**Duration Operation Information obtained**

minutes/hours

1. Select a suitable crystal and mount it for X-ray study

a, b, c, α, β, γ

crystal system, space group

Assign crystal system and lattice centering

2. Obtain unit cell geometry and preliminary symmetry information

minutes/hours

list of

*Ihkl (intensities)*

*σ(Ihkl) (standard deviations)*

hours/days

3. Measure intensity data

list of

⎜*Fhkl*⎜2 *(structure factors = corrected intensities)*

*σ(Fhkl) (standard deviations)*

4. Data reduction (various corrections applied to data)

minutes

symmetry of the structure based on systematic absences and intensity statistics

minutes

5. Assign possible Space Groups

approximate positions for some or all non-hydrogen atoms

from minutes upward

5. Solve the structure

possible atoms positions, atom types, H atom positions, disorder, twinning, etc

6. Fourier and difference syntheses: Find missing atoms in difference electron density maps



minutes-days

Iterate as often as needed

days-years

minutes-days

Exact atom positions, displacement parameter, weighting and extinction parameters, twin ratios, occupancy rates

Molecular geometry, packing

arrangement, etc.

7. Least square Refinement of structure model

8. Interpret the result