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Mass Spectrometry Study of Host-Guest Complexes between Angle-Strained Alkyne-Containing Cycloparaphenylenes and Fullerenes

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Cycloparaphenylenes (CPPs) are strained ring molecules, comprising only sp^2-hybridized carbon atoms. As a result of their both concave and convex extended π arrays, CPPs have been widely employed as ideal supramolecular hosts for fullerenes [1] and CPPs [2].
In this study, a variety of functionalized triazole-containing CPPs with an elliptic lasso-like shape are exploited as hosts for C_{60} and C_{70}. Host-guest complexes of these Lasso-CPPs and closely related [12]CPP with C_{60}/C_{70} are investigated by electrospray ionization mass spectrometry. The mass spectra show that [1:1] complexes of Lasso-CPPs with C_{60}/C_{70} are formed as radical cations and protonated species, while [2:1] complexes mainly exist as protonated molecules. Energy-resolved collision (MS^2) experiments reveal that Lasso-CPP⊃fullerene [1:1] complexes are more stable as radical cations than as protonated species. This is due to the fact that in the radical cation, the positive charge on Lasso-CPPs can be delocalized, thus enhancing the complex stability. Changes in the electron donating/-accepting nature of peripheral substituents on Lasso-CPPs, on the other hand, have little influence on the complex stability. Additionally, MS^2 experiments indicate that [2:1] and [1:1] complexes of Lasso-CPPs with C_{70} are more stable than the corresponding C_{60} analogue, as reported for CPP-based complexes [2]. However, complexes of Lasso-CPPs with C_{60}/C_{70} are found to be more stable than [12]CPP complexes.
Our results suggest that strain-promoted Lasso-CPPs with a series of unique properties are desirable host molecules for fullerenes. Mass spectrometry is a powerful tool for the study of these non-covalent host-guest complexes.

References

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