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Structural and spectroscopic studies of photo-switchable molecular capsule

M. Choudhari[a], C. Ritchie[a]

a: Monash University, Wellington Rd, Clayton VIC 3800.

manjiri.choudhari@monash.edu

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Photochromism is defined as the reversible conversion of two chemical species in response to light, with photochromic compounds being important due to their various real-world applications.[1] Among the different classes of photochromic compounds, diarylethenes (DAEs) offer thermal stability of the photogenerated isomers, fatigue resistance, and high quantum yields, proving them important for various applications.[2] The incorporation of DAEs in metal-organic frameworks, nanomaterials, and polymers has led to substances with novel properties.[3] Polyoxometalates (POMs) are inorganic discrete and nanosized metal-oxygen compounds of early transition metals commonly found in their highest oxidation with a range of structural and compositional diversity, making them suitable for various applications.[4] Functionalization of POMs with organic species results in various organic-inorganic hybrid materials with tunable properties.[5] In 2018, we reported a POM-DAE complex which showed modified photochromic properties compared to the parent DAE.[Based on these earlier findings, we extended our study and have since succeeded in obtaining a photochromic molecular capsule with the generic formula $[(POM)_2(DAE)_3]^{x-}$ **(1)**. The compound has been structurally characterized using single-crystal x-ray diffraction while also being studied extensively in solution using a suite of spectroscopic techniques.

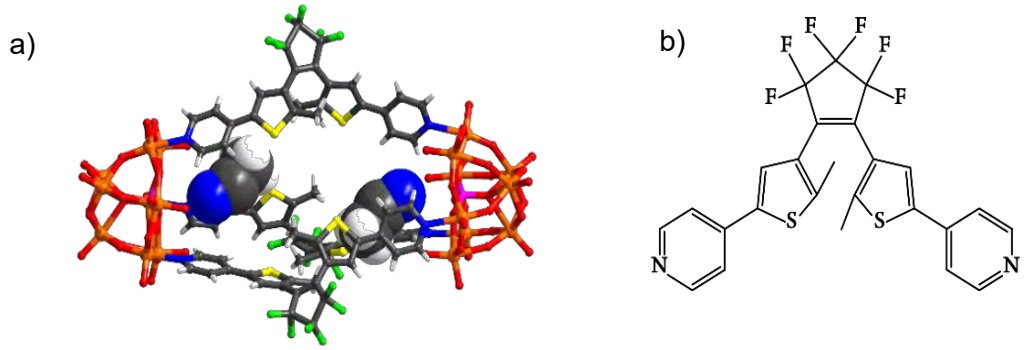

Figure 1: a) Graphical representation of the chiral molecular capsule **(1)** obtained from single-crystal X-ray diffraction structure determination b) Chemdraw representation of **DAE** ($C_{25}H_{16}N_2S_2F_6$).

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