13.5-04 A NEUTRON DIFFRACTION AND AN X-N DEFORMATION DENSITY STUDY OF LITHIUM HYDROGEN OXYDIACETATE AT 295 K. By H. Herbertsson, Dept of Engineering Materials, Luleå University of Technology, S-951 87 Luleå, Sweden, B. Hedman, Dept of Inorganic Chemistry, University of Umeå, S-901 87 Umeå, Sweden and R. Tellgren, Institute of Chemistry, University of Uppsala, Box 531, S-751 21 Uppsala, Sweden.

The crystal structure of lithium hydrogen oxydiacetate, $LiHO(CH_2COO)_2$, has been determined from X-ray data (Herbertsson, Acta Cryst. (1976) B32, 238). The crystals are monoclinic, space group $P2_1/n$, with a = 7.259(2), b = 5.468(1), c = 14.256(2) Å, β = 91.84(2)°. The structure consists of layers of infinite chains of hydrogen-bonded $O(CH_2COO^-)_2$ ions held together by Li^+ ions. The oxydiacetate residue forms a bidentate chelate with the Li^+ ion, which results in a fairly large conformational change in the two halves of the ligand.

In order to study the electron distribution around the ether oxygen and the atoms participating in the chelate a recollection of the X-ray data was made using MoKα radiation with sin Θ/λ < 1.15 $Å^{-1}$. Neutron diffraction data were collected at the Swedish R2 reactor at a wavelength of 1.210 Å with sin Θ/λ < 0.69 $Å^{-1}$.

Details of the structure and X-N maps showing the features of the electron distribution will be shown.