Single-crystal X-ray diffraction is the ideal method for solving crystal structures but suffer from obtaining quality crystals by growth methods. Powders are often available and so the ability to determine crystal structures from powder data is highly desirable.

The crystal structure of $K_2Al_2O_3F_2$ was solved from powder diffraction data by:

- optimized measurement up to high diffraction angles
- cell parameters and crystal lattice class determination
- a modified Pawley procedure to detect impurities
- the ab-initio structure determination procedure and structure model analysis
- empirical energy calculations to support the structure model