Fig.1 The 4f charge densities of Pr from point charge model calculations including quadrupolar (Q_2/a_0^2) and octupolar (Q_4/a_0^4) moments [1].

GT-13. Peculiarity of a magnetic structure in a quasi-one-dimensional columbite $Co_{0.4}Ni_{0.6}Nb_2O_6$. *P.W. Sarvezuk*[1], M.A. Gusmao[2], J.B. Marimon da Cunha[2] and O. Isnard[3] *1. Universidade Tecnológica Federal do Paraná, Campo Mourão, Brazil; 2. Universidade Federal do do Rio Grande do Sul, Porto Alegre, Brazil; 3. Institute Néel, Grenoble, France*

Quasi-one-dimensional (Q1D) spin chain systems have a great potential applications in high-density information storage devices, quantum: information and computers, given their quantum magnetic properties. The low-dimensional magnetic behavior have been investigated in ANb_2O_6, (A = Mn, Fe, Co or Ni) compounds, they structural and magnetic properties are very interesting because the system presents weakly interacting Ising chains, which leads to his quasi-one-dimensional magnetic order. Our investigation combines specific heat and magnetic measurements; x-ray and neutron diffraction (ND). In this work, we present a Co/Ni orthorhombic structure, called columbite, which crystallize with *Pbcn* space group, whose formula is $Co_{0.4}Ni_{0.6}Nb_2O_6$. Co for Ni substitution induces a continuous lattice volume decrease, preserving the orthorhombic crystal structure. Magnetic susceptibility and specific heat measurements reveals that antiferromagnetic order occurs at 3.4 K, as consequence of a weak interchain interactions. Partial substitution of the magnetic ion tends to change the magnetic ordering observed in the $CoNb_2O_6$ and $NiNb_2O_6$. Lastly, we present this magnetic structure changes with the Ni-Co substitution.

GT-14. Multiple Antiferromagnetic structures in $HoCoGa_5$ studied by X-ray resonant magnetic scattering. *C. Adriano*[1], R.M. Grossi[1], K.R. Pakuszewski[1], P. Pagliuso[1] and C. Giles[2] *1. DEQ, University of Campinas, Campinas, Brazil; 2. DFMC, University of Campinas, Campinas, Brazil*

The relationship between magnetism and superconductivity (SC) in strongly correlated electron systems is still a subject of investigation since the existence of series of structurally related compounds is a good opportunity to explore how the evolution of the physical properties along the series can affect the ground state of each compound. In this context, the isostructural family of intermetallic compounds R_nMX_{3n+2} (R = rare earth or actinides, M = transition metal, X = In, Ga and n = 1, 2) has allowed a remarkable opportunity to further explore the relationship between magnetism, SC, crystalline electrical field effects and crystal structure. Among this isostructural family the most important members are the heavy fermions superconductors $CeCoIn_5$ [1] and $PuCoGa_5$ [2] and their related compounds. The interesting properties arise from the interaction between the *4f* and *5f*, respectively, with the conduction electrons. In low temperatures the *f*-electrons start to interact with the conduction electrons and the ground state is mainly determined by an intricate balance between the RKKY (Ruderman-Kittel-Kasuya-Yosida) interactions and the Kondo Effect [3]. As the SC in these materials is believed to be magnetic mediated [4] the systematic study of the non-Kondo compounds within the R_nMX_{3n+2} family is very elucidative to investigate the evolution of the magnetism of the *4f* electrons. In this work we add new results to the Ga-based series, for which the trends observed in the magnetic properties along these series can be further explored. We report the solution of the magnetic structure of the intermetallic antiferromagnet $HoCoGa_5$ by means of the X-ray magnetic resonant technique. We found a magnetic structure consistent with a commensurate antiferromagnetic phase below 7.4 K with a magnetic propagation vector (1/2 0 1/2) and an incommensurate

antiferromagnetic ordering phase between 7.4 K and 9.7 K where the spins align in the ab-plane an rotate with an angle of around 65 degrees along the c direction and with a propagation vector (1/2 0 0.359). The spin reorientation found for this compound and existing in related *5f* compounds like $NpMGa_5$ with (M = Rh,Co) is further discussed in this work.

[1] R. Movshovich, M. Jaime, J. D. Thompson, C. Petrovic, Z. Fisk, P. G. Pagliuso, and J. L. Sarrao, Phys. Rev. Lett. 86, 5152 (2001). [2] J. L.Sarrao, L. A. Morales, J. D. Thompson, B. L. Scott, G. R. Stewart, F.Wastin, J. Rebizant, P. Boulet, E. Colineau, and G. H. Lander, Nature (London) 420, 297 (2002). [3] A. C. Hewson, The Kondo Problem to Heavy Fermions, (Cambridge University Press, Cambrige, 1993). [4] T. Park, F. Ronning, H. Q. Yuan, M. B. Salamon, R. preMovshovich, J. L. Sarrao and J. D. Thompson, Nature 440, 65 (2006).
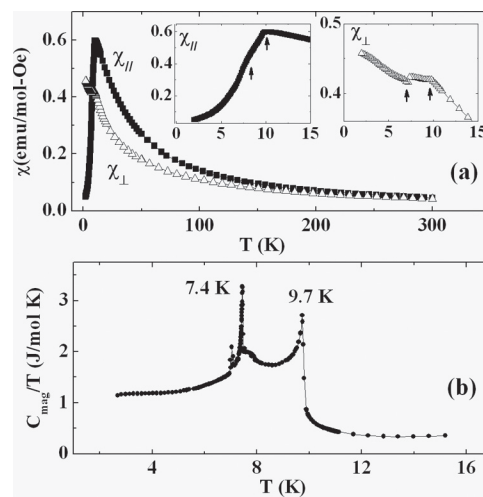

Fig.1 HoCoGa5 magnetic properties.

GT-15. Investigation of Local Magnetic Properties of CeCd as a Function of the Unit Cell Volume by means of First Principles Calculations. *L.F. Pereira*[1], L.M. Scalise[1], J. Mestnik-Filho[1], W.L. Ferreira[1], V.C. Gonçalves[1] and *A.W. Carbonari*[1] *1. Research Reactor Center, Nuclear and Energy Research Institute, São Paulo, Brazil*

In the work here reported magnetic hyperfine field (B_{hf}) at Cd site as well as the cerium magnetic moment (*m*-Ce) were calculated from simulation of the CeCd compound in many different unit cell volumes. Results are compared with the experimental values of B_{hf} (5.10 T) obtained with Perturbed Angular Correlation spectroscopy measurements [1] and *m*-Ce from magnetization measurements. The electronic structure calculations of the CeCd cubic cells (under normal conditions the space group is Pm-3m) were performed using density functional theory implemented on ELK and WIEN2k codes with "full-potential linearized augmented plane wave" method and the local density or generalized gradient approximations to estimate exchange-correlation energy. Three methodologies were carried out in our simulations: just spin polarized (SP); spin-orbit coupling (SO); and, SO plus *ad hoc U* parameter to treat the strong correlation in the cerium *4f* shell. The cell energy (CE), *m*-Ce and Fermi-contact contribution (B_{Fc}) of Cd-B_{hf} from electrons (labelled core and valence) inside the atomic spheres and others quantities were calculated for volume fractions varying from -14% to 5% of the experimental unit cell volume, in steps of 1%. The smallest energy and bestest Cd-B_{hf} agreement were reached when the volume is compressed by 12%. Results are discussed in terms of Ce-*4f* electron (de)localization and its strong correlation as well as hybridization effects between Cd and Ce observed through density of states plots to understand the dependence of Cd-B_{Fc} with the compression and relaxation of the cell. A brief comparison of Cd-B_{Fc} for 3 the methodologies and *m*-Ce and Cd-B_{Fc} versus volume (SP calculation) from WIEN2k are presented.

[1] F.H.M. Cavalcante, M. Forker and L.F.D. Pereira, PRB, Vol. 96, p. 064417-1 (2016)

	Contact Magnetic Hyperfine Field at Cadmium site (Tesla)					
	Experimental Volume (0 %)			Reduced Volume		
	SP	SP+SO	SP+SO+U	SP (-12%)	SP+SO (-10%)	SP+SO+U (-10%)
B_x core	-0.2255	-8.5098	-9.211	-0.1389	-0.1165	-0.0717
B_x valence	-9.462	-0.1945	-0.1504	-5.6056	-4.9785	-3.3734
B_x total	-9.6875	-8.7043	-9.3614	-5.7445	-5.095	-3.4451

Fig. 1. Fermi contact hyperfine field at Cd site from different methodologies.
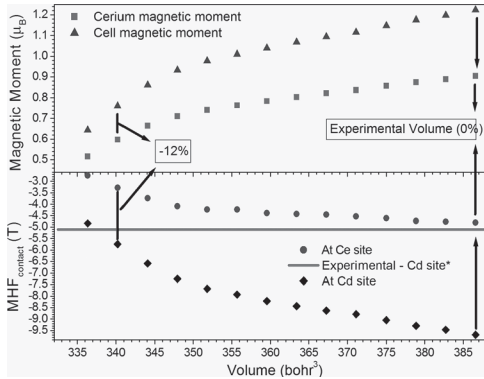

Fig. 2. Cerium and unit cell magnetic moment and Fermi contact hyperfine field at Cd site versus volume variation

GT-16. Magnetic-Field Driven Pr-Valence Change in $(Pr_{1-y}Sm_y)_{1-x}Ca_xCoO_3$.

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A metal-insulator transition (MIT) and spin-state transition (SST) is known to take place simultaneously in $(Pr_{1-y}RE_y)_{1-x}Ca_xCoO_3$ (RE=rare earth elements) system. This MI-SST originates from the fact that the spin-state of Co^{3+} changes between the intermediate (or high) and low spin states. Recently, several works revealed that the valence shift of a part of Pr ions from trivalent to tetravalent played an important role in the MI-SST by the X-ray absorption spectroscopy (XAS) at the Pr L_3 edge [1]. On the other hand, we have studied a magnetic-field effect on the MI-SST to control the SST, because the magnetic-field stabilizes the higher spin states and should influence the transition temperature. As a result, we found that the MI-SST temperature decreases with increasing magnetic-field, and finally the MI-SST is fully suppressed. For instance, the magnetic-field of 9 T wiped out the MI-SST in $(Pr_{0.9375}Y_{0.0625})_{0.7}Ca_{0.3}CoO_3$ sample with the transition temperature of 41 K at zero field [2]. In this paper, we have studied the XAS at the Pr L_3 edge in magnetic-field up to 10 T for $(Pr_{1-y}Sm_y)_{1-x}Ca_xCoO_3$ system to examine the relationship between the magnetic-field effect and the valence of Pr ions. For $(Pr_{0.8}Sm_{0.2})_{0.7}Ca_{0.3}CoO_3$ with the transition temperature of about 50 K, a $4f^2$ peak due to Pr^{3+} increases with increasing magnetic-field at 50 K, and returns to the starting spectrum at 0 T by removing the magnetic-field. The valence of Pr estimated from the XAS spectra changes from approximately 3.14 at 0T to 3.09 at 10 T. The decrease in Pr-valence by applying magnetic-field is consistent with the suppression of the MI-SST. We discuss the mechanism of the change in Pr-valence induced by the magnetic-field.

[1] H. Fujishiro et al., J. Phys. Soc. Jpn., Vol. 81, 064709 (2012) [2] T. Naito et al., J. Appl. Phys., Vol. 115, 233914 (2014)

GT-17. Co-site Substitution Effects on the Simultaneous Metal-Insulator and Spin-State Transition in $(Pr_{1-y}Gd_y)_{1-x}Ca_xCoO_3$.

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A metal-insulator transition (MIT) and spin-state transition (SST) is known to take place simultaneously in $(Pr_{1-y}RE_y)_{1-x}Ca_xCoO_3$ (RE=rare earth elements) system. This MI-SST originates from the fact that the spin-state of Co^{3+} changes between the intermediate (or high) and low spin states. Several works revealed that the valence shift of a part of Pr ions from trivalent to tetravalent played an important role in the MI-SST by the identification of the Pr^{4+}-related Schottky peak in heat capacity measurements [1] and by X-ray absorption spectroscopy (XAS) at the Pr L_3 edge [2]. The increase of the fraction of Co^{3+} by the valence change of Pr ions induced the MI-SST. In this paper, we have studied that a Co-site substitution effect by various metal elements (M=Mn, Fe, Ni, Ga, etc.) on the MI-SST in $(Pr_{1-y}Gd_y)_{1-x}Ca_x(Co_{1-z}M_z)O_3$, to clarify the relationship between the fraction of Co^{3+} and the MI-SST. For M=Mn, the transition temperature increased with increasing the amount of Mn. The introduction of Mn^{4+}, revealed by the XAS, increases the fraction of Co^{3+}, and resulted in the increase of the transition temperature. On the other hand, for M=Ni, the transition temperature decreased with the amount of Ni, and finally the MI-SST was fully suppressed at z=0.05. The results of the Ni-substitution is quite similar to the magnetic-field effect, in which the MI-SST disappeared above a strong magnetic field [3]. Although the valence of Ni was not determined by the XAS, we found that the ferromagnetic element also suppress this transition.

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GT-18. Withdrawn

GT-19. Withdrawn