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Observing and modeling the sequential pairwise reactions that drive solid-state ceramic synthesis

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Abstract:

Solid-state synthesis from powder precursors is the primary processing route to advanced multicomponent ceramic materials. Designing ceramic synthesis routes is usually a laborious, trial-and-error process, as heterogeneous mixtures of powder precursors often evolve through a complicated series of reaction intermediates. Here, we show that phase evolution from multiple precursors can be modeled as a sequence of pairwise interfacial reactions, with thermodynamic driving forces that can be efficiently calculated using *ab initio* methods. Using the synthesis of the classic high-temperature superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ (YBCO) as a representative system, we rationalize how replacing the common BaCO_3 precursor with BaO_2 redirects phase evolution through a kinetically-facile pathway. Our model is validated from *in situ* X-ray diffraction and *in situ* microscopy observations, which show rapid YBCO formation from BaO_2 in only 30 minutes. By combining thermodynamic modeling with *in situ* characterization, we introduce a new computable framework to interpret and ultimately design synthesis pathways to complex ceramic materials.

Solid-state ceramic synthesis involves heating a mixture of precursor powders at high temperatures (typically >700 °C) and has been used to realize countless functional materials (1-3). Recent *in situ* characterization studies have revealed that solid-state reactions often evolve through a variety of non-equilibrium intermediates prior to formation of the equilibrium phase (4-10). These complicated phase evolution sequences are currently difficult to understand, resulting in laborious trial-and-error efforts to optimize ceramic synthesis recipes. The ability to rationalize and anticipate which intermediate phases form would enable solid-state chemists to design crystallization pathways that target (or avoid) specific intermediates, accelerating the design of time- and energy-efficient ceramic synthesis recipes for new materials. The need for synthesis prediction encourages the use of computation as a guide, but computation has mostly been used only to evaluate thermodynamic stability or metastability (11-15). While useful, phase stability alone does not provide any mechanistic insights to help guide synthesis planning for experimentalists.

The complexity of phase evolution arises from the various pathways by which an initially heterogeneous mixture of precursor particles can transform to a homogeneous target phase. At the microscopic level, solid-state reactions initiate in the interfacial regions between precursors as the system is heated. Because these interfacial reactions occur between only two solid phases at a time, we hypothesize that reactions starting from three or more precursors can be modeled as being initially dominated by the most reactive interface between a single pair of precursors, as illustrated schematically in **Figure 1A**. Once two precursors react to form a new phase, this non-equilibrium intermediate will then react through its interface with other precursors and intermediate phases. By decomposing the overall phase evolution into a sequence of pairwise reactions, we can calculate the thermodynamics and analyze the kinetics of each reaction step separately, which provides a simplified theoretical picture to conceptualize and navigate ceramic synthesis (15-19).

We demonstrate how this concept of sequential pairwise reactions enables us to model phase evolution in the ceramic synthesis of the classic high-temperature superconductor, $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ (YBCO) (20-22). Following the discovery that YBCO remains superconducting above the boiling point of liquid N_2 (>77 K), YBCO has been synthesized many thousands of times in laboratories around the world. The typical synthesis recipe for YBCO calls for three precursors—a 0.5/2/3 molar ratio of $\text{Y}_2\text{O}_3/\text{BaCO}_3/\text{CuO}$ powders—which are ground in a mortar, then compacted, pelletized, and baked in air at 950 °C for >12 hours. Even after 12 hours, the synthesis reaction is often incomplete, so the pellets must be re-ground, re-pelletized, and re-baked until phase-pure YBCO is obtained (23).

It has been reported that replacing BaCO_3 with BaO_2 can shorten YBCO synthesis times to 4 hours and eliminate the need for regrinding (24, 25). This dramatic difference in synthesis times offers an ideal case study to explore how precursor selection governs phase evolution in solid-state synthesis (26). In **Figure 1B**, we show temperature-dependent Gibbs reaction energies, ΔG_{rxn} , for the formation of YBCO with either BaO_2 or BaCO_3 as the barium source. BaO_2 is less stable than BaCO_3 (27), so although both reactions are thermodynamically favorable ($\Delta G_{\text{rxn}} < 0$) above ~ 700 °C, the thermodynamic driving force (magnitude of ΔG_{rxn}) is much larger with BaO_2 .

Naively, one might anticipate that this larger driving force explains why YBCO synthesis with a BaO_2 precursor proceeds faster. Instead, we will show that it is actually the pairwise $\text{BaO}_2|\text{CuO}$ reaction that directs phase evolution through a low-temperature eutectic melt, producing a liquid self-

flux to facilitate rapid YBCO formation. BaO_2 is a relatively uncommon YBCO precursor, appearing in only 8 out of 237 synthesis recipes for YBCO (and related phases) as text-mined from the literature (28), whereas BaCO_3 is the most common Ba precursor, at 176 out of 237 recipes (Table S1 shows all extracted synthesis recipes). By better understanding how uncommon precursors promote kinetically-facile sequential pairwise reactions (26), we can build towards new design principles for precursor selection and rational synthesis planning.

Here, we use *in situ* synchrotron X-ray diffraction (XRD) to characterize the temperature-time-transformation process of YBCO formation, as well as *in situ* microscopy (SEM, DF-STEM) to directly observe the spatiotemporal microstructural evolution from the three initial precursors. By comparing these experimentally-observed phase evolution pathways against density functional theory (DFT)-calculated thermodynamics (29) aided by a machine-learned model for temperature-dependent Gibbs free energies (30), we conclusively verify the role of interfacial reactions in dictating phase evolution in solid-state synthesis. Our model provides a theoretical foundation to model phase evolution during solid-state synthesis from multiple precursors, integrating computation and experiment towards the long-standing goal of predictive solid-state synthesis.

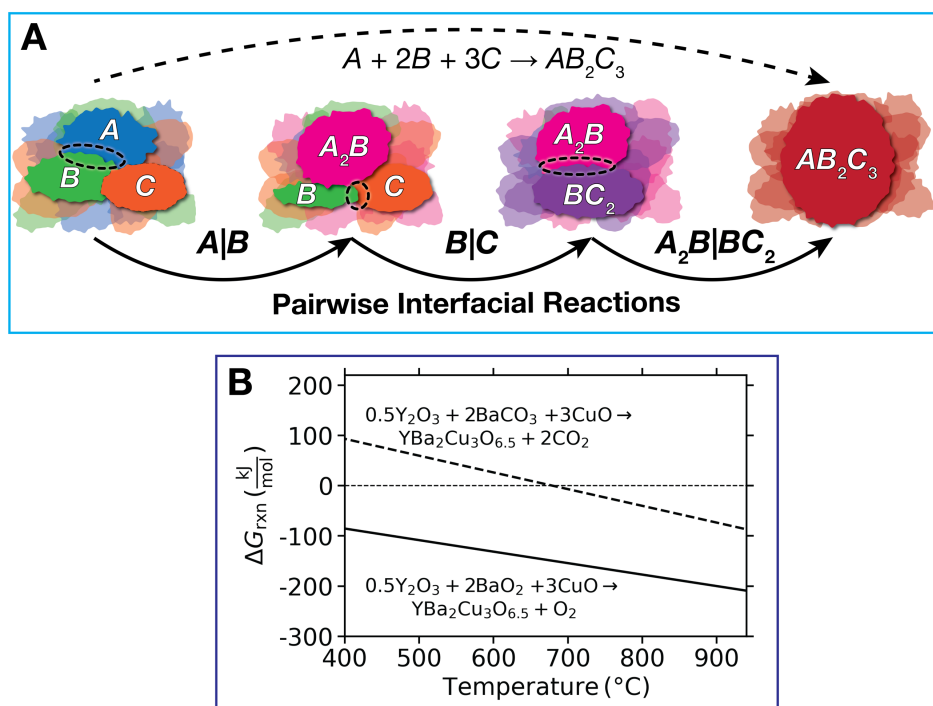


Figure 1. Schematic of sequential pairwise interfacial reactions and overall reaction energetics for YBCO synthesis. (A) Schematic of the pairwise reaction concept, illustrating that phase evolution from powder precursors must initiate at the shared interface between two precursor grains. (B) The temperature-dependent Gibbs reaction energies, ΔG_{rxn} , for the formation of YBCO from precursor mixtures utilizing BaCO_3 (dashed line) or BaO_2 (solid line) as the Ba source.

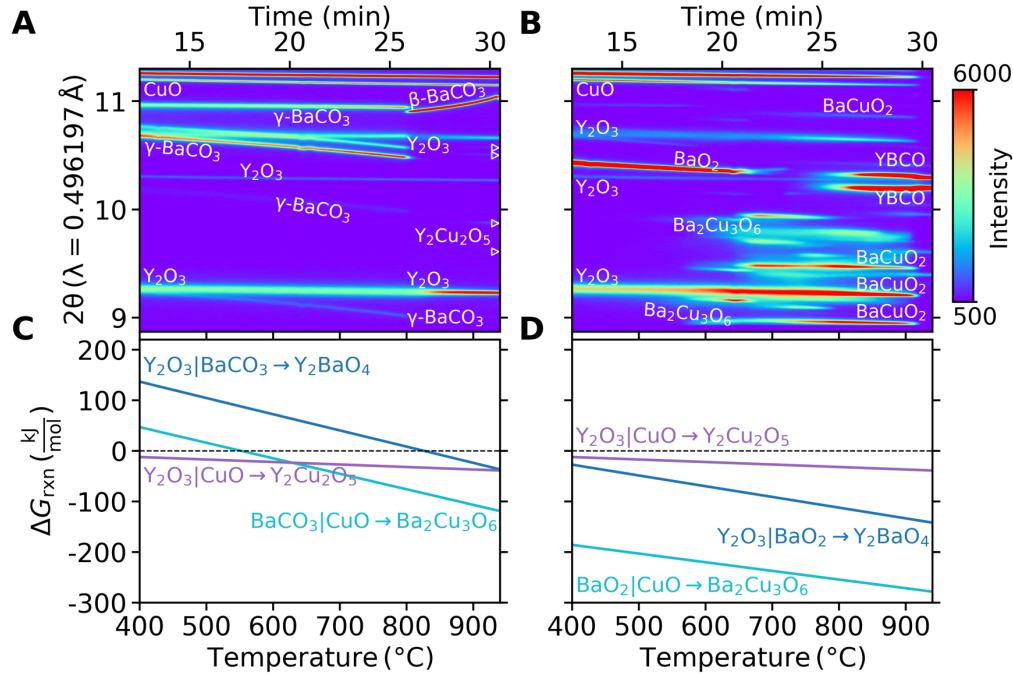


Figure 2. Phase evolution during YBCO synthesis compared to reaction thermodynamics. (A) *in situ* synchrotron XRD pattern for heating of the Y₂O₃ + BaCO₃ + CuO precursor mixture. The triangles mark peaks for Y₂Cu₂O₅. Individual XRD patterns at select temperatures are provided in **Supplementary Figure 1. (B)** *in situ* synchrotron XRD pattern for heating of the Y₂O₃ + BaO₂ + CuO precursor mixture. Individual XRD patterns at select temperatures are provided in **Supplementary Figure 2**. Mixed powders were heated in quartz tubes under air atmosphere at a heating rate of 30 °C/min. **(C)** Gibbs reaction energies for the lowest energy reactions at each interface in the Y₂O₃ + BaCO₃ + CuO precursor mixture. The reactions are Y₂O₃|BaCO₃ = 1.5 Y₂O₃ + 1.5 BaCO₃ → 1.5 BaY₂O₄ + 1.5 CO₂; Y₂O₃|CuO = 1.5 Y₂O₃ + 3 CuO → 1.5 Y₂Cu₂O₅; BaCO₃|CuO = 12/7 BaCO₃ + 18/7 CuO + 3/7 O₂ → 6/7 Ba₂Cu₃O₆ + 12/7 CO₂, **(D)** Gibbs reaction energies for the lowest energy reactions at each interface in the Y₂O₃ + BaO₂ + CuO precursor mixture. The reactions are Y₂O₃|BaO₂ = 2 Y₂O₃ + 2 BaO₂ → 2 BaY₂O₄ + O₂, Y₂O₃|CuO = 1.5 Y₂O₃ + 3 CuO → 1.5 Y₂Cu₂O₅, BaO₂|CuO = 2.4 BaO₂ + 3.6 CuO → 1.2 Ba₂Cu₃O₆ + 0.6 O₂. The coefficients of each reaction are normalized to be consistent with the formation of 1 mol of YBa₂Cu₃O_{6.5} in an atmosphere open to O₂. As such, the products of each reaction form 6 mol of non-oxygen atoms. See the **Supplementary Information** for more details.

In **Figure 2**, we show *in situ* synchrotron X-ray diffraction patterns for phase evolution in YBCO synthesis in air with either BaCO₃ (**Figure 2A**) or BaO₂ (**Figure 2B**) as the Ba source, which we compare to the thermodynamic driving force for new phase formation at each pairwise interface (**Figure 2C-D**). **Figure 2A** shows that when BaCO₃ is used, the precursors remain the dominant phases up to 940 °C, confirming the lack of rapid phase formation. In contrast, **Figure 2B** shows the formation of YBCO in 30 min when BaO₂ is used as the Ba source. In both cases, we have a three-precursor system, so the relevant interfaces are Y₂O₃|CuO, Y₂O₃|BaCO₃(BaO₂), and BaCO₃(BaO₂)|CuO. In the BaCO₃-containing system, no reaction has substantial driving force until >900 °C (**Figure 2C**). When BaCO₃ is replaced with BaO₂, the reaction thermodynamics change dramatically as the BaO₂|CuO

interface has large driving force ($\Delta G_{\text{rxn}} < -200$ kJ/mol) to form ternary Ba-Cu-oxides above 400 °C (**Figure 2D**). This is consistent with *in situ* XRD observations of barium copper oxides emerging at ~600 °C and the consumption of BaO₂ by ~700 °C (**Figure 2B**).

Synthesis of YBCO using a BaCO₃ precursor usually requires >12 hours with intermittent regrindings (23), so it is not surprising that YBCO did not form in our 30 min *in situ* experiment (**Figure 2A**). At temperatures >850 °C, traces of a Y₂Cu₂O₅ phase are observed, even though the BaCO₃|CuO interface has the larger thermodynamic driving force to react (**Figure 2C**). BaCO₃ decomposition is reported to have a substantial activation barrier of 305 kJ/mol (31), and the thermodynamic driving forces for all Y₂O₃-BaCO₃-CuO interfacial reactions have ΔG_{rxn} less negative than -100 kJ/mol up to 800 °C, which is evidently too small to overcome this kinetic barrier. These poor reaction kinetics, coupled with a small thermodynamic driving force, underlie the slow synthesis of YBCO when starting from a BaCO₃ precursor.

The fast formation of YBCO when starting from BaO₂ originates from the large driving force at the BaO₂|CuO interface, which is ~200 kJ/mol larger than at the BaCO₃|CuO interface at 600 °C. We previously demonstrated in the Na_xMO₂ (M = Co, Mn) system that the first phase to form in an interfacial reaction is the compound with the largest compositionally-unconstrained reaction energy from the precursors (10). Here, we confirm this theory in the YBCO system. We calculate that Ba₂Cu₃O₆ has the largest reaction energy to form at the BaO₂|CuO interface, and indeed this is the first observed ternary phase, which is accompanied by evolution of O₂ gas. Between 600 °C and 850 °C, Ba₂Cu₃O₆ decomposes to form BaCuO₂ and CuO (**Figure 2B**). The preferential reactivity of the BaO₂|CuO interface—instead of the Y₂O₃|BaO₂ or Y₂O₃|CuO interfaces—supports the theory that the first phase to form is the one with the largest thermodynamic driving force, and further asserts that when multiple competing interfaces exist, the interface with the most exergonic compositionally-unconstrained reaction energy will initiate the solid-state reaction. This provides a straightforward means by which computation can be integrated into synthesis planning to predict which pairwise interfaces will be the most reactive in a given precursor mixture and which phases will be most likely to form at those interfaces.

Whereas *in situ* XRD measurements track the temperature-time-transformation evolution of the system, *in situ* SEM/DF-STEM provides direct spatiotemporal observation of the microstructural evolution during the solid-state reaction. We monitored the synthesis of YBCO from Y₂O₃ + BaO₂ + CuO on a hot stage using *in situ* electron microscopy (SEM/DF-STEM: Hitachi HF5000). Although the *in situ* microscopy used here cannot identify crystal structure, the reaction conditions (temperature, heating rate, precursors) are the same as those characterized by *in situ* XRD (**Figure 2B**), so we anticipate that the temperature-time-transformation progression between the two methods are comparable. We also characterize the elemental distribution in the sample using energy-dispersive X-ray spectroscopy (EDX) before and after the *in situ* microscopy experiment (our EDX instrument can only operate at room temperature). In **Figure 3A**, we show DF-STEM snapshots of the particles during heating along with EDX before and after heating. A video of this reaction is also provided as **Supplementary File 1**.

At room temperature, EDX shows that the three precursor powders are in intimate contact. Importantly, it is clear from EDX that all three potential pairwise interfaces ($\text{Y}_2\text{O}_3|\text{BaO}_2$, $\text{Y}_2\text{O}_3|\text{CuO}$, and $\text{BaO}_2|\text{CuO}$) exist in the sample. As the stage is heated to 500 °C, the initial BaO_2 and CuO precursors react at the $\text{BaO}_2|\text{CuO}$ interface, which according to the *in situ* XRD experiments, results in $\text{Ba}_2\text{Cu}_3\text{O}_6$. Meanwhile, the Y_2O_3 particle remains inert, as does its interface with BaO_2 . From 650 °C to 800 °C, we observe the ejection of small bubble-like particles, which corresponds to the reaction: $\text{Ba}_2\text{Cu}_3\text{O}_6 \rightarrow 2 \text{BaCuO}_2 + \text{CuO} + 0.5 \text{O}_2$. In a separate *in situ* heating experiment, we confirm with SEM and EDX measurements that this initial reaction occurs strictly in the Ba-Cu-O subsystem. (**Supplementary Figure 3**). The observed reactivity of the $\text{BaO}_2|\text{CuO}$ interface and inertness of the Y_2O_3 -containing interface aligns with our thermodynamic predictions from **Figure 2D**.

From **Figure 1B**, we calculated the total thermodynamic driving force of $0.5 \text{Y}_2\text{O}_3 + 2 \text{BaO}_2 + 3 \text{CuO} \rightarrow \text{YBa}_2\text{Cu}_3\text{O}_{6.5} + \text{O}_2$ to be approximately -200 kJ/mol . For the formation of BaCuO_2 , we calculate a reaction energy of -130 kJ/mol ($2 \text{BaO}_2 + 2 \text{CuO} \rightarrow 2 \text{BaCuO}_2 + \text{O}_2$), meaning that $\sim 2/3^{\text{rd}}$ of total reaction driving force is consumed before Y_2O_3 becomes involved in the reaction. Only $\sim 70 \text{ kJ/mol}$ remain to drive the reaction to form YBCO. This is more or less comparable to the overall reaction energy from Y_2O_3 , BaCO_3 and CuO (**Figure 1B**), indicating this thermodynamic driving force does not account for the quick formation of YBCO when BaO_2 is used. Thus, we anticipate kinetic selection to play the primary role in the formation of the next phase. Indeed, this kinetic mechanism is provided by the melting of BaCuO_2 and CuO at $\sim 900 \text{ °C}$. This liquid Ba-Cu-O melt is then rapidly consumed into the Y_2O_3 particle to form YBCO. In the EDX taken after the experiment, the morphology of the Y region remains similar to the beginning of the experiment, but now Ba and Cu signals are found in the final particle.

In **Figure 3B**, we overlay the observed phase evolution sequence onto the pseudo-binary BaO_2 - CuO slice (32) of the overall Y_2O_3 - BaO_2 - CuO phase diagram to reveal how the BaO_2 precursor enables rapid YBCO synthesis. The first reaction occurs before 500 °C and proceeds at the $\text{BaO}_2|\text{CuO}$ interface to form $\text{Ba}_2\text{Cu}_3\text{O}_6$. This is consistent with our calculations in **Figure 2D**, where we found the $\text{BaO}_2|\text{CuO}$ interface to be the most reactive among the three precursor interfaces and $\text{Ba}_2\text{Cu}_3\text{O}_6$ to be the phase with the largest driving force to form at this interface. Above 700°C, $\text{Ba}_2\text{Cu}_3\text{O}_6$ undergoes peritectoid decomposition into BaCuO_2 and CuO , which was observed as the ejection of small bubble-like particles in **Figure 3**. BaCuO_2 and CuO are unreactive until the temperature is increased to their eutectic point at 890 °C, after which BaCuO_2 and CuO melt into one another. This liquid melt becomes a self-flux, providing fast kinetic transport of Ba and Cu into Y_2O_3 for the rapid formation of YBCO at the $\text{Y}_2\text{O}_3|\text{Ba-Cu-O(liquid)}$ interface.

If one consults the Y_2O_3 - CuO or Y_2O_3 - BaO_2 phase diagrams (33), the lowest liquidus temperatures in these systems are $\geq 1095 \text{ °C}$, which is above the temperature at which YBCO decomposes (1006 °C) (34). BaO_2 therefore plays a crucial role in directing the phase evolution through the pseudo-binary BaO_2 - CuO subsystem—where a low-temperature liquid self-flux provides the fast diffusion kinetics that facilitates the formation of YBCO in 30 minutes. This is in contrast to when BaCO_3 is used as the Ba source, where the slow decomposition reaction kinetics at the $\text{BaCO}_3|\text{CuO}$ interface forces the overall reaction to proceed through the Y_2O_3 - CuO subsystem, and a high liquidus temperature of 1095 °C obstructs any liquid-mediated transport kinetics for YBCO formation (33).

Although the overall reaction energies shown in **Figure 1B** suggest that the larger thermodynamic driving force is why a reaction with the BaO_2 precursor proceeds more quickly than with BaCO_3 , we emphasize here that the magnitude of the overall reaction energy is not the origin of the fast synthesis time. Instead, it is the initial selection of the BaO_2 - CuO subsystem, where there is a low-temperature eutectic below the decomposition temperature of YBCO, that enables rapid YBCO synthesis by forming a self-flux. This finding highlights the need to consider computations beyond the phase stabilities of the target or overall reaction energies in order to obtain mechanistic insights into the reaction pathways by which phases can evolve during synthesis.

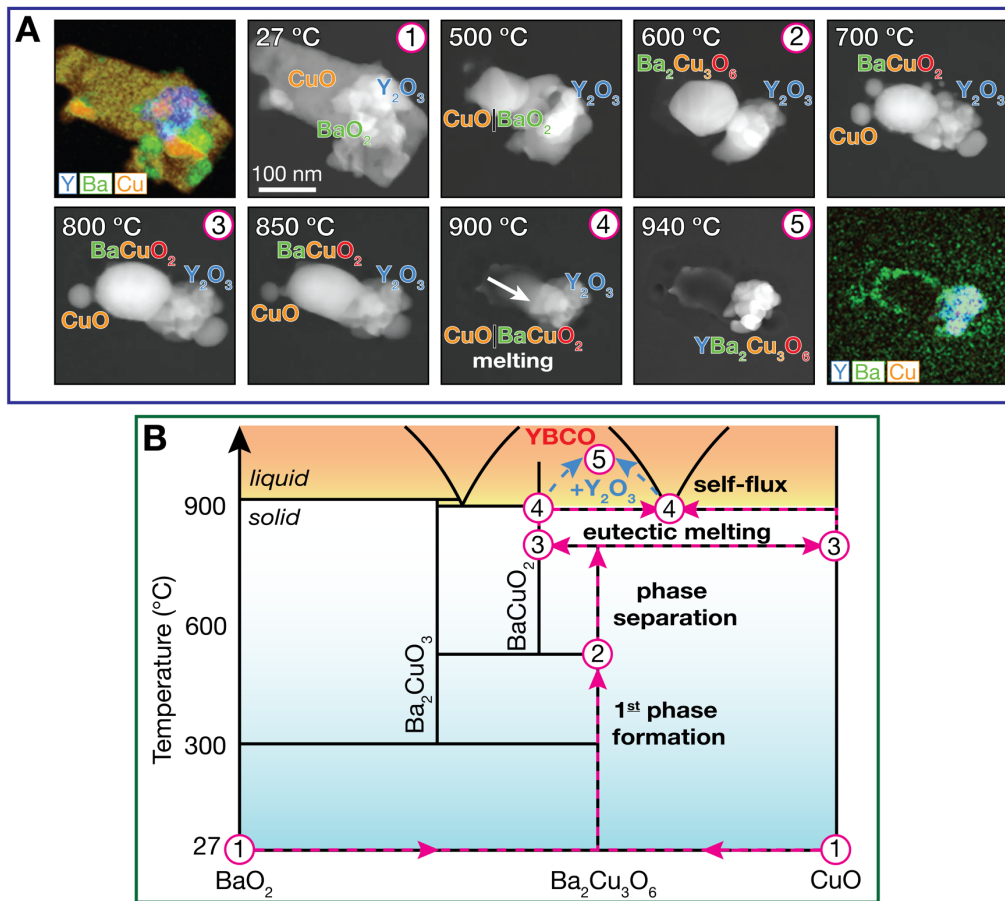
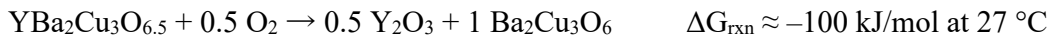


Figure 3. *In situ* microscopy of YBCO formation from Y_2O_3 , BaO_2 , and CuO particles and the observed phase evolution sequence mapped onto the BaO_2 - CuO phase diagram. **(A)** *In situ* DF-STEM and EDX images show the heating of $0.5 \text{ Y}_2\text{O}_3 + 2 \text{ BaO}_2 + 3 \text{ CuO}$ from 27 °C to 940 °C at 30 °C/min. The markers in the upper right corner of select panels are for comparison to panel B. A video of the reaction is provided in Supplementary File 1. *In situ* SEM and EDX for a shorter run to capture the initial formation of $\text{Ba}_2\text{Cu}_3\text{O}_6$ is also provided in Supplementary Figure 3. **(B)** Observed phase evolution sequence in the context of the pseudo-binary phase diagram for BaO_2 - CuO , adapted from Ref. (32).

Upon cooling the sample down from 940 °C at a rate of 5 °C/min, *in situ* XRD shows in **Figure 4** a structural transition from tetragonal to orthorhombic YBCO at 620 °C, indicating the uptake of ambient O_2 into $\text{YBa}_2\text{Cu}_3\text{O}_6$ to form $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$, consistent with reports from the literature (35, 36).

The synthesized product exhibits a strong diamagnetic signal below 77 K (**Figure 4C**), indicating the successful synthesis of superconducting YBCO. From a thermodynamic perspective, it is well-characterized that $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ is metastable at low temperature with respect to decomposition (37) by the reaction:



However, this solid-state decomposition is kinetically limited at room temperature. On the other hand, oxygen diffusion is highly mobile in the YBCO framework (38, 39), indicating that this final topotactic uptake of O_2 gas at the YBCO| O_2 interface is a kinetically-mediated non-equilibrium reaction.

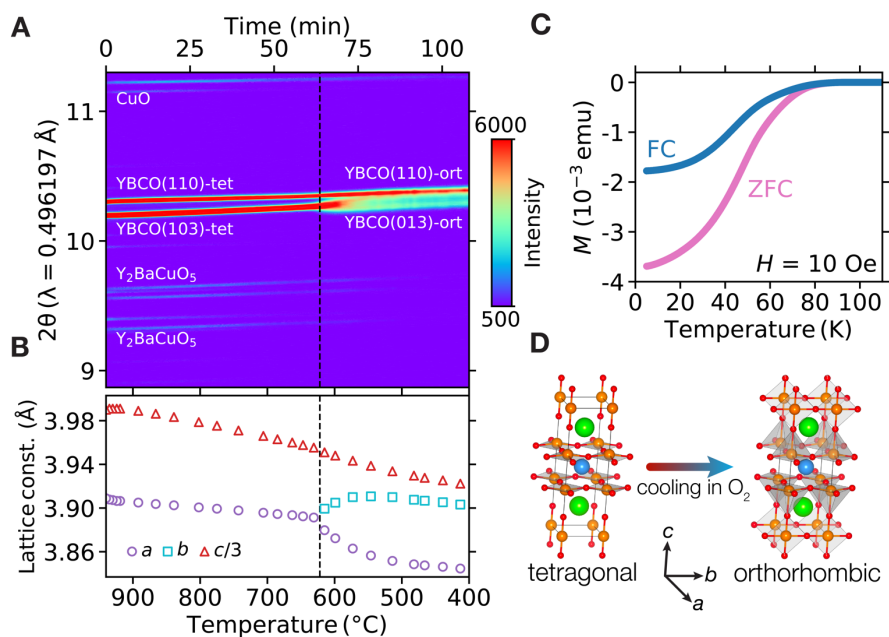


Figure 4. Topotactic O_2 uptake and phase transition during slow cooling. (A) *in situ* synchrotron XRD pattern for cooling of $\text{Y}_2\text{O}_3 + \text{BaO}_2 + \text{CuO}$ precursor from 940°C to 400°C at $5^\circ\text{C}/\text{min}$. “tet” refers to the tetragonal structure and “ort” to the orthorhombic structure. (B) Changes in lattice parameters during cooling. (C) Magnetic susceptibility of synthesized YBCO exhibiting superconductivity above liquidus nitrogen temperature. (D) The tetragonal and orthorhombic crystal structures for YBCO, where blue spheres are Y, green are Ba, orange are Cu, and red are O.

In **Figure 5**, we summarize how phase evolution during YBCO synthesis can be understood as a sequence of pairwise reactions that result from an interplay between thermodynamics and kinetics. The initial mixture of three precursors— Y_2O_3 , BaO_2 and CuO —produces three possible reactive interfaces. We calculated in **Figure 2D** that the $\text{BaO}_2|\text{CuO}$ interface possesses the largest thermodynamic driving force to react, and predicted $\text{Ba}_2\text{Cu}_3\text{O}_6$ to be the first reaction intermediate, which was confirmed by *in situ* XRD (**Figure 2B**) and microscopy (**Figure 3A, Supplementary Figure 3**). The formation of $\text{Ba}_2\text{Cu}_3\text{O}_6$ below 600°C consumes $\sim 2/3^{\text{rd}}$ of the overall reaction driving force, meaning the ensuing

reactions necessarily occur with smaller driving forces. Using *in situ* DF-STEM we observed that after the peritectoid decomposition of $\text{Ba}_2\text{Cu}_3\text{O}_6$ into $\text{BaCuO}_2 + \text{CuO}$, there is no further phase evolution in the system until the formation of a eutectic melt at the $\text{BaCuO}_2|\text{CuO}$ interface. This liquid melt serves as a self-flux, providing fast Ba and Cu transport into the thus-far immobile Y_2O_3 , forming $\text{YBa}_2\text{Cu}_3\text{O}_6$ (**Figure 3**). Finally, fast topotactic oxygen uptake at the $\text{YBa}_2\text{Cu}_3\text{O}_6|\text{O}_2$ interface upon cooling yields the superconducting $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ phase (**Figure 4**), which persists kinetically as a metastable phase to room temperature, instead of decomposing to the equilibrium $\text{Y}_2\text{O}_3 + \text{Ba}_2\text{Cu}_3\text{O}_6$ phases. In the Y_2O_3 - BaCO_3 - CuO precursor set, small $\text{BaCO}_3|\text{CuO}$ reaction driving forces and poor BaCO_3 decomposition kinetics drive the phase evolution down through the Y_2O_3 - CuO subsystem, where slow diffusion kinetics means manual regrinding is necessary to reintroduce interfaces between any unfinished reaction intermediates.

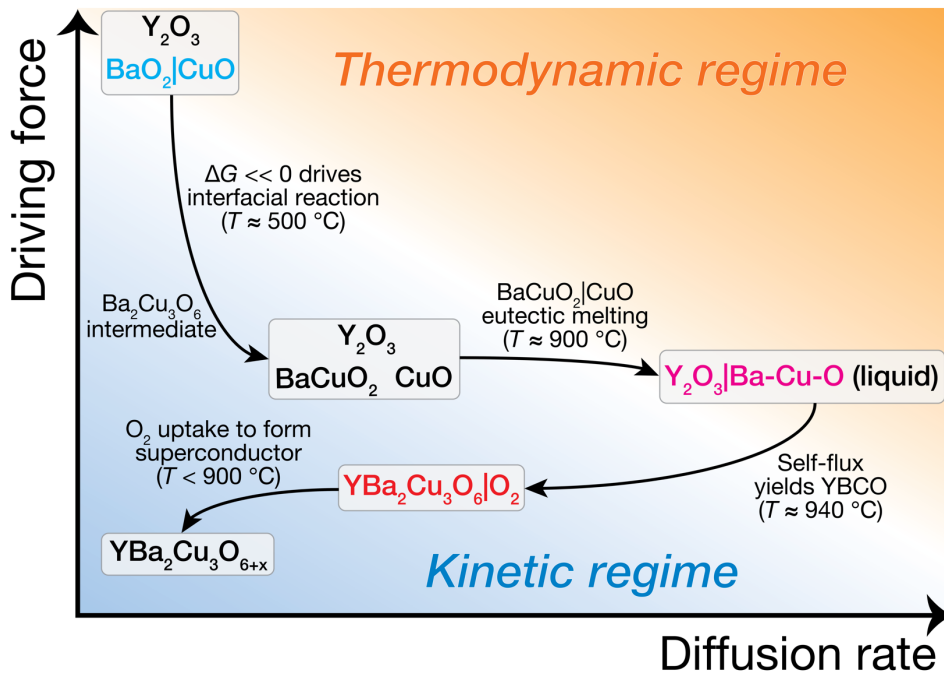


Figure 5. Phase evolution pathway for the formation of YBCO dictated by sequential pairwise reactions. The YBCO synthesis pathway is shown here along two qualitative axes – the thermodynamic driving force to form new phases along the vertical axis and the diffusion rate of reactive species along the horizontal axis. Within this framework, we understand reaction events occurring in either a thermodynamic regime, where driving forces or diffusion rates are sufficiently high that equilibrium products are observed, or a kinetic regime, where ion transport is sufficiently slow or driving forces sufficiently small such that the system becomes unreactive or non-equilibrium products are formed.

Our investigation here provides a general conceptual framework to understand the solid-state synthesis of complex multicomponent ceramics. A ceramic synthesis reaction that begins from N precursors will exhibit $N C_2$ pairwise reaction interfaces. We showed here that of the many possible pairwise interfaces, the first reaction will occur between the two precursors with the largest

compositionally-unconstrained reaction driving force. This initial reaction interface can be predicted from *ab initio* thermodynamics and determines which pseudo-binary subsystem the ensuing phase evolution proceeds from. By thoughtfully choosing the starting precursors (26) to control which pairwise interface is the most reactive, one can deliberately direct phase evolution through whichever pseudo-binary subsystem exhibits the best kinetic pathway to the target material. Today, it remains difficult to anticipate which kinetic mechanisms are available in a given subsystem, meaning that in the short term, *in situ* characterization will be the most productive approach for rationally designing solid-state synthesis recipes. In the future, a theoretical framework that embeds nucleation, diffusion, and crystal growth kinetics within a thermodynamic description of sequential pairwise reactions will pave the way towards a complete computational platform for predictive solid-state ceramic synthesis.

Materials and Methods

In-situ synchrotron powder X-ray diffraction

Y₂O₃ (>99.9%, Kojundo Kagaku), BaCO₃ (>99.9 %, Kojyundo Kagaku), BaO₂ (>80%, Jyunsei Kagaku), CuO (>99%, Wako Chemical) were weighed in a molar ratio of for Y/Ba/Cu =1/2/3, and loaded into a zirconia pot with zirconia balls with a diameter of 4 mm. The starting materials were mechanochemically milled by planetary ball milling for 3 h over 150 rpm. The mixed powder was loaded into a quartz capillary with a diameter of 0.3 mm.

The change in crystalline phases were examined using synchrotron powder X-ray diffraction at the *BL02B2* beamline of *SPring-8* (proposal numbers 2019A1101, 2019B1195 and 2020A1096). The quartz capillary with powder mixture was settled in a furnace in air atmosphere. Heating started after setting in the furnace operated at 100 °C at the heating rate of 30 °C /min till 940 °C. The sample kept 10 min at 940 °C and then started cooling at 5 °C /min till 400 °C. The diffraction data of 2θ range from 8.9° to 15.5° with a step of 0.02° were collected using a high-resolution one-dimensional semiconductor detector (MYTHEN)(40). The wavelength of the radiation beam was determined using a CeO₂ standard. The crystal structure was visualized using VESTA software.(41)

In-situ TEM measurement

In an Ar-filled glove box, BaO₂ powder (>80%, Jyunsei Kagaku) was mechanochemically milled by planetary ball milling for 8 h over 150 rpm. The powder was sieved to remove particles larger than 20 μm. In ambient atmosphere, Y₂O₃ (>99.9%, Kojundo Kagaku), CuO nanopowder (>99%, Alderich), and above BaO₂ powder were weighed in a molar ratio of for Y/Ba/Cu =1/2/3, and loaded again into a zirconia pot with φ 4 mm zirconia balls. The powder was mechanochemically mixed by planetary ball milling for 3 h over 150 rpm. The sample was dispersed in dehydrate ethanol, and ultrasonicated. This suspension was dropped onto a silicon nitride TEM grid.

Morphology and compositional change were observed by transmission electron microscopy (TEM: HF-5000 Hitachi High-Tech Corporation). The accelerate voltage was 200 kV, and pressure was approximately 2×10^{-5} Pa. The sample was initially heated at 300 °C, and then heated till 940 °C at 30 °C /min. The apparatus allows to record three images simultaneously: scanning electron microscope (SEM), bright-field scanning transmission electron microscopy (BF-STEM), and dark-field scanning transmission electron microscopy (DF-STEM) images. Before and after heating the sample, compositional distribution was examined by energy-dispersive X-ray (EDX) mapping at room temperature.

Magnetization measurement

Magnetization was measured using a superconducting quantum interference device (SQUID) magnetometer (Quantum Design MPMS-3) with an applied field of 10 Oe, in order to check Meissner effect of synthesized sample.

Computational

Standard Gibbs formation energies, $\Delta G_f^\circ(T)$, for gaseous species were obtained from NIST (42). To account for the synthesis atmosphere (air), Gibbs formation energies of a given gaseous species, $\Delta G_{f,i}^\circ(T)$, were obtained as:

$$\Delta G_{f,i}(T) = \Delta G_{f,i}^\circ(T) + RT \ln(p_i)$$

where R is the gas constant and p_i approximates the activity coefficient of gaseous species, i . The only gaseous species evolved or consumed in reactions discussed in this work are O_2 and CO_2 , where p_{O_2} was taken to be 0.21 atm and $p_{CO_2} = 0.0004$ atm.

For solid-state compounds, formation enthalpies (at 0 K) were obtained with density functional theory (DFT), utilizing the SCAN meta-GGA density functional (29). Each structure was obtained from the Materials Project database (43) and optimized using the Vienna Ab Initio Simulation Package (VASP) (44) and the projector augmented wave (PAW) method (45), a plane-wave energy cutoff of 520 eV, and 1000 k-points per reciprocal atom.

Standard Gibbs formation energies, $\Delta G_f^\circ(T)$, for each solid-state compound were then obtained by combining the DFT-calculated formation enthalpies, the machine-learned descriptor introduced in (30), and experimental Gibbs energy data for elemental phases as described in (30). The activity of all solid phases was taken to be 1, so $\Delta G_f(T) = \Delta G_f^\circ(T)$.

Gibbs reaction energies, $\Delta G_{rxn}(T)$ were obtained as:

$$\Delta G_{rxn}(T) = \sum_{products} \Delta G_f(T) - \sum_{reactants} \Delta G_f(T)$$

The coefficients of each reaction were selected such that 6 moles of non-oxygen atoms appear in the product side of each reaction. This was done to normalize the comparison of $\Delta G_{rxn}(T)$ across a diverse set of reactions, and because the reacting mixture was assumed to exchange freely with O_2 in the synthesis atmosphere.

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Supplementary Materials:

Supplementary Figures S1-3

Supplementary Table S1

Supplementary File S1

Supplementary information

Observing and modeling the sequential pairwise reactions that drive solid-state ceramic synthesis

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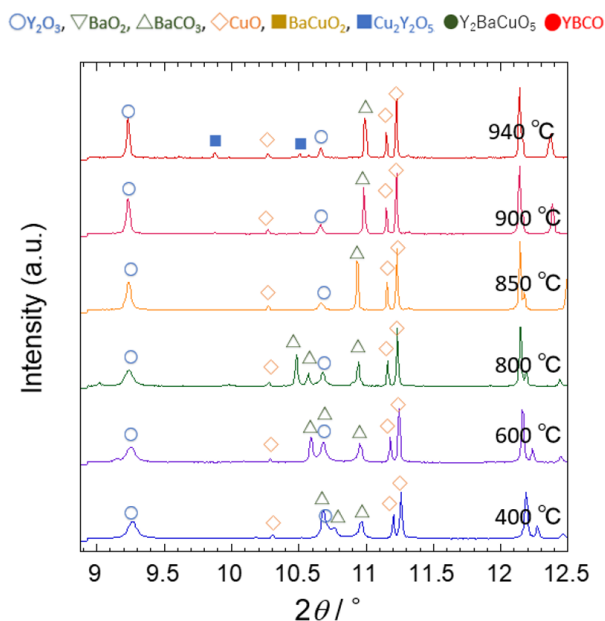


Figure S1. XRD patterns of the $\text{Y}_2\text{O}_3\text{-BaCO}_3\text{-CuO}$ mixture at 400, 600, 800, 850, 900, 940 °C upon heating. The sample was heated in air at a rate of 30 °C /min. $\lambda = 0.496197 \text{ \AA}$.

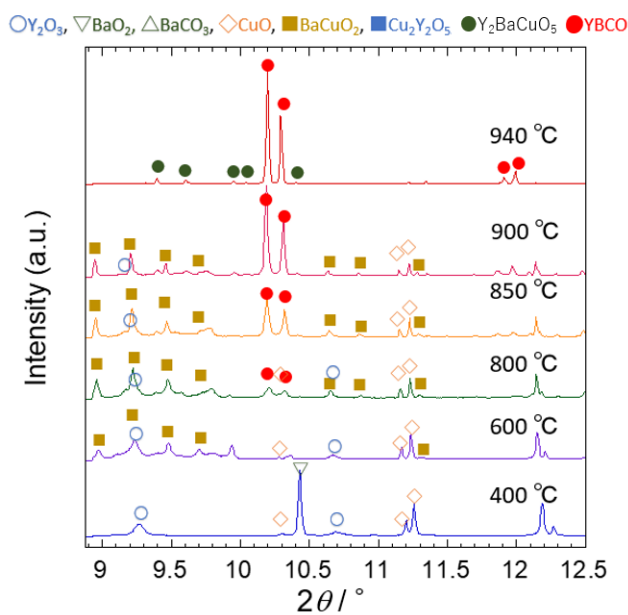


Figure S2. XRD patterns of the $\text{Y}_2\text{O}_3\text{-BaO}_2\text{-CuO}$ mixture at 400, 600, 800, 850, 900, 940 °C upon heating. The sample was heated in air at a rate of 30 °C /min. $\lambda = 0.496197 \text{ \AA}$.

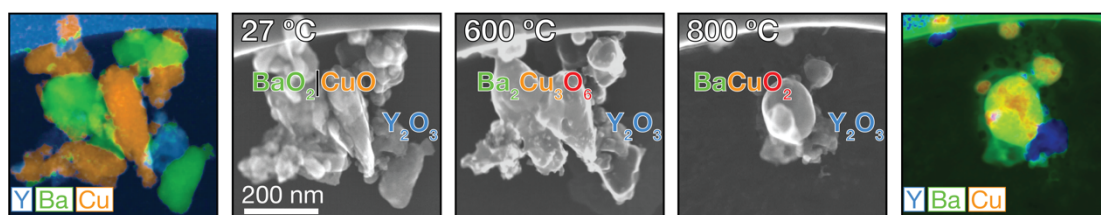


Figure S3. *In situ* SEM and EDX for the reaction of $0.5 \text{ Y}_2\text{O}_3 + 2 \text{ BaO}_2 + 3 \text{ CuO}$, heated from $27 \text{ }^\circ\text{C}$ to $800 \text{ }^\circ\text{C}$ at $30 \text{ }^\circ\text{C}/\text{min}$. The EDX map on the far left was taken before heating and the one on the far right taken after cooling down from $800 \text{ }^\circ\text{C}$ to room temperature. This provides further confirmation that the only reactive interface among the initial precursors is $\text{BaO}_2|\text{CuO}$ with Y_2O_3 remaining inert throughout this experiment.

Table S1. Synthesis recipes extracted for YBCO-related phases. Target = synthesis target; precursors = synthesis precursors; T = maximum temperature during synthesis; t = total time elapsed during heating operations; tag = Y-Ba-Cu-O if target elements are only these four elements or Y-Ba-Cu-O-* if these elements are present along with others; doi = digital object identifier for paper reporting synthesis. Note that “None” appears for T and t when synthesis operations were not successfully extracted. Recipes using BaO₂ as the Ba source are highlighted in yellow.

target	precursors	T (°C)	t (hr)	tag	doi
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	980	25	Y-Ba-Cu-O	10.1016/j.apcata.2006.03.034
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/S0167-577X(99)00202-5
Y _{1.5} Ba ₂ Cu ₃ O _x	Y ₂ O ₃ ; YBa ₂ Cu ₃ O ₇	None	None	Y-Ba-Cu-O	10.1016/j.jcrysgro.2012.04.029
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	938	24	Y-Ba-Cu-O	10.1016/S0167-577X(01)00562-6
Y ₂ BaCuO ₅	BaCO ₃ ; CuO; Y ₂ O ₃	1025	77	Y-Ba-Cu-O	10.1016/S0167-577X(02)00433-0
Y ₂ BaCuO ₅	BaCO ₃ ; CuO; Y ₂ O ₃	1025	77	Y-Ba-Cu-O	10.1016/S0167-577X(02)00433-0
YBaCuO	BaCO ₃ ; CuO; Y ₂ O ₃	950	20	Y-Ba-Cu-O	10.1016/S0038-1098(02)00714-7
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	930	24	Y-Ba-Cu-O	10.1016/S0921-5107(97)00213-4
YBa ₂ Cu ₃ O _{7-x}	Ba(CH ₃ COO) ₂ ; Cu(CH ₃ COO) ₂ ·H ₂ O Y(NO ₃) ₃ ·6H ₂ O	None	None	Y-Ba-Cu-O	10.1016/S0925-8388(99)00076-6
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/S0925-8388(99)00076-6
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	920	12	Y-Ba-Cu-O	10.1016/S0167-577X(02)00795-4
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	1000	34	Y-Ba-Cu-O	10.1016/j.elspec.2014.02.006
YBa ₂ Cu ₃ O ₇	BaCO ₃ ; CuO; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/j.radmeas.2004.01.005
YBa ₂ Cu ₄ O ₈	Ba(CH ₃ COO) ₂ ; Cu(CH ₃ COO) ₂ ·H ₂ O; Y ₂ O ₃	820	50	Y-Ba-Cu-O	10.1016/S0955-2219(00)00206-5

YBaCuO	BaCO ₃ ; CuO; Y ₂ O ₃	950	20	Y-Ba-Cu-O	10.1016/S0038-1098(02)00714-7
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	180	25	Y-Ba-Cu-O	10.1016/j.eurpolymj.2008.10.020
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	1060	28	Y-Ba-Cu-O	10.1016/s0040-6090(99)00717-8
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	940	78	Y-Ba-Cu-O	10.1016/s0925-4005(99)00089-1
YBa ₂ Cu ₃ O _{7-x}	Ba(NO ₃) ₂ ; Cu(NO ₃) ₂ ·3H ₂ O; Y(NO ₃) ₃ ·6H ₂ O; NH ₃	None	None	Y-Ba-Cu-O	10.1039/c2cp23046a
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	1060	28	Y-Ba-Cu-O	10.1016/S0040-6090(99)00717-8
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/s0167-577x(99)00202-5
Y Ba ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/j.ssc.2008.11.010
YBa ₂ Cu ₃ O _y	BaO ₂ ; CuO; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/j.physc.2004.01.088
Y ₂ BaCuO ₅	BaO ₂ ; CuO; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/j.physc.2004.01.088
Y _{1.8} Ba _{2.4} Cu _{3.4} O _x +0.5 CeO ₂ + 0.7 w% Sm ₂ O ₃	BaCO ₃ ; CeO ₂ ; CuO; Sm ₂ O ₃ ; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/j.jeurceramsoc.2018.01.026
YBa ₂ Cu ₃ O _{7-x}	BaCuO ₂ ; CuO; Y ₂ BaCuO ₅	None	None	Y-Ba-Cu-O	10.1007/s10854-007-9468-1
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/j.physc.2004.03.216
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	950	6	Y-Ba-Cu-O	10.1016/j.physc.2004.03.240
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	940	24	Y-Ba-Cu-O	10.1016/j.physc.2004.11.003
YBa ₂ Cu ₃ O _{7-x}	BaO ₂ ; CuO; Y ₂ O ₃	940	10	Y-Ba-Cu-O	10.1016/j.physc.2010.11.005
YBa ₂ Cu ₃ O _{7-x}	Ba(NO ₃) ₂ ; Cu(NO ₃) ₂ ·3H ₂ O; Y(NO ₃) ₃ ·6H ₂ O; NH ₃	None	None	Y-Ba-Cu-O	10.1039/C2CP23046A
Y ₂ BaCuO ₅	Ba(NO ₃) ₂ ; Cu(NO ₃) ₂ ·3H ₂ O; Y(NO ₃) ₃ ·6H ₂ O; NH ₃	None	None	Y-Ba-Cu-O	10.1016/j.physc.2013.04.064
YBa ₂ Cu ₃ O ₇	Ba(CH ₃ COO) ₂ ; Cu(CH ₃ COO) ₂ ; Y(OH) ₃	None	None	Y-Ba-Cu-O	10.1016/j.physc.2015.02.003

YBa ₂ Cu ₃ O ₇	Ba(CH ₃ COO) ₂ ; Cu(CH ₃ COO) ₂ ; Y(CH ₃ COO) ₃	None	None	Y-Ba-Cu-O	10.1016/j.physc.2016.04.004
YBa ₂ Cu ₃ O ₇	Ba(NO ₃) ₂ ; Cu(NO ₃) ₂ ·3H ₂ O; Y(NO ₃) ₃ - 6H ₂ O	930	43	Y-Ba-Cu-O	10.1016/j.physc.2018.02.010
Y ₃ Ba ₅ Cu ₈ O ₁₉	Ba(NO ₃) ₂ ; Cu(NO ₃) ₂ ·3H ₂ O; Y(NO ₃) ₃ +6H ₂ O	790	14	Y-Ba-Cu-O	10.1016/j.physc.2018.02.050
YBa ₂ Cu ₄ O ₈	Ba(CH ₃ COO) ₂ ; Cu(CH ₃ COO) ₂ ·H ₂ O; Y ₂ O ₃	800	70	Y-Ba-Cu-O	10.1016/s0040-6031(99)00285-3
YBa ₂ Cu ₃ O ₇	BaCO ₃ ; CuO; Y ₂ O ₃	800	20	Y-Ba-Cu-O	10.1016/j.physc.2005.09.005
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	980	21	Y-Ba-Cu-O	10.1016/j.memsci.2003.12.011
YBa ₂ Cu ₃ O _{6.71}	BaO; CuO; Y ₂ O ₃	950	30	Y-Ba-Cu-O	10.1016/j.physc.2006.03.088
YBa ₂ Cu ₃ O _{7-x}	BaO ₂ ; CuO; Y ₂ O ₃	1100	36	Y-Ba-Cu-O	10.1016/j.jpcc.2013.04.025
YBa ₂ Cu ₃ O _y	BaCO ₃ ; CuO; Y ₂ O ₃	950	32	Y-Ba-Cu-O	10.1016/j.physc.2007.01.033
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	950	32	Y-Ba-Cu-O	10.1016/j.physc.2007.03.108
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/j.physc.2007.04.234
YBa ₂ Cu ₄ O ₈	BaCO ₃ ; CuO; Y ₂ O ₃	935	110	Y-Ba-Cu-O	10.1103/PhysRevB.70.144515
YBa ₂ Cu ₃ O _{7-d}	BaCO ₃ ; CuO; Y ₂ O ₃	930	48	Y-Ba-Cu-O	10.1021/cm020747j
YBa ₂ Cu ₃ O _{7-x}	BaCuO ₂ ; CuO; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/j.physc.2007.05.001
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/j.jqsrt.2004.09.023
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	1045	200	Y-Ba-Cu-O	10.1016/j.physc.2007.07.010
Y ₂ BaCuO _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	1045	200	Y-Ba-Cu-O	10.1016/j.physc.2007.07.010
YBa ₂ Cu ₄ O ₈	Ba(CH ₃ COO) ₂ ; Cu(CH ₃ COO) ₂ ·H ₂ O; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/j.chemphys.2006.04.007

YBa ₂ Cu ₃ O _x	BaCO ₃ ; CuO; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/S0921-4534(00)01520-3
Y ₂ BaCuO ₅	BaCO ₃ ; CuO; Y ₂ O ₃	1050	12	Y-Ba-Cu-O	10.1016/s0925-8388(98)00427-7
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/j.physc.2008.01.007
Y ₂ BaCuO ₅	BaCO ₃ ; CuO; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/j.physc.2008.01.007
YBa ₂ Cu ₃ O _x	BaCO ₃ ; CuO; Y ₂ O ₃	900	8	Y-Ba-Cu-O	10.1016/s0925-8388(98)00664-1
YBa ₂ Cu ₃ O _x	BaCO ₃ ; CuO; Y ₂ O ₃	950	32	Y-Ba-Cu-O	10.1016/j.physc.2008.12.002
YBa ₂ Cu ₃ O ₇	BaCO ₃ ; CuO; Y ₂ O ₃	900	72	Y-Ba-Cu-O	10.1021/ja9706920
YBa ₂ Cu ₃ O _x	BaCO ₃ ; CuO; Y ₂ O ₃	945	16	Y-Ba-Cu-O	10.1016/s0925-8388(99)00115-2
Y ₂ BaCuO ₅	BaO; CuO; Y ₂ O ₃	880	24	Y-Ba-Cu-O	10.1016/j.physc.2009.05.019
YBa _{2-x} Na _x Cu ₃ O _y +40mol%Y ₂ BaCuO ₅	BaCO ₃ ; CuO; Na ₂ C ₂ O ₄ ; Y ₂ O ₃	1050	150	Y-Ba-Cu-O	10.1016/S0921-4534(01)00150-2
YBa ₂ Cu ₃ O _{7-y}	BaCO ₃ ; CuO; Y ₂ O ₃	950	30	Y-Ba-Cu-O	10.1016/j.physc.2009.05.106
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	930	72	Y-Ba-Cu-O	10.1016/j.cryogenics.2015.05.011
Y ₃ Ba ₅ Cu ₈ O ₁₈	BaCO ₃ ; CuO; Y ₂ O ₃	840	12	Y-Ba-Cu-O	10.1016/j.physc.2009.09.003
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	950	8	Y-Ba-Cu-O	10.1016/j.physc.2009.11.034
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	925	32	Y-Ba-Cu-O	10.1016/j.jmmm.2010.04.002
Y ₂ Ba ₅ Cu ₇ O _x	BaCO ₃ ; CuO; Y ₂ O ₃	850	48	Y-Ba-Cu-O	10.1016/j.ssc.2016.02.017
Y ₂ BaCuO ₅	BaCO ₃ ; CuO; Y ₂ O ₃	900	60	Y-Ba-Cu-O	10.1016/S0921-4534(01)00624-4
Y ₂ BaCuO ₅	BaCO ₃ ; CuO; YBa ₂ Cu ₃ O _{7-x}	None	None	Y-Ba-Cu-O	10.1016/j.physc.2010.05.012
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	950	16	Y-Ba-Cu-O	10.1016/S0921-4534(01)00831-0
YBa ₂ Cu ₄ O ₈	Ba(CH ₃ COO) ₂ ; Cu(CH ₃ COO) ₂ ·H ₂ O; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/S0924-2031(01)00157-6
YBa ₂ Cu ₃ O _y	BaO; CuO; Y ₂ O ₃	910	12	Y-Ba-Cu-O	10.1016/j.physc.2010.05.236

Y ₂ BaCuO ₅	BaO; CuO; Y ₂ O ₃	910	12	Y-Ba-Cu-O	10.1016/j.physc.2010.05.236
Y ₂ BaCuO ₅	BaCO ₃ ; CuO; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/j.jcrysgr.2005.01.094
YBa ₂ Cu ₃ O _y	Ba(NO ₃) ₂ ; Cu(NO ₃) ₂ ·3H ₂ O; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/j.mseb.2003.11.015
YBa ₂ Cu ₃ O ₇	BaCO ₃ ; CuO; Y ₂ O ₃	940	144	Y-Ba-Cu-O	10.1039/c4ta06767c
Y ₂ BaCuO ₅	BaCuO ₂ ; Y ₂ O ₃	820	20	Y-Ba-Cu-O	10.1016/S0921-4534(01)00968-6
YBa ₂ Cu ₃ O _{7-x}	BaO ₂ ; CuO; Y ₂ O ₃	940	10	Y-Ba-Cu-O	10.1016/j.physc.2010.11.005
YBa ₂ Cu ₃ O _y	BaCO ₃ ; CuO; Y ₂ O ₃	950	32	Y-Ba-Cu-O	10.1016/j.physc.2010.12.012
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	950	10	Y-Ba-Cu-O	10.1016/S0921-4534(02)01318-7
YBa ₂ Cu ₃ O _y	BaCO ₃ ; CuO; Y ₂ O ₃	950	20	Y-Ba-Cu-O	10.1016/j.physc.2011.10.003
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/j.physc.2012.05.012
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	938	24	Y-Ba-Cu-O	10.1016/S0167-577X(01)00562-6
YBa ₂ Cu ₃ O _{7-x}	BaO; CuO; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/j.solidstatesciences.2005.07.002
Y ₂ BaCuO ₅	BaCO ₃ ; CuO; Y ₂ O ₃	1025	77	Y-Ba-Cu-O	10.1016/S0167-577X(02)00433-0
Y ₂ BaCuO ₅	BaCO ₃ ; CuO; Y ₂ O ₃	1025	77	Y-Ba-Cu-O	10.1016/S0167-577X(02)00433-0
YBa ₂ Cu ₃ O _{7-x}	BaO; CuO; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/j.jssc.2010.01.006
Y _{1.5} Ba ₂ Cu ₃ O _{7-x}	Y ₂ O ₃ ; YBa ₂ Cu ₃ O ₇	None	None	Y-Ba-Cu-O	10.1016/j.physc.2013.04.028
Y _{1.5} Ba ₂ Cu ₃ O _{7-x}	Y ₂ O ₃ ; YBa ₂ Cu ₃ O ₇	None	None	Y-Ba-Cu-O	10.1016/j.physc.2013.04.084
YBa ₂ Cu ₃ O _y	BaCO ₃ ; CuO; Y ₂ O ₃	950	20	Y-Ba-Cu-O	10.1016/j.physc.2013.12.006
YBa ₂ Cu ₃ O _y	BaCO ₃ ; CuO; Y ₂ O ₃	900	94	Y-Ba-Cu-O	10.1016/S0921-4534(02)02058-0
Y ₃ Ba ₅ Cu ₈ O _{18±x}	BaCO ₃ ; CuO; Y ₂ O ₃	950	60	Y-Ba-Cu-O	10.1007/s00339-017-1547-4
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	950	60	Y-Ba-Cu-O	10.1007/s00339-017-1547-4
Y ₂ BaCuO ₅	BaCO ₃ ; CuO; Y ₂ O ₃	900	94	Y-Ba-Cu-O	10.1016/S0921-4534(02)02058-0

YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	980	34	Y-Ba-Cu-O	10.1016/j.ssc.2004.04.044
YBa ₂ Cu ₃ O _{7-x}	Ag ₂ O; BaO; CuO; Y ₂ O ₃	950	74	Y-Ba-Cu-O	10.1016/j.ssc.2004.05.015
Y ₂ BaCuO ₅	BaCO ₃ ; CuO; Y ₂ O ₃	900	24	Y-Ba-Cu-O	10.1016/j.physc.2014.05.009
Y _{1.6} Ba _{2.3} Cu _{3.3} O _y	BaCO ₃ ; CuO; Y ₂ O ₃	1400	26	Y-Ba-Cu-O	10.1016/S0921-4534(02)02539-x
YBa ₂ Cu ₃ O _{7-x}	BaCu ₃ ; CuO; Y ₂ O ₃	920	12	Y-Ba-Cu-O	10.1016/S0167-577X(02)00795-4
YBa ₂ Cu ₃ O _y	BaCO ₃ ; CuO; Y ₂ O ₃	925	74	Y-Ba-Cu-O	10.1016/j.physc.2016.11.003
YBa ₂ Cu ₃ O _{6+x}	BaCO ₃ ; CuO; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1103/PhysRevB.93.054523
Y ₃ Ba ₅ Cu ₈ O ₁₉	BaCO ₃ ; CuO; Y ₂ O ₃	840	24	Y-Ba-Cu-O	10.1016/j.physc.2018.02.050
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1111/j.1551-2916.2008.02900.x
Y ₃ Ba ₅ Cu ₈ O ₁₈	Ba(NO ₃) ₂ ; CuO; Y ₂ O ₃	900	72	Y-Ba-Cu-O	10.1016/j.solidstatesciences.2011.08.024
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	945	24	Y-Ba-Cu-O	10.1007/s10854-013-1212-4
YBa ₂ Cu ₃ O ₇	BaCO ₃ ; CuO; Y ₂ O ₃	900	72	Y-Ba-Cu-O	10.1021/ja9706920
YBa ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Y ₂ O ₃	980	21	Y-Ba-Cu-O	10.1016/j.ssi.2004.10.003
YBa ₂ Cu ₄ O ₈	Ba(CH ₃ COO) ₂ ; Cu(CH ₃ COO) ₂ ·H ₂ O; Y ₂ O ₃	None	None	Y-Ba-Cu-O	10.1016/s0924-2031(01)00157-6
Y _{1-x} Pr _x Ba ₂ Cu ₃ O _{7-x}	BaCO ₃ ; CuO; Pr ₆ O ₁₁ ; Y ₂ O ₃	935	36	Y-Ba-Cu-O-*	10.1016/s0167-577x(01)00577-8
Y ₂ Ba(Cu _{1-x} Mg _x)O ₅	BaCO ₃ ; CuO; MgO; Y ₂ O ₃	1000	12	Y-Ba-Cu-O-*	10.1016/s0955-2219(03)00548-x
YBa _{2-x} La _x Cu ₃ O _y	BaCO ₃ ; CuO; La ₂ O ₃ ; Y ₂ O ₃	920	42	Y-Ba-Cu-O-*	10.1016/S0038-1098(00)00360-4
(La _{1-x} Y _x) ₂ Ba ₂ CaCu ₅ O _z	BaCO ₃ ; CaCO ₃ ; CuO; La ₂ O ₃ ; Y ₂ O ₃	900	48	Y-Ba-Cu-O-*	10.1016/j.ssc.2006.03.035
Y _{1-y} Yb _y Ba ₂ Cu ₃ O _x	BaCO ₃ ; CuO; Y ₂ O ₃ ; Yb ₂ O ₃	None	None	Y-Ba-Cu-O-*	10.1103/PhysRevB.79.054519
Y ₂ Ba(Cu _{1-x} Ni _x)O ₅	BaCO ₃ ; CuO; NiO; Y ₂ O ₃	1300	32	Y-Ba-Cu-O-*	10.1016/S0921-5107(00)00566-3
Ba(Zr _{0.84} Y _{0.15} Cu _{0.01})O _{3-x}	BaCO ₃ ; CuO; Y ₂ O ₃ ; ZrO ₂	1300	2	Y-Ba-Cu-O-*	10.1007/s10008-013-2187-z

$Y(Ba_{1-x}Sr_x)_2Cu_3O_{7-x}$	BaCO ₃ ; CuO; SrCO ₃ ; Y ₂ O ₃	930	24	Y-Ba-Cu-O-*	10.1016/j.ssc.2006.07.026
$YBa_2(Cu_{1-x}Ni_x)_3O_{7-x}$	BaCO ₃ ; CuO; Ni ₂ O ₃ ; Y ₂ O ₃	None	None	Y-Ba-Cu-O-*	10.1016/S0038-1098(01)00490-2
$YBaCuFeO_5$	BaCO ₃ ; CuO; Fe ₂ O ₃ ; Y ₂ O ₃	1150	72	Y-Ba-Cu-O-*	10.1016/j.jcrysro.2014.12.020
$(La_{1-x}Y_x)_2Ba_2CaCu_5O_z$	BaCO ₃ ; CaCO ₃ ; CuO; La ₂ O ₃ ; Y ₂ O ₃	900	48	Y-Ba-Cu-O-*	10.1016/j.ssc.2006.09.008
$Y_{1-x}Nd_xBa_2Cu_3O_{7-x}$	BaCO ₃ ; CuO; Nd ₂ O ₃ ; Y ₂ O ₃	930	46	Y-Ba-Cu-O-*	10.1016/j.jmatprotec.2007.12.078
$Y_{1-x}Ca_xBa_2Cu_{2.85}Re_{0.15}O_z$	BaCO ₃ ; CaO; CuO; ReO ₃ ; Y ₂ O ₃	None	None	Y-Ba-Cu-O-*	10.1016/s0038-1098(99)00085-x
$YBaCuFeO_5$	BaCO ₃ ; CuO; Fe ₂ O ₃ ; Y ₂ O ₃	1150	100	Y-Ba-Cu-O-*	10.1038/ncomms13758
$YBa_2(Cu_{1-x}Mn_x)_4O_8$	Ba(CH ₃ COO) ₂ ; Cu(CH ₃ COO) ₂ ·H ₂ O; Mn(CH ₃ COO) ₂ ; Y ₂ O ₃	820	50	Y-Ba-Cu-O-*	10.1016/s0955-2219(00)00206-5
$Y_{0.7}Ca_{0.3}Ba_2Cu_3O_yF_x$	BaCO ₃ ; CaCO ₃ ; CaF ₂ ; CuO; Y ₂ O ₃	920	84	Y-Ba-Cu-O-*	10.1016/j.jmmm.2003.11.105
$Y_{0.5}Nd_{0.5}Ba_2Cu_3O_x$	BaCO ₃ ; CuO; Nd ₂ O ₃ ; Y ₂ O ₃	900	48	Y-Ba-Cu-O-*	10.1016/S0022-0248(99)00391-7
$(La_{2-x}Y_x)Ba_2(Ca_yCu_{4+y})O_z$	BaCO ₃ ; CaCO ₃ ; CuO; La ₂ O ₃ ; Y ₂ O ₃	950	84	Y-Ba-Cu-O-*	10.1016/s0167-577x(98)00067-6
$YBa_{2-x}La_xCu_3O_{7-x}$	BaCO ₃ ; CuO; La ₂ O ₃ ; Y ₂ O ₃	1203	72	Y-Ba-Cu-O-*	10.1016/s1293-2558(03)00187-0
$YBa_{2-x}La_xCu_3O_y$	BaCO ₃ ; CuO; La ₂ O ₃ ; Y ₂ O ₃	950	1000	Y-Ba-Cu-O-*	10.1016/j.physc.2003.09.002
$YBa_{2-x}Na_xCu_3O_{y+40}$	BaCO ₃ ; CuO; Na ₂ C ₂ O ₄ ; Y ₂ O ₃	1040	174	Y-Ba-Cu-O-*	10.1016/s0167-577x(99)00178-0
$Cu_{1-0.75x}(Sr_{2x}Ba_{2-2x})(Ca_{0.5x}Y_{1-0.5x})Cu_2O_y$	BaCO ₃ ; CaCO ₃ ; CuO; SrCO ₃ ; Y ₂ O ₃	970	15	Y-Ba-Cu-O-*	10.1016/s0022-3697(01)00117-2
$YBa_2Cu_3F_{0.4}O_x$	$YBa_2Cu_3F_4O_x$; $YBa_2Cu_3O_x$	900	8	Y-Ba-Cu-O-*	10.1016/S0924-0136(99)00474-4
$Y_{1-x}La_xBa_2Cu_3O_{7-x}$	BaCO ₃ ; CuO; La ₂ O ₃ ; Y ₂ O ₃	970	41	Y-Ba-Cu-O-*	10.1016/j.mseb.2006.12.007
$Y_{1-y}CaYBa_2Cu_3O_{7-x}$	BaCO ₃ ; CaCO ₃ ; CuO; Y ₂ O ₃	970	41	Y-Ba-Cu-O-*	10.1016/j.mseb.2006.12.007
$Y_{1-x}Ca_xBaCuFeO_{5+x}$	BaCO ₃ ; CaCO ₃ ; CuO; Fe ₂ O ₃ ; Y ₂ O ₃	None	None	Y-Ba-Cu-O-*	10.1016/j.solidstatesciences.2011.10.021
$Y_{1-x}Ca_xBa_2Cu_3O_z$	BaCO ₃ ; CaCO ₃ ; CuO; Y ₂ O ₃	950	48	Y-Ba-Cu-O-*	10.1016/j.physc.2004.01.002
$TlBa_2Y_{1-x}Ca_xCu_2O_{7+x}$	BaO ₂ ; CaO; CuO; Tl ₂ O ₃ ; Y ₂ O ₃	None	None	Y-Ba-Cu-O-*	10.1016/s0022-3697(02)00087-2

$Y_2Ba_4CuWO_{10.8}$	BaCO ₃ ; CuO; WO ₃ ; Y ₂ O ₃	None	None	Y-Ba-Cu-O-*	10.1016/j.jeurceramsoc.2018.01.026
$Y_2Ba_4CuWO_x$	BaCO ₃ ; CuO; WO ₃ ; Y ₂ O ₃	None	None	Y-Ba-Cu-O-*	10.1016/j.jeurceramsoc.2018.01.026
$Ba(Zr_{0.84}Y_{0.15}Cu_{0.01})O_{3-x}$	BaCO ₃ ; CuO; Y ₂ O ₃ ; ZrO ₂	1500	42	Y-Ba-Cu-O-*	10.1016/j.jpowsour.2016.09.129
$Y_{1-x}Ca_xBa_2Cu_3O_y$	BaCO ₃ ; CaCO ₃ ; CuO; Y ₂ O ₃	None	None	Y-Ba-Cu-O-*	10.1016/s0254-0584(01)00545-4
$YBa_2Cu_{3-x}GdxO_{7-x}$	BaCO ₃ ; CuO; Gd ₂ O ₃ ; Y ₂ O ₃	930	24	Y-Ba-Cu-O-*	10.1016/j.physc.2004.10.008
$(Y_{0.74}Ca_{0.26})Ba_2Cu_3O_{7-x}$	BaCO ₃ ; CaCO ₃ ; CuO; Y ₂ O ₃	980	102	Y-Ba-Cu-O-*	10.1016/j.jpcs.2010.10.079
$(Y_{0.84}La_{0.16})(Ba_{1.74}La_{0.26})Cu_3O_{7-x}$	BaCO ₃ ; CuO; La ₂ O ₃ ; Y ₂ O ₃	980	102	Y-Ba-Cu-O-*	10.1016/j.jpcs.2010.10.079
$YBa_2Cu_{3-x}GdxO_{7-x}$	BaCO ₃ ; CuO; Gd ₂ O ₃ ; Y ₂ O ₃	930	24	Y-Ba-Cu-O-*	10.1016/j.physc.2004.10.008
$Fe_{0.5}Cu_{0.5}Ba_2YCu_2O_{7.41}$	BaCO ₃ ; CuO; Fe ₂ O ₃ ; Y ₂ O ₃	930	110	Y-Ba-Cu-O-*	10.1016/j.physc.2004.11.002
$Y_{0.8}Ca_{0.2}Ba_2Cu_3O_y$	BaCO ₃ ; CaCO ₃ ; CuO; Y ₂ O ₃	920	96	Y-Ba-Cu-O-*	10.1016/j.physc.2004.11.006
$YBa_2(Cu_{1-x}Zn_x)_3O_{7-x}$	BaCO ₃ ; CuO; Y ₂ O ₃ ; ZnO	1050	148	Y-Ba-Cu-O-*	10.1016/j.physc.2010.01.032
$Y_{1-x}Ca_xBa_2Cu_3O_{7-x}$	BaCO ₃ ; CaO; CuO; Y ₂ O ₃	920	48	Y-Ba-Cu-O-*	10.1016/j.physc.2005.01.002
$(Hg_{0.5}Pb_{0.5})(Sr_{2-x}Ba_x)(Ca_{0.7}Y_{0.3})Cu_2O_{7-d}$	BaO ₂ ; CaO; CuO; HgO; PbO; SrO ₂ ; Y ₂ O ₃	970	24	Y-Ba-Cu-O-*	10.1021/ie9611249
$Y_2Ba_4CuNbO_y$	BaCO ₃ ; CuO; Nb ₂ O ₅ ; Y ₂ O ₃	None	None	Y-Ba-Cu-O-*	10.1016/j.physc.2005.02.060
$Y_{0.92}Ta_{0.08}Ba_2Cu_3O_y$	BaCO ₃ ; CuO; Ta ₂ O ₅ ; Y ₂ O ₃	900	36	Y-Ba-Cu-O-*	10.1016/j.physc.2005.03.010
$(Cu_{1-x}Co_x)(Ba_{1-y}Sr_y)_2(Y_{1-z}Ca_z)Cu_2O_{7+x}$	BaCO ₃ ; CaCO ₃ ; Co ₃ O ₄ ; CuO; SrCO ₃ ; Y ₂ O ₃	940	48	Y-Ba-Cu-O-*	10.1016/j.physc.2005.04.034
$YBaCuCoO_{5+x}$	Ba(NO ₃) ₂ ; Co(NO ₃) ₂ ·6H ₂ O; Cu(NO ₃) ₂ ·6H ₂ O; Y ₂ O ₃	1000	3	Y-Ba-Cu-O-*	10.1002/fuce.201400141
$Y_{1-x}Sb_xBa_2Cu_3O_z$	BaCO ₃ ; CuO; Sb ₂ O ₃ ; Y ₂ O ₃	800	20	Y-Ba-Cu-O-*	10.1016/j.physc.2005.09.005
$YBa_2Cu_{3-x}Ca_xO_{7-y}$	BaCO ₃ ; CaO; CuO; Y ₂ O ₃	940	72	Y-Ba-Cu-O-*	10.1016/j.sna.2012.06.015
$YBa_2Cu_{2.99}Li_{0.01}O_y + 0.4Y_2BaCuO_5$	BaCO ₃ ; CuO; Li ₂ CO ₃ ; Y ₂ O ₃	1035	48	Y-Ba-Cu-O-*	10.1016/j.physc.2006.02.012
$YBa_{2-x}K_xCu_3O_y$	BaCO ₃ ; CuO; K ₂ CO ₃ ; Y ₂ O ₃	920	40	Y-Ba-Cu-O-*	10.1016/j.physc.2006.03.093

$Y_{1-x}B_xBa_2Cu_3O_y$	B_2O_3 ; Ba_2CO_3 ; CuO ; Y_2O_3	950	28	Y-Ba-Cu-O-*	10.1016/j.physc.2006.03.135
$Y_{0.95}Pr_{0.05}Ba_2(Cu_{1-x}Mn_x)_3O_{7-x}$	$BaCO_3$; CuO ; MnO_2 ; Pr_6O_{11} ; Y_2O_3	915	24	Y-Ba-Cu-O-*	10.1016/j.physc.2006.08.002
$Cu_{1-0.75x}(Sr_{2x}Ba_{2-2x})(Ca_{0.5x}Y_{1-0.5x})Cu_2O_y$	$BaCO_3$; $CaCO_3$; CuO ; $SrCO_3$; Y_2O_3	970	15	Y-Ba-Cu-O-*	10.1016/S0022-3697(01)00117-2
$YBa_2(Cu_{1-x}Zn_x)_3O_{6+x}$	$BaCO_3$; CuO ; Y_2O_3 ; ZnO	None	None	Y-Ba-Cu-O-*	10.1016/S0921-4534(00)00118-0
$YBa_2Cu_{3-x}M_xO_y$	Al_2O_3 ; $BaCO_3$; CuO ; Y_2O_3	920	12	Y-Ba-Cu-O-*	10.1103/PhysRevB.69.224517
$YBa_2Cu_{3-x}M_xO_y$	$BaCO_3$; CuO ; Y_2O_3 ; ZnO	920	12	Y-Ba-Cu-O-*	10.1103/PhysRevB.69.224517
$Y_{0.38}La_{0.62}(Ba_{0.82}La_{0.18})_2Cu_3O_y$	$BaCO_3$; CuO ; La_2O_3 ; Y_2O_3	980	90	Y-Ba-Cu-O-*	10.1103/PhysRevB.86.045124
$TlBa_2Y_{1-x}Ca_xCu_2O_{7+x}$	BaO_2 ; CaO ; CuO ; Tl_2O_3 ; Y_2O_3	None	None	Y-Ba-Cu-O-*	10.1016/S0022-3697(02)00087-2
$HgBa_2(Ca_{1-x}Y_x)Cu_2O_y$	BaO ; CaO ; CuO ; HgO ; Y_2O_3	720	22	Y-Ba-Cu-O-*	10.1016/S0921-4534(00)00205-7
$YBa_2(Cu_{3-x}Sc_x)O_y$	$BaCO_3$; CuO ; Sc_2O_3 ; Y_2O_3	967	72	Y-Ba-Cu-O-*	10.1016/j.physc.2007.04.043
$Y_{(1-x)}Ce_xBa_2Cu_3O_7$	$BaCO_3$; CeO_2 ; CuO ; Y_2O_3	930	160	Y-Ba-Cu-O-*	10.1016/j.physc.2007.04.046
$YBa_{2-x}La_xCu_3O_{7-x}$	$BaCO_3$; CuO ; La_2O_3 ; Y_2O_3	1203	72	Y-Ba-Cu-O-*	10.1016/S1293-2558(03)00187-0
$Y(Ba_{2-x}Sr_x)Cu_3O_{6.95}$	$BaCO_3$; CuO ; $SrCO_3$; Y_2O_3	950	60	Y-Ba-Cu-O-*	10.1016/S0921-4534(00)00293-8
$Y_{1-x}Ca_xBa_2Cu_3O_y$	$BaCO_3$; $CaCO_3$; CuO ; Y_2O_3	750	15	Y-Ba-Cu-O-*	10.1103/PhysRevB.70.214517
$YBa_{2-x}M_xCu_3O_y$	$BaCO_3$; CuO ; $NaNO_3$; Y_2O_3	950	12	Y-Ba-Cu-O-*	10.1016/S0921-4534(00)00338-5
$Y_2Ba_4CuMO_x$	$BaCO_3$; CuO ; Y_2O_3 ; ZrO_2	None	None	Y-Ba-Cu-O-*	10.1111/j.1551-2916.2007.01771.x
$Y_2Ba_4CuMO_x$	$BaCO_3$; CuO ; Nb_2O_5 ; Y_2O_3	None	None	Y-Ba-Cu-O-*	10.1111/j.1551-2916.2007.01771.x
$Y_{1-x}Ca_xBa_2Cu_3O_{7-x}$	$Ba(NO_3)_2$; $CaCO_3$; CuO ; Y_2O_3	450	1	Y-Ba-Cu-O-*	10.1016/S0921-4534(00)01530-6
$Ba(Zr_{0.84}Y_{0.15}Cu_{0.01})O_{3-x}$	$BaCO_3$; CuO ; Y_2O_3 ; ZrO_2	None	None	Y-Ba-Cu-O-*	10.1016/j.ceramint.2013.05.081
$YBa_{1.8}La_{0.2}Cu_3O_y$	$BaCO_3$; CuO ; La_2O_3 ; Y_2O_3	950	20	Y-Ba-Cu-O-*	10.1016/S0921-4534(00)01549-5
$Ba(Nd_xY_{2-x})CuO_5$	$BaCO_3$; CuO ; Nd_2O_3 ; Y_2O_3	980	44	Y-Ba-Cu-O-*	10.1016/j.jssc.2008.08.002
$YBa_2Cu_{3-x}Zn_xO_{6+x}$	CuO ; Y_2O_3 ; ZnO ; $BaCO_3$	None	None	Y-Ba-Cu-O-*	10.1016/s0925-8388(98)00577-5

$Y_{1-x}Tb_xBa_2Cu_3O_{7-x}$	BaCO ₃ ; CuO; Tb ₂ O ₃ ; Y ₂ O ₃	950	60	Y-Ba-Cu-O-*	10.1016/j.physc.2008.04.012
$YBa_2Cu_{3-x}Zn_xO_{7-x}$	BaCO ₃ ; CuO; Y ₂ O ₃ ; ZnO	970	26	Y-Ba-Cu-O-*	10.1016/S0921-4534(00)01648-8
$(La_{1-x}Y_x)_2Ba_2CaCu_5O_z$	BaCO ₃ ; CaCO ₃ ; CuO; La ₂ O ₃ ; Y ₂ O ₃	900	24	Y-Ba-Cu-O-*	10.1111/j.1551-2916.2007.01845.x
$YBa_{2-x}Sr_xCu_3O_{7-x}$	BaCO ₃ ; CuO; SrCO ₃ ; Y ₂ O ₃	950	8	Y-Ba-Cu-O-*	10.1016/S0921-4534(00)01748-2
$YBa_{2-x}Sr_xCu_3O_{7-x}$	BaCO ₃ ; CaCO ₃ ; CuO; Y ₂ O ₃	950	8	Y-Ba-Cu-O-*	10.1016/S0921-4534(00)01748-2
$Y_{1-x}Sm_xBa_2Cu_3O_{7-x}$	Ba ₂ CO ₃ ; CuO; Sm ₂ O ₃ ; Y ₂ O ₃	940	90	Y-Ba-Cu-O-*	10.1016/s0025-5408(01)00539-6
$Y_{1-x}Pr_xBa_2Cu_3O_y$	BaCO ₃ ; CuO; Pr ₂ O ₃ ; Y ₂ O ₃	930	96	Y-Ba-Cu-O-*	10.1016/j.physc.2008.05.031
$(Y_{1-x}Ca_x)SrBaCu_{2.80}(PO_4)_{0.20}O_y$	BaO; CaCO ₃ ; CuO; NH ₄ H ₂ PO ₄ ; SrCO ₃ ; Y ₂ O ₃	1000	32	Y-Ba-Cu-O-*	10.1016/S0921-4534(01)00104-6
$Y_{1-x}Ca_xBa_{2-x}La_xCu_3O_y$	BaCO ₃ ; CaCO ₃ ; CuO; La ₂ O ₃ ; Y ₂ O ₃	930	72	Y-Ba-Cu-O-*	10.1016/j.physc.2009.05.010
$Y_{1-x}(Yb_{0.9}Nd_{0.1})_xBa_2Cu_3O_z$	BaO; CuO; Nd ₂ O ₃ ; Y ₂ O ₃ ; Yb ₂ O ₃	910	12	Y-Ba-Cu-O-*	10.1016/j.physc.2009.05.019
$Y_{1-x}Pr_xBa_2Cu_3O_y$	BaCO ₃ ; CuO; Pr ₂ O ₃ ; Y ₂ O ₃	930	96	Y-Ba-Cu-O-*	10.1016/j.physc.2009.05.119
$Y_2Ba_4CuNbO_y$	BaCO ₃ ; CuO; Nb ₂ O ₅ ; Y ₂ O ₃	None	None	Y-Ba-Cu-O-*	10.1016/j.physc.2009.05.194
$Y_xNd_{1-x+y}Ba_{2-y}Cu_3O_{6+x}$	BaCO ₃ ; CuO; Nd ₂ O ₃ ; Y ₂ O ₃	1070	174	Y-Ba-Cu-O-*	10.1016/S0921-4534(01)00351-3
$Y_{1-z}Ca_zBa_{2-z}La_zCu_3O_x$	BaCO ₃ ; CaCO ₃ ; CuO; La ₂ O ₃ ; Y ₂ O ₃	1010	24	Y-Ba-Cu-O-*	10.1016/S0921-4534(01)00366-5
$Y_{1-x}Ho_xBa_2Cu_3O_y$	$(Y_{1-x}Ho_x)_2BaCuO_5$; BaCuO ₂ ; CuO	550	40	Y-Ba-Cu-O-*	10.1016/S0921-4534(01)00368-9
$YBa_2Cu_3F_{0.4}O_x$	YBa ₂ Cu ₃ F ₄ O _x ; YBa ₂ Cu ₃ O _x	900	8	Y-Ba-Cu-O-*	10.1016/S0924-0136(99)00474-4
$YBa_2Cu_{3-x}In_xO_y$	BaCO ₃ ; CuO; In ₂ O ₃ ; Y ₂ O ₃	1233	24	Y-Ba-Cu-O-*	10.1016/j.physc.2010.05.073
$Y_{1-x}Pr_xBa_2Cu_3O_{7-d}$	BaCO ₃ ; CuO; Pr ₆ O ₁₁ ; Y ₂ O ₃	1213	183	Y-Ba-Cu-O-*	10.1021/cm9604928
$YBa_2Co_xCu_{3-x}O_{7-x}$	BaCO ₃ ; Co ₂ O ₃ ; CuO; Y ₂ O ₃	980	25	Y-Ba-Cu-O-*	10.1016/j.catcom.2006.11.029
$YBa_2Cu_{3-x}Co_xO_y$	BaCO ₃ ; Co ₂ O ₃ ; CuO; Y ₂ O ₃	900	48	Y-Ba-Cu-O-*	10.1016/S0921-4534(01)01286-2
$YBa_2Cu_{3-x}M_xO_y$	BaCO ₃ ; CuO; Fe ₂ O ₃ ; Y ₂ O ₃	900	48	Y-Ba-Cu-O-*	10.1016/S0921-4534(02)01268-6

$YBa_2Cu_{3-x}M_xO_y$	$BaCO_3; Co_3O_4; CuO; Y_2O_3$	900	48	Y-Ba-Cu-O-*	10.1016/S0921-4534(02)01268-6
$YBa_{2-x}La_xCu_{3-x}Al_xO_z$	$Al_2O_3; BaCO_3; CuO; La_2O_3; Y_2O_3$	940	66	Y-Ba-Cu-O-*	10.1016/j.physc.2012.01.013
$YxGd_{1-x}Ba_2Cu_3O_{7-x}$	$BaCO_3; CuO; Gd_2O_3; Y_2O_3$	950	58	Y-Ba-Cu-O-*	10.1016/S0921-4534(02)01441-7
$YBa_{2-x}La_xCu_{3-x}Zn_xO_z$	$BaCO_3; CuO; La_2O_3; Y_2O_3; ZnO$	940	66	Y-Ba-Cu-O-*	10.1016/j.physc.2012.01.013
$Y_{1-x}Ca_xBa_2Cu(Cu_{1-y}Mg_y)_3O_{7-x}$	$BaCO_3; CaCO_3; CuO; MgO; Y_2O_3$	940	24	Y-Ba-Cu-O-*	10.1016/j.physc.2012.02.031
$Y_{1-x}Sm_xBa_2Cu_3O_{7-x}$	$Ba_2CO_3; CuO; Sm_2O_3; Y_2O_3$	940	90	Y-Ba-Cu-O-*	10.1016/S0025-5408(01)00539-6
$YBaCuFeO_5$	$BaCO_3; CuO; Fe_2O_3; Y_2O_3$	1050	60	Y-Ba-Cu-O-*	10.1103/PhysRevB.91.064408
$Y_{1-x}Pr_xBa_2Cu_3O_{7-x}$	$BaCO_3; CuO; Pr_6O_{11}; Y_2O_3$	935	36	Y-Ba-Cu-O-*	10.1016/S0167-577X(01)00577-8
$Y_2Ba(Cu_{1-x}Zn_x)O_5$	$BaCO_3; CuO; Y_2O_3; ZnO$	950	30	Y-Ba-Cu-O-*	10.1016/s0955-2219(01)00097-8
$YBa_2Cu_{3-x}Gd_xO_{7-x}$	$BaCO_3; CuO; Gd_2O_3; Y_2O_3$	940	20	Y-Ba-Cu-O-*	10.1007/s10854-012-0917-0
$Ba(Zr_{0.84}Y_{0.15}Cu_{0.01})O_{3-x}$	$BaCO_3; CuO; Y_2O_3; ZrO_2$	1500	12	Y-Ba-Cu-O-*	10.1016/j.ijhydenc.2014.02.072
$Y_{2-x}Dy_xBaCuO_5$	$BaCO_3; CuO; Dy_2O_3; Y_2O_3$	1000	60	Y-Ba-Cu-O-*	10.1016/j.ssc.2004.02.026
$YBa_2Cu_{3-x}Al_xO_{7-x}$	$Al_2O_3; BaCO_3; CuO; Y_2O_3$	550	24	Y-Ba-Cu-O-*	10.1016/S0921-4534(02)02057-9
$Y_{0.85}Ca_{0.15}Ba_2Cu_3O_{7-x}$	$BaCO_3; CaCO_3; CuO; Y_2O_3$	930	24	Y-Ba-Cu-O-*	10.1016/j.ssc.2004.03.002
$(Y_{1-x-y}Pr_xCa_y)Ba_2Cu_3O_{7-x}$	$BaCO_3; CaCO_3; CuO; Pr_6O_{11}; Y_2O_3$	940	72	Y-Ba-Cu-O-*	10.1016/S0921-4534(02)02362-6
$Y_2Ba(Cu_{1-x}Ni_x)O_5$	$BaCO_3; CuO; NiO; Y_2O_3$	1300	32	Y-Ba-Cu-O-*	10.1016/s0921-5107(00)00566-3
$YBa_2Cu_{3-x}Gd_xO_{7-x}$	$BaCO_3; CuO; Gd_2O_3; Y_2O_3$	940	20	Y-Ba-Cu-O-*	10.1007/s10854-012-1022-0
$Tl_2Ba_2Ca_{1-x}Y_x(Cu_{1-y}Co_y)_2O_8$	$Ba_2Ca_{1-x}Y_x(Cu_{1-y}Co_y)O_{4+x}; CoO; CuO;$ Tl_2O_3	930	30	Y-Ba-Cu-O-*	10.1016/S0921-4534(03)00628-2
$Y_{1-x}Eu_xBa_2Cu_3O_{7-x}$	$BaCO_3; CuO; Eu_2O_3; Y_2O_3$	1015	32	Y-Ba-Cu-O-*	10.1016/S0921-4534(03)00704-4
$Y(Ba_{2-x}R_x)Cu_3O_{7-x}$	$BaCO_3; CuO; La_2O_3; Y_2O_3$	940	72	Y-Ba-Cu-O-*	10.1016/S0921-4534(03)00810-4
$Y(Ba_{2-x}R_x)Cu_3O_{7-x}$	$BaCO_3; CuO; Nd_2O_3; Y_2O_3$	940	72	Y-Ba-Cu-O-*	10.1016/S0921-4534(03)00810-4

$Y(Ba_{2-x}R_x)Cu_3O_{7-x}$	$BaCO_3$; CuO ; Pr_6O_{11} ; Y_2O_3	940	72	Y-Ba-Cu-O-*	10.1016/S0921-4534(03)00810-4
$YBa_{2-x}Sm_xCu_3O_{7-x}$	$BaCO_3$; CuO ; Sm ; Y_2O_3	935	24	Y-Ba-Cu-O-*	10.1016/j.physc.2018.02.026
$Y_{1-y-x}Co_yCa_xBa_2Cu_3O_{7-x}$	$BaCO_3$; $CaCO_3$; Co_3O_4 ; CuO ; Y_2O_3	None	None	Y-Ba-Cu-O-*	10.1016/j.physc.2018.02.029
$Y_{0.98-x}Co_{0.02}Ca_xBa_2Cu_3O_{7-x}$	$BaCO_3$; $CaCO_3$; Co_3O_4 ; CuO ; Y_2O_3	950	24	Y-Ba-Cu-O-*	10.1016/j.physc.2018.02.029
$YBa_2Cu_3(OH)_x$	$Ba(OC_3H_7)_2$; $Cu(CH_3COO)_2$; $Y(OC_3H_7)_3$	None	None	Y-Ba-Cu-O-*	10.1111/j.1551-2916.2008.02900.x
$YBa_2(Cu_{1-x}Cr_x)_4O_8$	$Ba(CH_3COO)_2$; $Cr(NO_3)_3 \cdot 9H_2O$; $Cu(CH_3COO)_2 \cdot H_2O$; Y_2O_3	800	50	Y-Ba-Cu-O-*	10.1016/j.chemphys.2006.12.001
$Y_3Ba_5Ca_2Cu_8O_{18}$	$Ba(NO_3)_2$; $CaCO_3$; CuO ; Y_2O_3	900	72	Y-Ba-Cu-O-*	10.1016/j.solidstatesciences.2011.08.024
$Y_{1-x}Ca_xBaSrCu_3O_y$	$BaCO_3$; $CaCO_3$; CuO ; $SrCO_3$; Y_2O_3	1233	24	Y-Ba-Cu-O-*	10.1016/S0921-4534(03)01167-5
$BaCe_{0.5}Zr_{0.3}Y_{0.08}Yb_{0.08}Cu_{0.04}O_{3-x}$	$BaCO_3$; CeO_2 ; CuO ; Y_2O_3 ; Yb_2O_3 ; ZrO_2	1400	3	Y-Ba-Cu-O-*	10.1016/j.ijhydene.2015.05.020
$Y_{1-x}Ca_xBa_{1.9}Nd_{0.1}Cu_3O_y$	$BaCO_3$; CaO ; CuO ; Nd_2O_3 ; Y_2O_3	950	36	Y-Ba-Cu-O-*	10.1016/S0921-4534(03)01275-9
$Fe_{0.5}Cu_{0.5}Ba_2YCu_2O_{7+x}$	$BaCO_3$; CuO ; Fe_2O_3 ; Y_2O_3	930	110	Y-Ba-Cu-O-*	10.1016/S0921-4534(03)01294-2
$YBa_{2-x}La_xCu_3O_y$	$BaCO_3$; CuO ; La_2O_3 ; Y_2O_3	920	42	Y-Ba-Cu-O-*	10.1016/s0038-1098(00)00360-4
$Fe_xCu_{1-x}Ba_2YCu_2O_{7+y}$	$BaCO_3$; CuO ; Fe_2O_3 ; Y_2O_3	930	110	Y-Ba-Cu-O-*	10.1016/j.ssc.2005.03.017
$(Y_{2-x}Sm_x)Ba(Cu_{1-y}Co_y)O_5$	$BaCO_3$; CoO ; CuO ; Sm_2O_3 ; Y_2O_3	850	32	Y-Ba-Cu-O-*	10.1016/s0955-2219(03)00179-1
$YBa_2Cu_3F_{0.4}O_x$	$YBa_2Cu_3F_4O_x$; $YBa_2Cu_3O_x$	900	8	Y-Ba-Cu-O-*	10.1016/s0924-0136(99)00474-4
$YBa_2(Cu_{1-x}Ni_x)_3O_{7-x}$	$BaCO_3$; CuO ; Ni_2O_3 ; Y_2O_3	None	None	Y-Ba-Cu-O-*	10.1016/s0038-1098(01)00490-2