

## W0045

**Crystallographic Studies of Phosphoenolpyruvate Carboxykinase.** Julien J.H. Cotelesage<sup>a</sup>, Louis T.J. Delbaere<sup>a</sup>, Hughes Goldie<sup>a</sup>, J. Gregory Zeikus<sup>b</sup>, <sup>a</sup>Dept. of Biochemistry, Univ. of Saskatchewan, <sup>b</sup>Dept. of Biochemistry and Molecular Biology, Michigan State Univ.

The K213S mutant of the enzyme phosphoenolpyruvate carboxykinase (PCK) from the bacterium *Escherichia coli* has been found to have the unusual kinetic property of being inhibited by divalent manganese. Normally ionic manganese enhances the activity of PCK. A 2.0 Å crystal structure of K213S complexed with ATP, Mg<sup>2+</sup>, Mn<sup>2+</sup> and substrate-analogue pyruvate might explain the inhibitory effect of Mn<sup>2+</sup>. The structure reveals that with the side chain of lysine at position 213 missing, pyruvate is able to take an alternate orientation when coordinating the manganese ion. If the substrate oxaloacetate is able to coordinate Mn<sup>2+</sup> differently as well, it may not be able to react, thus explaining the inhibitory effect of Mn<sup>2+</sup>.

A novel technique to put carbon dioxide in the active site of crystallized PCK has been designed. It is based on the techniques used to make heavy atom derivatives of crystals with xenon gas. PCK from *E. coli* and *Anaerobiospirillum succiniciproducens* have been crystallized under a pressurized atmosphere of carbon dioxide. The results of this experiment will be discussed.