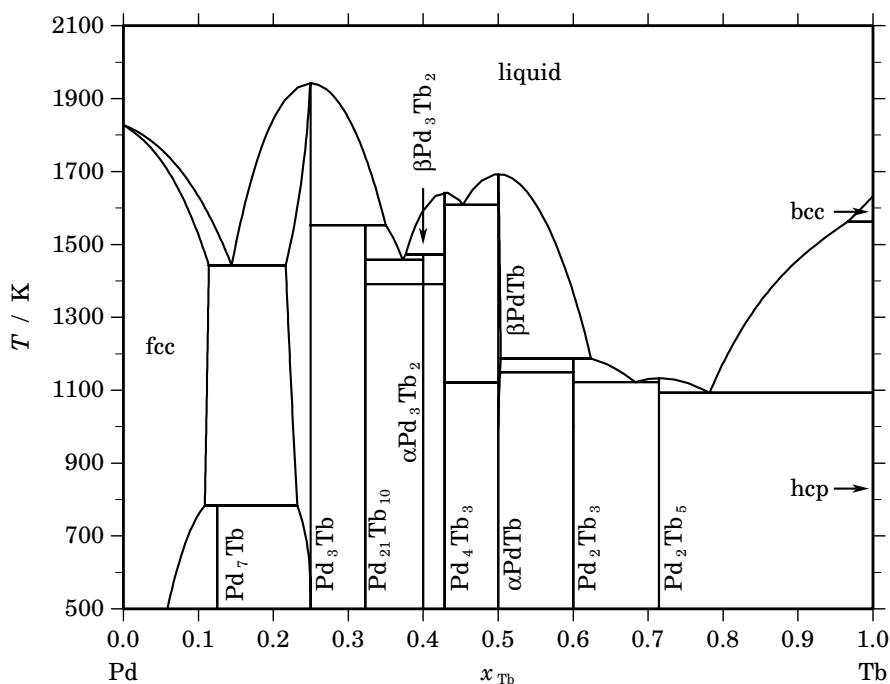


Pd – Tb (Palladium – Terbium)**Fig. 1.** Calculated phase diagram for the system Pd-Tb.

Intermetallic compounds of palladium with rare earth metals are of interest due to their potential use in hydrogen diffusion membranes for purification and isotope enrichment. Only few and insufficient experimental data are known of the Pd-Tb system. After comparing the phase diagrams of palladium with some of the heavier rare earth metals (Gd, Dy, Ho, Er) a phase diagram of Pd-Tb has been proposed by [1990Bor]. The melting temperatures of the intermetallic Pd-Tb compounds have been interpolated from series of known values for Pd-compounds with adjacent rare earth elements. The melting point of PdTb which has been measured by [1975Pal] is in agreement with the interpolation. The region of the phase diagram around the compound Pd_7Tb has been experimentally investigated by [1993Tak]. Enthalpies of formation have been determined for PdTb [1974Pal, 1995Guo] and Pd_2Tb_5 [1974Pal]. Based on these investigations a thermodynamic assessment has been prepared by [2000Du]. However, in view of the scarce available data it is much desired to verify the phase diagram and further thermodynamic properties by selected key experiments.

Table I. Phases, structures and models.

Phase	Struktur- bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	(Pd,Tb) ₁
fcc	A1	Cu	<i>cF4</i>	<i>Fm$\bar{3}m$</i>	FCC_A1	(Pd,Tb) ₁
Pd ₇ Tb	PD7TB	Pd ₇ Tb ₁
Pd ₃ Tb	L1 ₂	AuCu ₃	<i>cP4</i>	<i>Pm$\bar{3}m$</i>	PD3TB	Pd ₃ (Pd,Tb) ₁
Pd ₂₁ Tb ₁₀	PD21TB10	Pd ₂₁ Tb ₁₀
α Pd ₃ Tb ₂	PD3TB2_A	Pd ₃ Tb ₂
β Pd ₃ Tb ₂	PD3TB2_B	Pd ₃ Tb ₂
Pd ₄ Tb ₃	<i>hR14</i>	<i>R$\bar{3}$</i>	PD4TB3	Pd ₄ Tb ₃
α PdTb	B33	CrB	<i>oC8</i>	<i>Cmcm</i>	PDTB_A	(Pd,Tb) ₁ Tb ₁
β PdTb	B27	FeB	<i>oP8</i>	<i>Pnma</i>	PDTB_B	(Pd,Tb) ₁ Tb ₁
Pd ₂ Tb ₃	D5 _a	U ₃ Si ₂	<i>tP10</i>	<i>P4/mbm</i>	PD2TB3	Pd ₂ Tb ₅
Pd ₂ Tb ₅	<i>cF144</i>	<i>Fd$\bar{3}m$</i>	PD2TB5	Pd ₂ Tb ₅
bcc	A2	W	<i>cI2</i>	<i>Im$\bar{3}m$</i>	BCC_A2	(Pd,Tb) ₁
hcp	A3	Mg	<i>hP2</i>	<i>P6₃/mmc</i>	HCP_A3	(Pd,Tb) ₁

Table II. Invariant reactions.

Reaction	Type	<i>T</i> / K	Compositions / <i>x</i> _{Tb}			$\Delta_r H$ / (J/mol)
liquid \rightleftharpoons Pd ₃ Tb	congruent	1942.6	0.250	0.250		−20035
liquid \rightleftharpoons β PdTb	congruent	1693.3	0.500	0.500		−13376
liquid \rightleftharpoons Pd ₄ Tb ₃	congruent	1642.3	0.429	0.429		−9365
liquid \rightleftharpoons Pd ₄ Tb ₃ + β PdTb	eutectic	1609.1	0.453	0.429	0.500	−10202
liquid + bcc \rightleftharpoons hcp	peritectic	1562.0	0.966	1.000	1.000	−4381
Pd ₃ Tb + liquid \rightleftharpoons Pd ₂₁ Tb ₁₀	peritectic	1552.5	0.250	0.350	0.323	−6964
liquid + Pd ₄ Tb ₃ \rightleftharpoons β Pd ₃ Tb ₂	peritectic	1472.7	0.377	0.429	0.400	−4516
liquid \rightleftharpoons Pd ₂₁ Tb ₁₀ + β Pd ₃ Tb ₂	eutectic	1457.5	0.372	0.323	0.400	−8381
liquid \rightleftharpoons fcc + Pd ₃ Tb	eutectic	1442.6	0.144	0.114	0.217	−9155
β Pd ₃ Tb ₂ \rightleftharpoons α Pd ₃ Tb ₂	polymorphic	1391.5	0.400	0.400		−156
β PdTb + liquid \rightleftharpoons Pd ₂ Tb ₃	peritectic	1187.5	0.503	0.624	0.600	−21422
β PdTb + Pd ₂ Tb ₃ \rightleftharpoons α PdTb	peritectoid	1148.9	0.502	0.600	0.503	−90
liquid \rightleftharpoons Pd ₂ Tb ₅	congruent	1133.3	0.714	0.714		−17632
liquid \rightleftharpoons Pd ₂ Tb ₃ + Pd ₂ Tb ₅	eutectic	1122.2	0.683	0.600	0.714	−18458
Pd ₄ Tb ₃ + β PdTb \rightleftharpoons α PdTb	peritectoid	1120.9	0.429	0.500	0.500	−153
liquid \rightleftharpoons Pd ₂ Tb ₅ + hcp	eutectic	1093.1	0.782	0.714	1.000	−15719
fcc + Pd ₃ Tb \rightleftharpoons Pd ₇ Tb	peritectoid	783.0	0.109	0.232	0.125	−7586

Table IIIa. Integral quantities for the liquid phase at 2000 K.

x_{Tb}	ΔG_{m} [J/mol]	ΔH_{m} [J/mol]	ΔS_{m} [J/(mol·K)]	G_{m}^{E} [J/mol]	S_{m}^{E} [J/(mol·K)]	ΔC_P [J/(mol·K)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−32168	−41630	−4.731	−26763	−7.434	0.000
0.200	−53410	−69164	−7.877	−45089	−12.037	0.000
0.300	−66070	−84418	−9.174	−55912	−14.253	0.000
0.400	−71357	−89209	−8.926	−60166	−14.522	0.000
0.500	−70310	−85355	−7.523	−58783	−13.286	0.000
0.600	−63890	−74672	−5.391	−52698	−10.987	0.000
0.700	−53002	−58979	−2.988	−42844	−8.067	0.000
0.800	−38475	−40090	−0.808	−30154	−4.968	0.000
0.900	−20967	−19825	0.571	−15561	−2.132	0.000
1.000	0	0	0.000	0	0.000	0.000

Reference states: Pd(liquid), Tb(liquid)

Table IIIb. Partial quantities for Pd in the liquid phase at 2000 K.

x_{Pd}	ΔG_{Pd} [J/mol]	ΔH_{Pd} [J/mol]	ΔS_{Pd} [J/(mol·K)]	G_{Pd}^{E} [J/mol]	S_{Pd}^{E} [J/(mol·K)]	a_{Pd}	γ_{Pd}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−6126	−7351	−0.613	−4374	−1.489	0.692	0.769
0.800	−19961	−26982	−3.510	−16251	−5.366	0.301	0.376
0.700	−39695	−55258	−7.782	−33764	−10.747	0.092	0.131
0.600	−63540	−88546	−12.503	−55046	−16.750	0.022	0.037
0.500	−89756	−123211	−16.727	−78230	−22.490	0.005	0.009
0.400	−116687	−155618	−19.466	−101450	−27.084	0.001	0.002
0.300	−142859	−182135	−19.638	−122838	−29.648	0.000	0.001
0.200	−167292	−199126	−15.917	−140528	−29.299	0.000	0.000
0.100	−190943	−202958	−6.007	−152653	−25.152	0.000	0.000
0.000	−∞	−189996	∞	−157346	−16.325	0.000	0.000

Reference state: Pd(liquid)

Table IIIc. Partial quantities for Tb in the liquid phase at 2000 K.

x_{Tb}	ΔG_{Tb} [J/mol]	ΔH_{Tb} [J/mol]	ΔS_{Tb} [J/(mol·K)]	G_{Tb}^{E} [J/mol]	S_{Tb}^{E} [J/(mol·K)]	a_{Tb}	γ_{Tb}
0.000	−∞	−492842	∞	−312920	−89.961	0.000	0.000
0.100	−266552	−350141	−41.794	−228262	−60.939	0.000	0.000
0.200	−187205	−237890	−25.343	−160442	−38.724	0.000	0.000
0.300	−127613	−152456	−12.422	−107592	−22.432	0.000	0.002
0.400	−83083	−90204	−3.560	−67846	−11.179	0.007	0.017
0.500	−50863	−47499	1.682	−39337	−4.081	0.047	0.094
0.600	−28692	−20708	3.992	−20197	−0.256	0.178	0.297
0.700	−14492	−6197	4.147	−8560	1.182	0.418	0.598
0.800	−6271	−332	2.970	−2560	1.114	0.686	0.857
0.900	−2081	523	1.302	−329	0.426	0.882	0.980
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Tb(liquid)

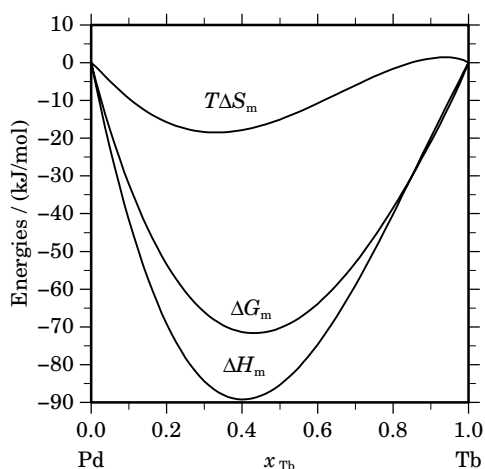


Fig. 2. Integral quantities of the liquid phase at $T=2000$ K.

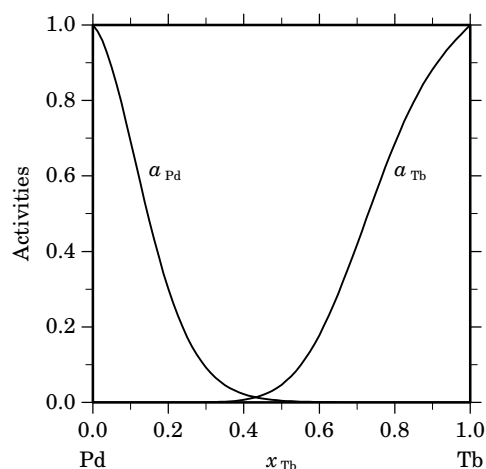


Fig. 3. Activities in the liquid phase at $T=2000$ K.

Table IV. Standard reaction quantities at 298.15 K for the compounds per mole of atoms.

Compound	x_{Tb}	$\Delta_f G^\circ / (\text{J/mol})$	$\Delta_f H^\circ / (\text{J/mol})$	$\Delta_f S^\circ / (\text{J}/(\text{mol}\cdot\text{K}))$	$\Delta_f C_P^\circ / (\text{J}/(\text{mol}\cdot\text{K}))$
Pd ₇ Tb ₁	0.125	-47937	-52022	-13.703	0.000
Pd ₃ Tb	0.250	-79090	-82053	-9.937	0.000
Pd ₂₁ Tb ₁₀	0.323	-80159	-82457	-7.710	0.000
α Pd ₃ Tb ₂	0.400	-81089	-82910	-6.105	0.000
β Pd ₃ Tb ₂	0.400	-80966	-82753	-5.993	0.000
Pd ₄ Tb ₃	0.429	-81420	-83082	-5.575	0.000
α PdTb	0.500	-81709	-83719	-6.742	0.000
β PdTb	0.500	-81597	-83566	-6.606	0.000
Pd ₂ Tb ₃	0.600	-79334	-84434	-17.105	0.000
Pd ₂ Tb ₅	0.714	-57901	-61113	-10.771	0.000

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