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Magnetic Structure of UPb_3

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UPb_3 shows a sharp minimum in the inverse magnetic susceptibility versus temperature curve indicating its antiferromagnetic origin (Fig. 1) (1). A neutron diffraction study has been therefore undertaken to determine the magnetic structure of UPb_3.

A polycrystalline sample has been synthetized from spectrally pure components in a berylia crucible sealed in evacuated quartz tube. The sample was first heated at 600 ^{o}C for 150 h annealed at 300 ^{o}C during next 300 h and finally cooled down to room temperature during one week.

X-ray and neutron patterns show strong lines due to a $AuCu_3$ type lattice, however, it is impossible to decide whether the atomic distribution is ordered or disordered at room temperature, because X-ray and neutron scattering amplitudes for uranium and lead are close to each other (neutron scattering amplitudes for U and Pb are 0.84×10^{-12} and 0.96×10^{-12} cm respectively (2)).

The crystal structure of UPb_3 is of the $AuCu_3$ type (3). The lattice constant was determined from X-ray patterns to be (4.793 ± 0.002) Å at room temperature.

On neutron diffraction patterns taken at 4.2 ^{o}K we found, apart from strong nuclear peaks, two superstructure reflections due to magnetic ordering. Both were

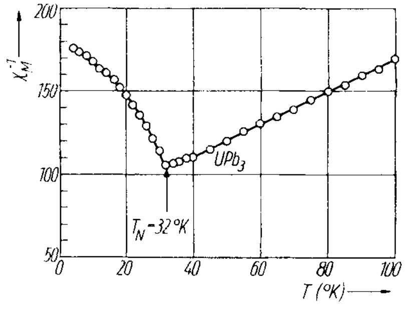

Fig. 1. Inverse molar susceptibility vs. temperature curve for UPb_3 (1)

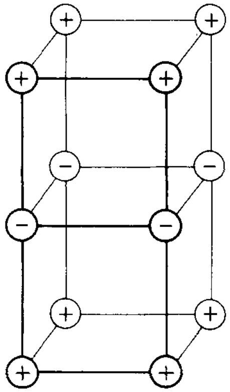

Fig. 2. The magnetic structure of UPb_3

indexed on a unit-cell of tetragonal symmetry with $a = a_o$ and $c = 2 a_o$ (a_o is the lattice constant of UPb_3). The proposed magnetic structure consists of uranium magnetic moments aligned oppositely in adjacent (001) ferromagnetic places (Fig. 2). The configurational symmetry is P4/mmm with

1 U (+)	at	1 (a)	0, 0, 0;
1 U (-)	at	1 (b)	0, 0, 1/2.

This model requires the presence of magnetic reflections with l odd only, as observed in experiment. For these reflections the magnetic structure factor is F(Mhkl) = 2p, where p is the magnetic scattering amplitude. The absence of the M 0 0 1/2 peak suggests that the alignment of uranium magnetic moments is along the fourfold axis. In this case

$$\langle q^2 \rangle_{00\frac{1}{2}} = 0 \ .$$

The mean value of the magnetic moment determined from the intensities of both observed M 1 0 $\frac{1}{2}$ and M 1 1 $\frac{1}{2}$ peaks is (1.7 ± 0.1) Bohr magnetons, using the magnetic form factor of uranium for the $5f^2$ configuration (4). An ordered distribution of U and Pb atoms at 4.2 ^oK is assumed.

The temperature dependence of the M 1 0 $\frac{1}{2}$ peak height gives the Néel temperature at 32 ^oK (Fig. 3).

The other two $AuCu_3$-type uranium compounds - UTl_3 and UIn_3 - which also show antiferromagnetic behaviour at low temperatures (5) are now investigated by

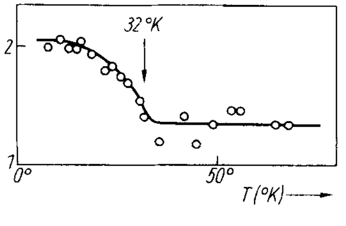

Fig. 3. The height of the M 1 0 $\frac{1}{2}$ peak as a function of temperature

neutron diffraction.

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