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Elements of X-RAY DIFFRACTION

SECOND EDITION

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be constructed which gives d directly as a function of line position when laid on the film or diffractometer chart; the accuracy obtainable by such a scale, although not very high, is generally sufficient for identification purposes. If the diffraction pattern has been obtained on film, relative line intensities are usually estimated by eye, on a scale running from 100 for the strongest line down to 10 or 5 for the weakest. On a diffractometer recording the intensity is taken as the maximum intensity measured above background.

After the experimental values of d and I/I_1 are tabulated, the unknown can be identified by the following procedure:

1. Locate the proper d_1 group in the numerical search manual.
2. Read down the second column of d values to find the closest match to d_2. (In comparing experimental and tabulated d values, always allow for the possibility that either set of values may be in error by ± 0.01 Å.)
3. After the closest match has been found for d_1, d_2, and d_3, compare their relative intensities with the tabulated values.
4. When good agreement has been found for the lines listed in the search manual, locate the proper data card in the file, and compare the d and I/I_1 values of all the observed lines with those tabulated. When full agreement is obtained, identification is complete.

14–5 EXAMPLES OF ANALYSIS

The unknown may consist of one or more phases, but the search procedure is initially the same for either case.

Single Phase

When the unknown is a single phase, the search procedure is relatively straightforward. Consider, for example, the pattern described in Table 14–1. It was obtained with Cu $K\alpha$ radiation and a Debye–Scherrer camera; line intensities were estimated. The experimental values of d_1, d_2, and d_3 are 2.82, 1.99, and 1.63 Å,

Table 14–1

Pattern of Unknown

d(Å)	I/I_1	d(Å)	I/I_1
3.25	10	1.00	20
2.82	100	0.95	5
2.18	5	0.94	20
1.99	60	0.89	20
1.71	5	0.86	5
1.63	30	0.85	20
1.42	20	0.82	10
1.25	30	0.79	10
1.15	30	0.78	20
1.09	5		