

Modeling in EMR spectroscopy - low symmetry aspects

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Paramagnetic centers with orthorhombic, monoclinic, and triclinic site symmetry occur often in various technologically important materials. For such centers intricate low symmetry aspects arise, which bear on meaningful interpretation of electron magnetic resonance (EMR) data and their correlation with structural data. The focus of this paper is on providing an overview of the modeling techniques for analysis and interpretation of EMR data, including the zero-field splitting parameters (ZFSPs) and g -factors, for transition ions at low symmetry sites in crystals worked out by us. Illustrative examples taken from our recent studies of low symmetry ion-host systems are discussed. This paper serves as a primer for experimentalists.