TABLE 1. X-Ray Data for the Phase Mg_2SnII at p = 70 ± 3 kbar at 25°C

hkl	*I*	d_{meas}, Å	d_{calc}, Å	*hkl*	*I*	d_{meas}, Å	d_{calc}, Å
300	s(b)	3.68	3.67	501	(b)		2.10
211			3.57	421	v w	1.99	1.96
311 + β-Sn	w-av	2.82	2.80	510	(b)		1.98
400	(b)		2.77	600	w	1.84	1.84
401	w-av	2.55	2.56	700	v w	1.59	1.57
302	(b)		2.52	522			1.58
330	w-av	2.11	2.12	630	w	1.39	1.40

Note: For Tables 1-3: s) strong; av) average; w) weak; v) very; b) broad.

with the behavior of Mg_2Sn is evidently observed for CdS [6].

It is known that Cannon et al. [7] first synthesized a new high-pressure modification of Mg_2Sn in an apparatus of the "belt" type at 30 to 65 kbar and 600 to 900°C; these experiments were also repeated by Seifert [8] who obtained this phase in a "belt" apparatus at 60-65 kbar and 600 to 1000°C. On this basis a number of experiments in a high-pressure chamber of large volume at fixed pressure and temperature (40-80 kbar, 50-1100°C) were carried out to synthesize the same metastable phase. Powder of the material to be investigated was placed in a container of stainless steel with a heater of spectrally pure graphite insulated from the container with lithographic stone. The pressure calibration was carried out using the fixed jumps in the electrical resistance of the reference metals Bi, Tl, and Ba (the pressures of the transitions are assumed equal in the NaCl scale [9]). The temperature was measured with a chromel-alumel thermocouple introduced into the high-pressure chamber. In order to avoid contaminating the product being investigated with material from the thermocouple, its junction was placed near the outer wall of the center section of the graphite heater. The time required for an experimental run varied from 20 min to several hours. Thus we could produce the metastable phase in sufficient quantity that we could determine its density pycnometrically: $\rho_e = 4.1 \pm 0.2$ g/cm^3. Annealing of the phase, just as in previous experiments, caused it to transform into the stable antifluorite phase Mg_2SnI under normal conditions.

Debye patterns of the metastable phase were made with filtered Cu, Cr, or Fe radiation in an RKU-114 camera. They contained more than 40 diffraction lines which were indexed in the hexagonal system by the method of differences. The unit-cell parameters are $a_0 = 13.18 \pm 0.02$ Å and $c_0 = 6.99 \pm 0.04$ Å.

The identical nature of the diffraction pattern of the metastable phase Mg_2Sn synthesized at 60 kbar and 900°C and the phase Mg_2SnII obtained in a high-pressure x-ray camera at 40 kbar and 400°C is illustrated in Table 2. Naturally x-ray patterns taken in high-pressure x-ray cameras contain a smaller number of reflections in comparison to ordinary Debye patterns (RKU-114) due to the substantial absorption in the boron disc.

Comparison with Cannon's data [7] (Table 3) showed that for the most part there was complete agreement of the strongest lines, but the pattern obtained in the present work is substantially richer. As seen from Table 3, the authors of [7] were generally not able to index some of the reflections to correspond to the hexagonal unit cell $a_0 = 13.09$ and $c_0 = 13.44$ Å.

Seifert [8], using his own data which were not published but according to the author are close to the data of Cannon [6] proposed that Mg_2SnII crystallizes in a rhombic structure of the Ni_2Si structure type (anti-$PbCl_2$) with parameters $a_0 = 6.25$, $b_0 = 4.82$, $c_0 = 9.14$ Å, z = 4, and $\rho_p = 4.03$ g/cm^3 with space group $D_{2h}^{16} = Pnma$.

Table 3 gives data from a comparison of the indexing in the rhombic and hexagonal systems.

The proposed rhombic model [8] gives good agreement of ρ_p and ρ_e (for the present work), but the structure of Mg_2SnII does not precisely correspond to the Ni_2Si type (the absence of extinction required by the $D_{2h}^{16} = Pnma$ space group symmetry and the presence of "extra" reflections). This model is based on crystal chemistry; actually one can think of the $PbCl_2$ structure as arising from the fluorite structure by displacement of the Cl atoms along a [111] direction. It is known that high-pressure phase transitions of the fluorite−$PbCl_2$ type are found in a number of compounds: CaF_2, SrF_2, BaF_2 [8, 10, 11], MnF_2 [11, 12], CdF_2 [11], and EuF_2 [8]. Polymorphic transitions of this kind occur with a volume jump of about 10% and are accompanied by a jump in the coordination number from 8 to 9.

On the other hand, it is known that compounds with the general formula $NaLnF_4$ and $Na(Ca, Ln)F_6$ where Ln is a lanthanide or rare earth, depending