

## Topology of spin Hamiltonian and crystal field tensors for Mn<sup>2+</sup> in ZnSeO<sub>4</sub>·6H<sub>2</sub>O crystal

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### Abstract

The expansion of the {B<sub>2</sub>} and {B<sub>4</sub>} tensors of the spin Hamiltonian (SH) for Mn<sup>2+</sup> (6S-state) is performed in terms of the irreducible tensor products {V<sub>L1</sub> ⊗ V<sub>L2</sub>}<sup>2</sup> and {V<sub>L1</sub> ⊗ V<sub>L2</sub>}<sup>4</sup> of the crystal field (CF) tensors {V<sub>L1</sub>} and {V<sub>L2</sub>}. The EPR spectra of Mn<sup>2+</sup> in the ZnSeO<sub>4</sub>·6H<sub>2</sub>O crystal are studied and the SH tensors {B<sub>2</sub>} and {B<sub>4</sub>} are calculated. The tensors {V<sub>4</sub> ⊗ V<sub>4</sub>}<sup>2</sup> and {V<sub>4</sub> ⊗ V<sub>4</sub>}<sup>4</sup> are computed using the point-charge model (PCM) of the [Zn(H<sub>2</sub>O)<sub>6</sub>] complex with the C<sub>2</sub> symmetry and are compared with the SH tensors {B<sub>2</sub>} and {B<sub>4</sub>}, respectively. The correct signs of the elements and the pseudo-symmetry axes of the tensors are obtained both for the {B<sub>2</sub>} tensor and {V<sub>4</sub> ⊗ V<sub>4</sub>}<sup>2</sup> and for the {B<sub>4</sub>} tensor and {V<sub>4</sub> ⊗ V<sub>4</sub>}<sup>4</sup>. It is concluded that the irreducible tensor products {V<sub>4</sub> ⊗ V<sub>4</sub>}<sup>2</sup> and {V<sub>4</sub> ⊗ V<sub>4</sub>}<sup>4</sup> provide the predominant contribution respectively to the SH tensors {B<sub>2</sub>} and {B<sub>4</sub>} of Mn<sup>2+</sup>. © 1994 Springer.

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