

## [Electron Density and Chemical Bonding I](#)

Experimental Charge Density Studies

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# Preface

Ever since Wilhelm Conrad Röntgen discovered X-rays in Würzburg and von Laue, Ewald, Friedrich, Knipping, and Bragg developed analytical methods to interpret X-ray diffraction patterns a hundred years ago in Göttingen, experimental single crystal structure analysis from diffraction data has become the most powerful analytical tool used to elucidate unequivocally the three dimensional structures of solid matter. Since that time the technique has contributed to many Nobel prizes in chemistry, physics and life sciences. From a knowledge of the connectivities at the atomic level and the arrangement in the solid phase many properties, both at the molecular and macroscopic scale, can be deduced. Currently X-ray sources in research laboratories and large facilities are getting more and more powerful, detectors more and more sensitive and crystallographic programs more and more sophisticated, so that the method continues to flourish and has been successfully applied to problems of increasing complexity. However, the most basic concept, the chemical bond, is still vigorously discussed and at times debated since its essential features were introduced by Lewis and put on a quantum mechanical basis by Pauling and Mulliken. Still there is room for interpretation, because single crystal structural analyses based on the independent atom model only provides the positions of the centroids of the atoms and the distances between the atoms. In the electron density maps there are no lines or dashes defining or even indicating the chemical bond and the nature of the bonding remains a matter of interpretation based on a bonding model. Hence the anecdote that *a bond is where the chemist draws the line* remains valid to a certain extent. Most of our understanding of the chemical bond is still deduced from the distances and angles, which are determined as a result of the crystallographic analysis, and represents a conclusion from a logical causal chain. For example, chemical intuition suggests that a short bond is a strong bond and possibly it has multiple bond character making it difficult to cleave, but nevertheless remaining reactive towards polar reagents. Hence we employ knowledge compiled from databases and statements of masterminds to indirectly deduce the nature of the bond. However, increasingly it has been recognised that there are exceptions to these simple generalisations, e.g. increasing ‘evidence’ that short bonds are not necessarily strong or multiple bonds and multiple bonds may at

times be longer than single bonds. Furthermore, there may be features of bonds which we cannot explain using current concepts.

This explains the increasing interest in looking at the bond directly and not by means of deductions and statistics. The Hansen and Coppens partitioning of the electron density in the aspherical atom model paved the way to describe the interference of X-rays with electrons from high resolution diffraction data more adequately. This density may then be analysed by Bader's Quantum Theory of Atoms in Molecules, directly providing more resilient and physically meaningful descriptions of chemical bonding than inferences from bond distances and angles.

The following collection of articles in Volumes 146 and 147 of the Structure and Bonding Series provides a state-of-the-art overview of the capacity of the method written by leaders in the field, which we hope will motivate more scientists to take advantage of the general approach.

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