

Supplementary Information

Reactions of thiocalix[4]arene 1,3-bistriflate: formation of thiocalix[2]phenoxathiins –structural and complexation studies

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and Paris E. Georghiou^{1*}

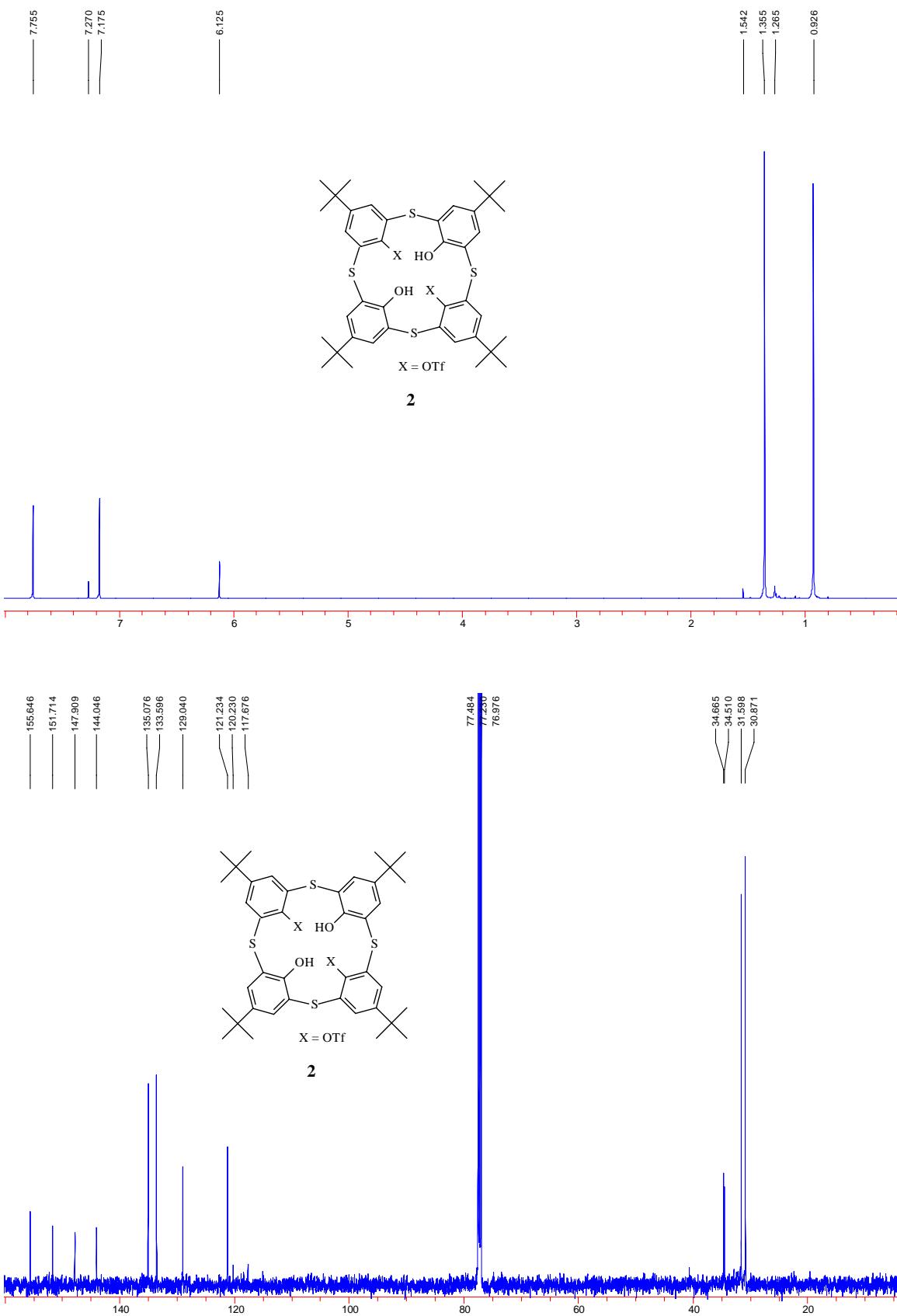
1. Department of Chemistry, Memorial University of Newfoundland, St. John's, Newfoundland, NL, Canada A1B 3X7.

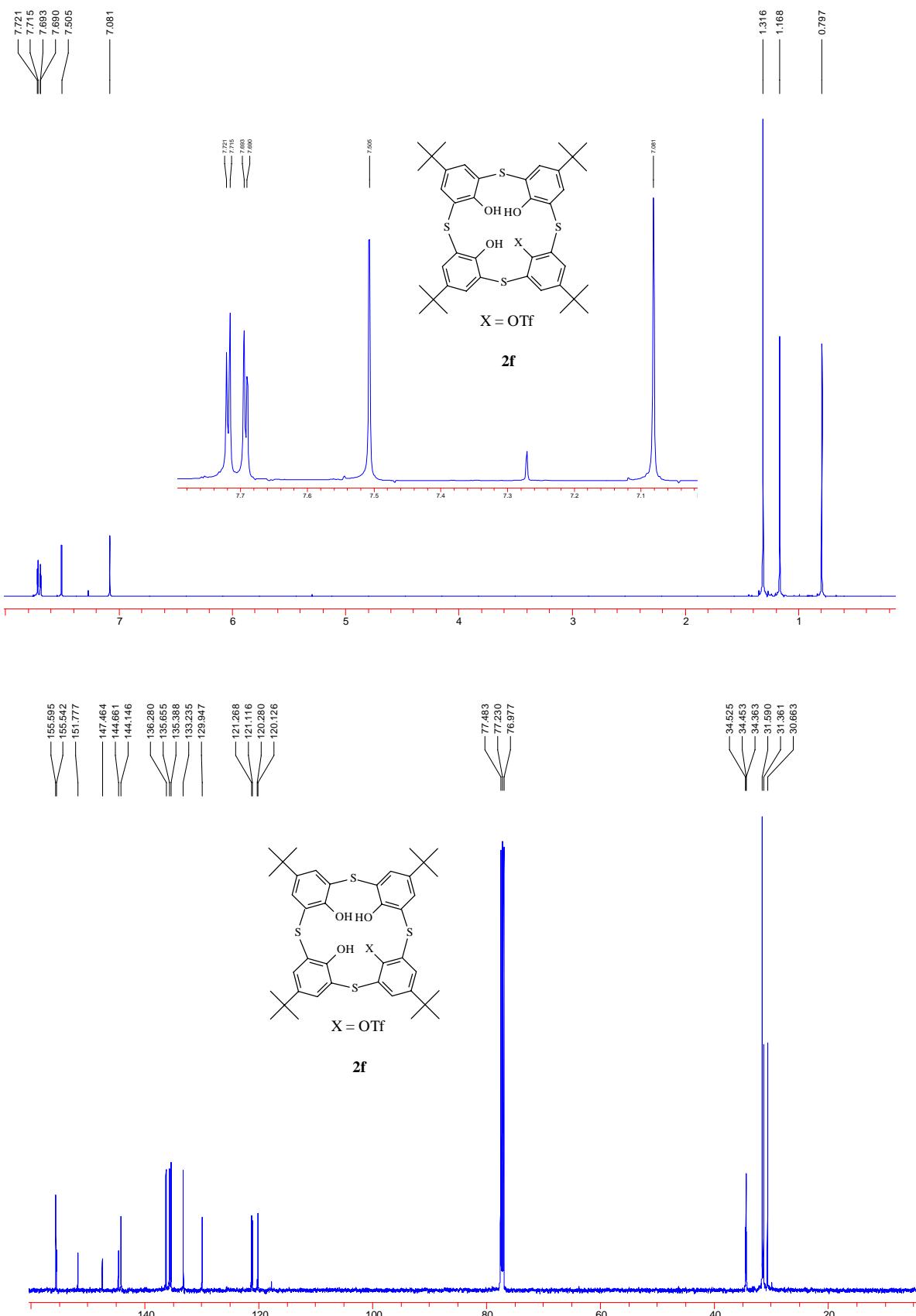
2. CREAIT, Memorial University of Newfoundland, St. John's, Newfoundland, NL, Canada A1B 3X7

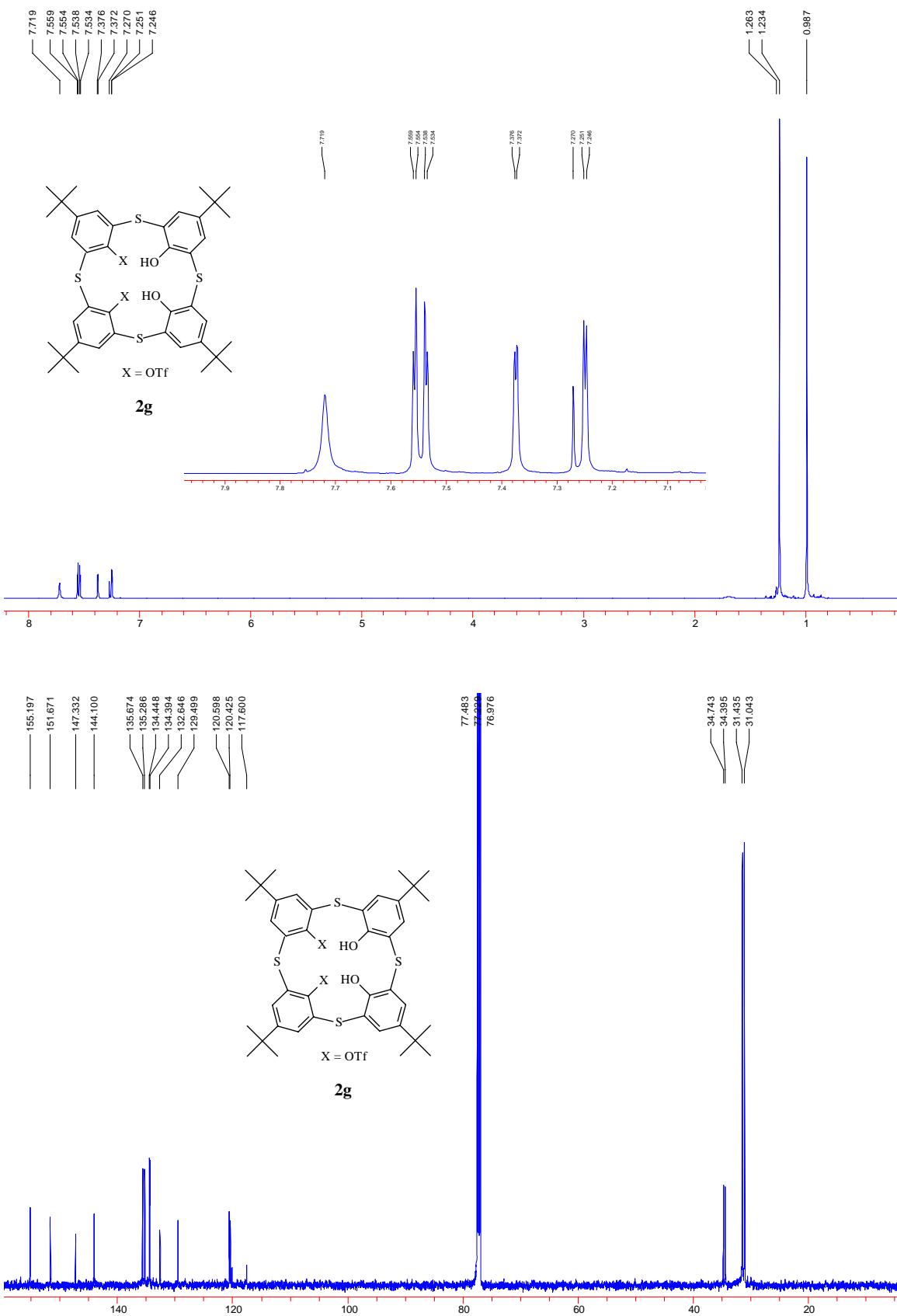
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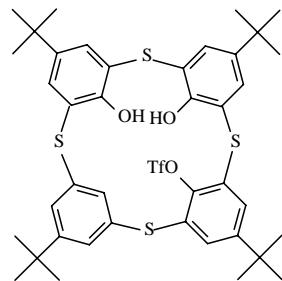
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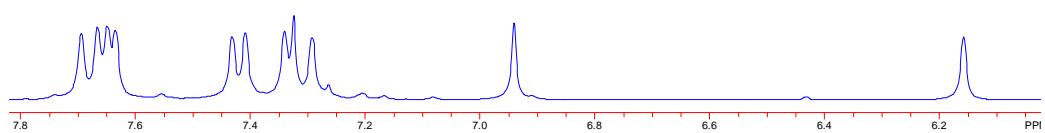
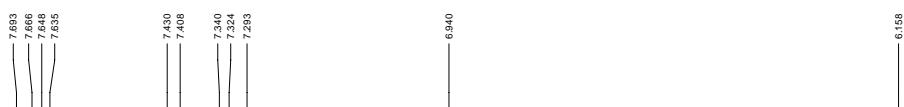
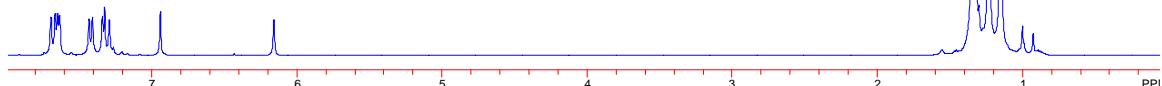


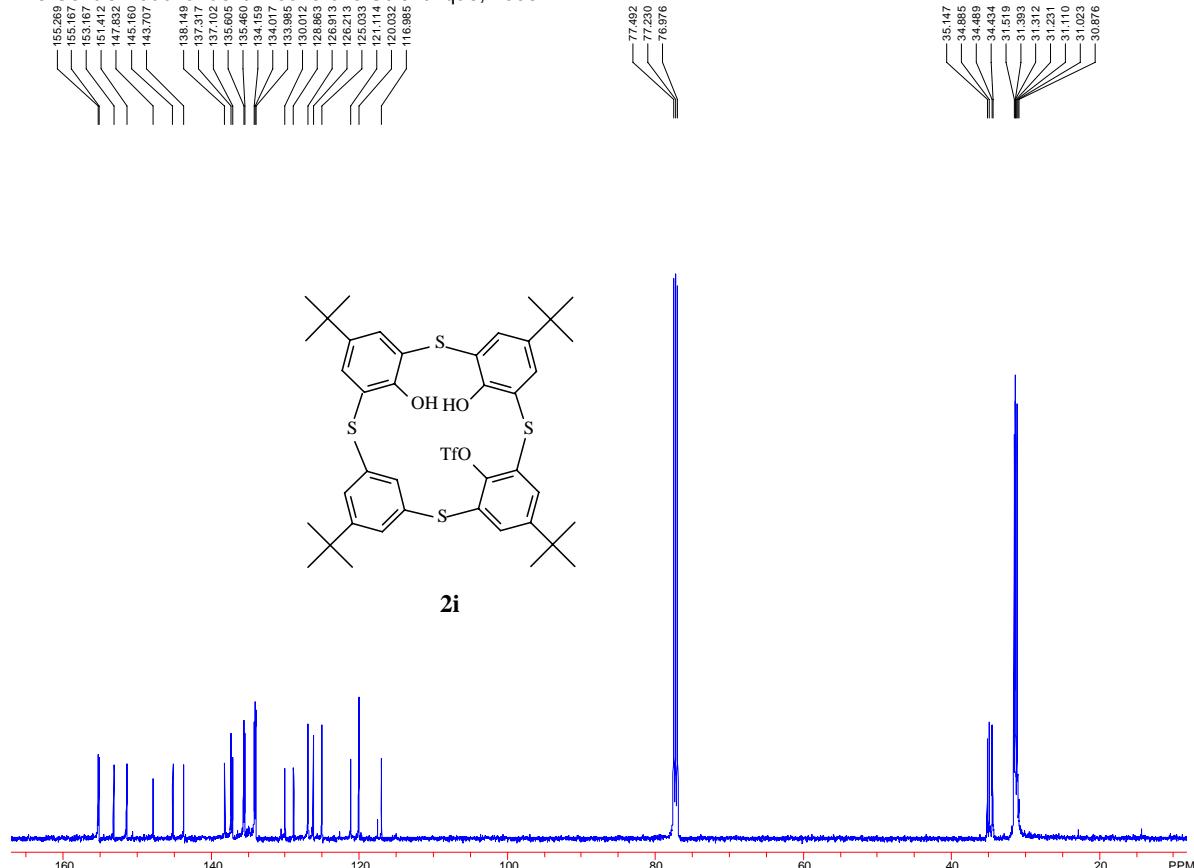


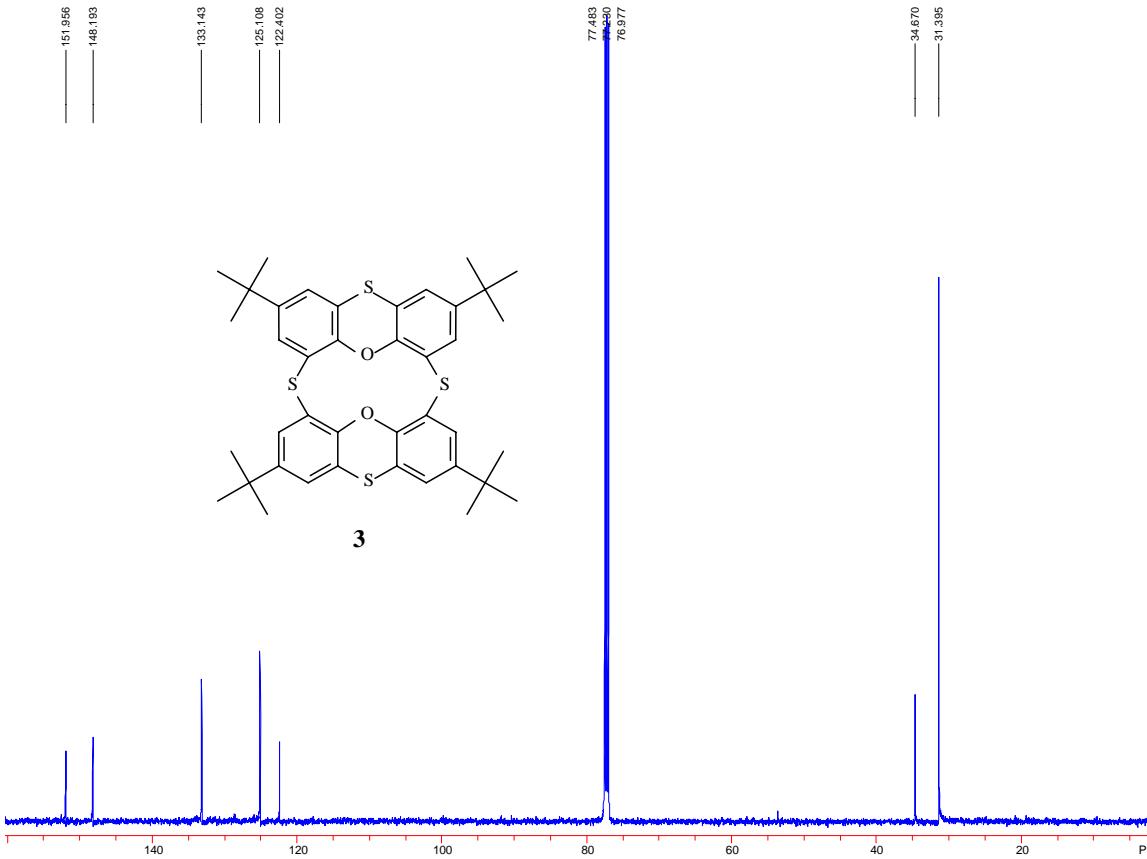
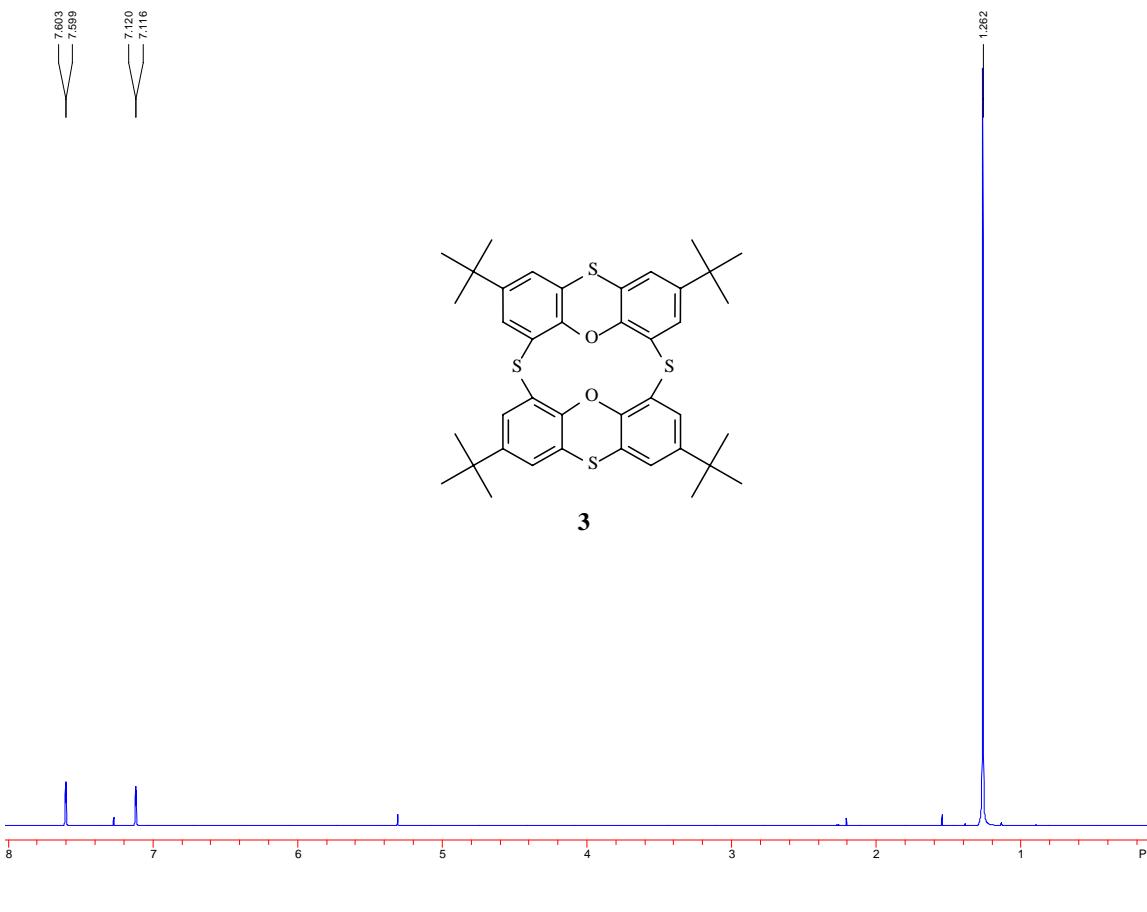


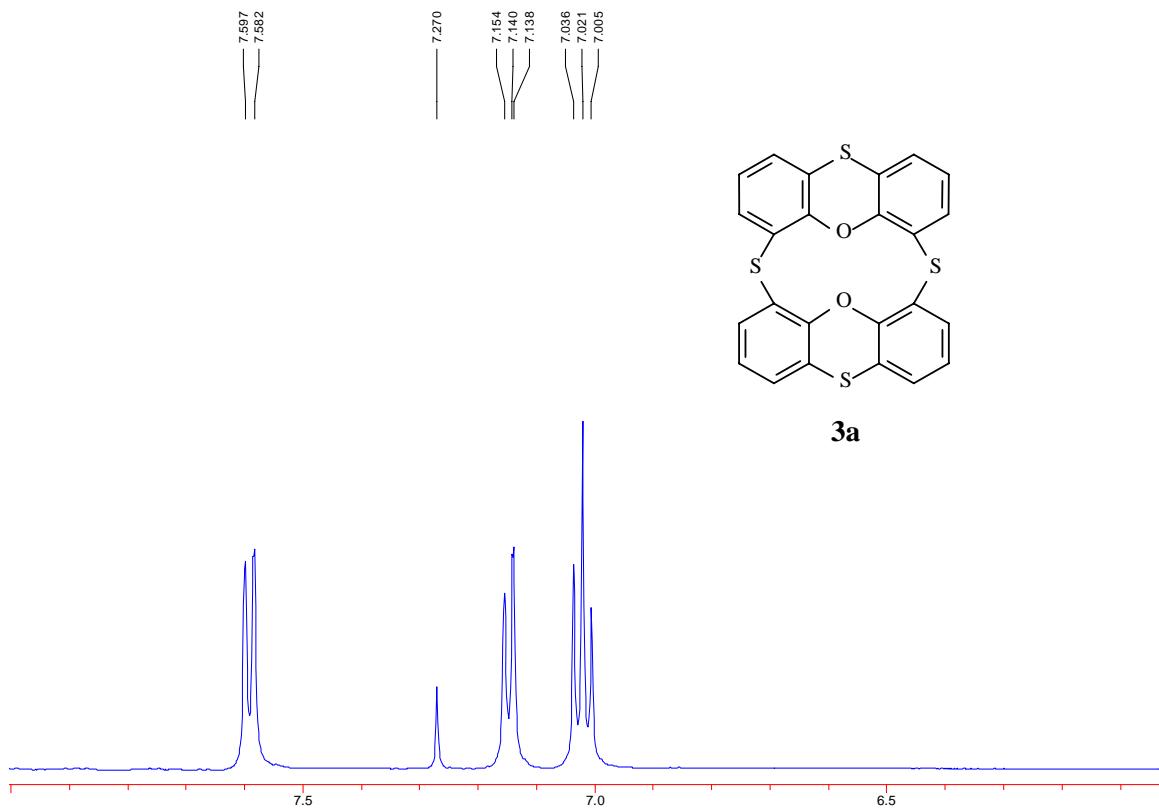


2i

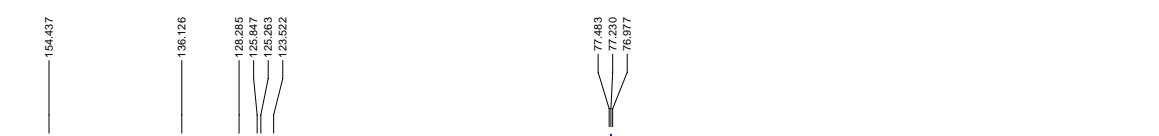




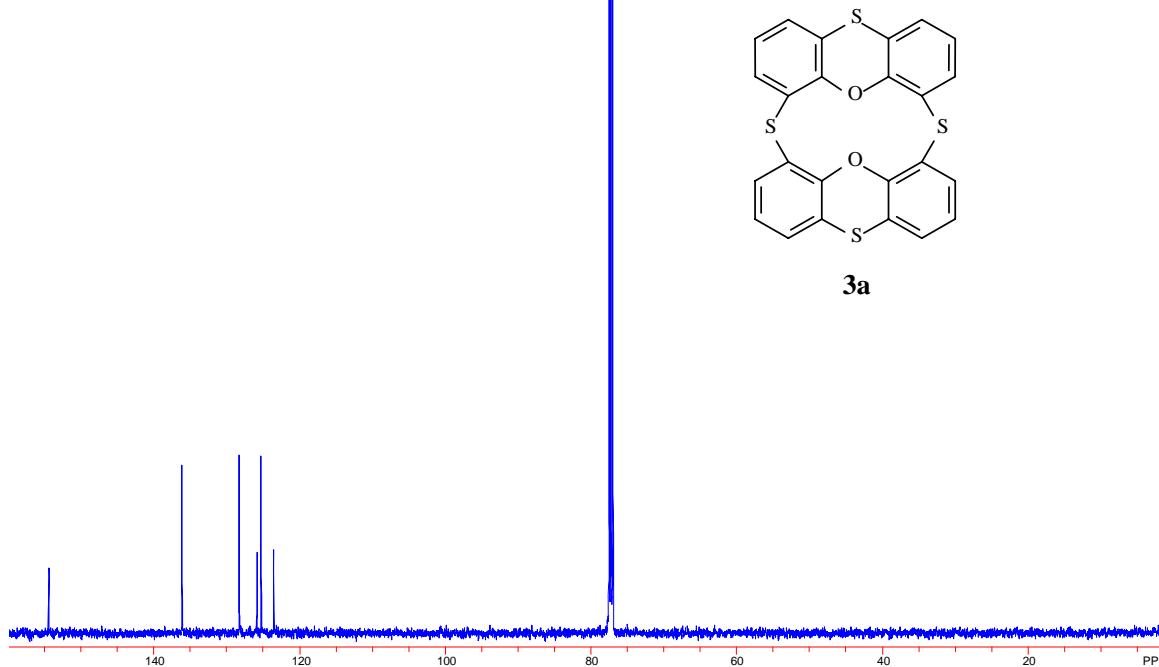


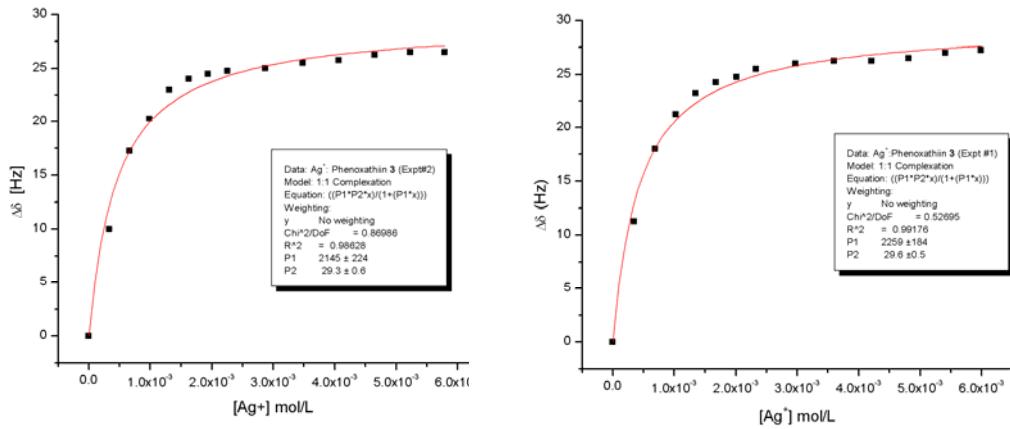


3a

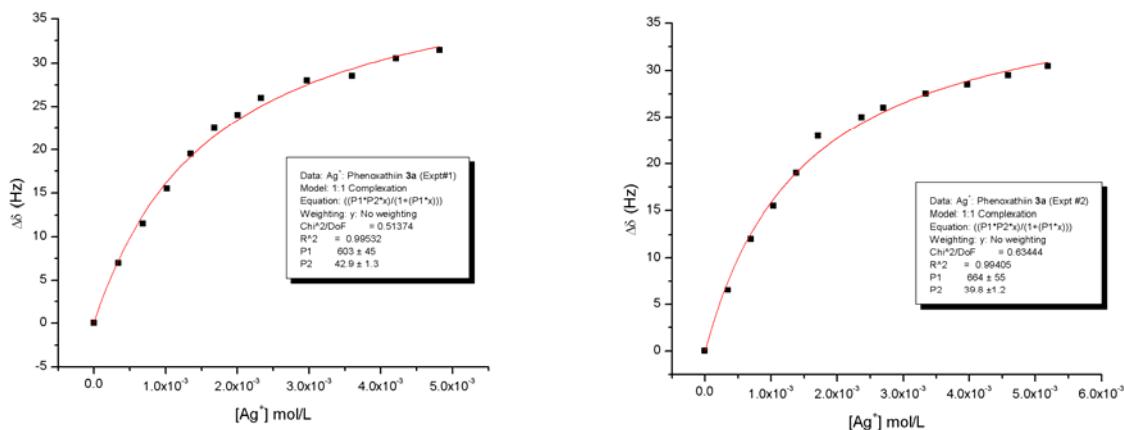


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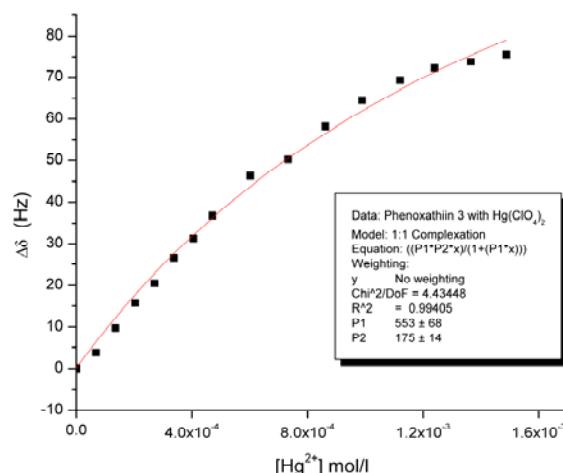
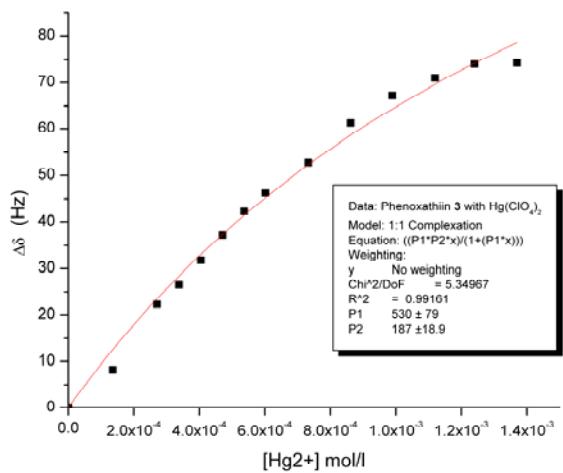




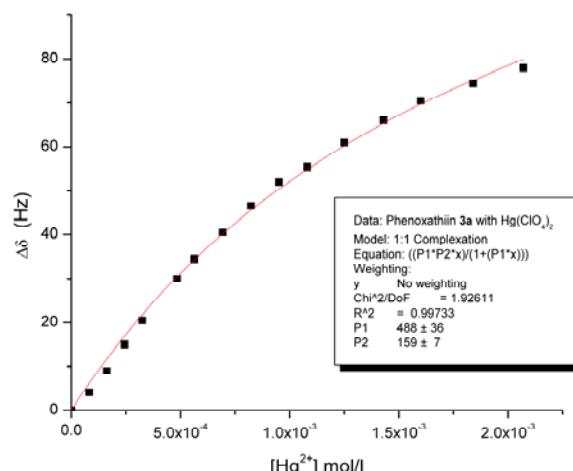
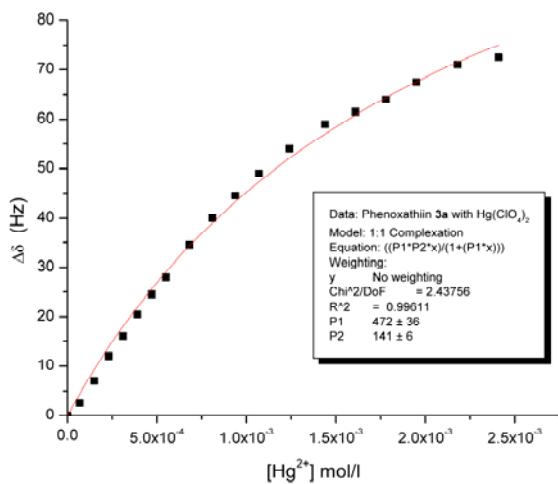
Binding isotherms from repeat experiments of titrations of aliquots of $[\text{AgO}_2\text{CCF}_3]$ added to solutions of *tert*-butylbisphenoxyxathiin **3** in 1:9 CDCN:CDCl_3 (v/v).



Binding isotherms from repeat experiments of titrations of aliquots of $[\text{AgO}_2\text{CCF}_3]$ added to solutions of bisphenoxyxathiin **3a** in 1:9 CDCN:CDCl_3 (v/v).



Binding isotherms from repeat experiments of titrations of aliquots of $[Hg(ClO_4)_2]$ added to solutions of bisphenoxathiin **3** in 1.5:9 D₃COD:CDCl₃ (v/v).



Binding isotherms from repeat experiments of titrations of aliquots of $[Hg(ClO_4)_2]$ added to solutions of bisphenoxathiin **3a** in 1.5:9 D₃COD:CDCl₃ (v/v).