Supplementary Materials

Exploration of AB_3Si_3 (A = Na/ K/ Rb/ Cs) Compounds under Moderate Pressure

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Table S1. The related materials used to compute formation energies of AB_3Si_3 (A = Na/ K/ Rb/ Cs) compounds.

Elemental materials	Space group	Pressure range (GPa)
Na	*Im*-3*m*	0 - 58.9
	Fm-3*m*	58.9 - 100
K	*Im*-3*m*	0 - 12.5
	Fm-3*m*	12.5 - 21.9
	$P6_3/mmc$ (*hP*4)	21.9 - 34.2
	Pnma (*oP*8)	34.2 - 45.3
	$I4_1/amd$	45.3 - 84.8
	Cmca	84.8 - 100
Rb	*Im*-3*m*	0 - 8.2
	Im-3*m*	8.2 - 15.1
	$I4_1/amd$	15.1 - 41.0
	Cmca	41.0 -100
Cs	*Fm*-3*m*	0 - 3.6
	$I4_1/amd$	3.6 - 10.7
	Cmca	10.7 - 49.5
	$P6_3/mmc$ (*dhcp*)	49.5 - 100
B	*R-3m*	0 - 17.7
	Pnnm (*γ*-B)	17.7 - 91.3
	Cmca (*α-Ga*)	91.3 -100
Si	*Fd*-3*m* (*dia-Si*)	0 - 8.9
	Imma	8.9 - 40.0
	$P6_3/mmc$ (*hcp*)	40.0 - 83.9
	Fm-3*m*	83.9 - 100

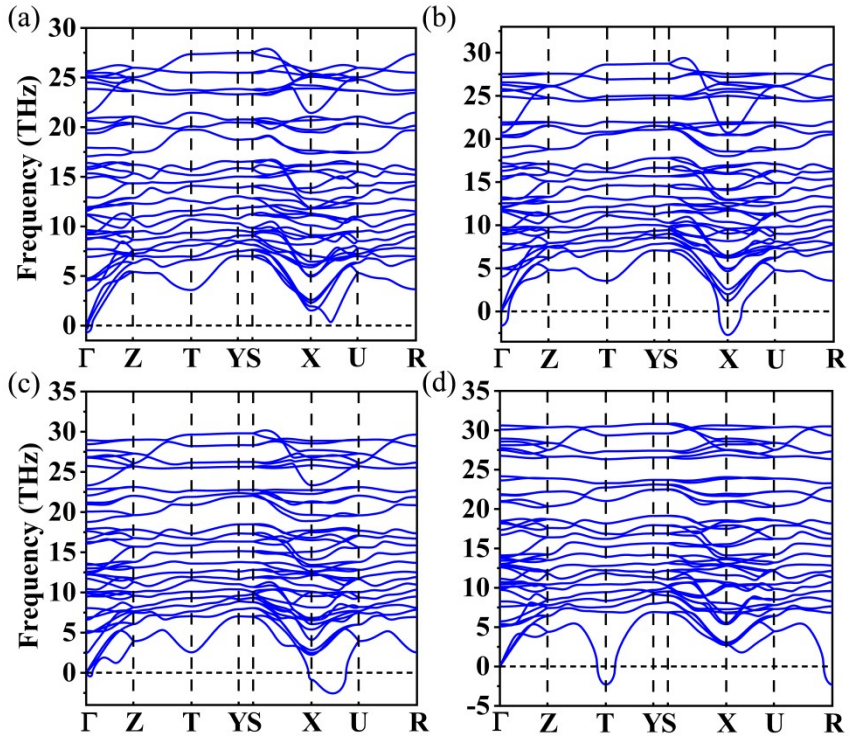

Fig. S1 Phonon dispersion curves of *Pmn*2$_1$ phase of NaB_3Si_3 compound at (a) 30 GPa, (b) 40 GPa, (c) 50 GPa and (d) 60 GPa.

Structural files

Below we provide POSCAR files for AB_3Si_3 (A= Na / K / Rb / Cs) compound calculations at ambient pressure.

1. *Pmn*2$_1$ structure of NaB_3Si_3

1.0

3.1777999401	0.0000000000	0.0000000000
0.0000000000	12.6159000397	0.0000000000
0.0000000000	0.0000000000	4.1154999733

Na	B	Si
2	6	6

Direct

0.500000000	0.238409996	0.107359998
0.000000000	0.761590004	0.607360005
0.500000000	0.413819999	0.402500004
0.000000000	0.586179972	0.902500033
0.000000000	0.907729983	0.185519993
0.500000000	0.092270017	0.685519993
0.000000000	0.153709993	0.554210007
0.500000000	0.846289992	0.054210007
0.500000000	0.934740007	0.549989998

0.000000000	0.065259993	0.049989998
0.000000000	0.327080011	0.601149976
0.500000000	0.672919989	0.101149976
0.000000000	0.436010003	0.084729999
0.500000000	0.563989997	0.584730029

2. *C*2/*m* structure (primitive cell) of NaB_3Si_3

1.0

9.6933002472	0.0000000000	0.0000000000
8.5238555905	4.6156208200	0.0000000000
-0.4809841336	-0.1218653670	4.7624217992

Na	B	Si
2	6	6

Direct

0.300320029	0.300320029	0.229259998
0.699679971	0.699679971	0.770740032
0.575260043	0.218259990	0.702759981
0.781740010	0.424739987	0.297240019
0.424739987	0.781740010	0.297240019
0.218259990	0.575260043	0.702759981
0.518769979	0.518769979	0.345099986
0.481229991	0.481229991	0.654900014
0.102469981	0.102469981	0.568970025
0.897530019	0.897530019	0.431029975
0.863460004	0.863460004	0.946120024
0.136539996	0.136539996	0.053879976
0.758310020	0.241689980	0.000000000
0.241689995	0.758310020	0.000000000

3. *Imm*2 structure of NaB_3Si_3

1.0

3.4839999676	0.0000000000	0.0000000000
0.0000000000	8.6724004745	0.0000000000
0.0000000000	0.0000000000	6.0082001686

Na	B	Si
2	6	6

Direct

0.500000000	0.000000000	0.670570016
0.000000000	0.500000000	0.170570016
0.000000000	0.000000000	0.366939992
0.500000000	0.500000000	0.866940022
0.000000000	0.813730001	0.486710012
0.000000000	0.186269999	0.486710012

0.500000000	0.313730001	0.986710012
0.500000000	0.686269999	0.986710012
0.000000000	0.000000000	0.040849999
0.500000000	0.500000000	0.540849984
0.000000000	0.238519996	0.830669999
0.000000000	0.761479974	0.830669999
0.500000000	0.738520026	0.330669999
0.500000000	0.261480004	0.330669999

4. *R*-3*m* structure (primitive cell) of KB_3Si_3

1.0

7.5149002075	0.0000000000	0.0000000000
4.6972233659	5.8659882186	0.0000000000
4.6972233659	2.2562707263	5.4147077659

K B Si

2 6 6

Direct

0.611819983	0.611819983	0.611819983
0.388180017	0.388180017	0.388180017
0.783959985	0.053490002	0.053490002
0.216040015	0.946510017	0.946510017
0.053490002	0.783959985	0.053490002
0.946510017	0.216040015	0.946510017
0.053490002	0.053490002	0.783959985
0.946510017	0.946510017	0.216040015
0.098920003	0.098920003	0.465600014
0.901080012	0.901080012	0.534399986
0.465600014	0.098920003	0.098920003
0.534399986	0.901080012	0.901080012
0.098920003	0.465600014	0.098920003
0.901080012	0.534399986	0.901080012

5. *R*-3 structure (primitive cell) of KB_3Si_3

1.0

6.9670000076	0.0000000000	0.0000000000
3.7728648417	5.8570111826	0.0000000000
3.7728648417	2.0575409354	5.4837127288

K B Si

2 6 6

Direct

0.325199991	0.325199991	0.325199991
0.674800038	0.674800038	0.674800038
0.185900003	0.054790001	0.880330026

0.814100027	0.945209980	0.119669974
0.880330026	0.185900003	0.054790001
0.119669974	0.814100027	0.945209980
0.054790001	0.880330026	0.185900003
0.945209980	0.119669974	0.814100027
0.171599999	0.556550026	0.845229983
0.828400016	0.443449974	0.154770017
0.845229983	0.171599999	0.556550026
0.154770017	0.828400016	0.443449974
0.556550026	0.845229983	0.171599999
0.443449974	0.154770017	0.828400016

6. $P2_12_12_1$ structure of KB_3Si_3

1.0

5.2678999901	0.0000000000	0.0000000000
0.0000000000	5.8123002052	0.0000000000
0.0000000000	0.0000000000	12.0914001465

K	B	Si
4	12	12

Direct

0.417070001	0.876479983	0.031789999
0.082929999	0.123520017	0.531790018
0.582929969	0.376479983	0.468210012
0.917070031	0.623520017	0.968209982
0.077689998	0.362610012	0.328550011
0.422309995	0.637390018	0.828549981
0.922309995	0.862609982	0.171449989
0.577690005	0.137389988	0.671450019
0.121560000	0.182640001	0.822239995
0.378439993	0.817359984	0.322239995
0.878440022	0.682640016	0.677760005
0.621559978	0.317359984	0.177760005
0.799939990	0.162570000	0.903180003
0.700060010	0.837430000	0.403180003
0.200060010	0.662570000	0.596819997
0.299939990	0.337430000	0.096819997
0.168369994	0.853389978	0.760529995
0.331629992	0.146610022	0.260529995
0.831629992	0.353389978	0.739470005
0.668370008	0.646610022	0.239470005
0.578869998	0.839529991	0.578660011
0.921130002	0.160470009	0.078660011
0.421130002	0.339529991	0.921339989
0.078869998	0.660470009	0.421339989

0.829299986	0.094310001	0.292479992
0.670700014	0.905690014	0.792479992
0.170700014	0.594309986	0.207520008
0.329299986	0.405690014	0.707520008

7. *P*1 structure of RbB_3Si_3

1.0

5.0682001114	0.0000000000	0.0000000000
2.4743492491	4.5166466295	0.0000000000
2.3391094731	-0.2616746290	10.7352033162

Rb	B	Si
2	6	6

Direct

0.836220026	0.831030011	0.397579998
0.300989985	0.161789998	0.145009995
0.117169999	0.178470001	0.512269974
0.205540001	0.298310012	0.829339981
0.555410028	0.325320005	0.830110013
0.853259981	0.239659995	0.923870027
0.867879987	0.577539980	0.931060016
0.512490034	0.580619991	0.941380024
0.035670001	0.810209990	0.013810000
0.913470030	0.879589975	0.796970010
0.254639983	0.806429982	0.607280016
0.247810006	0.336899996	0.634299994
0.714640021	0.332639992	0.632780015
0.473020017	0.839070022	0.787999988

8. *Cm* structure of CsB_3Si_3

1.0

6.5510001183	0.0000000000	0.0000000000
3.3770912362	5.6134532448	0.0000000000
1.3504833465	0.7635783005	5.9311572872

Cs	B	Si
2	6	6

Direct

0.475970000	0.475970000	0.972769976
0.712469995	0.712469995	0.272249997
0.947860003	0.227559999	0.635110021
0.227559999	0.947860003	0.635110021
0.192650005	0.192650005	0.055390000
0.356480002	0.356480002	0.522480011

0.830309987	0.830309987	0.736090004
0.967710018	0.967710018	0.824090004
0.438890010	0.027400000	0.775330007
0.027400000	0.438890010	0.775330007
0.730960011	0.160999998	0.494910002
0.160999998	0.730960011	0.494910002
0.211099997	0.211099997	0.375919998
0.011000000	0.011000000	0.141560003