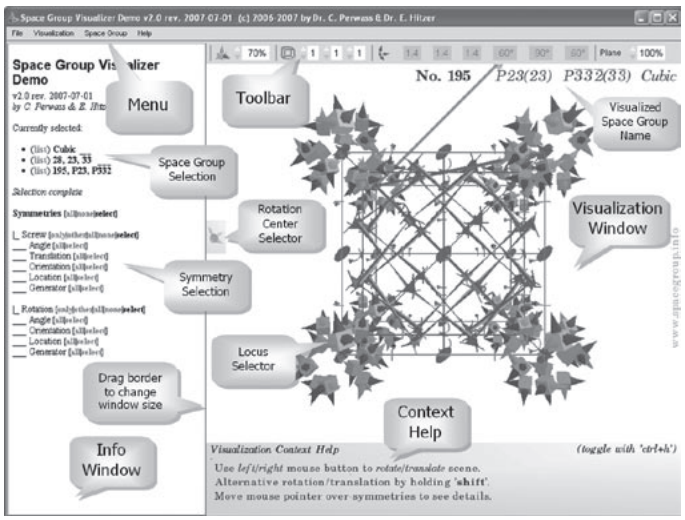
Browser selection panel for 7 crystal families, crystal classes (point groups), individual space groups;
Symmetry selection menu by type, angle, translation, orientation, location, generator;
Change cell type;
Mouse control to rotate/translate visualization and interactively animate, select, and remove single symmetries;
General position (mouse) interaction: rotation/motion of general position symbols;
Vary number of cells in view, vary cell angles and lengths;
Orthographic projection, stereo colors (cinema type stereo view);
Save visualization as image file.
We will present the unique mathematical and algorithmic structure underlying the visualization software using a coordinate free approach to symmetry with Geometric Algebra. We demonstrate the powerful set of interactive visualization tools made available by the SGV. Free demo at www.spacegroup.info



Keywords: space-group symmetry, interactive computer graphics, virtual reality

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In situ measurement of microorganisms metabolism under high hydrostatic pressure

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Many biotopes, e.g. deep-sea environments, subseafloor, are characterized by high hydrostatic pressure (HHP). Accordingly, most of the biosphere might live in high-pressure biotopes. Therefore, we aim at measuring microbial metabolic activities under high hydrostatic pressure, in particular to infer the contribution of microbial activity in the subsurface geochemical cycles. To avoid artifacts due to compression/decompression cycling on the behavior of microorganisms, we have developed an experimental set-up for in situ measurements at HHP in the 0-1 GPa range. This includes a low-pressure diamond anvil cell (DAC) optimized for imaging and spectroscopy, that is of interest for studying not only live microorganisms and related organic compounds, but also soft solids. A new accurate pressure gauge was also calibrated over the same pressure range. This high-pressure set-up was combined to Raman spectroscopy to investigate the alcoholic fermentation by the yeast Saccharomyces cerevisiae, as a function of pressure. Ethanol fermentation from glucose was monitored in the low-pressure DAC from ambient pressure up to 100 MPa. Our results show that below 10 MPa, fermentation proceeds three times faster than at ambient pressure and the fermentation yield is enhanced by 5 % after 24 hours. At higher pressure, the fermentation yield decreases linearly, and reaches 0 at 87(7) MPa. The respiration of selenite by a surface sediment bacterium, Shewanella oneidensis strain MR-1, could also be investigated under HHP by in situ microXANES at BM30B and ID22 beamlines of the European Synchrotron (ESRF, Grenoble) using a diamond anvil cell (ID22) or an autoclave (BM30B), to 150 MPa. We could show that Shewanella oneidensis strain MR-1 could reduce selenite into selenium to ca. 160 MPa.

Keywords: pressure, metabolism, spectroscopy

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High-pressure studies of pharmaceutical compounds

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This presentation will demonstrate how high-pressure techniques can provide a complementary method for exploring polymorphism and solvate formation in molecular solids, with a particular focus on pharmaceutical compounds. The techniques are proving useful for the identification and characterisation of new forms that do not appear in conventional polymorph screens performed under ambient conditions. This is particularly true for molecules that exhibit significant conformational flexibility. The presentation will highlight the range of strategies that have been developed for exploring polymorphism and solvate formation at high pressure, e.g. direct compression, recrystallisation from solution, effect of pressure-transmitting medium. Relationships between the effects of static compression and the effects of ball-milling will also be explored. These high-pressure methodologies are also well-suited for obtaining in a reproducible manner so-called disappearing or elusive polymorphs. Examples will be provided to demonstrate how new forms obtained at high pressure on a small scale can be recovered to ambient pressure and subsequently be used in seeding experiments under ambient conditions. The results provide insight into how the hierarchies of intermolecular interactions change with pressure and how the relative thermodynamic stabilities of different forms can change, with particular relevance to ab initio computational methods for crystal structure prediction. Furthermore, these methodologies may also have the potential to circumvent patents or enhance protection of intellectual property associated with pharmaceutical compounds.

Keywords: polymorphs, pharmaceutical compounds, high-pressure chemistry