

TABLE I. Lattice parameters of Gd, Tb, and Dy under 0- and 20- kbar hydrostatic pressure.

	Gd		Tb		Dy	
Pressure (kbar)	0	20	0	20	0	20
$a$ (a.u.)	6.867	6.745	6.811	6.694	6.784	6.676
$c$ (a.u.)	10.925	10.737	10.768	10.591	10.673	10.502

mesh of 60 points.

It seems appropriate at this point to discuss the limitations of this calculation. (a) The band calculation involves a whole series of approximations. There is no way to assess the accuracy of the result because of the lack of experimental Fermi-surface data. We took great care to do the zero-pressure and 20-kbar calculations in an identical manner in order to minimize random error. Also, by choosing a high enough pressure we hoped that the pressure shift would be large enough to be detectable above the noise level. (b) The  $\chi(\vec{q})$  calculation has a 3% noise content. This is not a serious problem because the peak in  $\chi(\vec{q})$  is usually broad enough so that the maximum can be picked out with little difficulty. (c) The susceptibility calculation is done with the paramagnetic band, so the conclusions apply only to the initial ordering properties. However, in reality the turn angle must be measured when there is a substantial amount of ordered moment. There is reasonable ground for comparing the theory with the experiment in case of Dy where the magnetoelastic effect is weak over most of the helical-ordering temperature range, but not so for Tb where we expect an important influence of magnetoelastic

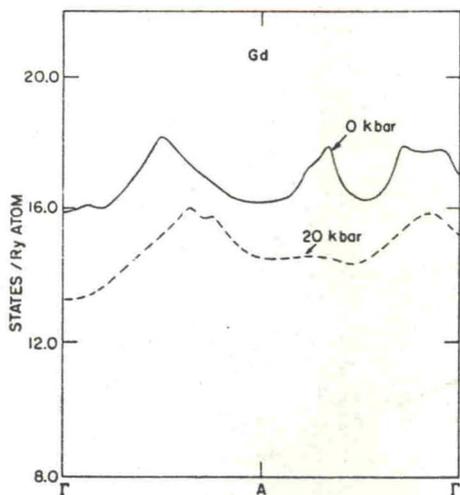


FIG. 1. Generalized susceptibility function for gadolinium in  $\Gamma A \Gamma$  direction at 0 and 20 kbar of hydrostatic pressure.

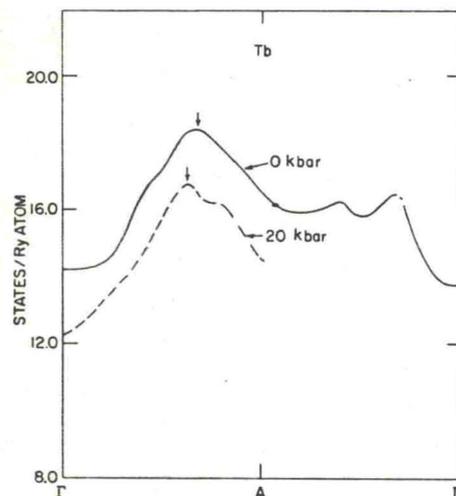


FIG. 2. Generalized susceptibility function for terbium in  $\Gamma A \Gamma$  direction at 0 and 20 kbar of hydrostatic pressure.

energy on the turn angle.<sup>9</sup> (d) The  $s$ - $f$  matrix element is assumed to be pressure independent purely because of our great ignorance about this quantity.

The results of this investigation are summarized in Figs. 1-3 and in Table II. In the figures we plot the susceptibility function per spin per atom along the  $\Gamma A \Gamma$  direction. From Figs. 2 and 3 one can see the peaks of  $\chi(\vec{q})$  for Tb and Dy shift to smaller  $q$  values when the pressure is applied and the sizes of the peaks are reduced. There is a small peak in the susceptibility function for Gd, but one should not take it seriously because it is probably wiped out by a  $q$ -dependent  $s$ - $f$  matrix element. The shift in  $T_c$  or  $T_N$  is obtained from

$$T_c(P)/T_c(0) = \chi_0(P)/\chi_0(0)$$

for Gd, and

$$T_N(P)/T_N(0) = \chi_{\max}(P)/\chi_{\max}(0)$$

for Tb and Dy.<sup>15</sup> Here  $\chi_{\max}$  is the size of the peak of  $\chi(\vec{q})$ , and  $\chi_0$  is the static susceptibility. Table II displays the numerical results alongside the experimental values. The range of the measured values is given in case there is slight disagreement among the various investigators. In view of all the uncertainties in the calculation, the agreement with the experimental values must be termed

TABLE II. Dependence of ordering temperature and turn angle of heavy rare earths on hydrostatic pressure.

	Gd		Tb		Dy	
	Expt	Calc	Expt	Calc	Expt	Calc
$dT/dP$ (K/kbar)	-1.56	-2.3	-0.8	-1.0	-0.4	-0.4
$d\omega/dP$ ( $^\circ$ /kbar)	...	...	~-1.1	~-0.6	?	-0.38