The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

2157-14

Workshop on Principles and Design of Strongly Correlated Electronic Systems

2 - 13 August 2010

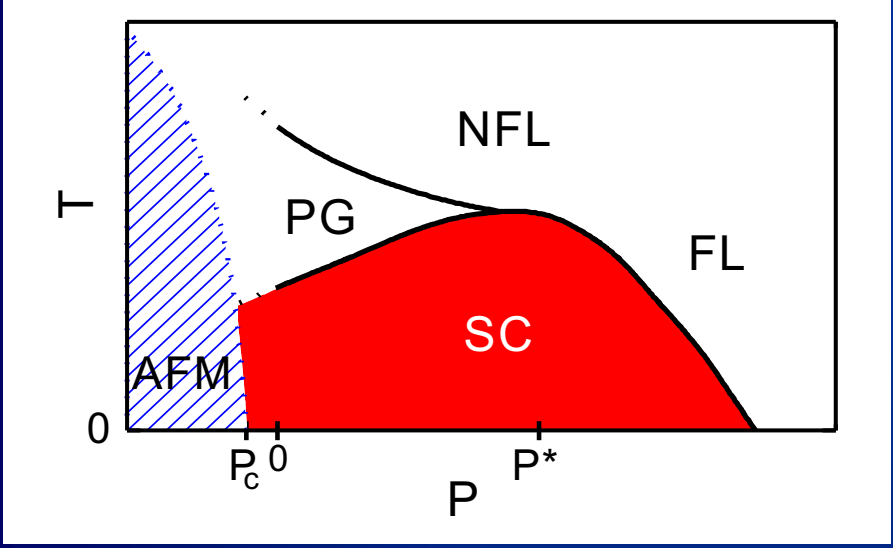
Low symmetry structures and hybridization: Key ingredients for finding new superconductors

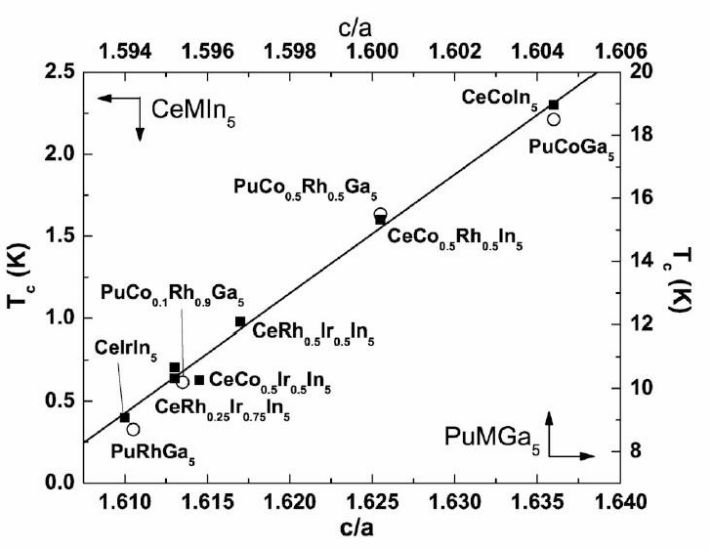
Pascoal G. PAGLIUSO

GPOMS, Instituto de Fisica "Gleb Wataghin"
UNICAMP. Campinas, SP
Brazil

Workshop on Principles and Design of Strongly Correlated Electronic Systems – Trieste - 08/10

Low symmetry structures and hybridization: key ingredients for finding new superconductors





GPOMS

Pascoal G. Pagliuso

Grupo de Propriedades Ópticas e Magnéticas dos Sólidos (GPOMS)
Instituto de Física ``Gleb Wataghin'', UNICAMP – Campinas -SP

UNICAMP

Los Alamos National Laboratory • Materials Science and Technology •
UC - Irvine
CBPF
NIST National Institute of Standards and Technology
LNLS
ESRF
FAPESP
CNPq 50 ANOS

Area
8.5 millions km^2

Sea shore
8,500 km

Population
176 millions
inhab.

São Paulo
15 millions
inhab.

Rio de Janeiro
~ 6 millions
inhab.

Campinas
~ 100 km NW
from SP
- 500 km from
Rio

Campinas City 1.5 million inhabitants

Universidade Estadual de Campinas “UNICAMP”

~ 4 km^2 - 35,000 Students (40 years old)

Magnetic and Optics Facilities GPOMS

PPMS-QD 9T, 0.3 K
14 T 50 mK

Cp(T,H)
M(T,H)
ρ(T,H) e R_H
κ(T,H)
0 < P < 25 kbar.

MPMS
SQUID-QD 7T
1.8 < T < 800 K
0 < P < 12 kbar.

RAMAN Lab
1.6 < T < 800 K
0 < H < 7 T.

10 K
-
1000 °C

X
-
R
A
Y

300 K

V
S
M

F
U
R
N
A
C
E
S

ESR Spectrometers

L (1.4 GHz); S (4.0 GHz); X (9.4 GHz) Q; (34.4 GHz)

(400 G) (1.200 G) (3.200 G) (12.000 G)

Bruker-ELEXSYS E-500

VARIAN

CAMPINAS SYNCHROTRON NATIONAL LABORATORY
EXAFS-XANES-XDR (structural and magnetic)

~ 10^{11} fótons/s @ 200 mA @ E = 8keV (ë ~1.5); D ~30 m

Outline

I. Review of structurally related physical properties of HFS families $Ce_mM_nIn_{3m+2}$ – the role of CEF tetragonal symmetry – layered structural

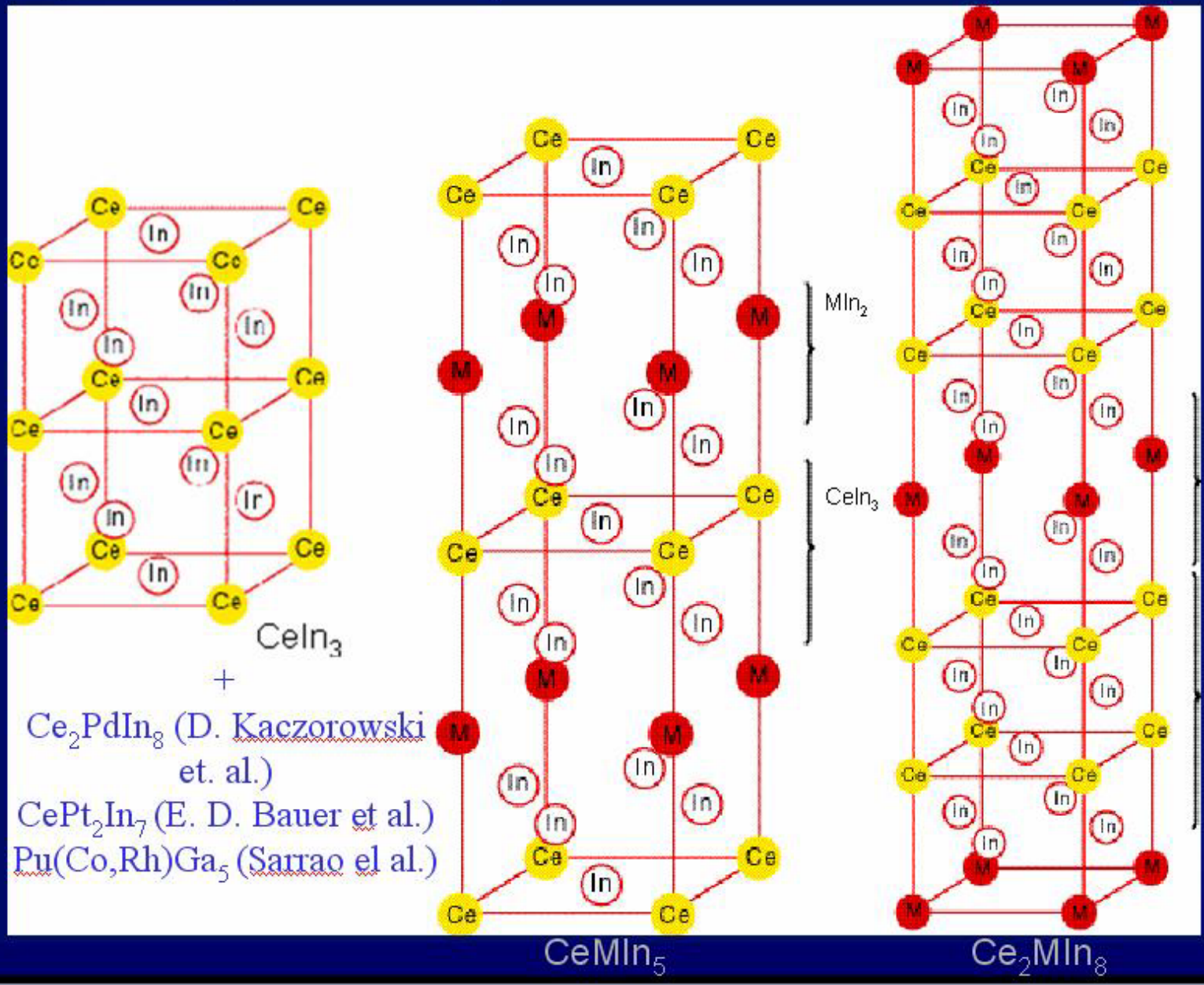
II. $CeRhIn_5$ doped with La and Sn

III. Cd-doped $Ce_2(Rh,Ir)In_8$

IV. Possible relationship to FeAs-based, Yb-based HFS

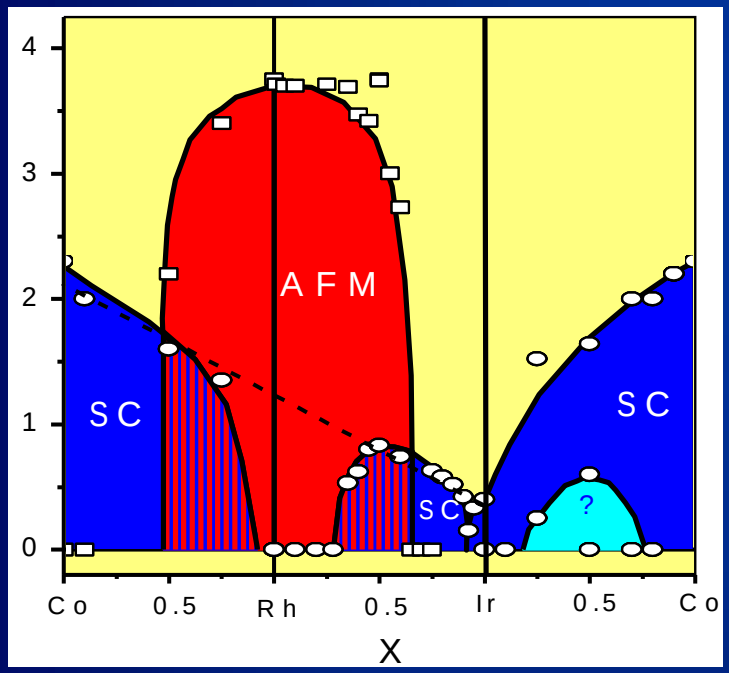
V. Implications in new materials search

6 HFS – What is special about these structures?

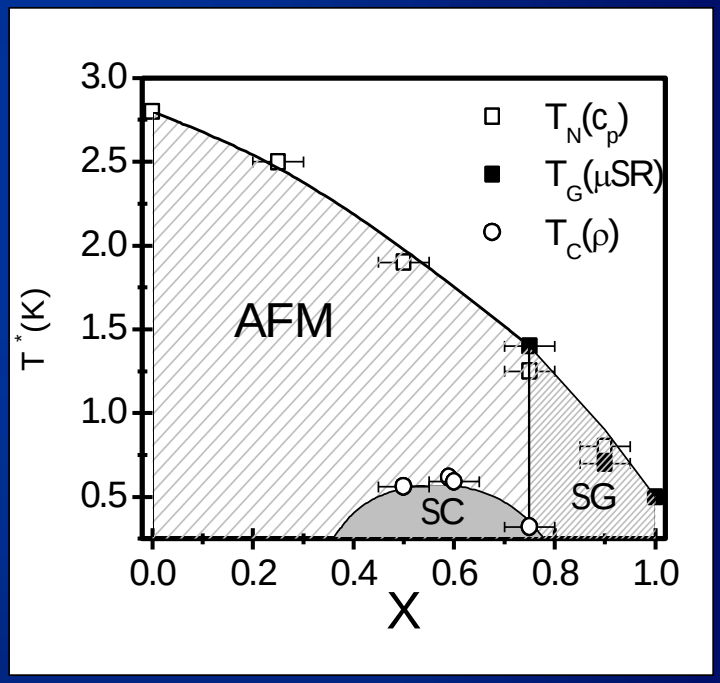


$Ce_mM_nIn_{3m+2n}$

$CeRh_{1-x}(Ir,Co)_xIn_5$ [1,2]



$Ce_2Rh_{1-x}Ir_xIn_8$ [3,4,5]



-Ce_2CoIn_8

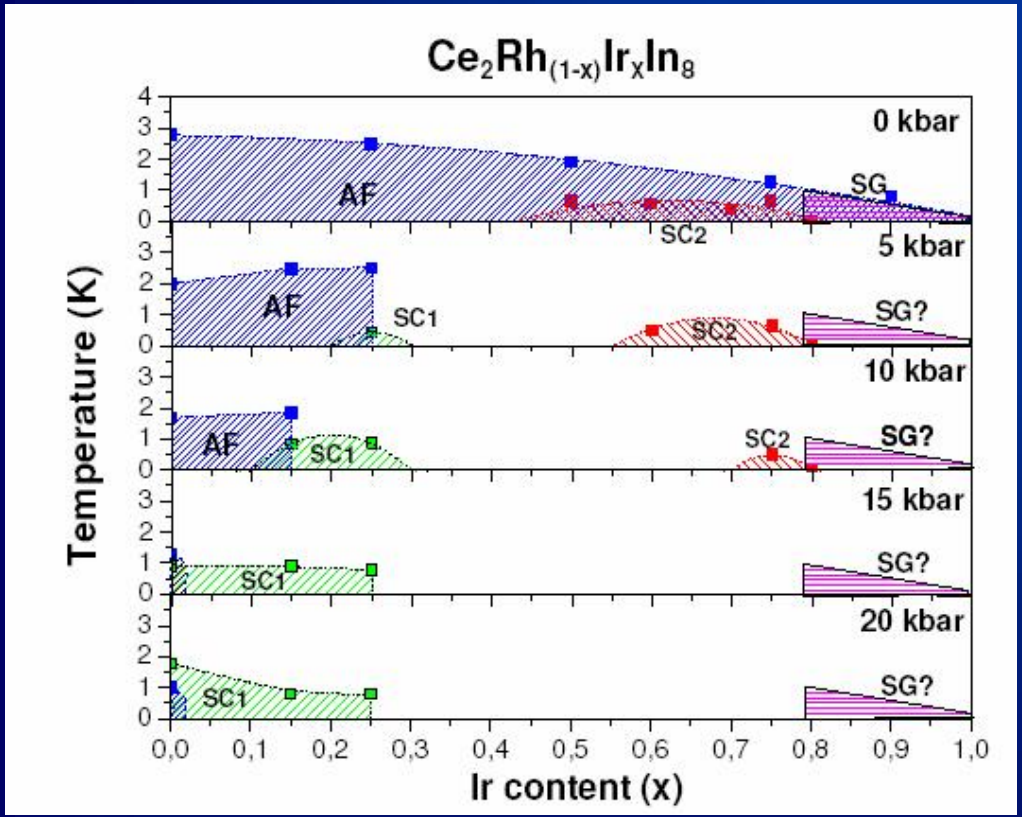
$T_C \approx 1.0$ K

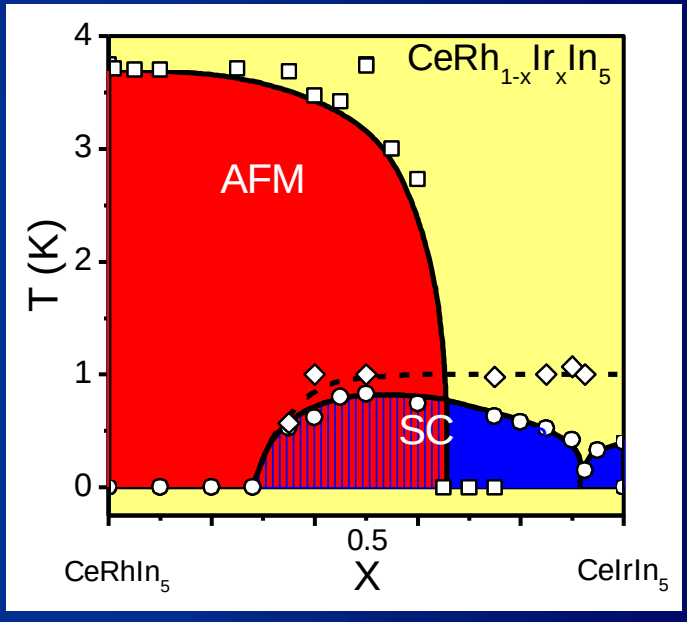
$\gamma \geq 600$ mJ/K^2 mole Ce

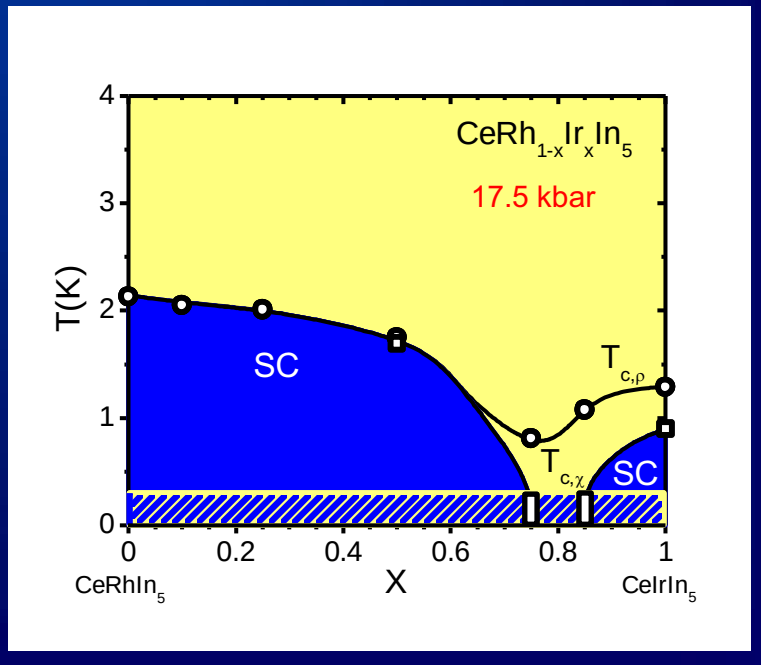
[1] Pagliuso et al, Physica B, 312, 129 (2002).
[2] Pagliuso et al, Phys.Rev B, 64, 100503(R) (2001).

[3] E.N. Hering et al Physica B, 378, 423 (2006).
[4] E.N. Hering, Physica B, 403, 780 (2008);
[5] E. N. Hering, C. Adriano, et al, submited to PRB (2010).

$Ce_2(Rh,Ir)_{1-x}Co_xIn_8$ – Phase Diagrams



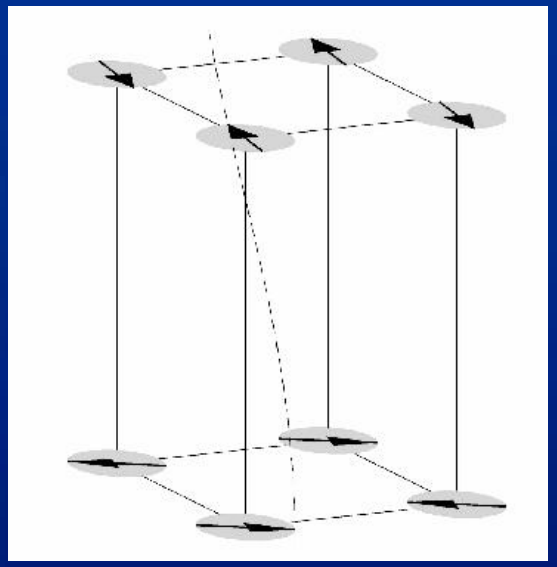




E. N Hering, et al
M. Nicklas et al.

Magnetic Structure

$CeRhIn_5$



$T_N = 3.8$ K

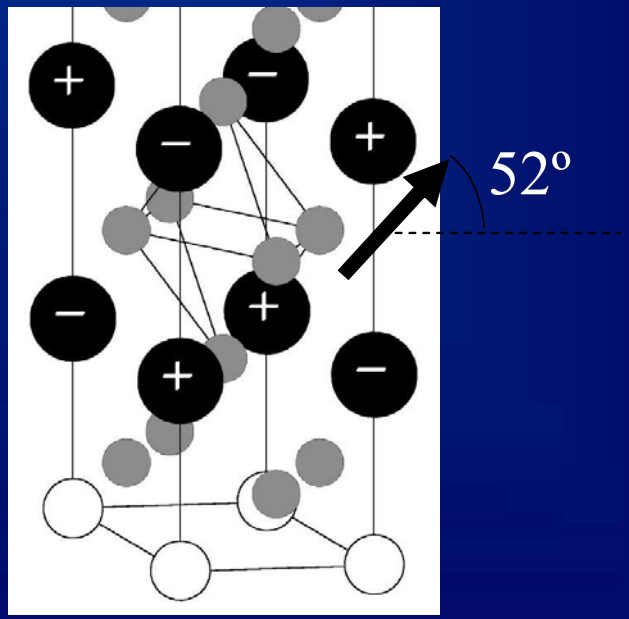
$\mu_{ord}=0.7\ \mu_B$ (in plane)

107° spiral layer-to-layer

Curro et al., PRB 62, R6100 (2000)
Bao et al., PRB 62, R14621 (2000)

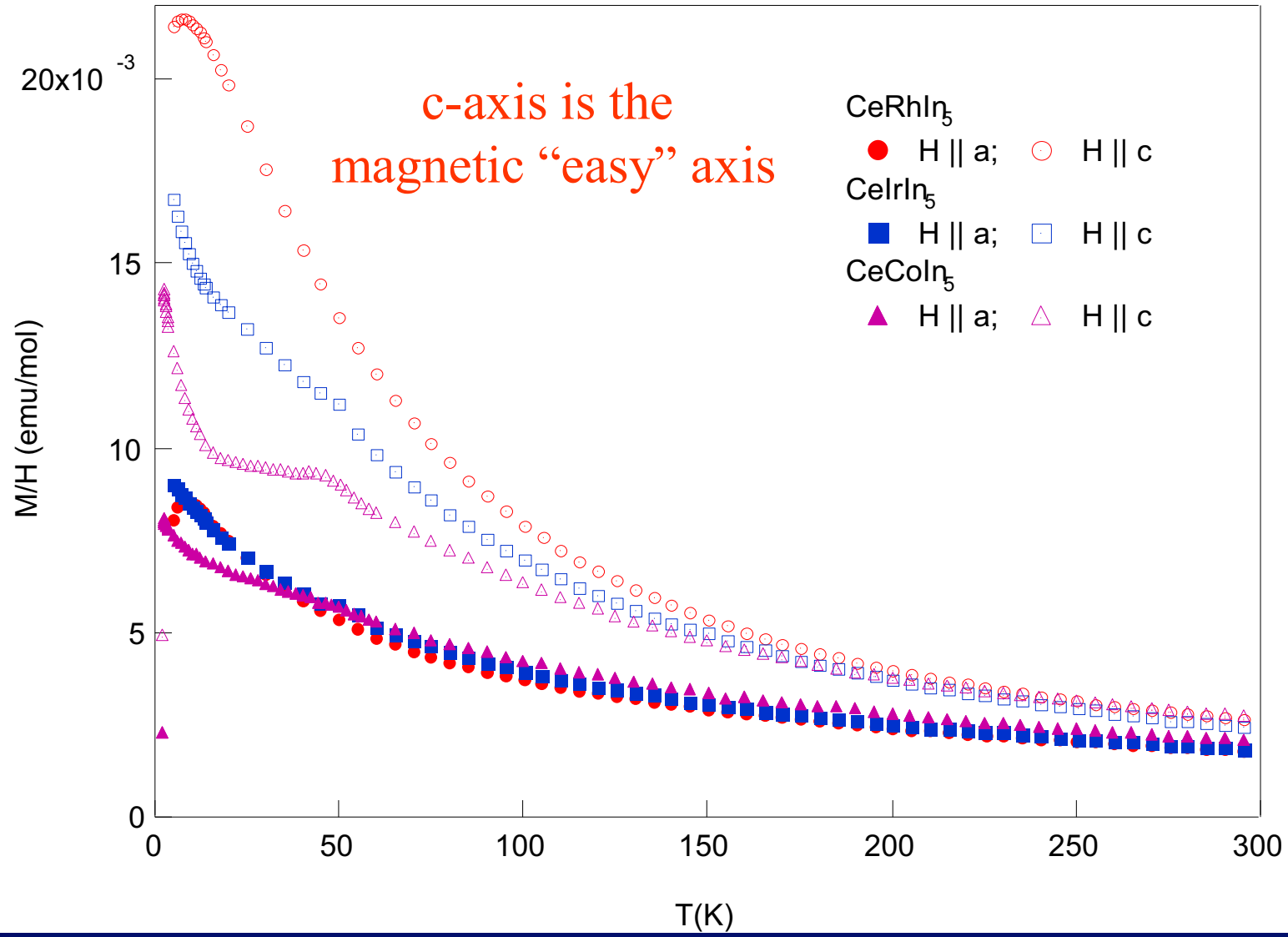
Ce_2RhIn_8

- AFM with $T_N = 2.8$ K
- $\varepsilon = (1/2, 1/2, 0)$ and $\eta = 52°$
- $\mu_{eff} = 0.55\ \mu_B$



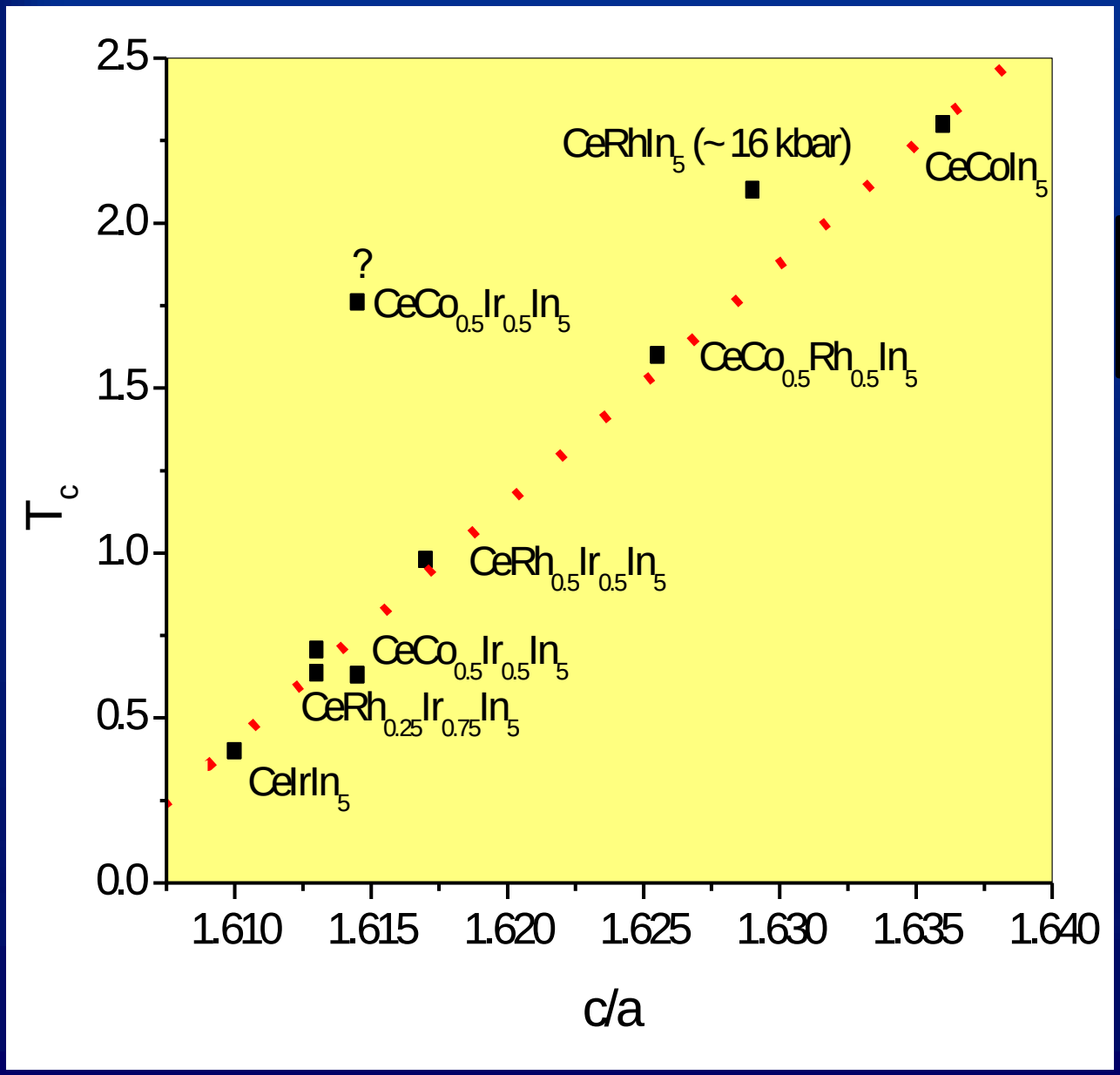
W. Bao et al Phys. Rev. B, 64 020401R (2001)

$CeMIn_5$ - $\chi(T)$ summary



C. Petrovic et al., J. Phys.: Cond Mat. 13 (2001) L337

c/a as control parameter for T_c



Is there an intrisic parameter in this plot, which depends on c/a and determines T_C?

Tuning:

- J_{RKKY}
- T_K
- CEF

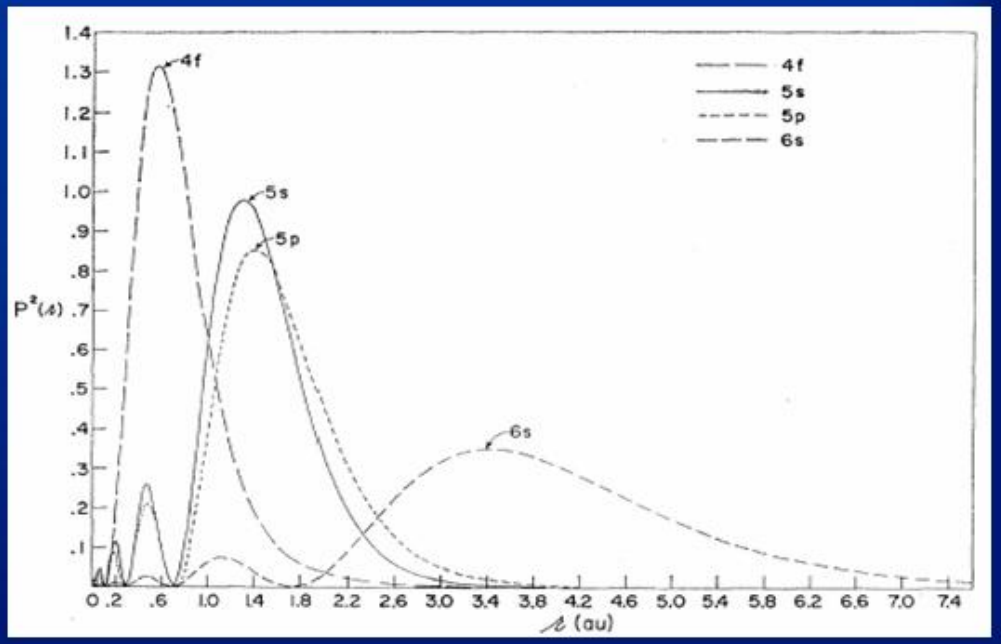
P.G. Pagliuso et al. PRB, 100503 (R) (2002); Physica B 312-313, 129 (2002).

The rare-earth ions

Electronic configuration:

- Incomplete 4*f* shells
- Chemically alike – valence 3+.

	Z	R
La	57	$[Xe]5d^16s^2$
Ce	58	$[Xe]4f^15d^16s^2$
Pr	59	$[Xe]4f^36s^2$
Nd	60	$[Xe]4f^46s^2$
Pm	61	$[Xe]4f^56s^2$
Sm	62	$[Xe]4f^66s^2$
Eu	63	$[Xe]4f^76s^2$
Gd	64	$[Xe]4f^75d^16s^2$
Tb	65	$[Xe]4f^96s^2$
Dy	66	$[Xe]4f^{10}6s^2$
Ho	67	$[Xe]4f^{11}6s^2$
Er	68	$[Xe]4f^{12}6s^2$
Tm	69	$[Xe]4f^{13}6s^2$
Yb	70	$[Xe]4f^{14}6s^2$
Lu	71	$[Xe]4f^{14}5d^16s^2$



- 4*f* shells are partially shielded by external orbitals.
- Spin-orbital coupling stronger than crystal field effects

The rare-earth ions

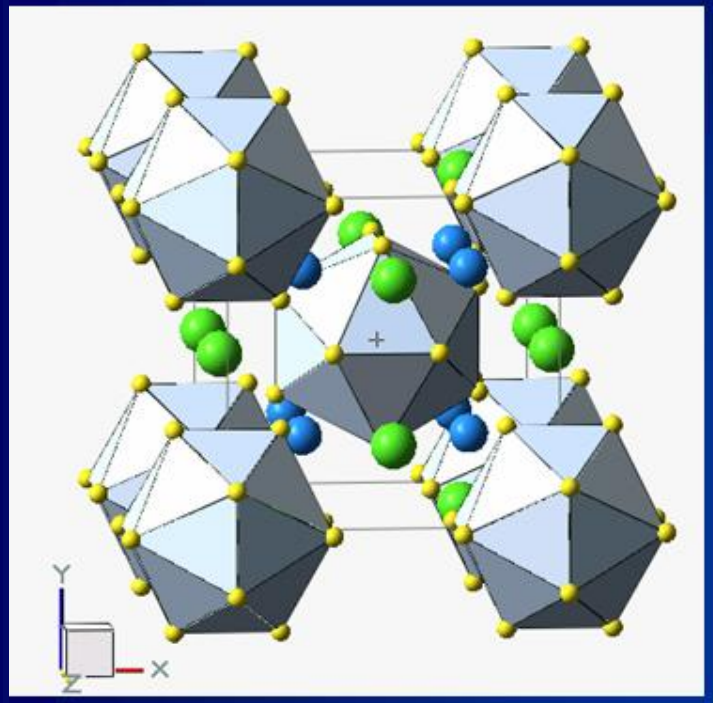
f-shell ($l = 3$)											
n	$l_z = 3,\ 2,\ 1,\ 0, -1, -2, -3$								S	$L = \lvert\Sigma l_z\rvert$	J	
1	↓							Ce^{3+}	1/2	3	5/2	$^2F_{5/2}$
2	↓	↓						Pr^{3+}	1	5	4	$^3H_4$
3	↓	↓	↓					Nd^{3+}	3/2	6	9/2	$^4I_{9/2}$
4	↓	↓	↓	↓					2	6	4	$^5I_4$
5	↓	↓	↓	↓	↓				5/2	5	5/2	$^6H_{5/2}$
6	↓	↓	↓	↓	↓	↓			3	3	0	$^7F_0$
7	↓	↓	↓	↓	↓	↓	↓	Gd^{3+}	7/2	0	7/2	$^8S_{7/2}$
8	↓↑	↑	↑	↑	↑	↑	↑		3	3	6	$^7F_6$
9	↓↑	↓↑	↑	↑	↑	↑	↑		5/2	5	15/2	$^6H_{15/2}$
10	↓↑	↓↑	↓↑	↑	↑	↑	↑		2	6	8	$^5I_8$
11	↓↑	↓↑	↓↑	↓↑	↑	↑	↑		3/2	6	15/2	$^4I_{15/2}$
12	↓↑	↓↑	↓↑	↓↑	↓↑	↑	↑		1	5	6	$^3H_6$
13	↓↑	↓↑	↓↑	↓↑	↓↑	↓↑	↑	Yb^{3+}	1/2	3	7/2	$^2F_{7/2}$
14	↓↑	↓↑	↓↑	↓↑	↓↑	↓↑	↓↑		0	0	0	$^1S_0$

$J = |L - S|$ (5/2, 4, 9/2, 4, 5/2, 0)

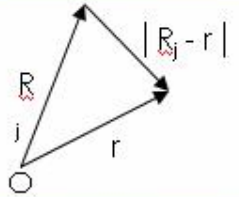
$J = L + S$ (6, 15/2, 8, 15/2, 6, 7/2)

[a] ↑ = spin $\frac{1}{2}$; ↓ = spin $-\frac{1}{2}$.

The rare-earth ions in solids

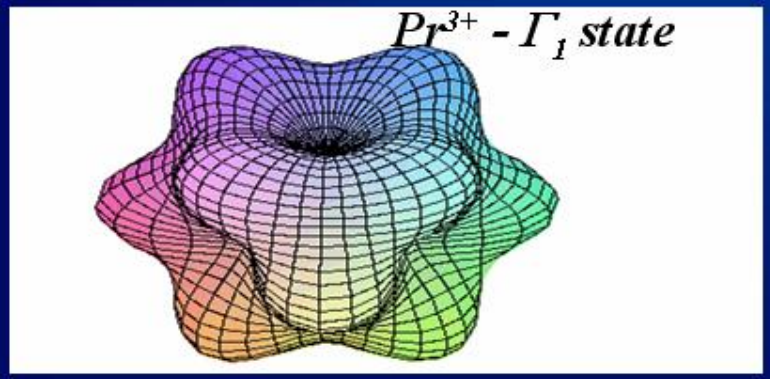


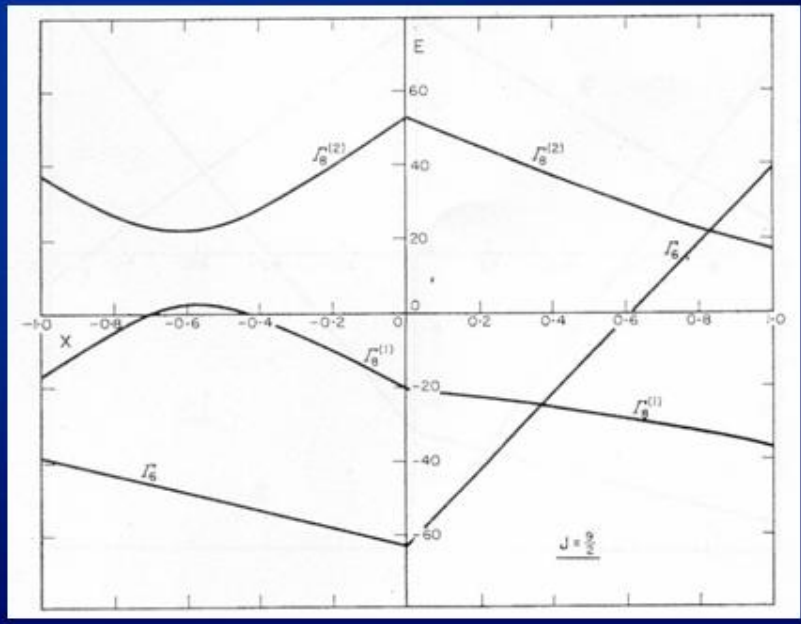
$$V(r,\theta,\phi) = \sum_j \frac{q_j}{\left|(\mathbf{R}_j - \mathbf{r})\right|}$$



$$H_{CEF} = B_4\left(O_4^0 + 5\cdot O_4^4\right) + B_6\left(O_6^0 - 21\cdot O_6^4\right)$$

(cubic CEF)





CEF defines single ion spin-anisotropy

Local f-electrons: Magnetic properties

f-shell ($l = 3$)

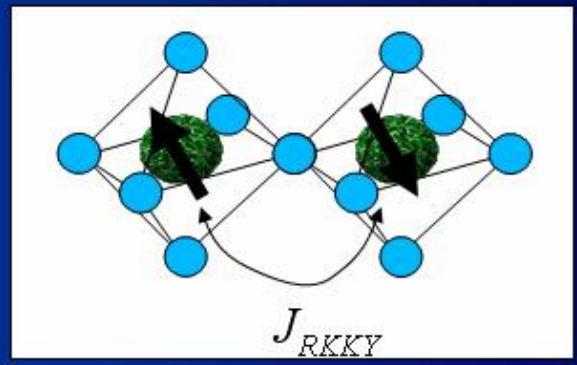
n	$l_z = 3, 2, 1, 0, -1, -2, -3$	S	$L = \lvert\Sigma l_z\rvert$	J	
1	↓	1/2	3	5/2	$^2F_{5/2}$
2	↓ ↓	1	5	4	$^3H_4$
3	↓ ↓ ↓	3/2	6	9/2	$^4I_{9/2}$
4	↓ ↓ ↓ ↓	2	6	4	$^5I_4$
5	↓ ↓ ↓ ↓ ↓	5/2	5	5/2	$^6H_{5/2}$
6	↓ ↓ ↓ ↓ ↓ ↓	3	3	0	$^7F_0$
7	↓ ↓ ↓ ↓ ↓ ↓ ↓	7/2	0	7/2	$^8S_{7/2}$
8	↕ ↑ ↑ ↑ ↑ ↑ ↑	3	3	6	$^7F_6$
9	↕ ↕ ↑ ↑ ↑ ↑ ↑	5/2	5	15/2	$^6H_{15/2}$
10	↕ ↕ ↕ ↑ ↑ ↑ ↑	2	6	8	$^5I_8$
11	↕ ↕ ↕ ↕ ↑ ↑ ↑	3/2	6	15/2	$^4I_{15/2}$
12	↕ ↕ ↕ ↕ ↕ ↑ ↑	1	5	6	$^3H_6$
13	↕ ↕ ↕ ↕ ↕ ↕ ↑	1/2	3	7/2	$^2F_{7/2}$
14	↕ ↕ ↕ ↕ ↕ ↕ ↕	0	0	0	$^1S_0$

$J = |L - S|$ (rows 1–6); $J = L + S$ (rows 8–13)

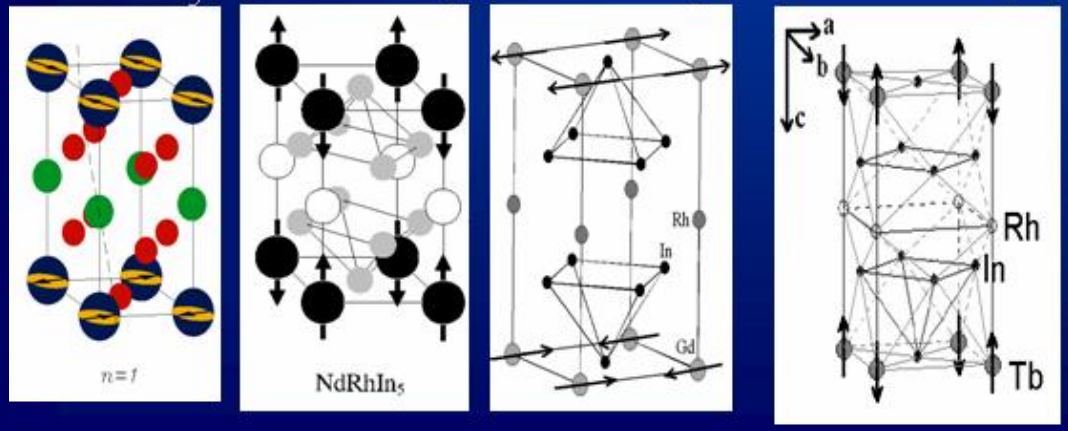
*↑ = spin ½; ↓ = spin −½.

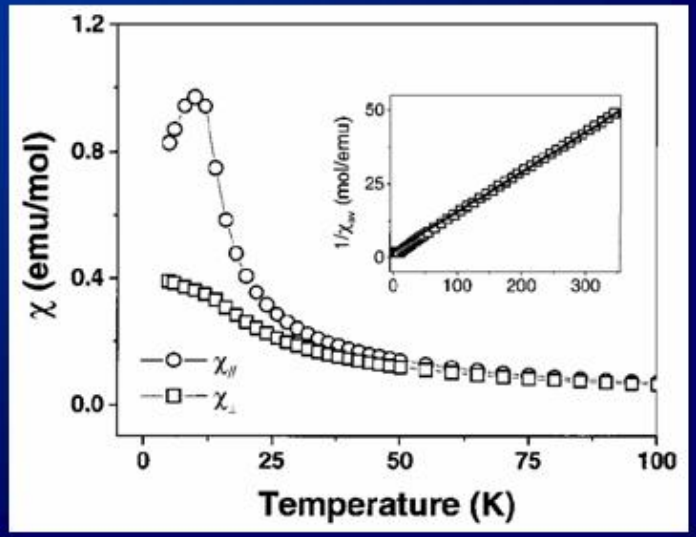
Magnetic susceptibility:

$$\chi = \frac{C}{T - \theta_{CW}} \therefore C \propto p^2 = g_j \sqrt{J(J(J+1)\mu_B^2}$$



$CeRhIn_5$ $NdRhIn_5$ $GdRhIn_5$ $TbRhIn_5$





Why are Ce and Yb specials?

Ce^{3+} - $4f^1$

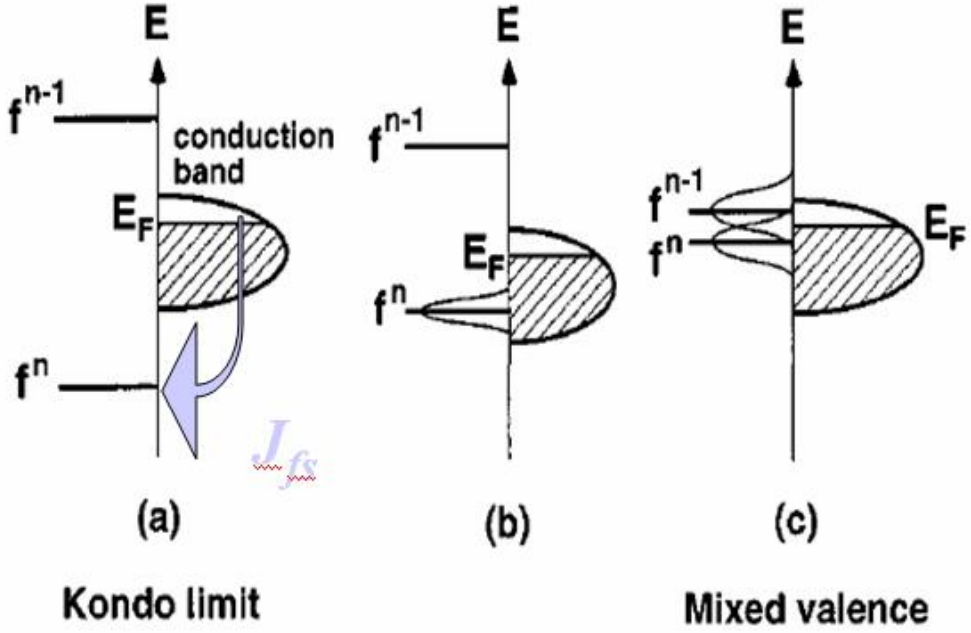
l	-3	-2	-1	0	+1	+2	+3
	↑						

Yb^{3+} - $4f^{13}$

l	-3	-2	-1	0	+1	+2	+3
	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑

spin/valence instability
due to desire
to fill/empty shell

Ce^{4+} - $4f^0$ and Yb^{2+} - $4f^{14}$
Non-magnetic ions
Pressure effects

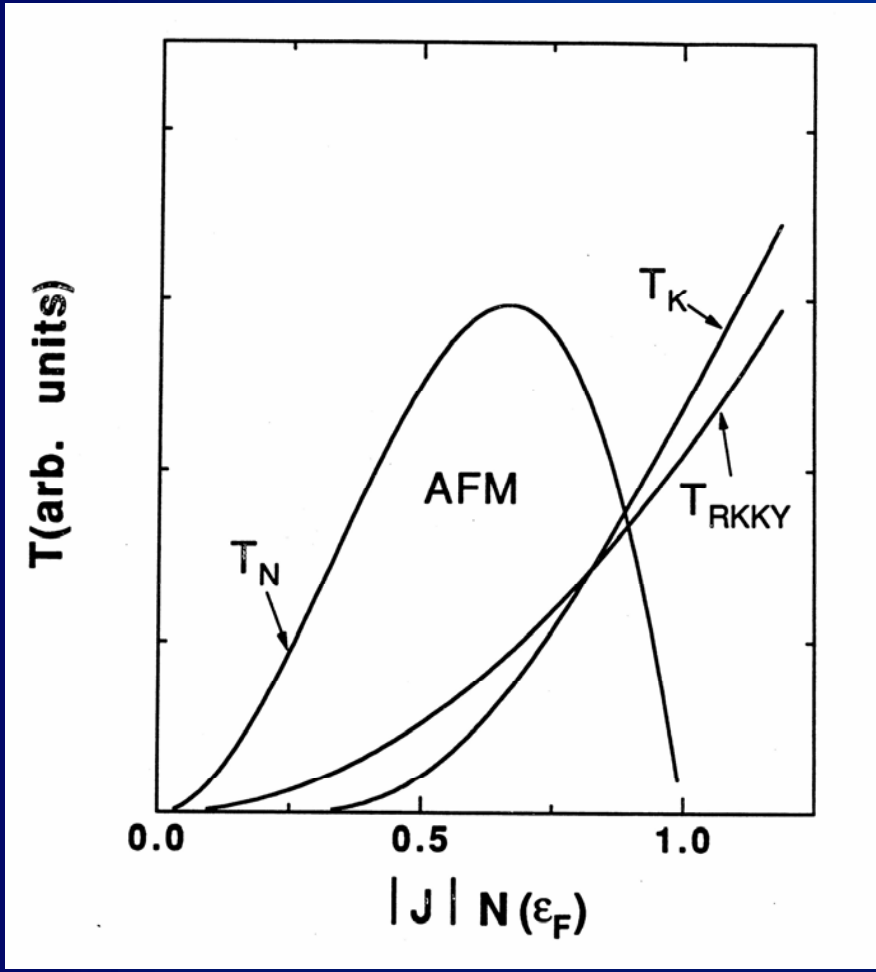


J_{fs} is strong and antiferromagnetic

f-s hybridization takes place

Tsunetsugu, Sigrist and Ueda, Rev. of Mod. Phys. 69, 809(1997).

Ground state competition



Competition between Kondo screening and magnetic order

- Tune J with doping or pressure
- Often find superconductivity where $T_N \rightarrow 0$: quantum critical point.

S. Doniach, in Valence Instabilities and Related Narrow Band Phenomena, ed. R.D. Parks (Plenum, New York, 1977) p. 169.

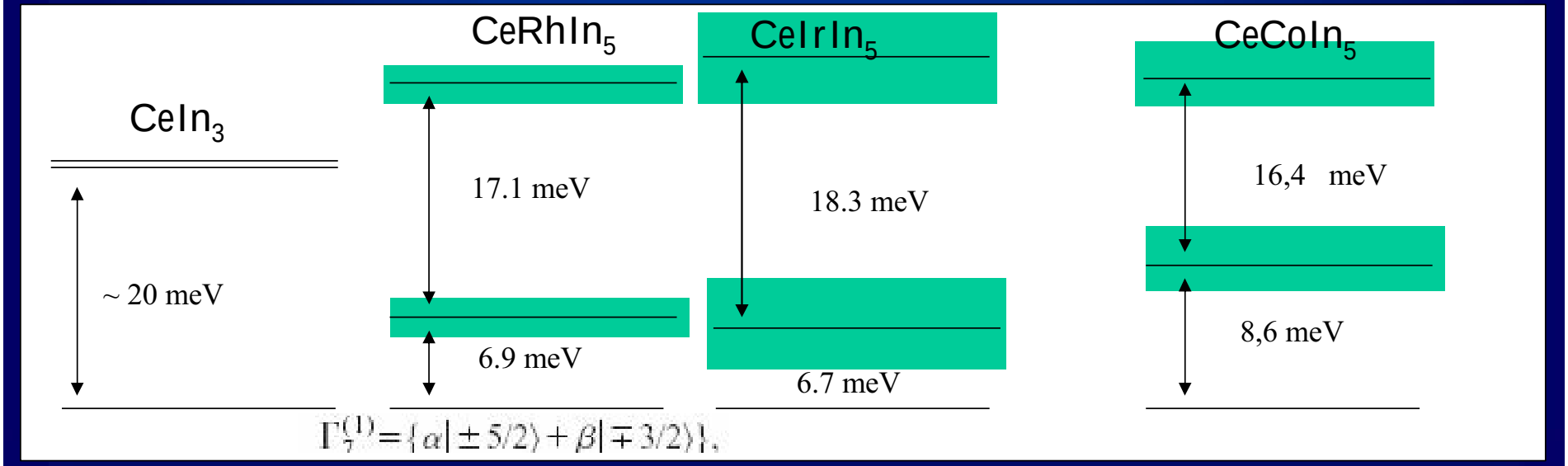
CEF effects on T_k

CEF effects in Ce-M-In_5:

Effective T_K in the presence of CEF:

$$T_K^{eff} = T_K^{J=5/2} / \Delta_{CEF}^2$$

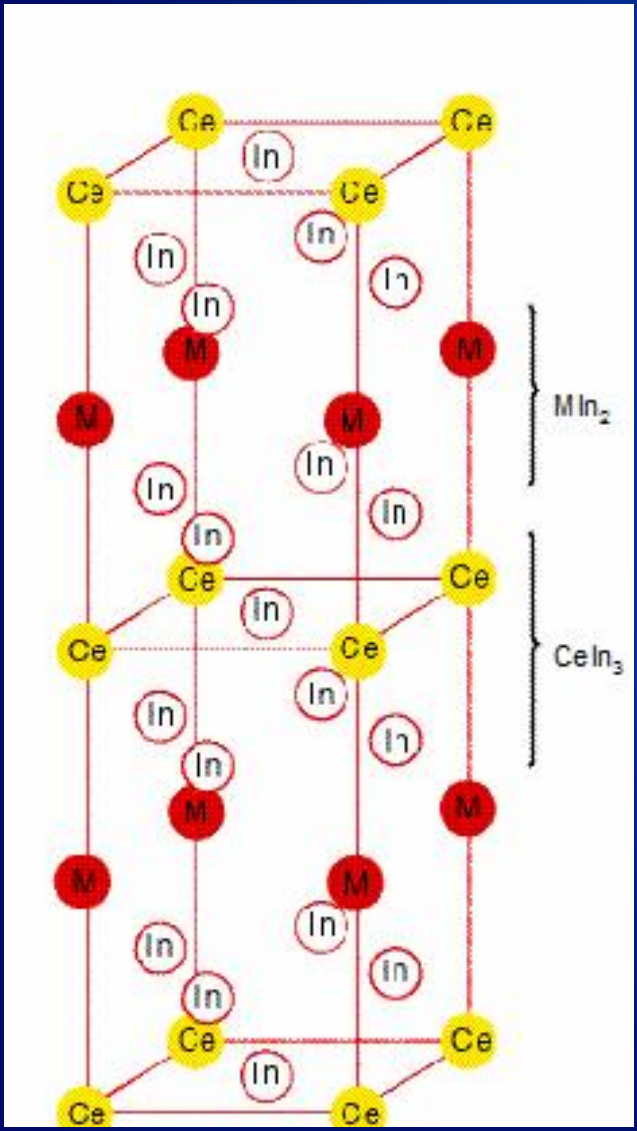
	$CeRhIn_5$	$CeCoIn_5$	$CeIrIn_5$
χ^2	0.69	0.52	0.83
B_2^0	-1.03	-.81	-1.2
B_4^0	0.044	0.058	0.06
B_4^4	0.122	0.139	0.12
β [NCA]	0.60 [0.6]	0.86 [0.95]	0.70 [0.71]
Γ_{ie}	2.3	6.6(4)	8.7
$E(\Gamma_7^2)$ [NCA]	6.9 [7]	8.6 [6.45]	6.7 [2]
$E(\Gamma_6)$ [NCA]	24 [25]	25 [21.44]	29 [22.56]
V	456	469	470
λ	35	40	70



H.-U. Desgranges, J. W. Rasul, PRB 36, 328 (1987).

A.D. Christianson et al PRB, 70 134505 (2004).

$CeMIn_5$ (M = Rh, Ir, Co) Family

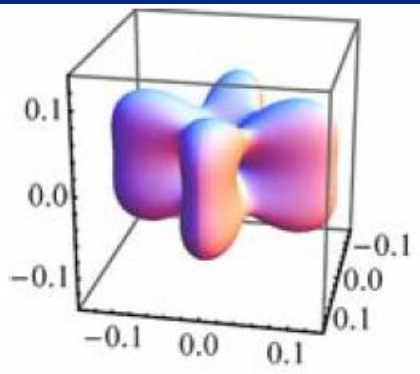


$$H_{CEF}^{tetrag} = B_2^0 O_2^0 + B_4^0 O_4^0 + B_6^0 O_6^0 + B_4^4 O_4^4 + B_6^4 O_6^4$$

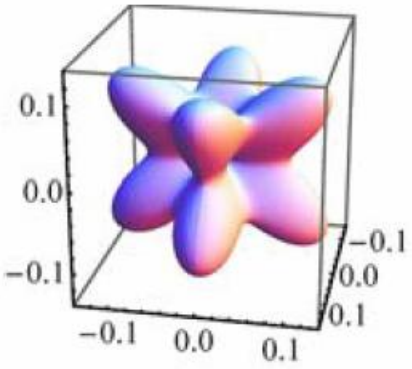
$$|2\rangle = \Gamma_6 = |\pm 1/2\rangle,$$

$$|1\rangle = \Gamma_7^1 = \beta|\pm 5/2\rangle - \alpha|\mp 3/2\rangle,$$

$$|0\rangle = \Gamma_7^2 = \alpha|\pm 5/2\rangle + \beta|\mp 3/2\rangle$$

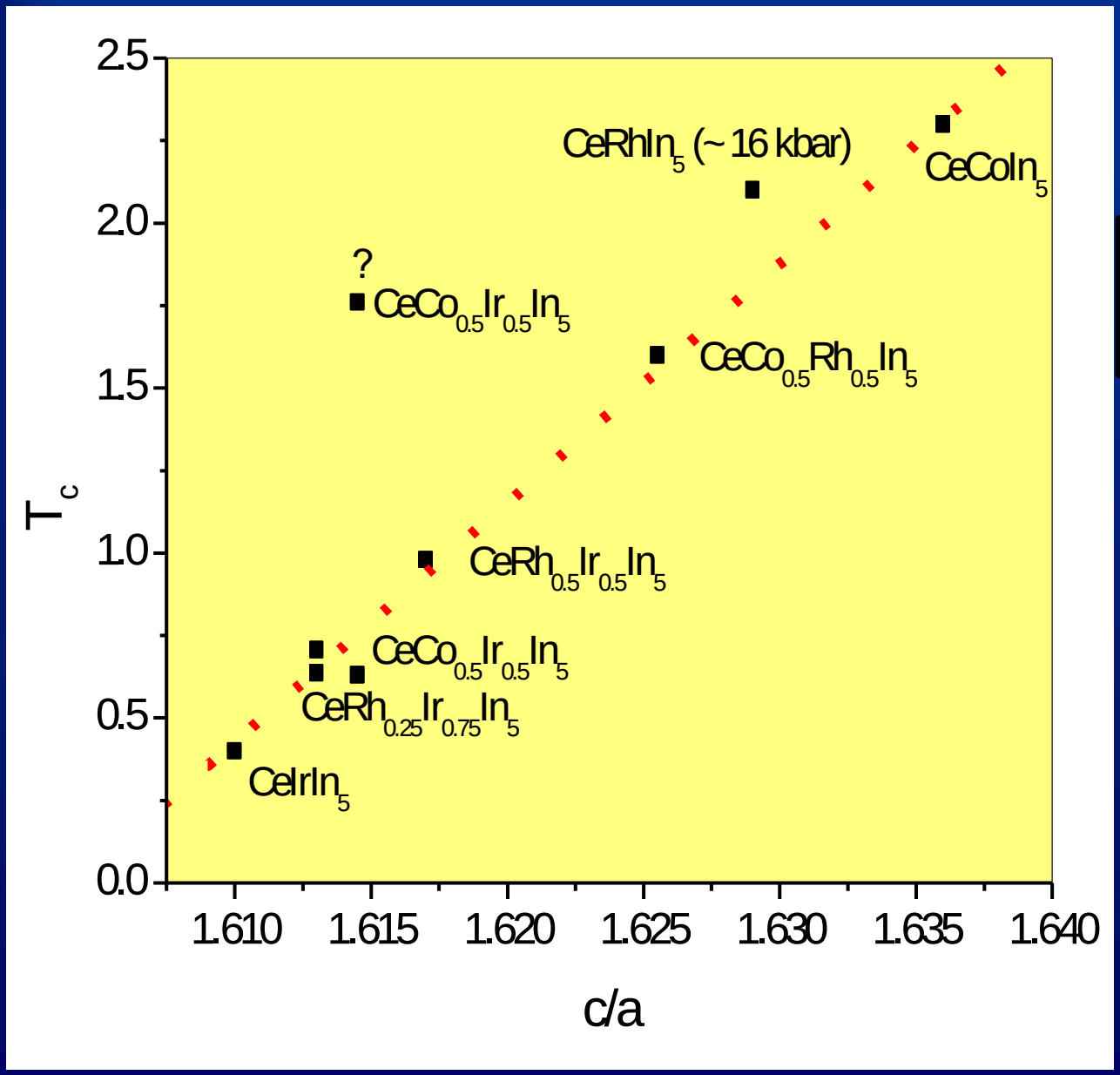


α=0.62



α=0.36

c/a as control parameter for T_c



Is there an intrisic parameter in this plot, which depends on c/a and determines T_C?

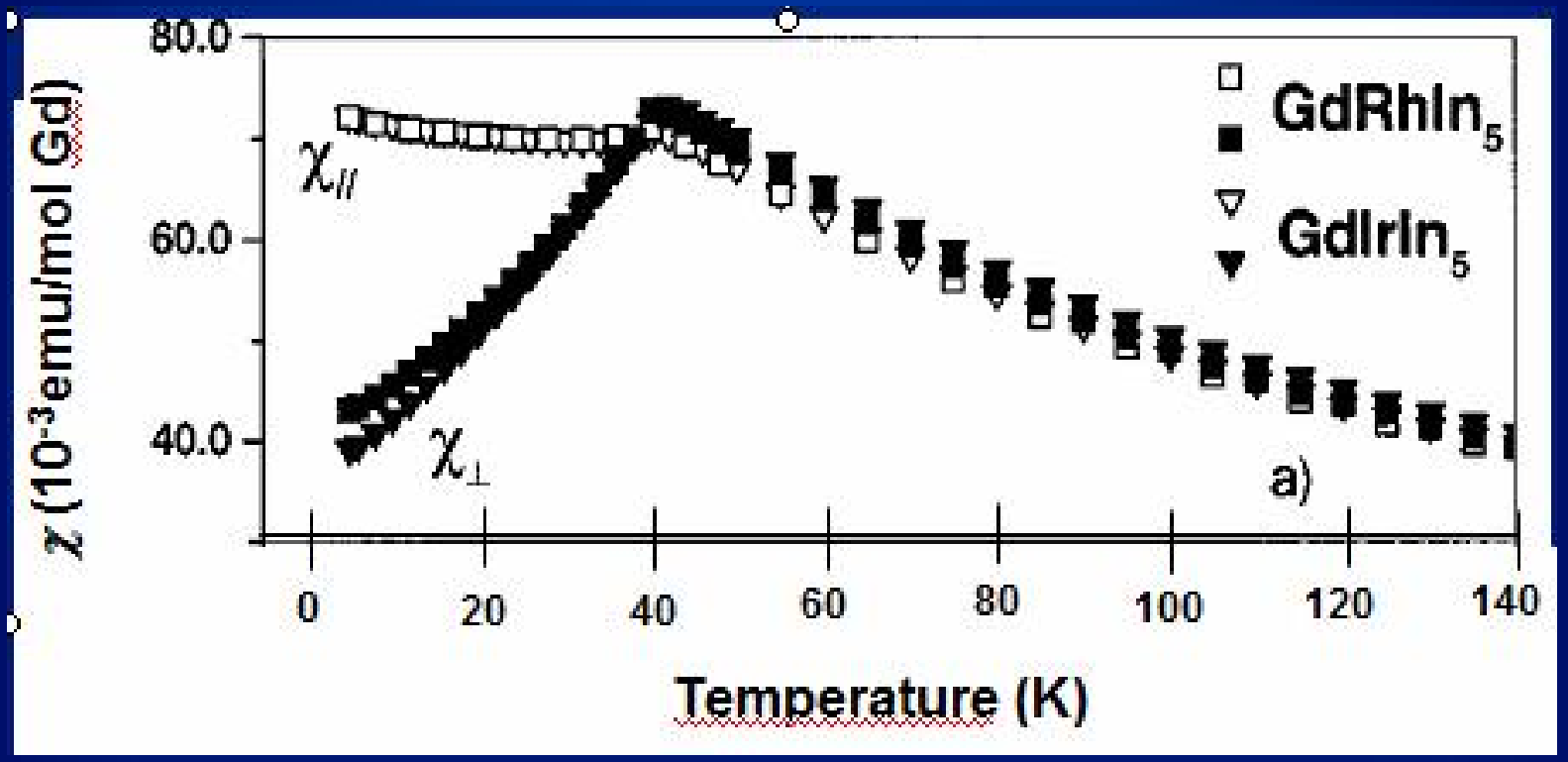
Tuning:

- J_{RKKY}
- T_K
- CEF

P.G. Pagliuso et al. PRB, 100503 (R) (2002); Physica B 312-313, 129 (2002).

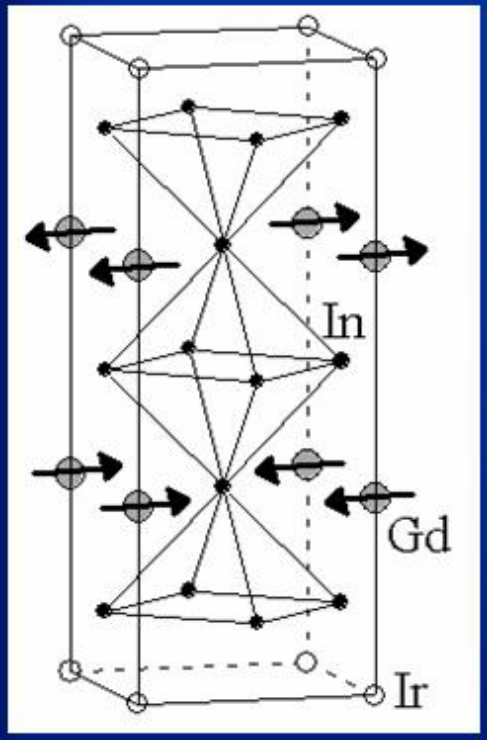
Tuning of J_{RKKY}?

Gd $4f^7$ → S=7/2, L=0

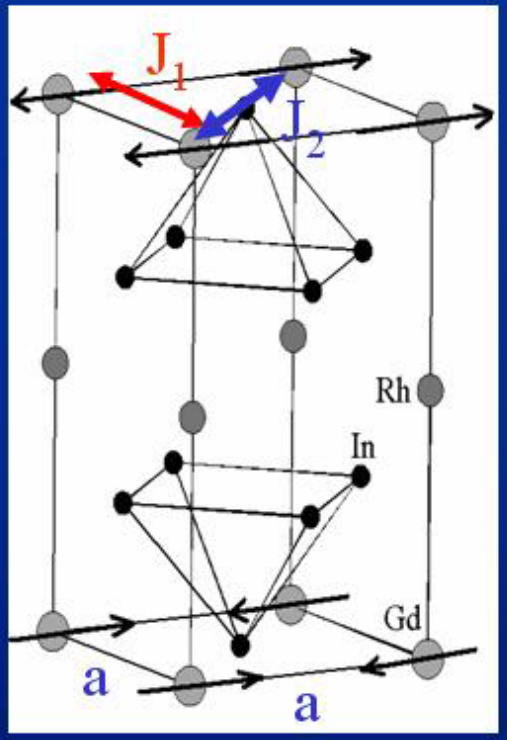


Pagliuso et al. PRB. 62, 12266 (2000); PRB (2001).

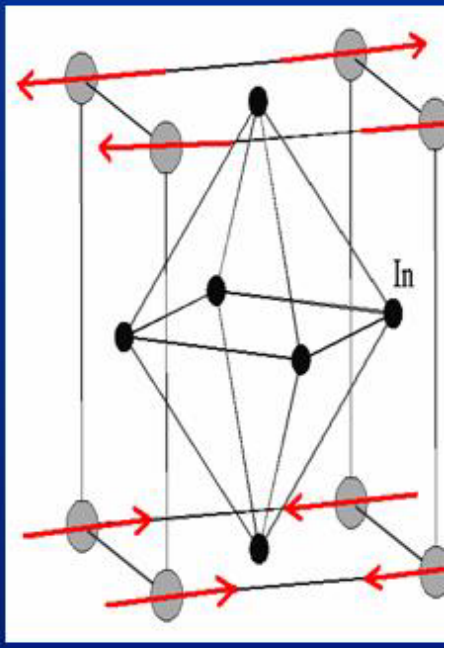
Tuning of J_{RKKY}?



2-1-8



1-1-5



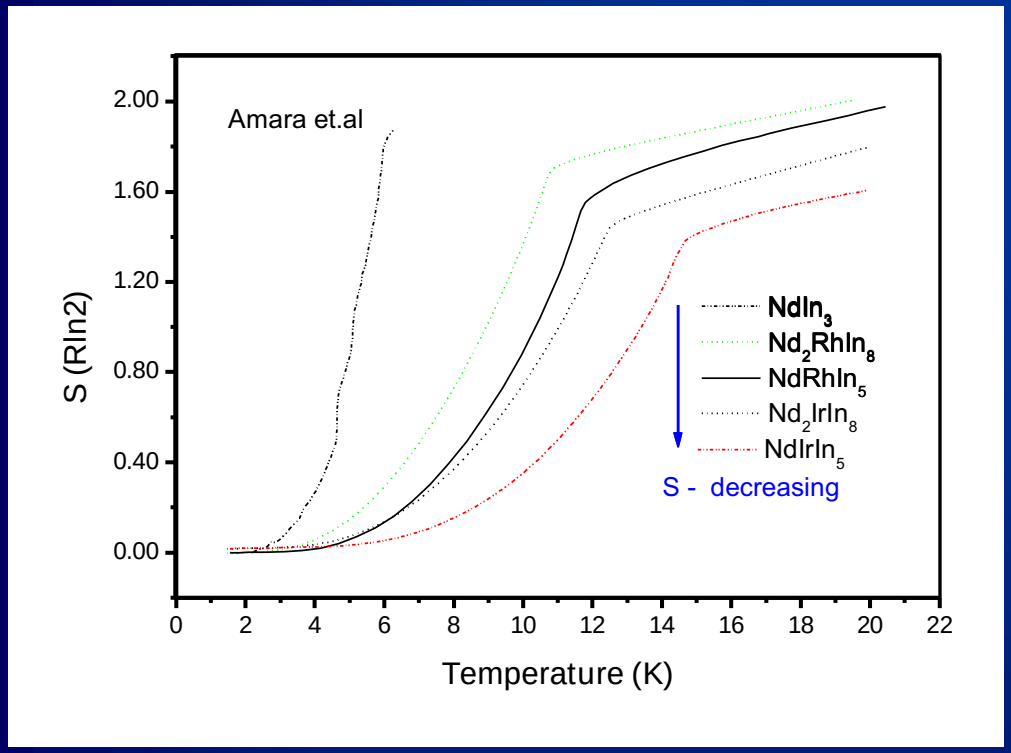
1-0-3

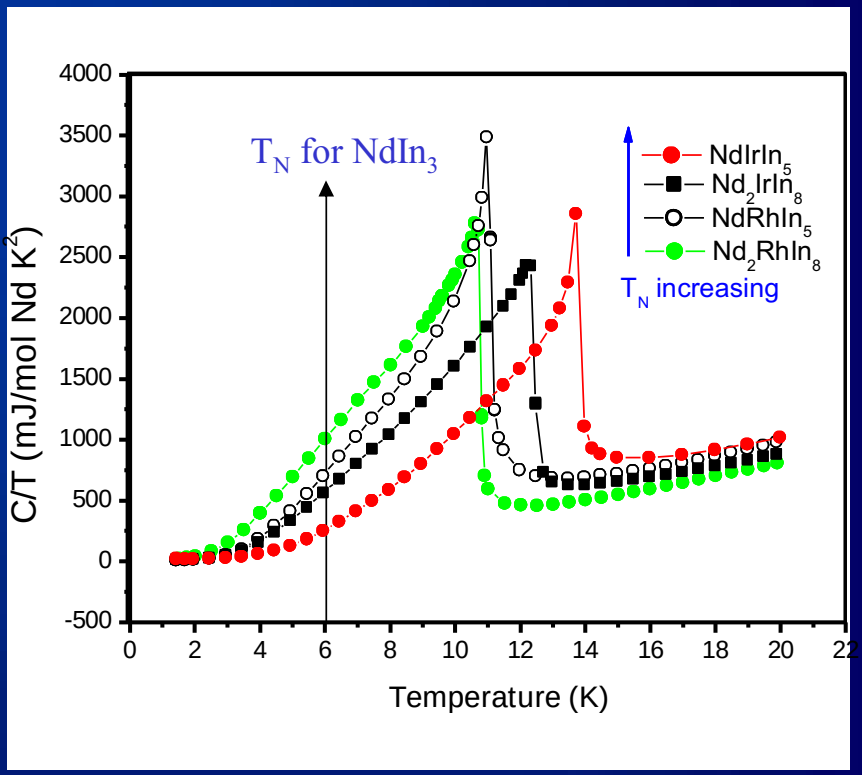
Same T_N and Magnetic Structures (ε = (1/2, 0,1/2) → same J_{RKKY}

θ_{CW} = 70 K and T_N = 40 K - $J_2 > J_1$
- frustrated first neighbor interaction

E. Granado, R. Lora Serr
PRB (2004) - PRB (20

Tuning the CEF?
Cp(T) and S(T) for Nd-based compounds

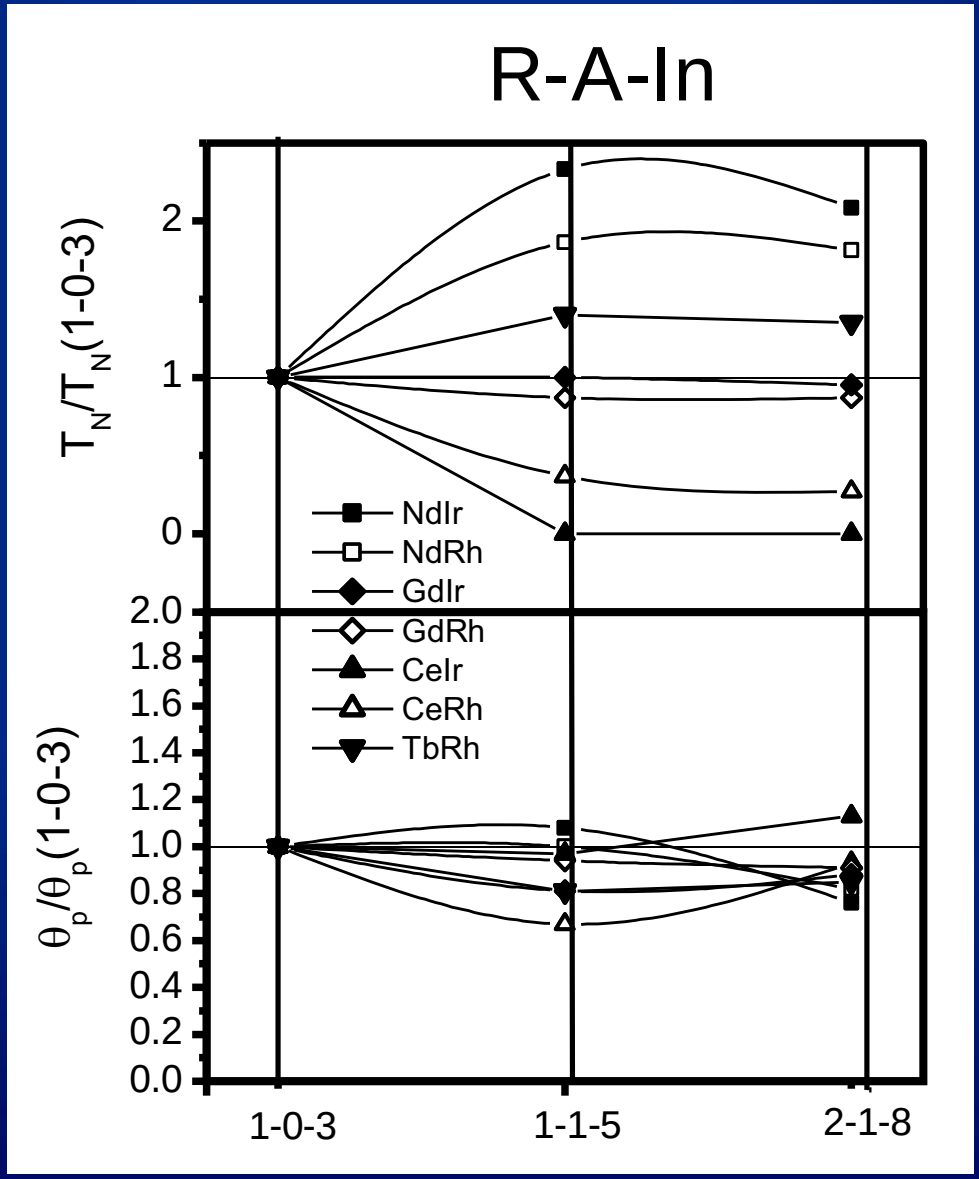




The larger Γ_8 CEF Splitting $\Rightarrow$ larger T_N

P.G. Pagliuso et al. Physical Review B. 62, 12266 (2000).

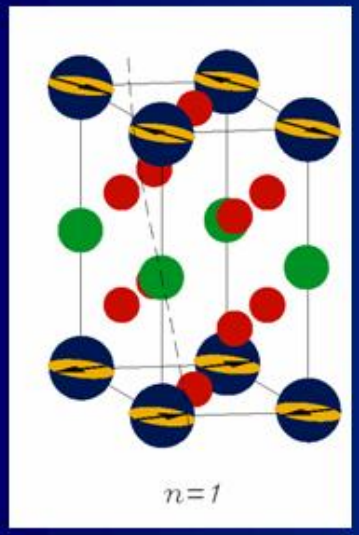
T_N evolution for $R_mA_nIn_{3m+2n}$(m = 1,2 ; n =0,1) (R = Nd, Tb, Gd, Sm)

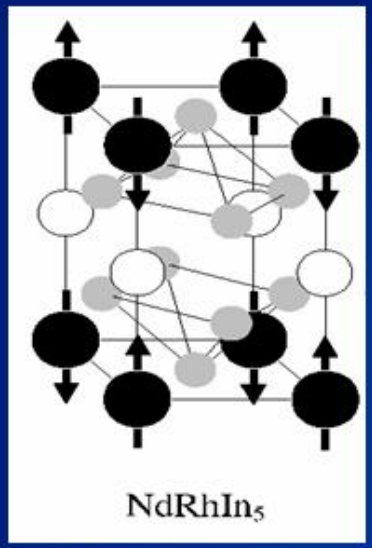


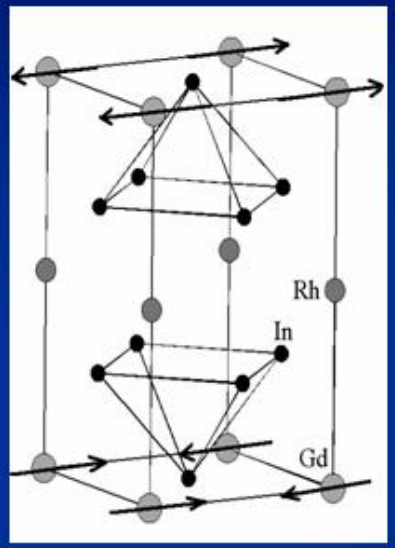
Pagliuso et al. PRB. 62, 12266 (2000); PRB (2001).

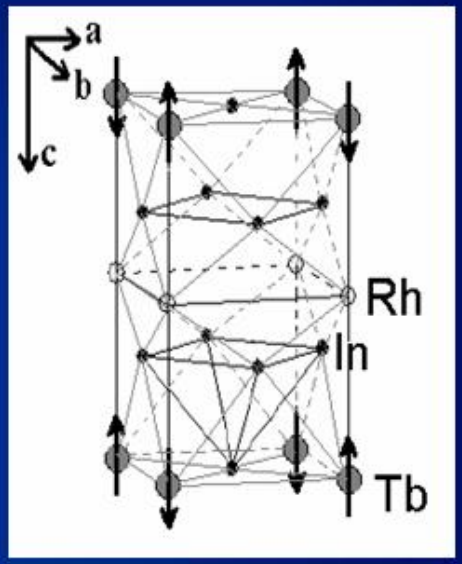
Summary of Experiments Facts

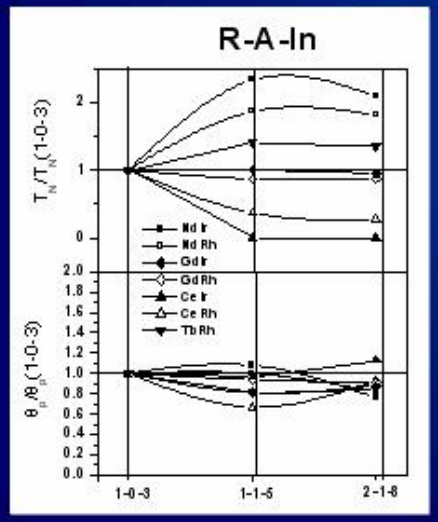
$CeRhIn_5$ $NdRhIn_5$ $GdRhIn_5$ $TbRhIn_5$

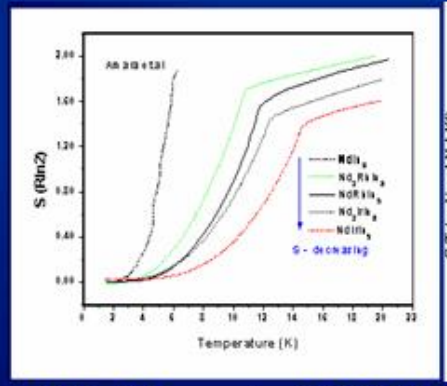


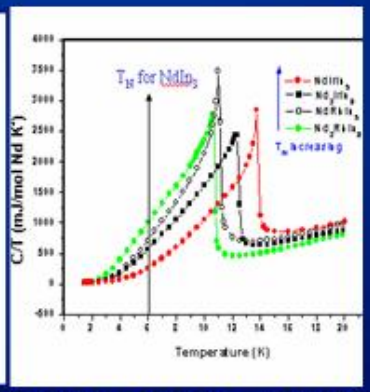


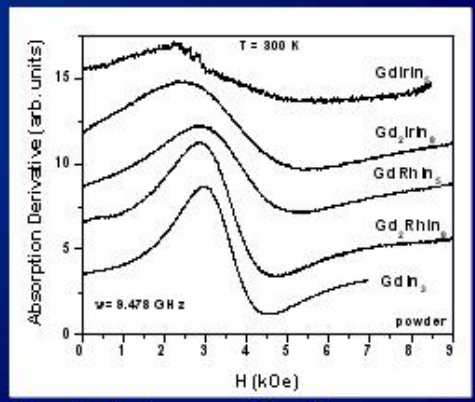












Wei Bao et al (PRB 2000, 2001, 2002) C. Adriano, R. Lora Serrano, C. Giles PRB (2007) - PRB (2008) – PRB (2009)

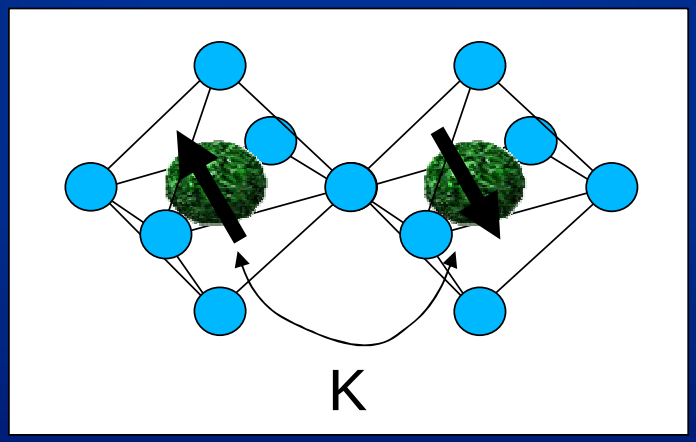
The model: Magnetic Interactions and Crystal Field Effects-

Simplest Magnetic Interaction:
(mimics RKKY interaction)

$$K\vec{J}_i \cdot \vec{J}_j$$

Crystal Field (CFE) Interaction:

$$B_{20}O_{20} + B_{40}O_{40} + B_{44}O_{44}$$



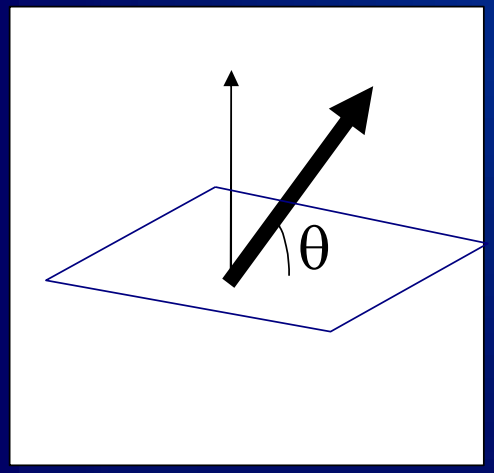
Can this simple model account for change in direction of the order moment along the series and for the T_N behavior?

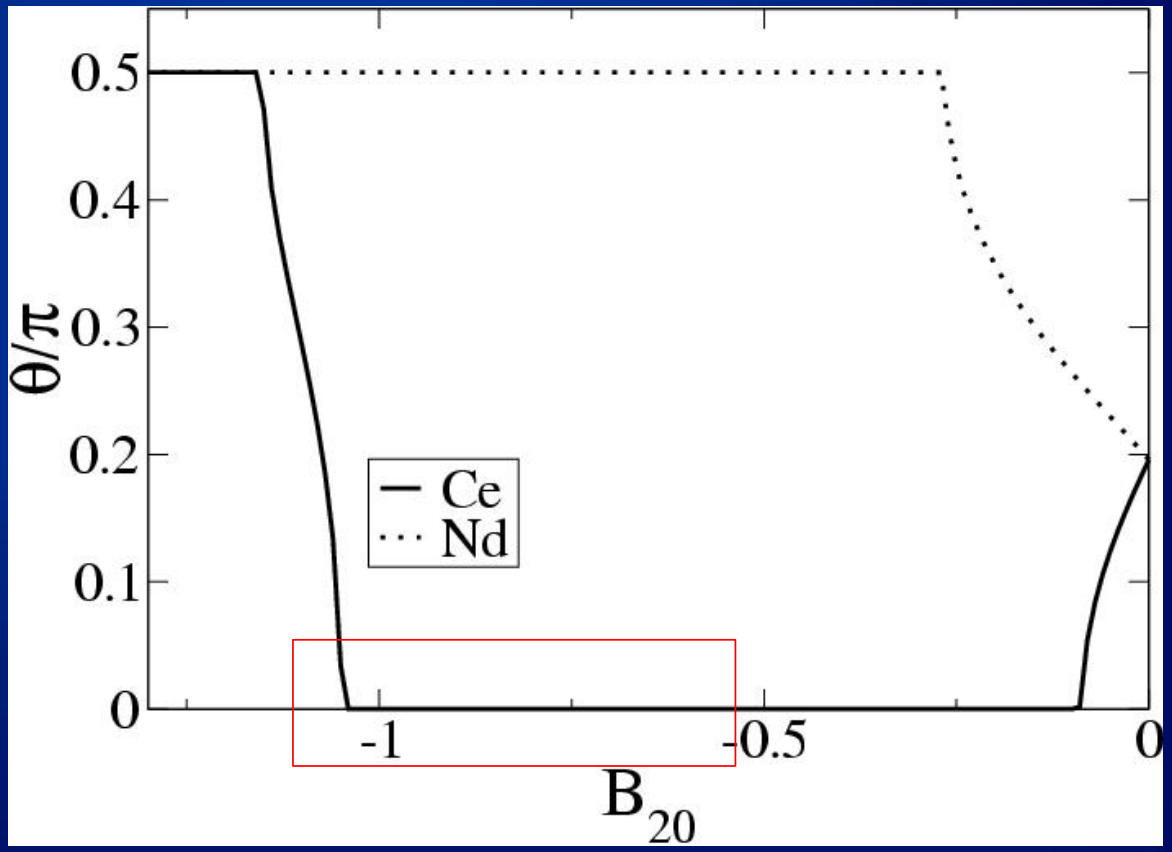
D. Garcia, E. Miranda, et al. JAP (2006)

Cristal Field Effects:

$$B_{20}O_{20} + B_{40}O_{40} + B_{44}O_{44}$$

Results for
(B44=5B40=0.25meV)



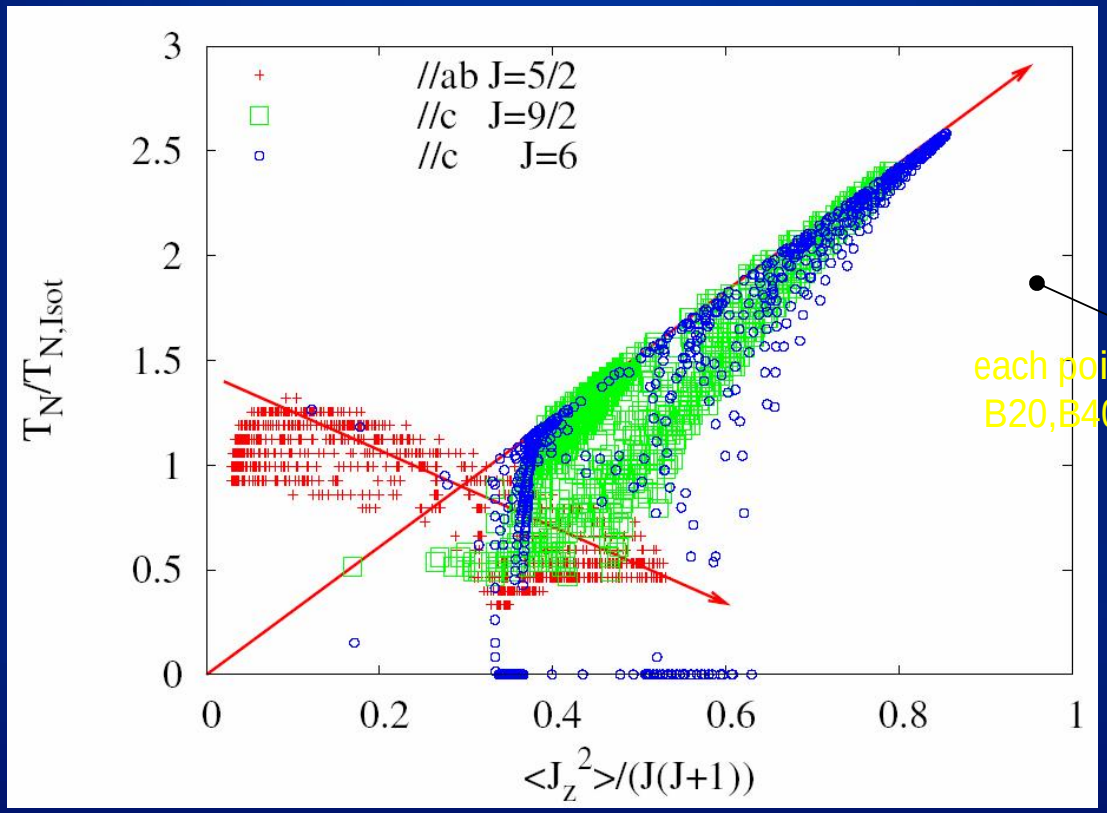


Interaction Effects on the order temperature T_N

Without CF: isotropic K

CEF enhanced order

CEF frustrated order



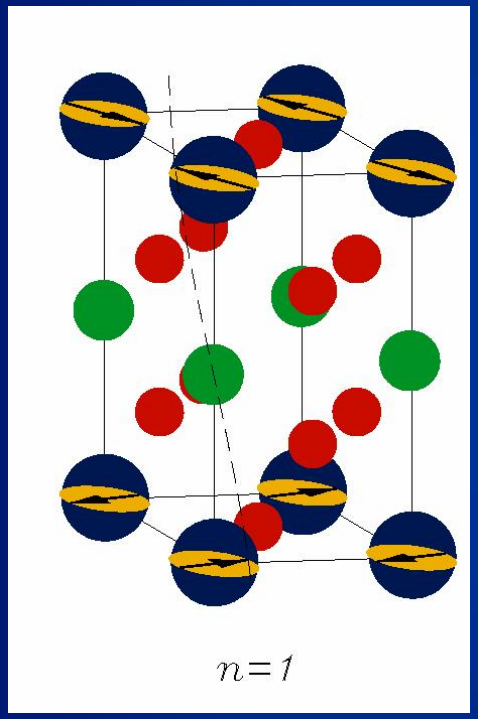
each point is obtained for specific B20,B40 and B44 parameters

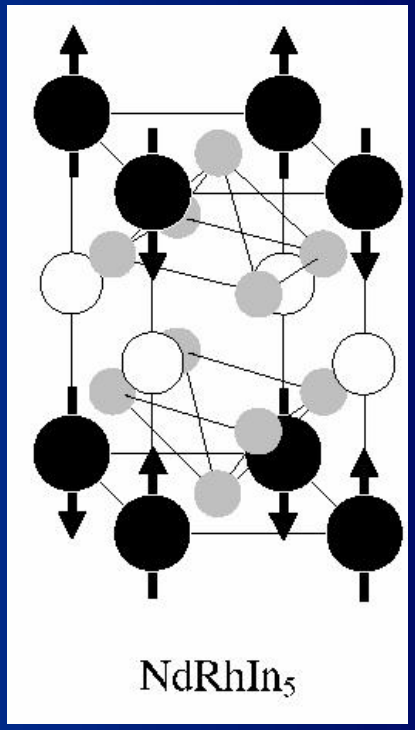
Diminished low-T c-susceptibility

Enhanced low-T c-susceptibility

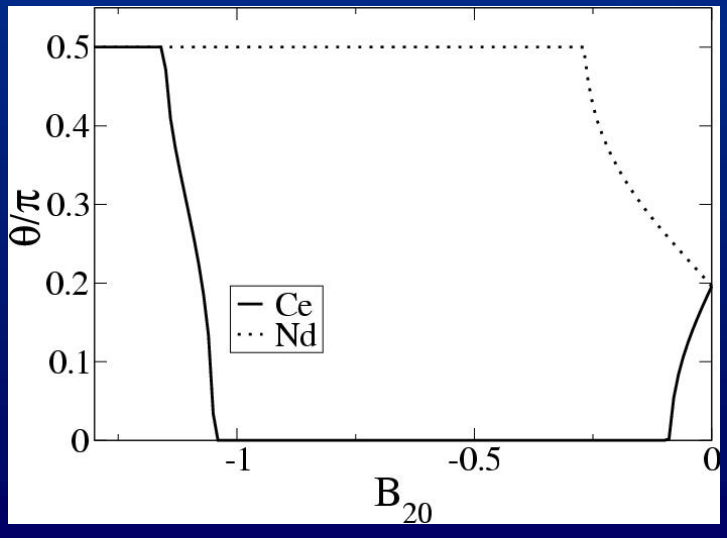
Isotropic susceptibility

R_nMIn_{3n+2} Magnetic Structures



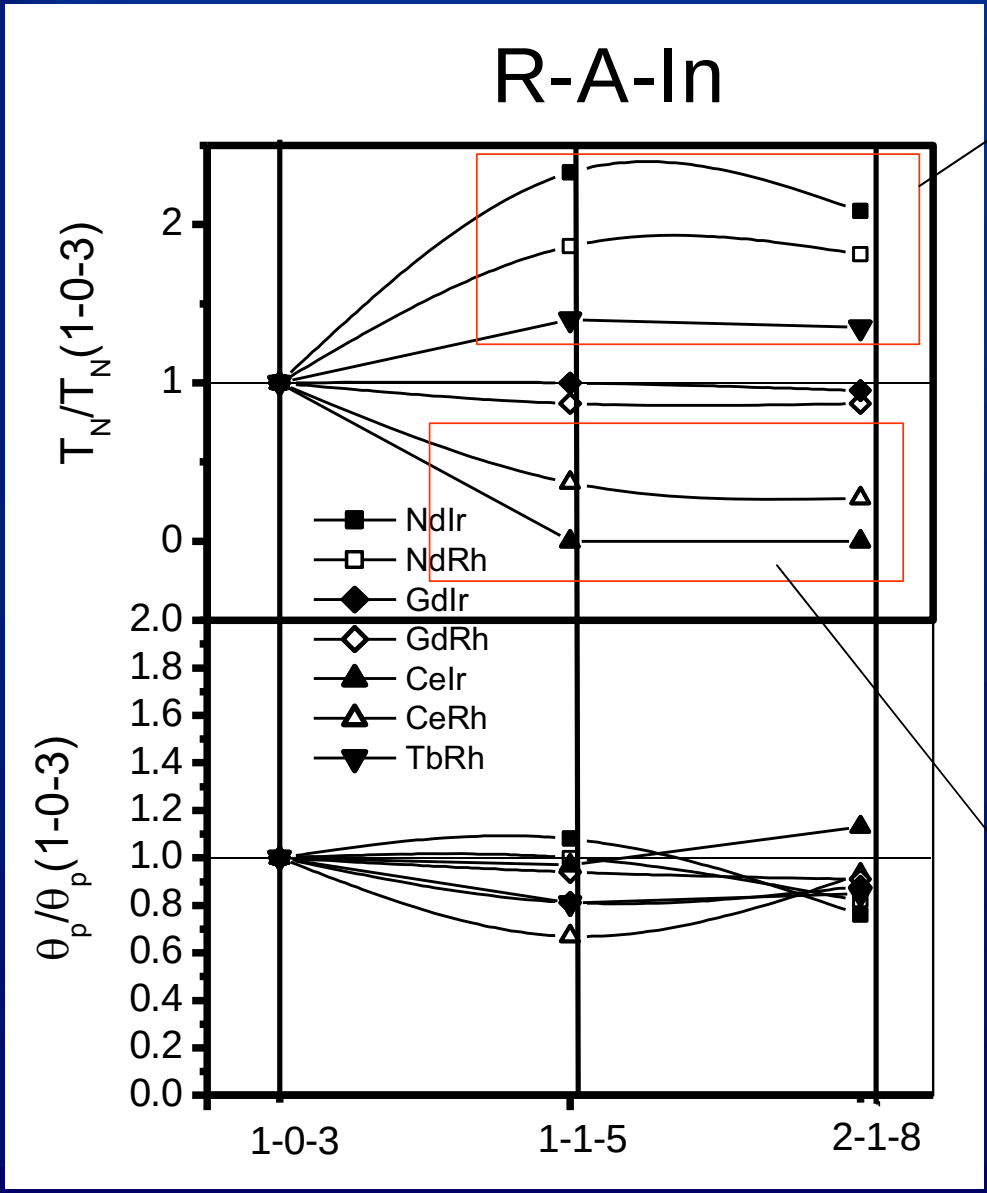


$CeRhIn_5$

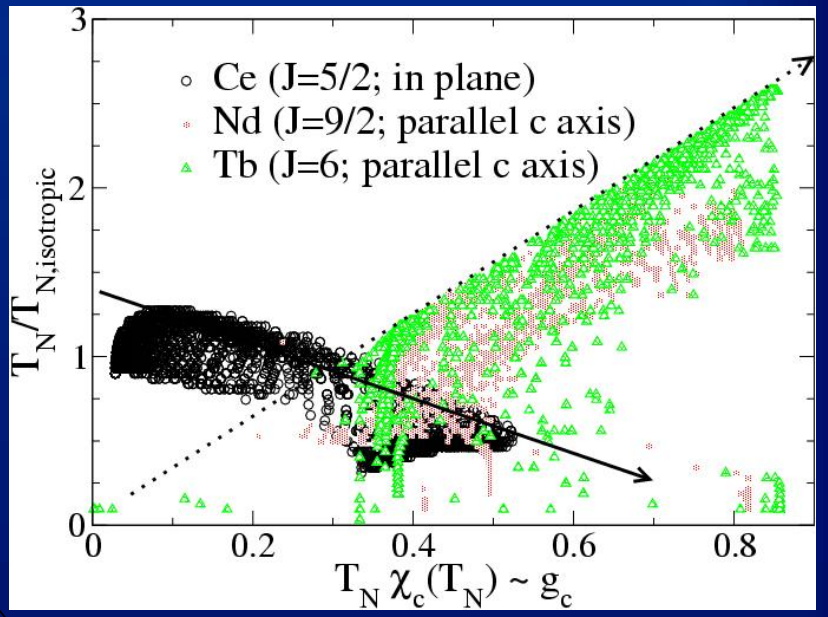


$NdRhIn_5$

T_N evolution for $R_mA_nIn_{3m+2n}$(m = 1,2 ; n =0,1)



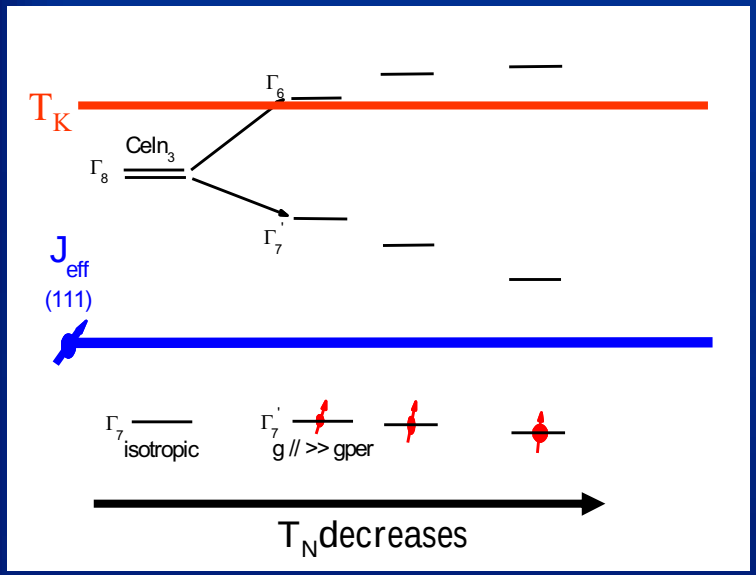
RE moments ordered along c-axis.



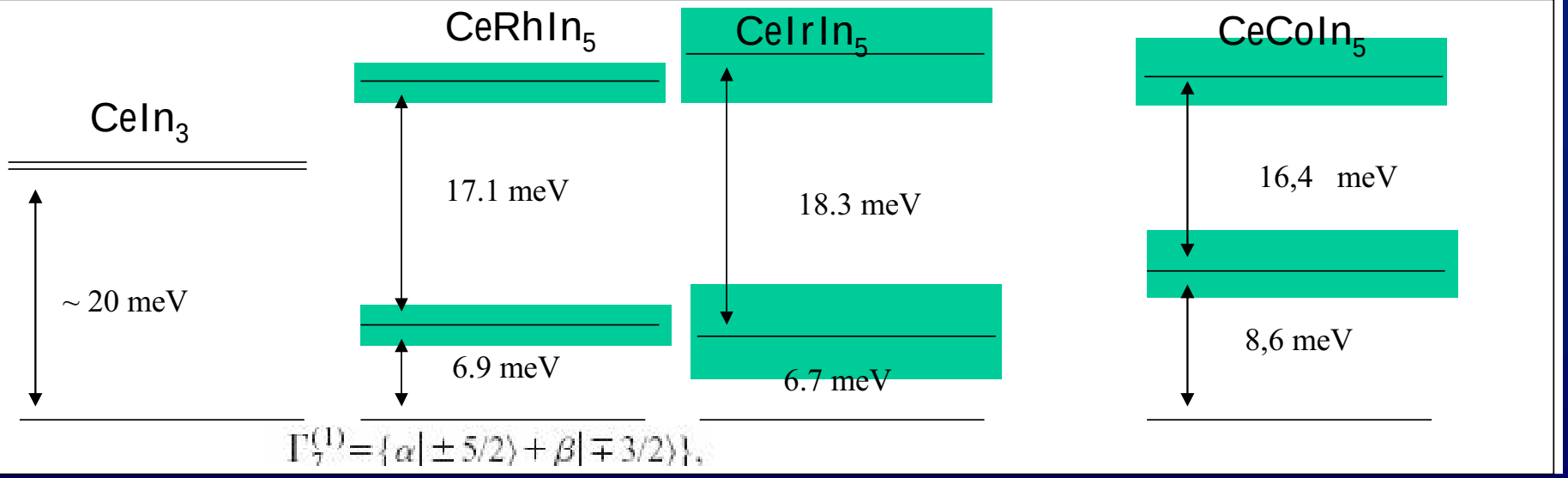
RE moments in the ab-plane.

P.G. Pagliuso et al. Physical Review B. 62, 12266 (2000).

Extrapolation of CEF trend to Ce-M-In



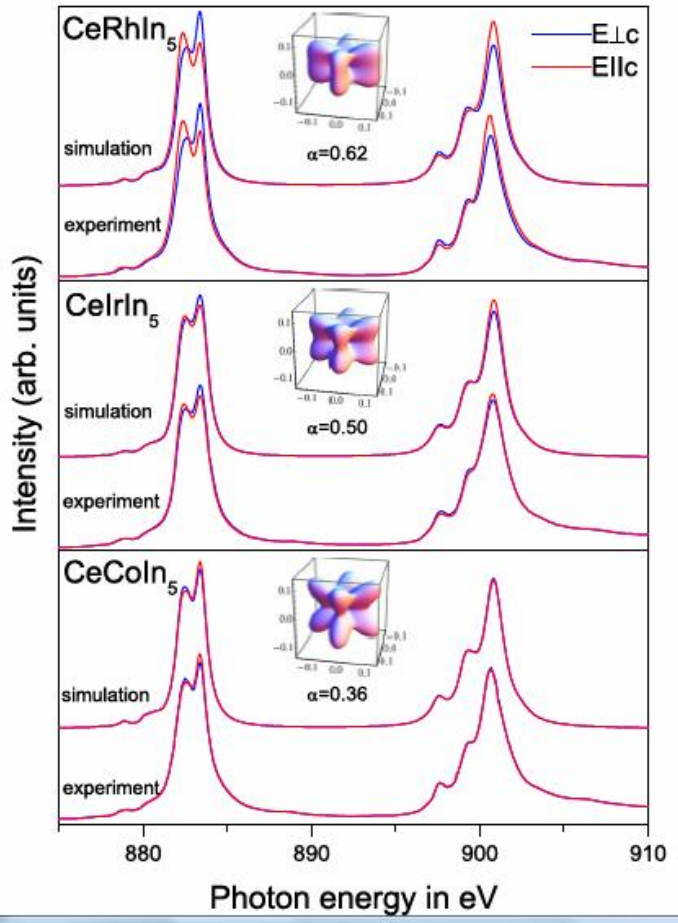
	$CeRhIn_5$	$CeCoIn_5$	$CeIrIn_5$
χ^2	0.69	0.52	0.83
B_2^0	-1.03	-.81	-1.2
B_4^0	0.044	0.058	0.06
B_4^4	0.122	0.139	0.12
β [NCA]	0.60 [0.6]	0.86 [0.95]	0.70 [0.71]
Γ_{ie}	2.3	6.6(4)	8.7
$E(\Gamma_7^2)$ [NCA]	6.9 [7]	8.6 [6.45]	6.7 [2]
$E(\Gamma_6)$ [NCA]	24 [25]	25 [21.44]	29 [22.56]
V	456	469	470
λ	35	40	70

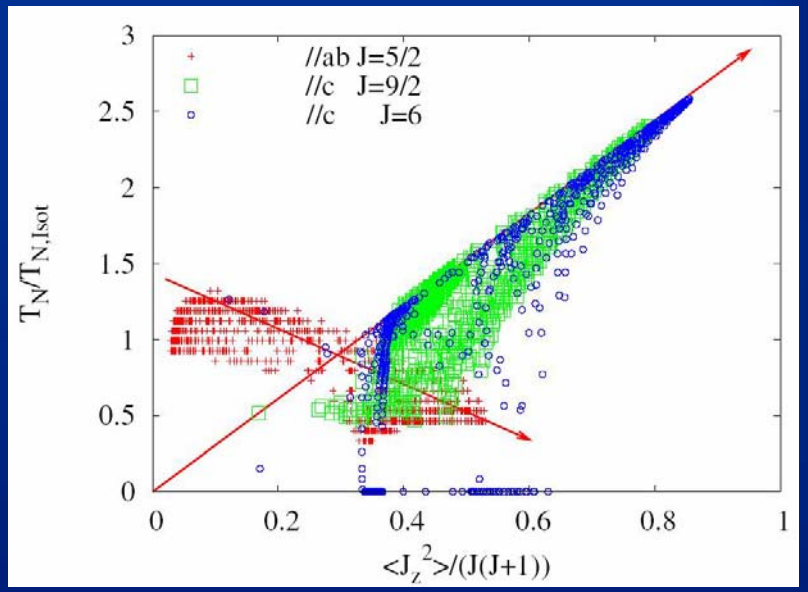


A.D. Christianson et al PRB (2004).

INS and XAS CEF study in Ce-M-In

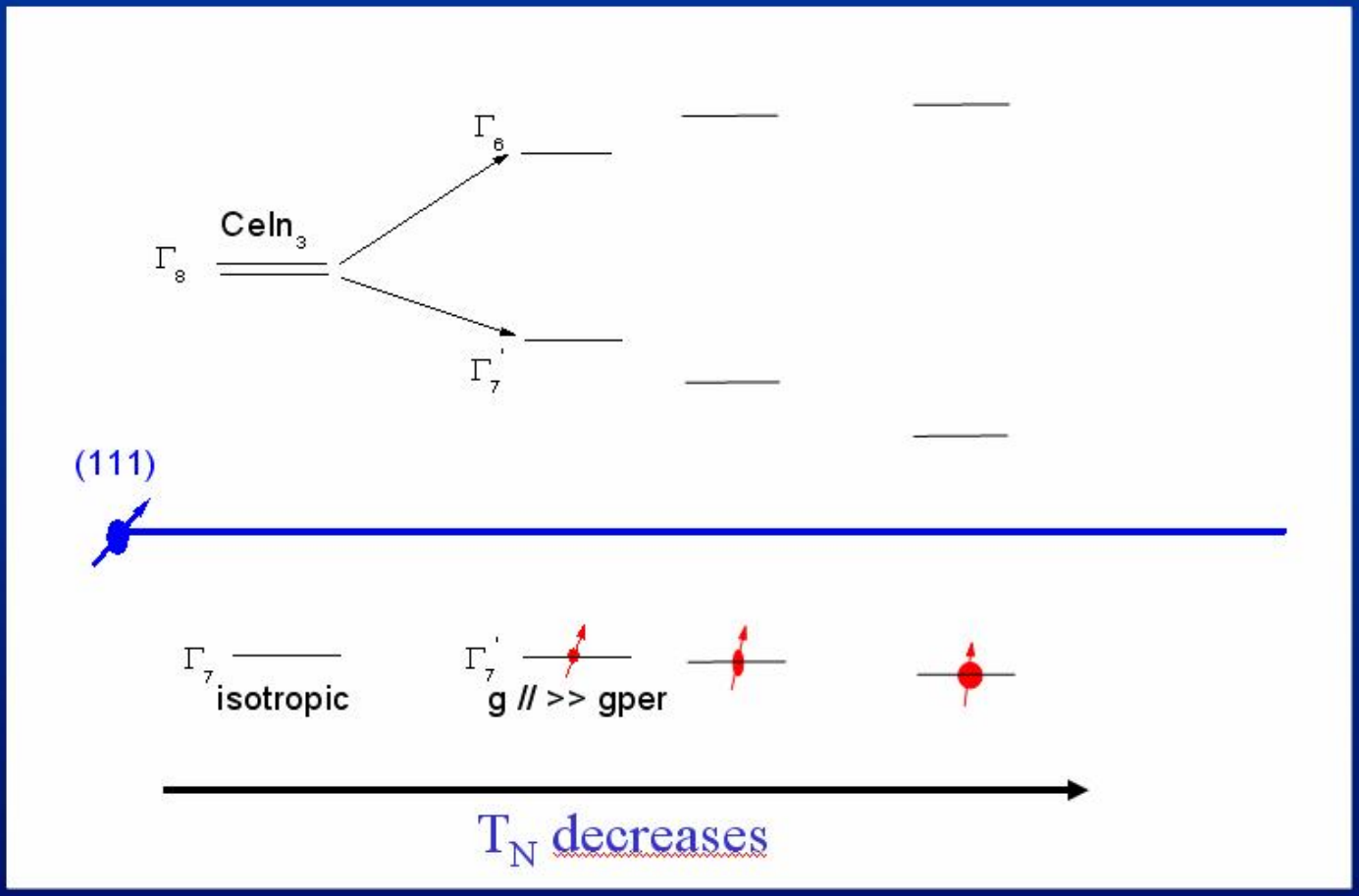
T. Willers et al. PHYSICAL REVIEW B **81**, 195114 (2010)





(meV)	$CeRhIn_5$	$CeIrIn_5$	$CeCoIn_5$	Instrument (meV)	$CeAu_2Si_2$ (Refs. 15 and 36)
$\Gamma_{qu}/2$ @ 8 K	1.2 ± 0.2			IN6 3.1	0.13
$\Gamma_{qu}/2$ @ 75 K	1.7 ± 0.2	2.7 ± 0.5	3.9 ± 0.5	IN6 3.1	0.43
E_1	7.0 ± 0.5	5.2 ± 1.0	6.8 ± 1.0	HET 20	16.5
E_2	24.7 ± 1.0	29.4 ± 1.5	25.0 ± 1.5	HET 60	21.0
$\Gamma^1_{in}/2$ @ 5 K	1.6 ± 0.5	3.0 ± 0.5	4.8 ± 0.8	HET 20/60	
$\Gamma^2_{in}/2$ @ 5 K	1.8 ± 0.5	3.4 ± 0.8	4.7 ± 0.8	HET 60	
$\Gamma^1_{in}/2$ @ 75 K	2.5 ± 0.5	3.7 ± 0.5	4.4 ± 0.8	IN6 3.1	
B_{20}	−0.928	−1.197	−0.856		
B_{40}	0.052	0.069	0.063		
$\lvert B_{44}\rvert$	0.128	0.088	0.089		

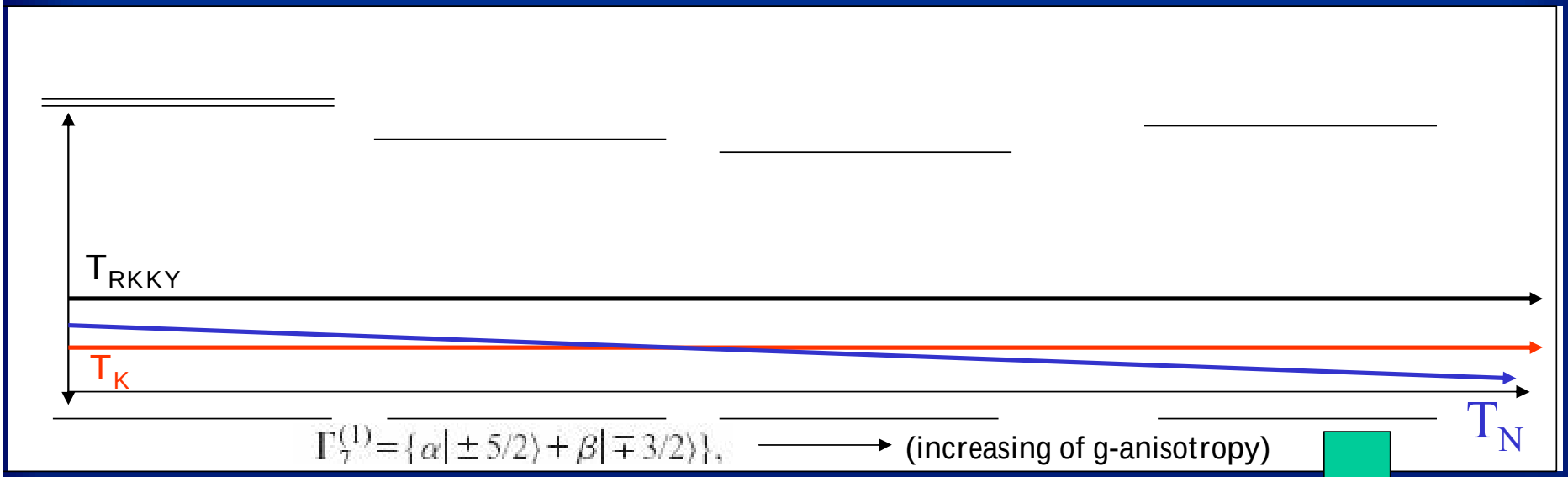
Extrapolation of CEF trend to Ce-M-In



$CeIn_3$ – $CeRhIn_5$ – Ce_2RhIn_8 – Ce_2IrIn_8 – $CeIrIn_5$ – Ce_2CoIn_8 - $CeCoIn_5$

$T_N = 10$ K $T_N = 3.8$ K $T_N = 2.8$ K $T_s \sim 0.8$ K $T_c = 0.4$ K $T_C \sim 1{,}6$ K $T_C = 2.3$ K

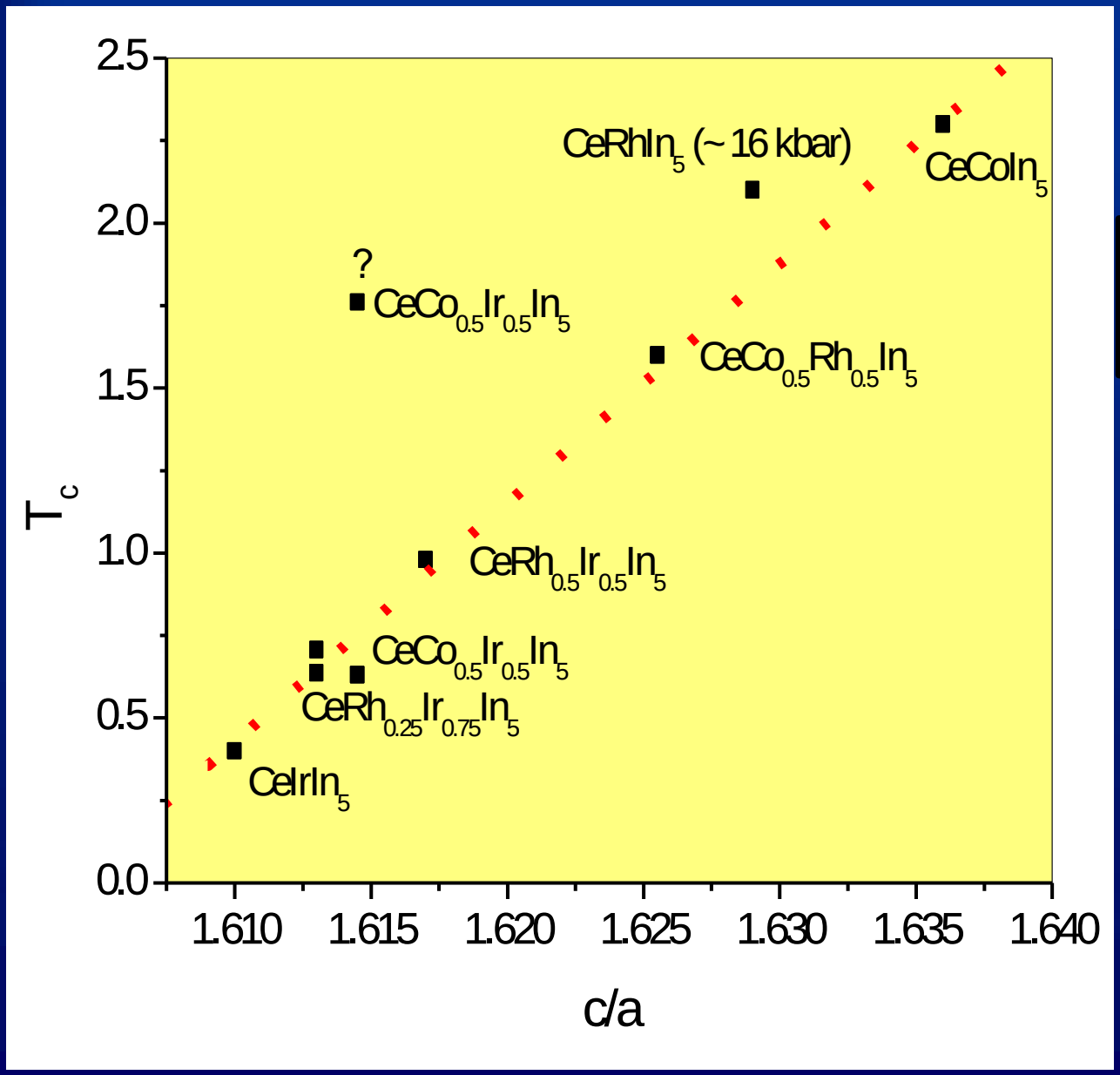
Extrapolation of CEF trend to Ce-based materials



Frustrated local moments + hybridization

Strong magnetic-fluctuations??

c/a as control parameter for T_c



Is there an intrisic parameter in this plot, which depends on c/a and determines T_C?

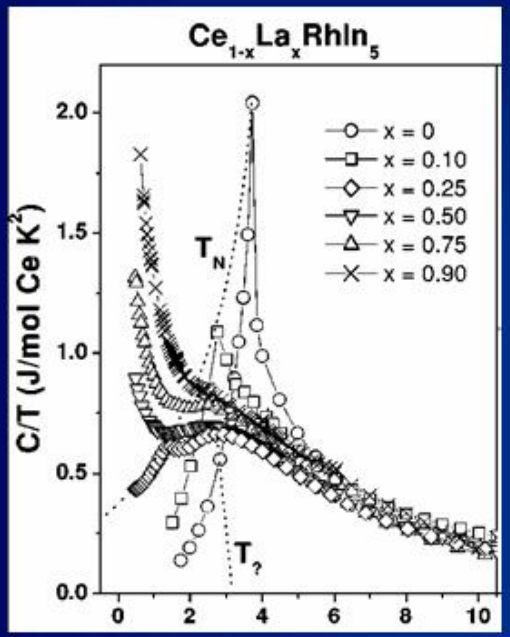
Tuning:

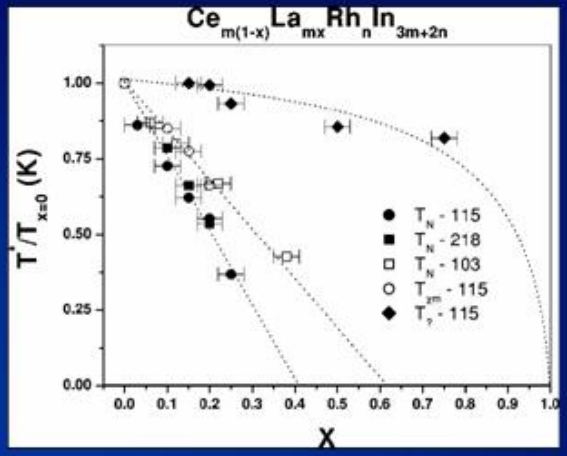
- J_{RKKY}
- T_K
- CEF

P.G. Pagliuso et al. PRB, 100503 (R) (2002); Physica B 312-313, 129 (2002).

La- and Sn-doped $CeRhIn_5$

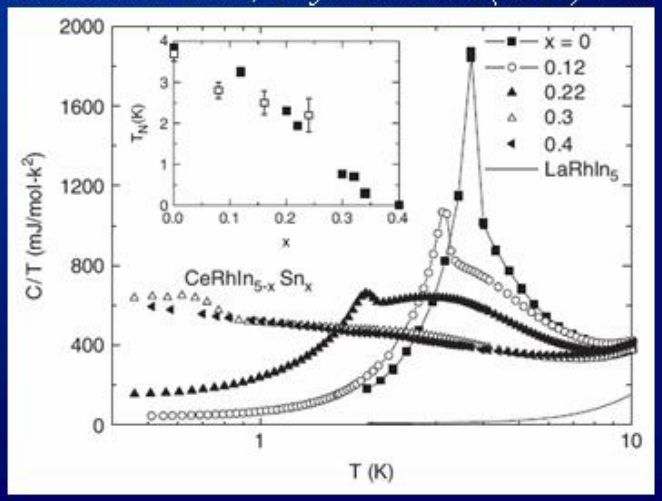
P. G. Pagliuso et al., Phys. Rev. B (2002) 054433.





- AFM is smoothly suppressed by La-doping;
- $T_N \rightarrow 0$ at $x_c \approx 0.40$;
- No SC is found around $x_c \approx 0.40$.

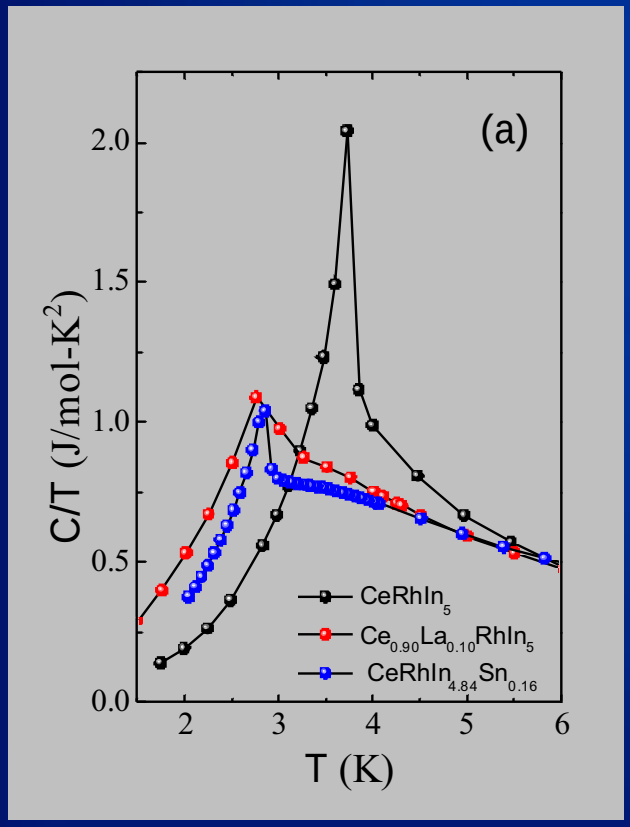
E. D. Bauer et al., Physica B 378 (2006) 142

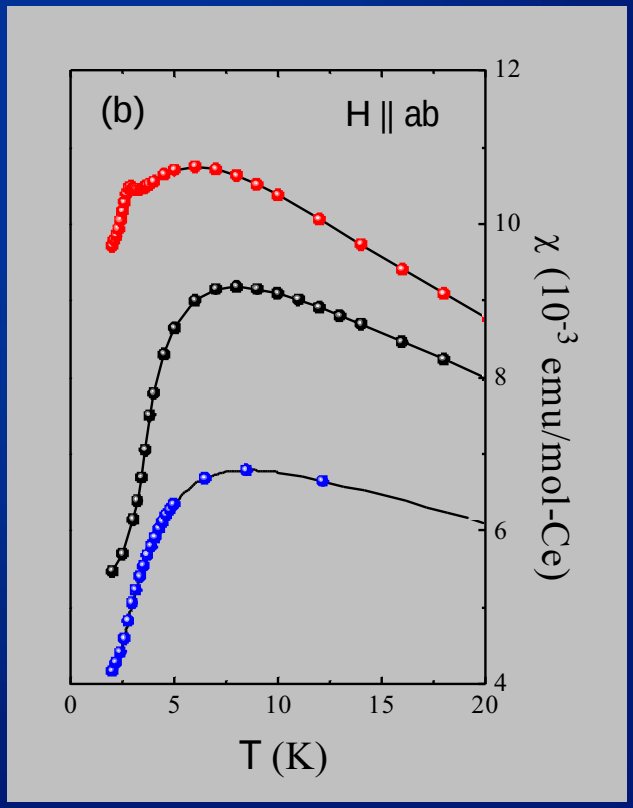


- AFM is suppressed by Sn-doping;
- $T_N \rightarrow 0$ at $x_c \approx 0.35$;
- No SC is found around $x_c \approx 0.35 <$ (10%)

La- and Sn-doped $CeRhIn_5$

- We have carefully chosen two specific compositions, $Ce_{0.90}La_{0.10}RhIn_5$ and $CeRhIn_{4.84}Sn_{0.16}$.



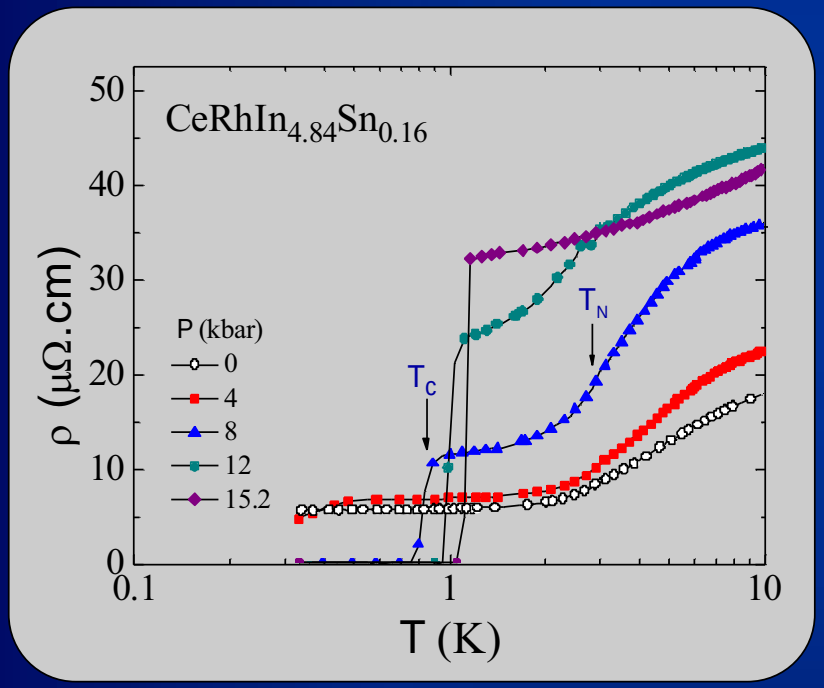


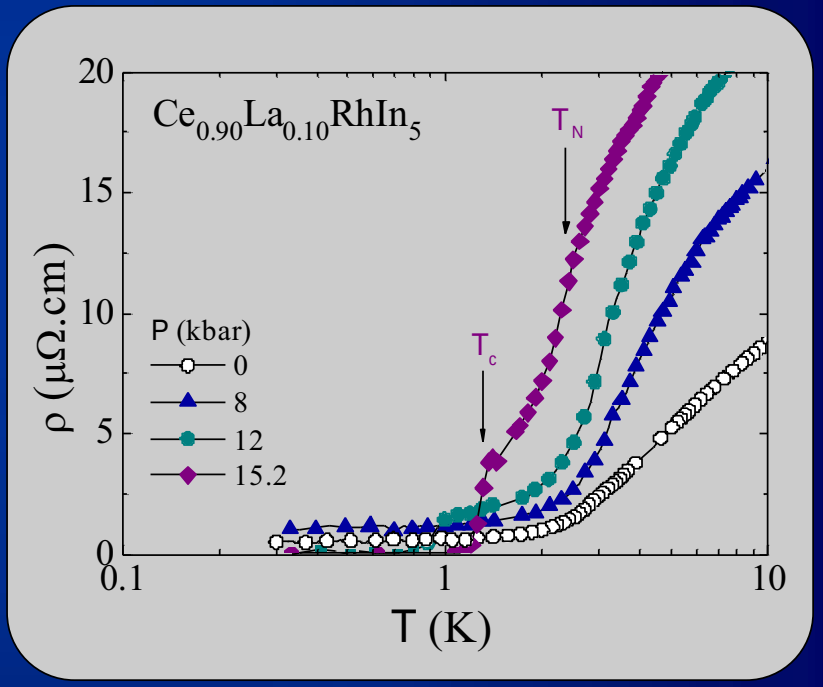
The ordering temperature T_N = 3.8 K of undoped $CeRhIn_5$ was suppressed to the same $T_N \approx 2.8$ K for both La and Sn doping in the studied concentrations.

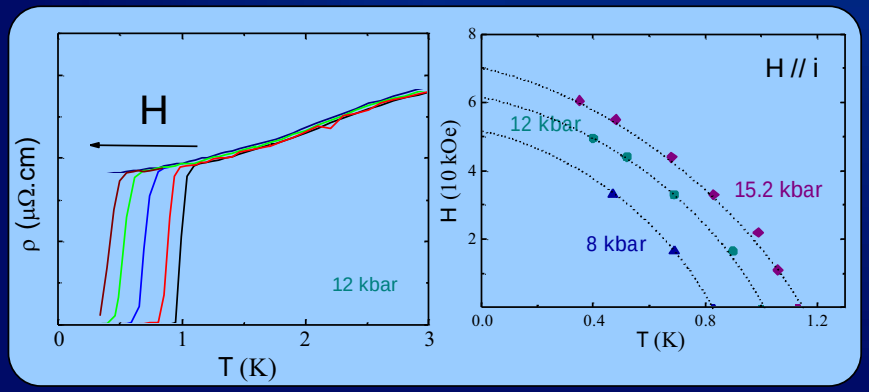
L. Mendonça-Ferreira et al. PRL 101, 017005 (2008)

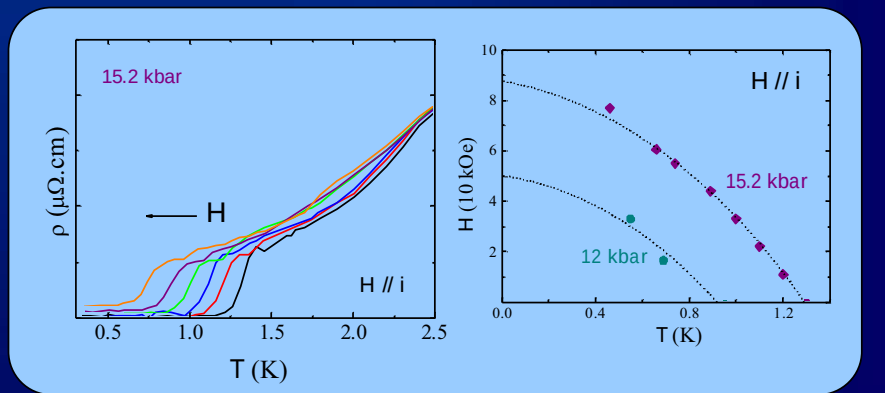
La- and Sn-doped $CeRhIn_5$

AC electrical resistivity under pressure



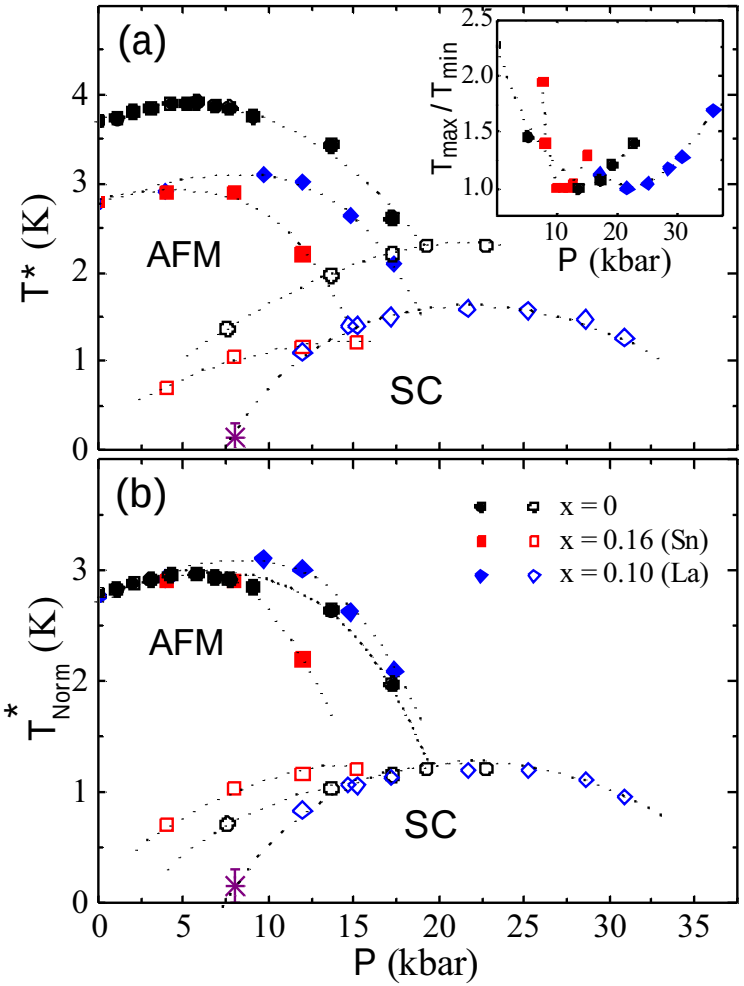






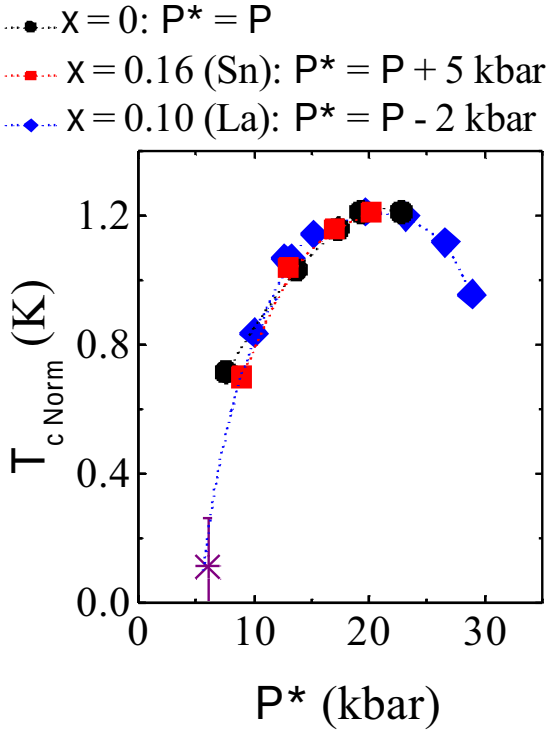
La- and Sn-doped $CeRhIn_5$

P – T phase diagram



- For the two doped samples, T_{max}, T_N and T_c follow the same qualitative evolution as a function of pressure found for pure $CeRhIn_5$.

- However, by comparing the P – T phase diagram of the three samples, one sees that the La-doping shifts the P – T phase diagram of $CeRhIn_5$ to higher pressure while the Sn-doping does exactly the opposite.



As the two doped samples have the same T_N at ambient pressure and similar strength of the Ce-Ce inter-site magnetic coupling, it is the strength of the intra-site Kondo-coupling which mainly determines the pressure evolution of the $CeRhIn_5$ ground state.

The suppression of the magnetism has to be associated with an increasing of T_K and a consequent crossover between localized and itinerant behavior of the Ce 4f.

If a given control parameter tunes T_N to zero by a local mechanism, such as dilution or magnetic frustration which are not necessarily associated with an increase of the Kondo-coupling, this tuning might in fact inhibit SC:

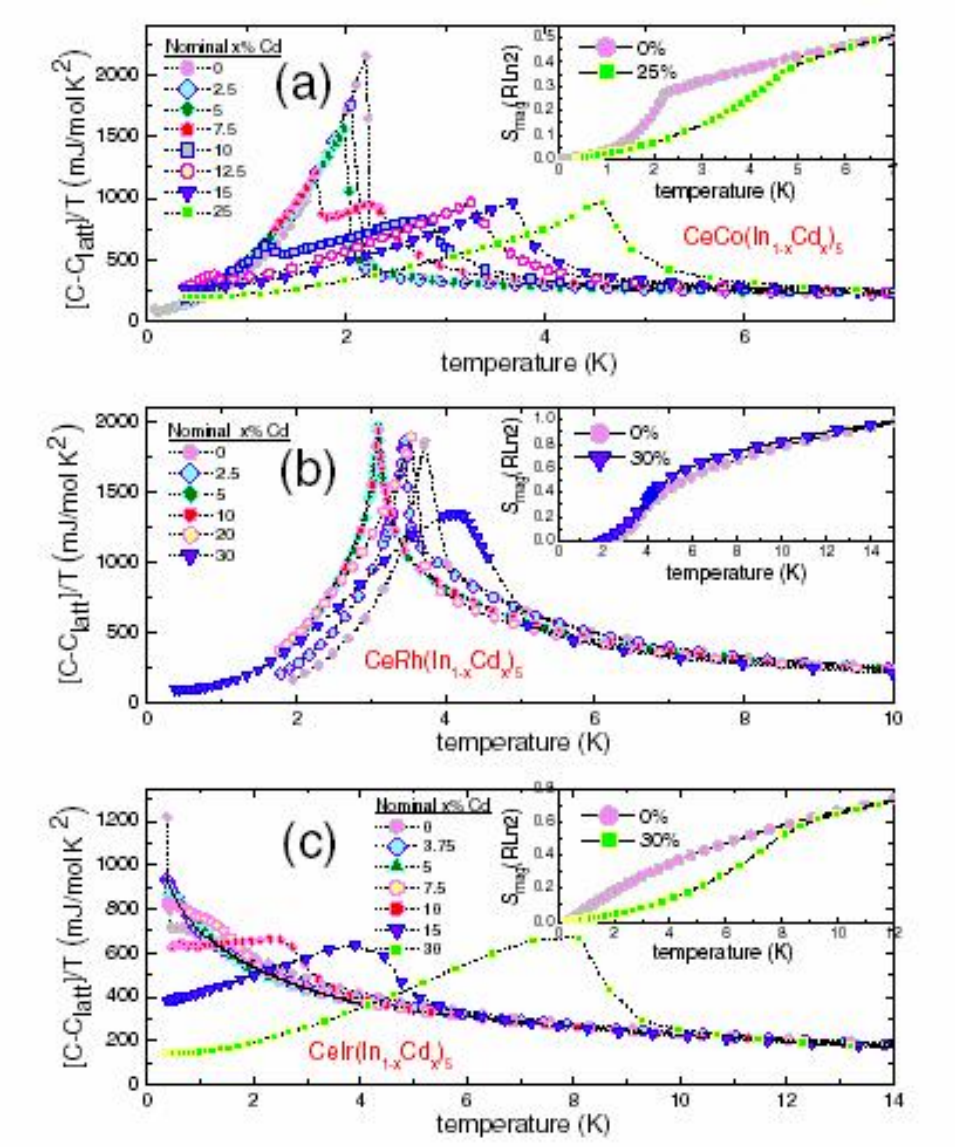
SC would not be expected at ambient pressure in $Ce_{1-x}La_xRhIn_5$, only at much higher P.

However, SC was not found at ambient pressure for $CeRhIn_{5-x}Sn_x$.

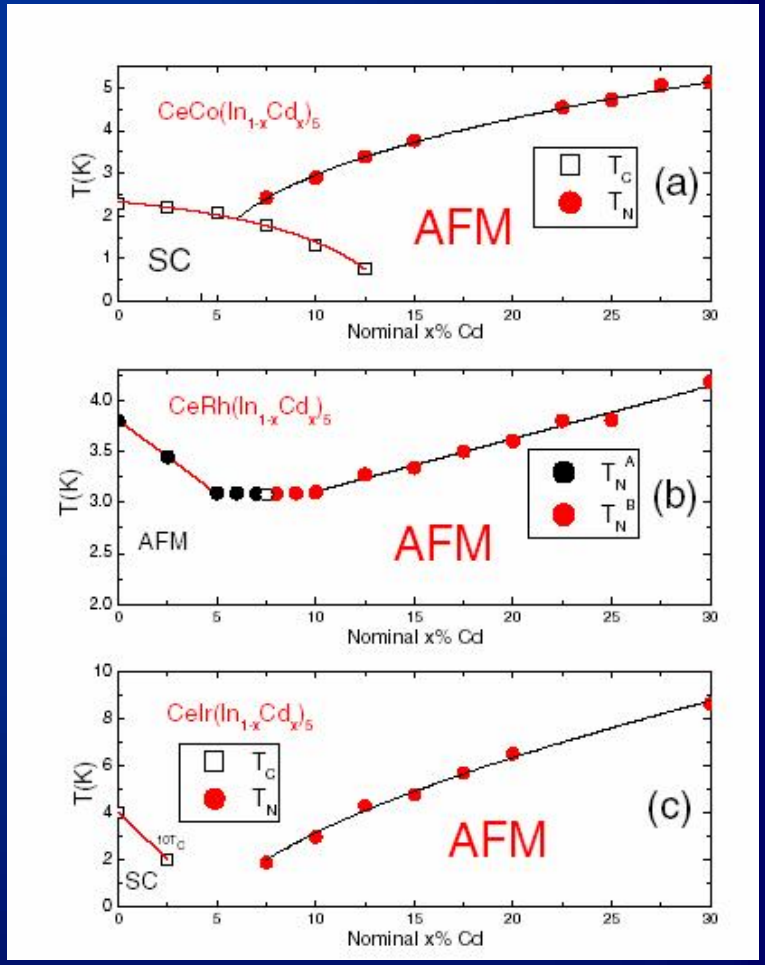
→ Disorder effects: T_{cmax} = 1.2 K for $CeRhIn_{4.84}Sn_{0.16}$ and T_{cmax} = 1.6 K for $Ce_{0.90}La_{0.10}RhIn_5$) is roughly a factor of two smaller than that for $CeRhIn_5$ (T_{cmax} = 2.3 K).

L. Mendonça-Ferreira et al. PRL 101, 017005 (2008)

Cd doping in $CeMIn_5$ – "in block" doping



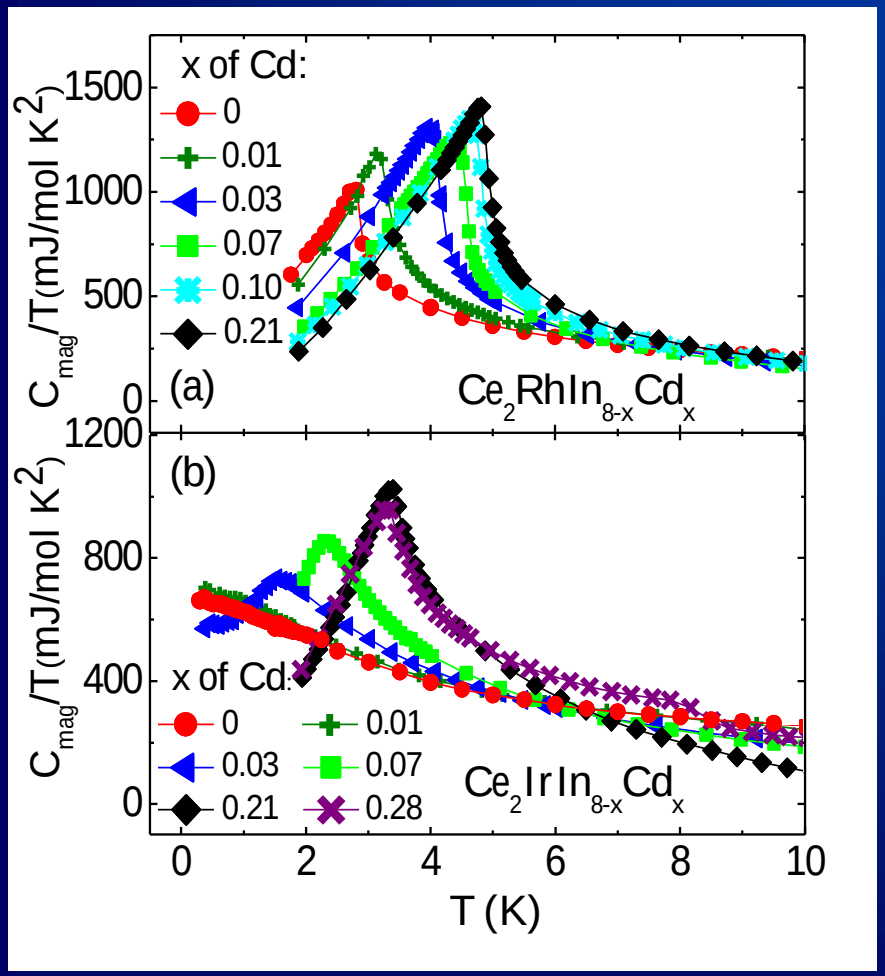
Cd has one p-electron less.
Hole doping – Fermi surface tuning

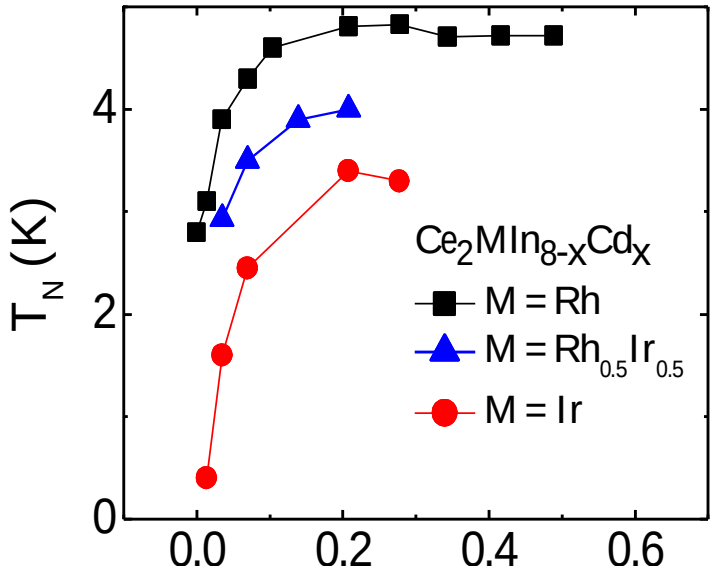


L. D. Pham et al. PRL 97, 056404 (2006).

$Ce_2MIn_{8-x}Cd_x$ phase diagram

Specif-heat divided by temperature and phase diagram for Cd-doped samples

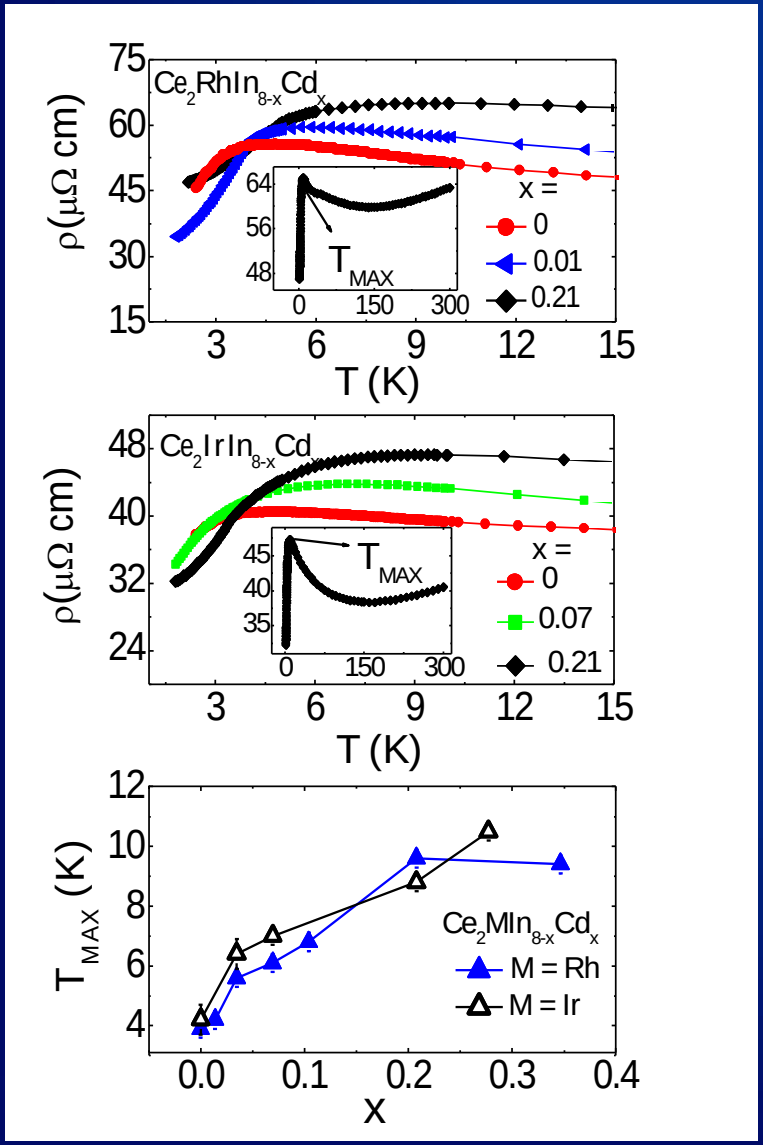




- Cd increases T_N for the 3 compounds;
- Cd induces long range order for M=Ir;

C. Adriano et al, PRB 81, 245115 (2010)

Resistivity results of $Ce_2MIn_{8-x}Cd_x$

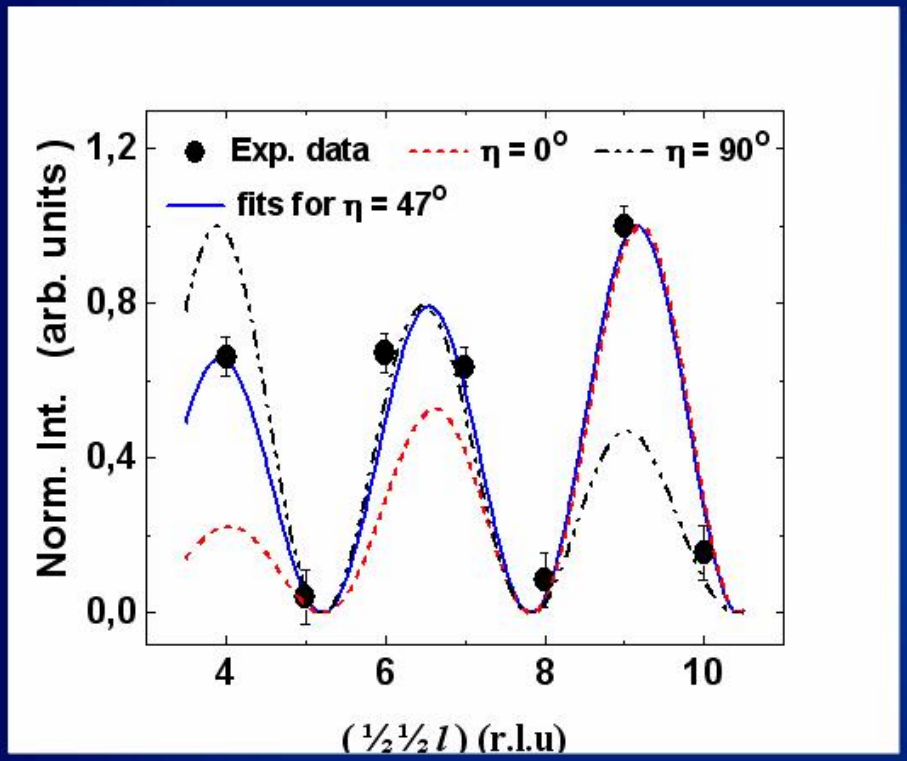


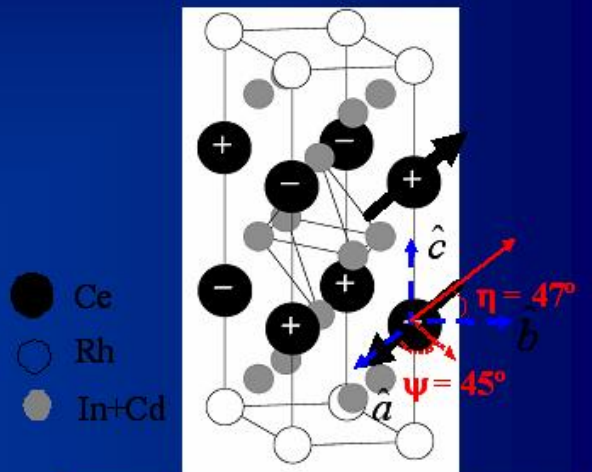
T_N obtained from $\rho(T)$ is in good agreement with specific heat measurements;

T_{MAX} shows an increase not consistent with the decrease of the Kondo coupling.

C. Adriano et al, PRB 81, 245115 (2010)

XRMD of $Ce_2RhIn_{7.79}Cd_{0.21}$ at ESRF and NCNR





η=47° from the ab-plane;
M= (0.9 ± 0.1) μ_B por Ce

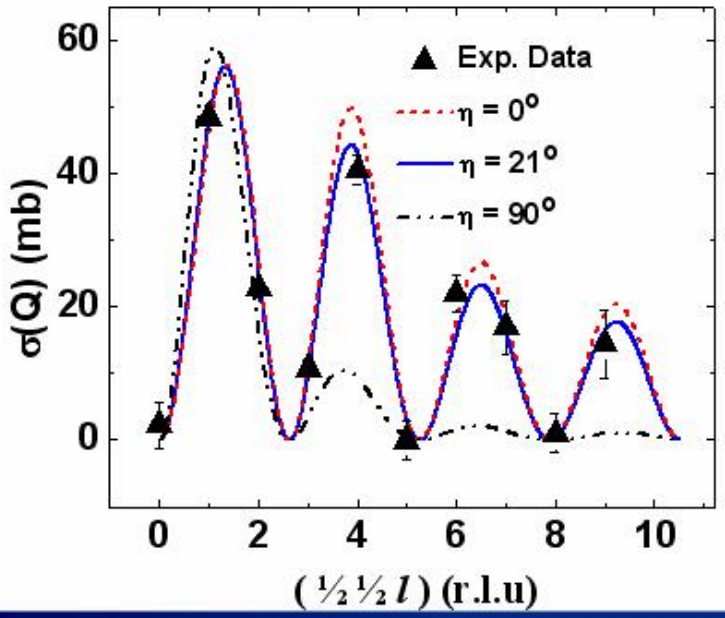
Cd-induces a small rotation of the ordered magnetic moment towards the ab-plane.

C. Adriano *et al*, PRB 81, 245115 (2010)

C. Adriano *et al*, Physica B, 404 3014 (2009).

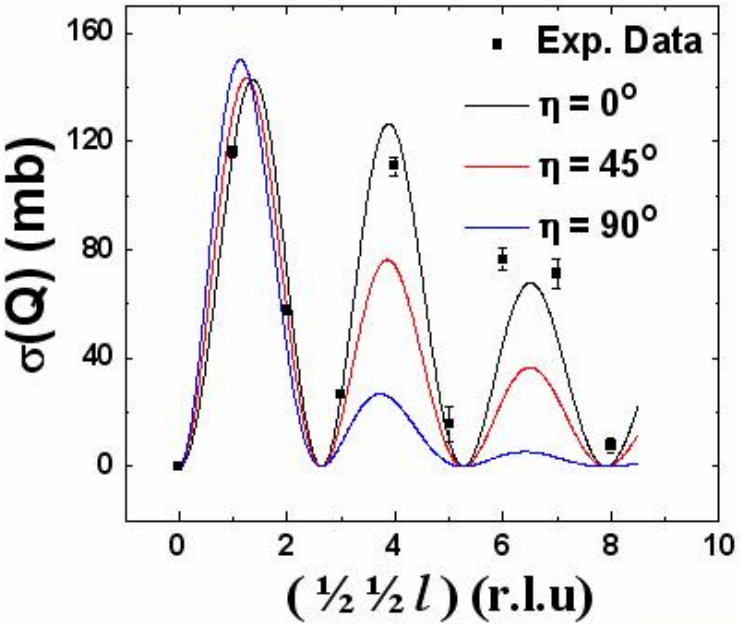
$Ce_2(Rh_{0.5}Ir_{0.5},Ir)In_{8-x}Cd_x$ at NCNR

$Ce_2IrIn_{8-x}Cd_x$



η=21° from the ab-plane;
M= (0.4 ± 0.1) μ_B por Ce

$Ce_2Rh_{0.5}Ir_{0.5}In_{8-x}Cd_x$

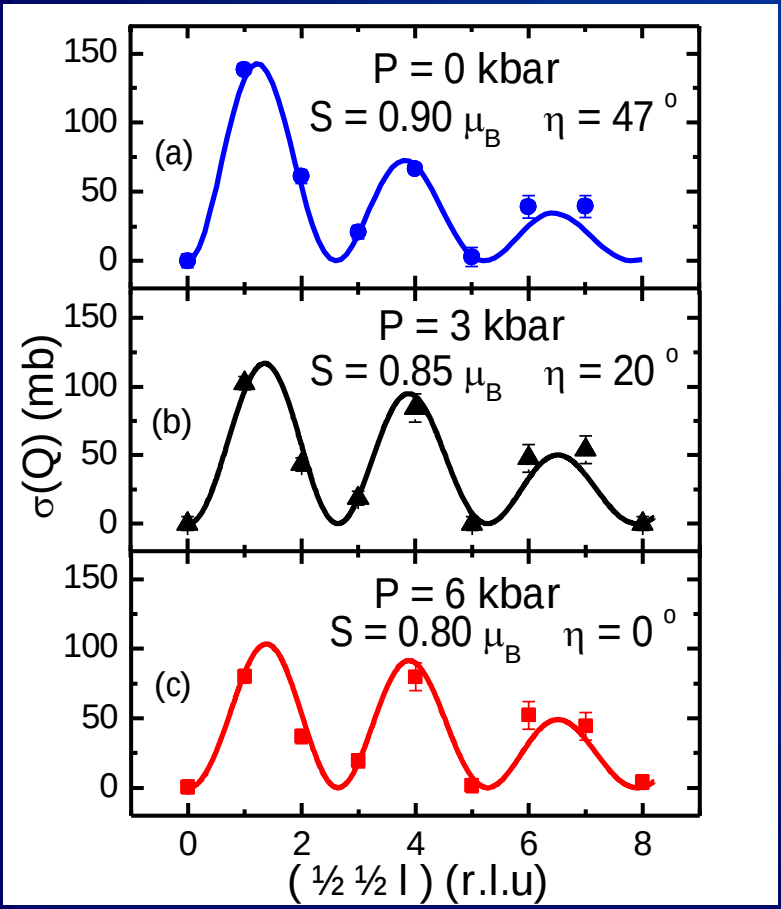


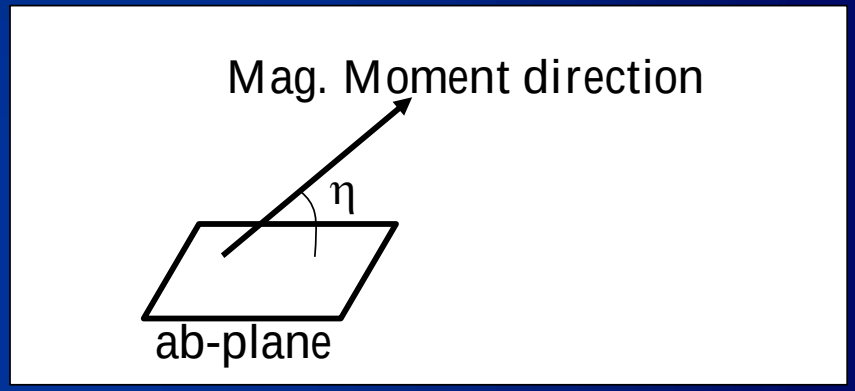
η=0° from the ab-plane;
M= (0.9 ± 0.1) μ_B por Ce

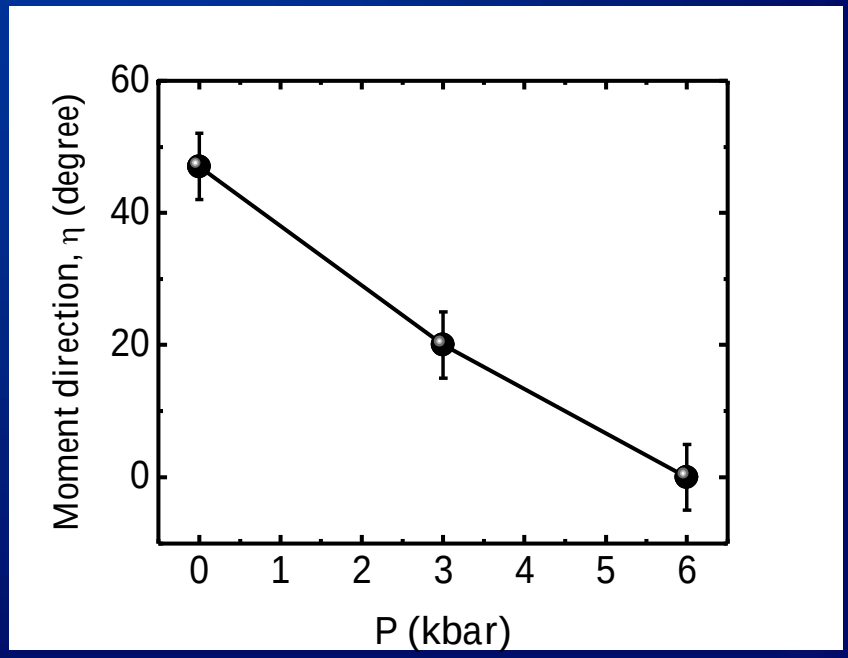
C. Adriano *et al*, PRB 81, 245115 (2010)

$Ce_2RhIn_{8-x}Cd_x$ under pressure

$Ce_2RhIn_{7.79}Cd_{0.21}$

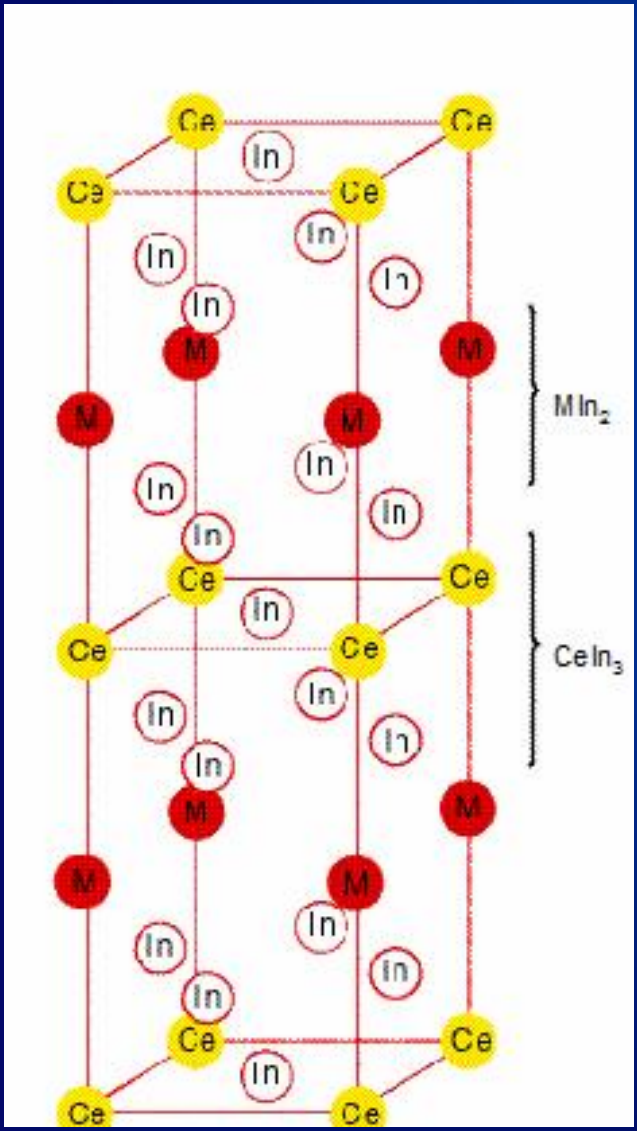






No SC up to ~ 23 kbar!!

$CeMIn_5$ (M = Rh, Ir, Co) Family

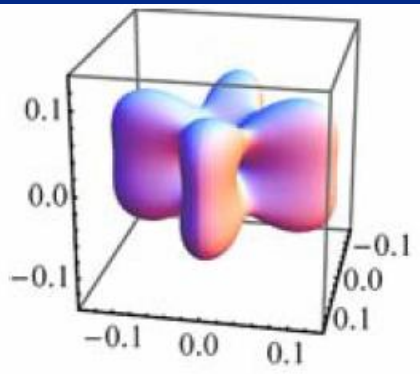


$$H_{CEF}^{tetrag} = B_2^0 O_2^0 + B_4^0 O_4^0 + B_6^0 O_6^0 + B_4^4 O_4^4 + B_6^4 O_6^4$$

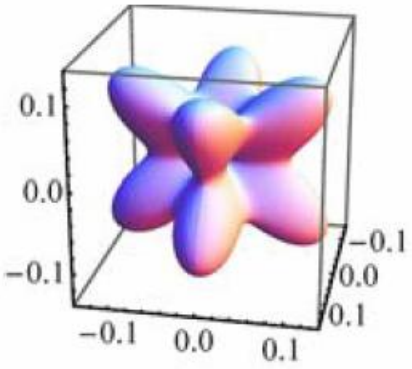
$$|2\rangle = \Gamma_6 = |\pm 1/2\rangle,$$

$$|1\rangle = \Gamma_7^1 = \beta|\pm 5/2\rangle - \alpha|\mp 3/2\rangle,$$

$$|0\rangle = \Gamma_7^2 = \alpha|\pm 5/2\rangle + \beta|\mp 3/2\rangle$$

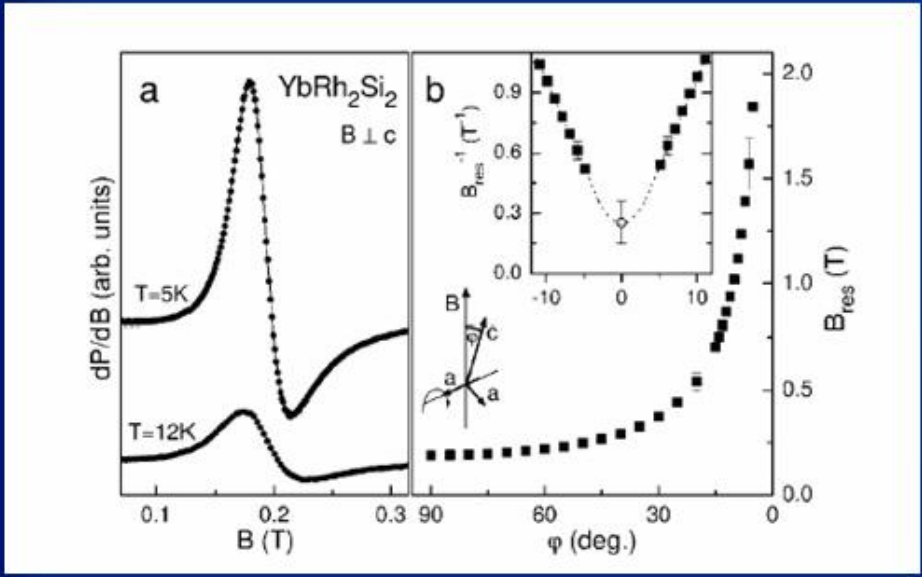


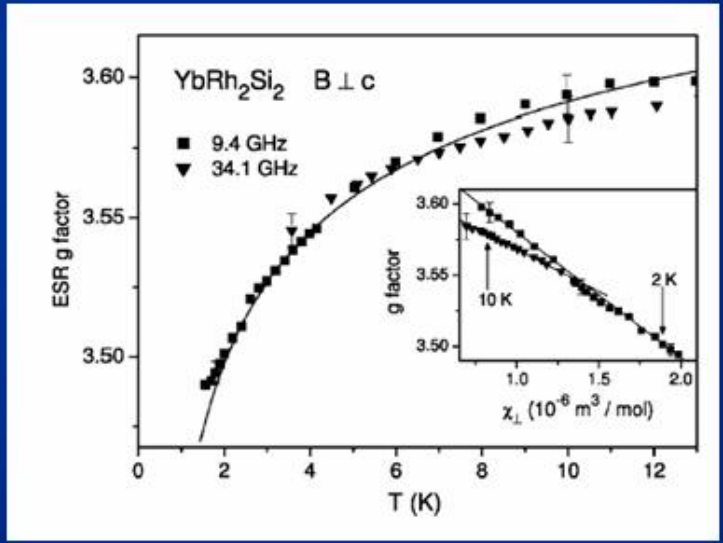
α=0.62



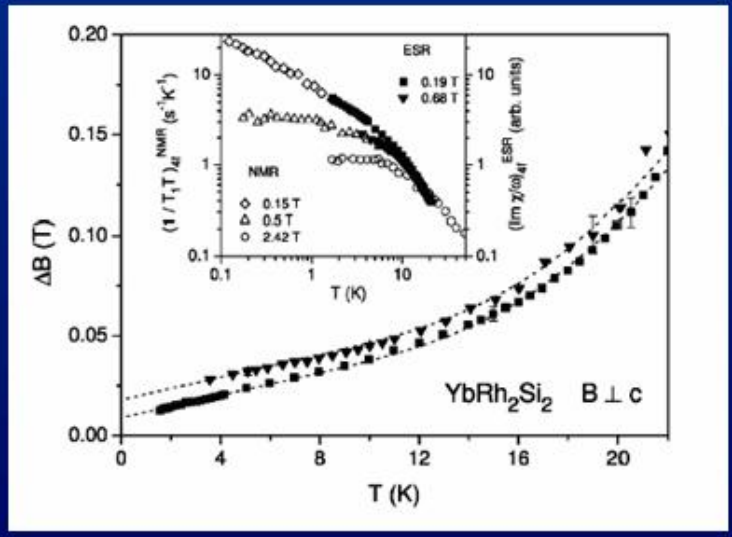
α=0.36

Probing the f-electron site: ESR in $YbRh_2Si_2$



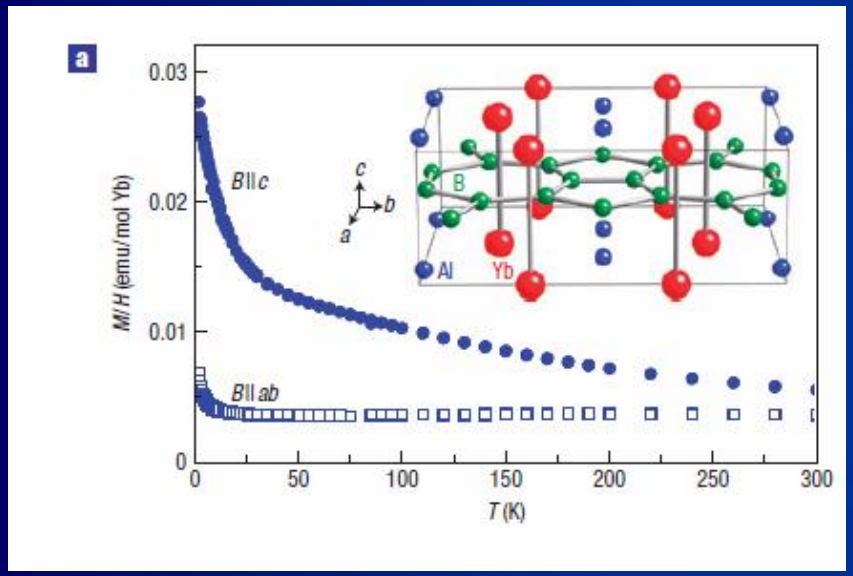


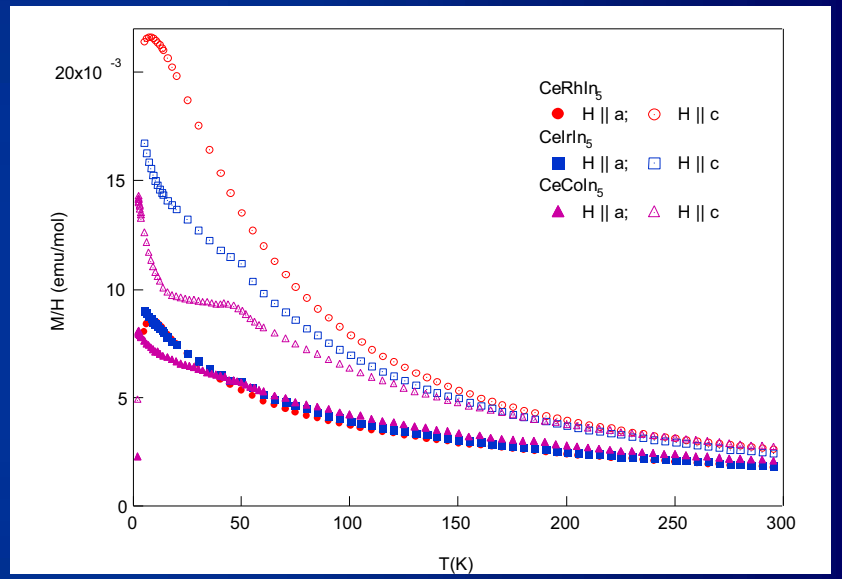
- ESR signal presumably arising from localized Yb^{3+} CEF ground state.
- Spin dynamics as measured by ESR seems consistent to the formation of a Kondo Lattice seen by remained localized *4f* electrons.

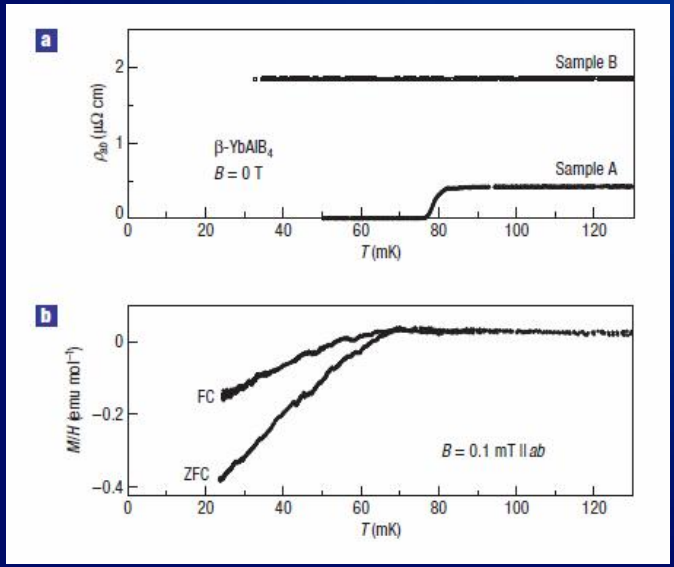


J. Sichelschimidt et al., PRL 2007.

Extrapolation to â-$YbAlB_4$ – IV – large T_{SF}







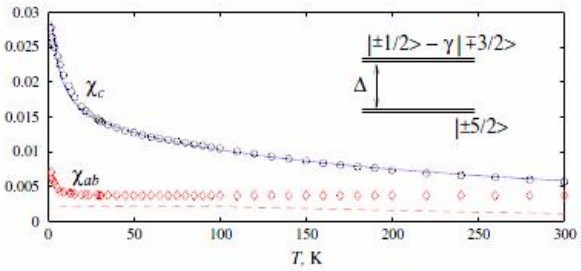
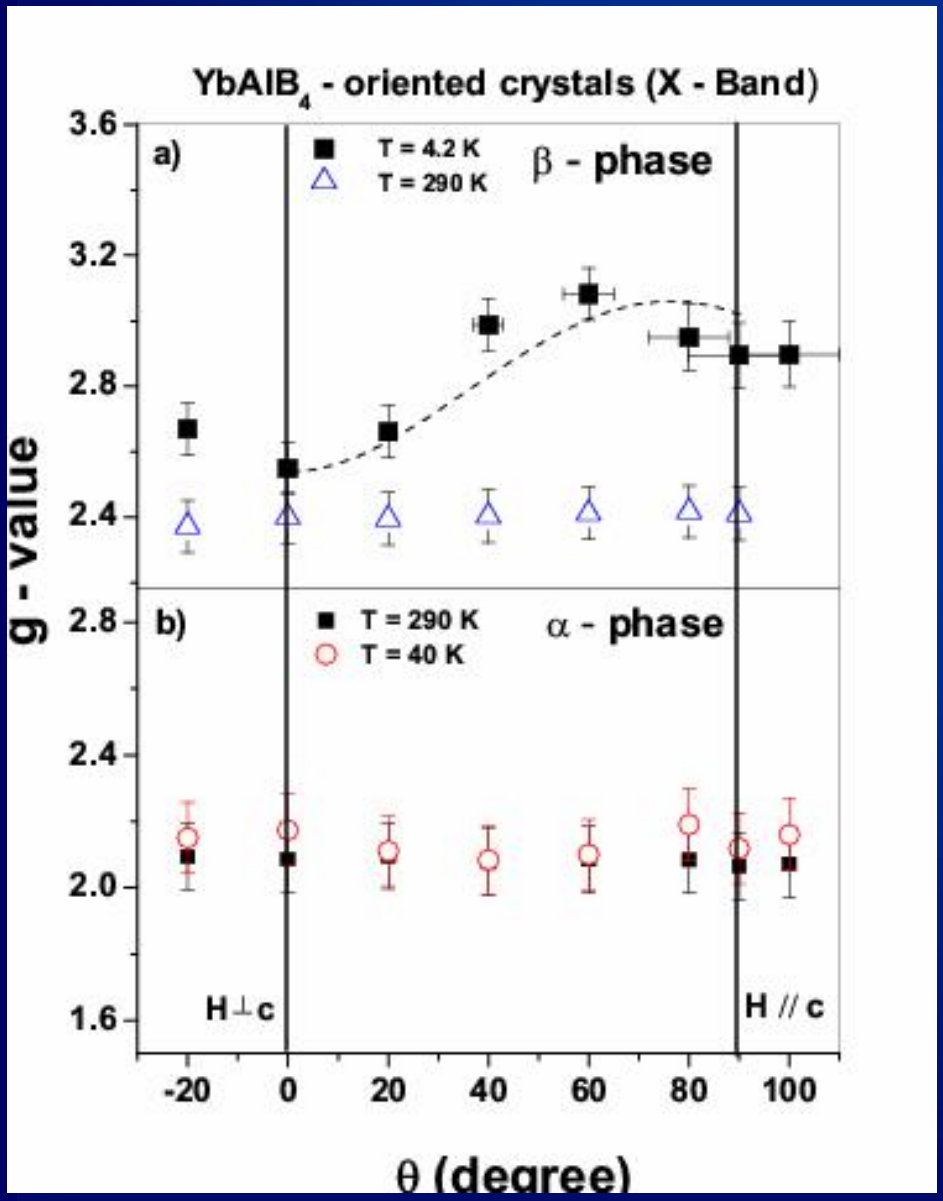


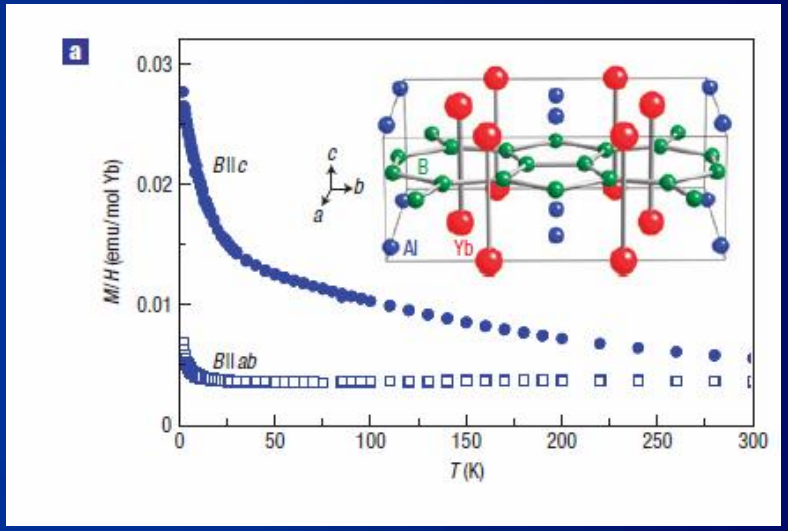
FIG. 4 (color online). (a) Theoretical fit to experimental susceptibility data [7] $\chi_c(T)$ (circles) and $\chi_{ab}(T)$ (rhombi) in the range 50–300 K using the single-ion model shown in the inset and the fitted Curie-Weiss temperature θ_{CW}. The best fit yields the lowest crystal field splitting $\Delta = 80$ K, the coefficient of admixture $\gamma \approx 0.28$ and $\theta_{CW}^{th} = -230$ K, close to the experimental value $\theta_{CW}^{exp} \sim -210$ K.

Nakatsuji S. et al. Nature 4, 603-607 (2008).

Andriy H. Nevidomskyy* and P. Coleman, PRL 102, 077202 (2009)

ESR g-anisotropy

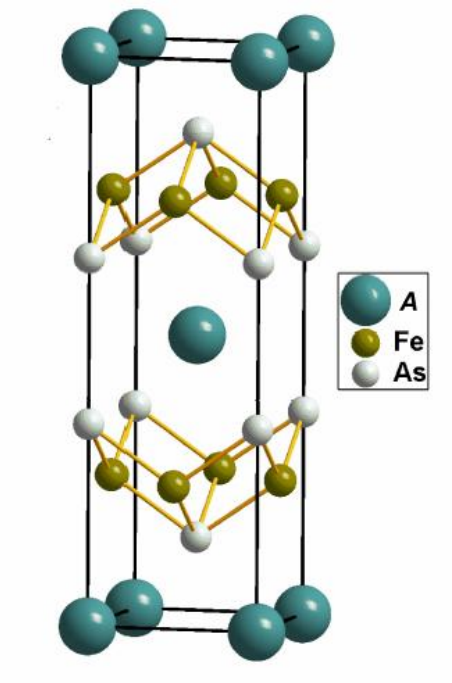


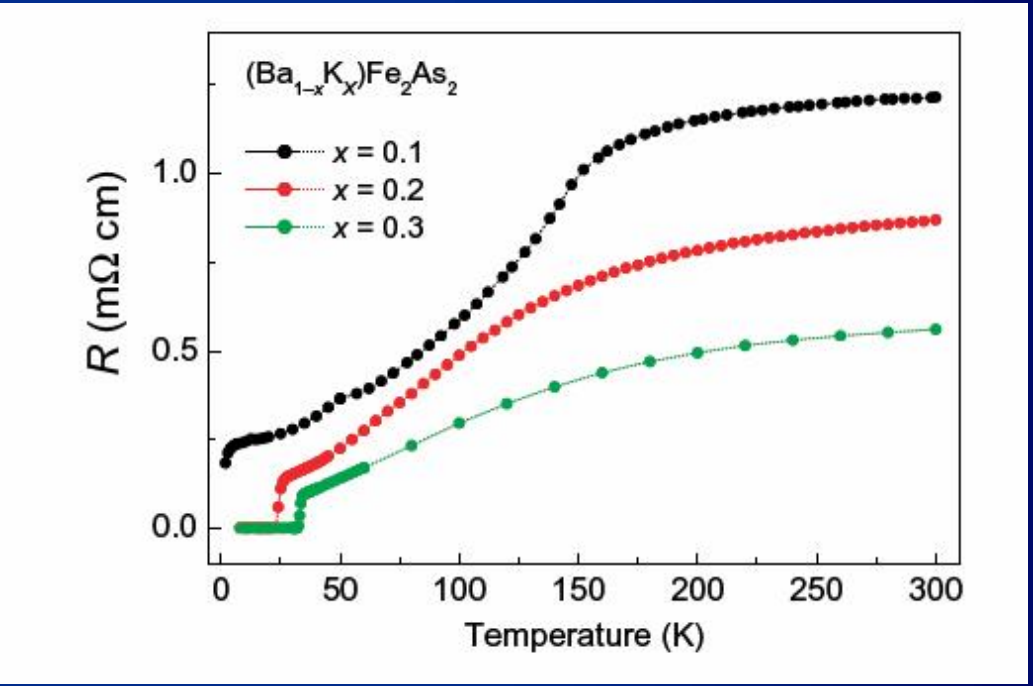


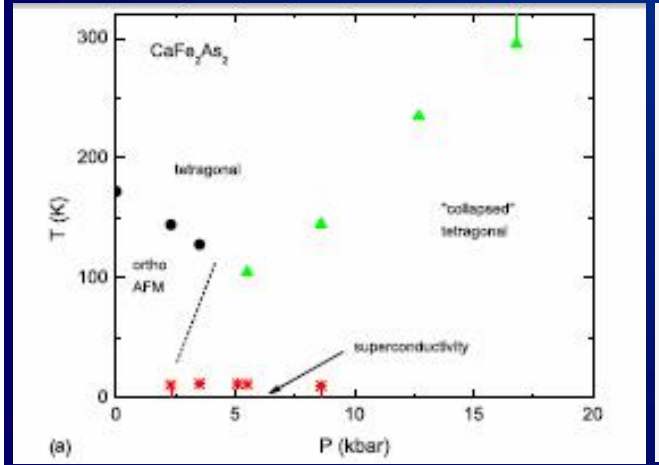
This remarkable and unprecedented ESR signal found in the HFS â-YbAlB4 behaves as a CESR at high temperatures and acquires characteristics of Yb3+ LM ESR at low temperature. This dual behavior in same ESR spectra strikes as an in situ unique observation of the Kondo localization of the f-electron at the quantum critical point (QCP) of â-YbAlB4.

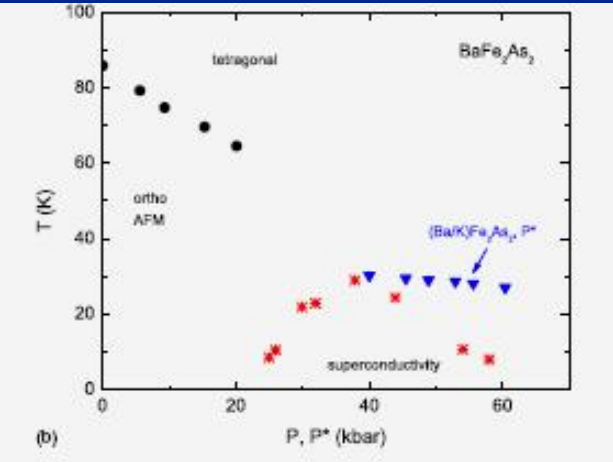
cond-mat 0908.0044

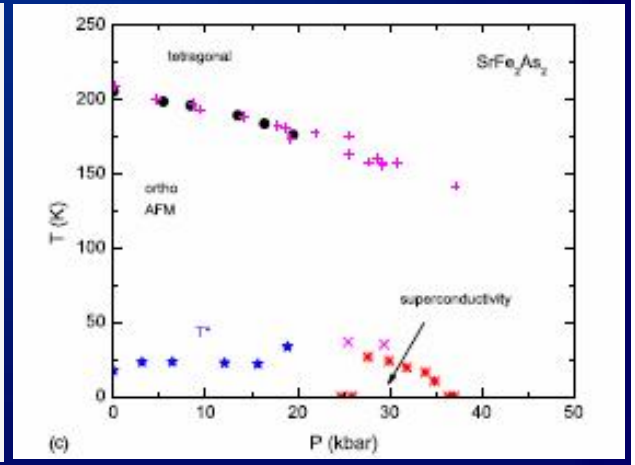
1-1-5 - $PuCoGa_5$ – FeAs-intermetallics ?











M. S. Torikachvilli et al. PRB 2008.

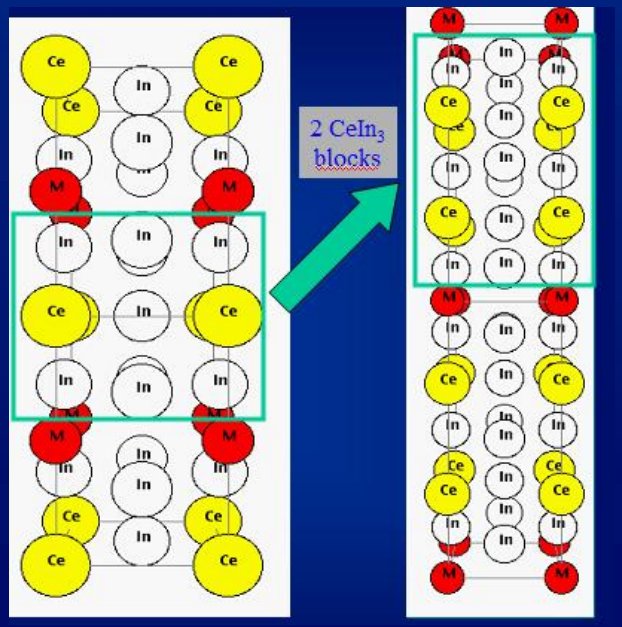
Marianne Rotter al. New J. of Phys. (2009).

Implications for designing materials

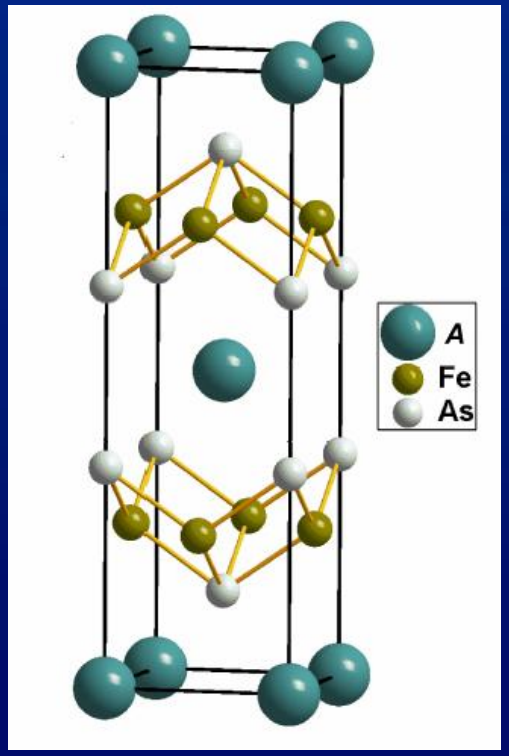
• To increase T_C for magnetically mediated SC:
Tsf, characteristic T for spin fluctuations high
Tunable carrier density

•Quasi 2-d helps a lot; maybe not much 2-d needed – increase c/a – tune CEF GS

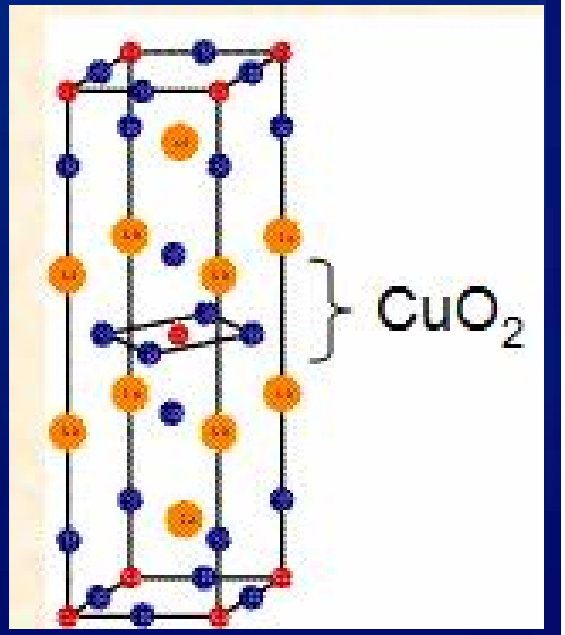
•Need bigger bandwidths to increase T_{sf}, but keep optimized T_c/T_{sf} - 3d spins in the active layer.



1-1-5 e 2-1-8

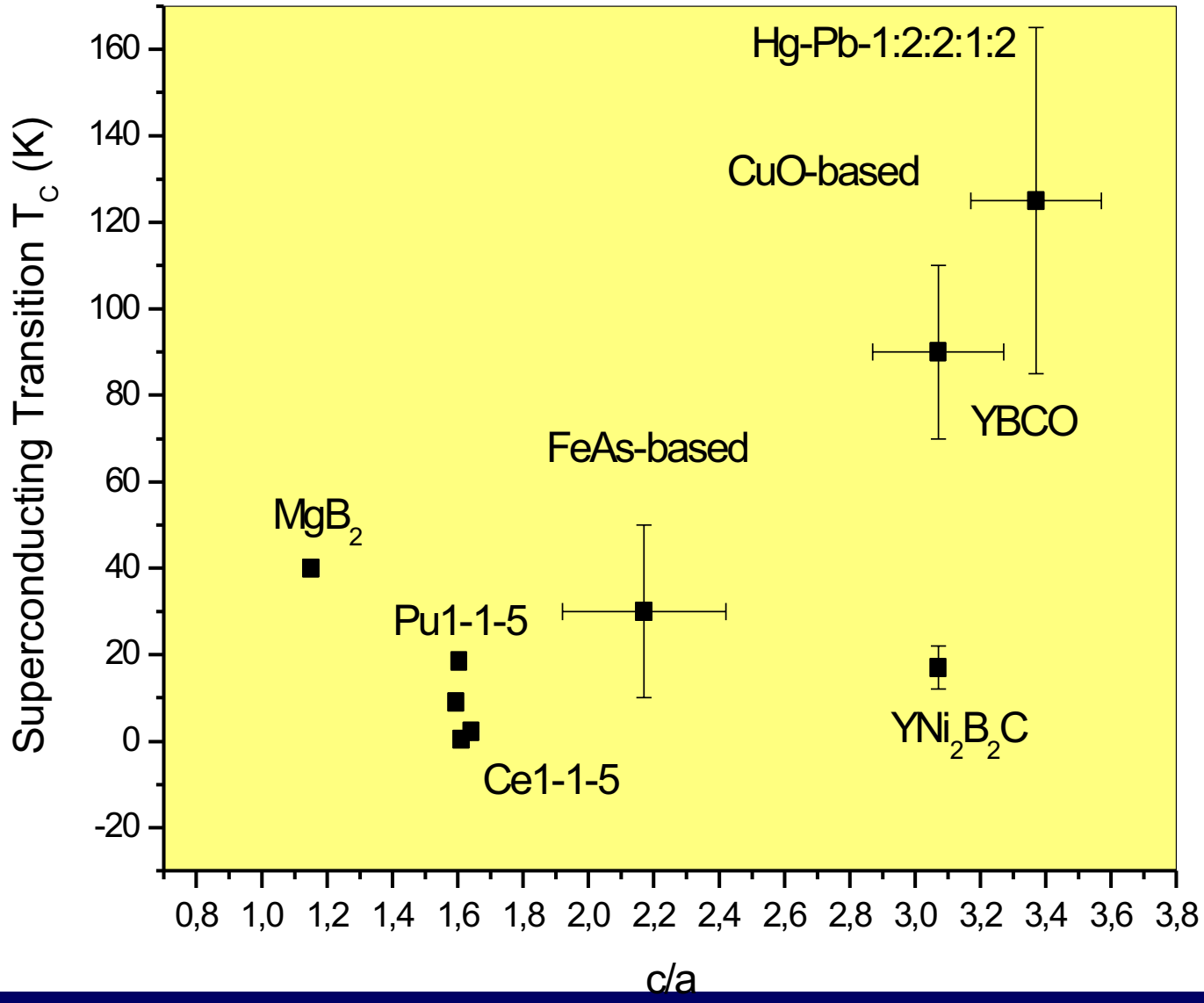


1-2-2

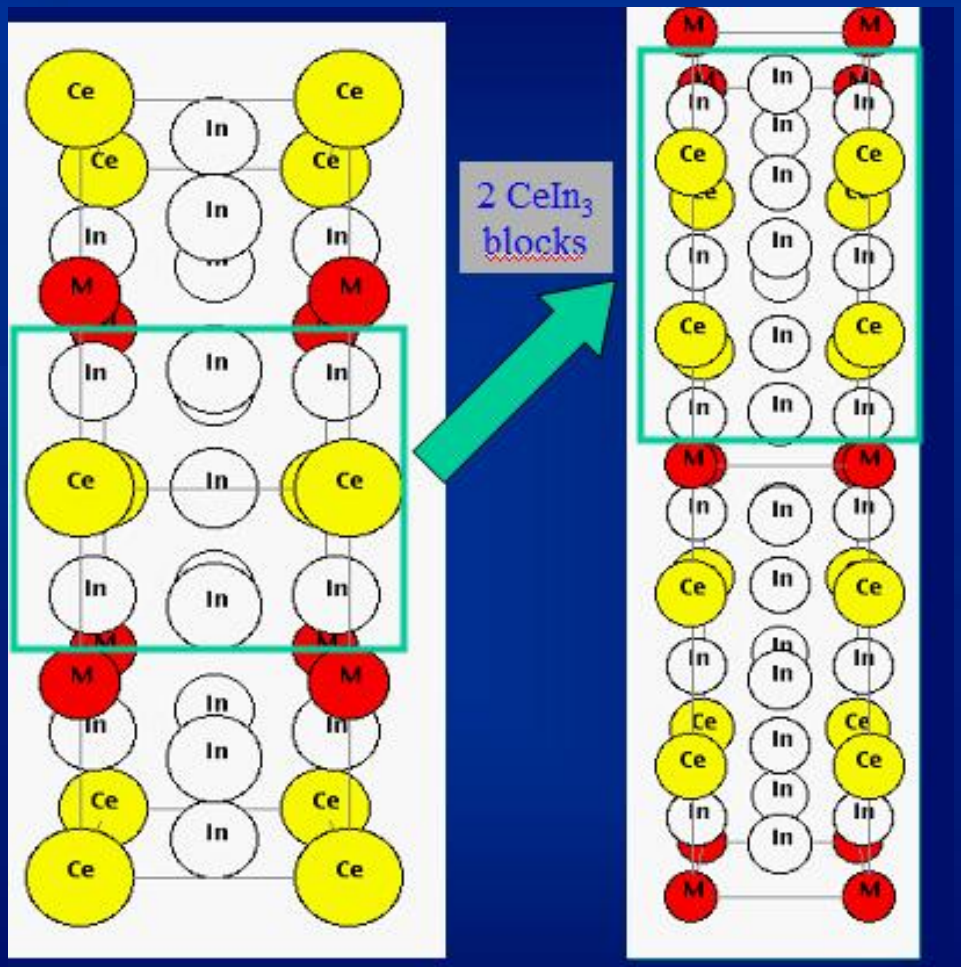


2-1-4, etc

Generalized c/a plot



Implications for designing materials



- 1-1-5: c/a ~ 1.6
- 2-1-8: c/a ~ 3.0 –

3d spins as the active layer.

- Examples: A_2MB_8

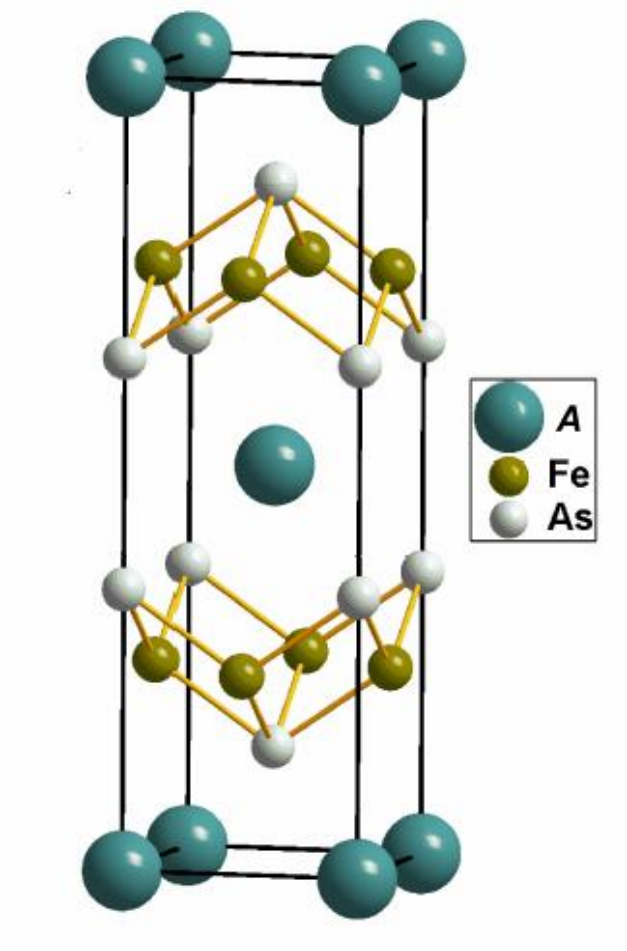
M = Cu, Fe, Co, Ni, Mn, Ru, Re, Mo…

A = La, Y, Ca, Sr, Ba, Mg, K

B = Bi, Sb, Ge, Sn, In, As, etc

1-1-5 e 2-1-8 1-2-2 2-1-4, etc

Implications for designing materials



•c/a ~ 2-3 - 3d spins as the active layer.

•Examples: AM_2B_2

M = Cu, Fe, Co, Ni, Mn, Ru, Re, Mo…

A = La, Y, Ca, Sr, Ba, Mg, K, Li, Mg

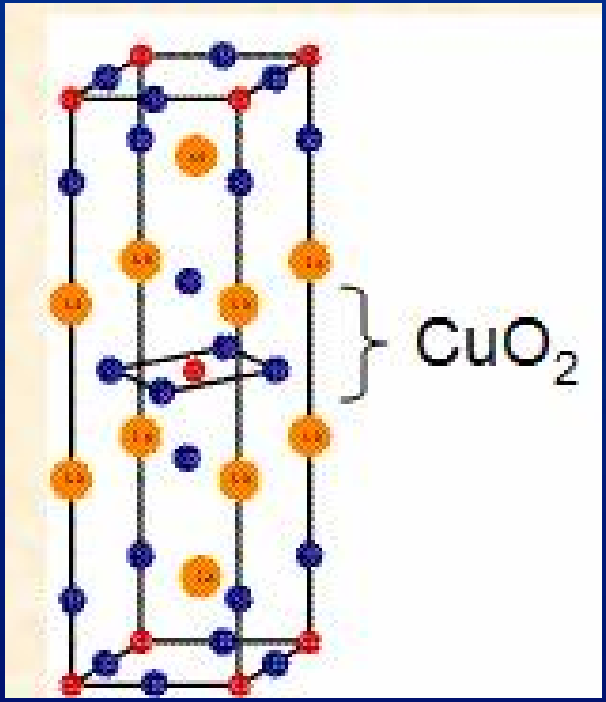
B = Bi, Sb, Ge, Sn, In, etc

1-1-5 e 2-1-8

1-2-2

2-1-4, etc

Implications for designing materials



•2-1-4: c/a ~ 3/4 - 3d spins as the active layer.

•Examples: A_2MB_4

M = Cu, Fe, Co, Ni, Mn, Ru, Re, Mo…

A = La, Y, Ca, Sr, Ba, Mg, K

B = Bi, Sb, Ge, Sn, In, Pb, etc

1-1-5 e 2-1-8

1-2-2

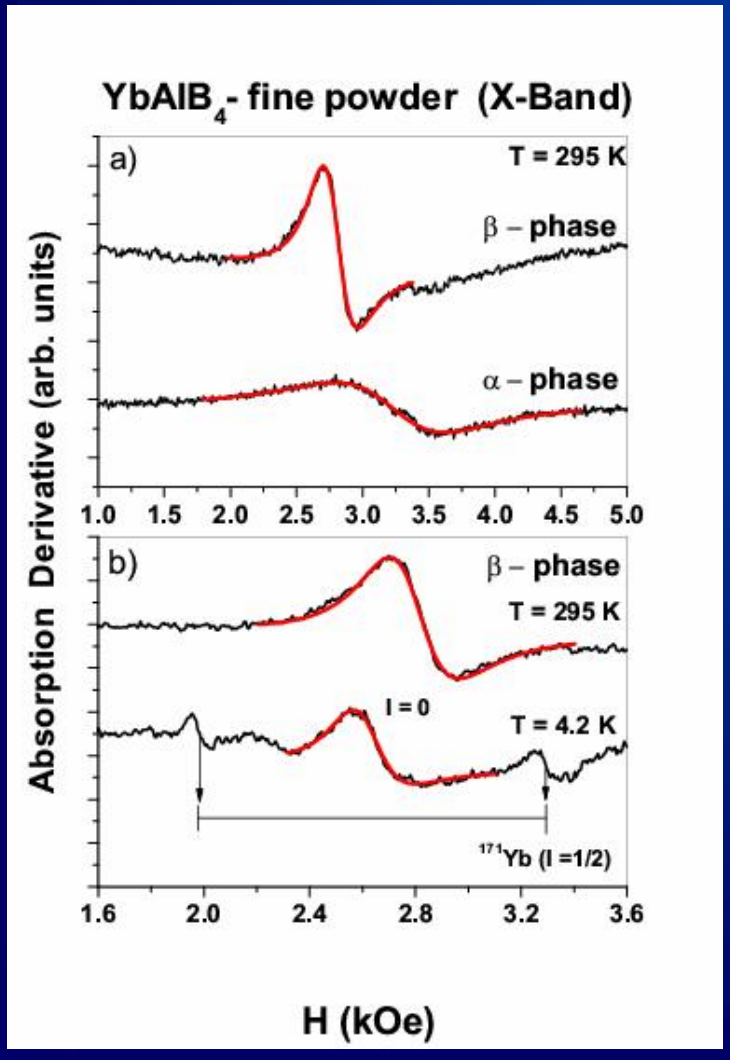
2-1-4, etc

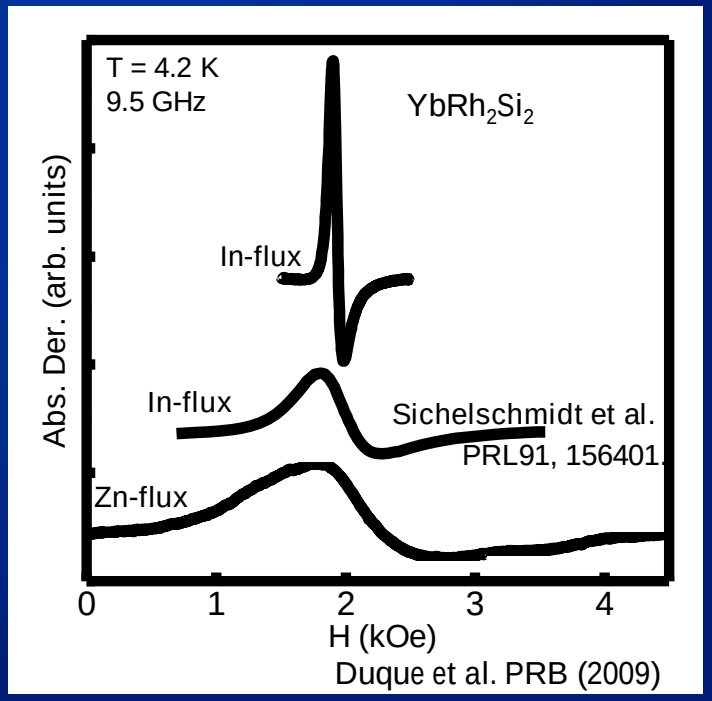
Thank you for your attention!

ESR signal in â-$YbAlB_4$: cond-mat 0908.0044

Evidence for the existence of *Kondo coupled resonant modes* in heavy fermions

L. M. Holanda [1], J. M. Vargas [1], C. Rettori [1], S. Nakatsuji [2], K. Kuga [2], Z. Fisk [3], S.B. Oseroff [4] and P. G. Pagliuso [1]
[1] *Instituto de Física "Gleb Wataghin", UNICAMP, Campinas-SP, 13083-970, Brazil.*
[2] *Institute for solid State Physics (ISSP), University of Tokyo, Kashiwa 277-8581, Japan.*
[3] *University of California, Irvine, California 92697-4573, U.S.A.*
[4] *San Diego State University, San Diego, California 92182, U.S.A.*





Abrahams, E., Wolfle, P. Phys. Rev. B 78 104423 (2008).

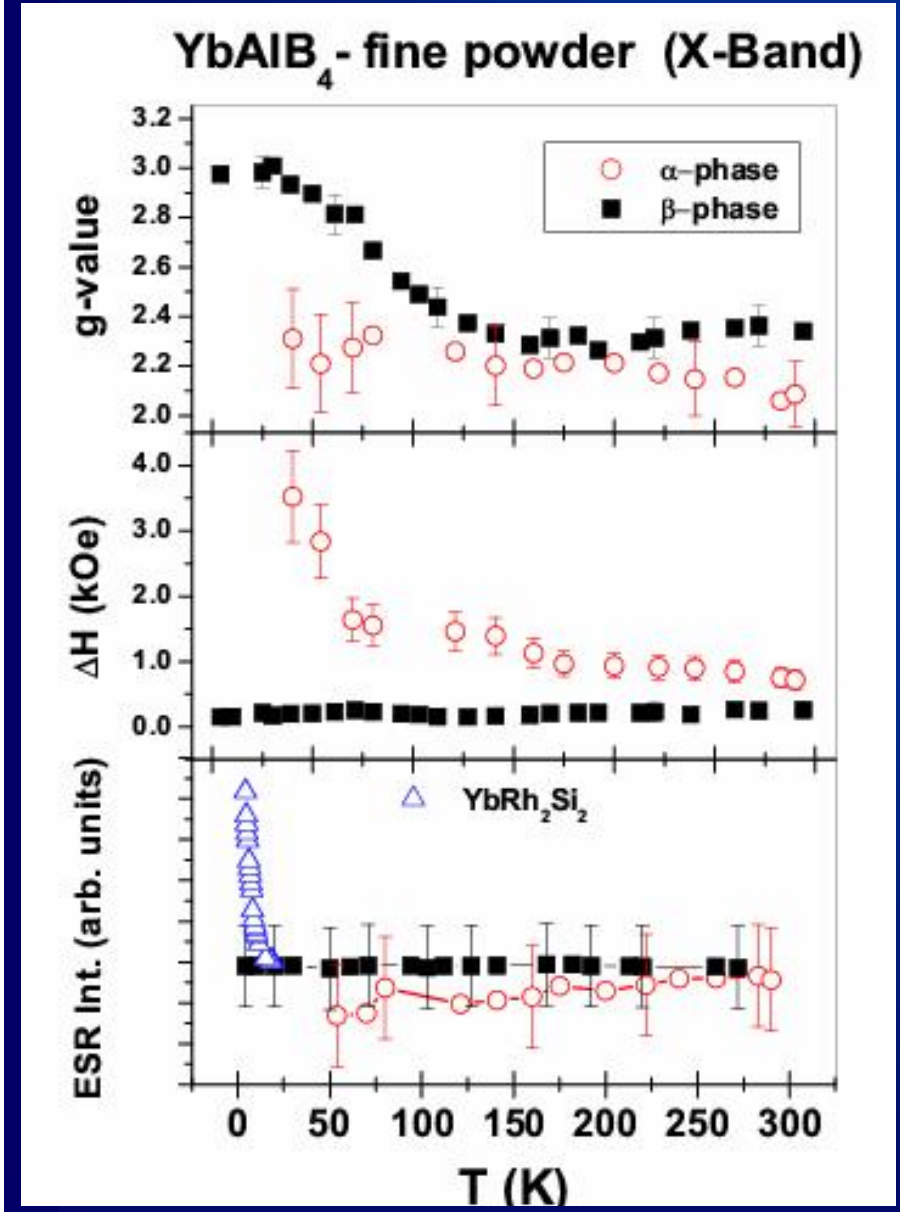
Schlottmann, P.Phys. Rev. B 79 045104 (2009).

Kochelaev, B. I. arXiv:0907.2074 (2009).

^{171}A ~ 1300 Oe which is of the order of the typical values found for ^{171}Yb in low symmetry systems.

Irrefutable indication that the ESR spectra found for â-YbAlB4 acquires the characteristic of the Yb^{3+} ions at low-T.

ESR temperature dependence

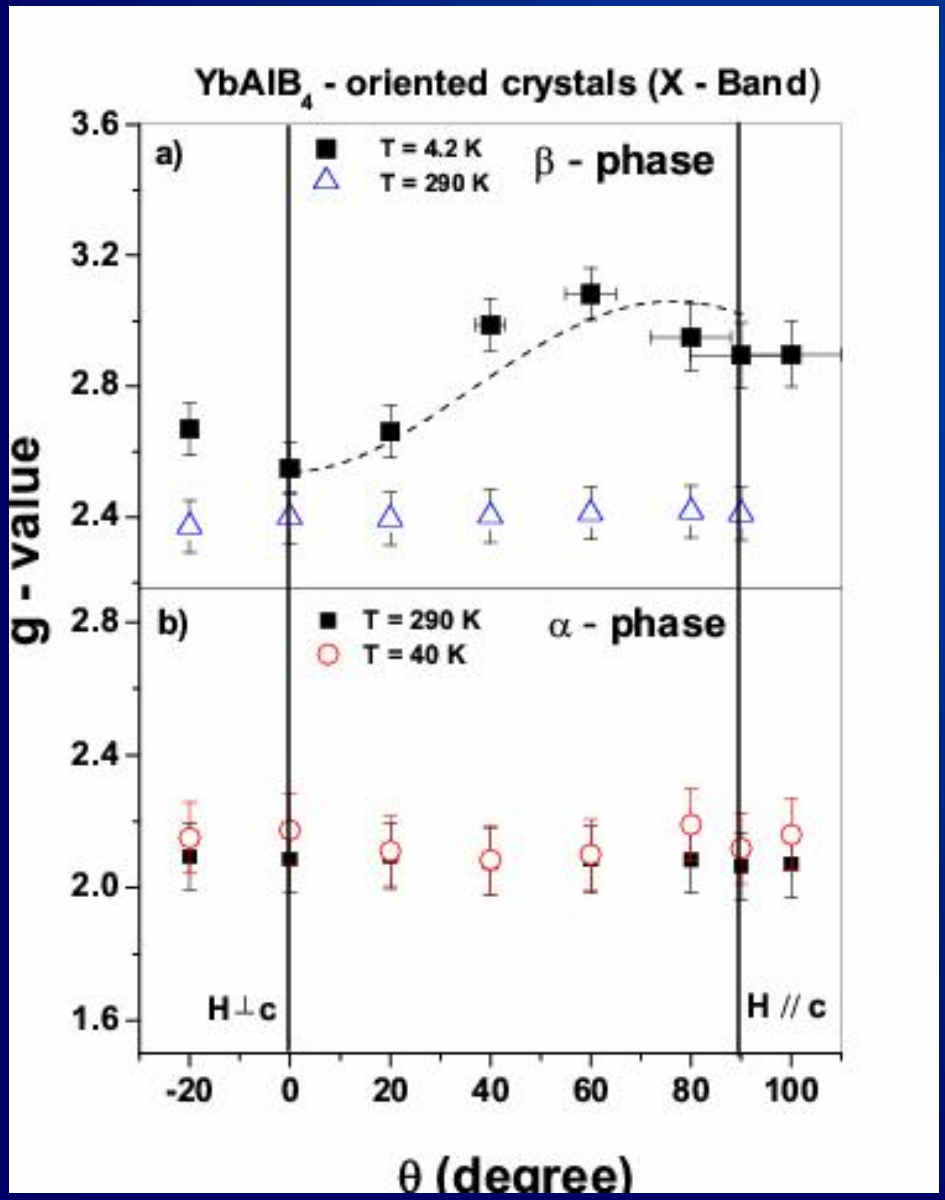


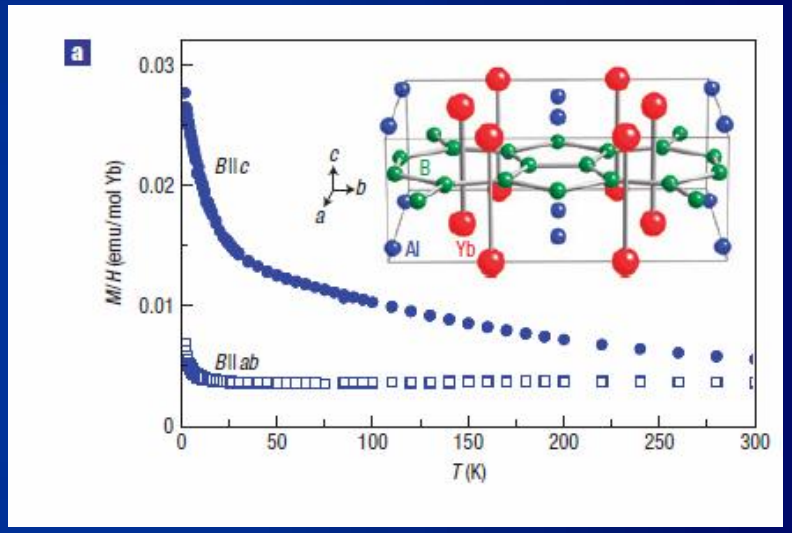
Both phases show T-independent ESR intensity – typical of CESR

g-value for the â-phase shifts to larger value at low-T (g ~ 3): typical for Yb^{3+} Krammers doublets)

For â-YbAlB4 ΔH(T) shows a weak non-monotonic increase as a function of temperature which results in an average linewidth broadening of ~ 0.4 Oe/K in the whole temperature range. This rate is much smaller than the linear Korringa-rate found for the ESR line observed at low-T for YbRh2Si2. In contrast, for α-YbAlB4 ΔH(T) increases dramatically with decreasing-T which avoid the observation of the resonance for T < 40 K.

g-anisotropy





This remarkable and unprecedented ESR signal found in the HFS â-YbAlB4 behaves as a CESR at high temperatures and acquires characteristics of Yb3+ LM ESR at low temperature. This dual behavior in same ESR spectra strikes as an in situ unique observation of the Kondo localization of the f-electron at the quantum critical point (QCP) of â-YbAlB4.