

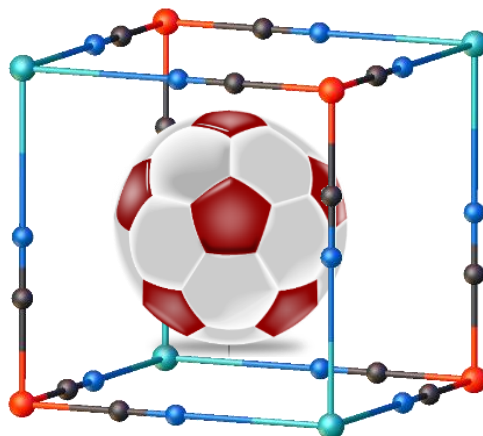
Thermal and spectroscopic properties of coordination polymers with a double perovskite structure



JINR



Uniwersytet
Wrocławski



Alicja Fabisiak

Supervisor: dr Magdalena Rok



Research Project Objectives



A – organic cation

B(1) – K^+ , Li^+ , Na^+

B(2) – Cr^{3+} , Fe^{3+} , Co^{3+}

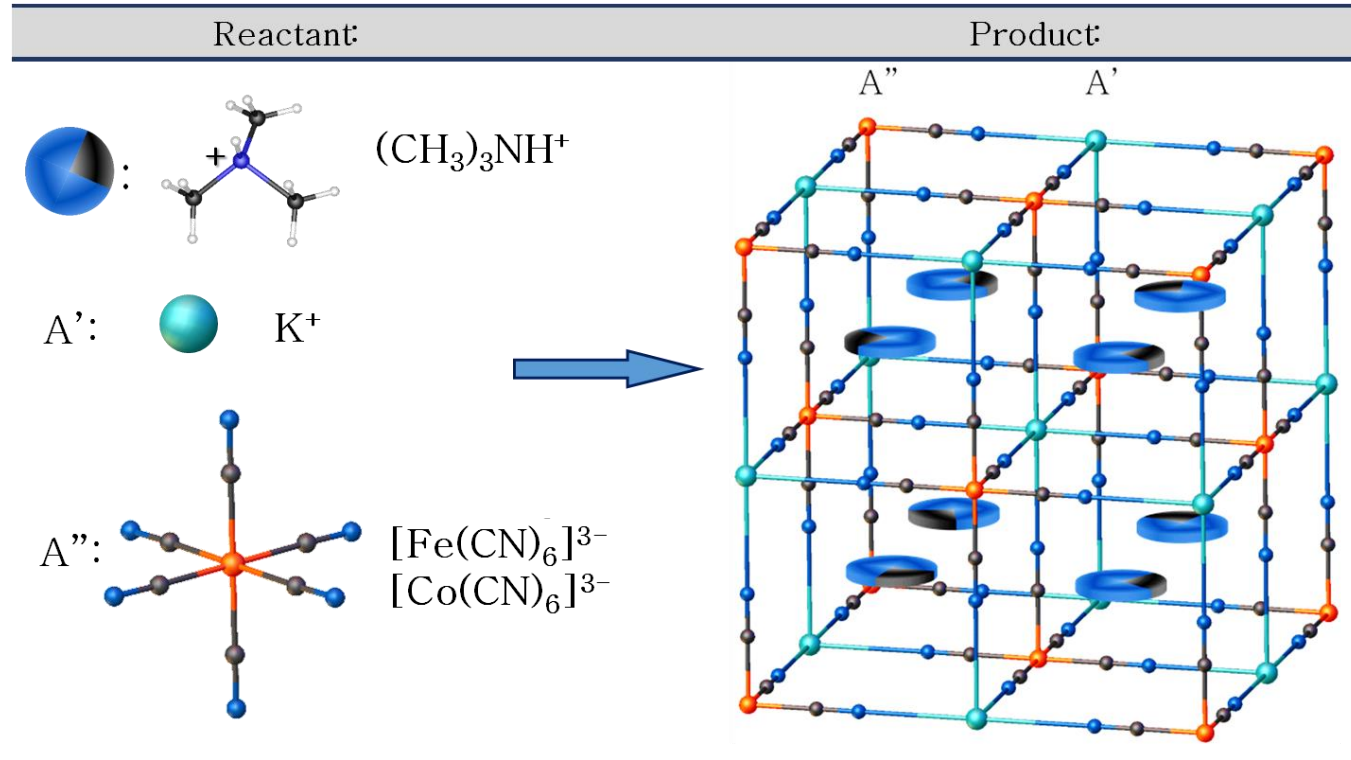
X – CN^-



- double perovskite-type structure
 - organic-inorganic hybrids, HOI
 - coordination polymers, CPs
 - host-guest system, H-G
 - tunable and switchable
 - ferroelastic properties
-

Research Project Objectives

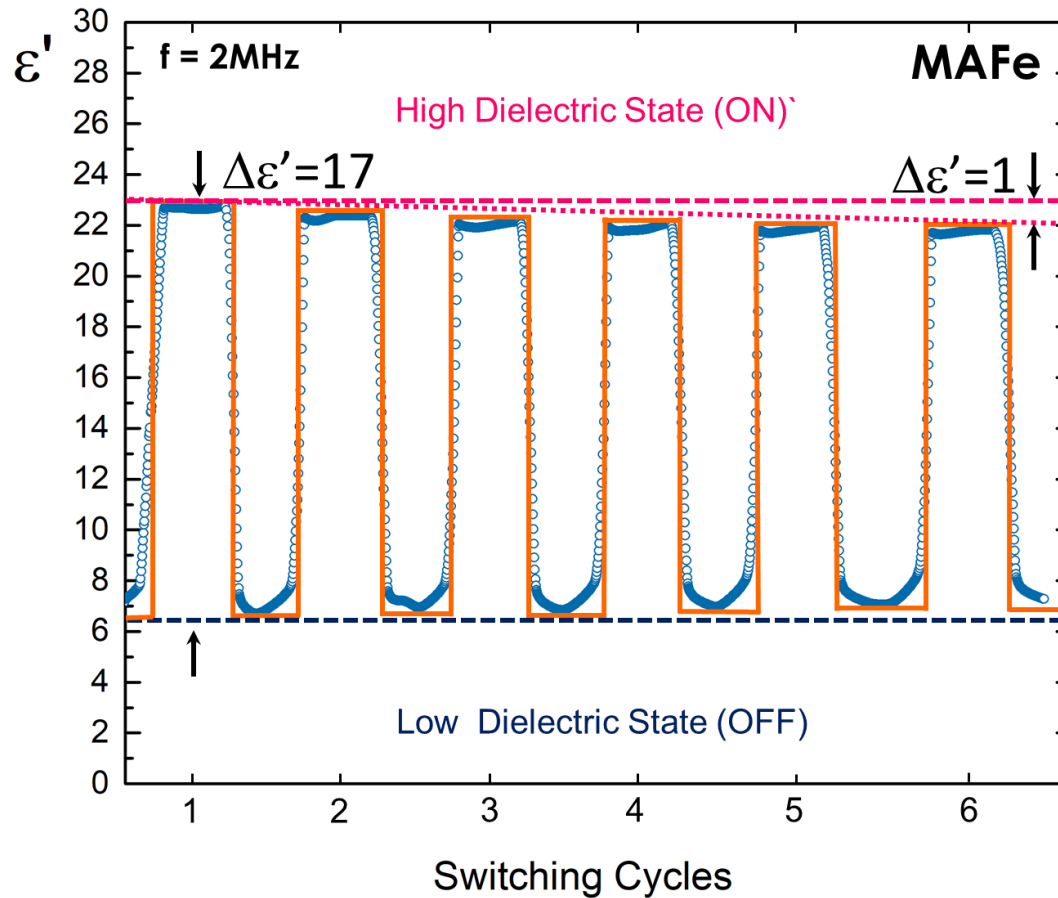
- HOI,
- CPs
- H-G



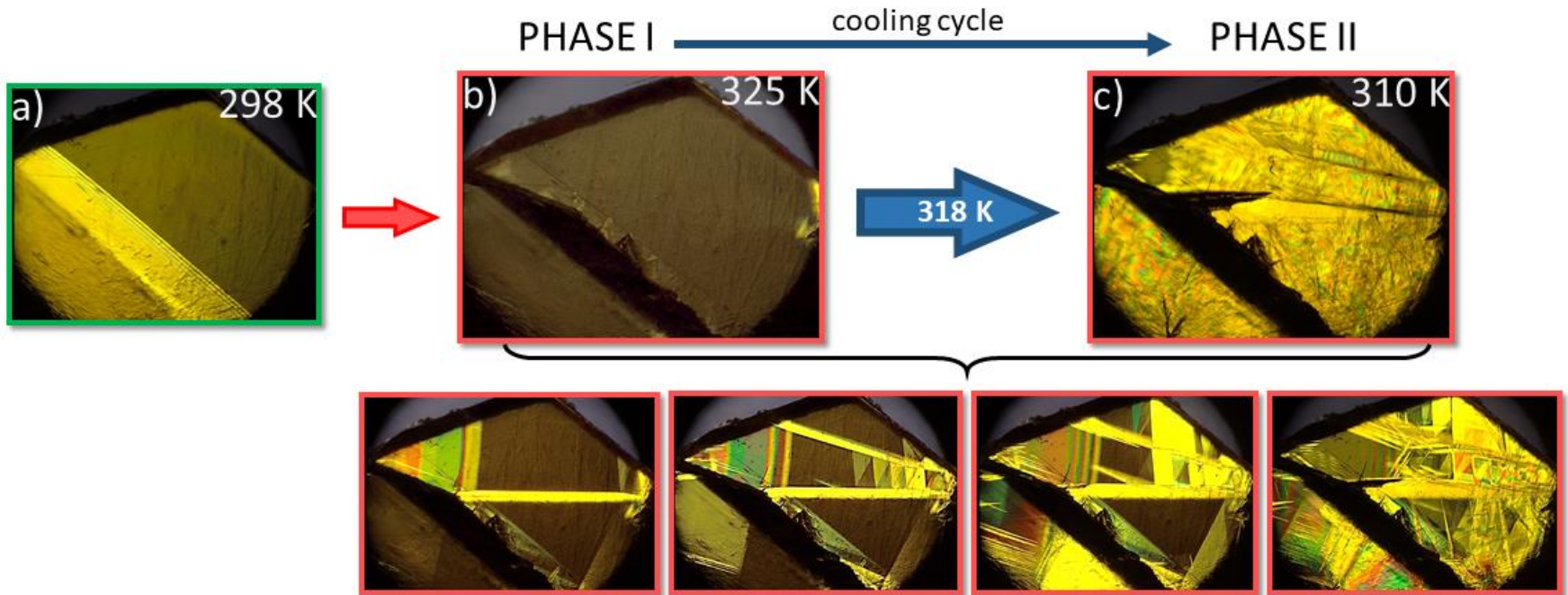
Scheme 1. Schematic procedure of the self-assembly CPs crystals in three-dimensional packed cages.



Tunable and switchable

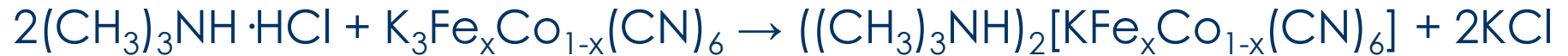


Ferroelastic properties





Sample preparation $\text{TrMAFe}_x\text{Co}_{1-x}$



TrMACo
 $x = 0.0$

$x = 0.2$

$x = 0.5$

$x = 0.8$

TrMAFe
 $x = 1.0$





Thermal analysis

Differential scanning calorimetry (DSC)

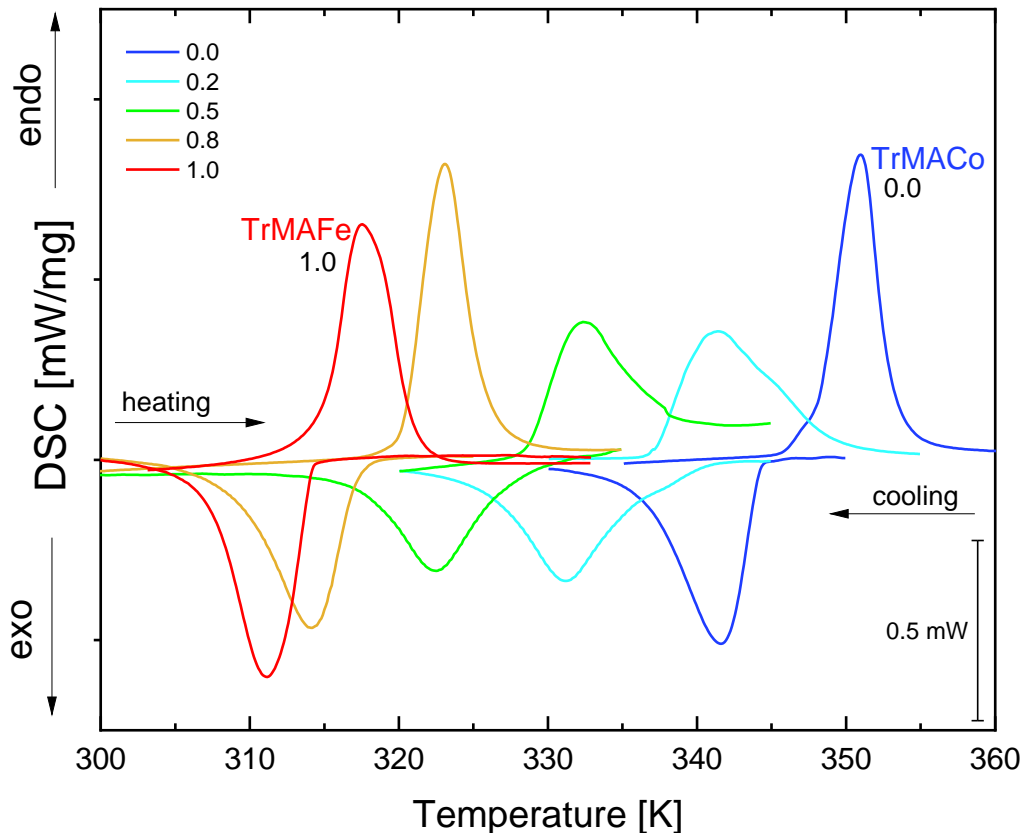
one solid-to-solid phase transitions

Temp. range: 298 - 393 K

Temp. ramp: 10K/min

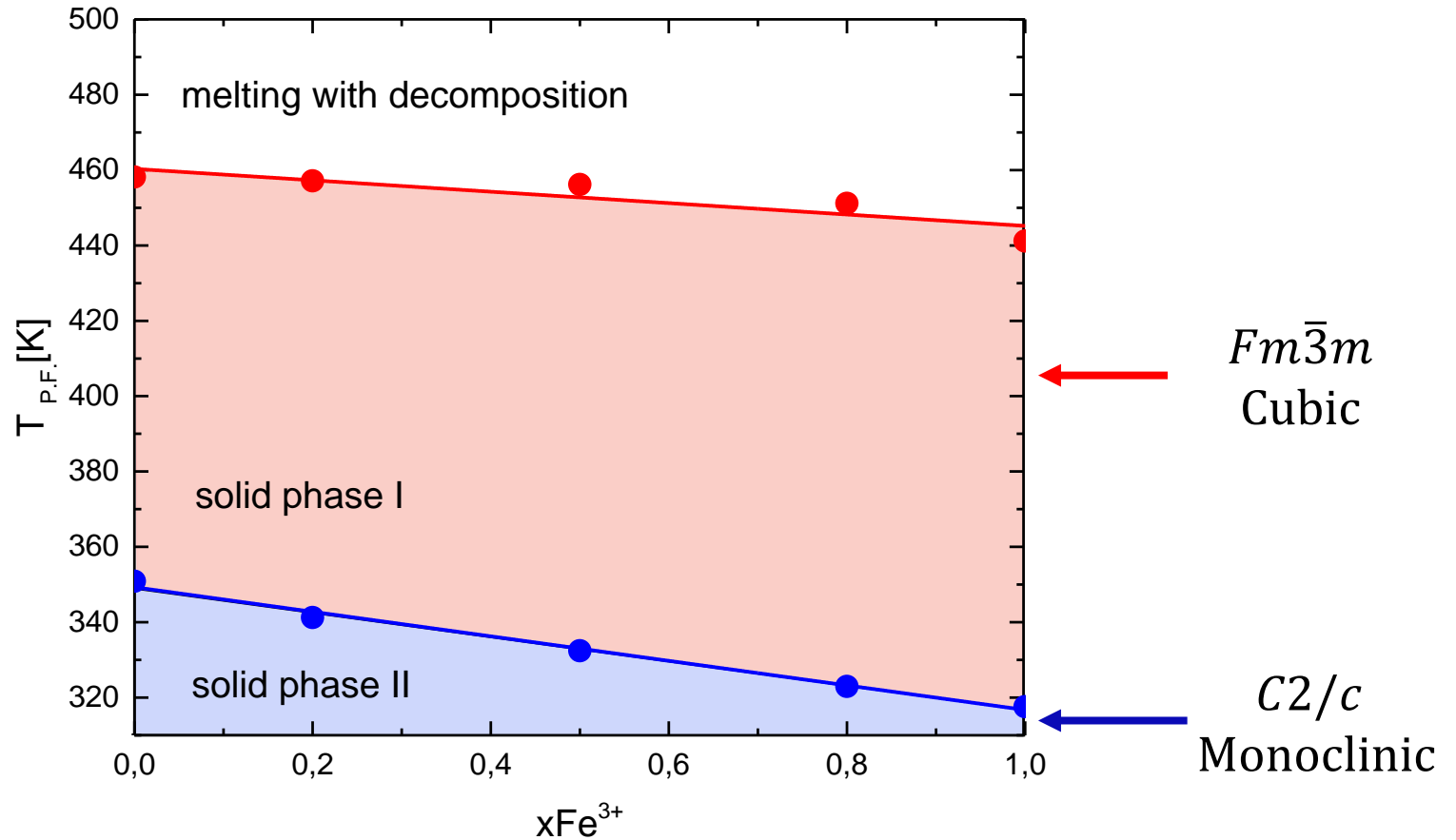


DSC 404 F1 Pegasus®





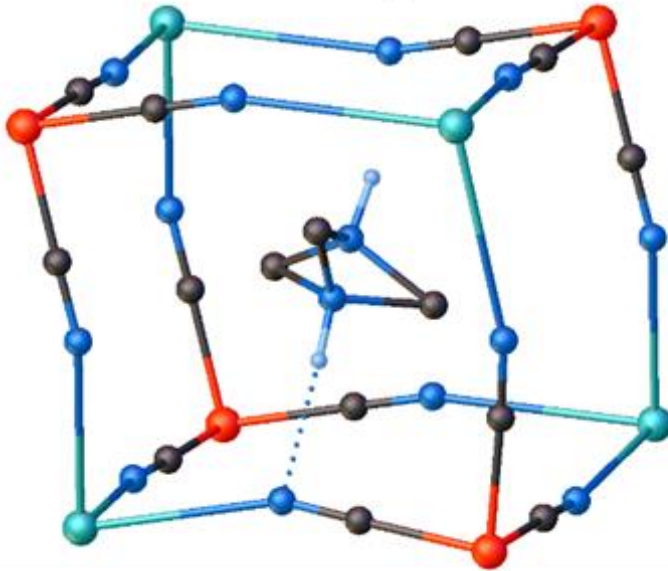
Phase diagram



X-Ray analysis

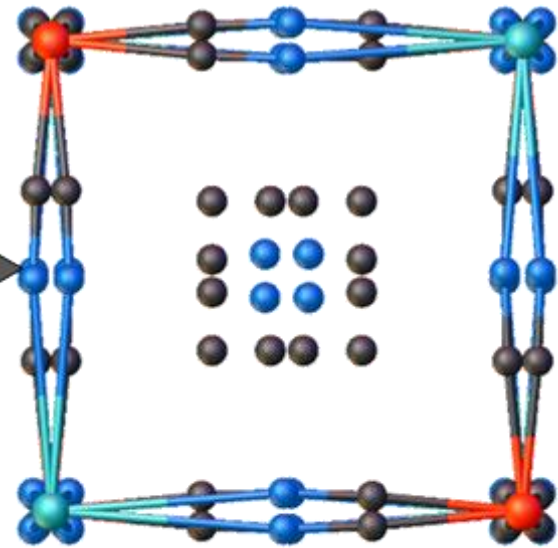
TrMAFe

$C2/c$



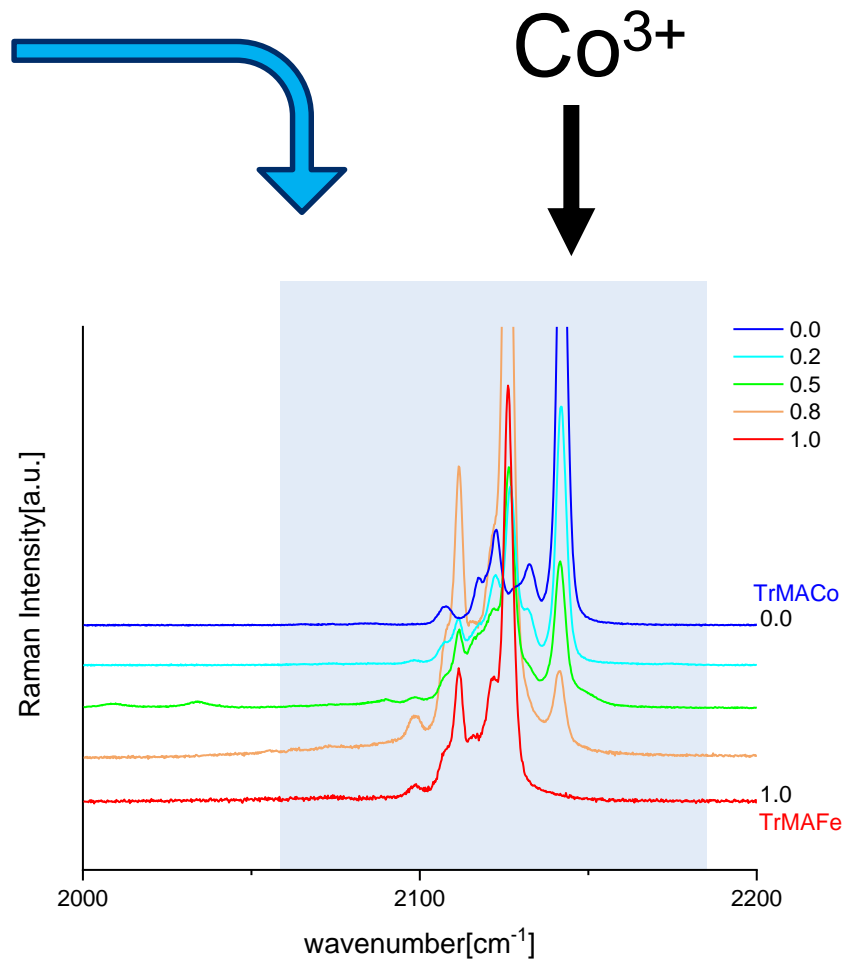
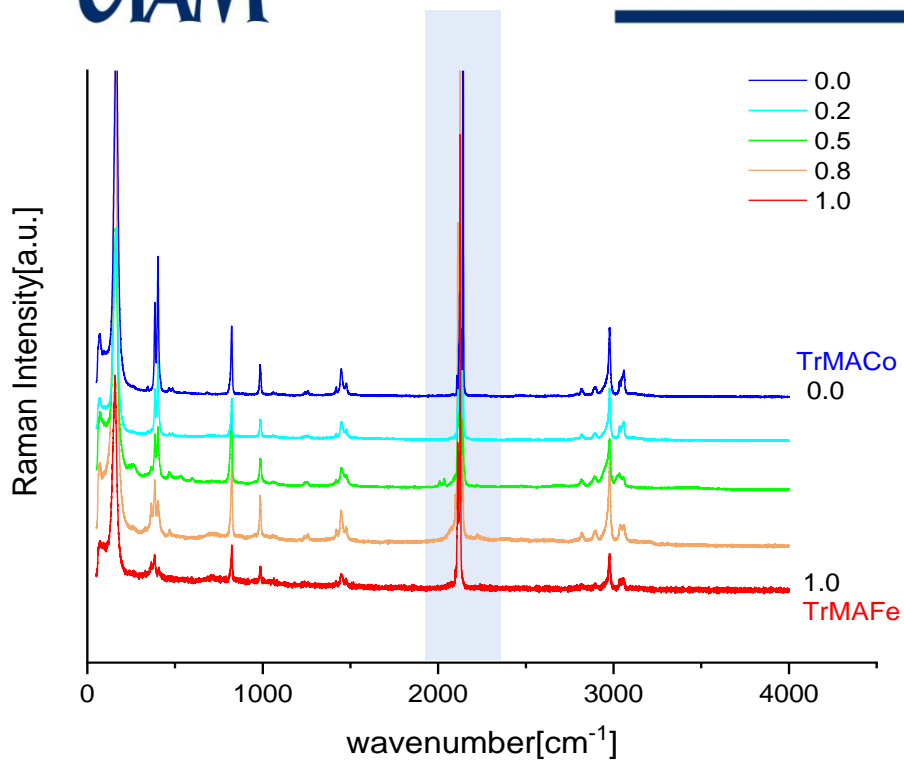
319K

$Fm\bar{3}m$



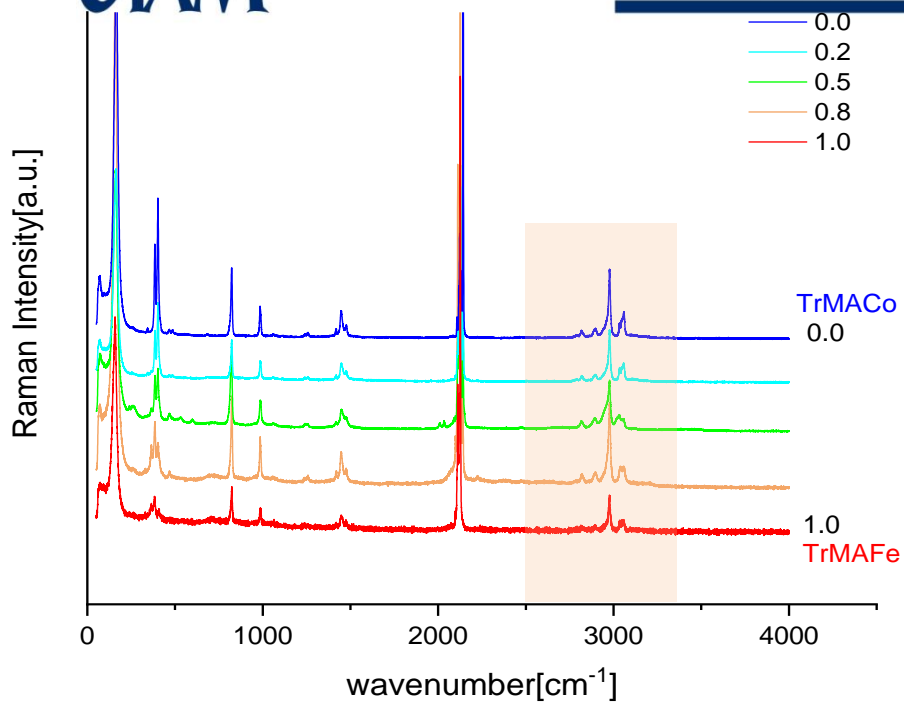


Raman analysis of inorganic cage/host



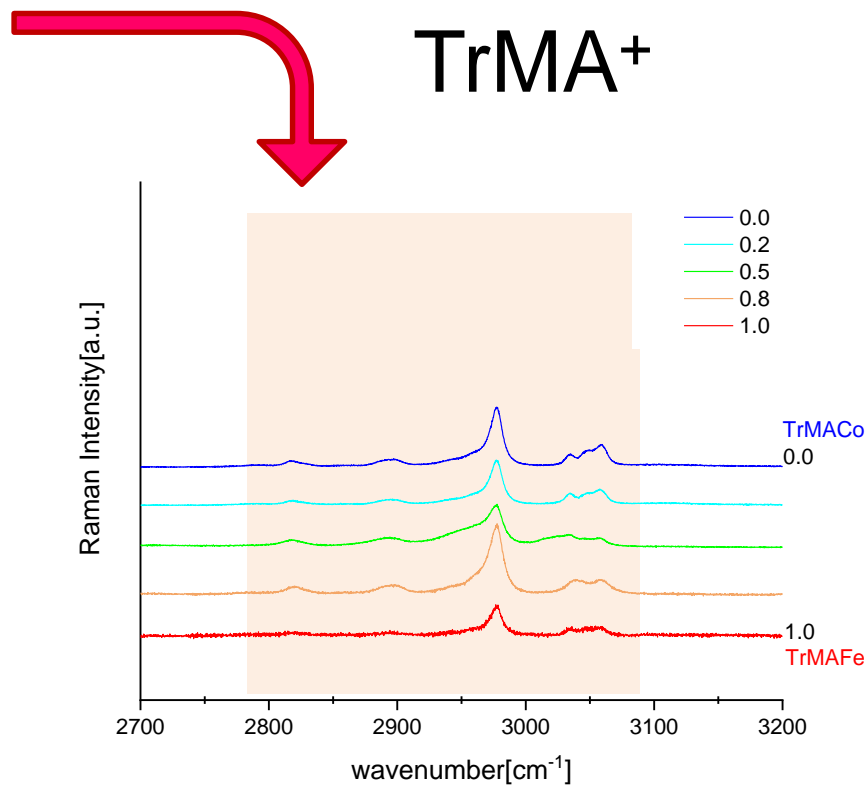


Raman analysis of organic guest



v C-H

v N-H





Conclusion

- The main objective of the project was to obtain 5 mixed crystals from the CPs group
 - The general formula: $((\text{CH}_3)_2\text{NH})_2[\text{KFe}_x\text{Co}_{1-x}(\text{CN})_6]$, $x=0.0, 0.2, 0.5, 0.8, 1.0$
 - For all crystal one solid-to-solid phase transition with the linear dependency of $T_{\text{P.F.}}$ versus x has been observed
 - The thermal stability of the crystal decreased with increasing x
 - Based on the thermal analysis the phase diagram has been constructed
 - The admixture of the Co^{3+} metallic cation has been detected by Raman spectroscopy
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The end.....

