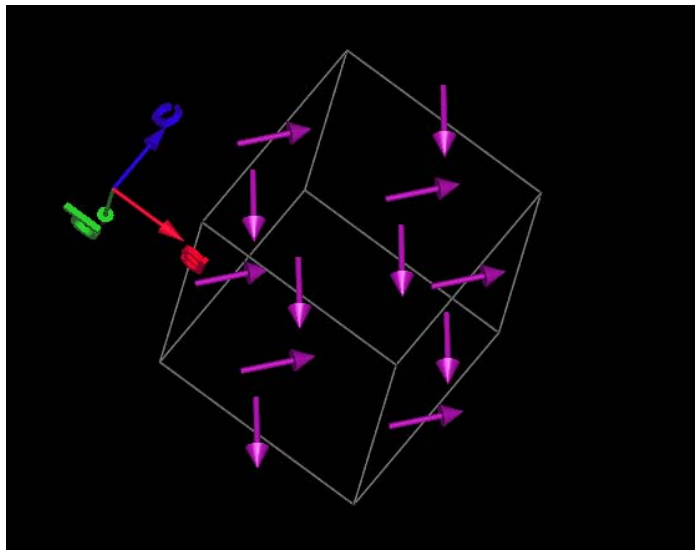
Magnetic structure of $La_{0.7}Ca_{0.3}Cr_xMn_{1-x}O_3$ ($x = 0.5, 0.7$) compounds: preliminary results

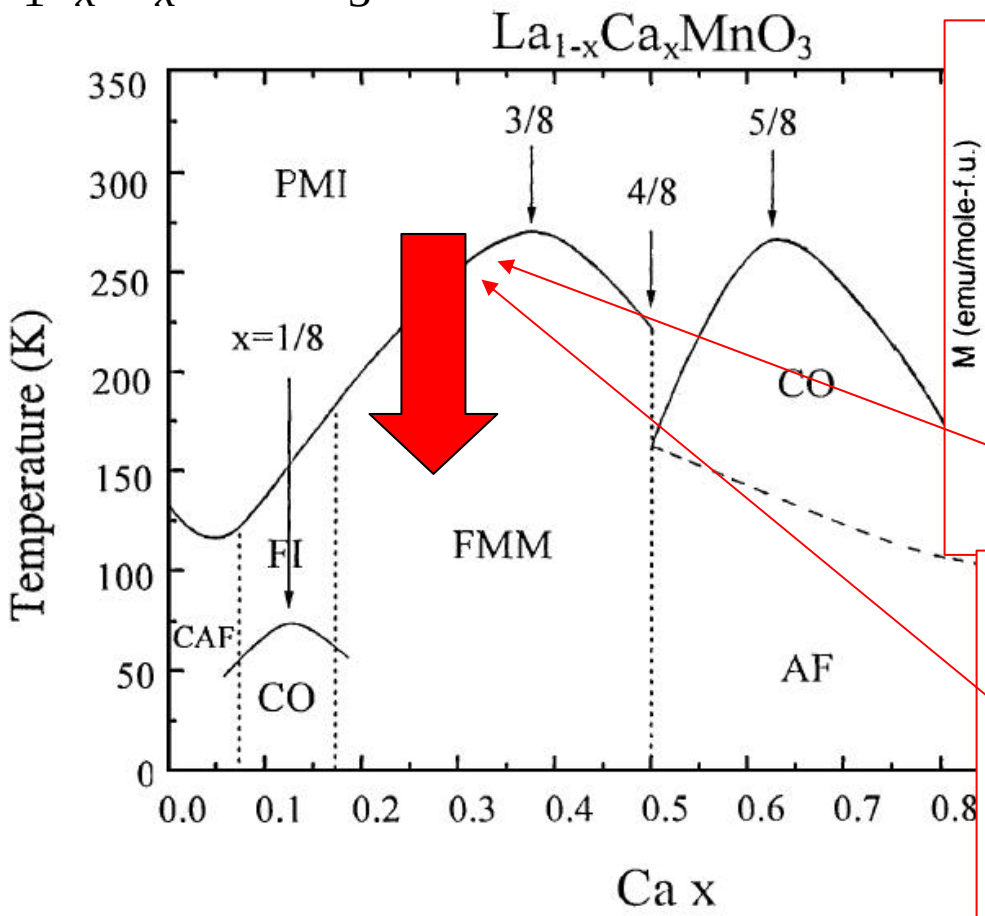


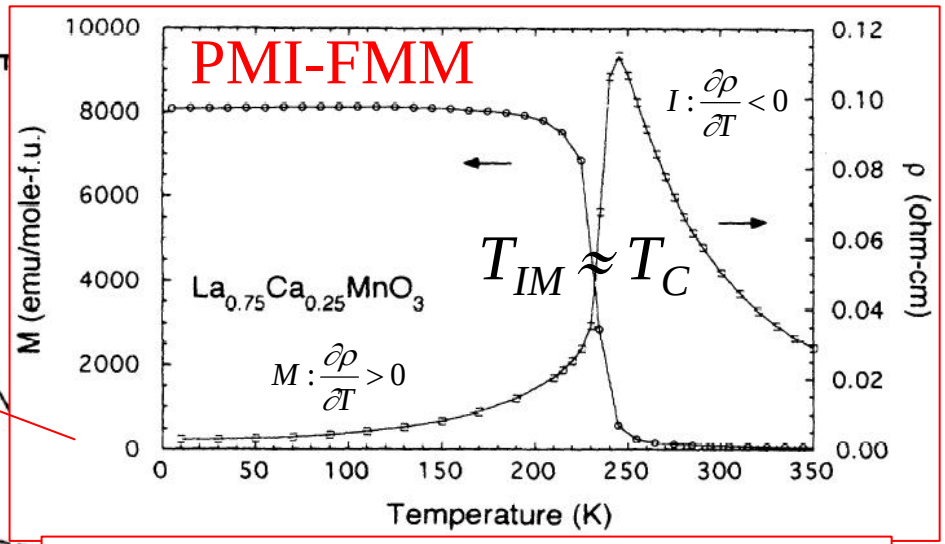
L. Capogna, ILL-Grenoble (France)
T. Corridoni & N. Pompeo, Università Roma Tre, Roma (Italy)

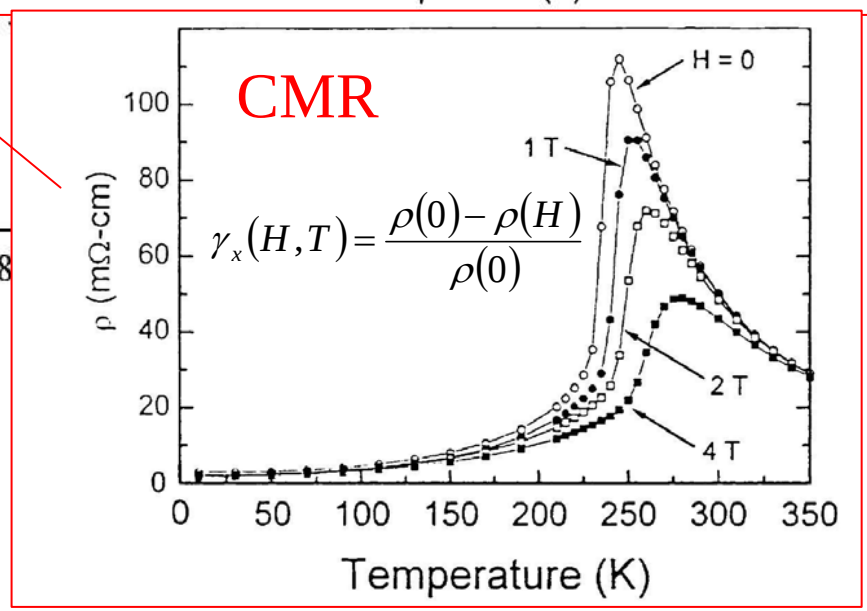
School of Neutron Scattering “F. P. Ricci”, VIII edition, Pula, 2006

Perovskite Manganites

$L_{1-x}R_xMnO_3 \qquad L = La, Pr, \ldots \qquad R = Ca, Sr, \ldots$





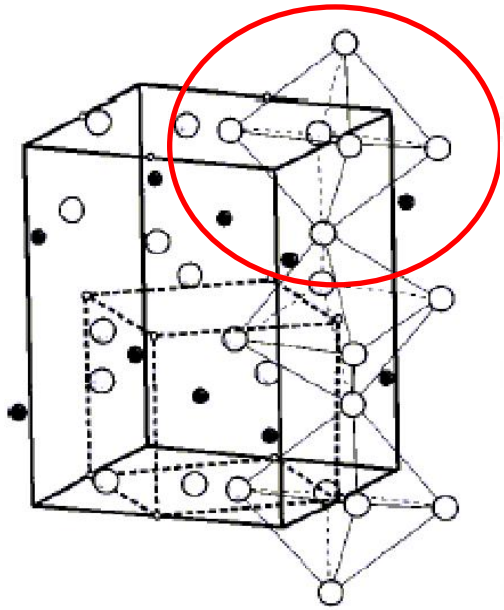


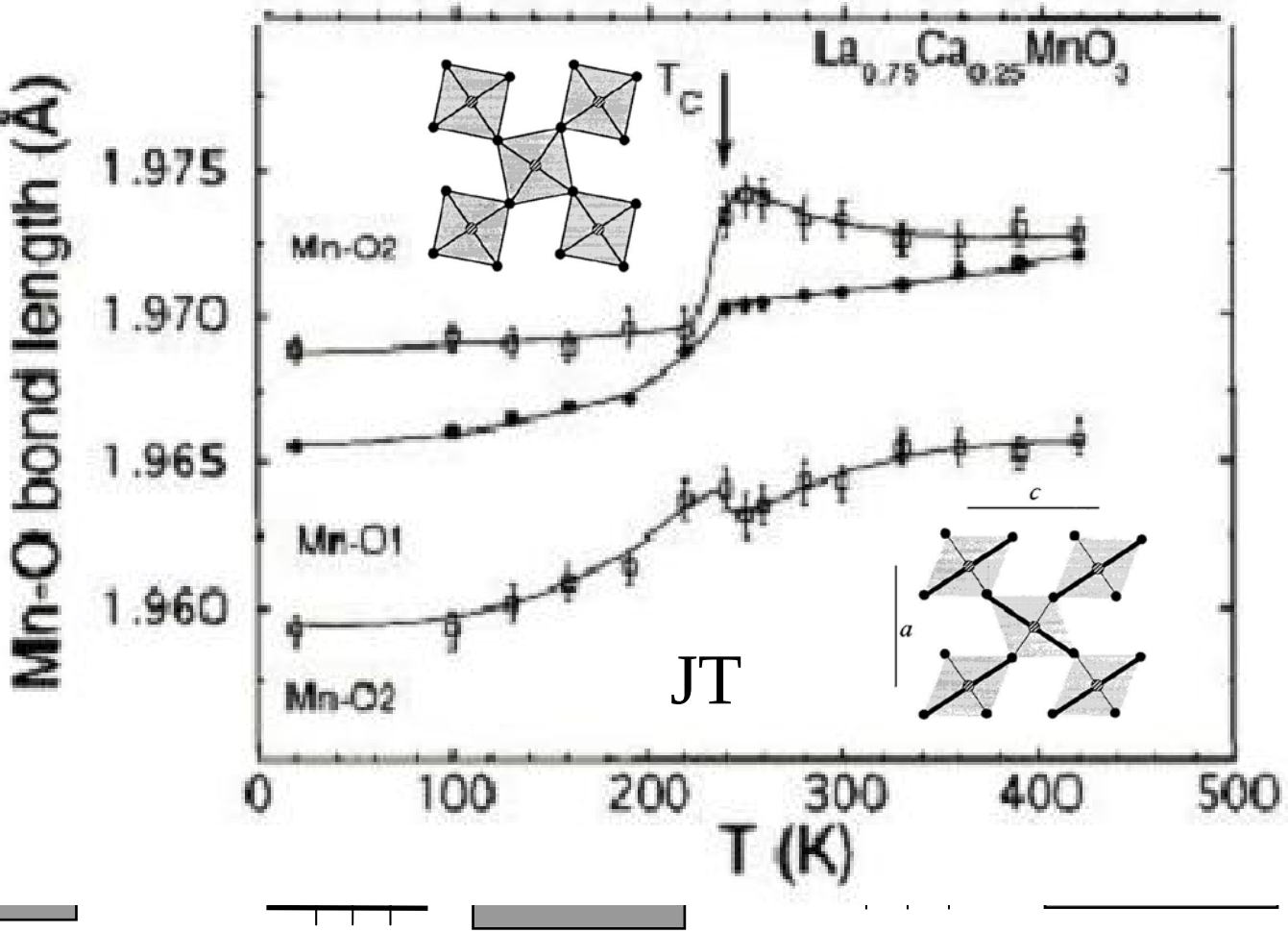
$\gamma_{LCMO,0.21}(H = 5T, T = T_C) \approx 92\%$

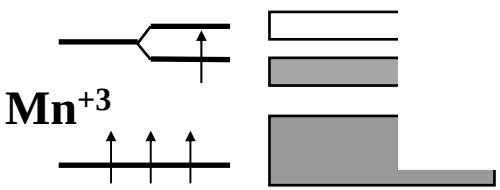
Colossal Magneto Resistence

Radaelli et al, PRB (1994-1998)

Localization/delocalization (DE, JT &…)







x = 0: all octahedra JT distorted: insulant behaviour

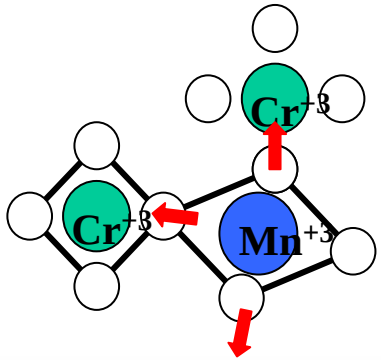
0.2 < x < 0.5: octahedra distorted and not: metallic behaviour

x = 1: simmetric octahedra only: insulant behaviour

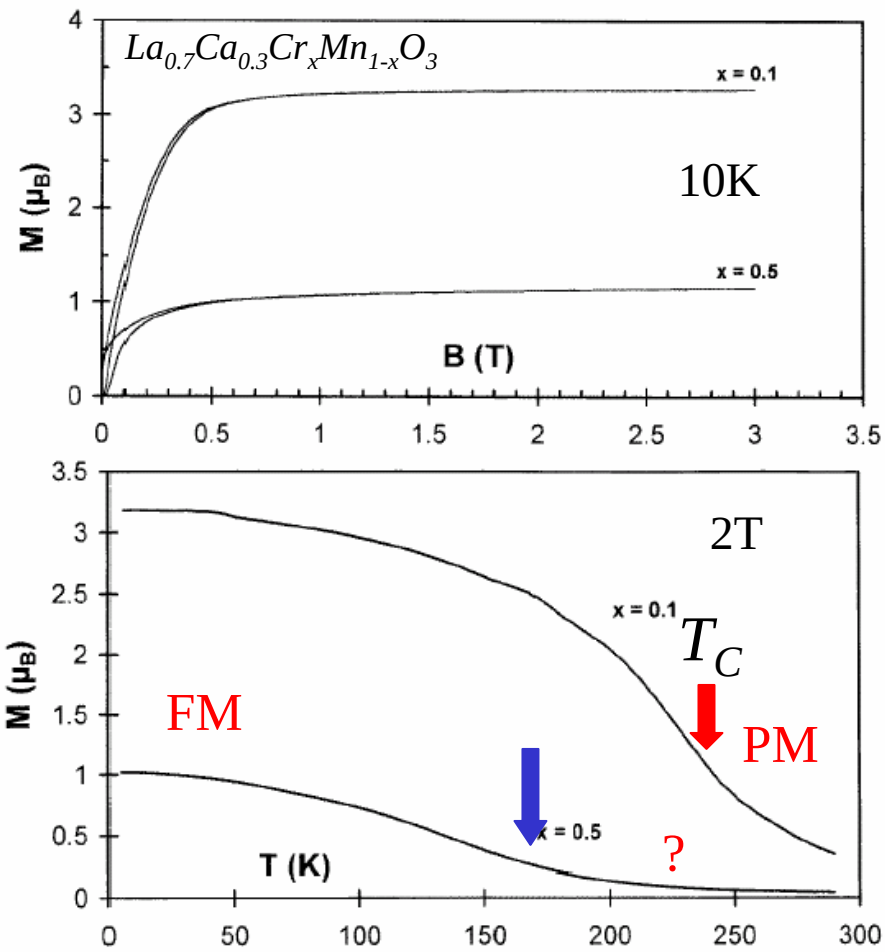
DE/JT competition, but AF interactions needed for low *x* doping transitions!

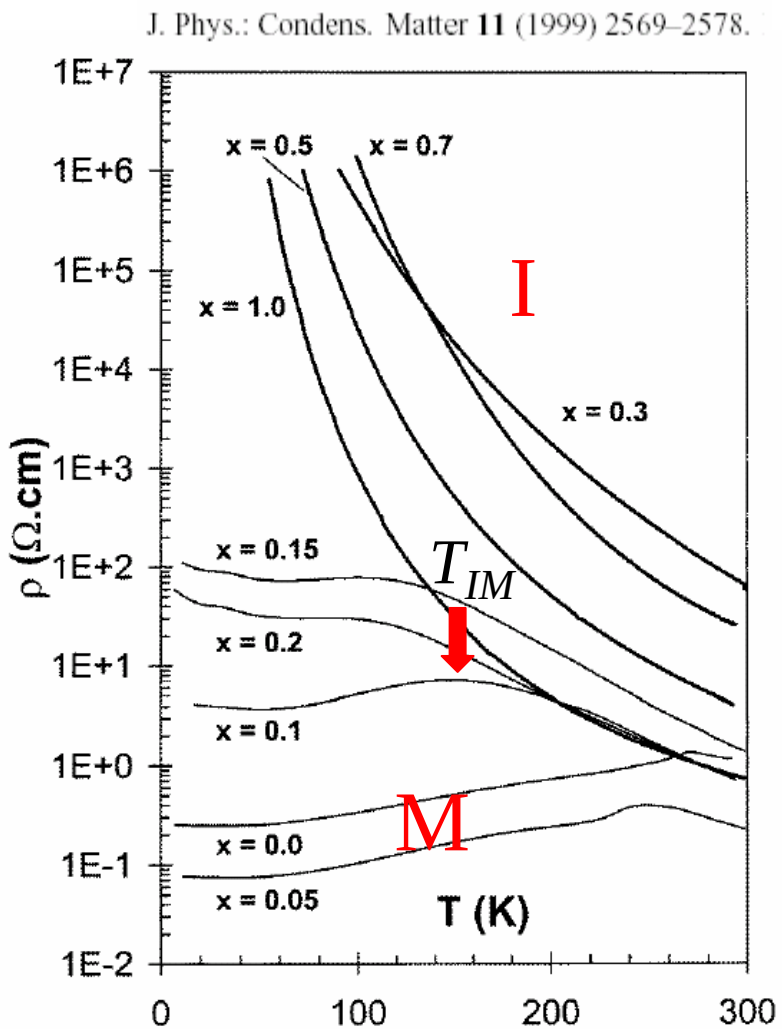
Where PMI-FMM transition is observed: DE > JT > X

Cr doping: motivations and results in $Ca_{0.3}$ samples

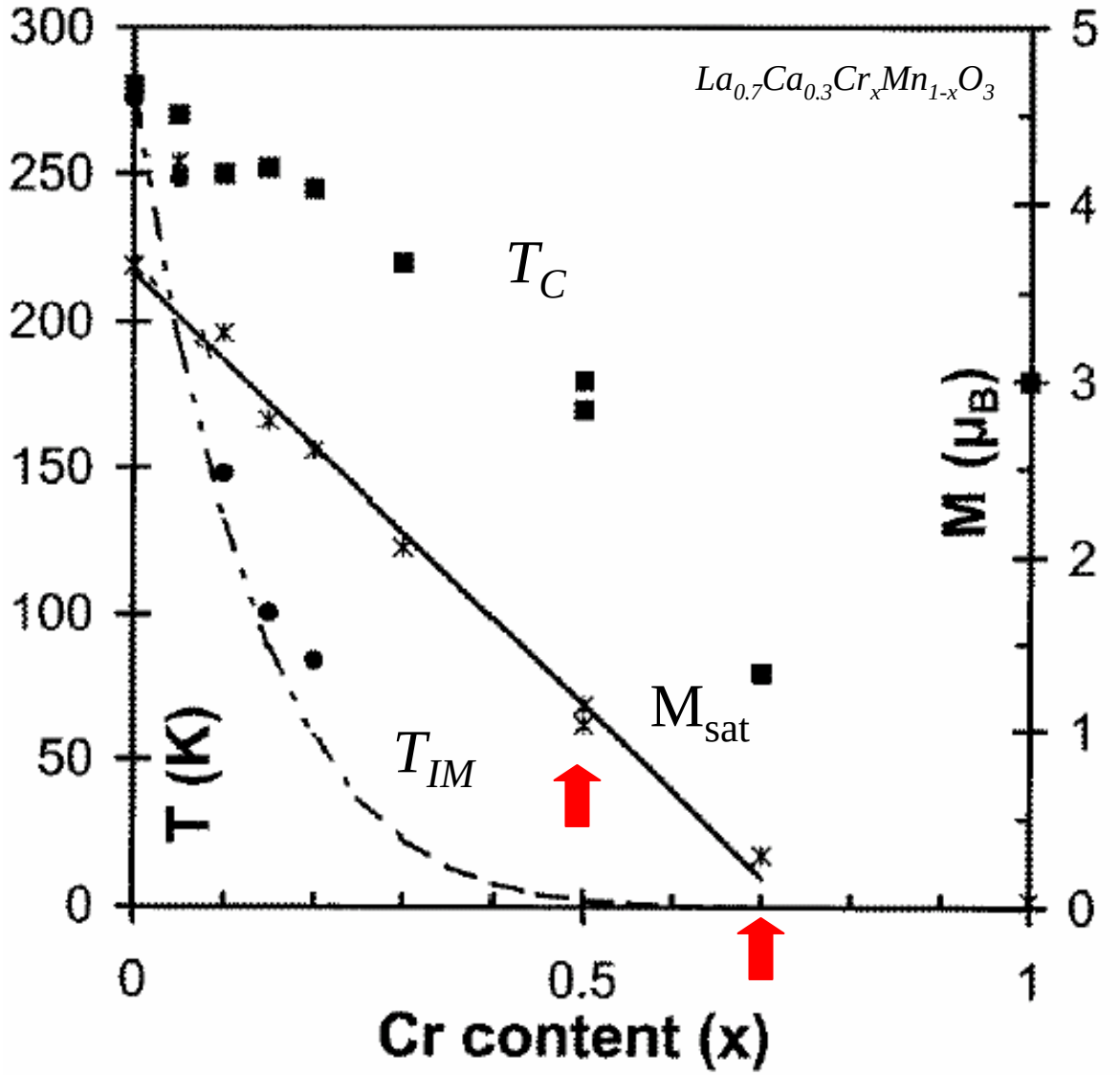


- *Electronic structure : **$Cr^{+3} \approx Mn^{+4}$**: empty e_g orbital*
- *Electronic structure : **$Cr^{+2} \approx Mn^{+3}$**: one e in e_g orbital, JT*
- *Cr/O hybridisation is stronger than Mn/O one: simmetrization of whole lattice ($Mn^{+3}O_6$ octahedra, above all)*
- *Decreasing JT effect*
- ***Enhancing DE ?***
- ***Configurational disorder…***





Need for a magnetic structure analysis



- $T_C \neq T_{IM}$: ***FM-PM / M-I*** **decoupling**
- $M_{sat} \propto -x$**: decreasing FM behaviour**
- $T_{IM} \approx P_{Mn\text{-}6Mn}$**: Metallic behaviour linked to the probability of having 6 Mn around a Mn site**

Perhaps

Cr doping stops DE coupling

Why ?

Let's analyse the magnetic structure of $La_{0.7}Ca_{0.3}Cr_xMn_{1-x}O_3$ for $x = 0.5$ and $x = 0.7$ ($x = 0.17$ in the future)

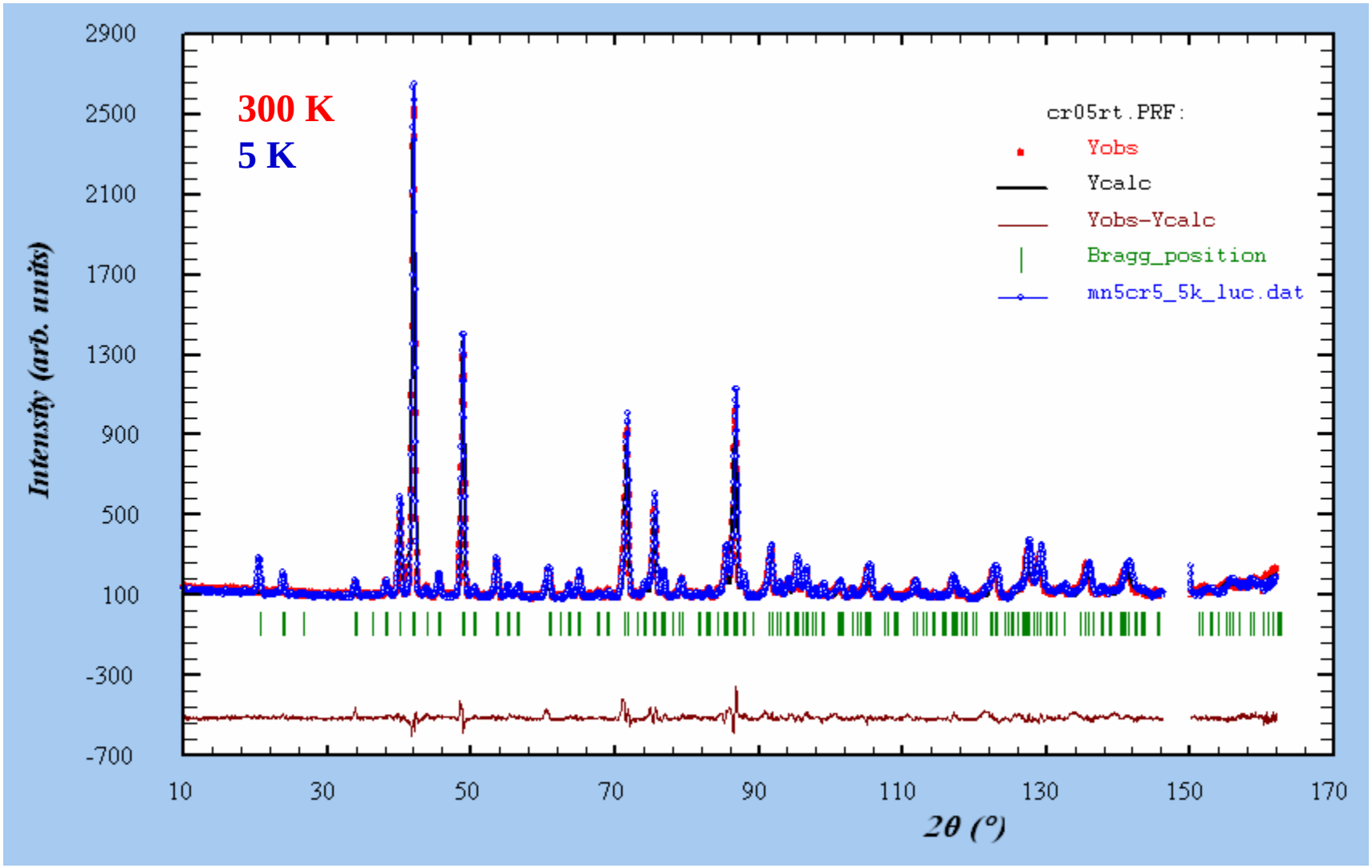
Samples

- $La_{0.7}Ca_{0.3}Mn_{1-x}Cr_xO_3$ with x=(0.17), 0.5, 0.7
  - Same samples as previous data
  - Space group: P M N A
  - Magnetic ions: Mn3+/Mn4+, partially substituted by Cr2+/Cr3+
  - Powder
  - synthesized by M.G. Francesconi

- Measurements:
  - ILL, D2B, Grenoble (L. Capogna, P.G. Radaelli)
  - Two temperatures: T=300 K , T=5 K

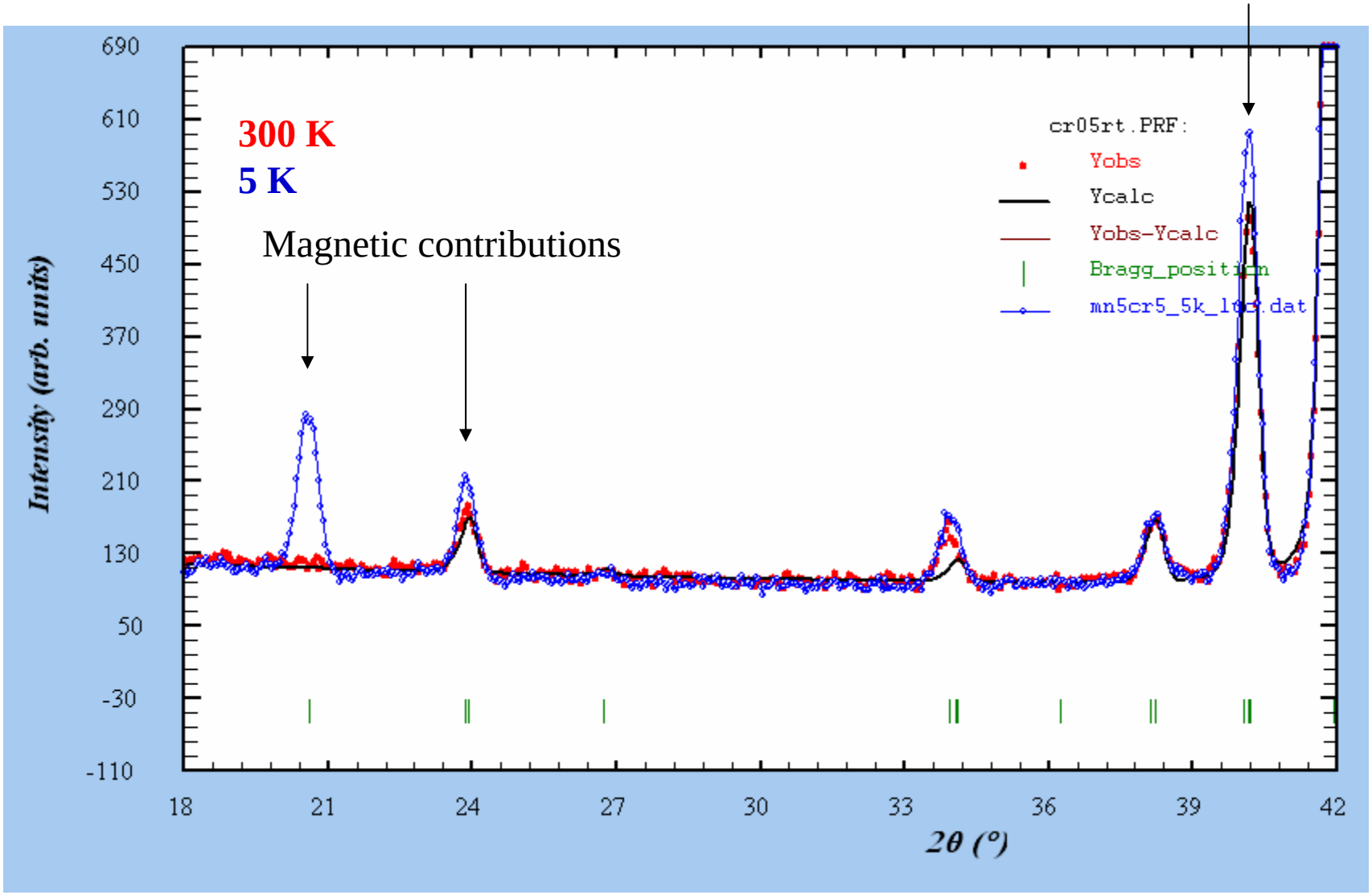
- Data analysis:
  - *Fullprof*
  - *SuperCell*
  - *BasIreps*

Data at doping x=0.5: structural phase



T=300K data: cell parameters determination; refined also at T=5 K

Data at doping x=0.5: magnetic contributions at T=5 K

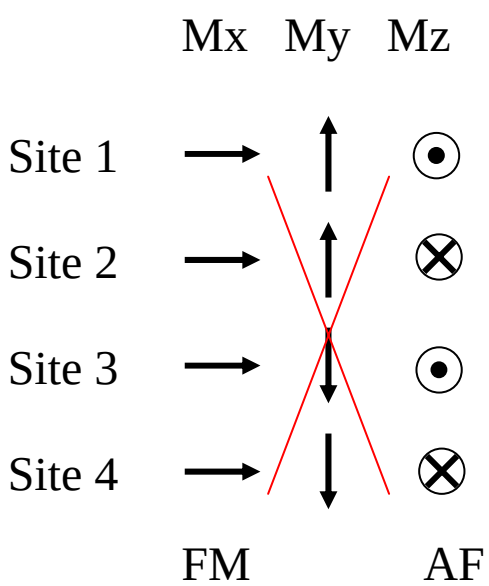


T=5 K: magnetic peak positions + cell parameters → *Supercell* → **k**=(0,0,0)

Data at doping x=0.5: determination of IRreps for the magnetic phase

- *BasIreps*
  - input: space group, **k**=(0,0,0), magnetic ion positions (4 sites)
  - output: 4 IRreps of dimension 1:
    - Eg: IRrep(7)

```
Atoms:      MN_1                MN_2                MN_3                MN_4
 1:Re (    1    0    0) (    1    0    0) (    1    0    0) (    1    0    0)
 2:Re (    0    1    0) (    0    1    0) (    0   -1    0) (    0   -1    0)
 3:Re (    0    0    1) (    0    0   -1) (    0    0    1) (    0    0   -1)
```

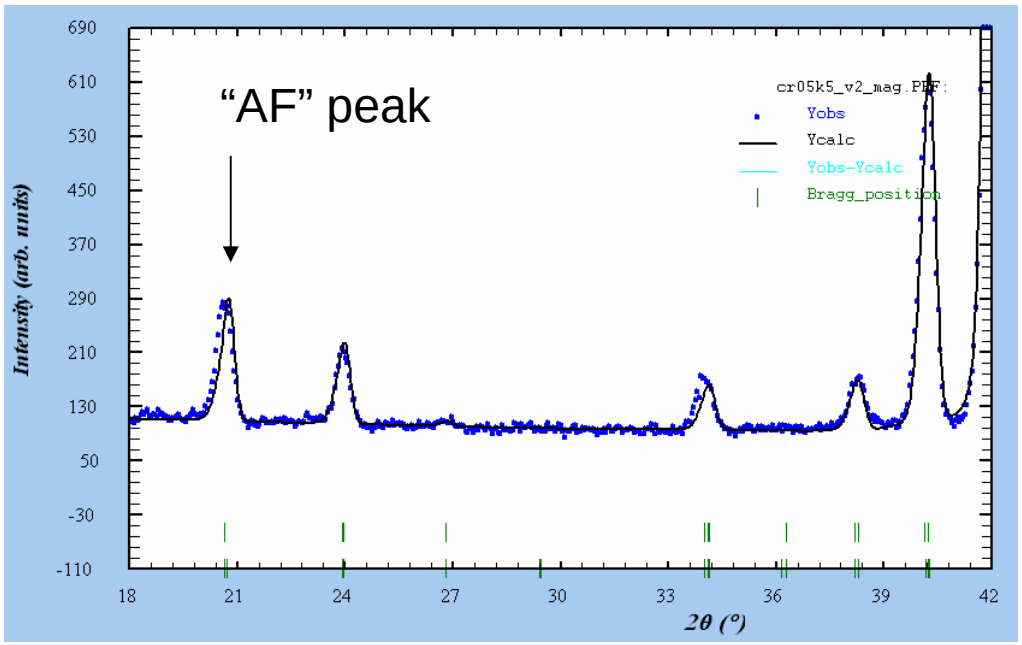


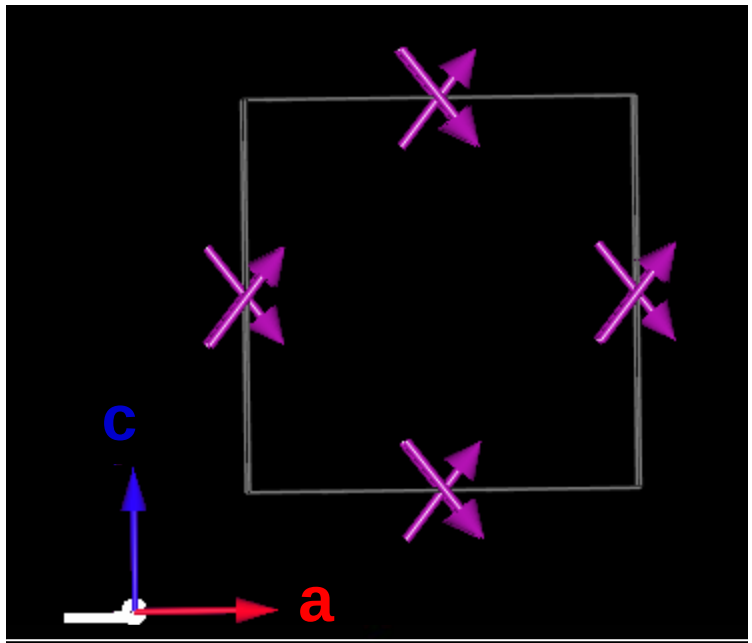
- IRrep(1) and IRrep(5): no AF components
- IRrep(3): like IRrep(7), x ↔ z

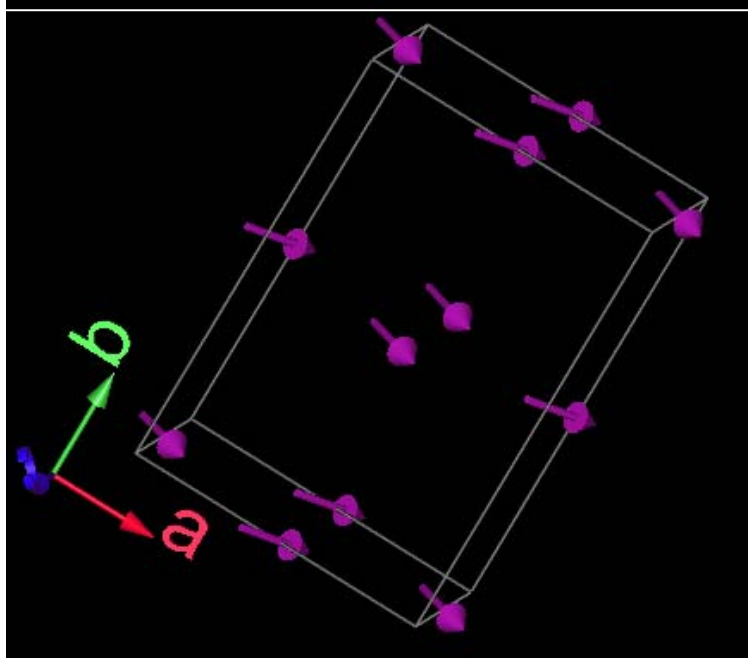
Data at doping x=0.5: refinement of the magnetic phase

- Fitting IRrep: no. 7
- Magnetic moments:
  - Mx=1.1 (FM like)
  - My=0.0
  - Mz=1.4 (AF like)

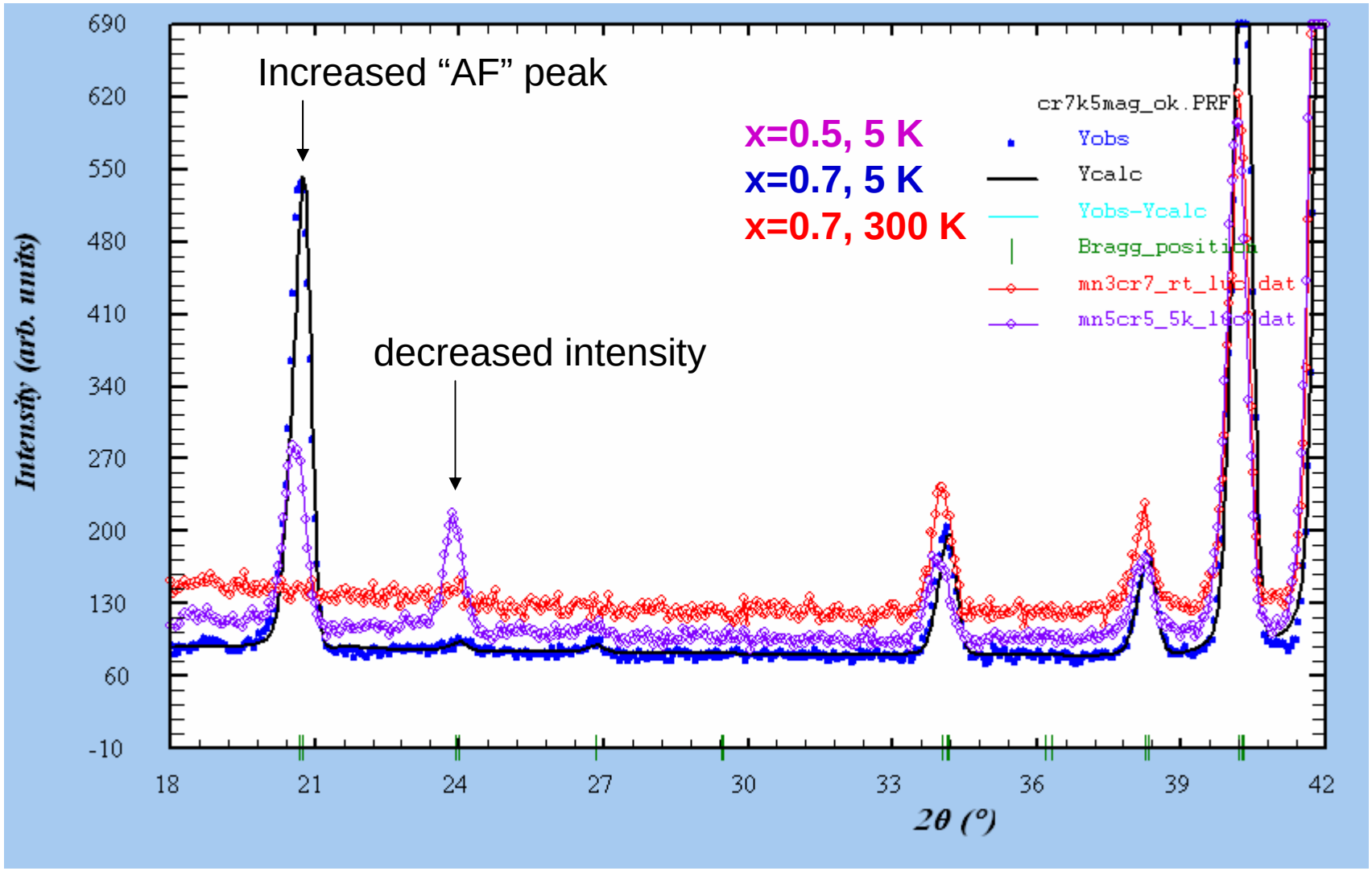
- IRrep(3): analogous results
- IRrep(1) and RIrep(5): no fit





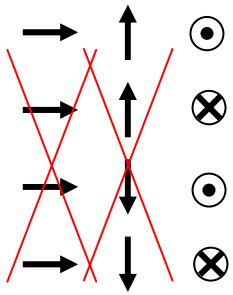


Data at doping x=0.7: magnetic phase at T=5 K

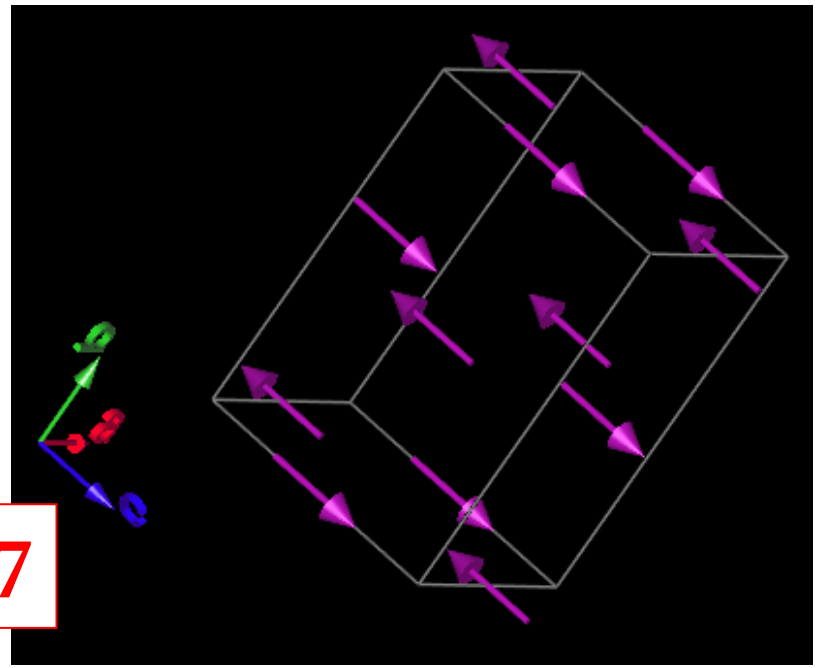


Data at doping x=0.7: magnetic phase at 5 K

- Fitting IRrep: no. 7
- Magnetic moments:
  - Mx=0.0
  - My=0.0
  - Mz=2.1 (AF like)



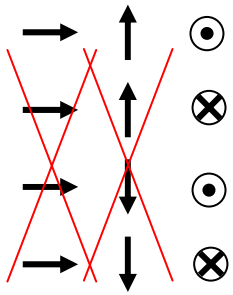
- IRrep(3): no fit
- IRrep(1) and RIrep(5): no fit



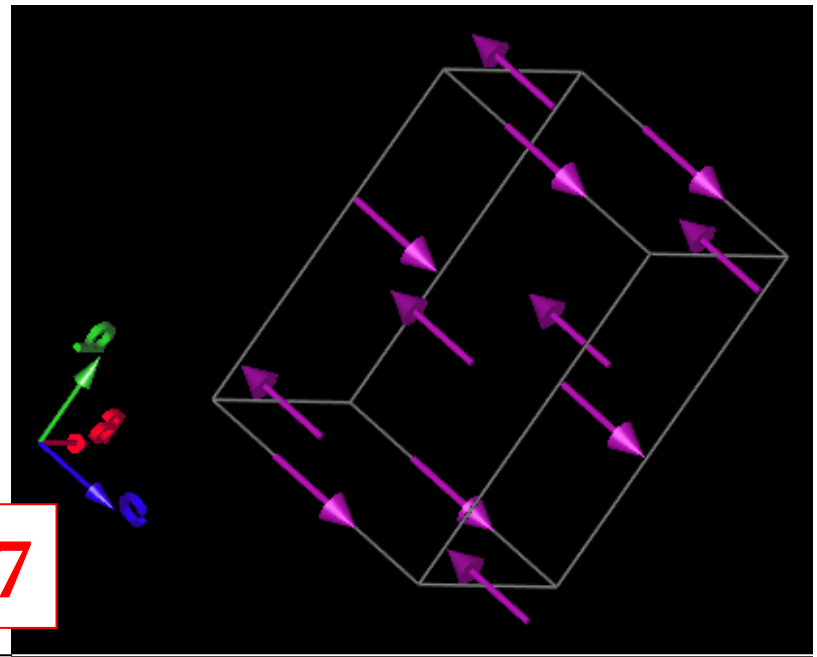
x=0.7

Data at doping x=0.7: magnetic phase at 5 K

- Fitting IRrep: no. 7
- Magnetic moments:
  - Mx=0.0
  - My=0.0
  - Mz=2.1 (AF like)

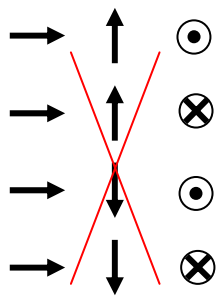


- IRrep(3): no fit
- IRrep(1) and RIrep(5): no fit

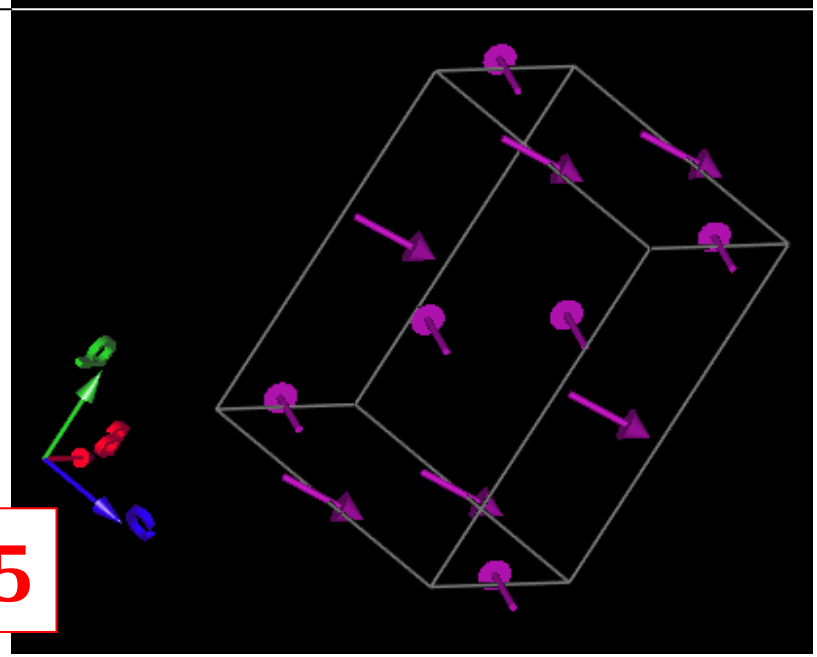


x=0.7

- Fitting IRrep: no. 7
- Magnetic moments:
  - Mx=1.1 (FM like)
  - My=0.0
  - Mz=1.4 (AF like)

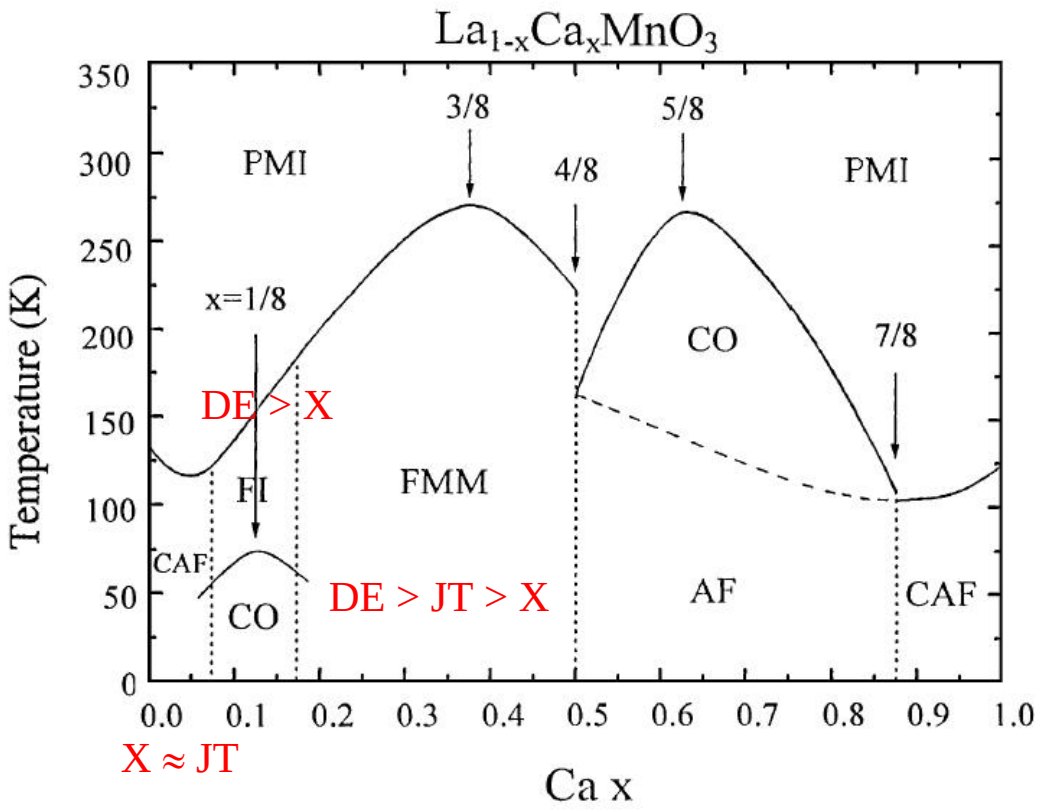


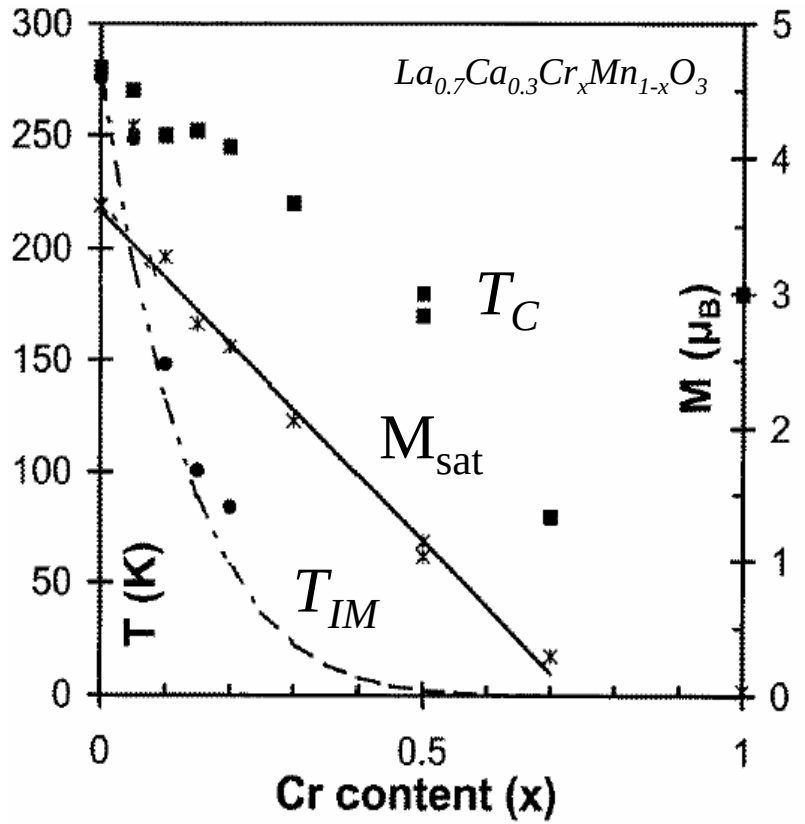
- IRrep(3): analogous results
- IRrep(1) and RIrep(5): no fit



x=0.5

Final considerations





Without Cr doping, Ca doping increase DE coupling, decreasing at the same time JT and possible magnetic couplings, stronger in low Ca-doping, low-T zone of the phase diagram.

These couplings are responsible for AF order, and perhaps are not ruled aut in FMM phase too: DE and JT distorsion “are not alone”.

With Cr doping, fixing Ca doping, DE decreases with JT distorsion: other couplings can so become stronger, and dominate the physics of the compound. An AF coupling, then, could destroy any metallic behaviour, because of the huge Hund coupling between tg and eg orbitals.

Acknowledgments

We would like to thank all the organisers, professors and participants of this school for useful lessons (even if at 22:00), discussions, exercises, dinners and breakfasts together.

We would like to thank also all sardinian people we met for their unique kindness.

Thank You !