Electronic Supplemental Information

Self-assembly of a family of suprametallomacrocycles: revisiting an o-carborane bisterpyridyl building block

James M. Ludlow III,a A. N. Masato Tominaga,d Yoshiki Chujo,d Anthony Schultz,b Xiaocun Lu,a Tingzheng Xie,a Kai Gao,a Charles N. Moorefield,c Chrys Wesdemiotis,*a,b and George R. Newkome*a,b

aDepartment of Polymer Science, bDepartment of Chemistry, and cThe Maurice Morton Institute for Polymer Science The University of Akron, Akron, OH 44325-4717 USA Tel: 330-972-6458
dDepartment of Polymer Chemistry, Graduate School of Engineering, Kyoto University, Katsura, Nishikyo-ku, Kyoto, 615-8510, Japan. Tel: +81-75-383-2604

E-mail: newkome@uakron.edu, wesdemiotis@uakron.edu

Table of Contents

1. 2D NMR Spectra .......................................................................................................................... S2
2. ESI-MS and ESI-TWIM-MS, data .......................................................................................... S5
3. Isotope patterns ........................................................................................................................ S7
4. van’t Hoff plot and table .......................................................................................................... S10
1. 2D NMR Spectra

Figure S1. COSY for bisterpyridyl o-carborane (1)
Figure S2. COSY for ZnC2-C3 mixture, aromatic region

Figure S3. COSY for FeC2, aromatic region
Figure S4. COSY for FeC3, aromatic region

Figure S5. NOESY for FeC3, aromatic region

NOESY
M(II) = Fe
2. ESI-MS and ESI-TWIM-MS data

Figure S6. ESI-MS plot of FeC3

Figure S7. ESI-TWIM-MS plot (m/z vs. drift time) for FeC3 at a traveling wave velocity of 350 m/s and a traveling wave height of 7.5V.
Figure S8. ESI-TWIM-MS plot (m/z vs. drift time) for ZnC2 at a traveling wave velocity of 350 m/s and a traveling wave height of 7.5V
3. Isotope patterns

ZnC₄ 3+

3+ Theoretical

3+ Experimental

Figure S9. Isotope pattern for ZnC₄ charge state 3+. 
Figure S10. Isotope patterns for ZnC3 charge states 4+ and 5+.
Figure S11. Isotope patterns for ZnC2 charge states 2+, 3+, and 4+.
4. van’t Hoff plot and table

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Figure S12. Column 2 contains temperature values calculated from the temperature calibration curve’s regression equation.

Figure S13. van’t Hoff plot
Figure S14. Temperature calibration curve.