TABLE 1

X-Ray Data on Forms of Li_3BN_2

Li_3BN_2(3) (1 atm. form)		Li_3BN_2* (1 atm. form)		Wentorf's phase(2) (quenched from high pressure)		Li_3BN_2(W)* (quenched from high pressure)	
d(Å)	I/I_o	d(Å)	I/I_o	d(Å)	I/I_o	d(Å)	I/I_o
3.81	m	3.73	10	5.60	m	5.57	20
				3.60	s	3.61	70
3.50	s	3.47	50	3.50	mw		
		3.27	10	3.34	mw		
2.82	vs	2.78	100	3.25	w	3.28	5
		2.67	20	3.08	ms	3.06	45
2.63	s	2.63	30	2.85	w	2.84	15
				2.78	s	2.78	100
2.24	w	2.22	5	2.67	m	2.67	40
				2.56	mw	2.59	15
2.07	vs	2.07	15	2.50	mw	2.50	5
		2.05	25	2.35	w		
1.93	w	1.91	5	2.25	m	2.27	10
				2.15	ms	2.15	10
1.83	vw			2.07	vw		
				2.03	m	2.03	15
1.74	m	1.74	10	1.96	w	1.97	5
		1.69	5	1.92	w	1.93	5
1.64	vs	1.64	20	1.85	mw	1.85	15
		1.63	10	1.73	mw	1.74	5
1.55	m	1.55	10	1.68	vw	1.69	5
				1.64	m	1.65	10
1.48	w			1.62	m	1.63	10
				1.60	m	1.61	5
1.42	w			1.53	m		
				1.50	vw		
1.40	w			1.44	w		
				1.41	w		

* X-ray results from present study; data taken on GE x-ray diffractometer with CrKα radiation; s=strong; m=medium; w=weak; v=very. Additional weak lines at smaller d-spacings are found in published data from references (2) and (3).

that of Li_3AlN_2 and the other members of an isomorphous series(6) formed by substitutions for Al^{3+} and for N^{3-}. Since the structures of these compounds are based on an anti-CaF_2 lattice (i.e., N^{3-} in Ca^{2+} sites), compression along <111> could result in a layer lattice of hexagonal symmetry with layers of close-packed N^{3-} ions perpendicular to the hexagonal "c" axis.

The lath-like morphology of this form is best developed between 1000°C and 1400°C above 40 kb. Quenched runs from the liquid region above the melting curve of the high pressure form are characterized by fine-grained clusters of equant crystals, and the x-ray patterns differ somewhat in peak intensity from those of crystals quenched from the stability region of the phase. These differences appear to be related to a more random orientation obtained when preparing an x-ray slide with the material quenched from the liquid.

Li_3BN_2(W) is also markedly less soluble in water at room temperature than the low pressure form.

Results and Discussion

General

Our interpretation of the results is summarized in the P-T representation of Fig. 2 in which a large area of stability of Li_3BN_2(W) exists. Some aspects of this interpretation need amplification.

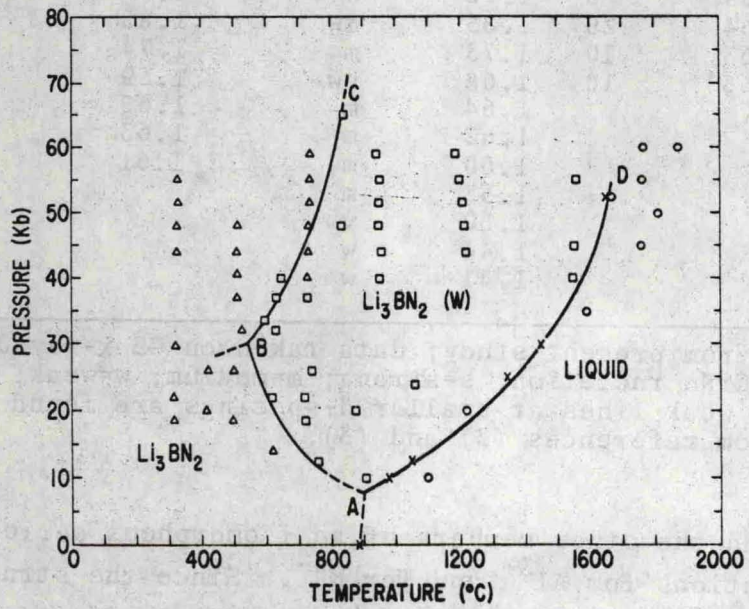

FIG. 2
P-T Diagram for the System Li_3BN_2 Quench data indicated by △,□,○; thermal analysis data by x

A clean separation of a homogeneous sample from the center of a cell in which a temperature gradient existed was sometimes difficult to obtain. Particularly near the P-T conditions where