S. GELLER, A. JAYARAMAN and G. W. HULL, Jr.

Table 3. Powder pattern for In₃Te₄ (CuKa radiation)

		d (Å)		Rel. I			d (Å)		Rel. I	
hk·l		obs.	calc.	obs.	calc.	hk•l	obs.	calc.	obs.	cale.
	00.3	13.5	13.53	· VW	60	12.17	1.205	1.203	VW	32
	00.6	6.78	6.79	VVW	20	11.30	1.142	1.142	VVW	23
	00.9	4.50	4.51	VW	65	02.31)		(1.068		(24
	00.12	3.386	3.382	VW	71	22.0	1.066	1.065	$W-M^*$	42
	10.7	3.093	3.110	VVS	1250	11.33)		1.065		1
	01.8	3.006	2.992	VW	39	30.21)		(1.037		(11
	10.10	2.729	2.732	W	76	03.21	1.039	1.037	VW	11
	01.14	2.272	2.278	M-S	342	22.9		1.036		15
	11.0	2.128	2.128	S	463	13.7	1.008	1.008	W-M	65
	11.3)		(2.109	777	(35	11.36)		(0.9963		(18
	10.16	2.098	2.097	W	65	30.24	0.9955	0.9945	W^*	134
	01.17	2.003	2.004	W-M	97	03.24)		0.9945		34
	00.21)		(1.932		(34	31.14	0.9648	0.9649	W	40
	11.9	1.934	11.935	W-M	137	21.31	0.9554	0.9544	W	40
	10.19	1.860	1.848	VVW	15	10.43		(0.9143	100 M	/12
	11.12)		(1.801	*****	(32	31.20		0.9136		5
	20.5	1.800	1.797	VW	6	40.7	0.9127	(0.9109	VW^*	130
	02.7	1.754	1.756	M-S	215	30.30		0.9100		6
	00.24	1.691	1.691	VW	33	03.30)		0.9100		6
	01.23	1.587	1.591	VW	35	00.45)		(0.9018	TTTTT	(3
	20.14	1.555	1.555	W-M	93	22.24	0.9021	0.9011	VW+	132
	· 20·17	1.458	1.459	VW	32	04.14	0.8785	0.8789	VW^*	19
	11.21	1.431	1.431	W	69	12.38	0.8491	0.8478	W*	38
	21.7)		(1.354		(166	01.47		10.8407		124
	00.30	1.355	1.353	M-S	5	02.43		0.8402		27
	10.28		1.349		10	04.20	0.8388	0.8396	M^*	1 3
	12.14	1.255	1.256	W-M	83	32.7		0.8375		69
	10.31)		(1.234		(38	22.30)		0.8368		14
	00.33	4 004	1.230	3.54	3	23.14	0.8130	0.8125	W^*	54
	30.0	1.231	1.229	· MT	66	13.31)	0.004	(0.8062	7 54	(60
	11.27		1.228		8	41.0	0.8064	0.8051	M^*	105
	2.)		1		10	0)		1		1200

* Broad line.

the powder photograph. The lattice constants determined from the powder photograph (CuK α radiation) are $a = 4.26 \pm 0.01$, $c = 40.6 \pm 0.1$ Å or in the rhombohedral description $\alpha = 13.75$ Å, $\alpha = 17.80^{\circ}$. The powder pattern indexed on the hexagonal basis is given in Table 3. Shown also are qualitatively estimated intensities and those calculated* from

$I_{\rm rel} = p |F|^2 \times 10^{-5} L \cdot P$

where p is the multiplicity, F, the structure factor

* The program used was originally derived by TREUT-ING⁽²⁰⁾ for the IBM 704 and modified for the IBM 7094 by N. V. Vaughan and A. R. Storm. and $L \cdot P$ the Lorentz-polarization factor. The positional parameters were those obtained from the single crystal analysis, and because the program* allows only individual isotropic temperature factors, In(1) and Te(2) were assigned values of 0.5 Å² and In(2) and Te(1) values of 1.0 Å².†

When this pressure-induced In_3Te_4 phase was heated at 200°C in an evacuated sealed fused silica tube for 67 hr, it decomposed into a mixture of the atmospheric pressure In_2Te_3 phase and an NaCltype phase with composition (determined from the

[†] Differences in vibration amplitudes of the atoms were indicated by the results from the single crystal analysis.

CRYSTAL

lattice const appears to f under a pre pressure rele NaCl-type a probable th contains exco The press conductor. T a transition tivity of this tion on the 1

SOME RESU

The press determined 1 the subject o we discuss t obtained afte and tempera leased. The difficult to un It appears In2Te3 phase known Bi2Te ably as a sing discern the patterns, be In₃Te₄-type tures of the t belong to th atoms on th In₃Te₄ has t Te-In-, divi in approxim must have tl dividing the approximatel two phases a one would ex (threefold ax In3Te4 is ve constants of

358