
Tris{[tris(2-hydroxymethyl)methyl]ammonium}D-3-phosphoglycerate at 150 K and tris(cyclohexylammonium) D-3-phosphoglycerate ethanol solvate at 85 K.

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Streszczenie

The structures of the D-3-phosphoglycerate trianion in the tris{[tris(2-hydroxymethyl)methyl]ammonium} salt, $3C_4H_{12}NO_3 \cdot 3C_3H_4O_6P^{3-}$, (I), and in the tris(cyclohexylammonium) ethanol solvate, $3C_6H_{14}N^+ \cdot C_3H_5O_6P^{3-} \cdot CzH_5OH$, (II), have been determined by X-ray analyses at 150 and 85 K, respectively. A notable feature of (I) is the shortest P-O(ester) bond [1.607 (2), Å] found so far for the completely ionized phosphate ester group. In contrast, in (II), this bond length is 1.627(2) Å, similar to that observed in doubly ionized phosphate ester groups. In (II), the carboxylate group is twisted by $-23.5 (4)^\circ$ relative to the ortho-hydroxyl group, as indicated by the O1-C1-C2-O2 torsion angle, whereas in (I), the O2-C2-C1-O1 system is almost planar. Both crystal structures are stabilized by hydrogen bonds utilizing all N and O atoms.

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