Supplementary Document

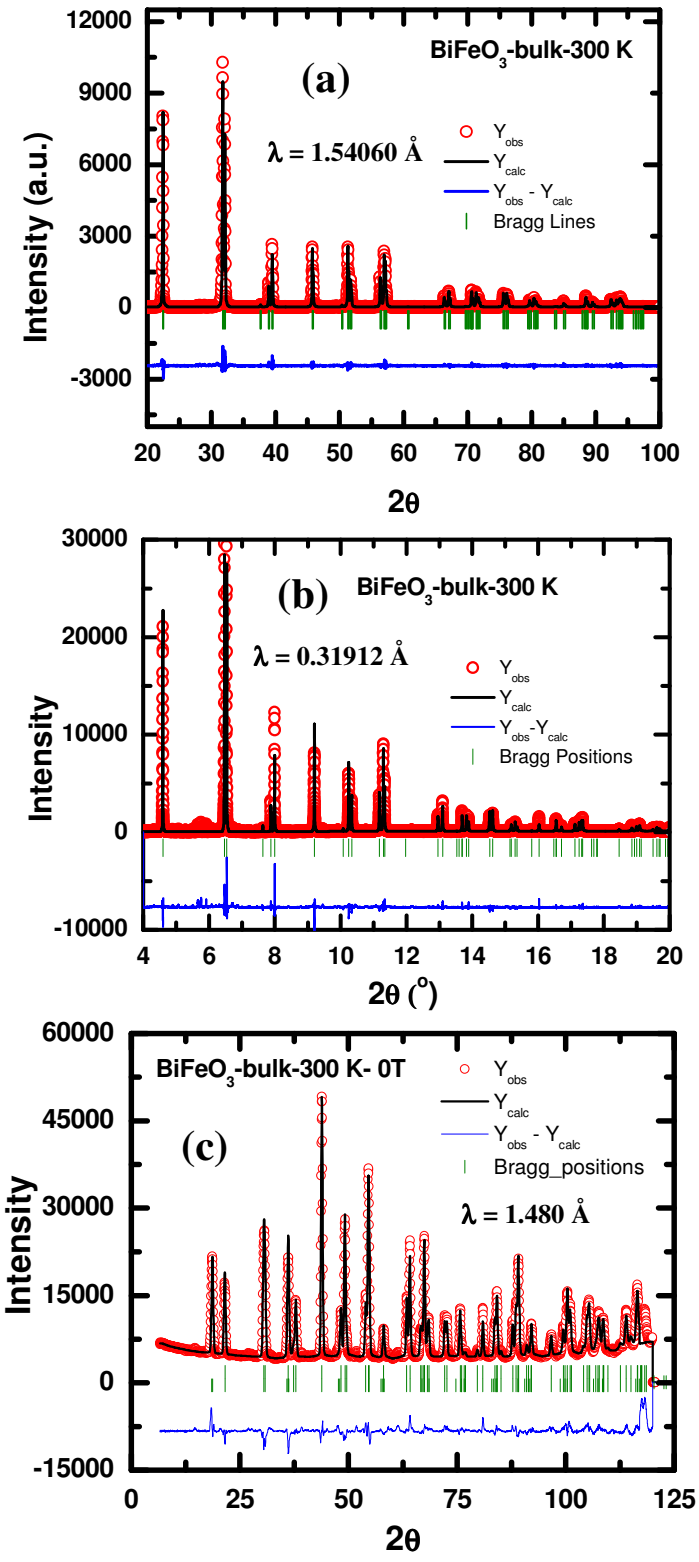

Fig. 1. The diffraction patterns obtained for bulk $BiFeO_3$ at room temperature from (a) laboratory x-ray, (b) synchrotron x-ray, and (c) neutron sources.

In this document, we discuss about how the atom positions determined from the laboratory x-ray, synchrotron x-ray, and neutron diffraction differ. We have carried out the measurements on a bulk sintered pellet of $BiFeO_3$ at room temperature under zero magnetic field. The synchrotron x-ray diffraction data have been recorded at the ID31 beamline of ESRF, Grenoble while the powder neutron diffraction data have been recorded at the PD-3 beamline of BARC, Mumbai. The data were refined by FullProf. In Figs.1a, b, and c, we show the diffraction patterns recorded at laboratory, synchrotron, and neutron sources, respectively. The results obtained from the refinement are given in the Table-I below.

It is important to note from the results that while the position of Fe ion differs by 1-3% when estimated from the laboratory x-ray, synchrotron x-ray, and powder neutron data, the position of oxygen ion differs a lot. While the O_x and O_z positions, determined from synchrotron and neutron diffraction data, differ by <1%, the O_y position differs by a staggering ~20% when estimated from neutron and synchrotron or lab x-ray data. This result shows that determination of the position of lighter ions such as oxygen could be grossly erroneous if estimated from the x-ray diffraction data. Since accurate determination of the position of oxygen ion is essential for accurate determination of the structural noncentrosymmetry, it is highly advisable to use neutron diffraction data. Therefore, in this work we used powder neutron

diffraction data both for bulk and nanoscale $BiFeO_3$ in order to determine the structural noncentrosymmetry and its anomaly around the magnetic transition point T_N.

Table-I. The lattice parameters, ion positions, bond lengths, angles, and the fit statistics obtained from the refinement of laboratory x-ray, synchrotron x-ray, and neutron diffraction patterns for the bulk $BiFeO_3$.

Experiment	**Lattice parameter (Å) and Lattice volume (Å^3)**	**Ions**	**Position**			**Bond length (Å)**		**Bond angle (°)**		**R_p**	**R_{wp}**	**χ^2**
			x	**y**	**z**							
Lab X-Ray	a=5.572620 c=13.850105 Vol=373.441	Bi	0	0	0	Bi-O	2.0527	Fe-O-Fe	148.24	16.8	21.9	12.0
		Fe	0	0	0.21512	Bi-O	2.6337	O-Bi-O	81.29			
		O	0.45015	0.02144	0.93091	Fe-O	1.8744					
						Fe-O	2.2447					
Synchrotron X-ray	a=5.596004 c=13.925158 Vol=377.648	Bi	0	0	0	Bi-O	2.2727	Fe-O-Fe	152.04	12.8	17.0	8.06
		Fe	0	0	0.22244	Bi-O	2.4944	O-Bi-O	73.12			
		O	0.43955	0.02135	0.95184	Fe-O	1.9690					
						Fe-O	2.1303					
Neutron	a=5.577308 c=13.863700 Vol=373.473	Bi	0	0	0	Bi-O	2.2823	Fe-O-Fe	154.56	4.47	6.09	26.7
		Fe	0	0	0.22000	Bi-O	2.5036	O-Bi-O	73.30			
		O	0.44138	0.01698	0.95259	Fe-O	1.9593					
						Fe-O	2.1035					