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Estimation and revision of some thermodynamic data in the YBaCuO system.
Part 3. Heat capacities

G. Moiseev [a],*, N. Vatolin [a] and J. Šesták [b]

[a] *Institute of Metallurgy, Ural Division of Russian Academy of Sciences, 101 Amundsen Str., GSP-812, Ekaterinburg 620219, Russian Federation*
[b] *Institute of Physics, Academy of Sciences of the Czech Republic, 10 Cukrovarnicka, 16200 Prague 6, Czech Republic*

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Abstract

By analysing the literature data for $YBa_2Cu_3O_7$ (123-O_7), $YBa_2Cu_3O_6$ (123-O_6), $YBa_2Cu_4O_8$ (124-O_8), $YBa_2Cu_{3.5}O_{7.5}$ (123.5-$O_{7.5}$), Y_2BaCuO_5 (211), $BaCuO_2$ (011), $Y_2Cu_2O_5$ (202), $YCuO_2$ (101), Y_2BaO_4 (210), $Y_4Ba_3O_9$ (430) and $BaCu_2O_2$ (012), the basic values of $C_p^\ominus(298)$ and the corrected temperature dependences of the heat capacity are suggested. It is shown that it is preferable to use the method of addition of the heat capacities of the simple oxides constituting the complex compounds (the method of Neumann–Kopp) for the calculation of the temperature dependences of the heat capacities of the compounds. In addition, the $C_p = f(T)$ dependences were also calculated for $Y_2Ba_2O_5$ (220), Ba_2CuO_3 (021). Ba_3CuO_4 (031), $YBa_4Cu_3O_{8.5}$ (143-$O_{8.5}$) and $YBa_2Cu_5O_9$ (125-O_9).

INTRODUCTION

Using different empirical and quasi-thermodynamic methods, we previously calculated [1–3] the temperature dependences of the heat capacities of 34 real and hypothetical compounds of the YBaCuO system. We have since collected some additional data (Table 1), allowing us to estimate the heat capacities of the compounds of this system more correctly.

The aim of the present paper is to attempt to systematize and evaluate the data available to authors for the heat capacities of compounds in the YBaCuO system, to correct them, to estimate the best calculation method for $C_p = f(T)$, and to revise the data, particularly for compounds whose existence has been demonstrated experimentally [17, 18].

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* Corresponding author.

TABLE 1

Standard heat capacities and temperature dependences of the heat capacity of some phases in the YBaCuO system

$C_p^\ominus$ 298 in J K^{-1} mol^{-1}	$C_p = f(T)$ in J K^{-1} mol^{-1}	Ref.	Remarks
123-O_X, $x \approx 7$			
282.1 $x = 7.0$	–	4	Experiment
285.8 $x = 7.0$	–	5	Experiment
285.03 $x = 7.0$	$319.82 + 52.02 \times 10^{-3}T - 45.55 \times 10^{5}T^{-2}$, 298–600 K	6	Experiment
283.52 $x = 6.9$	–	7	Experiment
285.7 $x = 7$	–	8	Experiment
282.7 $x = 6.98$	–	9	Experiment
287.12 $x = 7$	–	10	Experiment
283.00 $x = 7$	$302.19 + 71.219 \times 10^{-3}T - 35.882 \times 10^{5}T^{-2}$, $298 - T_m$ K	1–3	Calculated using empirical dependences
283.81 $x = 7$	$438–2387 \times T^{-0.5} - 18.15 \times 10^{5}T^{-2} + 11.97 \times 10^{7}T^{-3}$, 100–1200 K	11	Calculated from experimental data at low temp.
297.8 $x = 7$	$303.75 + 66.39 \times 10^{-3}T - 22.85 \times 10^{5}T^{-2}$, 298–$T_m$ K	12	Calculated with regard to known θ_D and $C_p^\ominus$ 298
295 $x = 6.9$	–	13	Experiment
123-O_x $x \approx 6$			
274.0 $x = 6$	$276.0 + 52.735 \times 10^{-3}T - 15.72 \times 10^{5}T^{-2}$, 298–$T_m$ K	1–3	Calculated with regard to known $C_p^\ominus$ 298
269.3 $x = 6.3$	–	9	Experiment
280.21 $x = 6$	–	10	Experiment
124-O_8			
319.5	–	8	Experiment
327.73	$345.0 + 55.83 \times 10^{-3}T - 30.11 \times 10^{5}T^{-2}$, $298 - T_m$ K	1, 2	Calculated using empirical dependencies
320.5	$473–2241T^{-0.5} - 22.59 \times 10^{5}T^{-2} + 16.24 \times 10^{7}T^{-3}$ 100–1200 K	11	Calculated from experimental data at low temperatures
123.5-$O_{7.5}$			
298.62	–	14	Experiment
304.26	$316.37 + 64.59 \times 10^{-3}T - 27.852 \times 10^{5}T^{-2}$, 298–$T_m$ K	1, 2	Calculated using empirical dependences
211			
202.5	$207.0 + 37.052 \times 10^{-3}T - 13.8 \times 10^{5}T^{-2}$, 298–$T_m$ K	1–3	Calculated using empirical dependences
185.35	$205.2 + 33.35 \times 10^{-3}T - 28.05 \times 10^{5}T^{-2}$, 300–1200 K	11	Calculated from experimental data at low temperatures

TABLE 1 (continued)

$C_p^{\ominus}$ 298 in J K^{-1} mol^{-1}	$C_p = f(T)$ in J K^{-1} mol^{-1}	Ref.	Remarks
011			
82.85	$82.84 + 2.927 \times 10^{-3}T$, $298-T_m$ K	15	Estimation calculation
91.80	$91.5 + 24.42 \times 10^{-3}T$ $-6.19 \times 10^5 T^{-2}$, $298-T_m$ K	1–3	Calculated using empirical dependences
89.33	$91.4 + 24.43 \times 10^{-3}T$ $-8.3 \times 10^5 T^{-2}$, 300–1200 K	11	Calculated from experimental data at low temperatures
202			
198.67	$207.0 + 34.63 \times 10^{-3}T$ $-16.56 \times 10^5 T^{-2}$, $298-T_m$ K	1, 2	Calculated using empirical dependences
186.6 ± 0.4	–	16	Experiment
195.78	$203.4 + 49.07 \times 10^{-3}T$ $-19.75 \times 10^5 T^{-2}$, 300–1200 K	11	Calculated from experimental data at low temperatures
101			
89.86	$92.0 + 16.35 \times 10^{-3}T$ $-6.23 \times 10^5 T^{-2}$, $298-T_m$ K	1, 2	Calculated using empirical dependences
87.57	$93.8 + 16.38 \times 10^{3}T$ $-9.87 \times 10^5 T^{-2}$, 300–1200 K	11	Calculated from data at low temperatures
210			
155.11	$161.0 + 27.81 \times 10^{-3}T$ $-12.59 \times 10^5 T^{-2}$, $298-T_m$ K	1, 2	Calculated using empirical dependences
140.67	$168.3 + 13.27 \times 10^{-3}T$ $-28.05 \times 10^5 T^{-2}$, 300–1200 K	11	Calculated from experimental data at low temperatures
358.90	$368.0 + 65.57 \times 10^{-3}T$ $-25.43 \times 10^5 T^{-2}$, $298-T_m$ K	1, 2	Calculated using of empirical dependences
358.18	$419.5 + 30.88 \times 10^{-3}T$ $-64.4 \times 10^5 T^{-2}$, 300–1200 K	11	Calculated from experimental data at low temperatures
012			
120.36	$121.3 + 28.2 \times 10^{-3}T$ $-8.3 \times 10^5 T^{-2}$, 300–1200, K	11	Calculated using experimental data at low temperatures
114.35	$115.3 + 25.974 \times 10^{-3}T$ $-7.716 \times 10^5 T^{-2}$, $298-T_m$ K	1, 2	Calculated by our methods

ANALYSIS OF LITERATURE DATA FOR THE HEAT CAPACITIES OF THE COMPOUNDS

From the data given in Table 1, the most valid $C_p^\ominus(298)$ values for each compound were selected applying principles described earlier [19], see Table 2, with average quadratic deviations from mean arithmetic values. The $C_p^\ominus(298)$ value for the phase 128-O_7 is estimated to be most reliable. For the phases 211 and 210, the mean quadratic deviations are maximal: ± 8.57 and ± 2.2 J K^{-1} mol^{-1} respectively. For the remaining compounds the average value of the average quadratic deviation is ± 2.1 J K^{-1} mol^{-1}.

TABLE 2

Basic values of the heat capacities of the compounds $\bar{C}_p^\ominus(298)$

Compound	$C_p^\ominus(298)$ in J K^{-1} mol^{-1}	Ref.	$\bar{C}_p^\ominus(298)$ in J K^{-1} mol^{-1}
123-O_7	282.1	4	283.71 ± 0.41
	285.8	5	
	285.03	6	
	283.52	7	
	284.7	8	
	282.7	9	
	283.0	1–3	
	283.81	11	
123-O_6	274.0	1–3	274.63 ± 3.05
	269.3	9	
	280.2	10	
124-O_8	319.5	8	322.58 ± 2.6
	327.73	1, 2	
	320.5	11	
123.5-$O_{7.5}$	298.62	14	301.44 ± 2.82
	304.26	1, 2	
211	202.5	1–3	193.93 ± 8.57
	185.35	11	
011	91.8	1–3	90.56 ± 1.24
	89.33	11	
202	198.67	1, 2	193.68 ± 3.64
	186.6	16	
	195.78	11	
101	89.86	1, 2	88.72 ± 1.14
	87.57	11	
210	155.11	1, 2	147.9 ± 7.2
	140.67	11	
430	358.90	1, 2	357.54 ± 1.36
	358.18	11	
012	120.36	11	117.36 ± 3.0
	114.35 [a]	–	

[a] Calculated by us using the methods in refs. 1 and 2.

TABLE 3

Deviations in the value of $C_p(T)$ calculated by different equations

Compound	ΔC_p in %, at T/K			
	298	500	1000	1200
123-O_7 [a]	−0.36	−1.27	+0.69	+1.6
	+0.08	−0.81	−1.77	−2.95
124-O_8 [b]	+2.26	−0.81	−0.48	−0.81
202	+1.48	−0.95	−4.1	−5.1
211	+9.25	+4.54	+3.0	+3.05
011	+2.76	+1.04	+0.36	+0.28
210	+10.26	+3.86	+5.02	+5.3
430	+0.76	−4.44	−2.82	−1.5
101	+2.62	−0.17	−1.22	−1.26
012	−5.0	−5.2	−5.4	−4.7
$\lvert\Delta \bar{C}_p\rvert$	1.875	1.445	1.785	2.098
$\Sigma\,\lvert\Delta \bar{C}_p\rvert = 1.8$				

[a] Comparison of $C_p(T)$ from refs. 1–3 and 11, with data of ref. 6, obtained by experiment and extrapolated to 1000 and 1200 K.

[b] For this and all the remaining compounds, there is comparison of the data obtained in refs. 1–3 with the data of ref. 11.

To estimate the correctness of the temperature dependences of the heat capacities of the compounds, data for 123-O_7 were omitted because no reliable experimental data are available for $T > 298$ K.

We compared the temperature dependences of the heat capacities of the compounds, as follows. Using the equation $C_p = f(T)$, given in Table 1 for a number of the compounds, for the temperatures 298, 500, 1000 and 1200 K, we calculated and compared the values of ΔC_p in %, see Table 3. For 123-O_7, the ΔC_p values were estimated from experimental data given in ref. 6 and extrapolated for 1000 and 1200 K. For the remaining compounds, we compared the data of refs. 1–3 with the results of ref. 11. The average value of the maximum deviation for all the compounds at different temperatures $|\Delta \bar{C}_p|$ is 1.8%. For phases 211, 210 and 012, $|\Delta C_p|$ is 3–10.3%, the maximum deviation, as a rule, being observed at 298 K. The agreement of the $C_p = f(T)$ dependences for 123-O_7 is good when the equations from refs. 1–3, 6 and 11 are used; for the rest of the compounds, it is satisfactory except for 211, 210 and 012.

In order to make the function $C_p = f(T)$ correct and smooth, we have to use the following procedures. For compounds, given in Table 3, coefficients a, b and c in the equation

$$C_p = a + bT - cT^{-2} \text{ in J K}^{-1}\text{ mol}^{-1} \qquad (1)$$

were established as mean arithmetic values and the coefficients obtained a', b' and c' were used to calculate $C_p^{\ominus\prime}(298)$. Thus, we determined the difference between this and the basic value of the standard heat capacity

$$\Delta C_p^{\ominus}(298) = C_p^{\ominus\prime}(298) - \bar{C}_p^{\ominus}(298) \tag{2}$$

The value of $\Delta C_p^{\ominus}(298)$ was used for the recorrection of coefficient a' so that the new value of a'' was obtained from

$$C_p = a'' + bT - cT^{-2} \tag{3}$$

and the value of $C_p^{\ominus}(298)$ is equal to the basic value, $\bar{C}_p^{\ominus}(298)$, for the under consideration.

For example, for phase 202 the averaged value of $C_p = f(T)$ with coefficients a', b' and c' is

$$C_p(T) = 205.2 + 41.85 \times 10^{-3}T - 18.155 \times 10^{5}T^{-2} \text{ in J K}^{-1}\text{ mol}^{-1} \tag{4}$$

to yield $C_p^{\ominus\prime}(298) = 197.23$ and $\bar{C}_p^{\ominus}(298) = 193.68$ J K^{-1} mol^{-1}. Then

$$\Delta C_p(298) = 197.23 - 193.68 = 3.55 \text{ J K}^{-1}\text{ mol}^{-1} \tag{5}$$

and the corrected value of coefficient a'' in eqn. (3) is

$$a'' = 205.2 - 3.55 = 201.65 \text{ J K}^{-1}\text{ mol}^{-1} \tag{6}$$

and the resulting corrected equation is

$$C_p(T) = 201.65 + 41.85 \times 10^{-3}T - 18.155 \times 10^{5}T^{-2} \text{ J K}^{-1}\text{ mol}^{-1} \tag{7}$$

All the coefficients of equations $C_p = f(T)$ given in Table 3 were corrected in a similar way.

RESULTS

Table 4 gives the corrected coefficients of the temperature dependence of the heat capacities of a wide variety of compounds. It is assumed that these dependences can be used in the temperature range from 298 K up to the temperatures of melting and/or decomposition. For the 123-O_7 phase, the equation $C_p = f(T)$ describes the heat capacity only relatively because this phase is metastable [20, 21]. During heating under equilibrium conditions, it loses oxygen (at $T > 600$–$700°C$ in oxygen and at $T > 500$–$650°C$ in air) on transition from the orthorhombic to the tetragonal form [22], the composition changing from 123-O_7 to 123-O_6 [22, 23]. This certainly influences the value of the heat capacity [24]. Clearly, the possibility of compositional changes due to oxygen losses on temperature increases cannot be excluded for the other compounds. Thus, one should bear in mind that the temperature dependences of the heat capacities of the compounds, given in Table 4, are estimated as being valid for the thermodynamically stable stoichiometric compounds ranging from 298 K up to their temperatures of melting and/or decomposition.

TABLE 4

Corrected temperature dependences of the heat capacities of some compounds

Compound	$C_p = a + bT - cT^{-2}$ in J K^{-1} mol^{-1}		
	a	$b \times 10^3$	$c \times 10^{-5}$
123-O_7	315.29	54.466	42.45
123-O_6	276.63	52.735	15.72
124-O_8	356.72	45.735	42.47
123.5-$O_{7.5}$	313.55	64.590	27.85
211	206.10	35.200	20.925
011	91.45	24.425	7.245
202	201.65	41.850	18.155
101	92.90	16.365	8.05
210	164.65	20.535	20.32
430	393.75	48.225	44.915
012	118.3	28.087	8.01

DISCUSSION

It would be interesting to determine which calculation method is the most correct. The equation $C_p = f(T)$ for 123-O_7, given in Table 4, can be used as a standard. With different empirical and quasi-thermodynamic methods, the values of the heat capacities at different temperatures can be calculated and compared with the value calculated from the standard dependence at the same temperatures.

For calculation of $C_p = f(T)$, several methods are of use, see Table 5. Deviations of $C_p(T)$, for the temperatures 298, 500, 1000 and 1200 K, are given in Table 6. Satisfactory agreement with standard $C_p(T)$ values is observed for methods A, B, and D.

It is expedient to use the rule of Neumann–Kopp (RNK) for further correction and additional checking of the dependences $C_p = f(T)$ for phases 211, 210, 012, 202, 123-O_6 and 123.5-$O_{7.5}$ (Table 4), and for the revision of $C_p = f(T)$ for phases 220, 021, 031 and 143-$O_{8.5}$ from refs. 1, 2 and for the estimation of the temperature dependence of the heat capacity of the 125-O_9 phase.

From Table 7, it follows that the agreement between the $C_p(T)$ values obtained using the RNK and the values given in Table 4 can be considered good, except for 123-O_6 and 123.5-$O_{7.5}$. The revision of the dependences $C_p = f(T)$ [1, 2] shown in Table 8 can be considered satisfactory except for 143-$O_{8.5}$. The difference is to do with a misprint in refs. 1 and 2 that was missed by the authors when checking the text: instead of $a = 184.1$ cal K^{-1} mol^{-1}, it should reach $a = 134.1$. With regard to this error $|\Delta \bar{C}_p|$ is 5.1%. For the phases of Table 8, however, it is better to use $C_p = f(T)$ on bases of the RNK.

TABLE 5

Methods used for the calculation of the $C_p = f(T)$ dependences for the phase 123-O_7

(A) Additive, using the $C_p(T)$ of simple oxides [26] and the Neuman–Kopp rule [25]

$C_p(T)\mathrm{BaO} = 12.74 + 1.04 \times 10^{-3}T - 1.984 \times 10^{5}T^{-2}$, 298–1270 K
$C_p(T)\mathrm{BaO_2} \approx 13.6 + 2 \times 10^{-3}T$
$C_p(T)\mathrm{Cu_2O} = 14.9 + 5.7 \times 10^{-3}T$, 298–1200 K
$C_p(T)\mathrm{CuO} = 9.27 + 4.8 \times 10^{-3}T$, 298–1250 K
$C_p(T)\mathrm{Y_2O_3} = 29.21 + 1.72 \times 10^{-3}T - 4.6 \times 10^{5}T^{-2}$, 286–1300 K,
All in cal K^{-1} mol^{-1} [25]. In particular, for 123-O_7 by summation:
$C_p(T) = 0.5C_p(T)[\mathrm{Y_2O_3}] + 1.5C_p(T)[\mathrm{BaO}] + 0.5C_p(T)[\mathrm{BaO_2}] + 3C_p(T)[\mathrm{CuO}]$
Converted into SI units:
$C_p(T)285.735 + 74.523 \times 10^{-3}T - 22.064 \times 10^{5}T^{-2}$ J K^{-1} mol^{-1}

(B) Utilizing known values of $C_p^\circ(298)$ and T_{melt} [25]; $C_p^\circ(298)$ [123-O_7] = 283.72 J K^{-1} mol^{-1} and $T_{\mathrm{melt}} = 1288$ K [17]

$a = \{T_m \times 10^{-3}[C_p^\circ(298) + 1.125n] - 0.298 \times 10^5 nT_m^{-2} - 2.16n\}/(T_m \times 10^{-3} - 0.298)$ cal K^{-1} mol^{-1}
$b = [6.125n + 10^5 \times nT_m^{-2} - C_p^\circ(298)]/(T_m \times 10^{-3} - 0.298)$ cal K^{-2} mol^{-1}
$c = -n$ cal K mol^{-1}
n is the number of atoms in a molecule of the compound. After the conversion:
$C_p(T) = 329.09 + 53.082 \times 10^{-3}T - 54.366 \times 10^{5}T^{-2}$ J K^{-1} mol^{-1}

(C) As for (B), but adding the Debye temperature, $\theta_D = 372.17$ K [28, 29]

$a = n[5.96 - 0.3C_p^\circ(298)\theta_D/(nT_m)]$ cal K^{-1} mol^{-1}
$b = 0.34C_p^\circ(298)/T_m$ cal K^{-2} mol^{-1}
$c = 0.9[a + b298 - C_p^\circ(298)n] \times 10^5$ cal K mol^{-1}
n is the number of atoms in a molecule of the compounds,
$C_p^\circ(298)$ is in (cal K^{-1} mol^{-1})/n
After the calculations and the conversation:
$C_p(T) = 322.15 + 5.763 \times 10^{-3}T\text{-}36.71 \times 10^{5}T^{-2}$ J K^{-1} mol^{-1}

(D) As for (B), but adding the derivative $(\partial C_p/\partial T)_{298}^\circ = 82 \times 10^{-3}$ cal K^{-2} mol^{-1} [5] to the known experimental dependence $C_p = f(T)$ in the range 0–298 K [30]

$b = 1/4[C_p^\circ(298)/T_m](T_m/298)^{1/4}]$ cal K^{-2} mol^{-1}
$c = 0.132 \times 10^8[(\partial C_p \partial T)_{p,298} - b]$ cal K mol^{-1}
$a = C_p^\circ(298) - b298 + c298^{-2}$ cal K^{-1} mol^{-1}
Yielding after conversion:
$C_p(T) = 299.23 + 79.404 \times 10^{-3}T - 34.86 \times 10^{5}T^{-2}$ J K^{-1} mol^{-1}

(E) As for (B), but using the characteristic temperature τ [27]

$a = 5.5$ (cal K^{-1} mol^{-1})/n
$b = 0.125/\tau$ (cal K^{-2} mol^{-1})/n
$c = [5.5 + 37.25/\tau - C_p(T)]\ 298^2$ (cal K mol^{-1})/n
Using the known value of $C_p^\circ(298) = 5.2187$ cal K^{-1} (g atom)$^{-1}$ (this work) and $\tau = 140.4$ [27], we obtain:
$C_p(T) = 299.0 + 48.402 \times 10^{-3}T - 26.39 \times 10^{5}T^{-2}$ J K^{-1} mol^{-1}

TABLE 6

Deviations of $C_p(T)$, calculated by the method given in Table 5 for the 123-O_7 phase

Method for Calculating $C_p(T)$	ΔC_p in % at T/K				Average absolute deviation $\lvert\Delta\bar{C}_p\rvert$ in %
	298	500	1000	1200	
A	−0.22	−3.5	−2.04	+1.08	1.70
B	0	+2.56	+3.07	+3.0	2.16
C	−0.42	−4.67	−11.3	−13.55	7.50
D	0	+0.16	+2.64	+3.8	1.65
E	0	−3.96	−5.67	−5.94	3.90
Using the mean arithmetic coefficients of the methods					
(A) + (B)	−0.11	−0.47	+0.52	+0.96	0.52
(A) + (D)	−0.11	−1.67	+0.3	+1.36	0.86

TABLE 7

Differences of $C_p(T)$ for 211, 210, 012, 202, 123-O_6 and 123.5-$O_{7.5}$, calculated by method A in Table 5 and by the equation in Table 4

Compound	ΔC_p in % at T/K				$\lvert\Delta\bar{C}_p\rvert$ in %
	298	500	1000	1200	
211	−0.2	+1.7	+1.6	+1.34	1.21
210	0	+2.0	+0.57	−0.27	0.71
012	−2.3	−1.76	−1.9	−0.9	1.72
202	−0.8	+0.2	+1.4	+1.80	1.05
123-O_6	+9.5	+13.0	+16.3	+17.23	14.0
123.5-$O_{7.5}$	+1.34	+1.15	+3.2	+4.1	2.45

TABLE 8

Differences in $C_p(T)$ for 220, 021, 031 and 143-$O_{8.5}$ calculated by the rule of Neumann–Kopp and by the equations in refs. 1 and 2

Compound	ΔC_p in % at T/K				$\lvert\Delta\bar{C}_p\rvert$ in %
	298	500	1000	1200	
220	−5.33	+1.63	+1.2	+0.21	2.1
021	−2.6	−2.44	−4.07	−4.16	3.32
031	−3.36	+2.63	+3.15	+2.78	3.0
143-$O_{8.5}$	−31.9	−29.06	−31.0	−32.1	31.0

TABLE 9

Temperature dependences of the heat capacities of the main compounds of the YBaCuO system at 298-$T_{\text{melt/decom}}$

Compound	$C_p = a + bT - cT^{-2}$ in J K^{-1} mol^{-1}		
	a	$b \times 10^3$	$c \times 10^{-5}$
123-O_7	315.29	54.466	42.45
123-O_6	307.48	76.28	26.213
124-O_8	356.72	45.735	42.47
123.5-$O_{7.5}$	305.12	84.56	22.064
125-O_9	363.27	114.67	22.064
143-$O_{8.5}$	312.96	41.067	42.81
211	206.10	35.20	20.925
202	201.65	41.85	18.155
101	92.9	16.365	8.06
210	164.65	20.535	20.32
220	227.88	22.048	36.734
430	393.75	48.225	44.915
011	91.45	24.425	7.245
012	118.3	27.087	8.01
021	145.32	28.772	16.594
031	198.6	33.12	24.90

The dependences for the main compounds in the YBaCuO system, see Table 9, are satisfactory until further data become available.

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