



## A study on host-guest complexation of octaprotonated octaaza macrocycles with selected PAHs towards the template-directed synthesis of mechanically interlocked molecules

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Template-directed synthesis (TDS) is one of the commonly used strategies in synthesis of mechanically interlocked molecules (MIMs). Inclusion complexes (ICs) of electron-deficient cationic macrocyclic ‘host’ and electron-rich ‘guest’ molecules have been used as donor-acceptor interactions driven ‘templates’ in TDS of MIMs. Among them, ‘templates’ consisting polycationic macrocyclic ‘host’ and polycyclic aromatic hydrocarbon (PAH) ‘guests’ are yet to be explored. Therefore, this research project focused on the study of IC formation between an octaprotonated octaazacyclophane (CP) ‘host’ and three selected PAH ‘guests’, naphthalene, anthracene and phenanthrene, separately with the intention to develop a potential ‘template’ for TDS of MIMs. The CP was synthesized by following [2+2] Schiff-base condensation between terephthalaldehyde with triethylenetetramine using lead nitrate as a template followed by the reduction of Schiff-base macrocycle with sodium borohydride, and the protonation using perchloric acid. After the characterization of CP and synthetic intermediates using FT-IR, UV-visible, and <sup>1</sup>H NMR spectroscopy, complexation studies of CP

and PAHs in acetonitrile were performed using UV-visible and fluorescence spectroscopy. A mixture of 1:1 CP and PAH exhibited an enhancement of UV-visible absorbance and fluorescence intensity with respect to the corresponding PAH which indicated the complexation of CP and PAH. Stoichiometry and binding constants of each combination of CP and PAHs were determined using Job’s plot method and dilution method, respectively. Each combination of CP and PAH exhibited 1:1 complexation stoichiometry. Among the three PAHs studied, the highest and the lowest binding constants with CP were demonstrated by anthracene and naphthalene, respectively. In summary, the geometrical compatibility between the cavity of CP and each PAH determined the stoichiometry and binding constant. The findings of this research could be used to develop TDS of MIMs using a CP and anthracene consisting ‘template’.

### Keywords:

Template-directed synthesis, mechanically interlocked molecules, polycyclic aromatic hydrocarbons, host-guest chemistry, inclusion complex