

# Investigations of the Spin Hamiltonian Parameters and the Local Structures of the Substitutional $V^{4+}$ Centres in Rutile-Type $MO_2$ ( $M = Sn, Ti, Ge$ )

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The spin Hamiltonian parameters and the local structures of the substitutional  $V^{4+}$  centres in rutile-type  $MO_2$  ( $M = Sn, Ti$  and  $Ge$ ) are theoretically investigated from the perturbation formulas of these parameters for a  $3d^1$  ion in a rhombically compressed octahedron. The oxygen octahedra around  $V^{4+}$  are found to transform from the original elongation on the host  $M^{4+}$  site to compression in the impurity centres due to the Jahn-Teller effect. The calculated spin Hamiltonian parameters based on the above local structures show good agreement with the experimental data.

*Key words:* Defect Structures; Electron Paramagnetic Resonance; Crystal- and Ligand-Fields;  $V^{4+}$ ; Rutile.