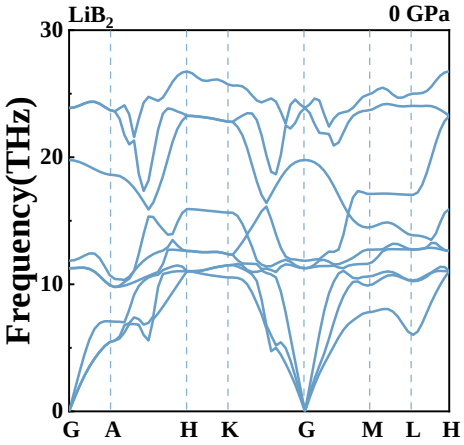
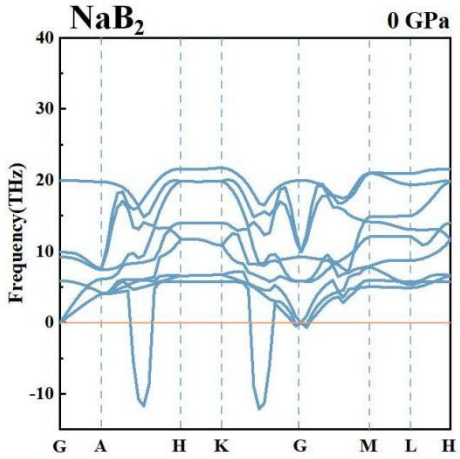
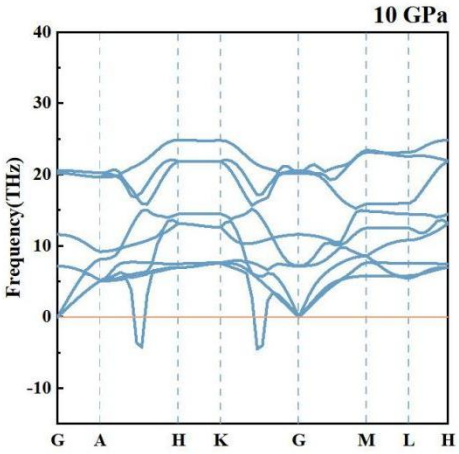
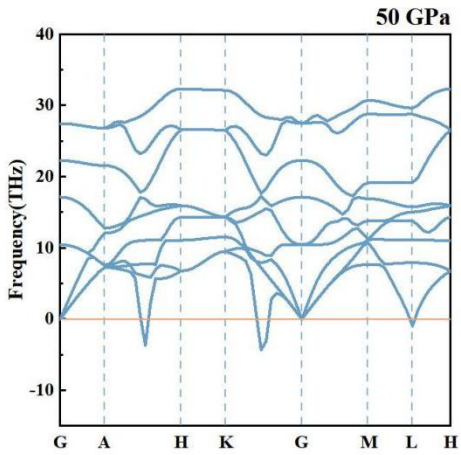
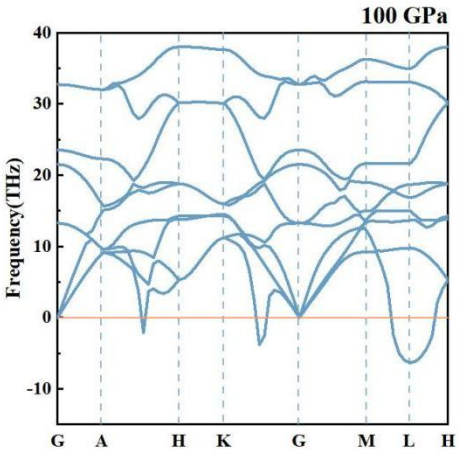
Phonon-mediated superconductivity in the metal diborides XB_2 under pressure

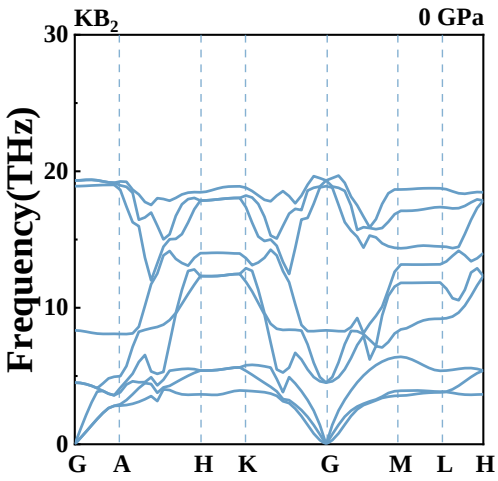


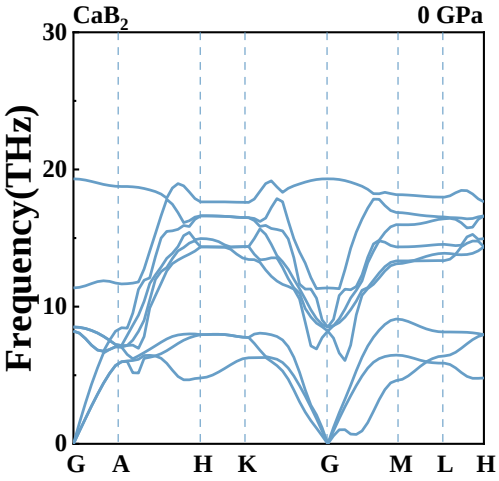


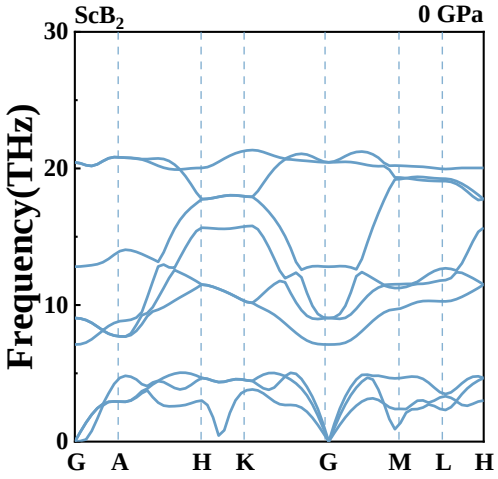







KB2
0 GPa
Frequency(THz)
30
20
10
0
G A H K G M L H


CaB2
0 GPa
Frequency(THz)
30
20
10
0
G A H K G M L H


ScB2
0 GPa
Frequency(THz)
30
20
10
0
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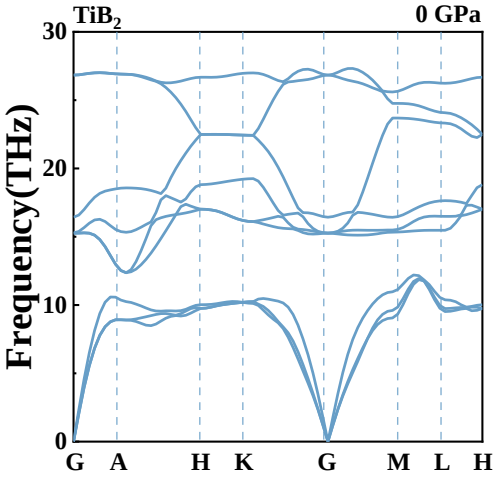
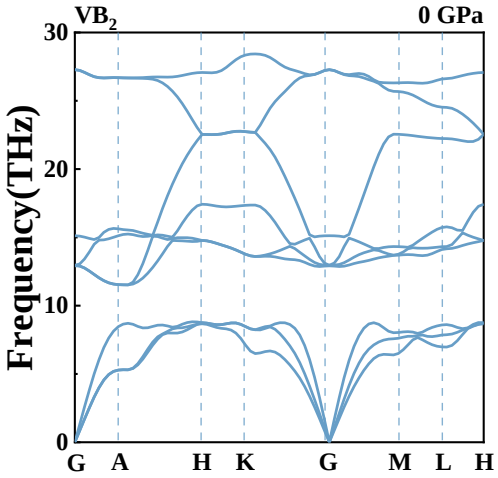
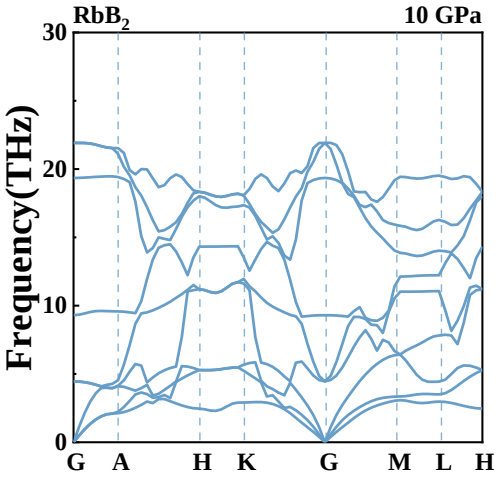
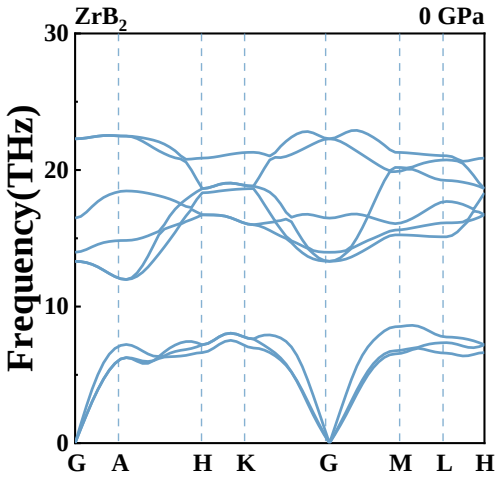
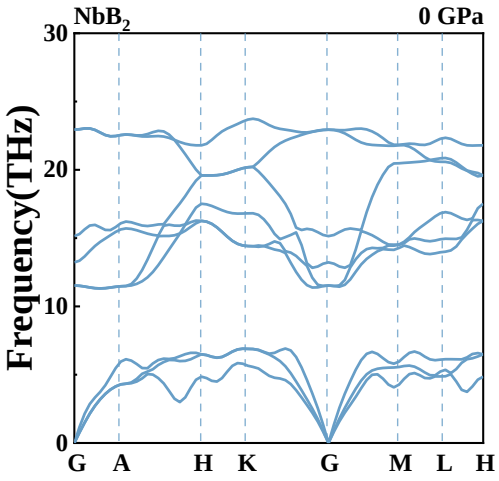
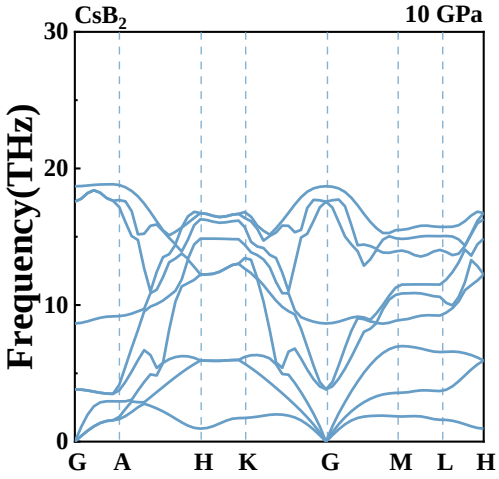

TiB2
0 GPa
Frequency(THz)
30
20
10
0
G A H K G M L H

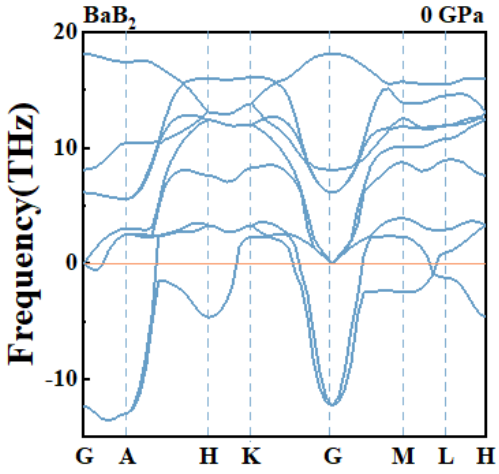

VB2
0 GPa
Frequency(THz)
30
20
10
0
G A H K G M L H

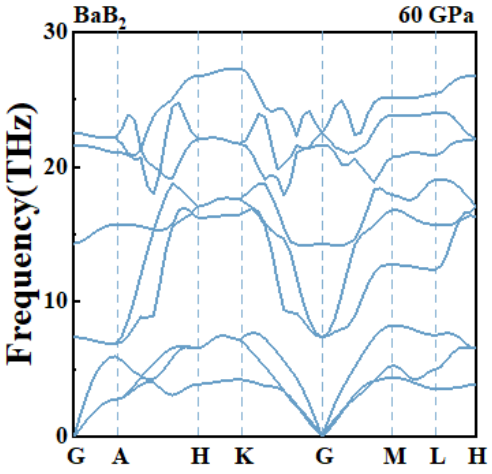

RbB2
10 GPa
Frequency(THz)
30
20
10
0
G A H K G M L H


ZrB2
0 GPa
Frequency(THz)
30
20
10
0
G A H K G M L H


NbB2
0 GPa
Frequency(THz)
30
20
10
0
G A H K G M L H


CsB2
10 GPa
Frequency(THz)
30
20
10
0
G A H K G M L H


BaB2
0 GPa
Frequency(THz)
20
10
0
-10
G A H K G M L H


BaB2
60 GPa
Frequency(THz)
30
20
10
0
G A H K G M L H

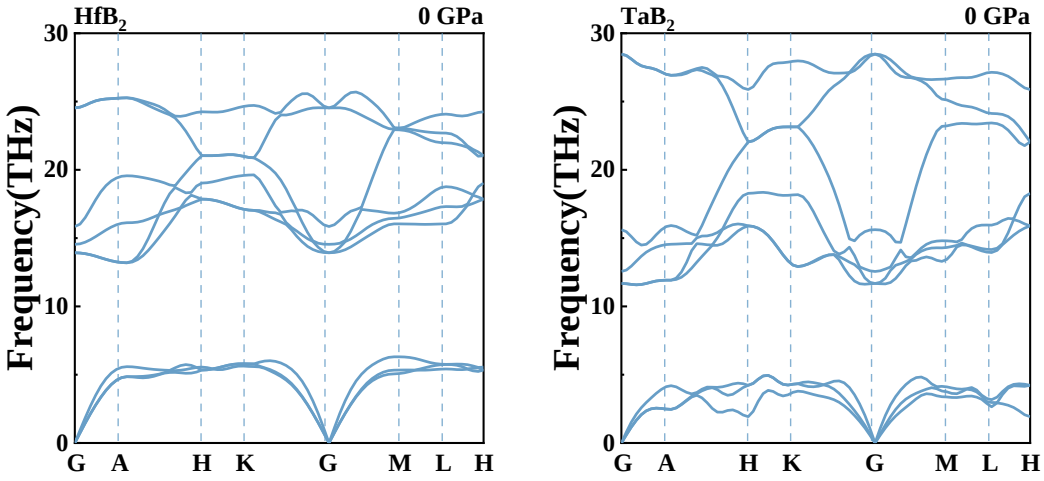


Figure S1. Phonon spectrum of 14 kinds of XB_2 under pressures.

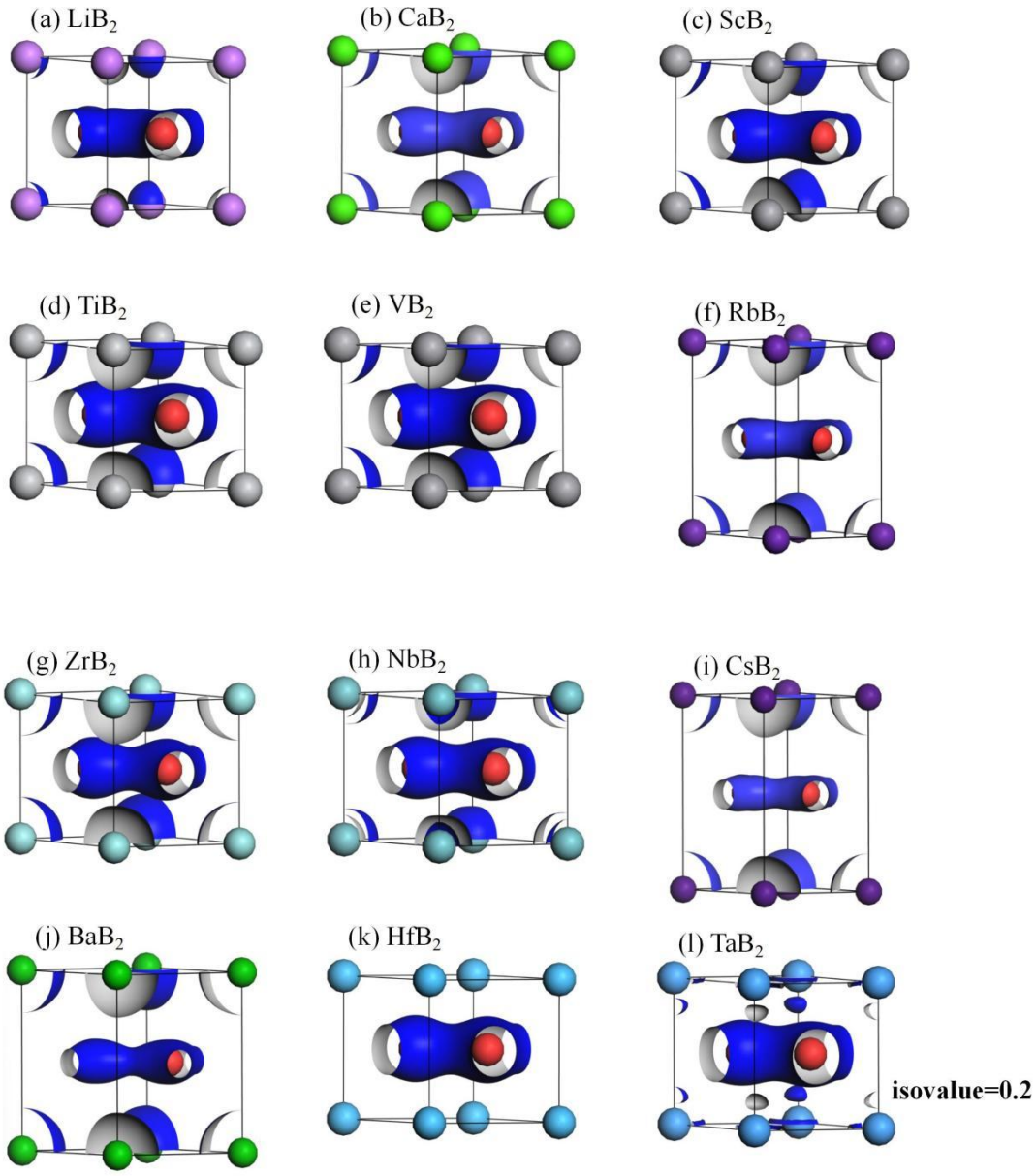


Figure S2. The three-dimensional electron density of XB_2 (*P6/mmm*).

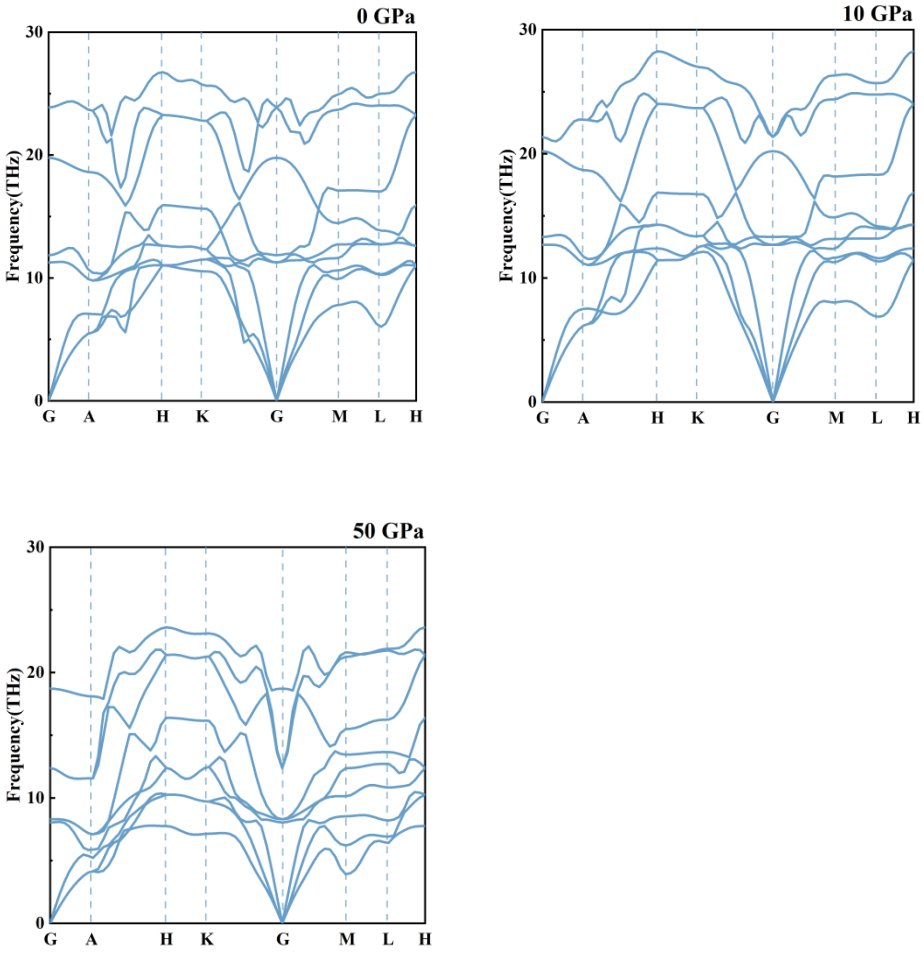


Figure S3. Phonon spectrum of LiB_2 under different pressures.

Table S1. 14 kinds of XB_2 formation energy

Materials	E_{form} (eV/atom)
LiB_2	-0.0420
KB_2	0.0149
CaB_2	-0.1400
ScB_2	-0.8637
TiB_2	-1.0473
VB_2	-2.2218
RbB_2	-0.6192
ZrB_2	-1.0282
NbB_2	-0.8011
CsB_2	-0.4301
BaB_2	-1.7007
HfB_2	-3.7230
TaB_2	-0.7372
NaB_2	0.2871

Table S2. Mulliken charge of XB_2 (*P6/mmm*).

Materials	Species	Ion	s	p	d	Total	Mulliken charges (e)
	B	1	1.00	2.48	0.00	3.49	-0.49
LiB_2	B	2	1.00	2.48	0.00	3.49	-0.49
	Li	1	1.57	0.46	0.00	2.03	0.97
	B	1	1.04	2.51	0.00	3.55	-0.55
CaB_2	B	2	1.04	2.51	0.00	3.55	-0.55
	Ca	1	1.90	6.19	0.80	8.90	1.10
	B	1	1.02	2.63	0.00	3.66	-0.66
ScB_2	B	2	1.02	2.63	0.00	3.66	-0.66
	Sc	1	0.07	-0.10	3.72	3.69	1.31
	B	1	0.91	2.64	0.00	3.55	-0.55
TiB_2	B	2	0.91	2.64	0.00	3.55	-0.55
	Ti	1	2.06	6.15	2.70	10.90	1.10
	B	1	1.05	2.76	0.00	3.81	-0.81
VB_2	B	2	1.05	2.76	0.00	3.81	-0.81
	V	1	0.19	-0.64	3.84	3.38	1.62
	B	1	1.07	2.40	0.00	3.47	-0.47
RbB_2	B	2	1.07	2.40	0.00	3.47	-0.47
	Rb	1	2.34	4.97	0.80	8.06	0.89
	B	1	0.98	2.60	0.00	3.58	-0.58
ZrB_2	B	2	0.98	2.60	0.00	3.58	-0.58
	Zr	1	2.10	5.96	2.79	10.85	1.15
	B	1	1.10	2.69	0.00	3.79	-0.79
NbB_2	B	2	1.10	2.69	0.00	3.79	-0.79
	Nb	1	0.68	-1.45	4.20	3.42	1.58
	B	1	1.11	2.30	0.00	3.40	-0.40
CsB_2	B	2	1.11	2.30	0.00	3.40	-0.40
	Cs	1	2.29	4.94	0.97	8.19	0.81
	B	1	1.03	2.47	0.00	3.50	-0.5
BaB_2	B	2	1.03	2.47	0.00	3.50	-0.5
	Ba	1	2.31	4.89	1.80	9.00	1.00
	B	1	1.10	2.80	0.00	3.90	-0.90
HfB_2	B	2	1.10	2.80	0.00	3.90	-0.90
	Hf	1	0.69	-1.57	3.08	2.20	1.80
	B	1	1.02	2.81	0.00	3.83	-0.83
TaB_2	B	2	1.02	2.81	0.00	3.83	-0.83
	Ta	1	0.60	-1.17	3.91	3.34	1.66