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Calculation of thermodynamic properties of the phases in the Y–Ba–Cu–O system

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Abstract

Enthalpy, entropy, specific heat, melting point and associated enthalpy change are calculated for 34 different phases considered to exist in the Y–Ba–Cu–O system. Polynomial coefficients for expressing the reduced Gibbs energy are also listed. Theoretically evaluated data are compared with the standard enthalpies of formation from their elements of the known compounds: Y_2BaCuO_5; $YBa_2Cu_3O_y$; $BaCuO_2$; $Y_2Cu_2O_5$; $YCuO_2$.

INTRODUCTION

According to the data given in refs. 1–10, in the system Y–Ba–Cu–O other phases have been found, besides the known compounds $BaCuO_2$, Y_2BaCuO_5, $Y_2Cu_2O_5$, $YCuO_2$ and $YBa_2Cu_3O_y$ (where y varies from 6 to 7) (Table 1).

Current data about phases are necessary to perform research based on thermodynamical simulation (TS) [11,12].

The purpose of this work is to estimate the thermodynamic and thermochemical properties of some phases, and to calculate their reduced Gibbs energies.

A comparison of calculated and experimental values of the properties of a number of substances has been made.

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TABLE 1

Phases in the system Y–Ba–Cu–O [a]

Phases	Ref.
Ba_2CuO_3, Ba_3CuO_4, $Y_2Ba_4O_7$, Y_2BaO_4	1
$Y_2Ba_4O_7$, $Y_2Ba_2O_5$, Y_2BaO_4, $Y_4Ba_3O_9$, $Y_3BaCuO_{7.5}$ [b]	2
Ba_2CuO_3, Y_2BaO_4, $Y_2Ba_2O_5$, $Y_2Ba_4O_7$, $YBa_3Cu_3O_{7.5}$ [b]	3
$YBa_2Cu_4O_8$ [c], $Y_2Ba_4Cu_7O_{14+x}$ [c]	4
$YBa_3Cu_2O_{6.5}$ [b], Y_2BaO_4, $Y_2Ba_4O_7$	5
Ba_2CuO_3, Y_2BaO_4, $Y_4Ba_3O_9$, $YBa_4Cu_3O_{8.5}$ [b], $YBa_5Cu_2O_{8.5}$ [b], $Y_3Ba_8Cu_5O_{17.5}$ [b]	6
Ba_2CuO_3, Ba_3CuO_4, Y_2CuO_4, Y_2BaO_4, $Y_2Ba_2O_5$, $Y_4Ba_3O_9$, $Y_2Ba_4O_7$, $YBa_2Cu_4O_8$, $YBaCu_2O_{4.5}$ [b], $YBa_4Cu_3O_{8.5}$ [b], $YBa_3Cu_2O_{6.5}$ [b], $YBa_4Cu_2O_{7.5}$ [b], $YBa_5Cu_3O_{9.5}$ [b], $YBa_3CuO_{5.5}$ [b], $YBa_2CuO_{4.5}$ [b], $Y_3Ba_8Cu_5O_{17.5}$ [b], $Y_4BaCu_5O_{17}$ [b]	7
Ba_2CuO_3, $Ba_2Cu_3O_{5+q}$, $YBa_4Cu_3O_{8.5}$ [b], $YBa_6Cu_3O_{10.5}$ [b], $Y_3Ba_8Cu_5O_{17.5}$ [b], Ba_2CuO_3, Ba_3CuO_4, Y_2BaO_4, $Y_2Ba_4O_7$, $Y_4Ba_3O_9$, $YBa_3Cu_3O_{7.5}$ [b],	8
$Y_2Ba_3Cu_5O_{11+q}$, $Y_2BaCu_3O_{7-q}$, $Y_2Ba_4Cu_3O_{8.5+q}$ [b], $YBa_4Cu_3O_8$, $Y_3Ba_8Cu_5O_{16.45}$, $YBa_5Cu_2O_{8.34}$	9
Y_2BaO_4, $Y_2Ba_2O_5$, $Y_2Cu_2O_5$, $YBa_4Cu_3O_{8.97}$, $Y_3Ba_8Cu_5O_{18}$, $YBa_5Cu_2O_{8.97}$, $Y_3Ba_8Cu_5O_{18}$	10

[a] The existence of phases $BaCuO_2$, Y_2BaCuO_5, $Y_2Cu_2O_5$, $YCuO_2$ and $YBa_2Cu_3O_y$ (where y varies from 6 to 7) is considered proved.

[b] The oxygen content is calculated on the assumption that the cations of yttrium, barium and copper have valencies 3, 2 and 2 respectively.

[c] Superconductors with $T_c = 80$ K ($YBa_2Cu_4O_8$) and 14–68 K ($Y_2Ba_4Cu_7O_{14+x}$) [5,13,14].

CALCULATIONS

Some preliminary explanations

In most papers [1–10] the oxygen index in compounds either is not estimated or is not mentioned. These indexes are calculated by proceeding from the valencies of yttrium, barium and copper, which are equal to 3, 2 and 2 respectively.

The algorithm of the program complex ASTRA [11] does not allow the use of formulae containing fractional numbers of atoms. We have therefore adjusted such numbers to integers wherever possible, and doubled the formulae of compounds whose oxygen index is, for example, 6.5 of 8.5, etc.

The estimation of the thermodynamic functions of the superconducting phases $YBa_2Cu_4O_8$ and $Y_2Ba_4Cu_7O_{14+x}$ is of special interest. According to ref. 13 $YBa_2Cu_4O_8$ has a narrow range of oxygen content (7.85–8.1) and $T_c \approx 80$ K. Thus, the group of formulae with oxygen index 8 describes this phase well enough. According to ref. 14, compounds $Y_2Ba_4Cu_7O_{14.3-15.02}$ are superconducting with $T_c = 14$–68 K. We had no possibility of describing these compounds by fractional oxygen indexes, so we estimated thermody-

namical functions for $Y_2Ba_4Cu_7O_{14}$ (non-SC phase) and $Y_2Ba_4Cu_7O_{15}$ (Sc phase).

According to various authors, some compounds have different oxygen indexes at equal cation compositions. We used those values of indexes that are found in several papers and/or obtained from the most reliable experiments. For some phases, which in our opinion, have not been analysed correctly, we did not make calculations of thermodynamic functions.

Calculations of thermodynamic and thermochemical properties were performed by using the methods described in refs. 15 and 16. The temperature dependence of the reduced Gibbs free energy was calculated using the sub-program TERMOS in ASTRA, in the form

$$\phi_n^* = y_1 + y_2(\ln x) + y_3 x + y_4 x^{-1} + y_5 x + y_6 x^2 + y_7 x^3 \quad (1)$$

where y_i are numerical coefficients, $x = T \times 10^{-4}$ (T in K) (technical system of units).

Table 2 shows properties of 34 phases. For compounds **1–4** properties have been calculated previously [15]; for the remainder, these properties are given for the first time.

COMPARISON WITH LITERATURE

We consider it necessary to compare calculated properties with known literature values. Such a comparison was made for $YCuO_2$, $YBa_2Cu_3O_{6.5}$ ($Y_2Ba_4Cu_6O_{13}$), $YBa_2Cu_3O_6$, $Yba_2Cu_3O_7$, $BaCuO_2$, Y_2BaCuO_5 and $Y_2Cu_2O_5$, mainly of standard enthalpies of formation from their elements. For the other phases we did not find any data about properties.

In a number of papers, the standard enthalpies of formation from oxides ($\Delta H^\circ_{298,\text{oxide}}$) were measured; conversion of those values to the enthalpies of formation from the elements was performed by the equation

$$\Delta H^\circ_{298}(i) = \Delta H^\circ_{298,\text{oxide}}(i) + \sum_{n=2} \Delta H^\circ_{298}(\text{oxide}) \quad (2)$$

$YBa_2Cu_3O_7$ (123–O_7): Standard enthalpy of formation from elements

The design value is 662.3 kcal mol^{-1}. In ref. 16 it is quoted as -663.6 kcal mol^{-1}. An approximation of data from ref. 17 made in ref. 18 gives the value of -651.3 kcal mol^{-1}. Averaging various data from ref. 18 leads to a value of -650.0 kcal mol^{-1}. Refs. 19 and 20 give values of -645.4 and -638.9 kcal mol^{-1}, respectively. In ref. 21 $\Delta H^\circ_{298,\text{oxide}}(123\text{–}O_7) = -45.48$ kcal mol^{-1} (in oxygen).

TABLE 2

Design values of thermodynamical and thermochemical properties of some superconducting and concomitant phases in the system Y–Ba–Cu–O

No.	Phase	$-\Delta H^{\circ}_{298}$ (kcal mol^{-1})	S°_{298} (cal K^{-1} mol^{-1})	$H^{\circ}_{298} - H^{\circ}_{0}$ (cal mol^{-1})	$C_p = a + b(10^{-3})T - c(10^5)T^2$ (cal K^{-1} mol^{-1})			T_{melt} (K)	ΔH_{melt} (cal mol^{-1})	$\Delta C_{p,melt}$ (cal K^{-1} mol^{-1})
					a	b	c			
1	$YBa_2Cu_3O_7$	662.3	78.12	12297	72.26	17.03	8.58	1503	41030	104.31
2	$YBa_2Cu_3O_6$	628.5	77.2	12433	66.0	12.61	3.76	1446	36440	90.3
3	Y_2BaCuO_5	659.8	53.9	8883	49.5	8.86	3.3	1545	29200	67.72
4	$BaCuO_2$	183.4	26.7	4250	21.88	5.84	1.48	1280	10750	31.36
5	Ba_2CuO_3	322.7	42.7	6068	33.0	6.72	1.62	1360	17140	45.21
6	Ba_3CuO_4	462.0	58.7	8233	44.0	9.28	1.92	1315	22090	60.28
7	$Y_2Ba_4O_7$	1010.3	91.3	13050	71.5	14.17	3.64	1400	38220	97.96
8	Y_2BaO_4	610.6	43.3	6499	38.5	6.65	3.01	1610	23670	52.75
9	$Y_2Ba_6Cu_4O_{13}$	1488.6	166.1	24278	137.5	25.50	8.50	1495	78490	188.38
10	$Y_2Ba_2O_5$	745.4	59.3	8693	49.5	9.0	3.15	1525	28820	67.82
11	$Y_4Ba_3O_9$	1357.2	102.6	15200	88.0	15.68	6.08	1555	52250	120.56
12	$YBa_2Cu_4O_8$	684.0	88.9	13548	82.5	13.35	7.20	1715	54020	113.03
13	$Y_2Ba_4Cu_6O_{13}$	1298.2	155.4	25330	137.5	25.4	4.25	1496	78540	188.38
14	$Y_2Ba_4Cu_8O_{15}$	1386.4	176.9	26691	159.5	26.97	13.05	1640	99880	218.52

15	$Y_2Ba_4Cu_7O_{14}$	1342.3	166.2	24988	148.5	25.11	14.85	1645	93270	203.45
16	$Y_6Ba_{16}Cu_{10}O_{35}$	4099.0	444.9	65028	368.5	68.34	22.78	1495	210350	504.85
17	Y_2CuO_4	520.5	38.0	5964	38.5	5.81	4.13	1840	27050	52.75
18	$Y_2Ba_2Cu_4O_9$	931.4	102.1	15496	93.5	15.47	7.82	1680	59980	128.10
19	$Y_2Ba_8Cu_4O_{15}$	1767.2	198.1	28629	159.5	30.45	8.99	1450	88310	218.52
20	$Y_2Ba_{10}Cu_6O_{19}$	2134.0	251.5	36415	203.5	38.85	11.47	1450	112670	278.80
21	$Y_2Ba_6Cu_2O_{11}$	1400.4	144.7	20840	115.5	22.26	6.3	1440	63500	158.24
22	$Y_2Ba_4Cu_2O_9$	1121.8	112.7	16482	93.5	17.17	5.95	1510	53910	128.10
23	$Y_2Ba_4Cu_7O_{15}$	1368.6	166.95	27500	151.3	30.89	13.32	1645	96726	216.34
24	$Y_2Ba_8Cu_6O_{17}$	1855.4	219.3	32519	184.1	36.76	18.00	1276	88427	247.26
25	$Y_4BaCu_5O_{12}$	1312.6	124.0	21706	119.3	25.89	10.64	1342	62000	164.95
26	$Y_2Ba_6Cu_6O_{15}$	1576.8	187.4	28587	160.4	33.65	15.03	1266	77100	217.27
27	$Y_2Ba_3Cu_5O_{11}$	1114.8	128.7	20723	114.64	25.55	10.08	1267	55875	157.38
28	$Y_2Ba_{12}Cu_6O_{21}$	2412.6	283.3	40383	225.4	40.59	23.94	1519	130786	307.49
29	$Y_2BaCu_3O_7$	748.0	75.3	12860	70.63	15.56	6.12	1309	35736	97.47
30	$Y_2Ba_{10}Cu_4O_{17}$	2045.8	229.9	30553	181.09	31.97	21.79	1092	71090	231.45
31	$Y_2Cu_2O_5$	526.3	48.7	7650	49.50	8.28	3.96	1500	28350	67.82
32	$YCuO_2$	261.3	23.9	3944	22.0	3.91	1.49	1560	13100	30.04
33	$Ba_2Cu_3O_5$	410.8	64.05	9910	53.29	1.648	3.968	1014	21294	74.87
34	$Ba_3Cu_5O_8$	638.4	101.42	15810	84.57	2.712	5.952	1011	33970	119.81

Conversion by eqn. (2)

$$\Delta H^{\circ}_{298}(123\text{–}O_7) = \Delta H^{\circ}_{298,\text{oxide}}(123\text{–}O_7) + 0.5\Delta H^{\circ}_{298}(Y_2O_3) + 1.5\Delta H^{\circ}_{298}(BaO) + 0.5\Delta H^{\circ}_{298}(BaO_2) + 3\Delta H^{\circ}_{298}(CuO) \quad (3)$$

gives the value -658.8 kcal mol^{-1}.

In the same paper, for an air atmosphere, $\Delta H^{\circ}_{298,\text{oxide}}(123\text{–}O_7) = -36.97$ kcal mol^{-1}. Conversion by eqn. (3) leads to the value of -650.2 kcal mol^{-1}.

According to ref. 8 the enthalpy of formation from oxides is -16.71 kcal mol^{-1}. Calculation by eqn. (3) gives the value -630.0 kcal mol^{-1}. Another possible way of estimating $\Delta H^{\circ}_{298}(123\text{–}O_7)$ is by eqn. (2).

In ref. 22 $\Delta H^{\circ}_{298}(Cu_2O_3)$ is calculated as -84.9 kcal mol^{-1}. With the use of these data and the enthalpy of formation of 123–O_7 from oxides, we can calculate $\Delta H^{\circ}_{298}(123\text{–}O_7)$ by the equation

$$\Delta H^{\circ}_{298}(123\text{–}O_7) = \Delta H^{\circ}_{298,\text{oxide}}(123\text{–}O_7) + 0.5\Delta H^{\circ}_{298}(Y_2O_3) + 2\Delta H^{\circ}_{298}(BaO) + 2\Delta H^{\circ}_{298}(CuO) + 0.5\Delta H^{\circ}_{298}(Cu_2O_3) \quad (4)$$

Conversion of data from refs. 8 and 21 by eqn. (4) leads to the values of -654.4 kcal mol^{-1} (in oxygen), -645.9 kcal mol^{-1} (in air) [21] and -625.7 kcal mol^{-1} [8].

The average of 11 values of $\Delta H^{\circ}_{298}(123\text{–}O_7)$ is -646.7 kcal mol^{-1}, which differs from the calculated value by about 2.4%.

Standard entropy of formation from elements $S^{\circ}_{298}(123\text{–}O_7)$

The design value is 78.12 cal mol^{-1} K^{-1}. According to data in refs. 9, $S^{\circ}_{298}(123\text{–}O_7) = 77.36$ or 76.92 cal mol^{-1} K^{-1}. According to ref. 23, $S^{\circ}_{298}(123\text{–}O_7) = -76.9$ cal mol^{-1} K^{-1}.

Heat capacity at 298 K $C_p(298)$

The design value is 67.67 cal mol^{-1} K^{-1}. According to refs. 9 and 23, values are 68.34, 67.5 and 67.46 cal mol^{-1} K^{-1}.

Value of $H^{\circ}_{298} - H^{\circ}_{0}$

According to calculation the value is 12 297 cal mol^{-1}. According to refs. 9 and 23, $-12\,250$, 12 140 and 12 146 cal mol^{-1}.

$Y_2Ba_4Cu_6O_{13}$ ($YBa_2Cu_3O_{6.5}$): Standard enthalpy of formation from elements

The design value is -1298.2 kcal mol^{-1}. According to ref. 17 for the composition 123–$O_{6.47}$, $\Delta H^{\circ}_{298} = -1277.4$ kcal mol^{-1} (after doubling). The

value according to ref. 19 is -1280 kcal mol^{-1}. In ref. 24, $\Delta H^{\circ}_{298,\text{oxide}}(123\text{–}O_{6.5}) = -34.19$ kcal mol^{-1}. After conversion by eqn. (2) and doubling, we obtain -1275.6 kcal mol^{-1}.

$YBa_2Cu_3O_6$: Standard enthalpy of formation from elements

The design value is -628.5 kcal mol^{-1}. An approximation of data from ref. 17, made in ref. 18, leads to the value of -640.7 kcal mol^{-1}. Averaging of values in ref. 18, leads to the value of -631.6 kcal mol^{-1}. According to data in ref. 9, $\Delta H^{\circ}_{298,\text{oxide}}(123\text{–}O_6) = -34.19$ kcal mol^{-1}. Conversion by eqn. (2) gives the value -621.4 kcal mol^{-1}.

$BaCuO_2$: Standard enthalpy of formation from elements

The design value is -183.4 kcal mol^{-1}. According to refs. 9 and 25 $\Delta H^{\circ}_{298,\text{oxide}}(BaCuO_2) = -23.45$ and -22.31 kcal mol^{-1}, respectively. Conversion by eqn. (2) gives the values -192.8 and -191.7 kcal mol^{-1}, respectively. According to ref. 25, $\Delta H^{\circ}_{298}(BaCuO_2) = -192$ kcal mol^{-1}.

In ref. 26 the standard enthalpies of formation from their elements of $BaCuO_{2.05}$, $BaCuO_{2.095}$ and $BaCuO_2$ were estimated, as -190.6, -193.5 and -187.7 kcal mol^{-1}, respectively.

Melting points, according to calculations and data in ref. 27, are 1280 and 1223 K, respectively.

Y_2BaCuO_5: Standard enthalpy of formation from elements

The design value is -659.8 kcal mol^{-1}. According to ref. 9, the enthalpy of formation from oxides is -18.72 kcal mol^{-1}. Conversion by eqn. (2) gives the value -643.5 kcal mol^{-1}. According to ref. 24, $\Delta H^{\circ}_{298}(Y_2BaCuO_5) = -647.3$ kcal mol^{-1}.

Melting points, according to calculations and data in ref. 27, are 1545 and 1423 K, respectively.

$Y_2Cu_2O_5$: Standard enthalpy of formation from elements

The design value is -526.3 kcal mol^{-1}. According to ref. 9 $\Delta H^{\circ}_{298,\text{oxide}}(Y_2Cu_2O_5) = 13.38$ kcal mol^{-1}. Conversion by ref. (2) gives the value -543 kcal mol^{-1}. According to the data in ref. 28 the enthalpy of formation is 549.3 kcal mol^{-1}. Melting points, according to calculations and data in ref. 27, are 1500 and 1423 K, respectively.

$YCuO_2$

Design values of ΔH°_{298} and S°_{298} are -261.3 kcal mol^{-1} and 23.9 cal mol^{-1} K^{-1}. According to ref. 28, these values are -255.9 kcal mol^{-1} and 21.76 cal mol^{-1} K^{-1}.

TABLE 3

Polynomial coefficients of reduced Gibbs energy [a]

No.	Substance	T (K)	Polynomial coefficients [b]				
			y_1	y_2	y_3	y_4	y_5
1	$YBa_2Cu_3O_7$	298–1503	260.307	76.4024	−0.0054411	1.46744	62.153
		1503–6000	326.156	101.8	0	0.1724	0
2	$YBa_2Cu_3O_6$	298–1446	241.434	66.0001	0.0018804	0.65333	63.053
		1446–6000	307.582	90.4202	0	−0.7519	0
3	Y_2BaCuO_5	298–1545	173.807	49.5	−0.00165	0.736877	44.303
		1545–6000	222.359	67.8202	0	−0.431503	0
4	$BaCuO_2$	298–1280	79.116	21.8801	−0.00074	0.302628	29.203
		1280–6000	105.043	31.3602	0	−0.048904	0
5	Ba_2CuO_3	298–1360	122.722	33	−0.00081	0.46081	33.5999
		1360–6000	156.658	45.21	0	-0.226014	0
6	Ba_3CuO_4	298–1315	165.436	44.0001	−0.00096	0.593534	46.403
		1315–6000	211.241	60.28	0	−0.291609	0
7	$Y_2Ba_4O_7$	298–1400	264.725	71.5	−0.00182	1.01077	70.853
		1400–6000	337.519	97.96	0	−0.5215	0
8	Y_2BaO_4	298–1610	136.383	38.5	−0.0015054	0.62794	33.253
		1610–6000	173.625	52.7502	0	−0.3254	0
9	$Y_2Ba_6Cu_4O_{13}$	298–1495	499.287	137.5	−0.00425	2.06817	127.503
		1495–6000	635.915	188.3801	0	−1.0808	0
10	$Y_2Ba_2O_5$	298–1525	179.25	49.5	−0.001575	0.75148	45.003
		1525–6000	228.074	67.82	0	−0.4039	0
11	$Y_4Ba_3O_9$	298–1555	315.67	88.0001	−0.00304	1.37606	78.403
		1555–6000	401.817	120.5601	0	−0.7207	0
12	$YBa_2Cu_4O_8$	298–1715	288.211	82.5	−0.0036	1.4046	66.752
		1715–6000	366.026	113.0302	0	−0.7668	0
13	$Y_2Ba_4Cu_6O_{13}$	298–1496	491.00	137.5	−0.0021254	1.81991	127.003
		1496–6000	627.384	188.3801	0	−1.2932	0
14	$Y_2Ba_4Cu_8O_{15}$	298–1640	562.378	159.5001	−0.0065254	2.64168	134.852
		1640–6000	715.435	218.5201	0	−1.3735	0

15	$Y_2Ba_4Cu_7O_{14}$	298–1645	523.573	148.5	−0.0074254	2.53632	125.552
		1645–6000	666.078	203.4502	0	−1.2391	0
16	$Y_6Ba_{16}Cu_{10}O_{35}$	298–1495	1337.839	368.4997	−0.0113904	5.54637	341.7
		1495–6000	1703.993	504.8498	0	−2.8937	0
17	Y_2CuO_4	298–1840	130.70	38.5	−0.0020654	0.7153	29.052
		1840–6000	166.028	52.7502	0	−0.3737	0
18	$Y_2Ba_2Cu_4O_9$	298–1680	328.076	93.5001	−0.0039104	1.56781	77.352
		1680–6000	417.025	128.1	0	−0.8471	0
19	$Y_2Ba_8Cu_4O_{15}$	298–1450	584.827	159.5	−0.0044945	2.32709	152.253
		1450–6000	745.045	218.52	0	−1.2091	0
20	$Y_2Ba_{10}Cu_6O_{19}$	298–1450	744.91	203.5	−0.0057354	2.98021	194.253
		1450–6000	949.324	278.8	0	−1.5315	0
21	$Y_2Ba_6Cu_2O_{11}$	298–1440	424.799	115.5	−0.0031504	1.66816	111.303
		1440–6000	541.19	158.2402	0	−0.879	0
22	$Y_2Ba_4Cu_2O_9$	298–1510	339.222	93.5	−0.0029754	1.41401	85.853
		1510–6000	431.791	128.1002	0	−0.7493	0
23	$Y_2Ba_4Cu_7O_{15}$	298–1645	530.499	151.3001	−0.0066604	2.34289	154.453
		1645–6000	692.706	216.3402	0	−0.8911	0
24	$Y_2Ba_8Cu_6O_{17}$	298–1276	660.899	184.1	−0.009	3.00153	183.8
		1276–6000	844.535	247.26	0	−0.915612	0
25	$Y_4BaCu_5O_{12}$	298–1342	410.124	119.3	−0.005321	1.85654	129.45
		1342–6000	537.398	164.95	0	−0.627859	0
26	$Y_2Ba_6Cu_6O_{15}$	298–1266	572.034	160.4	−0.0075154	2.575	168.253
		1266–6000	736.669	217.2702	0	−0.7506	0
27	$Y_2Ba_3Cu_5O_{11}$	298–1267	403.529	114.64	−0.0050404	1.79568	127.753
		1267–6000	525.873	157.3802	0	−0.507	0
28	$Y_2Ba_{12}Cu_6O_{21}$	298–1519	824.211	225.4	−0.0119704	3.66221	202.953
		1519–6000	1045.097	307.4902	0	−1.7873	0
29	$Y_2BaCu_3O_7$	298–1309	224.728	70.6301	−0.0030604	1.09324	77.803
		1309–6000	320.309	97.4702	0	−0.3469	0
30	$Y_2Ba_{10}Cu_4O_{17}$	298–1092	665.741	182.0901	−0.0108954	3.24415	159.854
		1092–6000	826.618	231.4502	0	−0.5804	0

TABLE 3 (continued)

No.	Substance	T (K)	Polynomial coefficients [b]				
			y_1	y_2	y_3	y_4	y_5
31	$Y_2Cu_2O_5$	298–1500	168.409	49.5001	−0.0019804	0.87976	41.403
		1500–6000	216.252	67.8202	0	−0.1652	0
32	$YCuO_2$	298–1560	77.187	22.0001	−0.0007454	0.32857	19.553
		1560–6000	98.612	30.0402	0	−0.2125	0
33	$Ba_2Cu_3O_5$	298–1014	195.304	53.2902	−0.0019844	0.53707	82.405
		1014–6000	260.632	74.8703	0	−0.2122	0
34	$Ba_3Cu_5O_8$	298–1011	309.235	84.5702	−0.0029764	0.85988	135.605
		1011–6000	415.48	119.8103	0	−0.3015	0

[a] From eqn. (1) (in cal K^{-1} mol^{-1}). [b] Coefficients y_6 and y_7 are equal to zero for all phases.

In general, calculated and measured properties show good agreement and suggest promising uses of these calculations of thermodynamic data.

Table 3 summarizes the coefficients y_i of the approximating polynomial ϕ_n^* in eqn. (1).

CONCLUSIONS

On the basis of analysis of data for the Y–Ba–Cu–O system 34 phases (stable, metastable of hypothetical) were chosen, and identified in it. Calculations were used to estimate ΔH°_{298}, S°_{298}, $H^\circ_{298} - H^\circ_0$, $C_p(T)$, T_{melting} and $\Delta H_{\text{melting}}$, in addition to the temperature dependence of the reduced Gibbs energy in the range 298–6000 K.

Calculated and experimentally measured properties of $YBa_2Cu_3O_7$, $YBa_2Cu_3O_{6.5}$, $YBa_2Cu_3O_6$, $BaCuO_2$, Y_2BaCuO_5, $Y_2Cu_2O_5$ and $YCuO_2$ are in satisfactory agreement.

The data presented can be found useful in the further classification of phase compatibilities [29] as well as of formation under non-equilibrium (interface curvature of stress) conditions [30].

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