

Theoretical Study of Glucose Transformation to 5-Hydroxymethylfurfural using RISM-SCF-SEDD

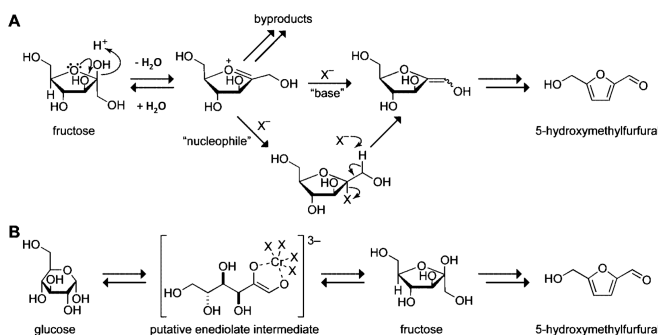
Arifin, Daisuke Yokogawa, Stephan Irle

Quantum Chemistry Group, Nagoya University, Japan

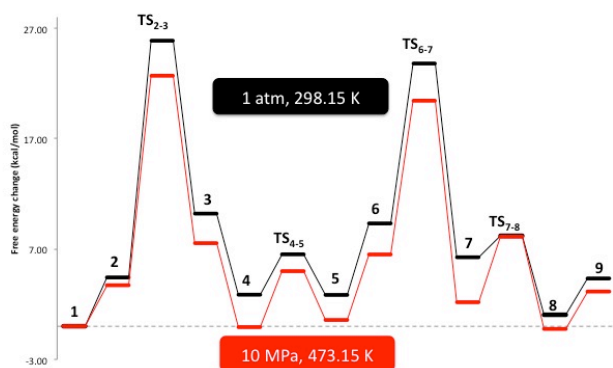
Email: arifin@b.mbox.nagoya-u.ac.jp

Hydrolysis of hexose into 5-(Hydroxymethyl)furfural (HMF) is believed to be one of the many key reactions for 'green chemistry'. Previous proposed mechanisms, as shown in Scheme 1, suggests that formation of HMF from glucose occurs after the isomerization into fructose (**B**), which would be directly dehydrated into HMF (**A**). [1] Open ring mechanism, also given in Scheme 1, is the most likely pathway of isomerization from glucose into fructose. Besides the open ring mechanism, cyclic or closed ring mechanisms have been proposed by experimental and theoretical works as the reaction pathway for transforming 6-membered ring pyranose xylose molecule into the 5-member ring furanose furfural. [2]

In the present work, we considered both open ring and cyclic mechanisms for the isomerization reaction and further dehydration to produce HMF. We applied the coupled-cluster level of theory using RISM-SCF-SEDD [3] as the solvation model. We found that our energetics produced by RISM-SCF-SEDD shown good agreement with experimental studies. Furthermore, RISM-SCF-SEDD allows to treat the system in high pressure and temperature conditions which shown in Scheme 2.



Scheme 1. Previous proposed mechanism via open ring



Scheme 2. Free energy surface of glucose isomerization for cyclic mechanism

[1] Binder, J. P., Raines, R. T., *J. Am. Chem. Soc.*, 131:1979-1985, 2009.

[2] Qian, X., Wei, X., *J. Phys. Chem. B*, 116:10898-10904, 2012.

[3] Yokogawa, D., Sato, H., Sasaki, S., *J. Chem. Phys.*, 126:244504, 2007.