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Preface

Special issue on High Pressure

The interactions between atoms at the atomic scale govern all physical and chemical properties. The application of pressure probes these interactions because it is these interactions that oppose the externally-applied pressure. High-pressure crystallography yields fundamental insights into the nature of the bonding and other interatomic interactions in the solid state by providing direct and unequivocal information about atomic structures and how they change with pressure. In molecular materials, for example, the application of pressure primarily probes the packing forces between molecules and thus leads to better understanding of polymorph stability, which is crucial for the pharmaceutical industry. For inorganic solids, and especially framework materials, pressure leads to new structural configurations which can be accessed through synthesis, and modified conformations that indicate the balance of bonding forces controlling the response of individual structures to pressure. Insights from high-pressure studies can then guide, for example, the design of new materials for electronics applications and catalysis. At even higher pressures the nature of the bonding and the electronic structure can change fundamentally, leading to new structures and structure types with novel physical and chemical properties.

The previous special issue of Zeitschrift für Kristallographie dedicated to high pressure was published a decade ago. The papers collected in that volume exhibited the same breadth of applications in chemistry and physics and materials science that characterises the contributions to the current issue; molecular compounds, metals, minerals, framework materials were all included. The previous issue also demonstrated the breadth of crystallographic methods that can be applied to study samples under high pressures – synthesis, spectroscopies, diffraction, and computer simulations at various levels. However, when one makes a comparison of the current contributions to those of the 2004 volume it quickly becomes apparent how much progress has been made in developing the techniques of high-pressure crystallography. Several of the new papers for example show that single-crystal diffraction measurements have become routine for all types of materials. The commercial availability and easy access to the equipment for sample preparation, loading and measurement with laboratory X-ray instruments has opened up opportunities for chemists and physicists to easily use pressure, outside of the specialist high-pressure groups. At the same time, there has been great progress in understanding the high-pressure environment within pressure-generating devices, and this has led to much improved and more reliable measurements towards the limits of pressure achievable; contributions include the description of single-crystal measurements at megabar pressures (100 GPa) and many 'routine' measurements in the 10–100 GPa pressure range, which were possible but rare, a decade ago.

In order for science in general to benefit from high-pressure crystallography in these, and many other ways, the experimental techniques must be widely known, easy to use, and should provide results of high precision and accuracy. Our aim in compiling this special issue was to help in this process by assembling a collection of contributions that were not simply just reviews. We have explicitly encouraged authors to explain their methodologies in more detail than is often possible in other publications, and thereby provide a tutorial aspect to the papers. Thus, in addition to demonstrating how much cutting-edge science can be done at elevated pressures, we hope that this collection of papers will encourage others to apply pressure to their own materials of interest. Lastly, we hope that it is clear that while the current contributions demonstrate that high-precision crystallography can be performed at the very highest pressures, new insights can be often obtained by measurements at 'modest' pressures ... what is 'very low pressure' for one material is often 'extreme conditions' for another, softer, crystal.

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