statistical accuracy, it is possible to identify very weak peaks with low $P/B$ as shown in Fig. 2.3.3.11.

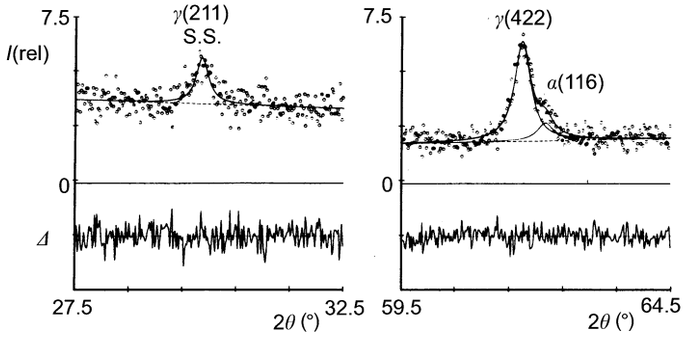


Fig. 2.3.3.11. Profile fitting of poor statistical data.

### 2.3.3.9. *Computer graphics for powder patterns*

An interactive graphics display program is a very important asset for interpreting and analysing powder diffraction data. If a colour graphics station is used, the display can be enhanced by using various colours. The simplest form is the VDU display of experimental points connected with straight lines, which appears similar to a strip-chart recording but has no time-constant error and is printed on page-size paper. It avoids storing large numbers of charts because hundreds of patterns can be stored on a diskette and displayed and printed at any time.

The basic parameters required in one of the published methods (Parrish, Huang & Ayers, 1984) are the $d$'s and $I$'s of the reflections, the wavelength and profile shapes ($\lambda * G$ instrument function). This makes it possible to produce a pattern exactly as it would appear on the user's diffractometer, aside from contributions arising from sample microstructure. The step size can be included if experimental patterns are to be reproduced or if patterns are to be subtracted. A section of the pattern can be enlarged to the full screen size by entering the desired angular range and highest peak intensity. A linear background can be added by entries at the low- and high-$2\theta$ points. Nonlinear background, *e.g.* from an amorphous substrate, can be transferred from a stored file. Counting statistical noise can be added to a simulated pattern by using a normally distributed random number with a standard deviation scaled to the calculated $I^{1/2}$. Noise in an experimental pattern can be smoothed. A profile broadening factor can be added to the $\lambda * G$ function. Quantitative synthesis of a mixture can be simulated by entering the relative weight percentage and reference intensity, the ratio of the intensities of the strongest lines of each pattern in a 50–50 mixture, or the ICDD values compared to $\alpha$-$Al_2O_3$ (de Wolff & Visser, 1988; Davis & Smith, 1988). The program has access to the ICDD file stored on disk so that any card can be reproduced as a pattern using any wavelength. Some examples are shown in Fig. 2.3.3.12.

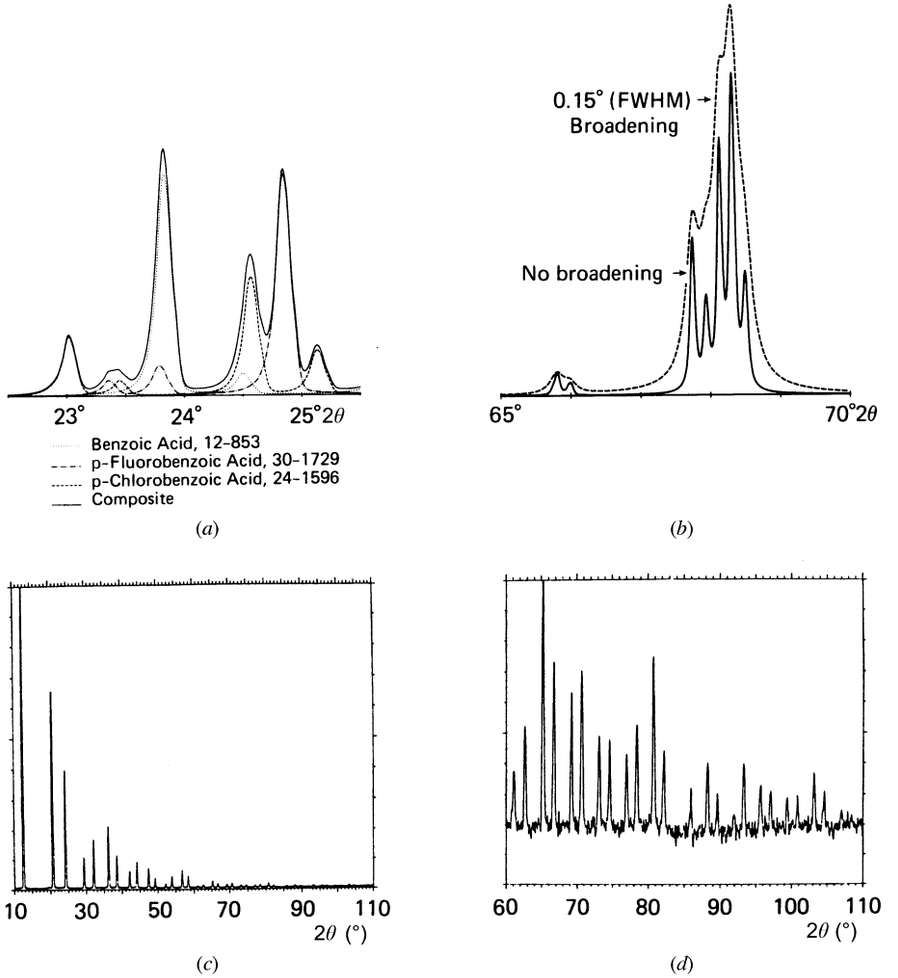


Fig. 2.3.3.12. Some examples of computer graphics of powder patterns. (*a*) Overlay of three patterns with ICDD card numbers. (*b*) Effect of adding 0.15° to FWHM. (*c*) Synchrotron 0.6888 Å radiation pattern of Si powder. (*d*) Low-intensity section enlarged and 11-point smoothing.





references