

Adenosine hypodiphosphate ester, an analogue of ADP : analysis of the adenine–hypodiphosphate interaction mode in hypodiphosphate nucleotides and adenine salts.

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Streszczenie

Adenosine diphosphate (ADP) plays a crucial role in cell biochemistry, especially in metabolic pathways and energy storage. ADP itself, as well as many of its analogues, such as adenosine hypodiphosphate (AhDP), has been studied extensively, in particular in terms of enzymatic activity. However, structural studies in the solid state, especially for AhDP, are still missing. An analogue of ADP, i.e. adenosine hypodiphosphate ester, has been synthesized and characterized in the crystalline form as two hydrated sodium salts of 2':3'-isopropylideneadenosine 5'-hypodiphosphate (H_3AhDP , $\text{C}_{13}\text{H}_{19}\text{N}_5\text{O}_9\text{P}_2$ for the neutral form), namely pentasodium tetrakis(2':3'-isopropylideneadenosine 5'-hypodiphosphate) tetracosahydrate, $5\text{Na}^+ \cdot 3\text{C}_{13}\text{H}_{18}\text{N}_5\text{O}_9\text{P}_2^- \cdot \text{C}_{13}\text{H}_{17}\text{N}_5\text{O}_9\text{P}_2^{2-} \cdot 24\text{H}_2\text{O}$ or $\text{Na}_5(\text{H}_2\text{AhDP})_3(\text{HAhDP}) \cdot 24\text{H}_2\text{O}$, (I), and sodium tetrakis(2':3'-isopropylideneadenosine 5'-hypodiphosphate) pentadecahydrate, $\text{Na}^+ \cdot \text{C}_{13}\text{H}_{20}\text{N}_5\text{O}_9\text{P}_2^+ \cdot 2\text{C}_{13}\text{H}_{18}\text{N}_5\text{O}_9\text{P}_2^- \cdot \text{C}_{13}\text{H}_{19}\text{N}_5\text{O}_9\text{P}_2 \cdot 15\text{H}_2\text{O}$ or $\text{Na}(\text{H}_4\text{AhDP})(\text{H}_3\text{AhDP})(\text{H}_2\text{AhDP})_2 \cdot 15\text{H}_2\text{O}$, (II). Crystal structure analyses of (I) and (II) reveal two nucleoside hypodiphosphate ions in the asymmetric units with different ionization states of the hypodiphosphate unit and adenine base. For all AhDP nucleotides, the same anti conformation about the N-glycosidic bond and similar puckering of the ribose ring have been found. AhDP geometry and interactions have been compared to ADP nucleotides deposited in the Cambridge Structural Database. The adenine-hypodiphosphate interactions, identified as defining nucleotide self-assembly, have been analysed in model systems, i.e. the adenine (Ade) salts of hypodiphosphoric acid, namely bis(adeninium) hypodiphosphate dihydrate, $2\text{C}_5\text{H}_6\text{N}_5^+ \cdot \text{H}_2\text{P}_2\text{O}_6^{2-} \cdot 2\text{H}_2\text{O}$ or $(\text{AdeH})_2(\text{H}_2\text{P}_2\text{O}_6) \cdot 2\text{H}_2\text{O}$, (III), and bis(adeninium) hypodiphosphate, $2\text{C}_5\text{H}_6\text{N}_5^+ \cdot \text{H}_2\text{P}_2\text{O}_6^{2-}$ or $(\text{AdeH})_2(\text{H}_2\text{P}_2\text{O}_6)$, (IV).

Słowa kluczowe

nucleotides, adenosine hypodiphosphate esters, ADP analogues, adenine salts, hypodiphosphate salts, sodium salts, nucleobase interactions, crystal structures, hypodiphosphoric acid, adenosine diphosphate

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