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Raman and X-Ray Diffraction Studies on Doped $LiMn_2O_4$ RAJEEV GUPTA, Department of Physics and Materials Science Programme, Indian Institute of Technology, Kanpur 208016, India, S.L. GUPTA, Department of Physics, Indian Institute of Technology, Kanpur 208016, India — We have carried out Raman and X-Ray diffraction measurements on polycrystalline Cr doped $LiMn_2O_4$. Structural analysis using the XRD data suggests that for less than 50% substitution of Cr at Mn sites the samples have the cubic spinel structure with Fd3m space group. The diffraction peaks shift towards higher angles with increasing Cr content suggesting contraction of the lattice with increasing Cr. We observe strong Raman modes near 630 cm^{-1} and 580 cm^{-1} corresponding to A_{1g} and F_{2g} symmetry respectively. Specifically, A_{1g} corresponds to the stretching of the $Mn^{3+}O_6$ octahedra and F_{2g} involves $Mn^{4+}O_6$ stretching. Thus their relative intensity as a function of doping can be considered as representative of the relative amount of Mn^{3+} and Mn^{4+}. We find that the intensity ratio I (F_{2g})/ I(A_{1g}) increases with increasing Cr doping clearly indicating the decrease in the Mn^{3+} content in $LiCr_xMn_{2-x}O_4$ for $0 \leq x \leq 1$. As Mn^{3+} is mainly responsible for the Jahn – Teller distortion, chromium substitution in $LiMn_2O_4$ on Mn sites suppresses the Jahn – Teller distortion. These results are also consistent with recent theoretical results of suppression of Jahn-Teller distortion on Cr doping done using density functional theory.

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