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Preface

Computational chemistry plays an ever increasing role in chemical research facilitated by the development of more sophisticated programmes capable of predicting chemical properties with remarkable accuracy and the emergence of very fast and inexpensive computer workstations. Computation is becoming regarded as a tool in parallel with other common tools such as NMR, vibrational, electronic and mass spectroscopy etc.

Most chemical projects could probably benefit from a computational component but there is still a fear of theory in many quarters. Further, the proliferation of 'friendly' programmes which can run on a desktop computer leads, potentially, to a 'black box' mentality where results are 'churned out' without a deep enough understanding of the methodology or boundary conditions.

This special issue of *Coordination Chemistry Reviews* is designed to illustrate how theory can be applied successfully to a wide range of chemical problems as a means of encouraging the use of chemical computation. This issue should also engender care in not pushing the theory beyond its current capabilities.

The issue spans a wide range of topics. Peter Day honors one of inorganic chemistry's outstanding early theorists, Christian Klixbull Jørgensen, a member of a small group of extremely influential spectroscopists who opened the door to our understanding of the electronic spectra of complex molecules from the middle of the last century.

Many of today's outstanding theorists have written the remaining chapters which cover a wide range of topics including chemical bonding, problems in organometallic, bioinorganic and surface chemistry, electronic spectroscopy, photoreactivity and electron transfer, magnetism, inorganic and bioinorganic molecular mechanics.

While Jørgensen very ably employed *crystal* and *ligand field theory* to interpret electronic spectra, it is clear from the chapters in this Volume that *Density Functional Theory* enjoys great popularity as the choice computational method of the early part of this century.

I am indebted to the many colleagues who have contributed their time, effort and expertise to produce this Volume which I trust will prove extremely valuable to the inorganic and physical inorganic community.

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