

An Excimer-based, Binuclear, On-off Switchable Calix[4]crown Chemosensor

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Page 3: UV Frontier molecular orbitals (HOMO, LUMO, LUMO2, and LUMO3) of (a) **1**, (b) **1**• Pb^{2+} , and (c) **1**• K^+ . (Figure S3)

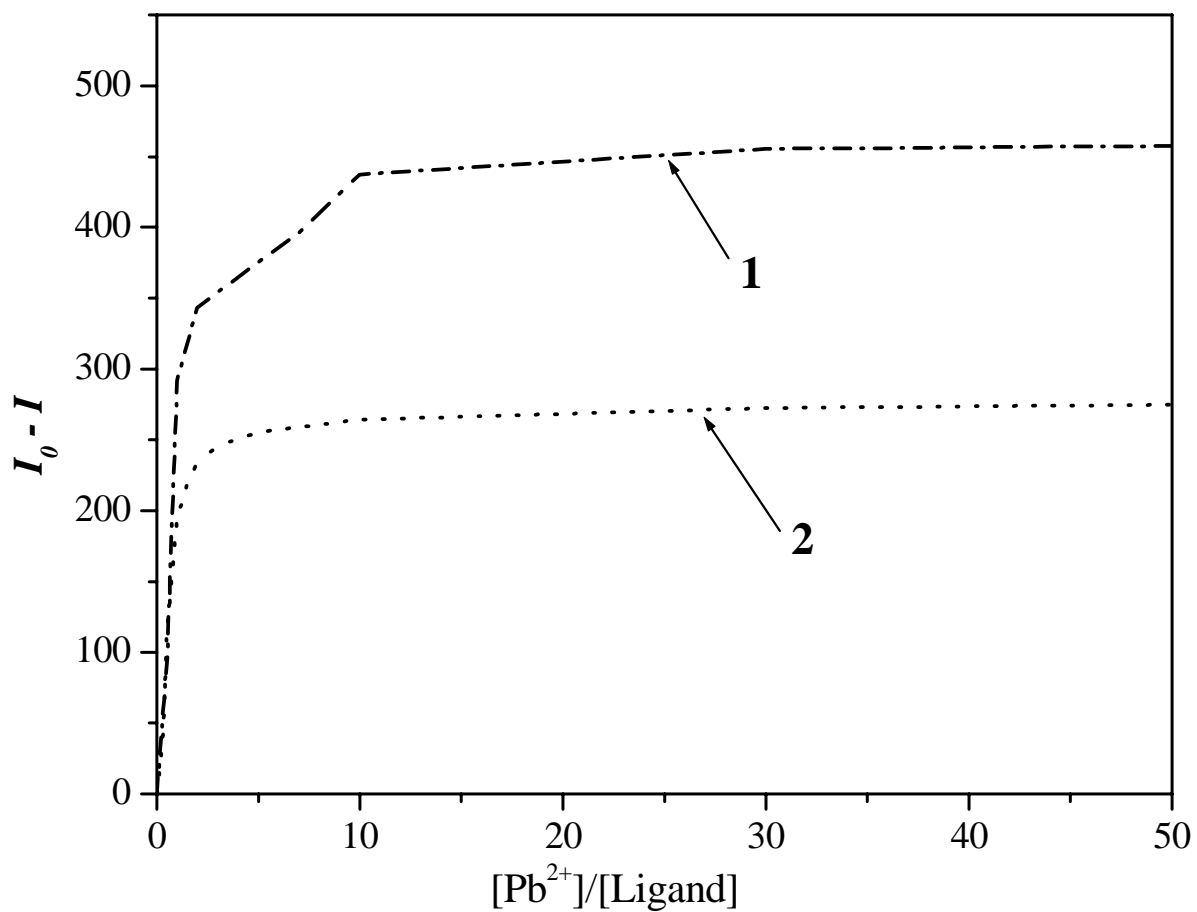


Figure S1. Fluorescence intensity changes ($I_0 - I$) of **1** and **2** with increasing Pb^{2+} ion concentrations in acetonitrile. I_0 : fluorescence emission intensity of uncomplexed **1** and **2**; I : fluorescence emission intensity of metal ion-complexed **1** and **2**

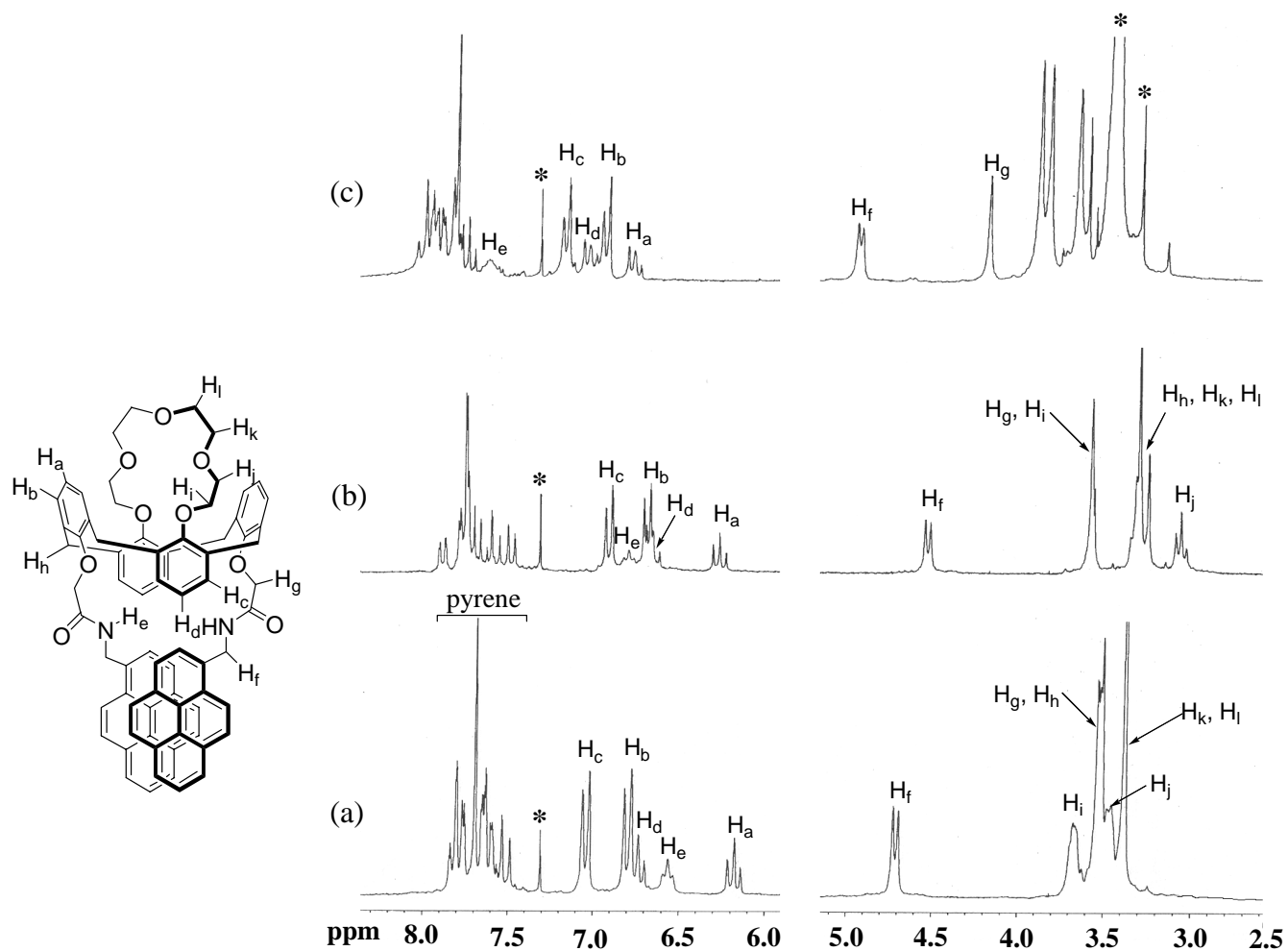


Figure S2. Metal ion-induced chemical shift changes of **1** in $\text{CD}_3\text{CN}/\text{CDCl}_3$ (4/1, v/v). (a): **1** only, (b): **1** + 10 equiv. of K^+ClO_4^- , (c): **1** + 10 equiv. of $\text{Pb}^{2+}(\text{ClO}_4^-)_2$. * denotes NMR solvent peaks.

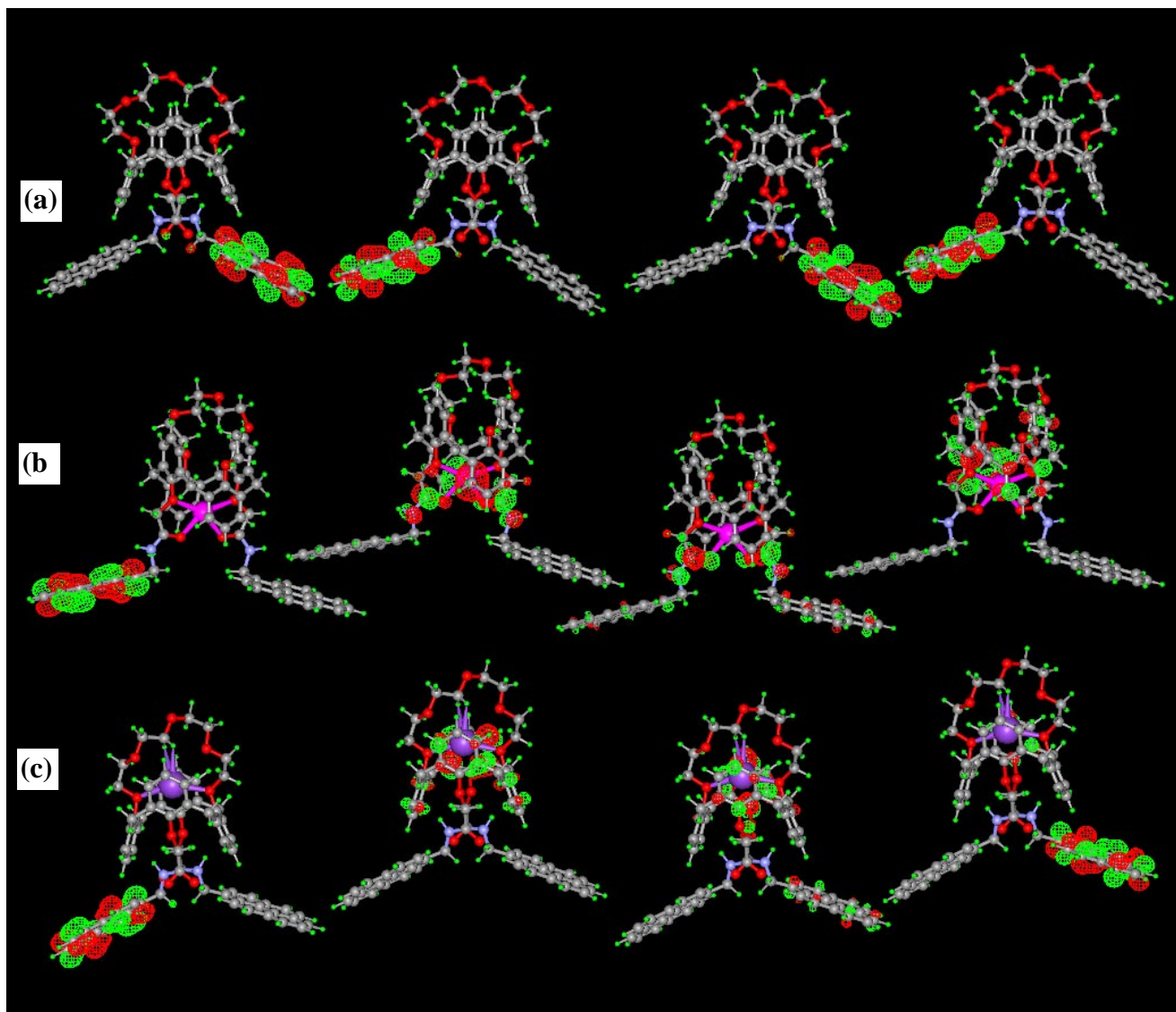


Figure S3. Frontier molecular orbitals (HOMO, LUMO, LUMO2, and LUMO3) of (a) **1**, (b) **1•Pb²⁺**, and (c) **1•K⁺**.