

Supporting Information for

Enhancement mechanism of electron-phonon coupling in XB_3 (X = K, Rb) compounds with Kagome lattice

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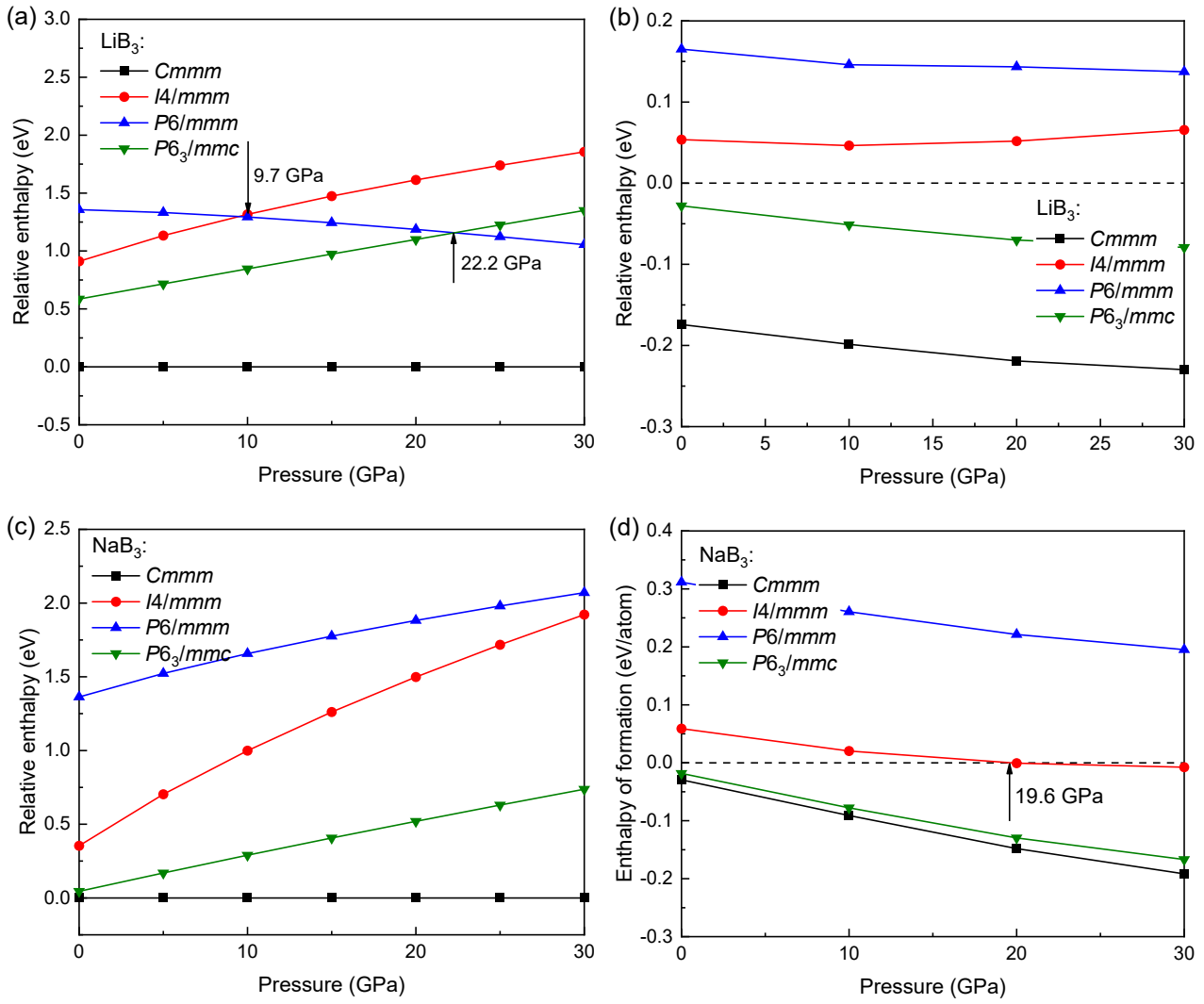
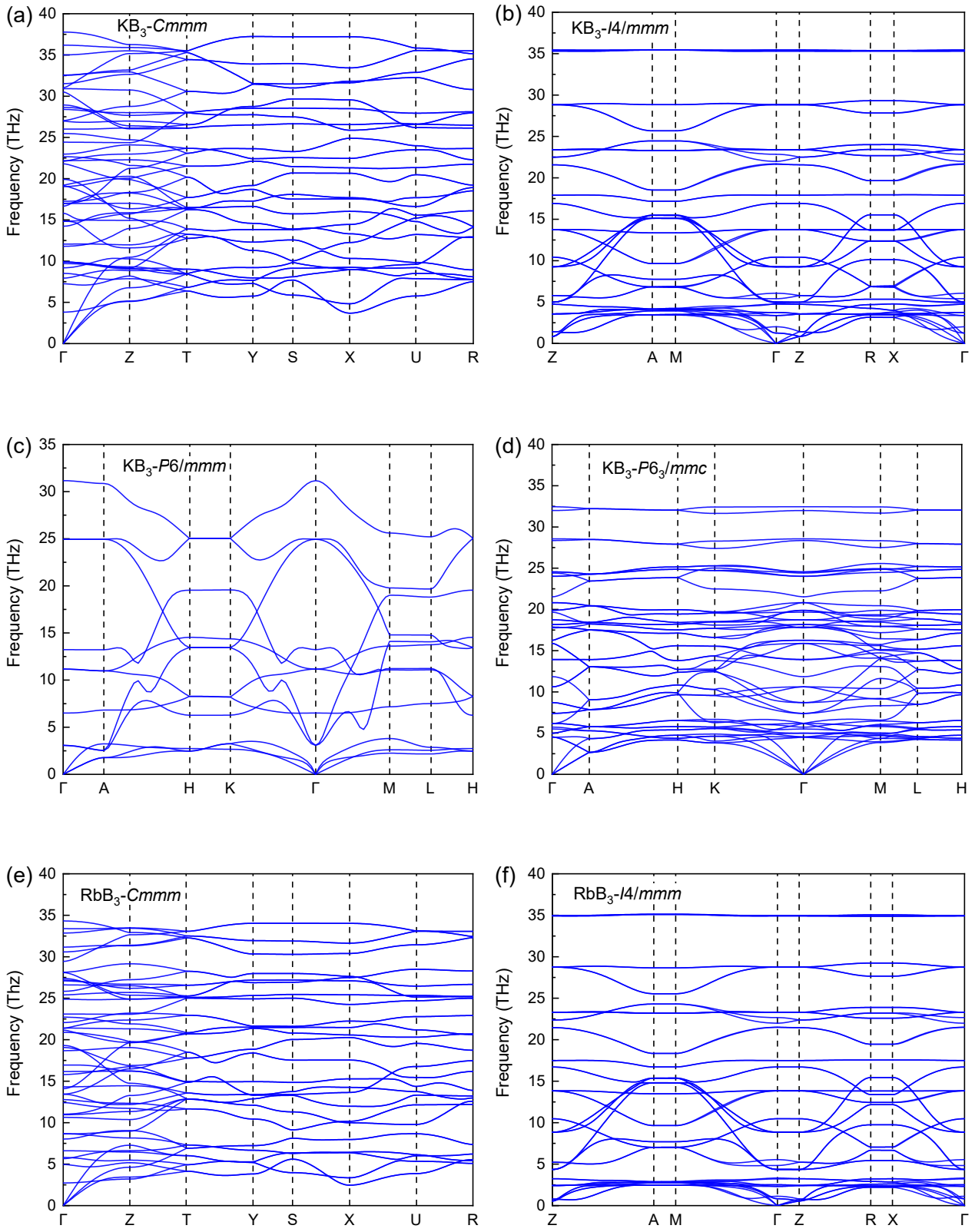


Fig. S1 Calculated phase transition pressures versus formation enthalpies for *Cmmm*, *I*4/*mmm*, *P*6/*mmm*, and *P*6$_3$/*mmc* phases for LiB_3 and NaB_3 compounds in the range of 0-30 GPa, where (a)-(b) are LiB_3 compounds and (c)-(d) are NaB_3 compounds.


(a)
KB3-Cmmm
Frequency (THz)
Γ Z T Y S X U R
(b)
KB3-I4/mmm
Frequency (THz)
Z A M Γ Z R X Γ
(c)
KB3-P6/mmm
Frequency (THz)
Γ A H K Γ M L H
(d)
KB3-P63/mmc
Frequency (THz)
Γ A H K Γ M L H
(e)
RbB3-Cmmm
Frequency (Thz)
Γ Z T Y S X U R
(f)
RbB3-I4/mmm
Frequency (THz)
Z A M Γ Z R X Γ

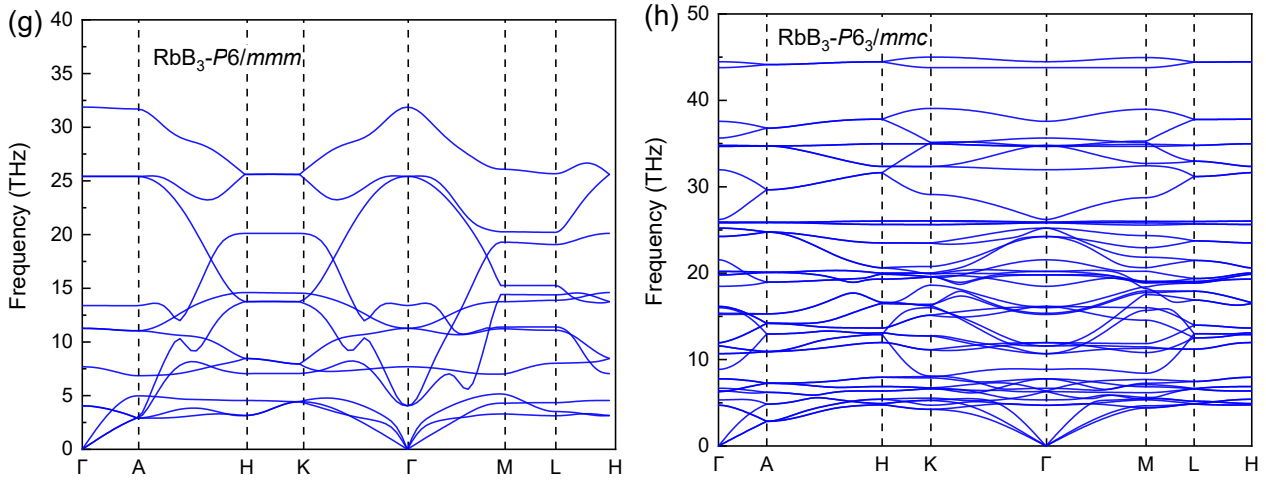
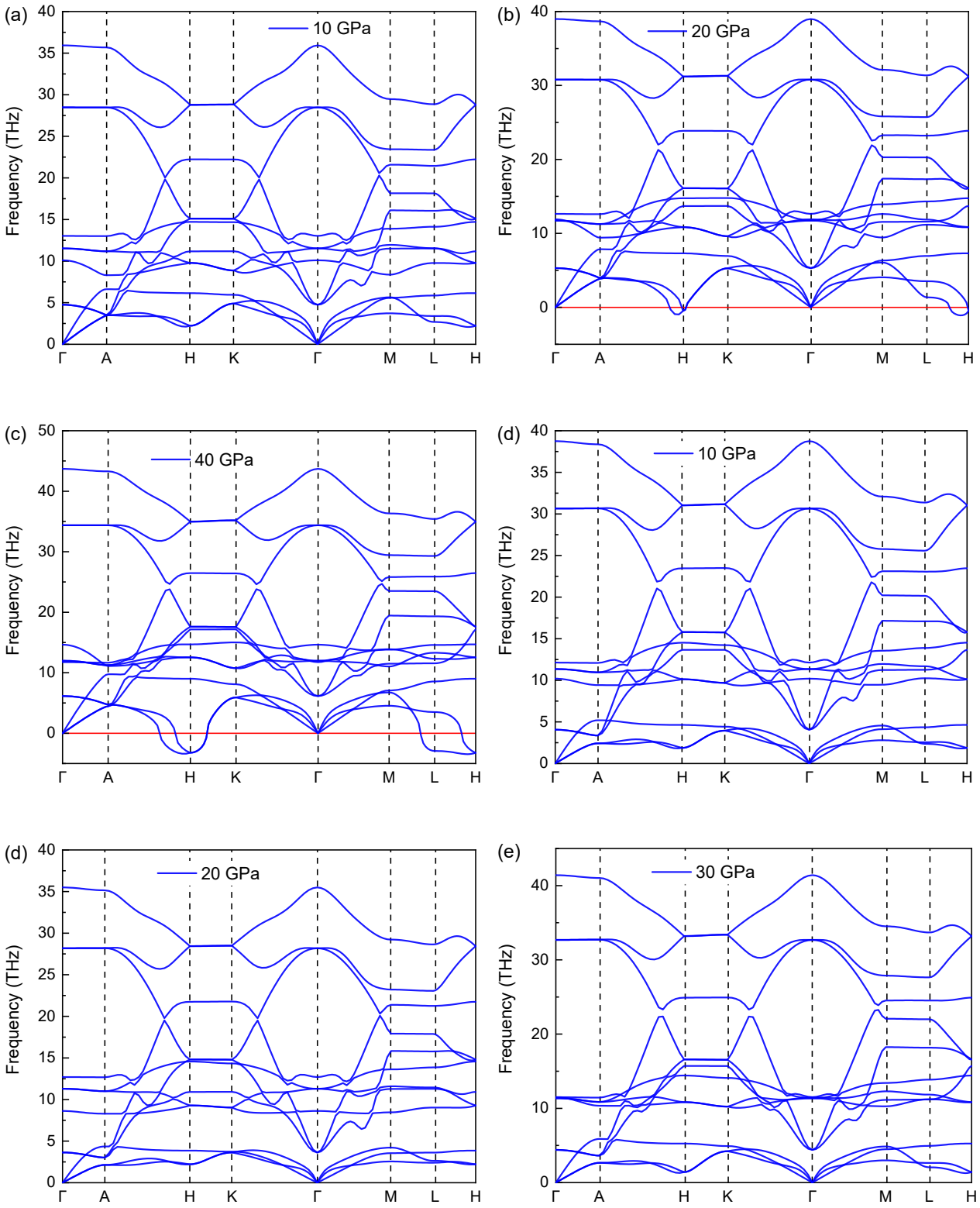


Fig. S2 Phonon dispersion curves of four structures *Cmmm*, *I*4/*mmm*, *P*6/*mmm*, and *P*6$_3$/*mmc* of KB_3 and RbB_3 compounds were calculated in the range of 0-30 GPa, where (a)-(e) are 30 GPa, (b)-(f) are 0 GPa, (c)-(g) are 0 GPa, and (d)-(h) are 0 GPa.


(a)
10 GPa
(b)
20 GPa
(c)
40 GPa
(d)
10 GPa
(d)
20 GPa
(e)
30 GPa
Frequency (THz)
Γ A H K Γ M L H

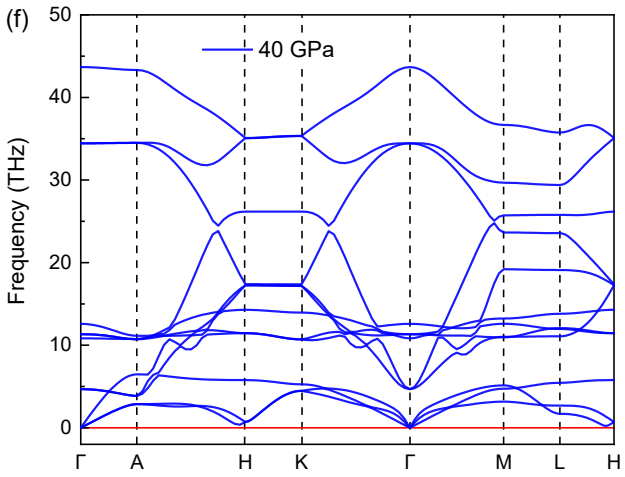


Fig. S3 Phonon dispersion curves of *P*6/*mmm* of KB_3 and RbB_3 compounds were calculated in the range of 10-40 GPa, where (a)-(c) are KB_3 compounds and (d)-(f) are RbB_3 compounds.

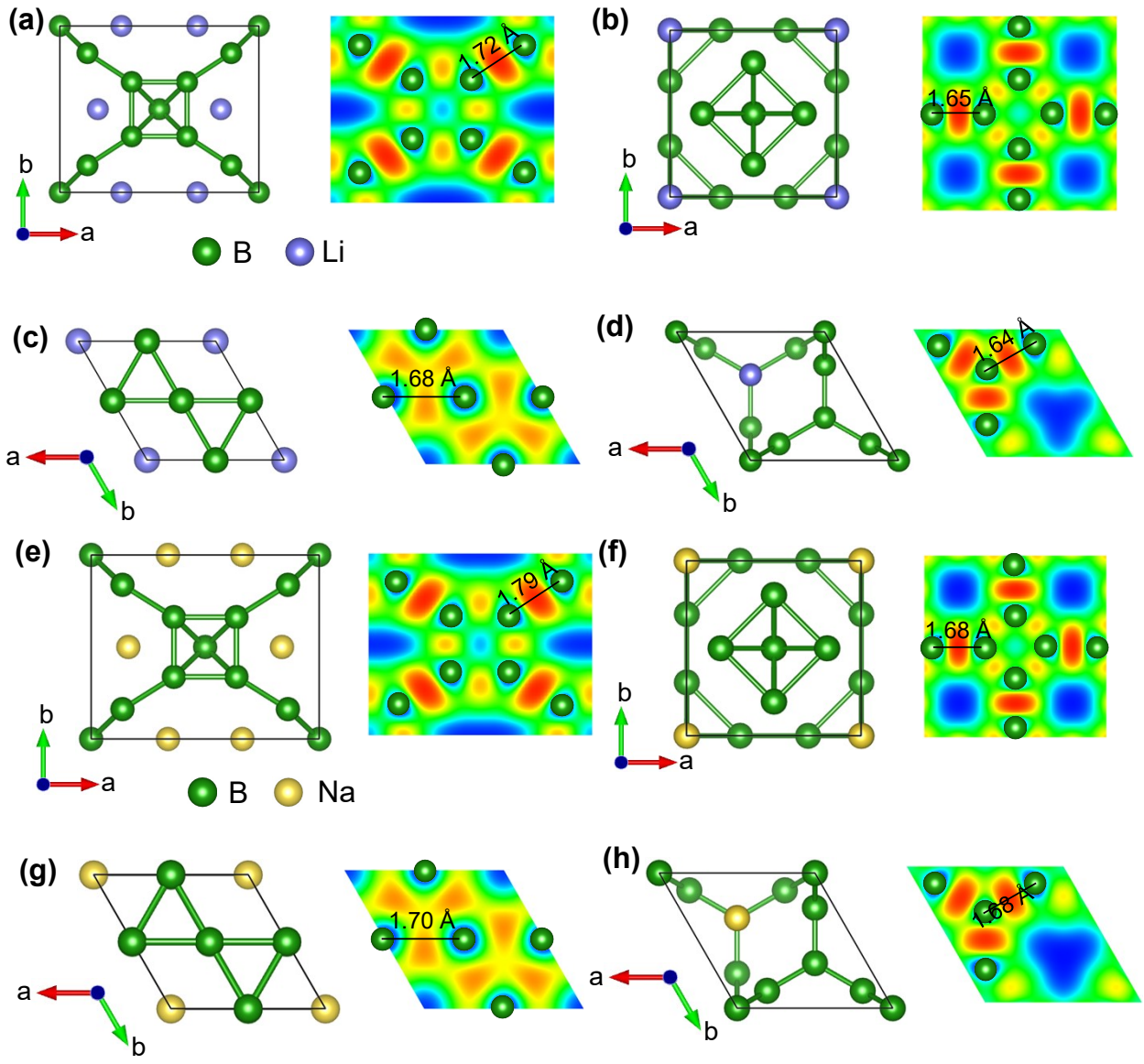


Fig. S4 Crystal structure of XB_3 (X = Li, Na) compounds along the (001) plane at 0 GPa with electron localization function (ELF). (a) *Cmmm*, (b) *I*4/*mmm*, (c) *P*6/*mmm*, and (d) $P6_3/mmc$ phases.

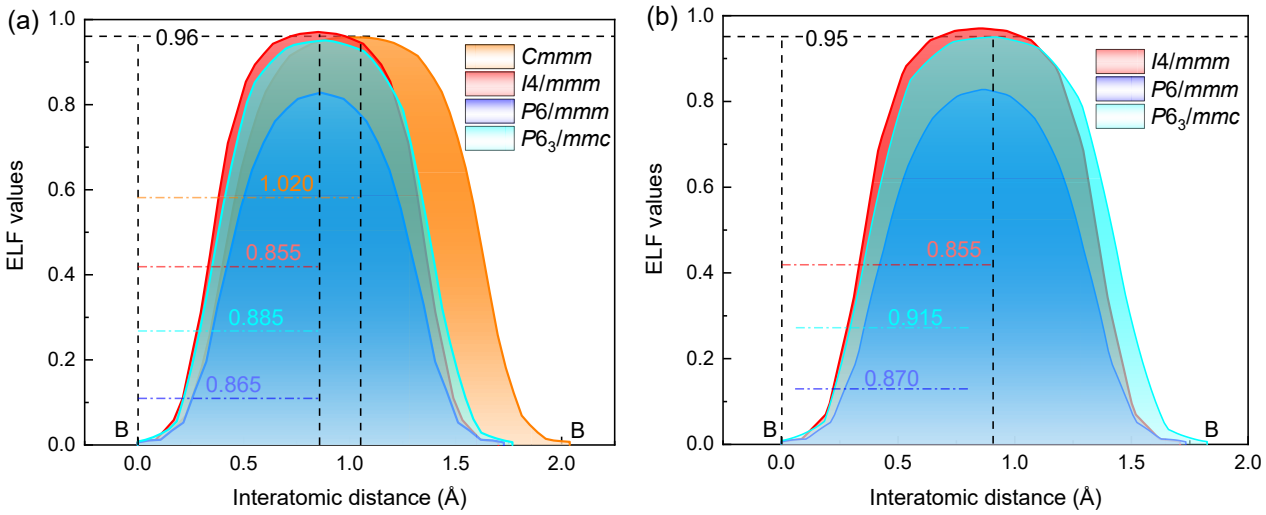


Fig. S5 Variation of ELF values of XB_3 (X = K, Rb) compounds along the (001) crystallographic plane with respect to the distance between B-B atoms at 0 GPa.

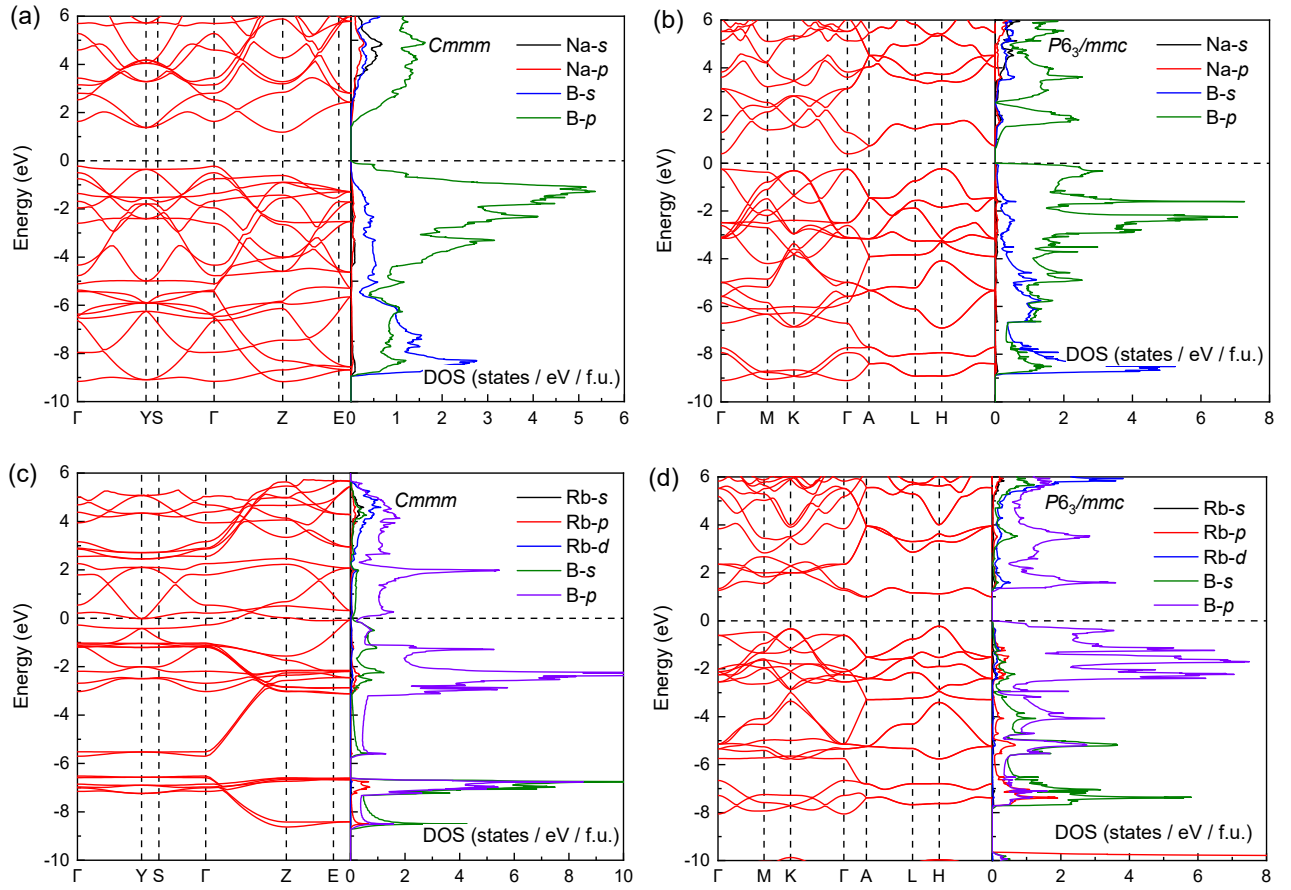


Fig. S6 Energy bands of the LiB_3 and NaB_3 system at 0 GPa using VASP package, (a) LiB_3-*Cmmm*, (b) LiB_3-*P*6_3/*mmc*, (c) NaB_3-*Cmmm* and (d) NaB_3-*P*6_3/*mmc*.

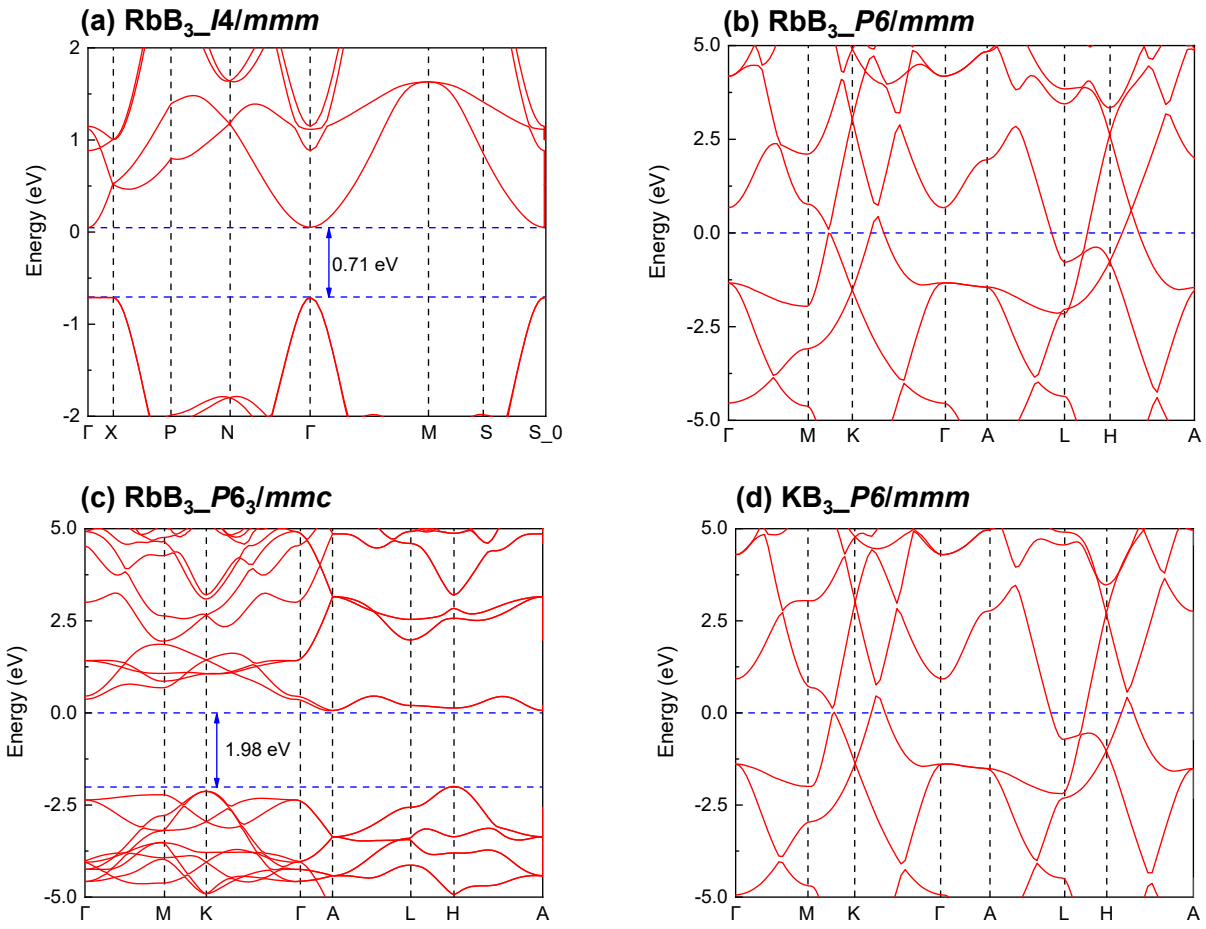


Fig. S7 Energy bands of KB_3 and RbB_3 compounds at 0 GPa calculated using the HSE06 method for (a) RbB_3_*I*4/*mmm*, (b) RbB_3_*P*6/*mmm*, (c) RbB_3-*P*6_3/*mmc*, and (d) KB_3_*P*6/*mmm*.

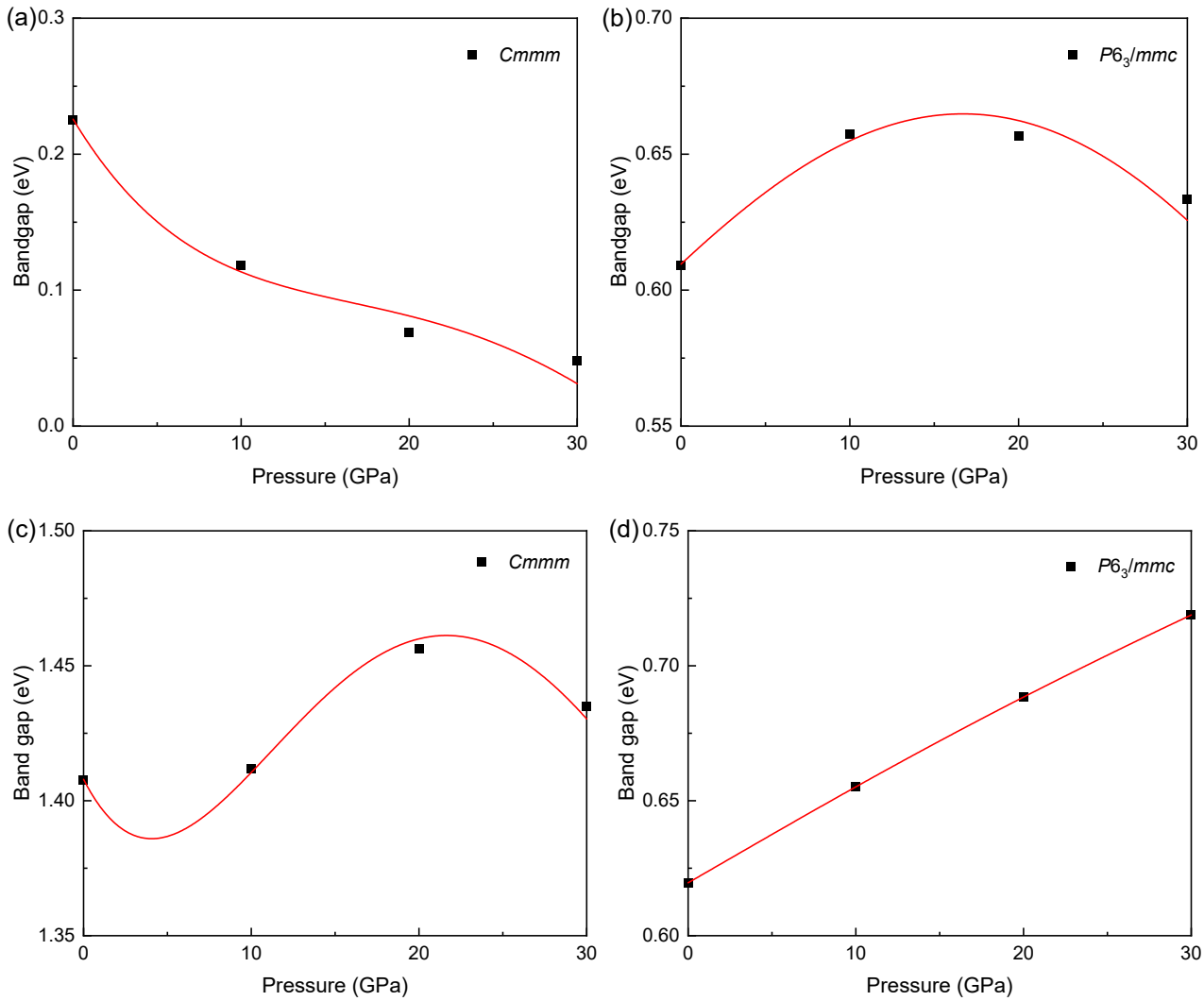


Fig. S8 Variation of the bandgap with pressure for the *Cmmm* and $P6_3/mmc$ phases in the XB_3 (X = Li, Na) systems calculated using VASP package in the range 0-30 GPa, and the curves represent the fitted data.

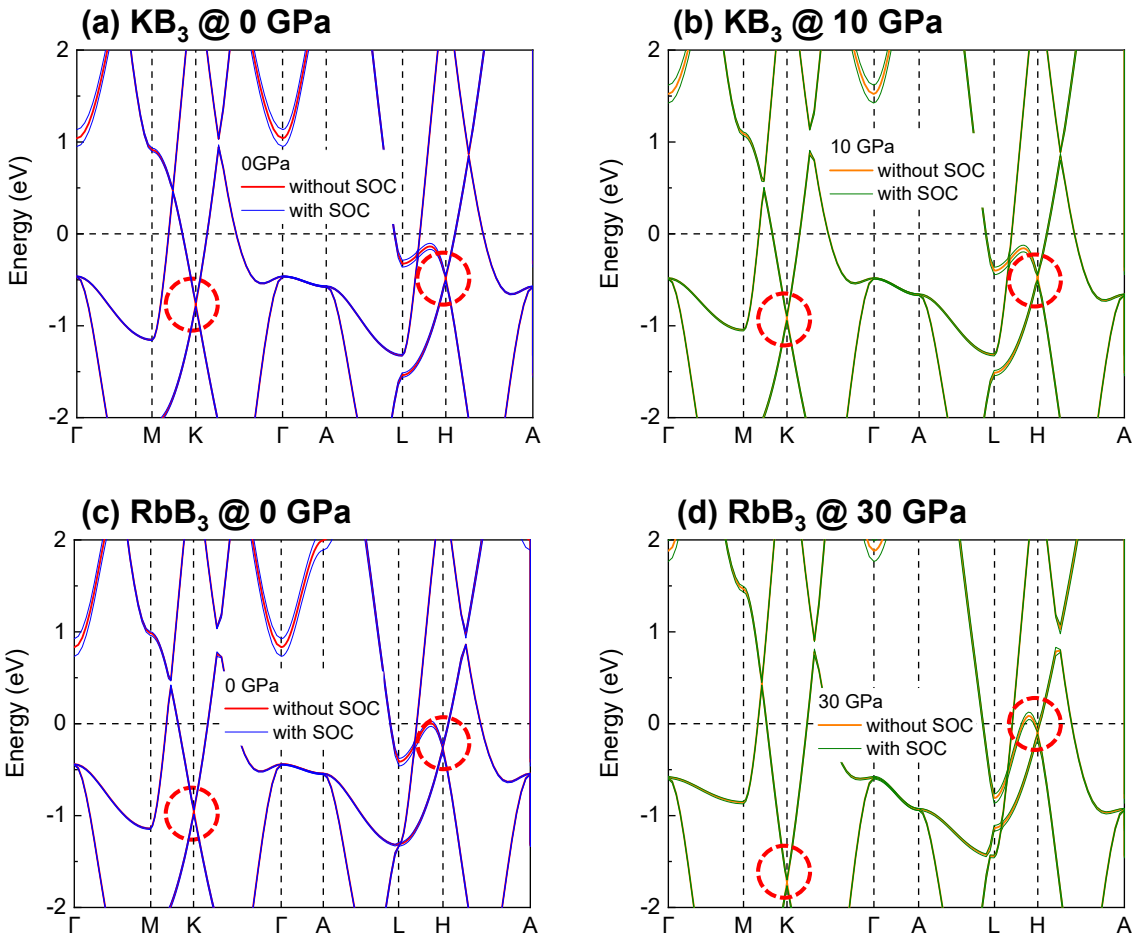


Fig. S9 Energy bands of the *P*6/*mmm* phase for KB_3 and RbB_3 compounds are calculated with and without SOC using HSE06 method. (a) KB_3 at 0 GPa, (b) KB_3 at 10 GPa, (c) RbB_3 at 0 GPa, (d) RbB_3 at 30 GPa.

Table S1. Lattice constants of the *Cmmm*, *I*4/*mmm*, and *P*6$_3$/*mmc* phases of the KB_3 and RbB_3 compounds using the PBE and HSE06 approaches.

Method	Lattice parameters (Å)	KB_3			RbB_3		
		*I*4/*mmm*	*P*6/*mmm*	*P*6$_3$/*mmc*	*I*4/*mmm*	*P*6/*mmm*	*P*6$_3$/*mmc*
PBE	*a*	4.356	3.454	4.956	4.374	3.467	5.087
	c	13.106	5.134	8.906	14.243	5.447	9.039
HSE	*a*	4.339	3.439	4.941	4.362	3.455	5.077
	c	13.075	5.130	8.870	14.235	5.447	9.013

Table S2. Lattice parameters, atomic coordinates, and equivalent isotropic displacement parameters of the predicted Na-Si phases as well as LiB_3, NaB_3, CsB_3, $LiSi_3$, $LiGe_3$, and $NaGe_3$ for *P*6/*mmm* phases.

Compounds & Pressures	Lattice parameters (Å, °)	Wyckoff positions	*x*	*y*	*z*
KB_3	a = 5.64720 α = 90	K1 (4j)	0.50000	0.83146	0.50000
Cmmm	b = 7.30980 β = 90	B1 (8p)	0.15696	0.86945	-0.00000
(0 GPa)	c = 4.45340 γ = 90	B2 (4k)	0.50000	0.50000	0.28383
KB_3	a = 4.35640 α = 90	K1 (4e)	0.50000	0.50000	0.65481
*I*4/*mmm*	b = 4.35640 β = 90	B1 (8j)	0.69533	-0.00000	0.50000
(0 GPa)	c = 13.1061 γ = 90	B2 (4e)	0.00000	0.00000	0.58164
KB_3	a = 3.45400 α = 90	K (1b)	0.00000	0.00000	0.50000
*P*6/*mmm*	b = 3.45400 β = 90	B (3f)	0.50000	0.00000	0.00000
(0 GPa)	c = 5.13350 γ = 120				
KB_3	a = 4.95570 α = 90	K1 (4f)	0.66667	0.33333	0.06771
*P*6$_3$/*mmc*	b = 4.95570 β = 90	B1 (2c)	0.66667	0.33333	0.75000
(0 GPa)	c = 8.90760 γ = 120	B2 (6h)	0.12738	0.25476	0.25000
		B3 (4e)	0.00000	0.00000	0.59817
RbB_3	a = 6.58440 α = 90	Rb1 (4j)	0.50000	0.82703	0.50000
Cmmm	b = 9.64350 β = 90	B1 (8p)	0.12783	0.91233	-0.00000
(0 GPa)	c = 4.33410 γ = 90	B2 (4k)	0.50000	0.50000	0.30509
RbB_3	a = 4.37410 α = 90	Rb1 (4e)	0.50000	0.50000	0.65468
*I*4/*mmm*	b = 4.37410 β = 90	B1 (8j)	0.69529	-0.00000	0.50000
(0 GPa)	c = 14.2426 γ = 90	B2 (4e)	0.00000	-0.00000	0.57477
RbB_3	a = 3.46690 α = 90	Rb (1b)	0.00000	0.00000	0.50000
*P*6/*mmm*	b = 3.46690 β = 90	B (3f)	0.50000	0.00000	0.00000
(0 GPa)	c = 5.44670 γ = 120				
RbB_3	a = 5.08660 α = 90	Rb1 (4f)	0.66667	0.33333	0.06748
*P*6$_3$/*mmc*	b = 5.08660 β = 90	B1 (2c)	0.66667	0.33333	0.75000
(0 GPa)	c = 9.03880 γ = 120	B2 (6h)	0.12624	0.25248	0.25000
		B3 (4e)	0.00000	0.00000	0.59977