First principles study and neutron diffraction investigation of $Y_3Ni_{13}B_2$, $Y_3Co_{13}B_2$ and $Y_3Ni_{10}Co_3B_2$; A comparison with related 1:5 systems

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DFT meets Solid State Chemistry & 8th Tutorial Hands-on-FPLO
MPI CPfS Dresden, October 25 - 29, 2009

Presentation layout:

1. Why the interest in $R_{m+n}\,T_{5m+3n}\,B_{2n}$ phases ?
2. Structure and magnetic properties of the title compounds.
3. Details on calculations and neutron exp..
4. Calculation results.
5. Neutron diffraction results.
6. Concluding remarks.

$R_{m+n}\ T_{5m+3n}\ B_{2n}$ series: P6/mmm (# 191) S:G: symmetry

YCo5 and SmCo5: exceptional ferromagnets !

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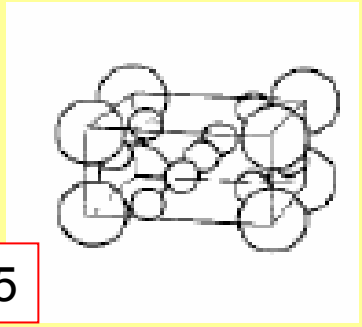
n=0



R T5

+

m=0
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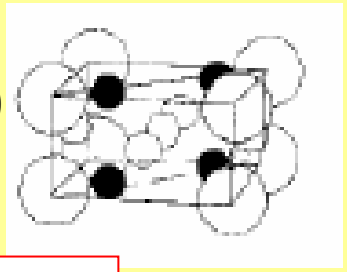
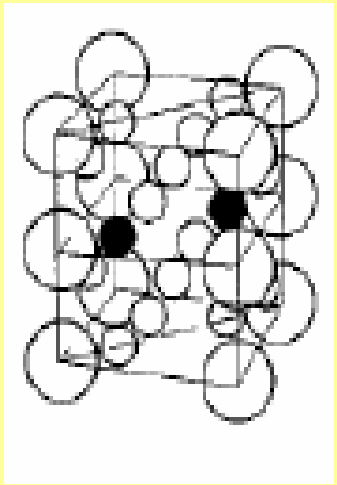


R T3 B2

=>



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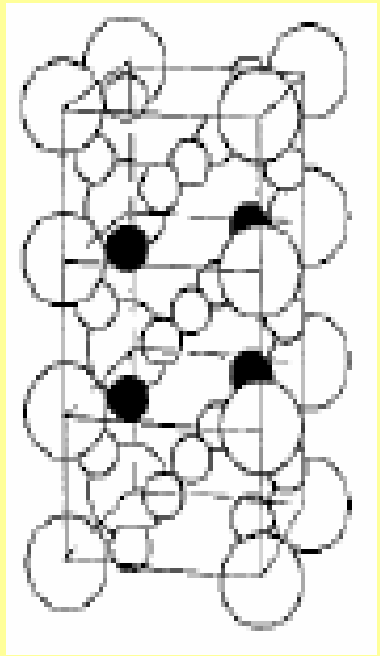
R Co4 B



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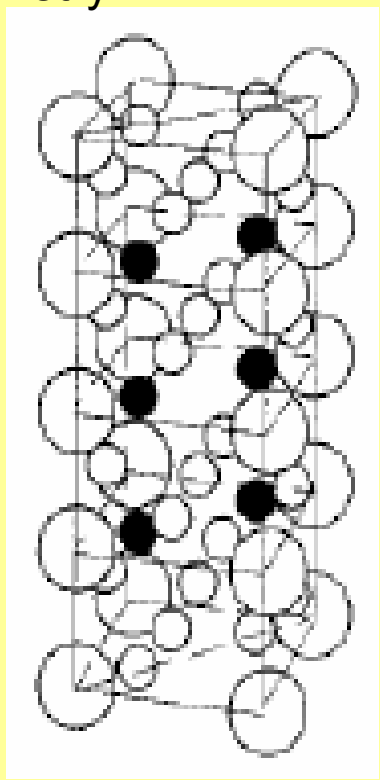
R3 Co11 B4



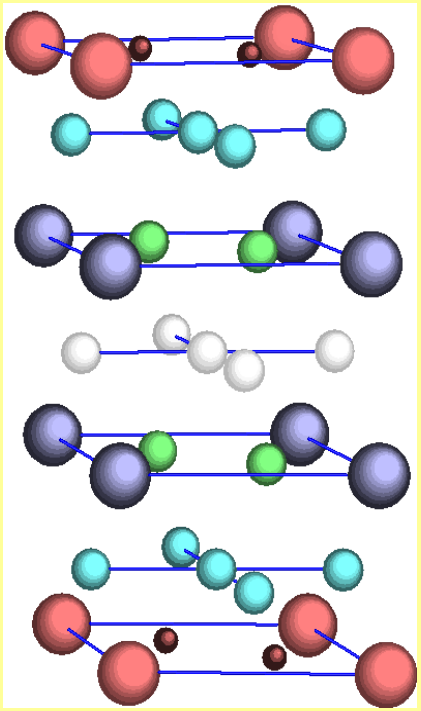
m=1
n=3

R2 Co7 B3

E. Parthé and B. Chabot, in Handbook on the Physics and Chemistry of Rare Earths, Elsevier Sci. Publ. B.V., Vol.6, North-Holland 1984.

2.1 CRISTAL STRUCTURE

m=2, n=1 => Nd3 Ni13 B2 -type cell:

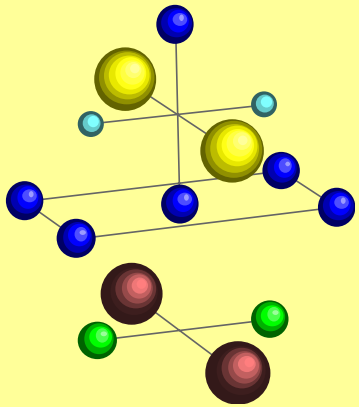


T(6i)

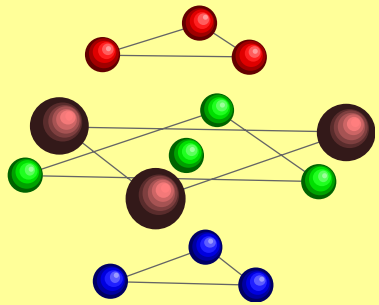
T(3g)

R(2e) T(4h)

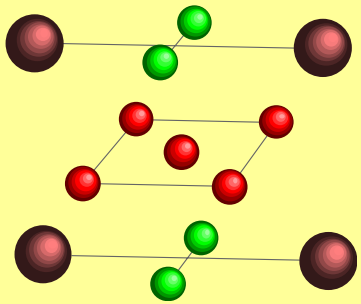
R(1a) B(2c)



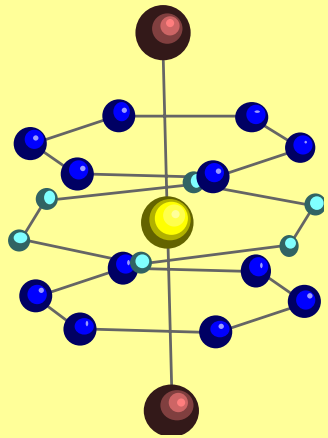
T(6i) 2mm



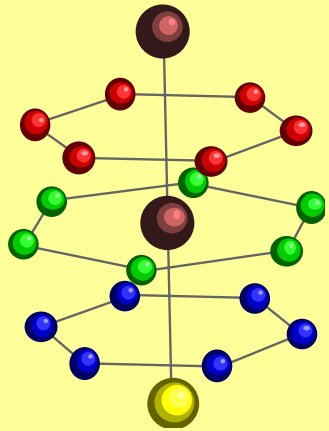
T(4h) 3m.



T(3g) mmm



R(1a) 6/mmm



R(2e) 6mm

1:5	**3:13:2**
2c	2c, 4h
3g	3g, 6i
1a	1a, 2e

2.2 MAGNETIC PROPERTIES

$Y_3Ni_{13}B_2$: Itinerant AF with T_N= 68 K, μ_{eff} = 0.71 μ_B/Ni at., r=6.8

(Plugaru et. al., Phys Rev.B 71, 024433 (2005))

La_2Ni_7 with T_N=54 K, - ref. K.H.J Buschow, JMMM 40, 224 (1983).

$Y_3Ni_{10}Co_3B_2$: Ferromagnet with T_C= 170 K, M= 2.4 μ_B/f.u..at 5 K.

$Y_3Co_{13}B_2$ No magnetic data reported..

Our (unpublished) results : T_C = 636 K.

3.1 CALCULATION APPROACH

- Full relativistic FPLO7 code.
- Exchange and correlations: Perdew and Wang 92.
- k-space integration:

  Y3T13B2 : 270 irreducible k-points from 4096 (16x16x16)

  YT5 : 793 irreducible k-points from 13824 (24x24x24)
- Structural optimization of Y3T13B2.
- Calculations at the exp. lattice constants of YT5.

(Kirchmayr and Burzo, Landolt-Bornstein N.S. III, Vol. 19d2, Springer, Berlin, 1990).

3.2 NEUTRON EXPERIMENTS

- Powder samples of $Y_3Ni_{13}B_2$ and $Y_3Ni_{10}Co_3B_2$
- Instrument D20 (wavelength 1.890 Å) at ILL Grenoble.
- Temperature range 1.8-250 K..
- Rietveld refinement using the FullProf Suite code.

  (J. Rodriguez-Carvajal, Physica B 192 (1993) 55.)
- Crystallographic-like magnetic unit cell for the magnetic phase refinement.
- Constraint of collinearity imposed on the type of magnetic ordering.
- Correction factor for neutron absorption by ^{10}B in samples.

Table. Structural parameters of $Y_3Ni_{13}B_2$ and $Y_3Ni_{10}Co_3B_2$ - refinement of neutron difraction spectra at 1.8 K and Y3 Co13 B2 - refinement of xrd data at RT.

	Y3 Ni13 B2	**Y3 Ni10 Co3 B2**	**Y3 Co13 B2**
a (Å)	4.9524(1)	4.9610(2)	5.0063(3)
c (Å)	10.9061(5)	10.9053(6)	10.853(1)
z, 6i	0.1345(3)	0.1340(2)	0.1441(9)
z, 4h	0.3181(6)	0.3189(4)	0.328(2)
z, 2e	0.3282(9)	0.3283(7)	0.316(1)
T, 6i occ.		Ni, 0.776 Co, 0.224	
T, 4h occ.		Ni, 0.822 Co, 0.178	
T, 3g occ.		Ni, 0.656 Co, 0.344	
c/a	2.202	2.198	2.168
$V_{u.c.}$ (Å^3)	231.65(1)	232.44(1)	235.57(4)

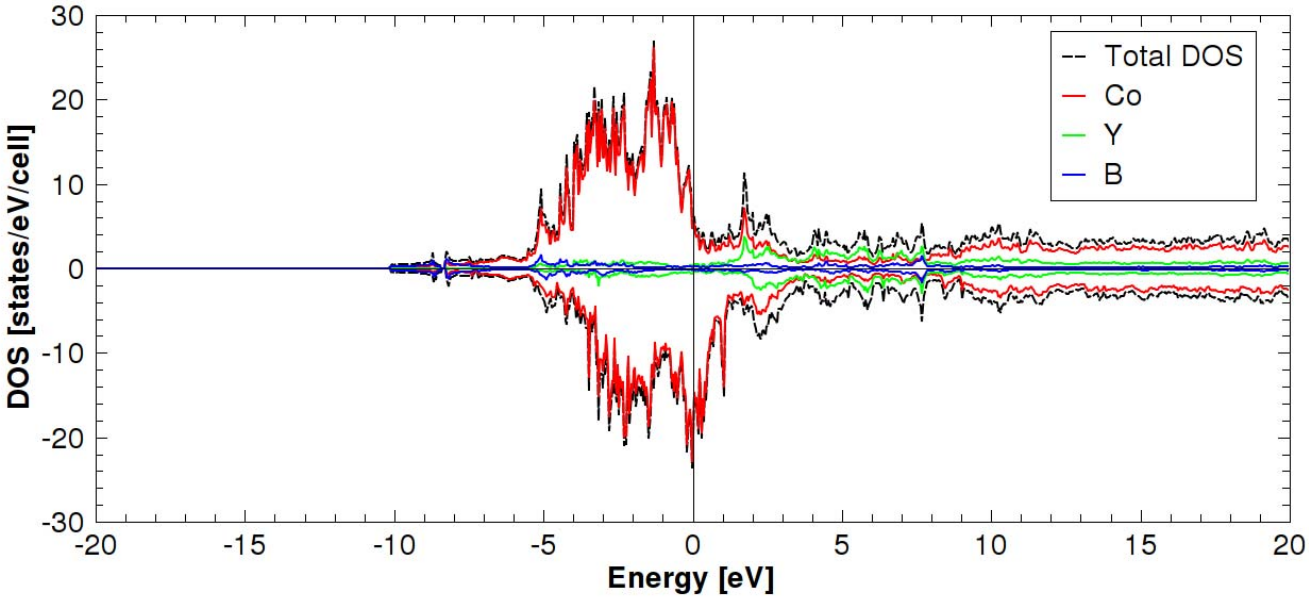
4. CALCULATION RESULTS

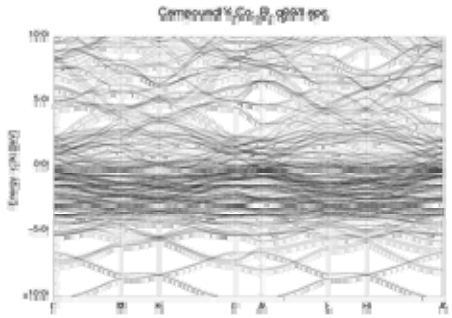
Table. Equilibrium structure parameters of $Y_3Ni_{13}B_2$ and $Y_3Co_{13}B_2$

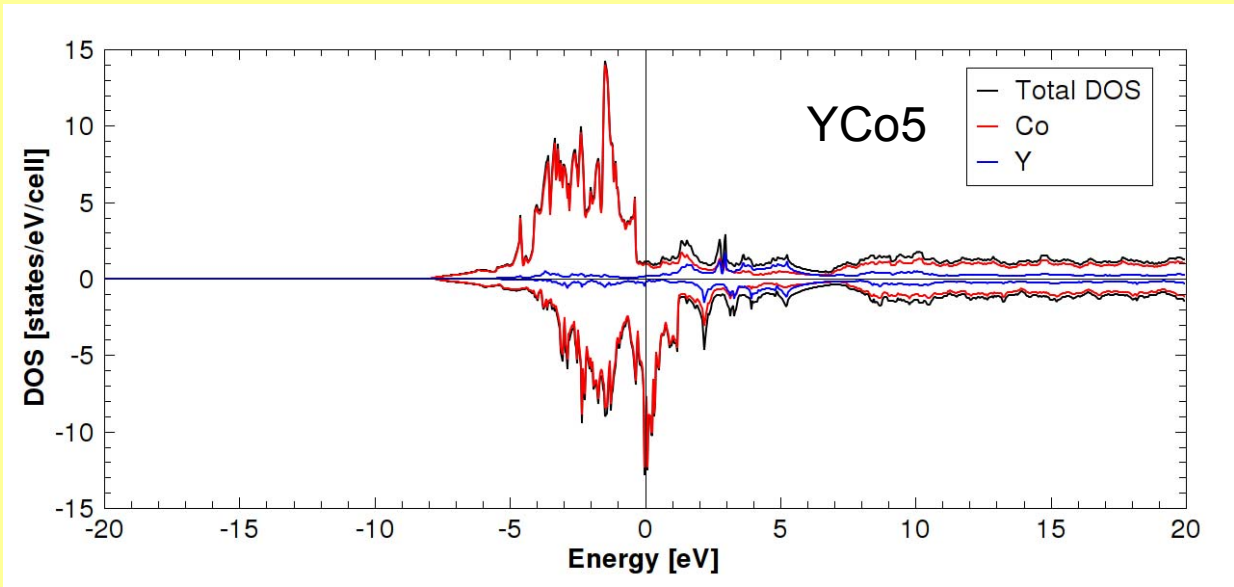
	Y3 Ni13 B2	**Y3 Co13 B2**
a (Å)	4.8386 **(-2.30 %)**	4.8281 **(-3.56 %)**
c (Å)	10.6652 **(-2.21 %)**	10.6067 **(-2.27 %)**
z, 6i	0.1354	0.1407
z, 4h	0.3192	0.3205
z, 2e	0.3279	0.3242
c/a	2.204	2.197
$V_{u.c.}$ (Å^3)	216.24 **(-6.65 %)**	214.12 **(-9.11 %)**

	Y3Ni13B2	**Y3Co13B2**
B(GPa)	194.8 +/- 0.5	190.2+/-3.2

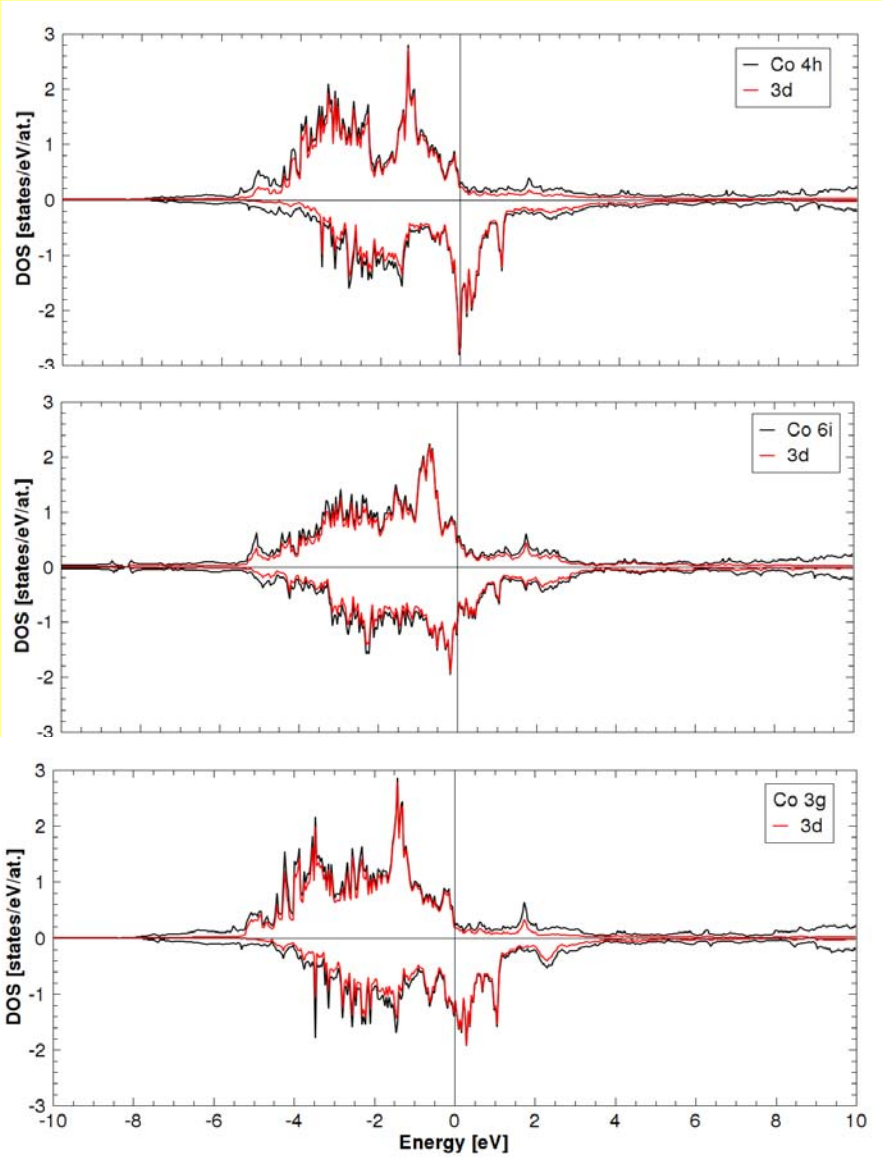
$Y_3Co_{13}B_2$ LSDA, Full Relativistic, OPC



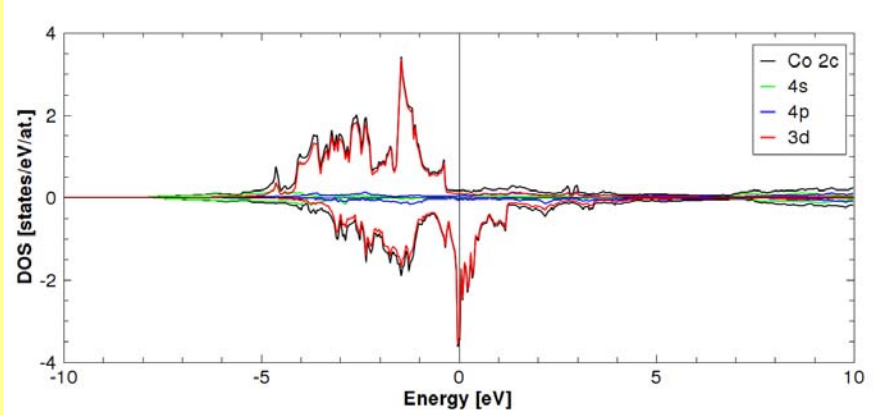




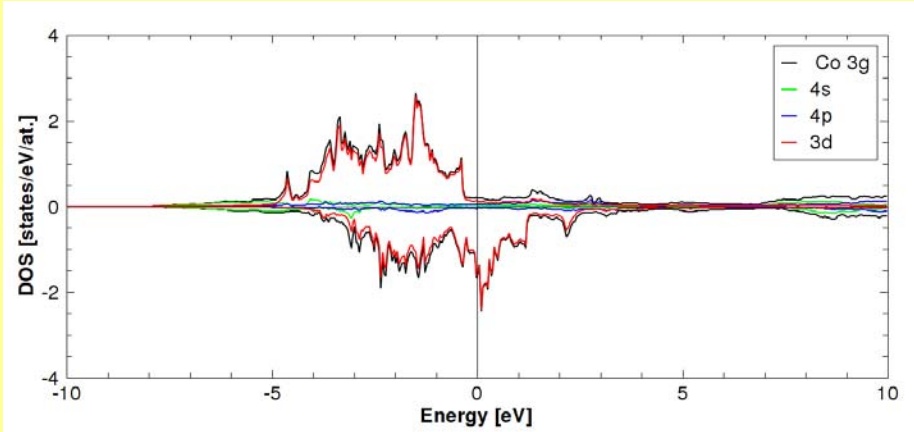
$Y_3Co_{13}B_2$ LSDA, Full Relativistic, OPC



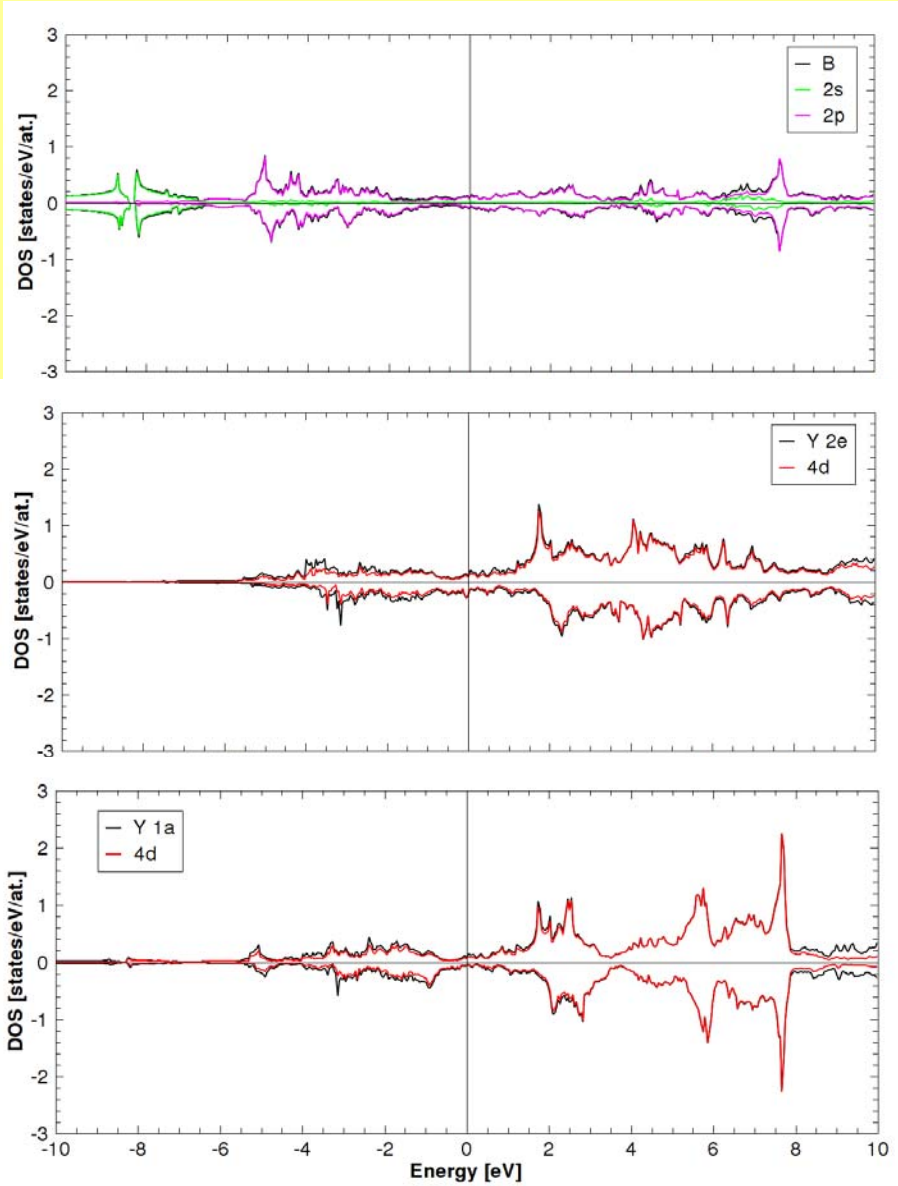
YCo5



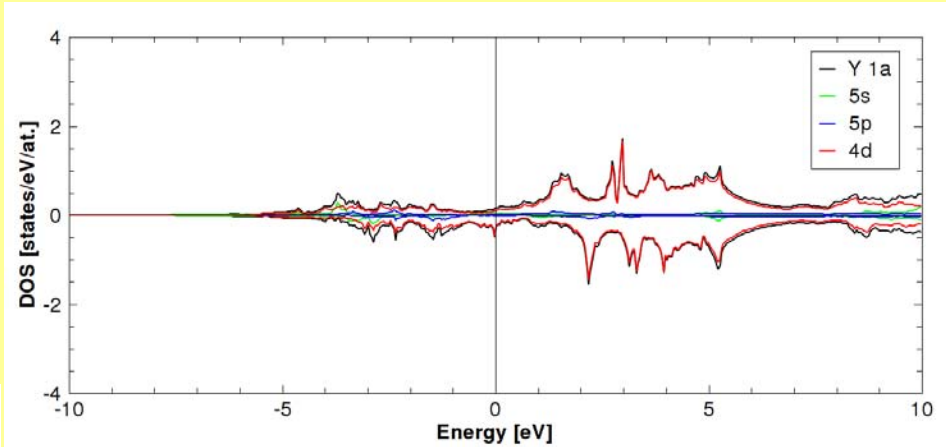
3:13:2	**1:5**
2c, 4h	2c
3g, 6i	3g
1a, 2e	1a



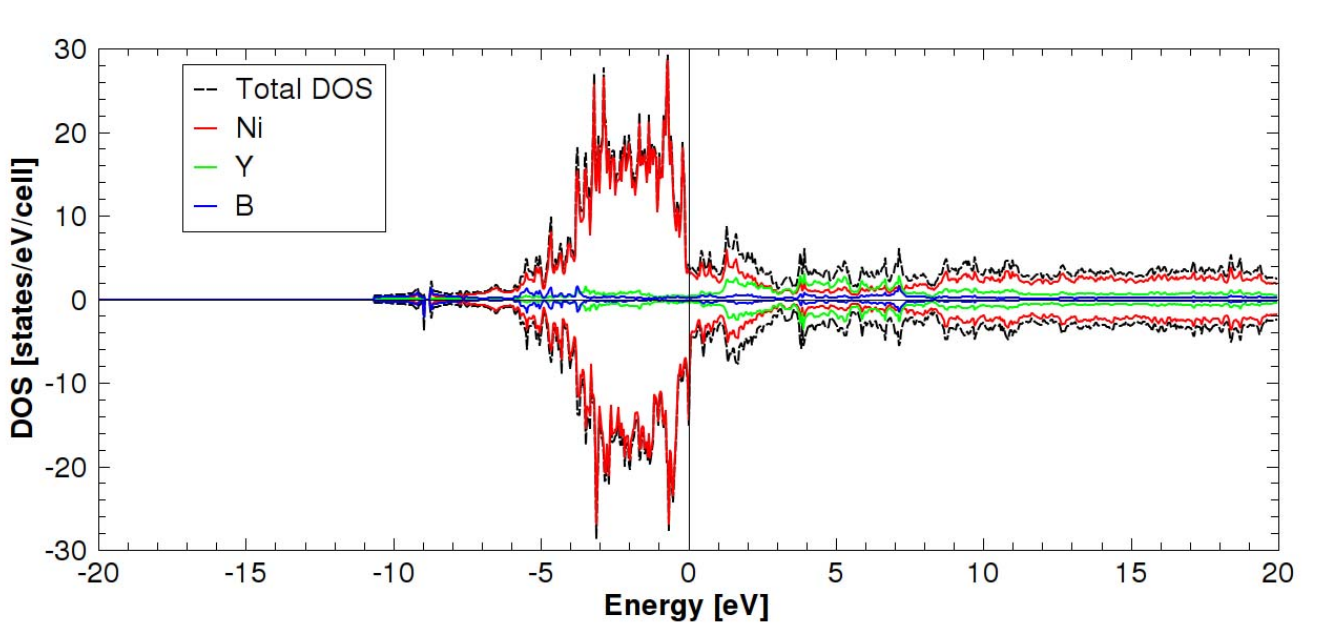
$Y_3Co_{13}B_2$ LSDA, Full Relativistic, OPC

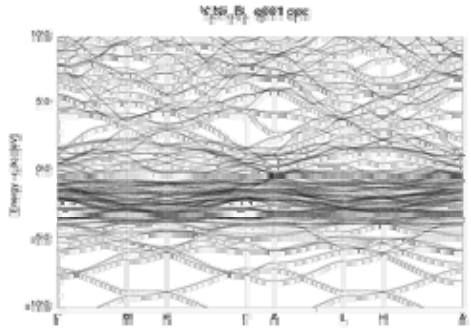


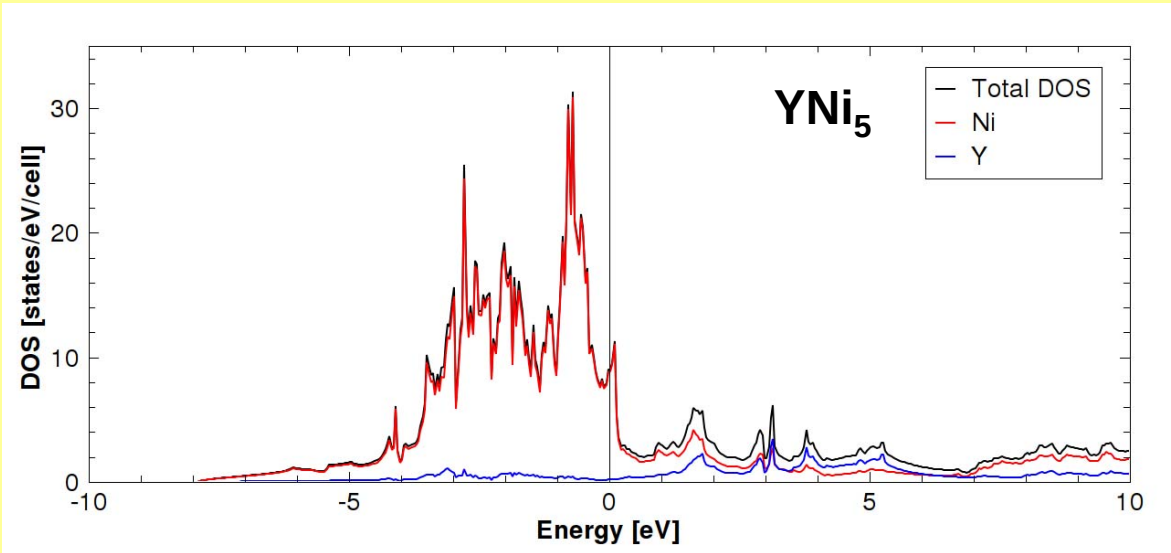
YCo5



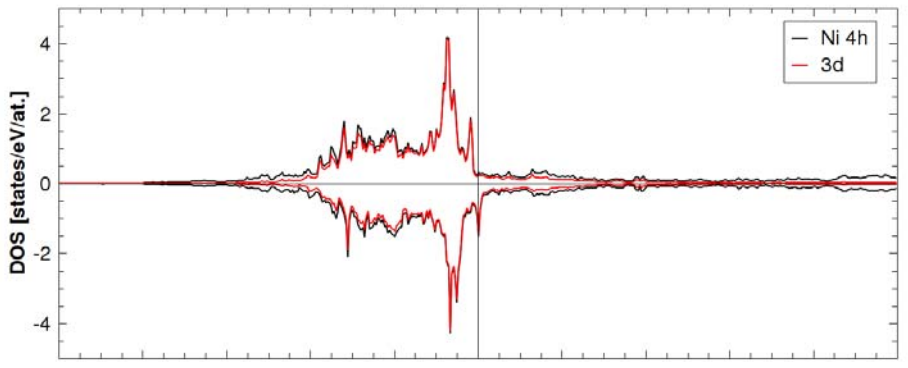
$Y_3Ni_{13}B_2$ LSDA, Full Relativistic, OPC

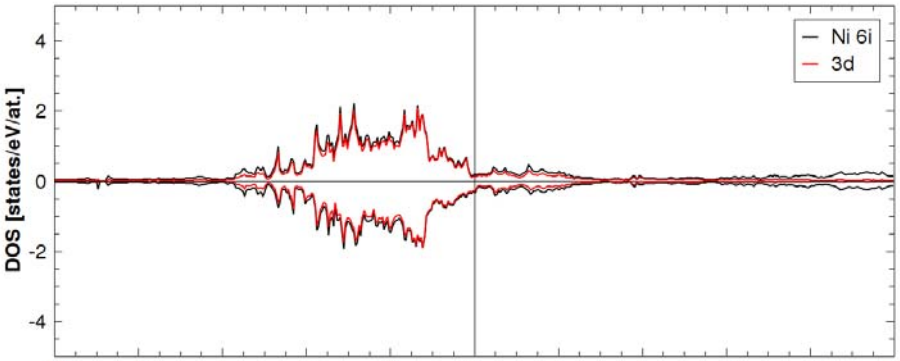


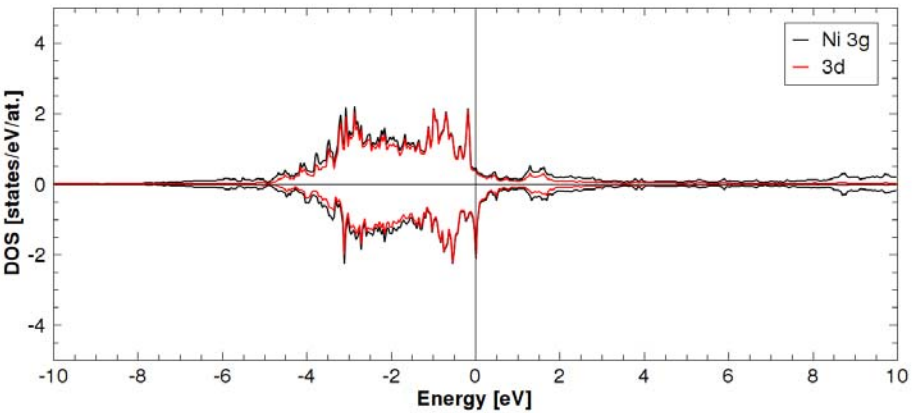




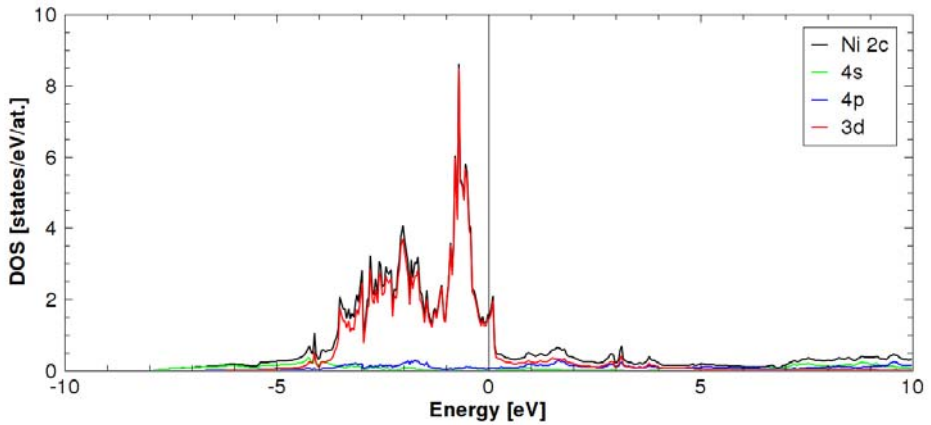
$Y_3Ni_{13}B_2$ LSDA, Full Relativistic, OPC

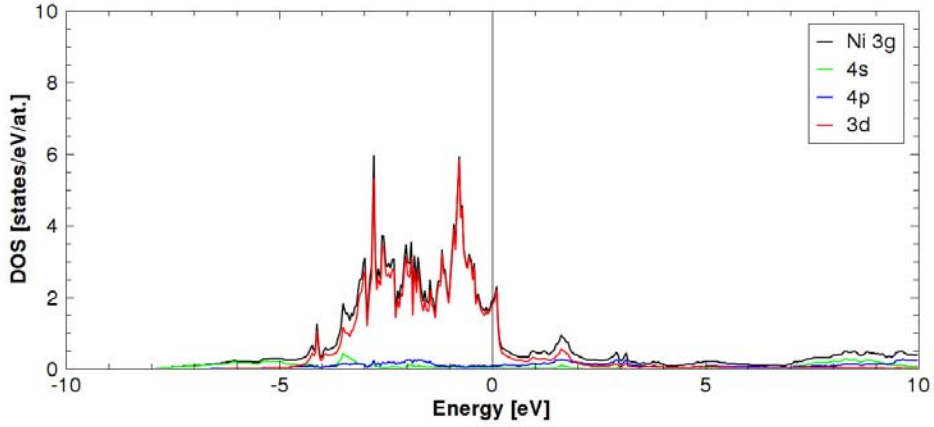




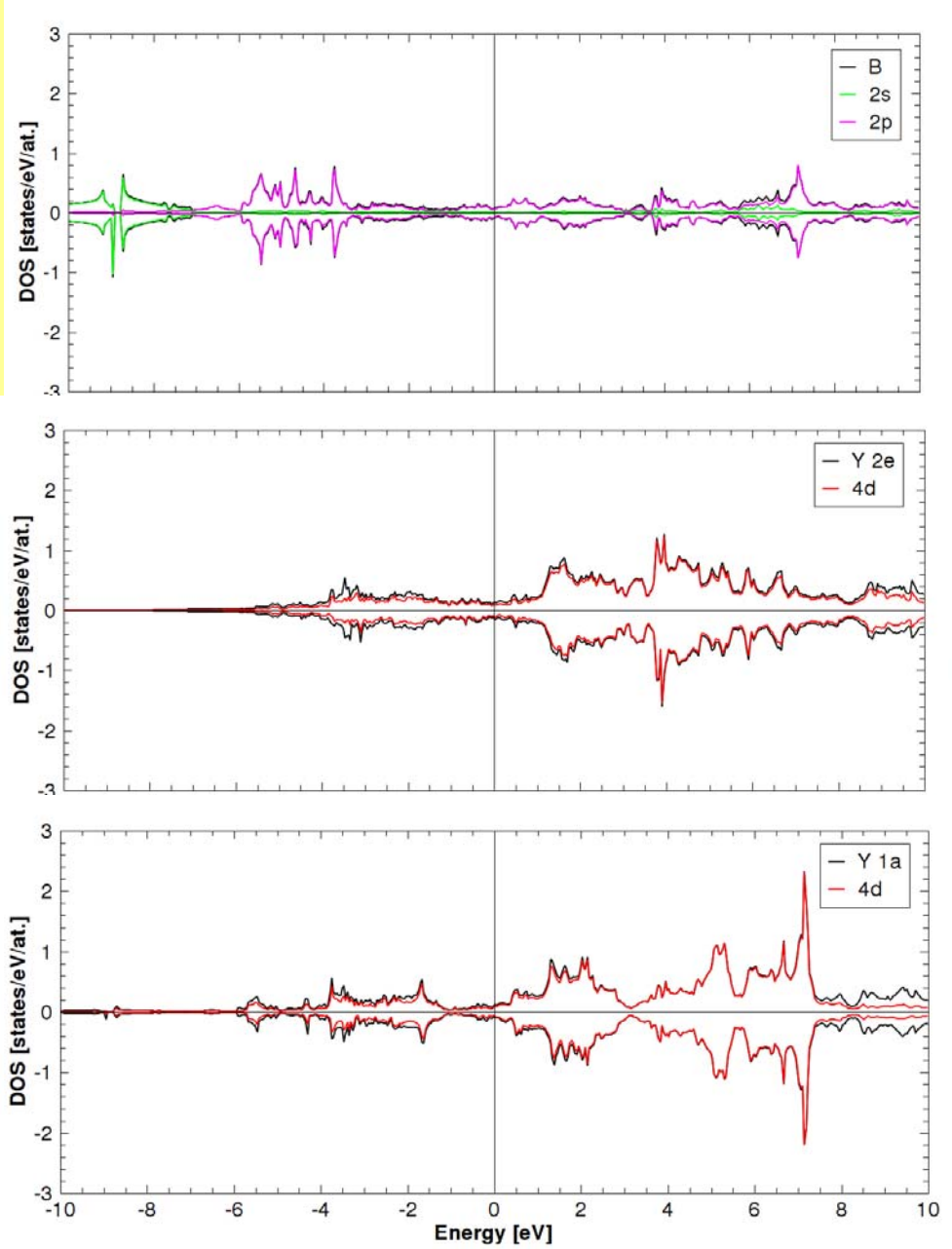


YNi_5





$Y_3Ni_{13}B_2$ LSDA, Full Relativistic, OPC



YNi_5

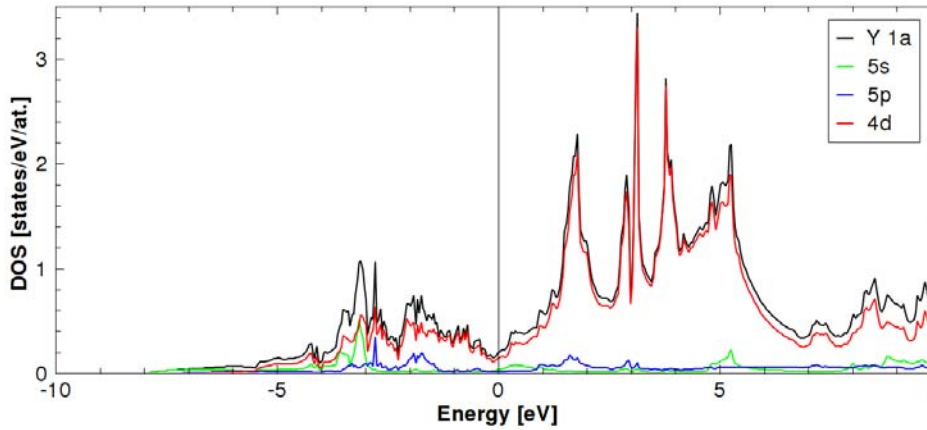


Table. On-site spin, m_s, and orbital, m_l, magnetic moments and the magnetic moment per formula unit, M, for $Y_3T_{13}B_2$. (Between paranthesis: m_l values without OPC.)

			site				
			T, 6i	**T, 4h**	**T, 3g**	**Y, 2e**	**Y, 1a**
m_s (μ_B)	$Y_3Ni_{13}B_2$		0.01	0.12	0.20	-0.02	-0.01
	$Y_3Co_{13}B_2$		0.51	1.35	1.33	-0.20	-0.12
m_l (μ_B)	$Y_3Ni_{13}B_2$		0.00	0.01	0.02	-	-
	$Y_3Co_{13}B_2$		0.04 (0.02)	0.30 (0.12)	0.22 (0.10)	-	-
M (μ_B/f.u.)	$Y_3Ni_{13}B_2$	1.03					
	$Y_3Co_{13}B_2$	11.80					

YCo5		2c	3g	1a
m_s (μ_B)		1.45	1.47	-0.31
m_l (μ_B)		0.37	0.30	0.04
M (μ_B/f.u.)	6.99			

MAE

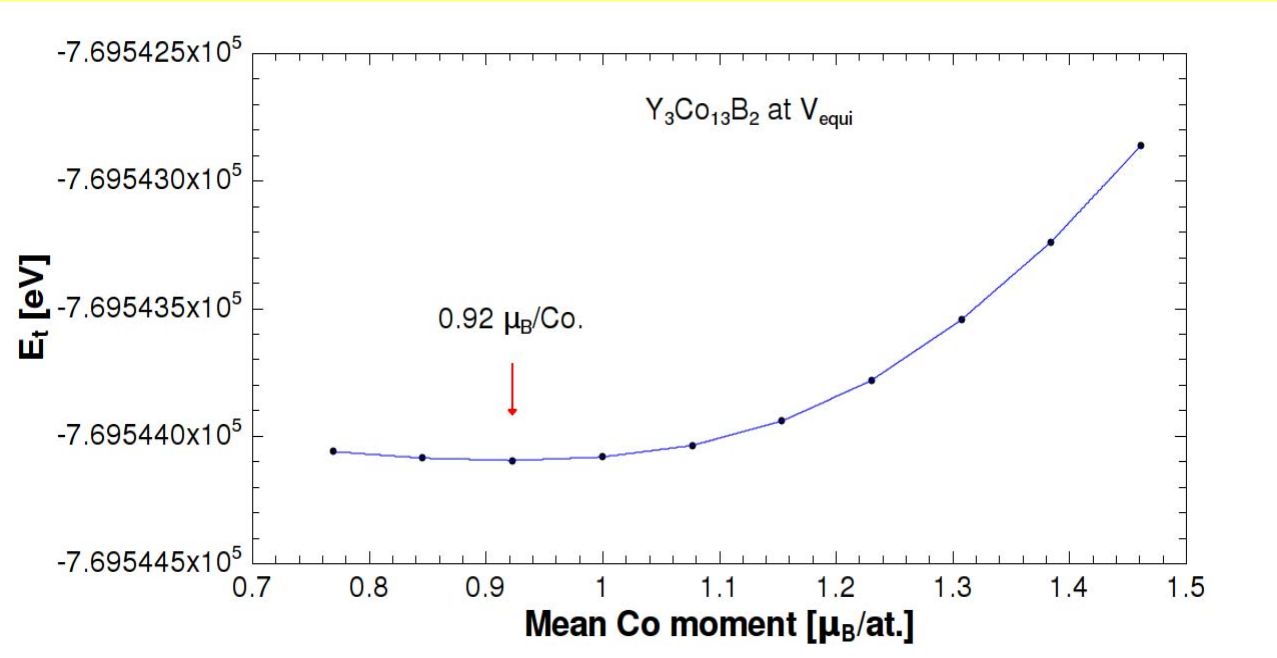
$Y_3Co_{13}B_2$ $E_{t(q100)} - E_{tq001)} = 5.84$ meV /f.u.

YCo_5 (FPLO7) = 5.23 meV /f.u.

YCo_5 (ste01) = 4.4 meV /f.u

[ste01] Steinbeck et al., Phys. Rev.B 63 184431 (2001) .

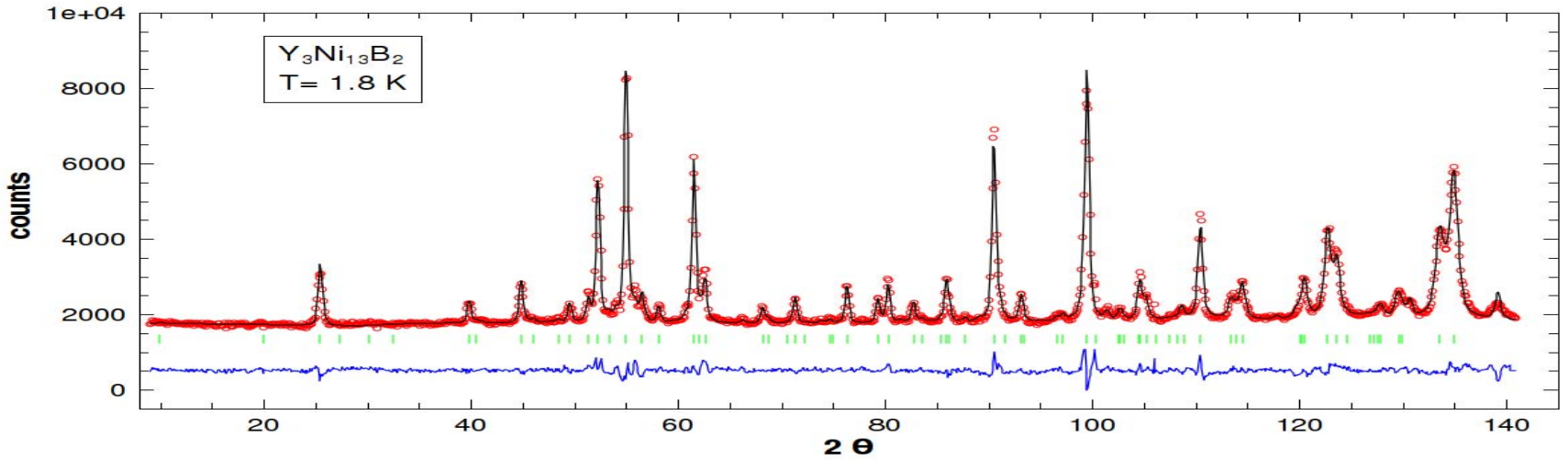
$Y_3Ni_{13}B_2$ = - 0.66 meV /f.u.

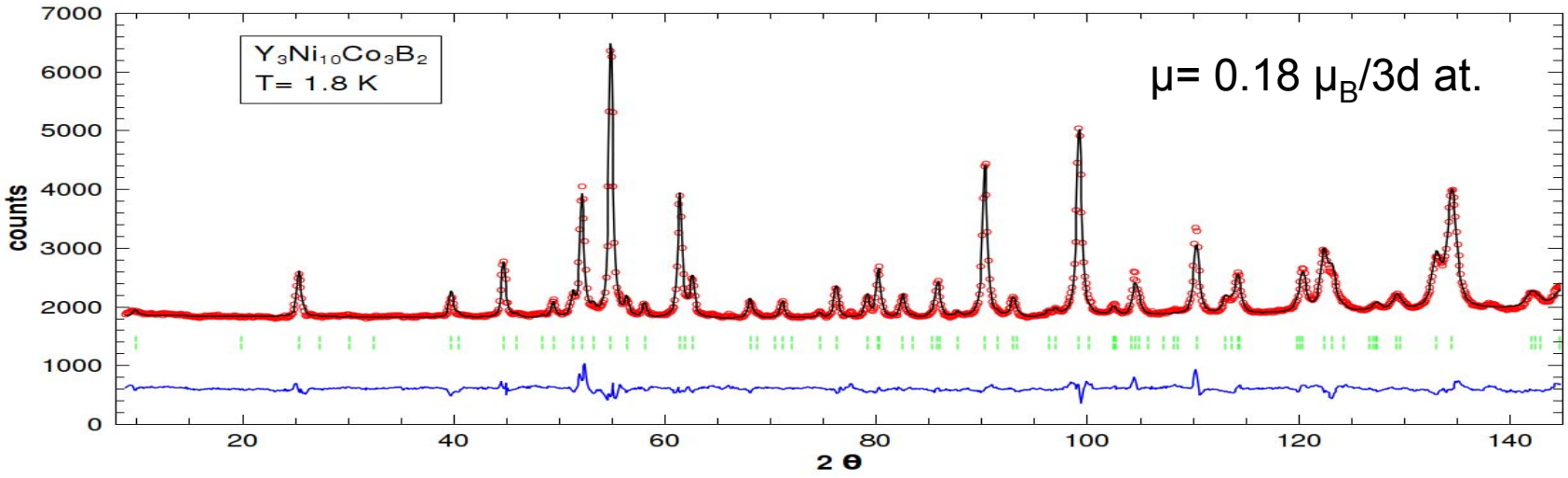


FSM calculation for $Y_3Co_{13}B_2$ at V_{equi}

5. NEUTRON INVESTIGATION RESULTS

T=1.8 K





6. SUMMARY

Full relativistic LSDA+OPC calculations show:

Y3Ni13B2

- **Ni magnetic moments in agreement with magnetic measurements data.**
- **μ(Ni) below the limit posed by the resolution of the neutron data.**
- **In-plane magnetic anisotropy.**

Outlook: further refinement of the magnetic structure is needed.

Y3Co13B2

- **Strong effect of B nn at Co(6i) and Y(1a) sites.**
- **MAE(Y3Co13B2) > MAE(YCo5)**
- **FSM test of the magnetic state: no metamagnetic transition at Co6i site**

Outlook: OMA to be analyzed.

Acknowledgments

Great support from

M. Richter
Ulrike Nitzsche
and many people from ITF-IFW Dresden

is gratefully acknowledged !