

m12.o05**Time-Resolved Fibre Diffraction on Human Arteries During Tensile Testing and Nanostructure Correlation to Mechanical Behavior**Heinz Amenitsch^a, F. Schmid^a, G. Sommer^{b,c}, M. Rappolt^a, P. Regitnig^d, G. Holzapfel^{b,c}, P. Laggner^a^aInstitute of Biophysics and X-ray Structure Research, Austrian Academy of Sciences, Graz 8010, Austria. ^bDepartment of Solid Mechanics, Royal Institute of Technology, Stockholm 10044, Sweden. ^cInstitute for Structural Analysis - Computational Biomechanics, University of Technology Graz, Graz 8010, Austria. ^dInstitute of Pathology, Medical University Graz, Graz 8036, Austria. E-mail: amenitsch@elettra.trieste.it**Keywords: biomaterial, mechanical properties, fibre diffraction**

The collagen diffraction patterns of human arteries under uniaxial tensile test conditions have been investigated by time resolved synchrotron small angle X-ray diffraction [1].

Different types of arteries were chosen according to their clinical interest and have been studied after dissection into their major layers (intima, media, adventitia).

Using a recently designed tensile testing device [2], the orientation and d-spacing of the collagen fibers in the layers have been measured *in situ* under physiological conditions, together with the macroscopic force and sample deformation. This allows reconstruction of true stresses and strains and the fitting of this data to a non linear mechanical model [3]. The results show a relation between the orientation/extension of the collagen fibers on the nanoscopic level and the macroscopic stress and strain. This is attributed first to a straightening, second to a reorientation of the collagen fibers, and third to an up-take of the increasing loads by the collagen fibers.

[1] F. Schmid, G. Sommer, M. Rappolt, C.A.J. Schulze-Bauer, P. Regitnig, G.A. Holzapfel, P. Laggner, and H. Amenitsch, *J. Synchrotron Rad.*, 2005, 12, 727.

[2] F. Schmid, G. Sommer, M. Rappolt, P. Regitnig, G.A. Holzapfel, P. Laggner, and H. Amenitsch, NIMB, in press.

[3] T. C. Gasser, R.W. Ogden and G.A. Holzapfel, *J. R. Soc. Interface*, 2005, doi:10.1098/rsif.2005.0073, published online

m13.o01**Halogen ...halogen interactions in hexahalogenated benzenes**

Gautam R. Desiraju

School of Chemistry, University of Hyderabad, Hyderabad 500 046, India

Hexahalogenated benzenes ($C_6Cl_{6-n}Br_n$, $C_6Cl_{6-n}I_n$, $C_6Br_{6-n}I_n$) crystallize in two packing modes with the monoclinic and triclinic space groups $P2_1/n$ and P , respectively. The former, which is isostructural to C_6Cl_6 , is more common. In C_6Cl_6 , the planar molecules form $Cl\cdots Cl$ contacts and $\Pi\cdots\Pi$ stacking interactions and when crystals are compressed mechanically along their needle length, a bending deformation takes place. This bending is related to the weakness of the $Cl\cdots Cl$ interactions vis-à-vis the stronger $\Pi\cdots\Pi$ stacking interactions. The triclinic packing which is less common is restricted to molecules that have a symmetrical (1,3,5 and 2,4,6) halogen substitution. It is characterized by specific, polarization induced $X\cdots X$ interactions which result in threefold-symmetrical X_3 -synthons, especially when $X = I$; this leads to a layered pseudo-hexagonal structure in which successive planar layers are inversion related. The triclinic crystals shear on application of mechanical stress because of mutual sliding of layers. The $X\cdots X$ interactions in the monoclinic group are non-specific while in the triclinic group, some $X\cdots X$ interactions are anisotropic, chemically specific and crystal structure directing.