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Carmelo Giacovazzo

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Direct methods are now used in a variety of cases: X-ray, neutron or electron data; single crystal and powder data; small molecules and macromolecules. While direct methods solved in practice the phase problem for small molecules, their application to macromolecules is recent and still undergoing development. This book describes the fundamental methods; in particular it is shown how the methods can be optimized for powder, neutron or electron data, and how they can be integrated with isomorphous replacement, molecular replacement and anomalous dispersion techniques. Maximum entropy methods are also described and discussed. Sets of test structures are used throughout the various chapters to verify the mathematical techniques and to provide practical examples. This book offers both a comprehensive description of direct methods in crystallography and an invaluable reference tool. The first three chapters provide an introduction to the field, with sufficient material to constitute a university course. Subsequent chapters are aimed at graduate students and working crystallographers. Basic results are described and discussed in the main body of the text, while the appendices complement these with in depth mathematical details. The quoted literature is extremely wide and the interested reader can find suggestions for future work and further reading throughout the book.

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