



Preface

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It is a pleasure to write the preface to this special edition of *Acta Crystallographica Section B*. The collection of papers is most impressive and shows how much the field has blossomed over the years. The contents range from high-quality charge- and spin-density studies (one of which is combined with X-ray absorption measurements), optimizing data and model quality, statistical analysis of the data, charge densities at high pressures, evaluation of pseudoatom density models, measuring the charge density in unusual bonding situations, a further extension of Bader's theory by applying the Source Function to spin localization and polarization mechanisms, and development of new detectors allowing accurate powder diffraction measurements of charge-density quality, as well as in-house time-resolved studies down to milliseconds resolution with a new gated detector, thus optimizing faster, in-house, dynamic studies. At the 2006 Sagamore meeting near Warwick, UK, inclusion of the field of structural dynamics into the Sagamore topics was discussed and accepted. It is very satisfying to find a series of papers in this issue with subjects overlapping in charge- and spin-dynamics analyses, including the relaxation dynamic of an excited spin state, showing that the fields are related and must often be considered together, vindicating the earlier decision made years ago.

It is well known that the Sagamore meetings were initiated in the 1960s by the unforgettable Dick Weiss, and have maintained their high standard over the years. They have attracted an increasing number of theoretical chemists, starting with Vedene Smith, who could always be relied on to explain difficult theoretical concepts. Richard Bader's atoms in molecules theory constituted a great advance as it made electron densities a central topic, stimulating much further analysis. The Sagamore conferences cover the wide range of techniques used in accurate crystallography, as well as the interrelation of the results with those of theory, providing an essential check, benefiting both experimentalists and theoreticians. It is important that this well defined framework of a field of fundamental importance be preserved.

I would like to thank my many collaborators over the years, who have shared the excitement with the new science created. I am grateful to the authors of the excellent contributions to this issue, and last but not least would like to warmly thank Claude Lecomte, who initiated this issue and served as its Editor, as well as Co-editors Jason Benedict and Yu-Sheng Chen.

