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Topology of spin Hamiltonian and crystal field tensors for Mn²⁺ in ZnSeO₄·6H₂O crystal

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Abstract

The expansion of the {B₂} and {B₄} tensors of the spin Hamiltonian (SH) for Mn²⁺ (6S-state) is performed in terms of the irreducible tensor products {VL₁ ⊗ VL₂}₂ and {VL₁ ⊗ VL₂}₄ of the crystal field (CF) tensors {VL₁} and {VL₂}. The EPR spectra of Mn²⁺ in the ZnSeO₄·6H₂O crystal are studied and the SH tensors {B₂} and {B₄} are calculated. The tensors {V₄⊗V₄}₂ and {V₄⊗V₄}₄ are computed using the point-charge model (PCM) of the [Zn(H₂O)₆] complex with the C₂ symmetry and are compared with the SH tensors {B₂} and {B₄}, respectively. The correct signs of the elements and the pseudo-symmetry axes of the tensors are obtained both for the {B₂} tensor and {V₄⊗V₄}₂ and for the {B₄} tensor and {V₄⊗V₄}₄. It is concluded that the irreducible tensor products {V₄⊗V₄}₂ and {V₄⊗V₄}₄ provide the predominant contribution respectively to the SH tensors {B₂} and {B₄} of Mn²⁺. © 1994 Springer.

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