Bi$_2$NaCaNb$_3$O$_{12}$ (BCNN) is an Aurivillius phase with [Bi$_2$O$_2$]$^{2+}$ sheets interleaved among perovskite-like blocks. Topochemical conversion to the protonated form may be achieved using simple acid treatment, and subsequent exfoliation into nanosheet suspensions is also possible. The XRD data for protonated BCNN shows two subtle features: anisotropic hkl-dependent peak broadening and shifts from the expected peak positions, especially at high angle. Both characteristics of the XRD pattern suggest disorder in the protonated form, either from stacking faults or topotactic stacking features. Multiple models were used in an attempt to correctly model the XRD data. Of these, only models which allow incommensurate shifts in the a-b plane of the perovskite sheets can successfully model the data.

Modeling was undertaken using the software TOPAS (Bruker-AXS) and supercells along the c-axis with rigid bodies representing the perovskite sheets. Supercells of 2, 4, 6, 8, 12, 18, and 36 layers were tested, with improved fitting achieved on reaching 12 layers and the finer details better modeled using 18 or 36 layers. Optimized models show that the interlayer shifts between successive perovskite blocks are centered on the expected commensurate value (0.25 along a- and b-axes) but with a broad distribution. Likewise, the interlayer spacings show a broad distribution, ranging from 1.80 to 4.13Å, with an average value of 2.37(53)Å.

with 1 H$_2$O per formula unit, but also with wide distribution.