PARAMAGNETIC SCATTERING OF NEUTRONS BY RARE-EARTH IONS: CALCULATED PARAMAGNETIC CROSS SECTIONS FOR Ce, Pr, Nd, Gd, Tb, Dy, Ho, Er, Tm and Yb.

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RESUMO

A teoria dada por Trammell foi usada para se calcular a secção de choque total de espalhamento paramagnético de nêutrons para os ions de terras raras. Os fatôres de forma magnéticos foram calculados usando-se as funções determinadas por Blume, Freeman e Watson, assumindo-se funções de onda de Hartree-Fock.

RESUMÉ

La théorie donnée par Trammell a été employée pour calculer la section efficace totale de diffusion paramagnétique des neutrons par les ions des terres rares. Les facteurs de forme magnétiques ont été calculés utilisant les fonctions determinées par Blume, Freeman et Watson, en supposant des fonctions d'onde de Hartree-Fock.

ABSTRACT

The theory given by Trammell has been used for calculating the total paramagnetic scattering cross section of neutrons for rare-earth ions. The magnetic form factors have been calculated using the functions determined by Blume, Freeman and Watson, assuming Hartree-Fock wave-functions.

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Paramagnetic Scattering of Neutrons by Rare-Earth Ions: Calculated Paramagnetic Cross Sections for Ce, Pr, Nd, Gd, Tb, Dy, Ho, Er, Tm, and Yb

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The theory given by Trammell[1] for the paramagnetic scattering of neutrons by rare-earth ions has been used.

The total paramagnetic cross section is given by[1,2]

$$\sigma_{pm}=\tfrac{2}{3}\pi(e^2/mc^2)^2\gamma^2\mu^2\bar{f}^2,$$

where e^2/mc^2 is the classical electronic radius, γ and μ are the magnetic moments of the neutron and of the atom, respectively, and $\bar{f}^2$ is the average over all scattering angles of the squared magnetic form factor.

The form factors were calculated assuming Hund ground state and Russell–Saunders coupling for the $4f$ electrons. The functions determined by Blume, Freeman, and Watson,[3] assuming Hartree–Fock wavefunctions were used for evaluating the orbital and spin contributions. For Pm, Sm, and Eu, the form factors have not been calculated because of the narrowness of the multiplet spacings and of contributions of J states other than the lowest[4–6] so that the assumption of Hund ground state is no longer valid. In this assumption there is no paramagnetic scattering for Eu. Since Gd^{3+} is in an S state, there is just the spin contribution to its form factor.

Table I gives the values of $\bar{f}^2$ as a function of wavelength, calculated by numerical integration for the rare earths. $\bar{f}^2$ reduces to unity for wavelengths large compared to the linear size of the $4f$ electron distribution and approaches zero for wavelengths comparable to the diameter of the $4f$ shell. Figure 1 shows the calculated curves of $\bar{f}^2$ for Nd^{3+} and Gd^{3+}, corresponding, respectively, to form factors having the largest and no orbital contribution. The other curves fall between these two.

For the calculation of σ_{pm} the measured values of the

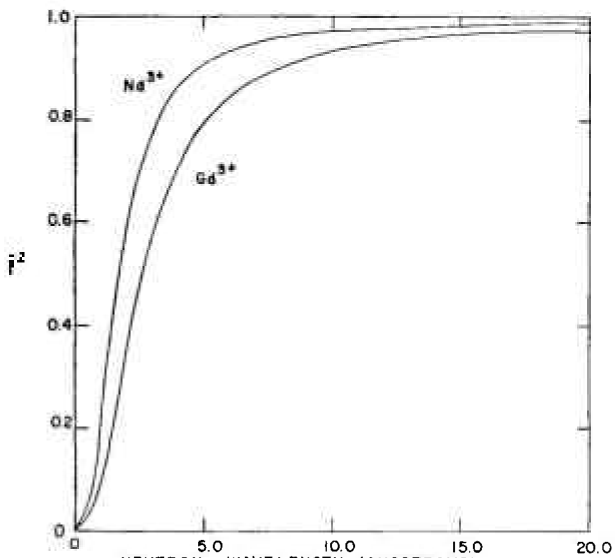

FIG. 1. Average squared magnetic form factors for Nd^{3+} and Gd^{3+}.

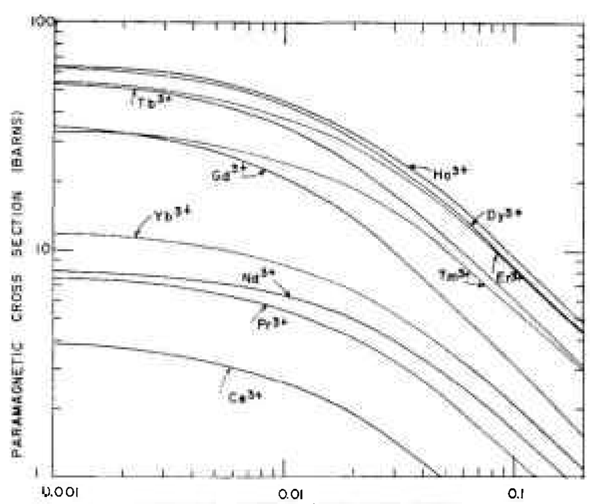

FIG. 2. Calculated total paramagnetic cross sections.

TABLE I. Values of $\bar{f}^2$ as a function of wavelength.

λ (Å)	Ce^{3+}	Pr^{3+}	Nd^{3+}	Gd^{3+}	Tb^{3+}	Dy^{3+}	Ho^{3+}	Er^{3+}	Tm^{3+}	Yb^{3+}
20.00	0.980	0.984	0.988	0.972	0.964	0.979	0.980	0.982	0.983	0.984
10.00	0.951	0.961	0.972	0.933	0.937	0.949	0.953	0.957	0.960	0.962
5.00	0.849	0.877	0.909	0.797	0.825	0.844	0.856	0.866	0.873	0.880
2.86	0.646	0.701	0.764	0.554	0.607	0.641	0.656	0.683	0.698	0.712
2.00	0.466	0.521	0.596	0.357	0.416	0.454	0.478	0.505	0.524	0.541
1.54	0.327	0.379	0.449	0.231	0.283	0.318	0.342	0.367	0.386	0.403
1.25	0.232	0.275	0.334	0.155	0.196	0.230	0.246	0.267	0.283	0.299
1.00	0.154	0.185	0.230	0.099	0.128	0.152	0.164	0.180	0.193	0.206
0.87	0.117	0.142	0.177	0.075	0.097	0.116	0.126	0.138	0.149	0.159
0.74	0.085	0.103	0.130	0.055	0.070	0.084	0.091	0.101	0.109	0.116

magnetic moments[7] of the rare-earth ions in the form of oxide have been used. Figure 2 shows the calculated total paramagnetic cross sections of the rare earths as a function of energy. The curves for Pr, Ho, Er, Tm, and Yb have already been published[8] and are presented here for completeness.

The agreement verified in the comparison[8] of calculated and experimental form factors for Ho^{3+} and Tm^{3+} indicates that the calculated total paramagnetic cross sections presented in Fig. 2 for the rare-earth ions can be used in the analysis of data obtained by total neutron cross-section measurements.

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