The Structure of BaFeO$_{2.8-\delta}$ Prepared by Thermal Decomposition of BaFe[(CN)$_5$NO].3H$_2$O

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Beamline(s): X3B1

Introduction: BaFeO$_{2.8-\delta}$ was prepared by a low temperature method of synthesis, based on the oxidative thermal decomposition of BaFe[(CN)$_5$NO].3H$_2$O. For catalytic purposes, low temperatures of synthesis are needed in order to produce a high surface area catalyst with a high content of Fe$^{+4}$.

Methods and Materials: The high resolution X-ray diffraction pattern of BaFeO$_{2.8-\delta}$ was collected at the X3B1 beamline, N.S.L.S.. The crystal structure was solved with the program EXPO.

Results: The structure is shown in Figure 1. The material belongs to the space group P6$_3$/mmc, cell parameters $a=b=5.77944(1)$ Å, $c=24.60871(6)$ Å, $\alpha=90^\circ$, $\beta=90^\circ$, $\gamma=120^\circ$, $Z=10$.

The structure consists of 10H close packed (hchch)$_2$ stacking of BaO$_n$ layers (8 BaO$_3$ layers and 2 oxygen deficient BaO$_2$ layers). Additional oxygen deficiencies are randomly distributed on the h BaO$_3$ layers.

This new polytype in the system BaFeO$_y$ is believed to be stabilized only at this low temperature of synthesis (850°C) and atmospheric oxygen pressure, since it has not been described for samples prepared with other methods.

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Figure 1. The structure of BaFeO$_{2.8-\delta}$