

Impurity Effects on the Local Structure in the Mixed Hexachlorometallate (A_2BCl_6 : A = K, Rb, B = Sn, Re, and Pb) Studied by the Chlorine NQR

Y. M. Seo, S. K. Song, and J. Pelzl^a

Department of Physics, Myongji University, Yongin Kyunggi-do, 449-728, Korea

^a Institut für Experimentalphysik 3, Ruhr Universitaet, D-44801 Bochum

Reprint requests to Prof. S. K. S.; Fax: +82-335-335-7248; E-mail: sksong@wh.myongji.ac.kr

Z. Naturforsch. **55 a**, 207–211 (2000); received August 23, 1999

Presented at the XVth International Symposium on Nuclear Quadrupole Interactions, Leipzig, Germany, July 25 - 30, 1999.

Chlorine NQR was studied for the isostructural hexachlorometallate mixed system. The study shows that Isomorphic hexachlorometallate solid solutions exhibit often impurity induced local structural order because of their relatively clear local site symmetry. This is manifested in the formation of a few satellite lines near the original resonance line and results from the random distribution of impurities on the lattice sites of the corresponding counterpart ions. Using the point charge model and a simple binomial function for the occupation probability of the guest ions on the host lattice sites, the position and the line intensity could be determined, the results of which are in good agreement with the NQR-observation. The temperature region of lattice dynamics in the crystal seems to shift in proportion to the impurity content. This fact explains the gradual change of the transition temperature in the mixed crystal between two starting materials.

Key words: NQR; Hexahalmetallates; Phase Transition; Mixed Crystals.