Disodium D-3-phosphoglycerate (a reinvestigation at 80 K) and bis(cyclohexylammonium) D-3-phosphoglycerate dihydrate at 85 K.

Autorzy

Tadeusz Lis

Lucjan B. Jerzykiewicz

Rok wydania

1996

Czasopismo

Acta Crystallographica Section C: Structural Chemistry

Numer woluminu

C52

Strony

129-134

DOI

10.1107/S0108270195009905

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The structure of the D-3-phosphoglycerate dianion in the disodium salt $2Na^{+}.C_3H_5O_7P^{2-}$ [Na_2H(3-PGA), (I)], and the hydrated bis(cyclohexylammonium) salt $2C_6H_{14}N^{+}.C_3H_5O_7P^{2-}.2H_2O$ [$(CHA)_2H$(3-PGA)·$2H_2O$, (II)] [H(3-PGA) = $^{-}HO_3POCH_2CH(OH)COO^{-}$, CHA = $C_6H_{11}NH_3^{+}$] has been determined by X-ray analyses at 80 and 85 K, respectively. A room-temperature study of (I) was previously desribed by Fewster & Fenn [*Acta Cryst.* (1982), B**38**, 282-284]. The dianions in (I) and (II) differ in the orientations of the carboxylate and phosphate groups with respect to the carbon backbone. The P-O ester bond lengths are 1.606 (2) and 1.608 (2) Å in (I) and (II), respectively. The crystal structure of (I) is governed by NaO interactions. The two crystallographically independent Na^{+} cations are seven- and six-coordinate, respectively, with NaO distances in the range 2.275 (2)-2.822 (2) Å. The crystal structure of (II) is stabilized by hydrogen bonds which utilize all N and O atoms.