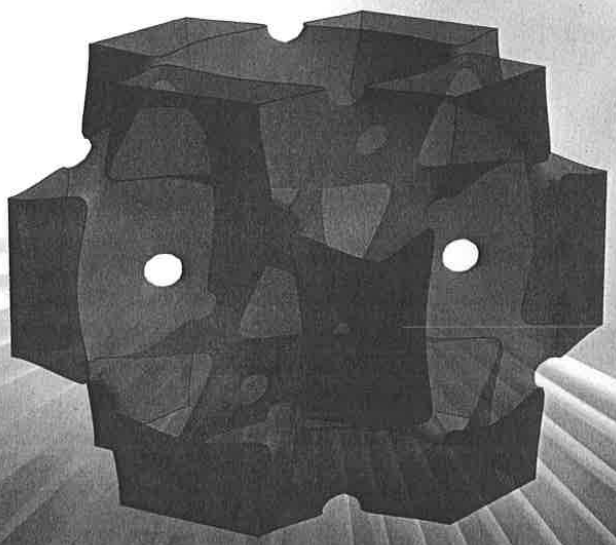
Inorganic Materials Series



Structure from Diffraction Methods

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Finally, as a summary comparison between single-crystal XRD and powder XRD, the following generalisations may be made:

(i) *Sample preparation*: Preparation of a single crystal of suitable size and quality for single-crystal XRD can be straightforward, challenging or impossible, depending on the material of interest, whereas preparation of a suitable powder sample for powder XRD is usually straightforward.

(ii) *Data collection*: The time required to record a complete set of single-crystal XRD data is generally longer than the time required to record a good-quality powder XRD pattern for the same material (although the development of area detectors for single-crystal XRD has improved considerably the rapidity of data collection).

(iii) *Structure determination*: Structure determination from single-crystal XRD data is generally very rapid and routine, whereas structure determination from powder XRD data is substantially more time-consuming and challenging; nevertheless, the methodology for analysis of powder XRD data has advanced significantly in recent years and the prospects for achieving successful structure determination from powder XRD data are continually improving.

1.3 QUALITATIVE ASPECTS OF POWDER XRD: 'FINGERPRINTING' OF CRYSTALLINE PHASES

A crucially important, yet very straightforward, application of powder XRD is the identification ('fingerprinting') of crystalline phases, based on the fact that different crystal structures give rise to distinct powder XRD patterns. This type of qualitative characterisation of crystalline materials is exploited in all areas of materials preparation and is also widely utilised in industrial protocols, including quality control, polymorph screening and the characterisation of products from rapid-throughput crystallisation experiments.[27,28]

In utilising powder XRD for 'fingerprinting' of crystalline phases, the aim is to compare the experimental powder XRD pattern of a sample prepared by materials synthesis with those of known materials (either experimental powder XRD patterns recorded for materials prepared by other synthetic routes or powder XRD patterns simulated from known crystal structures that have been determined previously). An example of this type of comparison is given in Figure 1.3. In some cases, the

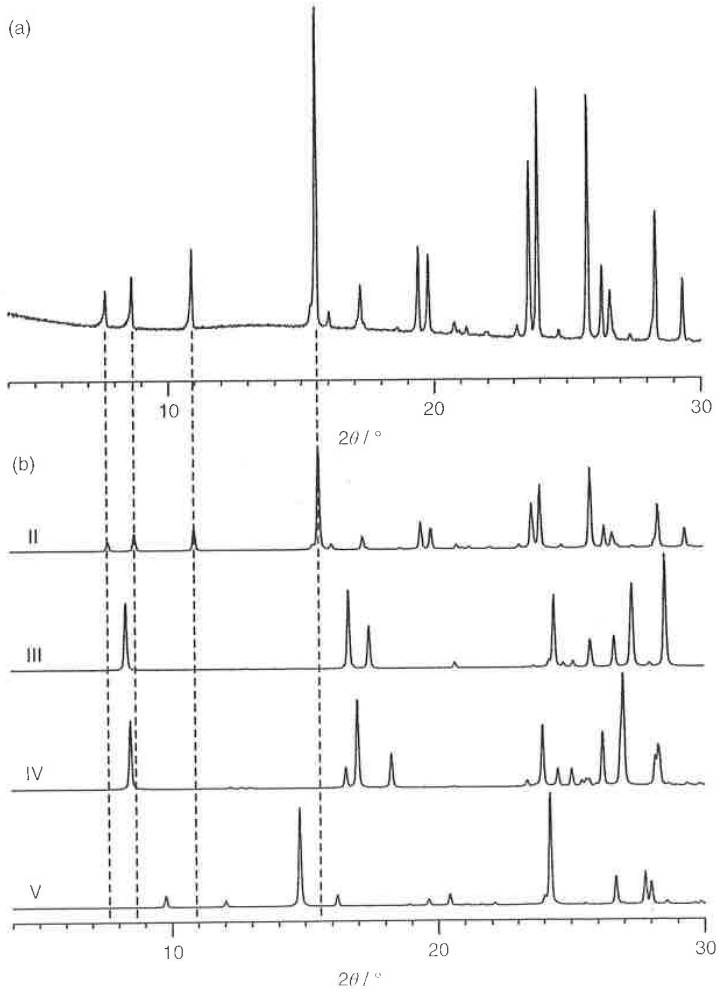

Figure 1.3 Comparison of (a) the experimental powder XRD pattern for a sample of *m*-aminobenzoic acid and (b) the simulated powder XRD patterns for all polymorphs of *m*-aminobenzoic acid with known crystal structures (Forms II, III, IV and V). From this comparison (see the matching of the vertical dashed lines), the sample of *m*-aminobenzoic acid with the powder XRD pattern shown in (a) is readily identified as Form II.

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