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NOTES

$Ln_2Cu_2O_5$ Compounds [*Ln*: Lu, Yb, Tm, Ho, Er, Dy, Tb, and Y]

In the process of establishing the phase diagram of the Yb_2O_3–Fe_2O_3–CuO system in air at 1000°C, Kimizuka and Takayama prepared a new compound, $Yb_2Cu_2O_5$, and reported its *d*-spacings and relative intensities of powder X-ray diffraction (*1*). Uhlig and Hahn (*2*) synthesized the $Cu_2Y_2O_5$ compound at 1000°C in air and reported its crystal data (space group: P_2, a = 13.60 (Å), b = 3.27 (Å), c = 13.60 (Å), and β = 133.15°, z = 4, Dx = 5.79). In the present note, we report crystal data of $Yb_2Cu_2O_5$ and its isostructural compounds, $Ln_2Cu_2O_5$ [*Ln*: Lu, Yb, Tm, Ho, Er, Dy, Tb, and Y], and their synthesis conditions.

Ln_2O_3 (99.9%) and CuO (reagent grade) were used as starting materials. Prior to mixing, each Ln_2O_3 was heated at 1200°C for 2 days and CuO was heated at 1000°C in air for 1 day. Each mixture of Ln_2O_3 : CuO = 1 : 2 (in mole ratio) was fully mixed in an agate mortar and was placed in a Pt crucible. Every sample was heated at 1000°C in air for 1 week. After heat treatment, each sample was rapidly cooled to room temperature. The sample weights were checked before and after heat treatment. No weight change due to reduction of CuO to Cu_2O was detected (*3*). The X-ray powder diffraction patterns of the samples thus obtained showed that they were isostructural compounds. Each compound has blue-green color. Based upon Uhlig and Hahn's conclusion, we tried to index each X-ray powder diffraction peak of $Ln_2Cu_2O_5$, but we could not index all of them. Using Ito's method (*4*), we successfully indexed the powder diffraction patterns of each compound. For instance, the results for $Yb_2Cu_2O_5$, assuming an orthorhombic system with a = 10.721(1) Å, b = 3.4323(2) Å, c = 12.344(1) Å, are shown in Table I. In order to assure the above results, we took electron diffractions of $Y_2Cu_2O_5$ by means of a 1000-keV microscope. The crystal was tilted in the electron microscope to examine the distribution of the diffraction spots. They showed that the above unit cell was a reduced one with a possible space group of *Pnma* (No. 62) or $Pna2_1$ (No. 33) (extinc-

TABLE I

POWDER X-RAY DATA FOR $Yb_2Cu_2O_5$

h k l	d_{obsd} (Å)	d_{calcd} (Å)	I (%)
0 0 2	6.168	6.1718	4
2 0 1	4.912	4.9167	12
2 0 2	4.046	4.0470	50
0 1 1	3.306	3.3069	1
2 0 3	3.262	3.2639	26
1 1 1	3.159	3.1599	2
0 0 4	3.085	3.0859	9
2 1 0	2.8901	2.8905	27
2 1 1	2.8148	2.8144	100
2 0 4	2.6749	2.6744	80

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TABLE I—*Continued*

h k l	d_{obsd} (Å)	d_{calcd} (Å)	*I* (%)
0 1 3	2.6345	2.6357	60
4 0 1	2.6188	2.6191	24
1 1 3	2.5594	2.5594	3
3 1 1	2.4270	2.4271	3
2 1 3	2.3649	2.3652	4
3 1 2	2.2975	2.2975	3
2 0 5	2.2421	2.2423	8
2 1 4	2.1099	2.1096	5
0 0 6	2.0566	2.0573	12
4 1 2	1.9997	1.9986	46
2 0 6	1.9214	1.9207	5
4 1 3	1.8791	1.8792	34
4 0 5	1.8158	1.8158	8
6 0 1	1.7678	1.7683	1
4 1 4	1.7434	1.7431	23
6 0 2 0 2 0	1.7160	1.7163 1.7162	15
1 2 0	1.6943	1.6946	2
2 1 6	1.6757	1.6761	7
0 2 2	1.6537	1.6534	1
6 0 3	1.6388	1.6389	18
2 2 1	1.6205	1.6203	1
6 1 0	1.5848	1.5849	13
2 2 2	1.5803	1.5800	15
0 1 7	1.5683	1.5685	10
6 0 4	1.5461	1.5463	2
0 0 8	1.5426	1.5430	5
6 1 2 3 2 1	1.5349	1.5351 1.5350	5
2 2 3	1.5187	1.5190	5
2 1 7	1.5054	1.5054	19
2 0 8	1.4826	1.4827	3
6 1 3	1.4792	1.4790	4
4 0 7	1.4731	1.4731	7
2 2 4	1.4443	1.4444	13
4 2 1	1.4353	1.4355	6
6 1 4	1.4099	1.4098	5
2 2 5	1.3628	1.3628	2
4 1 7	1.3537	1.3537	2
4 0 8	1.3371	1.3372	2
8 0 1	1.3324	1.3323	7
0 2 6	1.3179	1.3178	4
8 0 2	1.3095	1.3096	4
0 1 9	1.2735	1.2736	2
6 1 6	1.2556	1.2555	8
4 1 8	1.2465	1.2460	9
8 1 2	1.2235	1.2235	3
2 0 10	1.2029	1.2029	2

TABLE II

LATTICE CONSTANTS OF $Ln_2Cu_2O_5$

	a (Å)	*b* (Å)	*c* (Å)
$Y_2Cu_2O_5$	10.793(1)	3.4933(2)	12.450(1)
$Tb_2Cu_2O_5$	10.855(1)	3.5444(4)	12.532(2)
$Dy_2Cu_2O_5$	10.833(1)	3.5180(2)	12.477(1)
$Ho_2Cu_2O_5$	10.798(1)	3.4921(3)	12.463(1)
$Er_2Cu_2O_5$	10.775(Å)	3.4703(4)	12.439(1)
$Tm_2Cu_2O_5$	10.737(1)	3.4527(2)	12.373(1)
$Yb_2Cu_2O_5$	10.721(1)	3.4323(2)	12.344(1)
$Lu_2Cu_2O_5$	10.695(1)	3.4088(2)	12.356(1)

tion rule: $k + 1 \neq 2n$ for $0kl$, and $h \neq 2n$ for $h0l$). Observed specific gravity of $Y_2Cu_2O_5$ by means of a pycnometric method was 5.45 ± 0.02 at 20°C, which agrees with the calculated one of 5.45 based on the assumption of four $Y_2Cu_2O_5$ in one unit cell.

The lattice constants of $Lu_2Cu_2O_5$, $Tm_2Cu_2O_5$, $Er_2Cu_2O_5$, $Ho_2Cu_2O_5$, $Dy_2Cu_2O_5$, $Tb_2Cu_2O_5$, and $Y_2Cu_2O_5$ are shown in Table II.

In order to grow single crystals of $Yb_2Cu_2O_5$, we heated the $Yb_2Cu_2O_5$ powder at 1000°C under 20 kbar for 11 hr and obtained single crystals which made it possible to measure intensities of a single-crystal X-ray diffraction. Maximum size of a single crystal grown by means of this method was about $20 \times 50 \times 50$ μm. The Weissenberg and precession photographs of a single crystal showed the same crystal data as those in electron diffraction. The cyrstal structure analysis of $Yb_2Cu_2O_5$ is in progress.

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