TABLE 1

Observed and Calculated d-apacings and Unit Cell Dimensions of $BaWO_4$-II

h	k	l	d_{obs}	d_{calc}	I_{obs}
2	0	0	6.588	6.565	M
0	1	1	5.188	5.174	VW
$\bar{2}$	1	1	4.163	4.154	M
2	1	1	3.980	3.977	VW
0	2	0	3.582	3.581	VW
$\bar{2}$	0	2	3.349	3.346	S
4	0	0	3.284	3.283	S
0	2	1	3.232	3.230	S_-
2	0	2	3.162	3.163	S_+
$\bar{1}$	2	1		3.157	
4	1	0	2.985	2.984	M
$\bar{2}$	2	1	2.933	2.931	M_-
2	1	2	2.895	2.893	M_-
2	2	1	2.868	2.866	M
$\bar{4}$	1	1	2.831	2.830	M_-
4	1	1	2.717	2.717	W
3	2	1	2.565	2.564	W
$\bar{5}$	1	1	2.387	2.386	VW
$\bar{4}$	2	1	2.336	2.336	W

$a=13.159\pm0.012$Å , $b=7.161\pm0.003$Å , $c=7.499\pm0.006$Å
$\beta=93.76\pm0.05°$, $V=705.2\pm1.0$Å^3 , $Z=8$
Space group ; $P2_1/n$

these patterns as depicted in Fig.1, between the wolframite structure($CdWO_4$) and the present high pressure $BaWO_4$ and also $PbWO_4$ of high pressure form. In the figure, I and II stand for the high pressure forms of $BaWO_4$ and $PbWO_4$, respectively, and III for $CdWO_4$. The pattern of $PbWO_4$ is similar to that of $BaWO_4$. These patterns strongly suggest that the structure of high pressure $BaWO_4$ is different from the wolframite one. We, therefore, tentatively name the present high pressure product as $BaWO_4$-II.

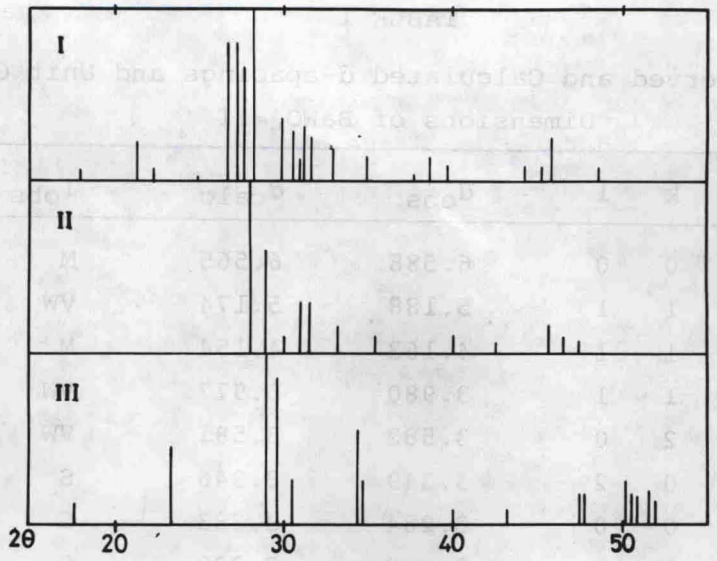

FIG. 1

Comparison between the powder patterns (CuKα) of $BaWO_4$-II, high pressure form of $PbWO_4$ (3) and the wolframite structure ($CdWO_4$) (6).

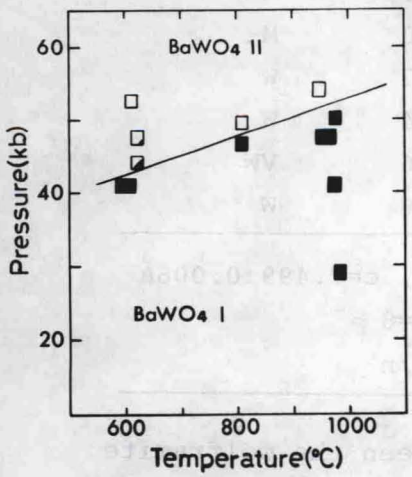

FIG. 2

Pressure-Temperature diagram of $BaWO_4$

These statements are further confirmed by the structure analysis based on the four circle goniometer data. Although the details of the structure will be reported in a separate paper, it is worthwhile noting here that the average coordination number of the cations has increased as compared with that of either the wolframite- or the scheelite-structure.

Although $BaWO_4$-II was quenchable as described above, this was completely transformed to $BaWO_4$-I upon heating in air at 800°C. This suggests that the transformation is reversible.

Phase diagram: Throuout the entire experimental runs, the product was always either a mixture of the I and II forms or a single phase of the respective one. This enables us to establish