Borides of Rhenium and the Platinum Metals

The Crystal Structure of Re$_7$B$_3$, ReB$_3$, Rh$_7$B$_3$, RhB $_{\sim 1.1}$, IrB$_{\sim 1.1}$ and PtB

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Some features of the binary systems of boron with rhenium and the platinum metals are reported. Re$_7$B$_3$ and Rh$_7$B$_3$ are isomorphous with Ru$_7$B$_3$ (Th$_7$Fe$_3$ ($D10_2$)-type). The structure of ReB$_3$ is closely related to those of Mo$_2$B$_5$ and W$_2$B$_5$. RhB$_{\sim 1.1}$ and PtB crystallize in the anti-NiAs structure, and a phase with the approximate composition IrB$_{\sim 1.1}$ is isomorphous with ThSi$_2$ (C_c-type).

A s mentioned in an earlier communication [1] studies on the borides of the platinum metals are in progress at this Institute. In the previous paper the crystal structure of Ru$_7$B$_3$ was dealt with. In this paper we shall discuss some general features of the binary systems of boron with rhenium and the platinum metals and also described the crystal structures of Re$_7$B$_3$, ReB$_3$, Rh$_7$B$_3$, RhB$_{\sim 1.1}$, IrB$_{\sim 1.1}$ and PtB.

EXPERIMENTAL

Rhenium, ruthenium, rhodium and osmium (powder) were obtained from Heraeus (Hanau, Germany) and iridium and platinum from Johnson, Matthey & Co (London). Crystalline boron powder was kindly donated by Borax Consolidated (London). The manufactures have given the following information about their products:

Re : ca. 99.8 %
Ru : ca. 99.9 % — 99.95 %, traces of Cu, Fe, Ca, Mg and Si
Rh : ca. 99.95 %, traces of Ru, Fe, Ca and Mg
Os : ca. 99.5 %, main impurity: oxygen, traces of alkali and Fe
Ir : min. 99.8 %
Pt : min. 99.9 %
B : 99.0 — 99.7 %, main impurities: Fe, Si, O.

All phases reported in this paper were prepared by arc melting weighed amounts of metal and boron powders. Some borides of ruthenium, rhodium, and platinum were also synthesized by sintering in crucibles of recrystallized alumina (Degussit Al 23 from Degussa, Frankfurt).

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* *Note on authorship.* E. Stenberg and J. Åselius have collaborated with the main author in the crystal structure determinations of Rh$_7$B$_3$, RhB$_{\sim 1.1}$, IrB$_{\sim 1.1}$ and PtB.

No chemical analyses were made. Since the vapour pressures of boron and the metals involved are not very different, we believe that the compositions are not changed much when the samples are melted.

Powder photographs were taken in cameras of the Guinier type (CuKα-radiation) with CaF$_2$ ($a = 5.4630$ Å) and NaCl ($a = 5.6401$ Å) as internal standards. Since the expression for the intensities of powder lines is somewhat different for cameras of the Guinier type than for the ordinary Debye-Scherrer cameras we have also given the calculated $p|F|^2$ values. Single crystals of the phases RhB$_{\sim 1.1}$, IrB$_{\sim 1.1}$ and PtB were examined in Weissenberg cameras. We used MoKα radiation and the multiple film technique with thin iron foils between the films. The intensities were visually estimated by comparison with an intensity scale. The structure factors of Re$_7$B$_3$ and Rh$_7$B$_3$ were computed on the digital electronic computer BESK with a program devised by Åsbrink et al. [2]. The scattering factors were computed with the formula:

$$f_i = A_i \exp\left(-\frac{a_i}{\lambda^2}\sin^2\Theta\right) + B_i\exp\left(-\frac{b_i}{\lambda^2}\sin^2\Theta\right) + C_i \exp\left(-\frac{c_i}{\lambda^2}\sin^2\Theta\right) + D_i$$

The following constants A_i, B_i, C_i, a_i, b_i and c_i were calculated by Dr. K. Appel at the Quantum Chemistry Group of this University on basis of the scattering factor tables by Tomas and Umeda [3] (rhenium, rhodium) and Ibers [4] (boron):

	A	B	C	a	b	c
Re	25.854	28.303	19.925	0.170	1.885	15.175
Rh	15.520	16.977	12.024	0.237	2.600	20.057
B	1.644	0.406	2.878	0.6069	4.5832	33.019

In the calculations of the structure factors of ReB$_3$, RhB$_{\sim 1.1}$ and IrB$_{\sim 1.1}$ we used the mentioned scattering factor tables [3,4].

No corrections for dispersion (D_i) absorption or thermal movement were made.

RESULTS

A great number of intermediate phases were observed in the arcmelted alloys. We could characterize some phases by determining their crystal structures or unit cells (Table 1). We have confirmed the observation of Buddery and Welch [5] that many borides of the platinum metals are also easily prepared by sintering in silica tubes. Thus, Ru$_7$B$_3$, RuB$_{\sim 1.0}$, Rh$_7$B$_3$, RhB$_{\sim 1.1}$, and PtB

Table 1. Crystallographic constants of borides of rhenium and the platinum metals.

	Structure type	Lattice parameters in Å			Unit cell volume in Å³
Re$_3$B	(orthorhombic)	$a = 2.89_4$	$b = 9.31_7$	$c = 7.26_4$	
Re$_7$B$_3$	Th$_7$Fe$_3$	$a = 7.50_4$	$c = 4.77_2$	$c/a = 0.6506$	238.1
ReB$_3$	ReB$_3$	$a = 2.900$	$c = 7.475$	$c/a = 2.578$	54.44
Ru$_7$B$_3$	Th$_7$Fe$_3$	$a = 7.46_9$	$c = 4.71_4$	$c/a = 0.631_1$	227.6
RuB$_{\sim 1.0}$	(cubic?)	$a = 6.98$			
Rh$_7$B$_3$	Th$_7$Fe$_3$	$a = 7.47_1$	$c = 4.77_7$	$c/a = 0.639_4$	230.9
RhB$_{\sim 1.1}$	anti-NiAs	$a = 3.30_9$	$c = 4.22_4$	$c/a = 1.27_7$	40.0$_5$
OsB$_{\sim 1.0}$	(cubic ?)	$a = 7.04$			
IrB$_{\sim 1.1}$	ThSi$_2$	$a = 2.81_0$	$c = 10.26_3$	$c/a = 3.65_2$	81.0$_4$
PtB	anti-NiAs	$a = 3.35_8$	$c = 4.05_8$	$c/a = 1.20_8$	39.6$_3$

were successfully synthesized in alumina crucibles which had been inserted in evacuated and sealed silica tubes. As pointed out by Rundqvist and Jellinek [6] and also ourselves [7] borides prepared in this way may be contaminated through reactions with the silica tubes. It seems as if the risk of contamination is

Table 2. Powder photograph of an arcmelted alloy with the nominal composition Re_2B-($CuK\alpha$ radiation).

$h\ k\ l$ for Re_7B_3	$\sin^2\Theta_{obs}$	$\sin^2\Theta_{calc}$ for Re_7B_3	I_{obs}	I_{calc} for Re_7B_3	$pF^2_{calc} \times 10^{-4}$ for Re_7B_3
101	0.0392	0.0390	m	4	2.0
110	0.0425	0.0422	w+	2	0.8
?	0.0531		w+		
200	0.0563	0.0563	w	7	4.8
201	0.0814	0.0812	st	49	53.0
(ReB₃)	0.0942		vw		
210	0.0987	0.0985	st	69	90.0
002	0.0998	0.0998	m	20	26.9
(ReB₃)	0.1049		m+		
?	0.1090		vw		
102	0.1137	0.1138	st+	93	138.8
211	0.1234	0.1234	vst	241	382.0
300	0.1268	0.1266	m+	19	31.1
(ReB₃)	0.1369		vw		
112	0.1421	0.1420	m	8	14.1
301	0.1517	0.1516	st+	64	121.1
202	0.1560	0.1560	st	48	93.6
220	0.1689	0.1689	st−	27	57.5
310	0.1830	0.1829	vw	1	2.0
(ReB₃)	0.1902		w		
212	0.1983	0.1983	m	11	27.8
311	0.2079	0.2079	m	13	33.8
400	} 0.2255	0.2251	} w+	4	10.3
302		0.2264		8	2.1
103	0.2384	0.2385	vw	2	4.6
401	0.2500	0.2500	m+	19	52.6
222	0.2684	0.2686	w+	8	24.4
203	0.2808	0.2807	st−	29	86.2
321	0.2921	0.2923	m−	10	31.6
410	0.2953	0.2955	w−	4	13.4
411	0.3205	0.3204	w+	7	21.9
213	0.3229	0.3229	(m−) *	11	33.2
402	0.3257	0.3249	(w+) *	3	9.9
303	} 0.3512	0.3511	} vst	92	274.0
500		0.3518		18	54.0
322	0.3673	0.3674	vst	109	310.0
501	0.3768	0.3767	st+	84	235.8
330	0.3800	0.3799	st+	76	212.4
412	0.3956	0.3953	w+	8	22.6
004	0.3990	0.3990	m−	15	39.9
313	0.4074	0.4074	m+	19	50.2
104	0.4127	0.4131	m−	22	55.7

* A powder line of ReB₃ overlaps 213 and 402.

Table 3. Powder photograph of an arcmelted alloy with the nominal composition Rh_7B_3. (CuKα radiation.)

h k l Rh_7B_3	$\sin^2\Theta_{obs}$	$\sin^2\Theta_{calc}$ for Rh_7B_3	I_{obs}	I_{calc} for Rh_7B_3	$pF^2_{calc} \times 10^{-4}$ for Rh_7B_3
200	0.0568	0.0568	vw	2.0	1.4
201	0.0829	0.0829	st	14.4	16.0
210	0.0995	0.0995	st +	21.8	28.6
002	0.1042	0.1043	st −	6.0	8.3
102	0.1185	0.1185	st +	29.0	44.7
(Rh)	0.1234		st		
211	0.1256	0.1255	vst	76.2	122.9
300	0.1279	0.1279	m	6.6	10.8
112	0.1471	0.1469	w	2.5	4.7
301	0.1539	0.1540	st	20.7	39.8
202	0.1613	0.1611	st −	15.4	30.7
(Rh)	0.1644		m		
220	0.1706	0.1705	m +	9.0	19.2
212	0.2034	0.2038	w	3.7	9.2
311	0.2107	0.2108	w −	4.3	11.0
400	0.2272	0.2274	vw	1.3	3.4
302	0.2323	0.2322	w −	2.4	6.6
401	0.2532	0.2534	w +	6.0	16.6
222	0.2749	0.2748	w −	2.4	6.9
203	0.2913	0.2915	m	8.8	26.6
(Rh)	0.3286		m		
500	0.3553	0.3553	w	5.4	15.9
303	0.3623	0.3626	st +	28.4	83.5
322	0.3742	0.3743	st +	31.3	89.5
501	⎱ 0.3820	0.3813	⎱ vst	26.1	72.6
330	⎰	0.3837	⎰	23.6	65.5
004	⎱ 0.4180	0.4172	⎱ w	5.1	12.3
313	⎰	0.4194	⎰	6.5	15.2
104	0.4311	0.4314	w +	6.9	16.8

reduced when direct contact between sample and silica is avoided, but without complete chemical analyses we can make no quantitative statements on this point.

The lattice parameters (l.p.) of rhenium, ruthenium, rhodium, osmium, iridium and platinum in two-phase metal-boron alloys were not significantly (that is not more than 0.05 %) different from those reported for the pure metals. This indicates that the solubility of boron is small in the solid phases of the metals mentioned.

In arc-melted rhenium-boron alloys only three rhenium borides were observed. Their unit cells are given in Table 1. We could not detect the tetragonal phase Re_2B which Neshpor et al.[8] reported to exist in sintered alloys. The other binary systems certainly contain several more intermediate phases than those in Table 1. We have confirmed the observation [5] that the powder photographs of $RuB_{\sim1.0}$ and $OsB_{\sim1.0}$ could be indexed with a cubic unit cell. As far as we are aware the other phases of Table I have not been properly characterized before.

The formulæ of Re_7B_3, ReB_3, Ru_7B_3, Rh_7B_3 and PtB are based on the structures of these phases but seem to agree well with their real compositions. The ideal structural formulae of $RhB_{\sim1.1}$ and $IrB_{\sim1.1}$ are RhB (or possibly RhB_2) and IrB_2 respectively. In both cases, other phases not yet characterized may have the same ideal composition. It is suggested that the notations $RhB_{\sim1.1}$ and $IrB_{\sim1.1}$ be used until the Rh-B and Ir-B systems have been clarified.

The l.p. variations of the phases of Table 1 are small. The largest variations (0.1—0.2 %) were observed for $RhB_{\sim1.1}$ and PtB. Thus, the reported phases probably have narrow ranges of homogeneity.

The crystal structures of Re_7B_3, ReB_3, Rh_7B_3, $RhB_{\sim1.1}$, $IrB_{\sim1.1}$ and PtB: The powder photographs of Re_7B_3 and Rh_7B_3 were very similar to that of Ru_7B_3. When we assumed the atomic parameters to be the same in Re_7B_3 and Rh_7B_3 as in Ru_7B_3 we obtained good agreement between observed and calculated intensities (Tables 2 and 3). Thus, Re_7B_3 and Rh_7B_3 are isomorphous with Ru_7B_3.

The powder photograph of ReB_3 (Table 4) could be indexed with a hexagonal cell. From the size of the unit cell we concluded that it contained two rhenium atoms. The only systematic extinction was observed for $hh\bar{2}hl$ reflexions which only appeared for l even. Thus, the possible space groups are: $P6_3/mmc$ $P\bar{6}2c$, $P6_3mc$, $P\bar{3}1c$ and $P31c$. Assuming the rhenium atoms to occupy two-fold positions 1/3, 2/3, 1/4 (or 1/3, 2/3, z) excellent agreement between observed and calculated intensities is obtained (Table 4). Because of the

Table 4. Powder photograph of an arcmelted alloy with the nominal composition ReB_3. (Cu$K\alpha$ radiation.)

$h\ k\ l$ for ReB_3	$\sin^2\Theta_{obs}$ for ReB_3	$\sin^2\Theta_{calc}$ for ReB_3	I_{obs}	I_{calc}* for ReB_3	$\|pF^2_{calc} \times 10^{-4}$ for ReB_3
002	0.0425	0.0426	st +	6.6	3.26
?	0.0530	—	vw	—	
100	0.0942	0.0942	m —	1.9	2.34
101	0.1048	0.1049	vst	10.0	13.7
102	0.1367	0.1368	m	2.4	4.20
004	0.1702	0.1702	m —	1.2	2.73
103	0.1898	0.1900	st +	4.8	11.3
104	0.2644	0.2644	w +	1.1	3.30
110	0.2827	0.2827	m	2.1	6.42
112	0.3251	0.3252	st	3.9	12.0
105	0.3602	0.3602	m +	2.9	8.62
200	0.3770	0.3769	w —	0.5	1.41
006	0.3830	0.3829	w	0.7	1.87
201	0.3876	0.3876	m +	3.0	8.34
202	0.4197	0.4195	w	1.1	2.66
114	0.4530	0.4529	st	4.6	10.2
203	0.4731	0.4727	st —	3.6	7.54
106	0.4775	0.4773	w +	1.2	2.49

* Only the rhenium contributions have been accounted for in the calculations of pF^2_{calc} and I_{calc}.

Table 5. Interatomic distances in ReB$_3$ (in Å).

$$
\begin{array}{llll}
\text{Re} & -\ 6\ \text{Re} & : & 2.90\ (6). \\
          & -\ 8\ \text{B}_I & : & 2.24\ (2);\ 2.24\ (6). \\
          & -\ 6\ \text{B}_{II} & : & 2.51\ (6). \\
\\
\text{B}_I & -\ 4\ \text{Re} & : & 2.24,\ 2.24\ (3). \\
          & -\ 3\ \text{B}_I & : & 1.83\ (3). \\
          & -\ 3\ \text{B}_{II} & : & 1.71\ (3). \\
\\
\text{B}_{II} & -\ 6\ \text{Re} & : & 2.51\ (6). \\
          & -\ 6\ \text{B}_I & : & 1.71\ (6). \\
\end{array}
$$

great differences in scattering power of rhenium and boron, the boron atoms have to be located from space considerations. If we make the plausible assumptions that Re-B distances are > 2.2 Å and B-B distances > 1.6 Å, six boron atoms can be situated in one four-fold position 1/3, 2/3, z and one two-fold position 0,0,0 (or 0,0,z). The only other boron arrangement which does not seem very improbable is to place the boron atoms in one six-fold position x,0,0 ($x \sim 1/3$). In this second alternative the shortest B$-$B distances have the normal value of 1.68 Å but the shortest Re$-$B distance is only 2.10 Å. Therefore, the first proposed structure is considered to be the most probable one. This structure has the symmetry of space group $P6_3/mmc$ with the following atomic positions:

2 Re in 2(c)
4 B$_I$ in 4(f) with $z = 0.55$
2 B$_{II}$ in 2(a)

Interatomic distances are given in Table 5. [The second, less probable structure has the symmetry of space group $P\bar{6}2c$ with two rhenium atoms in 2(c) and six boron atoms in 6(g) with $x \sim 1/3$].

Table 6. Power photographs of arcmelted alloys with the nominal compositions RhB$_{1.5}$ and PtB, respectively. (Cu$K\alpha$ radiation.) Since the relative values of I_{calc} are very similar for RhB$_{\sim 1.1}$ and PtB, they have only been computed for RhB$_{\sim 1.1}$.

$h\ k\ l$ for NiAs-type	RhB$_{1.5}$					PtB		
	$\sin^2\Theta_{obs}$	$\sin^2\Theta_{calc}$ for RhB$_{\sim 1.1}$	I_{obs}	I_{calc} for RhB$_{\sim 1.1}$	$pF'^2 \times 10^{-3}$ for RhB$_{\sim 1.1}$	$\sin^2\Theta_{obs}$	$\sin^2\Theta_{calc.}$ for PtB	I_{obs}
?			—			0.0531	—	vw
100	0.0723	0.0723	st −	6.3	5.88	0.0703	0.0703	st
101	0.1057	0.1056	vvst	32.6	44.9	0.1064	0.1064	vst
?			—			0.1158	—	w
002	0.1332	0.1332	m	5.0	7.98	0.1445	0.1444	m
102	0.2058	0.2056	m +	6.0	14.9	0.2143	0.2146	st
110	0.2169	0.2170	st	9.8	25.8	0.2110	0.2108	st
200	0.2896	0.2894	w	1.3	3.80	0.2806	0.2810	w
201	0.3226	0.3227	st	9.3	28.2	0.3168	0.3171	st
112	0.3501	0.3502	st +	10.6	31.6	0.3551	0.3551	st +
103	0.3720	0.3721	st −	9.2	26.3	0.3950	0.3951	m +
202	0.4224	0.4226	m	4.2	10.3	0.4254	0.4254	m

Table 7. Interatomic distances in RhB$_{\sim1.1}$ and PtB (in Å).

Rh	—	12 Rh	: 2,85 (6); 3.31 (6).	Pt	—	12 Pt	: 2.81 (6); 3.36 (6)
	—	6 B	: 2.18 (6).		—	6 B	: 2.19 (6).
B	—	6 Rh	: 2.18 (6).	B	—	6 Pt	: 2.19 (6).
	—	2 B	: 2.21 (2).		—	2 B	: 2.03 (2).

The powder photographs of RhB$_{\sim1.1}$ and PtB were very similar indicating that these phases were isomorphous. From the systematic extinction of $h\,h\,\overline{2h}l$ reflexions with l odd and the unit cell dimension we suspected that the structure of these phases was of the anti-NiAs (*B*8) type. With this assumption (space group $P\overline{6}_3/mmc$, two metal atoms in 2(c) and two boron atoms in 2(a)), good agreement between observed and calculated intensities was obtained (Table 6). A single crystal of each of RhB$_{\sim1.1}$ and PtB was also studied. The agreement between observed and calculated structure factors for $h\,0\,\overline{h}\,l$ reflexions is satisfactory — the R value was 9.4 % (45 observed reflexions) for RhB$_{\sim1.1}$ and 10.0 % (29 observed reflexions) for PtB. Interatomic distances are given in Table 7. (In a preliminary communication [5] we described the structure of RhB$_{\sim1.1}$ and PtB using the orthorhombic space-group *C m c m*. We have found, however, that there are no significant deviations from hexagonal symmetry.)

The single crystal and powder photographs of IrB$_{\sim1.1}$, finally, could be indexed with a tetragonal unit cell. Since $h\,k\,l$ reflexions were only observed when $h + k + l = 2n$ and $2k + l = 2n + 1$ or $4n$, the only possible space group was $I4_1/amd$. In order to adhere to convention we have chosen the

Table 8. Powder photograph of an arc-melted alloy with the nominal composition IrB$_{1.15}$ (Cu$K\alpha$ radiation).

$h\,k\,l$ for IrB$_{\sim1.1}$	$\sin^2\Theta_{obs}$	$\sin^2\Theta_{calc}$ for IrB$_{\sim1.1}$	I_{obs}	I_{calc}** IrB$_{\sim1.1}$	$pF^2 \times 10^{-4}$** for IrB$_{\sim1.1}$
* 101	0.0809	0.0809	vst	23.0	25.2
004	0.0903	0.0903	m	10.6	12.7
103	0.1260	0.1260	st	15.0	24.4
112	0.1732	0.1731	st +	21.4	45.6
105	0.2165	0.2163	m —	8.0	21.1
* 200	0.3011	0.3010	st	6.2	18.9
107	} 0.3539	0.3517	} st	5.9	17.4
116		0.3536		10.2	30.6
008	0.3609	0.3611	w	2.7	7.8
* 211	0.3824	0.3819	st	10.7	29.8
204	0.3915	0.3913	m	11.2	30.4
213	0.4267	0.4270	m +	12.3	30.1

* The strongest lines of a neigbouring phase, traces of which are present in this alloy coincide with 101, 200 and 211. Therefore, the observed intensities of these lines are stronger than expected.

** In the computations of I_{calc} and pF^2 it has been assumed that the 8(e) positions are statistically occupied by four boron atoms.

Table 9. Interatomic distances in $IrB_{\sim 1.1}$ (in Å).

$$Ir \quad - \quad 8 \ Ir \quad : \ 2.81 \ (4); \ 2.92 \ (4).$$
$$- \ 12 \ B * : \ 2.16 \ (8); \ 2.22 \ (4).$$

$$B* \ - \quad 6 \ Ir \quad : \ 2.16 \ (4); \ 2.22 \ (2).$$
$$- \quad 3 \ B* \quad : \ 1.66 \ (2); \ 1.68 \ (1).$$

* The boron positions are occupied to only about 50 %.

origin at $\bar{4}m2$. From the size of the unit cell we concluded that it contained four iridium atoms which were placed in $4(a)$. As in the case of ReB_3 the boron atoms had to be located from space considerations. It seems unlikely that the boron atoms occupy the positions $4(b)$, $8(c)$ or $8(d)$ since with boron in any of these positions $Ir-B$ distances of about 2.0 Å or shorter would be formed. The most probable boron position is in $8(e)$ with $z = 0.41_8$. The agreement between observed and calculated intensities for the proposed structure is good (Table 8). With the boron atoms in $8(e)$, $IrB_{\sim 1.1}$ is isomorphous with $ThSi_2$[9] (C_c type according to the handbooks of Smithells[10] and Pearson[11]). Interatomic distances are shown in Table 9.

DESCRIPTIONS OF THE STRUCTURES AND COMMENTS

The Ru_7B_3 structure was discussed at some length in the previous paper[1]. Somewhat unexpectedly the Me_7B_3 borides are isomorphous with Th_7Fe_3[12] ($D \ 10_2$-type [10,11]). (In this connection we wish to point out that the structure[12] of ThCo is also isomorphous with a common boride structure, namely the CrB structure).

The rhenium skeleton of ReB_3 is built up of close packed layers arranged in a close packed hexagonal structure ($ABAB\ldots$). The shortest intermetallic distance within the layers is 2.90 Å whereas atoms of neighbouring layers only have a remote contact (4.10 Å) with each other. Between the metal layers there are slightly puckered hexagonal sheets of boron atoms with the shortest $B-B$ distances 1.71 Å and 1.83 Å. The distances between atoms of neighbouring boron layers are also quite large (> 3.0 Å). Thus the cohesion in the c-direction must be mainly due to metal-boron bonds.

The structures which Kiessling[13] has suggested for W_2B_5 and Mo_2B_5 contain the same building elements as ReB_3. In addition to the puckered boron sheets there are also plane boron layers in W_2B_5 and Mo_2B_5. With the usual notations the sequences of close packed hexagonal metal layers in ReB_3, W_2B_5 and Mo_2B_5 are: $ABAB\ldots$, $AABBAABB\ldots$, and $AABBCCAABBCC\ldots$, respectively. If, following Kiessling, we denote the puckered boron sheets with K and the plane boron sheets in W_2B_5 and Mo_2B_5 with H, the complete stacking sequences along the c direction of the three structures are as follows:

$$ReB_3 \quad : \quad AKBK\ldots$$
$$W_2B_5 \quad : \quad AHAKBHBK\ldots$$
$$Mo_2B_5 \quad : \quad AHAKBHBKCHCK\ldots$$
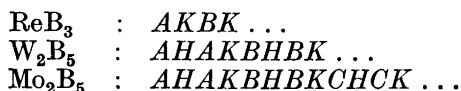
Thus, these structures are very closely related.

$IrB_{\sim 1.1}$ is of interest because of its apparent deviation from the ideal formula IrB_2. It should be noted that other compounds with structures closely related to that of $ThSi_2$ also show deviations from the ideal formula. Thus, Perri et al.[14] found that a gadolinium silicide with the ideal formula $GdSi_2$ had the composition $GdSi_{1.4}$.

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