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Disentangling intricate web of interrelated notions at the interface between the*physical* (crystal field) Hamiltonians and the*effective* (spin) Hamiltonians.

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Streszczenie

This review provides a summary of distinct Hamiltonians used to describe magnetic and spectroscopic properties of paramagnetic and magnetic coordination compounds. Based on the origins and the underlying physical principles, clear recommendations are formulated on when these Hamiltonians are appropriate and how they relate to each other. The interface, denoted CF (LF) ↔ SH (ZFS), encompasses the *physical* Hamiltonians, which include the crystal field (CF) [or equivalently ligand field (LF)] Hamiltonians, and the *effective* spin Hamiltonians (SH), which include the zero-field splitting (ZFS) Hamiltonians, as well as, to a certain extent, also the notion of magnetic anisotropy (MA). Survey of recent literature has revealed that the intricate web of interrelated notions has become dangerously entangled over the years. A given crucial notion is often referred to by one of the three names that are not synonymous: CF (LF), SH (ZFS), or MA, each having a well-defined and established meaning in optical spectroscopy, electron magnetic resonance (EMR), and magnetism, respectively. The terminological confusions occurring in literature call for in-depth clarifications, which are provided in this review. For this purpose, crucial notions are systematically defined and their logical interrelationships illustrated by concept maps. The operator types used to express the CF (LF) and SH (ZFS) Hamiltonians, i.e. the Stevens and Wybourne ones, are classified and their distinct properties discussed. Several key aspects are considered in the nutshell: basic forms of Hamiltonians and definitions of the associated parameters, distinct properties of the Stevens and Wybourne CF (LF) parameters and implications for conversion relations, distinctions and interrelationships between the CF (LF) and SH (ZFS) Hamiltonians or parameters, conversion relations between the Stevens ZFS parameters and conventional ones. The general focus is on the fundamental aspects underlying

physics and chemistry of single transition ($4f^N$ and $3d^N$) ions in coordination compounds as well as the novel single-ion and polynuclear magnetic systems. This includes the single-ion magnets and the exchange coupled systems (ECS) based on transition ions, especially the single molecule magnets (SMM) or molecular nanomagnets (MNM). The general aim is to provide deeper understanding of the major intricacies involved in the CF (LF) ↔ SH (ZFS) interface. The level of presentation is geared toward experimentalists with background in chemistry or physics.

Słowa kluczowe

Electron magnetic resonance (EMR), Optical spectroscopy, Magnetism, Crystal/ligand field (CF/LF) Hamiltonian, Zero-field splitting (ZFS), Single molecule magnets (SMM)

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