Co – Y (Cobalt – Yttrium)

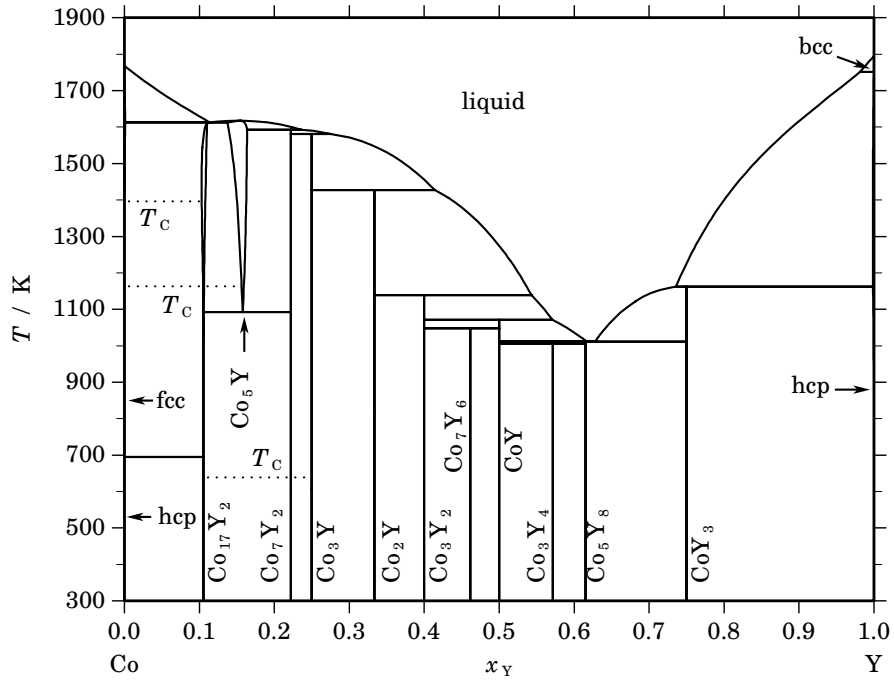

Fig. 1. Calculated phase diagram for the system Co-Y.

The Co-Y system is of interest for permanent magnets ($Co_{17}Y_2$) and for its potential use as hydrogen storage materials. A survey on the literature of the Co-Y system and a thermodynamic assessment has been been given by [2004Du]. The optimisation is based on experimental data on the phase diagram which are taken mainly from [1974Kha, 1991Wu] and on thermochemical data for the intermetallic compounds [1985Sub, 1987Col, 1987Mey]. For the liquid, no data have been available. A polymorphic transformation between $\alpha Co_{17}Y_2$ and $\beta Co_{17}Y_2$ at about 1573 K has been omitted in the assessment. At higher temperature the compounds $Co_{17}Y_2$ and Co_5Y deviate from their stoichiometric compositions due to an excess of Y in $Co_{17}Y_2$ and excess Co in Co_5Y. Since their crystal structures are closely related, [2004Du] have described both compounds as a single phase with a miscibility gap. However, since both structures are different, the phases are still denoted as different compounds in the present diagrams and tables. The dataset should not be used at too high temperatures because an artificial inverse miscibility gap opens in the liquid above 3800 K.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Co,Y)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Co,Y)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Co,Y)_1$
$\alpha Co_{17}Y_2$	$\cdots$	Th_2Zn_{17}	$hR19$	$R\overline{3}m$	CO17RE2	$Co_{15}(Co_2,Y)_2(Co_2,Y)_1$
$\beta Co_{17}Y_2$	$\cdots$	$Ni_{17}Th_2$	$hP38$	$P6_3/mmc$	CO17RE2	$Co_{15}(Co_2,Y)_2(Co_2,Y)_1$
Co_5Y	$D2_{\mathrm{d}}$	$CaCu_5$	$hP6$	$P6/mmm$	CO17RE2	$Co_{15}(Co_2,Y)_2(Co_2,Y)_1$
Co_7Y_2	$\cdots$	Co_7Er_2	$hR18$	$R\overline{3}m$	CO7Y2	Co_7Y_2
Co_3Y	$\cdots$	Be_3Nb	$hR12$	$R\overline{3}m$	CO3Y	Co_3Y_1
Co_2Y	$C15$	Cu_2Mg	$cF24$	$Fd\overline{3}m$	CO2Y	Co_2Y_1
Co_3Y_2	$\cdots$	$\cdots$	$cP*$	$\cdots$	CO3Y2	Co_3Y_2
Co_7Y_6	$\cdots$	$\cdots$	$\cdots$	$\cdots$	CO7Y6	Co_7Y_6
CoY	$B33$	CrB	$oC8$	$Cmcm$	COY	Co_1Y_1
Co_3Y_4	$\cdots$	Co_3Ho_4	$hP22$	$P6_3/m$	CO3Y4	Co_3Y_4
Co_5Y_8	$\cdots$	$\cdots$	$mP52$	$P2_1/c$	CO5Y8	Co_5Y_8
CoY_3	$D0_{11}$	Fe_3C	$oP16$	$Pnma$	COY3	Co_1Y_3
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Co,Y)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_Y			$\Delta_r H$ / (J/mol)
liquid + bcc $\rightleftharpoons$ hcp	peritectic	1751.2	0.981	1.000	1.000	−4896
liquid $\rightleftharpoons$ Co_5Y	congruent	1617.5	0.155	0.155		−33578
fcc + liquid $\rightleftharpoons$ $Co_{17}Y_2$	peritectic	1613.3	0.001	0.114	0.110	−31923
liquid $\rightleftharpoons$ $Co_{17}Y_2$ + Co_5Y	eutectic	1613.3	0.114	0.110	0.137	−32696
Co_5Y + liquid $\rightleftharpoons$ Co_7Y_2	peritectic	1593.0	0.164	0.236	0.222	−28455
Co_7Y_2 + liquid $\rightleftharpoons$ Co_3Y	peritectic	1580.8	0.222	0.275	0.250	−18188
Co_3Y + liquid $\rightleftharpoons$ Co_2Y	peritectic	1427.0	0.250	0.414	0.333	−16225
liquid + hcp $\rightleftharpoons$ CoY_3	peritectic	1161.9	0.736	0.999	0.750	−16777
Co_2Y + liquid $\rightleftharpoons$ Co_3Y_2	peritectic	1139.0	0.333	0.543	0.400	−10918
Co_5Y $\rightleftharpoons$ $Co_{17}Y_2$ + Co_7Y_2	eutectoid	1092.0	0.158	0.106	0.222	−1372
Co_3Y_2 + liquid $\rightleftharpoons$ CoY	peritectic	1071.0	0.400	0.571	0.500	−16986
Co_3Y_2 + CoY $\rightleftharpoons$ Co_7Y_6	peritectoid	1048.0	0.400	0.500	0.462	−2465
CoY + liquid $\rightleftharpoons$ Co_5Y_8	peritectic	1012.6	0.500	0.616	0.615	−20645
liquid $\rightleftharpoons$ Co_5Y_8 + CoY_3	eutectic	1011.3	0.628	0.615	0.750	−20133
CoY + Co_5Y_8 $\rightleftharpoons$ Co_3Y_4	peritectoid	1005.0	0.500	0.615	0.571	−595
fcc + $Co_{17}Y_2$ $\rightleftharpoons$ hcp	peritectoid	695.0	0.000	0.105	0.000	−428

Table IIIa. Integral quantities for the liquid phase at 1800 K.

x_{Y}	ΔG_{m} [J/mol]	ΔH_{m} [J/mol]	ΔS_{m} [J/(mol·K)]	$G_{\mathrm{m}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{m}}^{\mathrm{E}}$ [J/(mol·K)]	ΔC_P [J/(mol·K)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−11761	1932	7.607	−6896	4.905	0.000
0.200	−20390	−4115	9.042	−12901	4.881	0.000
0.300	−26679	−12995	7.602	−17537	2.523	0.000
0.400	−30533	−20885	5.360	−20461	−0.236	0.000
0.500	−31841	−25284	3.643	−21467	−2.120	0.000
0.600	−30556	−25014	3.079	−20484	−2.517	0.000
0.700	−26719	−20221	3.610	−17577	−1.469	0.000
0.800	−20436	−12373	4.479	−12947	0.319	0.000
0.900	−11796	−4261	4.186	−6930	1.483	0.000
1.000	0	0	0.000	0	0.000	0.000

Reference states: Co(liquid), Y(liquid)

Table IIIb. Partial quantities for Co in the liquid phase at 1800 K.

x_{Co}	ΔG_{Co} [J/mol]	ΔH_{Co} [J/mol]	ΔS_{Co} [J/(mol·K)]	$G_{\mathrm{Co}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Co}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Co}	γ_{Co}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1931	4958	3.827	−354	2.951	0.879	0.977
0.800	−5463	12308	9.872	−2123	8.017	0.694	0.868
0.700	−11398	13741	13.966	−6060	11.000	0.467	0.667
0.600	−20153	4918	13.929	−12508	9.682	0.260	0.434
0.500	−31781	−14531	9.583	−21407	3.820	0.120	0.239
0.400	−46000	−41009	2.773	−32287	−4.845	0.046	0.116
0.300	−62289	−66949	−2.589	−44270	−12.599	0.016	0.052
0.200	−80159	−80815	−0.364	−56072	−13.746	0.005	0.024
0.100	−100462	−67104	18.532	−66001	−0.612	0.001	0.012
0.000	$-\infty$	−6341	∞	−71957	36.453	0.000	0.008

Reference state: Co(liquid)

Table IIIc. Partial quantities for Y in the liquid phase at 1800 K.

x_{Y}	ΔG_{Y} [J/mol]	ΔH_{Y} [J/mol]	ΔS_{Y} [J/(mol·K)]	$G_{\mathrm{Y}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Y}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Y}	γ_{Y}
0.000	$-\infty$	79683	∞	−71480	83.979	0.000	0.008
0.100	−100230	−25296	41.630	−65769	22.485	0.001	0.012
0.200	−80098	−69804	5.719	−56011	−7.663	0.005	0.024
0.300	−62336	−75379	−7.246	−44317	−17.257	0.016	0.052
0.400	−46103	−59590	−7.493	−32390	−15.111	0.046	0.115
0.500	−31900	−36037	−2.298	−21527	−8.061	0.119	0.237
0.600	−20260	−14351	3.283	−12615	−0.964	0.258	0.430
0.700	−11475	−195	6.267	−6137	3.301	0.465	0.664
0.800	−5505	4737	5.690	−2165	3.835	0.692	0.865
0.900	−1944	2721	2.592	−367	1.716	0.878	0.976
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Y(liquid)

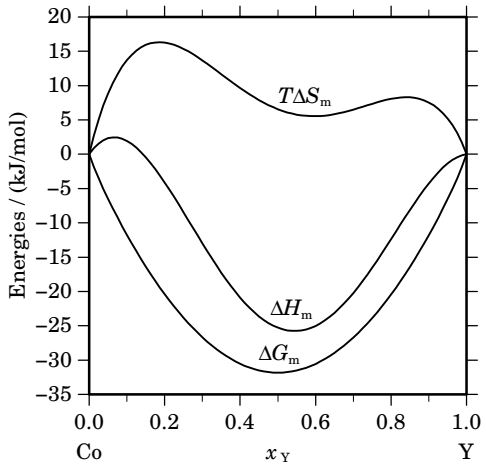

Fig. 2. Integral quantities of the liquid phase at T=1800 K.

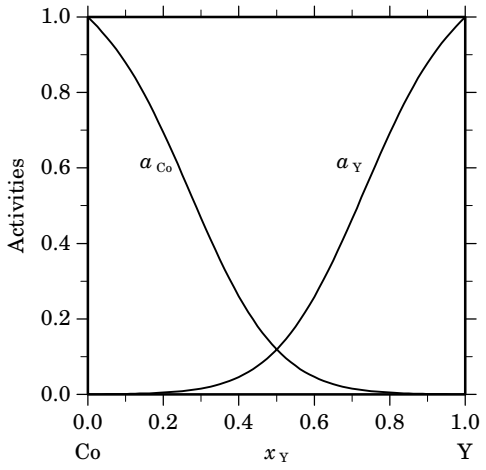

Fig. 3. Activities in the liquid phase at T=1800 K.

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

Compound	x_Y	$\Delta_f G^\circ$ / (J/mol)	$\Delta_f H^\circ$ / (J/mol)	$\Delta_f S^\circ$ / (J/(mol·K))	$\Delta_f C_P^\circ$ / (J/(mol·K))
$Co_{17}Y_2$	0.105	−10488	−10226	−0.878	−0.078
Co_7Y_2	0.222	−19841	−19935	−0.314	0.307
Co_3Y_1	0.250	−21765	−21643	0.407	5.028
Co_2Y_1	0.333	−27238	−27815	−1.935	−0.097
Co_3Y_2	0.400	−30600	−32522	−6.446	−0.087
Co_7Y_6	0.462	−33450	−36853	−11.412	−0.078
Co_1Y_1	0.500	−32365	−35553	−10.693	−0.072
Co_3Y_4	0.571	−29319	−32133	−9.437	−0.062
Co_5Y_8	0.615	−26768	−29066	−7.708	−0.056
Co_1Y_3	0.750	−18245	−18892	−2.171	−0.036

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