

## Structural aspects of dehydration and rehydration in the adenosine 5'-diphosphate (ADP)–potassium–water system

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### Rok wydania

2023

### Czasopismo

CrystEngComm

### Numer woluminu

25

### Strony

4592-4603

### DOI

10.1039/d3ce00395g

### Kolekcja

Naukowa

### Język

Angielski

### Typ publikacji

Artykuł

### Streszczenie

This work presents the solution crystallization, post-crystallization dehydration and structural studies of hydrated and anhydrous potassium salts of adenosine 5'-diphosphate obtained in this way. ADP is crucial for cellular energy processes.  $K^+$  is the most abundant metal cation in cells. However, both ADP and nucleotide–K systems are poorly understood in terms of crystal structure. We report three hydrated salts:  $K(ADP) \cdot 4H_2O$ ,  $K(ADP) \cdot 2H_2O$ , and  $(H_5O_2)K(ADP)_2 \cdot 4.25H_2O$  and one anhydrous salt,  $K(ADP)$ , formed by dehydration of  $K(ADP) \cdot 2H_2O$ , proceeding as a single crystal to single crystal (SC-to-SC) process, which were tested by single crystal XRD, variable temperature micro-PXRD and TGA/DTA methods. The phase transition in  $(H_5O_2)K(ADP)_2 \cdot 4.25H_2O$  was observed. The structural description of the dehydration–rehydration process in the ADP–potassium–water system was presented. The most important interaction types and structural motifs as well as the function of water molecules in the studied ADP crystals were identified.

### Adres publiczny

<http://dx.doi.org/10.1039/d3ce00395g>

### Strona internetowa wydawcy

<https://www.rsc.org/>