

## CHAPTER 5

### CONCLUSION

The structural and electronic properties of Pd(II) tetraaza macrocyclic ligand has been determined with B3LYP exchange-correlation using 6-311G basis set at ground state. The structure of tetraaza macrocyclic ligand behaves as tetradentate chelating to Pd(II) atom that portrays a square planar geometry of the cationic complex structure. Based on the NBO analysis, there is no hybridisation of two nitrogen atoms or known as lone pair atoms in the tetraaza macrocyclic ligand. This allows Pd(II) atom to form coordination bond with nitrogen atoms in the Pd(II) tetraaza macrocyclic ligand structure. The stability of tetraaza macrocyclic ligand is mainly contributed by lone pair orbitals while the stability of Pd(II) complex promoted by metal-ligand interactions. The electrostatic potential surface map reveals that the Pd(II) tetraaza macrocyclic ligand possesses characteristics such as low electron distribution, a low tendency for electron donation, and high stability.

The optical properties of the Pd(II) tetraaza macrocyclic ligand were calculated through TD-DFT with hybrid functional B3LYP using LANL2DZ basis set of triplet state in gas phase. In the ultraviolet region, the intense band was observed at 275 nm and the weak band was observed at 389 in the visible region. On the other hand, the small energy gap in Pd(II) tetraaza macrocyclic ligand shows that the complex has high electron mobility since only little energy is required for the electron transfer process.

Subsequently, the optical properties of the Pd(II) tetraaza macrocyclic ligand were measured through TD-DFT with hybrid functional B3LYP using LANL2DZ basis set in different solvents. The dielectric constant value for each solvent are water (78.3553), acetonitrile (35.688), methanol (32.613), chloroform (4.7), toluene (2.37) and hexane (1.88). Based on the analysis, Pd(II) tetraaza macrocyclic complex in solvent phase has better optical properties compared to gas phase. The presence of methanol as solvent improved the optical properties by increasing the absorption wavelength, lowering the energy gap and enhancing the first hyperpolarizability of Pd(II) tetraaza macrocyclic ligand. However, the NLO properties of the Pd(II) tetraaza macrocyclic ligand in all solvents are lower than those of standard NLO materials due to its non-conjugated system, which limits intramolecular charge transfer capability

The theoretical results provide a benchmark for the synthesis of the protonated tetraaza macrocyclic ligand and cationic Pd(II) complex. In the future, the non-linearity of the Pd(II) tetraaza macrocyclic ligand can be enhanced by introducing conjugated bonds (double or triple bonds) between the atoms in the molecule. This will create a continuous pathway of  $\pi$ -electrons, allowing for their delocalization across the entire molecular framework.