

TABLE 3. Various Ways of Indexing the Metastable Phase Mg_2SnII

Canon's data [6]			Data from the present work					
hexagonal unit cell, $a_0 = 13.09$, $c_0 = 13.44$ Å			hexagonal unit cell, $a_0 = 13.18$, $c_0 = 6.99$ Å			rhombohedral, Ni_2Si type, Pbnm; $a_0 = 9.19$, $b_0 = 6.20$, $c_0 = 4.81$ Å		
hkl	I	d_{meas} Å	hkl	I	d_{meas} Å	d_{calc} Å	d_{calc} Å	hkl
			110	v w	6.60 ₆	6.58 ₆		
003	w	4.50						
300	av	3.80	300	v s	3.80 ₁	3.80 ₂	3.80 ₂	011 *
112	av	3.70	211	av	3.66 ₉	3.67 ₉	3.69 ₁	210
213	w	3.11	112	w	3.10 ₃	3.11 ₇	3.09 ₉	020
			$\beta\text{-Sn} + 311$	w-av	2.89 ₃	2.88 ₈	2.92 ₉	211
			400	w	2.80 ₇	2.83 ₀		
			$\beta\text{-Sn} + 212$	w	2.78 ₅	2.73 ₅	2.74 ₆	310
223	av	2.65	401	s	2.64 ₁	2.64 ₅	2.60 ₃	
320	av	2.60	302	w-av	2.58 ₄	2.59 ₃		
304	w	2.50	410	w	2.49 ₂	2.48 ₉	2.50 ₇	121
323	w	2.26	500	w	2.26 ₀	2.27 ₁	2.26 ₇	221
	av	2.20	330	s	2.19 ₆	2.19 ₅	2.18 ₀	112; 320
404	av-w	2.16	501	av	2.16 ₈	2.17 ₃	2.15 ₄	410
			331	w	2.09 ₈	2.09 ₆	2.07 ₅	401 *
			421	v w	2.05 ₀	2.05 ₄		
			412	v w	2.03 ₂	2.02 ₉		
			303	v w	2.00 ₇	2.00 ₀	2.01 ₆	130; 121
007	av-w	1.91	600	av	1.90 ₃	1.90 ₁	1.89 ₉	031 *
117	w	1.84	601	v w	1.83 ₆	1.83 ₆	1.83 ₇	500 *
521	w	1.80	004; 431	w	1.79 ₆	1.81 ₈	1.81 ₀	312
			611	w-av	1.68 ₉	1.68 ₉		
416	w	1.66	432	w	1.65 ₅	1.65 ₇	1.66 ₂	402
			700; 522	v w	1.62 ₃	1.62 ₃	1.61 ₇	322
			701	v w	1.59 ₃	1.58 ₉	1.58 ₁	103
			612; 224	av	1.55 ₉	1.56 ₂	1.55 ₃	013 *
			621; 314	v w	1.53 ₂	1.53 ₇		
			710	v w	1.51 ₁	1.51 ₀	1.51 ₅	203 *
703	av-w	1.44	630	av	1.43 ₆	1.43 ₇		
			105; 631	v w	1.40 ₉	1.40 ₈	1.40 ₈	123
			205	v w	1.38 ₄	1.37 ₈	1.38 ₄	313; 340
			712			1.38 ₉		
731	w	1.35	542; 215	v w	1.34 ₇	1.34 ₉		
			802	v w	1.32 ₂	1.32 ₃		
			640; 722	v w	1.30 ₁	1.30 ₃	1.30 ₃	042
			900	w-av		1.26 ₇	2.26 ₆	701
			405		1.26 ₉	1.27 ₁		
			812	w	1.24 ₉	1.24 ₉		
823	av	1.22	444; 732	w	1.20 ₆	1.20 ₇	1.20 ₉	503
			723	w	1.20 ₀	1.20 ₀	1.20 ₀	051 *
			714	v w	1.14 ₇	1.15 ₀		

*Forbidden reflections.

on the radius of the Ln ion, crystallize either in the fluorite-type structure with a random distribution of Na, Ca, and Ln or in a hexagonal structure of the NaNdF_4 type [13] also with a random distribution of the Na and Ln cations. Moreover, a poly-

morphic transformation from the fluorite modification into the hexagonal NaNbF_4 type has been found at high pressures for NaYbF_4 [8]. It is also known that the compounds NaYF_4 [14, 15], NaHoF_4 , and NaErF_4 [16] are dimorphous with the high-temper-