Preface

Bond valence theory has developed slowly over the last 100 years as a method of analyzing and validating the structures of inorganic materials. The various rules of the model have hitherto been strictly empirical, having grown out of the ionic model and the bonding rules proposed by Linus Pauling in the early part of the last century. The remarkable success of the model, however, suggests that it must reflect some underlying theory. Such a theory is developed in the first part of this volume. Classical electrostatics applied to a simple, but physically correct, picture of the atom provides a chemical bond definition that can be used to derive not only the theorems of the bond valence model but also the rules of the traditional ionic and covalent ball-and-stick models.

Recent developments have seen applications of bond valence theory extended from the simple validation of crystal structure determinations to the prediction of the structure and bonding geometry of complex materials, to the exploration of structure-related properties such as ionic conduction, and to the study of the chemistry of surfaces and interfaces. These topics are the subject of the contributions to the second part of this volume.

It is our hope in producing this volume that supplying a theoretical base for the bond valence model, and illustrating some of its more recent applications, will inspire a greater interest in, and appreciation of, the underlying concepts and applications of this powerful bonding model.

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