# Structural Optimization of a Macrocyclic Supramolecule

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A 728 atoms-formed macrocyclic metal complex was found to self-assemble through hexacoordinate bonding between 14 Ni atoms and flexible tripeptide ligands.[1] In the previous studies including a model calculation of the macrocyclic metal complex,[2] the isomerization pathways had been effectively explored using the global reaction route mapping (GRRM) method.[3]

In the former research, we tried structural optimization of this supramolecule of +28 (=14$Ni^{2+}$) charge with one of semi-empirical molecular orbital methods, PM6. The obtained results have dissimilarity with the initial structure, indicating an expanded wavy shape (Fig.1).[2] Neither the calculated structure of 0 charge met our demand. Fig.1 indicates increased bond distance of the hexacoordination. The diameter of the 0 charge complex tends to shrink.

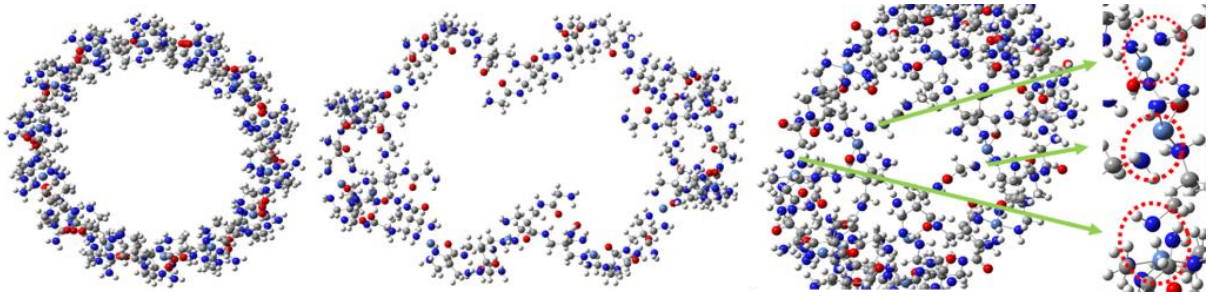

Fig 1. Left: Initial structure (728 atoms, ca. 30Å diameter);
Middle: A calculated structure of optimization with +28 charge (ca.46Å diameter);
Right: A calculated structure of optimization with 0 charge.

In order to include the effects by counter anions in a solvent at the geometry optimization, we need adjustment process of the effective charge of Ni ions. Starting from +14 (=14$Ni^{+}$) charge, we have tried some calculations of geometry optimization for a 728 atoms-formed macrocyclic metal complex. Details will be shown in our poster presentation.

**References**

[1] R. Miyake, A. Ando, M. Ueno, T. Muraoka. *J. Am. Chem. Soc.*, 2019, **141**, 8675-8679.

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