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To cite this version:

HAL Id: jpa-00218858
https://hal.archives-ouvertes.fr/jpa-00218858
Submitted on 1 Jan 1979

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CoU$_2$S$_5$ — magnetic structure and properties

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Résumé. — Le composé CoU$_2$S$_5$ s’ordonne magnétiquement à 270 K avec un arrangement antiferromagnétique simple des moments du cobalt et une configuration non colinéaire des moments de l’uranium. Ces derniers forment deux réseaux d’Ising couplés par une faible interaction d’échange aux moments du cobalt.

Abstract. — CoU$_2$S$_5$ exhibits below 270 K a pure colinear antiferromagnetic structure for the Co moments and a canted one for the U moments. These later can be described by two Ising sublattices weakly coupled to the cobalt ones.

1. Introduction. — The new compound CoU$_2$S$_5$ belongs to the series MX-(AX)$_n$ (M = 3d-metal, A = 5f-metal, X = S or Se, n = 1, 2) [1]. It crystalizes in space-group C2/c with $a = 14.685$ Å, $b = 6.259$ Å, $c = 7.020$ Å and $\beta = 96.42^\circ$ as parameters of the monoclinic cell. Its crystal structure is derived from that of the Hagg carbide Fe$_5$C$_2$ with the 3d-metal located in the octahedral site of Fe$_5$C$_2$. The uranium coordination polyhedron is a bicapped trigonal prism [2]. Co and U atoms are respectively in position 4d and 8f and numbered as following:

\[\begin{align*}
\text{Co} & : 1/4, 1/4, 0; \\
\text{Co2} & : 1/4, 1/4, 1/4; \\
\text{U1} & : x, y, z; \\
\text{U2} & : x, -y, -z; \\
\text{U3} & : x, y, -z; \\
\text{U4} & : x, -y, 1/2+z.
\end{align*}\]

2. Magnetic properties. — The magnetic susceptibility of CoU$_2$S$_5$ follows a Curie-Weiss law above 300 K with a Curie constant of 4.76 K$\mu$m-Oe/mole and indicates an ordering with a weak ferromagnetic component below 270 K [3].

Below the Curie point, the magnetic behaviour of powder samples in high magnetic fields is quite similar to that of many compounds of the MUX$_n$ series like CrUS$_3$ [4], CrUSe$_3$ or VUSe$_3$ [5]. We observe critical fields for the irreversible increase of magnetization and long after effect time constants which are characteristic of the propagation of narrow domain walls (Fig. 1). These phenomena are due mainly to the existence of a large magnetocrystalline anisotropy [6].

When the temperature is lowered the remanent magnetization increases as indicated in figure 2 and reaches the value of 0.65 $\mu_n$ by CoU$_2$S$_5$ formula at 4.2 K.

3. Neutron diffraction. — From the high resolution diagrams obtained at 300, 125 and 4.2 K with multidetector D1B of Institute Laue-Langevin, accurate nuclear and magnetic intensities have been deduced. At 125 and 4.2 K all magnetic lines can be indexed in the chemical unit-cell with the condition $h+k=2n$.

The application of the macroscopic method of Bertaut [7] to the space group C2/c with q = 0 provides the four different possible models which are indicated in table I.
with a sharp increase of uranium moments [8], in CoU₂S₅ there is no significant change of the directions of moments from $T_c$ down to 4.2 K (table II).

![Magnetic structure of CoU₂S₅](image)

Fig. 3. — Magnetic structure of CoU₂S₅.

Table II. — Magnetic structures at 125 K and 4.2 K.

<table>
<thead>
<tr>
<th>Temperatures</th>
<th>Atoms</th>
<th>Components ($\mu_0$)</th>
<th>Configurations</th>
<th>Moment ($\mu_0$)</th>
<th>Veracity factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>125 K</td>
<td>Co</td>
<td>${ x \ 2.3, y \ 1.9, z \ 1.9 }$</td>
<td>$G_x$</td>
<td>3.03</td>
<td>R = 0.038</td>
</tr>
<tr>
<td></td>
<td>U</td>
<td>${ x \ -0.1, y \ 0.1, z \ 0.2 }$</td>
<td>$c_x$</td>
<td>0.36</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Co</td>
<td>${ x \ 2.4, y \ 1.7, z \ 1.7 }$</td>
<td>$G_z$</td>
<td>3.07</td>
<td></td>
</tr>
<tr>
<td>4.2 K</td>
<td>U</td>
<td>${ x \ -0.4, y \ 0.6, z \ 1.5 }$</td>
<td>$c_z$</td>
<td>1.77</td>
<td>R = 0.007</td>
</tr>
</tbody>
</table>
state and half the spontaneous magnetization is just the expected value for an assembly of particles with a quasi-infinite uniaxial anisotropy. As the directions of the moments do not vary significantly, the curve of spontaneous magnetization versus temperature reflects almost exactly the variation of the uranium moment with the temperature.

On the other hand, the value of the Co moment is in good agreement with a Co$^{3+}$ state and the Curie constant per U atom deduced from the experimental one is $C_U = 1.44$. Assuming an Ising-like behaviour for uranium with an effective spin $S = \frac{1}{2}$, it leads to an effective $g$ factor of 3.92 and an ordered moment of $1.96 \mu_B$ at 0 K, in good agreement with the observed value: $1.77 \mu_B$ at 4.2 K. The exchange interaction between U and Co atoms can be estimated as 32 K in terms of U level splitting at 0 K. The variation of the spontaneous magnetization versus temperature computed in a simple molecular field model is very close to the observed one. The uranium-uranium interaction seems therefore to be very small and probably negligible.

5. Conclusion. — The compound Co$_2$U$_3$S$_7$ can be described in first approximation as a colinear Co antiferromagnet with strong internal interactions giving a high ordering temperature, weakly coupled to a paramagnetic-like system of Ising-like uranisms with two inequivalent easy directions.

References