elastic constants from low pressure), or we estimate a range of possible values for α and compute the transition pressure, again using extrapolations of the elastic constants. In all cases, the extrapolations were based on the measured pressure derivatives of the elastic constants. For the NaCl-type alkali-halides, we used a NNN lattice model extrapolation formula [*Demarest*, 1972*a*], while in all other cases we assumed that the elastic constants are linear with pressure. We conclude from earlier calculations [*Demarest*, 1972*b*] that this type of extrapolation is adequate for the present purposes up to reduced pressures of $P/K_O \approx 0.5$.

TABLE 5. Evaluations of α and predictions of Phase Transition

Compound	Structure	Soft Shear Mode	Transition Pressure, kbar		α	
			Predicted	Experiment	Assumed	Measured
NaF	NaCl→CsCl	C_{44}		~300		0.14
NaCl				290		0.14
NaBr			>120		<0.20	
NaI			-		<0.20	
KF				17.3		0.26
KCl				19.3		0.20
KBr				17.4		0.19
KI				17.8		0.16
RbF				9.4		0.13
RbCl				5.2		0.22
RbBr				4.5		0.21
RbI				3.4		0.19
MgO	NaCl→CsCl	C_{44}	-		<0.26	
CaO			275-400		0.15-0.20	
SrO			1000-2200		0.15-0.20	
AgCl	NaCl→HgS	C_{44}		76		0.06
AgBr	NaCl→HgS			82		0.05
AgI	NaCl→tetragonal			97		-
Si	Diamond→white Sn	C_S*		110		0.36
Ge				90		0.37
Diamond			-	-		-
CaF_2	Fluorite→$PbCl_2$	C_S		80		0.54
BaF_2				20		0.36
CdS	Wurtzite→NaCl	C_{44}		25		0.18
ZnS	Wurtzite→Sphalerite	C_{66}		45		(0.29)
	→NaCl	C_{44}		117		0.18
TiO_2	Rutile→Dist. Fluorite	C_S		50		0.16
SnO_2			30-90		0.14-0.18	
GeO_2			150-250		0.14-0.18	
SiO_2	αQuartz→coesite	$\frac{1}{2}\lambda_7$*		20		0.59
	αQuartz→stishovite	$\frac{1}{2}\lambda_7$		85		0.25
$MgAl_2O_4$	Spinel→	C_S	300-700		0.15-0.20	
$MgO \cdot 2.6Al_2O_3$	Spinel→		1000-2000		0.15-0.20	

*$C_S = \frac{1}{2}(C_{11}-C_{12})$ $\qquad \lambda_7 = C_S + C_{44} - \sqrt{(C_S-C_{44})^2 + 4C_{14}^2}$

Estimates of α for the NaCl→CsCl transition in the alkali-halides range from 0.13 (RbF) to 0.26 (KF). Most of the data seems to be centered in the range 0.15-0.20. The seven alkali halides for which no transition has been found will probably not transform to the CsCl structure. NaBr may transform above 120 kbar, but this is not clear since C_{44}/K never dips much below 0.20. MgO will probably not have a transformation of this type. SrO may transform to the CsCl structure at extreme pressures, and we think that CaO will probably transform between 270 and 400 kbar.

The silver halides transform to the cinnabar (HgS) structure with $\alpha \cong 0.05$. This transformation is not a pure shear, but it does involve a smaller shift of atom positions than does the NaCl-CsCl transition.

The metallic transitions in Si and Ge are among those which we do not expect to conform well with our theory, because of the change in electronic structure. Here $\alpha = 0.36$. There is no prediction of diamond going through this transition at high pressure. Our theory also fails to predict the high pressure transition in the fluorite structure.

The wurtzite → NaCl transition in CdS and ZnS is in perfect agreement with this theory ($\alpha = 0.18$). We neglect the complication of the sphalerite structure, which for ZnS is stable in an intermediate pressure range, depending upon the temperature and stoichiometry.

The transformation of rutile to distorted fluorite is in excellent agreement ($\alpha = 0.16$). We predict transitions in the range 30-90 kbar for SnO_2 and 150-250 kbar for GeO_2.

Our method fails to predict the α-quartz → Coesite transition. However even in this case, our method shows its usefulness. The Born criterion predicts a lattice instability at 180 kbar, while the modified Born criterion predicts the transition at 95-115 kbar. This is not too far from the transition to Stishovite at 85 kbar.

We have deliberately omitted from Table 5 elements or compounds for which all the shear moduli increase rapidly with pressure. We have selected an assortment of crystal structures for which there was sufficient readily available data to make a test of the modified Born criterion.

Table 5 confirms our theories concerning the interrelationship of pressure-induced phase changes and weak shear constants. Values of α tend to be similar for a particular transformation. In no case is α very small, and the smallest value here is 0.05. The modified Born criterion does not work when the transformation involves a change in the electronic structure of the compound, or when the transformation is in no way related to a shear (these cases were not included in the table). However, in many cases this method will permit good estimates of phase transition pressures with very little effort.