# CHAPTER 6

# CONCLUSION

## 6.1 The Structure-Property Relationships of Selectivity

From the study, the distance between Cp planes is the best parameter for predicting the % isotacticity of zirconocene catalyst because it doesn't have exception for all structure. The % isotacticity increases as the distance between Cp plane as well as the angle between Cp plane increases. However, the relation with other parameters is also worth noted although there is no clear relation observed. We found that in exception of **structure 4**, the % isotacticity increases as the gap aperture increases, the zirconocene with small negative obliquity has high selectivity, the zirconocene which has negative or small positive twisted angle yields polypropylene with high % isotacticity, and the % isotacticity increases with the increases of the cavity distance and cavity angle.

## 6.2 The Structure-Property Relationships of Reactivity

The cavity distance and cavity angle are recommended for predicting the reactivity of zirconocene catalyst. The productivity increases as the cavity distance and cavity angle increases. Similar trend was observed for gap aperture. Other than that we also found the zirconocene catalyst with large negative obliquity having lower activity than that with less negative obliquity (around –16° to -17°). The zirconocene catalyst, with large negative value of twisted angle yields higher productivity. The productivity increases as the cavity distance and cavity angle increases. Finally, the zirconocene which has more positive charge on zirconium will has higher productivity.

## 6.3 The Effect of Substituents Group and Bridging Group to Cp ring Opening

The zirconocene structures with the silano-bridged have larger Cp ring opening than that with the ethano-bridged. The opening is described by the distance between Cp ring, angle between Cp plane, gap aperture, cavity distance, and cavity angle. For the silano-bridged zirconocene, the zirconocene structure which has larger bulky group at the β position of Cp ring has larger ring opening and twisted angle than the one with smaller bulky group at the same position. The zirconocene that has good electron donating group at α and β-position also has high productivity.

## 6.4 The Optimum Method for Calculated Zirconocene Structure

The bond distances, bond angles and bond torsions obtained from B3LYP/LANL2DZ agree with the B3LYP/DZVP. Except for bond torsions, bond distances and bond angles obtained from ONIOM (B3LYP/DZVP:UFF) are in good agreement with those from B3LYP/DZVP. The structure parameters such as distance between Cp plane, angle between Cp plane, gap aperture, obliquity, cavity distance, and cavity angle that obtained from B3LYP/LANL2DZ are slightly smaller than those from B3LYP/DZVP. On the other hand, these structural parameters from ONIOM (B3LYP/DZVP:UFF) which only acceptable for few cases are larger than those from B3LYP/DZVP. The minimal time-saving of B3LYP/LANL2DZ and the inaccuracy of ONIOM (B3LYP/DZVP:UFF) do not encourage these methods to replace B3LYP/DZVP. However, the QM/MM method with other force fields which better described the bridge torsion of metallocene needs further exploration.