

s13.m37.o6 **In situ pressure crystallization: an alternative to crystallization by cooling.** Andrzej Katrusiak, Armand Budzianowski and Kamil Dziubek, *Faculty of Chemistry, Adam Mickiewicz University, Grunwaldzka 6, 60-780 Poznan., Poland.* E-mail: [katran@amu.edu.pl](mailto:katran@amu.edu.pl)

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*In situ* crystallization of liquids is usually connotated with the crystallization by lowering temperature, which started to be routinely applied in the 1950's [e.g. 1-4], and was perfected in the 1980's [5,6]. *In situ* temperature crystallization is routinely applied in neutron diffraction. In fact the low-temperature diffraction studies are regarded as the most accurate structural data. At the same time the crystallization of liquids can be achieved by elevating pressure. Therefore soon after the inception of the high-pressure diamond cell (DAC) the pressure technique was applied for *in situ* crystallization [7-9], and has been used for a number of studies [e.g. see 10]. However the precision of the high-pressure data is still inferior than the low-temperature results, even though in a small number of studies a comparable accuracy of the pressure results was demonstrated for laboratory [11] and synchrotron [12] studies on organic compounds. Most recently we have implemented a series of data correcting programs [13] and methods [14] which facilitate *in situ* pressure crystallization and considerably improve the accuracy of single-crystal high-pressure results measured with a DAC and a CCD diffractometer. The methods will be outlined, and the quality of the measured data exemplified. The primary aim of our pressure structures are intermolecular interactions in crystals and conformational transformations of molecules.

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s13.m38.o1 **Continuous Symmetry and Continuous Chirality Analyses: Coordination Compounds, Proteins, Quartz and More.** David Avnir, *Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel.* E-mail: [david@chem.ch.huji.ac.il](mailto:david@chem.ch.huji.ac.il)

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Many molecular and material properties are inherently associated with their symmetry or chirality. Whereas the treatment of symmetry/property relations has been carried out mainly in terms of exact symmetry groups, quite often these symmetries are only approximate. We have introduced a novel structure-analysis tool that enables the measurement of *the degree of symmetry or chirality on a continuous level*. This tool opens the possibility to identify trends in the variability of geometrical features of large families of compounds – such as the coordination complexes – and to identify quantitative correlations between symmetry/chirality and molecular or material properties. The continuous symmetry measure (CSM) and chirality measure (CCM) used for this purpose are of global nature, and take into account all angles and bond lengths of the molecular building blocks. The measure is a special distance function which evaluates the minimal distance of a given structure to (an a-priori unknown reference structure which has) the desired exact symmetry. In this lecture, I will provide a general overview of the approach, providing representative examples based mainly on crystallographic data, which include (as time will allow) [1]:

- Detailed quantitative symmetry and chirality analysis of selected families of coordination compounds, including homoleptic hexacoordinated  $D_3$ -symmetric complexes, hexacoordinated tris-chelated metal complexes and more
- Correlations between the degree of symmetry of tetracoordinated copper complexes, and a variety of their chemical and physical properties, including spectral Jahn-Teller splitting, enantioselective catalytic activity, and more.
- The use of quantitative symmetry and quantitative chirality to establish correlations between pressure or temperature and the degree of these structural properties for the molecular building blocks of low quartz.
- Applications of the CSM and CCM approach to the analysis of enzymatic activities (of cholinesterases and HIV-proteases).

**Programs availability:** Programs for computing the degree of symmetry or chirality, are available upon request from the author: [david@chem.ch.huji.ac.il](mailto:david@chem.ch.huji.ac.il)

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