Magnetism in Unconventional Superconductors

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Rio de Janeiro

Jacques Danon

Collaboration with

Dalber Sanchez

Mariella Alzamora, Julian Munevar , Y. Xing: Fe-As

Hans Micklitz: RNi_nB_nC

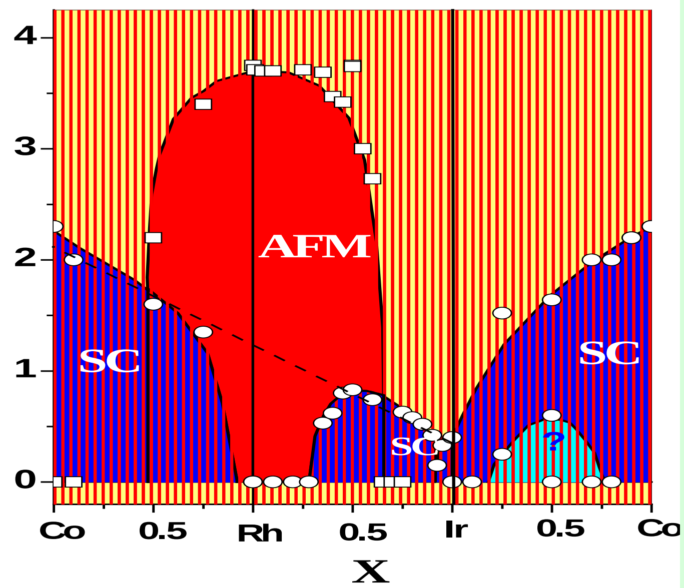
T. Uemura: µSR

N. L. Wang , S. L. Budko: samples Fe-As

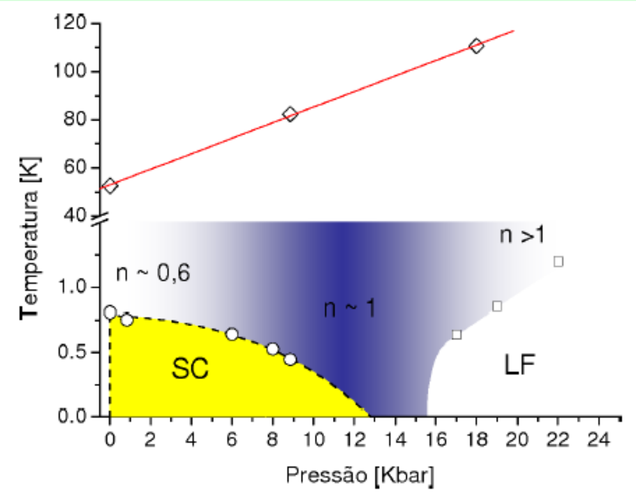
Unconventional Superconductors

Ce(Rh,Ir,Co)In_5 and $CeCoIn_{5-x}Sn_x$ Phase Diagram

Ce(Rh,Ir,Co)In5



$CeCoIn_{5-x}Sn_x$



No Fe in H-Tc

P.G. Pagliuso et al.

Outline

- Structural Features and Pair Breaking Field in RNi_2B_2C and RNiBC Compounds as Seen by Local Method
- Fe Probing Magnetism in Fe-As families of SC

Structural Features and Pair Breaking Field in RNi_2B_2C and RNiBC Compounds as Seen by Local Method

Phys. Rev. Lett. 72, 274 - 277 (1994)

Bulk superconductivity at an elevated temperature ($T_c \approxeq 12$ K) in a nickel containing alloy system Y-Ni-B-C

R. Nagajan,
Chandan Mazumdar, Zakir Hossain, S.K. Dhar, K. V. Gopalakrishnan,
L.C. Gupta, C. Godart, B. D. Padalia and R. Vijayaraghavan

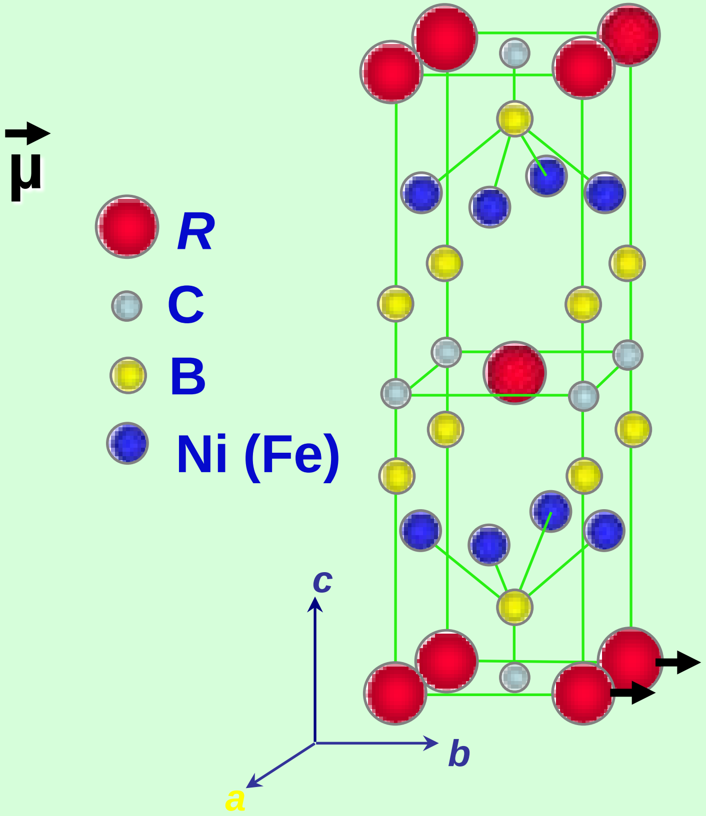
Tate Institute of Fundamental Research, Bombay, India 400 005
Indian Institute of Technology, Bombay

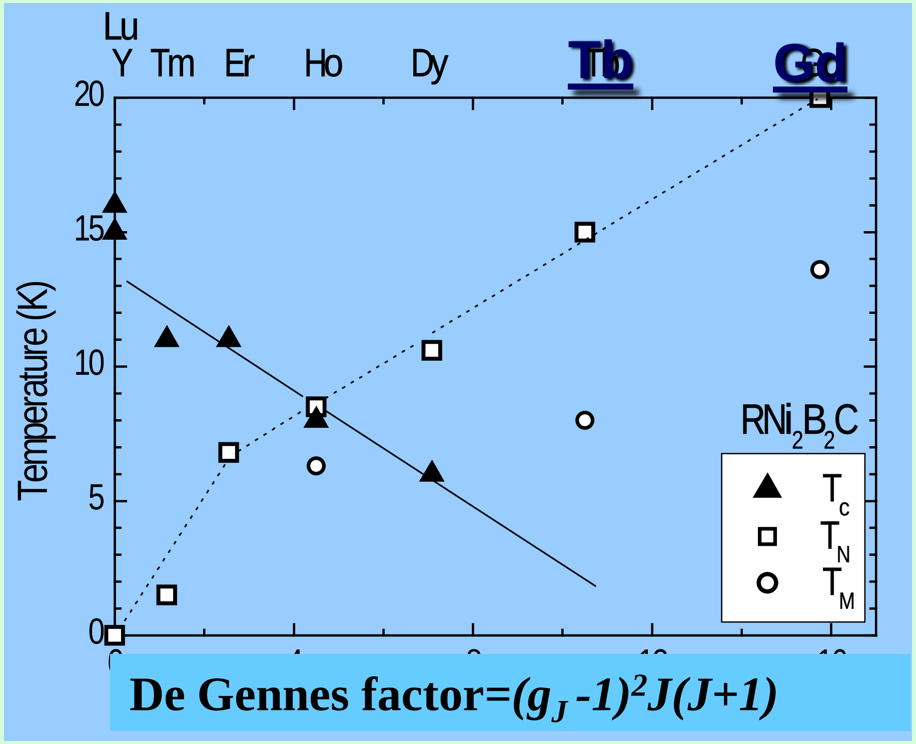
Received 24 September 1993

R. Cava

RNi$_2$B$_2$C

Physical Properties





✓**Magnetism is due exclusively to R magnetic moments:**

AF, FM, WFM, and SDW determined by coupling of R layers

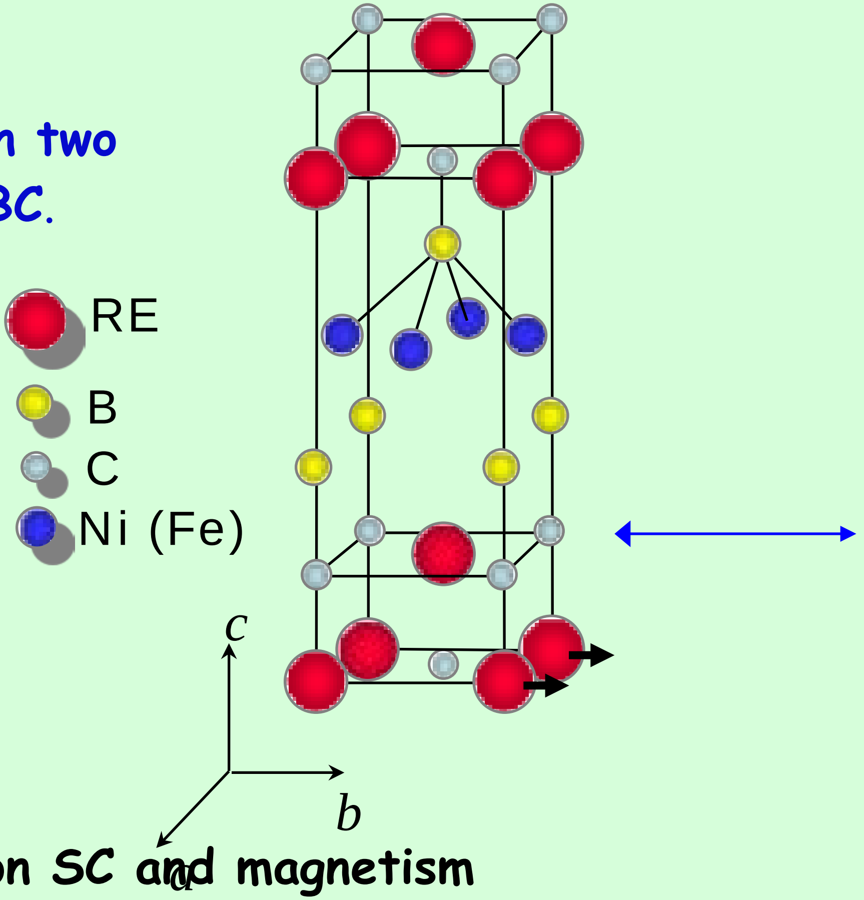
✓**Interplay between Superconductivity and Magnetism**

TbNi$_2$B$_2$C and GdNi$_2$B$_2$C are not superconductors

RNiBC

Physical Properties

Insertion of one more R-C layer between two adjacent Ni_2B_2 blocks, gives rise to RNiBC.



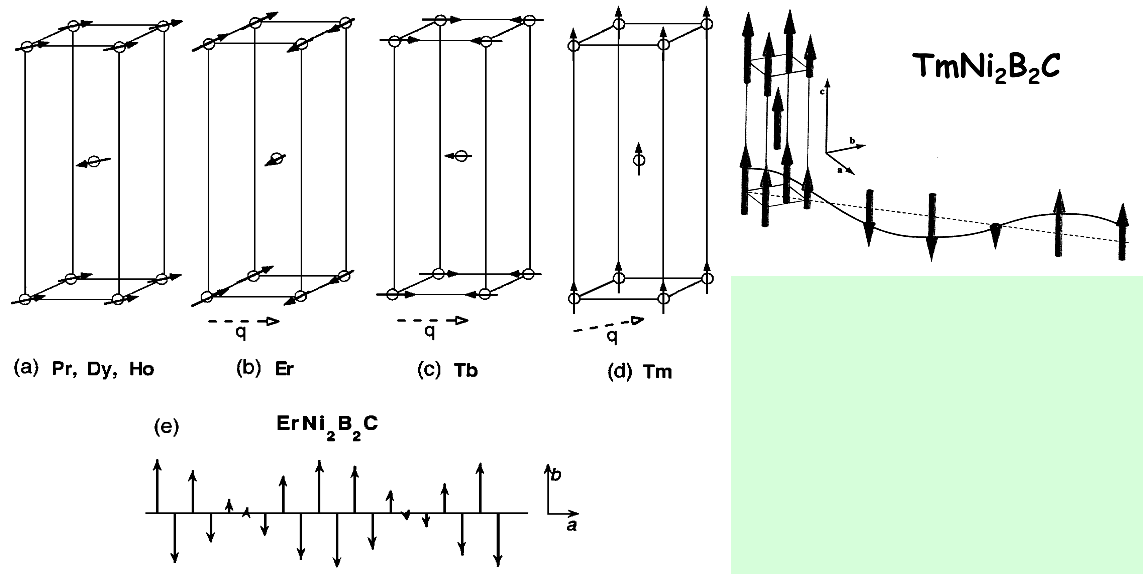
✓Double R-C layers: dramatic effects on SC and magnetism

✓Only the LuNiBC is superconducting with T_c =2.9 K

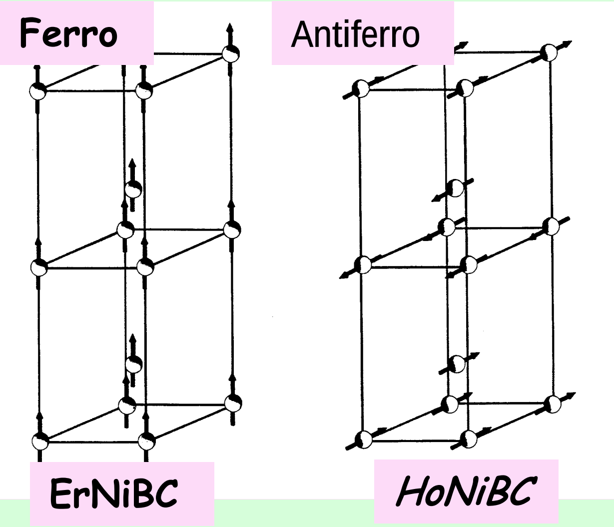
✓FM (ErNiBC) and AF (HoNiBC)

Magnetic structures

RNi_2B_2C →



$RNiBC$ →



RNi_2B_2C and RNiBC

- ✓ Superconductivity in RNi_2B_2C: interplay of superconductivity and magnetism with moderated Tc ~ 16K.

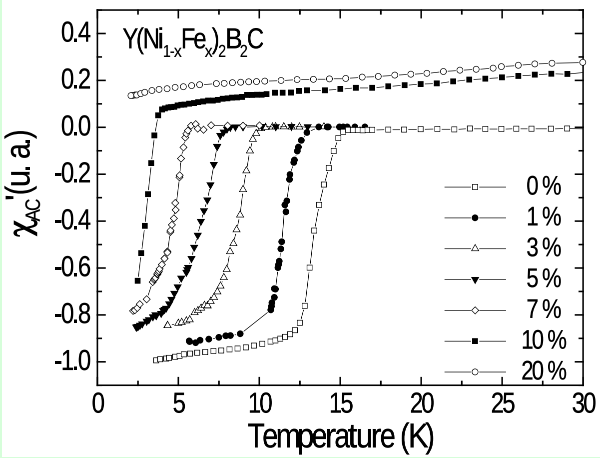
- ✓ The RNiBC series only R = Lu is SC with low T_c

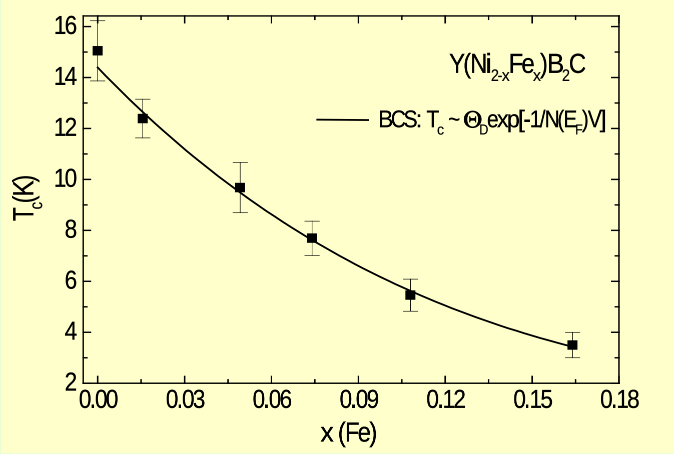
- ✓ The ^{57}Fe at the Ni site is an ideal probe to study the interplay of superconductivity and magnetism:

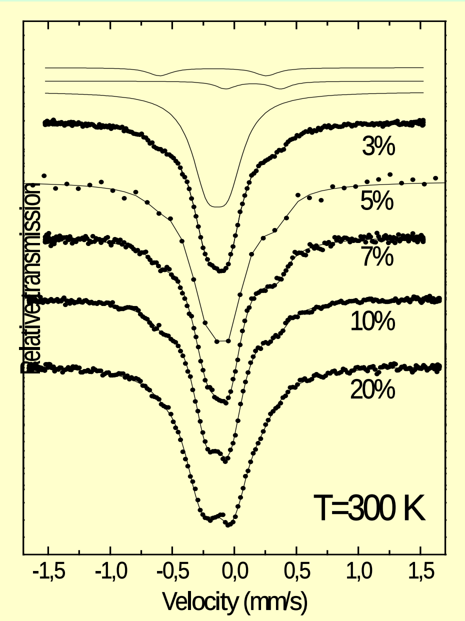
  - Why other members of the RNiBC series are not superconductors?

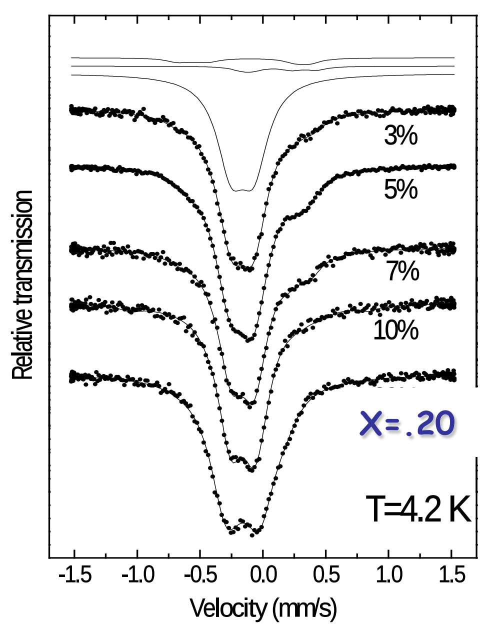
  - Role of structural features on the physical properties of RNi_2B_2C

Non magnetic $Y(Ni_{1-x}Fe_x)_2B_2C$









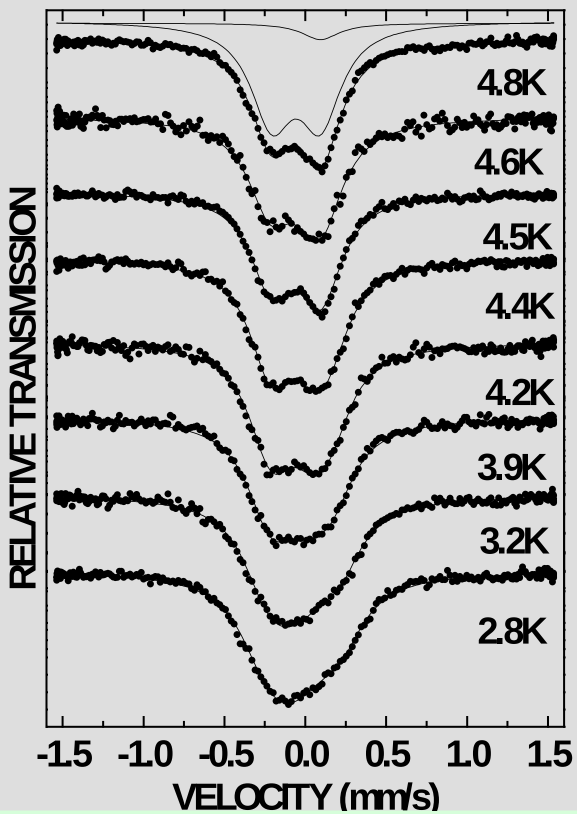
Variation of T_c determined mainly by $N(E_F)$

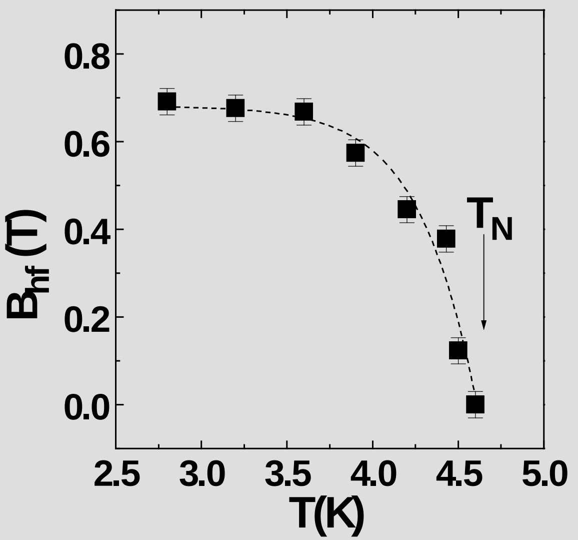
No magnetic hyperfine field at the Ni (Fe) site, for x=0.20.

Our sampes have ~1.5 % Fe

Fe has no magnetic moment

Magnetism in ErNiBC





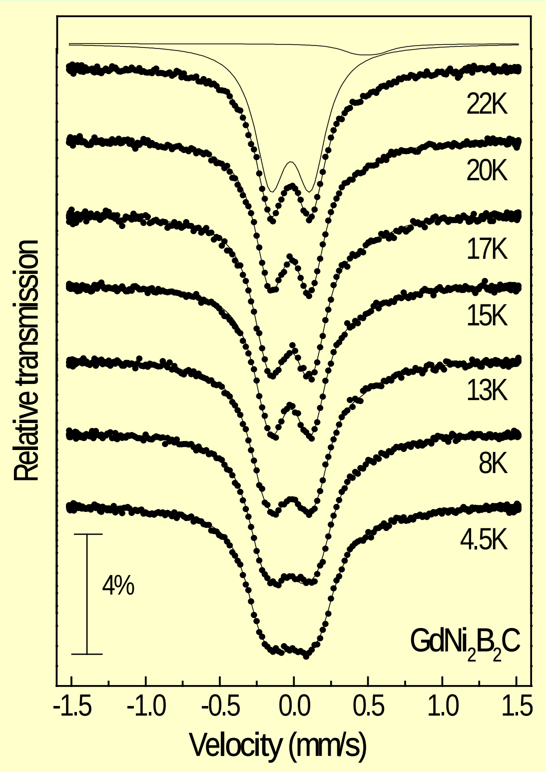
The ErNiBC orders ferromagnetically at 4.5 K,

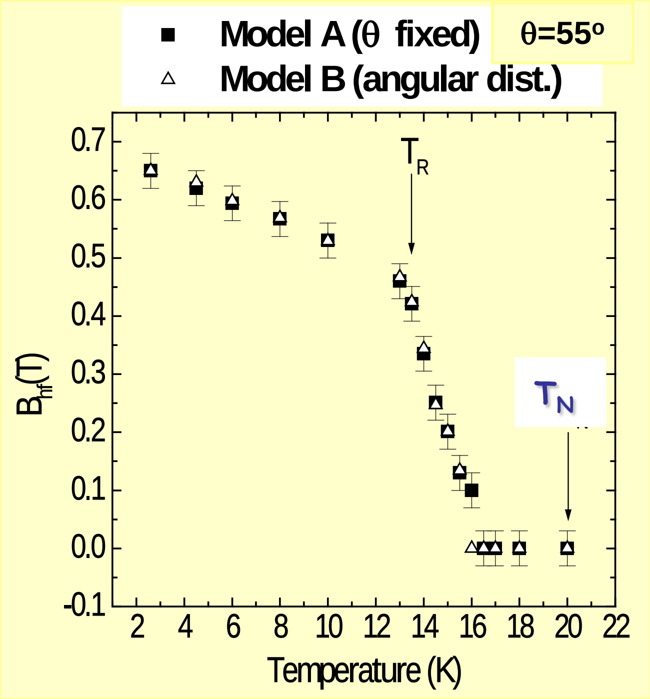
this order can be observed in the ^{57}Fe ME

$GdNi_2B_2C$

T_N=20K : incommensurate AFM

T_R~13.6K : second magnetic transition

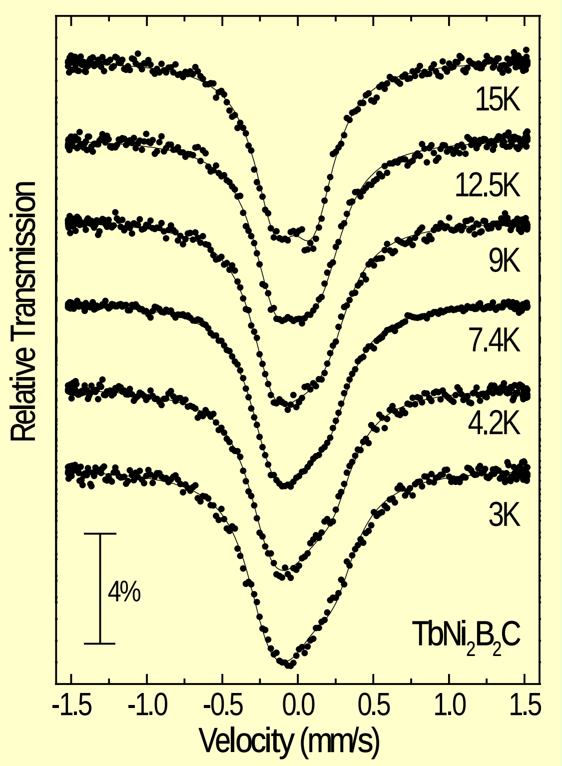


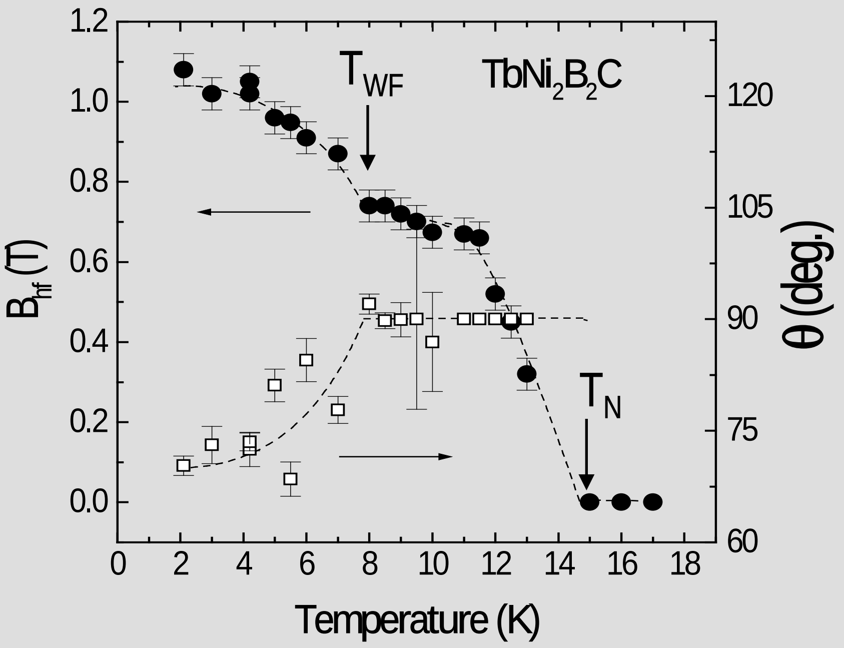


* D. R. Sánchez, H. Micklitz, M. B. Fontes and E. Baggio Saitovitch, J. Phys. Condens. Matter 9 L299(1997)

Magnetismo em $TbNi_2B_2C$ (Fe)

T_N~15K:AF





T<8K : Weak Ferro

8 K< T < 10 K: Vzz< 0 and θ ~90º

(planar AFM structure)

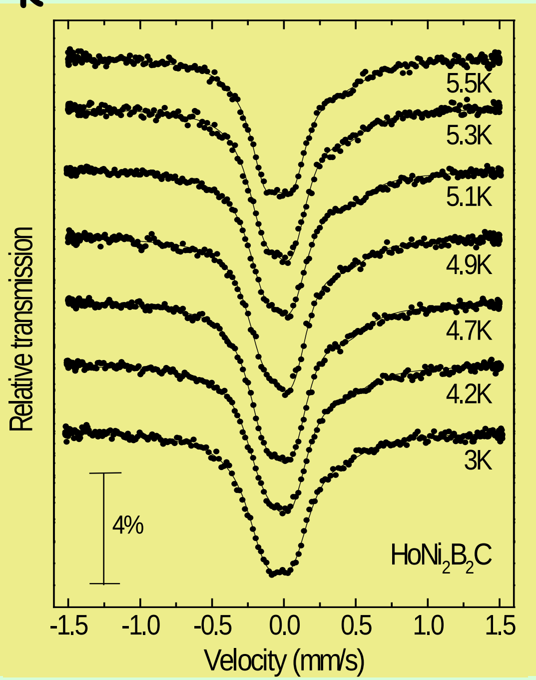
Below 8 K: θ decreases to ~ 70º

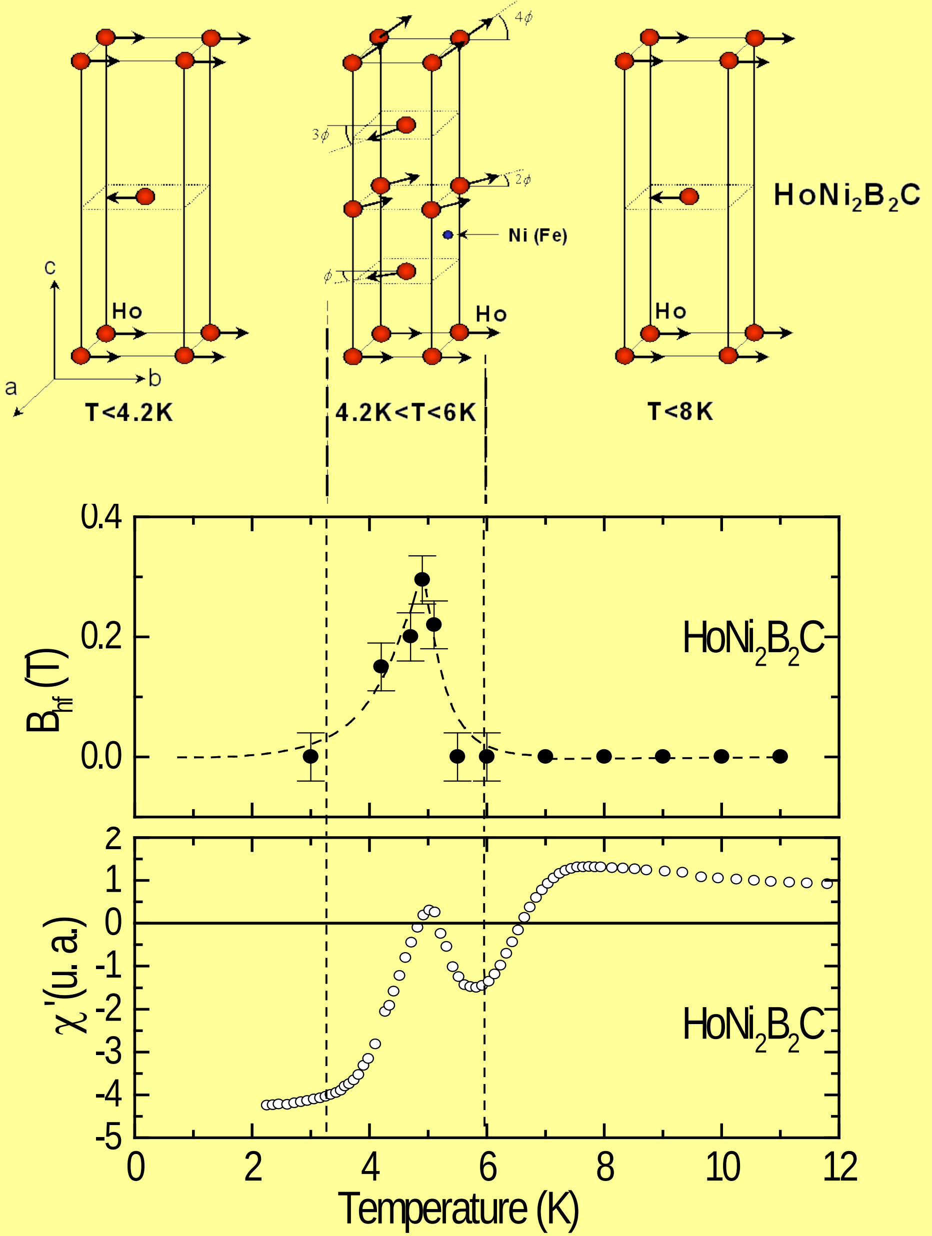
We relate these observations to a WFM component below 8 K (magnetization and neutron data only see this in single crystals).

D. R. Sánchez, S. L. Bud'ko, E. Baggio Saitovitch, Phys. Rev. B 57, (1998)

Superconductivity and Magnetism in $HoNi_2B_2C$

Reentrant behavior and incommensurate modulated magnetic structure for 4.6≤T≤6 K

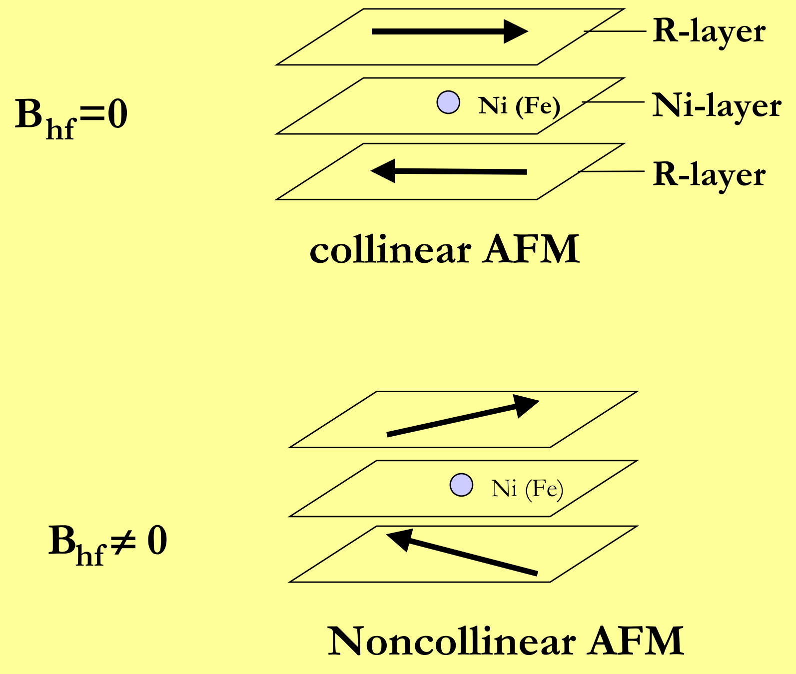


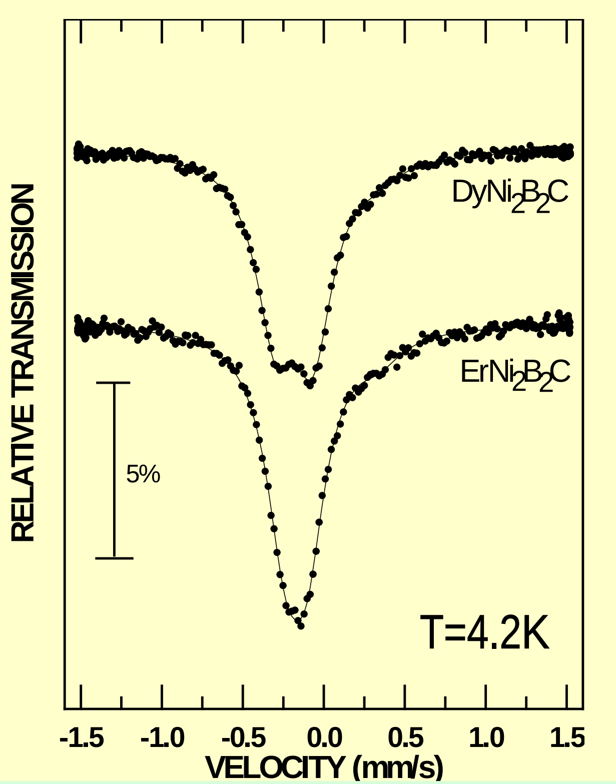


Evidence of pair-breaking field at the Ni (^{57}Fe)

D. R. Sánchez, H. Micklitz, M. B. Fontes, S. L. Bud’ko and E. Baggio Saitovitch, Phys. Rev. Lett. 76, 507 (1996)

$$B_{hf} = B_{thf} = \sum_i \alpha_i \vec{s}_i$$



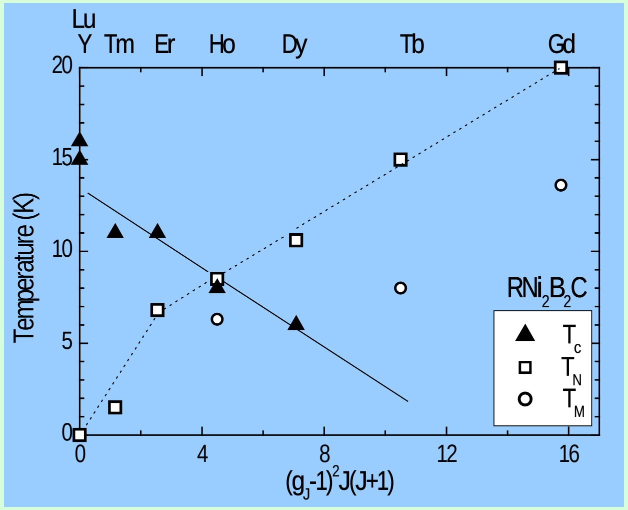


No magnetic hf field was observed at any temperature below T_N for the AFM *superconductors* $ErNi_2B_2C$ and $DyNi_2B_2C$

T_c scaling with de Gennes factor and/or Structural Effects in RNi_2B_2C

De Gennes scaling works quite well in:

- $(R_{1-x}R'_x)Ni_2B_2C$ if one of them (R or R') is magnetic, T_c will decrease according to Abrikosov-Gorkov theory.



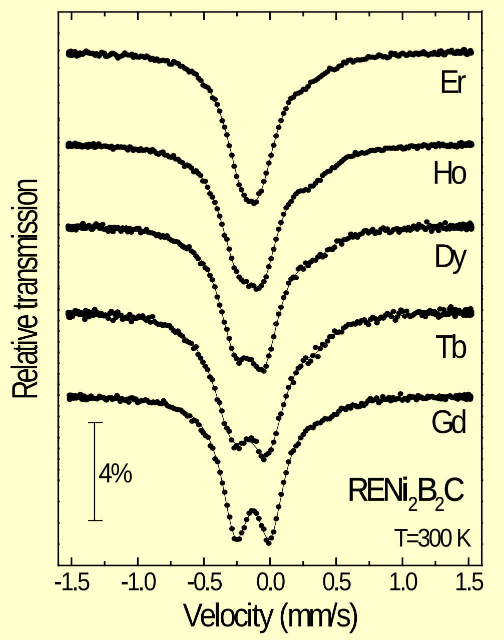
Issues that de Gennes scaling can not explain:

- High T_c of $LuNi_2B_2C$
- Absence of superconductivity in $LaNi_2B_2C$
- The decrease of T_c in the non-magnetic $(Y_{1-x}La_x)Ni_2B_2C$

We will address the structural aspects comparing RNi_2B_2C **with** RNiBC

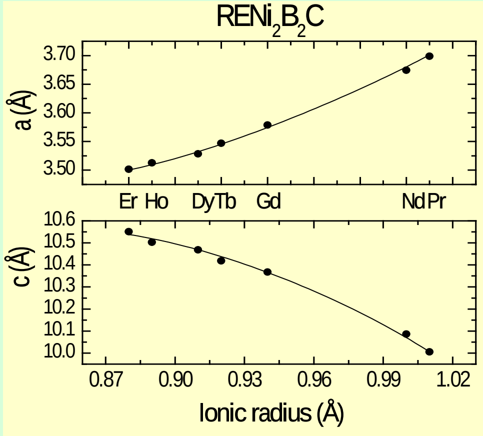
Structural Aspects

RNi$_2$B$_2$C

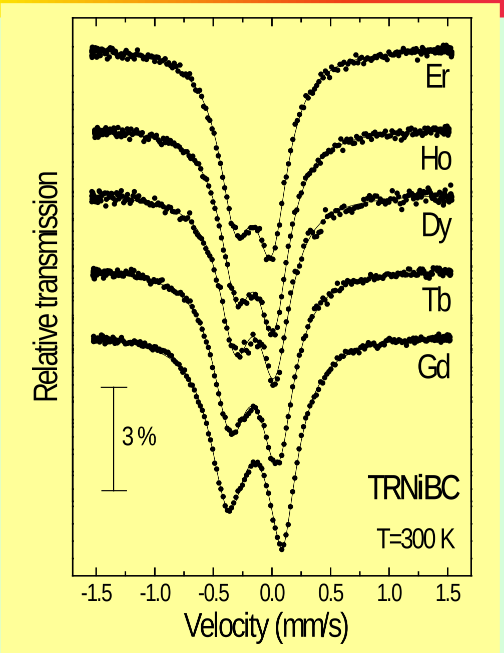


a

c

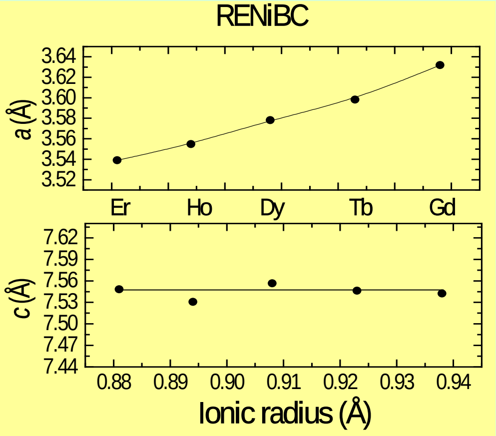


RNiBC



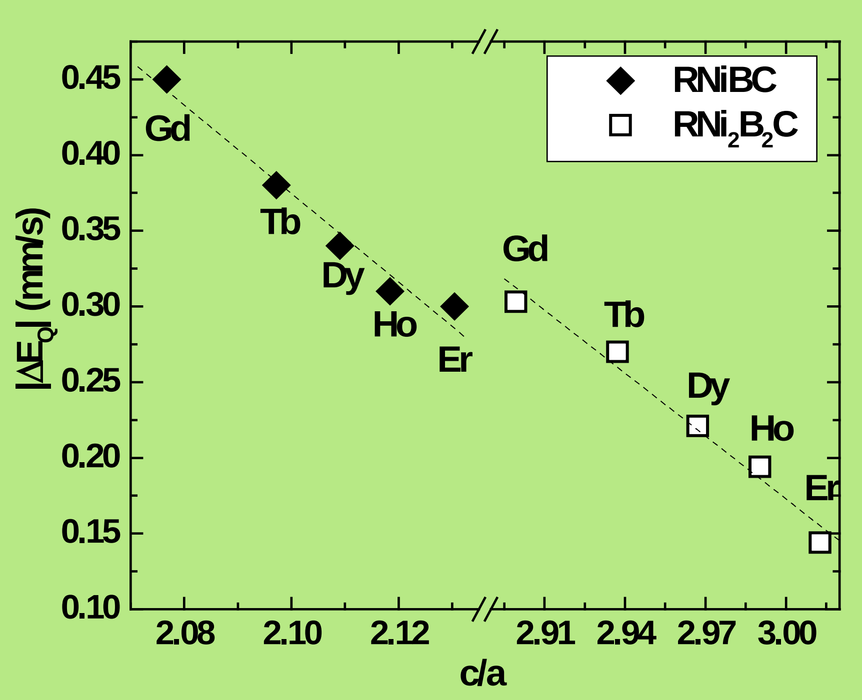
a

c

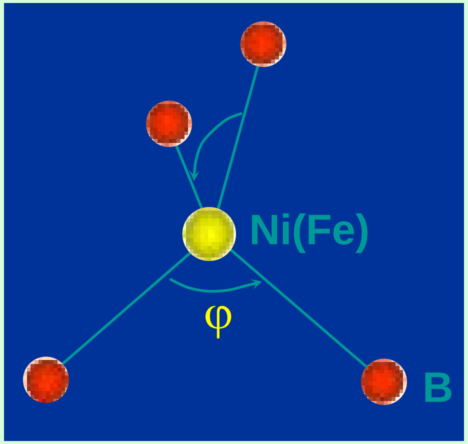


$|\Delta E_Q|$ vs c/a

$|\Delta E_Q|$ varies along the two series reflecting some correlation with the structure



$|\Delta E_Q|_{RNiBC} > |\Delta E_Q|_{RNi2B2C}$



First principles density-functional calculations (D. Ellis et al): Fe atomic charges and orbital populations are quite similar in the RNi_2B_2C series (IS~cte)

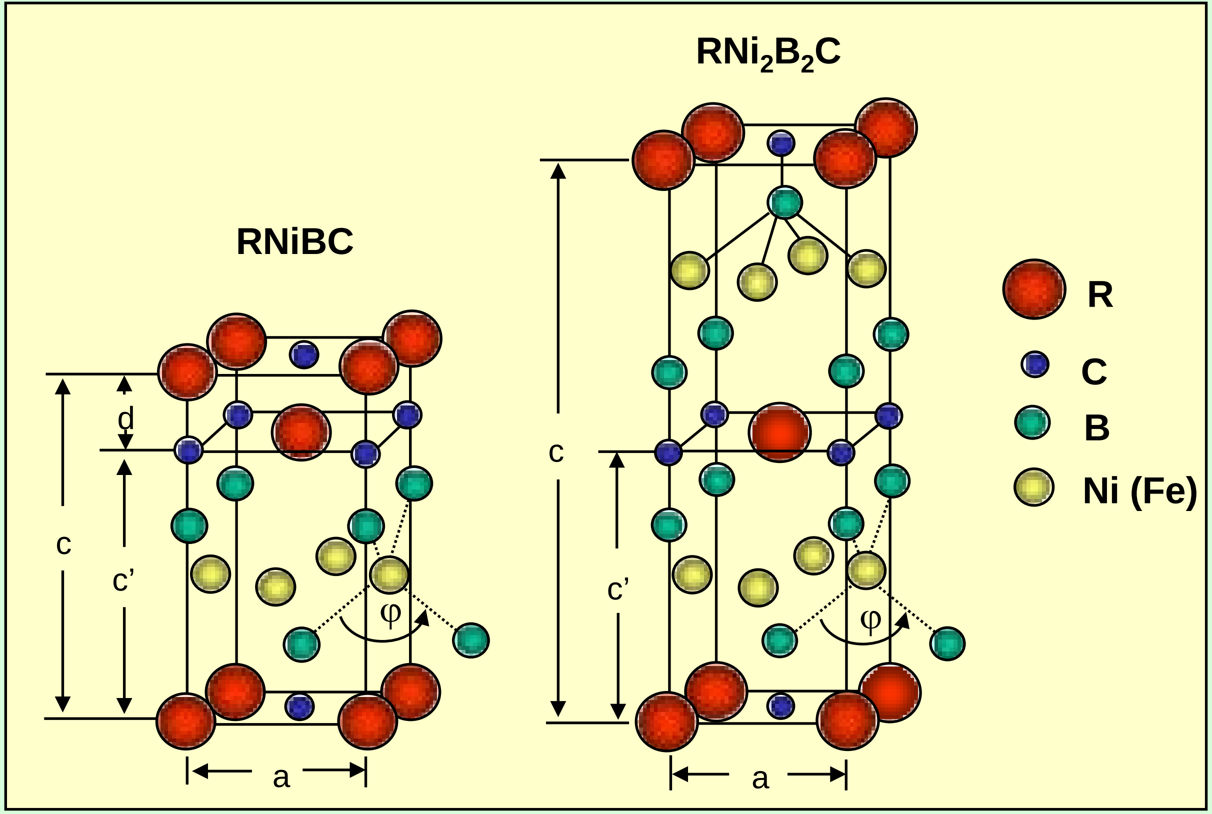
Thus geometrical effects induces changes in $|\Delta E_Q|$

Structures

The Ni_2-B_2 layers are essentially similar in both series of compounds.

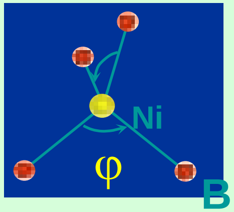
RNiBC : $c'=c-d$

RNi_2B_2C: $c'=c/2$



d is the spacing between two adjacent R-C layers

(*c'/a*) is a measure for the bonding angles φ of the NiB_4 tetrahedra.



$|\Delta E_Q|$ and T_c vs c'/a

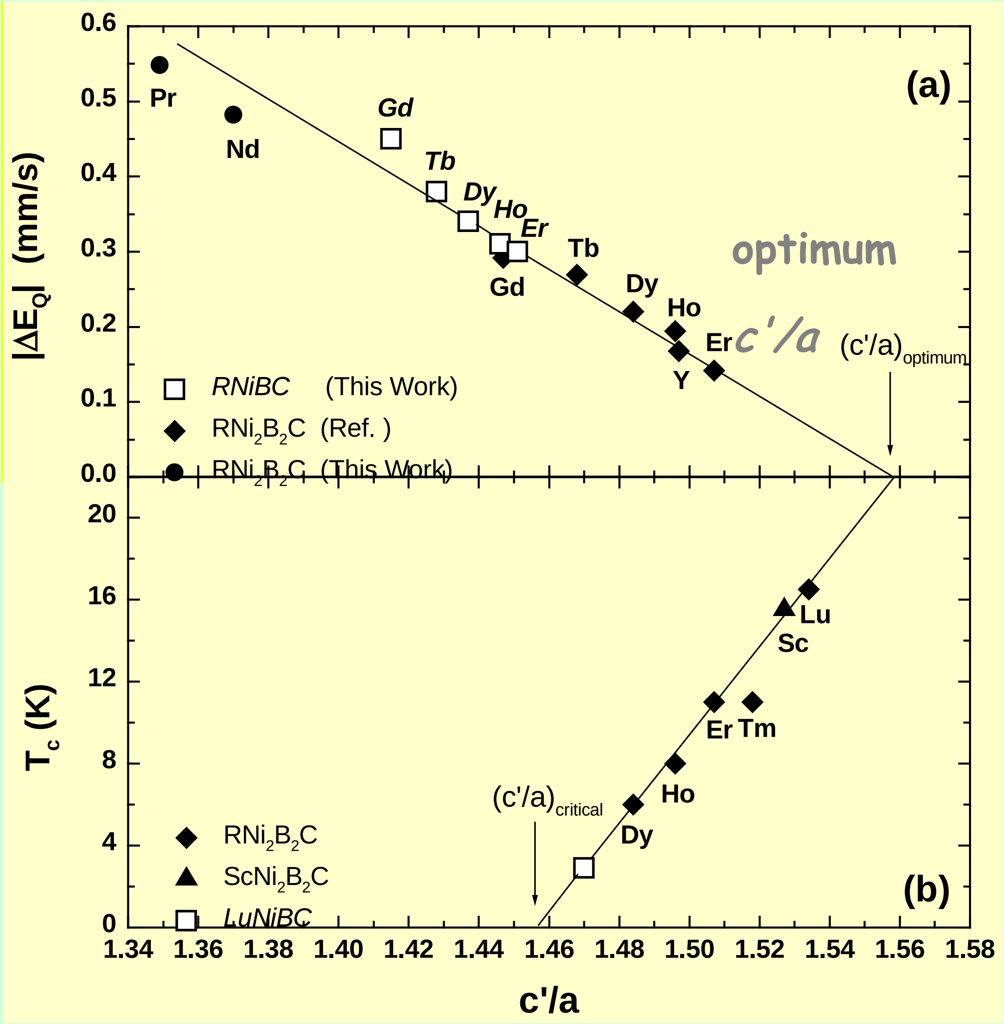
For RNiBC $(c'/a) < (c'/a)_{crit}$

except LuNiBC

$LuNi_2B_2C$ is not at optimum

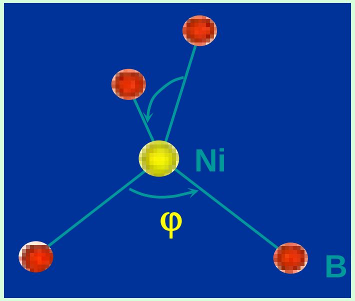
(c'/a) and

T_c could still go higher



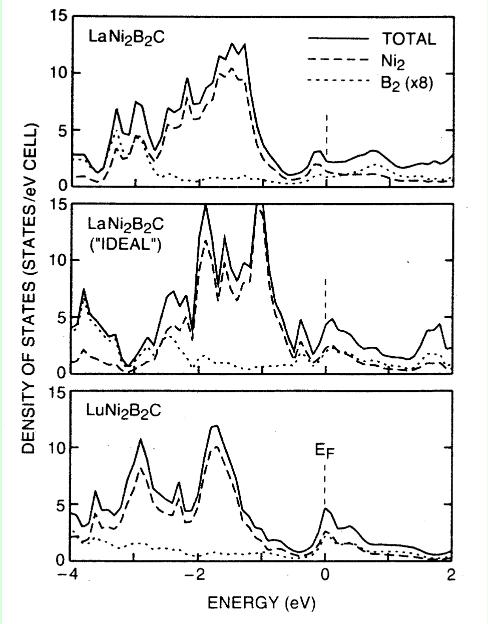
Superconductivity and Structural Features

DOS depends on the bonding angles in the Ni_2-B_2 tetrahedra.



Ideal tedrahedral symmetry at the Ni site

happens to be also “ideal” for superconductivity



Conclusions

- ^{57}Fe at the Ni site gives information about local symmetry and magnetic order in the RNi_2B_2C and RNiBC

- B_{hf} at the ^{57}Fe nucleus, resulting from the non collinear AF spin structure of the RE moments, acts as a pair-breaking field at the Ni site

- A new parameter (c'/a) determined by the Ni-B bonding angles was introduced to understand the geometrical variation between the two series

- Correlation between T_C and (c'/a) for both series explains why RNiBC series are non superconductors, except for Lu

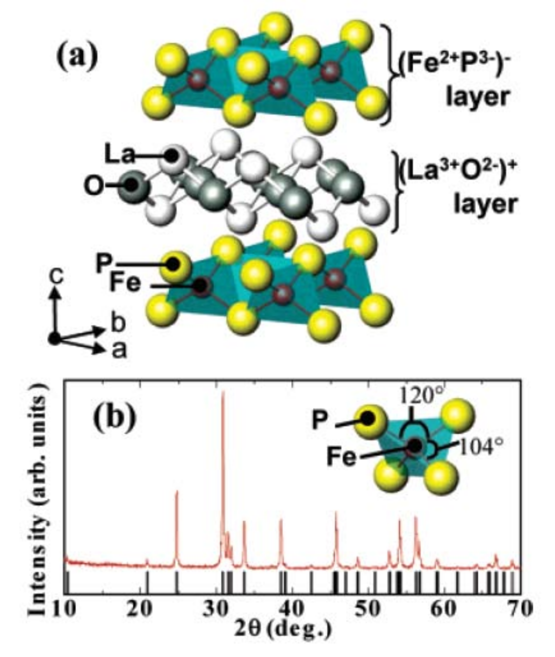
Magnetism and Superconductivity in the iron-based layered compounds: $RFeAsO_{1-x}F_x$ (R=Nd, CeSm) and $CaFe_2As_2$

D. R. Sánchez, M. Alzamora, J. Munevar , Y. Xing,
N. L. Wang , S. L. Budko***

*Beijing National Laboratory for Condensed Matter Physics, Institute of Physics,
Chinese Academy of Sciences, Beijing 100080, Peoples Republic of China
**Ames Laboratory, U.S. DOE and Department of Physics and Astronomy, Iowa State
University, Ames, USA

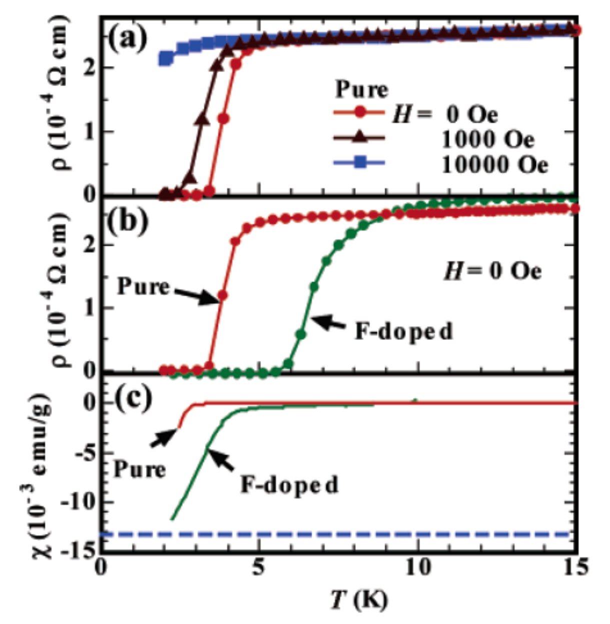
Iron-Based Layered Superconductor: LaOFeP

The compounds RFeXO
R=La...Gd,
X=P - 1995
X=As - 2000.



Tetragonal structure P4/nmm

Only in 2006 a report appeared for superconductivity in LaFePO,



Tc ~ 4K

Kamihara, Y. et al.
J. Am. Chem. Soc. 128, 10012-10013 (2006)

- Oxygen deficiency or
- Impurities: *$LaFe_4P_{12}$* → Tc=4.1 K
  La → Tc=6.9 K

*B. I. Zimmer, et al., J. Alloys Compd. 229, 238 (1995).
**P. Quebe, et al., J. Alloys Compd. 302, 70 (2000).

Iron-arsenide-oxides layered Superconductor $LaO_{1-x}F_xFeAs$

The recent discovery of superconductivity in doped iron-arsenide-oxides has generated enormous interests in the community of superconductivity.

J|A|C|S
COMMUNICATIONS

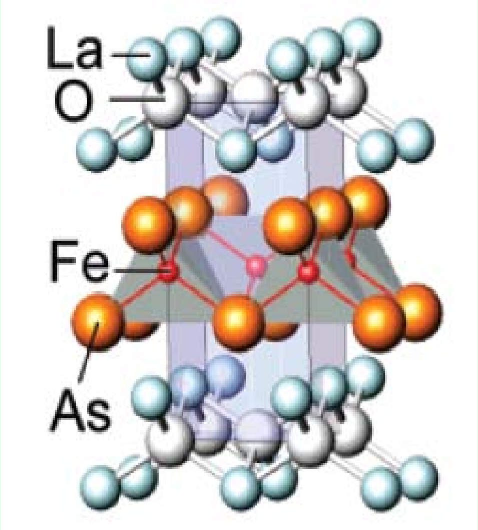
Published on Web 02/23/2008

Iron-Based Layered Superconductor La[$O_{1-x}F_x$]FeAs (x = 0.05−0.12) with T_c = 26 K

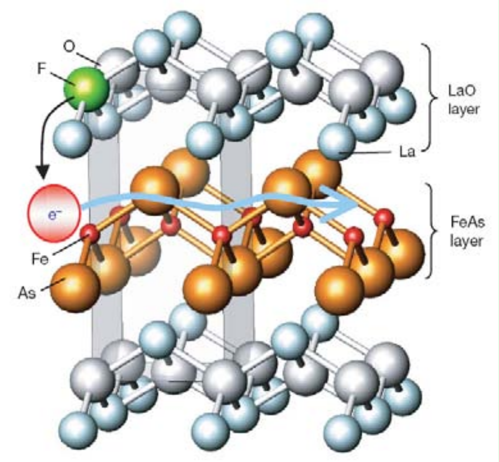
Yoichi Kamihara,[*,†] Takumi Watanabe,[‡] Masahiro Hirano,[†,§] and Hideo Hosono[†,‡,§]

LaOFeAs -> SC under
- doping with F^-
- oxygen deficiency

carrier doping in the FeAs layer due ion substitution in the insulating layers



Tetragonal structure (P4/nmm).



The crystal is composed of a stack of alternating LaO and FeAs layers.

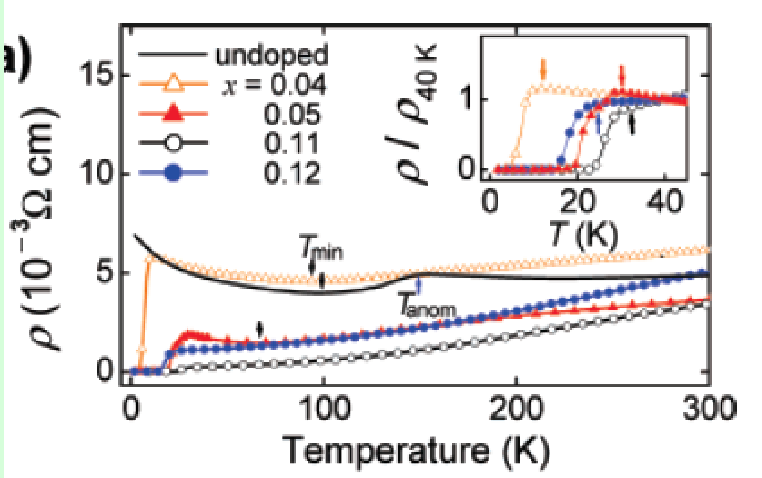
ROFeAs 1111 R=La……Gd

AFe_2As_2 122 A=Ba, Ca Sr, Eu

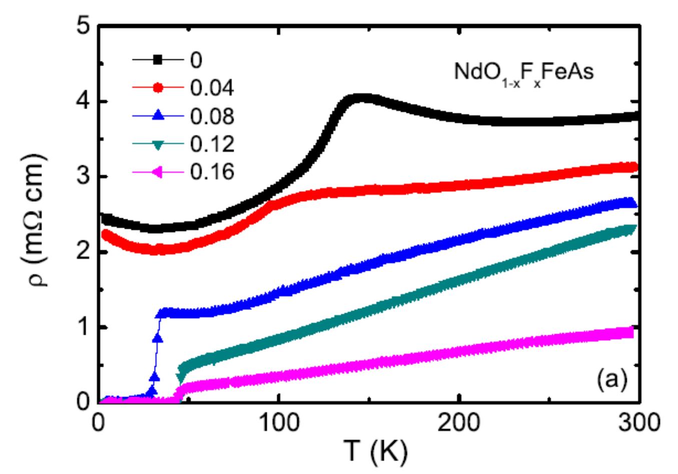
*D. Johrendt and R. Pottgen, Angew. Chem. Int. Ed. 47, 4782 (2008).

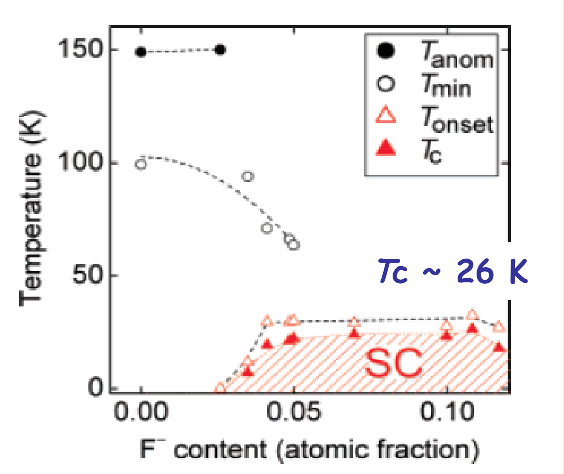
Superconductivity under F doping and pressure: T_C and T_N

LaOFFeAs



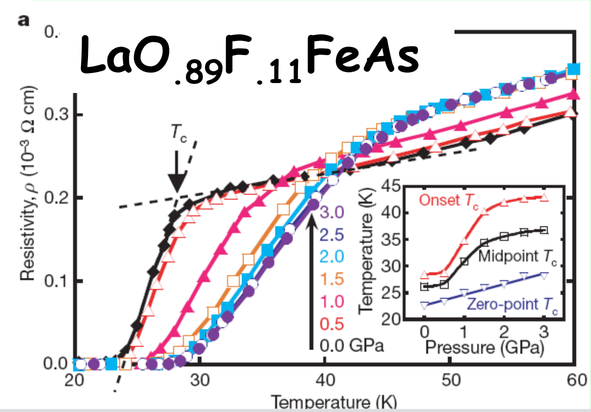
NdOFFeAs



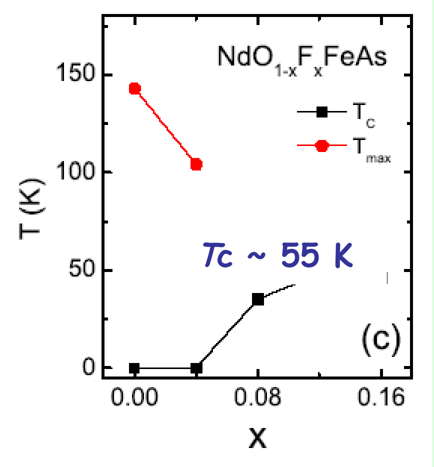


Tc ~ 26 K

$LaO_{.89}F_{.11}FeAs$



Vol 453|15 April 2008|**doi:10.1038/nature06972**



Tc ~ 55 K

D. Johrendt & R. Pottgen, Angew. Chem. Int. Ed. 47, 4782 (2008)

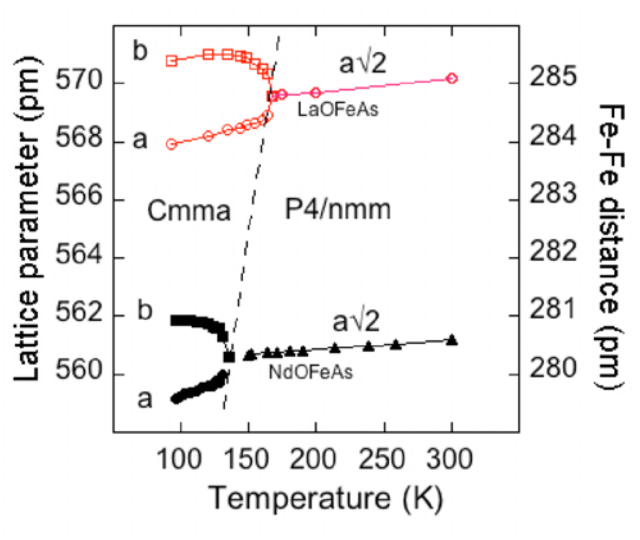
G. F. Chen, et al., arXiv:0803.4384v1 (2008)
Y. Qiu, et al., arXiv:0806.2195v2 (2008)

Structural phase transition ROFeAs

tetragonal → orthorhombic phase,

LaOFeAs
$T_{T/O}$~155K

NdOFeAs
$T_{T/O}$~147K



From X ray and neutron diffrction

$T_{T/O}$ decreases with F doping

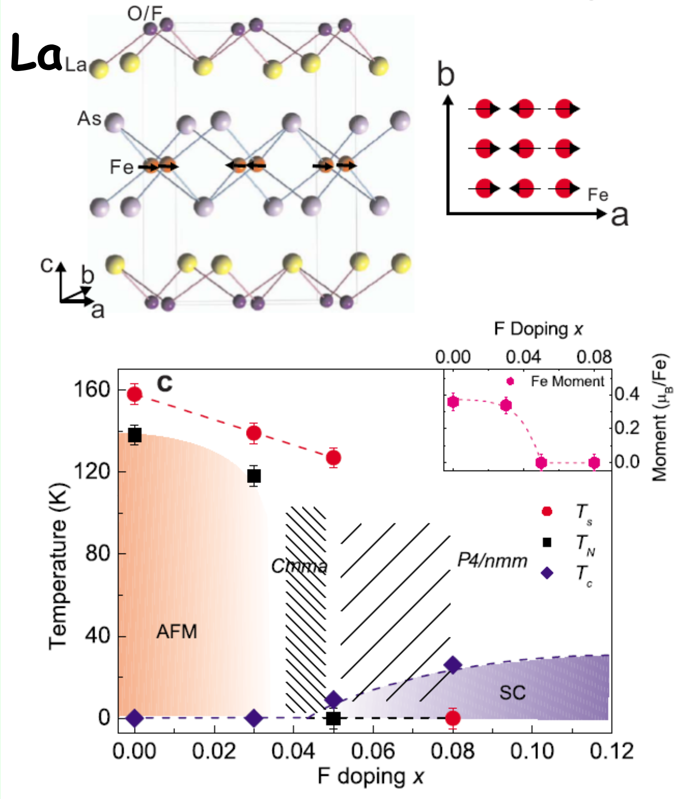
and disappears before SC

Fratini M et al Supercond. Sci. Technol. 21, 092002 (2008)
[Ying Chen et al., B 78, 064515 (2008)

[10] Fratini M et al Supercond. Sci. Technol. 21, 092002 (2008)
[11] Ying Chen et al., B 78, 064515 (2008)

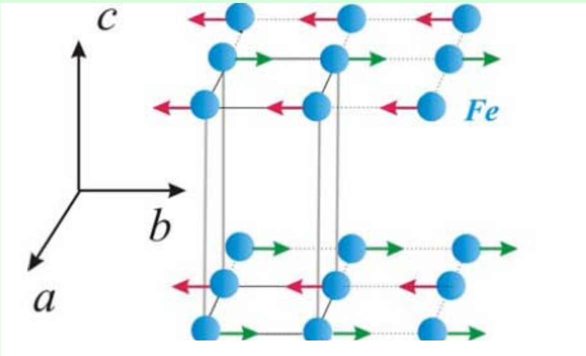
[10] Fratini M et al Supercond. Sci. Technol. 21, 092002 (200

Magnetic order $LaO_{1-x}F_xFeAs$ $NdO_{1-x}F_xFeAs$



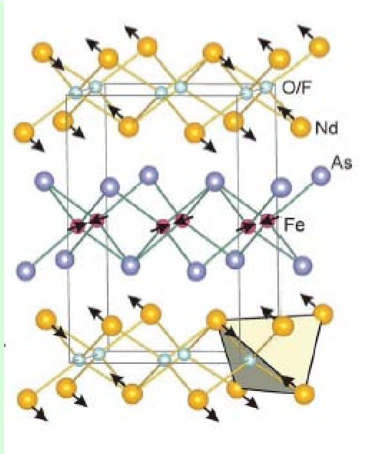
Neutron diffraction

Nd



T_N ~ 141K

T ~ 2K order of Nd moments



long range *SDW-type antiferromagnetic order* at T_N~137 K with Fe small moment

μ_{Fe}=0.36(5) μ_B **for x~0.04**

μ_{Fe}=0.25(7) μ_B

C. de la Cruz, et al. Nature 453(2008).
Nomura T, et al. , 2008 *preprint* arXiv:0804.3569
Q. Huang, et al., Phys Rev 78, 054529 (2008)

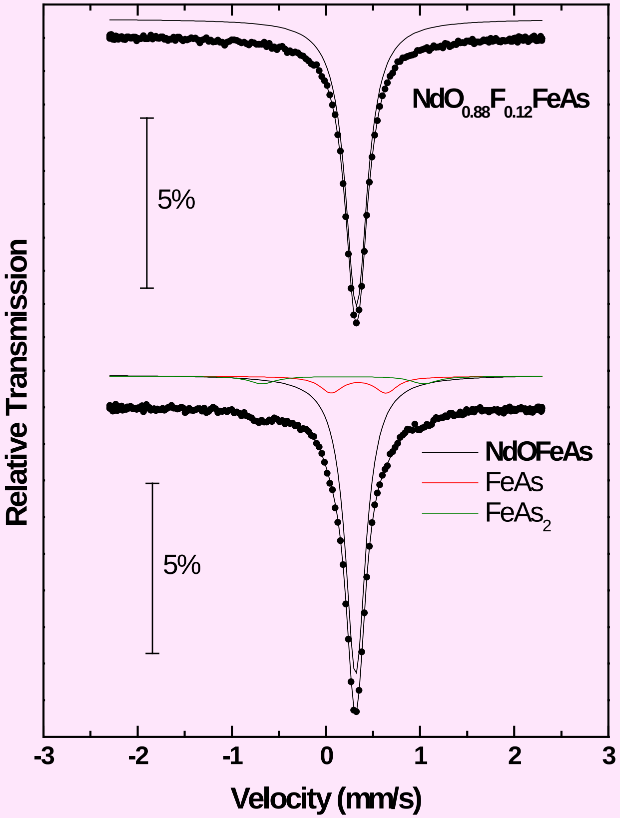
EXPERIMENTAL

Ceramic samples of NdOFeAs and $NdO_{0.88}F_{0.12}FeAs$ polycrystals were synthesized at *Institute of Physics, Chinese Academy of Sciences, Beijing, China.*

Ternary iron-arsenide samples of AFe2As2 Ames Laboratory, Iowa State University, Ames, USA

Magnetization, Mössbauer and XRD measurements were performed at CBPF

Room temperature Mössbauer Spectroscopy: NdOFeAs



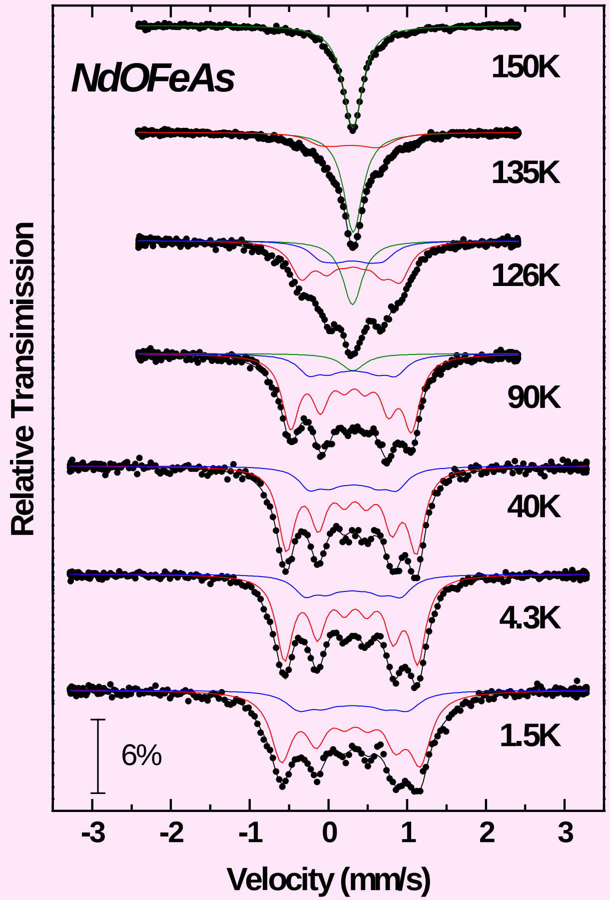
Doublet with ΔE_Q=0.02(2) *mm/s* and δ_{IS}=*0.44 mm/s*, indicating a unique phase for Fe. These values are similar to that found for LaOFeAs [12]

Small **impurities of FeAs** (absorption area A~ 8%) and $FeAs_2$ (~5%)
The main component (doublet) is attributed to Fe in NdOFeAs phase and their hyperfine parameters are almost the same as for $NdO_{0.88}F_{0.12}FeAs$

The δ_{IS} (*~0.44 mm/s*)

[12] H.-H. Klauss et al., Phys. Rev. Lett. 101, 077005 (2008)

Low temperature MS for NdOFeAs



Below T_N~ 140K a fraction of paramagnetic component begins to broaden magnetically showing the onset of the magnetic ordering

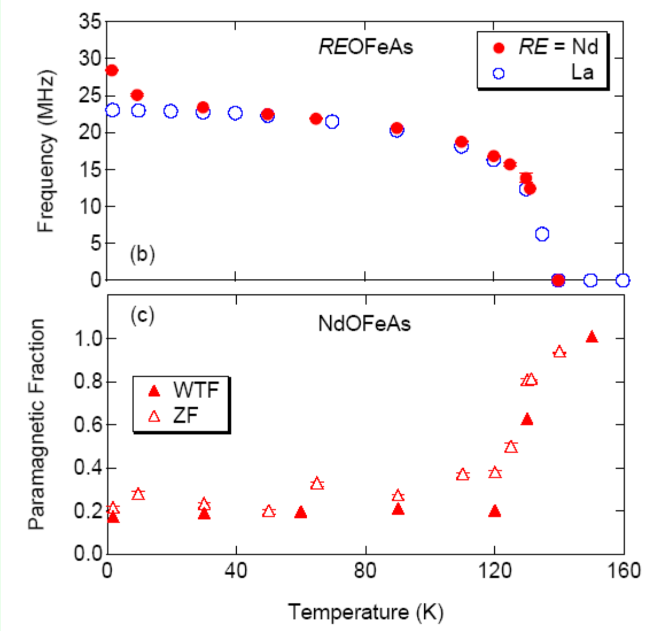
Below T_N the spectra were fitted with two components: one singlet and one sextet.

Below 126K an additional sextet was included in the fit.

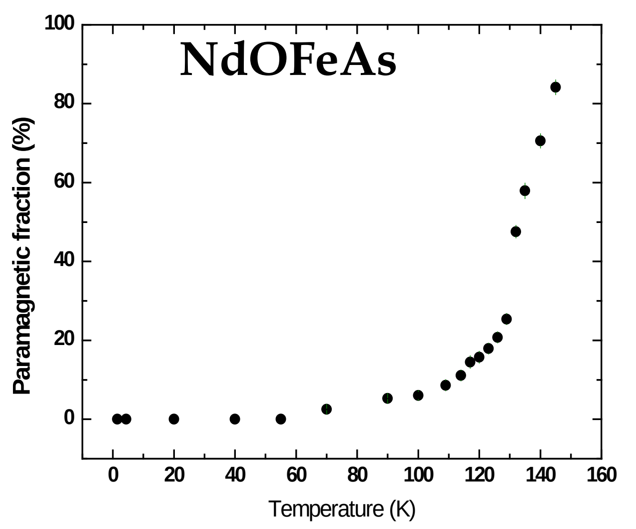
ΔE_Q=0.15(2) *mm/s* for the magnetic components.

Increase of ΔE_Q below T_N is caused by the orthorhombic distortion due structural phase transition.
(ΔE_Q → reflects the lattice distortion)

Mossbauer and µSR in the same NdOFeAs sample



muons in paramagnetic environment [6]



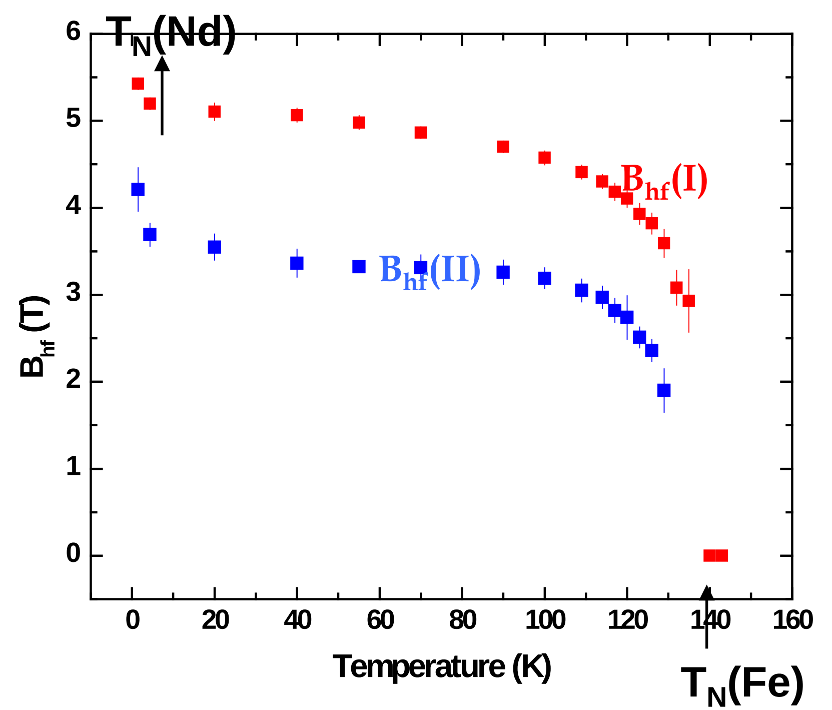
Mössbauer

Fraction of Fe ions in paramagnetic state

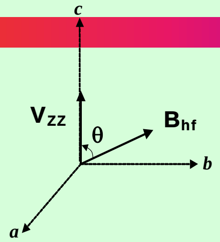
µSR results [6] support the Mössbauer data.

[6]A. A. Aczelet al. arxiv:0807.1044 (2008)

NdOFeAs



θ: angle between V_{zz} and B_{hf}



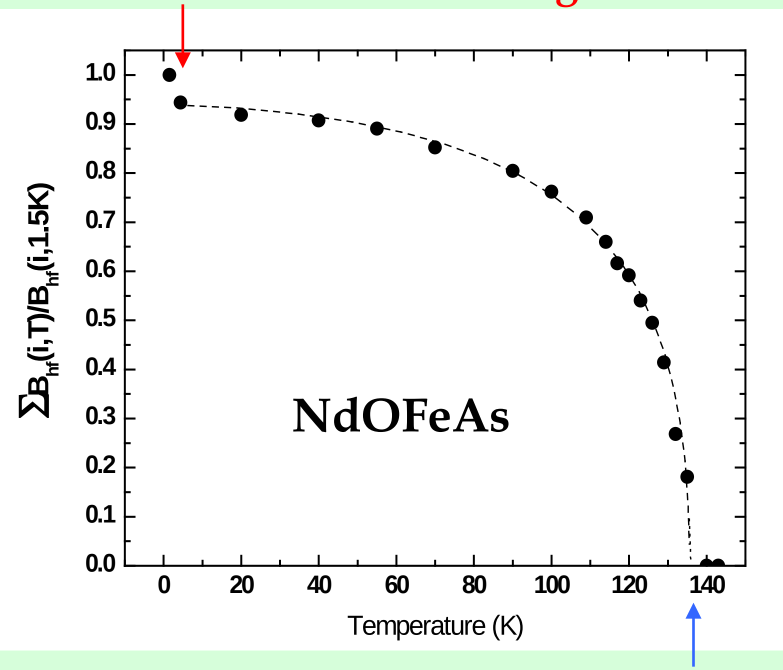
For main magnetic component (I) (A~ 80%): θ(I)~90º

For the minor component (II): θ(II)≈55º
magic angle or angle distribution (0≤ θ ≤90º)

These results speak for a **commensurate antiferromagnetic order** below T_N in agreement with recent μSR results [6].

The minor magnetic component could also be related with small variations of the oxygen content.

*an incommensurate SDW should lead to a very broad hyperfine field distribution ranging from zero to a maximum field value



Nd moments ordering

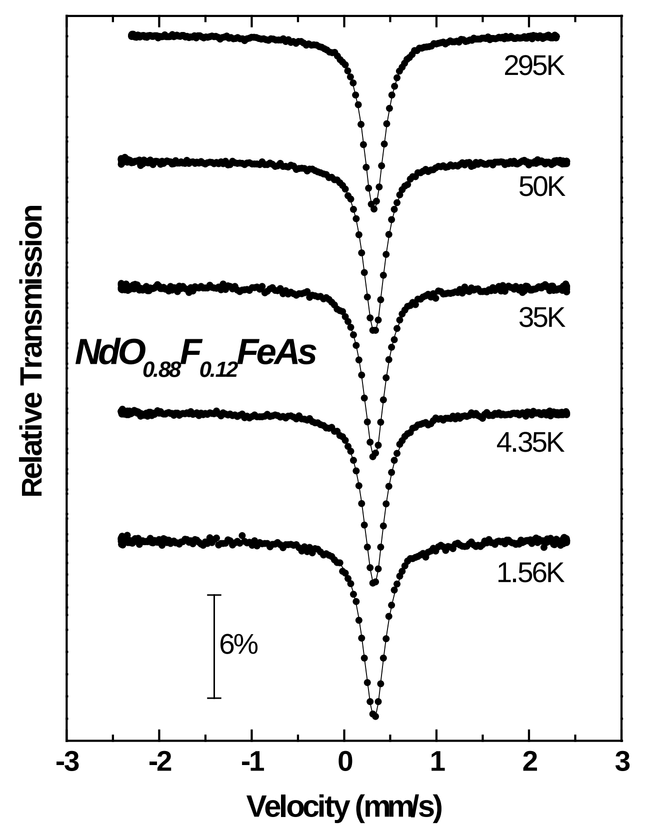
T_N (Fe moments ordering)

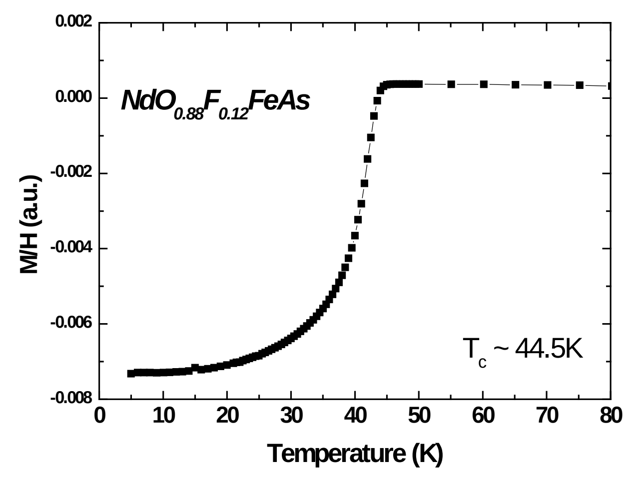
<u>Total magnetization curve</u>,
each Fe ion is contributing according with its relative intensity in the Mössbauer spectra.

The increase of B_{hf} at 1.5 K is due to magnetic order of the Nd moments (observed by neutron diffraction below 2K [5]).

From this curve NdOFeAs: $\mu_{Fe} \approx 0.34\ \mu_B$ (from neutron $\mu_{Fe} \approx 0.35\ \mu B$)

Low temperature MS for superconducting $NdO_{0.88}F_{0.12}FeAs$ (T_c~44.5K)





No change with different temperatures

No **hyperfine magnetic field was observed at ^{57}Fe nucleus [$B_{hf}(1.5K) \leq 0.1T$] of Fe in superconducting $NdO_{0.88}F_{0.12}FeAs$ down to 1.5K**

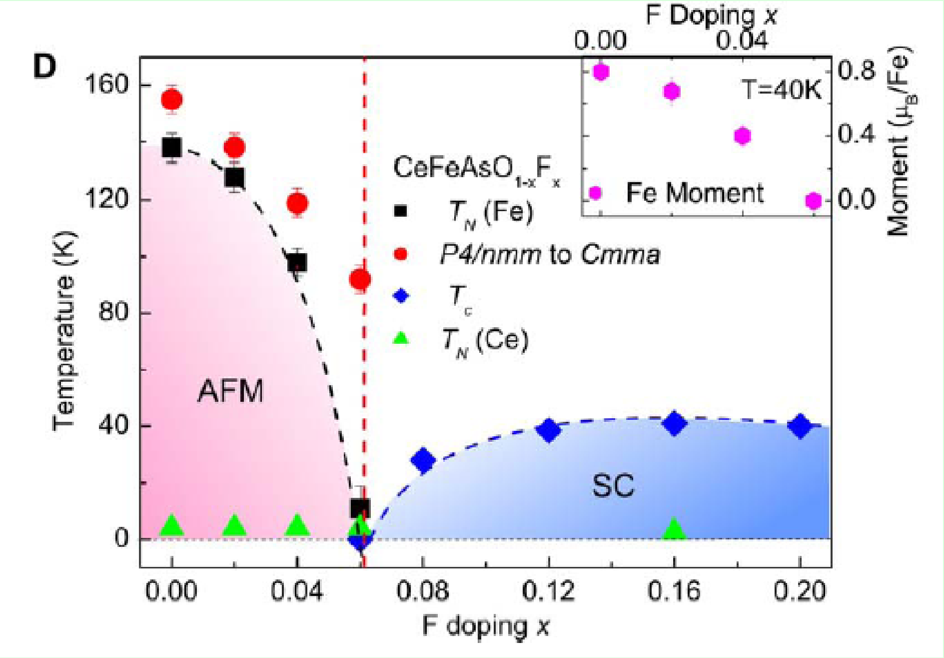
CONCLUSION

The peculiar hyperfine parameters found for **NdOFeAs** could be associated with a commensurate SDW antiferromagnetic order below 141K. The magnetic moment of the Fe was estimated to be ~0.34 μ_B in this compound.

No hyperfine magnetic field was observed at ^{57}Fe nucleus of Fe in superconducting **$NdO_{0.88}F_{0.12}FeAs$** at any temperature indicating absence of magnetism in this compound

Doping the system with F suppresses both the magnetic order and structural distortion in favor of superconductivity

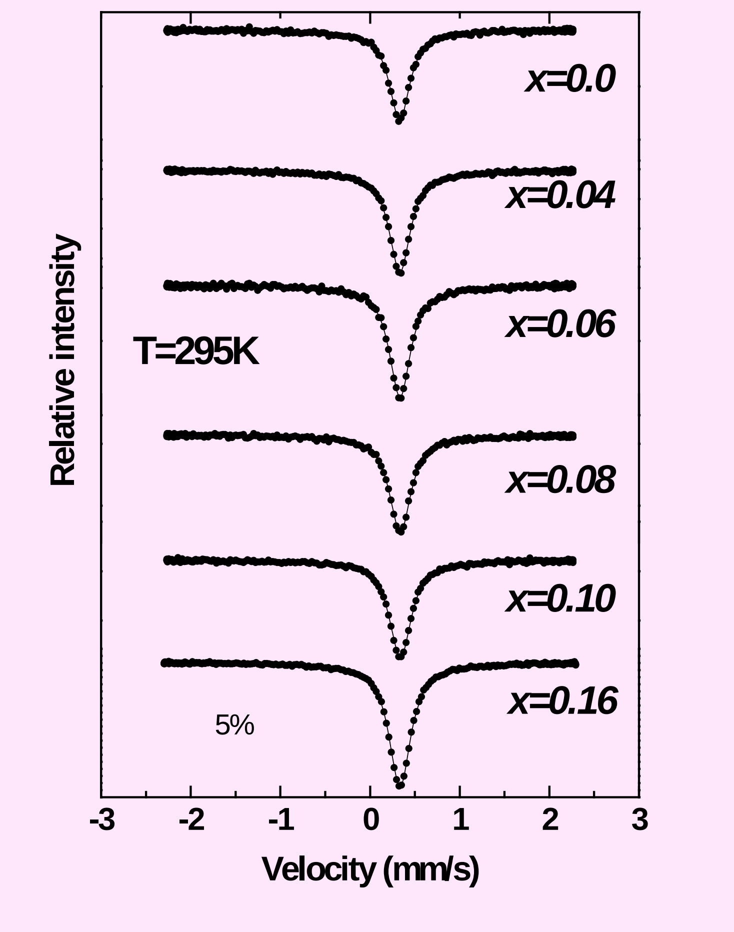
$CeO_{1-x}F_xFeAs$

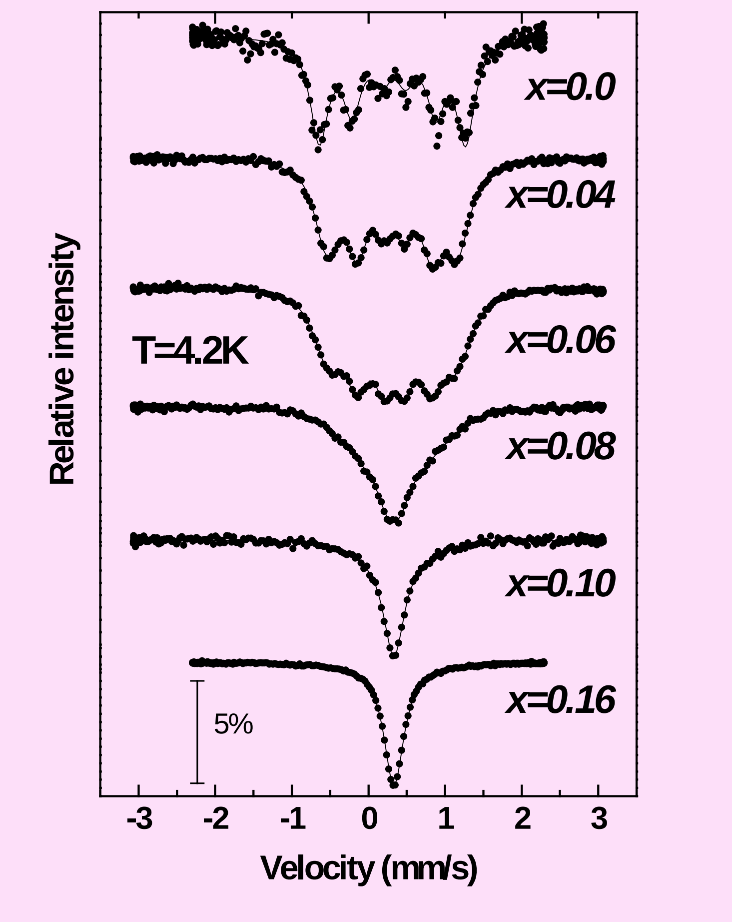


Neutron studies

[13] Jun Zhao Cond-mat arXiv:0806.2528 (2008).

Mössbauer studies in $CeO_{1-x}F_xFeAs$



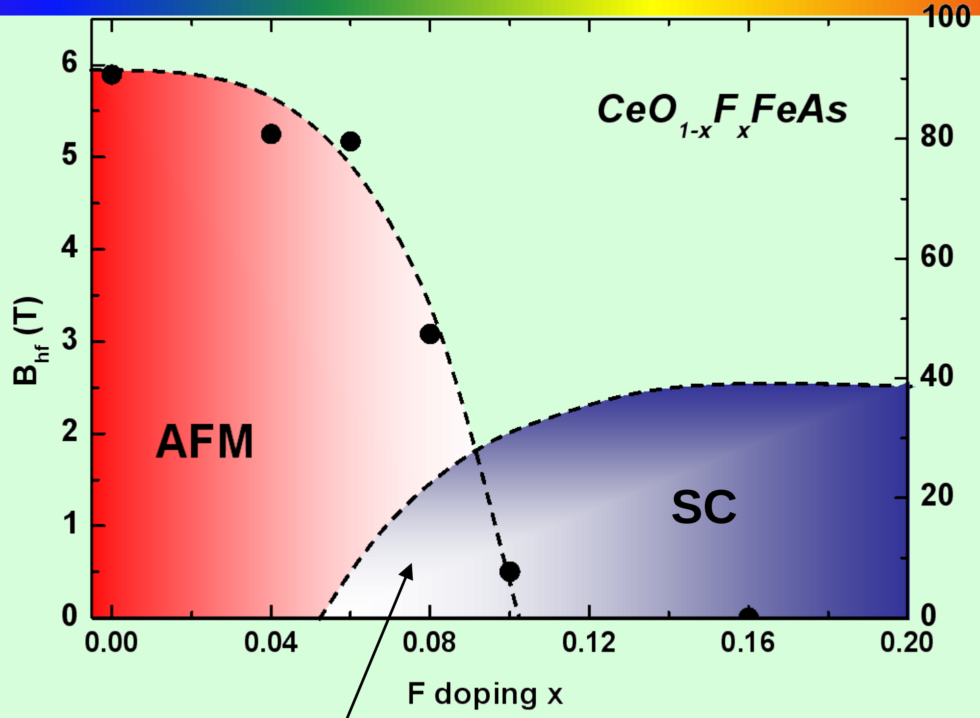


Room temperature: single lines with almost the same hyperfine parameters.

4.2 K: hyperfine magnetic field at Fe nucleus decrease with the increase of F content. Magnetism suppressed by F doping.

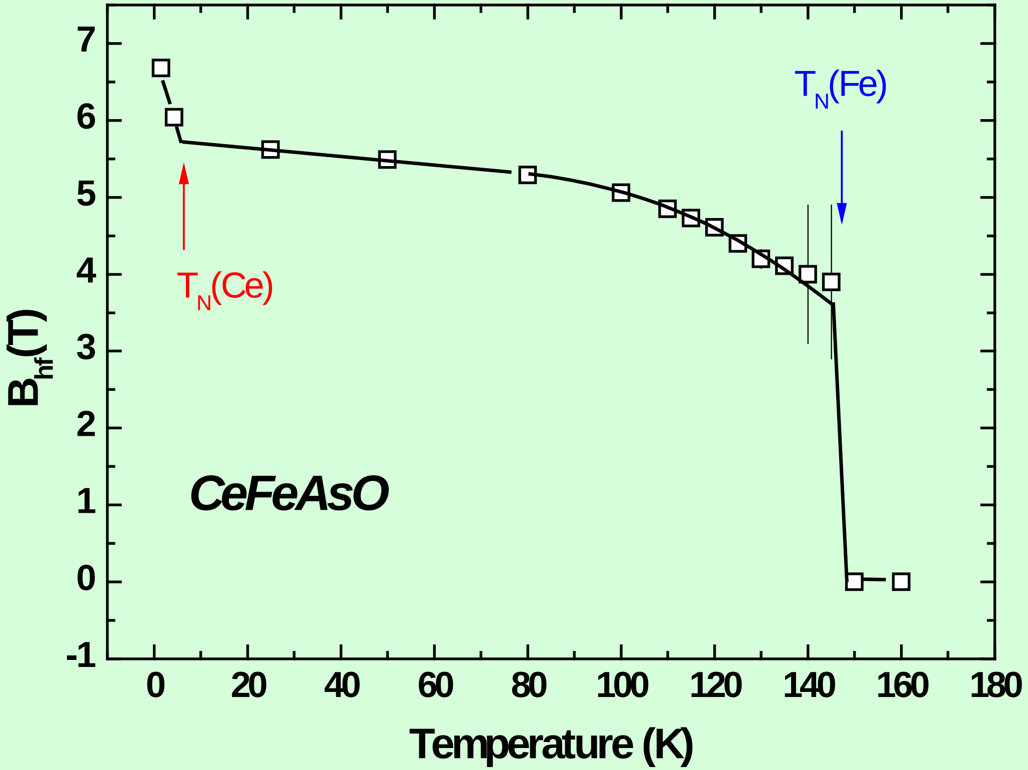
Preliminary results for $CeO_{1-x}F_xFeAs$

CeOFeAs:
$\mu_{Fe} \approx 0.39\ \mu_B$



Our preliminary Mössbauer results shown a region of coexistence of superconductivity and magnetism

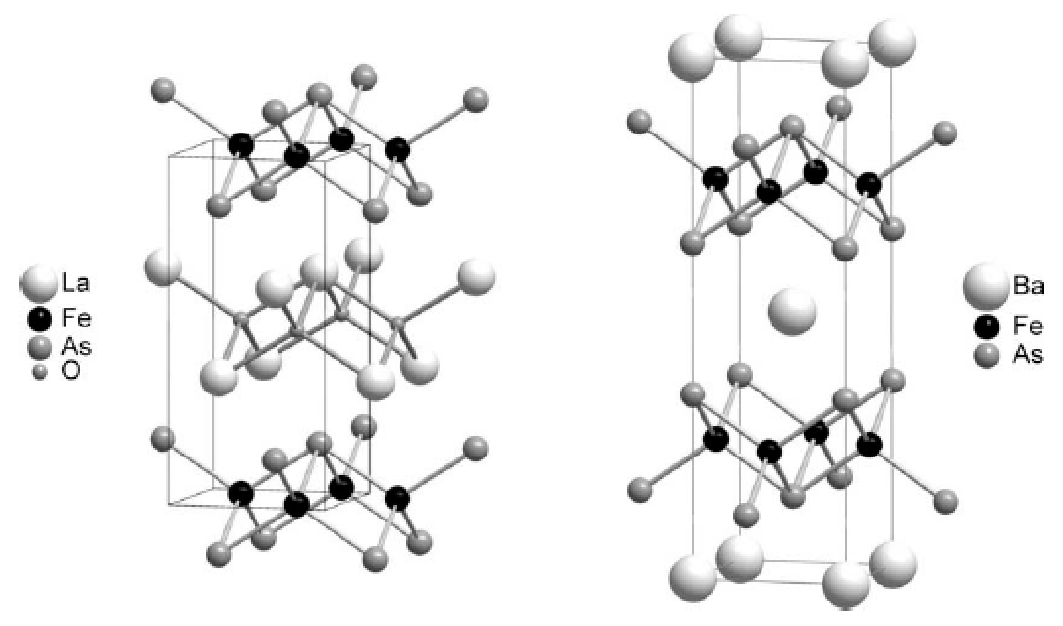
A strong covalency, i.e., a possible delocalization of spin density from the Fe 3*d* to adjacent As atoms could, in principle, reduce the measured hyperfine field at the iron nucleus as determined by Mossbauer spectroscopy.



The magnetic transition at ~ 147K is due to ordering of Fe moments.
The increase of Bhf below ~ 6 K is due to magnetic order of the Ce moments

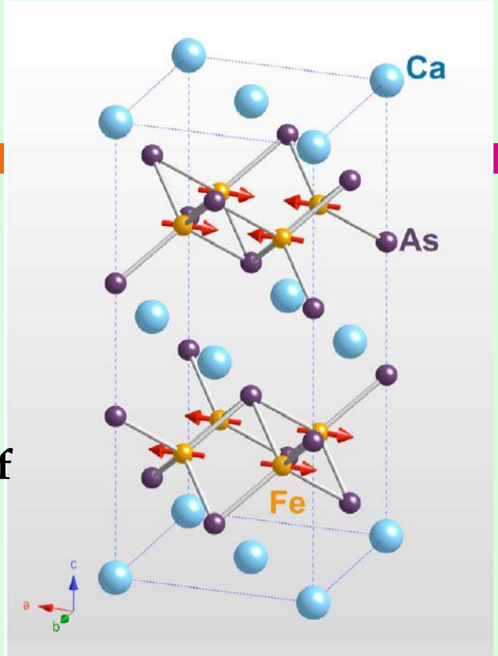
*Jun Zhao, et al., arXiv:0806.2528 (2008)

Ternary iron-arsenide AFe_2As_2 (A=Ba, Ca, Sr) 122 family



	LaOFeAs	$BaFe_2As_2$
Structure:	tetragonal *P4/nmm*	Tetragonal *I4/mmm*
Structural transition:	below ~ 140K	below ~ 140K
Magnetic ordering:	below ~ 155K	below ~ 140K
Superconducting transition:	under F doping	under K doping

Ternary iron-arsenide $CaFe_2As_2$



Recent neutron studies in $CaFe_2As_2$ [14]:

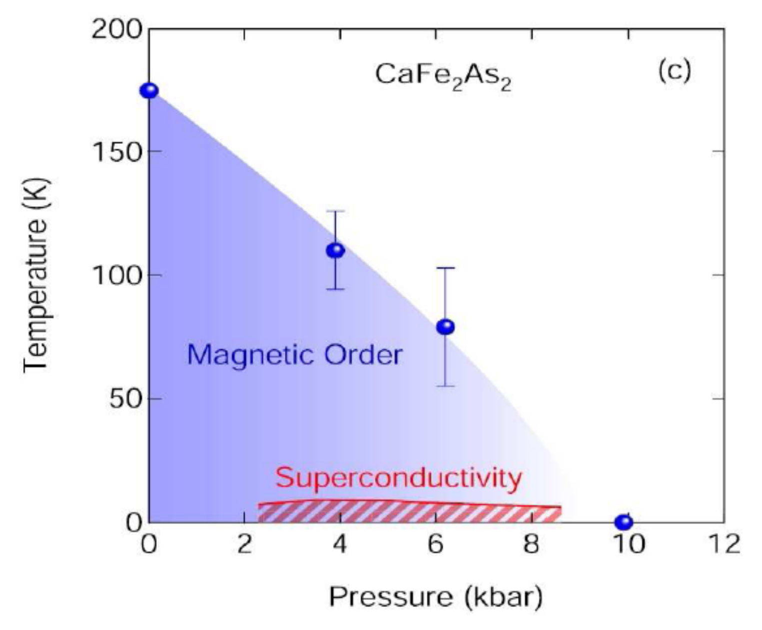
- Structural transition (tetragonal to orthorhombic) at ~ 170K

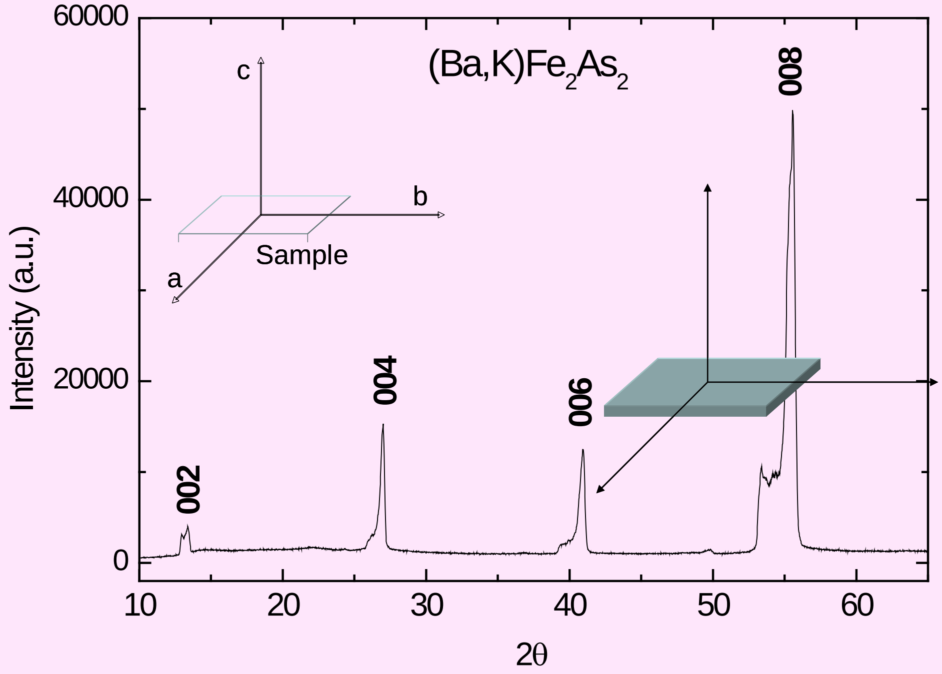
- Coincident with the structural transition was observed ordering of the Fe moments, in a commensurate antiferromagnetic structure.

[14] A.I. Goldman et al., Cond-mat arXiv:0807.1525 (2008).

***Pressure Induced Superconductivity in $CaFe_2As_2$ [15,16**

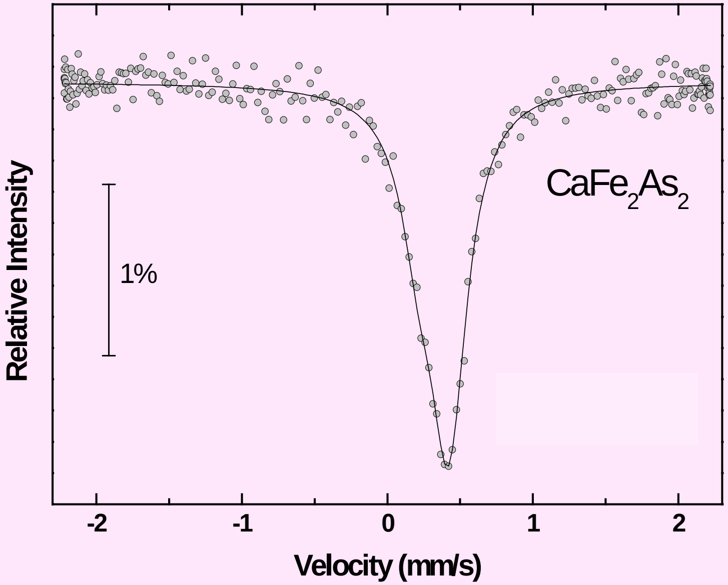
[15] Milton S. Torikachvili et al., PRL 101, 057006 (2008)
[16] T. Goko, et al., arXiv 0808.1425 (2008)



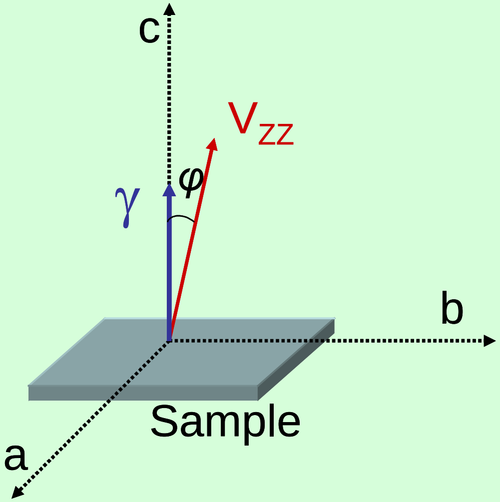


60000
40000
20000
0
10
20
30
40
50
60
Intensity (a.u.)
2θ
(Ba,K)Fe$_2$As$_2$
c
b
a
Sample
002
004
006
008

Mössbauer studies in single crystal $CaFe_2As_2$



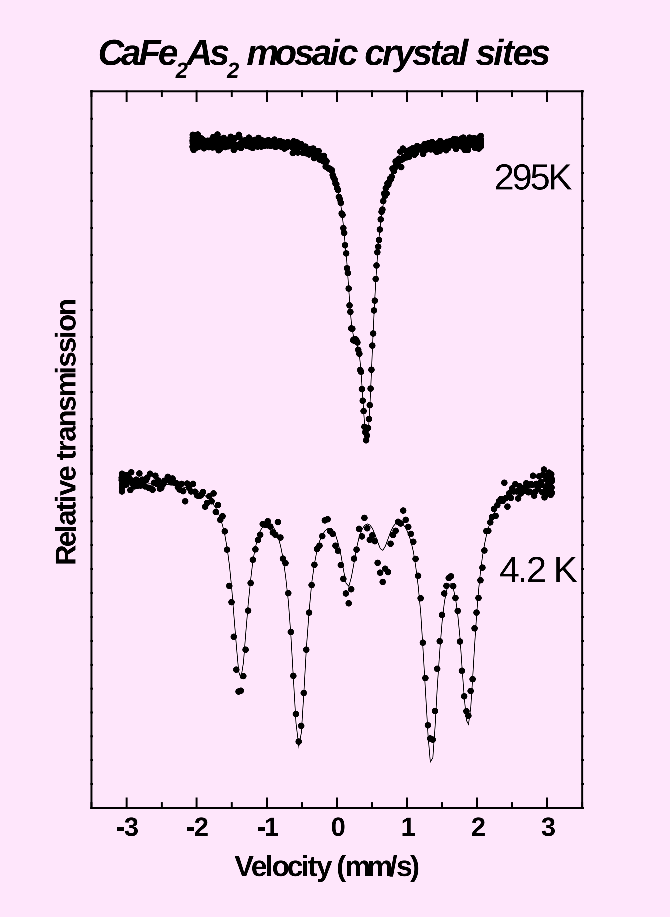
^{57}Co point source



ΔE_Q=0.207 mm/s
IS=0.44 mm/s
Γ=0.30 mm/s
$\varphi \approx 0^o$

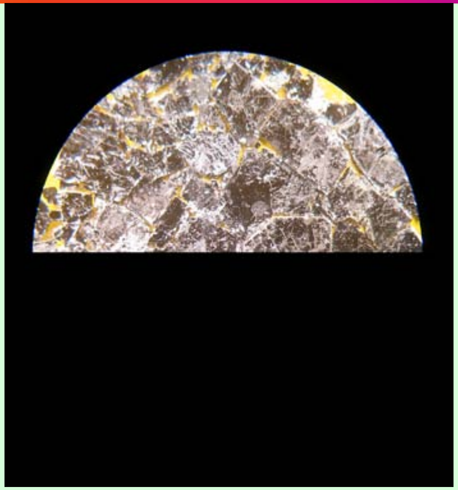
Main component of electric field gradient:
V_{zz} // c

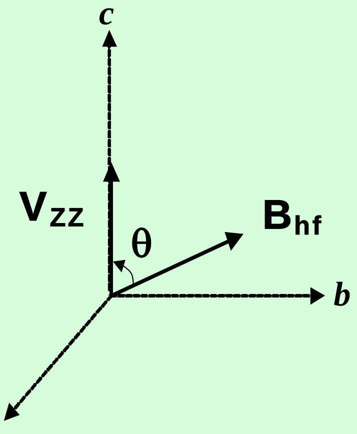
Mössbauer studies in single crystal $CaFe_2As_2$



$CaFe_2As_2$ mosaic crystal sites

$\Delta E_Q = 0.207$ mm/s
IS=0.44 mm/s
$\Gamma = 0.26$ mm/s
$\varphi \approx 10^o$





$\Delta E_Q = 0.339$ mm/s
$B_{hf} = 9.95T$
$\theta \approx 80^o$

$\mu_{Fe} \approx 0.66\ \mu_B$ and lie in *a-b* plane
(In agreement with neutron results)

Perspectives for Mössbauer in the studies of Unconventional SC

Follow details at local level of magnetic transitions

Determine the structural phase transition and any special feature related with

In the cases of Fe:NiB and FeAs tetrahedral their high symmetry favor SC

The correlation between c/a and T_c is valid for
- H-Tc SC
- RNi_nB_nC
- $CeCoIn_5$

Should it occur for the Fe As Sc compounds?

There is any new information for the Fe containing SC?

c/a as control parameter for T_c

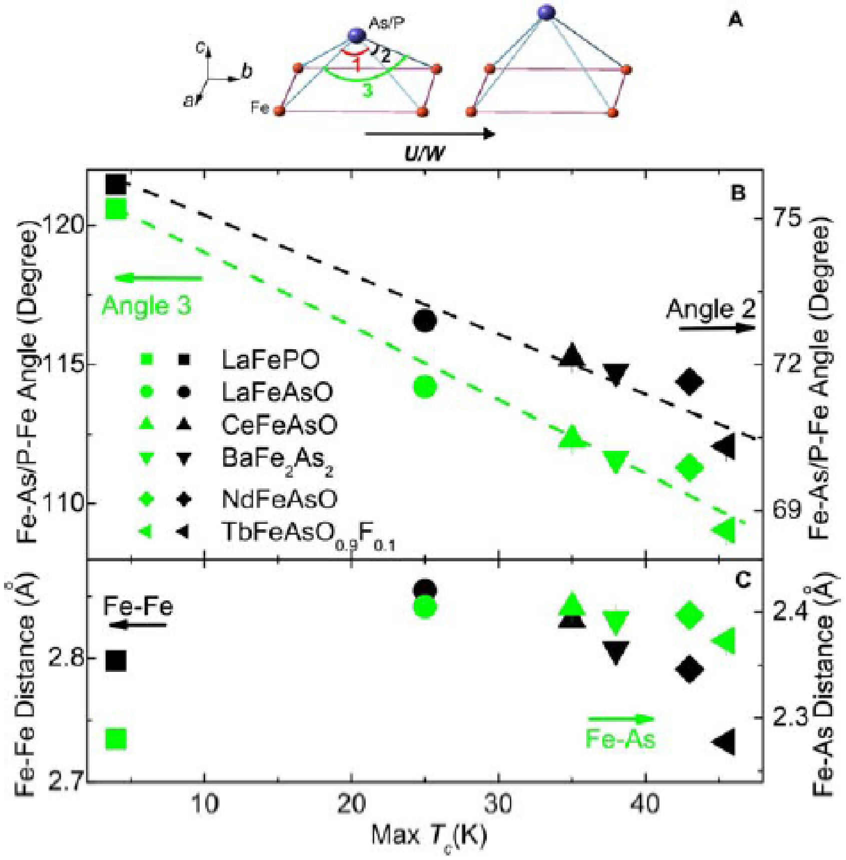
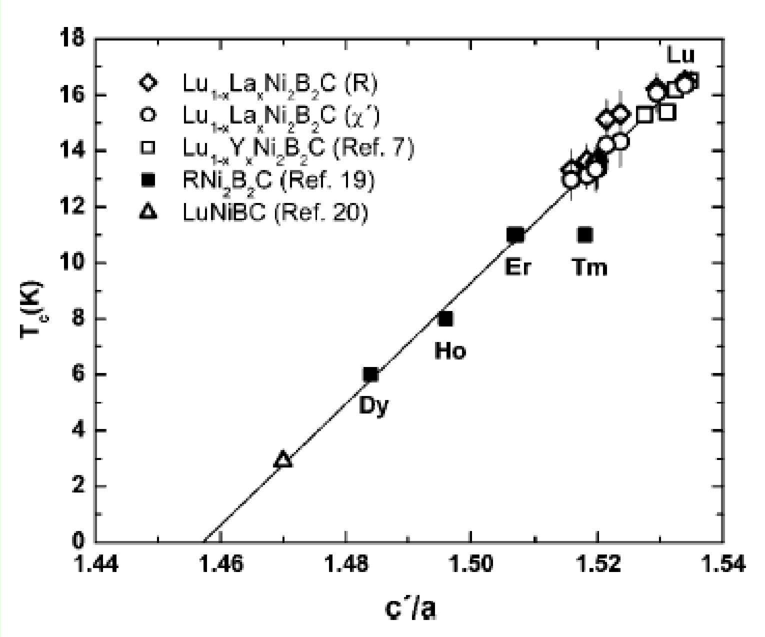
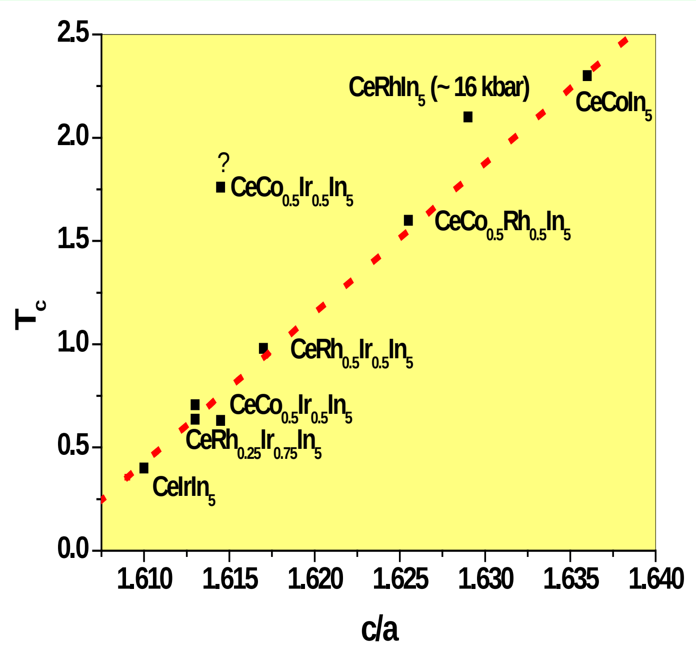


Figure 4. Fe-As(P)-Fe bond angles, Fe-Fe, and Fe-As(P) distances for different Fe-

Jun Zhao**, et al., arXiv: 0806.2528**

C/A

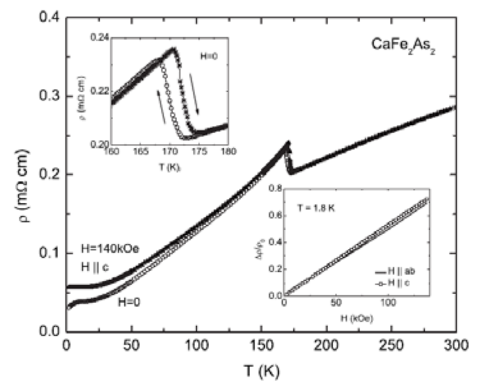


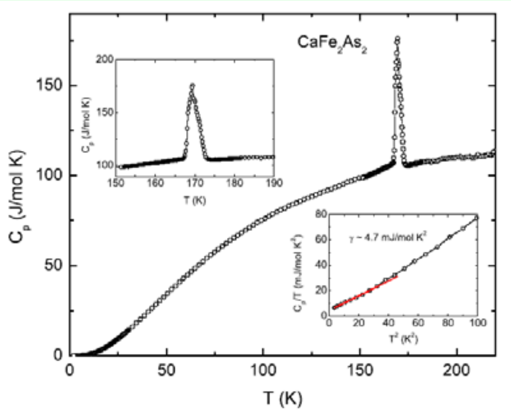


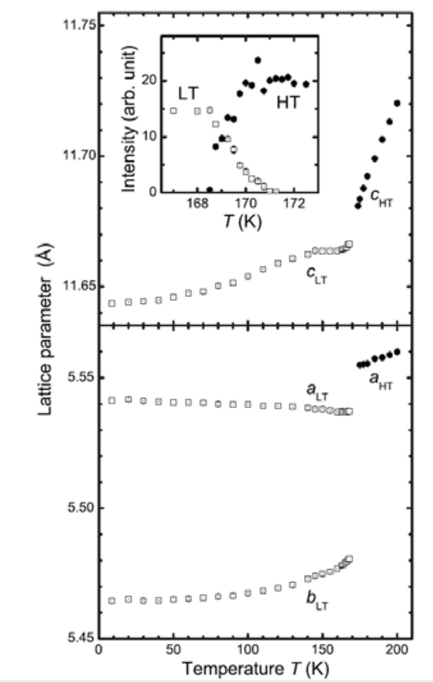
D. R. Sánchez, H. Micklitz, and E. M. Baggio-Saitovitch
PHYSICAL REVIEW B **71**, 024509 (2005)

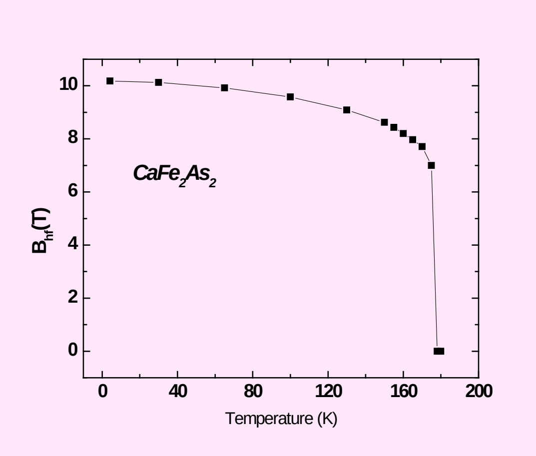
D. R. Sánchez, H. Micklitz, and E. M. Baggio-Saitovitch
PHYSICAL REVIEW B **71**, 024509 (2005)

Below 170 K, $CaFe_2As_2$ undergoes a first-order structural phase transition to a low-temperature orthorhombic phase with a 2–3 K range of hysteresis.



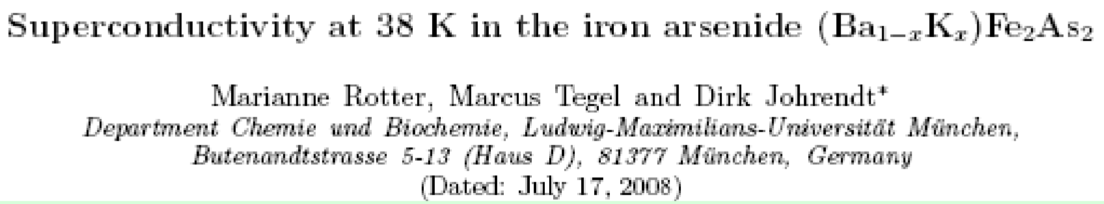






Discontinuous jump in B_{hf} at ~170K: typical for a first-order transition

N. Ni, et al., Phys. Rev. B **78**, 014523 (2008)



Superconductivity at 38 K in the iron arsenide $(\mathrm{Ba}_{1-x}\mathrm{K}_x)\mathrm{Fe}_2\mathrm{As}_2$

Marianne Rotter, Marcus Tegel and Dirk Johrendt*
Department Chemie und Biochemie, Ludwig-Maximilians-Universität München,
Butenandtstrasse 5-13 (Haus D), 81377 München, Germany
(Dated: July 17, 2008)

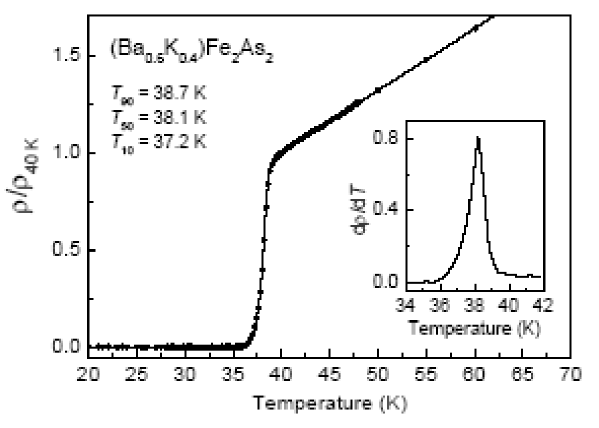
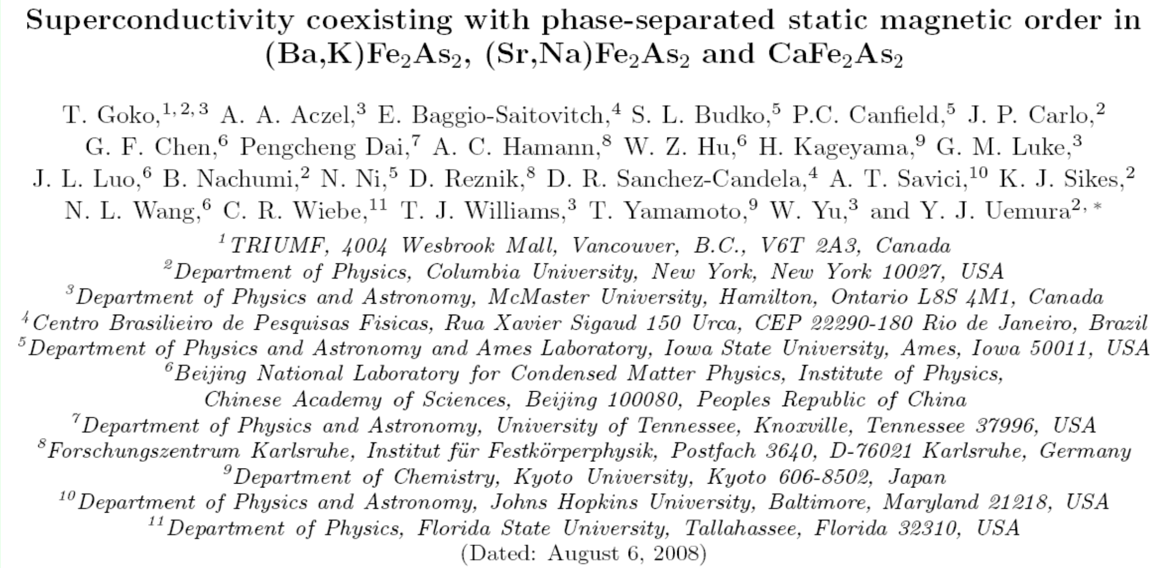


FIG. 4: Resistivity transition of $(\mathrm{Ba}_{0.6}\mathrm{K}_{0.4})\mathrm{Fe}_2\mathrm{As}_2$.



Superconductivity coexisting with phase-separated static magnetic order in $(\mathrm{Ba,K})\mathrm{Fe}_2\mathrm{As}_2$, $(\mathrm{Sr,Na})\mathrm{Fe}_2\mathrm{As}_2$ and $\mathrm{CaFe}_2\mathrm{As}_2$

T. Goko,[1,2,3] A. A. Aczel,[3] E. Baggio-Saitovitch,[4] S. L. Budko,[5] P.C. Canfield,[5] J. P. Carlo,[2]
G. F. Chen,[6] Pengcheng Dai,[7] A. C. Hamann,[8] W. Z. Hu,[6] H. Kageyama,[9] G. M. Luke,[3]
J. L. Luo,[6] B. Nachumi,[2] N. Ni,[5] D. Reznik,[8] D. R. Sanchez-Candela,[4] A. T. Savici,[10] K. J. Sikes,[2]
N. L. Wang,[6] C. R. Wiebe,[11] T. J. Williams,[3] T. Yamamoto,[9] W. Yu,[3] and Y. J. Uemura[2,*]

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[8] *Forschungszentrum Karlsruhe, Institut für Festkörperphysik, Postfach 3640, D-76021 Karlsruhe, Germany*
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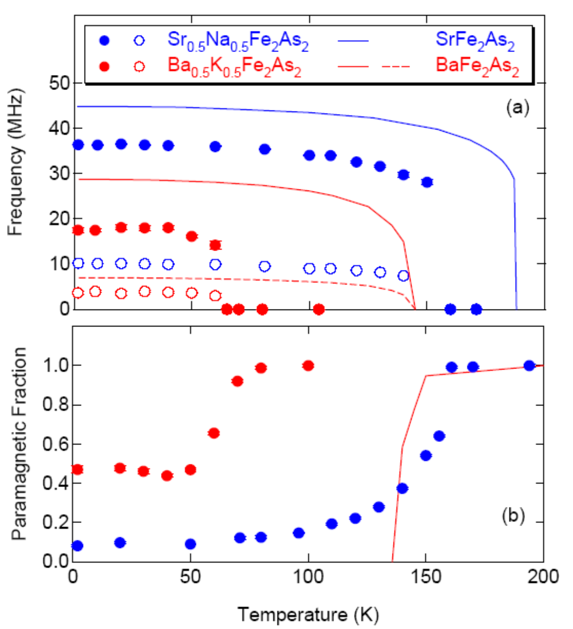
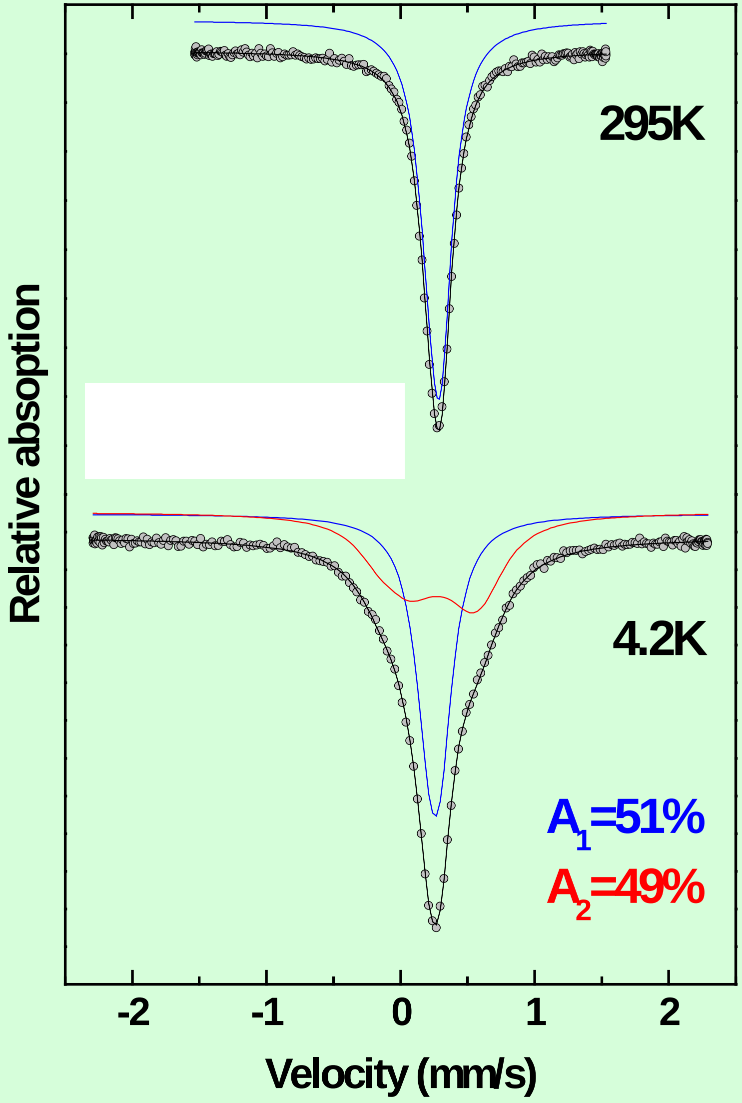
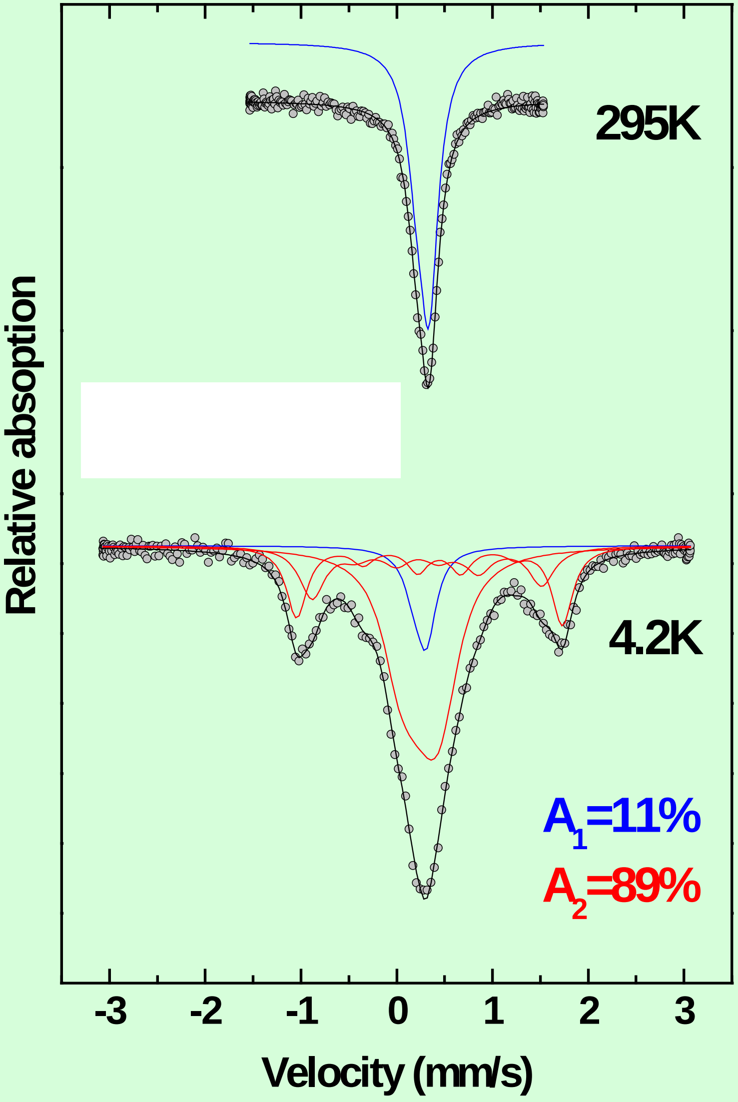
[11] *Department of Physics, Florida State University, Tallahassee, Florida 32310, USA*
(Dated: August 6, 2008)

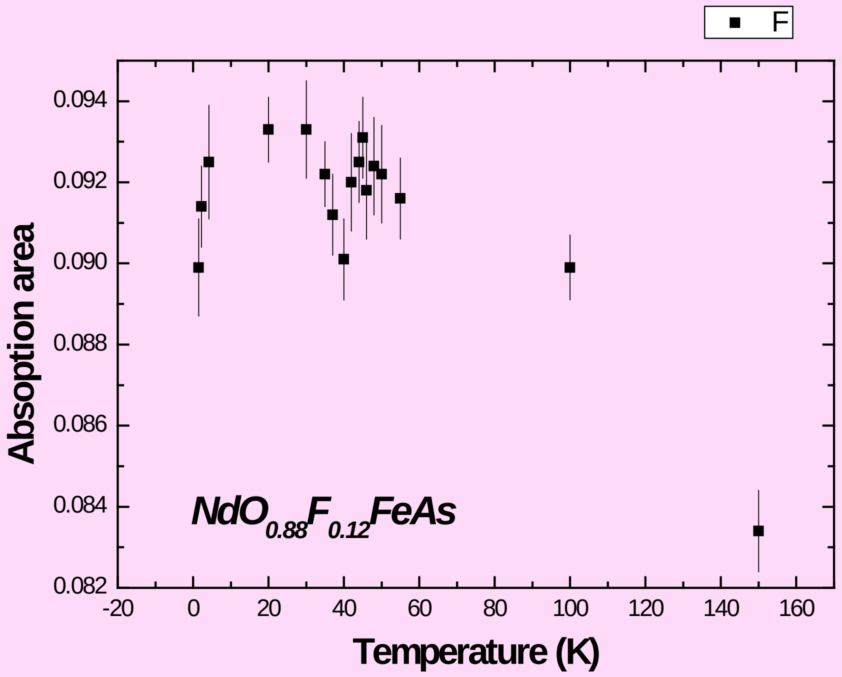


$(Ba_{0.5}K_{0.5})Fe_2As_2$



$(Sr_{0.5}Na_{0.5})Fe_2As_2$




■ F
Absoption area
0.094
0.092
0.090
0.088
0.086
0.084
0.082
-20
0
20
40
60
80
100
120
140
160
Temperature (K)
NdO0.88F0.12FeAs

The quaternary borocarbides RNi2B2C have been classified as conventional s-wave superconductors with a strongly anisotropic energy gap.*

Andreev spectroscopy study in SmFeAsO0.85F0.15 with Tc~54.2 classify it as a nodeless, BCS-type gap (s-wave).&

* K-H Müller and V N Narozhnyi, Rep. Prog. Phys. 64 (2001) 943–1008

& T. Y. Chen, Z. Tesanovic, R. H. Liu, X. H. Chen & C. L. Chien, Nature 453, 1224 (2008)