

Electronic Supplemental Information

**Self-assembly of a family of suprametallomacrocycles: revisiting
an *o*-carborane *b*isterpyridyl 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

^d Department of Polymer Chemistry, Graduate School of Engineering, Kyoto University,
Katsura, Nishikyo-ku, Kyoto, 615-8510, Japan

Tel: +81-75-383-2604

E-mail: chujo@chujosynchem.kyoto-u.ac.jp

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1. 2D NMR Spectra

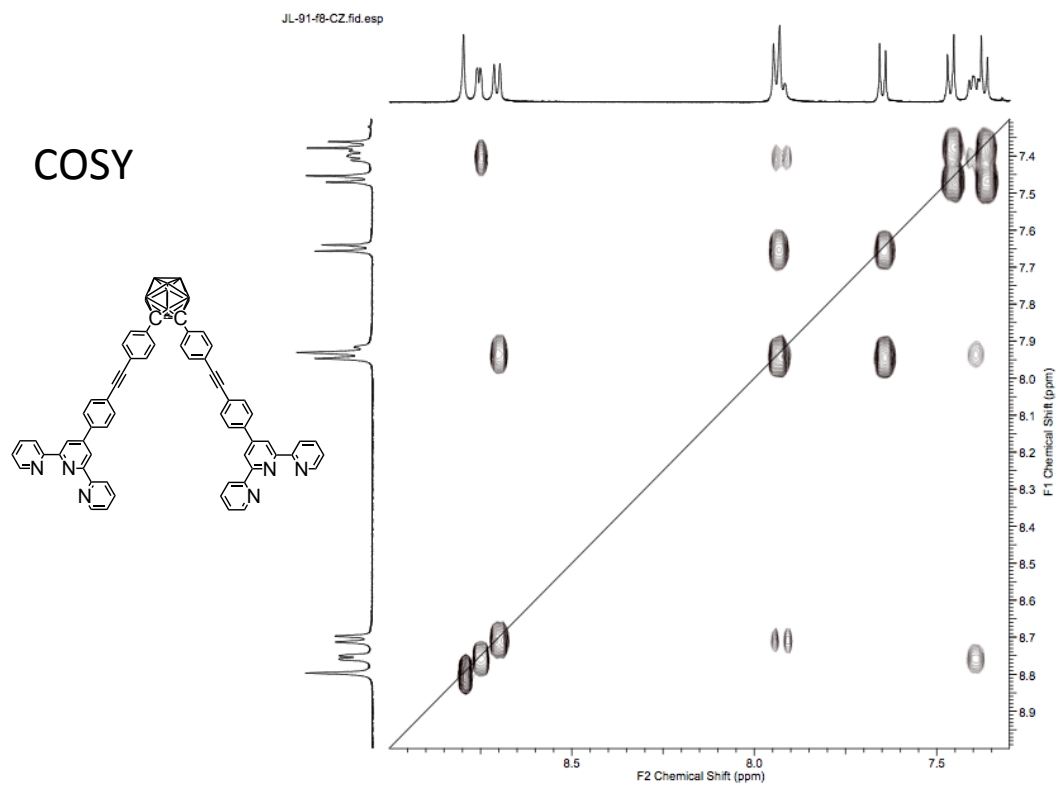


Figure S1. COSY for *bisterpyridyl o-carborane* (**1**)

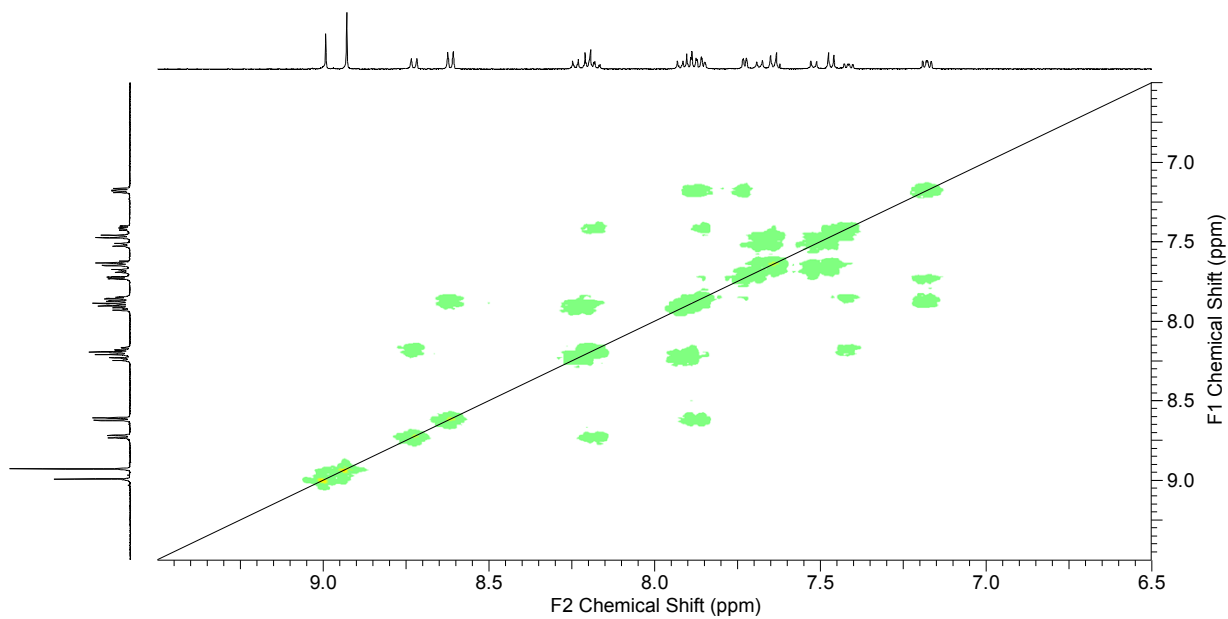


Figure S2. COSY for ZnC2-C3 mixture, aromatic region

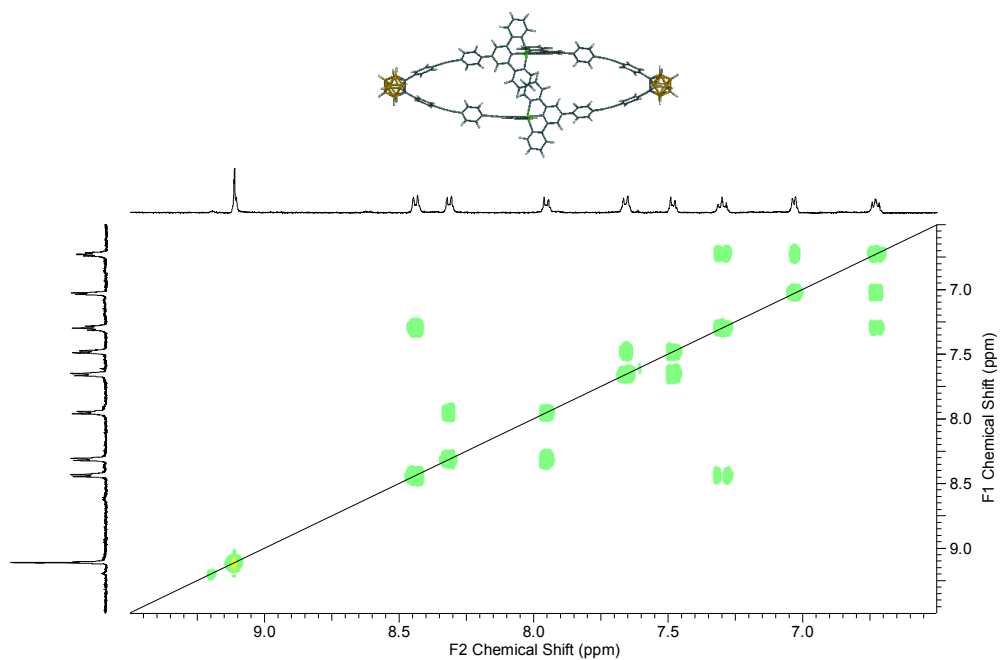


Figure S3. COSY for FeC2, aromatic region

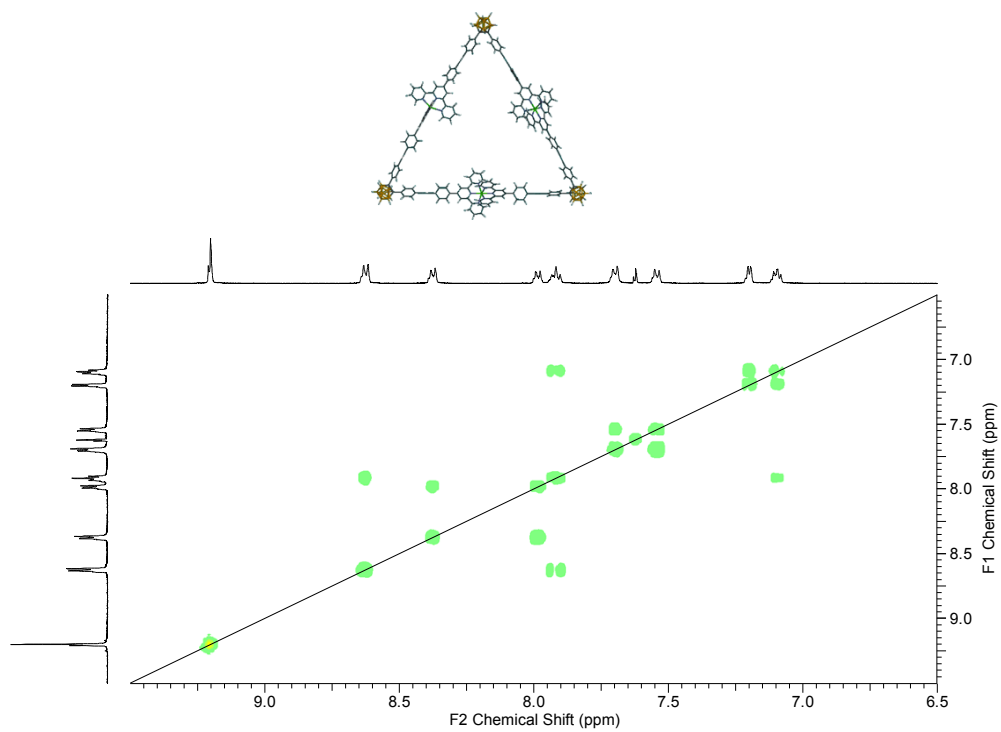


Figure S4. COSY for FeC3, aromatic region

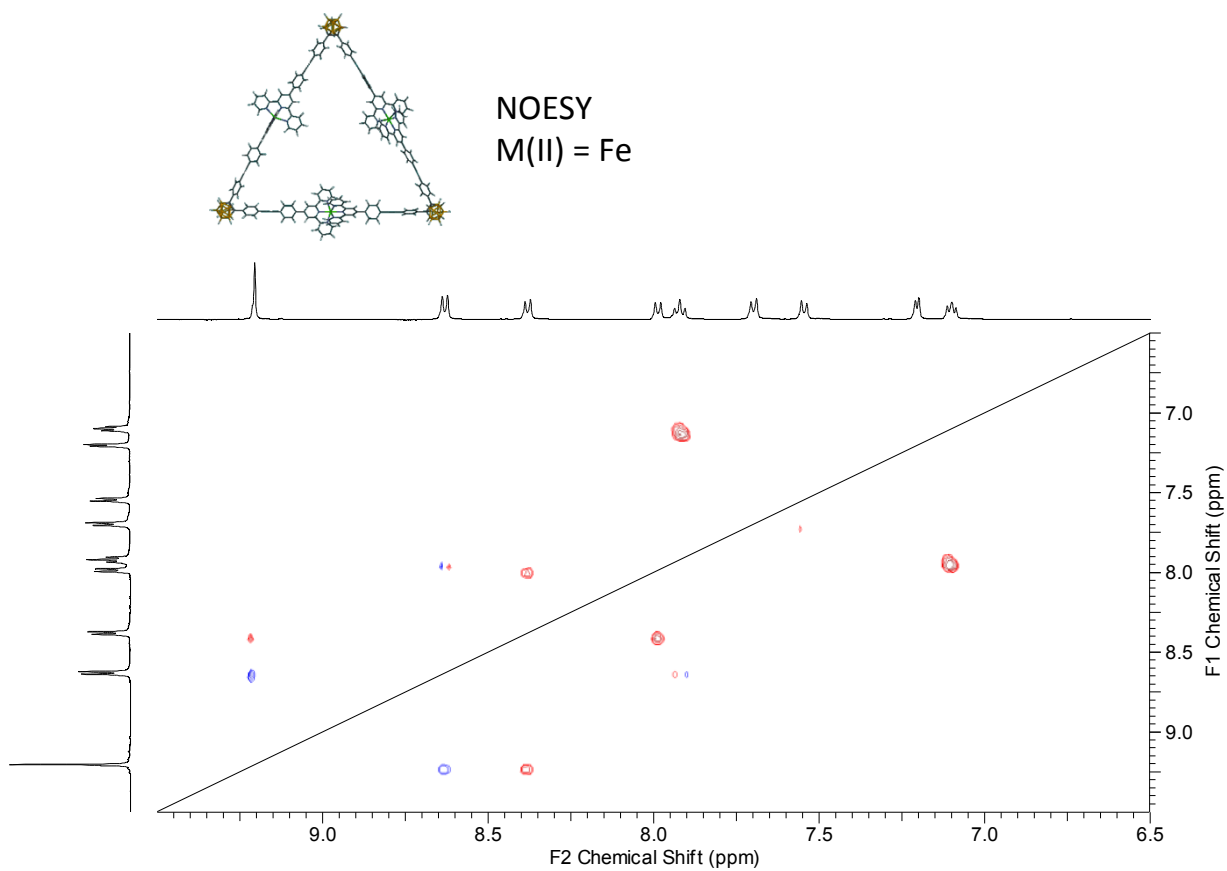
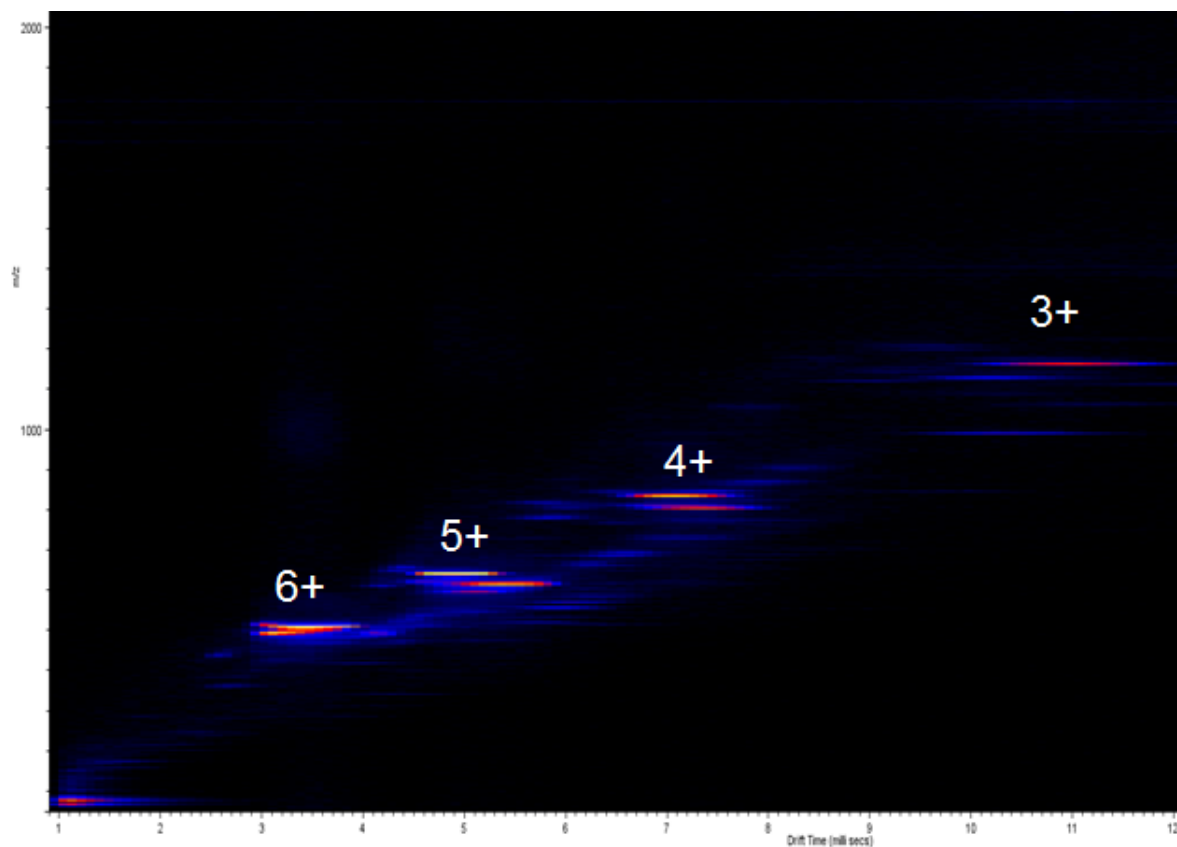
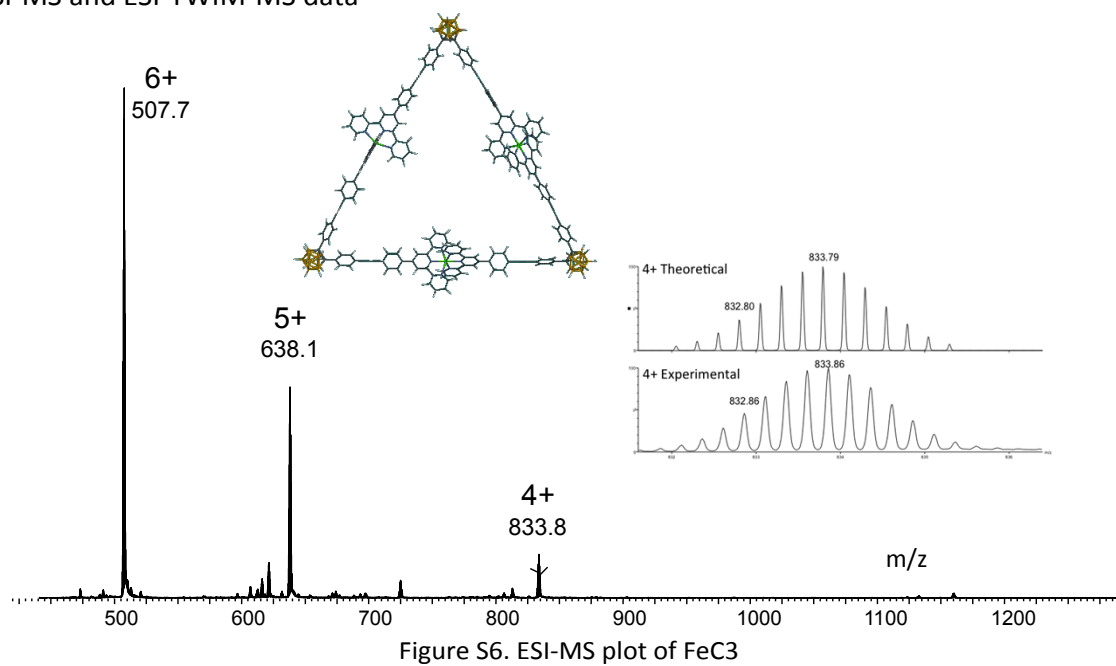


Figure S5. NOESY for FeC3, aromatic region

2. ESI-MS and ESI-TWIM-MS data



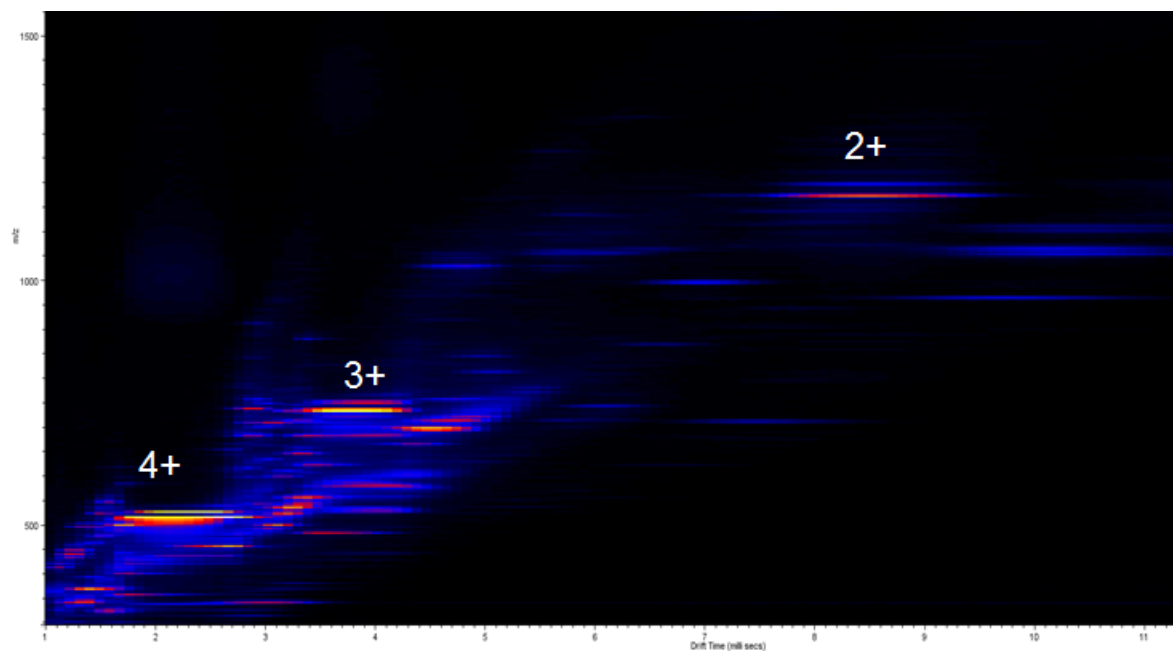


Figure S8. ESI-TWIM-MS plot (m/z vs. drift time) for ZnC_2 at a traveling wave velocity of 350 m/s and a traveling wave height of 7.5V

3. Isotope patterns

ZnC4 3+

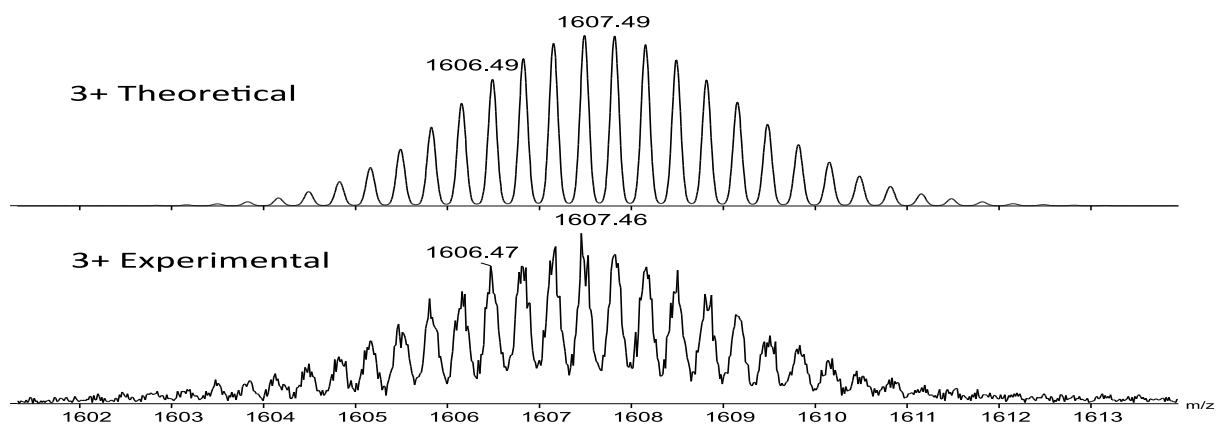
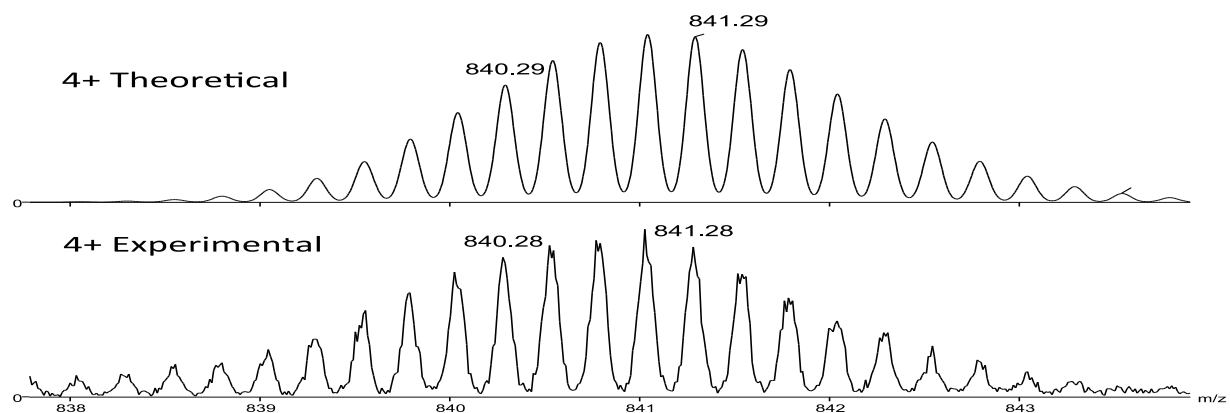


Figure S9. Isotope pattern for ZnC4 charge state 3+.

ZnC3 4+



ZnC3 5+

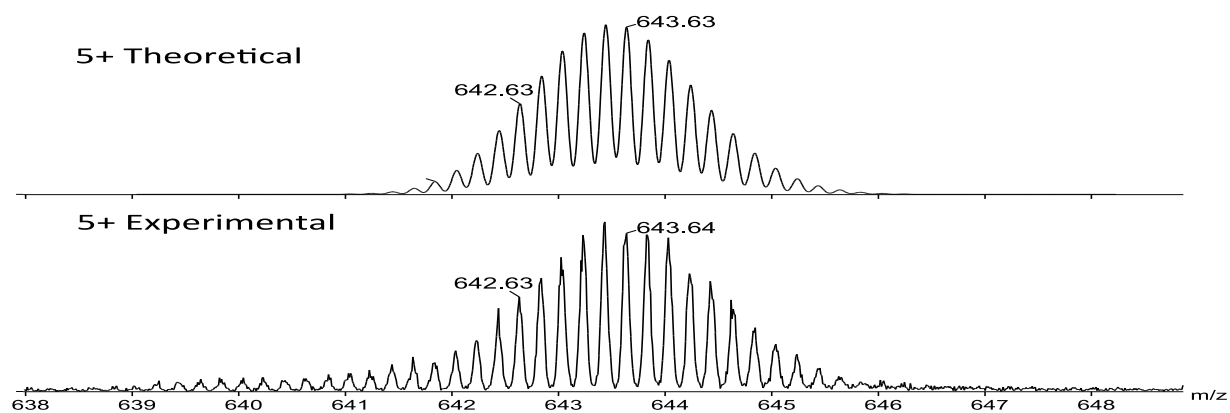
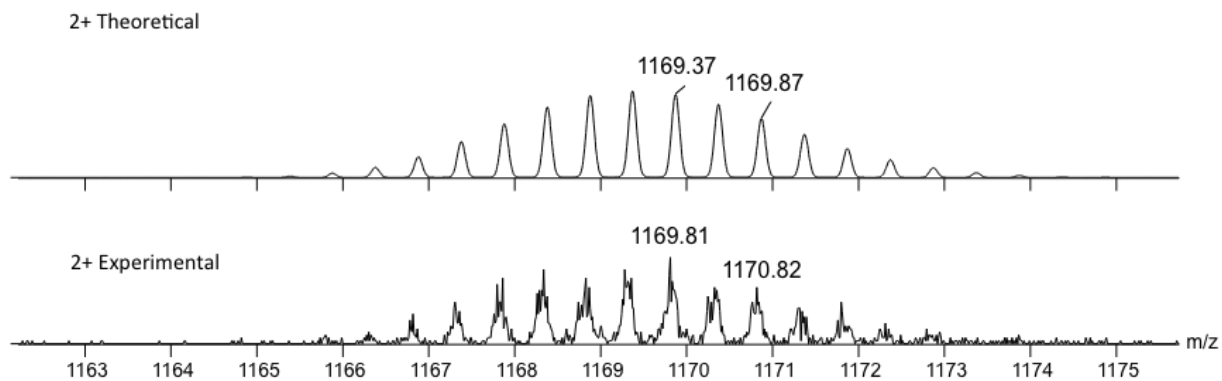
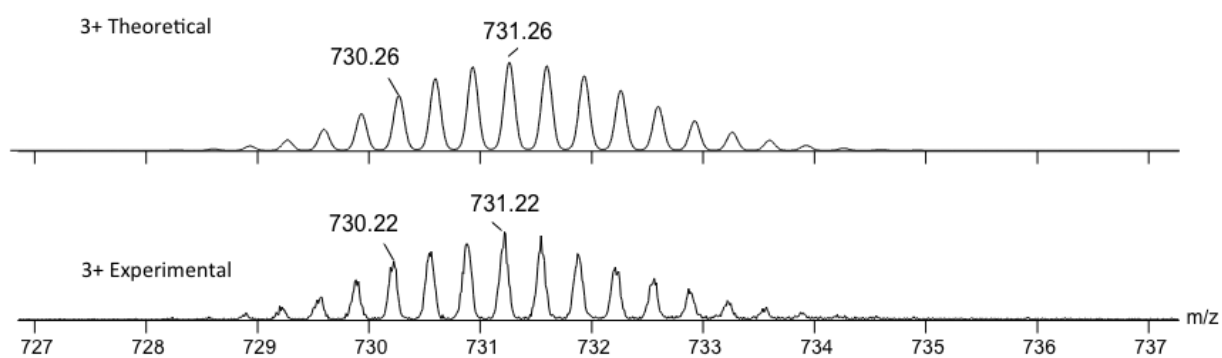


Figure S10. Isotope patterns for ZnC3 charge states 4+ and 5+.

ZnC2 2+



ZnC2 3+



ZnC2 4+

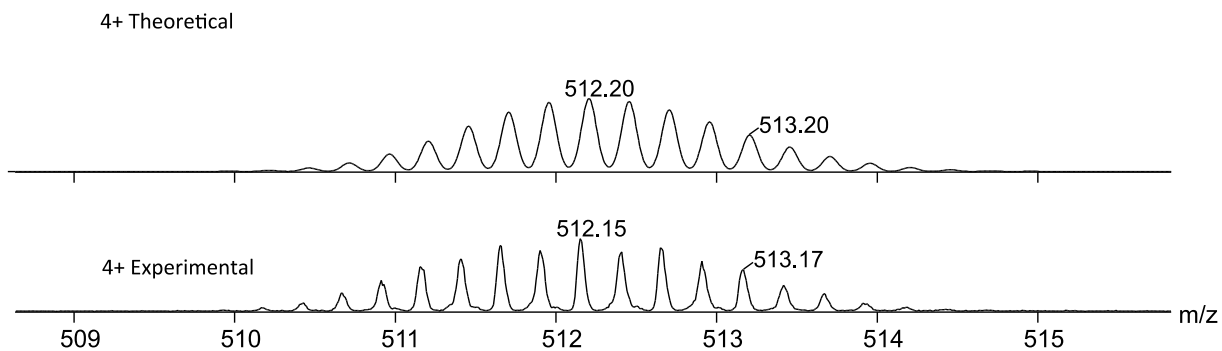


Figure S11. Isotope patterns for ZnC2 charge states 2+, 3+, and 4+.

4. van't Hoff plot and table

Set	T(K)	3'5' dimer	3'5' outer	Dimer mol frac	outer mol frac	K	1/T	lnK
343	345.521	1	0.83	0.64	0.36	2.1	0.0029	0.7
333	335.44	1	0.85	0.64	0.36	2.0	0.0030	0.7
323	325.359	1	0.92	0.62	0.38	1.6	0.0031	0.5
313	315.278	1	0.97	0.61	0.39	1.5	0.0032	0.4
303	305.197	1	1.06	0.59	0.41	1.2	0.0033	0.2
293	295.116	1	1.12	0.57	0.43	1.0	0.0034	0.0
283	285.035	1	1.17	0.56	0.44	0.9	0.0035	-0.1

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

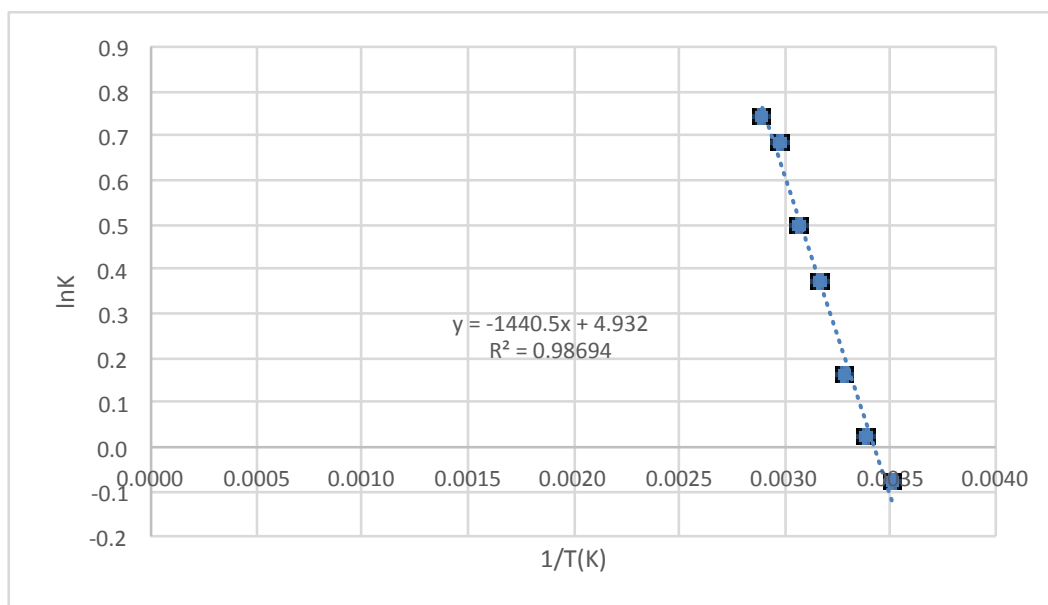


Figure S13. van't Hoff plot

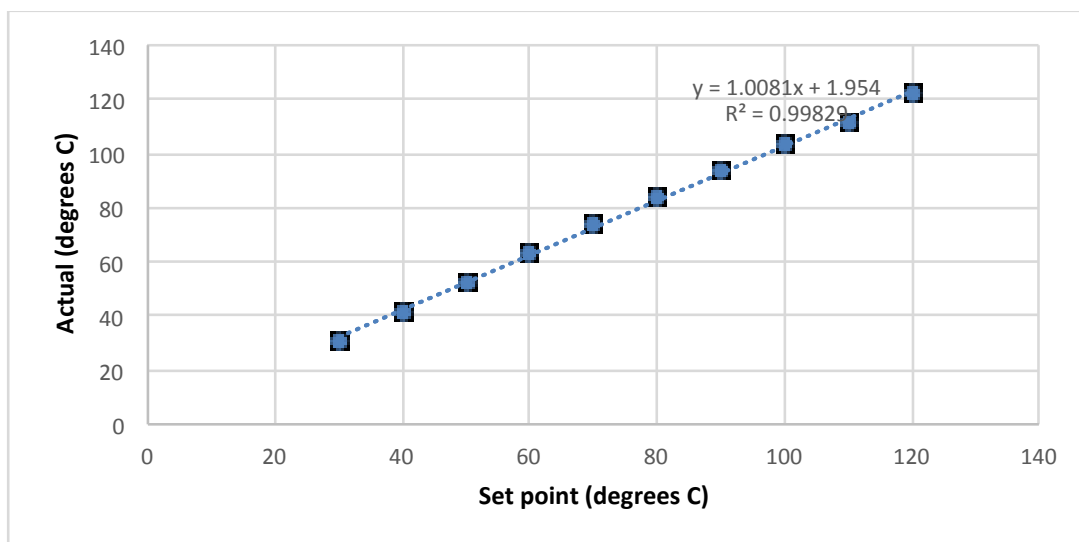


Figure S14. Temperature calibration curve.