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The art of solving a structure from powder diffraction data has developed rapidly over the last ten years to the point where numerous crystal structures, both organic and inorganic, have been solved directly from powder data. However, it is still an art and, in contrast to its single crystal equivalent, is far from routine. The art lies not only in the correct application of a specific experimental technique or computer program, but also in the selection of the optimal path for the problem at hand. Written and edited by experts active in the field, and covering both the fundamental and applied aspects of structure solution from powder diffraction data, this book guides both novices and experienced practitioners alike through the maze of possibilities.
Describes methods for determining the unknown structure of a material from powder diffraction data. The 17 contributions discuss choosing a radiation source and instrument geometry, indexing the diffraction pattern, adapting conventional crystalline approaches, and global optimization algorithms. The use of X-ray diffractometers, synchrotron radiation, and neutron powder diffraction for collecting data is explained. The phase problem is solved by Direct, Patterson, and maximum-entropy methods that have been modified to address the deficiencies inherent to powder diffraction data. The final chapter illustrates how other chemical information and intuition can facilitate structure determination and refinement.