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

Damith D. Lekamge and Isurika R. Fernando*

Department of Chemistry, Faculty of Applied Sciences, University of Sri Jayewardenepura, Nugegoda 10250, Sri Lanka.

**Corresponding author: isurika.fernando@sjp.ac.lk*

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 ^{1}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

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Qualitative and quantitative detection of peanut oil adulteration in sesame oil

Selvaluxmy Kathirgamanathar, B.A.W. Sahara, M.M.N.P. Gunasekara and T.D.C.M.K. Wijeyasiriwardena

MRDC, Industrial Technology Institute, 503A, Halbarawa Gardens, Thalahena, Malabe,Sri Lanka.

**Corresponding author: selvaluxmy@iti.lk*

The present study was focused on developing rapid, cost-effective, and straightforward methods for qualitative and quantitative detection of peanut oil (PO) adulteration in sesame oil (SO). In Sri Lanka, due to the higher price and demand of SO, merchants intentionally add cheaper and lower quality edible oils mainly the PO for economic gains. Intentional adulteration using pure SO and PO was done in the laboratory. Two approaches were established using UV spectrophotometric analyses and chromogenic tests. Under UV spectrophotometric analysis, the absorbance was measured with and without developing colours. First the absorption spectra in the

UV range obtained for PO adulterated SO samples were compared with that of pure SO and PO. Pure SO and PO recorded maximum absorbance, 4.2030±0.08 and 3.3530±0.04 at 305.6±0.00 nm and 290.2±0.00 nm respectively. The maximum absorbance for 5%, 10%, 20%, 30%, 40%, 50%, 60%, 70%, 80%, and 90% PO adulterated samples were 4.1870±0.10, 4.1360±0.08, 4.0940±0.12, 4.0260±0.06, 4.0090±0.05, 3.8830±0.10, 3.8010±0.05, 3.7550±0.06, 3.6890±0.09, and 3.5730±0.08 respectively. A significant variation in both maximum absorbance and corresponding wavelength was observed starting from 40% adulteration. The detection can be simply done for 40 – 90% adulteration levels by this method. Secondly, the absorbance measured for the colour complex formed by the reaction between SO and ethanolic furfural solution to represent the SO level. The absorbance recorded for pure SO at 520 nm was 0.7376±0.0201 and 0.6466±0.0550, 0.5576±0.0404, 0.3956±0.0136, 0.3386±0.0116 and 0.2056±0.0185 for 10%, 20%, 30%, 40%, and 50% PO adulterations respectively. Absorbances exhibited a strong correlation with the SO percentage up to 50% adulteration tested in the laboratory. The simple chromogenic test was developed using 0.5M KMnO4 and 0.25M $K_2Cr_2O_7$ solutions separately using 5% - 95% PO adulterated SO samples as a second approach. The colour change in both chromogenic tests indicated promising results and this method could be used to detect a minimum 5% peanut oil adulteration level as there is a visible change in colour compared to the colour given for pure oils.

Key Words:
Sesame oil, Adulteration, Chromogenic reaction, Rapid test, UV Spectrophotometry

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Inhibition of Corrosion of Mild Steel by Polyaniline – Cinnamon Oil Composite Layers

Sathya S Srirajan[1] and Namal Priyantha[1,2]*

[1] *College of Chemical Sciences, Institute of Chemistry Ceylon, Rajagiriya 10107, Sri Lanka.*

[2] *Department of Chemistry, University of Peradeniya, Peradeniya, Sri Lanka.*

**Corresponding author: namal.priyantha@yahoo.com*

Mild steel is used in many industrial applications. However, its tendency toward corrosion has limited its applications. Consequently, inhibition of corrosion of mild steel, especially through environmentally friendly and cost-effective means has become a necessity. Composite coating of polished mild steel samples coated with polyaniline via electrochemical polymerization with the aid of cyclic voltammetry followed by a layer of cinnamon oil deposited by dipping for 21 hours has shown tremendous corrosion inhibition properties. More importantly, the composite layer results in much increased corrosion inhibition efficiency as compared to cinnamon oil and polyaniline coating alone, demonstrating the synergistic effect. The percentage corrosion inhibition efficiency of mild steel in 0.10 M HCl with polyaniline coating, with cinnamon oil coating and with polyaniline-cinnamon oil composite was quantitatively determined by mass loss measurements and found to be 20.9%, 34.8% and 45.9% respectively. Based on the results, polyaniline-cinnamon oil composite was found to be the effective inhibitor compared to polyaniline and cinnamon oil alone. Further, these results were supported by Tafel plots and Electrochemical Impedance Spectra. The percentage corrosion inhibition efficiencies of the composite layer is shown within the concentration range of aqueous HCl solutions between 0.1 M and 1.0 M, and within the solution temperature range between 303 K and 318 K. Percentage corrosion inhibition efficiency of the polyaniline-cinnamon oil composite layer in 0.1 M, 0.3 M, 0.5 M and 1.0 M HCl found to be 45.9%, 47.97%, 50.63% and 52.27% respectively. Percentage corrosion inhibition efficiencies of the polyaniline-cinnamon oil composite layer at 303 K, 308 K, 313 K and 318 K found to be 48.26%, 42.33%, 38.45% and 34.32% respectively. The results showed that polyaniline-cinnamon oil composite works effectively in 1.0 M HCl at 303 K. Scanning electron microscopy (SEM) was used to investigate the surface morphology of mild steel specimens without any coating and with polyaniline-cinnamon oil composite layer coating after immersion in 0.5 M HCl for 2 hours.