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CRYSTAL AND MOLECULAR STRUCTURE OF PHOSPHOENOLPYRUVATE SALTS

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Phosphoenolpyruvate (PEP) plays central role in the storage and transfer of energy in biological systems. Its free energy of hydrolysis ($-58.5 \text{ kJ mol}^{-1}$) is the highest known for monoesterified phosphate esters. Depending on pH PEP can occur as monoanion, dianion and trianion or as tri-basic acid. Studying PEP salts in different crystal forms provides additional information on its molecular flexibility, phosphate group conjugation with the enolpyruvate residue and kind of binding to different cations.

We have determined the crystal and molecular structure of two polymorphic forms of the PEP monocyclohexylammonium salt. The orthorhombic form (I) was obtained from water and the monoclinic form (II) from alcohol solutions. The forms differ from each other in molecular conformation. The phosphate group is *trans* to the carboxyl group in I and perpendicular to the enolpyruvate system in II. In I the hydroxyl oxygen in carboxyl group is *trans* planar and in II *syn* planar with respect to the ester O atom. The enolpyruvate system in I and II is very deviated from planarity. The comparison of I and II with structures of monosodium¹ and monopotassium² PEP salts suggests that the differences in the PEP monoanion geometry depend upon the cation as well as upon the polarity and the kind of the solvent used.

The detailed account of this work will be published in *Acta Crystallographica*, C.

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2. T.Lis, *Acta Cryst.* C43, 1898-1900, (1987).