The crystal structure of lithium hydrogen oxodiacetate, LiHO(CH₂COO)₂, has been determined from X-ray data (Herbertsson, Acta Cryst. (1976) B32, 238). The crystals are monoclinic, space group P2₁/n, with a = 7.259(2) Å, b = 5.468(1) Å, c = 14.256(2) Å, β = 91.84(2)°. The structure consists of layers of infinite chains of hydrogen-bonded O(CH₂COO⁻)₂⁻ ions held together by Li⁺ ions. The oxodiacetate 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.