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A new Li-Mn-Ge-O phase solved by combining 3D electron diffraction methods

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Pyroxene compounds are a common form of natural minerals and have been studied as such for a long time. More recently the research on quasi-one-dimensional magnetic and multiferroïc materials has renewed the interest in pyroxenes of the stoichiometry AMX2O6 (A = alkali metal, M = transition metal, X = Si or Ge), since the magnetic M3+ ions form chains. Chemical substitution on the A and M sites can change the magnetic coupling along these chains making this system a rich field for the exploration of new phases of interesting magnetic properties [1]. In this work we report the discovery of a new phase in the Li-Mn-Ge-O system. A HP-HT solid state reaction was performed on a mixture of nominal stoichiometry LiMnGe2O6 during 1 h at a temperature of 850°C and a pressure of 3 GPa in a belt press. Powder X-ray diffraction yielded a diffractogram that could not be indexed by known phases of this system. An electron diffraction study in a transmission electron microscope was conducted in order to identify any unknown phases. In the case of structures that promise interesting properties a more targeted synthesis can then be undertaken. For the purpose of this work, we studied one of several unknown phases in the powder in more detail. From standard selected area electron diffraction the unit cell was determined to be triclinic with cell parameters a = 2.51 nm, b = 1.30 nm, c = 1.30 nm, α = 96.0°, β = 98.8° and γ = 80.8°. No comparable unit cell could be found in the databases neither in this system nor with different A, M or X ions. Intensities were recorded by in-zone axis precession electron diffraction and by electron diffraction tomography. Combining the data from both methods yielded the first model of the structure which we will present here.

[1] *J. Cheng, W. Tian, J. Zhou et al., 2013, J. American Chem. Soc., 135, 2776-2786*

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