

Self-Assembly of Molecular Prisms *via* Pt₃ Organometallic Acceptors and a Pt₂ Organometallic Clip

Sushobhan Ghosh, Bappaditya Gole, Arun Kumar Bar, and Partha Sarathi Mukherjee*

Department of Inorganic and Physical Chemistry, Indian Institute of Science,

Bangalore-560 012, India. Fax: 91-80-2360-1552; Tel: 91-80-2293-3352

E-mail: psm@ipc.iisc.ernet.in

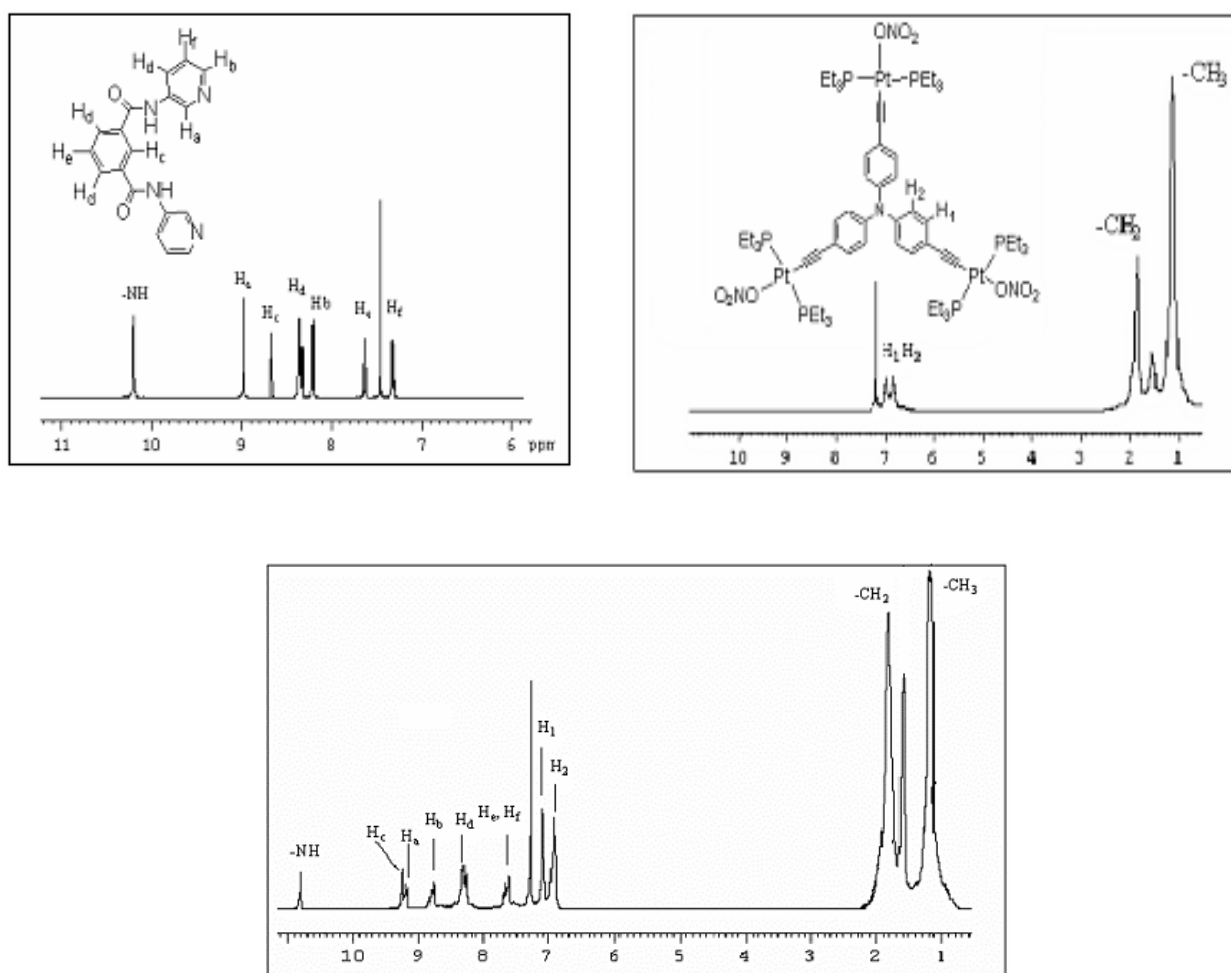


Fig. S1: ¹H NMR spectra of **2a**, (top left) **1a** (top right) and **3a** (bottom).

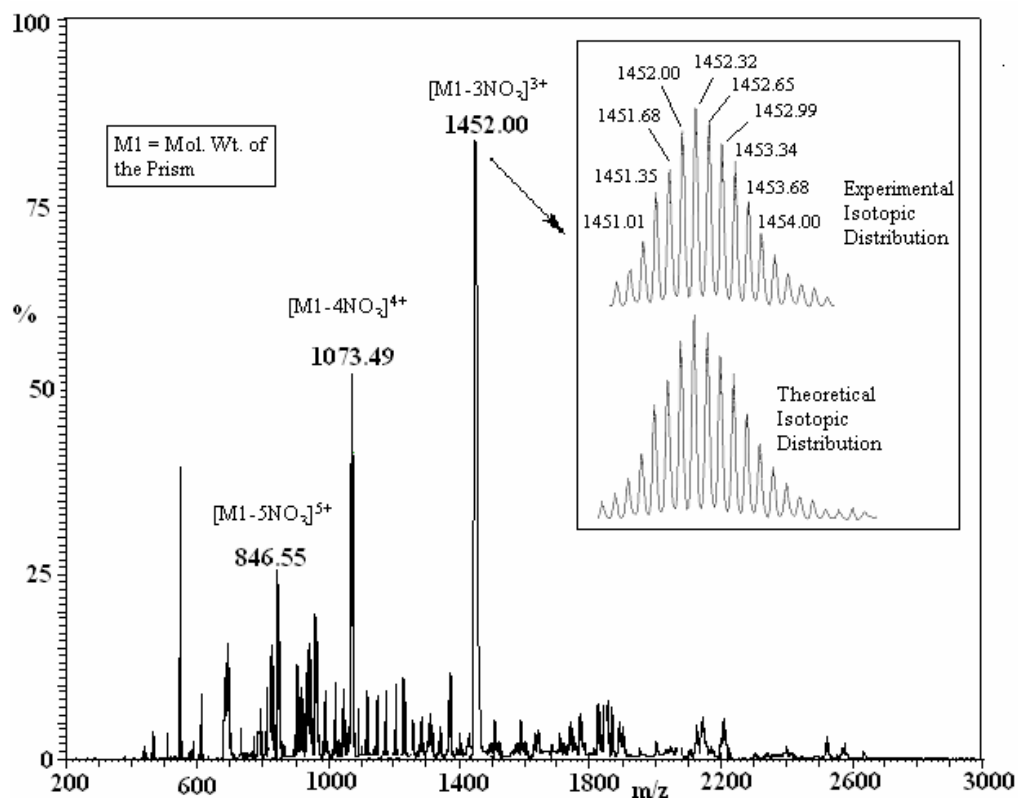
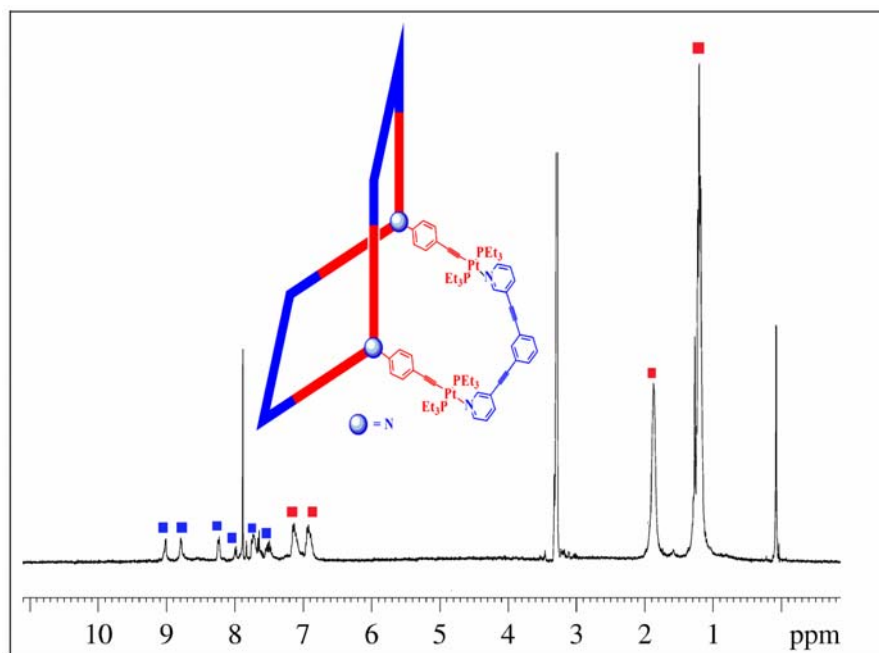


Fig. S2: ESI-MS spectrum of **3a** in MeOH. Inset: Theoretical and experimental isotopic distribution patterns of the $[M-3NO_3]^{3+}$ peak.



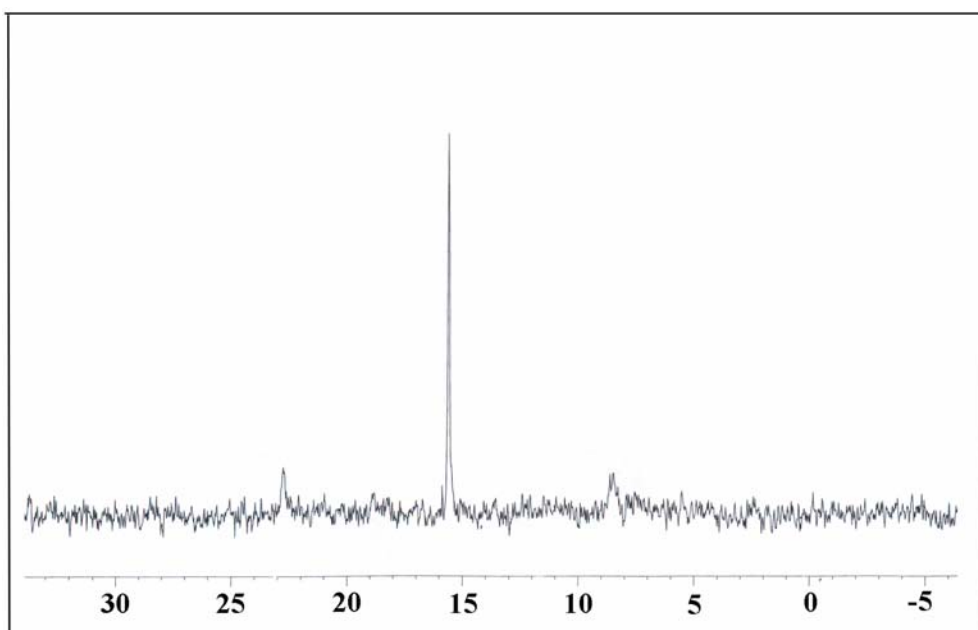


Fig. S3. ^1H NMR (above) and ^{31}P NMR (below) of the supramolecular prism **3b**.

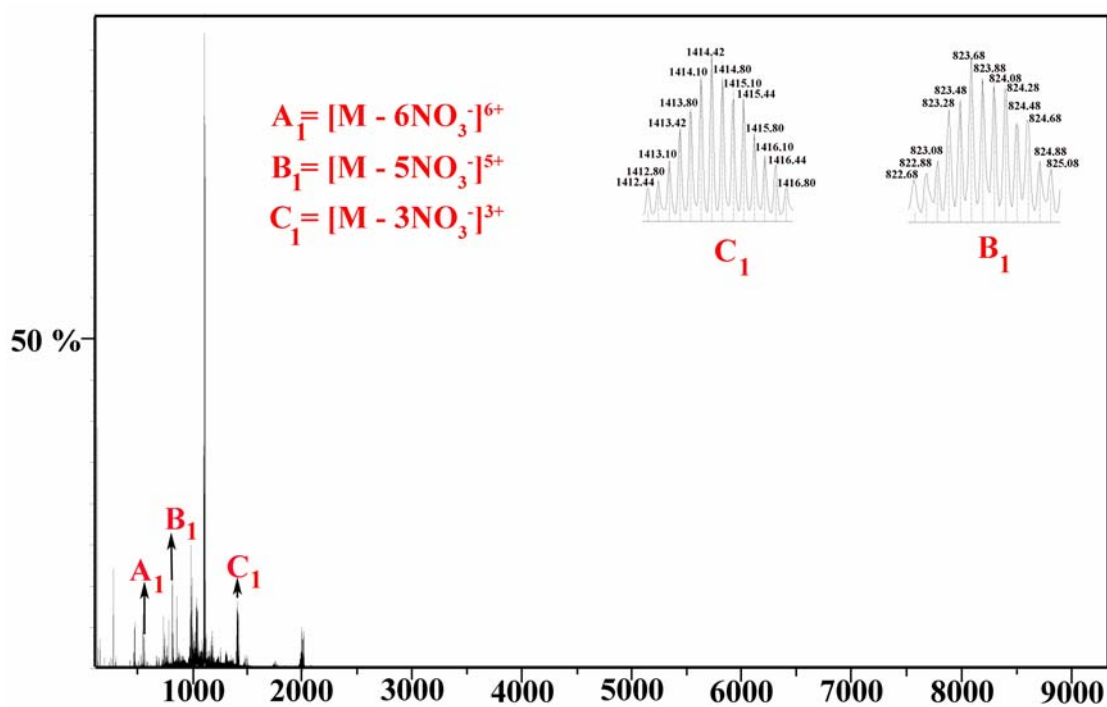


Fig. S4. ESI MS of the supramolecular prism **3b** and the experimental isotropic distribution pattern of the peaks.

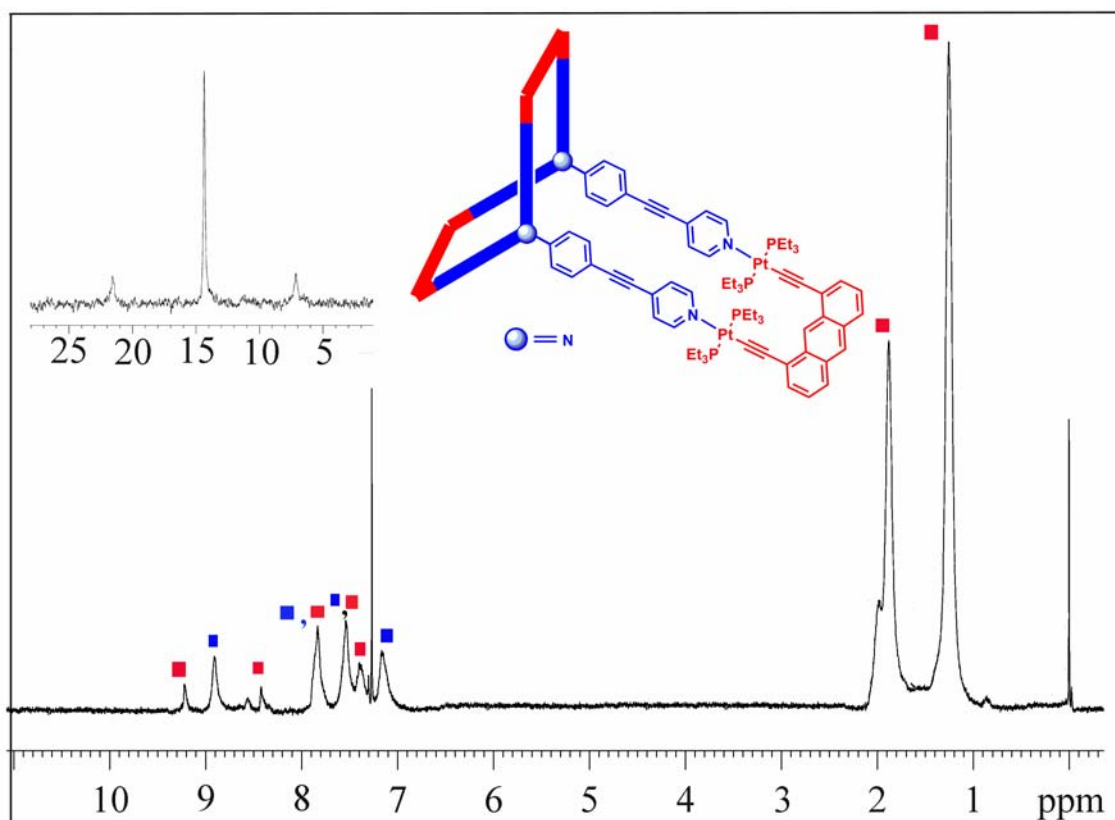


Fig. S5: ^1H and $^{31}\text{P}\{^1\text{H}\}$ (inset) NMR spectra of the prism **3c** in CDCl_3 .

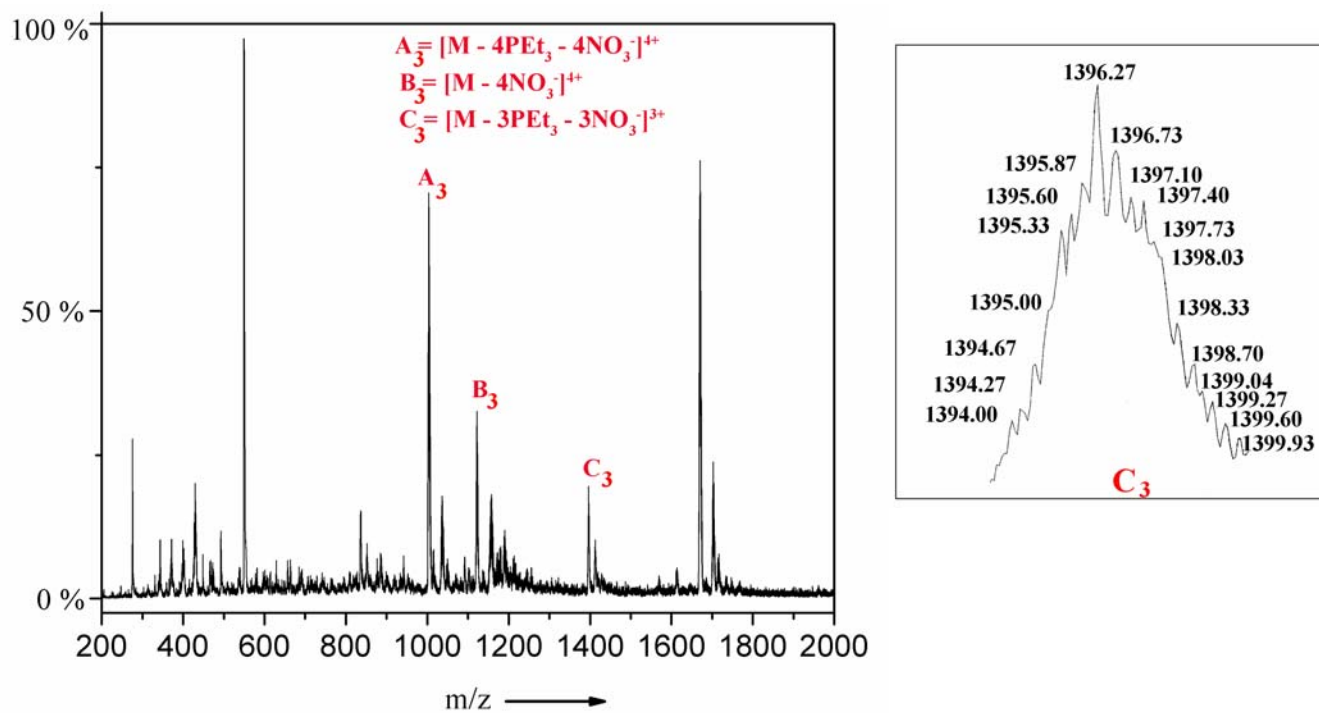


Fig. S6: ESI mass spectrum (left) of **3c** and the experimental isotopic distribution pattern of the peak C_3 (right).

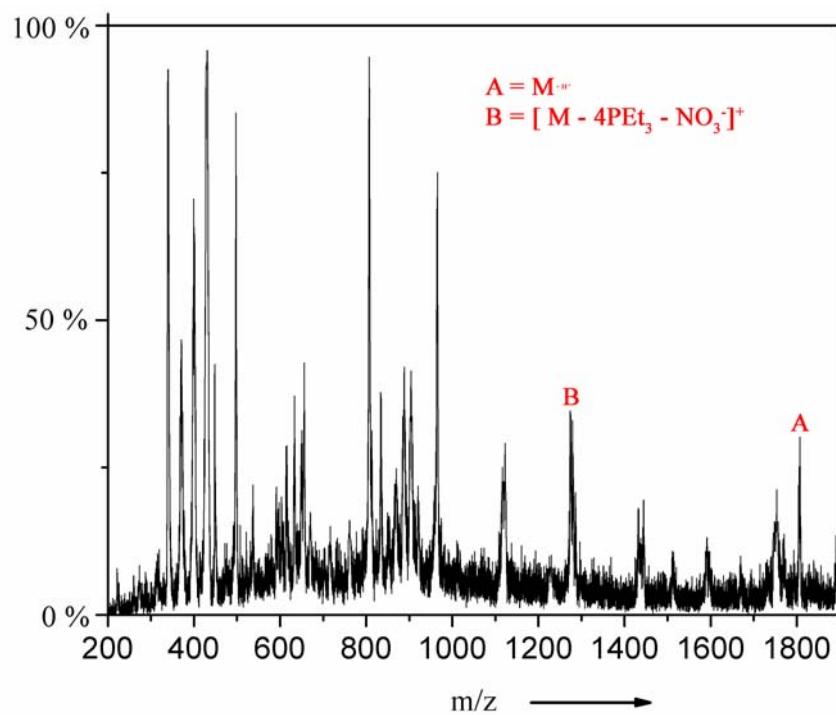


Fig. S7: ESI-Mass spectrum of **1c** in methanol.

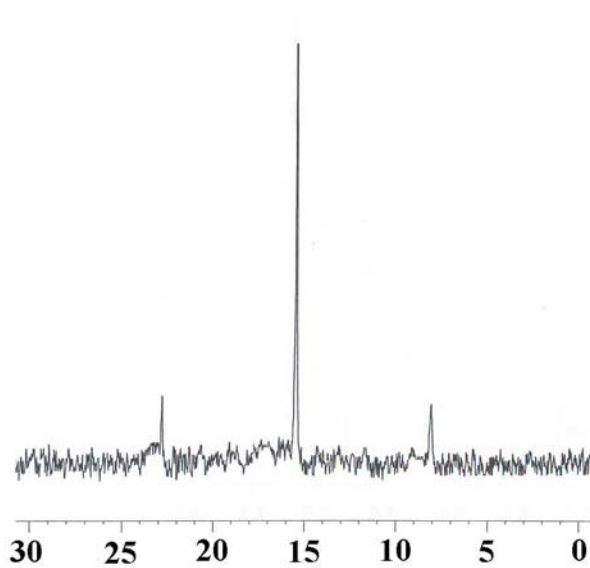


Fig. S8: ^{31}P NMR spectrum of **3d** in $CDCl_3$.

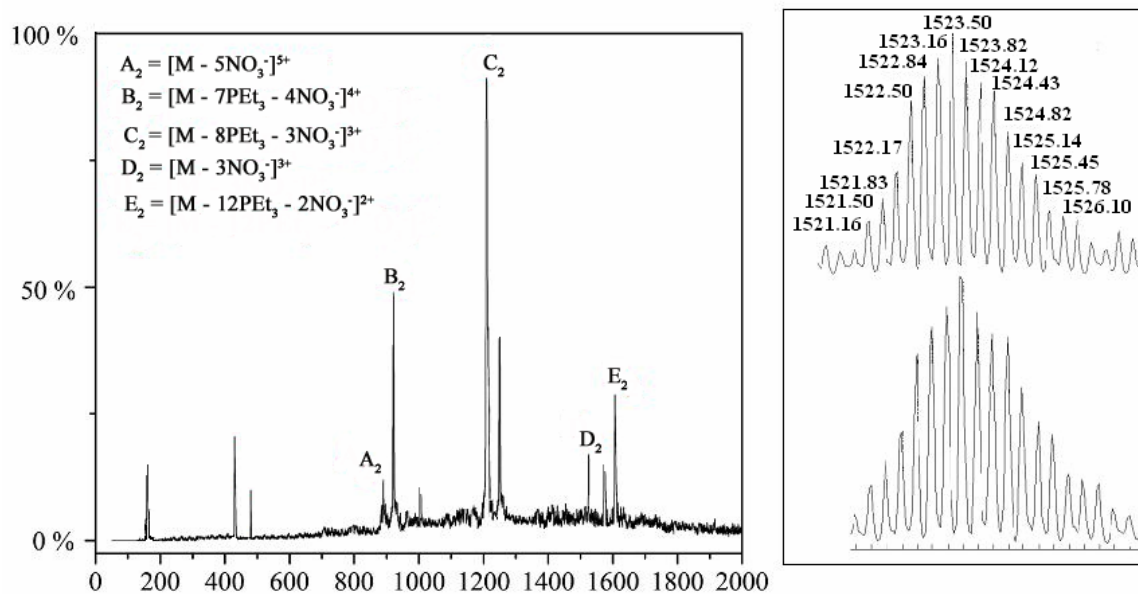


Fig. S9: ESI mass spectrum of **3d** (left) and the isotopic distribution pattern of the peak due to [M-3NO₃]³⁺ (right).

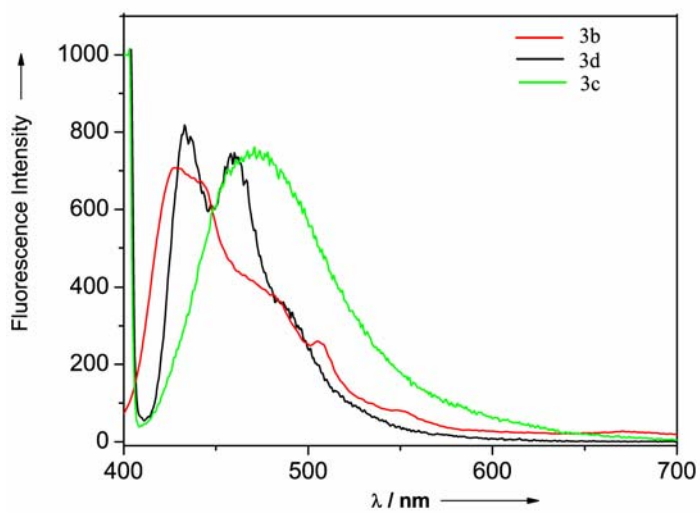


Fig.S10: Fluorescence spectra of the prisms **3b-d** in DMF.

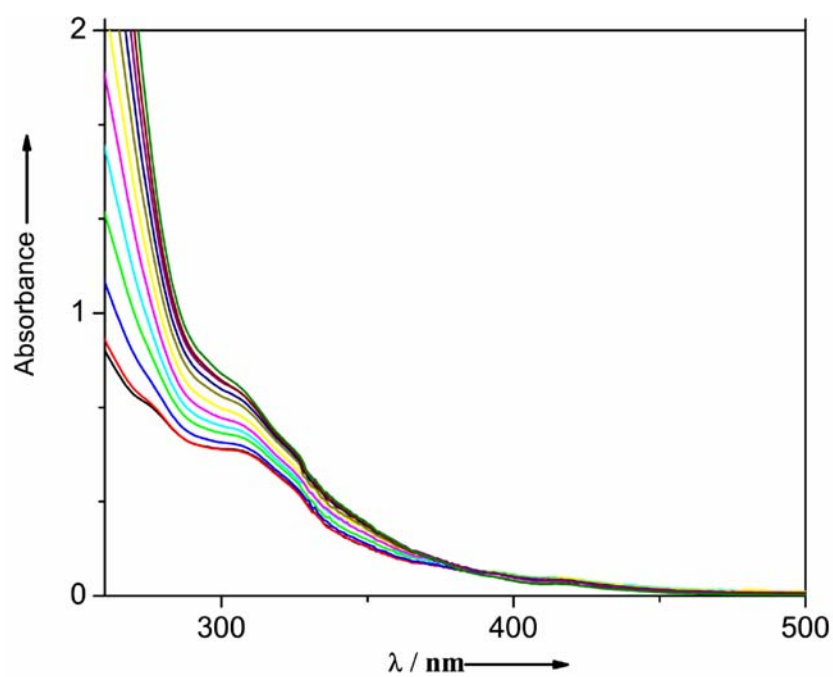


Fig. S11. Binding study of supramolecular prism **3d** by titration of molecular prism **3d** with TNT (from 0.5×10^{-3} M to 2.5×10^{-3} M) and monitoring the change in absorption spectra.

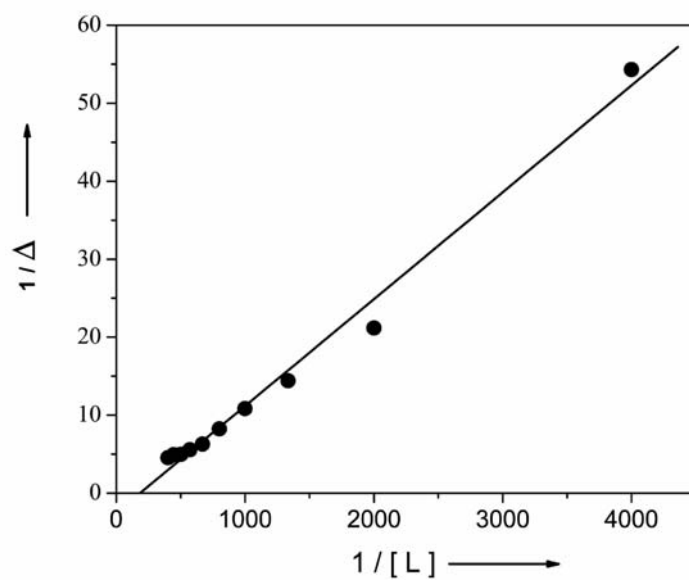


Fig. S12. Plot of inverse of the change of absorption of supramolecular prism **3d** vs the inverse of concentration of TNT to determination the binding constant for the binding of supramolecular prism **3d** and TNT.

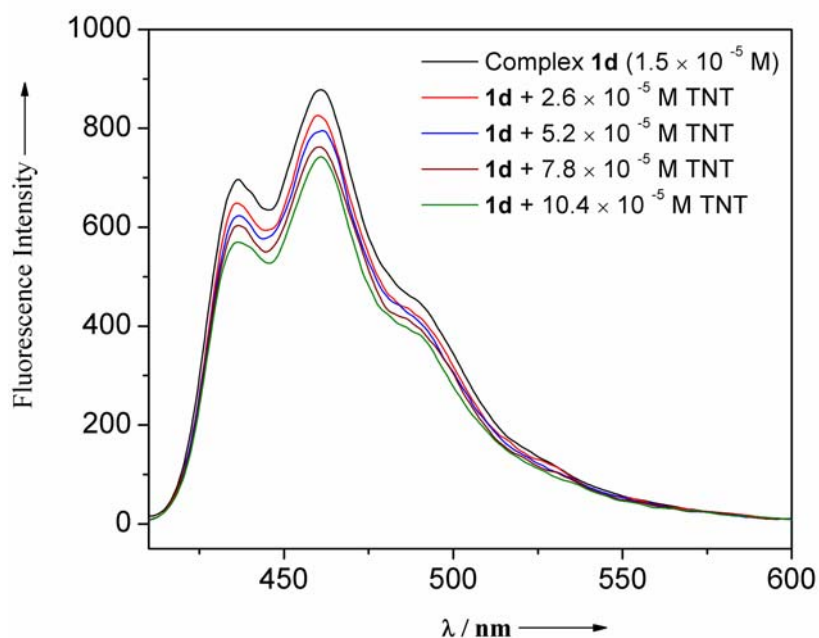


Fig. S13. Quenching of fluorescence intensity of **3d** ($1.5 \times 10^{-5} \text{ M}$) on gradual addition of dilute TNT solution ($\sim 10^{-5} \text{ M}$).

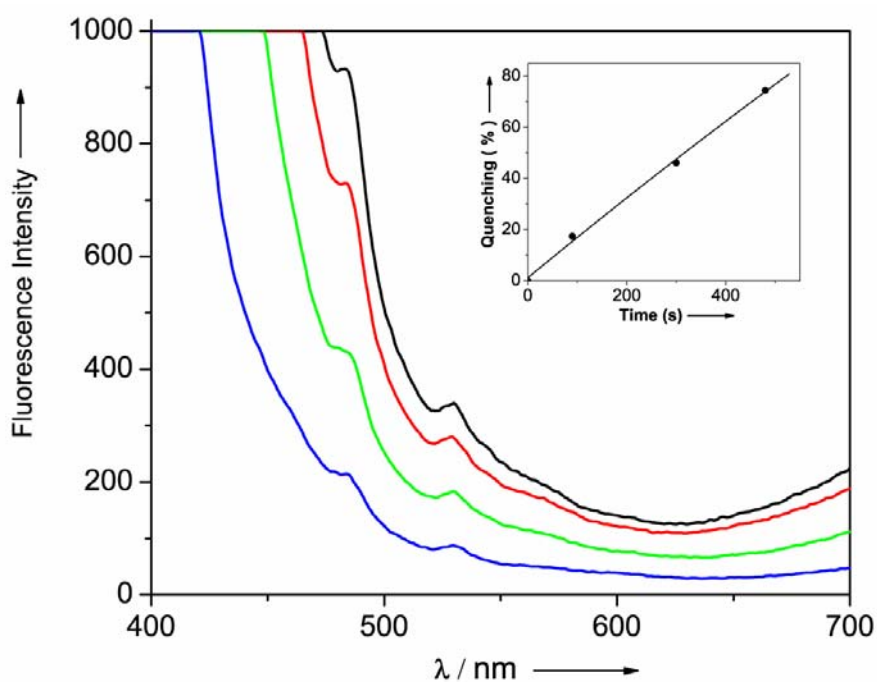


Fig. S14: Fluorescence quenching of the spin cast film of **3d** after exposing to TNT vapour. Plot of percentage of fluorescence quenching *vs* time (inset).

Table S1. Photophysical Data of the Supramolecular Prisms (**3b-d**).

| Complex | Solvent | Absorbance | Fluorescence | Φ_F |
|-----------|---------|-----------------------------|-----------------------------|----------|
| | | $\lambda_{\max}(\text{nm})$ | $\lambda_{\max}(\text{nm})$ | |
| 3b | DMF | 283, 365 | 425 | 0.04 |
| 3c | DMF | 430, 383, 270 | 472 | 0.48 |
| 3d | DMF | 421, 398, 309. | 430, 460 | 0.35 |