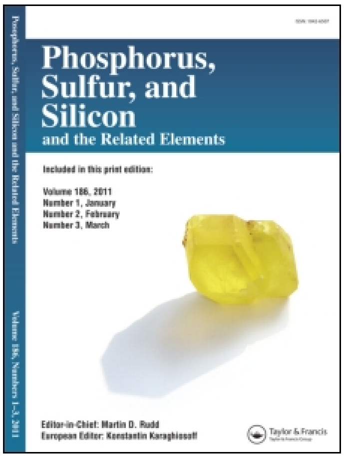

Phosphorus, Sulfur, and Silicon and the Related Elements
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713618290

Crystal and Molecular Structure of Phosphoenolpyruvate Salts

A. Weichsel[a]; T. Lis[a]
[a] Institute of Chemistry, University, Wroclaw, Poland

To cite this Article Weichsel, A. and Lis, T.(1990) 'Crystal and Molecular Structure of Phosphoenolpyruvate Salts', Phosphorus, Sulfur, and Silicon and the Related Elements, 51: 1, 300

To link to this Article: DOI: 10.1080/10426509008040834

URL: http://dx.doi.org/10.1080/10426509008040834

Phosphorus, Sulfur, and Silicon, 1990, Vols. 51/52, p. 300
Reprints available directly from the publisher
Photocopying permitted by license only

CRYSTAL AND MOLECULAR STRUCTURE OF PHOSPHOENOLPYRUVATE SALTS

A.WEICHSEL and T.LIS
Institute of Chemistry, University, 50-383 Wrocław,
Poland

Phosphoenolpyruvate (PEP) plays central role in the storage and transfer of energy in biological systems. Its free energy of hydrolysis (-58.5 kJ mol^{-1}) is the highest known for monoesterified phosphate esters. Depending on pH PEP can occur as monoanion, dianion and trianion or as tribasic 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 monosodium[1] and monopotassium[2] 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.

1. S.K.Katti, M.V.Hosur and M.A.Viswamitra, Acta Cryst. B37, 834-838 (1981).
2. T.Lis, Acta Cryst. C43, 1898-1900, (1987).