of  $\text{Cr}^{3+}$  ions at various orthorhombic symmetry sites in  $\text{LiKSO}_4$  by Pandey and Kripal is critically commented on. We argue that the crystal field parameters,  $B_{kq}$ , in the Wybourne notation, which were calculated using the superposition model for  $\text{Cr}^{3+}$  ions in  $\text{LiKSO}_4$ , may only be converted into the crystal field parameters in the Stevens notation. Regrettably, the authors have also converted the latter parameters supposedly into the zero-field splitting parameters  $D$  and  $E$  in the conventional notation. Such direct conversions are fundamentally incorrect and constitute factual invalid usage of the conversion relations between the crystal field (ligand field) parameters and the zero-field splitting ones. The cases of an implied usage of the invalid conversion relations between the crystal field parameters and the zero-field splitting parameters occurring in recent literature are also outlined. Pandey and Kripal have found the zero-field splitting parameters theoretically evaluated in this way to be in good agreement with the experimental values. However, the faulty methodology renders the conclusion that  $\text{Cr}^{3+}$  ions enter into the  $\text{LiKSO}_4$  lattice at the substitutional  $\text{K}^{+}$  sites unjustified. Several other conceptual problems arising from misinterpretations of the crucial notions identified therein are also discussed and clarified.

### Adres publiczny

<http://dx.doi.org/10.12693/APhysPolA.125.1215>

### Strona internetowa wydawcy

<http://www.ifpan.edu.pl>