

## The Structure of BaFeO<sub>2.8-δ</sub> Prepared by Thermal Decomposition of BaFe[(CN)<sub>5</sub>NO].3H<sub>2</sub>O

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Beamline(s): X3B1

**Introduction:** BaFeO<sub>2.8-δ</sub> was prepared by a low temperature method of synthesis, based in the oxidative thermal decomposition of BaFe[(CN)<sub>5</sub>NO].3H<sub>2</sub>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<sup>+4</sup> <sup>1</sup>.

**Methods and Materials:** The high resolution X-ray diffraction pattern of BaFeO<sub>2.8-δ</sub> was collected at the X3B1 beamline, N.S.L.S.. The crystal structure was solved with the program EXPO <sup>2</sup>.

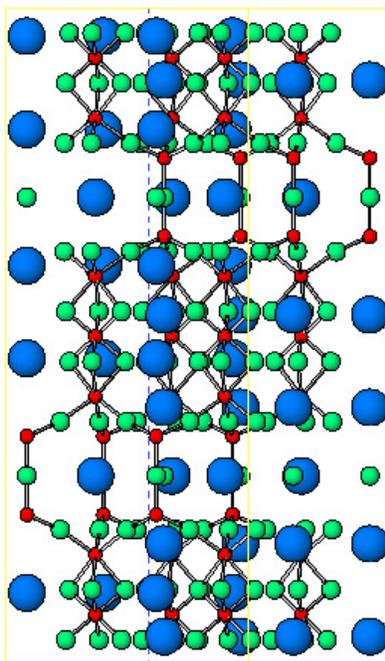
**Results:** The structure is shown in **Figure 1**. The material belongs to the space group P6<sub>3</sub>/mmc, cell parameters a=b=5.77944(1) Å, c=24.60871(6) Å, α=90°, β=90°, γ=120°, Z=10.

The structure consists of 10H close packed (hch)<sub>2</sub> stacking of BaO<sub>n</sub> layers (8 BaO<sub>3</sub> layers and 2 oxygen deficient BaO<sub>2</sub> layers). Additional oxygen deficiencies are randomly distributed on the h BaO<sub>3</sub> layers.

This new polytype in the system BaFeO<sub>y</sub> 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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**References:** <sup>1</sup> M. I. Gómez, G. Lucotti, J. A. de Morán, P. J. Aymonino, S. Pagola, P. W. Stephens and R. E. Carbonio, "Ab-initio Structure Solution of BaFeO<sub>3.δ</sub>, a new polytype in the System BaFeO<sub>y</sub> (2.5 ≤ y ≤ 3.0) Prepared from the Oxidative Thermal Decomposition of BaFe[(CN)<sub>5</sub>NO].3H<sub>2</sub>O", *J. Solid State Chem.*, submitted for publication. <sup>2</sup> A. Altomare, M. C. Burla, M. Camalli, B. Carrozzini, G. L. Casciarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori and R. Rizzi, "EXPO: A Program for Full Powder Pattern Decomposition and Crystal Structure Solution", *J. Appl. Cryst.* 32, p. 339-340, 1999.



**Figure 1.** The structure of BaFeO<sub>2.8-δ</sub>