

# Conformational aspects of the *O*-acetylation of *C*-tetraphenylcalixpyrogallol[4]arene

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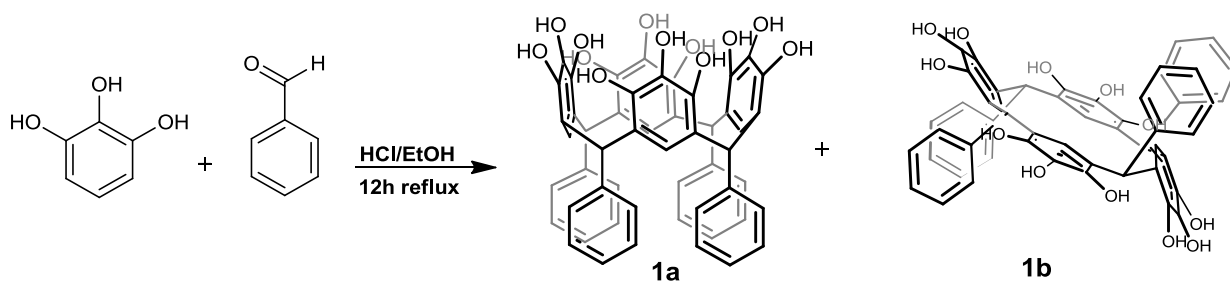
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## Synthesis of tetraphenylpyrogallol[4]arene



Scheme S1. Synthesis of C-tetra(phenyl)pyrogallol[4]arene

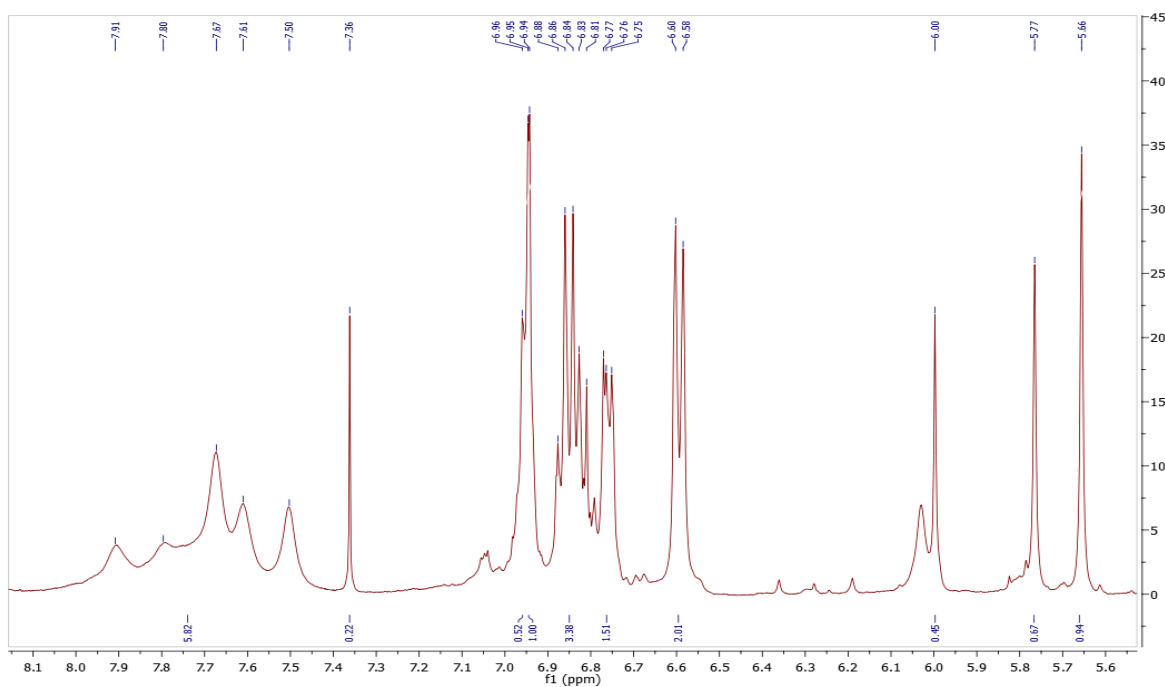


Figure S1. <sup>1</sup>H-NMR spectrum - DMSO-*d*<sub>6</sub> conformational mix (**1a** and **1b**)

## 1. Crown conformer

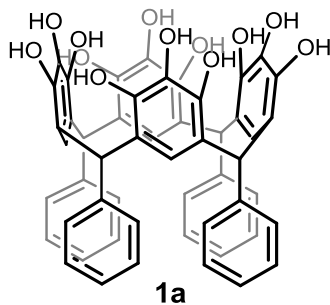


Figure S2. Tetra(phenyl)pyrogallol[4]arene (*crown*)(**1a**)

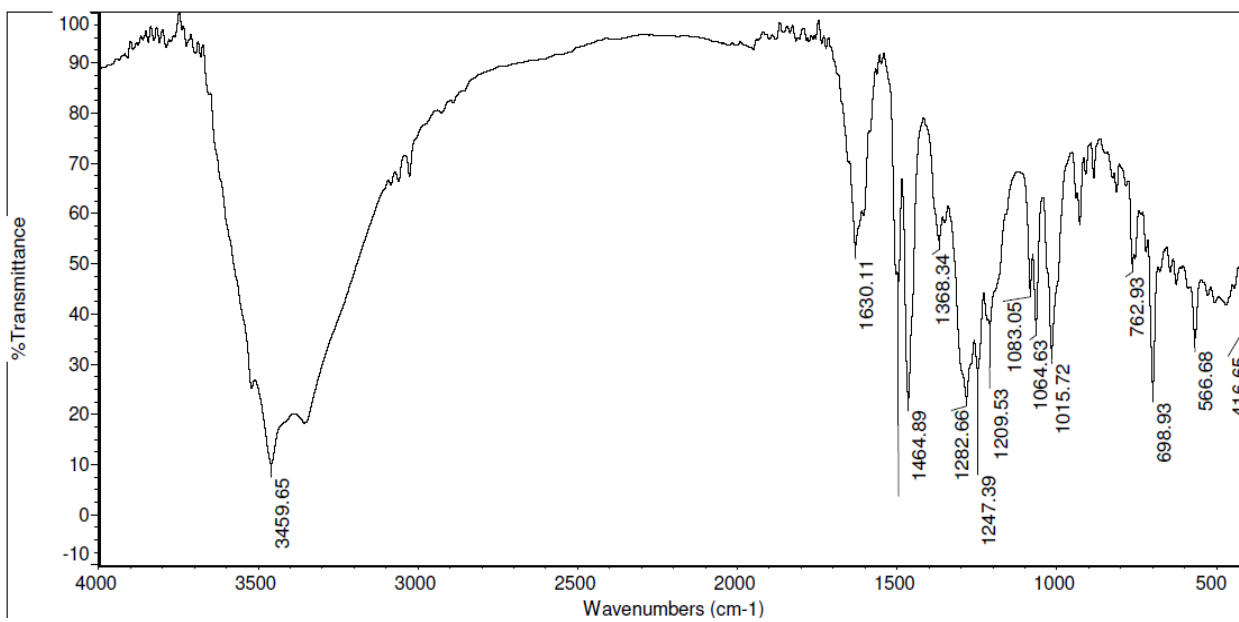


Figure S3. IR Spectrum of compound **1a**

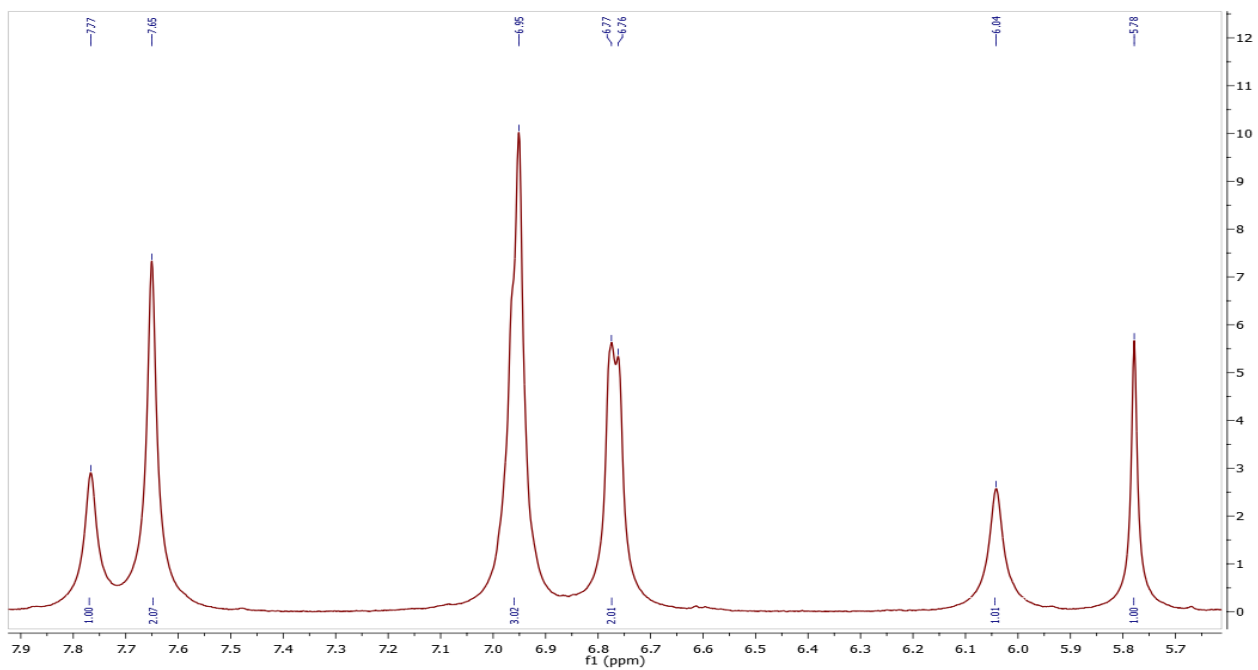


Figure S4.  $^1\text{H-NMR}$  spectrum  $\text{DMSO-}d_6$  of boat conformer(1a)

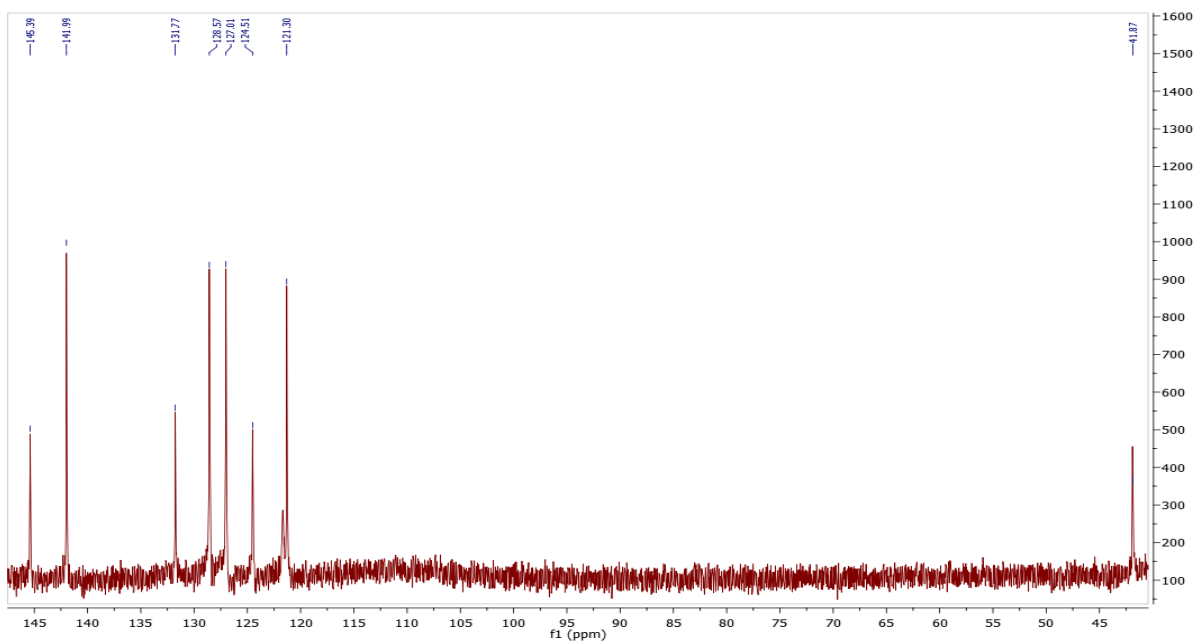


Figure S5. Spectrum  $^{13}\text{C-NMR}$  - $\text{DMSO-}d_6$  boat conformer(1a)

## 2. Chair conformer

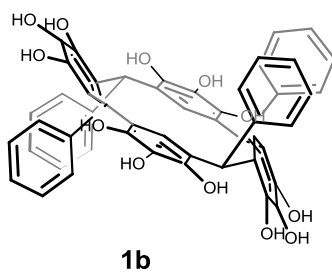


Figure S6. Tetra(phenyl)pyrogallo[4]larene (*chair*)(**1b**)

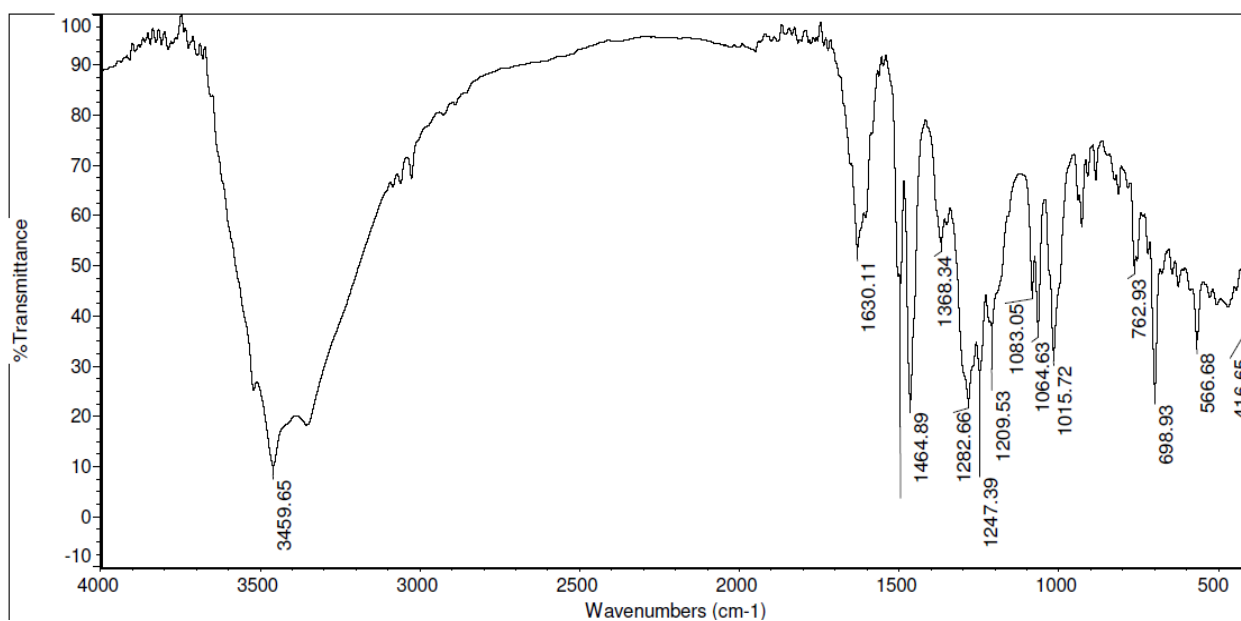


Figure S7. IR Spectrum of compound **1b**

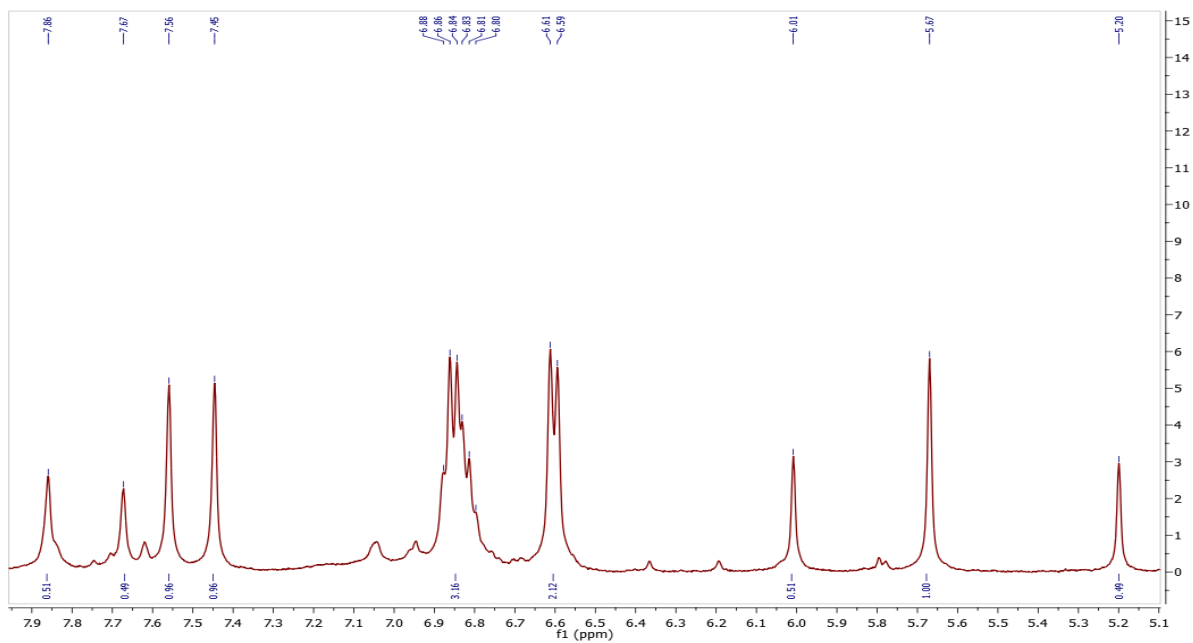


Figure S8. <sup>1</sup>H-NMR of chair conformer(1b)

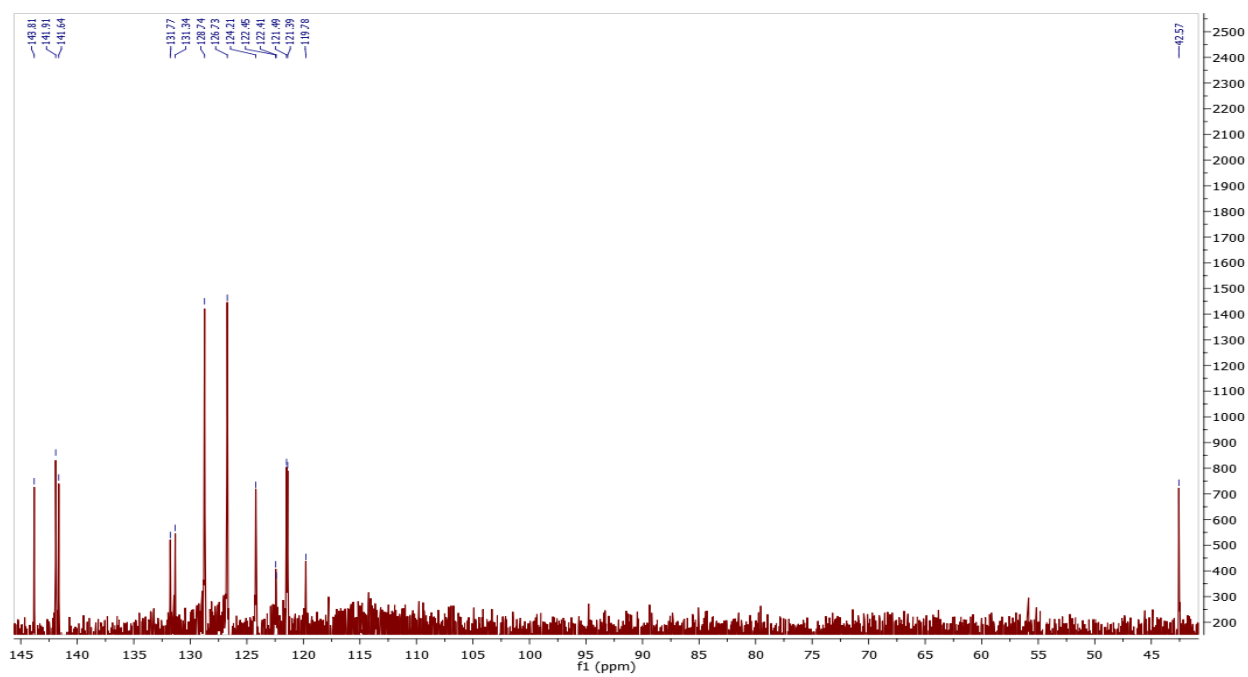
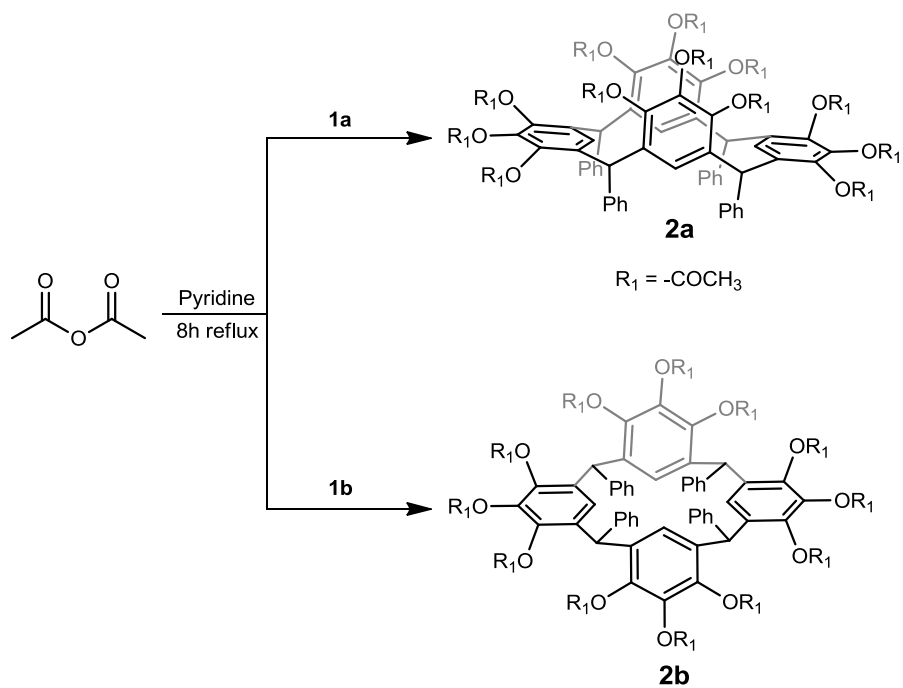


Figure S9. <sup>13</sup>C-NMR of chair conformer(1b)

## Synthesis of the acylated phenylpyrogallol[4]arene



Scheme S2. Synthesis of C-tetraphenylpyrogallol[4]arene acetylated (**2a** and **2b**)

### 1. Boat conformer

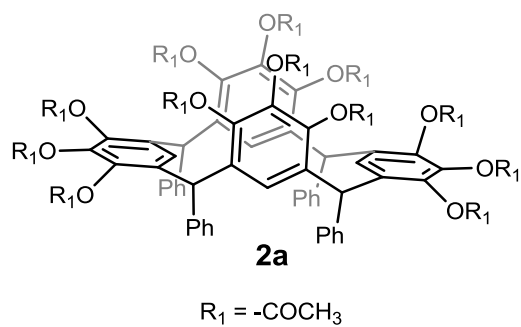


Figure S10. Dodecaacetyl-tetra(phenyl)pyrogallol[4]arene (*Boat*)(**2a**)

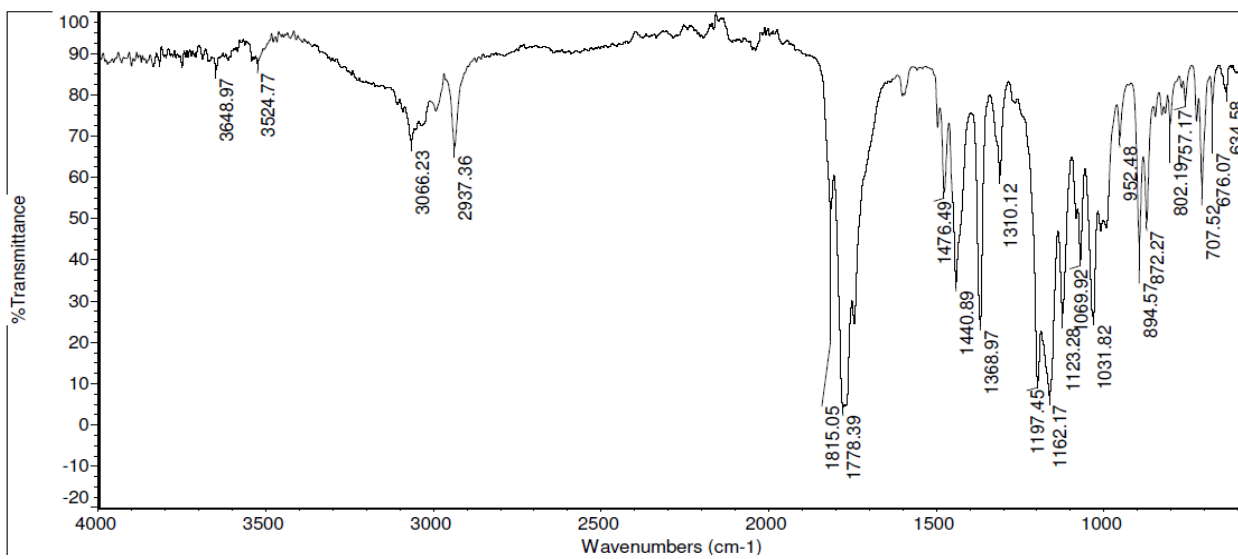


Figure S11. IR spectrum of compound 2a

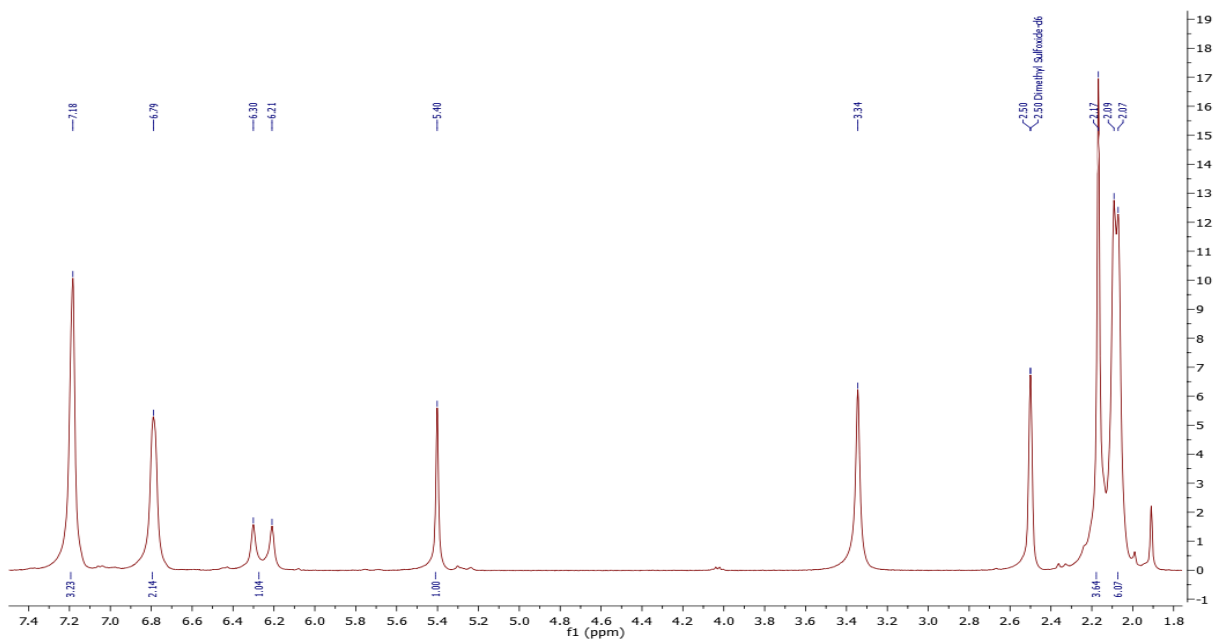


Figure S12. <sup>1</sup>H-NMR spectrum boat isomer (2a)



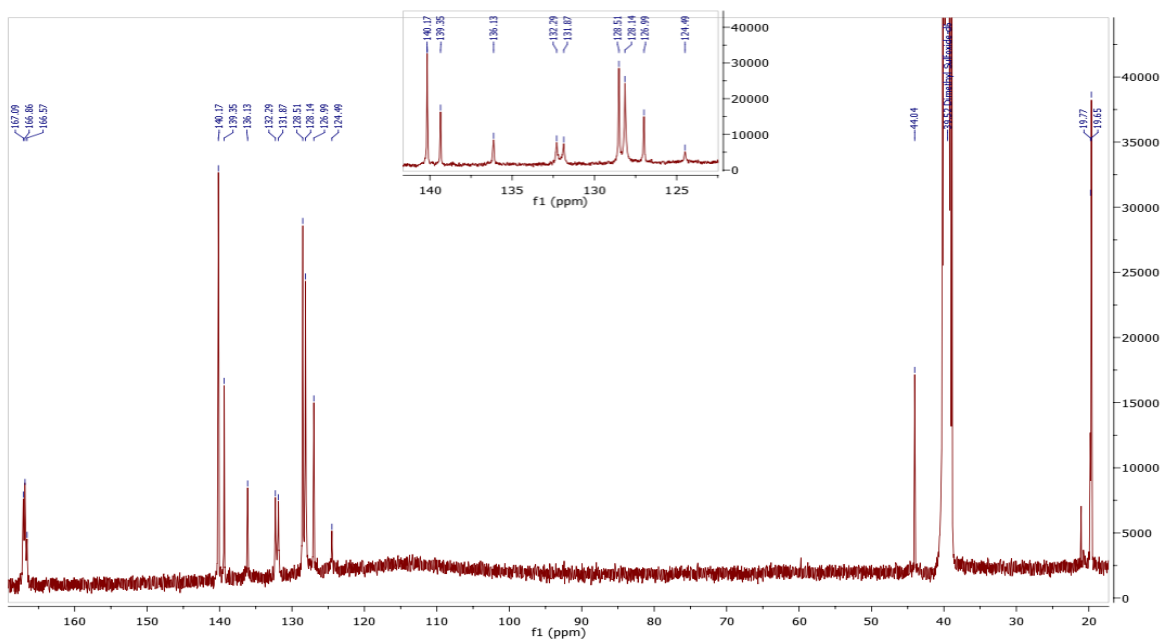


Figure S13.  $^{13}\text{C}$ -NMR boat conformer(2a)

## 2. Chair isomer

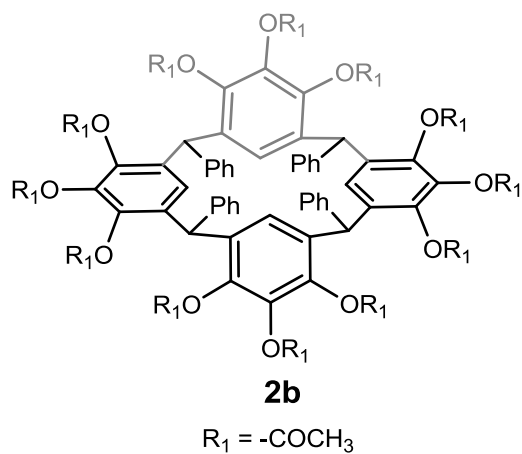


Figure S14. Dodecaacetyl-tetra(phenyl)pyrogallol[4]arene (*chair*) (2b)

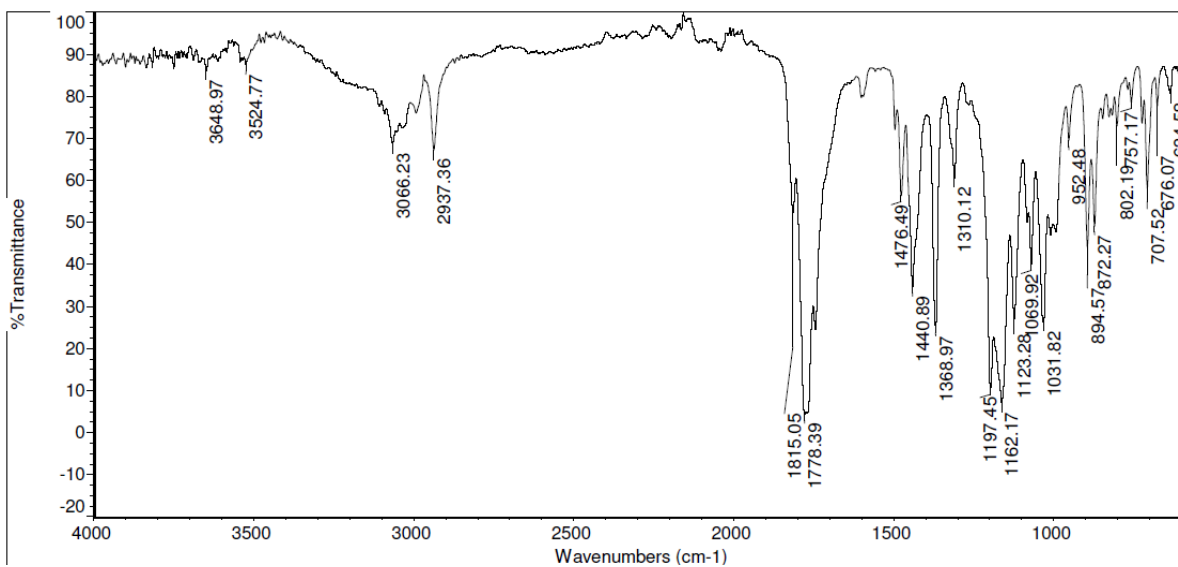


Figure S15. IR of compound **2b**

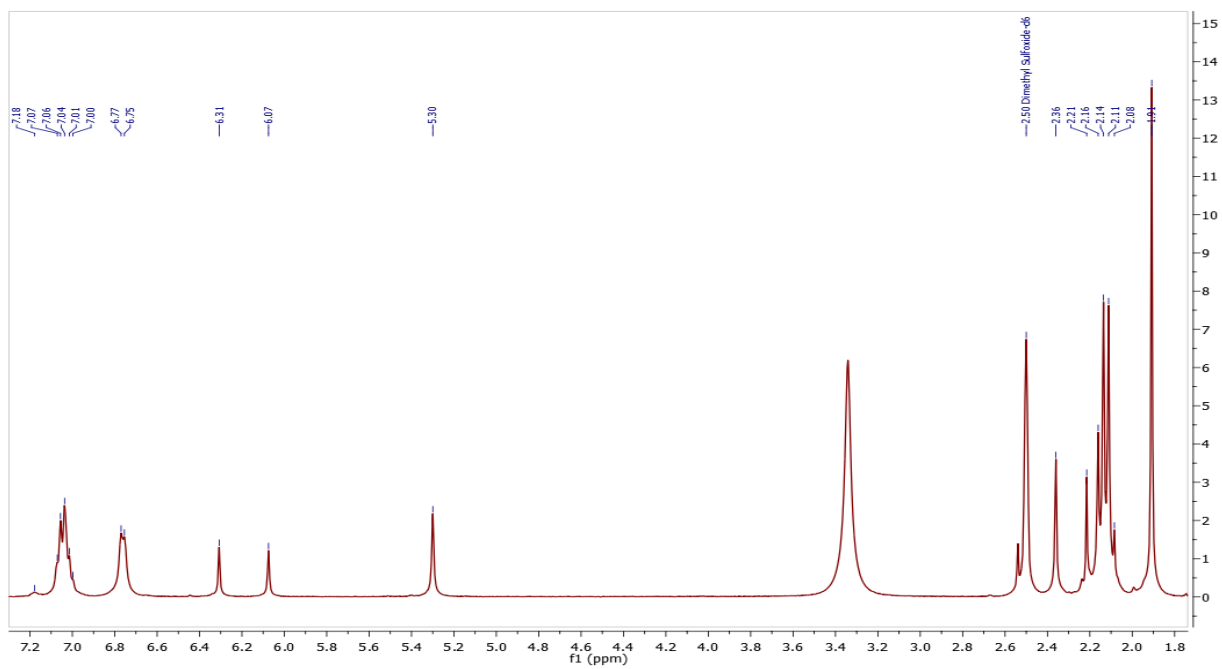


Figure S16. <sup>1</sup>H-NMR spectrum of chair isomer (**2b**)

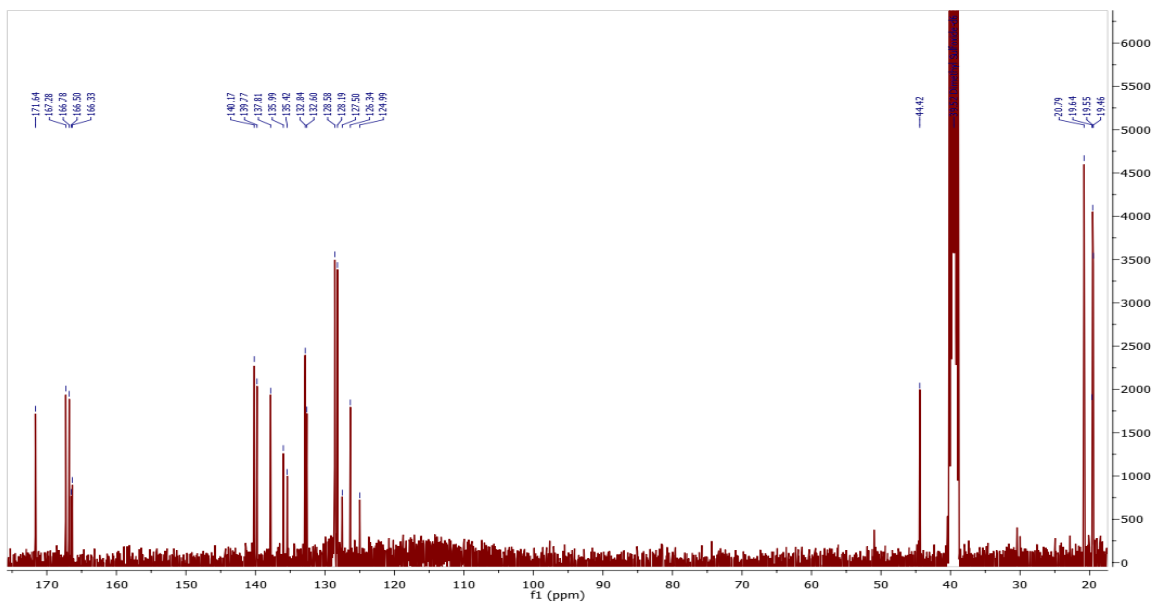


Figure S17.  $^{13}\text{C}$ -NMR spectrum of chair isomer(2b)