Anomalous electrical transport in frustrated intermetallic YbCuAs$_2$: the role of spin

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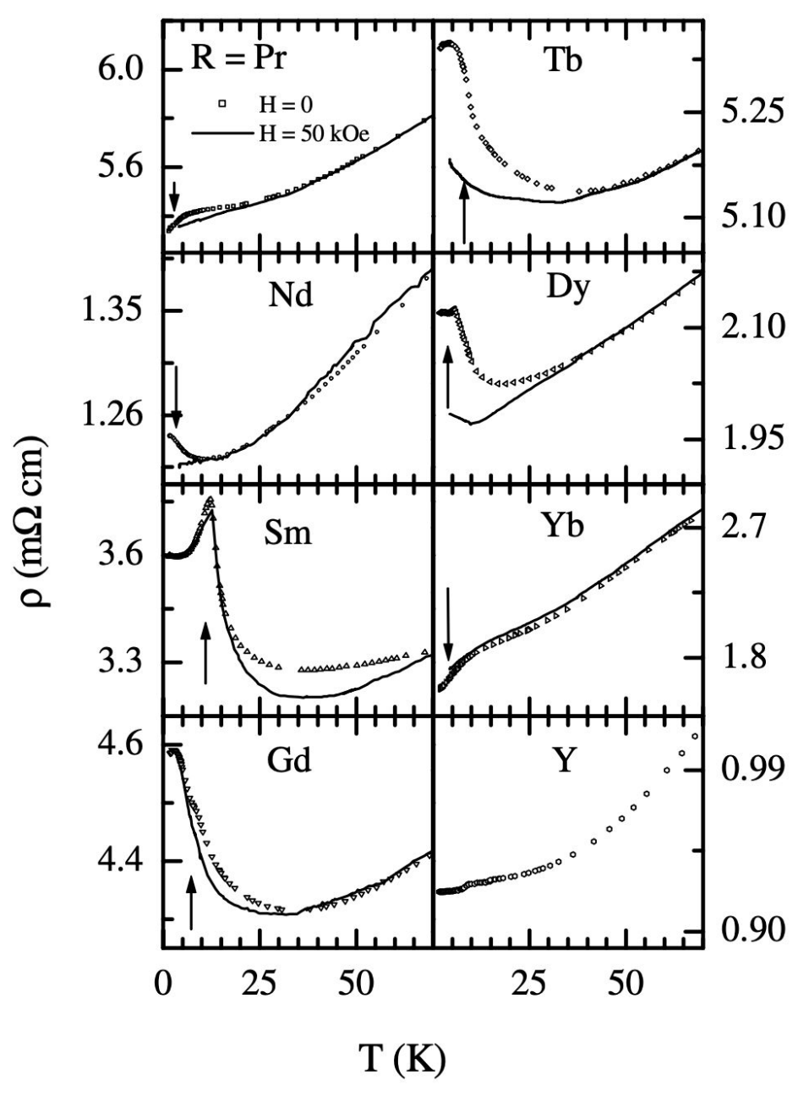
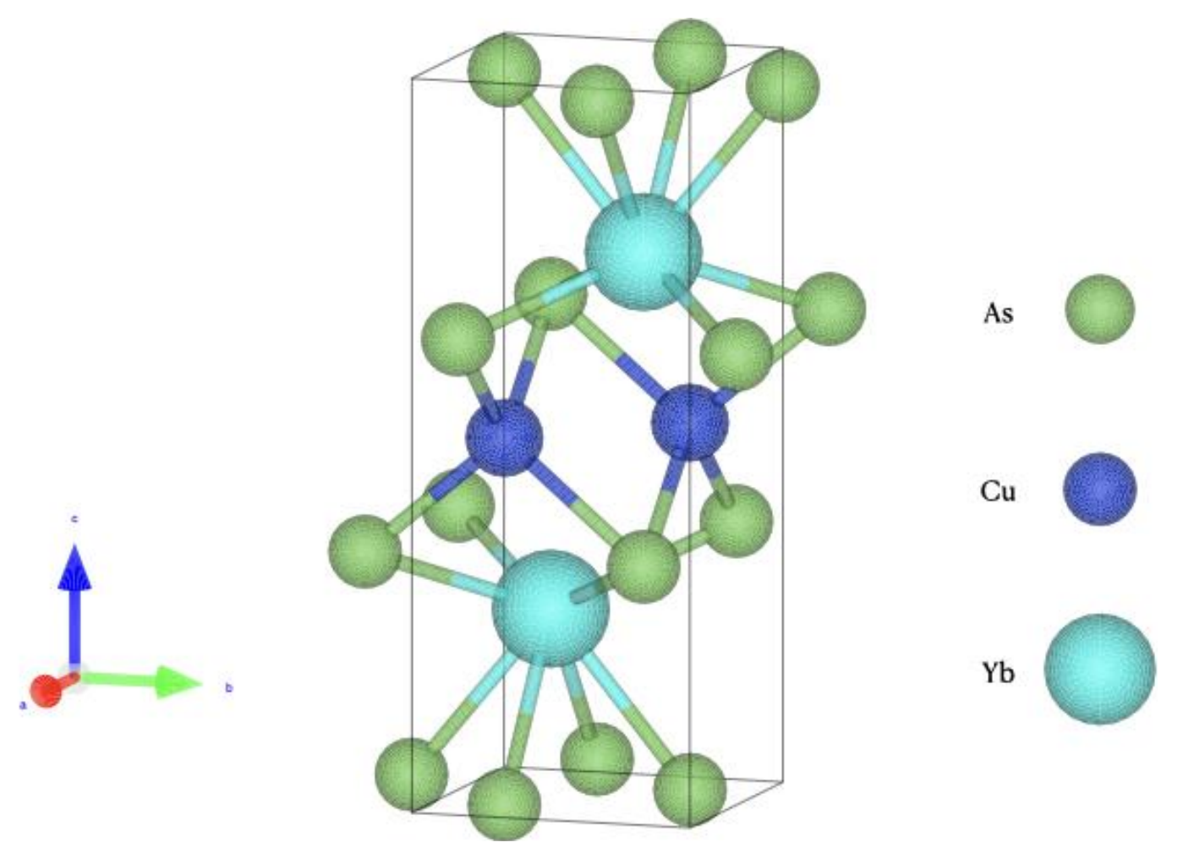
The competition between the Kondo effect and Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction characterize heavy Fermion systems. The Kondo effect is the screening of the localized magnetic moments by the spin of conduction electrons and leads to the formation of the spin-singlet. A characteristic low-temperature electrical resistivity minimum can happen in metals containing magnetic impurities due to the Kondo effect. The RKKY interaction is a long-range interaction between localized moments that is mediated by conduction electrons.

The ternary intermetallic compounds of RCuAs$_2$ with rare earth (R) ions like Sm, Gd, Tb, and Dy exhibit resistivity minima well above their respective Neel temperature. The Kondo effect is not anticipated in these ions as they have strictly localized 4f electrons. In contrast, for rare earth ions like Yb, where the Kondo effect is expected, the resistivity minimum is suppressed. Muon Spin Relaxation (μSR) measurements, as a probe of local magnetism, can help to shed light on the origin of this unanticipated phenomenon.

Transport and Thermodynamic Properties

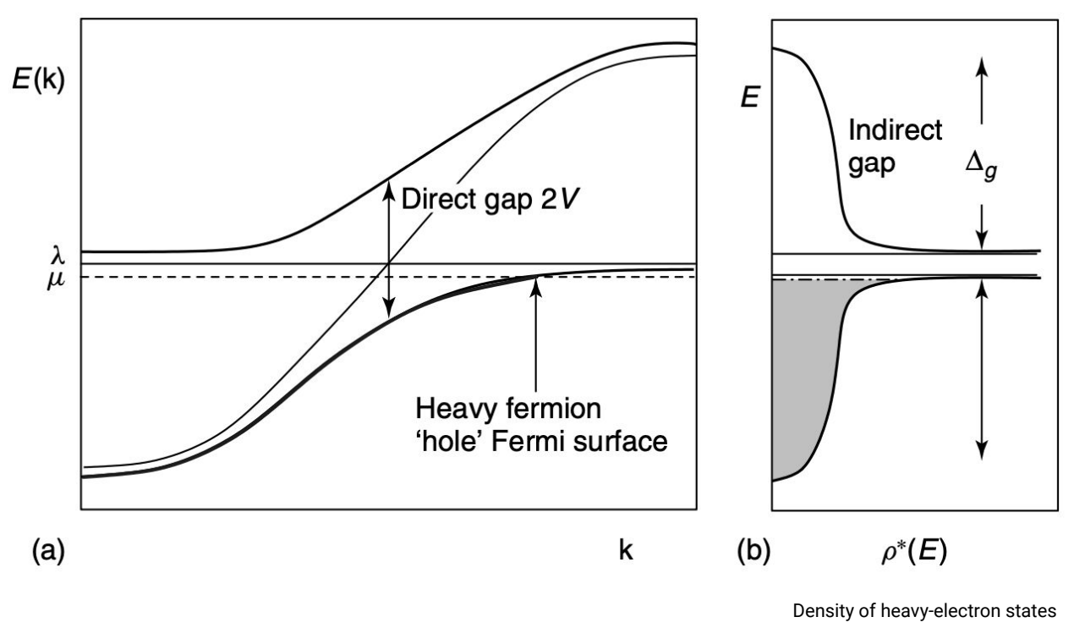


Sampathkumaran et. al. [1] investigated electrical resistivity in RCuAs2 intermetallic compounds. Some rare earths showed a distinct resistivity minimum above their Neel temperature, but others with strong 4f electron hybridization and Kondo effect did not exhibit this behavior.



YbCuAs$_2$:

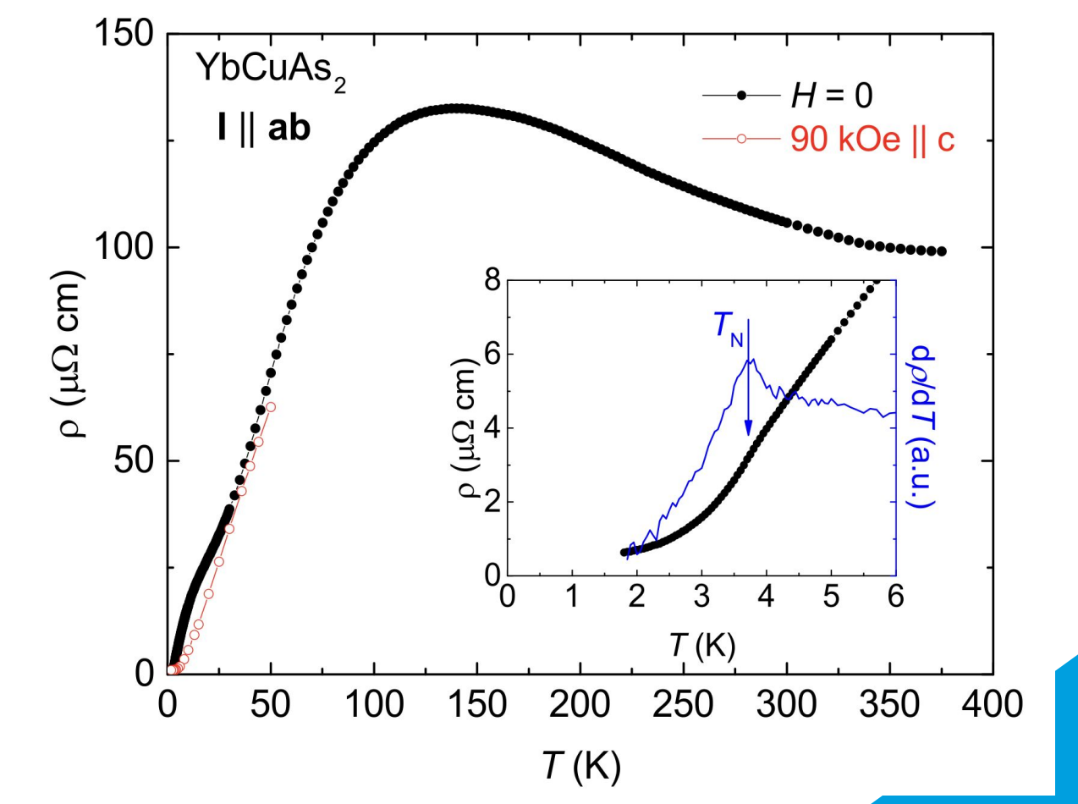
- Crystallise in the HfCuSi$_2$-type layered tetragonal form.
- 4f electrons are mostly localized.
- Magnetic properties influenced by Kondo and RKKY interactions, and CEF effect.

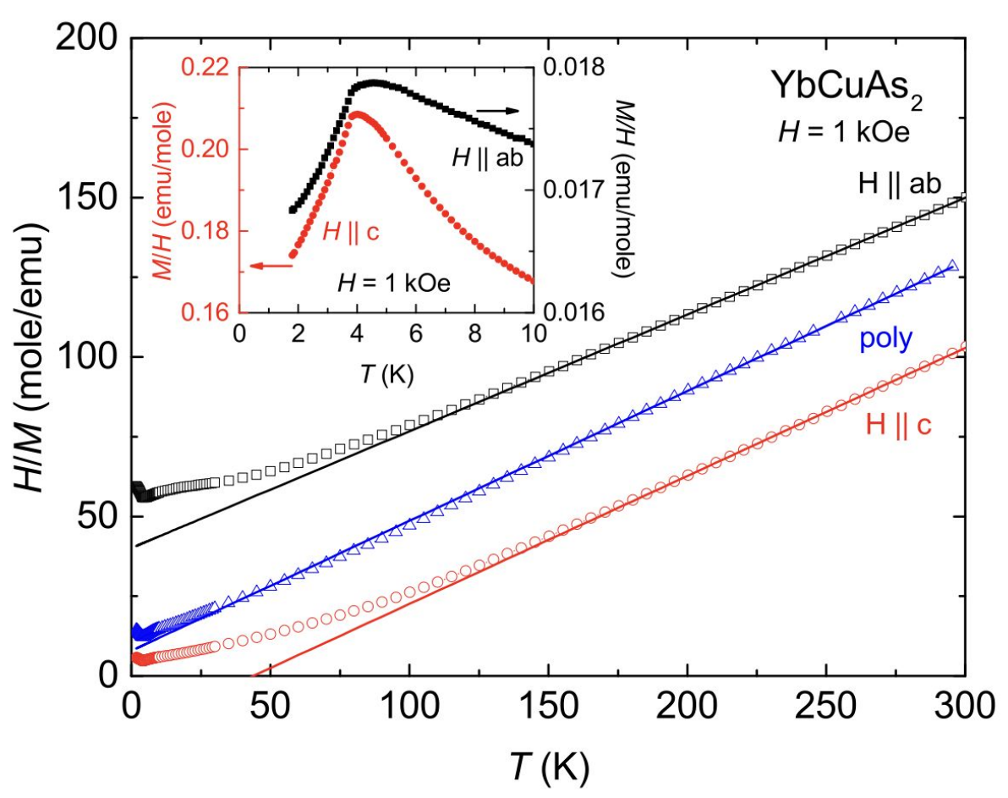


[8] (a) Electronic band structure showing hybridization between the f-electron states and the conduction electrons results in the formation of an upper and lower Fermi band. These bands are separated by an indirect hybridization. (b) Renormalized density of states showing hybridization gap: $\Delta_g = E_g(+) - E_g(-) \sim T_{K(\text{Kondo temp.})}$

[6] Resistivity (ρ) measurements for single crystal YbCuAs$_2$:

- maximum at T~125 K followed by -log(T) dependence in lower temperatures due to Kondo scattering in the presence of CEF splitting
- Broad hump at T~20 K due to Kondo scattering within the ground state
- Rapid drop below T_N~3.7 K due to Antiferromagnetic ordering
- Note the dramatically reduced resistivity compared with powder samples of [1]



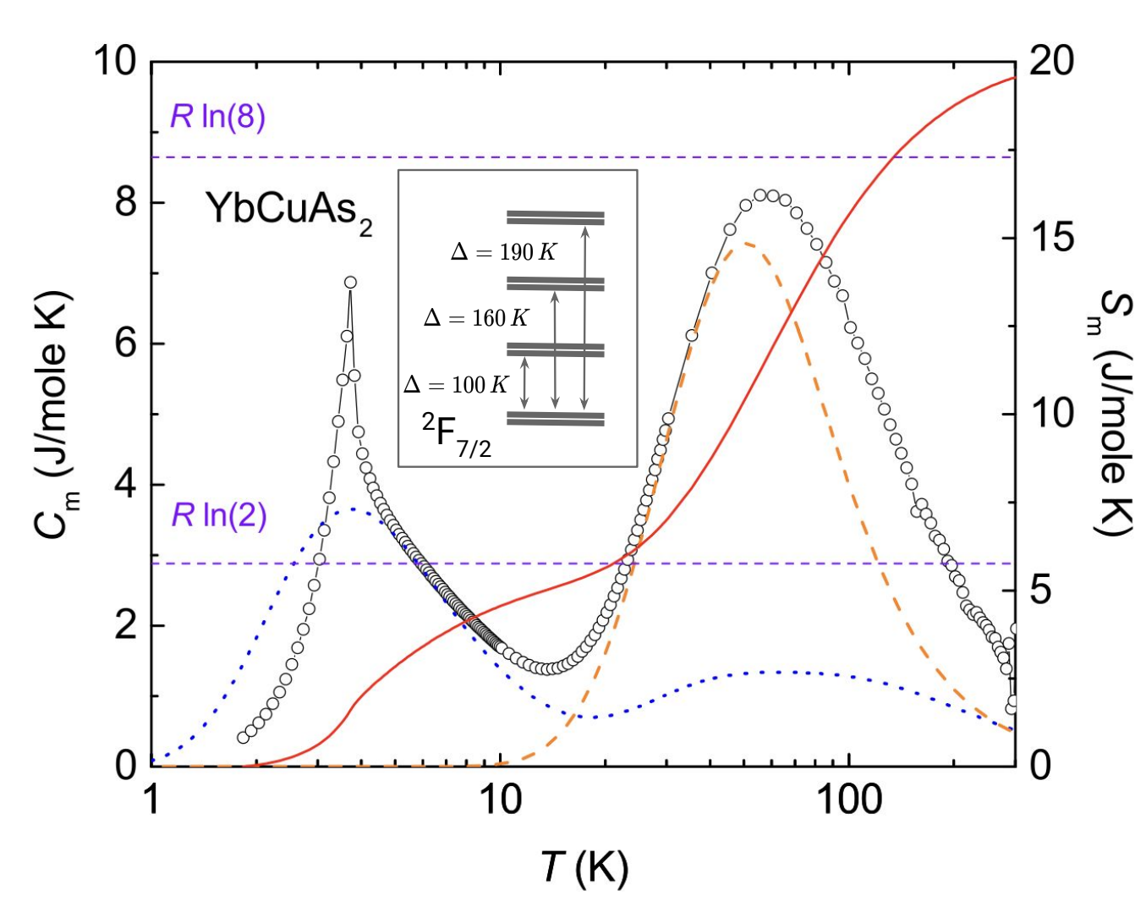


Inverse bulk magnetic susceptibility H/M [6] :

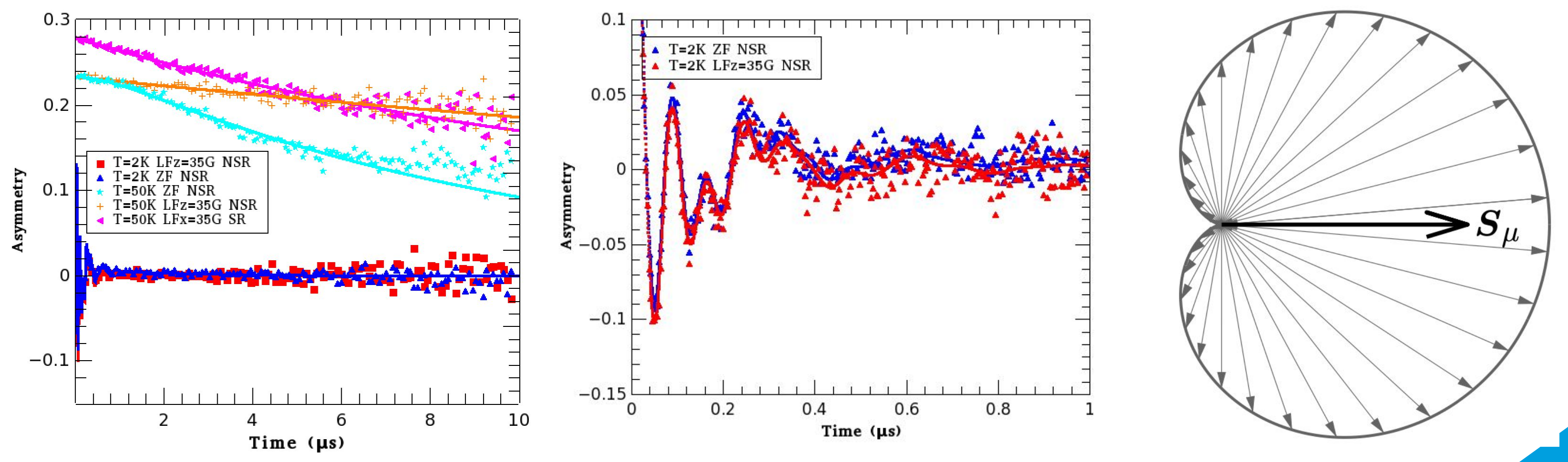
- A large magnetic anisotropy as shown by differences in the susceptibility parallel to the c axis and within the ab plane.
- Antiferromagnetic ordering at T = 3.7 K.

Magnetic contribution to the specific heat C_m:

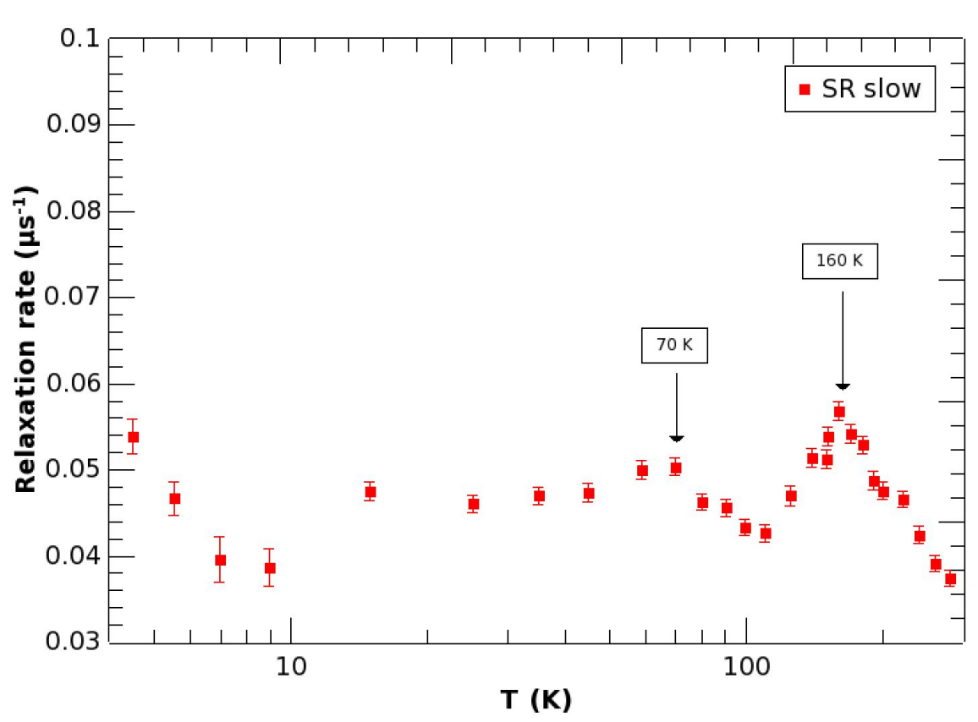
- Phase transition at T = 3.7 K.
- A sharp rise below T = 10 K and a broad maximum at T~55 K, which are suggestive of Schottky contribution due to crystal electric field (CEF) or enhanced magnetic fluctuations.
- The dashed line shows the Schottky contribution calculated from a four doublets configuration (inset).



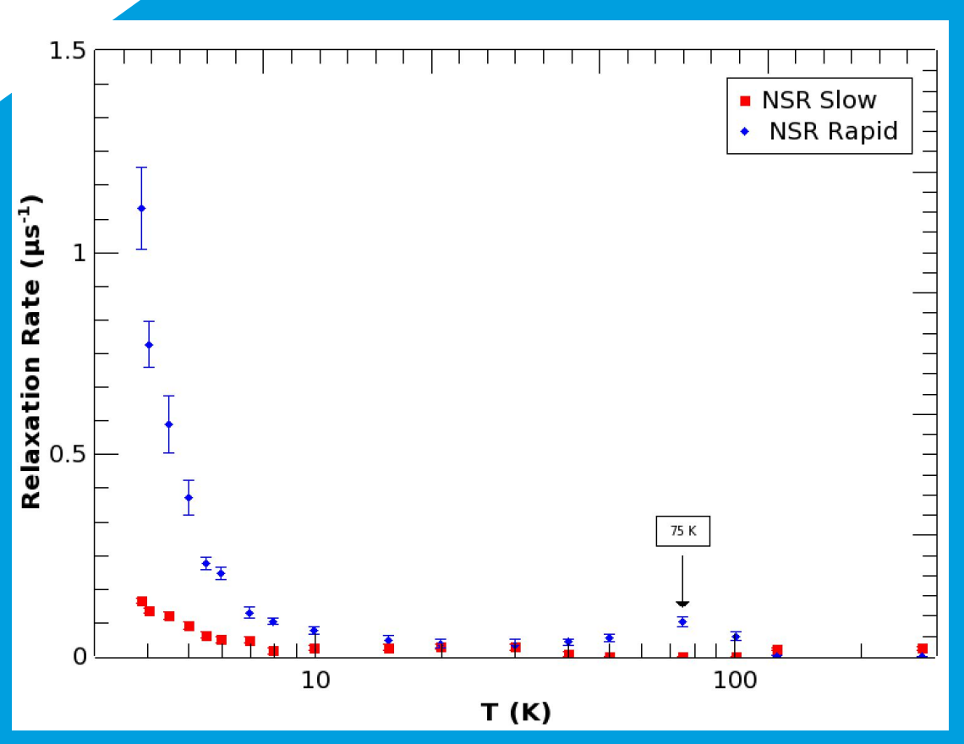
Muon Spin Relaxation



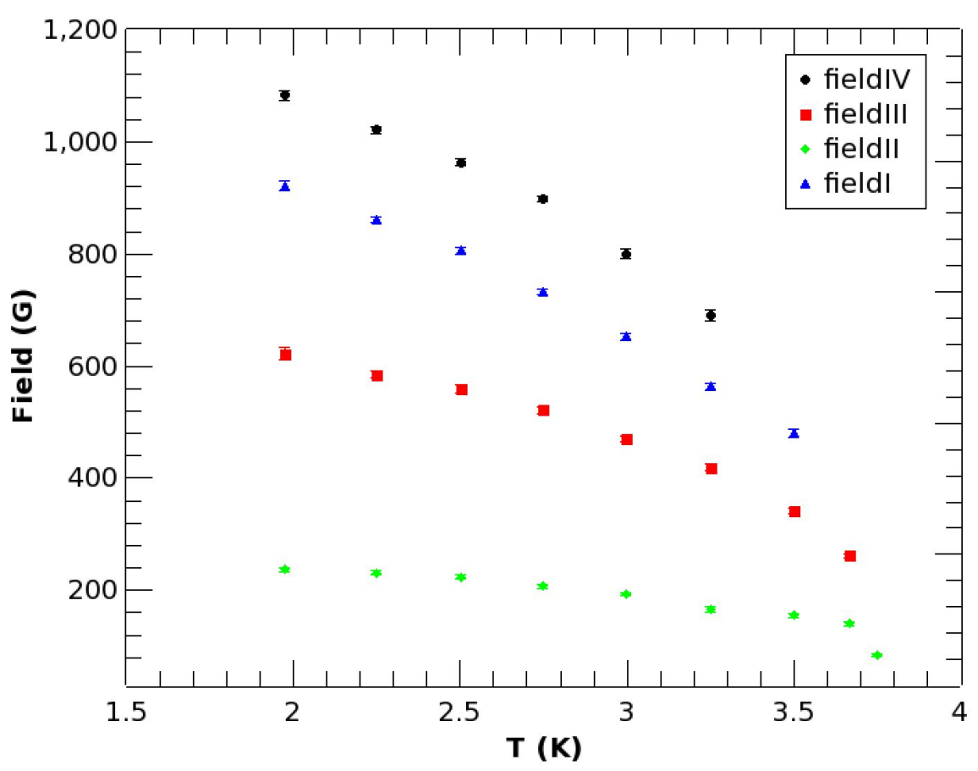
Left: Asymmetry in positron emission spectra for various experimental setups (ZF, LF).
Middle : Early times of the spectra below transition temperature: We can see spontaneous muon precession indicating magnetic ordering below 3.7 K. Surprisingly, Neutron diffraction scattering did not detect magnetic ordering down to 1.5 K for this compound.
Right : Asymmetric emission of positrons associated with weak beta decay of muon [9].

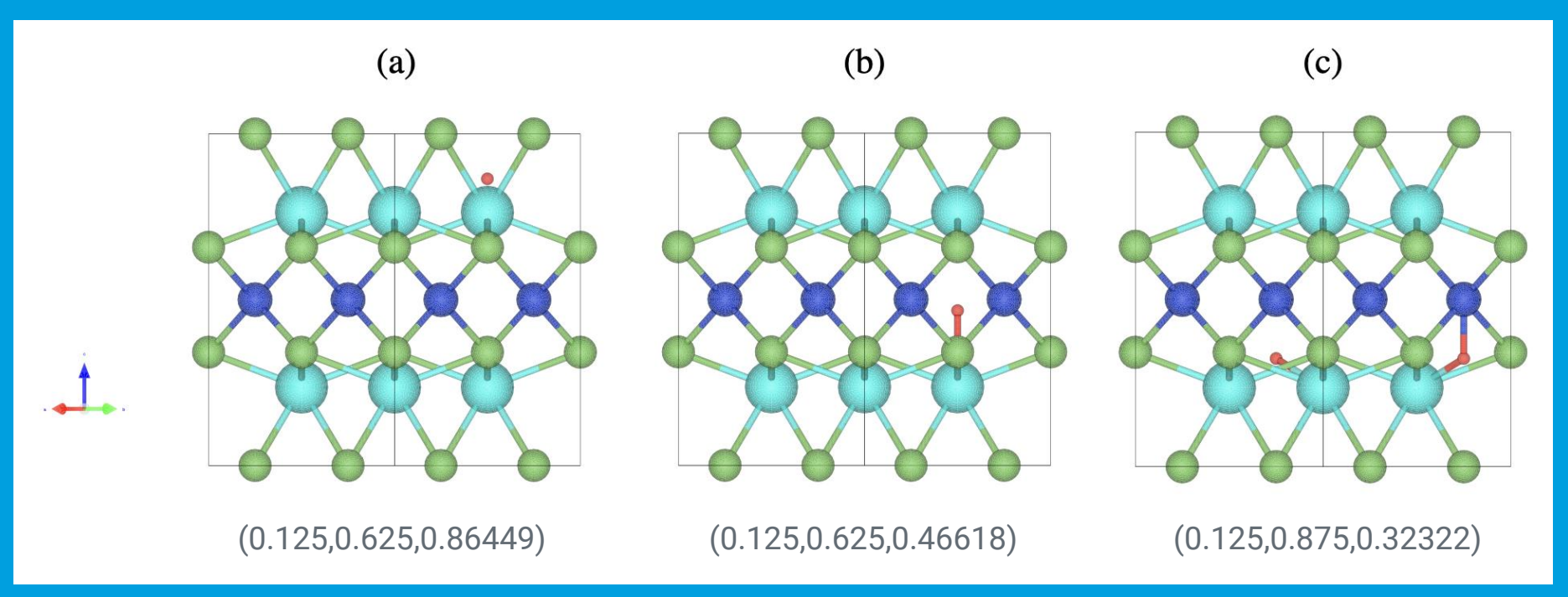


Relaxation rate (muon spin depolarization rate) vs. temperature above T_N

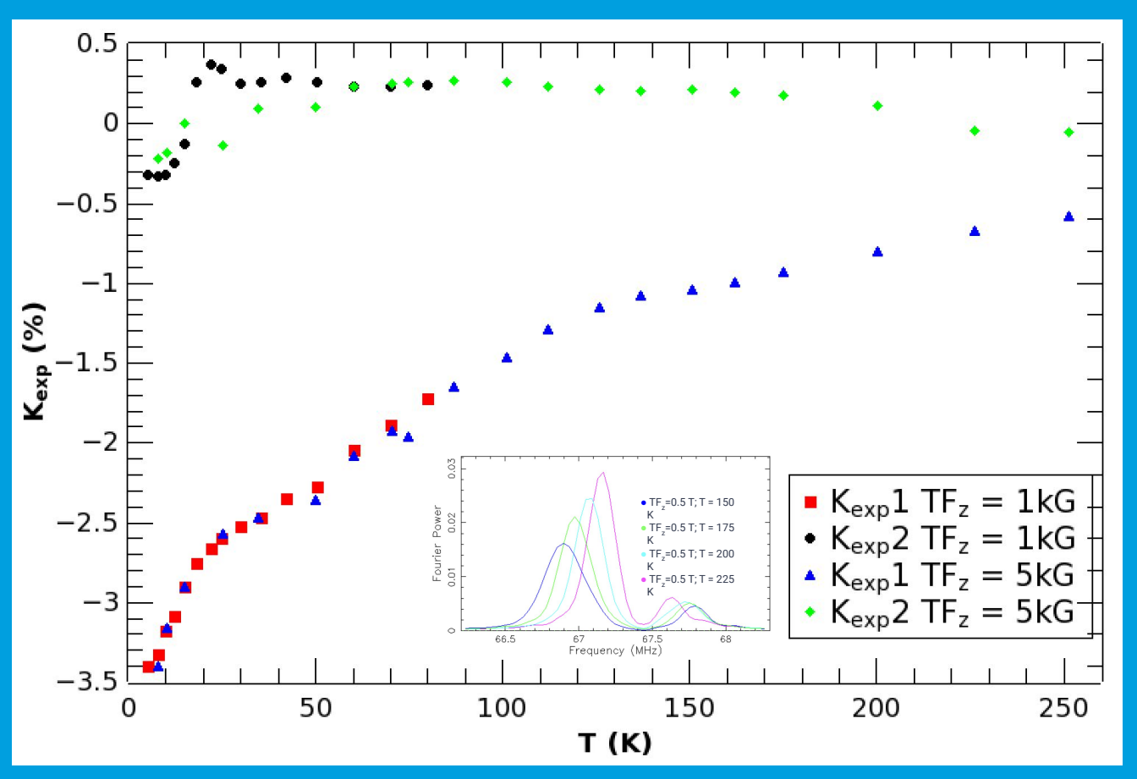


- Rapid relaxation rate growth below 10 K happens at the same temperature as the sharp rise in specific heat data.
- Broad maxima in the relaxation rate in the left panel roughly coincide with the analogous maxima in C_m and ρ.





Left: Precession frequencies below transition temperature, indicating four magnetically inequivalent Muon sites.
Right: DFT+μ calculations reveal three crystallographically inequivalent muon sites.

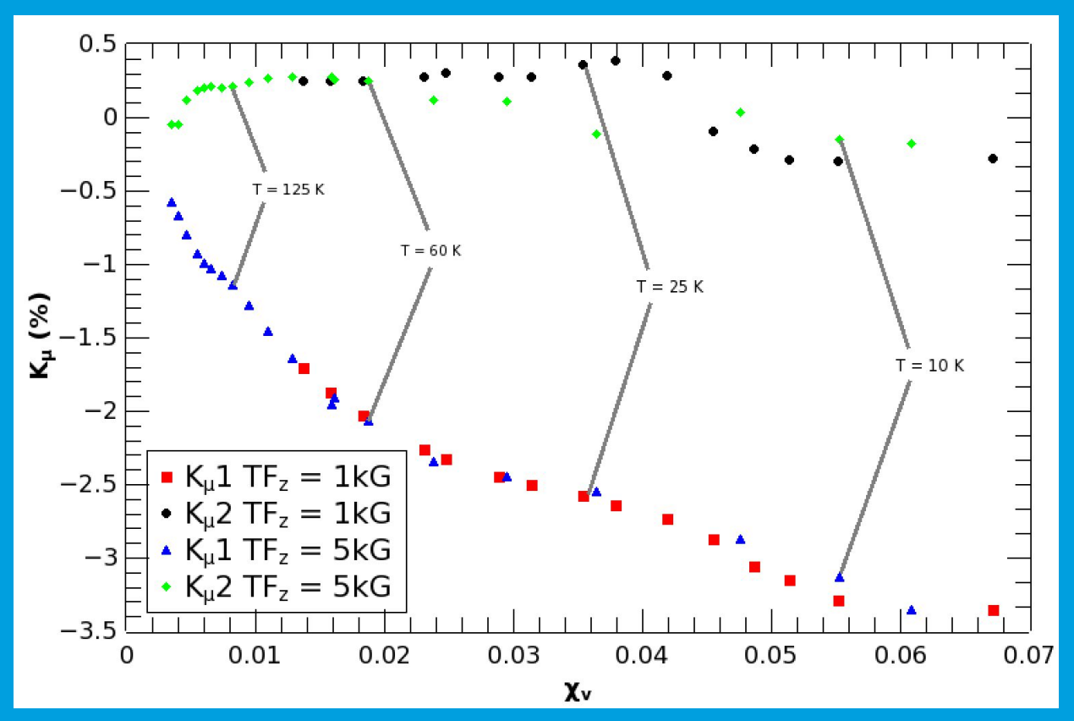


Fractional shift in the muon spin precession frequency vs. temperature :

- Both 5 kG and 1 kG field data follow the same trend.
- The fractional shift is a measure of the local susceptibility
- Inset: Fast Fourier Transform of the TF asymmetry spectra

Fractional shift corrected for demagnetization effects as a function of bulk susceptibility :

- Marks on the plot indicates deviations from linearity at ~125 K, ~25 K, and ~10 K. Deviations are happening at the same temperature scale as the features within resistivity and specific heat data.



In conclusion, our study has successfully confirmed the presence of magnetic ordering, even though it was not apparent through Neutron diffraction. By utilizing newly calculated Muon sites and precession signals, we will embrace the increasing trend within the μSR community of employing computational packages to explore the magnetic structure further. More generally, knowledge of the muon site(s) enables more detailed quantitative interpretation of the data. The muon spin depolarization rate, $1/T_1$, in the fast fluctuation limit, can be described by $2\Delta^2$ / ν, where Δ^2 represents the instantaneous internal field at the muon site, dependent on the moment's size and position. On the other hand, ν is influenced by transitions between different energy levels, determined by the exchange coupling. The observed Schottky contribution in the specific heat data below 10 K, signifying the depopulation of a doublet system, indicates the freezing out of spin fluctuations. As fluctuations slow down, the relaxation rate, $1/T_1$, increases inversely. In more complex heavy fermion systems with Kondo behavior, understanding the eigenfunctions of the crystal electric field (CEF) Hamiltonian will aid in calculating $1/T_1$. In the future, our goal is to differentiate between the impacts of CEF and the Kondo effect on the system, furthering our understanding of these magnetic phenomena.

Acknowledgments: Dr. Sarah Dunsiger, Dr. Jeff Sonier, Dr. Shayan Gheidi, Dr. Shyam Sundar, Nasrin Azari, Mariah Goeks, Michael Yakovlev, Katherine Curvelo, Isabelle St.-Martin, Dr. Eundeok Mun, David Evans, Dr. Gerald Morris, Dr Bassam Hitti, Dr Donald Arseneau, Rahim Abasalti, Deepak Vyas, Dr. Leandro Liborio.

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