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MAGNETIC STRUCTURES OF DYSPROSIUM OXYSULFIDE AND DYSPROSIUM OXYSELENIDE

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The magnetic structures of Dy_2O_2S and Dy_2O_2Se have been determined by neutron diffraction experiments at 1.5 K. For these two antiferromagnetic compounds the magnetic unit cell is orthohexagonal and doubled along the c-axis. The antiferromagnetic direction is parallel to the c-axis; the values of the Dy^{3+} magnetic moment in Dy_2O_2S and Dy_2O_2Se are $7.2 \pm 0.5\ \mu_B$ and $9.0 \pm 0.5\ \mu_B$, respectively.

THIS WORK is a part of systematic magnetic studies, on powder samples, of rare earth oxysulfides and oxyselenides.[1–5] The magnetic structure of Dy_2O_2S has been already determined,[1] but further magnetic[6] and Mössbauer effect[7] experiments on single crystals are in disagreement with the moment orientation. To remove this discrepancy we redetermined the magnetic structure of Dy_2O_2S which is presented here together with that of its isomorphous oxyselenide Dy_2O_2Se.

The dysprosium oxysulfide and oxyselenide order antiferromagnetically at 5.8 and 8.5 K respectively.[4] They crystallize in the space group $P\bar{3}m - D^3_{3d}$. Figure 1 gives the atomic positions in the hexagonal unit cell. The lattice and position parameters have been determined from the neutron diffraction patterns obtained at room temperature.

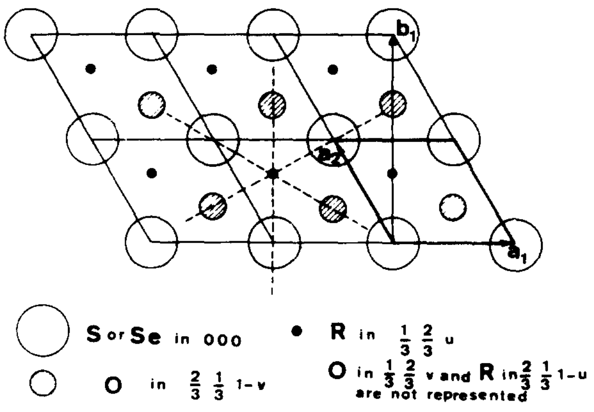

FIG. 1. Projection in the basal plane of the crystallographic structure of the rare earth oxychalcogenides R_2O_2S and R_2O_2Se.

In the nuclear structure factor

$$F_N(\mathbf{h}) = \sum_j b_j e^{2\pi i \mathbf{h} \cdot \mathbf{r}_j}$$

the following scattering lengths b_j were used for the calculation[8] $b_{Dy} = 1.69$; $b_O = 0.577$; $b_S = 0.28$ and $b_{Se} = 0.78$ in units of 10^{-12} cm/atom. The results are given in Table 1.

For the two compounds Dy_2O_2S and Dy_2O_2Se magnetic neutron diffraction patterns have been

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Table 1.

	a(Å)	c(Å)	u	v
Dy_2O_2S	3.792	6.587	0.272 ± 0.006	0.64 ± 0.005
Dy_2O_2Se	3.855	6.825	0.283 ± 0.004	0.622 ± 0.006

Table 2. Comparison of calculated and observed magnetic intensities of Dy_2O_2S *at* 1.5 K

hkl	Calculated intensities		Observed intensities
011		198	228
101 013	284 102	386	377
103		48	52
015 121	16 352	386	340
031 105 123	224 131 372	727	730

Reliability factor $R = \Sigma|I_{obs} - I_{cal}|/\Sigma I_{obs} = 4.3\%$

Table 3. Comparison of calculated and observed magnetic intensities of Dy_2O_2Se *at* 1.5 K

hkl	Calculated intensities		Observed intensities
011		629	708
101 013	1006 369	1376	1359
103		80	127
015 121	48 1101	1149	1186
105 131 123	413 792	2537	2535
033		84	obscured by $Al(200)$
117 125 211	57 281 860	1198	1105
107 035 213	20 570 1148	1738	1755

Reliability factor (defined as in Table 2) $R = 3.4\%$

recorded at $T = 1.5$ K. As the absorption cross-section of dysprosium is very large we have diluted the compounds with aluminium powder in order to obtain reasonable intensities. The neutron diffraction diagrams of Dy_2O_2Se obtained at room temperature and $T = 1.5$ K are reported on Fig. 2. In the case of Dy_2O_2S magnetic peaks are observed at analogous positions but with different intensities. The magnetic unit cell is therefore the same for the two compounds: the magnetic reflections can be indexed in an orthohexagonal cell doubled along the **c** axis (a, $b = a\sqrt{(3)}$, $2c$), i.e. the propagation vector is $\mathbf{k} = (0\ 0\ \frac{1}{2})$.

In the orthohexagonal description ($l = (2n+1)/2$), the magnetic structure factor can be written as:

$$\mathbf{F}_M = 2\eta f(\mathbf{m}_1\, e^{2\pi i(k/3 + lu)} - \mathbf{m}_2\, e^{-2\pi i(k/3 + lu)})$$

where

$$\eta = \frac{e\gamma^2}{mc^2} = 0.27 \cdot 10^{-12}\ \text{cm}\ \mu B^{-1}$$

f is the form factor.[9]

$\mathbf{m}_1$ and $\mathbf{m}_2$ are the magnetic moments (in μ_B) of the Dy^{3+} ion at the coordinates u and $1 - u$ in the crystallographic cell. For the two compounds the comparison between the observed and calculated intensities (Tables 2 and 3) indicates that $\mathbf{m}_1$ and $\mathbf{m}_2$ are coupled ferromagnetically i.e. $\mathbf{m}_1 = \mathbf{m}_2$ and that antiferromagnetic direction is parallel to the c-axis.

For Dy_2O_2S and Dy_2O_2Se the magnetic moment values of the Dy^{3+} ion at 1.5 K are $7.2 \pm 0.5\ \mu_B$ and $9.0 \pm 0.5\ \mu_B$, and the reliability factors are 4.3% and 3.4% respectively.

The magnetic structure of Dy_2O_2S and Dy_2O_2Se is represented on Fig. 3.

For Dy_2O_2S the moment direction and value are to be compared with the crystal field determination and Mössbauer effect results. Optical experiments and crystal field calculations[10] indicate that the first excited doublet lies at about 30 K above the ground

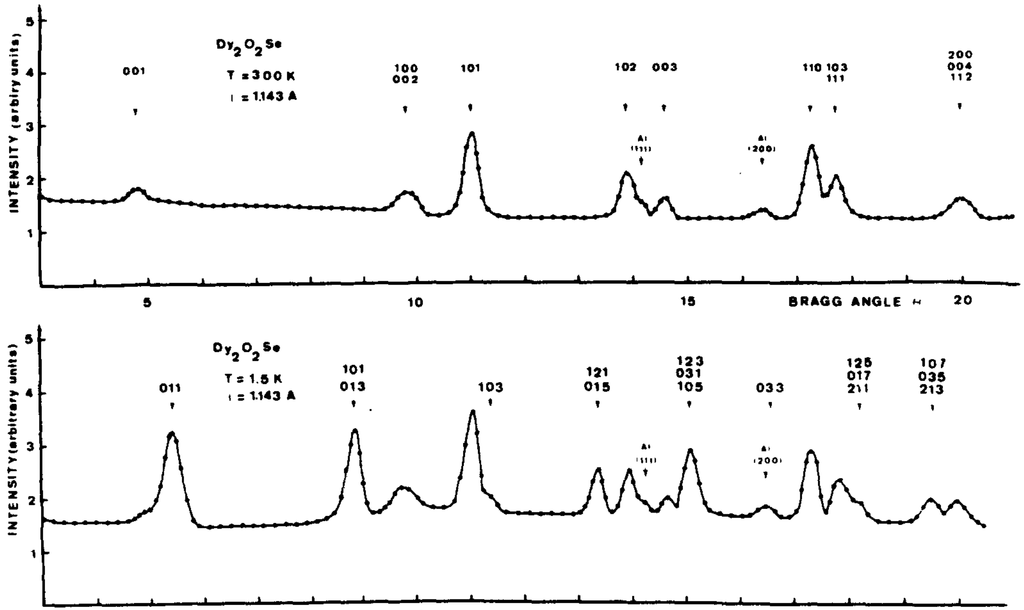

FIG. 2. Neutron diffraction patterns of Dy_2O_2Se at 300 K and 1.5 K. The magnetic peaks are indexed in an orthohexagonal unit cell doubled along the c-axis.

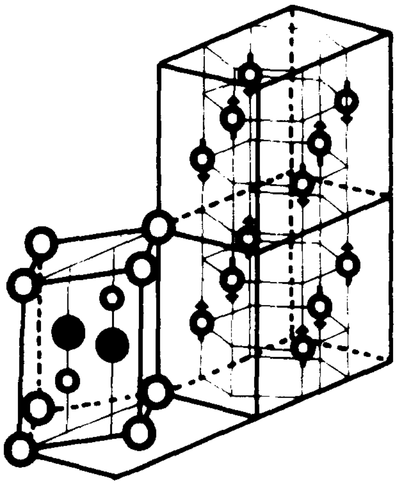

FIG. 3. The magnetic structure of Dy_2O_2S and Dy_2O_2Se.

state and thus the magnetic moment anisotropy in the antiferromagnetic state, depends only on the wave function of the ground state doublet. The nature of the irreducible representation associated with this doublet impose an Ising behaviour with the magnetic moment along the *c*-axis; the moment value at $T = 0$ K deduced from the calculated wave function is $8.2\ \mu_B$. Mössbauer experiments indicate also that the magnetic moments are along the c-axis with a value of $(8.2 \pm 0.4)\ \mu_B$.[7]

We can see that all these results are in good agreement concerning the moment direction. However the moment deduced from neutron diffraction data is smaller than the value given by crystal field calculations and Mössbauer experiments. This slight discrepancy can perhaps be related to the high neutron absorption cross-section of dysprosium.

In the oxyselenide, the wave function of Dy^{3+} ground state is probably of the same nature as in the oxysulfide but with a higher 15/2 component, because of the higher magnetic moment value.

Also the magnetic anisotropy of Dy_2O_2Se should be greater than that of Dy_2O_2S which is actually observed by susceptibility measurements.[4]

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Nous avons déterminé les structures magnétiques des composés antiferromagnétiques Dy_2O_2S et Dy_2O_2Se grâce à des expériences de diffraction neutronique effectuées à 1.5 K. Dans ces deux composés la maille magnétique est orthohexagonale doublée selon l'axe c, et les moments magnétiques sont paralléles à l'axe c. Le moment magnétique de l'ion Dy^{3+} vaut $7.2 \pm 0.5\ \mu_B$ dans Dy_2O_2S et $9.0 \pm 0.5\ \mu_B$ dans Dy_2O_2Se.