

s13.m37.p5 **First Observation of Helical Bundles in Crystal Structure of Helical Peptide Scaffolds Containing a, b-Dehydrophenylalanine Residue.** M. Gupta, Rudresh, S. Ramakumar, V. S. Chauhan. *International Center for Genetic Engineering and Biotechnology, New Delhi- 110067 India.* E-mail: g\_madhvi@hotmail.com

**Keywords:** Del-phe; DMSO; F-moc

De novo designed peptide based super secondary structures can provide scaffolds for the incorporation of functional sites as in proteins. Weak interactions leading to the self-association of helices (containing  $\Delta$ Phe residue) of similar screw sense have been probed by the structure determination in crystals of two peptides:

Ac-Gly<sup>1</sup>-Ala<sup>2</sup>- $\Delta$ F<sup>3</sup>-Leu<sup>4</sup>-Val<sup>5</sup>- $\Delta$ F<sup>6</sup>-Leu<sup>7</sup>-Val<sup>8</sup>- $\Delta$ F<sup>9</sup>-Ala<sup>10</sup>-Gly<sup>11</sup>-NH<sub>2</sub>, I; Ac-Gly<sup>1</sup>-Ala<sup>2</sup>- $\Delta$ F<sup>3</sup>-Leu<sup>4</sup>-Ala<sup>5</sup>- $\Delta$ F<sup>6</sup>-Leu<sup>7</sup>-Ala<sup>8</sup>- $\Delta$ F<sup>9</sup>-Ala<sup>10</sup>-Gly<sup>11</sup>-NH<sub>2</sub>, II. X-ray diffraction studies reveal that both the peptides adopt 310-helical conformation in the solid state. The crystal structures of the two peptides have been determined to atomic resolution and refined to R-factor of 8.15% and 4.01% respectively. An interesting finding is that a packing motif could be identified in both the structures, in which a given 3<sub>10</sub>-helix is surrounded by six other helices reminiscent of transmembrane seven helical bundles. This arrangement resulted in two kinds of interfaces, Leu-Leu and Val-Val in peptide I and Leu-Leu and Ala-Ala in peptide II. The angle between antiparallel helices are 161° and 164° in peptides I and II, respectively. The outer helices are orientated either parallel or antiparallel to central helix. The parallel helices interact through C-H...O and C-H... $\pi$  hydrogen bonds while the antiparallel helices are interacting via C-H... $\pi$  hydrogen bonds. Common to both the structures is the hydrophobic interaction between the pairs of leucine residues. The results of the packing of the helices in the solid state may help in achieving the ambitious design strategy for designing super secondary structural motifs such as helical hairpin and three or four helix bundles by connecting them through suitable linkers such as tetraglycine segments.

s13.m37.p6 **Influence of the Electrical Field on Crystal Growth in the System Li<sub>3</sub>PO<sub>4</sub> - Li<sub>4</sub>GeO<sub>4</sub> - Li<sub>2</sub>MoO<sub>4</sub> - LiF.** Dmitry A. Ksenofontov<sup>a</sup>, Ludmila N. Demianets<sup>a</sup>, Alexei K. Ivanov-Schits<sup>a</sup>, Vsevolod V. Kireev<sup>a</sup>, <sup>a</sup>Institute of Crystallography of Russian Academy of Sciences 59 Leninsky pr. Moscow 119333, Russia. E-mail: ksenofant@rambler.ru

**Keywords:** Crystal growth; Electrocrystallization; Superionic compounds

The simultaneous influence of heat and electrical fields on the crystal growth was studied for the system Li<sub>3</sub>PO<sub>4</sub> - Li<sub>4</sub>GeO<sub>4</sub> - Li<sub>2</sub>MoO<sub>4</sub> - LiF. The special set-up was constructed which allowed applying a direct electrical current for the system "growing crystal-melt". The Pt-rod and Pt-crucible served as cathode and anode respectively. Parameters of the crystallization process were as following: temperature of system melting was 970°C, temperature decrease rate in the range 970-950 °C was 0.1 °C/h, starting chemical components were 40.11g Li<sub>3</sub>PO<sub>4</sub>, 56.95g Li<sub>4</sub>GeO<sub>4</sub>, 73.53g Li<sub>2</sub>MoO<sub>4</sub>, and 23.53g LiF. Crystallization without electrical field application led to the formation of bulk crystals of superionic compound Li<sub>3+x</sub>P<sub>1-x</sub>Ge<sub>x</sub>O<sub>4</sub> (x=0.31). Growth occurs on the Pt-rod immersed into the flux due to temperature change (low temperature decrease during 3-4 weeks). Application of direct electrical current (voltage  $V=0.08$  and  $0.15V$ ) proved to control the growth process. The electrical current was found to control the compositions and growth conditions of crystallizing phases in the system under study. Applying the electrical field led to the change of the composition of the growing crystals. Lithium molybdates Li<sub>2</sub>MoO<sub>4</sub> and Li<sub>1.3</sub>Mo<sub>3</sub>O<sub>8</sub> were crystallized onto the Pt-rod at  $V=0.08V$  while the crystals of lithium germanate Li<sub>2</sub>GeO<sub>3</sub> were grown onto the cathode at  $V=0.15V$ . Phosphorus remained in the flux forming the vitreous phase. Thus the presence of the electrical field provides the directional ion migration in the melt. The local change of the melt composition and the crystallization of the compounds with various compositions depended on the magnitude of applied voltage. The change of the strength of the current was noticed during the process of crystal growth. At the beginning of the process, when Pt-rod was immersed into the flux,  $I=10$  mA; at the end of the crystallization it was one order higher. The explanation of that phenomenon was suggested based on the electrophysical characteristics of the melt; the composition of the melt and its properties were changing due to the growth of crystals with definite composition. Crystal growth under simultaneous action of heat and electrical fields may be represented as a novel method of crystal growing, which is based on the main principles of the flux growth and electrocrystallization.

The work was performed at partial financial support of Russian Foundation for Basic Researches, Grant N 02-02-16958 and Russian Federation President Grant for supporting the leading scientific school N 1954.2003.2.