Table 1. Observed and calculated *d*-spacings for high-pressure trigonal phase of Cd_3As_2.

from diffraction pattern at ~55 kbar				from parameters reported for retained phase[b]	
Int. (obs)	*d*(obs)	*d*(calc)[a]	*hkl*	*d*(calc)[b]	*hkl*
<0·5	3·415	3·435	20.0	3·435	00.2
<0·5	3·205	3·204	00.4	3·271	10.1
0·5	3·028	3·025	20.2		
10	2·851	2·901	10.4		
4	2·707	2·679	20.3		
<0·5	2·469	2·494	11.4	2·519	10.2
5	2·236	2·220	21.3		
8	2·015	2·018	21.4		
4	1·862	1·865	30.4	1·863	20.0
1 (broad)	1·720	1·720	40.0	1·720	00.4
0·5	1·513	1·515	40.4		
0·5	1·426	1·425	00.9	1·408	21.0
1	1·312	1·313	30.8	1·303	21.2
1	1·232	1·232	51.1	1·222	30.1

[a] Calculated from $a_0 = 7{\cdot}94$ Å, $c_0 = 12{\cdot}82$ Å.
[b] Katzman *et al.* (1968) give $a_0 = 4{\cdot}30$ Å, $c_0 = 6{\cdot}87$ Å. No line positions or intensities are given.

Table 2. Observed and calculated *d*-spacings for high-pressure phases of Zn_3As_2.

trigonal phase (est. 70 kbar)				'f.c.c.' phase (est. 55 kbar)			
Int.(obs)	*d*(obs)	*d*(calc)[a]	*hkl*	Int.(obs)	*d*(obs)	*d*(calc)[b]	*hkl*
1	3·319	3·388	10.3	10	3·417	3·419	222
4	3·157	3·153	20.0	0·5	2·988	2·961	400
10	2·644	2·702	11.3	2	2·726	2·717	331
3	2·514	2·482	20.3	8	2·097	2·090	440
5	2·078	2·052	21.3	5	1·791	1·783	622
10	1·873	1·865	30.3	2	1·478	1·479	800
5	1·726	1·728	00.7	2	1·358	1·358	662
0·5	1·615	1·622	31.3	0·5	1·309	1·299	911
0·5	1·314	1·313	10.9	4	1·205	1·208	844
1	1·218	1·218	33.0	1	1·146	1·139	1022
1	1·144	1·143	42.3				

[a] Calculated from $a_0 = 7{\cdot}27$ Å, $c_0 = 12{\cdot}08$ Å.
[b] Calculated from $a_0 = 11{\cdot}82$ Å.

The X-ray patterns for Zn_3As_2 at pressures above ~70 kbar are similar to those obtained for the high-pressure trigonal phase of Cd_3As_2. Since these pressures are attained routinely (without diamond fracture) only in the Bassett unit, they are not known to the same accuracy as the values for the gas-loaded cameras. The *d*-spacings observed in patterns obtained at an estimated 55 kbar and an estimated 70 kbar are listed in Table 2. The pattern obtained at ~70 kbar is indexed on a trigonal structure, with $a_0 = 7{\cdot}27$ Å, $c_0 = 12{\cdot}08$ Å, and $c/a = 1{\cdot}66$. As in the case of trigonal Cd_3As_2, the agreement between calculated and observed *d*-values is quite good. The calculated density, assuming $Z = 6$, is 6·2 g cm^{-3}, an increase of 11% over the tetragonal phase at one atmosphere. The pattern at ~55 kbar (Figure 4) cannot be indexed as either tetragonal or trigonal. This pattern can be indexed, with very good *d*-values, on an f.c.c. cell with $a_0 = 11{\cdot}82$ Å. However, the assignment of this structure is questionable for reasons which will be discussed below.

The positions of the reflection peaks in the Cd_3As_2 diffractometer patterns obtained at low temperatures were in good agreement among the various samples. The only difference was in the relative intensity of the peaks, particularly in the sample annealed at 1000°C with its sizable grains. The lines observed could all be accounted for by the trigonal high pressure structure determined from the X-ray

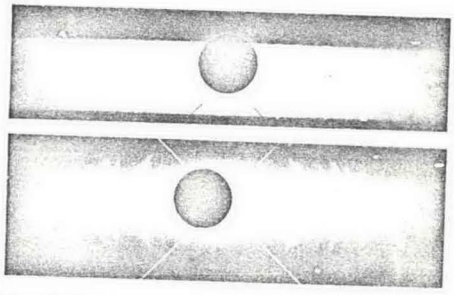

Figure 2. Diffraction patterns of Cd_3As_2 in gas-loaded diamond-anvil pressure unit: (a) tetragonal, ~20 kbar; (b) trigonal, >50 kbar.

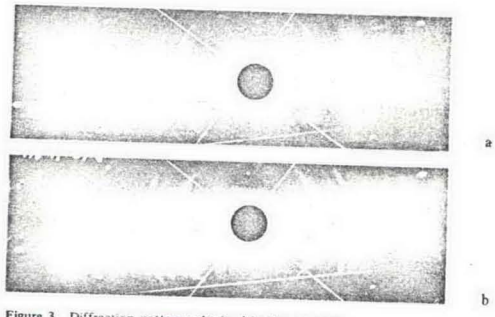

Figure 3. Diffraction patterns obtained in Bassett unit: (a) Zn_3As_2-trigonal; (b) Cd_3As_2-trigonal.

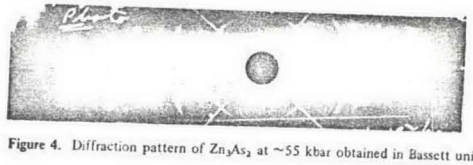

Figure 4. Diffraction pattern of Zn_3As_2 at ~55 kbar obtained in Bassett unit.