There is a great interest in the multiferroic compounds and in mechanisms of the magnetic-ferroelectric coupling in view of promising wide technological applications of such materials. Recently, a cascade of the magnetic and structural phase transitions were discovered in new multiferroic GdFe\(_2\)(BO\(_4\))\(_3\) [1], [2], [3]. A single-crystal X-ray structural study [2] showed the presence of two different iron helicoidal chains at 90 K, which becomes identical at room temperature. However, the relationship between magnetism and structure of GdFe\(_2\)(BO\(_4\))\(_3\) is still unclear.

In this work, the single-crystal of gadolinium iron borate GdFe\(_2\)(BO\(_4\))\(_3\) was investigated by the \(^{57}\)Fe Mössbauer spectroscopy and X-ray diffraction in the temperature range between 5 and 295 K. Computer analysis of the Mössbauer data shows the presence of two close but nonequivalent sites for the Fe ions in the whole temperature range 5 - 295 K. Temperature dependences of the hyperfine parameters of the Mössbauer spectra indicate some structural and magnetic anomalies at T < T\(_{K}\) and near the structural phase transition points, that are well correlated with our single-crystal X-Ray data.

The unit cell parameters of GdFe\(_2\)(BO\(_4\))\(_3\) single crystal were determined in a temperature range from room temperature to 30 K on a HUBER-5042 four-circle X-ray diffractometer equipped with a DISPLEX DE-202 two-stage closed-cycle cryostat (ADP Cryogenics Inc.), which affords the temperature stabilization within ±0.05 K. The accuracy of setting the angular positions of the goniometer is 0.001°. The unit cell parameters were measured at T = 295 K and in the 220 - 30 K range with the 5 - 10 K intervals. The measurements were based on 32 diffraction reflections at 19° < \(\theta\) < 22°. It was found that the a and b init cell parameters do not change until the phase transition at 155 K, and then they decrease dramatically with lowering temperature. After that they reduce as a ~ T\(^{-1}\)-law. Yet, the c parameter decreases uniformly from the room temperature down to 155 K, and then some anomalies appear near 80 K when it starts to increase. The unit cell volume shows properly the phase transition at 155 K and has some anomalies in the 80 - 60 K interval.

Acknowledgments: This work is supported by the Russian Foundation for Basic Research Grant and 11-02-00636-a and by the Program of Russian Academy of Sciences under the Project “Strongly correlated electronic systems”.


Keywords: multiferroics, phase transitions, low temperature
Poster Sessions

MS81.P52

**Acta Cryst.** (2011) A67, C722

**Diffraction methods for investigation of the real structure of langasite family**

Elena Domoroshchina,
Irina Kauraova,
Galina Kuz’micheva,
Viktor Rybakov,
Alain Cousson,
Oksana Zaharko,
Lomonosov State Academy of Fine Chemical Technology, Moscow, (Russia).

The crystallographic investigations of langasite family family, represented by general chemical formula Al2BCO6O18, are excellent candidates for piezoelectric and high temperature applications. However, the application of these compounds depends on the type and concentration of point defects, which does not coincide with the composition of the initial charge.

The real structures of langasite family family, represented by general chemical formula Al2BCO6O18, are excellent candidates for piezoelectric and high temperature applications. However, the application of these compounds depends on the type and concentration of point defects, which does not coincide with the composition of the initial charge.

**Keywords:** silienates, composition, structure

MS81.P53

**Acta Cryst.** (2011) A67, C722–C723

**Structure elucidation and aqueous speciation of water-soluble M,Si,M= (Mo,W) clusters bearing hydroxypropyl diphosphine ligands**

Tomas P. Beltrán,
Manuel G. Basallote,
M. Jesús Fernández-Trujillo,
Jose Angel Pino,
Carolina Corao,
Rosa Llusar,
Maxim Sokolov,
Cristian Vicent,
Department of Química Física e Analítica, Universitat Jaume I, Campus de Riu Sec, 12071 Castelló, (Spain).

The chemistry of water-soluble transition-metal complexes containing phosphine ligands is of interest because of the potential usefulness of these complexes in biphagic (aqua-organic) catalysis and biomedicine.[1] Two-phase catalysis can solve basic problems in homogeneous catalysis such as the separation and further recycling of the catalyst, making these processes environmentally friendly.

In particular, phosphines with hydroxyalkyl groups such as 1,2-bis(bis(hydroxypropyl)-phosphin)ethane (dhppe) have enabled the development of a wide spectrum of water-soluble transition/organometallic complexes.[2]

Here we present the structural characterization of new group six trinuclear [M,SiX3(dhppe)], (M= Mo, W; X=Cl, Br) clusters combining x-ray diffraction and spectroscopic techniques. A water speciation study is also shown. Depending on pH, new cluster structures are obtained as a result of dhppe ligand deprotonation.

C722