o.m13.p7 **Crystal Structure of the Solid Solutions in the Li-Mg-Ca and Li-Mg-Gd ternary systems.** V.V. Pavlyuk[1], G.S. Dmytriv[1], D.G. Kevorkov[1], O.I. Bodak[1], R.Schmid-Fetzer[2], J.Gröbner[2]. [1]*Department of Inorganic Chemistry, Ivan Franko Lviv National University, Kyryla & Mefodiastr.6, 79005 Lviv Ukraine, e-mail: gregor@ipm.lviv.ua* [2]*Electronic Materials Group, Department of Physics, Materials Science and Engineering at the TU Clausthal, Robert-Koch-Str.42, 38678 Clausthal-Zellerfeld, Germany, e-mail: Schmid-Fetzer@tu-clausthal.de.*
Keywords: crystal structure, phase diagram, lithium.

During investigation of the ternary systems Li-Mg-Ca and Li-Mg-Gd at 250°C existence of continuous solid solution between the binary compounds $CaLi_2$ and $CaMg_2$ in Li-Mg-Ca system and limited solid solutions based on Gd-Mg binary compounds in Li-Mg-Gd system were established.

Alloys were prepared from pure elements by arc-melting in argon atmosphere and then annealed at 250°C for 400 h. X-ray powder pattern were obtained using a DRON-2.0 powder diffractometer with FeKα-radiation for phase analysis. For more detailed structural investigation the X-ray measurements were performed using the Siemens powder diffractometer with CoKα-radiation. The XPD data were analysed with the Rietweld profile refinement method using the DBWS-9006PC program [1].

Forming of the continuous solid solution between the binary compounds $CaLi_2$ and $CaMg_2$ in the Li-Mg-Ca system explained by te same structure of these compounds [2] ($MgZn_2$ structure type, $P6_3/mmc$ space group) and small difference between atomic radia and electron structure of Li and Mg atoms. Lattice parameters oh this unlimited solid solution increasing from a=6.244(2) and c=10.195(4) Å to a=6.262(2) and c=10.208(4) with substitution Li atoms by Mg atoms. Also forming of this solid solutions explained by similar character of interaction Li and Mg with Ca.

In opposite to the Li-Mg-Ca system, in the Li-Mg-Gd system binary systems Li-Gd and Mg-Gd very differed. As results only limited solid solutions based on the Gd-Mg binary compounds (MgGd, Mg_3Gd and Mg_2Gd) are formed in the Li-Mg-Gd system. The extents of the homogeneity ranges and the change of lattice parameters for these solid solutions are listed in the Table.

Characteristics of solid solutions in Li-Mg-Gd system

Solid solution	Homogeneity range	a, Å
$GdMg_{1-x}Li_x$	0<x<0.1	3.833(2)-3.807(1)
$GdMg_{2-x}Li_x$	0<x<0.09	8.640(1)-8.562(5)
$GdMg_{3-x}Li_x$	0<x<0.2	7.315(5)-7.305(2)

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o.m13.p8 **Structural Study of Cerium Chromates**. B. Casari, V. Langer, *Department of Inorganic Chemistry, Göteborg University, SE-41296 Göteborg, Sweden. Department of Environmental Inorganic Chemistry, Chalmers University of Technology, SE-41296 Göteborg, Sweden.*
Keywords: cerium chromate hydrates, cerium oxygen coordination, single crystal X-ray diffraction.

Investigations of the crystalline phases of the system $CeO_2{\cdot}CrO_3{\cdot}H_2O$ were started by O. Lindgren in connection with studies on the cerium oxygen coordination. Crystal structure determination of only one of those compounds, $Ce(CrO_4)_2{\cdot}2H_2O$, was reported. The structure is described by Lindgren[1] as built up by layers of $Ce(CrO_4)_2$ components, held together by hydrogen bonds. The cerium(IV) coordination polyhedron is a bicapped trigonal prism, consisting of six chromate and two water oxygens.

The crystal structure of a cerium dichromate hydrate, $Ce(CrO_4)_2{\cdot}H_2O$ has been determined, from three dimensional X-ray data collected at low temperature, -100°C. The symmetry is orthorhombic, space group *Pbca*, with a = 10.9648(2), b = 11.4554(2), c = 22.0568(4) Å, Z = 16 and ρ_c = 3.72 gcm^{-3}. The cerium dichromate hydrate crystallises as very dark red crystals with the shape of an octahedron elongated along one axis.

The structure of $Ce(CrO_4)_2{\cdot}H_2O$ is essentially different from the one described by Lindgren. This compound is more polymerised and consequently its density is slightly higher. The structure extends through chromate bridges between cerium polyhedra to form infinite strings, joined by chromate groups forming thus an infinite three dimensional network. Cerium exhibits both eight and nine-fold oxygen coordinations. The eight and nine-vertex cerium polyhedra, form puckered layers alternating in the **c** direction. The hydrogen bonds play a minor role in the structural properties.

Nine coordination is quite common for the trivalent cerium ions while for oxygen coordinating cerium(IV) compounds eight coordination is normal but higher coordination numbers are also encountered[2,3].

Cerium(IV) is a strong oxidiser and considering the thermodynamic equilibrium between cerium(IV) and cerium(III) in acidic aqueous solutions and the thermodynamic equilibrium between oxygen and water, cerium(IV) in acidic aqueous solutions is metastable with regard to the oxidation of water. The attainment of equilibrium is kinetically controlled but mixed Ce(III) - Ce(IV) solutions tend to occur if heated, since the glass vessel walls act as the catalytic agent. Attempts to prepare different mixed Ce(III) - Ce(IV) compounds are in progress.

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