

Post-crystallization Rearrangement of Crystal Architecture, Intermolecular Interactions, and Nucleotide Conformation in Adenosine Monophosphates Crystals Induced by Single Crystal-to-Single Crystal Dehydration

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Rok wydania

2025

Czasopismo

Crystal Growth and Design

Numer woluminu

25

Strony

4586-4600

DOI

10.1021/acs.cgd.5c00490

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

In this paper, we present the results of structural studies of three adenosine monophosphates: 5'-AMP, 3'-AMP, and 2'-AMP. They concern extensive experiments to obtain new crystalline forms of the indicated nucleotides by both solution crystallization and temperature-induced dehydration. Recognizing the need for a more complete description of the nature of these systems in the solid state, as very poorly known in terms of structure compared to other nucleotides, we obtained several hydrated and anhydrous crystalline varieties in the acid form. Through a detailed analysis of the architecture of the crystals as well as the intermolecular interactions, we identified the main supramolecular tendencies of these compounds in the solid state as well as their particular preferences for the formation of hydrogen bonds, especially through adenine and phosphate groups. Among other things, it takes into account the role of water molecules in creating individual interactions between nucleotides. At the same time, we perceived an extraordinary conformational flexibility of adenylyl nucleotides upon partial or complete loss of water from the crystals. Many of the geometries appear to be extremely rare and have not been observed before in these systems. We emphasize the uniqueness of hydrated adenylyl nucleotide crystals in the context of the dehydration experiments (following the single crystal-to-single crystal transformation) and point out the extraordinary usefulness of this technique in the light of the search for new crystal forms and structural studies.

Słowa kluczowe

Crystal structure, Crystals, Dehydration, Monomers, Noncovalent interactions

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Adres publiczny

<http://dx.doi.org/10.1021/acs.cgd.5c00490>

Strona internetowa wydawcy

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