Poster

Structural description of dehydration and polymerization in cGMP crystals in light of the origins of life.

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In a prebiotic context, supramolecular ordering, such as liquid crystal self-assembly, adsorption on solid surfaces and, finally, crystallization, is believed to promote selection and non-enzymatic polymerization of nucleotides, thus providing an effective pathway to the emergence of the RNA World on the primordial Earth [1-3]. Laboratory simulations of the prebiotic hot springs (wet-dry cycling, 80 °C) were shown to give enough energy for nucleotide condensation and polymerization. What may be surprising is that guanosine 3′:5′-cyclic monophosphate (cGMP, a cyclic nucleotide known for its significant polymerization potential) was found to polymerize exclusively in solid crystalline form. Long poly-G RNA strands were then formed, and only time and elevated temperature (80 °C) were needed, without the use of enzymes or other catalysts [4]. cGMP was also shown to crystallize very easily upon drying its aqueous solution [3].

The polymerization of cGMP is believed to be favoured by its unique crystal structure. Crystalline cGMP, like almost all nucleotide crystals, contains water molecules [3, 5]. Therefore, heating it first leads to dehydration. What structural changes accompany crystal dehydration? Is it possible to capture and describe them? How do the initial crystal structure and structural changes accompanying dehydration affect the efficiency of polymerization in wet-dry cycling? These seem to be the most interesting questions both from the point of view of structural research and in the prebiotic context, from the perspective of the origins of life.

The poster will present the results of SC XRD and VT PXRD analyses, showing a step-by-step structural description of dehydration of various hydrates of cGMP. The effectiveness of polymerization for individual crystal forms of cGMP will be shown and an attempt will be made to explain them on the basis of structural studies. An exceptionally extensive conformational diversity will be presented, that had never been previously observed in nucleotide crystals obtained by crystallization from solutions (Fig. 1).

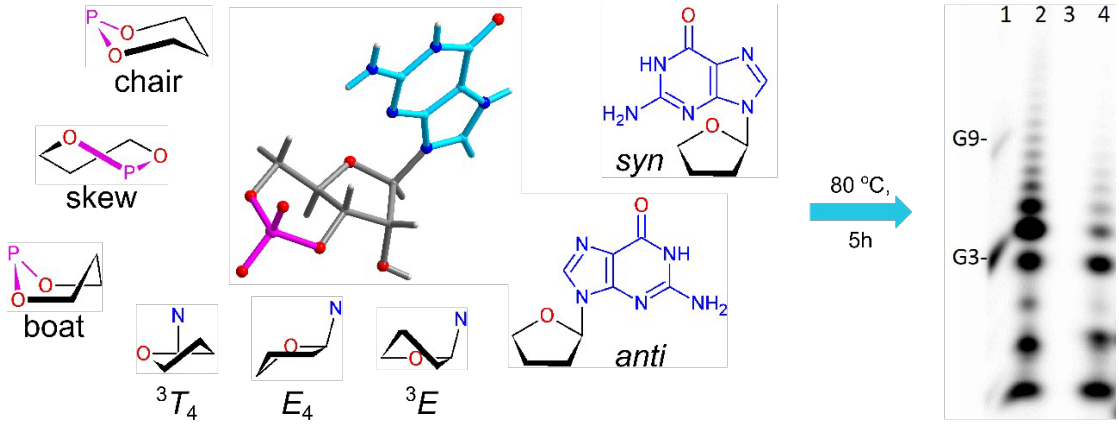

Figure 1. Conformational diversity of cGMP obtained by its crystallization and dehydration of its hydrates, which is the initial stage of polymerization.

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