Software package SIMPRE-Revisited.

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Streszczenie

This article elucidates the pitfalls identified in the software package SIMPRE recently developed by Baldoví et al. (J. Comput. Chem. 2013, 34, 1961) for modeling the spectroscopic and magnetic properties of single ion magnets as well as single-molecule magnets. Analysis of the methodology used therein reveals that the crystal field parameters (CFPs), expressed nominally in the Stevens formalism, exhibit features characteristic for the CFPs expressed in the Wybourne notation. The resemblance of the two types of CFPs introduces a serious confusion that may lead to wrong comparisons of the CFPs taken from various sources. To clarify this confusion, the properties of the CFPs (,) associated with the Stevens operators ($\boldsymbol{X = S}$, $\boldsymbol{J}$, or $\boldsymbol{L}$), which belong to the class of the tesseral-tensor operators, are contrasted with those of the CFPs B_{kq} associated with the Wybourne operators , which belong to the class of the spherical-tensor operators. Importantly, the confused properties of Stevens and Wybourne operators may bear on reliability of SIMPRE calculations. To consider this question independent calculations are carried out using the complete approach and compared with those of the restricted approach utilized earlier. It appears that the numerical results of the package SIMPRE are formally acceptable, however, the meaning of the CFPs must be properly reformulated. Several other conceptual problems arising from misinterpretations of the crucial notions and the CFP notations identified therein are also discussed and clarified.