Solid-State 87Rb NMR Study in Powdered RbMnCl₃

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RbMnCl₃ has received considerable attention in recent years due to its ferroelastic and optical properties. RbMnCl₃ has been found to undergo para–ferroelastic structural phase transition from a monoclinic with the space group C_{2h}^2 to a hexagonal structure with the space group D_{2h}^4 at $T_c(=272K)$. Solid–state ⁸⁷Rb NMR spectroscopy is utilized for the detection of the structural phase transition at 290K in powdered RbMnCl₃. Quadrupole coupling constants (e^2qQ/h) and the asymmetry parameters (7) for two physically nonequivalent Rb sites, Rb(I) and Rb(II), are determined from nonlinear least–squares fits to the ⁸⁷Rb powder patterns in the temperature range of 260K to 330K. Quadrupole parameters are examined for the detection of structural phase transition owing to the significant change in Rb(II) site. DSC and XRD data in RbMnCl₃ and ¹³³Cs NMR powder patterns in CsMnCl₃ are also carried out to confirm above results.