

s1.m2.p6

Application of a dual-source Weissenberg type diffractometer. H. Borrmann, H. Zhang, Yu. Prots, M. Schmidt and W. Schnelle, *Max Planck Institute for Chemical Physics of Solids, Noethnitzer Str. 40, 01187 Dresden, Germany.* E-mail: hzhang@cpfs.mpg.de

Keywords: Dual-source diffractometer; High resolution imaging plate; Zinc ferrite

An additional X-ray source along with a Johansson type monochromator is installed on a Weissenberg type diffractometer with a large imaging plate detector (Rigaku R-Axis RAPID) [1]. This enables two sets of intensity data to be collected at the very same sample setting but using two different X-ray beams, i.e. beams of different wavelengths and/or different beam shapes. For example, an optimal refinement on the structure parameters of the hydrogen atom in $\text{Ca}_2[\text{BN}_2]\text{H}$ (space group $Pnma$, No. 62, $a = 9.2015(8) \text{ \AA}$, $b = 3.6676(2) \text{ \AA}$, $c = 9.9874(12) \text{ \AA}$, $Z = 4$) has been investigated by analyzing the data collected using various primary beam sources. Moreover, additional specific information can be gained from data collected from a resonance experiment applying a wavelength very close to an absorption edge of a compositional element. We have tried to analyze the cation distribution in zinc ferrite (ZnFe_2O_4) [2] using high resolution data along with such a resonance experiment applying $\text{Co K}\beta$ radiation.

- [1] Borrmann, H., Armbruster, M., Burkhardt, U., Leithe-Jasper, A., Zhang, H. & Grin, Yu. (2002). *Acta Cryst.* **A58**, C261.
 [2] O'Neill, H. St. C. (1992). *Eur. J. Mineral.* **4**, 571-580.

s1.m3.p1

On Pentavalent Phosphorus Intermediates of Enzymatic Phosphoryl Transfer Reactions. Imre Berente and Gábor Náray-Szabó, *Department of Theoretical Chemistry, Eötvös Loránd University and Protein Modelling Group, Hungarian Academy of Sciences - Eötvös Loránd University H-1117 Budapest, Pázmány Péter st. 1A, Hungary.* E-mail: imre@chem.elte.h

Keywords: Transition State, Enzyme, Phosphorane

On the basis of ab initio molecular orbital calculations with a large basis set on extended models of the active site (cf.

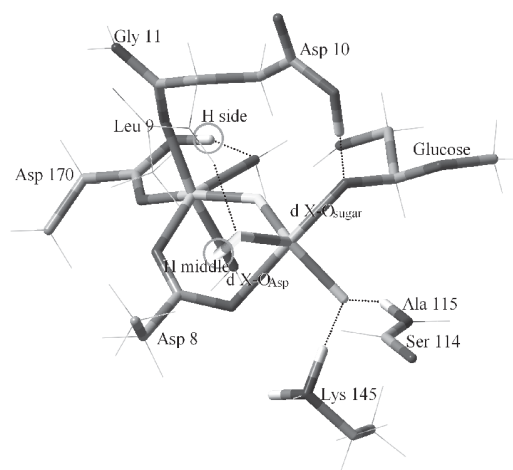


Figure) we question the existence of a symmetric trigonal bipyramidal oxyphosphorane species assumed to be present in the complex of phosphoglucomutase with glucose-6-phosphate substrate. In contrast to this suggestion by Lahiri et al. [1], we located two flat, distorted tetragonal structures on the potential surface, which may represent both the initial and final states of the reaction. Our calculations give also support to another interpretation [2] stating that instead of an oxyphosphorane species a $\text{MgF}_3(-)$ transition-state analogue binds to the active site. Both alternative structures provide electron density patterns similar to that obtained from X-ray diffraction experiments.

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 [2] G.M. Blackburn, N.H. Williams, S.J. Gamblin, S.S. Smerdon, *Science* **301**, 1184c (2003).