Crystal and Magnetic Structure of Potentially Multi-Ferroic PbFeO$_3$


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Multi-ferroics are materials that exhibit spontaneous electric and magnetic polarizations simultaneously. In the search for new multi-ferroic compounds, a popular strategy is to modify known ferroelectric materials by substitutions that introduce magnetic ions. For example,

PbTiO$_3$ is a well-known ferroelectric but is diamagnetic. Substitution of Ti with Fe will introduce magnetic properties. PbFeO$_3$ can be prepared only at high pressure (6 – 7 GPa) and temperature (1275 – 1575 K) in an anvil apparatus [1]. XPS data indicate that Pb$^{2+}$, Pb$^{4+}$ and Fe$^{3+}$ are present in this material. X-ray powder data are consistent with an orthorhombic pseudo cubic sub-cell with $a_c \sim 3.90$ Å, but a complex supercell of $6a_c \times 2a_c \times 2a_c$ was found from electron diffraction. It was the goal of this study to determine the critical temperature for magnetic order and, if possible, the crystal and magnetic structures. The sample size was only $\sim 700$ mg. Data were taken from 2.8 K to 610 K. For measurements above room temperature, the sample was contained in a quartz tube backfilled with $\sim 1$ atm of oxygen as the sample is known to decompose above 720K in air. To search for magnetic reflections, the difference plot 296 K – 610 K was constructed as shown in Figure 1. Three magnetic reflections are marked with an asterix (*) at $2\theta = 30.484(3)^\circ$, 59.89(1)$^\circ$ and 60.921(8)$^\circ$. These can be indexed on the primitive orthorhombic cell as $(1/2 \ 1/2 \ 1/2)$, $(3/2 \ 1/2 \ 1/2)$ and $(1/2 \ 1/2 \ 3/2)$ which indicates a G-type antiferromagnetic structure as was found for the related material, PbFeO$_2$F [2]. The temperature dependence of the strongest magnetic peak (2$\theta = 30.48^\circ$) is shown in the inset which indicates $T_c = 605(3)$ K.

Fig. 1 The difference plot 296 K – 610 K for PbFeO$_3$. Magnetic reflections are marked with an asterix (*). The temperature dependence of the strongest magnetic peak at 30.48 deg ,$(1/2 \ 1/2 \ 1/2)$, is shown in the inset which indicates $T_c = 605(3)$ K.

References
