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Substitution and Disorder Effects in Ternary Intermetallics

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SUBSTITUTION AND DISORDER EFFECTS IN TERNARY INTERMETALLICS

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I am grateful for my family and loved ones, thank you for the love and support.
To GOD, thank you for blessing me and allowing me to do your will.

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Table of Contents

Abstract

The focal point of this dissertation is the investigation of substitution and disorder effects in ternary intermetallics. The crystal growth, crystal structure, and physical properties are reported on single crystals of $Ln_6W_{4-x}Al_{43-y}T_{x+y}$ (Ln = Gd, Yb; T= Mn, Fe), $LnCr_2Fe_xAl_{20-x}$ (Ln = Yb, Gd), $Sm_{1.33}Pd_3Ga_8$, and $CeCo_{2-x}M_xAl_8$ (M = Mn, Fe, Ni; $0 \leq x < 1$). The reported compounds were grown via the flux growth method with the strategic synthetic parameters described. Correlations between the structural and physical properties in relation to substitution and disorder of $Ln_6W_{4-x}Al_{43-y}T_{x+y}$ (Ln = Gd, Yb; T= Mn, Fe), $LnCr_2Fe_xAl_{20-x}$ (Ln = Yb, Gd), $Sm_{1.33}Pd_3Ga_8$, and $CeCo_{2-x}M_xAl_8$ (M = Mn, Fe, Ni; $0 \leq x < 1$) are discussed.

The synthesis and characterization of Mn- and Fe- substituted $Ln_6W_4Al_{43}$ (Ln = Gd, Yb) are reported. The compounds adopt the $Ho_6Mo_4Al_{43}$ structure type with lattice parameters of $a \sim 11$ Å and $c \sim 17.8$ Å with structural site preferences for Mn and Fe. The magnetization of $Yb_6W_4Al_{43}$ is sensitive to Mn and Fe doping, which is evident by an increase in the field dependent magnetization. $Gd_6W_4Al_{43}$, $Gd_6W_4Al_{42.31(11)}Mn_{0.69(11)}$, and $Gd_6W_4Al_{41.69(12)}Fe_{1.30(12)}$ order antiferromagnetically in the *ab*- and *c*-direction at 15, 14, and 13 K, respectively, with positive Weiss constants, suggesting the presence of ferromagnetic exchange interactions. Anisotropic magnetization data of $Gd_6W_4Al_{43-y}T_y$ (T= Mn, Fe) analogs are discussed.

Crystal growth, structure determination, and magnetic properties of $LnCr_2Al_{20-x}Fe_x$ (Ln = La, Gd, Yb) adopting the $CeCr_2Al_{20}$ structure type with space group $Fd\bar{3}m$, $a \sim 14.5$ Å, type are reported. Single crystal X-ray diffraction and Mössbauer spectroscopy are employed to fully characterize the crystal structure of $LnCr_2Al_{20-x}Fe_x$ (Ln = La, Gd, Yb). $LnCr_2Al_{20-x}Fe_x$ (Ln = La, Gd, Yb) are the first pseudo-ternaries adopting the $CeCr_2Al_{20}$ structure type with a transition metal occupying the main group site. The Yb analogues are Pauli paramagnets with the Yb ion adopting

an electronic configuration close to Yb^{2+}, while the Gd analogues show paramagnetic behavior with no magnetic order down to 3 K.

The synthesis and characterization of $Sm_{1.33}Pd_3Ga_8$ is reported. $Sm_{1.33}Pd_3Ga_8$ adopts a disordered variant of the $Er_4Pt_9Al_{24}$-structure type with lattice parameters of a = 4.353(5) and c = 38.98(4) Å and V = 639.70(12) $Å^3$. The structure of $Sm_{1.33}Pd_3Ga_8$ is composed of three distinct building blocks: Pd_2Ga_4, $PdGa_2$, and $Sm_{0.67}Ga$. The $Sm_{0.67}Ga$ slab does not magnetically order, which directly affect the structure. $Sm_{1.33}Pd_3Ga_8$ is a temperature independent paramagnet. Field dependent magnetization of $Sm_{1.33}Pd_3Ga_8$ displays anisotropic behavior.

Single crystals of $CeCo_{2-x}M_xAl_8$ (M = Mn, Fe, Ni; $0 \leq x < 1$) were grown and crystallize in the $CaCo_2Al_8$ structure type with space group *Pbam*. Single crystal X-ray diffraction data suggest that the Ce *4f*-state is valence fluctuating as Fe concentration increases, whereas the Ni-doped analogues do not exhibit valence fluctuating. The results suggest that hole doping leads to an admixture of Ce^{3+}/Ce^{4+}.

Chapter 1. Introduction

1.1 Motivation

Determining the structure and physical properties of materials is one important area of solid state research. Pinpointing the structural features that are responsible for unique physical properties can lead to targeted structure types to consider for optimizing desired properties. Identifying promising candidates that possess the desired properties is approached by first selecting compounds with unique structural motifs. For example, $CeIn_3$ of the $AuCu_3$-structure type orders antiferromagnetic, $T_N \sim 11$ K, and upon application of pressure, the compound become superconducting at ~ 2.3 K.[1] The related homologous series Ce_nMIn_{3n+2} (n = 1, 2; M = Co, Rh, Ir)[2-7] also exhibit magnetically mediated superconductivity and adopt the $HoCoGa_5$- and Ho_2CoGa_8-structure type,[8] respectively. $CeMIn_5$ (M = Co, Rh, Ir) is composed of $CeIn_3$ cuboctahedra layers stacked periodically with alternating rectangular polyhedra of MIn_2 layers along the *c*-axis, while Ce_2MIn_8 (M = Co, Rh, Ir) is composed of $CeIn_3$ cuboctahedra layers stacked along the *c*-axis with two intervening rectangular polyhedra of MIn_2 layers.[8] Another example is the AlB_2 type MgB_2 that exhibit superconductivity at $T_c \sim 39$ K[9] MgB_2 is composed of honeycomb boron planar nets stacked along the *c*-axis with Mn atoms located in the hexagonal voids like intercalated graphite.[9] The cause of superconductivity in MgB_2 has been attributed to the metallic nature of the covalently bonded 2D boron sheets and attributed as phonon-mediated BCS-type mechanism.[10]

Intermetallic compounds with atoms arranged in a triangular motifs can exhibit magnetic frustration, which can lead to exotic properties. Geometric frustration is correlated to the geometry of the network of spins and inherent to the nearest neighbor antiferromagnetic interactions. Frustrated sublattices are constructed by triangles made of magnetic ions as seen in triangular and

tetrahedral motifs. Triangles and tetrahedra motifs can be packed by corner sharing or edge sharing in two or three dimensions as seen in hexagonal and Kagome networks and pyrochlore lattices, respectively.[11, 12] The nearest neighbors of any spins in the aforementioned arrangements are themselves nearest neighbors of each other thus making it intrinsically impossible to build a consistent antiferromagnetic configuration leading to numerous degenerate manifolds of spin configurations. Magnetic frustration arises when magnetic ions cannot arrange in favorable interactions causing suppression of long range magnetic ordering to temperature considerably lower than the Weiss constant.[12, 13] As result exotic behavior can persist such as spin glass behavior. Spin glass system is where the magnetic moments freeze at a temperature into random orientations without long-range order leading to exotic properties such as isothermal time-dependent relaxation.[14, 15] There are three factors linked to magnetic frustration such as the symmetry of the magnetic sublattice, site disorder, and the dimensionality of the magnetic sublattice. These parameters are attached in extended solids. Intermetallic compounds that adopt the $Ho_6Mo_4Al_{43}$-[16] and $CeCr_2Al_{20}$-structrue type[17] have Kagome and pyrochlore like networks made up of rare earth atoms or transition metals, respectively. It is of interest to investigate compounds of the aforementioned structure types and to study the effects of substitution on the magnetic ions interactions to discover competing and exotic properties.

Substitution of one element for another or introducing disorder in the structure has been successful in affecting the physical properties of materials. For instance, the $LaCo_2B_2$ of the $ThCr_2Si_2$ structure type[18] and is composed of layers of CoB_4 edge sharing tetrahedra alternating with layers of isolated La atom along the *c*-axis.[19] $LaCo_2B_2$ exhibits metallic resistivity and paramagnetic behavior down to 2 K. Upon isovalent substitution of Y for La, $La_xY_xCo_2B_2$, bulk superconductivity was observed at 4.2 K which is attributed to chemical pressure.[20] Hole

substitution studies, Fe for Co, led to $La(Co_{1-x}Fe_x)_2B_2$ that superconducts at ~ 4 K caused by Fe raising the hole concentration to an optimal level for the appearance of superconductivity. Electron doping Si for B, led to $LaCo_2Bi_{2-x}Si_x$ with no superconducting behavior presence.[20] Recently quantum criticality has been observed without tuning any control parameters such as pressure in β-$YbAlB_4$, an intermediate valent heavy fermion compound with a Sommerfeld coefficient of ~300 mJ/mol K^2.[21, 22] Its counterpart, α-$YbAlB_4$, has a Sommerfeld coefficient of ~130 mJ/mol K^2.[22] Heavy fermion behavior is a consequence of the *f*-electrons coupling with conduction electrons, which results in the electrons behaving as if they have an increased mass that results in a large Sommerfeld coefficient, γ, where $C_p = \gamma T + \beta T_3$ (γ > 200 mJ/mol-K^2). Both α- and β-$YbAlB_4$ exhibits Kondo behavior, which can be described as the screening of the local magnetic moment by conduction electrons. In α- and β-$YbAlB_4$, the Yb and Al atoms lie in the *ab*-plane, which is in the middle of two boron networks consisting of pentagonal and heptagonal rings.[22] Substitution of Fe for Al led to a volume contraction indicating that Fe substitution applies chemical pressure in α and β-$YbAlB_4$. As a result the Kondo temperature is suppressed and antiferromagnetic ordering persist at ~ 7 and 9 K for α-$YbAlB_4$ and β-$YbAlB_4$, respectively.[23]

1.2 Synthesis

The growth of high quality single crystals is necessary to determine the structure of materials and allows the determination of intrinsic properties of materials necessary to study the physics of materials. The single crystalline compounds presented in this dissertation are grown via the flux growth method.[24-27] The flux growth method uses metals with relatively low melting points such as gallium (m.p. 30 °C), aluminum (m.p. 660 °C), tin (m.p. 232 °C), lead (m.p. 327 °C), indium (m.p. 157 °C) and zinc (m.p. 420 °C).[24] The metallic flux can serve as an inert flux (non-reactive) or reactive (incorporated into the products) flux. Taking advantage of the relatively

low temperature of main group elements, the reaction can be slow-cooled to yield high quality single crystals. This does not discount the possibility of crystal formation during the ramp-up and ramp-down sequence or during dwelling at high temperature. In the flux-growth method, reaction ratios and temperature profiles can be varied to target the growth of the product. The synthetic parameters are strategically mapped out by first consulting the binary phase diagrams.[28] An example of a phase diagram is shown in Figure 1. 1.

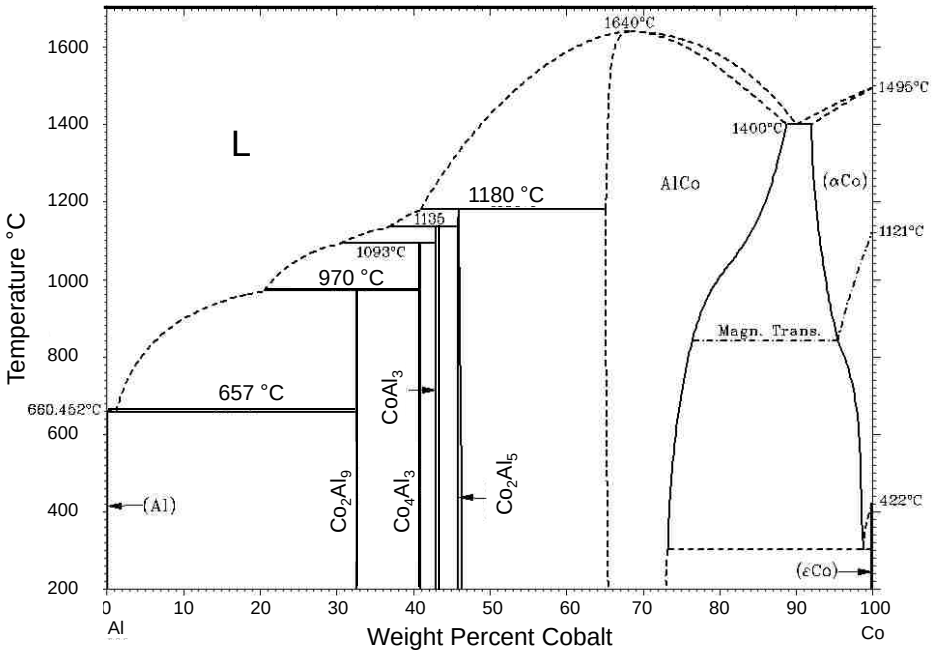

Figure 1.1. Binary phase diagram of Al and Co, as obtained from reference 33.

The binary phase diagram shows the conditions at which a compound is thermodynamically favorable at a specific composition of the two elements.[29] Phase boundary lines separate these areas indicating which phase will be stable in that particular region. Every point within this area represents a specific temperature and composition of the respective elements. For the flux growth method, the starting ratios of reactants are chosen to a certain ratio composition in the phase diagram which is often close to the targeted composition of the desired ternary or

binary compound. A typical temperature profile is shown in Figure 1.2. The temperature profile is strategically chosen considering variables such as temperature rates, dwell temperatures, dwell times, and the spin temperature which is typically above the melting point of the metallic flux. All variables in the temperature profile are important and have an effect on the final product. The heating and cooling rates can be adjusted to avoid undesirable phases and change the rate of nucleation and growth.

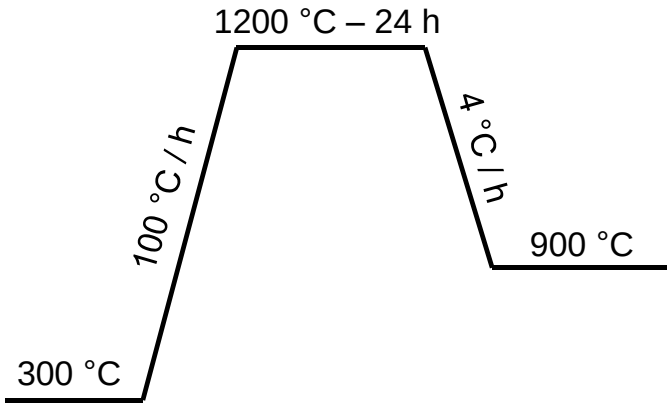

Figure 1.2. A generic temperature profile.

1.3 Characterization

Structure determination in crystalline materials can be achieved by X-ray diffraction. Both powder X-ray diffraction and single crystal X-ray diffraction are used for structural determination. Crystalline samples are bombarded by X-rays, which are scattered in all possible directions by the electrons in the material. The scattered X-rays can be in phase or out of phase given the distance traveled between the X-rays from the source to the sample. When the distance travel between the scattered waves are integral numbers of the wavelength, the X-rays are interacting constructively (in phase). This can be rationalized by Bragg's law, $2d\sin\theta = n\lambda$, where d is the interplanar spacing, θ is the angle between the X-ray beam and the reflecting lattice, n is an integer, and λ is the X-ray wavelength.[30] The scattered X-rays are observed in an array of reflection which is

known as the diffraction pattern.[31] The diffraction pattern provides information by the location and intensity of each reflection. The symmetry and dimensions of the crystalline material is determined by the symmetry of the diffraction pattern and the space separating the reflections. A unique atom and the position of that atom in a crystalline material is determined by the intensity and position of the reflections in the diffraction pattern. The interactions between atoms in the material under investigation are determined through refinement of the crystal structure and is based on the number of electrons of that particular atom. The interatomic distances and angles are determined by the refinement of the structural model, which can lead to insight of the nature of the atoms in a material. Powder and single crystal X-ray diffraction provides an average picture of the crystal structure. The structure can have irregular order of atoms known as disorder.[32, 33] Disorder in materials can be evident in the structural model by anomalous atomic displacement parameters, unrealistic interatomic distances, and residual electron density peaks. Structural elucidation of the disorder present in a material is essential to the investigation of the structure-property relationship due to the fact the properties are dependent on the particular atom at a unique position and its nearest contacts.

Site disorder in a crystalline material can be rationalized as an irregularity at a specific crystallographic sites from an ordered atomic arrangement in a crystalline material.[32, 33] Disorder can have a direct effect on the intrinsic physical properties of a material because disorder at one site will alter its nearest neighbors. Disorder can be categorized as dynamic or statistical disorder. Dynamic disorder can be classified as a physical motion in a crystal structure. Statistical disorder can be subdivided into positional and substitutional disorder.[32, 33] Positional disorder can be classified as the statistical distribution of an atom at different crystallographic sites in a unit cell, while substitutional disorder can be classified as the statistical occupation of the same

crystallographic site by different of atoms.[32, 33] Both dynamic and statistical disorder are often exhibited in disordered structures, which is observed in their X-ray diffraction pattern by directional and irregularly shaped reflections. The extent of dynamic and statistical disorder can be studied by collecting data at high and low temperatures and comparing the refined models. Dynamic disorder is not significantly affected by thermal fluctuations, so the structural models refined from the high and low data will be similar. However, statistical disorder is affected by thermal fluctuations that is evident in the structural models obtain from the refinement of different temperatures.

The research presented is focused on the investigation of how disorder affects the properties in ternary intermetallics, specifically substitutional disorder.[32] By strategically substituting specific elements the carrier concentration can be systematically changed as well as the nearest neighbors contact. One can then investigate the structural and magnetic properties of these compounds to draw general conclusions about the subtle changes caused by substitution.

In addition to X-ray diffraction, scanning electron microscope equipped with an energy dispersive X-ray detector was used to confirm the composition of our products. Mössbauer spectroscopy is a non-destructive technique and can provide information such as electron structure, symmetry, magnetism, phase transition, and lattice dynamics.[34-36] In particular, ^{57}Fe Mössbauer spectroscopy was also used to determine the chemical nature of the Fe-substituted compounds.

1.4 Properties

Our goal is to determine the first-order physical properties of materials including temperature and field dependent magnetic measurements and electrical resistivity. Magnetic behavior of most materials can be classified by the following: diamagnetism, paramagnetism, ferromagnetism, and antiferromagnetism. Magnetic susceptibility, χ, is the ratio of magnetization,

M, to the magnetic field, H. The modified Curie-Weiss law $\chi = \chi_o + (C/(T-\Theta))$ where χ_o is the diamagnetic contribution, C is the Curie Constant and Θ represents the Weiss constant describes the temperature dependency of the magnetic susceptibility of a material. The Curie constant directly relates to the magnetic moment of a sample and is described by the equation $C = (N\mu_B^2\mu_{eff}^2)/3k_B$, where N, μ_B, μ_{eff}, and k_B represents Avagadro's number, Bohr magneton, effective moment, and the Boltzmann constant, respectively.[29] The experimental effective moment can be obtained by a Curie-Weiss fit of the paramagnetic region in the susceptibility. The Weiss constant is related to the strength of the magnetic interactions. The temperature dependence of the resistivity of a material can suggest whether the material is metallic, semiconducting, or superconducting. The resistivity is related to this equation $\rho = R \times (A/l)$, where R is the measured resistance, A is the area of the sample, and *l* is the length of the sample. The quality of the sample can be evaluated by the residual resistivity ratio (RRR) and strongly dependent on disorder. The magnetic and electrical properties of ternary intermetallics depend on the interactions between the local magnetic moments and conduction electrons.

1.5 Substitution Effects in Rare Earth Intermetallics

The focus on the structural and physical properties of high quality crystalline materials through disorder sets the scope for the body of work presented in this dissertation. Ternary intermetallics can display highly correlated electron behavior such as superconductivity, Kondo behavior, and heavy fermion behavior due to the strong interactions of the conduction electrons with the local magnetic moment. The idea is to study the effects of chemical substitution and disorder in highly correlated extended solids. Four projects will be given to illustrate the effects of disorder in rare earth ternary intermetallics.

The first project involves investigating Mn and Fe in $Ln_6W_4Al_{43}$ (Ln = Gd, Yb) that adopts the $Ho_6Mo_4Al_{43}$-structure type.[16] We were motivated to investigate Mn and Fe substitution in $Ln_6W_4Al_{43}$ (Ln = Gd, Yb) because of the Kagome network of the Ln atoms. Single crystals of the pseudo-ternary compounds $Ln_6W_{4-x}Al_{43-y}M_{x+y}$ (Ln = Gd, Yb; M = Mn, Fe) were grown using excess Al-flux.[37] The Yb analogs are nonmagnetic consistent with the Yb adopting the divalent configuration, Yb^{2+}. Temperature dependent magnetization of $Gd_6W_4Al_{43-y}T_y$ (T = Mn, Fe) was measured in the *ab*- and *c*-direction. The easy axis is the *ab*-plane which constitutes the Kagome lattice. The Gd-analogues exhibit antiferromagnetic ordering in the *ab*- and *c*- with T_N decreasing in the order of ~ 15, 14, and 13 K for $Gd_6W_4Al_{43}$, $Gd_6W_4Al_{42.31(11)}Mn_{0.69(11)}$, and $Gd_6W_4Al_{41.69(12)}Fe_{1.30(12)}$, respectively. The Gd-analogues also show positive Weiss suggesting net ferromagnetic exchange interaction.

For the second project, we investigated $LnCr_2Al_{20}$ (Ln = La, Gd, Yb) adopting the $CeCr_2Al_{20}$-structure type[17] because of their Frank-Kasper cages formed by the main group element and pyrochlore like network formed by the transition metals. By means of single crystals X-ray diffraction and ^{57}Fe Mössbauer spectroscopy, we determined that Fe incorporation in $LnCr_2Al_{20}$ and this is the first pseudo-ternary of the $CeCr_2Al_{20}$-structure type where the transition metal dopant (Fe) substitutes for the main group element: $LnCr_2Al_{20-x}Fe_x$ (Ln = Yb, Gd). Single crystals of $GdCr_2Al_{20}$ and $GdCr_2Al_{19.7}Fe_{0.3}$ exhibit paramagnetic behavior down to 3 K with no magnetic ordering contrary to the polycrystalline $GdCr_2Al_{20}$ that display antiferromagnetic ordering at 3.90(5) K. $GdCr_2Al_{20}$ and $GdCr_2Al_{19.7}Fe_{0.3}$ show negative Weiss constant which indicate a dominate antiferromagnetic exchange interaction between the Gd ions.

For the third project we targeted $Sm_2Pd_3Ga_9$ because of the structural complexity of $Yb_2Pd_3Ga_9$.[27] However, we grew $Sm_{1.33}Pd_3Ga_8$ that adopts a disordered variant of the $Er_4Pt_9Al_{24}$-

structure type.[38] The structure of $Sm_{1.33}Pd_3Ga_8$ is composed of three distinct building blocks: Pd_2Ga_4 + 2 x [$Sm_{0.67}Ga$] + $PdGa_2$. The disorder, $Sm_{0.67}Ga$, plays a critical role in the structure by not ordering magnetically. As a result $Sm_{1.33}Pd_3Ga_8$ adopts a trigonal symmetry instead of a triclinic symmetry like the $Er_4Pt_9Al_{24}$-structure type. The crystal structure of $Sm_{1.33}Pd_3Ga_8$ is highly anisotropic given the $(Sm\text{-}Sm)_{ab}$, 4.353(5) Å, and $(Sm\text{-}Sm)_c$, ~ 5.3391 Å and 8.1846 Å, distances. Single crystals of $Sm_{1.33}Pd_3Ga_8$ exhibit temperature independent paramagnetic behavior. Field dependent of $Sm_{1.33}Pd_3Ga_8$ exhibits anisotropic behavior.

For the fourth project, we investigated the Fe and Ni substitution in $CeCo_2Al_8$. The motivation of this project stems from the fact that $CeCo_2Al_8$ exhibits Curie Weiss behavior with an effective moment consistent with Ce^{3+}, whereas $CeFe_2Al_8$ exhibits valence fluctuation consistent with Ce^{3+}/Ce^{4+} and Fe not carrying a local moment. The Fe and Ni-doped compounds adopt the $CaCo_2Al_8$-structure type which is very robust. Single crystal X-ray diffraction data suggest that the Ce *4f*-state is valence fluctuating as Fe concentration increases, whereas the Ni-doped analogues do not exhibit valence fluctuating.

Herein, detailed studies of the synthesis, crystal structure, and physical properties of $Ln_6W_{4-x}Al_{43-y}M_{x+y}$ (Ln = Gd, Yb; T= Mn, Fe),[37] $LnCr_2Al_{20-x}Fe_x$ (Ln = La, Gd, Yb),[39] $Sm_{1.33}Pd_3Ga_8$, and $CeCo_{2-x}M_xAl_8$ (M = Fe, Ni; $0 \leq x < 1$) are presented, along with the magnetic and structural effects of chemical substitution and disorder.

Chapter 2. The physical properties of $Ln_6W_4Al_{43}$ and substitution studies of Mn and Fe in $Ln_6W_4Al_{43}$ (Ln = Gd, Yb)*

2.1 Introduction

Substitution of elements in rare earth intermetallics can lead to the discovery of competing structural and physical property behavior.[40-47] Recently, α-$YbAlB_4$[48] was reported to form a heavy Fermi liquid state with the specific heat coefficient of $\gamma \sim 130$ mJ mol^{-1} K^{-2}, while the β-$YbAlB_4$ analog[21, 49] exhibits quantum criticality without tuning of any control parameters. Motivated by the role of chemical pressure on both polymorphs of $YbAlB_4$, it was discovered that Fe substitution leads to a suppression of the Kondo temperature and induces magnetism with α-$YbAlB_4$ and β-$YbAlB_4$ antiferromagnetically order at ~ 7 and 9 K, respectively.[23] The concentration of the dopants can also lead to the stability of different structures types, as evident by our recent work on $Yb(Mn,M)_xAl_{12-x}$ (M = Fe, Ru; $x \leq 2.5$),[50] where low concentrations of Fe leads to $ThMn_{12}$[51] and $CaCr_2Al_{10}$[52] and higher concentrations of Fe leads to $YbFe_2Al_{10}$ structure type.[53]

Recently, doping and substitution studies on compounds that adopt the $CeCr_2Al_{20}$ structure type have been investigated because of their structural motif, specifically the Frank-Kasper cages formed by the main group element and interpenetrating rare earth and transition metal sublattices. In particular, $GdFe_2Zn_{20}$ orders ferromagnetically at 86 K, while $GdCo_2Zn_{20}$ orders antiferromagnetically at 5.7 K. Doping of Co for Fe in $GdFe_2Zn_{20}$ leads to a competition between ferromagnetism and antiferromagnetism based on the filling of the electronic states.[54] Also, substitution of transition metals in RT_2Zn_{20} can greatly impact ordering temperatures as seen in $TbCo_2Zn_{20}$ ($T_N \sim 2.5$ K) and ferromagnetic $TbFe_2Zn_{20}$ ($T_c \sim 66$ K).[55] Furthermore, such studies

*Reprinted with permission from Treadwell, L. J.; Watkins-Curry, P.; McAlpin, J. D.; Prestigiacomo, J.; Stadler, S.; Chan, J. Y., Substitution studies of Mn and Fe in $Ln_6W_4Al_{43}$ (Ln=Gd, Yb) and the structure of $Yb_6Ti_4Al_{43}$. *J. Solid State Chem.* **2014,** *210*, 267-274.Copyright 2014 Elsevier.

have led to the first pseudo-ternaries, $LnCr_2Al_{20-x}Fe_x$ (Ln = La, Gd, Yb), adopting the $CeCr_2Al_{20}$ structure type with a transition metal occupying the main group site.[39]

The $CeCr_2Al_{20}$ and $Ho_6Mo_4Al_{43}$ structure types share similar structural motifs such as interpenetrating rare earth and transition metal sublattices as well as one unique rare earth site.[56, 57] The $Ho_6Mo_4Al_{43}$ structure type can be adopted for small lanthanides and mid transition metals (Ln = Y, Nd, Sm, Gd-Lu, U, and M = Ti, V, Nb, Ta, Cr, W, and Mo).[16] Motivated by the structural motif of the $Ho_6Mo_4Al_{43}$ structure type, we have chosen to synthesize and characterize $Ln_6W_4Al_{43}$ (Ln = Gd, Yb) and investigate Fe and Mn site preference and the influence of doping on the magnetic properties. Herein, we report the synthesis, crystal structure, and anisotropic magnetic properties of $Ln_6W_4Al_{43}$ and pseudo-ternary compounds $Ln_6W_{4-x}Al_{43-y}M_{x+y}$ (Ln = Gd, Yb; M = Mn, Fe).

2.2 Experimental

2.2.1 Synthesis

The flux growth technique was selected to grow single crystals of $Ln_6W_{4-x}Al_{43-y}M_{x+y}$ (Ln = Gd, Yb; M = Mn, Fe), as shown in Figure 2.1, and a summary of all reaction ratios and temperature profiles for $Ln_6W_{4-x}Al_{43-y}M_{x+y}$ (Ln = Gd, Yb; M = Mn, Fe) are provided in Table 2.1. This technique uses a low-melting metal as a solvent (flux) which enables metals with higher melting points to dissolve at relatively low temperatures.[25-27] Single crystals of $Ln_6W_4Al_{43}$ (Ln = Gd, Yb) were grown with excess Al flux. Ln, W, and Al were weighed in atomic ratios of 1:2:50 and placed in alumina crucibles. The crucibles were placed into a fused silica tube, which were then evacuated (50–70 mTorr) and sealed. The evacuated silica tubes were placed into a furnace, and heated at a rate of 160 °C/h to 1000 °C, where they dwelled for 5.2 h. Then the vessels were cooled to 700 °C at a ramp down rate of 5.5 °C/h. After this temperature was reached, the silica

tubes were centrifuged to separate crystals from the aluminum flux. The single crystal with approximate dimensions of ~1 x 1 x 2 mm^3 were etched in dilute NaOH until aluminum flux was removed from the surface of the metallic crystals and then cleaned with dilute (~ 0.1 M) HNO_3.

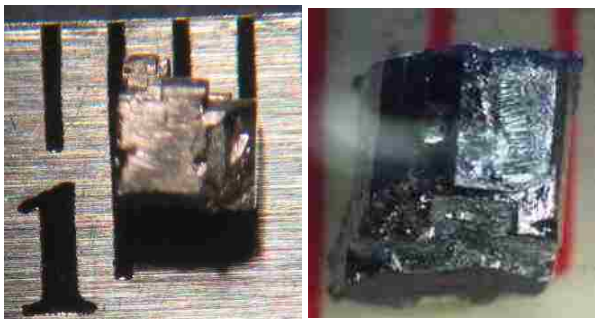

Figure 2.1. Aggregates of single crystal $Yb_6W_{4-x}Al_{43-x}Mn_{x+y}$ (left) and $Gd_6W_{4-x}Al_{43-x}Mn_{x+y}$ (right) are shown.

Table 2.1 $Ln_6W_{4-x}Al_{43-y}M_{x+y}$ (M = Mn, Fe) Reaction Profile

Targeted compound	Ratio (Ln:M:Al:T)	Ramp rate up (°C/h)	Dwell temp. (°C)	Dwell time (h)	Ramp rate down (°C/h)	Spin temp. (°C)	Product(s)
$Ln_6W_{4-x}Al_{43-y}T_{x+y}$ (Ln = Gd, Yb; T = Mn, Fe)	1:1:50:1	160	1000	5.2	5.5	700	Single crystals of $Ln_6W_{4-x}Al_{43-y}T_{x+y}$ (Ln = Gd, Yb; T = Mn, Fe), $LnAl_3$ (Ln = Gd, Yb), and LnT_2Al_{10} (Ln = Gd, Yb; T = Mn, Fe)
	1:1.5:50:0.5	160	1000	5.2	5.5	700	

2.2.2 Single-Crystal X-ray Diffraction

For crystal structure determinations, fragments of single crystals with approximate dimensions of ~0.05 x 0.07 x 0.08 mm^3 were chosen and glued onto glass fibers with epoxy. The fibers were mounted on a Nonius Kappa CCD X-ray diffractometer equipped with a Mo Kα radiation source (λ = 0.72073 Å) at room temperature. Crystal structures were solved by direct methods with SIR92[58] and refined with SHELXL97.[59] The atomic positions, Wyckoff symmetries, displacement parameters, site occupancies, and interatomic distances of $Ln_6W_4Al_{43}$ and $Ln_6W_{4-x}Al_{43-y}M_{x+y}$ (Ln = Gd, Yb; M = Mn, Fe) are provided in Tables 2.2-2.7.

Table 2.2. Crystallographic Parameters of $Ln_6W_4Al_{43}$ (Ln = Gd, Yb)

Compound	$Gd_6W_4Al_{43}$	$Yb_6W_4Al_{43}$
Crystal system	Hexagonal	Hexagonal
Space group	$P6_3/mcm$	$P6_3/mcm$
a (Å)	11.0240(10)	11.0040(3)
b (Å)	11.0240(10)	11.0040(3)
c (Å)	17.7780(19)	17.7280(7)
V (Å^3)	1871.1(3)	1859.05(10)
Z	2	2
Crystal dimensions (mm^3)	0.05 x 0.07 x 0.1	0.05 x 0.08 x 0.1
θ range (º)	2.13 - 30.01	3.14 - 30.01
μ (mm^{-1})	23.735	23.36
Data Collection and Refinement		
Measured reflections	6054	5974
Independent reflections	1026	1017
Reflections with I>2σ(I)	955	878
R_{int}	0.0349	0.0779
h	-15 to 15	-15 to 15
k	-12 to 12	-12 to 12
l	-18 to 24	-24 to 21
R_1[a]	0.0221	0.0285
wR_2[b]	0.0522	0.0573
Reflections	1026	1017
Parameters	54	54
$\Delta\rho_{max}$	1.475	1.314
$\Delta\rho_{min}$	-1.836	-1.713
Extinction coefficient	0.00056(5)	0.00085(9)
GOF	1.214	1.067

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$

[b] $R_w = [\Sigma [w(F_o^2 - F_c^2)^2]/\Sigma [w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (0.0393\ P)^2 + 22.11\ P]$, $[\Sigma [w(F_o^2 - F_c^2)^2]/\Sigma [w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (0.0227\ P)^2 + 25.53\ P]$, and $[\Sigma [w(F_o^2 - F_c^2)^2]/\Sigma [w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (0.0291\ P)^2]$ for, $Yb_6W_4Al_{43}$ and $Gd_6W_4Al_{43}$, respectively.

Table 2.3. $Ln_6W_4Al_{43}$ Atomic Positions (Ln = Gd, Yb)

Element	Wyckoff position	Symmetry	x	y	z	Occupancy	U_{eq}[a]
$Gd_6W_4Al_{43}$							
Gd1	12*k*	*m*	0.53199(6)	0	0.09572(3)	1.00	0.01237(16)
W1	6*g*	*mm*	0.73173(4)	0	1/4	1.00	0.00620(12)
W2	2*b*	$\bar{3}m$	0	0	0	1.00	0.00648(16)
Al1	24*l*	1	0.15864(19)	0.39462(18)	0.16372(10)	1.00	0.0111(3)
Al2	12*k*	*m*	0.1605(2)	0	0.61382(14)	1.00	0.0101(5)
Al3	12*k*	*m*	0.2537(2)	0	0.03015(15)	1.00	0.0100(5)
Al4	12*j*	*m*	0.1469(3)	0.5962(3)	1/4	1.00	0.0107(5)
Al5	12*i*	2	0.24714(13)	0.4943(3)	0	1.00	0.0118(5)
Al6	8*h*	3	1/3	2/3	0.12831(13)	0.939(3)	0.0123(7)
W6	8*h*	3	1/3	2/3	0.12831(13)	0.061(3)	0.0123(7)
Al7	6*g*	*m*2*m*	0.1486(3)	0	1/4	1.00	0.0096(9)
$Yb_6W_4Al_{43}$							
Yb1	12*k*	*m*	0.46896(4)	0	0.09475(2)	1.00	0.01041(15)
W1	6*g*	*mm*	0.26884(4)	0	1/4	1.00	0.00655(16)
W2	2*b*	$\bar{3}m$	0	0	0	1.00	0.0069(2)
Al1	24*l*	1	0.2369(2)	0.3944(2)	0.16349(12)	1.00	0.0110(4)
Al2	12*k*	*m*	0.1610(3)	0	0.11401(16)	1.00	0.0113(6)
Al3	12*k*	*m*	0.2544(3)	0	0.53107(17)	1.00	0.0110(6)
Al4	12*j*	*m*	0.1464(3)	0.5502(3)	1/4	1.00	0.0107(6)
Al5	12*i*	2	0.24704(15)	0.4941(3)	0	1.00	0.0117(6)
Al6	8*h*	3	1/3	2/3	0.12613(19)	0.673(12)	0.0088(6)
Al7	6*g*	*m*2*m*	0.8520(4)	0	1/4	1.00	0.0103(8)

[a] U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Table 2.4. Selected Interatomic Distances of $Ln_6W_4Al_{43}$ (Ln = Gd, and Yb)

	$Gd_6W_4Al_{43}$	$Yb_6W_4Al_{43}$
Ln (17 coordinate)		
Al11 x 2	3.0680(18)	3.059(2)
Al4 x 2	3.0877(13)	3.0825(14)
Al5 x 2	3.1017(4)	3.0872(4)
Al3 x 1	3.260(3)	3.246(3)
Al3 x 1	3.267(2)	3.248(3)
Al6 x 2	3.2535(5)	3.2442(6)
Al1 x 2	3.3259(24)	3.331(2)
Al5 x 2	3.3991(30)	3.38(3)
Al2 x 2	3.0877(13)	3.0825(14)
Ln1 x 1	3.4574(6)	3.422(7)
W1 x 1	3.5309(5)	3.5212(5)
W1 (12coordinate)		
Al7 x 2	2.7271(18)	2.730(2)
Al2 x 2	2.697(2)	2.683(3)
Al4 x 2	2.697(2)	2.683(3)
Al1 x 4	2.7271(18)	2.730(2)
Ln1 x 2	3.5661(5)	3.5675(5)
W2 (12 coordinate)		
Al2 x 6	2.688(2)	2.685(3)
Al3 x 6	2.847(2)	2.854(3)
Ln-Ln Network		
Ln-Ln NN[a] // c	3.4574(6)	3.422(7)
Ln-Ln NNN[b] //c	5.4987(8)	5.4940(7)
Ln-Ln //ab	5.5432(6)	5.54(4)

[a] Nearest Neighbor
[b] Next Nearest Neighbor

Table 2.5. $Ln_6W_{4-x}Al_{43-y}M_{x+y}$ (M = Mn, Fe) Crystallographic Parameters

Compound	$Gd_6W_4Al_{42.31(11)}Mn_{0.69(11)}$	$Gd_6W_4Al_{41.69(12)}Fe_{1.30(12)}$	$Yb_6W_{3.86(7)}Al_{41.76(7)}Mn_{1.39(7)}$	$Yb_6W_4Al_{41.76(12)}Fe_{1.24(12)}$
Crystal System	Hexagonal	Hexagonal	Hexagonal	Hexagonal
Space Group	$P6_3/mcm$	$P6_3/mcm$	$P6_3/mcm$	$P6_3/mcm$
a (Å)	11.005(3)	10.993(1)	10.975(1)	10.971(3)
c (Å)	17.746(8)	17.726(3)	17.611(3)	17.612(5)
V (Å^3)	1861.3(1)	1855.1(4)	1837.06(4)	1835.8(8)
Z	2	2	2	2
Crystal dimensions (mm^3)	0.05 x 0.05 x 0.05	0.05 x 0.05 x 0.05	0.05 x 0.05 x 0.05	0.05 x 0.05 x 0.05
θ range (º)	3.14 – 30.97	3.14 – 32.00	2.55 – 32.03	3.15 – 32.03
μ (mm^{-1})	24.068	24.398	28.592	29.076
Data Collection				
Measured Reflections	3693	3742	4005	4000
Independent Reflections	1100	1201	1192	1191
Reflections with I>2σ(I)	1053	1098	1048	1160
R_{int}	0.0193	0.0494	0.0326	0.0187
h	-15 to 15	-16 to 16	-16 to 16	-16 to 16
k	-13 to 13	-13 to 13	-13 to 13	-13 to 13
l	-25 to 25	-21 to 26	-26 to 26	-26 to 26
Refinement				
R_1 (F)[a]	0.0212	0.0316	0.0224	0.0196
wR_2[b]	0.0565	0.0734	0.0496	0.0452
Reflections	1100	1201	1192	1191
Parameters	54	54	55	54
$\Delta\rho_{max}$ (e Å^{-3})	1.455	1.955	1.83	1.295
$\Delta\rho_{min}$ (e Å^{-3})	-2.698	-3.171	-1.531	-1.337
Extinction coefficient	0.00158(8)	0.00126(9)	0.00049(4)	0.00059(4)
GOF	1.114	1.138	1.06	1.219

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$

[b] $_wR_2 = [\Sigma [w(F_o^2 - F_c^2)^2]/\Sigma [w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (0.0341\ P)^2 + 8.6856\ P]$, $[\Sigma [w(F_o^2 - F_c^2)^2]/\Sigma [w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (0.0407\ P)^2 + 2.0640\ P]$, and $[\Sigma [w(F_o^2 - F_c^2)^2]/\Sigma [w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (0.0278\ P)^2 + 4.8451\ P]$, and $[\Sigma [w(F_o^2 - F_c^2)^2]/\Sigma [w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (0.0163\ P)^2 + 15.2874\ P]$, $[\Sigma [w(F_o^2 - F_c^2)^2]/\Sigma [w(F_o^2)^2]]^{1/2}$ for $Gd_6W_4Al_{42.31(11)}Mn_{0.69(11)}$, $Gd_6W_4Al_{41.69(12)}Fe_{1.30(12)}$, $Yb_6W_{3.86(7)}Al_{41.76(7)}Mn_{1.39(7)}$, and $Yb_6W_4Al_{41.76(12)}Fe_{1.24(12)}$ respectively.

Table 2.6. $Ln_6W_{4-x}Al_{43-y}M_{x+y}$ (M = Mn, Fe) Atomic Positions

Element	Wyckoff position	Symmetry	x	y	z	Occupancy	U_{eq}[a]
$Gd_6W_4Al_{42.31(11)}Mn_{0.69(11)}$							
Gd1	12*k*	*m*	0.46913(3)	0	0.095410(15)	1.00	0.01031(10)
W1	6*g*	*mm*	0.26799(3)	0	1/4	1.00	0.00699(10)
W2	2*b*	$\bar{3}m$	0	0	0	1.00	0.00691(12)
Al1	24*l*	1	0.23586(13)	0.39526(13)	0.16377(7)	1.00	0.0116(2)
Al2	12*k*	*m*	0.16061(16)	0	0.11402(10)	1.00	0.0110(3)
Al3	12*k*	*m*	0.25427(16)	0	0.53023(11)	1.00	0.0108(3)
Al4	12*j*	*m*	0.14763(19)	0.55050(18)	1/4	1.00	0.0110(3)
Al5	12*i*	2	0.24748(9)	0.49497(19)	0	1.00	0.0161(4)
Al6	8*h*	3	1/3	2/3	0.12809(11)	0.826(11)	0.0123(5)
Mn6	8*h*	3	1/3	2/3	0.12809(11)	0.174(11)	0.0123(5)
Al7	6*g*	*m*2*m*	0.8512(2)	0	1/4		0.0094(4)
$Gd_6W_4Al_{41.69(12)}Fe_{1.30(12)}$							
Gd1	12*k*	*m*	0.46896(3)	0	0.09546(2)	1.00	0.01055(12)
W1	6*g*	*mm*	0.26736(3)	0	1/4	1.00	0.00654(12)
W2	2*b*	$\bar{3}m$	0	0	0	1.00	0.00648(15)
Al1	24*l*	1	0.23586(16)	0.39665(16)	0.16311(10)	1.00	0.0122(3)
Al2	12*k*	*m*	0.1610(2)	0	0.11382(14)	1.00	0.0109(4)
Al3	12*k*	*m*	0.25491(19)	0	0.53025(14)	1.00	0.0109(4)
Al4	12*j*	*m*	0.1491(2)	0.5510(2)	1/4	1.00	0.0113(4)
Al5	12*i*	2	0.24855(13)	0.4971(3)	0	1.00	0.0226(6)
Al6	8*h*	3	1/3	2/3	0.13049(14)	0.673(12)	0.0156(7)
Fe6	8*h*	3	1/3	2/3	0.13049(14)	0.327(12)	0.0156(7)
Al7	6*g*	*m*2*m*	0.8500(3)	0	1/4	1.00	0.0096(6)
$Yb_6W_{3.86(7)}Al_{41.76(7)}Mn_{1.39(7)}$							
Yb1	12*k*	*m*	0.46796(2)	0	0.095272(14)	1.00	0.01039(9)
W1	6*g*	*mm*	0.26692(3)	0	1/4	0.952(3)	0.00692(11)
Fe1	6*g*	*mm*	0.26692(3)	0	1/4	0.048(3)	0.00692(11)
W2	2*b*	$\bar{3}m$	0	0	0	1.00	0.00671(12)
Al1	24*l*	1	0.23643(14)	0.39665(13)	0.16249(8)	1.00	0.0112(3)

(Table 2.6. continued)

Element	Wyckoff position	Symmetry	x	y	z	Occupancy	U_{eq}[a]
Al2	12*k*	*m*	0.16010(16)	0	0.11427(10)	1.00	0.0096(3)
Al3	12*k*	*m*	0.25532(16)	0	0.53060(11)	1.00	0.0105(4)
Al4	12*j*	*m*	0.1485(2)	0.54950(18)	1/4	1.00	0.0117(4)
Al5	12*i*	2	0.24838(10)	0.4968(2)	0	1.00	0.0205(5)
Al6	8*h*	3	1/3	2/3	0.12932(11)	0.688(10)	0.0145(5)
Fe6	8*h*	3	1/3	2/3	0.12932(11)	0.312(10)	0.0145(5)
Al7	6*g*	*m*2*m*	0.8496(2)	0	1/4	1.00	0.0098(5)
$Yb_6W_4Al_{41.76(12)}Fe_{1.24(12)}$							
Yb1	12*k*	*m*	0.46819(2)	0	0.095210(13)	1.00	0.00830(7)
W1	6*g*	*mm*	0.26727(2)	0	1/4	1.00	0.00420(7)
W2	2*b*	$\bar{3}m$	0	0	0	1.00	0.00424(10)
Al1	24*l*	1	0.23658(13)	0.39730(12)	0.16246(7)	1.00	0.0098(2)
Al2	12*k*	*m*	0.16069(16)	0	0.11393(9)	1.00	0.0086(3)
Al3	12*k*	*m*	0.25599(15)	0	0.53066(10)	1.00	0.0095(3)
Al4	12*j*	*m*	0.14877(19)	0.55033(17)	1/4	1.00	0.0097(3)
Al5	12*i*	2	0.24844(10)	0.49689(19)	0	1.00	0.0199(4)
Al6	8*h*	3	1/3	2/3	0.13003(10)	0.673(12)	0.0131(5)
Fe6	8*h*	3	1/3	2/3	0.13003(10)	0.327(12)	0.0131(5)
Al7	6*g*	*m*2*m*	0.8493(2)	0	1/4	1.00	0.0087(4)

[a] U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor

Table 2.7. $Ln_6W_{4-x}Al_{43-y}M_{x+y}$ (M = Mn, Fe) Selected Interatomic Distances

	$Gd_6W_4Al_{42.31(11)}Mn_{0.69(11)}$	$Gd_6W_4Al_{41.69(12)}Fe_{1.30(12)}$	$Yb_6W_{3.86(7)}Al_{41.76(7)}Mn_{1.39(7)}$	$Yb_6W_4Al_{41.76(12)}Fe_{1.24(12)}$
Ln (17 coordinate)				
Al1 x 2	3.0649(14)	3.0588(16)	3.0519(13)	3.0482(13)
Al4 x 2	3.0843(13)	3.0865(12)	3.0699(9)	3.0720(11)
Al5 x 2	3.0969(7)	3.0950(4)	3.0797(2)	3.0793(6)
Al3 x 1	3.2499(17)	3.2407(19)	3.2186(18)	3.2147(18)
Al3 x 1	3.2563(14)	3.2481(14)	3.2436(18)	3.2325(19)
Al6 x 2	3.2472(8)	3.2515(6)	3.2436(4)	3.2447(8)
Al1 x 2	3.3136(17)	3.2944(17)	3.2829(18)	3.2808(13)
Al5 x 2	3.0969(7)	3.3893(21)	3.3838(20)	3.3812(20)
Al2 x 1	3.4113(13)	3.4010(12)	3.3953(9)	3.3897(13)
Ln1 x 1	3.4538(15)	3.4524(7)	3.4286(3)	3.4255(10)
M1 x 1	3.5250(10)	3.5236(5)	3.5062(2)	3.5058(8)
W1 (12 coordinate)				
Al7 x 2	2.5593(6)	2.5516(30)	2.5438(2)	2.5463(19)
Al2 x 2	2.6869(19)	2.6822(23)	2.6623(17)	2.6665(17)
Al4 x 2	2.6935(18)	2.7015(19)	2.6870(18)	2.6906(18)
Al1 x 4	2.7213(13)	2.7258(16)	2.7278(13)	2.7287(13)
Ln1 x 2	3.5250(10)	3.5236(5)	3.5062(2)	3.5058(8)
W2 (12 coordinate)				
Al2 x 6	2.6866(19)	2.6839(24)	2.6716(17)	2.6710(17)
Al3 x 6	2.8492(18)	2.8531(12)	2.8535(18)	2.8599(18)
Ln-Ln Network				
Ln-Ln NN //*c*[a]	3.4538(15)	3.4524(7)	3.4286(3)	3.4255(10)
Ln-Ln NNN //*c*[b]	5.4867(25)	5.4788(11)	5.4498(4)	5.4523(16)
Ln-Ln //*ab*	5.5339(14)	5.5282(4)	5.5212(1)	5.5187(14)

[a]Nearest neighbors
[b]Next nearest neighbor

An unusually small atomic displacement parameter (ADP) on the Al6, in comparison to the others Al sites, coupled with residual electron density was observed in $Gd_6W_4Al_{43}$ and $Ln_6W_{4-x}Al_{43-y}M_{x+y}$ (Ln = Gd, Yb; M = Mn, Fe). Therefore, in $Gd_6W_4Al_{43}$ and $Ln_6W_{4-x}Al_{43-y}M_{x+y}$ (Ln = Gd, Yb; M = Mn, Fe), the parent transition metal (W) and the dopant (M = Mn, Fe) were modeled on the Al6 site to identify the best statistical model. First, the parent transition metal (W) was modeled on the Al6 site, which resulted in suitable ADP for $Gd_6W_4Al_{43}$ and unusually large ADP in $Ln_6W_{4-x}Al_{43-y}M_{x+y}$ (Ln = Gd, Yb; M = Mn, Fe) signifying excessive electron density. As a result, the dopant (M) was modeled on the Al6 site which resulted in a well behaved ADP, concluding that the dopant (M = Mn, Fe) is occupying the Al6 site. There was no residual electron density observed on the Al6 site during refinement of $Yb_6W_4Al_{43}$, indicative of a fully occupied Al-site. The structural refinement of Mn in $Ln_6W_4Al_{43}$ led to $Gd_6W_4Al_{43-y}Mn_y$ and $Yb_6W_{4-x}Al_{43-y}Mn_{x+y}$ as the best statistical models. For $Ln_6W_4Al_{43-y}Fe_y$ (Ln = Gd, Yb), the Fe was only modeled on the Al6 site because refining Fe on either transition metal site led to an unstable refinement model. This behavior is consistent with the fact that the latter transition metals do not form in the $Ho_6Mo_4Al_{43}$ structure type.[17]

2.2.3 Elemental Analysis

Elemental analysis was performed via energy dispersive spectroscopy (EDS) using a EDAX detector equipped with a FEI Quanta 200 scanning electron microscope with an accelerating voltage of 20 kV. Spectra were integrated for 60 seconds and the results from 7-10 spots were averaged and normalized to Ln. The approximate compositions obtained by normalizing the EDS composition to the lanthanide are $Gd_6W_{3.5(1)}Al_{40.2(6)}$, $Yb_6W_{4.2(2)}Al_{46.5(2)}$, $Gd_6W_{3.76(14)}Al_{44.23(25)}Mn_{0.3(1)}$, $Gd_6W_{4.03(2)}Al_{45.33(26)}Fe_{1.29(3)}$, $Yb_6W_{4.2(2)}Al_{46.5(2)}$, $Yb_6W_{3.43(7)}Al_{41.68.33(18)}Mn_{1.12(3)}$, and $Yb_6W_{3.9(4)}Al_{46.33(25)}Fe_{0.2(1)}$.

2.2.4 Physical Properties

Magnetic data were collected on oriented single crystals using a Quantum Design Magnetic Property Measurement System (MPMS). The temperature-dependent susceptibility was measured under zero-field (ZFC) and field-cooled (FC) conditions between 1.8 and 300 K with an applied magnetic field of 0.1 T in the *ab*- and *c*-direction. Also, temperature-dependent susceptibility was measured in ZFC and FC conditions between 1.8 K and 50 K with 0.01 T in the *ab*- and *c*-directions. Field-dependent magnetization data were measured at 1.8 K with fields up to 9 T for all Gd-analogues and at 3 K with applied fields up to 7 T for the Yb-analogues.

2.3 Results and Discussion

2.3.1 Crystal Structure

$Ln_6W_{4-x}Al_{43-y}M_{x+y}$ (Ln = Gd, Yb; M = Mn, Fe) adopts the $Ho_6Mo_4Al_{43}$ structure type (space group $P6_3/mcm$) with $a \sim 11$ Å and $c \sim 17$ Å. The crystal structure of $Yb_6W_4Al_{43}$ is shown in Figure 2.2. Each W1 polyhedron is surrounded by 10 Al and 2 Yb atoms, with W-Al interatomic distances ranging from 2.6027(9) to 2.7304(10) Å and a W-Yb interatomic distance of 3.5339(4) Å. The W1 icosahedra are corner-sharing with each other by Al atoms. W2 atoms are surrounded by 12 Al atoms with interatomic distances of 2.7047(14) Å and 2.8538(14) Å. Yb is 17 coordinate with Yb-Al distances ranging from 3.07454(10) Å for Al1 to 3.4966(7) Å for Al2 and Yb-W1 contact of 3.5339(4) Å, and Yb-Yb distance of 3.4709(3) Å. The Yb atoms form two pairs of Kagome lattices stacked in the *c*-direction shown in Figure 2.3. All triangular networks are equilateral with an in-plane distance of 5.54(4) Å separating Yb atoms. The two sets of triangular networks are separated by 3.422(7) Å, while 5.4940(7) Å separates the individual triangular nets. Instead of the triangular networks lining parallel in the *c*-direction, the latter pair is twisted by ~ 4 degrees, illustrated in Figure 2.3. All Al environments are 12 coordinate forming distorted

icosahedra around Al4, Al5, and Al6 and distorted bi-capped pentagonal prisms around Al1, Al2, Al3, and Al7. Uniquely, the Al6 position resides directly in-plane and in the voids of the triangular network formed by Yb atoms. Therefore, Al6 distorted icosahedron is capped with three Yb atoms making it the center piece of the Kagome network shown in Figure 2.4. The best statistical models of $Ln_6W_{4-x}Al_{43-y}M_{x+y}$ (Ln = Gd, Yb: M = Mn, Fe) consist of a dopant (M = Mn, Fe) occupying the Al6 site. The un-doped analog $Yb_6W_4Al_{43}$ consist of a fully occupied Al6 site whereas a mix-occupancy on the Al6 site (92.9 % Al and 6.1 % W) is observed for $Gd_6W_4Al_{43}$. As a result of Mn and Fe occupying the Al6 site, the Yb-Yb distance should increase and Gd-Gd should decrease. The Yb-Yb in-plane distance of the un-doped analog is 3.4209(7) Å, while the Yb-Yb distance in $Yb_6W_{4-x}Al_{43-y}M_{x+y}$ (M = Mn, Fe) is 3.4286(3) and 3.4255(10) Å, respectively. The Gd-Gd in-plane distance in $Gd_6W_4Al_{43}$ and $Gd_6W_4Al_{43-y}M_y$ (M = Mn, Fe) is 3.4575(6) Å and 3.4538(15) Å and 3.4524(7) Å, respectively. Overall, all the bond distances in $Ln_6W_{4-x}Al_{43-y}M_{x+y}$ (Ln = Gd, Yb; M = Mn, Fe) decrease with the presence of the dopant (M = Mn, Fe), except Yb-Yb, in comparison to $Ln_6W_4Al_{43}$ (Ln = Gd, Yb). Also, there is a systematic decrease in volume from $Gd_6W_4Al_{43} > Gd_6W_4Al_{43-y}Mn_y > Gd_6W_4Al_{43-y}Fe_y$, likewise for the Yb-analogs. The bond distance and volume trends are consistent and as expected.

2.3.2 Magnetic Properties

Temperature dependent magnetic susceptibility data of $Gd_6W_4Al_{43-y}M_y$ (M = Mn, Fe) with an applied field of 0.1 T are shown in Figure 2.5. With the field oriented in the *ab*-plane, the magnetic susceptibility increases with decreasing temperature until $T_N \sim 16$ K, followed by a decrease in magnetization. Interestingly, when the field is parallel to the *c*-direction there is a steady increase in susceptibility with decreasing temperature. All compounds exhibit Curie-Weiss behavior above T_N and were fitted to a modified Curie Weiss equation, $\chi = \chi_o + (C/(T-\theta))$, where

χ_o is the temperature independent contribution, θ is the Weiss constant, and C is the Curie constant.

The constants from the Curie Weiss fit are provided in Table 2.8.

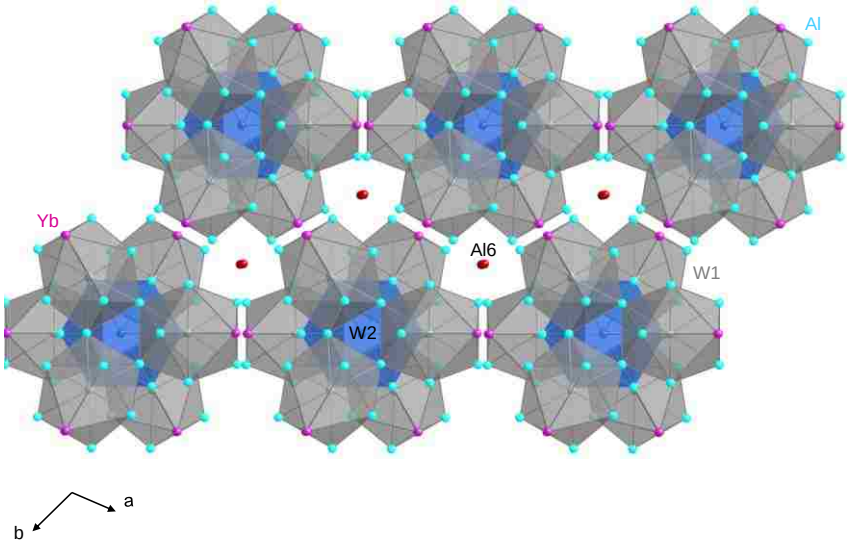

Figure 3.2. Transition metal sublattices of $Yb_6W_4Al_{43}$ viewed down the *c*-direction. W1 are shown as grey translucent icosahedra and W2 are blue icosahedra. Aluminum atoms are light blue spheres except Al6 which is represented as red spheres, while Yb are pink spheres forming Kagome lattice in the *ab*-plane and stacking in the *c*-direction.

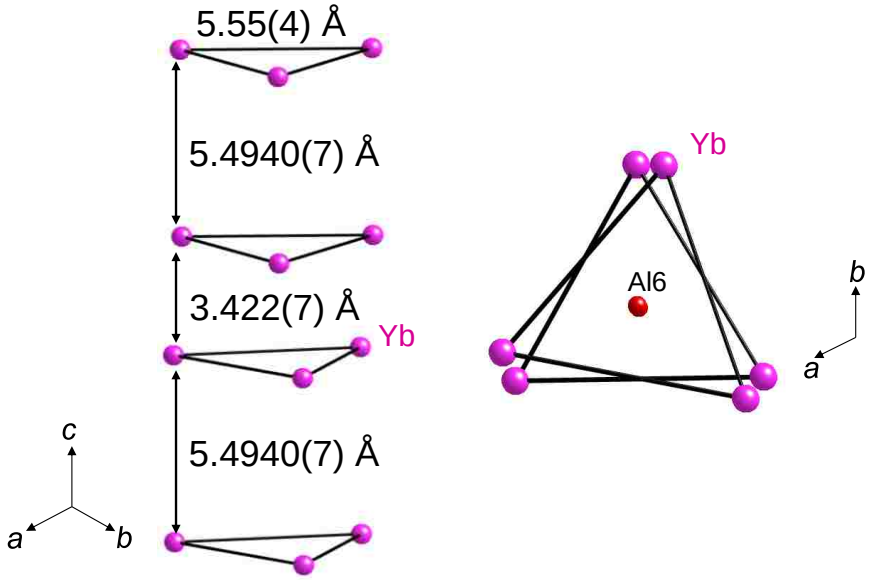

Figure 2.4. The Yb-network viewed in the *ab*- and *c*-direction. The Yb atoms (pink spheres) form equilateral triangles in the *ab*-direction, and stacking along the *c*-direction.

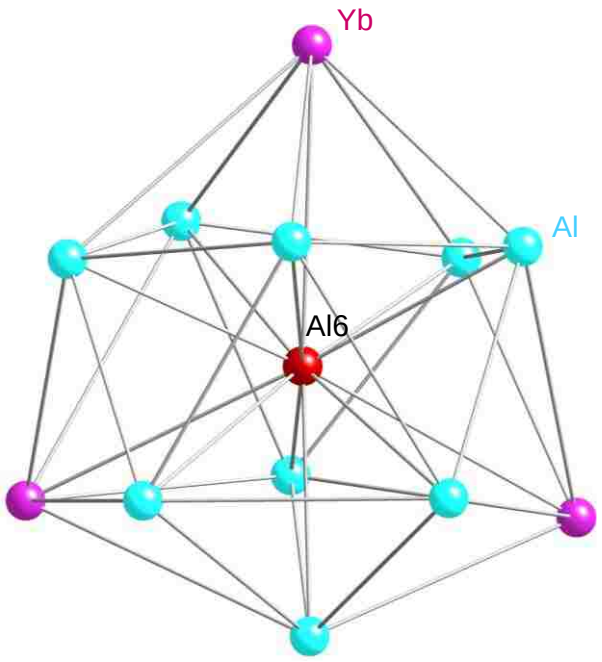

Figure 2.5. The local environment of Al6 is shown.

Table 2.8. Magnetic Properties of $Gd_6W_4Al_{43}$, $Gd_6W_4Al_{43-y}Mn_y$, $Gd_6W_4Al_{43-y}Fe_y$

Compound	$H_{direction}$	Fit range (K)	χ_o x10^{-2} (emu/mol Gd)	θ_W (K)	T_N (K)	μ_{eff} (μ_B/mol Gd)
$Gd_6W_4Al_{43}$	H//*ab*	>50	-0.1406(6)	13.62(7)	15	7.92(3)
$Gd_6W_4Al_{43}$	H//*c*	>45	-0.0562(8)	17.4(2)	15	7.93(2)
$Gd_6W_4Al_{42.31(11)}Mn_{0.69(11)}$	H//*ab*	>50	-0.1773(6)	9.91(6)	14	7.94(1)
$Gd_6W_4Al_{42.31(11)}Mn_{0.69(11)}$	H//*c*	>40	-0.0658(3)	11.82(5)	14	7.94(1)
$Gd_6W_4Al_{41.69(12)}Fe_{1.30(12)}$	H//*ab*	>50	-0.0731(2)	7.56(5)	13	7.78(5)
$Gd_6W_4Al_{41.69(12)}Fe_{1.30(12)}$	H//*c*	>50	-0.1251(4)	9.05(5)	13	7.96(1)

The ordering of spins in an antiferromagnet (AFM) can occur in a number of different configurations depending on the coordination of the magnetic ions. This is especially true in layered compounds, such as [(1-x)La, xCa]MnO_3, where the spins may order ferromagnetically (FM) within the slab while ordering antiferromagnetically between neighboring slabs (A-type), or vice versa (C-type).[60] Furthermore, because the Weiss constant represents the global exchange

interaction of the system, it is possible for an AFM to yield values which are positive rather than negative when its high temperature susceptibility data are fitted.[61, 62] The anisotropic behavior of $Gd_6W_4Al_{43-y}M_y$ (M = Mn, Fe) in Figure 2.5 implies that, if the peak is indeed associated with an AFM transition, the easy-axis of the magnetization lies in the *ab*-plane. This is interesting because in $Gd_6W_4Al_{43-y}M_y$ (M = Mn, Fe) the *ab*-plane constitutes a Kagome lattice. Thus, the possibility of observing glassy spin-dynamics in the ground-state arises because of the geometrical frustration present in this scenario. Although it is difficult to say for sure whether or not FM ordering exists between the slabs of magnetic ions (Gd) without having neutron diffraction data, this would help to explain the positive Weiss constants obtained from the fits of the modified Curie-Weiss equation and the increase in susceptibility with decreasing temperature when the field is applied parallel to the *c*-axis.

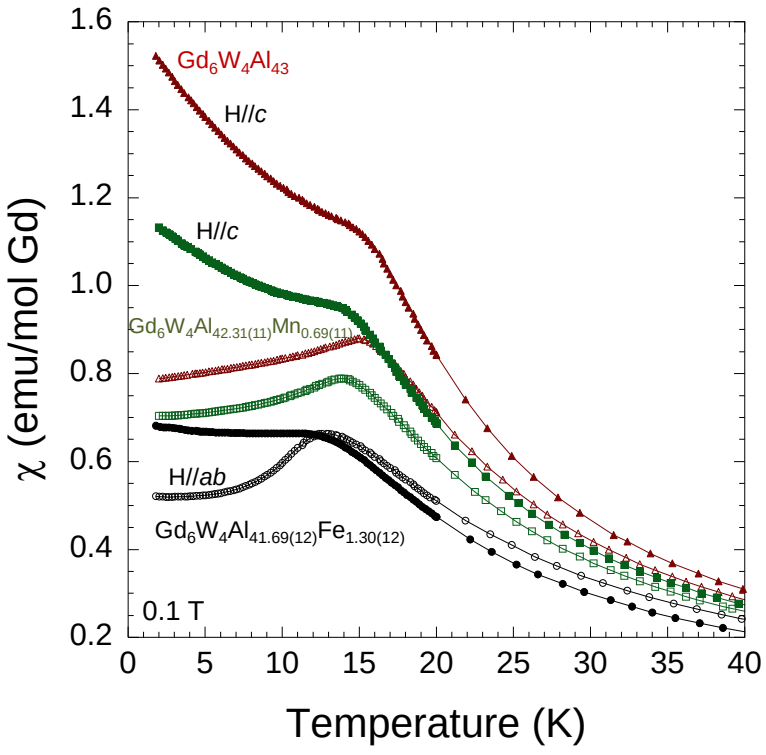

Figure 2.6. Temperature dependent ZFC magnetization of $Gd_6W_4Al_{43-y}M_y$ (M = Mn, Fe). $G_6W_4Al_{43}$, $Gd_6W_4Al_{43-y}Mn_y$, $Gd_6W_4Al_{43-y}Fe_y$ are depicted as triangle, squares, circles, respectively, with the filled shapes representing the H//*c* and unfilled shapes representing H//*ab*.

Field dependent magnetization of $Gd_6W_4Al_{43-y}M_y$ (M = Mn, Fe) at 2 K in applied fields up to 7 T are shown in Figure 2.6. The magnetization of all samples is linear at low fields followed by a change in slope at ~ 4.5 T. With the exception of $Gd_6W_4Al_{41.69(12)}Fe_{1.30(12)}$ (H//*c*), the magnetic moment saturates at ~ 6.3 μ_B/mol Gd for all compounds. Though this value is slightly less than the calculated spin-only Gd^{3+} ion, it is consistent with the previously reported magnetic data on single crystals and polycrystalline samples of $Gd_6W_4Al_{43}$. The anisotropy seen in the field dependent magnetization of $Gd_6W_4Al_{41.69(12)}Fe_{1.30(12)}$ is puzzling since the Gd^{3+} ion has a spherically symmetric spin state. However, the low M_s suggest antiparallel type of coupling between Gd (4*f*) and Fe (3*d*) in the *c*-plane, similar to $Gd(Ni_{1-x}Fe_x)_3$.[63]

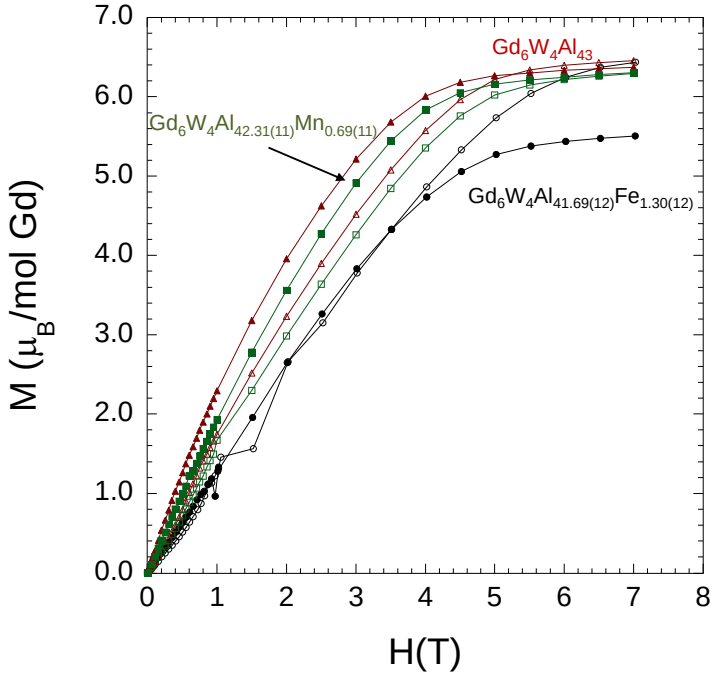

Figure 2.7. Field dependent magnetization of $Gd_6W_4Al_{43-y}M_y$ (M = Mn, Fe) are shown at 1.8 K. $Gd_6W_4Al_{43}$, $Gd_6W_4Al_{43-y}Mn_y$, $Gd_6W_4Al_{43-y}Fe_y$ are depicted as triangles, squares, and circles, respectively, with the filled shapes representing the H//*c* and unfilled shapes representing H//*ab*.

Figure 2.7 shows the field-dependent magnetization of $Yb_6W_{4-x}Al_{43-y}M_{x+y}$ (M = Mn, Fe) at 3 K. The field-dependent magnetization of $Yb_6W_4Al_{43}$ exhibits a small increase in magnetization between 0 – 0.05 T followed by a decrease in magnetization. The high field portion is consistent

with the Yb ions adopting the non-magnetic divalent configuration and the increase in low field could be due to a weak paramagnetic contribution of the sample or the background due to geometry of the sample holder. $Yb_6W_4Al_{41.76(12)}Fe_{1.24(12)}$ shows similar behavior as the un-doped analog with the exceptions that the magnetization increases between 0 – 0.8 T and the negative slope at high field is less pronounced. However, $Yb_6W_{3.86(7)}Al_{41.76(7)}Mn_{1.39(7)}$ exhibits an increase in magnetization between 0 – 4 T followed by saturation which is typical paramagnetic response. Magnetic susceptibility, not shown, for $Yb_6W_4Al_{43}$ and $Yb_6W_4Al_{41.76(12)}Fe_{1.24(12)}$ is consistent with nearly temperature independent paramagnets, whereas $Yb_6W_{3.86(7)}Al_{41.76(7)}Mn_{1.39(7)}$ exhibits a small Curie tail at low temperatures.

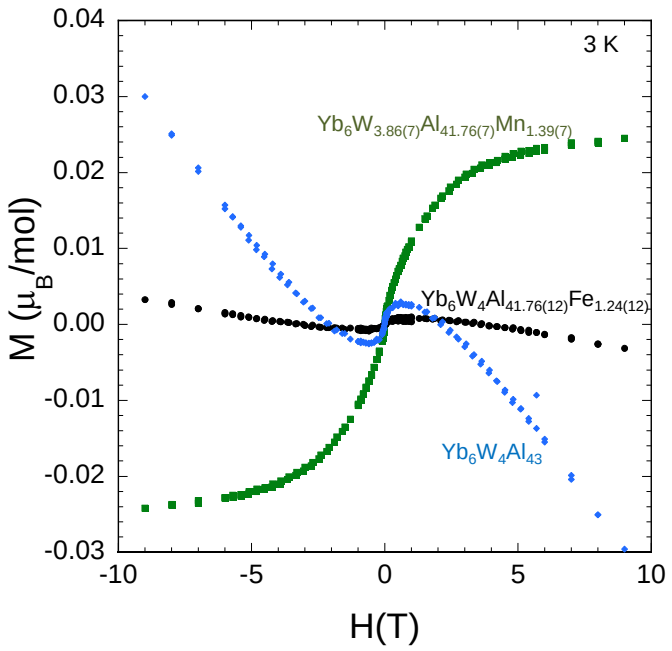

Figure 2.8. Field dependent magnetization of $Yb_6W_{4-x}Al_{43-y}M_{x+y}$ (M = Mn, Fe) are shown at 3 K.

2.4 Conclusion

Herein, we mapped out the synthetic conditions to grow $Ln_6W_{4-x}Al_{43-y}M_{x+y}$ (Ln = Gd, Yb; M = Mn, Fe). The ability to control certain variables such as the flux, reaction ratios, and reaction profiles while utilizing the flux growth method allows for the growth of the desired compound

over competing ternaries and binaries. We successfully grew single crystals of the $Ln_6W_4Al_{43}$ and pseudo-ternary compounds, $Ln_6W_{4-x}Al_{43-y}M_{x+y}$ (Ln = Gd, Yb; M = Mn, Fe). Refinement of the X-ray diffraction data of Fe- and Mn- doped GdW_4Al_{43} shows that the dopants prefer to substitute for Al as opposed to W, similar to previously published $LnCr_2Al_{20-x}Fe_x$.[39] For the $Yb_6W_{4-x}Al_{43-y}M_{x+y}$ (M = Mn, Fe) phase, Mn occupies both W1 and Al6 site, while Fe prefers to occupy the Al6 site only. Furthermore, Mn prefers to occupy the W1 instead of W2 site because W1-Al distances have shorter contacts (2.5438(2), 2.6624(16), 2.6870(17), and 2.7278(13) Å) than W2-Al (2.6716(14) and 2.8535(9) Å. The cell volume in $Gd_6W_4Al_{43}$ (1871.2(3) $Å^3$) is larger than $Yb_6W_4Al_{43}$ (1856.2(3) $Å^3$) and therefore it is plausible to infer that Mn prefers to occupy the Al6 site in $Gd_6W_4Al_{43}$. The results indicate that $Ln_6M_4Al_{43}$ can be adopted for late lanthanides and early/mid transition metals and can be rationalized by both atomic volume and valence electron count arguments similar to LnT_2Al_{20} compounds.[64]

This first report of anisotropic magnetic behavior on compounds adopting the $Ho_6Mo_4Al_{43}$ structure type ($Gd_6W_4Al_{43-y}M_y$; M = Mn, Fe) demonstrates the importance of growing single crystals to determine the intrinsic and anisotropic magnetic properties of materials.[27] The effective moments (μ_{eff}) of the Gd-analogs are close to the magnetic moment for a free Gd^{3+} ion (7.94 μ_B). However, there is a decreases in saturation magnetization M_s from $Gd_6W_4Al_{43}$ > $Gd_6W_4Al_{43-y}Mn_y$ > $Gd_6W_4Al_{43-y}Fe_y$, which suggest the dopant (Mn/Fe (3*d*)) spins are participating in an antiparallel arrangement with Gd (4*f*).[63, 65] The magnetization curves of the Yb-analogs are sensitive to doping with magnetic elements.

Chapter 3. Investigation of Fe incorporation in $LnCr_2Al_{20}$ (Ln = La, Gd, Yb) with ^{57}Fe Mössbauer and single crystal X-ray diffraction

3.1 Introduction

The study of intermetallics containing rare earth, transition metal, and group 13 elements has attracted much attention due to the strong interaction of the conduction electrons with the local magnetic moments.[27] This can lead to interesting magnetic and electrical properties, including superconductivity, Kondo behavior, valence instability, heavy fermion behavior, and quantum criticality. Ytterbium-containing compounds are particularly intriguing due to the potential valence instability between the Yb^{3+} (f^{13}) and Yb^{2+} (f^{14}) states, and heavy fermion behavior has recently been observed in YbSi (ThAl structure type),[66, 67] $YbCu_2Si_2$ ($ThCr_2Si_2$ structure type),[68, 69] and YbT_2Zn_{20} (T = Fe, Co, Ru, Rh, Os, Ir; $CeCr_2Al_{20}$ structure type).[56, 70] In addition, other members of the LnT_2Zn_{20} (Ln = lanthanides; T = Fe, Co, Ru, Rh, Os, Ir) series have been investigated, and it was found that the magnetic properties greatly depend on the transition metal present and the valence electron count.[40, 55, 56, 71]

Isostructural LnT_2Al_{20} (Ln = lanthanides; T = Ti-Cr, Nb, Mo, Ta, W) compounds have also been reported.[17, 72] Recently it was found that $PrTi_2Al_{20}$ and PrV_2Al_{20} exhibits quadrupolar order at 2 K and 0.6 K, respectively, while $PrCr_2Al_{20}$ shows Kondo behavior at low temperatures.[73-75] The SmT_2Al_{20} (T = Ti-Cr) analogues show valence fluctuations and order antiferromagnetically below 7 K.[76] GdV_2Al_{20} and $GdCr_2Al_{20}$ have also been shown to order antiferromagnetically at 2.35(5) and 3.90(5) K,[77] respectively, while CeT_2Al_{20} (T = Ti-Cr) and $YbCr_2Al_{20}$ are temperature independent paramagnets consistent with Ce^{4+} and Yb^{2+}, respectively.[78-80]

*Reprinted with permission from Treadwell, L. J.; McAlpin, J. D.; Schmitt, D. C.; Kangas, M. J.; Sougrati, M. T.; Haldolaarachchige, N.; Young, D. P.; Jumas, J.-C.; Chan, J. Y., Investigation of Fe incorporation in $LnCr_2Al_{20}$ (Ln = La, Gd, Yb) with ^{57}Fe Mössbauer and single crystal X-ray diffraction. *Inorg. Chem.* **2013,** *52*, 5055-5062.

Due to the robust structure of the $CeCr_2Al_{20}$ structure type and the Frank-Kasper cages formed by the main group element, several different doping atoms have been incorporated onto different sites to investigate the effect on magnetic and electronic properties. $GdFe_2Zn_{20}$ has an abnormally high Curie temperature T_c at 86 K, while $GdCo_2Zn_{20}$ orders antiferromagnetically at 5.7 K. A doping study of Co for Fe, $Gd(Fe_xCo_{1-x})_2Zn_{20}$, was performed to study the ferromagnetic to antiferromagnetic ordering associated with the filling of the electronic states.[54] Also, Al was doped for Zn in $GdFe_2Zn_{20}$, which leads to a ferromagnetic ordering, but T_c decreases with increasing Al doping.[40] We focus our efforts on doping Fe into $LnCr_2Al_{20}$ (Ln = La, Gd, Yb) in order to investigate Fe site preferences. The parent analogues of La and Yb adopting the $CeCr_2Al_{20}$ structure type are diamagnetic and Pauli paramagnetic, respectively, while the Gd analogue shows antiferromagnetic ordering at 3.90(5) K.[77, 81] Herein, we report the synthesis, crystal structure, Mössbauer results, and magnetic properties of the first pseudo-ternary of the $CeCr_2Al_{20}$-structure type where the transition metal dopant (Fe) substitutes for the main group element: $LnCr_2Fe_xAl_{20-x}$ (Ln = La, Gd, Yb).

3.2 Experimental Section

3.2.1 Synthesis

Single crystals of $LnCr_2Al_{20-x}Fe_x$ (Ln = La, Gd, Yb) were prepared using the molten metal flux technique using Ln (99.9%), Cr (99.996 %), Fe (99.998 %), and Al (99.999%) in various ratios. A ratio of 1:1.5:0.5:50 and 1:1:1:50 Ln:Cr:Fe:Al were used to prepare Yb and Gd analogues, respectively. The ratios of 1:1.5:0.5:100 and 1:1:1:100 for La:Cr:Fe:Al, respectively, were used to synthesize the La-analogue. For all reactions, the elements were placed in an alumina crucible, topped with a second alumina crucible, and then sealed inside an evacuated fused-silica tube. The samples were placed in an oven and heated to 1000 °C at 100 °C/h, dwelled for 24 h,

and slowly (2 °C/h) cooled to 800 °C. The samples were then removed from the oven and centrifuged to remove excess flux. Residual flux was etched using (~ 1 M) NaOH. For the Yb-reactions, the lower Fe concentration (1:1.5:0.5:50) only yielded crystals adopting the $CeCr_2Al_{20}$ structure type (space group $Fd\bar{3}m$, a ~ 14.5 Å), with octahedral morphology up to 3 mm in length.[17] The larger Fe concentration (1:1:1:50) produced smaller crystals (≤ 1 mm^3) adopting the $CeCr_2Al_{20}$ structure type and bar-shaped crystals of the $YbFe_2Al_{10}$ structure type (space group *Cmcm*, a ~ 8.966 Å, b ~ 10.153 Å, c ~ 9.003 Å)[82] which could be separated based on morphology. As a result, higher concentrations of Fe were not attempted due to the presence of $YbFe_2Al_{10}$. The higher Fe-ratio of the Gd-synthesis yielded flat plates crystals (≤ 2.5 mm^3) adopting the $CeCr_2Al_{20}$ structure type, while the lower Fe-concentration yielded compounds adopting the $Ho_6Mo_4Al_{43}$ structure type (space group $P6_3/mcm$, a ~ 10.975 Å, c ~ 17.611 Å),[80] which was determined by single crystal X-ray diffraction. As a result, only one Fe doped Gd-compound is reported. Single crystals of the La-analogue were synthesized with an increase Al concentration to avoid the $Ho_6Mo_4Al_{43}$ structure type in order to stabilize the $CeCr_2Al_{20}$ structure type.

3.2.2 Structural Characterization

Single crystals of Fe-doped $LnCr_2Al_{20}$ (Ln = La, Gd, Yb) were cleaved and attached to a glass fiber. The fiber was then mounted on the goniometer of a Nonius Kappa CCD diffractometer with Mo Kα radiation (λ = 0.71073 Å). The diffraction pattern was indexed to a face-centered cubic unit cell with the lattice parameter a ~ 14.5 Å, consistent with the $CeCr_2Al_{20}$ structure type.[17] A multi-scan absorption correction was applied to all data sets. The crystal structure was solved using SIR97[58] and refined with SHELXL97.[59] The final models were corrected for extinction, and atomic displacement parameters were modeled anisotropically. Collection and refinement parameters, atomic positions, and interatomic distances are provided in Tables 3.1-3.6,

respectively. Refinement of the iron occupancies is discussed in the Results and Discussion section below.

Table 3.1. Crystallographic parameters of $YbCr_2Al_{20-x}Fe_x$

Formula	$YbCr_2Al_{20}$ [a]	$YbCr_2Al_{19.9}Fe_{0.1}$	$YbCr_2Al_{19.8}Fe_{0.2}$
Crystal System	Cubic	Cubic	Cubic
Space Group	$Fd\bar{3}m$	$Fd\bar{3}m$	$Fd\bar{3}m$
a (Å)	14.473(13)	14.450(4)	14.444(4)
V (Å^3)	3032(5)	3017.2(14)	3013.4(14)
Z	8	8	8
Crystal dimensions (mm)	0.03 x 0.03 x 0.03	0.05 x 0.08 x 0.1	0.05 x 0.08 x 0.1
Temperature (K)	293(2)	296(1)	296(1)
θ range (º)	2.44 - 29.85	3.99 - 29.91	3.99 - 29.92
μ (mm^{-1})	8.666	8.794	8.909
Data Collection			
Measured Reflections	701	1785	1552
Unique Reflections	248	247	247
Reflections with I>2σ(I)	224	223	230
R_{int}	0.0409	0.0384	0.0296
h	$-20 \le h \le 20$	$-20 \le h \le 20$	$-20 \le h \le 20$
k	$-14 \le k \le 14$	$-14 \le k \le 14$	$-14 \le k \le 14$
l	$-13 \le l \le 13$	$-13 \le l \le 13$	$-13 \le l \le 13$
Refinement			
$\Delta\rho_{max}$ (eÅ^{-3})/$\Delta\rho_{min}$ (eÅ^{-3})	0.816 / -1.24	0.862 / -0.744	0.694 / -0.769
GoF	1.167	1.062	1.185
Extinction coefficient	0.00011(5)	0.00035(5)	0.00023(3)
Reflections	248	247	247
Parameters/Restraints	17 / 0	21 / 3	21 / 3
R_1 ($F^2 > 2sF^2$) [b]	0.0295	0.0215	0.0198
wR_2 (F^2) [c]	0.0553	0.0456	0.0337

[a] Crystallographic data from reference.[40]

[b] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$

[c] $R_w = [\Sigma [w (F_o^2 - F_c^2)^2]/ \Sigma [w (F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (0.0137P)^2 + 20.00\ P]$, $w = 1/[\sigma^2(F_o^2) + (0.0188P)^2 + 14.48P]$, $w = 1/[\sigma^2(F_o^2) + (0.0055P)^2]$; $P = (F_o^2 + 2\ Fc^2)/3$ for $YbCr_2Al_{20}$, $YbCr_2Fe_{0.1}Al_{19.9}$, and $YbCr_2Fe_{0.2}Al_{19.8}$, respectively.

Table 3.2. Crystallographic parameters of $LnCr_2Al_{20-x}Fe_x$ (Ln = La, Gd)

Formula	$LaCr_2Al_{20}$	$GdCr_2Al_{20}$	$GdCr_2Al_{19.7}Fe_{0.3}$
Crystal System	Cubic	Cubic	Cubic
Space Group	*Fd-3m*	*Fd-3m*	*Fd-3m*
a (Å)	14.552(1)	14.460(3)	14.431(1)
V (Å^3)	3081.5(6)	3023.5(11)	3005.3(5)
Z	8	8	8
Crystal dimensions (mm)	0.05 x 0.08 x 0.1	0.05 x 0.08 x 0.1	0.05 x 0.08 x 0.1
Temperature (K)	293(2)	293(2)	293(2)
θ range (º)	3.96 - 30.93	3.99 - 30.87	3.99 - 30.94
μ (mm^{-1})	5.229	6.89	7.8
Data Collection			
Measured Reflections	796	744	774
Unique Reflections	272	266	266
Reflections with I>2σ(I)	260	243	257
R_{int}	0.0133	0.0303	0.0135
h	-21 ≤ h ≤ 21	-20 ≤ h ≤ 20	-20 ≤ h ≤ 20
k	-14 ≤ k ≤ 14	-14 ≤ k ≤ 14	-14 ≤ k ≤ 14
l	-13 ≤ l ≤ 13	-13 ≤ l ≤ 13	-13 ≤ l ≤ 13
Refinement			
$\Delta\rho_{max}$ (eÅ^{-3})/$\Delta\rho_{min}$ (eÅ^{-3})	0.827 / -1.283	0.525 / -0.761	0.634 / -0.766
GoF	1.17	1.103	1.245
Extinction coefficient	0.00032(5)	0.00029(4)	0.00036(5)
Reflections	272	266	266
Parameters/Restraints	17 / 0	16 / 0	18 / 0
R_1 ($F^2 > 2sF^2$) [a]	0.0247	0.0216	0.0161
wR_2 (F^2) [b]	0.0649	0.0472	0.0418

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$

[b] $R_w = [\Sigma [w (F_o^2 - F_c^2)^2]/ \Sigma [w (F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (0.0137P)^2 + 20.00\ P]$, $w = 1/[\sigma^2(F_o^2) + (0.0188P)^2 + 14.48P]$, $w = 1/[\sigma^2(F_o^2) + (0.0055P)^2]$; $P = (F_o^2 + 2\ Fc^2)/3$ for $LaCr_2Al_{20}$, $GdCr_2Al_{20}$, and $GdCr_2Fe_{0.3}Al_{19.7}$, respectively.

Table 3.3. Atomic Positions of $YbCr_2Al_{20-x}Fe_x$

Atom	Site	Symmetry	x	y	z	Occ. [b]	U_{eq} (Å^2) [c]
$YbCr_2Al_{20}$ [a]							
Yb1	8*a*	$\bar{4}3m$	1/8	1/8	1/8	1	0.0139(3)
Cr1	16*d*	$\bar{3}m$	1/2	1/2	1/2	1	0.0078(4)
Al1	96*g*	*mm*	0.48698(14)	1/8	1/8	1	0.0091(4)
Al2	48*f*	2*mm*	0.05900(7)	0.05900(7)	0.32511(10)	1	0.0117(4)
Al3	16*c*	$\bar{3}m$	0	0	0	1	0.0182(8)
$YbCr_2Al_{19.9}Fe_{0.1}$							
Yb1	8*a*	$\bar{4}3m$	1/8	1/8	1/8	1	0.0113(2)
Cr1	16*d*	$\bar{3}m$	1/2	1/2	1/2	1	0.0091(3)
Al1	96*g*	*mm*	0.05899(5)	0.05899(5)	0.32525(8)	0.996(3)	0.0121(3)
Fe1	96*g*	*mm*	0.05899(5)	0.05899(5)	0.32525(8)	0.004(3)	0.0121(3)
Al2	48*f*	2*mm*	0.4867(1)	1/8	1/8	0.992(5)	0.0099(4)
Fe2	48*f*	2*mm*	0.4867(1)	1/8	1/8	0.008(5)	0.0099(4)
Al3	16*c*	$\bar{3}m$	0	0	0	1	0.0204(7)
$YbCr_2Al_{19.8}Fe_{0.2}$							
Yb1	8*a*	$\bar{4}3m$	1/8	1/8	1/8	1	0.01002(16)
Cr1	16*d*	$\bar{3}m$	1/2	1/2	1/2	1	0.0081(2)
Al1	96*g*	*mm*	0.05900(4)	0.05900(4)	0.32519(6)	0.988(2)	0.0119(3)
Fe1	96*g*	*mm*	0.05900(4)	0.05900(4)	0.32519(6)	0.012(2)	0.0119(3)
Al2	48*f*	2*mm*	0.48672(8)	1/8	1/8	0.988(4)	0.0093(4)
Fe2	48*f*	2*mm*	0.48672(8)	1/8	1/8	0.012(4)	0.0093(4)
Al3	16*c*	$\bar{3}m$	0	0	0	1	0.0194(5)

[a] Crystallographic data from reference.[40]
[b] Site occupancy
[c] U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tenso

Table 3.4. Atomic Positions of $LnCr_2Al_{20-x}Fe_x$ (Ln = La, Gd)

Atom	Site	Symmetry	x	y	z	Occ. [a]	U_{eq} (Å^2) [b]
$LaCr_2Al_{20}$							
La1	8*a*	$\bar{4}3m$	1/8	1/8	1/8	1	0.0123(2)
Cr1	16*d*	$\bar{3}m$	1/2	1/2	1/2	1	0.0096(3)
Al1	96*g*	*mm*	0.05818(4)	0.05818(4)	0.32698(6)	1	0.0133(3)
Al2	48*f*	2*mm*	0.48822(8)	1/8	1/8	1	0.0106(3)
Al3	16*c*	$\bar{3}m$	0	0	0	1	0.0272(6)
$GdCr_2Al_{20}$							
Gd1	8*a*	$\bar{4}3m$	1/8	1/8	1/8	1	0.0134(2)
Cr1	16*d*	$\bar{3}m$	1/2	1/2	1/2	1	0.0099(2)
Al1	96*g*	*mm*	0.05875(4)	0.05875(4)	0.32577(6)	1	0.0122(2)
Al2	48*f*	2*mm*	0.48703(8)	1/8	1/8	1	0.0106(3)
Al3	16*c*	$\bar{3}m$	0	0	0	1	0.0251(5)
$GdCr_2Al_{19.7}Fe_{0.3}$							
Yb1	8*a*	$\bar{4}3m$	1/8	1/8	1/8	1	0.0133(1)
Cr1	16*d*	$\bar{3}m$	1/2	1/2	1/2	1	0.0113(2)
Al1	96*g*	*mm*	0.05884(3)	0.05884(3)	0.32565(5)	0.97(2)	0.0147(3)
Fe1	96*g*	*mm*	0.05884(3)	0.05884(3)	0.32565(5)	0.03(2)	0.0147(3)
Al2	48*f*	2*mm*	0.48682(7)	1/8	1/8	1	0.0113(2)
Al3	16*c*	$\bar{3}m$	0	0	0	1	0.0278(5)

[a] Site occupancy

[b] U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor

Table 3.5. Select Interatomic Distances (Å) of $YbCr_2Al_{20-x}Fe_x$

Compound	$YbCr_2Al_{20}$ [a]	$YbCr_2Al_{19.9}Fe_{0.1}$	$YbCr_2Al_{19.8}Fe_{0.2}$
Yb - 16 coordinate			
Yb-Al3 (x4)	3.133(3)	3.1285(9)	3.1269(9)
Ln-Al1 (x12)	3.196(3)	3.1929(15)	3.1912(13)
Cr - 12 coordinate			
Cr-Al2 (x6)	2.565(2)	2.5615(7)	2.5605(7)
Cr-Al1 (x6)	2.804(3)	2.7977(14)	2.7965(12)
Al1 - 12 coordinate			
Al1-Al2	2.702(2)	2.6945(19)	2.6941(16)
Al1-Al1	2.705(3)	2.699(2)	2.6972(19)
Al1-Al1 (x2)	2.745(3)	2.7434(19)	2.7418(16)
Al1-Cr	2.804(3)	2.7977(14)	2.7965(12)
Al1-Al2 (x2)	2.838(3)	2.8316(13)	2.8307(12)
Al1-Al1 (x2)	2.923(2)	2.9155(15)	2.9143(13)
Al1-Al3 (x2)	3.091(3)	3.0869(11)	3.0852(9)
Al1-Yb	3.196(3)	3.1930(13)	3.1913(11)
Al2 – 12 coordinate			
Al2-Cr (x2)	2.565(2)	2.5615(7)	2.5602(7)
Al2-Al1 (x2)	2.705(3)	2.5615(7)	2.6941(16)
Al2-Al2 (x4)	2.825(3)	2.826(2)	2.824(2)
Al2-Al1 (x4)	2.838(3)	2.8316(13)	2.8306(12)
Al3 – 14 coordinate			
Al3-Al1 (x12)	3.091(3)	3.0869(11)	3.0852(11)
Al3-Ln (x2)	3.133(3)	3.1287(9)	3.1269(9)

[a] Crystallographic data obtained from reference.[40]

Table 3.6. Select Interatomic Distances (Å) of $LnCr_2Al_{20-x}Fe_x$ (Ln = La, Gd)

Compound	$LaCr_2Al_{20}$	$GdCr_2Al_{20}$	$GdCr_2Al_{19.7}Fe_{0.3}$
Ln - 16 coordinate			
Ln-Al3 (x4)	3.1505(16)	3.1307(6)	3.1244(3)
Ln-Al1 (x12)	3.2446(10)	3.2037(11)	3.1949(8)
Cr - 12 coordinate			
Cr-Al2 (x6)	2.5780(13)	2.5631(5)	2.5581(3)
Cr-Al1 (x6)	2.7882(17)	2.7912(10)	2.7880(8)
Al1 - 12 coordinate			
Al1-Al2	2.7197(19)	2.6968(14)	2.6894(12)
Al1-Al1	2.750(2)	2.7097(17)	2.7005(14)
Al1-Al1 (x2)	2.781(2)	2.7508(15)	2.7447(12)
Al1-Cr	2.7882(10)	2.7912(10)	2.7880(8)
Al1-Al2 (x2)	2.8373(10)	2.8292(10)	2.8248(7)
Al1-Al1 (x2)	2.9076(18)	2.9092(11)	2.9054(9)
Al1-Al3 (x2)	3.0896(8)	3.0935(8)	3.0859(5)
Al1-Yb	3.2017(1)	3.2037(1)	3.1949(7)
Al2 - 12 coordinate			
Al2-Cr (x2)	2.5780(13)	2.5631(5)	2.5581(3)
Al2-Al1 (x2)	2.8373(10)	2.6968(14)	2.8248(7)
Al2-Al2 (x4)	2.8202(18)	2.8215(18)	2.8201(15)
Al2-Al1 (x4)	2.8373(10)	2.8292(10)	2.6894(12)
Al3 - 14 coordinate			
Al3-Al1 (x12)	3.0915(7)	3.0935(8)	3.0859(5)
Al3-Ln (x2)	3.1508(4)	3.1307(4)	3.1244(3)

3.2.3 Elemental Analysis

Elemental analysis was performed via energy dispersive X-ray spectroscopy (EDXS) using a JEOL JSM-5600 scanning electron microscope with an accelerating voltage of 15 kV. For all compounds, two polished crystals were measured four times each, and the results were averaged. The compositions, normalized to Ln, were $YbCr_{2.03(12)}Al_{25.01(18)}Fe_{0.10(3)}$, $YbCr_{1.77(23)}Al_{20.11(33)}Fe_{0.18(2)}$, $GdCr_{2.19(11)}Al_{24.23(17)}Fe_{0.28(6)}$, and $LaCr_{2.1(3)}Al_{25.1(6)}Fe_{0.2(1)}$. The crystals selected for EDS were also characterized by X-ray diffraction.

3.2.4 Magnetization and Electrical Transport

Single crystals selected for physical property measurements were first characterized by X-ray diffraction and EDS. Magnetic data were collected using a Quantum Design Physical Property Measurement System (PPMS). The temperature-dependent susceptibility data were measured under zero-field cooled (ZFC) conditions between 3 K and 390 K with an applied field of 0.1 T. Field-dependent magnetization data were measured at 3 K with applied fields up to 9 T.

3.2.5 Mössbauer Spectroscopy

Single crystals used for physical property measurements were also used for Mössbauer spectroscopy. Powdered $YbCr_2Al_{20-x}Fe_x$ samples (x = 0.1 and 0.2) were analyzed at room temperature and at 77 K. The spectra were measured at two velocities (+/- 2 and +/- 10 mm/s) with a constant-acceleration spectrometer which utilized a rhodium matrix cobalt-57 source and was calibrated at 300 K with α-iron powder. The Mössbauer spectral absorbers contained 20 mg/cm^2 of sample powder mixed with boron nitride. The quoted errors for the Mössbauer spectral parameters are the relative statistical errors.

3.3 Results and Discussion

3.3.1 Crystal Structure

The crystal structure of $GdCr_2Al_{20}$ is shown in Figure 3.1 and consists of a diamond-like network of Gd polyhedra and a pyrochlore-like network of Cr polyhedra. The $GdCr_2Al_{20}$ lattice parameter is 14.460(3) Å, and upon substitution of Fe for Al ($GdCr_2Fe_{0.3}Al_{19.7}$), the lattice parameter decreases to 14.4310(15) Å. The lattice parameter of $YbCr_2Al_{20}$ is 14.473(3) Å and decreases to 14.450(4) Å and 14.444(4) Å for $YbCr_2Fe_{0.1}Al_{19.9}$ and $YbCr_2Fe_{0.2}Al_{19.8}$, respectively, with the incorporation of the smaller iron atoms. The contraction of lattice parameters is a strong indication and consistent with Fe incorporated in the compounds. The $GdCr_2Al_{20}$ crystal structure

has one Gd site (8*a*), one Cr site (16*d*) and three Al sites (96*g*, 48*f*, 16*c*). The local environments of the five sites are depicted in Figure 3.2. The Gd polyhedron is 16 coordinate and is made up of 4 Al3 and 12 Al1 atoms with Gd-Al bond distances of 3.1307(6) and 3.2037(11) Å, respectively. The Gd polyhedron corner shares with 4 other Gd polyhedra with Gd-Gd distances of 6.269(6) Å. The Cr environment is 12-coordinate, forming a distorted icosahedron and is surrounded by 6 Al1 and 6 Al2 atoms with Cr-Al distances of 2.5631(5) and 2.7912(10) Å, respectively. Al1 (12-coordinate), Al2 (12-coordinate), and Al3 (14-coordinate) polyhedra, respectively, can be described as a distorted bi-capped pentagonal prism, a bi-capped pentagonal prism, and a bi-capped hexagonal prism, respectively. The Al-Al distances range from 2.6968(14) to 3.0935(8) Å, and are longer than the expected distance of 2.42 Å from covalent radii.[83]

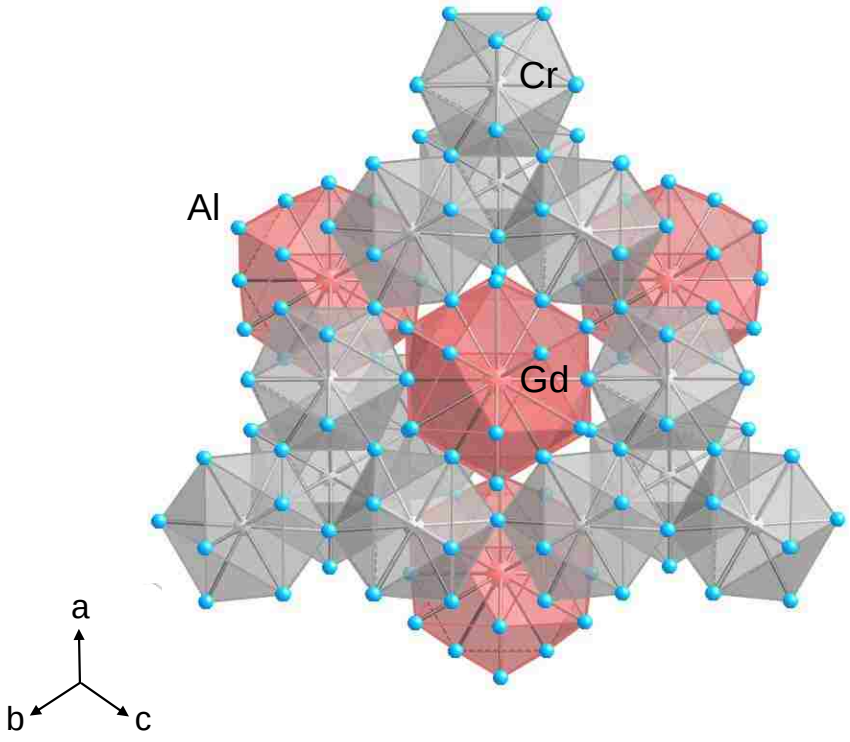

Figure 3.9. The crystal structure of $GdCr_2Al_{20}$ showing the interpenetrating network of the Gd and Cr polyhedra. The Gd polyhedra are shown as light pink and the Cr polyhedra are shown as grey. Aluminum atoms are depicted as small light blue spheres.

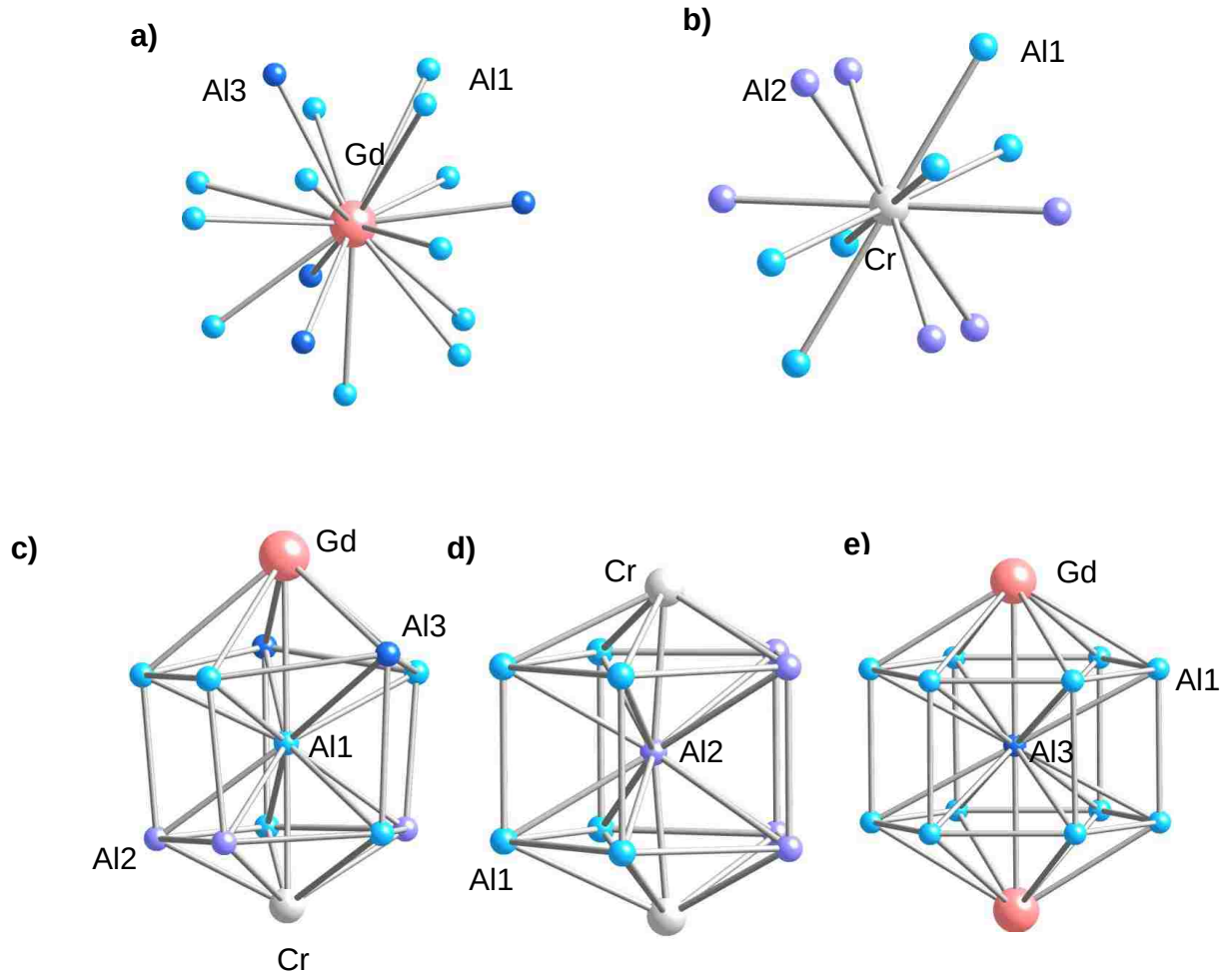

Figure 3.10.The local environments of Gd, Cr, Al1, Al2, and Al3 are shown in a-e, respectively. Gd atoms and Cr atoms are depicted as light pink spheres and grey spheres, respectively, while the Al1, Al2, and Al3 atoms are depicted as light blue.

3.3.2 Mössbauer spectroscopy

Mössbauer spectra for $YbCr_2Al_{20-x}Fe_x$ (x = 0.1 and 0.2) are shown in Figure 3.3. An attempt to fit the data with only one iron site using one asymmetric doublet (Model 1) leads to a difference in the experimental model and the calculated fit (misfit). The second attempt to fit the data with considering two iron sites (Model 2), leads to a minuscule misfit compared to Model 1, which suggests that our compound has two unique Fe-sites. In this case, the isomer shifts are quite

similar while the quadrupole splittings corresponding to the two sites are clearly different, indicating that electronic charges are different for the two iron sites. Schematically, the quadrupole splitting is indicative of the site distortion, an iron atom occupying a regular geometry site will have a smaller quadrupole splitting and vice-versa. Whichever the model used to fit the experimental data, the isomer shifts and the quadrupole splittings (provided in Table 3.7) are in the range of iron atoms in an intermetallic environment rich in aluminum[41, 84-88] concluding that the Fe is substituting on Al sites.

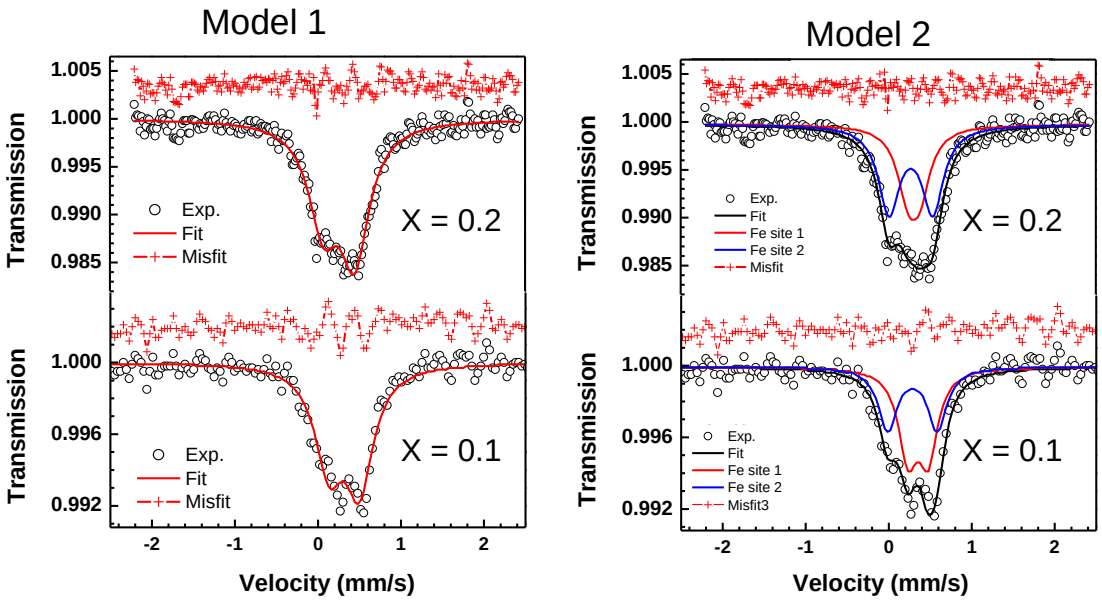

Figure 3.11. Room temperature Mössbauer data for $YbCr_2Al_{20-x}Fe_x$ samples (with x = 0.1 and 0.2) fitted with two different models as described in the text.

Table 3.7. Fitted Mössbauer parameters for spectra measured at room temperature. IS, QS, LW, and R.A. are the isomer shift (relative to a-Fe at 300 K), the quadrupole splitting, the line width and the relative areas, respectively.

Sample	IS (mm/s)	QS (mm/s)	LW (mm/s)	R.A. (%)
Fe = 0.2	0.31(1)	0.14(5)	0.31(3)	40(7)
	0.27(1)	0.53(3)	-	60(7)
Fe = 0.1	0.35(2)	0.24(3)	0.27(4)	57(6)
	0.28(2)	0.60(5)	-	43(6)

Since Model 2 has the best statistical data, we can conclude that there are two iron sites present. Model 2 suggests that the two iron sites can be distinguish based on distortion in both compositions (x = 0.1 and 0.2). The site having the bigger quadrupole splitting (in blue shown in Figure 3.3) should correspond to the most distorted site. This model can only be explained if we assume that iron atoms go simultaneously into two aluminum crystallographic sites. Finally, Mössbauer spectra have been recorded at 77 K and 300 K in a larger velocity range (Figure 3.4). The interest of recording spectra at such velocity (10 mm/s) is to check if there is any iron oxide. In fact, iron oxides give absorption peaks at around 8-9 mm/s which are not present in our spectra. From the results, we can also confirm the absence of any magnetic ordering between 77 K and 300 K.

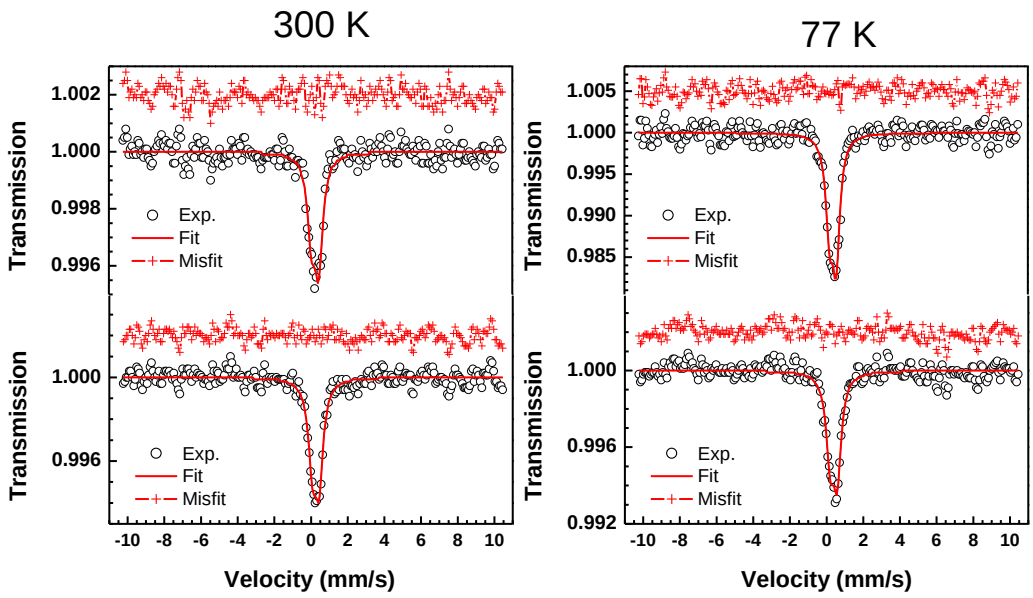

Figure 3.12. Mössbauer spectra at 300 K and 77 K for $YbCr_2Al_{20-x}Fe_x$ samples (with x = 0.1 and 0.2).

3.2.3 Crystal Structure Refinements

Because the Mössbauer results indicate two aluminum sites are occupied with iron, the X-ray diffraction models were re-examined to determine those sites. Bond lengths, atomic

displacement parameters (ADP), and site occupancies can be useful in determining partial or mixed occupancy in extended solids. As shown in Table 3.5, all bond lengths decrease as a function of iron content, so the iron sites could not be identified in this manner. Similarly, no ADP values were found to be anomalous, and all refined sites were within ~1% of fully occupied. Therefore, to identify the Fe occupied sites, refinements were conducted with Fe occupying pairs of atomic positions. The total Fe in the unit cell was constrained to the EDS values, and the SUMP command in SHEXL was used to refine the iron occupancy of the two sites. Seven of the 10 possibilities were successfully refined and gave similar quality metrics (R factors, goodness of fit, and residual electron density). The remaining three refinements were unstable or resulted in negative site occupancies. Sites were designated as more ordered (higher symmetry) or disordered (lower symmetry) to compare to the Mössbauer results. The model with iron occupying the Al1 and Al2 sites gave the best agreement with the site occupancies of the more ordered and disordered sites obtained from Mössbauer spectroscopy. This analysis assumes that the Fe occupies the same two crystallographic sites in each of the two doping levels.

The Fe doped Gd-analogue has a site preference for iron that is different from the Yb-analogues. The Fe can only be refined for the Al1 site for the Gd-analogue. Modeling other Al sites with Fe leads to an unstable refinement model, thus, we cannot conclusively determine the presence of Fe on the Al2 site for the Gd-analogue. As far as the La-analogue, no Fe was modeled on any sites, indicating that Fe was not successfully substituted for Al or that the concentration of Fe is so minuscule that we are not able to distinguish it. Modeling Fe on any site in the La-analogue leads to an unstable refinement of the model.

3.2.4 Magnetization

Temperature dependent magnetic susceptibility data for $GdCr_2Al_{20-x}Fe_x$ are shown in Figure 3.5. The susceptibility for the three Yb compounds is nearly temperature independent consistent with non-magnetic Yb^{2+}. This is similar to CeT_2Al_{20} (T = Ti-Cr) compounds,[78-80] which were also reported to be nearly temperature independent paramagnets. The doped and undoped Gd-analogues show no magnetic ordering down to 3 K, which is in contrast with previous literature that reported an antiferromagnetic ordering at 3.90(5) for $GdCr_2Al_{20}$.[77] A reason for the discrepancy is that previous magnetic data were measured on polycrystalline $GdCr_2Al_{20,}$ and our present work is on single crystalline material, which allows us to directly measure intrinsic properties. Both the doped and undoped Gd-compounds yield μ_{eff} = 7.69(8) and 7.67(6) μ_B/Gd and Weiss constants of -8.22(6) and -5.31(2) K, respectively, by using the modified Curie Weiss equation from 80 to 370 K. Although no magnetic ordering is apparent, the negative Weiss temperatures indicate a dominate antiferromagnetic exchange interaction between the Gd magnetic moments. The magnetic susceptibility of $LaCr_2Al_{20}$ is essentially temperature independent, which would indicate that Cr is non-magnetic. There is no indication of magnetic ordering down to 3 K in any of the $LnCr_2Al_{20-x}Fe_x$ (Ln = La, Gd, Yb) analogues.

Field dependent magnetization data (3 K) for $GdCr_2Al_{20-x}Fe_x$ are shown in Figure 3.6. The magnetization of $YbCr_2Al_{19.8}Fe_{0.2}$ and $YbCr_2Al_{19.9}Fe_{0.1}$ is very low and saturates at ~0.005- 0.007 μ_B/mol at 9 T. The $GdCr_2Al_{20}$ and $GdCr_2Al_{19.7}Fe_{0.3}$ magnetization data show linear dependence as a function of field at low field (< 3 T), which is typical of paramagnetic samples, then begin to deviate around 6 μ_B/mol Gd, which is close to the saturation magnetization of Gd^{3+} (7 μ_B/mol) . The nearly identical form and magnitude of the field dependent magnetization data for both Gd analogues is a good indication that the Fe is non-magnetic in the sample.

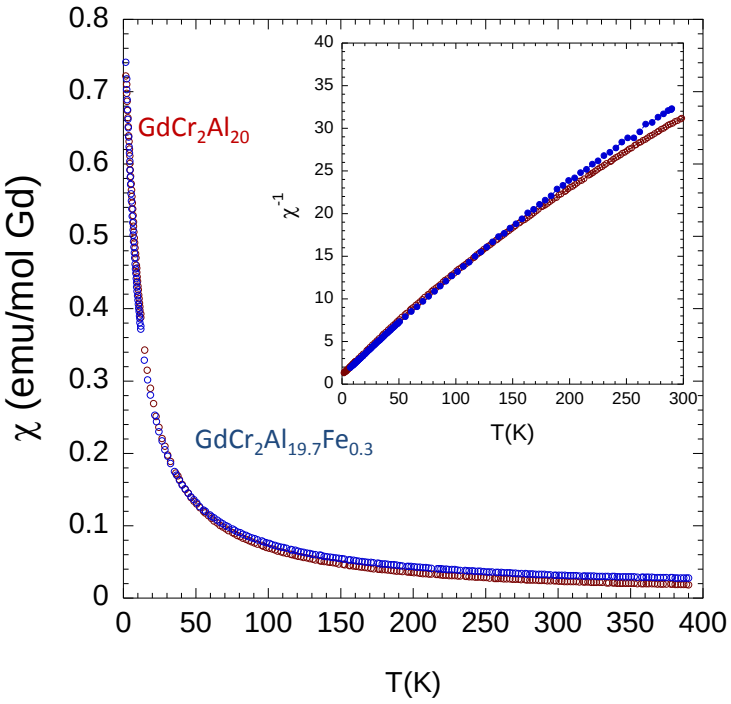

Figure 3.13. Temperature dependent magnetic susceptibility data for $GdCr_2Al_{20}$ and $GdCr_2Al_{19.7}Fe_{0.3}$.

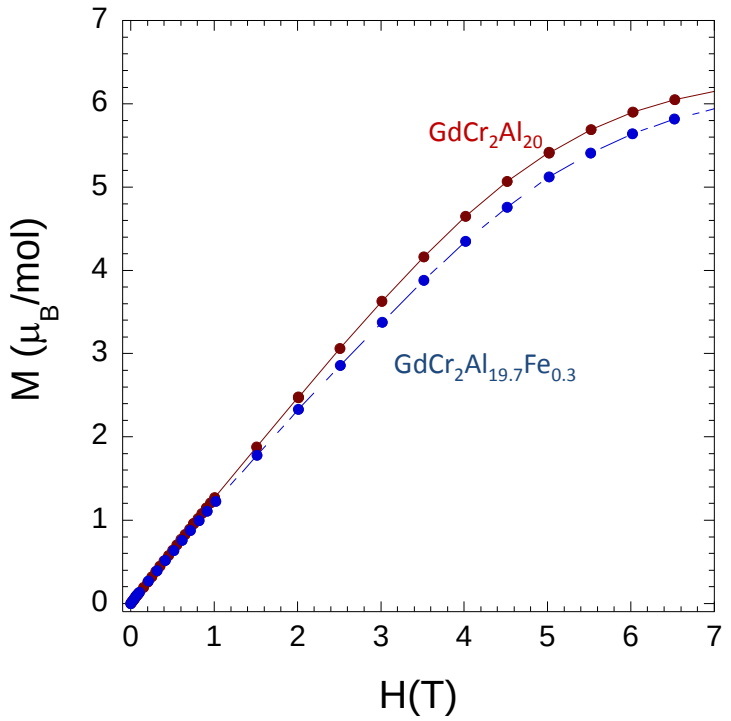

Figure 3.14. Field dependent magnetization data at 3 K are shown for $GdCr_2Al_{20}$ and $GdCr_2Al_{19.7}Fe_{0.3}$.

3.4 Conclusions

Single crystals of $LnCr_2Al_{20-x}Fe_x$ (Ln = La, Gd, Yb) were grown with molten aluminum flux. ^{57}Fe Mössbauer spectroscopy was essential in determining which sites the iron atoms occupied and indicated that the iron atoms occupied two distinct crystallographic sites. Crystallographic models were refined with Fe occupying each pair of crystallographic sites, and the best agreement with the Mössbauer spectroscopy was achieved when the Fe atoms partially occupied the Al1 (96*g*) and Al2 (48*f*) sites. The iron occupancy of the Al2 site remained fairly constant between the doping levels, while the iron occupancy of the Al1 site increased from ~0.5% to ~1.3% for the larger doping level. Single crystal X-ray diffraction data of the Fe doped Gd-analogues showed that Fe prefers to substitute for Al as opposed to a transition metal. Given the volume change with Fe substitution and the difference in atomic radii of the elements, it is reasonable to conclude that our model is suitable. Based on the atomic radii of Cr (1.249) and Fe (1.241), if Fe substitutes onto the transition metal site, we would expect a negligible change in volume. However, in our experiments, the volume of $GdCr_2Al_{20}$ (3023.5(11) Å^3) shows a decrease in volume upon substitution (3005.3(5) Å^3). This trend is also consistent with the Fe-doped Yb compounds as well. Due to the results of ^{57}Fe Mössbauer spectroscopy and single crystal X-ray diffraction data, we have successfully characterized the first pseudo ternary intermetallic of the $CeCr_2Al_{20}$ structure type, where the Fe substitutes for the main group element. The results indicate that the latter transition metals (≥ Fe) do not form LnT_2Al_{20} compounds adopting the $CeCr_2Al_{20}$ structure type, which can be rationalized by both atomic volume and valence electron count arguments.[80]

Like $YbCr_2Al_{20}$, both $YbCr_2Al_{20-x}Fe_x$ and $LaCr_2Al_{20}$ compounds display temperature independent magnetism. Due to the relative size of Gd, Fe can only be substituted on the Al1 site

for $GdCr_2Al_{20-x}Fe_x$, unlike $YbCr_2Al_{20-x}Fe_x$ where the Fe substitutes on both the Al1 and Al2 sites. Single crystals of $GdCr_2Al_{20}$ and $GdCr_2Al_{19.7}Fe_{0.3}$ exhibit paramagnetic behavior down to 3 K with no magnetic ordering, while previously reported polycrystalline $GdCr_2Al_{20}$ displayed antiferromagnetic ordering at 3.90(5) K. This shows the importance of growing single crystals to determine the intrinsic magnetic properties of materials.

Chapter 4. Crystal growth and physical properties of $Sm_{1.33}Pd_3Ga_8$, a disordered variant of the $Er_4Pt_9Al_{24}$-structure type

4.1 Introduction

Over the last decade, there has been significant interest in the single crystal growth of highly correlated materials. Recently, we have reviewed and highlighted several highly correlated Ce-based intermetallics with unusual properties such as magnetically mediated superconductivity, unusual forms of magnetism, and heavy fermion behavior.[27] Heavy fermion compounds are materials whose conduction electrons interact strongly with the local magnetic moments.[89] This phenomenon results in the electrons behaving as if they have an increased mass and is identified by a large Sommerfeld coefficient, γ, where $C_p = \gamma T + bT^3$ ($\gamma > 200$ mJ/mol-K^2). For example, the homologous series Ce_nMIn_{3n+2} (n = 1, 2; M = Co, Rh, Ir) is a family of heavy-fermion compounds that exhibit magnetism and superconductivity.[2-4, 90, 91] The report of Ce_nMIn_{3n+2} (n = 1, 2; M = Co, Rh, Ir) and their interesting physical properties stimulated our investigation in the Ce-Pd-Ga-based single crystals, which led to the discovery of $CePdGa_6$[92] and Ce_2PdGa_{12}.[93] Both materials were found to be tetragonal and composed of Ce-Ga and $PdGa_{8/2}$ layers. Physical property measurements determined each to also be heavy fermion antiferromagnets with $\gamma \sim 300$ mJ/K^2 mol and $\gamma \sim 72$ mJ/K^2 mol, respectively, and exhibit metamagnetic transitions at 2 T and 2.5 T, respectively.

In addition, the search for rare earth intermetallics has led to the discovery of the quadrupolar Kondo effect in Pr- and Sm-based intermetallics adopting the $CeCr_2Al_{20}$ structure type.[94] PrM_2Al_{20} (M = Ti, V, Cr) exhibits a decrease in electron scattering in resistivity below 5 K due to Kondo interactions with quadrupolar ordering.[95] It has been found that by increasing the conduction and *f*-electron hybridization (*c*-*f*) strength, magnetic ordering can be suppressed leading to greater Kondo interactions. For example, SmM_2Al_{20} (M = Ti, V, Cr) exhibits a

systematic increase in both Kondo temperature and valence fluctuating temperature from M = Ti to Cr, which is consistent with the enhancement of the *c-f* hybridization.[95, 96] More Recently, $SmTa_2Al_{20}$ was reported to exhibit Kondo behavior and a suppressed effective magnetic moment of 0.09 μ_B/Sm indicating strong *c-f* hybridization.[97]

Due to the unusual physical properties of Sm-containing intermetallics and the discovery of the layered compounds $CePdGa_6$ and Ce_2PdGa_{12}, we were motivated to grow Sm-Pd-Ga-based single crystals that led to the discovery of $Sm_{1.33}Pd_3Ga_8$. Several isostructural analogues $R_{1.33}Pt_3Al_8$ (R = Ce, Gd) have been reported.[98, 99] $Gd_{1.33}Pt_3Al_8$ orders antiferromagnetically at 20 K, but upon doping with silicon to yield $Gd_{1.33}Pt_3(Al,Si)_8$, the ordering temperature decreases to 7 K.[98] The structure of $Ln_{1.33}Pt_3Al_8$ (Ln = Ce, Gd) is composed of two dimensional layers consisting of a Pt_2Al_4 layer, R-Al disordered layer, and $PtAl_2$ layer stacked along *c*-direction. The Ln atoms are located in a 2-*d* triangular net with an interatomic distance of ~ 4 Å, resembling a Kagome network. Samarium intermetallics with similar rare-earth geometry have shown unusual magnetism such as spin glass and frustration as seen in $SmNiGeAl_4$[100] and $SmPd_2Al_3$.[101, 102] Herein, we report the synthesis, crystal structure, and physical properties of $Sm_{1.33}Pd_3Ga_8$.

4.2 Experimental

4.2.1 Synthesis

The flux-growth method was selected to grow single crystals, which uses a low melting metal as a flux.[25-27] Initially, we targeted $Sm_2Pd_3Ga_9$ due to our recent report of $Yb_2Pd_3Ga_9$.[27] Therefore, the elements Sm, Pd, and Ga were weighed in the same atomic ratios of 1:2:5 and loaded into an alumina crucible. The crucible was placed in a fused-silica tube topped with silica wool. The fused-silica tube was then evacuated (50-70 mTorr) and sealed. The vessel was heated to 1150 °C at a rate of 170 °C/h, and dwelled for 2 h. The vessel was then cooled to 500 °C at a

rate of 150 °C/h, and subsequently cooled to 400 °C at a rate 8 °C/h, followed by centrifugation to remove the excess Ga. Hot water was used to separate the aggregate crystals from the gallium flux and 3M DMF/I_2 solution was employed to clean residual gallium on the surfaces of the single crystals. The single crystals dimensions were ~ 0.5 x 0.5 x 3 mm^3.

4.2.2 Powder and Single Crystal X-ray Diffraction

Ground aggregates of crystals were characterized by X-ray powder diffraction using a Bruker AXS D8 Advance diffractometer with Cu $K\alpha_1$ radiation (λ = 1.540562 Å). The diffraction pattern is consistent with the calculated powder diffraction pattern of $Sm_{1.33}Pd_3Ga_8$. Single crystals of $Sm_{1.33}Pd_3Ga_8$ were cut to suitable sizes for data collection and mounted onto a glass fiber with epoxy. The fiber was then placed on a Nonius Kappa CCD diffractometer equipped with Mo Kα radiation (λ = 0.71073 Å). Data was collected up to θ = 32 ° at 298 K. The crystal structure was solved by direct methods with SIR92[58] and refined with SHELXL97.[59] The atomic positions, selected interatomic distances, and crystallographic parameters of $Sm_{1.33}Pd_3Ga_8$ are provided in Tables 4.1-4.3.

4.2.3 Structural Refinement

Following the initial refinement of $Sm_{1.33}Pd_3Ga_8$ using the previously reported atomic positions of $Gd_{1.33}Pt_3Al_8$, unusually large atomic displacement parameters (ADP) for Sm1 and Ga4 were observed possibly indicating that a lighter atom or no atom at all should occupy the site or disorder/partial occupancy is present. No other ADP values were found to be anomalous, and all refined sites were within ~ 1 % of fully occupied. A residual electron density of 127.24 e $Å^{-3}$ and deepest minimum of -10.00 e $Å^{-3}$ were observed. These Q peaks were located ~ 0.03 Å and 0.45 Å away from the Sm and Ga4 site, respectively. Because of the large atomic displacement parameters and the location of the Q peaks it was believed that the Sm and Ga4 site were partially

occupied. Therefore, to identify the occupancy of Sm and Ga4 sites, their occupancy were refined freely and found to be ~ 67 and 33 % occupancy, respectively.

Table 4.1. Atomic Positions

Atom	*x*	*y*	*z*	Occ.	U_{eq} (Å^2)[a]
Sm1	0	0	0.269775(13)	0.670(2)	0.00699(19)
Pd1	0	0	0	1.00	0.00806(17)
Pd2	0	0	0.120867(13)	1.00	0.00931(16)
Ga1	0	0	0.44354(2)	1.00	0.01176(19)
Ga2	0	0	0.18643(2)	1.00	0.0107(2)
Ga3	0	0	0.35195(2)	1.00	0.00900(19)
Ga4	0.53713(19)	0.46287(19)	0.39464(3)	0.330(2)	0.01004(4)

[a] U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Table 4.2. Selected Interatomic Distance (Å)

	$Sm_{1.33}Pd_3Ga_8$
Sm	
-Ga1 (x3)	3.1020(4)
-Ga2 (x1)	3.2488(7)
-Ga3 (x4)	3.0635(4)
Pd1	
-Ga3 (x6)	2.7071(16)
-Ga4 (x2)	2.6027(9)
Pd2	
-Ga1 (x3)	2.5473(6)
-Ga2 (x3)	2.5556(5)
-Ga2 (x1)	2.7104(5)
-Ga4 (x1)	2.5202(4)

Table 4.3. Crystallographic Parameters

Crystal System	Trigonal
Space Group	$R\bar{3}m$
a (Å)	4.353(5)
c (Å)	38.98(4)
V (Å^3)	639.70(12)
Z	3
Crystal dimensions (mm^3)	0.02 x 0.02 x 0.03
θ range (º)	4.71 – 30.98
μ (mm^{-1})	37.651
Data Collection	
Measured Reflections	917
Independent Reflections	313
Reflections with I>2σ(I)	296
R_{int}	0.0245
h	-6 to 6
k	-4 to 4
l	-55 to 52
Refinement	
R_1 (F)[a]	0.0178
wR_2[b]	0.0396
Reflections	313
Parameters	27
$\Delta_{\rho max}$ (e Å^{-3})	0.992
$\Delta_{\rho min}$ (e Å^{-3})	-1.736
Extinction coefficient	0.00108(10)
GOF	1.194

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$

[b] $_wR_2 = [\Sigma [w(F_o^2 - F_c^2)^2]/\Sigma [w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (0.0123\ P)^2 + 7.4140\ P]$, $[\Sigma [w(F_o^2 - F_c^2)^2]/\Sigma [w(F_o^2)^2]]^{1/2}$.

4.2.4 Physical Properties

Magnetic data were collected on grounded polycrystalline samples using a Quantum Design Magnetic Property Measurement System (MPMS). The temperature-dependent susceptibility was measured under zero-field conditions (ZFC) between 2 and 300 K with an applied magnetic field of 0.5 and 3 T. Field-dependent magnetization data was measured at 2 and 300 K with fields up to 7 T. The electrical resistivity measurement was performed on a single crystal by the standard four-probe AC technique.

4.3 Results and Discussion

4.3.1 Crystal Structure

$Sm_{1.33}Pd_3Ga_8$ crystallizes in the space group $R\bar{3}m$ with lattice parameters a = 4.353(5) Å and c = 38.98(4) Å and V = 639.70(12) Å^3. The crystal structure of $Sm_{1.33}Pd_3Ga_8$ is shown in Figure 4.1. There are seven crystallographic positions in $Sm_{1.33}Pd_3Ga_8$, including Sm, Pd1, Pd2, Ga1-3, and Ga4 occupying the 6*c*, 3*a*, 6*c*, 6*c*, and 18*h* sites, respectively. The crystal structure of $Sm_{1.33}Pd_3Ga_8$ can be viewed as a disordered variant of the triclinic $Er_4Pt_9Al_{24}$ structure type which has cell dimensions a = 7.462(2), b = 12.940(2), and c = 13.044(2) Å.[38] The rhombohedral dimensions can be related to the triclinic unit cell by the following relationships: $a_r = a_t/\sqrt{3}$ and $c_r = 3c_t$ (where r = rhombohedral and t = triclinic).

The structure of $Sm_{1.33}Pd_3Ga_8$, as shown in Figure 4.2, is composed of three distinct slabs: Pd_2Ga_4 + 2 x [$Sm_{0.67}Ga$] + $PdGa_2$. The slabs stack in the *c*-direction in an ABCBABC′BA′BC″B sequence, where A is a Pd_2Ga_4 slab, B is a disordered $Sm_{0.67}Ga$ slab, and C is a $PdGa_2$ slab, and the position of the slabs with respect to each other is indicated by A′, A″. Similarly, $Er_4Pt_9Al_{24}$ is formed by three distinctive slabs leading to 2 x [Er_2Al_3] + 3 x [$PdAl_2$ + Pd_2Al_4] that stack in the *c*-direction. The $Sm_{0.67}Ga$ slab can be related to three superimposed Er_2Al_3 slabs offset by $a_t/\sqrt{3}$ as shown in Figure 4.3. Due to the partially occupied Ga4 site (~ 33 %) in the $Sm_{0.67}Ga$ slab, three superimposed Er_2Al_3 slabs must be used to account for the near tripling of the *c*-dimension of the $Sm_{1.33}Pd_3Ga_8$ phase.

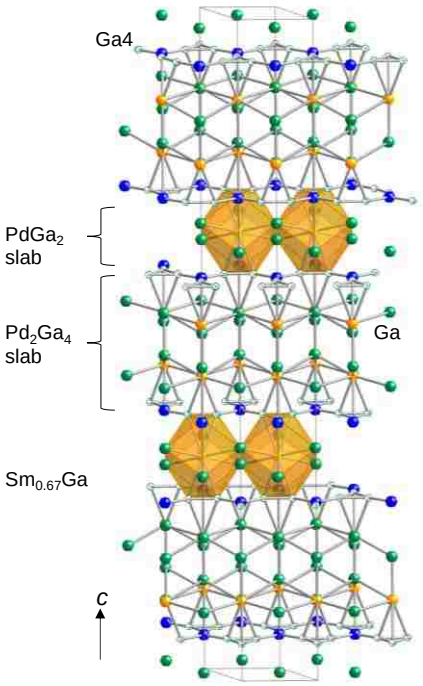

Figure 4.15. The crystal structure of $Sm_{1.33}Pd_3Ga_8$ viewed along the *c*-axis. Sm atoms are shown as blue spheres. Pd1 atoms are represented as orange polyhedra, and Pd2 atoms are orange spheres. Gallium atoms are shown as solid green spheres, while Ga4 atoms are represented as green hatch spheres.

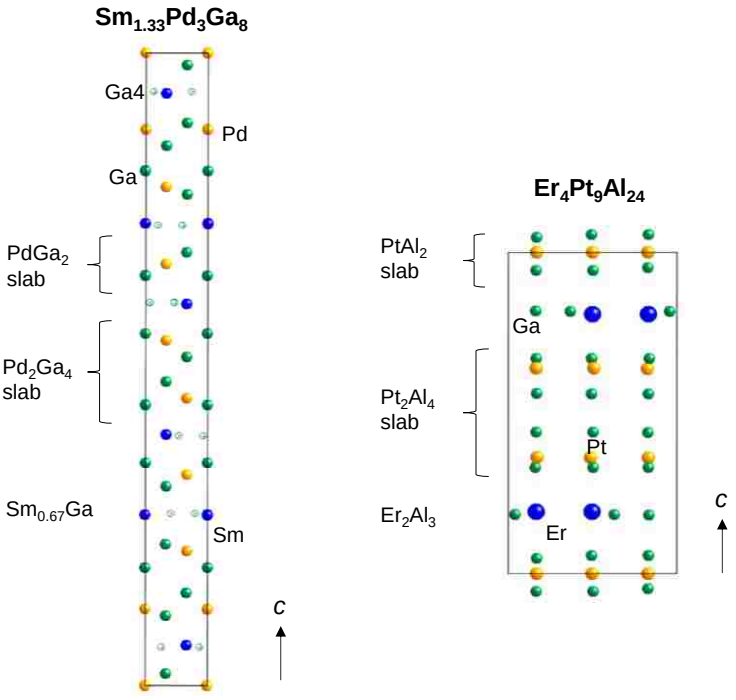

Figure 4.16. The unit cell projection of $Sm_{1.33}Pd_3Ga_8$ and $Er_4Pt_9Al_{24}$ along the *c*-axis are shown.

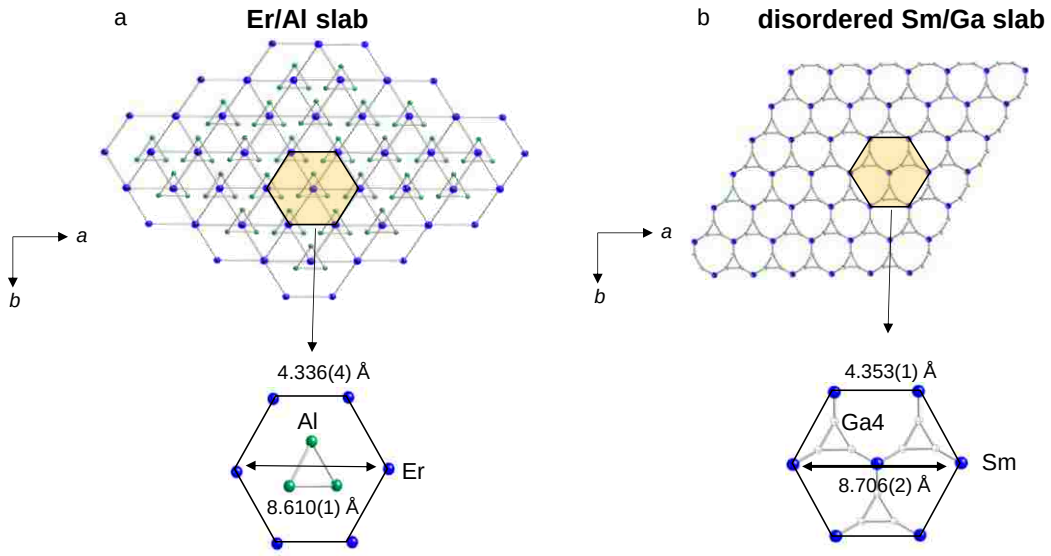

Figure 4.17. Projections of the $Er_4Pt_9Al_{24}$ and $Sm_{1.33}Pd_3Ga_8$ crystal structure down the *c*-plane are shown.

Figure 4.4 shows the $Sm_{0.67}Ga$ segment which consists of a triangular mesh of partially occupied Ga4 (33 %) atoms with the Sm (67 %) atoms residing in the center. The Sm-Ga distances are 1.539(2) Å and the Ga-Ga distances are 1.692(3) Å, which are too close to be considered an interatomic distance given the sum of Sm and Ga atomic radii. As a result, Sm and Ga4 atomic sites were refined with partial occupancy. Similar contacts of 1.5381(7) and 1.5505(5) Å were also found in $Gd_{1.33}Pt_3Al_8$ and $Ce_{1.33}Pt_3Al_8$ [99], respectively. Isostructural analogues $Ln_{1.33}Pt_3Al_8$ (Ln = Gd, Ce)[98, 99] also yielded partial occupancy of Ln ~ 66 and Al ~ 33 % where 1/3 of the Ln atoms are exchanged by Al-triangles. An attempt to explain the unique relationship between the disordered Ln-Al slab and the ordered Ln-Al slab was previously made between $Gd_{1.33}Pt_3Al_8$ and $Er_4Pt_9Al_{24}$.[98] The $Er_4Pt_9Al_{24}$-structure type is considered to be the supercell of the $Gd_{1.33}Pd_3Al_8$-structure type. The partially occupied Gd and Al atoms allow the $GdAl_{0.67}$ slab to coincide in the *c*-direction retaining the 3-fold rotational symmetry, whereas in $Er_4Pt_9Al_{24}$, the Er/Al slabs do not coincide due to the Er and Al being fully occupied and ordered, destroying the 3-fold axis of rotation. The $Ln_{0.67}X$ (Ln = rare earth; X = Al, Si, Ga) slab is very robust, which is evident in that

it has been observed in various compounds such as $Gd_{0.67}Pt_2Al_5$[98] and $La_xCe_{1.33-x}Pt_4Ga_{10}$,[103] where the Ln atoms are situated in a triangle mesh of X atoms (X = Ga or Al).

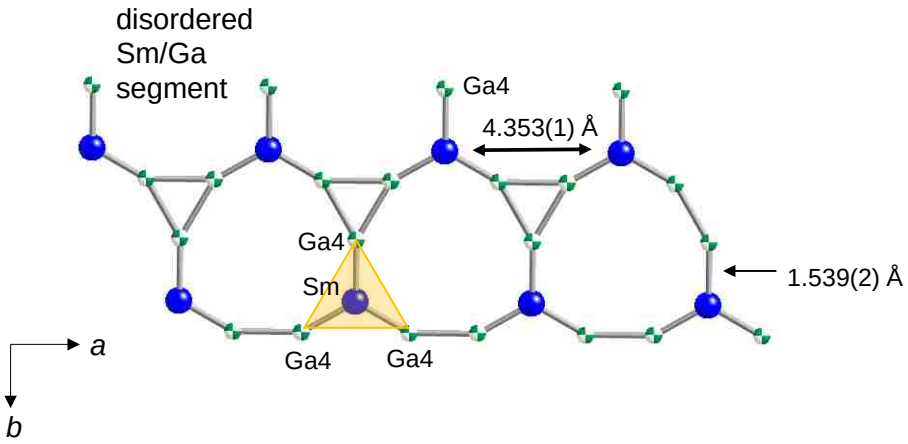

Figure 4.18. The Sm/Ga disordered slab viewed parallel to *c*-direction.

There are three distinct Sm-Sm distances in $Sm_{1.33}Pd_3Ga_8$: one Sm-Sm distance along the *ab*-plane and two Sm-Sm distances along the *c*-direction. The $(Sm\text{-}Sm)_{ab}$ interatomic spacing is 4.353(5) Å, which is comparable to previously reported Sm-compounds and isostructural analogues $Ln_{1.33}Pt_3Al_8$ (Ln = Gd, Ce) with $(Gd\text{-}Gd)_{ab}$ and $(Ce\text{-}Ce)_{ab}$ interatomic spacing of 4.309(1) Å and 4.361(2) Å, respectively. The $(Sm\text{-}Sm)_c$ distances are ~ 5.3391 Å parted by the $PdGa_2$ slab and ~ 8.1846 Å separated by the Pd_2Ga_4 slab, while $(Gd\text{-}Gd)_c$ and $(Ce\text{-}Ce)_c$ interatomic distances in $Ln_{1.33}Pt_3Al_8$ (Ln = Gd, Ce) are ~ 5.5197 and ~ 9.3528 and ~ 5.5989 and ~ 9.4522 Å. The three different Sm-Sm distances in $Sm_{1.33}Pd_3Ga_8$ may lead to anisotropic magnetic behavior.

Figure 4.5a shows the $PdGa_2$ segment consisting of Pd1, Ga2, and Ga3 and can be described as hexagonal close-packed layers with the Pd atoms residing between the gallium networks. This arrangement has been found in $Y_2Co_3Ga_9$ and isostructural analogs[104-106] as well as $SmNiAl_4Ge_2$ [100], $Yb_2Pd_3Ga_9$,[27] $CePdGa_6$,[92] and Ce_2PdGa_{12}.[93] Pd1 is surrounded by eight gallium atoms (six Ga4 partially occupied (33%) atoms), as shown in Figure 4.5b, with Pd-Ga

distances of 2.6027(9) and 2.7071(16) Å, which are slightly greater than the sum of the atomic radii of Ga (1.22 Å) and Pd (1.37 Å) as well as the interatomic distances in Pd-Ga binaries Pd_5Ga_2[107] and PdGa.[108] The Pd_2Ga_4 segment, as shown in Figure 4.5c, consists of Pd2, Ga1, Ga2, and Ga4 forming two $PdGa_2$ nets that are connected by Ga-Ga bonds. Pd2 is surrounded by a total of 8 gallium atoms (three Ga4 partially occupied (33%) atoms), as shown in Figure 4.5d, with Pd-Ga distances 2.5473(6), 2.5556(5), 2.7104(5), and 2.5202(4) Å.

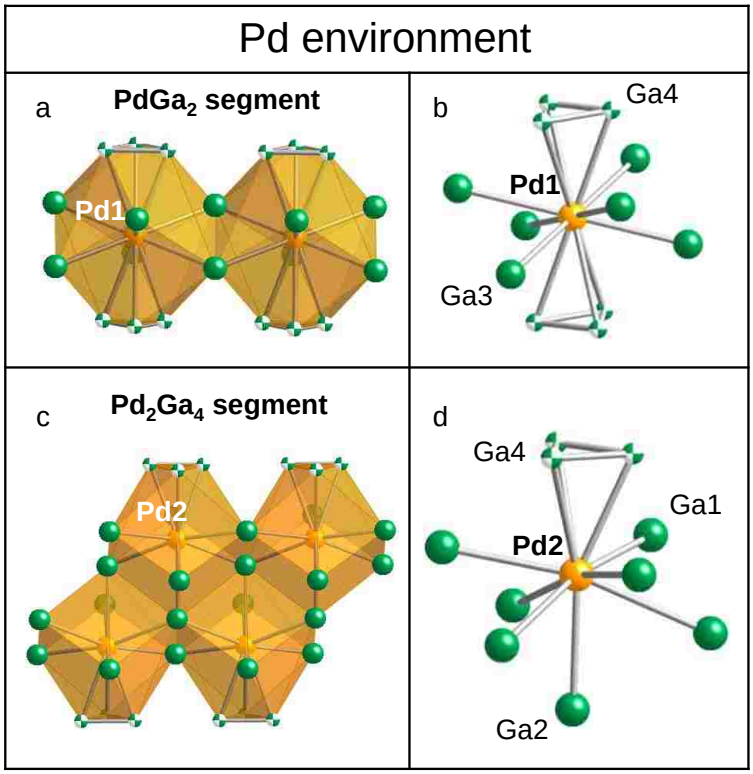

Figure 4.19. The $PdGa_2$ (a) and Pd_2Ga_4 (c) segments and the local environments of Pd1 (b) and Pd2 (d) are shown.

4.3.2 Magnetization and Electrical Transport

The temperature dependent magnetic susceptibility of $Sm_{1.33}Pd_3Ga_8$, not shown, is nearly temperature independent consistent with the presence of Sm^{2+} ions. The field-dependent magnetization measurements were measured at 3 K up to 9 T to characterize $Sm_{1.33}Pd_3Ga_8$. Anisotropic field dependent magnetization of $Sm_{1.33}Pd_3Ga_8$ is shown in Figure 4.6. When the

applied field is parallel to the *c*-direction the magnetization initially increases until 0.5 T where there is a change in slope. Subsequently, the magnetization increases to 0.015 μ_B/mol Sm at 9 T, which is below the expected value for free Sm^{3+} ions (μ_{sat} = 0.71 μ_B/mol). When the field is parallel to the *ab*-plane the magnetization displays linear behavior over the field measured up to 0.27 μ_B/mol Sm, well below the expected value for free Sm^{3+} ions (μ_{sat} = 0.71 μ_B/mol). The magnetization increases to 0.27 μ_B/mol Sm at 9 T when the field is oriented *ab*-plane, which is two times greater than the magnetization when the field is oriented in the *c*-direction. Therefore, the magnetic correlation is stronger in the *ab*-direction.

The magnetic anisotropy observed in the field dependent magnetization coincides with differences in Sm-Sm distances in $Sm_{1.33}Pd_3Ga_8$. For the $Sm_{1.33}Pd_3Ga_8$, the Sm-Sm distances are 4.353(5) Å along the *ab*-plane, while the Sm-Sm distances are ~ 5.3391 Å and 8.1846 Å for the *c*-direction. In considering the differences in the Sm-Sm distances, the magnetic correlations in the *ab*-plane should be stronger than those along the *c*-axis. Similar behavior has been reported for $CePdGa_6$[92] and Ce_2PdGa_{12},[93] where there are two unique Ce-Ce distances in the *ab*- and *c*-direction. In $CePdGa_6$, the Ce-Ce interatomic distances are 4.350(3) Å and 7.922(6) Å for the *ab*- and *c*-direction,[92] while the Ce-Ce interatomic distances in the *ab*-plane are 4.318(6) Å and 7.664(5) Å and 7.882(6) Å for the *c*-direction in Ce_2PdGa_{12}.[93] The magnetic correlations are stronger in the *ab*-plane for $CePdGa_6$ and Ce_2PdGa_{12} given the shorter Ce-Ce distances.[92, 93] Figure 4.7 shows the resistivity of $Sm_{1.33}Pd_3Ga_8$ as a function of temperature from 2 to 300 K. $Sm_{1.33}Pd_2Ga_8$ displays metallic behavior in the electrical resistivity.

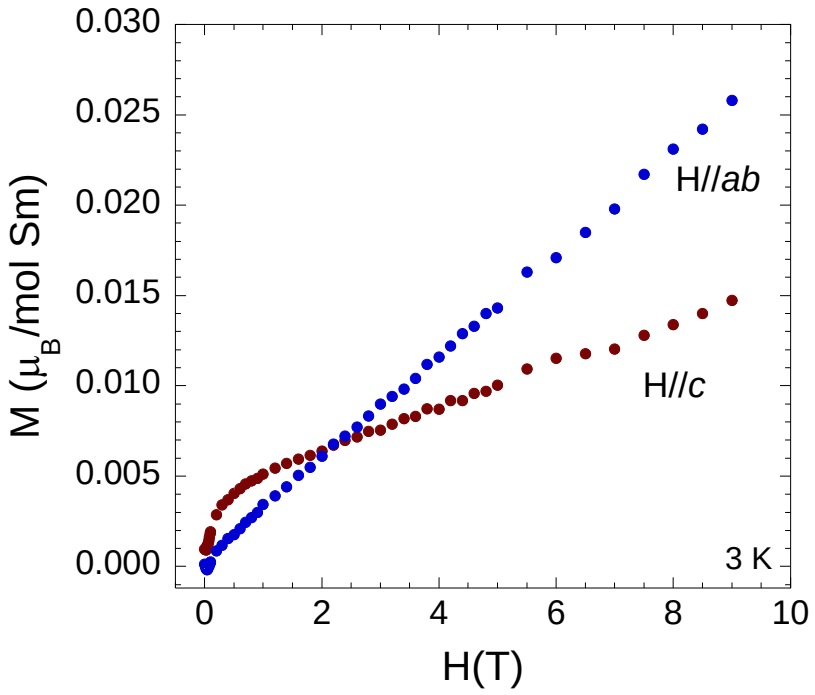

Figure 4.20. Magnetization as a function of applied field, measured at 3 K. Blue and red circles represent data collected for fields applied parallel to the crystallographic *c*- and *ab*-direction, respectively.

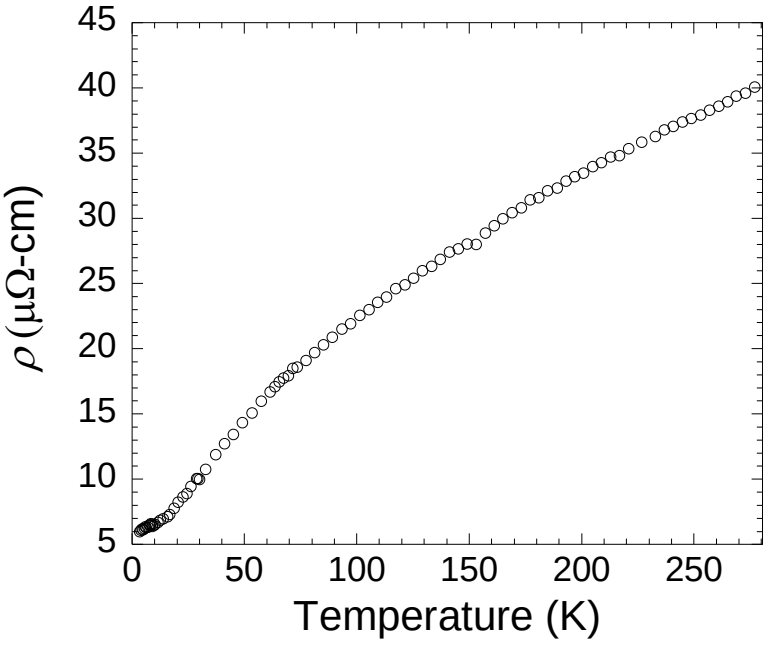

Figure 4.21. Electrical resistivity of $Sm_{1.33}Pd_3Ga_8$.

4.4 Conclusion

The crystal structure of $Sm_{1.33}Pd_3Ga_8$ adopts a disordered variant of $Er_4Pt_9Al_{24}$-structure type with the building blocks: $PdGa_2$, Pd_2Ga_4, $Sm_{0.67}Ga$ slabs. The crystal structure of $Sm_{1.33}Pd_3Ga_8$ is anisotropic given the lattice parameters and the magnetic behavior. Considering the structural motifs, unusual properties may exist in the compounds adopting the $Sm_{1.33}Pd_3Ga_8$ phase. Further exploration to grow isostructural analogues are of interest to study the anisotropic and disorder effects.

Chapter 5. Investigation of Fe and Ni incorporation in $CeCo_2Al_8$

5.1 Introduction

The growth of single crystalline Ce and Yb intermetallic compounds has attracted our interest in recent years because of the possibility of magnetically mediated superconductivity and unusual magnetism.[27] Our effort to study materials with competing magnetic interactions such as RKKY and Kondo interactions[109] has led us to grow and characterize compounds with valence instability. In particular, compounds such as $CeCo_2Al_8$,[110] an intermetallic phase adopting the $CaCo_2Al_8$ structure type,[111] follows Curie Weiss behavior with an effective moment consistent with Ce^{3+} with a θ = -136(1) K, while neither Ce or Fe carry a magnetic moment in $CeFe_2Al_8$.[110, 112] The electrical resistivity of the cerium compounds are remarkably different, with the Co analogue showing a maxima near 45 K, while the Fe analogue near 200 K, which is consistent with the strongly hybridized Ce ion with conduction electrons.

FeS_2 an insulator with ~ 1 eV band gap and CoS_2 an itinerant ferromagnet was previously reported.[113] Inspired by the carrier-doped magnetic semiconductor $Fe_{1-x}Co_xS_2$[114] and compounds exhibiting insulator-to-metal transition, we set out to grow single crystals of $CeCo_{2-x}M_xAl_8$ (M = Fe, Ni; $0 \leq x < 1$). Herein, we report the synthesis, crystal structure, magnetic and electrical properties of $CeCo_{2-x}M_xAl_8$ (M = Fe, Ni; $0 \leq x < 1$).

5.2 Experimental

5.2.1 Synthesis

Single crystals of $CeCo_{2-x}M_xAl_8$ (M = Fe, Ni; $0 \leq x < 1$) were prepared using the molten flux technique.[26, 27] Ce (rod, 99.9 %), Co (powder, 99.9 %), M (Fe, Ni powder, 99.9 %), and Al (shots, 99.9 %) were used as received. For $CeCo_2Al_8$, the elements Ce:Co:Al in atomic ratios 1:2:20, respectively, were placed in an alumina crucible, topped with another crucible, and sealed in an evacuated (50-70 mTorr) fused silica tube filled with argon. The silica tube was heated to

1200 °C at a rate of 100 °C/h, and dwelled for 24 h. The ampoule was subsequently cooled to 900 °C at a rate of 4 °C/h, followed by centrifugation to separate crystals from the aluminum flux. Single crystals of $CeCo_2Al_8$ were etched in dilute NaOH (~ 0.1 M) and then cleaned with dilute HNO_3 (~ 0.1 M). The nominal ratios of the elements weighed to grow single crystals of $CeCo_{2-x}M_xAl_8$ (M = Fe, Ni; $0 \leq x < 1$) are provided in Table 5.1.

5.2.2 Elemental Analysis

Elemental analysis was conducted via electron dispersive spectroscopy (EDS) using a FEI Quanta 200 scanning electron microscope equipped with an EDAX detector at an accelerating voltage of 20 kV. Spectra were integrated for 30 seconds and the results from 5 spots were averaged and normalized to Ln to determine the atomic percentage of each element. The compositions are $Ce_{1.00(3)}Co_{1.48(6)}Fe_{0.29(1)}Al_{9.43(9)}$, $Ce_{1.00(7)}Co_{1.30(6)}Fe_{0.55(3)}Al_{8.42(15)}$, $Ce_{1.00(5)}Co_{1.14(11)}Fe_{1.06(10)}Al_{7.58(25)}$, $Ce_{1.00(3)}Co_{1.73(2)}Ni_{0.24(3)}Al_{9.52(5)}$, and $Ce_{1.00(3)}Co_{1.31(15)}Ni_{0.62(9)}Al_{8.48(18)}$.

5.2.3 Single-Crystal X-ray Diffraction

Fragments of $CeCo_{2-x}M_xAl_8$ (M = Fe, Ni; $0 \leq x < 1$) single crystals were cut to suitable sizes and glued onto glass fibers with epoxy. The fibers were mounted on a Nonius Kappa CCD X-ray diffractometer equipped with a Mo Kα radiation source (λ = 0.71073 Å) at room temperature. Also, fragments of $CeCo_{2-x}M_xAl_8$ (M = Fe, Ni; $0 \leq x < 1$) single crystals were mounted on a Bruker D8 Quest Kappa single crystal X-ray diffractometer equipped with a IμS microfocus source (λ = 0.71073 Å) operating at 50 kV and 1 mA for multiple unit cell determinations. A starting model of the crystal structures was first obtained using SIR92[58] and refined with SHELXL97.[59] The atomic positions, Wyckoff symmetries, displacement parameters, site occupancies, and interatomic distances of $CeCo_{2-x}M_xAl_8$ (M = Fe, Ni; $0 \leq x < 1$) are provided in Tables 5.2-5.7.

5.2.4 Structure Refinement

Because scattering factors of Fe, Co, and Ni are similar, the composition obtained from EDX data were fixed during refinement of single crystal X-ray data. In all refinements the dopant (M) was only modeled on the Co1 and Co2 sites, except for $CeCo_{2-x}Fe_xAl_8$ (x = 0.33) where Fe was only modeled on the Co1 site. For the refinement of $CeCo_{2-x}M_xAl_8$ (M = Fe, Ni; $0 \leq x < 1$), we used the atomic positions of $CeCo_2Al_8$ and observed that the atomic displacement parameters (ADP) of the Co1 site was greater than Co2 site. Therefore, the dopant M was first modeled on the Co1 site and subsequently on the Co2 site. The dopant M in all refined models favored the Co1 position over the Co2 site, which is different than the previously reported $YbNi_{2-x}Fe_xAl_8$ (x = 0.91).[115] The structural refinement of $CeCo_{2-x}M_xAl_8$ (M = Fe, Ni; $0 \leq x < 1$) led to M composition provided in Table 5.1.

Table 5.1. Compositions of $CeCo_{2-x}M_xAl_8$ (M = Fe, Ni)

	Fe			Ni		
Nominal (x)	0.33	0.67	1.00	0.33	0.67	1.00
XRD (x)	0.23(7)	0.52(6)	0.70(4)	0.29(5)	0.60(8)	0.80(7)
EDS (x)	0.30(1)	0.61(3)	1.06(10)	0.24(2)	0.62(2)	0.80(4)

5.3 Results and Discussion

5.3.1 Crystal Structure

$CeCo_{2-x}M_xAl_8$ (M = Fe, Ni; $0 \leq x < 1$) adopts the $CaCo_2Al_8$ structure type[111] with the orthorhombic space group, *Pbam*. This structure type has also been reported for $LnRu_2Ga_8$ (Ln = Ce, Pr),[116] $PrCo_2Al_8$,[117] and $YbNi_{2-x}Fe_xAl_8$ (x = 0.91).[115] There are 12 unique crystallographic positions in $CeCo_2Al_8$ consisting of one Ce, two Co, and nine Al atoms. The crystal structure of $CeCo_2Al_8$ is shown in Figure 5.1 and consists of Ce atoms encapsulated in channels created by the Co-sublattice.

Table 5.2. $CeCo_{2-x}Fe_xAl_8$ ($0 \leq x < 1$) Crystallographic Parameters

Compound	$CeCo_2Al_8$	$CeCo_{1.77(7)}Fe_{0.23(7)}Al_8$	$CeCo_{1.48(4)}Fe_{0.52(6)}Al_8$	$CeCo_{1.30(4)}Fe_{0.70(4)}Al_8$
Crystal System	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
Space Group	*Pbam*	*Pbam*	*Pbam*	*Pbam*
a (Å)	12.4720(2)	12.4770(5)	12.4820(5)	12.4591(5)
*b (*Å)	14.3870(3)	14.391(2)	14.401(3)	14.3798(6)
c (Å)	4.0220(5)	4.027(2)	4.029(3)	4.024(1)
V (Å^3)	721.69(9)	723.1(4)	724.2(5)	720.96(5)
Z	4	4	4	4
θ range (º)	2.83 – 31.01	3.27 – 31.00	2.83 – 30.99	2.83 – 30.45
μ (mm^{-1})	11.613	11.303	11.285	10.828
Data Collection				
Measured Reflections	2191	2194	2144	11930
Independent Reflections	1297	1300	1300	1237
Reflections with I>2σ(I)	1141	1033	1092	1137
R_{int}	0.0243	0.0284	0.0263	0.0422
h	-17 to 17	-17 to 18	-17 to 18	-17 to 18
k	-20 to 20	-20 to 20	-20 to 20	-20 to 20
l	-5 to 5	-5 to 5	-5 to 5	-5 to 5
Refinement				
R_1 (F)[a]	0.0256	0.0266	0.0298	0.0211
wR_2[b]	0.0564	0.0583	0.0696	0.0492
Reflections	1297	1300	1300	1237
Parameters	70	71	74	74
$\Delta\rho_{max}$ (e Å^{-3})	1.119	2.459	1.318	1.417
$\Delta\rho_{min}$ (e Å^{-3})	-2.148	-1.272	-2.199	-1.923
Extinction coefficient	0.0045(3)	0.0076(3)	0.0293(11)	0.0225(6)
GOF	1.179	1.039	1.163	1.248

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$

[b] ${}_wR_2 = [\Sigma [w(F_o^2 - F_c^2)^2]/\Sigma [w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (0.0243\ P)^2 + 3.6274\ P]$, $[\Sigma [w(F_o^2 - F_c^2)^2]/\Sigma [w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (0.03119\ P)^2 + 0.6661\ P]$, $[\Sigma [w(F_o^2 - F_c^2)^2]/\Sigma [w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (0.0388\ P)^2 + 3.0837\ P]$, and $[\Sigma [w(F_o^2 - F_c^2)^2]/\Sigma [w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (0.0239\ P)^2 + 0.5008\ P]$, and $[\Sigma [w(F_o^2 - F_c^2)^2]/\Sigma [w(F_o^2)^2]]^{1/2}$ for $CeCo_2Al_8$, $CeCo_{1.72(2)}Fe_{0.28(2)}Al_8$, $CeCo_{1.37(4)}Fe_{0.63(4)}Al_8$, and $CeCo_{0.98(4)}Fe_{1.00(4)}Al_8$, respectively.

Table 5.3. $CeCo_{2-x}Ni_xAl_8$ ($0 < x < 1$) Crystallographic Parameters

Compound	$CeCo_{1.71(5)}Ni_{0.29(5)}Al_8$	$CeCo_{1.40(8)}Ni_{0.60(8)}Al_8$	$CeCo_{1.20(8)}Ni_{0.80(7)}Al_8$
Crystal System	Orthorhombic	Orthorhombic	Orthorhombic
Space Group	*Pbam*	*Pbam*	*Pbam*
a (Å)	12.4770(10)	12.4710(5)	12.4654(5)
*b (*Å)	14.393(4)	14.386(2)	14.3872(6)
c (Å)	4.023(4)	4.022(3)	4.022(1)
V (Å^3)	722.5(7)	721.6(5)	721.30(6)
Z	4	4	4
θ range (º)	2.83 – 31.19	2.83 – 31.01	2.83 – 30.50
μ (mm^1)	11.91	11.925	11.93
Data Collection			
Measured Reflections	2149	2197	8692
Independent Reflections	1303	1297	1249
Reflections with I>2σ(I)	942	1053	1070
R_{int}	0.0488	0.0299	0.0279
h	-17 to 18	-17 to 17	-17 to 17
k	-20 to 20	-20 to 20	-20 to 20
l	-5 to 5	-5 to 5	-5 to 5
Refinement			
R_1 (F)[a]	0.0366	0.0298	0.0181
wR_2[b]	0.0628	0.0696	0.0308
Reflections	1303	1297	1249
Parameters	72	72	74
$\Delta\rho_{max}$ (e Å^{-3})	1.301	1.915	1.381
$\Delta\rho_{min}$ (e Å^{-3})	-1.392	-1.416	-0.677
Extinction coefficient	0.00235(17)	0.0050(3)	0.00005(6)
GOF	1.06	1.015	1.095

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$

[b] ${}_wR_2 = [\Sigma [w(F_o^2 - F_c^2)^2]/\Sigma [w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (0.0112\ P)^2 + 7.2986\ P]$, $[\Sigma [w(F_o^2 - F_c^2)^2]/\Sigma [w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (0.0382\ P)^2 + 0.7057\ P]$, $[\Sigma [w(F_o^2 - F_c^2)^2]/\Sigma [w(F_o^2)^2]]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (0.0136\ P)^2 + 0.0005\ P]$, and $[\Sigma [w(F_o^2 - F_c^2)^2]/\Sigma [w(F_o^2)^2]]^{1/2}$ for $CeCo_{1.71(3)}Ni_{0.29(3)}Al_8$, $CeCo_{1.38(3)}Ni_{0.60(3)}Al_8$, $CeCo_{1.26(3)}Ni_{0.73(3)}Al_8$, respectively.

Table 5.4. $CeCo_{2-x}M_xAl_8$ (M = Fe, Ni; $0 \leq x < 1$) Atomic Positions

Element	Symmetry	x	y	z	Occupancy	$^aU_{eq}$ (Å^2)
$CeCo_2Al_8$						
Ce1	*m*	0.34038(2)	0.31841(2)	0	1	0.00837(11)
Co1	*m*	0.03488(6)	0.40566(5)	0	1	0.00693(16)
Co2	*m*	0.15166(5)	0.09643(5)	0	1	0.00565(15)
Al1	*m*	0.09584(12)	0.25276(10)	0	1	0.0078(3)
Al2	*m*	0.33993(12)	0.04446(11)	0	1	0.0097(3)
Al3	*m*	0.15953(12)	0.37939(11)	1/2	1	0.0075(3)
Al4	*m*	0.45285(13)	0.17938(10)	1/2	1	0.0070(3)
Al5	*m*	0.23625(13)	0.17238(10)	1/2	1	0.0077(3)
Al6	*m*	0.33139(13)	0.49140(11)	1/2	1	0.0080(3)
Al7	*m*	0.02559(13)	0.13168(11)	1/2	1	0.0075(3)
Al8	*2/m*	0	1/2	1/2	1	0.0076(4)
Al9	*2/m*	0	0	0	1	0.0082(4)
$CeCo_{1.77(7)}Fe_{0.23(7)}Al_8$						
Ce1	*m*	0.34072(2)	0.318513(19)	0	1	0.01055(11)
Co1	*m*	0.03456(5)	0.40589(5)	0	0.77(6)	0.0092(2)
Co2	*m*	0.15116(5)	0.09671(4)	0	1	0.00808(15)
Al1	*m*	0.02558(12)	0.13172(10)	1/2	1	0.0097(3)
Al2	*m*	0.15961(12)	0.37917(11)	1/2	1	0.0095(3)
Al3	*m*	0.23606(12)	0.17258(10)	1/2	1	0.0096(3)
Al4	*m*	0.33146(12)	0.49159(10)	1/2	1	0.0106(3)
Al5	*m*	0.45250(12)	0.17965(10)	1/2	1	0.0095(3)
Al6	*m*	0.09581(12)	0.25304(9)	0	1	0.0096(3)
Al7	*m*	0.33940(12)	0.04452(10)	0	1	0.0111(3)
Al8	*2/m*	0	1/2	1/2	1	0.0096(4)
Al9	*2/m*	0	0	0	1	0.0104(4)
$CeCo_{1.48(6)}Fe_{0.52(6)}Al_8$						
Ce1	*m*	0.34100(3)	0.31861(2)	0	1	0.01057(15)
Co1	*m*	0.03428(7)	0.40657(6)	0	0.79(7)	0.0100(3)
Fe1	*m*	0.03428(7)	0.40657(6)	0	0.21(8)	0.0100(3)
Co2	*m*	0.15082(6)	0.09679(6)	0	0.56(7)	0.0088(3)
Fe2	*m*	0.15082(6)	0.09679(6)	0	0.46(8)	0.0088(3)
Al1	*m*	0.02569(15)	0.13175(13)	1/2	1	0.0098(4)
Al2	*m*	0.15971(15)	0.37927(14)	1/2	1	0.0098(4)
Al3	*m*	0.23578(15)	0.17252(13)	1/2	1	0.0101(4)
Al4	*m*	0.33141(15)	0.49210(13)	1/2	1	0.0100(4)
Al5	*m*	0.45241(15)	0.17966(13)	1/2	1	0.0103(4)
Al6	*m*	0.09557(15)	0.25327(12)	0	1	0.0101(4)
Al7	*m*	0.33858(14)	0.04441(14)	0	1	0.0118(4)
Al8	*2/m*	0	1/2	1/2	1	0.0101(5)
Al9	*2/m*	0	0	0	1	0.0112(5)
$CeCo_{1.30(4)}Fe_{0.70(4)}Al_8$			0			
Ce1	*m*	0.340544(12)	0.318648(12)	0	1	0.00855(9)
Co1	*m*	0.03460(3)	0.40615(3)	0	0.68(4)	0.00687(15)
Fe1	*m*	0.03460(3)	0.40615(3)	0	0.30(4)	0.00687(15)
Co2	*m*	0.15020(3)	0.09724(3)	0	0.29(5)	0.00581(16)
Fe2	*m*	0.15020(3)	0.09724(3)	0	0.72(6)	0.00581(16)
Al1	*m*	0.02542(7)	0.13185(6)	1/2	1	0.00673(17)
Al2	*m*	0.15966(6)	0.37884(7)	1/2	1	0.00741(19)
Al3	*m*	0.23543(7)	0.17269(6)	1/2	1	0.00767(18)
Al4	*m*	0.33146(7)	0.49203(7)	1/2	1	0.00750(18)
Al5	*m*	0.45229(7)	0.17998(6)	1/2	1	0.00733(18)
Al6	*m*	0.09522(6)	0.25318(5)	0	1	0.00754(18)

(Table 5.4. continued)

Element	Symmetry	x	y	z	Occupancy	$^{a}U_{eq}$ (Å^2)
Al7	*m*	0.33860(6)	0.04479(7)	0	1	0.0094(2)
Al8	*2/m*	0	1/2	1/2	1	0.0071(2)
Al9	*2/m*	0	0	0	1	0.0077(2)
$CeCo_{1.71(5)}Ni_{0.29(5)}Al_8$						
Ce1	*m*	0.34044(4)	0.31848(3)	0	1	0.01117(14)
Co1	*m*	0.03473(9)	0.40571(8)	0	0.91(11)	0.0098(4)
Ni1	*m*	0.03473(9)	0.40571(8)	0	0.09(11)	0.0098(4)
Co2	*m*	0.15175(9)	0.09640(7)	0	0.80(10)	0.0087(4)
Ni2	*m*	0.15175(9)	0.09640(7)	0	0.20(10)	0.0087(4)
Al1	*m*	0.0253(2)	0.13172(17)	1/2	1	0.0099(5)
Al2	*m*	0.1597(2)	0.37958(17)	1/2	1	0.0101(5)
Al3	*m*	0.2366(2)	0.17235(18)	1/2	1	0.0105(5)
Al4	*m*	0.3318(2)	0.49155(16)	1/2	1	0.0099(5)
Al5	*m*	0.4523(2)	0.17948(18)	1/2	1	0.0104(5)
Al6	*m*	0.0961(2)	0.25286(18)	0	1	0.0105(5)
Al7	*m*	0.3399(2)	0.04426(17)	0	1	0.0114(5)
Al8	*2/m*	0	1/2	1/2	1	0.0098(8)
Al9	*2/m*	0	0	0	1	0.0109(7)
$CeCo_{1.40(8)}Ni_{0.60(8)}Al_8$						
Ce1	*m*	0.34035(2)	0.31849(2)	0	1	0.01152(11)
Co1	*m*	0.03469(5)	0.40569(5)	0	0.4858(17)	0.0100(2)
Ni1	*m*	0.03469(5)	0.40569(5)	0	0.4858(17)	0.0100(2)
Co2	*m*	0.15185(5)	0.09639(5)	0	0.89(8)	0.0089(3)
Ni2	*m*	0.15185(5)	0.09639(5)	0	0.11(8)	0.0089(3)
Al1	*m*	0.09608(12)	0.25288(11)	0	1	0.0110(3)
Al2	*m*	0.33977(12)	0.04458(12)	0	1	0.0122(3)
Al3	*m*	0.15972(12)	0.37922(12)	1/2	1	0.0107(3)
Al4	*m*	0.45256(13)	0.17966(11)	1/2	1	0.0109(3)
Al5	*m*	0.23631(13)	0.17248(11)	1/2	1	0.0110(3)
Al6	*m*	0.33148(13)	0.49133(11)	1/2	1	0.0109(3)
Al7	*m*	0.02525(13)	0.13192(11)	1/2	1	0.0109(3)
Al8	*2/m*	0	1/2	1/2	1	0.0110(4)
Al9	*2/m*	0	0	0	1	0.0111(4)
$CeCo_{1.20(7)}Ni_{0.80(7)}Al_8$						
Ce1	*m*	0.340227(13)	0.318594(11)	0	1	0.00855(5)
Co1	*m*	0.03483(3)	0.40579(3)	0	0.66(4)	0.00740(12)
Ni1	*m*	0.03483(3)	0.40579(3)	0	0.34(3)	0.00740(12)
Co2	*m*	0.15196(3)	0.09630(3)	0	0.73(4)	0.00634(12)
Ni2	*m*	0.15196(3)	0.09630(3)	0	0.27(4)	0.00634(12)
Al1	*m*	0.09611(7)	0.25282(6)	0	1	0.00818(17)
Al2	*m*	0.33977(7)	0.04459(6)	0	1	0.01066(18)

(Table 5.4. continued)

Element	Symmetry	x	y	z	Occupancy	$^{a}U_{eq}$ (Å^2)
Al3	*m*	0.15982(7)	0.37920(6)	1/2	1	0.00797(17)
Al4	*m*	0.45238(7)	0.17951(6)	1/2	1	0.00779(17)
Al5	*m*	0.23642(7)	0.17233(6)	1/2	1	0.00835(18)
Al6	*m*	0.33142(7)	0.49123(6)	1/2	1	0.00814(17)
Al7	*m*	0.02547(7)	0.13188(6)	1/2	1	0.00757(17)
Al8	*2/m*	0	1/2	1/2	1	0.0077(2)
Al9	*2/m*	0	0	0	1	0.0081(2)

$^{a}U_{eq}$ is defined as one-third of the trace of the orthogonalized U_{ij} tensor

Table 5.5. $CeCo_{2-x}Fe_xAl_8$ ($0 \leq x < 1$) Selected Interatomic Distances

	$CeCo_2Al_8$	$CeCo_{1.77(7)}Fe_{0.23(7)}Al_8$	$CeCo_{1.48(6)}Fe_{0.52(6)}Al_8$	$CeCo_{1.30(4)}Fe_{0.70(4)}Al_8$
Ce				
Al1 x 2	3.1457(16)	3.1443(14)	3.1438(17)	3.1402(7)
Al2 x 2	3.1467(14)	3.1500(13)	3.1531(17)	3.1427(6)
Al3 x 2	3.1851(15)	3.1891(13)	3.1952(17)	3.1889(7)
Al4 x 2	3.2017(16)	3.2049(14)	3.2116(17)	3.2058(8)
Al5 x 2	3.1643(15)	3.1611(13)	3.1617(17)	3.1564(7)
M1				
Al2 x 2	2.5698(14)	2.5761(13)	2.5814(16)	2.5749(5)
Al5 x 2	2.5667(14)	2.5726(12)	2.5777(16)	2.5756(6)
Al6 x 1	2.3275(16)	2.3287(15)	2.337(2)	2.3257(9)
Al7 x 2	2.5349(17)	2.5375((16)	2.543(2)	2.5438(10)
Al8 x 2	2.4649(17)	2.4646(9)	2.4600(11)	2.4608(2)
M1 x 1	2.8505(13)	2.8426(13)	2.8236(17)	2.8336(8)
M2				
Al1 x 2	2.6026(15)	2.6005(13)	2.5983(16)	2.5909(6)
Al3 x 2	2.5201(14)	2.5236(13)	2.5243(16)	2.5205(6)
Al4 x 2	2.5243(14)	2.5278(13)	2.5260(16)	2.5277(6)
Al6 x 1	2.3543(16)	2.3532(15)	2.357(2)	2.3447(9)
Al7 x 1	2.4643(17)	2.4658(16)	2.462(2)	2.4655(9)
Al9 x 1	2.3457(7)	2.3439(6)	2.3424(8)	2.3360(4)

Table 5.6. $CeCo_{2-x}Ni_xAl_8$ ($0 < x < 1$) Selected Interatomic Distances

	$CeCo_{1.71(5)}Ni_{0.29(5)}Al_8$	$CeCo_{1.40(8)}Ni_{0.60(8)}Al_8$	$CeCo_{1.20(8)}Ni_{0.80(8)}Al_8$
Ce			
Al1 x 2	3.143(2)	3.1417(16)	3.1403(7)
Al2 x 2	3.148(3)	3.1436(16)	3.1438(6)
Al3 x 2	3.186(2)	3.1843(16)	3.1853(7)
Al4 x 2	3.204(2)	3.1998(16)	3.1977(7)
Al5 x 2	3.162(2)	3.1609(16)	3.1627(6)
M1			
Al2 x 2	2.573(2)	2.5730(16)	2.5726(5)
Al5 x 2	2.570(2)	2.5693(16)	2.5702(6)
Al6 x 1	2.330(3)	2.3278(17)	2.3296(9)
Al7 x 2	2.535(3)	2.5383(18)	2.5360(9)
Al8 x 2	2.4646(18)	2.4641(13)	2.4636(2)
M1 x 1	2.849(2)	2.8480(15)	2.8465(7)
M2			
Al1 x 2	2.607(2)	2.6073(16)	2.6062(6)
Al3 x 2	2.522(2)	2.5203(16)	2.5198(6)
Al4 x 2	2.522(2)	2.5242(16)	2.5242(6)
Al6 x 1	2.356(3)	2.3563(17)	2.3571(9)
Al7 x 1	2.465(3)	2.4593(17)	2.4565(9)
Al9 x 1	2.3437(12)	2.3471(7)	2.3468(4)

Each Ce atom is located in a pentagonal prism of Al atoms with distances of ~ 3.1 Å. All the faces of the pentagonal prisms are capped by Al atoms with Ce-Al distances ranging from 3.3 to 4.0 Å. The transition metal sublattice of $CeCo_2Al_8$ forms a closed packed arrangement around the Ce atoms. The Co1 and Co2 environments are nine coordinate consisting of Al atoms forming monocapped rectangular prisms. The Co1 monocapped rectangular prisms are face-sharing with Co1 polyhedra forming dimers with Co1-Co1 distance of 2.8506(3) Å. The Co-Al distances in the $[CoAl_{8+1}]$ prisms range from ~ 2.3 to 2.5 Å. The Co-Al distances in $CeCo_2Al_8$ are comparable to the sum of the covalent radii of Co (1.26) and Al (1.18),[83] which suggest strong atomic interactions. The Co-Al interatomic distances are comparable to the bond interaction in binary

Co_2Al_9,[118, 119] with Co-Al distances ranging from 2.3 to 2.5 Å. The shortest Ce-Al distances and Co-Al distances in $[CoAl_{8+1}]$ prisms are comparable to the sum of the covalent radii (3.25 Å Ce+Al and 2.47 Å Co+Al). This suggests strong interactions are present in $CeCo_2Al_8$. Previously, spin-polarized band structure calculations of isostructural $EuRh_2Ga_8$ revealed the formation of a 3D $[Rh_2Ga_8]$ polyanion by Ga-Ga and polar Ga-Rh bonds. The Eu atoms interact with the $[Rh_2Ga_8]$ polyanion by ionic and covalent interactions.[120]

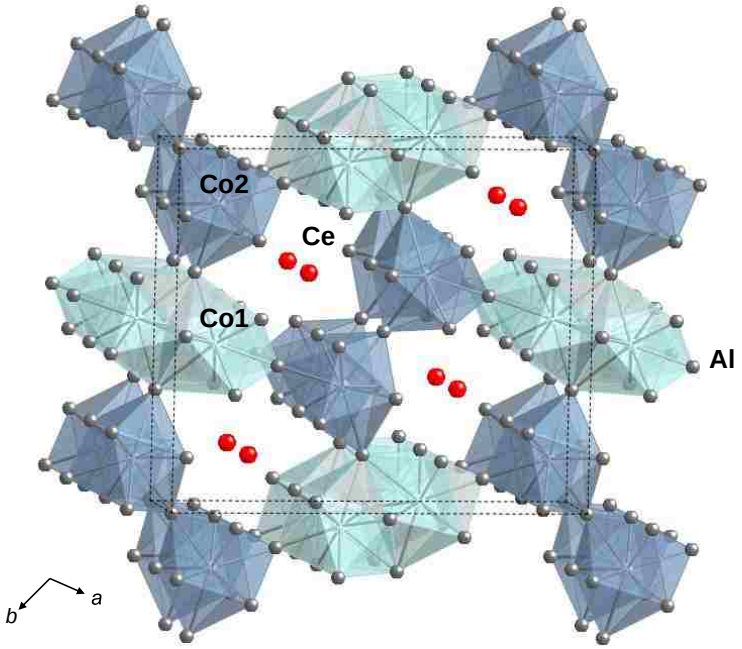

Figure 5.1. Crystal structure of $CeCo_2Al_8$ down the *c*-direction Co1 and Co2 are represented as light blue and dark blue polyhedra, respectively.

A plot of the volume as a function of dopant in $CeCo_{2-x}M_xAl_8$ (M = Fe, Ni; $0 \leq x < 1$) is shown in Figure 5.2. For the Fe-doped compounds, the volumes increase as a function of concentration until x = 0.70(4) where the volume decreases. This behavior can be attributed to valence fluctuation of Ce caused by the substitution of Fe consistent with the valence fluctuating $CeFe_2Al_8$. In the Ni-doped $CeCo_2Al_8$, a slight increase in volume is observed for x = 0.23(1), then followed by a decrease in volume as Ni concentration increases.

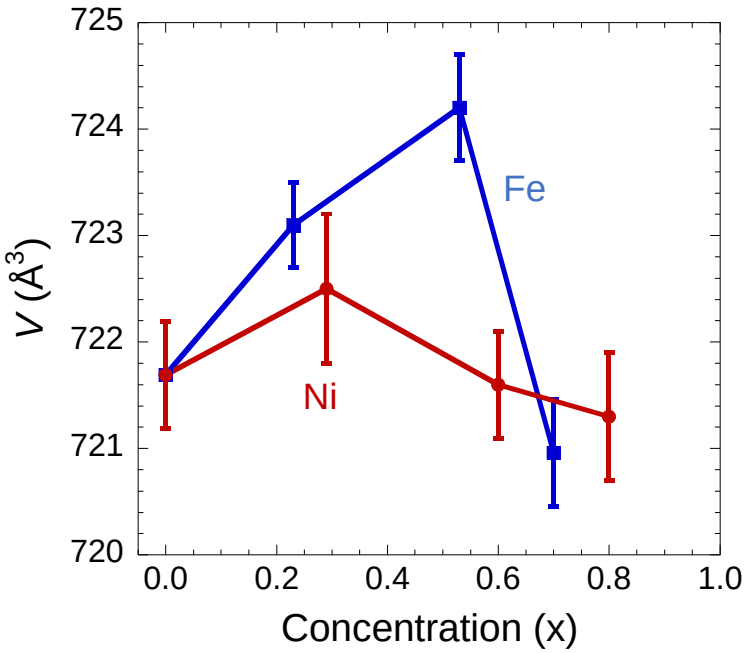

Figure 5.2. Volume $CeCo_{2-x}M_xAl_8$ (M = Fe, Ni; ($0 \leq x < 1$) as function of concentration.

5.4 Conclusion

We have successfully grown single crystals of $CeCo_{2-x}M_xAl_8$ (M = Fe, Ni; $0 \leq x < 1$). Hybridization between the 4*f*- and conduction electrons and the rare-earth valence state can change by applying chemical pressure to a strongly correlated intermetallic with an unstable ground state. By substituting and controlling the amount of dopant (M) in $CeCo_{2-x}M_xAl_8$ (M = Fe, Ni; $0 \leq x < 1$), we can systematically investigate the effects in substitution effect on the structural and physical properties of $CeCo_2Al_8$. The expansion and contraction of the volume of $CeCo_{2-x}M_xAl_8$ (M = Fe, Ni; $0 \leq x < 1$) follows the expected trend given the respective dopant (M), except for $CeCo_{2-x}Fe_xAl_8$ (x = 0.70(4)) which marks the critical concentration of Fe needed to induce valence instability in the Ce 4*f*-electronic state. Considering the variation in Ce valence on the basis of the single crystal data indicates that the size of the substituting elements does not affect the 4*f*-electronic state of Ce.

Chapter 6. Conclusion and Future Work

6.1 Summary

Chemical substitution in rare earth intermetallics can affect the coupling between the conduction and 4*f*-electrons that can lead to the discovery of competing structural and physical properties in rare earth intermetallics. For example, $YbNi_3Ga_9$ exhibits intermediate valency, +2.46, with a high Kondo temperature of T_K = 570 K.[121] Hole substitution studies, Co for Ni, led to $Yb(Ni_{1-x}Co_x)_3Ga_9$ causing a decrease in the Kondo temperature, T_k = 540 – 220 K for $0 \leq x \leq 0.3$, and an increase in the Sommerfeld coefficient, γ, indicating a mass enhancement.[122] At ambient pressure, $CeRhIn_5$ orders antiferromagnetic at 3.8 K. Upon application of pressure, 19 kbar, $CeRhIn_5$ exhibits superconductivity suppressing the antiferromagnetic transition.[2] Sn substitution in $CeRhIn_5$, led to $CeRhIn_{5-x}Sn_x$ and a suppression of the antiferromagnetic transition while inducing a quantum critical point at the critical concentration of x = 0.35.[123]

The work in this dissertation illustrates the effects of substitution on the structural and physical properties in rare earth intermetallics with unique structural motifs and competing interactions. $Ln_6W_4Al_{43}$ (Ln = Gd, Yb) adopts the $Ho_6Mo_4Al_{43}$-structure type[16] and can be describe as two interpenetrating networks of Ln and W atoms with the Ln atoms forming Kagome network in the *ab*-plane. $Gd_6W_4Al_{43}$ orders antiferromagnetically at T_N = 15 K with a θ = 13.62(7) K that suggests the presence of ferromagnetic exchange interactions.[124] The effect moment of $Gd_6W_4Al_{43}$ (7.92(3) μ_B) is close to the magnetic moment for a free Gd^{3+} ion (7.94 μ_B). $Yb_6W_4Al_{43}$ exhibits temperature independent paramagnetism with the Yb atoms adopting the nonmagnetic divalent configuration.[124] We aimed to substitute Mn and Fe in $Ln_6W_4Al_{43}$ (Ln = Gd, Yb) because of the arrangement of the Ln atoms and the nonmagnetic nature of W. Only a relatively small amount of Mn or Fe (x < 1.5) was able to substitute in $Ln_6W_4Al_{43}$ (Ln = Gd, Yb). Unexpectedly,

Mn and Fe prefers to substitute for Al only in $Gd_6W_4Al_{43}$.[37] However, Mn prefers to substitute for W and Al in $Yb_6W_4Al_{43}$, while Fe prefers to substitute for Al only. The site preference of Mn in $Ln_6W_4Al_{43}$ (Ln = Gd, Yb) can be attributed to the difference in the cell volume of the parent analogues ($Yb_6W_4Al_{43}$ (1856.2(3) $Å^3$) and $Gd_6W_4Al_{43}$ (1871.2(3) $Å^3$)). The Gd-analogues order antiferromagentically with the ordering temperatures decreasing from $Gd_6W_4Al_{43}$ (T_N = 15 K) > $Gd_6W_4Al_{43-y}Mn_y$ (T_N = 14 K) > $Gd_6W_4Al_{43-y}Fe_y$ (T_N = 13 K). All three analogues show positive Weiss constant that decreases from $Gd_6W_4Al_{43}$ (θ = 13.62(7) K) > $Gd_6W_4Al_{43-y}Mn_y$ (θ = 9.91(6) K) > $Gd_6W_4Al_{43-y}Fe_y$ (θ = 7.56(5) K).[37] The trend in magnetic behavior is unusually given the decrease in cell volumes, $Gd_6W_4Al_{43}$ (1871.1(3) Å) > $Gd_6W_4Al_{43-y}Mn_y$ (1861.3(1) Å) > $Gd_6W_4Al_{43-y}Fe_y$ (1855.1(4) Å), and Gd-Gd interatomic distances that should lead to stronger magnetic interactions. A plausible explanation for the magnetic trend is the presence of competing interactions of the magnetic ions in the *ab*- and *c*-direction. Like $Yb_6W_4Al_{43}$, Mn and Fe substituted $Yb_6W_4Al_{43}$ exhibit temperature independent magnetism, which indicate that Mn and Fe are nonmagnetic.

Compounds of the $Ho_6Mo_4Al_{43}$-[16] and $CeCr_2Al_{20}$-structure type[17] share similar structural motifs such as interpenetrating rare earth and transition metal sublattices. In $LnCr_2Al_{20}$ (Ln = La, Gd, Yb) of the $CeCr_2Al_{20}$ structure type,[17] the Ln ions are surrounded by 16 Al atoms forming Frank-Kasper cages that form triangular networks by corner sharing Al atoms. The Cr sublattice can be viewed as tetrahedral network of vertex sharing distorted icosahedra that is similar to the pyrochlore lattice. Polycrystalline $GdCr_2Al_{20}$ orders antiferromagnetically at 3.90(5) K.[77] Single crystals of $LnCr_2Al_{20}$ (Ln = La, Yb) are temperature independent paramagnets suggesting that the transition metal is nonmagnetic.[78] We targeted Fe incorporation in $LnCr_2Al_{20}$ (Ln = La, Gd, Yb) because of the arrangement of the Ln and Cr atoms and to induce unique magnetism. Based on

the similar atomic radii of Cr (1.249) and Fe (1.241), we expected the Fe to substitute for Cr in $LnCr_2Al_{20}$ (Ln = La, Gd, Yb). Through elemental analysis, we were able to determine that only a small amount of Fe, x ~ 0.1 and 0.2, was substituted in $LnCr_2Al_{20}$ (Ln = Gd, Yb), while no Fe was substituted in $LaCr_2Al_{20}$. As a result of the small concentration of Fe incorporation in $LnCr_2Al_{20}$ (Ln = Gd, Yb), we were not able to identify the site presence of Fe solely by X-ray diffraction. Therefore, ^{57}Fe Mössbauer spectroscopy was used to determine the nature of Fe in our compounds. The refinement of the ^{57}Fe Mössbauer data suggested that Fe substituted on two Al sites. As a result, crystallographic models were refined with Fe occupying each pair of crystallographic Al sites, and the best agreement with the Mössbauer spectroscopy was achieved when the Fe atoms partially occupy the Al1 and Al2 sites. Based on the volume change between the undoped and doped compounds, we concluded that Fe substitutes for Al rather than Cr.[39] The results suggest that the latter transition metals do not adopt the $CeCr_2Al_{20}$-structure type.[17] Single crystals of $GdCr_2Al_{20}$ and $GdCr_2Al_{20-x}Fe_x$ exhibit paramagnetic behavior down to the lowest temperature measured with no magnetic ordering contrary to the previously reported polycrystalline $GdCr_2Al_{20}$ that display antiferromagnetic ordering at 3.90(5) K.[77] Like $YbCr_2Al_{20}$, both $YbCr_2Al_{20-x}Fe_x$ and $LaCr_2Al_{20}$ compounds display temperature independent magnetism which indicate that the small concentration of Fe did not change the magnetic behavior.[39]

Because of the structural complexity in $Yb_2Pd_3Ga_9$,[27] we set out to target the samarium analogue due to the fact that Sm ions can exist in multiple electronic configuration ($4f^6$ and $4f^5$). However, with our flux growth conditions, we stabilized $Sm_{1.33}Pd_3Ga_8$ that adopts a disordered variant of the $Er_4Pt_9Al_{24}$-structure type.[38] The crystal structure of $Sm_{1.33}Pd_3Ga_8$ is composed of three distinct building block and is highly anisotropic. The temperature dependent susceptibility of $Sm_{1.33}Pd_3Ga_8$ display temperature independent paramagnetism, indicating Sm atoms adopting

the nonmagnetic divalent configuration. Field dependent magnetization of $Sm_{1.33}Pd_3Ga_8$ exhibits anisotropic behavior. When the field is perpendicular to the *c*-direction $Sm_{1.33}Pd_3Ga_8$ exhibits a change in slope at 0.5 T, followed by an increase in magnetization to a maximum of ~ 0.015 μ_B/mol Sm at 9 T. The field dependent magnetization in the *ab*-direction is linear up to 9 T with a maximum of ~ 0.028 μ_B/mol Sm. The magnetic anisotropy, observed in the field dependent magnetization, originates from the different Sm-Sm interatomic distances in the *ab*- and *c*-direction, which is similar to previously published $CePdGa_6$[92] and Ce_2PdGa_{12}.[93]

Strongly correlated Ce-intermetallic compounds exhibiting unusual behavior are highly dependent on the coupling of rare earth *f*-electrons and conduction electrons, which is greatly affected by substitution of transition metals.[27, 125-127] We expect the properties of $CeCo_{2-x}M_xAl_8$ (M = Fe, Ni; $0 \leq x < 1$) to change based on the dopant M and previously reported magnetic and electrical properties of CeM_2Al_8 (M = Fe, Co).[110] Single crystal data of $CeCo_{2-x}M_xAl_8$ (M = Fe, Ni; $0 \leq x < 1$) suggests Ce ground state changes as a function of Fe, which is evident by a deviation in the cell volume. However, the Ce ground state is stable as a function of Ni concentration given the consistent trend in the cell volume. This suggests that hole doping (Fe) or an increase in the cell volume plays a significant role in the oxidation state of Ce in $CeCo_2Al_8$. Future work will include measuring the magnetization and the electrical resistivity. By measuring the properties of $CeCo_{2-x}M_xAl_8$ (M = Fe, Ni; $0 \leq x < 1$), we will be able to investigate the ground state of Ce and determine how hole doping and electron doping effects the electrical resistivity. The results can lead to general conclusions on how the properties are affected by hole and electron doping, which in turn can be applied to future research with Yb-based compounds given their unstable ground state similar to Ce.

6.2 Future Work

The work presented in this dissertation illustrates how chemical substitution effects the structural and physical properties of rare earth intermetallics. Another way to influence the structure and magnetic properties of materials is to consider simple binary compounds and the insertion of guest atoms in the interstitial sites. A recent example of this strategy has been shown to be an effective method to discover new materials. Our research group recently reported Mn-insertion into the well-known $AuCu_3$-structure type.[128] This structure type is of particular interest because of the $CeIn_3$ compound that orders antiferromagnetic at $T_N \sim 11$ K. Upon the application of pressure (25 kbar), the $CeIn_3$ compound exhibits superconductivity at ~ 0.2 K.[1] $LnMn_xGa_3$ (Ln = Ho-Tm; $x < 0.2$) adopts the stuffed variant of the $AuCu_3$-structure type where Mn partially occupies the body center position of the unit cell.[128] Magnetic properties of $LnGa_3$ (Ln = Ho-Tm) change with the insertion of Mn. The Mn-containing Ho and Er analogues order antiferromagnetic at 7.7 K and 3.1 K, which is higher than the parent analogues that order at 6.2 K and 2.9 K.[128] This can be attributed to the increase in Ln-Ln distance due to the guest atom. The Mn containing $TmGa_3$ analogues exhibit paramagnetic behavior down to 3 K, however the $TmGa_3$ exhibits antiferromagnetic ordering at 4.2 K due to crystal electric field affects. DFT-chemical pressure analysis was performed to study the chemical pressure of $LnMn_xGa_3$ (Ln = Ho-Tm; $x < 0.2$). The results suggests that M guest atoms provide structural support when the Ln atoms are large so the Ga-Ga contacts of the $AuCu_3$-structure type are significantly stretched.[128] Given the physical properties of $LnMn_xGa_3$ (Ho, Tm; $x < 0.2$), it is of interest to study the effects of inserting Fe and Co in $LnGa_3$ (Ln = Ho-Tm). We have grown single crystals of ErM_xGa_3 (Fe, Co; $x < 0.2$) and currently optimizing the single crystal growth of LnM_xGa_3 (Ho, Tm; M = Fe, Co; $x < 0.2$) to investigate the chemical stability and magnetic behavior as a function of M.

The work in this dissertation illustrates that the geometry, magnetic ions interactions, elemental composition, and concentration of the substituting component is essential to achieve unique magnetic behavior. Substitution studies of the compounds reported led to the discovery of serendipitous as well as the desired pseudo ternary compounds. We have successfully grown and characterized Yb-containing compounds and performed substitution studies. There are relatively few studies of substitution effects in Yb-based compounds as compared to Ce-based compounds, due to the difficulty in growing Yb-based compounds because of the high vapor pressure of ytterbium. Unfortunately, we did not induce valence instability in Yb-based compounds which is most likely due to the low concentration of the substituting element; however mixed valent behavior in $CeCo_2Al_8$ was induced with high concentration of Fe. There is a lack in researchers' ability to predict how a substituting element will affect the magnetic properties of a host compound. Identification of structural motifs in materials that correlate with certain physical properties and how they are affected by substitution is a vital step to obtain a more profound understanding about the physics of materials. The most effective way to advance our understanding in the field of solid state chemistry is by continuing to search for new materials and perform substitution studies.

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Appendix A. Investigating the chemical stability and physical properties of ErM_xGa_3 (M = Fe, Co; x < 0.2)

A.1 Objective

To investigate the chemical stability and physical properties of ErM_xGa_3 (M = Fe, Co; x < 0.2). Single crystals of ErM_xGa_3 (M = Fe, Co; x < 0.2) were grown.

A.2 Synthesis

Single crystals of ErM_xGa_3 (M = Fe, Co; x < 0.2) were grown using the flux growth method. The elements Er: M: Ga were weighed in atomic ration of 1:0.1:20 and 1:0.2:20, respectively, to investigate the effect of varying M concentration. The respective elements Er: M: Ga were placed in an alumina crucibles, topped with another crucible, and sealed in an evacuated silica tubes. All vessels were heated to 1150 °C at a rate of 100 °C/h, and dwelled for 5 hr. Subsequently, the ampoules were cooled to 550 °C at a rate of 5 °C/h, and finally cooled to 300 °C at a rate of 100 °C/h. The samples were removed from the furnace and centrifuged to remove excess Ga flux. The excess Ga flux on the single crystals was removed by repeated sonication in hot water. Synthesis yielded large single crystals ~ 5 mm long.

A.3 Elemental Analysis

Elemental analysis of ErM_xGa_3 (M = Fe, Co; x < 0.2) single crystals was performed via energy-dispersive spectroscopy (EDS) using an EDAX detector with an accelerating voltage of 19 kV. Single crystals of ErM_xGa_3 (M = Fe, Co; x < 0.2) were polished prior to analysis in order to minimize the presence of possible surface impurities. Spectra were integrated for 60 seconds and results from 6 spots were averaged and normalized to Er. The compositions are $Er_{1.00(6)}Fe_{0.08(1)}Ga_{2.27(7)}$, $Er_{1.00(1)}Fe_{0.11(1)}Ga_{2.91(1)}$, and $Er_{1.00(1)}Co_{0.14(1)}Ga_{3.06(1)}$.

A.4 Physical Properties

Magnetic data were collected on single crystals of ErM_xGa_3 (M = Fe, Co; x < 0.2) using a Quantum Design Magnetic Property Measurement System (MPMS). The temperature-dependent susceptibility was measured under zero-field (ZFC) conditions between 3 and 300 K with an applied magnetic field of 0.01 T. Also, the field-dependent magnetization data were measured at 3 K with fields up to 7 T for all analogues.

A.5 Results and Discussion

Powder diffraction data was collected on ground single crystals of ErM_xGa_3 (M = Fe, Co; x < 0.2) using a Bruker D8 Advance X-ray diffractometer equipped with a Lynxeye detector with Cu Kα radiation. The diffraction patterns were indexed to $AuCu_3$-structure type. All diffraction patterns exhibit a shift in 2θ consistent with the insertion of the guest atom M. Fragments of ErM_xGa_3 (M = Fe, Co; x < 0.2) were cut to appropriate sizes and mounted on a Bruker D8 Quest Kappa single crystal X-ray diffractometer equipped with a IμS microfocus source (λ = 0.71073 Å) operating at 50 kV and 1 mA for data collections. The single crystal diffraction data were indexed to a primitive cubic cell with dimension a ~ 4.25 Å, consistent with the $AuCu_3$-structure type.[1] A starting model of the crystal structure was first obtained using SIR97[2] and was refined using SHELXL97.[3] After implementing the atomic position that corresponds to the $AuCu_3$-structure type, residual electron density was observed at ~ 0.11 ½ ½, which is really close to the elongated Ga1 site. Therefore, the Ga site was split to a Ga and Ga′ site. Subsequently, another Q peak at ½ ½ ½ was present corresponding to the middle of the unit cell. This position was modeled M with partial occupancy. The atomic positions, Wyckoff symmetries, displacement parameters, site occupancies, and interatomic distances of ErM_xGa_3 (M = Fe, Co; x < 0.2) are provided in Tables A.1-3.

Table A.1. Crystallographic Parameters of ErM_xGa_3 (M = Fe, Co; x < 0.2)

Crystal data			
Formula	$ErFe_{0.06(1)}Ga_3$	$ErFe_{0.11(2)}Ga_3$	$ErCo_{0.06(2)}Ga_3$
Space group	$Pm\bar{3}m$	$Pm\bar{3}m$	$Pm\bar{3}m$
a (Å)	4.2227(4)	4.2263(5)	4.2201(7)
V (Å^3)	75.296(12)	75.489(15)	75.16(2)
Z	1	1	1
Crystal size (mm^3)	0.04 x 0.04 x 0.12	0.04 x 0.04 x 0.10	0.10 x 0.10 x 0.15
θ Range (°)	4.83-30.33	4.82-30.30	4.83-30.35
μ (mm^{-1})	58.423	58.274	59.223
Data Collection and Refinement			
Collected reflections	734	756	745
Unique reflections	41	41	41
R_{int}	0.0217	0.0226	0.0236
h	$-4 \le h \le 6$	$-6 \le h \le 4$	$-5 \le h \le 5$
k	$-5 \le k \le 5$	$-5 \le k \le 5$	$-5 \le k \le 5$
l	$-6 \le l \le 5$	$-5 \le l \le 6$	$-5 \le l \le 5$
$\Delta\rho_{max}$ (e Å^{-3})	0.895	1.026	1.226
$\Delta\rho_{min}$ (e Å^{-3})	-0.681	-1.845	-1.102
GoF	1.416	1.269	1.529
Extinction coefficient	0.181(12)	0.001(6)	0.046(4)
[a] $R_1(F)$ for $F_o^2 > 2\sigma(F_o^2)$	0.0099	0.0184	0.0212
[b] $R_w(F_o^2)$	0.0204	0.0392	0.0495

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$

[b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$; w = $1/[\sigma^2(F_o^2) + (0.00005\ P)^2 + 0.0026\ P]$, w = $1/[\sigma^2(F_o^2) + 0.6347\ P]$, and w = $1/[\sigma^2(F_o^2) + (0.0168\ P)^2 + 0.5117\ P]$; P = $(F_o^2 + 2\ Fc^2)/3$ for $ErFe_{0.06(1)}Ga_3$, and $ErFe_{0.11(2)}Ga_3$, and $ErCo_{0.06(2)}Ga_3$ respectively.

Table A.2. Atomic Positions of ErM_xGa_3 (M = Fe, Co; x < 0.2)

Atom	Wyckoff position	Symmetry	x	y	z	Occupancy	[a] U_{eq} (Å^2)
$ErFe_{0.06(1)}Ga_3$							
Er	1*a*	*m*3*m*	0	0	0	1	0.0082(5)
Fe	1*b*	*m*3*m*	1/2	1/2	1/2	0.062(8)	0.005(7)
Ga	3*c*	4/*mmm*	0	1/2	1/2	0.76(8)	0.0110(14)
Ga′	6*f*	4*mm*	0.082(2)	1/2	1/2	0.171(10)	0.0082(13)
$ErFe_{0.11(2)}Ga_{2.92(8)}$							
Er	1*a*	*m*3*m*	0	0	0	1	0.0037(9)
Fe	1*b*	*m*3*m*	1/2	1/2	1/2	0.128(4)	0.002(8)
Ga	3*c*	4/*mmm*	0	1/2	1/2	0.684(13)	0.007(2)
Ga′	6*f*	4*mm*	0.070(9)	1/2	1/2	0.145(6)	0.004(4)
$ErCo_{0.06(2)}Ga_{2.9(1)}$							
Er	1*a*	*m*3*m*	0	0	0	1	0.0083(8)
Co	1*b*	*m*3*m*	1/2	1/2	1/2	0.104(5)	0.02(3)
Ga	3*c*	4/*mmm*	0	1/2	1/2	0.678(16)	0.010(2)
Ga′	6*f*	4*mm*	0.080(2)	1/2	1/2	0.141(8)	0.015(11)

Table A.3. Selected interatomic distances (Å) for ErM_xGa_3 (M = Fe, Co; x < 0.2)

Interatomic distance	$ErFe_{0.06(1)}Ga_3$	$ErFe_{0.11(2)}Ga_3$	$ErCo_{0.06(2)}Ga_{2.9(1)}$
Ln-Ga (x12)	2.9859(2)	2.9884(4)	2.9841(4)
Ln-Ga′ (x12)	2.9970(4)	3.0031(8)	2.0031(10)
Ln-M (x8)	3.6570(2)	3.6601(3)	3.6547(4)
Ln-Ln (x6)	4.2227(4)	4.2263(5)	4.2201(7)
M-Ga (x6)	2.1114(2)	2.1131(3)	2.1100(4)
M-Ga′ (x6)	1.8538(2)	1.8173(2)	1.7724(3)

Table A.4. Magnetic properties of ErM_xGa_3 (M = Fe, Co; $0 \leq x < 2$)

Compound	T_N (K)	θ_W (K)	μ_{eff} (μ_B/mol Er)
$ErGa_3$	2.9	-33.48(3)	10.095(4)
$ErFe_{0.06(1)}Ga_3$	5.2	-10.35(9)	10.78(7)
$ErFe_{0.11(2)}Ga_3$	6.2	-8.65(6)	10.44(5)
$ErCo_{0.06(2)}Ga_3$	3.3	-9.65(5)	10.34(3)

A.6 Crystal Structure

ErM_xGa_3 (M = Fe, Co; x < 0.2) crystallizes in the space group Pm3m with a = ~ 4.2 Å. The unit cell of $ErFe_{0.07}Ga_3$ is shown in Figure A.1. The crystal structure can be described as stuff variant of the $AuCu_3$-structure type. The lanthanide atoms occupy the corners of the unit cell, while the Fe atom partially occupies the center of the unit cell. As a result of Fe insertion, the Ga atoms that resides on the face was elongated as shown in Figure A.1. Therefore, the Ga1 position was refined to two partially occupied position, Ga and Ga′. Similar behavior was observed in $Er_4Fe_{0.67}Ga_{12}$ that adopts the Y_4PdGa_{12} structure type, where two gallium position were observed on the face of the cube and on an extended position due to Fe vacancies.[4]

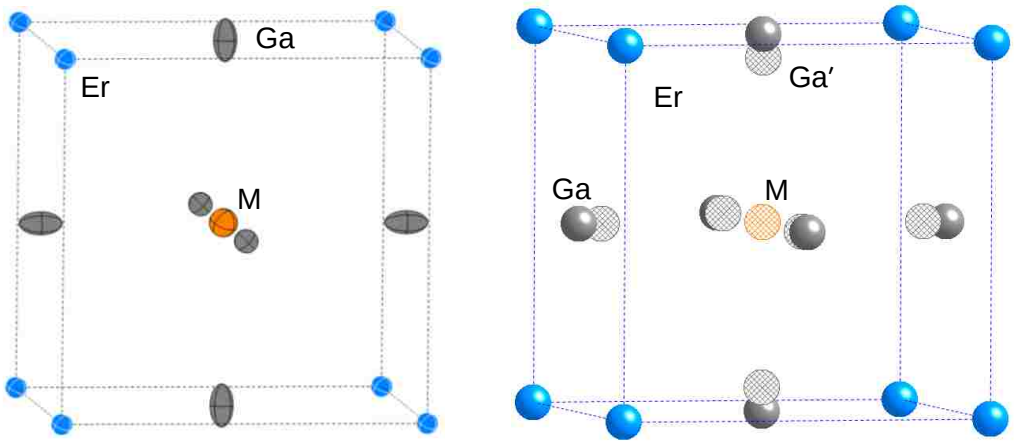

Figure A.1. a) Unit cell of $ErFe_{0.07}Ga_3$, where Er, Fe, and Ga atoms are blue, orange, and grey ellipsoids, (left) respectively. b) Unit cell of $ErFe_{0.07}Ga_3$, where Er, Fe, and Ga atoms are blue, orange, and grey spheres, (right) respectively.

A.7 Magnetism

The temperature dependent magnetic susceptibility of ErM_xGa_3 (M = Fe, Co) with an applied field of 0.1 T are shown in Figure A.2. The magnetic susceptibility increases with decreasing temperature until T_N ~ 5.2, 6.2, and 3.3 K for $Er_{1.00(6)}Fe_{0.08(1)}Ga_{2.27(7)}$, $Er_{1.00(1)}Fe_{0.11(1)}Ga_{2.91(1)}$, and $Er_{1.00(1)}Co_{0.14(1)}Ga_{3.06(1)}$, respectively, followed by a decrease in magnetization. The Neèl temperature are considerably different than the parent analogue $ErGa_3$ T_N ~ 2.9 K. The difference All compounds exhibit Curie-Weiss behavior above T_N and were fitted to a modified Curie-Weiss equation $\chi = \chi_o + (C/(T-\theta))$, where χ_o is the temperature independent contribution, θ is the Weiss constant, and C is the Curie constant. The constants from the Curie Weiss fit are provided in Table A.4. The magnetic moments are higher than the calculated mangetic moments of Er^{3+} ions (9.58 m_B), but it is comparable to the parent analogue $ErGa_3$ as shown in Table A.4. The Weiss constant of $Er_{1.00(6)}Fe_{0.08(1)}Ga_{2.27(7)}$, $Er_{1.00(1)}Fe_{0.11(1)}Ga_{2.91(1)}$, and $Er_{1.00(1)}Co_{0.14(1)}Ga_{3.06(1)}$ are significantly lower than $ErGa_3$, which could be due to the decrease in the interaction strengthen between the Er atoms caused by the increase in Er-Er distance as a result of M insertion. Figure A.2 shows the field-dependent magnetization of ErM_xGa_3 (M = Fe, Co) at

3 K. The magnetization of all samples is linear at low fields followed by a curvature at ~ 2 T with no signs of saturation.

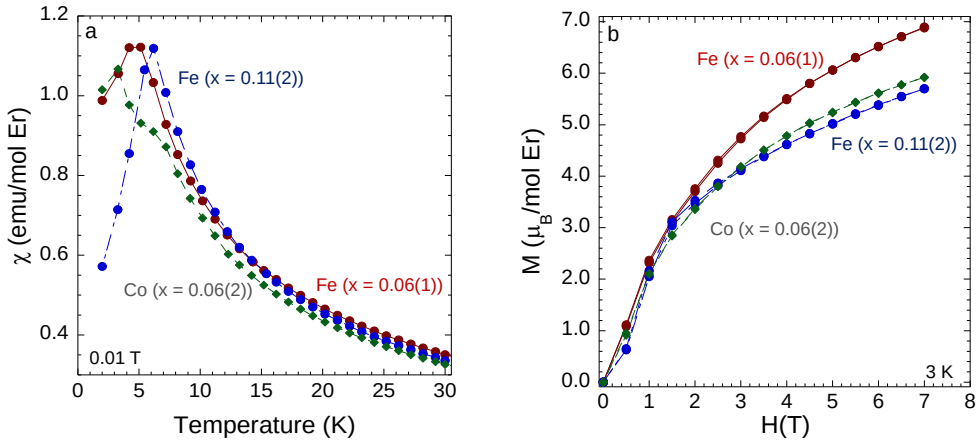

Figure A.1. Temperature (a) and field (b) dependent magnetization of ErM_xGa_3 (M = Fe, Co; x < 0.2).

A.8 References

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Appendix B. Investigation of Ce and Yb intermetallics

B.1 Introduction

Discovering exotic properties based on structure-property relationship is an extensive research area in solid state chemistry. Ce and Yb – intermetallics can be used to study the magnetic properties as a function of a tunable parameter, such as disorder, coordination, and atomic size. The AlB_2 and $ThSi_2$-structure types of Ce-analogues have been characterized structurally and magnetically based on the tunable parameter disorder.[1] $CeGa_2$ has been characterized as a Kondo lattice (Ce^{3+}) and exhibits multiple magnetic transitions between 8.4 and 11.4 K with a Sommerfeld parameter of approximately 32 mJ/mol K^2.[2] The $CeSi_2$ has been reported as a mixed $Ce^{3+/4+}$ and heavy fermion compound ($\gamma \sim 100$ mJ/mol K^2) with strong ferromagnetic interactions ($\theta \sim 302$ K).[3] The fully ordered phases of $CeGa_2$ and $CeSi_2$ have been magnetically tuned by doping in Ag to characterize their magnetic correlation based on a change in the electronic structure, which has been highlighted and extensively reviewed.[1, 4] Our group has recently grown single crystals of $CeAg_ySi_xGa_{2-x-y}$ adopting the AlB_2 and $ThSi_2$-structure types. The $ThSi_2$-structure type of $CeAg_ySi_xGa_{2-x-y}$ behaves as a Ce^{3+} Kondo system with no ordering down to 3 K but is more metallic than $ThSi_2$-structure type of $Ce(Si,Ga)_2$, which could be partly due to the addition of Ag.[1, 4] The AlB_2-structure type of $CeAg_ySi_xGa_{2-x-y}$ exhibits a paramagnetic state down to 3 K and mix valent character.[1, 4]

Relative to Ce-based intermetallic compounds, there are very few Yb-based analogues. A summary of $Yb(AgSiGa)_2$ pseudo binary compounds adopting the AlB_2 and $ThSi_2$-structure types are shown in Figure 5. The AlB_2-structure type has been reported for $YbGa_xSi_{2-x}$ ($1.12 < x < 1.49$) where Yb was determined to be mixed valent with an oxidation state of +2.23.[5, 6] $YbGa_xSi_{2-x}$ was observed to be superconducting as x varies from 1.12 - 1.49.[5, 6] However, neither of the parent phases, $YbGa_2$ and $YbSi_{2-x}$, are superconducting at any temperature.[7, 8] The Ga-containing parent compound $YbGa_2$ adopts the $CaIn_2$-structure type, unlike the Ce-analogue, $CeGa_2$, which adopts the AlB_2-structure type.[2] The Si-containing parent $YbSi_{2-x}$ adopts the AlB_2-structure type, unlike the Ce-analogue that adopts the $ThSi_2$-structure type.[3] By considering the previously reported superconductor, the AlB_2-type $Yb(Si,Ga)_2$,[9] and the physical properties of the AlB_2 and $ThSi_2$-structure types of $CeAg_{0.01(1)}Si_{0.1(1)}Ga_{1.9(1)}$, we have focused our efforts on the growth of $YbAg_ySi_xGa_{2-x-y}$ that adopts the $ThSi_2$ and AlB_2-structure types.

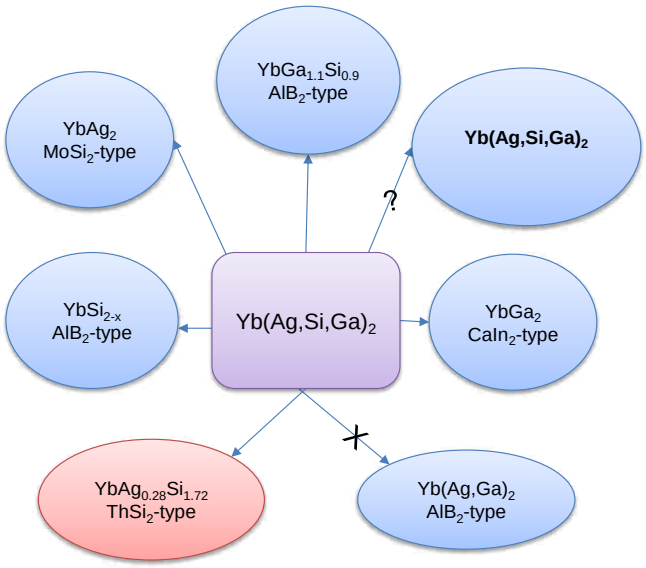

Figure B.1. This bubble diagram depicts a summary of Yb-Ag-Si-Ga pseudo binaries.

The self-flux growth method was attempted to synthesize the $Yb(Ag,Si,Ga)_2$ adopting the AlB_2 and $ThSi_2$-structure types. The initial reaction profile was similar to the reaction profile for the synthesis of $CeAg_ySi_xGa_{2-x-y}$ that adopts the AlB_2 and $ThSi_2$-structure types via different reaction ratio.[1, 4] The Yb:Ag:Si:Ga reaction ratios of 2:1:1:20 and 2:1:0.5:20 were attempted for the growth of pseudo-binaries of $YbAg_ySi_xGa_{2-x-y}$ because these particular ratios were used in the growth of $CeAg_ySi_xGa_{2-x-y}$. The elements were placed in alumina crucibles, topped with silica wool, and then sealed inside evacuated fused-silica tubes. Silica wool was placed on the brim of the alumina crucible to serve as a filter for excess flux during centrifugation. The initial reaction profile required heating the elements (Yb:Ag:Si:Ga) to 900 °C at a rate of 200 °C/h, dwelling for 24 h, then cooling to 650 °C at a rate of 150 °C/h, followed by dwelling for 2 days, and finally spinning to remove the excess flux. After the reaction, no single crystals were recovered. Subsequently, several attempts to grow pseudo binaries of $YbAg_ySi_xGa_{2-x-y}$ by systematically varying the heating rate, dwelling time, and cooling rate were unsuccessful. The heating rate was decreased from 200 °C/h to 25 °C/h, to decrease the volatility of Yb. The dwell time at 900 °C was varied from 9 h, 12 h, and 120 h to allow mixing. The spin temperature was also varied from 750 °C, 650 °C, and 500 °C, and the dwell time at low temperature (500 °C) from 2 days to 5 days. In all the growths attempted, the only product that was identified was the $Yb(AgGa)_4$, that adopts the $BaAl_4$-structure type, which was identified by using powder X-ray diffraction and EDS. In another attempt to grow pseudo-binaries of $YbAg_ySi_xGa_{2-x-y}$ the reaction ratios were changed to 6:1:1.5:20 and 6:1:2:20 to make sure that the silicon reacted with the other elements. The reactions were heated to 1000 °C at a rate of 25 °C/h, followed by a dwell for 24 h, and then cooling to 650 °C at a rate of 25 °C/h. The final synthesis yielded small crystals, which preliminary composition calculated from EDS measurements was $YbAg_{0.13(5)}Si_{0.03(2)}Ga_{2.0(5)}$. However, due to

low yield and poor crystal quality the structure could not be determined with these particular crystals. In order to grow the crystals with high yield and good crystal quality, the temperature profile was varied consisting of heating to 1000 °C at a rate of 25 °C/h, followed by a dwell for 96 h, and then cooling to 750 °C at a rate of 5 °C/h. Single crystals, in the shape of rods ~5 mm long, were obtained from this reaction. The rods were etched in diluted (~0.01 M) HCl and hot water to remove the excess gallium. X-ray powder diffraction technique was employed on the product, which is depicted in Figure 6. The X-ray powder diffraction pattern was compared to a calculated powder pattern of AlB_2-structure type of $YbAg_ySi_xGa_{2-x-y.}$ The powder patterns match up well with each other indicating that the AlB_2-structure type was synthesized. Crystallographic parameters of $YbAg_{0.10(2)}Si_{0.83(8)}Ga_{1.07(3)}$ were determined and provided in Appendix B.1. Crystal structures were solved by direct methods with SIR97 and refined with SHELXL97.[10, 11] The atomic positions, Wyckoff symmetry, displacement parameters, and occupancies of atoms for $YbAg_{0.10(2)}Si_{0.83(8)}Ga_{1.07(3)}$ are provided in Appendix B.2.

B.2 Results and Discussion

The hexagonal AlB_2-structure type, shown in Figure 7, has been well described for a vast number of intermetallics. The crystal structure can be described as honeycomb $[Ga_{2-x-y}Si_xAg_y]$ planar nets stacked along the *c*-axis with Yb atoms located in hexagonal voids between them. The M-M interatomic distances are 2.39831(17) Å, consistent with covalently bonded M-M contacts of ~2.5 Å.

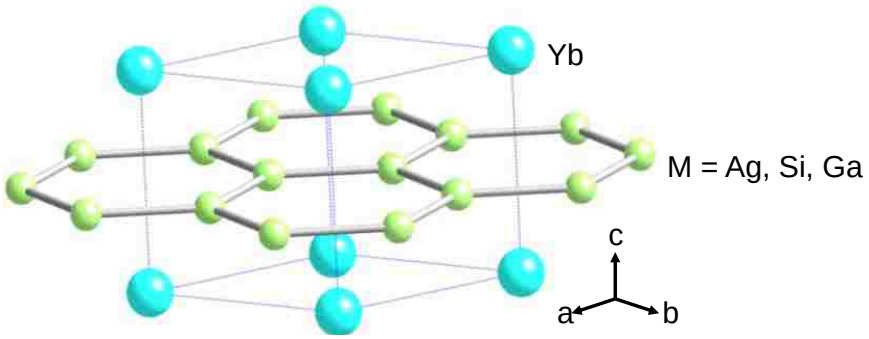

Figure B.2. Crystal structure of AlB_2-type of $YbAg_xSi_yGa_{2-x-y}$ is along the *c*-axis, with the Yb atoms represented as blue spheres and the M-atoms represented as green spheres.

Table B.1. Crystallographic Parameters of $YbAg_ySi_{2-x-y}Ga_x$

Crystal data	
Composition	$CeAg_{0.01(1)}Si_{0.1(1)}Ga_{1.9(1)}$
Crystal System	Hexagonal
Space group	*P*6/*mmm*
a (Å)	4.1540(3)
c (Å)	4.2500(2)
V (Å^3)	63.511(7)
Z	1
Crystal dimensions (mm^3)	0.05 x 0.05 x 0.05
θ range (˚)	1.00-30.85
μ (mm^{-1})	34.530
Data Collection	
Measured reflections	648
Independent reflections	61
Reflections with I > 2σ(I)	61
R_{int}	0.085
h	-6 to 14
k	-6 to 0
l	-5 to 23
R_1[a]	0.0158
wR_2[b]	0.0332
Parameters	9
Δp_{max} (e Å^{-3})	1.759
Δp_{min} (e Å^{-3})	-0.799
Extinction coefficient	0.19(2)
GOF	1.09

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$

[b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_0^2)^2]^{1/2}$; $P = (F_o^2 + 2F_c^2)/3$; $w = 1/[\sigma^2(F_o^2) + 0.0182\ P^2]$ for $YbAg_xSi_yGa_{2-x-y}$.

Table B.2. Atomic Positional & Displacement of AlB_2-type $YbAg_ySi_yGa_{2-x-y}$ at 298 K

Atom	Wyckoff position	*x*	*y*	*z*	Occ.[a]	U_{eq} (Å^2)[b]
$YbAg_{0.01(1)}Si_{0.9(1)}Ga_{1.0(1)}$						
Ce	1*a*	1	0	1	1.00	0.0127(4)
[†]*M*	2*d*	1/3	2/3	1/2	1.00	0.0190(6)

[†]*M* = Ag (0.5 %) + Si (45 %) + Ga (54.5 %)
[a]Occupancy
[b]U_{eq} is defined at one third of the trace of the orthogonalized U_{ij} tensor.

B.3 References

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 ?
;
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 _atom_type_scat_dispersion_imag
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_cell_length_b                    4.353(5)
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_cell_angle_beta                  90.00
_cell_angle_gamma                 120.00
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_cell_measurement_theta_min       ?
_cell_measurement_theta_max       ?

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;

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_diffrn_reflns_theta_max         30.98
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_reflns_threshold_expression     >2sigma(I)

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_computing_cell_refinement       ?
_computing_data_reduction        ?
_computing_structure_solution    'SHELXS-97 (Sheldrick,
1990)'
_computing_structure_refinement   'SHELXL-97
(Sheldrick, 1997)'
_computing_molecular_graphics    ?
_computing_publication_material  ?

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The
weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-
factors R are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-
factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_matrix_type           full
_refine_ls_weighting_scheme      calc
_refine_ls_weighting_details
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P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary   difmap
_atom_sites_solution_hydrogens   geom
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_refine_ls_number_parameters     27
_refine_ls_number_restraints     2
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_refine_ls_R_factor_gt           0.0178
_refine_ls_wR_factor_ref         0.0405
_refine_ls_wR_factor_gt          0.0397
_refine_ls_goodness_of_fit_ref   1.196
_refine_ls_restrained_S_all      1.203
_refine_ls_shift/su_max          0.000
_refine_ls_shift/su_mean         0.000

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 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_U_iso_or_equiv
 _atom_site_adp_type
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 _atom_site_symmetry_multiplicity
 _atom_site_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_assembly
 _atom_site_disorder_group
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0.652(2) 6 d SP . .
Pd1 Pd 0.0000 0.0000 0.0000 0.00803(17) Uani 1 12 d S . .
Pd2 Pd 0.0000 0.0000 0.120867(13) 0.00928(16) Uani 1 6
d S . .
Ga3 Ga 0.0000 0.0000 0.35195(2) 0.00897(19) Uani 1 6 d
S . .
Ga4 Ga 0.0000 0.0000 0.44354(2) 0.0117(2) Uani 1 6 d S .
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 are estimated using the full covariance matrix.  The cell
esds are taken
 into account individually in the estimation of esds in
distances, angles
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and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
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Appendix E. CIF of $CeCo_{2-x}M_xAl_8$ (M = Fe, Ni; $0 \leq x < 1$)

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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Fe'  'Fe'   0.3463   0.8444
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Al'  'Al'   0.0645   0.0514
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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 '-x, -y, -z'
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 'x-1/2, -y-1/2, z'

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(Sheldrick, 2008)'
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 Refinement of F^2^ against ALL reflections.  The
weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-
factors R are based
```

```
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2\s(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
;

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P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_hydrogens    geom
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0.23(6) 2 d SP . .
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distances, angles
 and torsion angles; correlations between s.u.'s in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
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involving l.s. planes.
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(Sheldrick, 2008)'
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 Refinement of F^2^ against ALL reflections.  The
weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-
factors R are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2\s(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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 'calc w=1/[\s^2^(Fo^2^)+(0.0388P)^2^+3.0837P] where
P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_hydrogens geom
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0.56(7) 2 d SP . .
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Al9 Al 0.0000 0.0000 0.0000 0.0112(5) Uani 1 4 d S . .
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 into account individually in the estimation of s.u.'s in
distances, angles
 and torsion angles; correlations between s.u.'s in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell s.u.'s is used for estimating s.u.'s
involving l.s. planes.
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(Sheldrick, 2008)'
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 Refinement of F^2^ against ALL reflections.  The
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factors R are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2\s(F^2^) is used only for calculating R-factors(gt)
etc. and is
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on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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distances, angles
 and torsion angles; correlations between s.u.'s in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
 treatment of cell s.u.'s is used for estimating s.u.'s
involving l.s. planes.
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expression of
 F^2^ > 2\s(F^2^) is used only for calculating R-factors(gt)
etc. and is
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factors based
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on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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Ni2 0.0095(6) 0.0094(5) 0.0073(5) 0.000 0.000 -0.0002(5)
Co2 0.0095(6) 0.0094(5) 0.0073(5) 0.000 0.000 -0.0002(5)
Al1 0.0096(12) 0.0105(11) 0.0096(12) 0.000 0.000
0.0001(10)
Al2 0.0072(11) 0.0136(11) 0.0094(11) 0.000 0.000
0.0004(10)
Al3 0.0093(12) 0.0119(12) 0.0103(11) 0.000 0.000 -
0.0012(10)
Al4 0.0119(13) 0.0079(10) 0.0100(11) 0.000 0.000 -
0.0009(10)
Al5 0.0105(12) 0.0108(11) 0.0100(11) 0.000 0.000 -
0.0001(10)
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0.0011(9)
Al7 0.0074(11) 0.0152(12) 0.0115(12) 0.000 0.000
0.0033(11)
Al8 0.0126(19) 0.0096(16) 0.0072(16) 0.000 0.000
0.0008(13)
Al9 0.0100(18) 0.0119(17) 0.0107(17) 0.000 0.000 -
0.0027(14)

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;
All s.u.'s (except the s.u. in the dihedral angle between two
l.s. planes)
are estimated using the full covariance matrix. The cell
s.u.'s are taken
into account individually in the estimation of s.u.'s in
distances, angles
and torsion angles; correlations between s.u.'s in cell
parameters are only
used when they are defined by crystal symmetry. An
approximate (isotropic)
treatment of cell s.u.'s is used for estimating s.u.'s
involving l.s. planes.
;

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Ni1 Al6 2.330(3) . ?
Ni1 Al8 2.4649(18) . ?
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Ni1 Al7 2.535(3) 3_455 ?
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Al9 Ni2 2.3473(12) 5 ?
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Al8 Ni1 Al2 145.60(8) 1_554 . ?
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Al5 Ni1 Al2 63.95(8) 3_456 . ?
Al6 Ni1 Al2 70.28(7) . 1_554 ?
Al8 Ni1 Al2 145.60(8) . 1_554 ?
Al8 Ni1 Al2 63.19(7) 1_554 1_554 ?
Al7 Ni1 Al2 74.99(7) 7_665 1_554 ?
Al7 Ni1 Al2 128.50(6) 3_455 1_554 ?
Al5 Ni1 Al2 63.95(8) 3_455 1_554 ?
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Al8 Ni1 Ni1 54.69(3) 1_554 5_565 ?
Al7 Ni1 Ni1 55.82(7) 7_665 5_565 ?
Al7 Ni1 Ni1 55.79(7) 3_455 5_565 ?
Al5 Ni1 Ni1 109.43(7) 3_455 5_565 ?
Al5 Ni1 Ni1 109.43(7) 3_456 5_565 ?
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expression of
 F^2^ > 2\s(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
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All s.u.'s (except the s.u. in the dihedral angle between two
l.s. planes)
are estimated using the full covariance matrix. The cell
s.u.'s are taken
into account individually in the estimation of s.u.'s in
distances, angles
and torsion angles; correlations between s.u.'s in cell
parameters are only
used when they are defined by crystal symmetry. An
approximate (isotropic)
treatment of cell s.u.'s is used for estimating s.u.'s
involving l.s. planes.
;

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_diffrn_radiation_monochromator  graphite
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(Sheldrick, 2008)'
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 Refinement of F^2^ against ALL reflections.  The
weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-
factors R are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2\s(F^2^) is used only for calculating R-factors(gt)
etc. and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based
on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_matrix_type           full
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 'calc w=1/[\s^2^(Fo^2^)+(0.0136P)^2^+0.0000P] where
P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      SHELXL
_refine_ls_extinction_coef        0.00000(8)
_refine_ls_extinction_expression
 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
_refine_ls_number_reflns          1249
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Al9 Al 0.0000 0.0000 0.0000 0.0081(2) Uani 1 4 d S . .
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d S . .
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All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell s.u.'s are taken
into account individually in the estimation of s.u.'s in distances, angles
and torsion angles; correlations between s.u.'s in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.
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Appendix F. CIF of ErM_xGa_3 (M = Fe, Co; x < 0.2)

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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Fe'  'Fe'   0.3463   0.8444
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Ga'  'Ga'   0.2307   1.6083
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_computing_cell_refinement       ?
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1990)'
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1997)'
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 Refinement of F^2^ against ALL reflections.  The weighted
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 goodness of fit S are based on F^2^, conventional R-
factors R are based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-
factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.
R-factors based
 on F^2^ are statistically about twice as large as those
based on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_weighting_details
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P=(Fo^2^+2Fc^2^)/3'
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_refine_ls_extinction_coef       0.17(2)
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SP . .
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 Refinement of F^2^ against ALL reflections. The weighted R-factor wR and
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 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement. R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
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distances, angles
 and torsion angles; correlations between esds in cell
parameters are only
 used when they are defined by crystal symmetry.  An
approximate (isotropic)
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 Refinement of F^2^ against ALL reflections.  The weighted
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factors R are based
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expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-
factors(gt) etc. and is
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R-factors based
 on F^2^ are statistically about twice as large as those
based on F, and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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Vita

LaRico Juan Treadwell was born in 1987, in Batesville, Mississippi to Stephen and Adrienne Robinson. He is the oldest of five children (Brycen, Byron, Bryen, and Melissa) and has one child (Latrell Treadwell). LaRico received his high school diploma from South Panola High School in Batesville, Mississippi, in May of 2006. In August of 2006, he began his studies in chemistry at The University of Mississippi, where he became an Ole Miss First Scholar, AGEM Scholar, and the Ronald E. McNair Scholar. He completed The University of Mississippi with a Bachelor of Science in Chemistry in 2010.

LaRico began his graduate career at Louisiana State University in August of 2010, under the direction of Professor Julia Y Chan. At LSU, he received the Board of Regents Fellowship and made significant contributions to the chemistry of materials that can be seen in various publications. Also, LaRico has attended numerous national scientific meeting. In 2012, he presented a poster at the NOBCChE conference in Washington D.C. and attended a neutron powder diffraction workshop at Oak Ridge National Laboratory. In 2013, LaRico presented a poster at the ACS National Meeting in New Orleans and NOBCChE in Indianapolis and gave an invited talk the ACS Southwest Regional Meeting in Waco, TX. In 2014, he gave an invited talk at the ACS National Meeting in Dallas, TX. In his graduate career, he has participated in numerous outreach programs (SuperScience Saturday, X-ray Crystallography Demonstration, chemistry demonstration at K-12 schools), organized a poster session, and held presidential positions for the local LSU NOBCChE chapter and chemistry graduate student council (CGSC). Also, he has organized/hosted a poster symposium for LSU STEM majors, South Louisiana Organic Symposium, and recruitment/collaborative efforts with LSU-Morehouse.

In December of 2014, LaRico J Treadwell will graduate and be awarded with a Doctor of Philosophy degree in chemistry.