Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for the paper entitled "*Predicted superhard phases of Zr-B compounds under pressure*"

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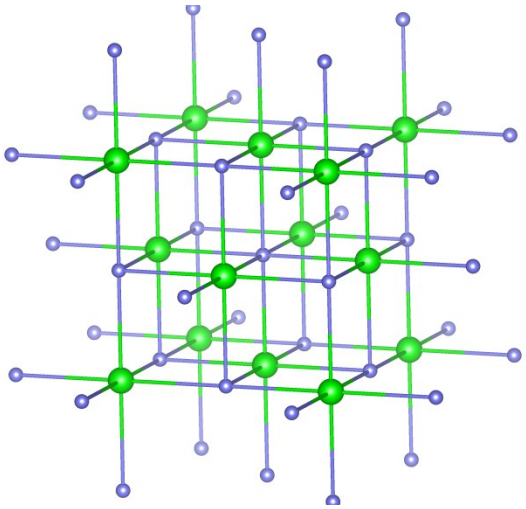

Fig.S1The crystal structure of Fm-3m-ZrB

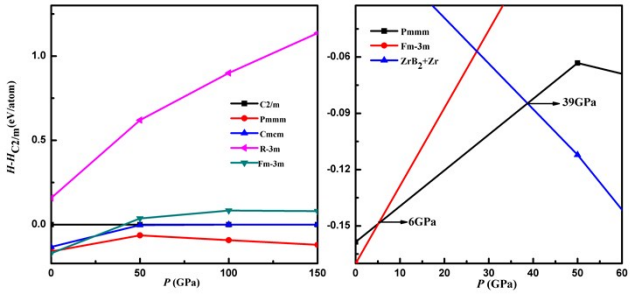

Fig.S2The phase stability of ZrB

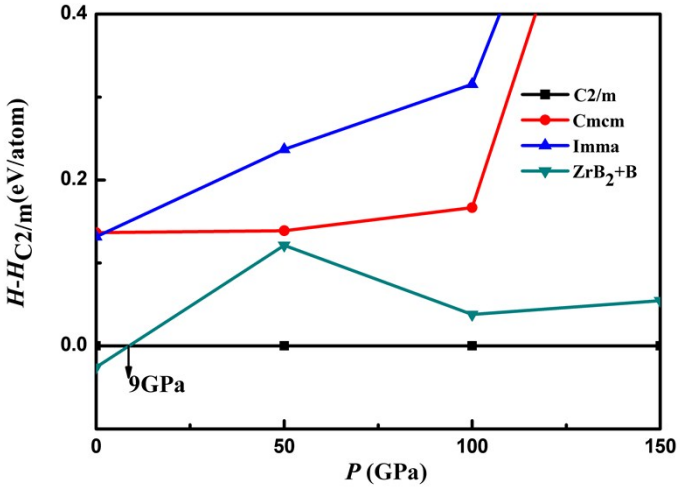

Fig.S3 The phase stability of ZrB_3

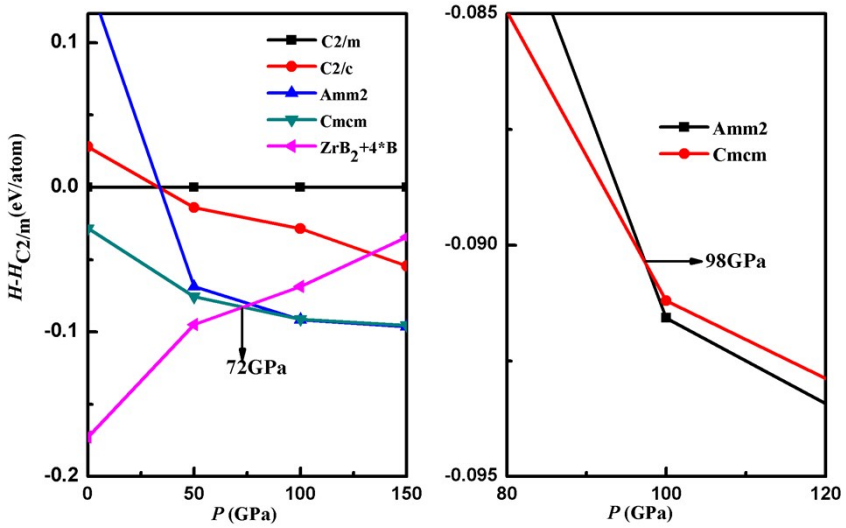

Fig.S4 The phase stability of ZrB_6

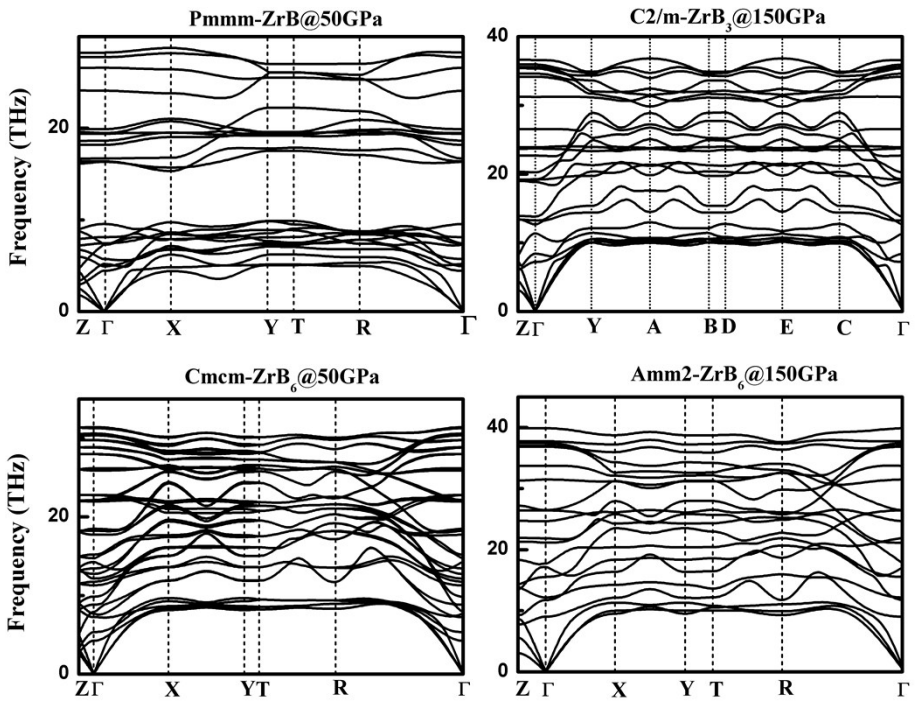

Fig.S5 The phonon dispersion curves of Zr-B system under pressure

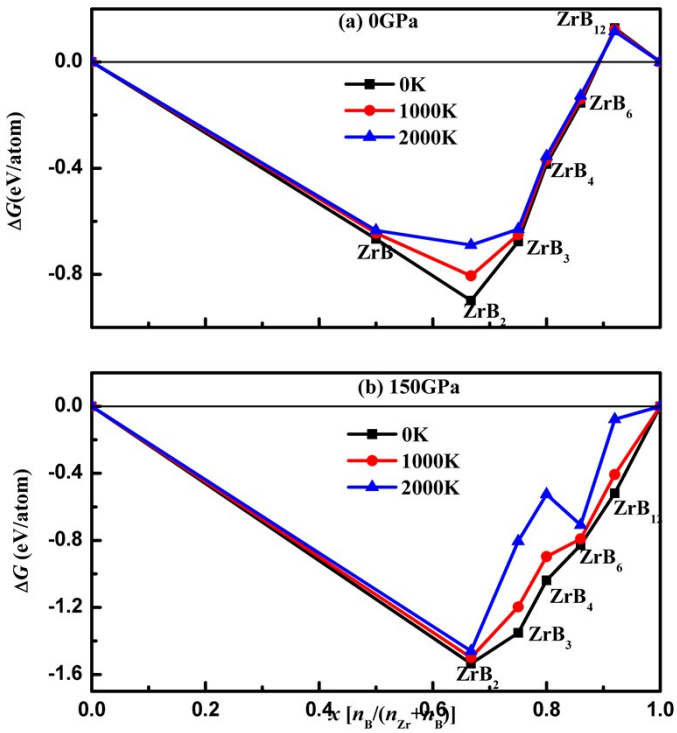

Fig.S6 The formation enthalpies of Zr-B compounds at different temperature and pressure

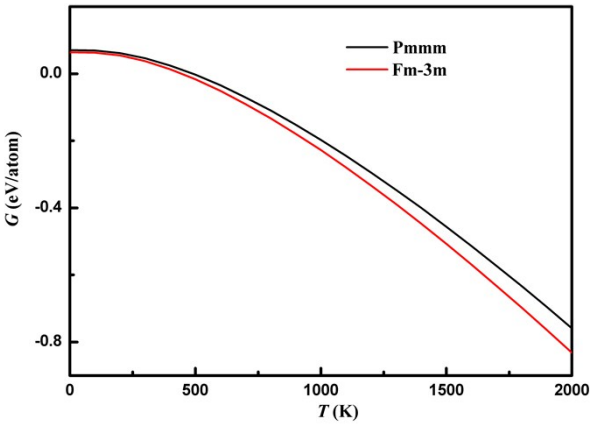

Fig.S7 The gibbs free energy of Fm-3m and Pmmm phases of ZrB at different temperature at 0GPa.

Table S1 The structure parameters of stable Zr-B compounds

						Site
Pmmm-ZrB	10	*a*=2.912	0.5	0.5	0.295	B (2t)
		b=3.145	0	0.5	0.603	B (2t)
		c=8.295	0	0	0.809	Zr (2q)
		V=75.95	0.5	0	0.5	Zr (1d)
			0.5	0.5	0	Zr (1f)
*C*2/*m*-ZrB_3	30	*a*=3.053	0.705	0.831	0.194	B (8j)
		b=2.251	0.5	0.333	0.5	B (4h)
		c=8.781	0.664	0	0.702	Zr (4i)
		V=135.2				
Cmcm-ZrB_6	50	*a*=5.041	0.168	0.487	0.133	B (8f)
		b=2.983	0.164	0.215	0.75	B (4e)
		c=12.781	0	0	0	Zr (2a)
		V=192.1				
*Amm*2-ZrB_6	150	*a*=6.019	0.734	0.167	0.628	
		b=4.763	0.5	0.337	0.44	
		c=2.802	0	0	0.142	
		V=80.3				

Table S2 the relevant elastic parameter and hardness of stable

Str.		C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{23}	*B*	*G*	*E*	*v*	H_V
Pmmm-ZrB	this work	426	343	263	135	118	149	83	92	113	177	128	308	0.21	25.3
Fm-3m-ZrB	Ref [1]	363			60			60			161	88	223	0.27	10.5
C2/m-ZrB_3	this work	500	578	582	270	245	225	54	114	112	246	236	537	0.137	43.5
Cmcm-ZrB_6	this work	660	669	601	220	283	139	66	86	94	269	231	540	0.165	24.6
Amm2-ZrB_6	this work	683	698	623	215	295	125	65	94	101	280	230	543	0.178	40.1

[1] G.T. Zhang, T.T. Bai, Y.R. Zhao and Y.F. Hu, *Materials*, 2016, **9**, 703.