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Self-assembly of trigonal prismatic metallocages encapsulating BF_4^- or CuI_3^{2-} as anionic guests: Structures and mechanism of formation

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^{13}C NMR data for Ligand MSTBim:

^{13}C NMR (CDCl_3): $\delta = 143.87 (C_2)$, $141.08 (C_{4a})$, $139.81 (C_{7a})$,
 $133.85 (C_9)$, $130.74 (C_{10})$, $123.38 (C_4)$, $122.77 (C_7)$, 120.64 ,
 (C_5) , $109.34 (C_6)$, $44.15 (C_8)$, $16.52 (C_{11})$.

Fig. S1. Top view of the $[\text{Ag}_3(\text{MSTBim})_2]^{2+}$ cage in complex $[\text{Ag}_3(\text{MSTBim})_2](\text{CF}_3\text{SO}_3)\cdot(\text{BPh}_4)_2$ showing locations of anions CF_3SO_3^- and BPh_4^- at the windows of the cage.

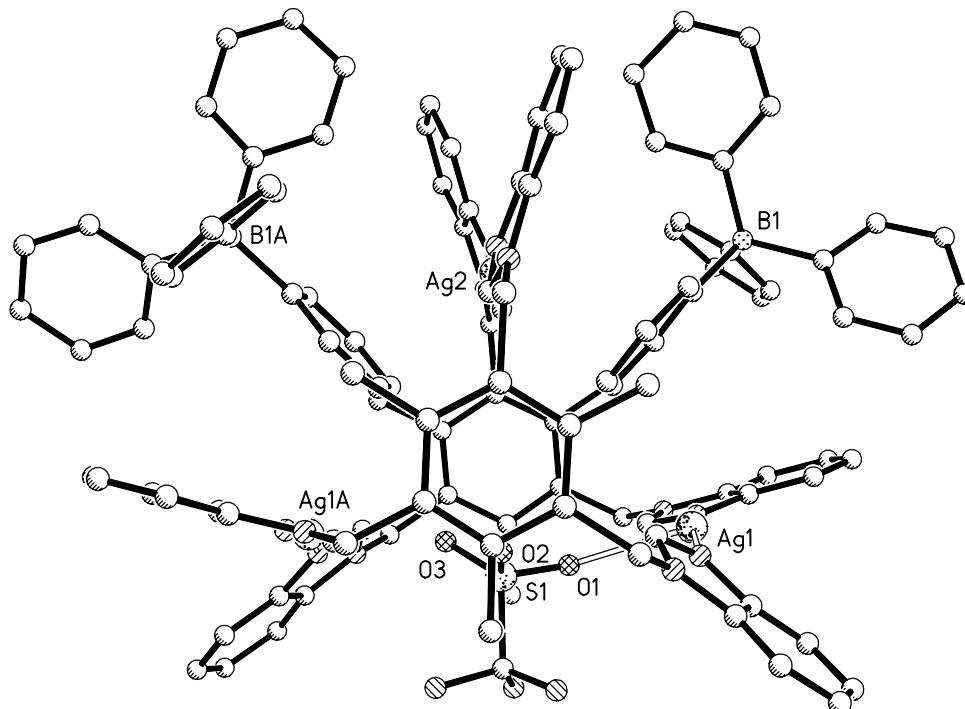


Fig. S2. Side view of the empty $[\text{Ag}_3(\text{MstBim})_2]^{2+}$ cage in complex $[\text{Ag}_3(\text{MstBim})_2](\text{CF}_3\text{SO}_3)\cdot(\text{BPh}_4)_2$.

