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CRYSTAL STRUCTURE OF Li_2TbF_6 AND MAGNETIC STUDY UNDER HIGH MAGNETIC FIELD

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The crystal structure of Li_2TbF_6 was solved ab-initio at 300 and 5 K using X-ray and neutron powder diffraction data respectively. This compound crystallizes in the monoclinic system, space group $P2_1/C$ (n° 14), Z = 4, with a = 7.585(1) Å, b = 4.965(1) Å, c = 11.116(1) Å and β = 106.96(1)° at 300 K.

The structure was solved and refined using direct methods and Rietveld profile refinement techniques. Li_2TbF_6 exhibits a completely new structural type for A_2MF_6 compounds with Tb^{4+} in bicapped trigonal prisms. Lithium ions in this structure adopt two types of coordination polyhedra : octahedra and unusual square pyramids. Relationships with γ-Na_2UF_6 and $CaTa_2O_6$ structural types will be presented.

The saturation magnetization measured in a 200 kθe magnetic field at 4.2 K has been found to be equal to 6.9 μ_B, what provides confirmation of the degree 4+ of the terbium which is isoelectronic with Gd^{3+} and exhibits a $^8S_{7/2}$ ground state.

The Curie law is not found to be obeyed at low temperatures. This behaviour will be discussed in terms of magnetic interactions or splitting of the ground state level in zero-field.