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Nota di contenuto	Contents; 1 Introduction to diffraction; 1.1 Introduction; 1.2 X-ray scattering from electrons; 1.3 X-ray scattering from atoms; 1.4 X-ray scattering from a unit cell; 1.5 The effects of the crystal lattice; 1.6 X-ray scattering from the crystal; 1.7 The structure-factor equation; 1.8 The electron-density equation; 1.9 A mathematical relationship; 1.10 Bragg's law; 1.11 Resolution; 1.12 The phase problem; 2 Introduction to symmetry and diffraction; 2.1 The relationship between a crystal structure and its diffraction pattern; 2.2 Translation symmetry in crystalline solids 2.3 Symmetry of individual molecules, with relevance to crystalline solids2.4 Symmetry in the solid state; 2.5 Diffraction and symmetry; 2.6 Further points; Exercises; 3 Crystal growth and evaluation; 3.1 Introduction; 3.2 Protect your crystals; 3.3 Crystal growth; 3.4 Survey of methods; 3.4.1 Solution methods; 3.4.2 Sublimation; 3.4.3 Fluid-phase growth; 3.4.4 Solid-state synthesis; 3.4.5 General comments; 3.5 Evaluation; 3.5.1 Microscopy; 3.5.2 X-ray photography; 3.5.3 Diffractometry; 3.6 Crystal mounting; 3.6.1 Standard procedures; 3.6.2

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4 Space-group determination4.1 Introduction; 4.2 Prior knowledge and information other than from diffraction; 4.3 Metric symmetry and Laue symmetry; 4.4 Unit cell contents; 4.5 Systematic absences; 4.6 The statistical distribution of intensities; 4.7 Other points; 4.8 A brief conducted tour of some entries in International Tables for Crystallography, Volume A; Exercises; 5 Background theory for data collection; 5.1 Introduction; 5.2 A step-wise theoretical journey through an experiment; 5.3 The geometry of X-ray diffraction; 5.3.1 Real-space considerations: Bragg's law
5.3.2 Reciprocal-space considerations: the Ewald sphere5.4 Determining the unit cell: the indexing process; 5.4.1 Indexing: a conceptual view; 5.4.2 Indexing procedure; 5.5 Relating diffractometer angles to unit cell parameters: determination of the orientation matrix; 5.6 Data-collection procedures and strategies; 5.6.1 Criteria for selecting which data to collect; 5.6.2 How best to measure data: the need for reflection scans; 5.7 Extracting data intensities: data integration and reduction; 5.7.1 Background subtraction; 5.7.2 Data integration; 5.7.3 Crystal and geometric corrections to data Exercises6 Practical aspects of data collection; 6.1 Introduction; 6.2 Collecting data with area-detector diffractometers; 6.3 Experimental conditions; 6.3.1 Radiation; 6.3.2 Temperature; 6.3.3 Pressure; 6.3.4 Other conditions; 6.4 Types of area detector; 6.4.1 Multiwire proportional chamber (MWPC); 6.4.2 Phosphor coupled to a TV camera; 6.4.3 Image plate (IP); 6.4.4 Charge-coupled device (CCD); 6.5 Some characteristics of CCD area-detector systems; 6.5.1 Spatial distortion; 6.5.2 Non-uniform intensity response; 6.5.3 Bad pixels; 6.5.4 Dark current; 6.6 Crystal screening
6.6.1 Unit cell and orientation matrix determination

Sommario/riassunto

This text focuses on the practical aspects of crystal structure analysis, and provides the necessary conceptual framework for understanding and applying the technique. By choosing an approach that does not put too much emphasis on the mathematics involved, the book gives practical advice on topics such as growing crystals, solving and refining structures, and understanding and using the results. The technique described is a core experimental method in modern structural chemistry,and plays an ever more important role in the careers of graduate students, postdoctoral and academic staff in chemis