

00147

Poster 4

Degenerate aspects of EPR and NMR spectra from the respective point defects and nuclei in hexagonal crystals

Sang Won Ahn, Jung Ho Kim², and Dae Il Hong¹

¹Department of Chemistry, Keimyung University, Teagu 704-701

²Department of Physics, Keimyung University, Teagu 704-701

Observable sets and degenerate aspects of EPR and NMR spectra arising from the respective point defects and nuclei at chemically equivalent but magnetically inequivalent sites have been systematically investigated for the point groups 6 , $\bar{6}$, 622 , $6mm$, $\bar{6}m2$, $\frac{6}{m}$, and $\frac{6}{m}mm$ in hexagonal crystals. The sets and their degenerate aspects depend on symmetry of the point groups and the nearest neighbors around point defects as well as orientation of the applied magnetic field. On the basis of them, we will initially provide the following important criteria, not being clarified experimentally and theoretically; *i*) for aligning the sample crystal accurately with respect to the applied magnetic field, *ii*) for properly classifying the spectra from point defects and nuclei at chemically equivalent but magnetically inequivalent sites, which make it possible to distinct their relative sites of the point defects and nuclei, *iii*) for examining the equivalency between several centers with very similar EPR and NMR parameters, *iv*) for determining a certain crystallographic axis parallel to two-, three-, four-, and six-fold axes of local structures around point defects and nuclei