Table 3. *Measured values of* $dc_{ij}/dP = c'_{ij}$ *at* 298°K, *for Gd, Dy and Er*

	Gd	Dy	Er
c'_{11}	3·018 ± 0·02	3·092 ± 0·006	4·768 ± 0·020
c'_{33}	5·726 ± 0·05	5·331 ± 0·008	5·448 ± 0·018
c'_{44}	0·185 ± 0·012	0·434 ± 0·001	0·949 ± 0·005
c'_{66}	0·377 ± 0·002	0·408 ± 0·002	0·853 ± 0·012
c'_H	0·435 ± 0·028	0·457 ± 0·070	1·663 ± 0·033
c'_{12}	2·26 ± 0·02	2·277 ± 0·006	3·062 ± 0·044
c'_{13}	3·53 ± 0·05	3·32 ± 0·1	2·16 ± 0·04
K'_s	3·320 ± 0·039	3·214 ± 0·054	3·302 ± 0·02
K'_T		3·228 ± 0·044	3·256 ± 0·25

but become considerably sharper when the derivatives are normalized with respect to initial values of the c_{ij} and volume compressibility. The two types of parameters are related as follows:

$$\pi_{ij} = \frac{\mathrm{d} \ln c_{ij}}{\mathrm{d} \ln V} = \frac{V}{c_{ij}}\left(\frac{\mathrm{d}c_{ij}}{\mathrm{d}P}\right)\frac{\mathrm{d}P}{\mathrm{d}V} = -\frac{K_T}{c_{ij}}\left(\frac{\mathrm{d}c_{ij}}{\mathrm{d}P}\right). \quad (5)$$

The 298°K values of π_{ij} for c_{11}, c_{33}, c_{44}, c_{66}, c_H, K_s and K_T computed from the above equation with the zero pressure values of K_T and c_{ij}, are given in Table 4. The probable errors given in Table 4 are based on the probable errors in $\mathrm{d}c_{ij}/\mathrm{d}P$ and estimated probable errors of 1 per cent total in each of the (K_T/c_{ij}) factors. The values of π_{33}, π_{K_s}, and π_{K_T} show only small variations between all 3 metals, with the values of Gd being slightly larger in magnitude. The π_{11} values for Gd and Dy are identical as are the values of π_{66} and π_{C_H}. In sharp contrast, π_{11} and π_{66} for Er are considerably greater. The π_{44} values are distinguished by the large differences in this parameter among the 3 metals.

Since we will be concerned with the possibility that the π_{ij} values for Gd are influenced by the spatial coherent magnetic order fluctuations at 298°K, measurements of c_{ij} for Gd were also carried out in the ferromagnetic phase, at 273°K. The results for ferromagnetic Gd are given in Table 5. By comparison with Table 4, it is noted that the magnetic order at 273°K reduces π_{11}, π_{33} and π_{K_s} very significantly, but the effects on π_{44} and π_{66} are quite small. The π_{44} values at 273°K and at 298°K are the same within the quoted errors.

4. DISCUSSION

The values of $\mathrm{d}K_s/\mathrm{d}P$ for all three metals and $\mathrm{d}K_T/\mathrm{d}P$ for Dy and Er are clearly smaller than Anderson's [19] 'lower limit' of 3·5 and are indeed smaller than reliable published values of $\mathrm{d}K_s/\mathrm{d}P$ for any solid including that for Na, where the ultrasonic data [2] gives $\mathrm{d}K_s/\mathrm{d}P \sim 3{\cdot}3$. The significance of the small $\mathrm{d}K_s/\mathrm{d}P$ is that one can be reasonably assured that the short range ion core repulsive contribution to the other compressional moduli, the shear moduli and their volume derivatives are relatively minor. We can then be fairly confident that an analysis of the values for $\mathrm{d}c_{44}/\mathrm{d}P$, $\mathrm{d}c_{66}/\mathrm{d}P$, and $\mathrm{d}C_H/\mathrm{d}P$ in terms of electrostatic and band structure contributions alone is a reasonably good model for Gd, Dy and Er metals. In view of the almost identical values for $\mathrm{d}K_s/\mathrm{d}P$ for the three metals it seems reasonably safe to conclude that the small core model holds for the elastic moduli and cohesive energy of all the heavy rare earth metals.

(a) *Analyses of* π_{44}, π_{66}, *and* π_{C_H}

The values of the electrostatic contributions to the volume derivatives of the shear moduli

Table 4. *Measured values of* $\pi_{ij} = d \ln c_{ij}/d \ln V$ *at* 298°K, *for Gd, Dy and Er*

	π_{11}	π_{33}	π_{44}	π_{66}	π_{C_H}	π_{K_s}	$\pi_{K_T=K'_T}$
Gd	−1·713 ± 0·03	−3·013 ± 0·06	−0·339 ± 0·025	−0·690 ± 0·10	0·648 ± 0·05	−3·283 ± 0·39	
Dy	−1·701 + 0·02	−2·783 ± 0·03	−0·734 ± 0·010	−0·690 ± 0·01	0·674 ± 0·10	−3·214 ± 0·054	−3·228 ± 0·044
Er	−2·510 ± 0·03	−2·895 ± 0·04	−1·538 ± 0·02	−1·390 ± 0·03	2·28 ± 0·068	−3·266 ± 0·021	−3·256 ± 0·025

Table 5. Values of $dc_{ij}/dP = c'_{ij}$ and $\pi_{ij} = d\ln c_{ij}/d\ln V$ for ferromagnetic Gd at 273°K, no external magnetic field. $(K_T)_{P=0} =$ 372·1 kbar

Modulus →	c_{11}	c_{33}	c_{44}	c_{66}
c'_{ij}	2·436 ± 0·016	3·841 ± 0·017	0·209 ± 0·011	0·338 ± 0·003
π_{ij}	−1·338 ± 0·023	−1·989 ± 0·028	−0·369 ± 0·024	−0·596 ± 0·012

	c_{12}	c_{13}	K_s	C_H
c'_{ij}	1·75 ± 0·016	2·01 ± 0·06	2·67 ± 0·03	0·042
π_{ij}	−2·56 ± 0·05	−5·36 ± 0·16	−2·64 ± 0·03	

of Gd, Dy and Er are given in Table 6 as calculated from equation (3). The values of M_{ij} and $(\partial M_{ij}/\partial[c/a])_V$ are taken directly from Cousins' computations [5]. For $c/a < 1{\cdot}65$ the M_{44}, M_{66} and M_{C_H} are linearly related to c/a and $(\partial M_{44}/\partial[c/a])_V$ is a factor of four larger than the next highest derivative, $(\partial M_{C_H}/\partial[c/a])_V$. The calculated values for four other hcp metals, Mg, Be, Zr and Ti are listed for comparison and the absolute differences between the electrostatic and observed values of π_{44}, π_{66} and π_{C_H} are also given [4, 20, 13, 10]. We note that the observed π_{44} and π_{66} values for Er (Table 4) are within 5 per cent of being the same as the respective electrostatic contributions. In contrast, the $(\pi_{44} - \pi^e_{44})$ values for Gd and Dy are about 1/3 and 2/3, respectively, of π^e_{44}. The $(\pi_{66} - \pi^e_{66})$ values for Gd and Dy are identical and about 50 per cent of π^e_{66}. The contrast between Er and the other two rare earths is further emphasized in the π_{C_H} values where the $(\pi_{C_H} - \pi^e_{C_H})$ are positive and identical within the errors, given in Table 4, for Gd and Dy, but negative for Er.

If we assume that electrostatic and band structure contributions to the shear moduli give clearly independent contributions to the c_{ij} values we have the following equation:

$$\pi_{ij} = \frac{\pi^e_{ij} \cdot c^e_{ij} + \pi^b_{ij} c^b_{ij}}{c_{ij}} \qquad (6)$$

where c^b_{ij} and π^b_{ij} represent the band structure contributions. If equation (6) is used, the weighted contribution of π^e_{ij} to the observed π_{ij} depends on the value of c^e_{ij}, computed from equation (1). It is thus necessary to define the effect valence, Z, making the partition between weighted π^e_{ij} and weighted π^b_{ij} somewhat arbitrary. It is nevertheless of some value to

Table 6. Electrostatic contributions to π_{44}, π_{66} and π_{C_H} for several hcp metals, as calculated from equation (3)

	π^e_{44}	$\pi_{44} - \pi^e_{44}$	π^e_{66}	$\pi_{66} - \pi^e_{66}$	$\pi^e_{C_H}$	$\pi_{C_H} - \pi^e_{C_H}$
Gd	−1·388	1·049	−1·337	0·647	−1·340	0·692
Dy	−1·303	0·569	−1·333	0·642	−1·329	0·655
Er	−1·609	0·071	−1·360	0·03	−1·378	−0·902
Mg	−1·513	−1·807	−1·341	−1·445	−1·346	−2·500
Be	−1·103	−0·60	−1·312	−0·447	−1·298	−0·289
Zr	−0·945	1·60	−1·300	0·602	−1·282	0·837
Ti	−1·491	0·296	1·341	0·01	−1·348	−0·458