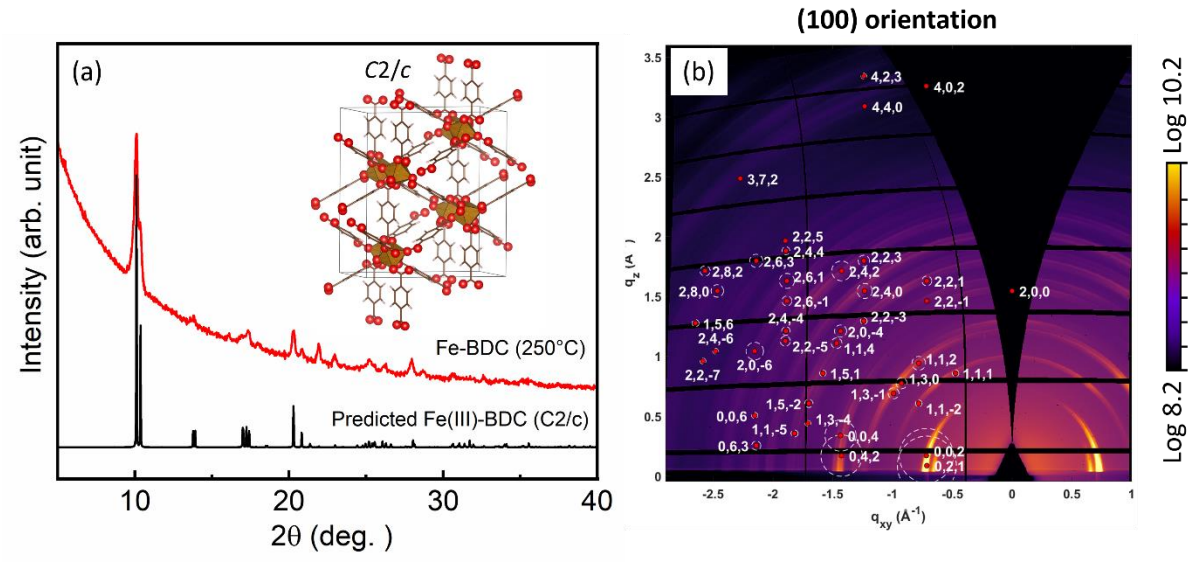

Figure 1. (a) XRD pattern for the computationally predicted Fe(III)-BDC crystal phase (C2/c) and experimentally measured in-house GIXRD pattern. (b) Reciprocal space map image from synchrotron GIXRD with simulated positions of Bragg peaks for a (100) orientation of the predicted C2/c structure. Red points at the center of circles give the expected positions of the diffraction peaks, and the areas inside the circles give the square of the structure factors, which are proportional to the expected intensities. Both figures clearly show the excellent match between the measured and the predicted novel crystal structure.