

TABLE 1
Observed and Calculated d-spacings and Unit Cell
Dimensions of BaWO₄-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		3.163	
$\bar{1}$	2	1	3.162	3.157	S ₊
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

$$a=13.159\pm 0.012\text{\AA}, b=7.161\pm 0.003\text{\AA}, c=7.499\pm 0.006\text{\AA}$$

$$\beta=93.76\pm 0.05^\circ, V=705.2\pm 1.0\text{\AA}^3, Z=8$$

Space group ; P2₁/n

these patterns as depicted in Fig.1, between the wolframite structure (CdWO₄) and the present high pressure BaWO₄ and also PbWO₄ of high pressure form. In the figure, I and II stand for the high pressure forms of BaWO₄ and PbWO₄, respectively, and III for CdWO₄. The pattern of PbWO₄ is similar to that of BaWO₄. These patterns strongly suggest that the structure of high pressure BaWO₄ is different from the wolframite one. We, therefore, tentatively name the present high pressure product as BaWO₄-II.

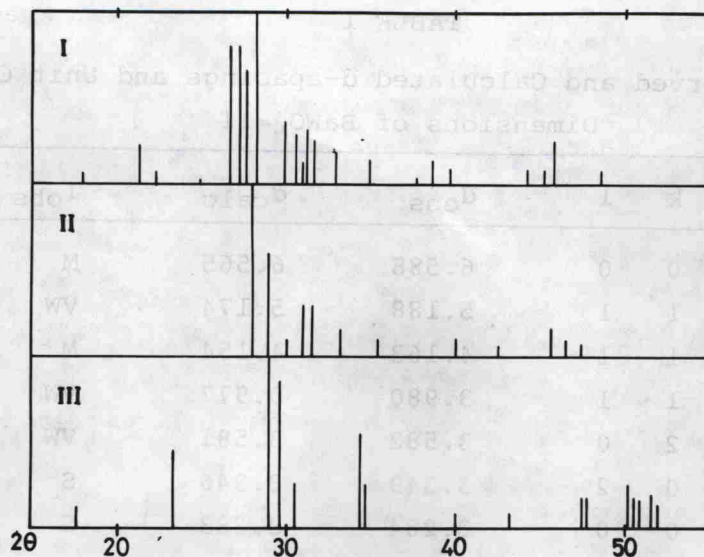


FIG. 1

Comparison between the powder patterns ($\text{CuK}\alpha$) of BaWO_4 -II, high pressure form of PbWO_4 (3) and the wolframite structure (CdWO_4) (6).

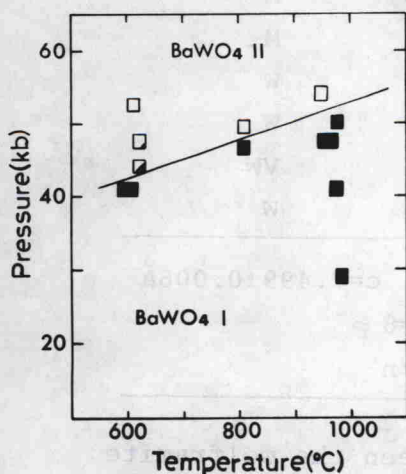


FIG. 2

Pressure-Temperature diagram of BaWO_4

suggests that the transformation is reversible.

Phase diagram: Throughout 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

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