Sadoway's Five-step Program for Determining Crystal Structure

Step 1 Start with 2θ values and generate a set of $\sin^2\theta$ values.

Step 2 Normalize the $\sin^2\theta$ values by generating $\sin^2\theta_n / \sin^2\theta_1$.

Step 3 Clear fractions from "normalized" column.

Step 4 Speculate on the *hkl* values that, if expressed as $h^2+k^2+l^2$, would generate the sequence of the "clear fractions" column.

Step 5 Compute for each θ the value of $\sin^2\theta / (h^2+k^2+l^2)$ on the basis of the assumed *hkl* values. If each entry in this column is identical, then the entire process is validated.