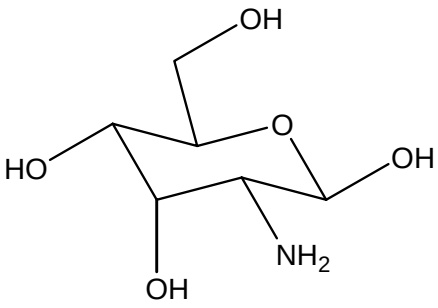
METHODS

Molecular Modeling is a way to determine any molecular structures and also transport mechanism during the operation. This technique has many advantages, for example, it eliminates the need of use real chemicals; saving not only resources but also reducing researcher exposure to toxic chemicals that is called greener science. The widespread availability and use of personal computer has resulted in molecular modeling and simulation techniques become a common research tools.

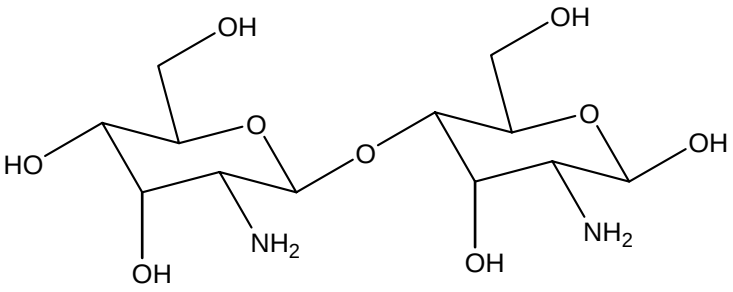
1. Geometrical Parameters

The geometries of the chitosan oligomers were constructed by GaussView 3.0 software in this case. Then, all calculations were carried out by the GAUSSIAN 03 software running on Windows PC, which is capable of predicting many properties of molecules and reactions.

The chitosan molecule is considered in many forms; chitosan-monomer; dimer; trimer; tetramer; and pentamer as shown in figure 3. Chitosan oliogomers was firstly studied to extrapolate the results into chitosan polymer. The molecule of chitosan monomer consists of carbon 6 atoms, oxygen 4 atoms, hydrogen 13 atoms, and nitrogen 1 atom in form of covalent single bond hexagonal. When chitosan dimer was formed, 1 hydrogen of chitosan monomer will be bonded with OH of another monomer. This phenomenon will occur repeatedly. The result of this phenomenon is chitosan polymer. The product of this reaction is water formed by condensation polymerization reaction. In this article, optimization of chitosan oligomers will be studied to geometrical parameter of these chitosan for integrating to determine the geometrical parameters of chitosan polymer. Therefore, the prediction of geometrical parameters of chitosan polymer can de drawn formthese results. Optimized bond lengths and angles of chitosan molecule calculated with the semiempirical PM3, AM1 and *ab inito* HF/6-31G* (Hehre et al., 1999) and comparison with X-ray crystallographic data was studied.



(a)



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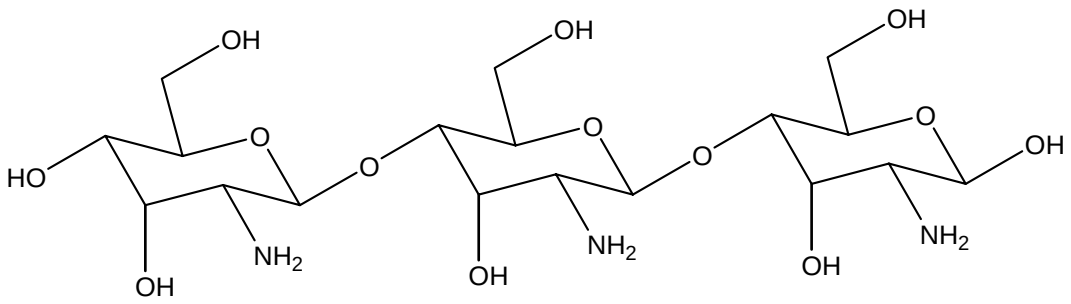
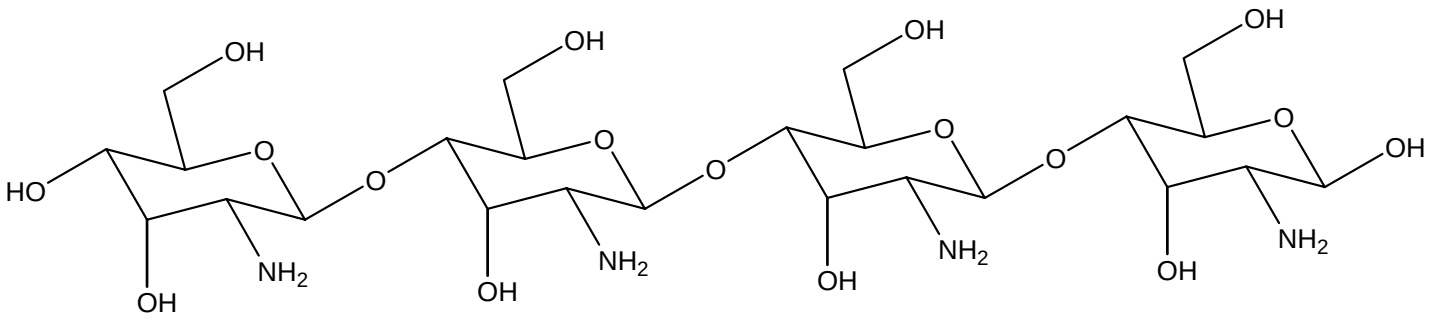
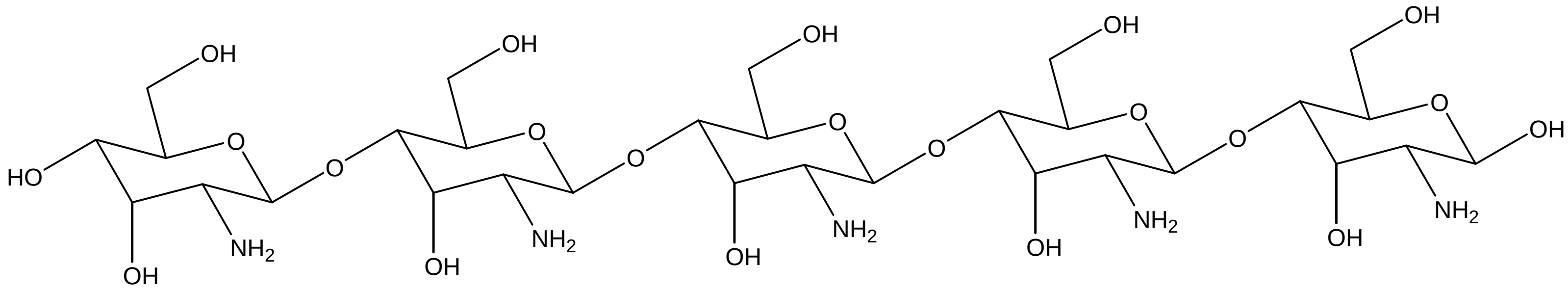


(c)



(d)



(e)

<u>Figure 3</u> Molecular structures of chitosan oligomers; (a) Chitosan monomer, (b) Chitosan dimer, (c) Chitosan trimer, (d) Chitosan tetramer, (e) Chitosan pentamer

2. The electronic property of conducting polymer

The conductivity of any conducting polymers depends on their electronic property. The property, in this case, is energy gap or band gap. Metal is known in sense of giving the best conductivity. The energy gap of metal is equal to zero as shown in fig. 4. Hence, the energy gap of any conducting polymers should be nearly zero. The method determining energy gap is HOMO-LUMO energy differences.

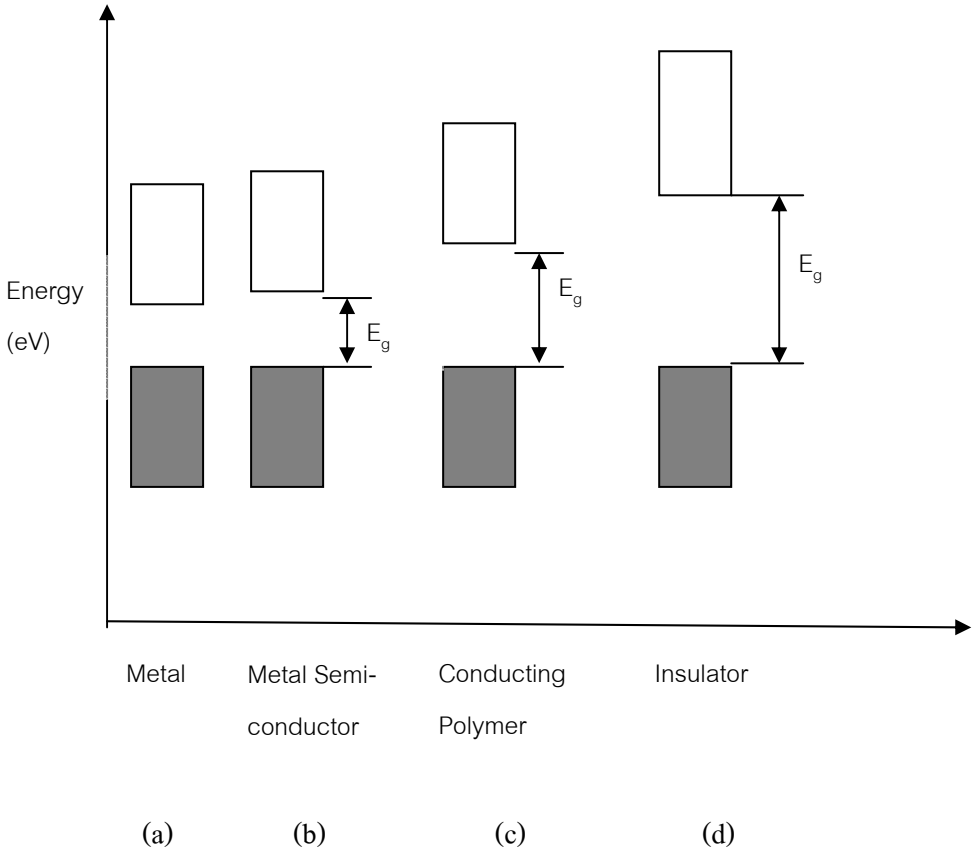


Figure 4 The energy gap of (a) Metal (b) Metal semiconductor (c) Conducting polymer (d) Insulator

In this study, The energy gap of chitosan oligomers will be studied using the best conformation of each oligomers. HOMO-LUMO energy differences is determined by 2 methods, AM1, PM3 and *ab inito* HF/6-31G*.

3. Proton Transfer Mechanism

The proton transfer mechanism is the way to determine phenomena within the membrane of PEM fuel cell. It can help us to better understand the pathway of proton transferring through the membrane.

In this study, the mechanism will be determined by Hyperchem 7.0 software. The variation of this study is the water content in the membrane. Thus, the amount of water has a significant effect on the mechanism. The water content will be varied into 3 classes; 10, 35, 90% water. The proton hopping mechanism, where the proton hops from one water molecule to another, is investigated. Hence, the behavior of protons and hydronium ions will have a great influence on the electrolyte's performance. These discovery will increase the understanding of the behavior of protons and hydronium ions through the electrolyte, which will, in turn, lead to design of improved electrolytes and better fuel cell performance.