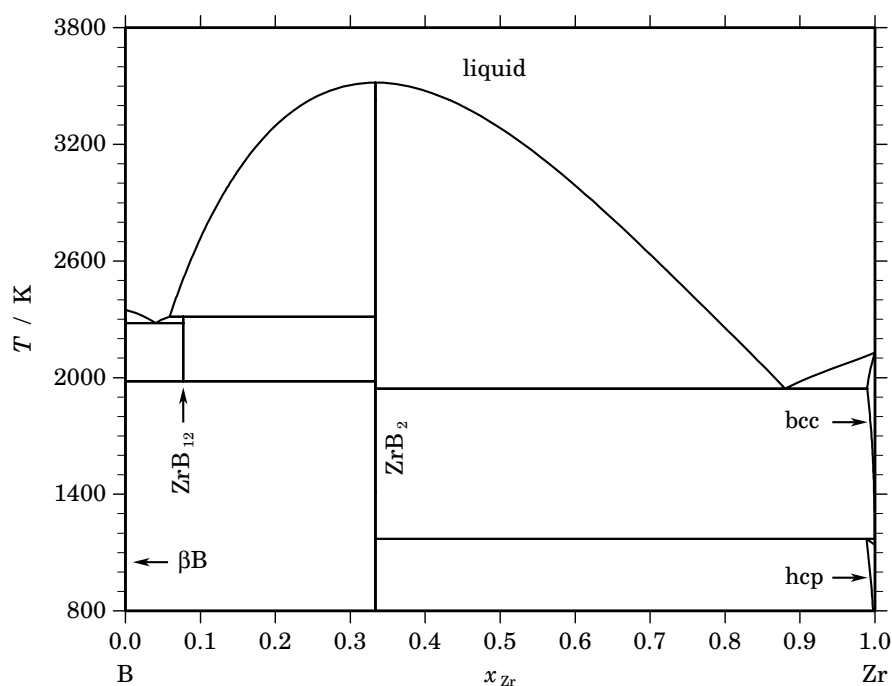


**B – Zr (Boron – Zirconium)****Fig. 1.** Calculated phase diagram for the system B-Zr.

A review and a thermodynamic assessment for the system B-Zr has been published in [1988Rog] which has been revised later [1998Dus]. The data for the phase diagram are based mostly on the results from [1966Rud] and from [1970Por]. The liquidus data show a very high scatter due to the aggressive attack of the B-melt on the crucible materials. Thermodynamic properties have been determined only for  $\text{ZrB}_2$ . The experimental data for this compound have been reviewed by [1976Alc] and recommended values have been given which are used in the assessment [1998Dus].

**Table I.** Phases, structures and models.

Phase	Struktur- bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(\text{B,Zr})_1$
$\beta\text{B}$	...	$\beta\text{B}$	$hR105$	$R\bar{3}m$	BETA_RHOMBO_B	$\text{B}_{93}\text{B}_{12}$
$\text{ZrB}_{12}$	$D2_f$	$\text{UB}_{12}$	$cF52$	$Fm\bar{3}m$	ZRB12	$\text{Zr}_1\text{B}_{12}$
$\text{ZrB}_2$	$C32$	$\text{AlB}_2$	$hP3$	$P6/mmm$	ZRB2	$\text{Zr}_1\text{B}_2$
bcc	$A2$	W	$cI2$	$Im\bar{3}m$	BCC_A2	$\text{Zr}_1(\text{B},\square)_3$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$\text{Zr}_2(\text{B},\square)_1$

**Table II.** Invariant reactions.

Reaction	Type	$T / \text{K}$	Compositions / $x_{\text{Zr}}$			$\Delta_r H / (\text{J/mol})$
liquid $\rightleftharpoons$ ZrB <sub>2</sub>	congruent	3518.0	0.333	0.333		–99035
liquid + ZrB <sub>2</sub> $\rightleftharpoons$ ZrB <sub>12</sub>	peritectic	2312.9	0.059	0.333	0.077	–39109
liquid $\rightleftharpoons$ $\beta$ B + ZrB <sub>12</sub>	eutectic	2280.1	0.040	0.000	0.077	–45880
ZrB <sub>12</sub> $\rightleftharpoons$ $\beta$ B + ZrB <sub>2</sub>	eutectoid	1980.7	0.077	0.000	0.333	–8121
liquid $\rightleftharpoons$ ZrB <sub>2</sub> + bcc	eutectic	1942.9	0.880	0.333	0.989	–22987
ZrB <sub>2</sub> + bcc $\rightleftharpoons$ hcp	peritectoid	1169.7	0.333	1.000	0.989	–3541

**Table IIIa.** Integral quantities for the liquid phase at 3600 K.

$x_{\text{Zr}}$	$\Delta G_{\text{m}}$ [J/mol]	$\Delta H_{\text{m}}$ [J/mol]	$\Delta S_{\text{m}}$ [J/(mol·K)]	$G_{\text{m}}^{\text{E}}$ [J/mol]	$S_{\text{m}}^{\text{E}}$ [J/(mol·K)]	$\Delta C_P$ [J/(mol·K)]
0.000	0	0	0.000	0	0.000	0.000
0.100	–28519	–28323	0.054	–18789	–2.649	0.000
0.200	–45818	–47791	–0.548	–30840	–4.708	0.000
0.300	–55400	–59363	–1.101	–37115	–6.180	0.000
0.400	–58719	–64000	–1.467	–38574	–7.063	0.000
0.500	–56926	–62664	–1.594	–36179	–7.357	0.000
0.600	–51033	–56314	–1.467	–30889	–7.063	0.000
0.700	–41950	–45913	–1.101	–23665	–6.180	0.000
0.800	–30447	–32419	–0.548	–15469	–4.708	0.000
0.900	–16990	–16795	0.054	–7260	–2.649	0.000
1.000	0	0	0.000	0	0.000	0.000

Reference states: B(liquid), Zr(liquid)

**Table IIIb.** Partial quantities for B in the liquid phase at 3600 K.

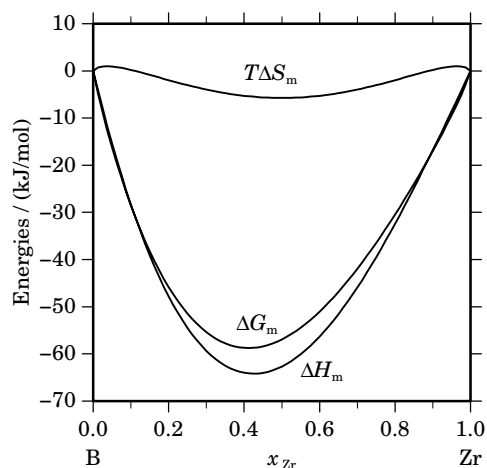
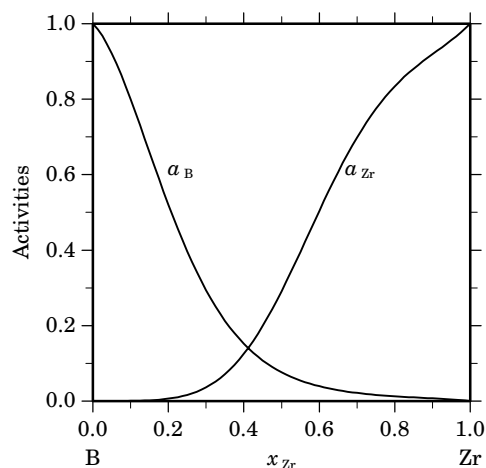
$x_{\text{B}}$	$\Delta G_{\text{B}}$ [J/mol]	$\Delta H_{\text{B}}$ [J/mol]	$\Delta S_{\text{B}}$ [J/(mol·K)]	$G_{\text{B}}^{\text{E}}$ [J/mol]	$S_{\text{B}}^{\text{E}}$ [J/(mol·K)]	$a_{\text{B}}$	$\gamma_{\text{B}}$
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	–6682	–4588	0.582	–3529	–0.294	0.800	0.889
0.800	–19513	–17072	0.678	–12834	–1.177	0.521	0.651
0.700	–36670	–35529	0.317	–25994	–2.649	0.294	0.420
0.600	–56378	–58038	–0.461	–41088	–4.708	0.152	0.253
0.500	–76941	–82679	–1.594	–56194	–7.357	0.076	0.153
0.400	–96817	–107529	–2.976	–69390	–10.594	0.039	0.098
0.300	–114793	–130667	–4.409	–78756	–14.420	0.022	0.072
0.200	–130543	–150172	–5.452	–82369	–18.834	0.013	0.064
0.100	–147231	–164121	–4.692	–78309	–23.837	0.007	0.073
0.000	– $\infty$	–170595	$\infty$	–64654	–29.428	0.000	0.115

Reference state: B(liquid)

**Table IIIc.** Partial quantities for Zr in the liquid phase at 3600 K.

$x_{\text{Zr}}$	$\Delta G_{\text{Zr}}$ [J/mol]	$\Delta H_{\text{Zr}}$ [J/mol]	$\Delta S_{\text{Zr}}$ [J/(mol·K)]	$G_{\text{Zr}}^{\text{E}}$ [J/mol]	$S_{\text{Zr}}^{\text{E}}$ [J/(mol·K)]	$a_{\text{Zr}}$	$\gamma_{\text{Zr}}$
0.000	$-\infty$	−330715	$\infty$	−224774	−29.428	0.000	0.001
0.100	−225049	−241940	−4.692	−156128	−23.837	0.001	0.005
0.200	−151039	−170667	−5.452	−102865	−18.834	0.006	0.032
0.300	−99102	−114975	−4.409	−63064	−14.420	0.036	0.122
0.400	−62231	−72943	−2.976	−34804	−10.594	0.125	0.313
0.500	−36911	−42649	−1.594	−16164	−7.357	0.291	0.583
0.600	−20511	−22171	−0.461	−5221	−4.708	0.504	0.840
0.700	−10731	−9589	0.317	−55	−2.649	0.699	0.998
0.800	−5422	−2981	0.678	1257	−1.177	0.834	1.043
0.900	−2519	−425	0.582	634	−0.294	0.919	1.021
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Zr(liquid)

**Fig. 2.** Integral quantities of the liquid phase at  $T=3600$  K.**Fig. 3.** Activities in the liquid phase at  $T=3600$  K.**Table IV.** Standard reaction quantities at 298.15 K for the compounds per mole of atoms.

Compound	$x_{\text{Zr}}$	$\Delta_f G^\circ$ / (J/mol)	$\Delta_f H^\circ$ / (J/mol)	$\Delta_f S^\circ$ / (J/(mol·K))	$\Delta_f C_P^\circ$ / (J/(mol·K))
Zr <sub>1</sub> B <sub>12</sub>	0.077	−18871	−18306	1.897	0.000
Zr <sub>1</sub> B <sub>2</sub>	0.333	−107409	−108899	−5.000	0.142

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