united nations educational, scientific and cultural organization
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SMR 1232 - 22

XII WORKSHOP ON
STRONGLY CORRELATED ELECTRON SYSTEMS

17 - 28 July 2000

CDW in $RE_5Ir_4Si_{10}$ Compounds

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These are preliminary lecture notes, intended only for distribution to participants.

ELECTRONIC

MAGNETIC AND

STRUCTURAL PROPERTIES

OF $(RE)_5(TM)_4Si_{10}$

INTERMETALLIC COMPOUNDS

- CDW, SUPERCONDUCTIVITY AND MAGNETISM

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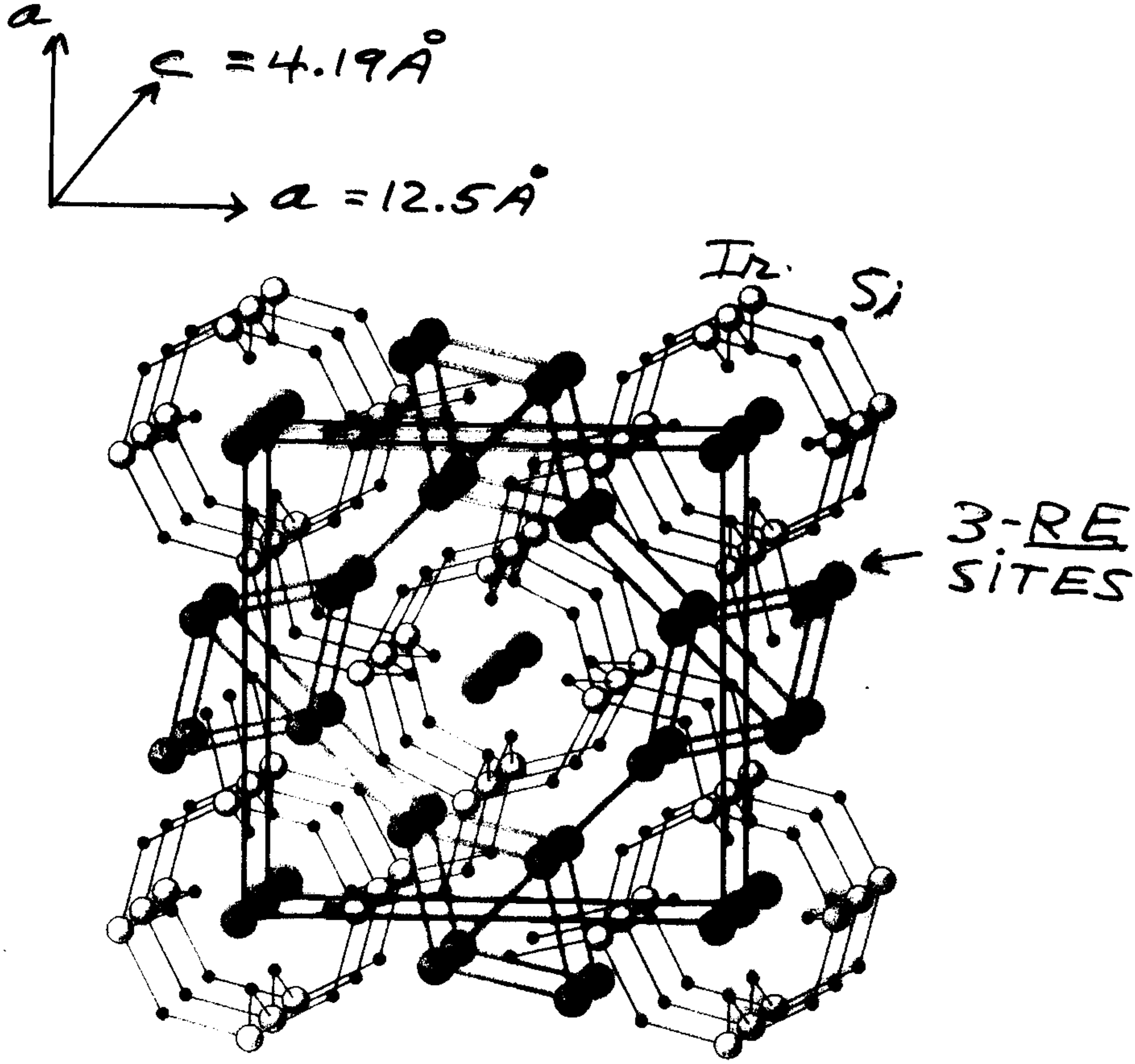


5 4 10 TETRAGONAL

P4/mbm

RE	Ir	Si
	Rh	Sn
	Os	Ge

$RE_5T_4X_{10}$			
compound	T_N (K)	T_C (K)	T_{CDW} (K)
$Sc_5Ir_4Si_{10}$	–	8.5	–
$Lu_5Ir_4Si_{10}$	–	3.9	83
$Yb_5Ir_4Si_{10}$	–	–	49
$Tm_5Ir_4Si_{10}$	0.8, 1.8	–	100, 133
$Er_5Ir_4Si_{10}$	1.3, 2.8	–	55, 155
$Ho_5Ir_4Si_{10}$	2.0	–	180
$Dy_5Ir_4Si_{10}$	5.0	–	210
$Ce_5Ir_4Sn_{10}$	4.2	–	– ?
$Pr_5Ir_4Sn_{10}$	–	–	–
$Ce_5Rh_4Sn_{10}$	4.4	–	–
$Pr_5Rh_4Sn_{10}$	5.5	–	–
$Nd_5Rh_4Sn_{10}$	6.5, 7	–	–
$Gd_5Rh_4Ge_{10}$	6.5, 9, 11, 14	–	–
$Tb_5Rh_4Ge_{10}$	2.5, 3.5, 5, 11.5	–	–
$Dy_5Rh_4Ge_{10}$	6	–	–
$Ho_5Rh_4Ge_{10}$	5	–	–
$Er_5Rh_4Ge_{10}$	4.2, 5.6	–	–
$Tm_5Rh_4Ge_{10}$	6, 6.9	–	–
$Lu_5Rh_4Ge_{10}$	–	2.4	–
$Yb_5Rh_4Ge_{10}$	–	–	–
$Lu_5Rh_4Si_{10}$	–	3.7	145
$Ho_5Os_4Ge_{10}$	2.1	–	–

H.F. BRAUN (1984, 1986)

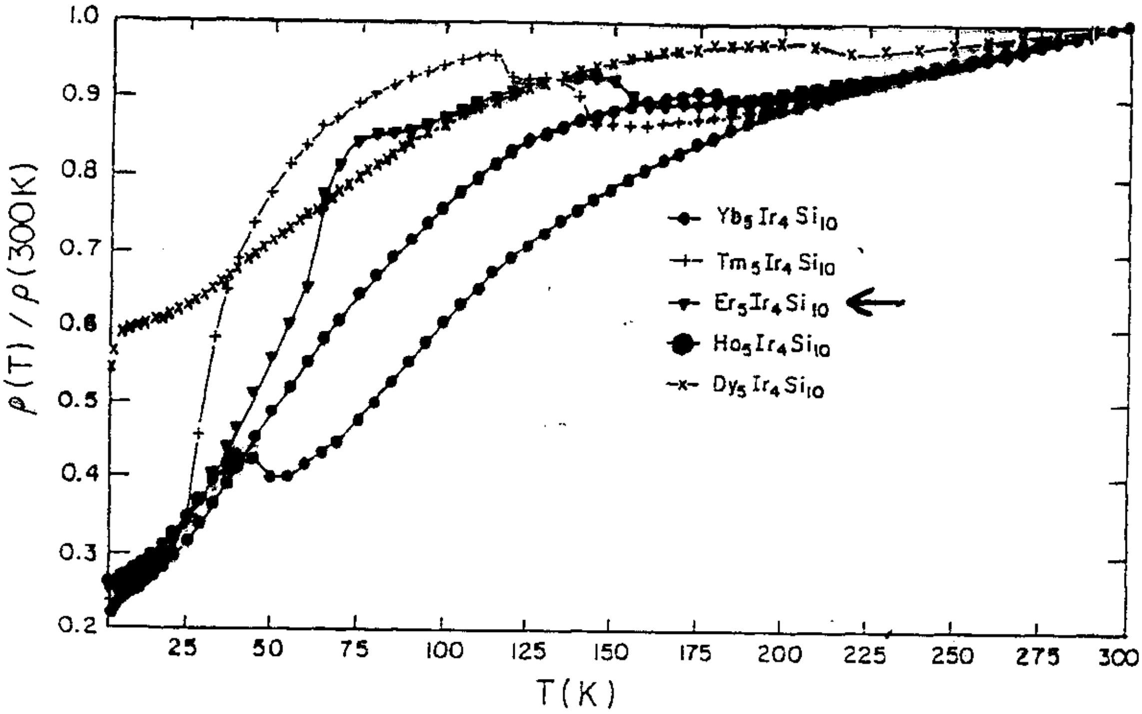
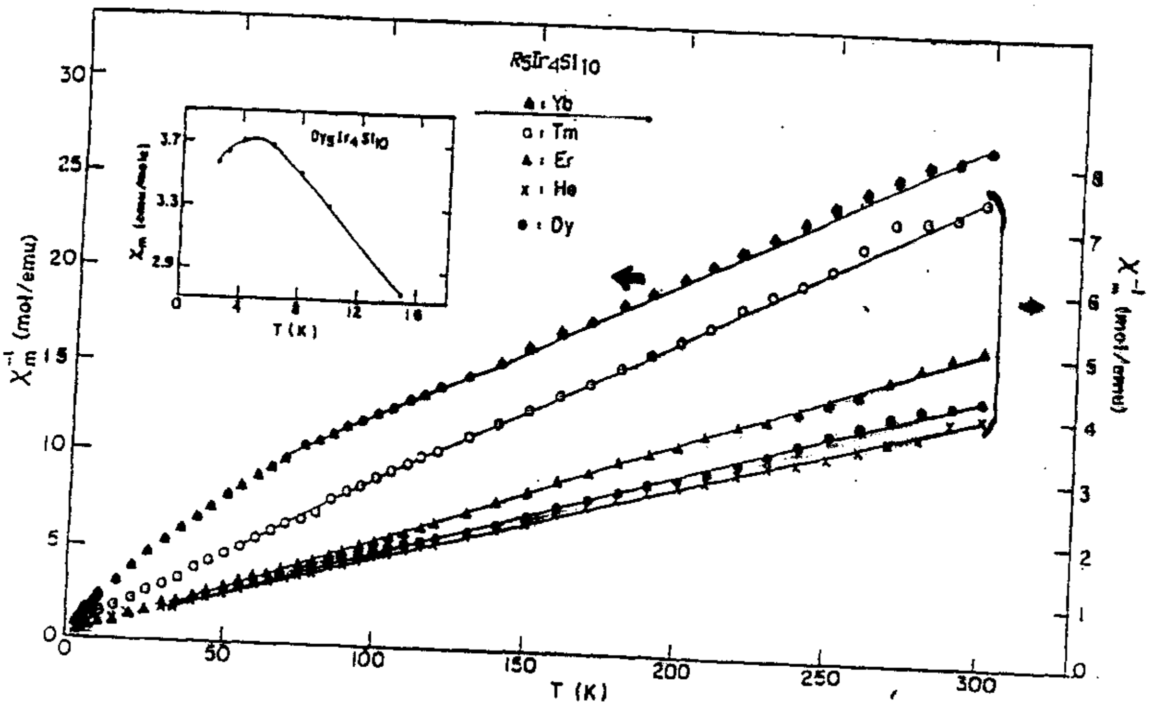
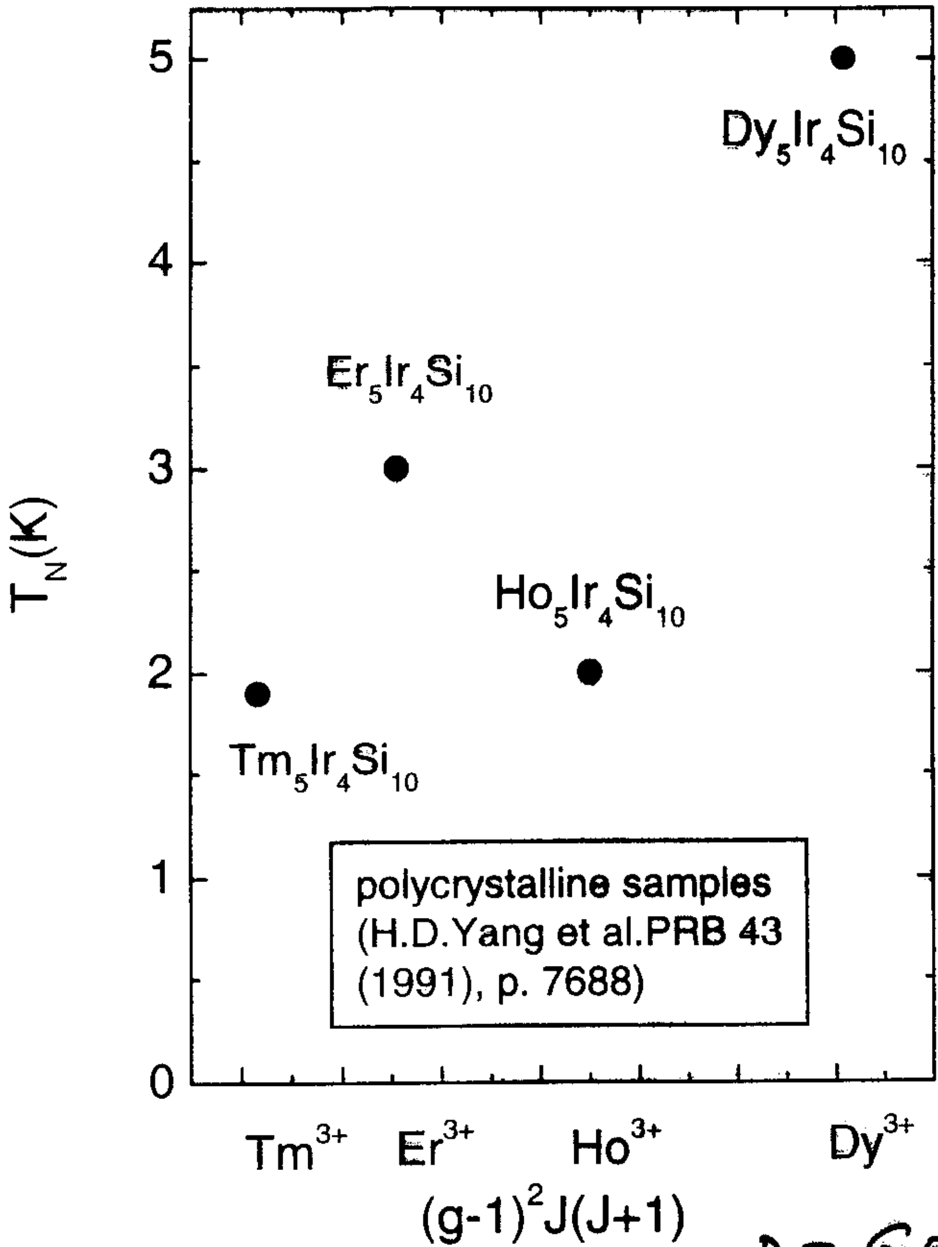


FIG. 3. Normalized resistivity as a function of temperatures between 2.6 and 300 K for $R_5Ir_4Si_{10}$ (R = Dy–Yb).

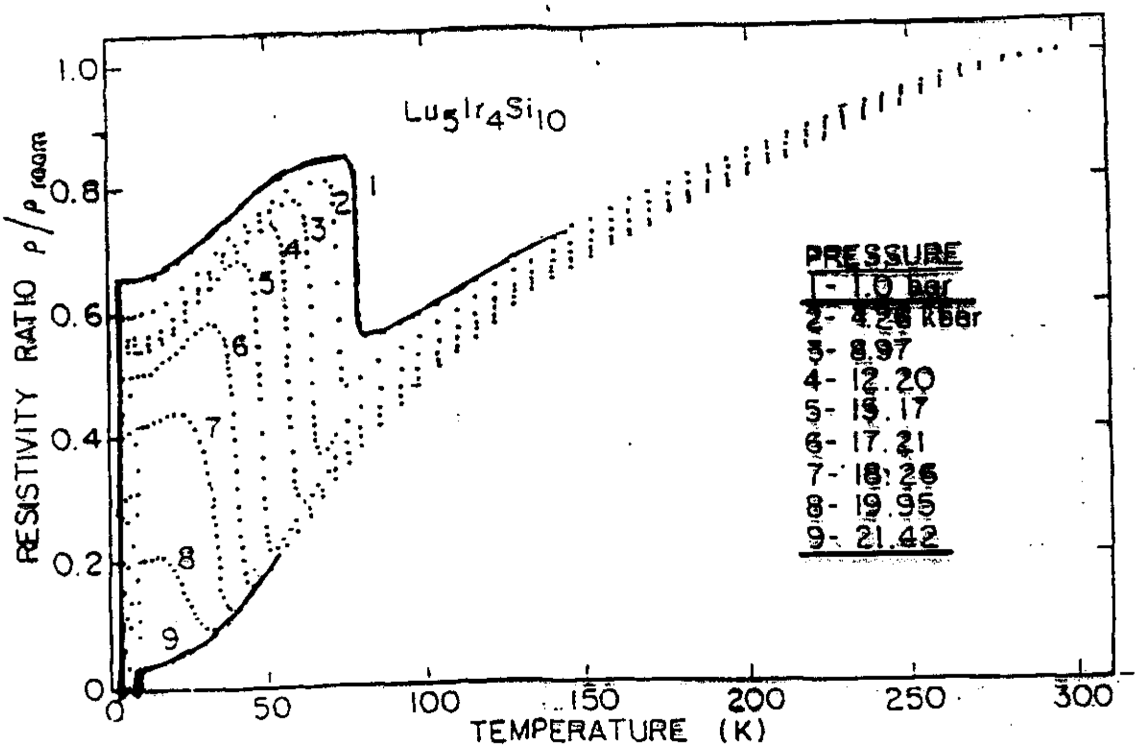
H. D. YANG et al. PRB. 43 (1991), 7688

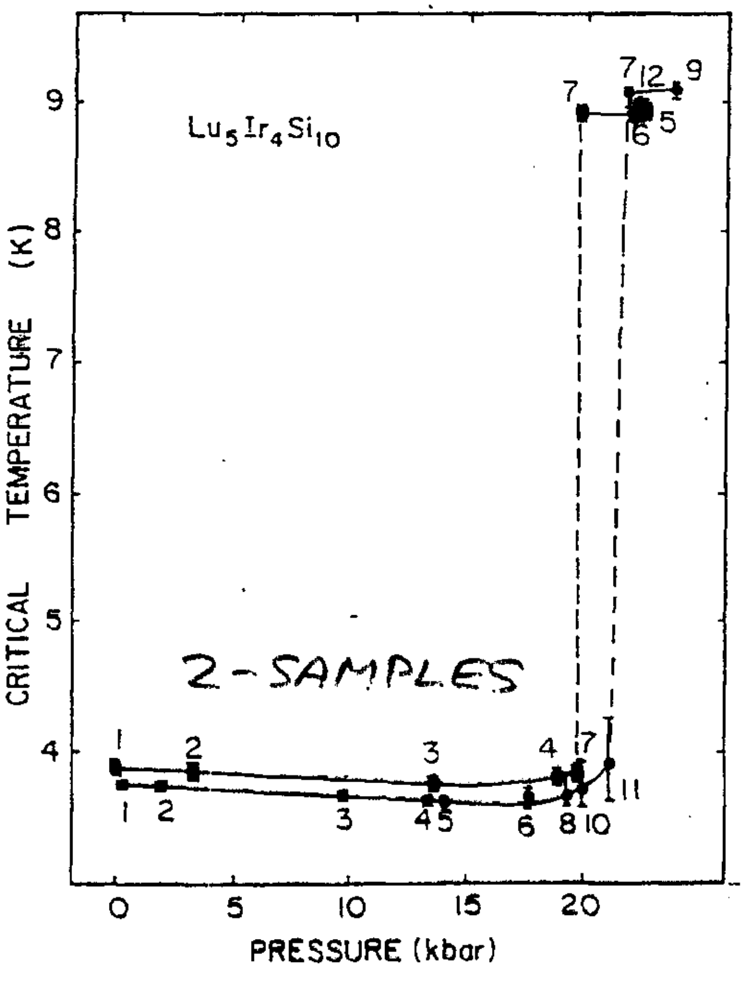


H. D. YANG et al. PRB 43 (1991), 7688



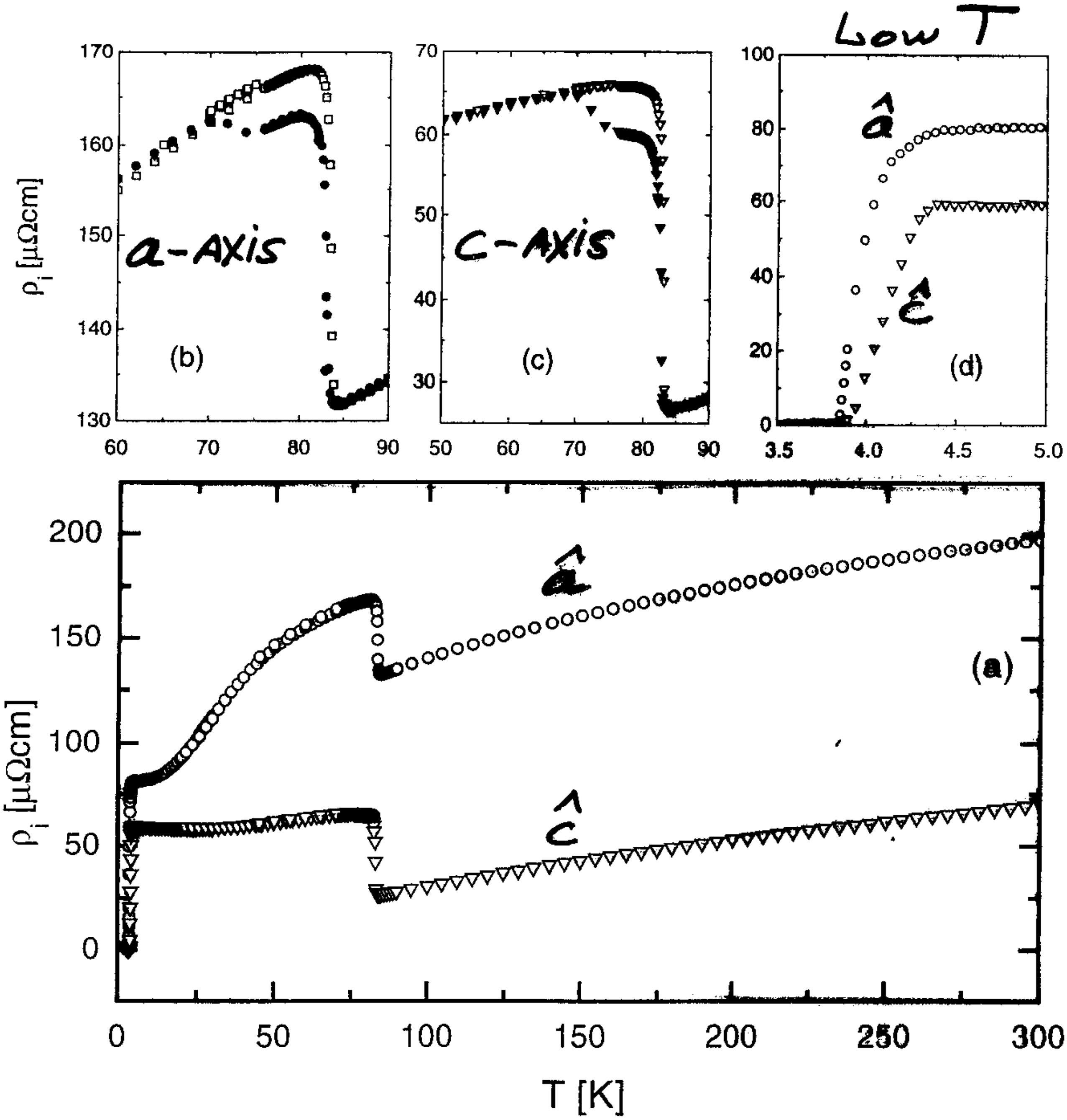
DE GENNES FACTOR





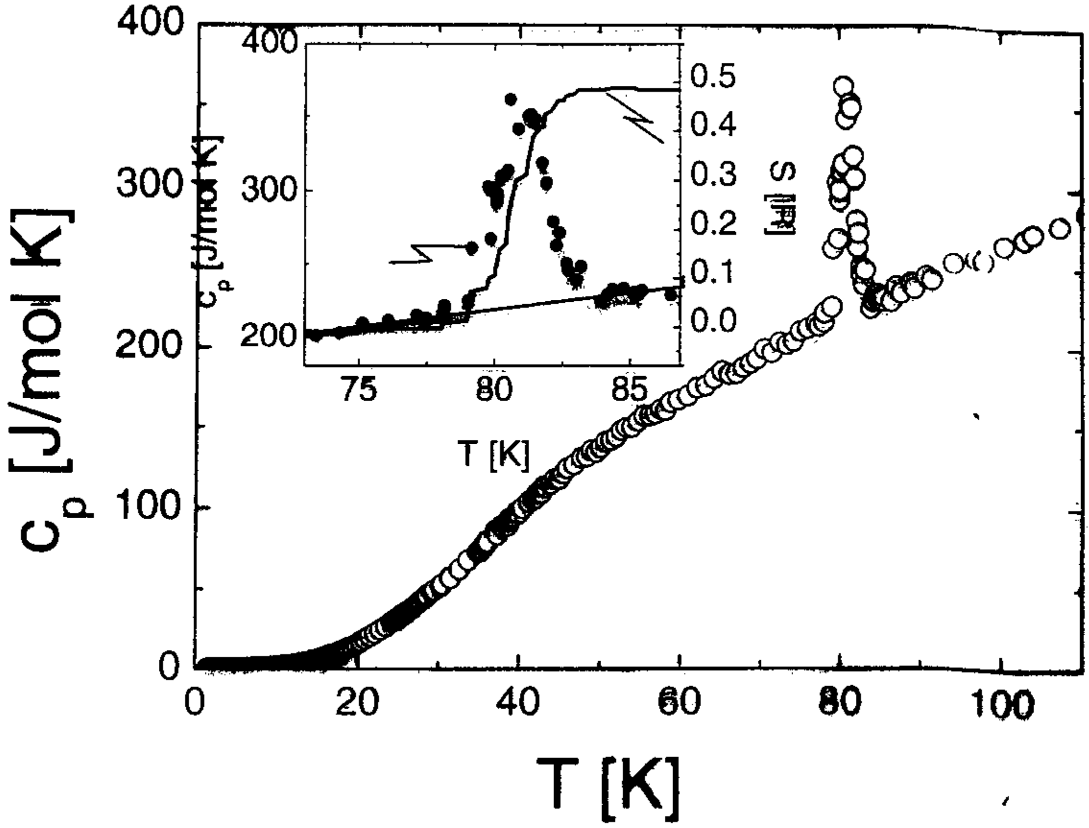
R.N. SHELTON et al.
PRB 34 (1986), 4590

$Lu_5Ir_4Si_{10}$ (single crystal): resistivity vs. temperature



B. Becker et al. (1999)

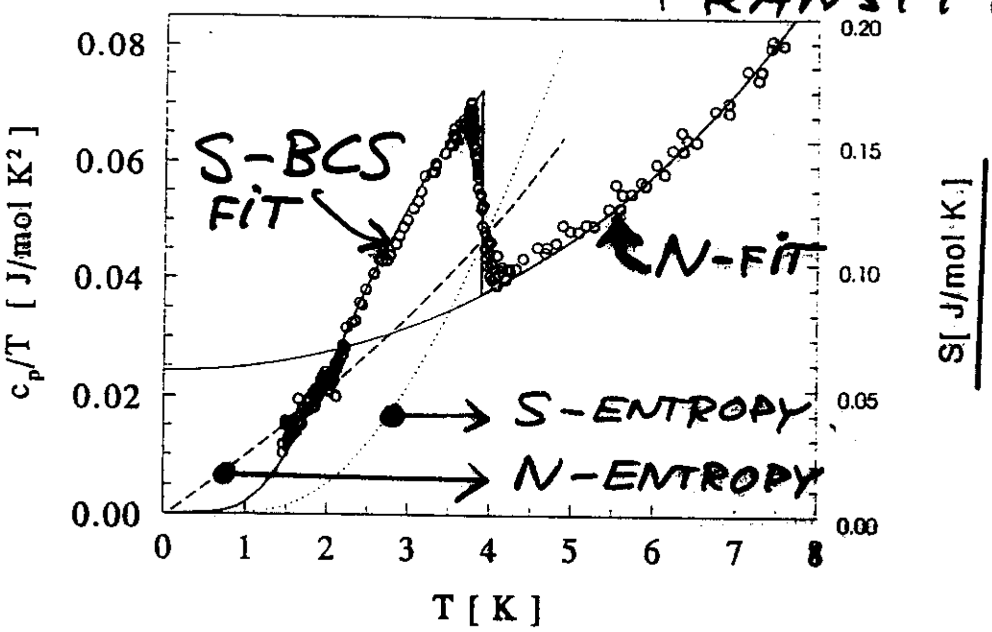
$Lu_5Ir_4Si_{10}$ (single crystal): high-temperature specific-heat



B. Becker *et al.*, PRB **59**, 7266 (1999).

Specific heat cusp in different CDW systems			
compound	T_{CDW}	$\Delta T/T_{CDW}$	ΔS
TTF-TCNQ	54 K	10%	≈0.03 R
$NbSe_3$	145 K	4.8%	≈0.01 R
	58 K	1.7%	≈0.005 R
$K_{0.3}MoO_3$	83 K	7%	≈0.11 R
purple bronzes			
$Li_{0.9}Mo_6O_{17}$	24 K	25%	0.03 R
$K_{0.9}Mo_6O_{17}$	120 K	20%	0.064 R
$TlMo_6O_{17}$	113 K	18%	0.038 R
molybdenum bronzes			
η-Mo_4O_{11}	30 K	8%	0.004 R
	109 K	14%	0.07 R
γ-Mo_4O_{11}	98 K	not measurable	–
$Lu_5Ir_4Ir_{10}$	83 K	1%	≈0.5 R
$Er_5Ir_4Ir_{10}$	155 K	2%	≈0.55 R
	55 K	–	–
$Tm_5Ir_4Ir_{10}$	138 K	2%	≈0.8 R
	115 K	–	–

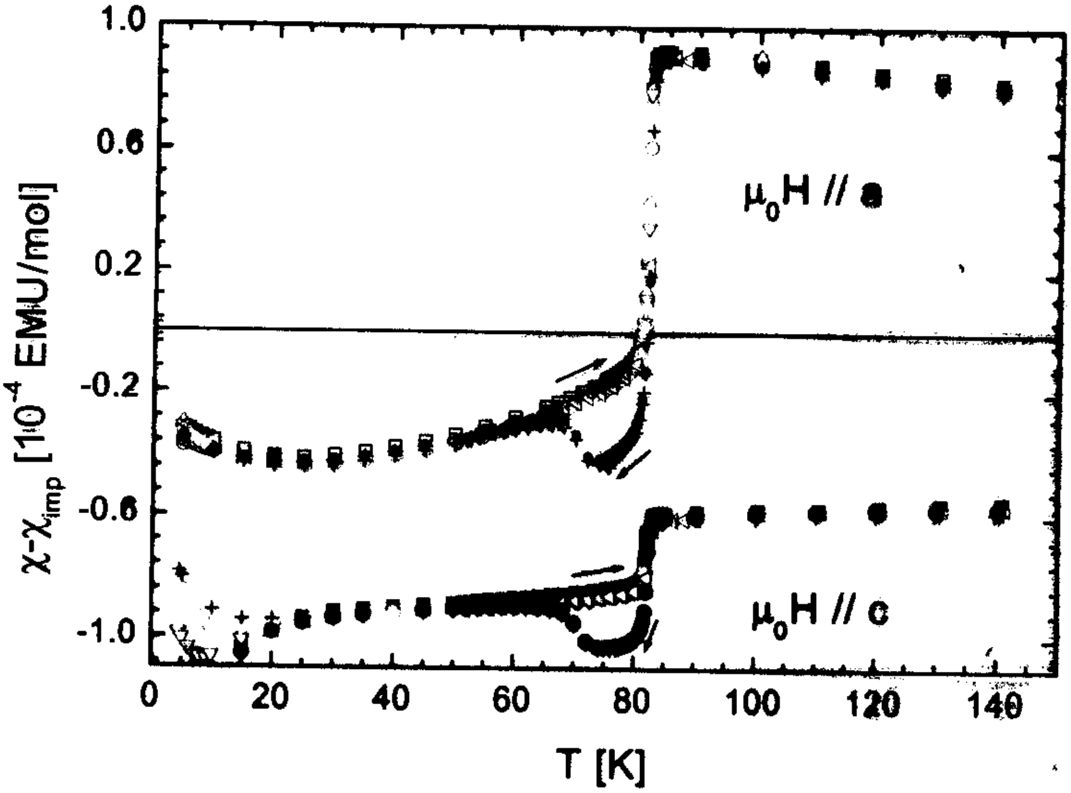
$Lu_5Ir_4Si_{10}$ - SUPERCONDUCTING TRANSITION



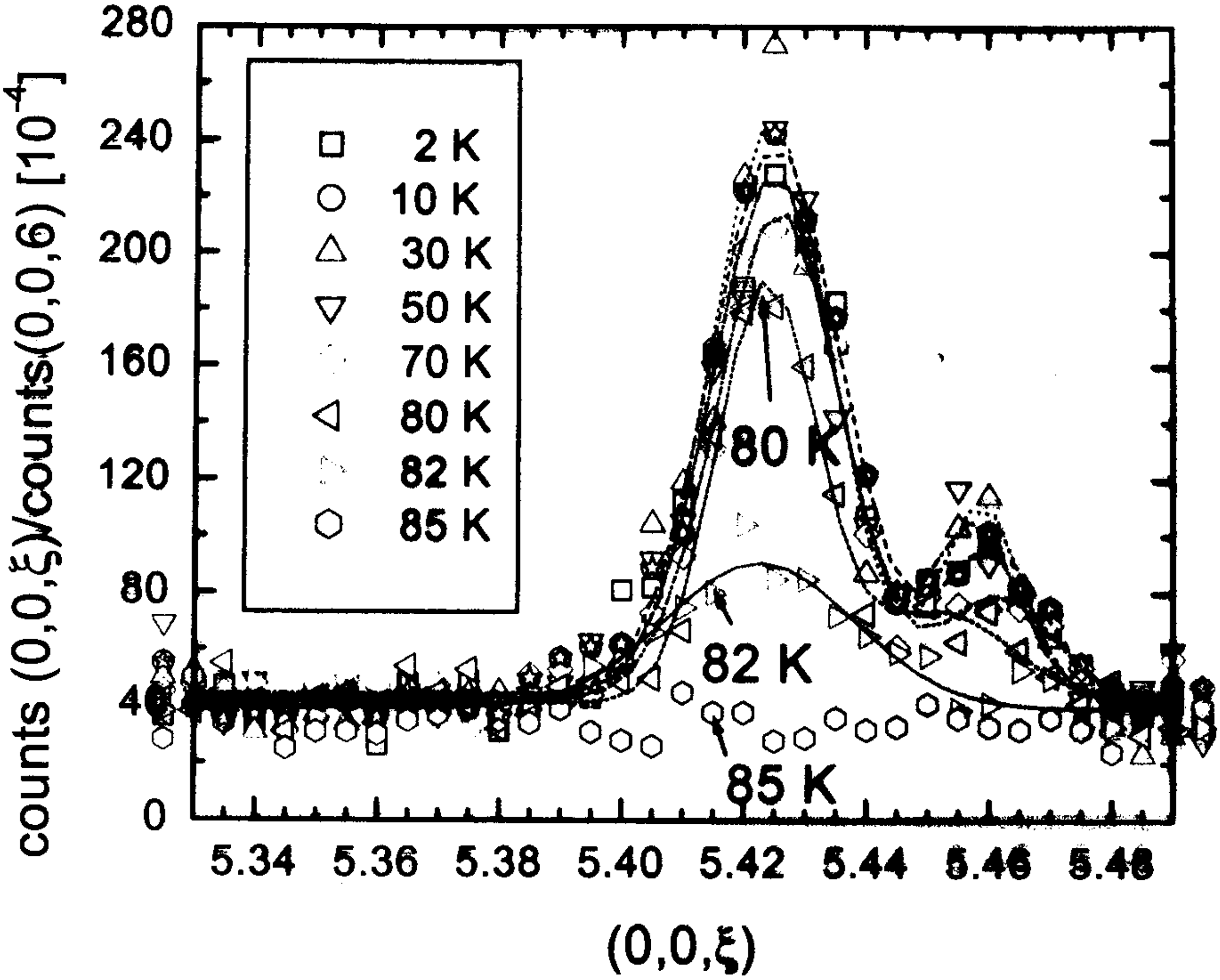
$$\frac{\Delta(0)}{k_B T_c} = 1.82 \quad (1.76)_{BCS}$$

$$\Delta C_p / \gamma T_c = 1.45 \quad (1.41)_{BCS}$$

$Lu_5Ir_4Si_{10}$ (single crystal): dc-susceptibility vs. temperature

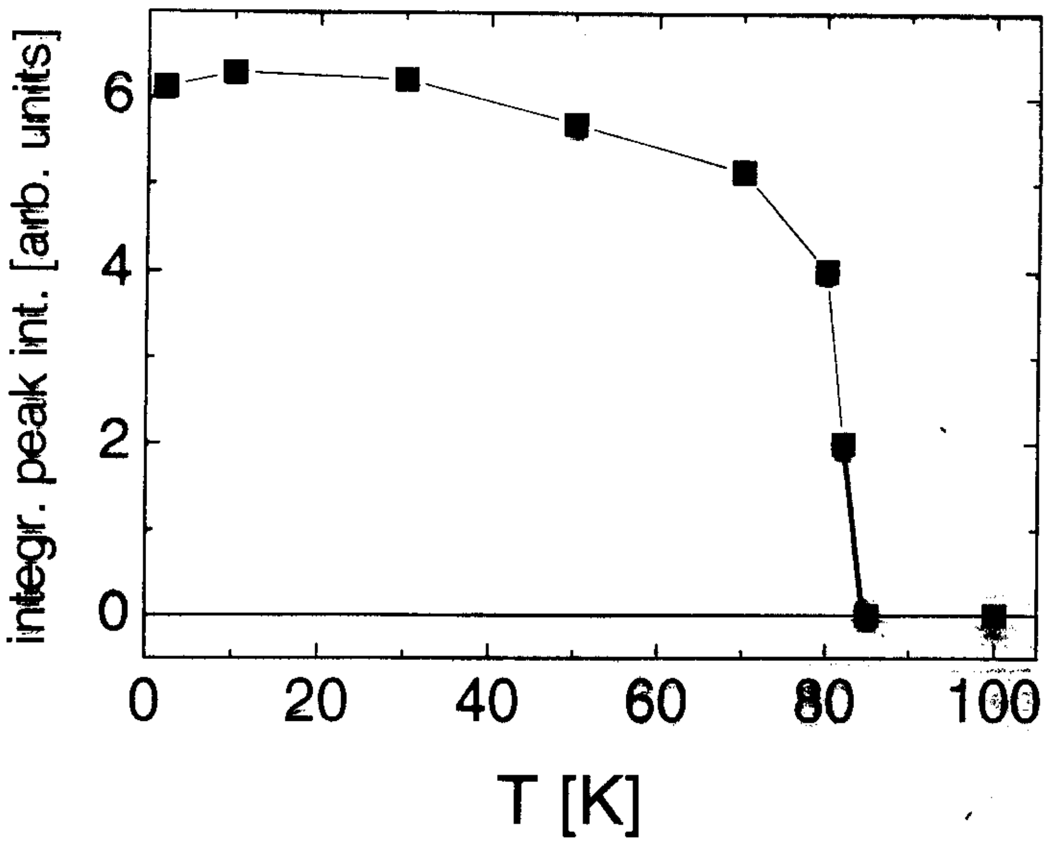


$Lu_5Ir_4Si_{10}$ (single crystal): temperature dependence of the superlattice reflections (high-res. x-ray data (*))



(*)M. Koghi. Tokyo Metropolitan Univ.

$Lu_5Ir_4Si_{10}$ (single crystal): intensity vs. temperature



EICHLER et al.

pressure ∥ c-axis

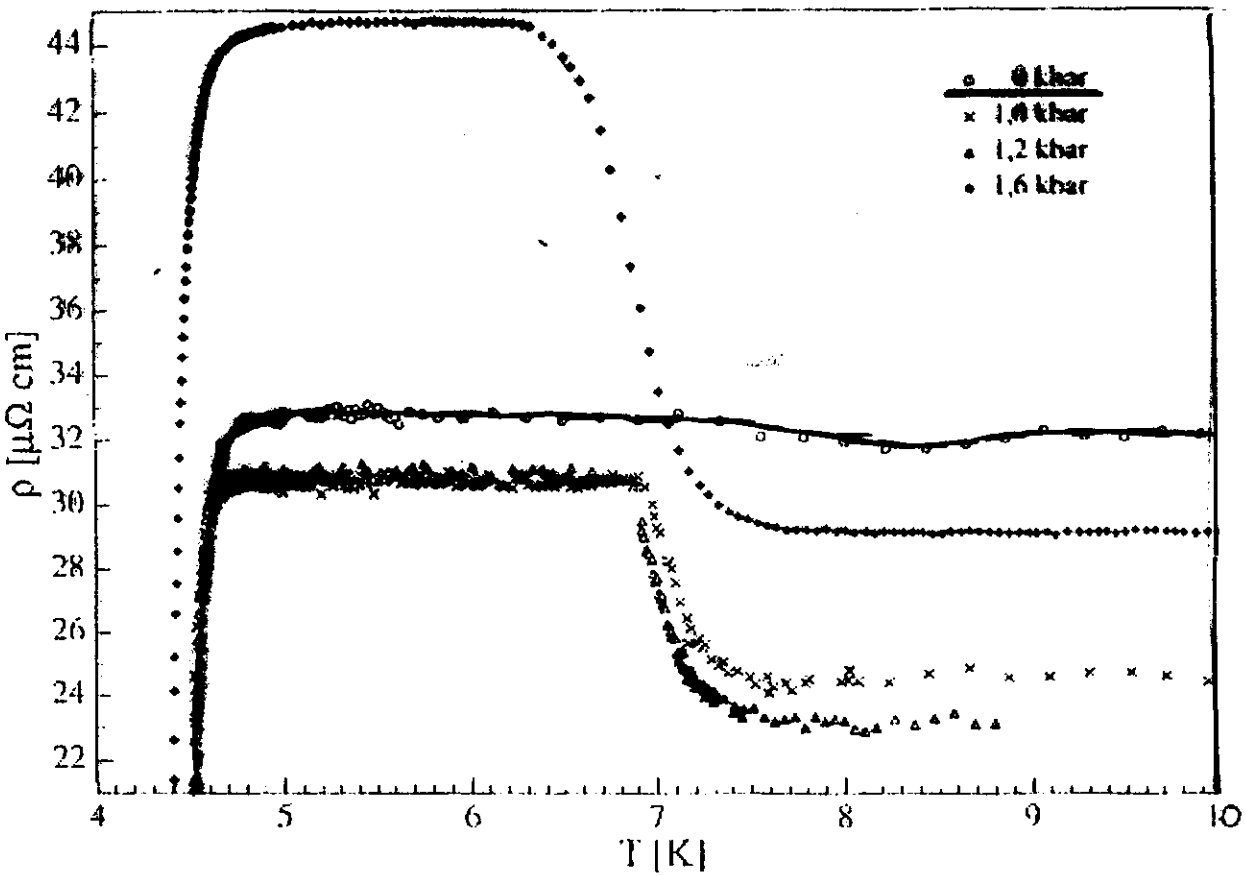
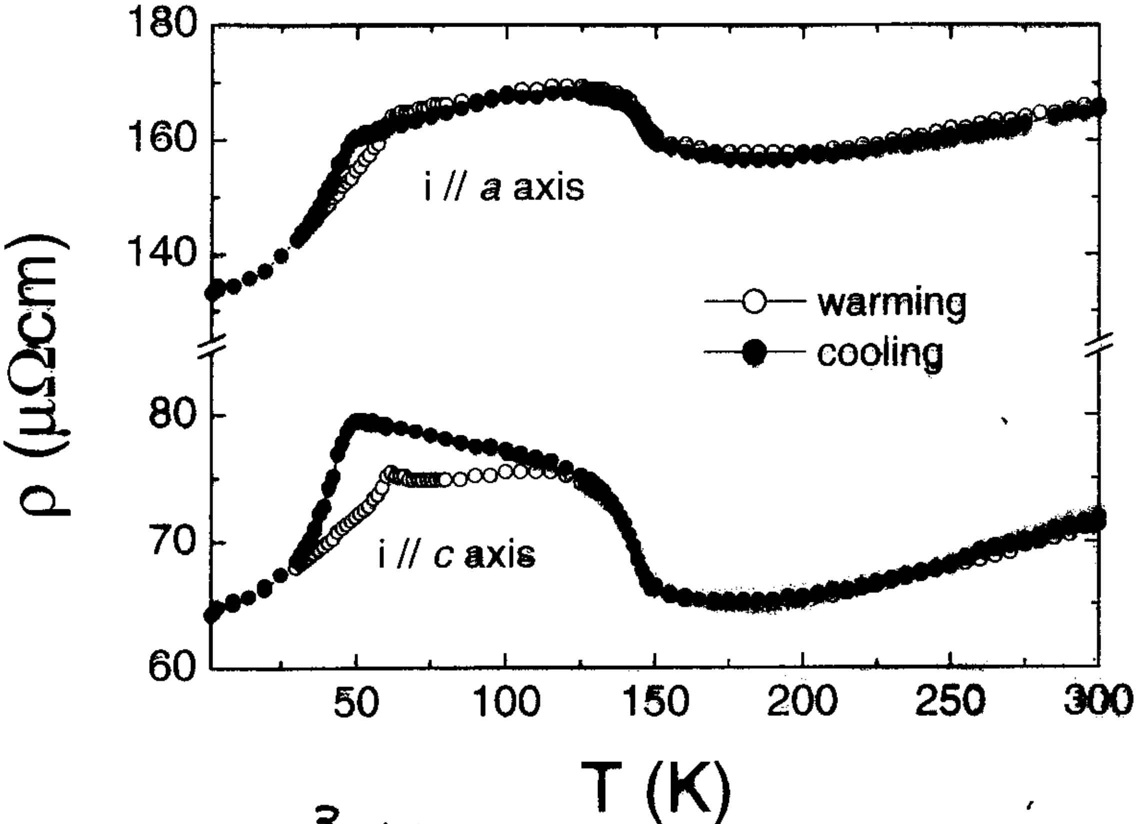


Abbildung 6.5: Anomalie im Widerstandsverlauf bei 7 Kelvin

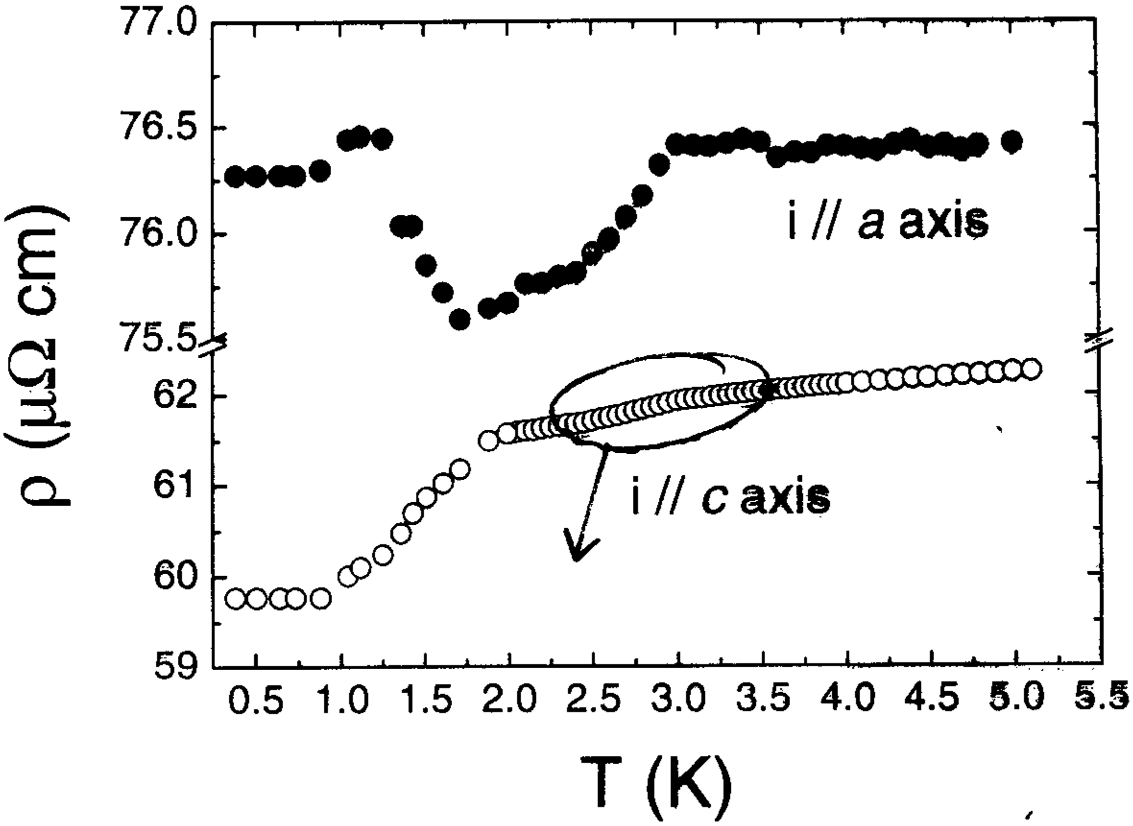
MAGNETIC RE 5-4-10's

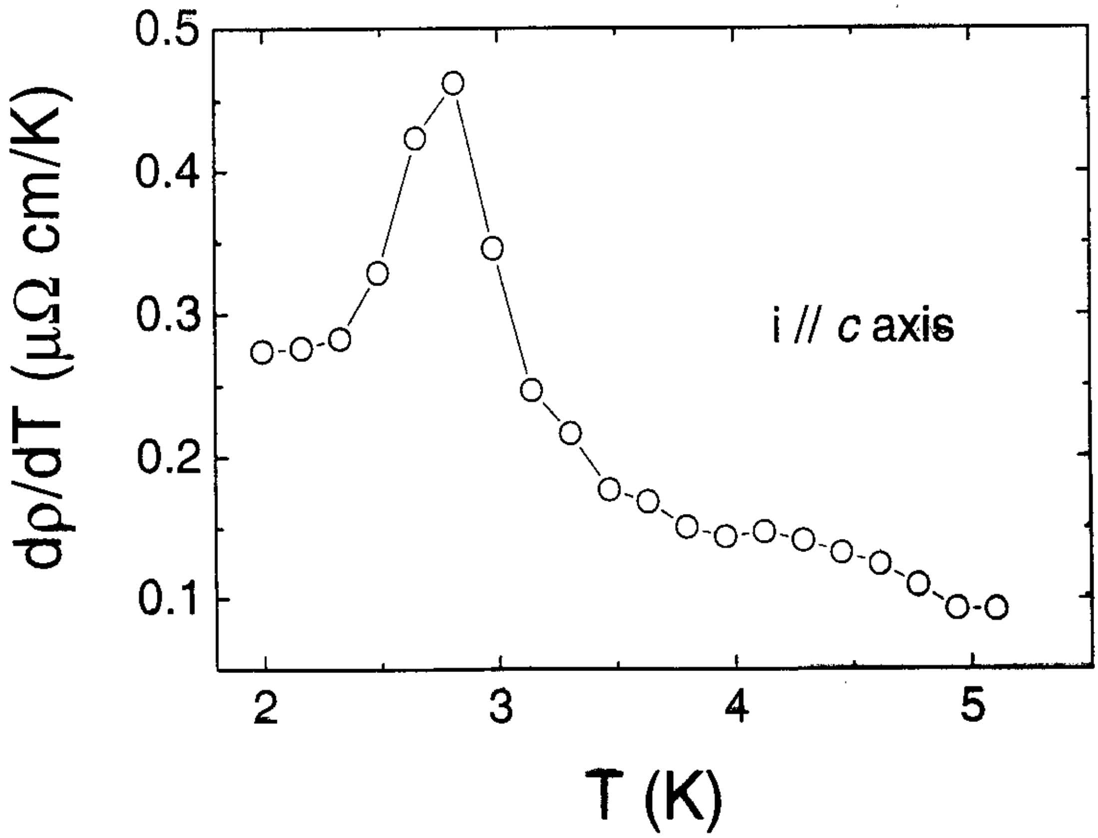
$Er_5Ir_4Si_{10}$ (single crystal): resistivity vs. temperature



3 LY
F. Galli *et al.*, PRL (Ju 2000).

$Er_5Ir_4Si_{10}$ (single crystal): low temperature resistivity





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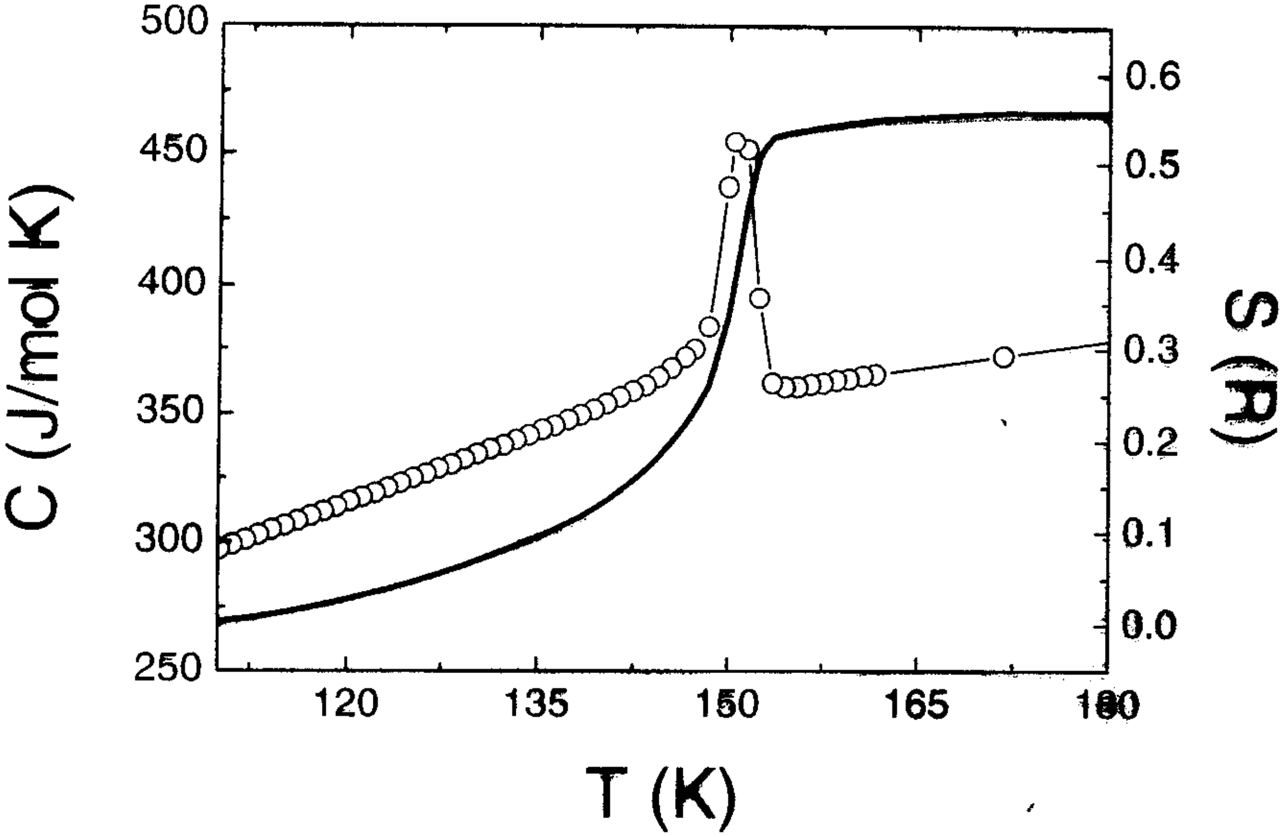
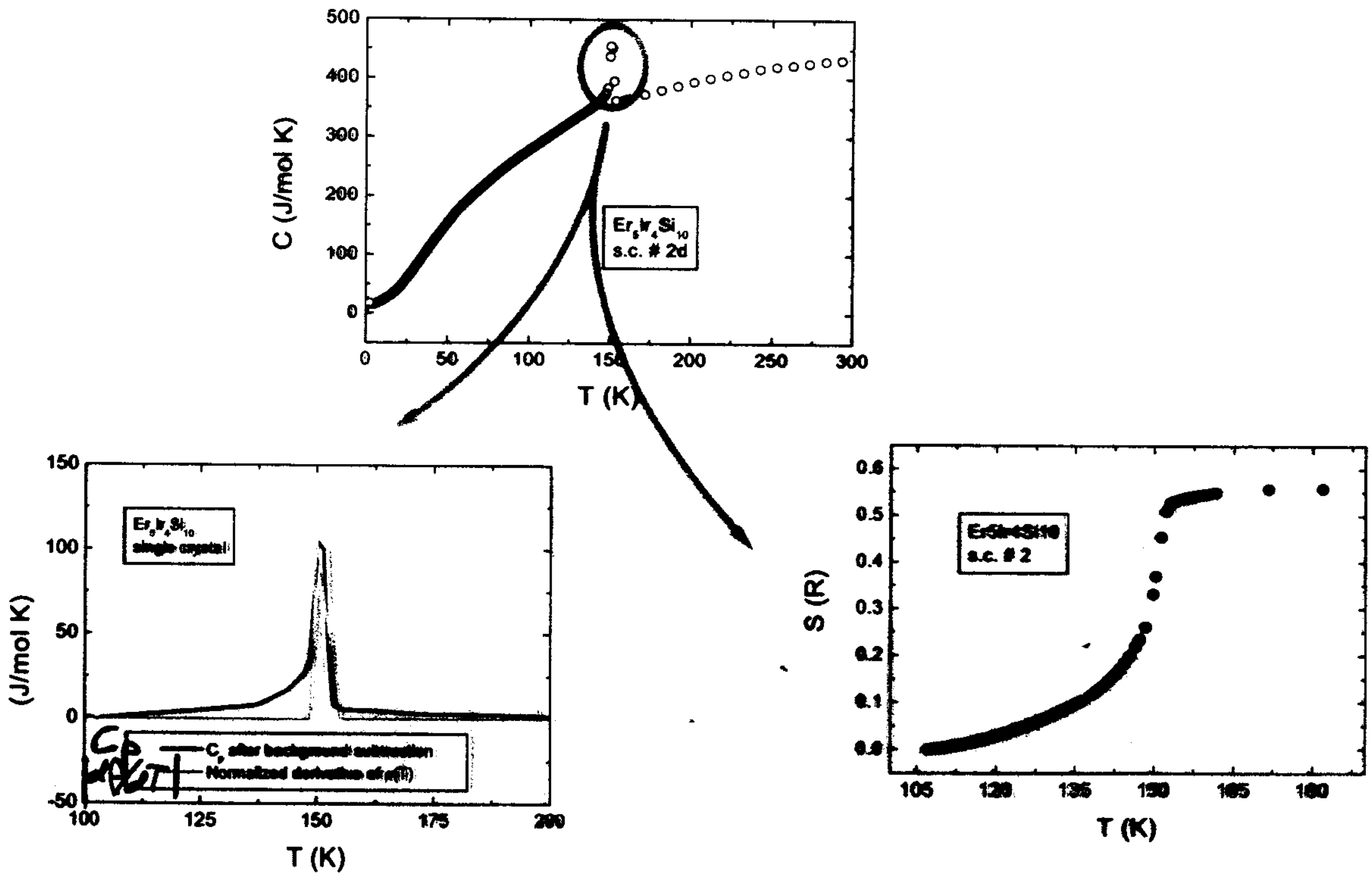
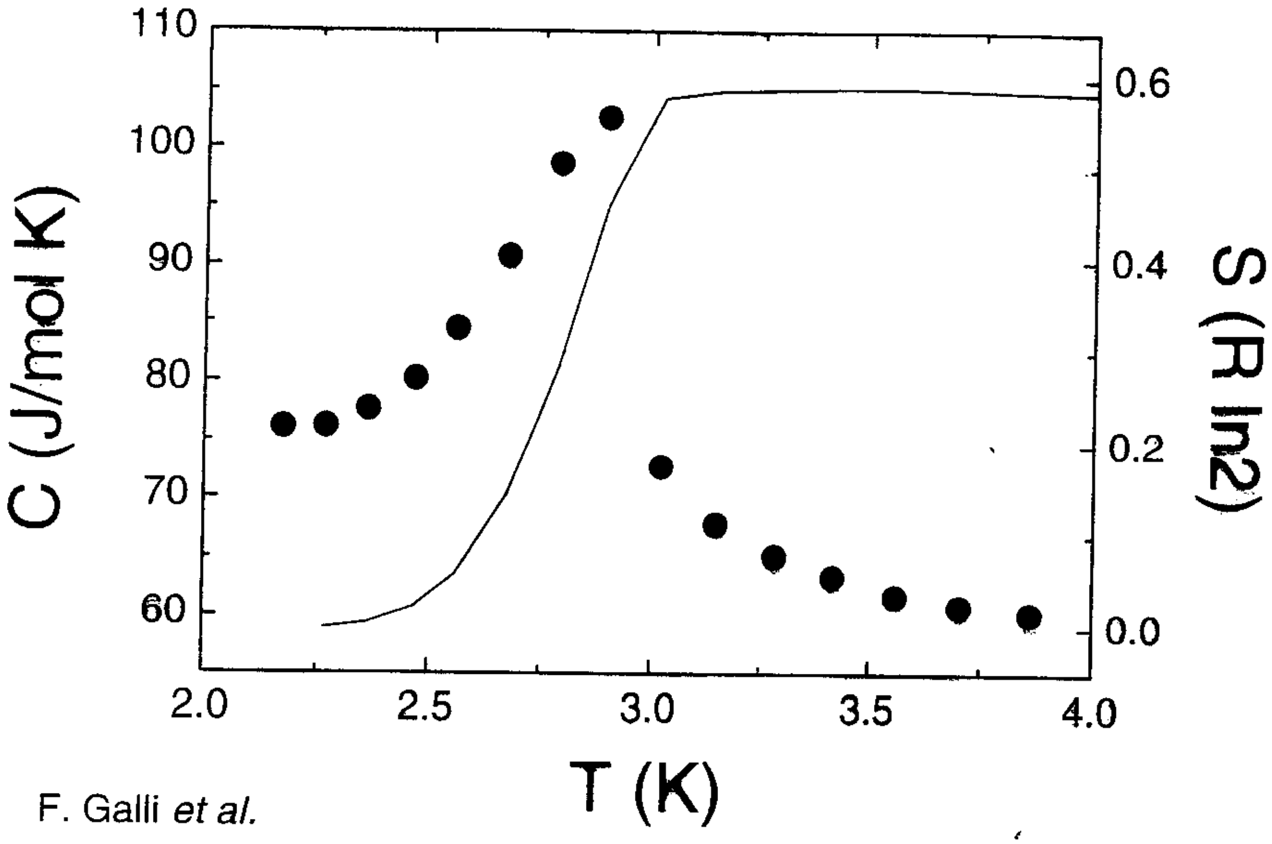
$Er_5Ir_4Si_{10}$ (single crystal): high-temperature specific-heat



Single Crystal of $Er_5Ir_4Si_{10}$: C_p vs T

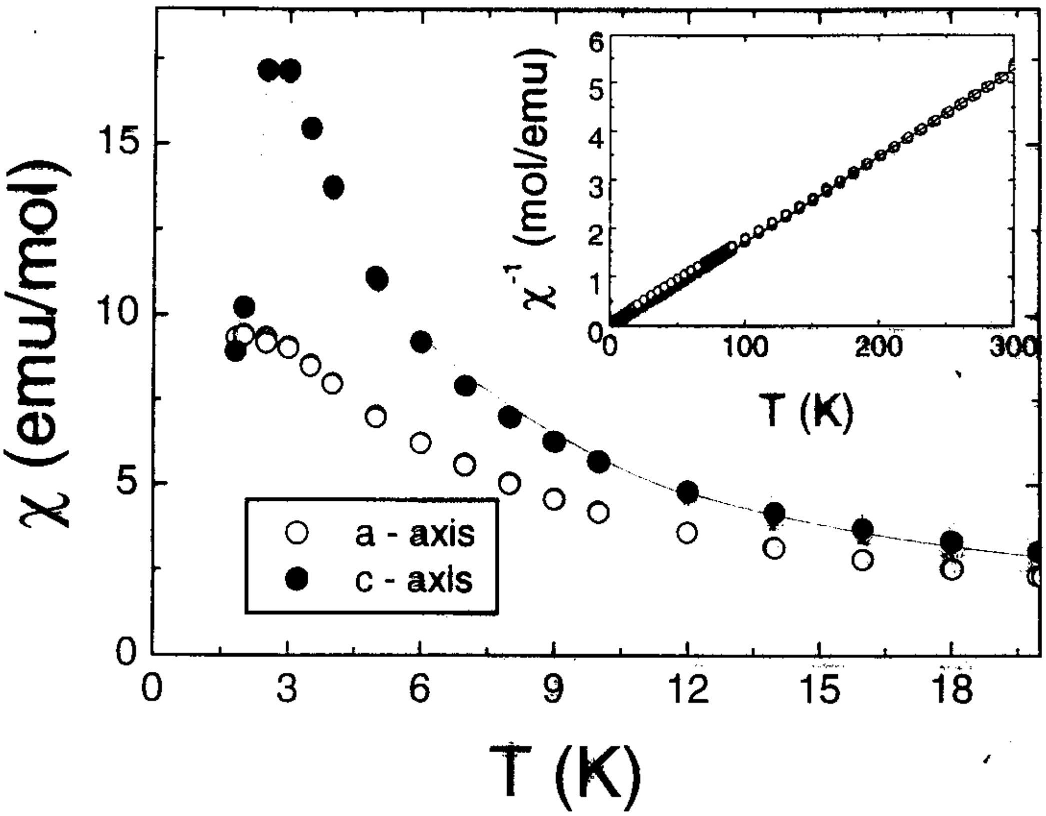


$Er_5Ir_4Si_{10}$ (single crystal): low-temperature specific-heat

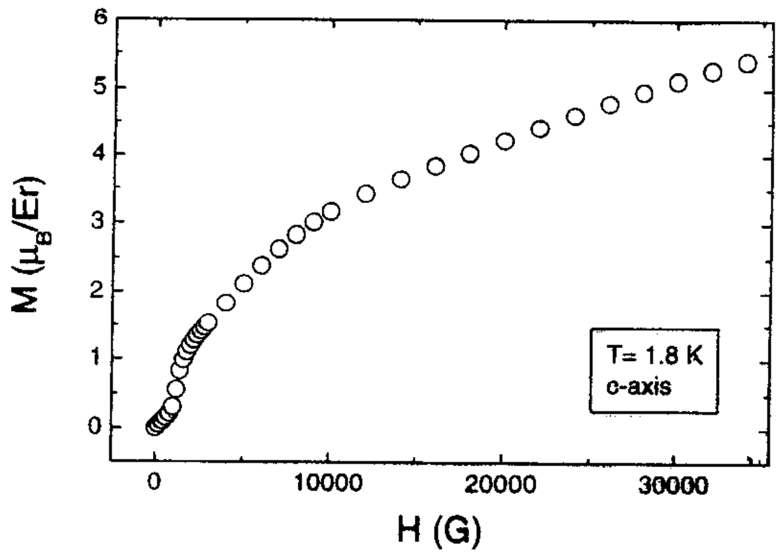


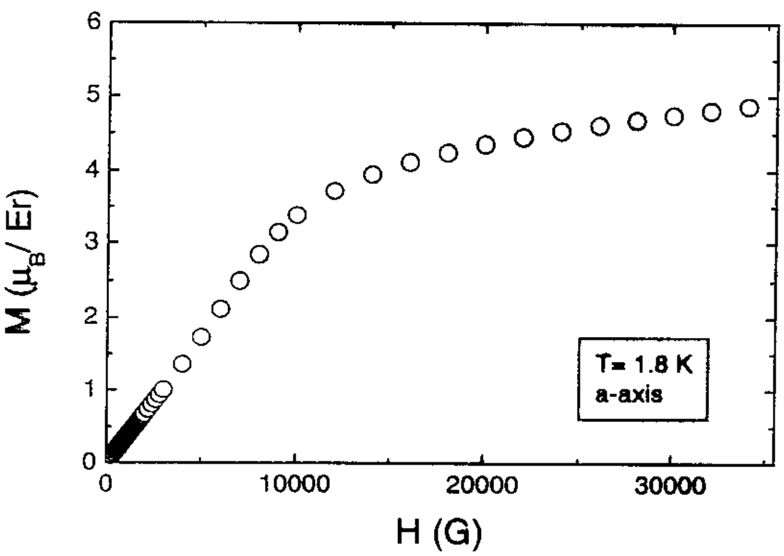
F. Galli *et al.*

$Er_5Ir_4Si_{10}$ (single crystal): magnetic susceptibility vs. temperature

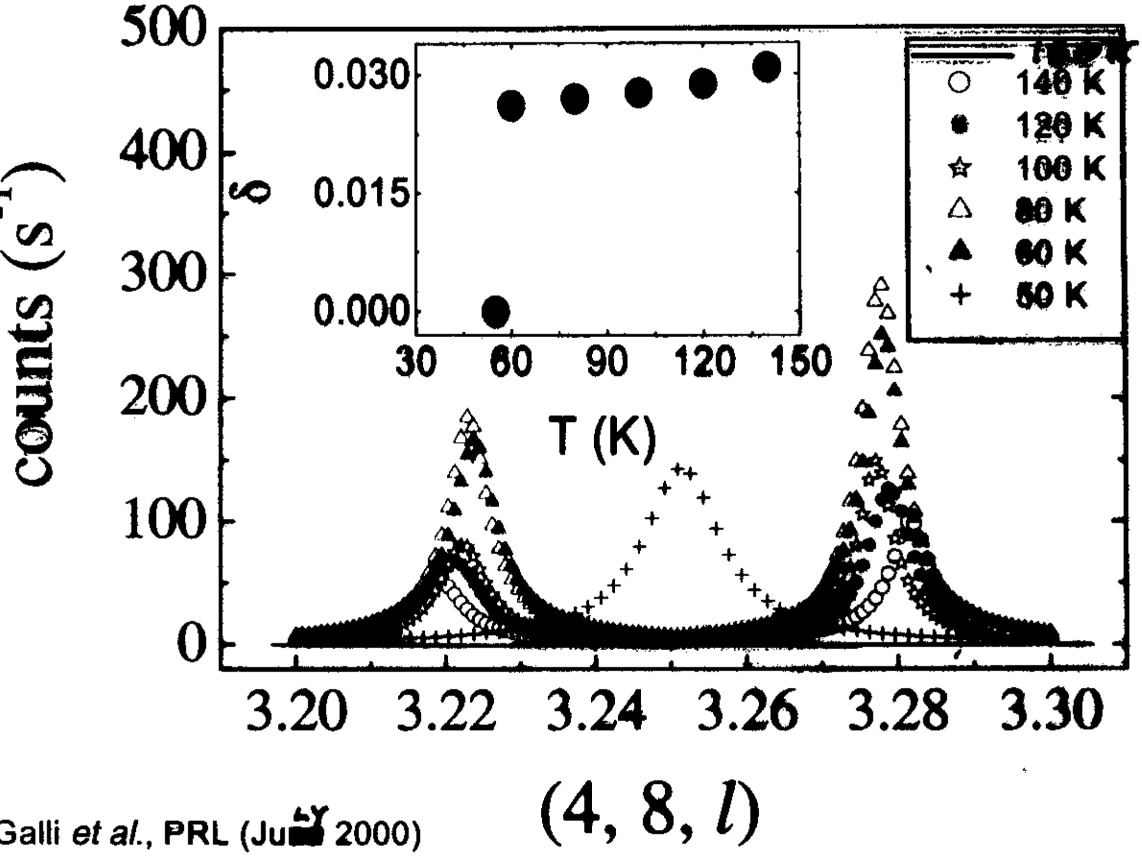


$Er_5Ir_4Si_{10}$ (single crystal): magnetization at 1.8 K





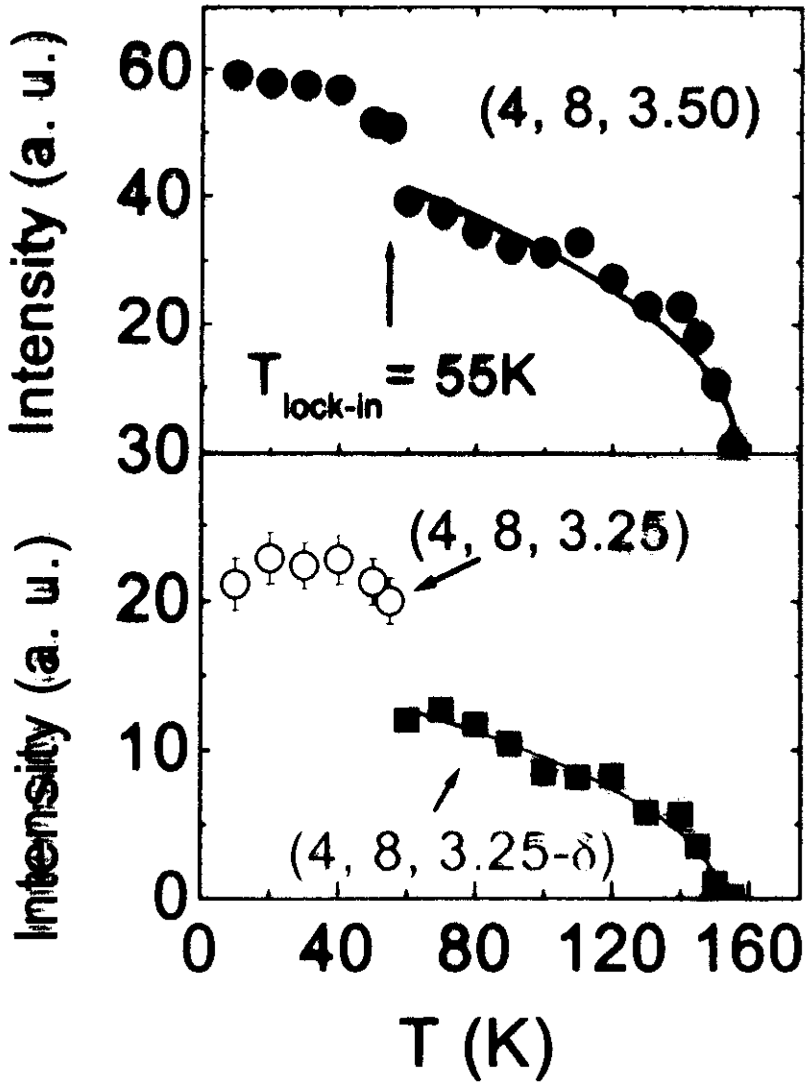
$Er_5Ir_4Si_{10}$ (single crystal): temperature dependence of the superlattice reflections (high-res. x-ray data (*))



F. Galli *et al.*, PRL (July 2000)

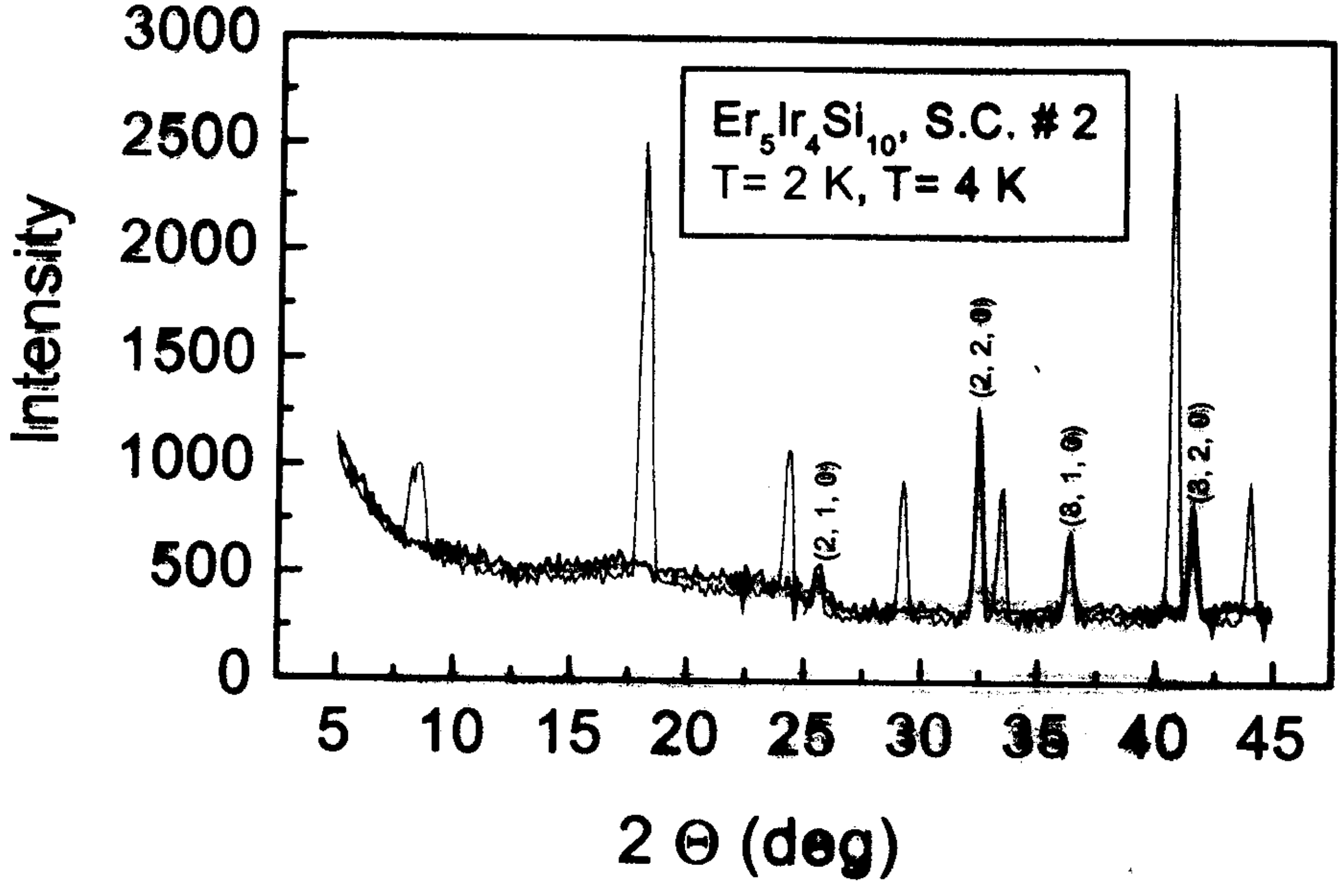
(*) DESY lab., Hamburg

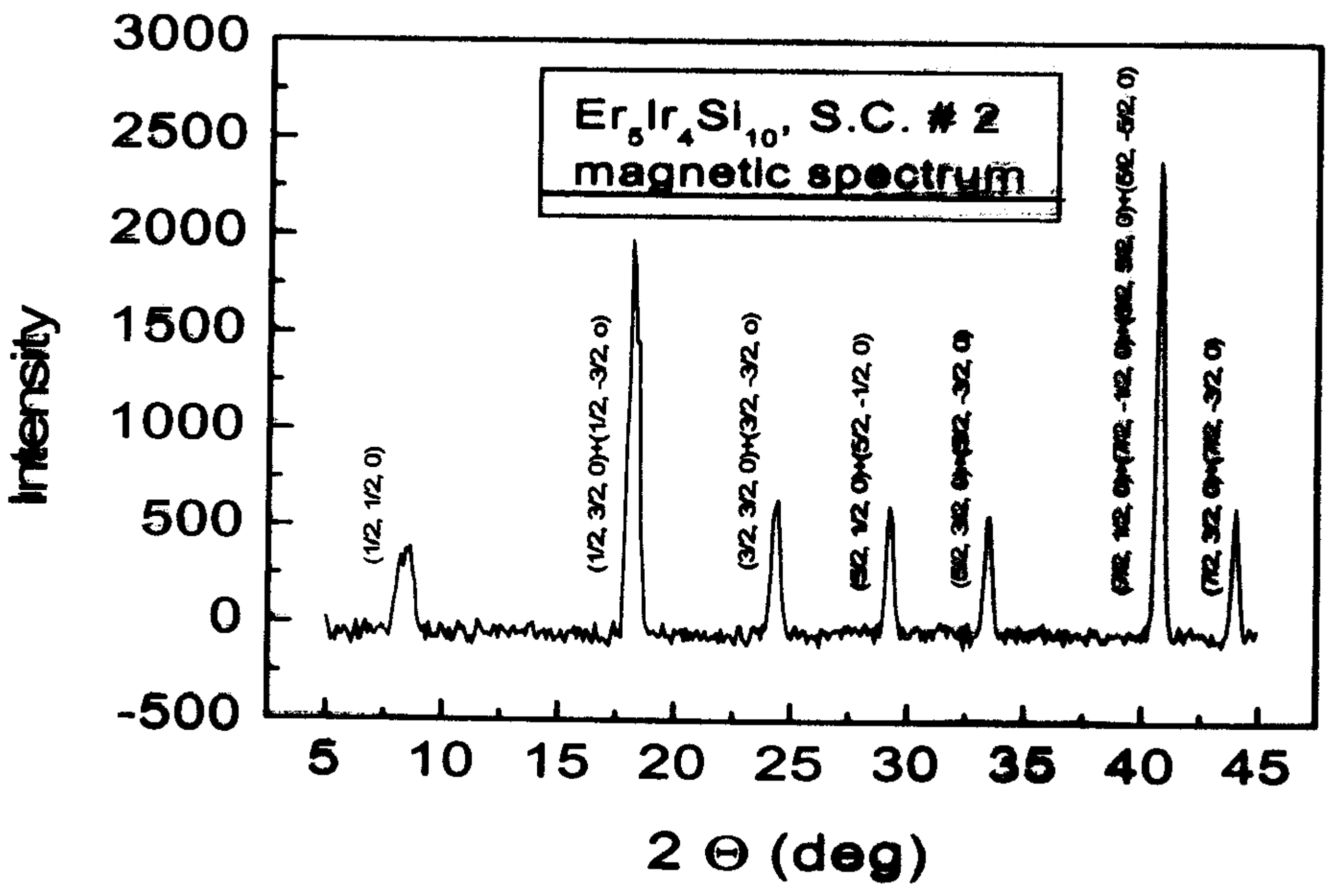
$Er_5Ir_4Si_{10}$ (single crystal): Intensities vs. temperature (high-res. x-ray data(*))



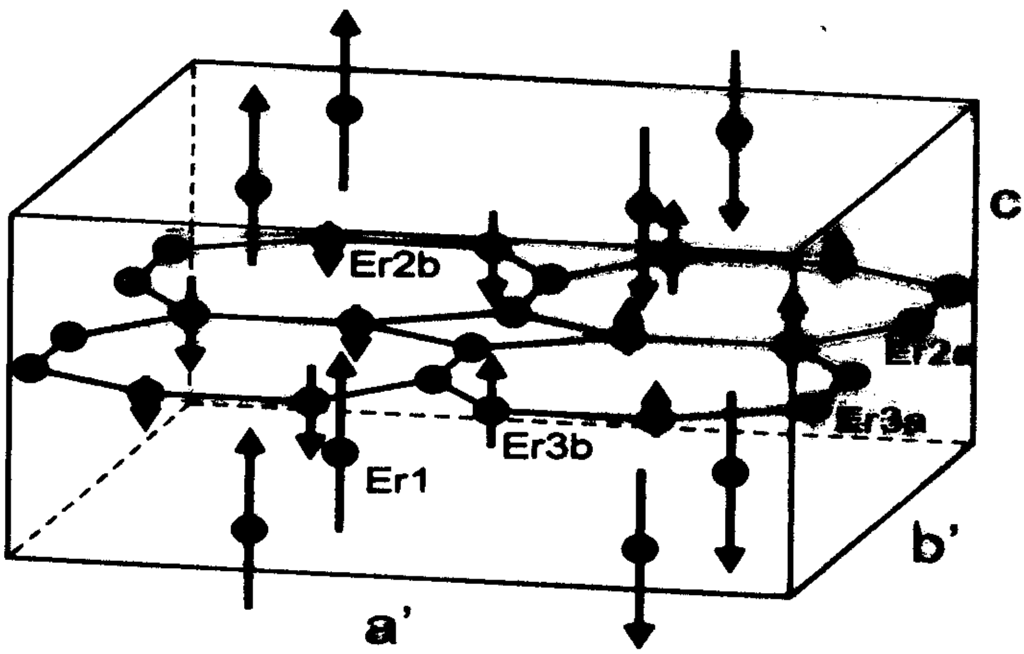
(*): DESY lab., Hamburg

SINGLE CRYSTAL NEUTRON DIFFRACTION DATA: MAGNETIC STRUCTURE DETERMINATION





$Er_5Ir_4Si_{10}$(single crystal): <u>magnetic unit cell</u>

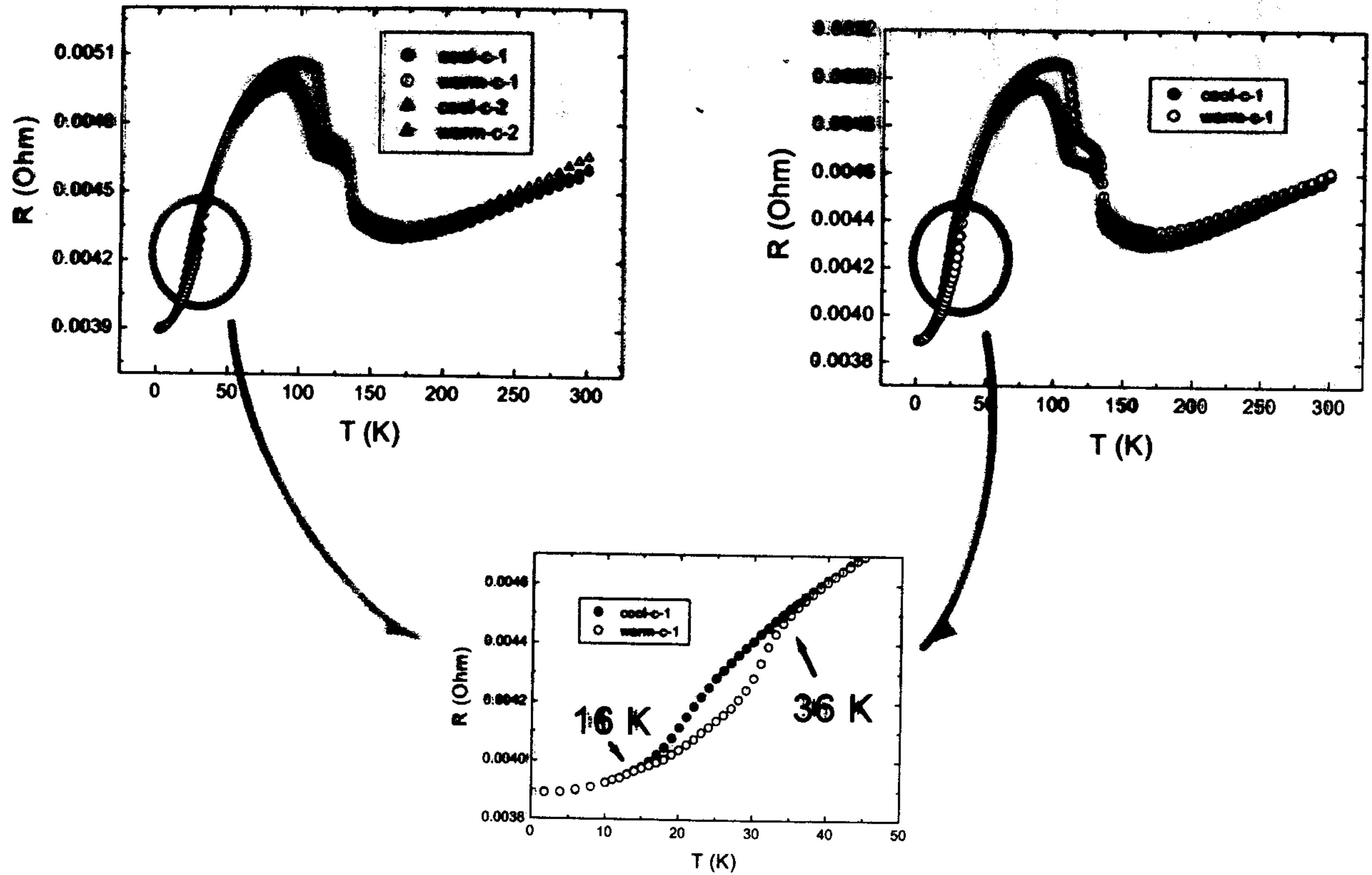


MAGNETIC UNIT CELL IS ROTATED BY 45° AND HAS CELL PARAMETERS: $a' = b' = \sqrt{2}a$

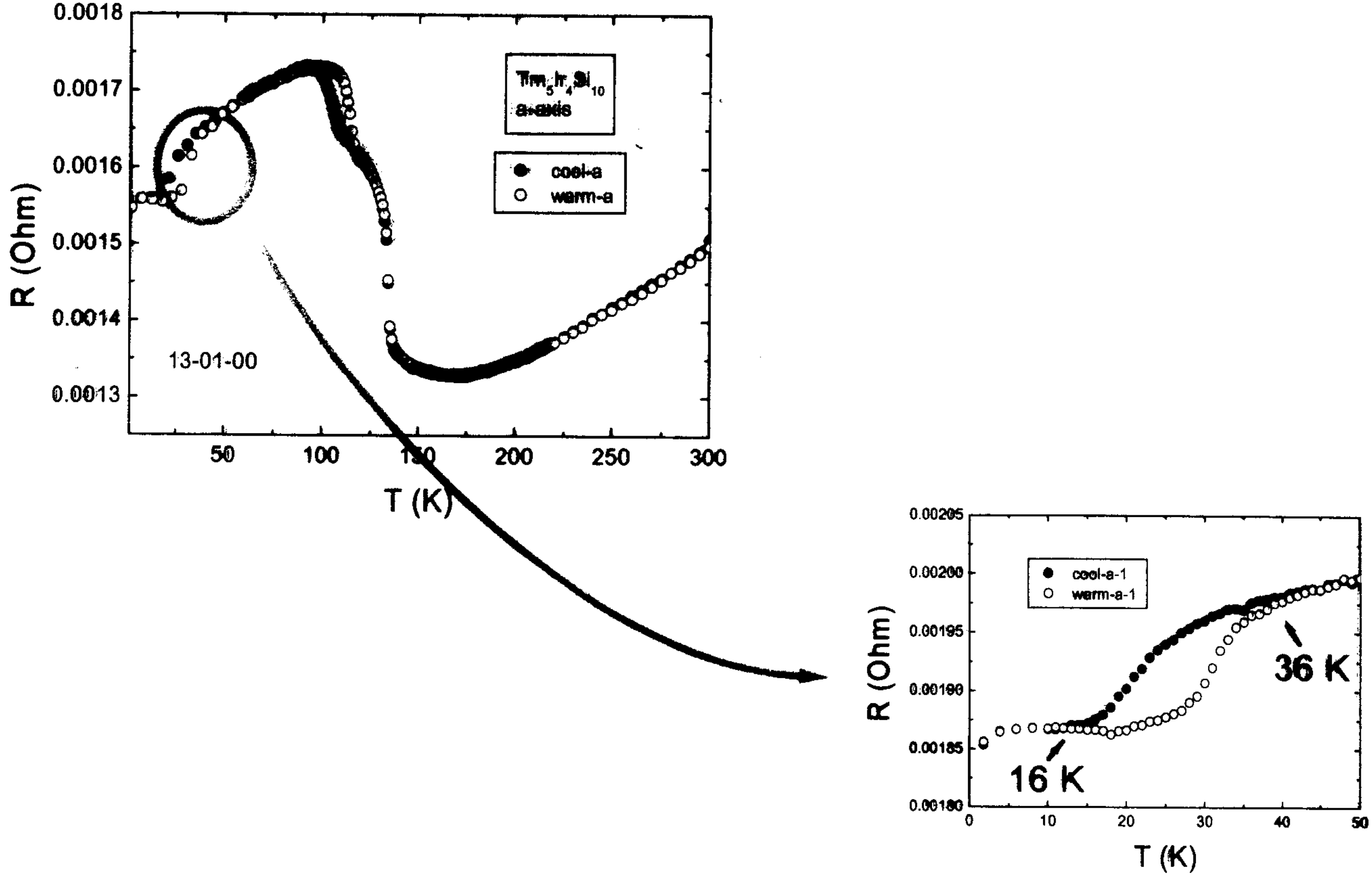
$\vec{Q} = (\frac{1}{2}, \frac{1}{2}, 0)$

Er1 → 9.0 μ_B
Er2a → 0, Er2b → 1.4 μ_B
Er3a → 0, Er3b → 2.0 μ_B

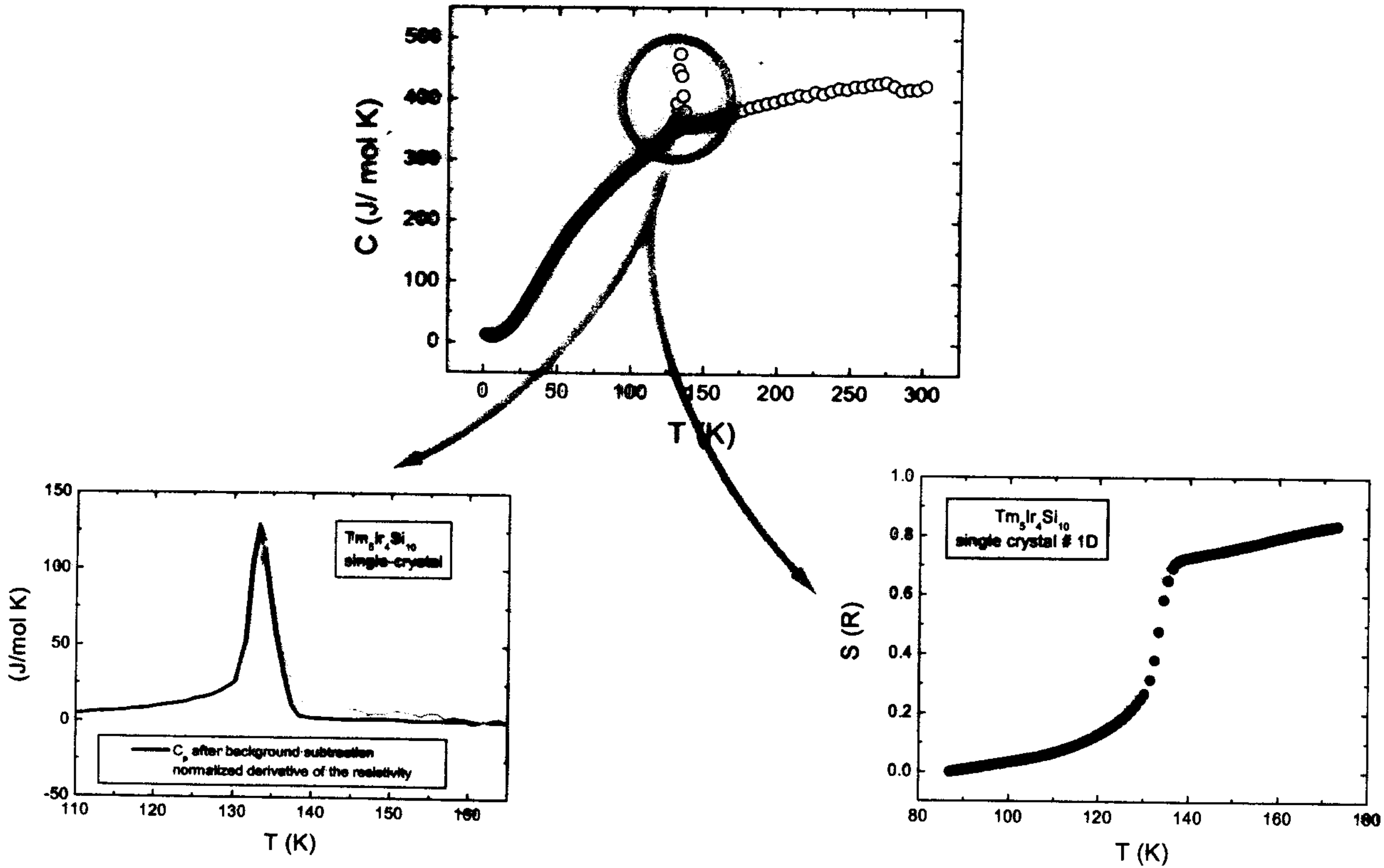
Single Crystal of $Tm_5Ir_4Si_{10}$: R vs T with current along c-axis



Single Crystal of $Tm_5Ir_4Si_{10}$: R vs T with current along a-axis



Single Crystal of $\underline{Tm_5Ir_4}Si_{10}$: $C_{\underline{p}}$ vs T



CONCLUSIONS

$RE_5Ir_4Si_{10}$ - INTERMETALLIC COMPOUNDS

INTERPLAY / COEXISTENCE

STRUCTURE

CDW

Q_{CDW}, $Q_{LOCK\text{-}IN}$
ALONG C-AXIS

LOCAL MOMENTS

ANTIFERRO. LRMO

M(3 Er SITES)
ALONG C-AXIS
$Q_M = (\frac{1}{2}\, \frac{1}{2}\, 0)$

QUESTIONS:

1) Tuning with E, H Fields?

2) Driven CDW?

3) Meta Magnetic Transition?

4) Interaction of CDW and Magnetism?

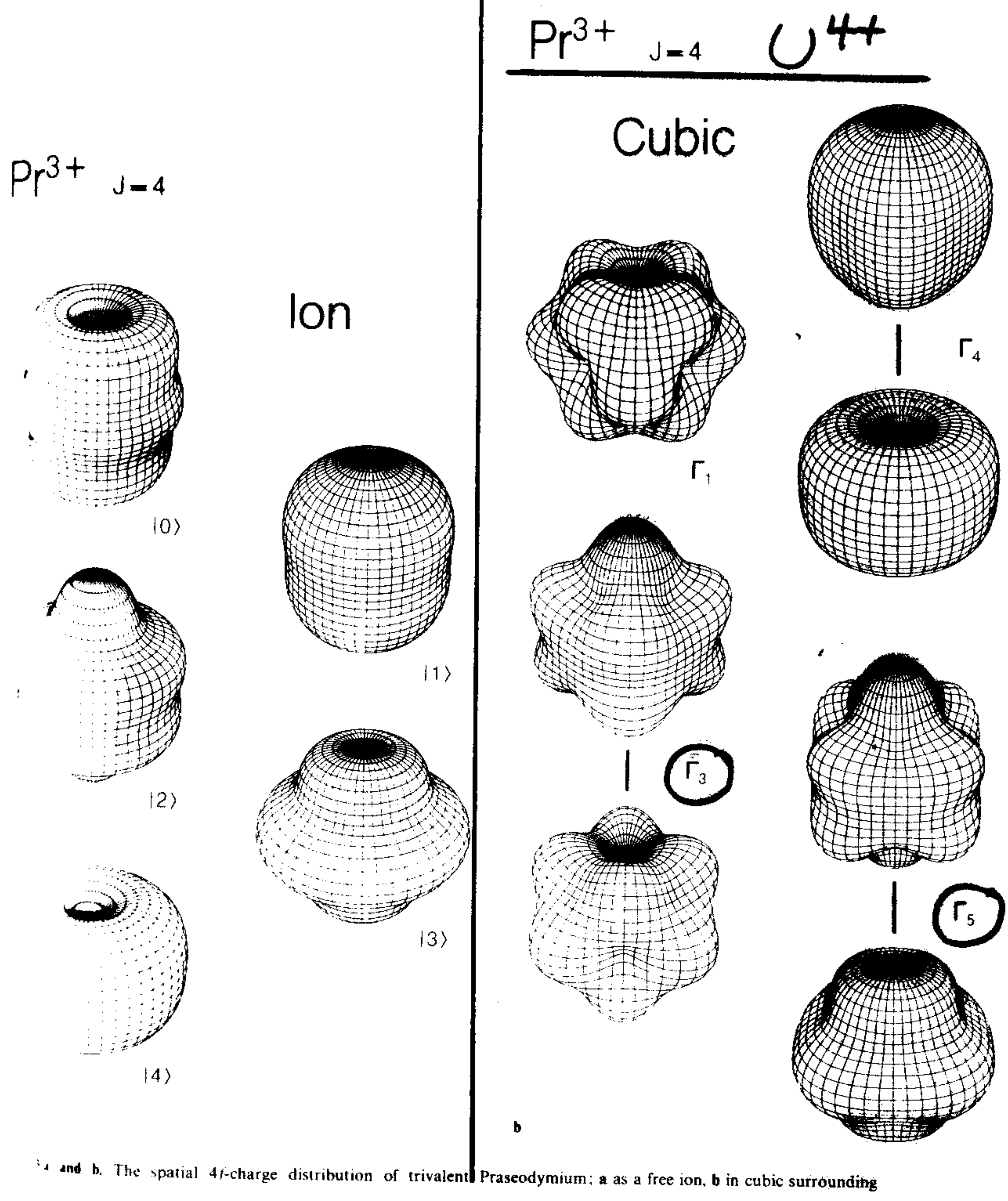
Perspective

Spin (dipole)/lattice (quadrupole) transitions in uranium compounds

- **4f/5f charge densities, e.g.** $\begin{cases} Pr^{3+}(4f^2) \\ J=4 \end{cases}$ (VG)
- **Quadrupolar interactions** $\mathcal{H} = -\frac{1}{2}\sum_{ij} K_\Gamma(i,j) O_\Gamma(i) O_\Gamma(j)$ **(aspherical Coulomb scattering)**
- **Cooperative Jahn-Teller effect**
  Quadrupolar Phase Transitions (1^{st} order)
  Lattice Distortions
- **e.g. I) UO_2 (insulating) fcc-structure single 1^{st} order phase transition at $T_N =$ 30.8 K. Distortion of oxygen sublattice and antiferromagnetic ordering of U.**
- **e.g. II) UPd_3 (metallic) dhcp-structure**
  $T_1 = 6.5$ K quadrupolar ordering
  $T_2 = 4.5$ K also magnetic ordering

$U^{4+}5f^2$ (J = 4) with quadrupolar active states, e.g. Γ_5 (triplets) and Γ_3 (doublets) interact and couple with dipolar (spin) antiferro magnetism.

↓ $U_2Rh_3Si_5$



a and b. The spatial 4f-charge distribution of trivalent Praseodymium; **a** as a free ion, **b** in cubic surrounding

…quation is valid not only for CF-states but …lso for the Hund's rule states. In that case the …tes have to be substituted by $|JM\rangle$. This …es Eq. (12) to

$$\rho_M(\underline{r}) = R_{nl}^2(r) \sum_{\substack{k=0\\ \text{even}}}^{\min(2l,2J)} \sqrt{\frac{2k+1}{4\pi}}\,\theta_k \cdot b_{k0} \langle JM|O_k^0|JM\rangle\, Y_k^0(\Omega). \tag{13}$$

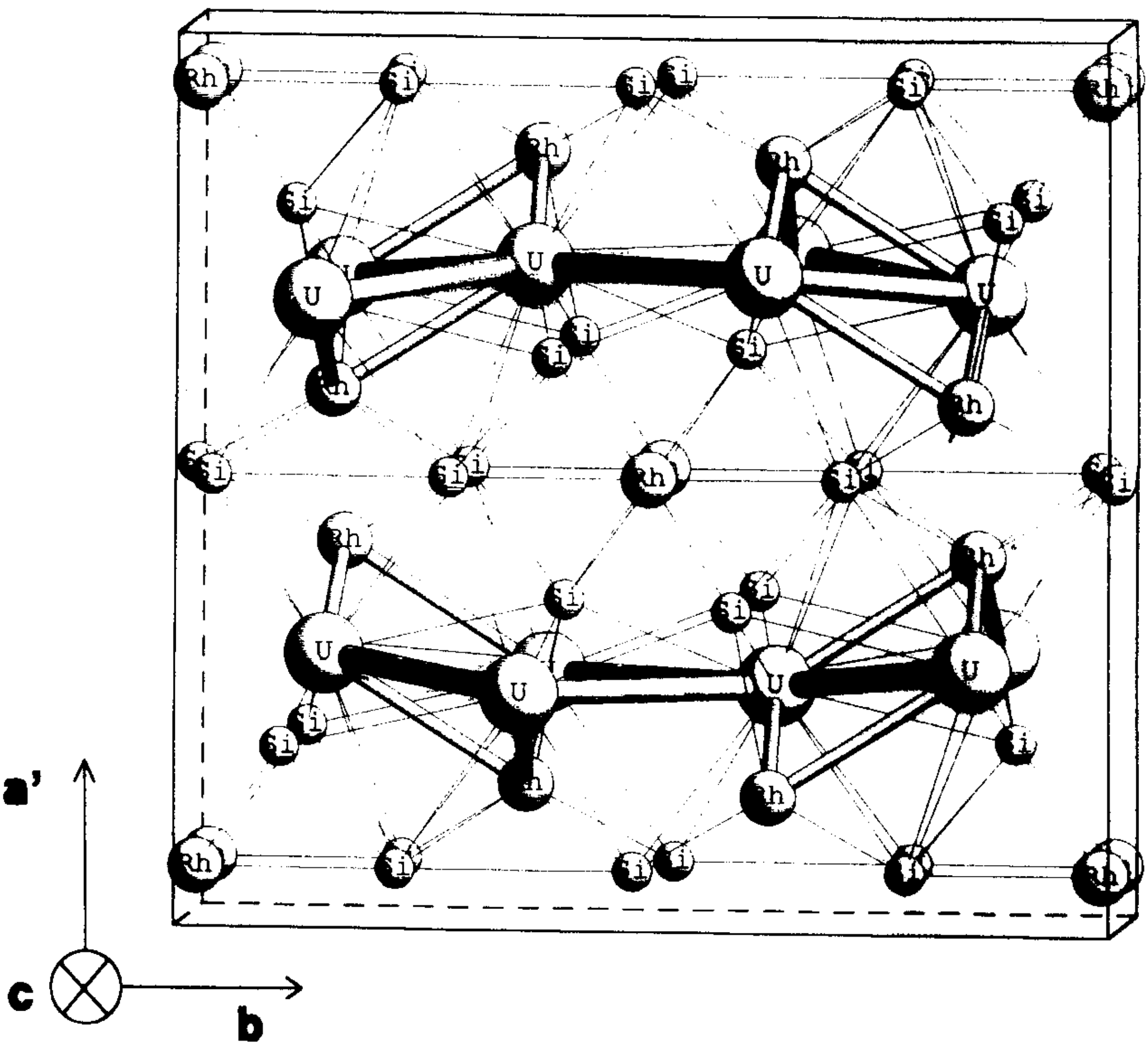


Fig. 1

QUASI ORTHORHOMBIC

CORRUGATED PLANES OF U-ATOMS

$U_2Rh_3Si_5$

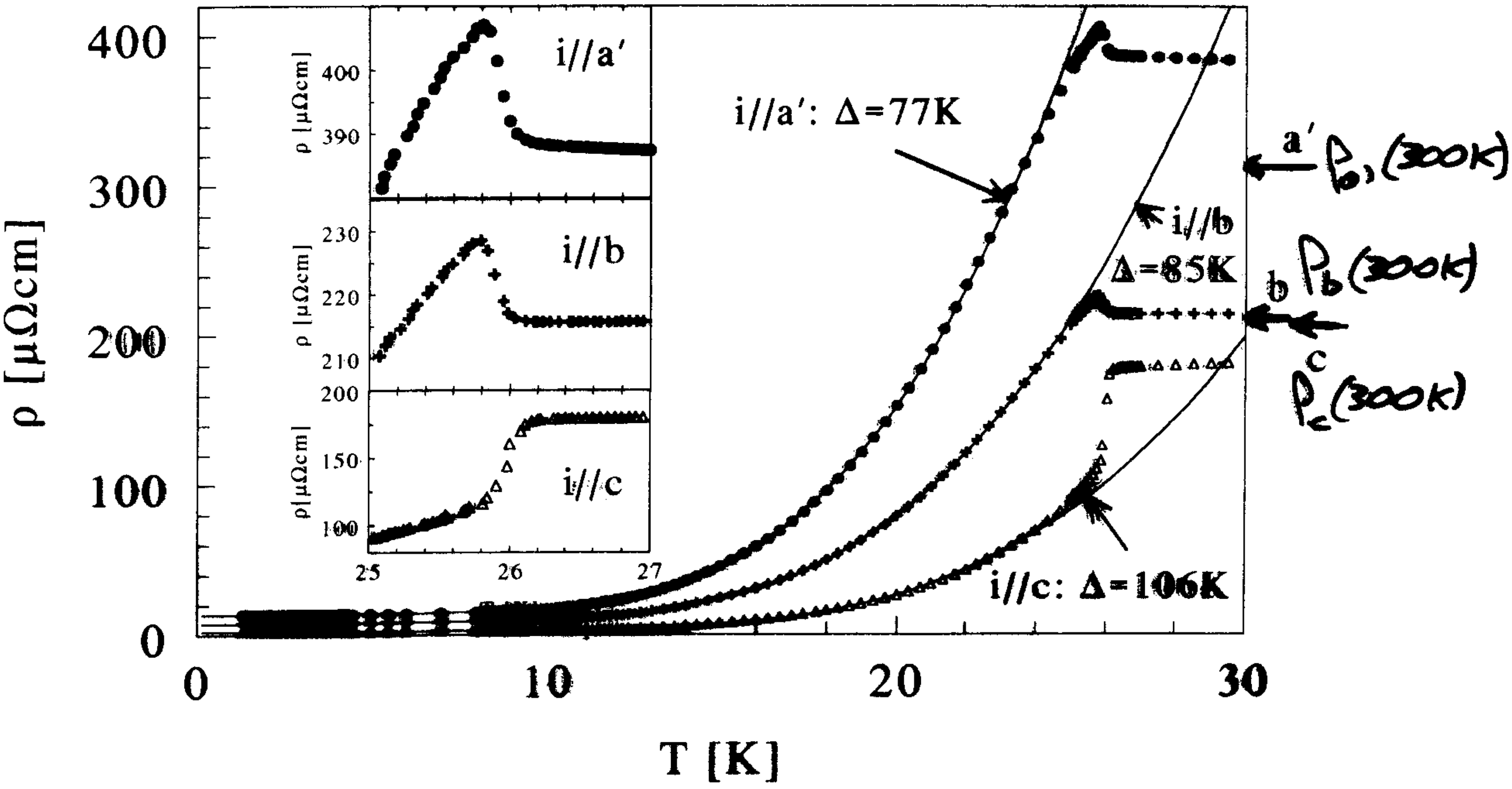
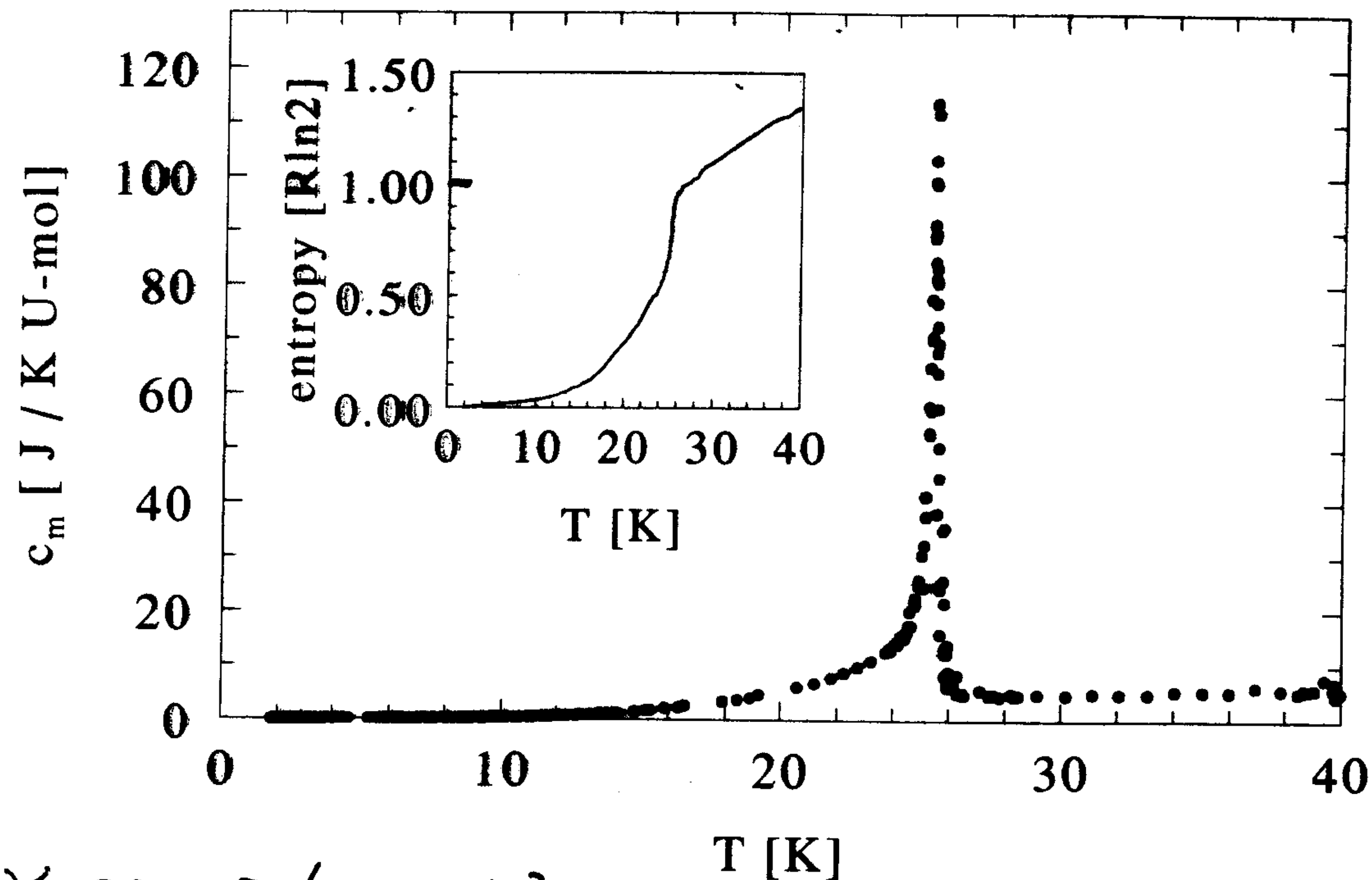


Fig. 4

$U_2 Rh_3 Si_5$



$\gamma = 22\ mJ/U\text{-}mol\ K^2$

Fig. 2

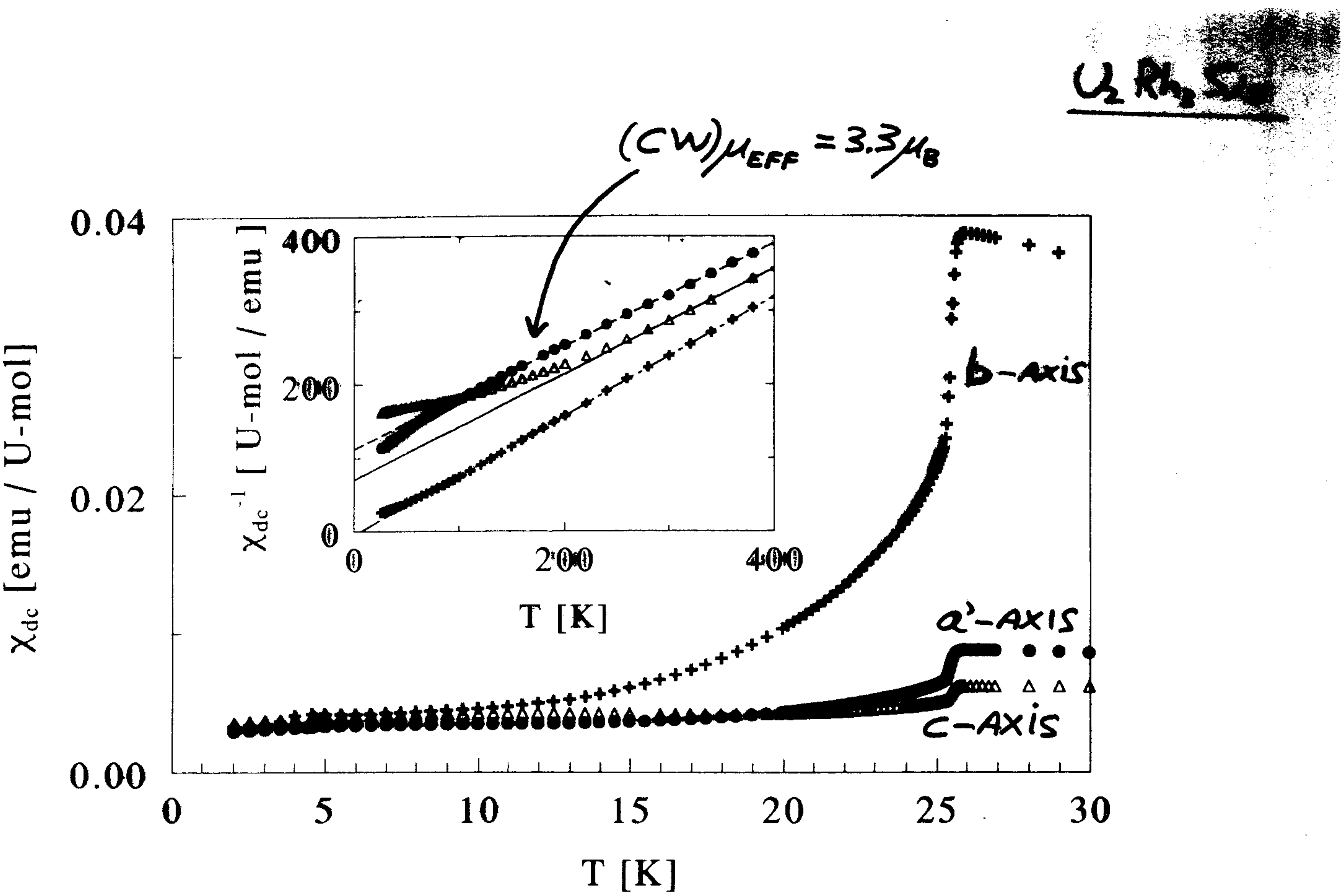

U2 Rh3 Si5
(CW) μEFF = 3.3 μB
0.04
0.02
0.00
χdc [emu / U-mol]
0
5
10
15
20
25
30
T [K]
χdc-1 [U-mol / emu]
400
200
0
T [K]
b-AXIS
a'-AXIS
c-AXIS

Fig. 3

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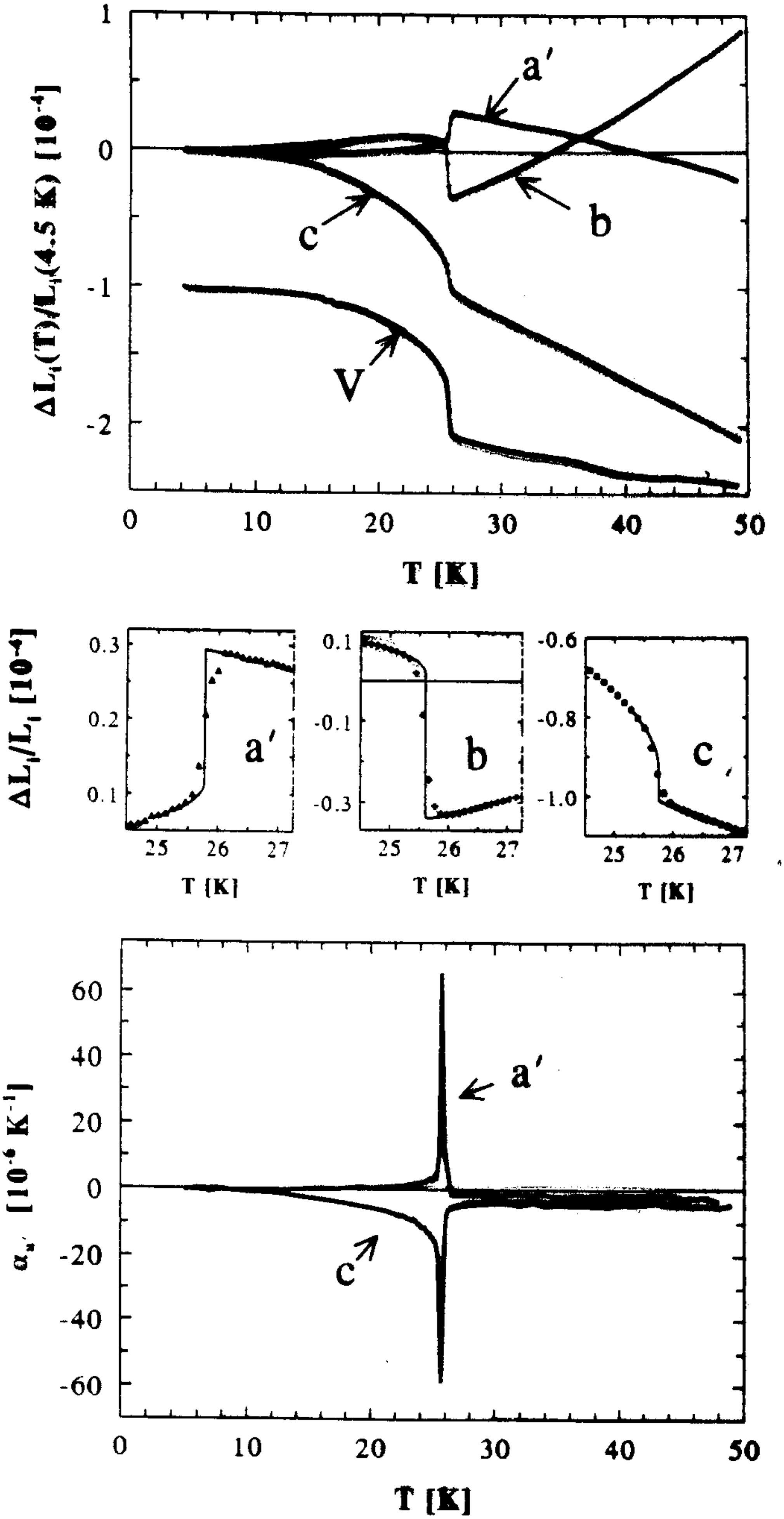
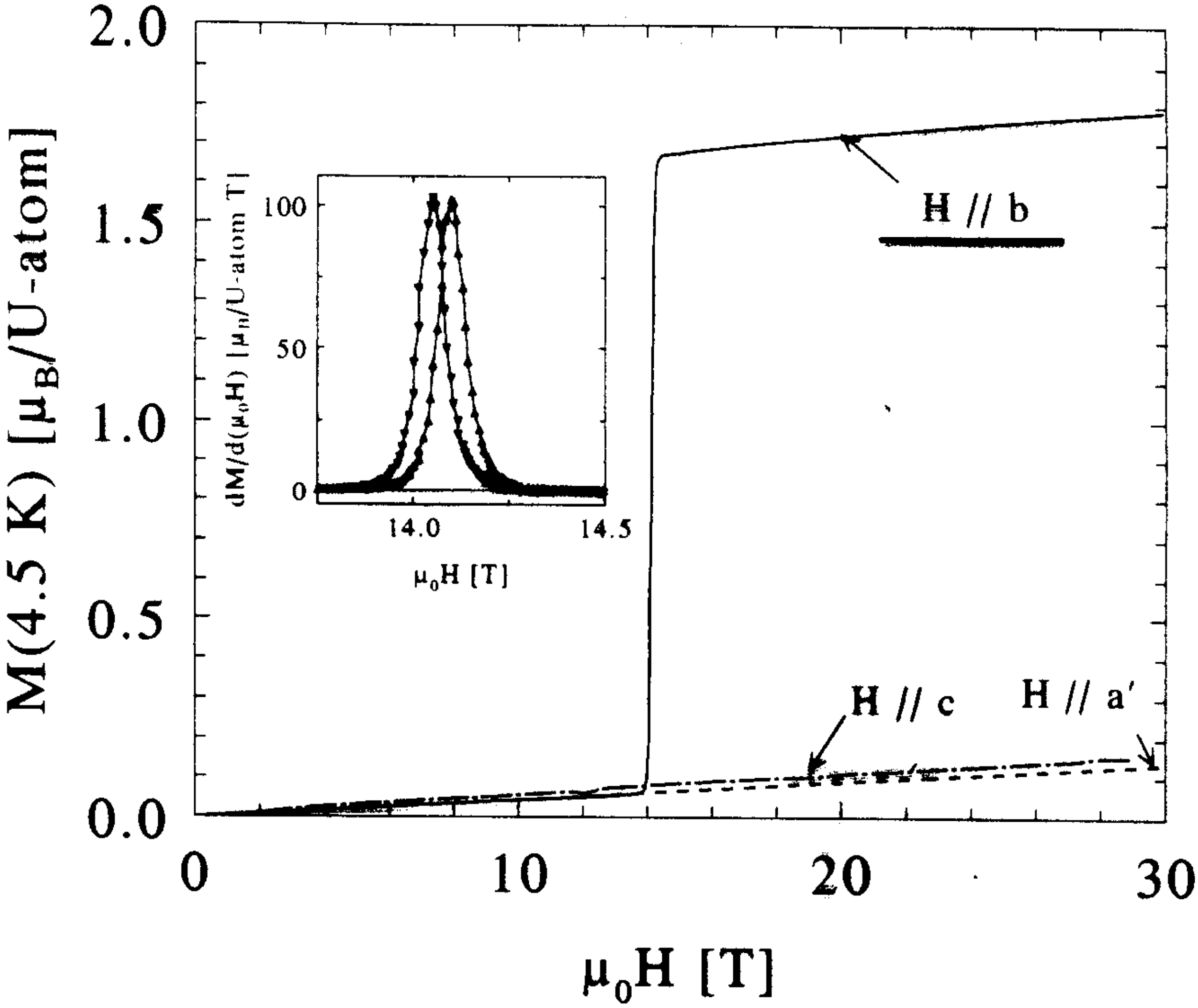
$U_2Rh_3Si_5$



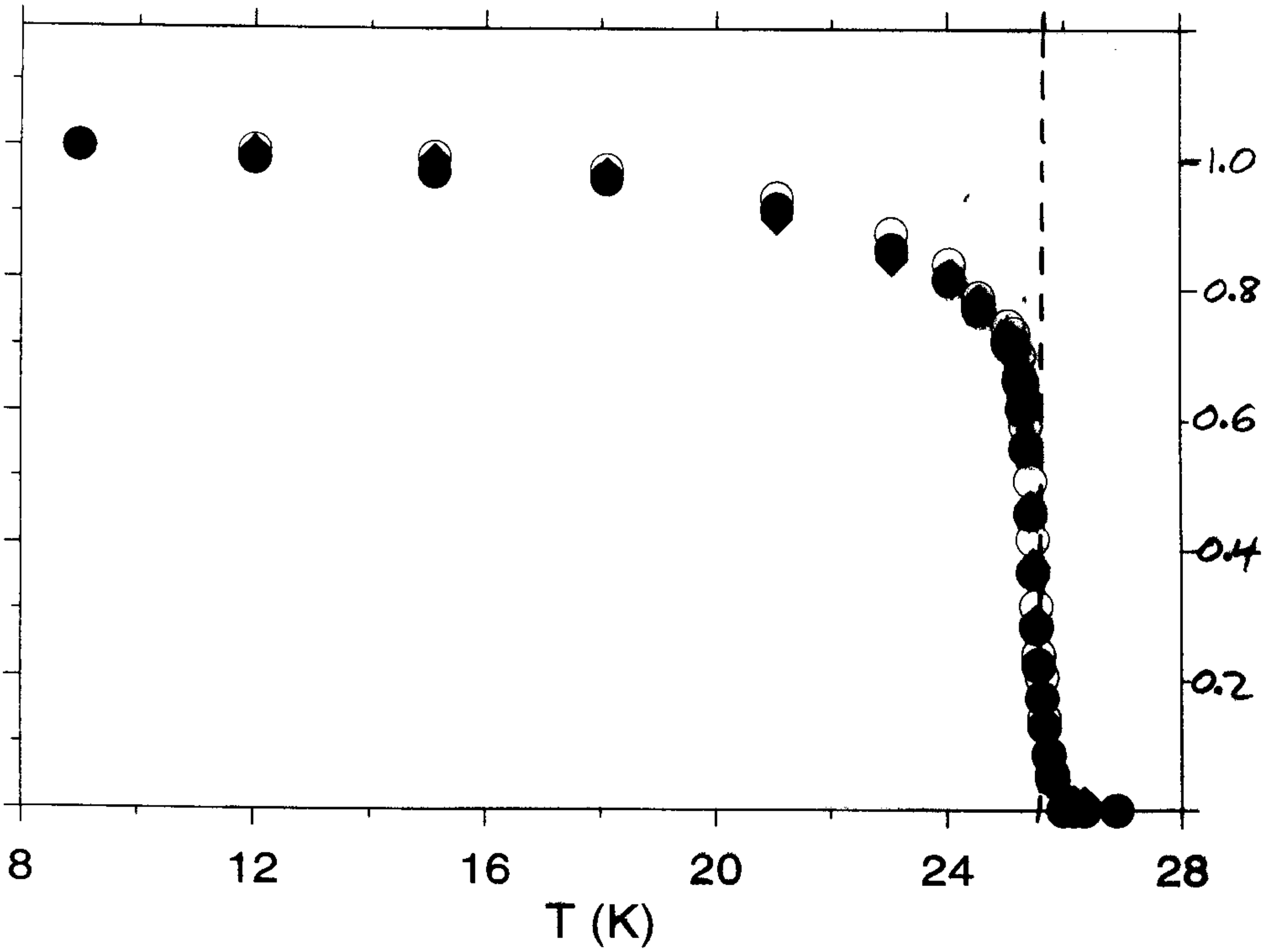


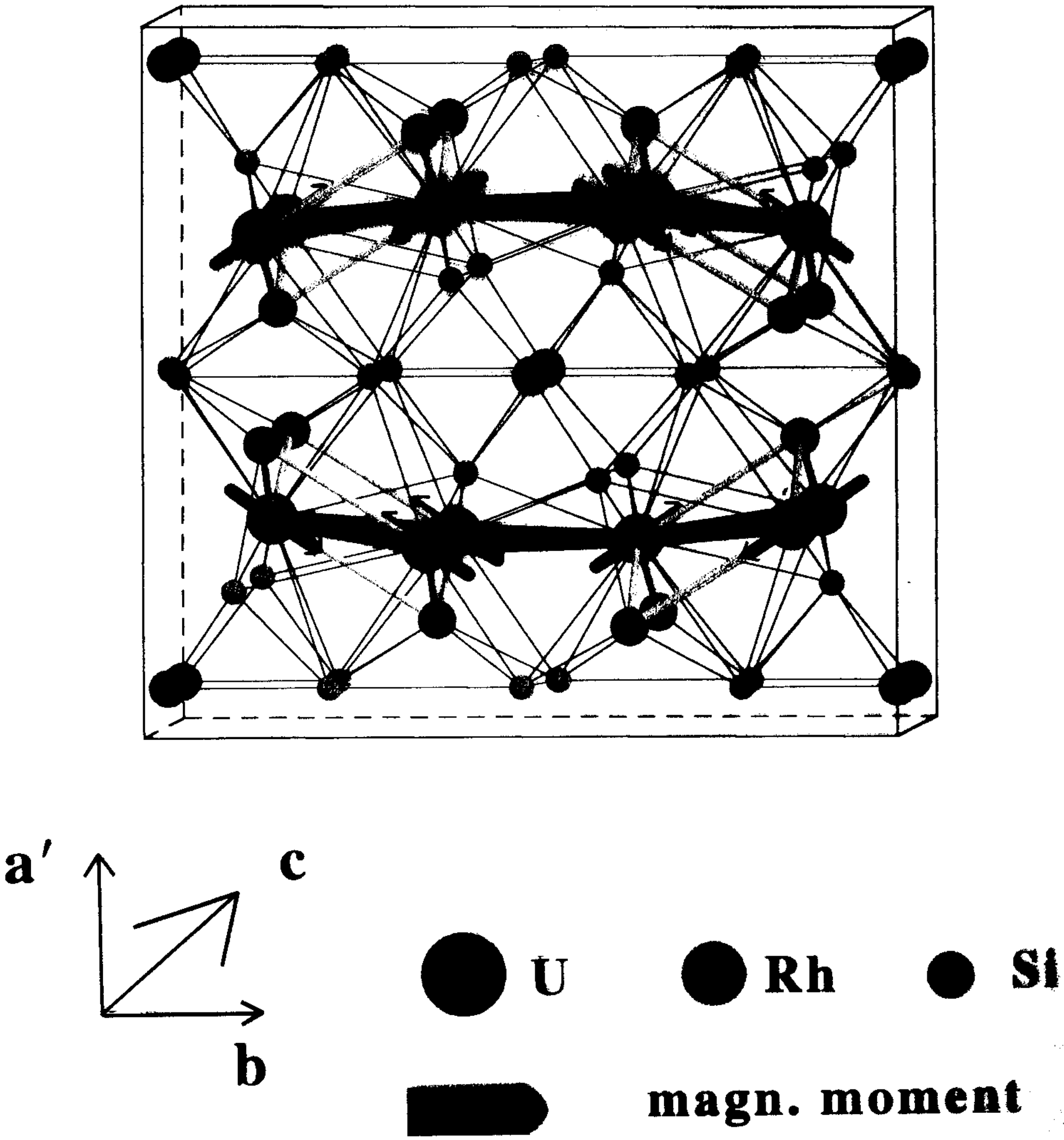
2.0
1.5
1.0
0.5
0.0
0
10
20
30
M(4.5 K) [μB/U-atom]
μ0H [T]
H // b
H // c
H // a'
100
50
0
14.0
14.5
dM/d(μ0H) [μB/U-atom T]

$U_2Rh_3Si_5$

$\mu/\mu(8.5K)$ FROM 2 BRAGG PEAKS

Drop of magnetic moment in U2Rh3Si5, single crystal




a′
c
b
U
Rh
Si
magn. moment

CONCLUSIONS $U_2Rh_3Si_5$

COMBINATION OF SPIN (DIPOLES)
CHARGE (QUADRUPOLES),

LONG-RANGE ORDERING AT SINGLE $T_0 = 25.6\,K$,
VIA FIRST-ORDER PHASE-TRANSITION.

- MAGNETIC STRUCTURE ✓ OK
- QUADRUPOLE ORDERING ? CEF ?

  (FUTURE WORK) ↓ LATTICE DEFORMATION, ↓ VOLUME DISTORTION.

- METALLIC SYSTEM ↓ RECONSTRUCTION OF FERMI-SURFACE?

  (BAND STRUCTURE)