MS20-P14 High-pressure study of *R,S*-ibuprofen

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R,S-Ibuprofen is an important non-steroidal anti-inflammatory drug used for relieving pain, helping with fever and reducing inflammation.[1] It crystallizes at varied pressure (0.1 MPa – 4.00 GPa) in the monoclinic, space group $P2_1/c$.[2] It is an optically active compound with both *s* and *r*-isomers. The *S*-ibuprofen is more active and hence desired for pharmaceutical applications. Its structure is monoclinic, space group $P2_1$.[3] Single crystals of *r,s*-ibuprofen have been grown *in situ* at isothermal and isochoric conditions in a modified Merrill-Bassett[4] diamond-anvil cell (DAC) from different achiral and chiral solutions. Their structures were determined by X-ray diffraction. High-pressure crystallizations of *R,S*-ibuprofen lead to the same crystal phase as the one at ambient conditions. It is a carboxylic acid with molecules linked by double OH•••O bridges into dimers. At 4.0 GPa the crystal is compressed to about 80% of its ambient-pressure volume. *r,s*-Ibuprofen crystal structure is stabilized by C-H···O contacts. The crystal compression and thermal expansion as well as shortest H···O distances comply with the inverse-relationship rule of pressure and temperature changes.

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MS20-P15 High-pressure polymorphism of α-D-glucose

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Carbohydrates create group of compounds most important for all living organisms. They are widely used in food, pharmaceutical, construction and other industries. One of the most significant representative of sugars is glucose. It is main energy carrier in human organism and takes part in many important biochemical processes. Processing and recognition of glucose is based on the unique structural pattern of hydroxyl groups that allows creation of multiple hydrogen bonds and intermolecular contacts. Recently we have shown how pressure can influence the solid-state preferences of bonding pattern of other well-known sugar, (+)-sucrose.[1] Compression of crystalline sucrose leads to its isostructural phase transition, and thorough reorganization of O-H•••O hydrogen bonds and C-H•••O contacts. Herein we present study of α-D-glucose crystals behavior at high-pressure and the first high-pressure monosaccharide polymorph ever reported.[2]

Crystals of α-D-glucose were either mounted in the Merrill-Bassett diamond-anvil cell (DAC)[3] and compressed or recrystallized isochorically at high-pressure. Obtained crystals were measured using 4-circle X-ray diffractometer in the 0.2 -6.2 GPa pressure range.

Collected data shown discontinuity of a-D-glucose unit-cell volume and parameters at 5.40 GPa which was later proven to be an evidence of its isostructural phase transition. α-D-Glucose preserves its orthorhombic symmetry, space group $P2_12_12_1$ (Z'=1) on transformation from phase I to phase II. During the transition, its molecules rearrange their aggregation due to compression which in turn leads to modification of intermolecular interactions. Role of strong O-H•••O hydrogen-bonds diminish, their number decrease after phase transition, and weaker interactions such as C-H•••O contacts increase their number and therefore importance in phase II.

Structural modification observed for α-D-glucose coincide to some point with those reported for (+)-sucrose. It makes us believe that structural similarities of carbohydrates can be reflected in their high-pressure behavior.

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