Laves phase compounds belong to the class of Frank – Kasper phases showing topologically close-packed structures. They are categorized primarily into three parent members: the *C*14 hexagonal $MgZn_2$ – type (*P6₃/mmc*), the *C*15 cubic $MgCu_2$ – type (*Fd-3m*) and the *C*36 hexagonal $MgNi_2$ – type structures (*P6₃/mmc*). The family have the general composition AB_2 with the larger *A* atoms in the center of a 16-atom Frank – Kasper polyhedron and the smaller *B* atoms in the centers of icosahedra. The *C*15 – type cubic structure is illustrated in Figure 1. The coordination number is 12 for the smaller *B* atoms (Fig. 1(b)) and 16 for the larger *A* atoms (Fig. 1(c)).

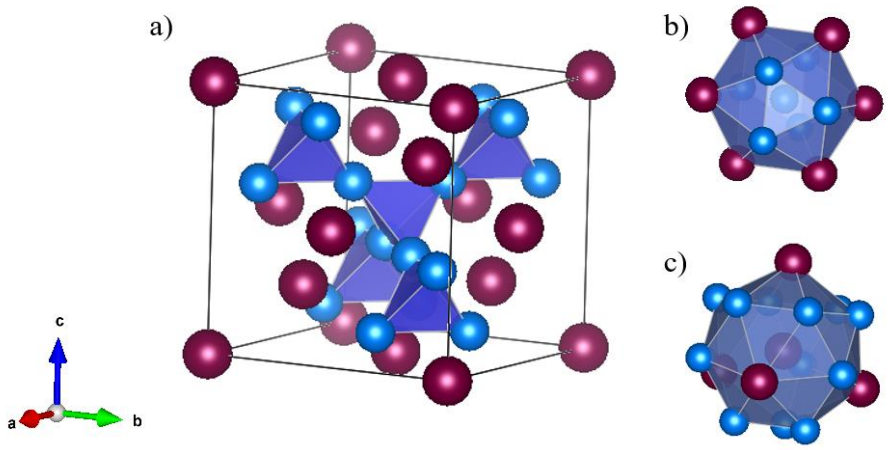

Figure 1. a) the cubic $MgCu_2$ – type structure with tetrahedra emphasized. b) the icosahedron surrounding the *B* atom. c) Frank – Kasper polyhedron with the larger *A* atom in the center. The crystal structure was created in the crystal structure visualization program VESTA.

The discussion on the special properties of Laves phases started in the 1920s and 1930s. Laves's work gave the first valuable insight into the characteristics of this class of materials. Especially in the last 30 years AB_2 – type Laves phase compounds have been a subject of particular interest in solid state physics due to the variety of their physical properties. In this system a geometrically frustrated magnetic arrangement, structural phase transition, a large magnetocrystalline anisotropy and a huge magnetostrictions at room temperature with a relatively high Curie temperature and a high magnetic saturation have been found. Additionally, many of the pseudobinary Laves compounds (e.g. $Ho_{1-x}Mn_xCo_2$) have a high hydrogen absorption capacity even at lower pressure. Several Laves compounds are also known as superconductors with critical temperatures ranging from 0.07 K for $HfMo_2$ to above 10 K for $V_2Hf_{0.5}Zr_{0.5}$. Today, over a thousand binary and ternary Laves phase intermetallics have been synthesized and characterized, of which about 60% contain a rare earth metal atom. Although this family is well known since long time, there are still unsolved problems concerning factors controlling the Laves phase stability.

The motivation for the research is a rather small number of reported Laves phase compounds containing an alkaline earth metal (Mg, Ca, Sr or Ba). Moreover, the detailed experimental characterization for almost all known superconductors with alkaline earth metal in this group is still lacking in the literature.

This project is designed to address some important aspects of new materials research in solid state physics and chemistry. In particular we will be searching for new compounds that exhibit interesting properties, especially superconductivity.