Table 1. *Effect of pressure on band structure of semiconductors*

Compound	ΔE_g(eV)* (1 atm)	P(10^3 atm)	Speculated transition direction†	$d\Delta E_g/dP$‡ (10^{-6}eV/atm)	$d\Delta E_g/dr$§ (eV/Å)	Max. blue shift (eV)
Si	1·08	0–140	(100)[10,11]	−2·0	−1·12	
Ge	0·70	0–50 50–129	(111)[11] (100)[3]	+8·0 −1·2	3·8 −0·6	0·15
GaP	2·34	0–20 20–50	(111) or (000) (100)	1·8 −1·7		0·02
GaAs	1·47	0–60 60–130	(000) or (111)[12,13] (100)	+9·4 −8·7		0·47
GaSb	0·70	0–50 50	(000) or (111) (100)	+12·3 ?		0·35
ZnS	3·54	0–180	(000) or (111)[4]	+5·7	6·2	0·50
ZnSe	2·57	0–130 130–210	(000) or (111) (100)	+6·0 −2·0	4·6	0·50
ZnTe	2·26	0–45	(000) or (111)	+6·0	3·2	0·22
ZnO	3·14 (wtz) (Znbl)	0–130 130–220	(111) or (000) (111) or (000)	0·6–1·9 1·9		0·15 0·20
CdS	2·50 (wtz) 1·7 (Znbl)	0–27·5 27·5–50 50–10	(000) or (111) ? ?	+3·3 ≈0 ≈0		0·08 ≈0 ≈0

*Zero point from which shift was measured.

†More probable direction is given first in uncertain cases. Where no reference is given, the estimate is based on the direction and magnitude of the pressure shift found in this paper.

‡Slope of shift at 1 atm, or average slope after a reversal of shift direction. These are, in general, estimated for $\alpha = 20$–65 cm^{-1}, since in only a few cases are values available for $\alpha = 0$. E.g., at $\alpha = 0$ for germanium the slope is $5{\cdot}0 \times 10^{-6}$ eV/atm.[10]

§Based on bond length.

the rise of the (111) minimum in the conduction band and the lowering of the (100) minimum, relative to the maximum of the valence band. The 50:50 germanium–silicon alloy has an energy gap of 1·05 eV, due to the transition to the (100) minimum, and the (111) minimum is about 0·35 eV higher, or 1·4 eV above the valence band, according to the data of JOHNSON and CHRISTIAN[7].

The effect of increasing asymmetry in this sequence seems to be a general rise in the conduction band relative to the valence band, the rate of rise being greatest for the minimum in the (100) direction. In ZnS, the (apparent) (100) minimum is at least 0·5 eV above the lowest conduction band level, thus explaining the fact that ZnS has an initial blue shift while GaP shifts red. Following this trend, one would expect the next member of this sequence, CuCl, to have a large blue shift with pressure before the red shift which should eventually follow.

(b) Ge, GaAs *and* ZnSe

In this sequence, the bond length is between 2·43 and 2·45 Å, with a total of 32 electrons per atom. The conduction-band minimum rises relative to the valence band, with the (100)