Phase Transition of YBO₃

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**Introduction**

YBO₃ is one of the members of the orthoborate family and a widely applied host material for luminescent dopants, such as Eu³⁺ and Tb³⁺. The rare earth borates REBO₃ constitute a group of compounds isostructural with the minerals of calcium carbonate CaCO₃. Depending on the cation size of RE, the orthoborates crystallize with the aragonite, vaterite, or calcite type structure. Yttrium orthoborate exhibits the vaterite structure and shows a phase transition (LT→HT) with a pronounced thermal hysteresis during the cooling. The hexagonal structure consists of a three-dimensional network made up of 8-fold coordinated yttrium atoms and 4- or 3-fold coordinated boron atoms. The LT-phase of YBO₃ consists of tetrahedral polyborate groups B₃O₉⁹⁻ and the HT-phase triangular comprises borate group BO₃⁻. During the phase transition the borate groups changes from B₃O₉⁹⁻ ring to BO₃⁻ single units.

**Powder Preparation and Characterization**

All investigated samples have been made from Y₂O₃ and H₃BO₃ (excess 10%) by using conventional solid state-reaction at 1100°C and 1350°C for 4 h in air. The formation of the ortho-borate phase can be identified by an exothermic reaction at about 712°C and by the change in the XRD patterns. The yttrium orthoborate shows a thermal stability up to about 1200°C and undergoes the phase transition into the HT-Phase at 980.9°C with \( \Delta H° = 12.1 \pm 1.3 \) kJ/mol. The powder shows x-ray high purity and IR spectra exhibit that no three coordinate boron is present due to the lack of an absorption line at 1200 cm⁻¹.

The extrapolation of the experimental data to zero \( \beta \) give true transition points at 986.8°C for heating and at 596.5°C for cooling, respectively (\( T_{\text{onset}} = a + b \ln(\beta + 1) \)).

**The True Transition Points**

The values of \( E_a \) evaluated using Kissinger’s equation are: \( E_a = 1386 \) kJ/mol for heating and \( E_a = 568 \) kJ/mol for cooling, respectively.

**The cyclic thermal treatment (heating/cooling) of YBO₃**

The ytrrium orthoborate shows a thermal stability up to about 1200°C and undergoes the phase transition into the HT-Phase at 980.9°C with \( \Delta H° = 12.1 \pm 1.3 \) kJ/mol.

The peak shifts toward higher (heating) and lower (cooling) temperature with the cycle number.

**Thermogramm of YBO₃ sample**

The powder shows x-ray high purity and IR spectra exhibit that no three coordinate boron is present due to the lack of an absorption line at 1200 cm⁻¹.

**X-ray pattern (left) and IR spectrum (right) of YBO₃ sample**

For samples with a different “thermal history” other phase transition temperatures are observed.

**SEM images of YBO₃ powder**

**For samples with a different “thermal history” other phase transition temperatures are observed.**

**Morphological observation of the real phenomenon occurring during phase transition**

**Transition temperature vs. ionic radii of the REBO₃.**

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