

Potassium D-3-phosphoglycerate and cyclohexylammonium D-3-phosphoglycerate hydrate.

Autorzy

Tadeusz Lis

Lucjan B. Jerzykiewicz

Rok wydania

1995

Czasopismo

Acta Crystallographica

Section C: Structural

Chemistry

Numer woluminu

C51

Strony

1001-1005

DOI

10.1107/S0108270194010474

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The structures of the D-3-phosphoglycerate mono- anions in the potassium $[\text{KH}_2(3\text{-PGA})]$ and cyclohexyl- ammonium $[(\text{CHA})\text{H}_2(3\text{-PGA})]$ salts $[\text{H}_2(3\text{-PGA}) = -\text{HO}_3\text{POCH}_2\text{CH}(\text{OH})(\text{CO}_2\text{H})]$ have been determined by X-ray analysis at 297 and 85 K, respectively. The C--C--C--OH torsion angles which define the relationship of the carboxylic group to the carbon backbone are $-120.2(2)$ and $60.1(3)^\circ$, and the P--O(ester) bond lengths are $1.596(2)$ and $1.600(2)$ Å for $\text{KH}_2(3\text{-PGA})$ and $(\text{CHA})\text{H}_2(3\text{-PGA})$, respectively. There are extensive networks of hydrogen bonds in both crystals in which all H atoms of the hydroxyl and ammonium groups are involved. The K⁺ ion is octacoordinate.

Adres publiczny

<https://doi.org/10.1107/S0108270194010474>