

Supporting Information

Study of the host-guest interaction between N,N' -bis[4-(dimethylaminophenyl)methyl]butane-1,4-diamine and the cucurbit[n]urils ($n = 6, 7$)

Zhiyou Xiao,^a Yang Zhou,^b Weitao Xu,^c Timothy J. Prior,^d Bing Bian,^e Carl Redshaw,^{d*} Zhu Tao,^c and Xin Xiao,^{c*}

^a *School of Chemical Engineering, Guizhou Institute of Technology, Guiyang 550003, China*

^b *College of Chemistry, Chemical Engineering and Materials Science, Shandong Normal University, Jinan 250014, China*

^c *Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang 550025, China*

^d *Department of Chemistry & Biochemistry, University of Hull, Hull HU6 7RX, U.K.*

^e *College of Chemistry and Environmental Engineering, Shandong University of Science and Technology, Qingdao 266590, China.*

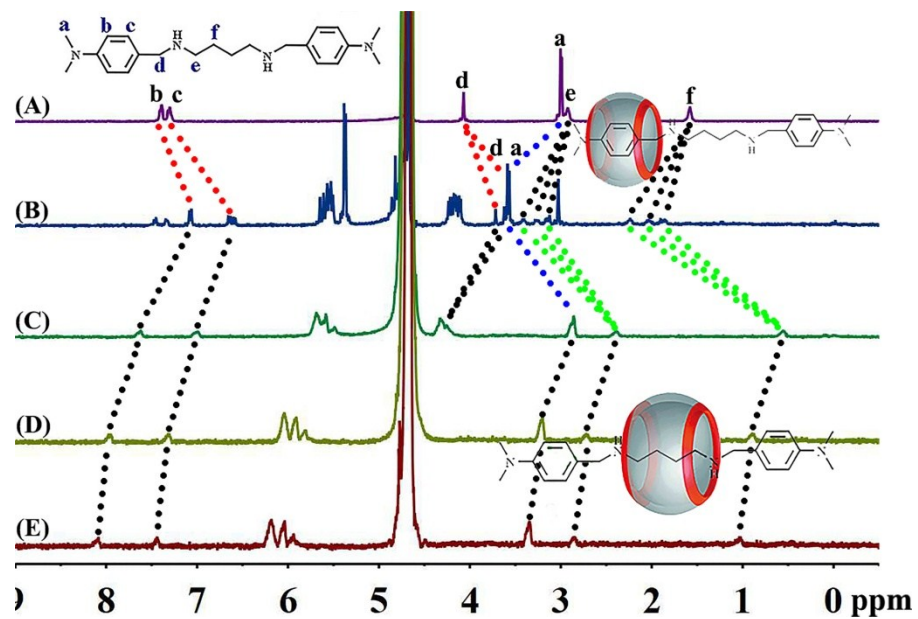


Figure S1 Interaction of **G** and Q[6] (D₂O): ¹H NMR spectra of **G** (ca. 2 mM) in the absence of Q[6] (A); in the presence of 1.949 equiv. of Q[6] at 20°C (B); in the presence of 1.949 equiv. of Q[6] at 40°C (C); in the presence of 1.949 equiv. of Q[6] at 60°C (D); in the presence of 1.949 equiv. of Q[6] at 80°C (E).

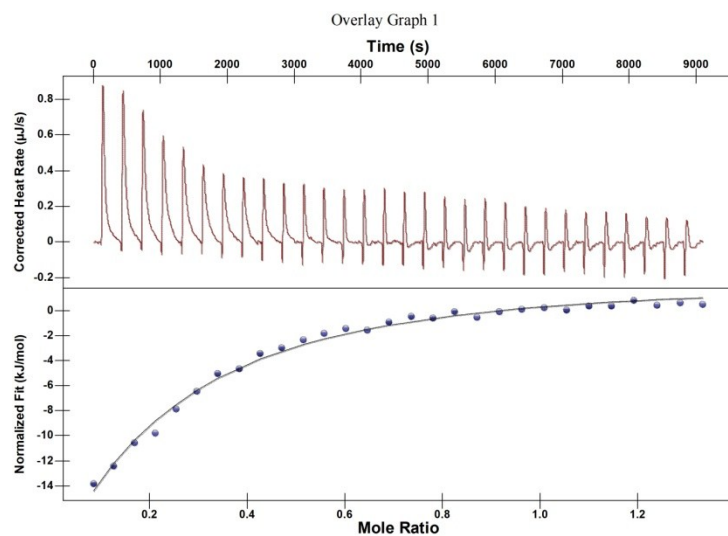


Figure S2. ITC data for the binding of Q[6] with G in aqueous solution at 298.15 K.

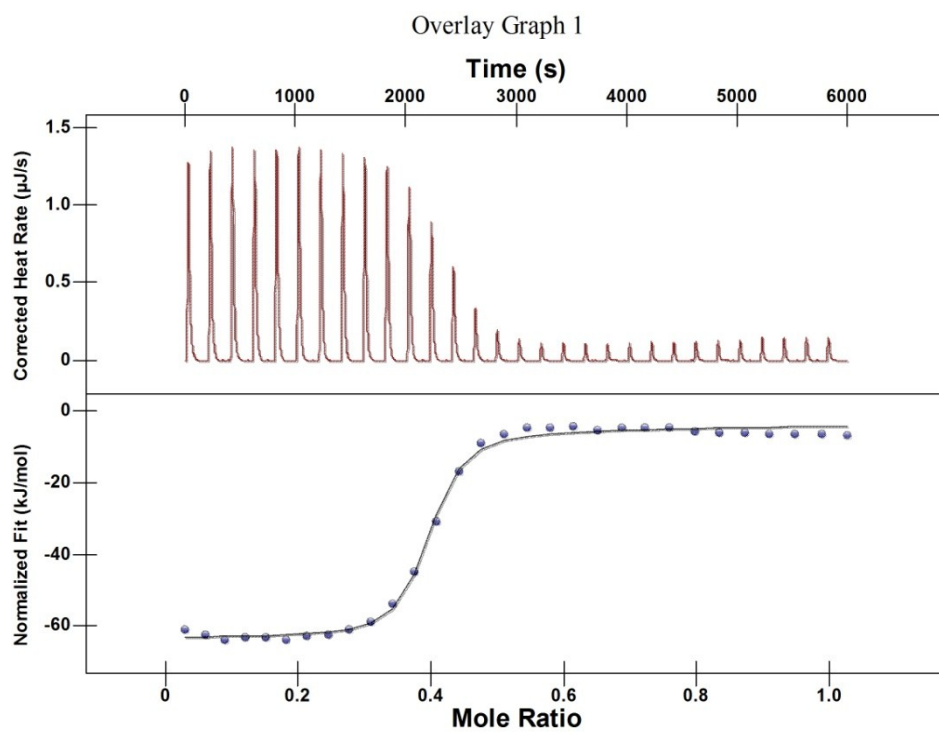


Figure S3. ITC data for the binding of Q[7] with G in aqueous solution at 298.15 K.

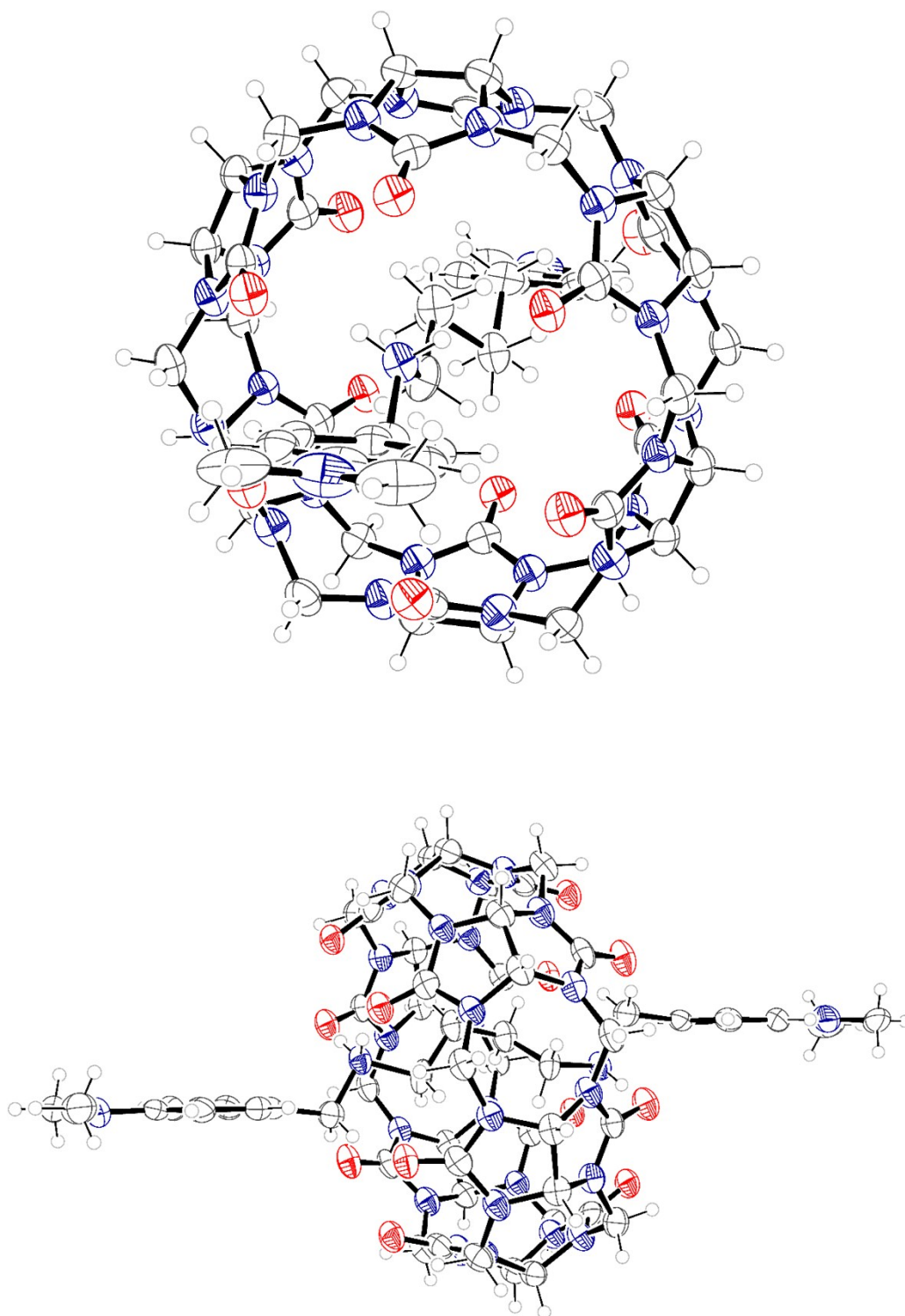


Figure S4. Alternative views of the molecular structure of **1**.

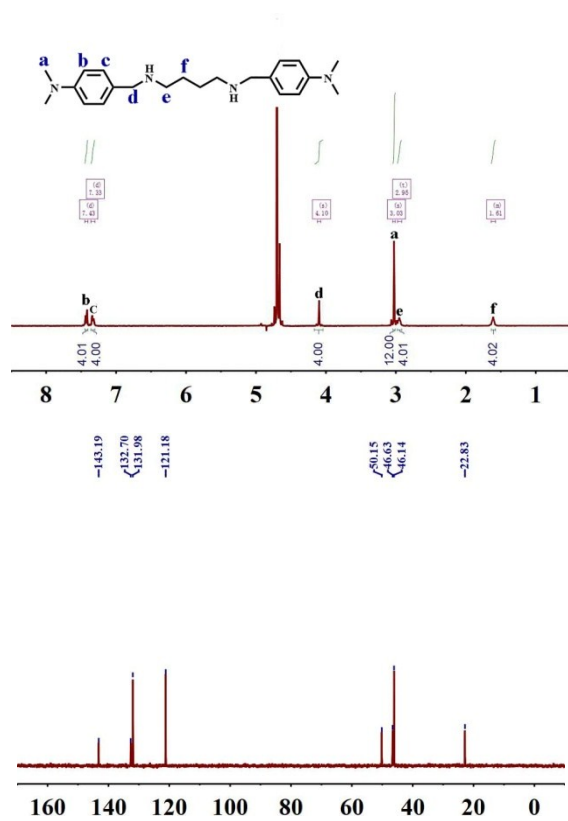


Figure S5. ^1H and ^{13}C NMR spectra of G.