Terminological confusions and problems at the interface between the crystal field Hamiltonians and the zero-field splitting Hamiltonians–Survey of the CF=ZFS confusion in recent literature.

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The single transition ions in various crystals or molecules as well as the exchange coupled systems (ECS) of transition ions, especially the single molecule magnets (SMM) or molecular nanomagnets (MNM), have been extensively studied in recent decades using electron magnetic resonance (EMR), optical spectroscopy, and magnetic measurements. Interpretation of magnetic and spectroscopic properties of transition ions is based on two physically distinct types of Hamiltonians: the *physical* crystal field (CF), or equivalently ligand field (LF), Hamiltonians and the effective spin Hamiltonians (SH), which include the zero-field splitting (ZFS) Hamiltonians. Survey of recent literature has revealed a number of terminological confusions and specific problems occurring at the interface between these Hamiltonians (denoted CF (LF)↔SH (ZFS)). Elucidation of sloppy or incorrect usage of crucial notions, especially those describing or parameterizing crystal fields and zero field splittings, is a very challenging task that requires several reviews. Here we focus on the prevailing confusion between the CF (LF) and SH (ZFS) quantities, denoted as the CF=ZFS confusion, which consists in referring to the parameters (or Hamiltonians), which are the true ZFS (or SH) quantities, as *purportedly* the CF (LF) quantities. The inverse ZFS=CF confusion, which pertains to the cases of labeling the true CF (LF) quantities as *purportedly* the ZFS quantities, is considered in a follow-up paper. The two reviews prepare grounds for a systematization of nomenclature aimed at bringing order to the zoo of different Hamiltonians. Specific cases of the CF=ZFS confusion identified in the recent textbooks, review articles, and SMM (MNM)- and EMR-related papers are surveyed and the pertinent misconceptions are outlined. The consequences of the terminological confusions go far beyond simple semantic issues or misleading keyword classifications of papers in journals and scientific databases. Serious consequences include misinterpretation of data from a wide range of experimental techniques and, most recently, have lead to pitfalls and errors of substance bearing on understanding of physical properties. Clarification of the incorrect terminology may prevent further proliferation of the problems and confusions, and thus bringing about better understanding of the physical principles involved.

Słowa kluczowe

Electron magnetic resonance (EMR), Magnetism, Crystal (Ligand) field (CF/LF) Hamiltonian Zero-field splitting (ZFS), Transition ions in crystals, Single molecule magnets (SMM)

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