BAND:

**File: REFORMATTED\_BAND.dat** (or BAND.dat if the reformatted one isn't available or is problematic)

Why Essential: This file contains the actual energy values (y-axis) for each band versus the k-path distance (x-axis). Without this, you can't draw the band lines.

Parser Needed: parse\_reformatted\_band\_dat()

**File: KLABELS**

Why Essential: This file provides the (Label, k-coordinate) pairs. The "k-coordinate" from this file tells you precisely where on your REFORMATTED\_BAND.dat's x-axis (k\_distance) each high-symmetry label (like Γ, X, M) should be placed. This makes the plot interpretable.

Parser Needed: parse\_klabels\_manual() (or the pandas one if it works reliably for your labels)

**File: HIGH\_SYMMETRY\_POINTS**

Why Useful (but secondary to KLABELS for plotting this specific 1D path): This file gives the fractional coordinates (3D coordinates in reciprocal space) for each high-symmetry point and its label. While KLABELS already gives you the 1D k-path distance for the labels, this file:

Confirms the labels if they match KLABELS.

Provides the underlying 3D definition, which is good for completeness if someone wanted to, say, plot the Brillouin zone itself (which is beyond your current scope but good data to have).

Parser Needed: parse\_high\_symmetry\_points\_fractional\_manual()

Priority: If KLABELS successfully gives you the 1D k-coordinates for your labels, that's often sufficient for marking up the x-axis of your REFORMATTED\_BAND.dat plot. This file is more for completeness or advanced uses.

Priority: Lower than REFORMATTED\_BAND.dat and KLABELS if those two give you enough info to make a good plot.