

## Supporting Information

### A large spin-crossover $[\text{Fe}_4\text{L}_4]^{8+}$ tetrahedral cage

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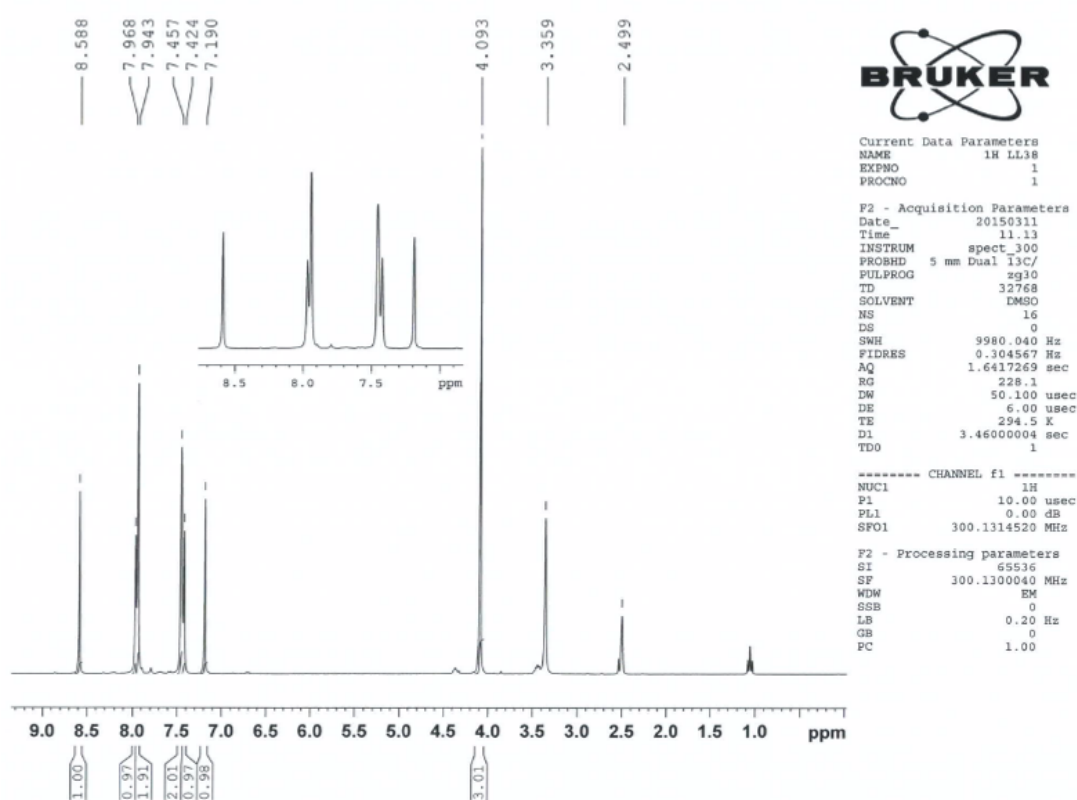
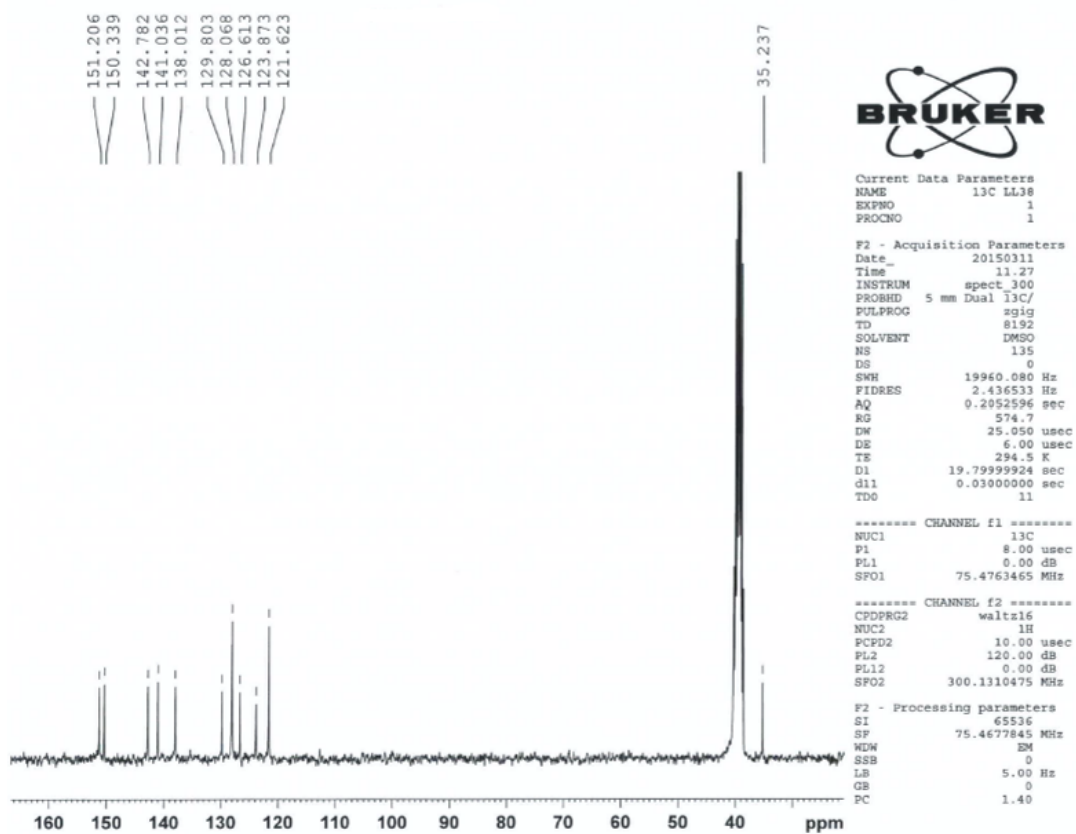
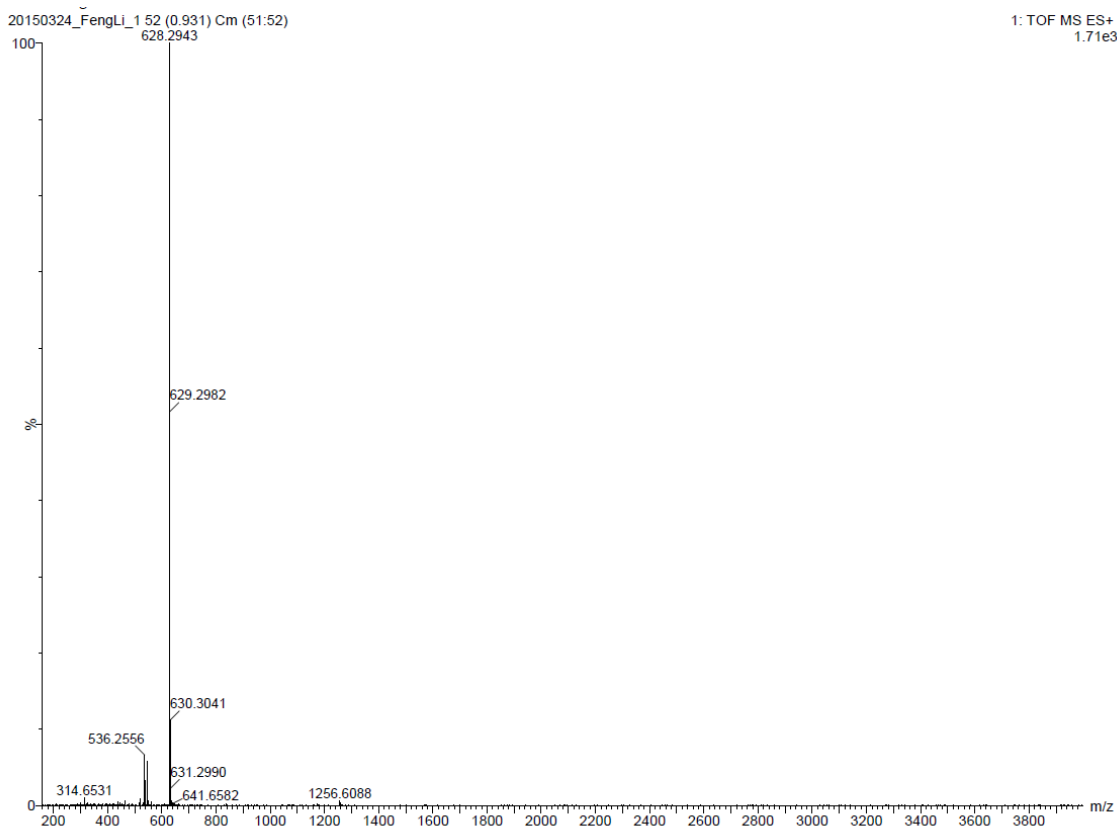


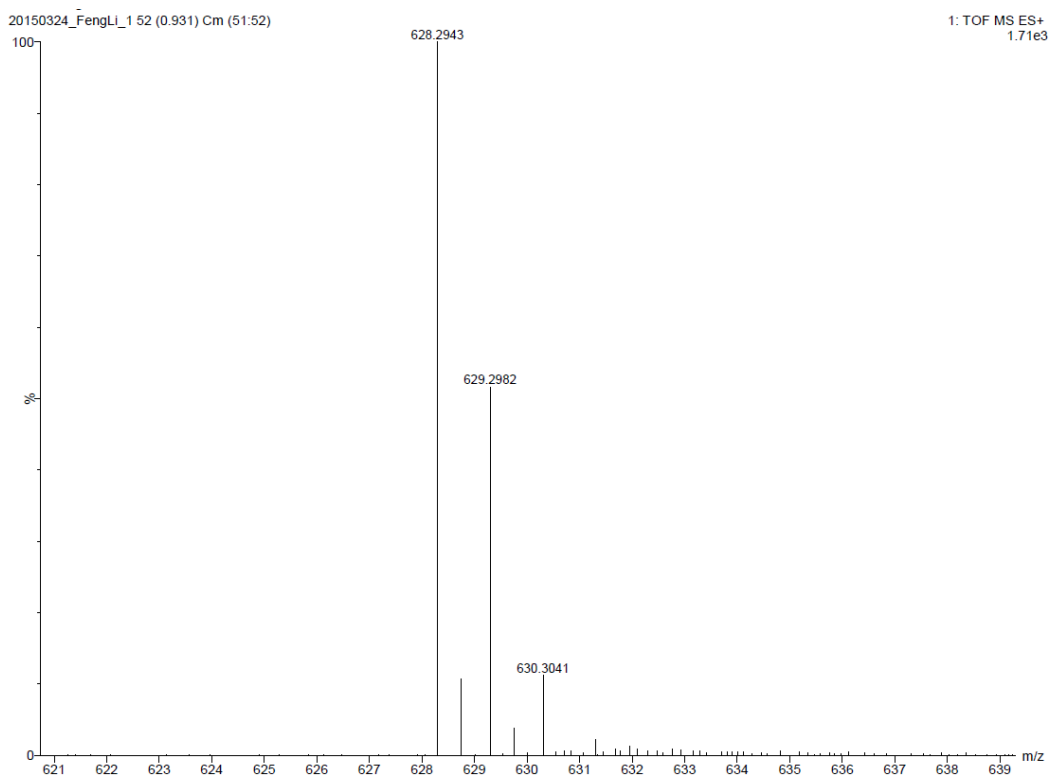
Figure S1:  $^1\text{H}$ -NMR spectrum of L



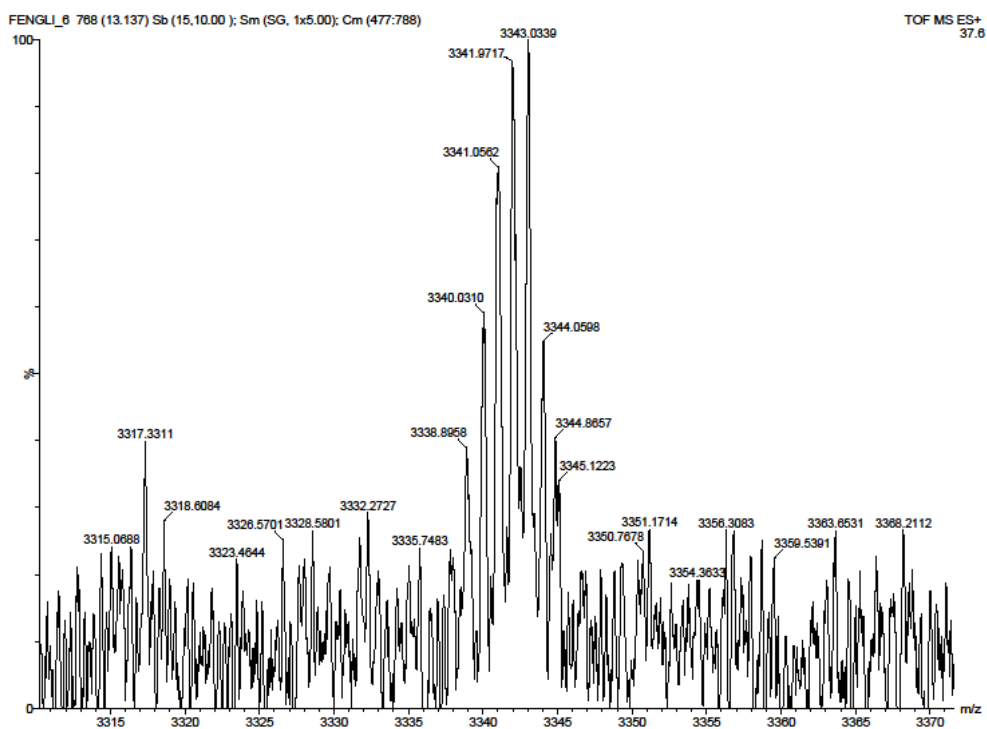
**Figure S2:**  $^{13}\text{C}$ -NMR spectrum of **L**



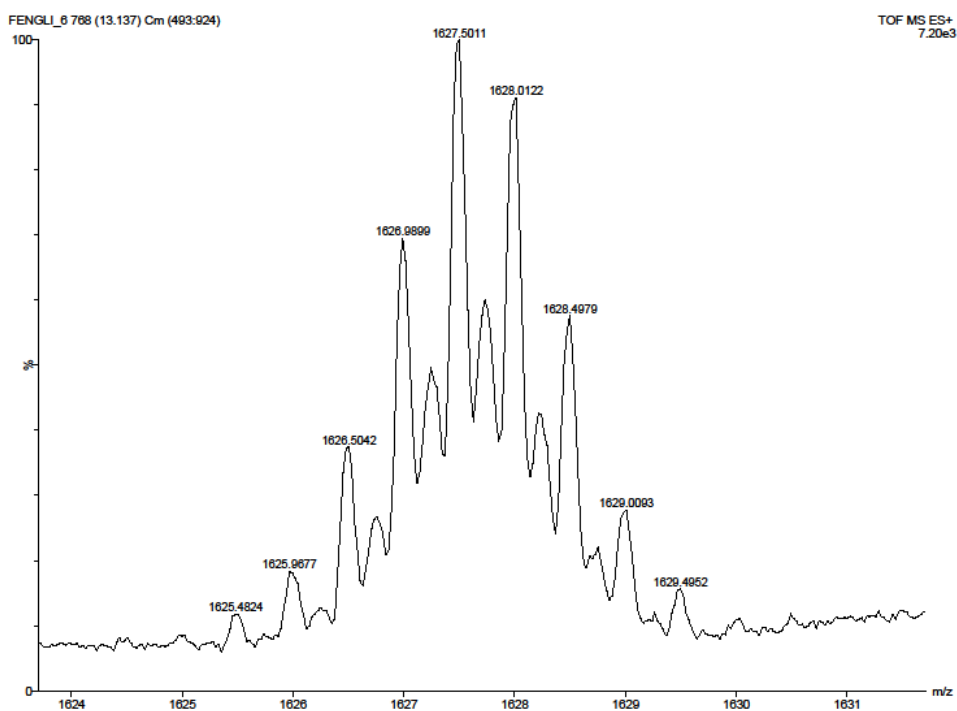
**Figure S3.** High resolution ESI-Mass spectrum of  $[\text{L}+\text{H}]^+$



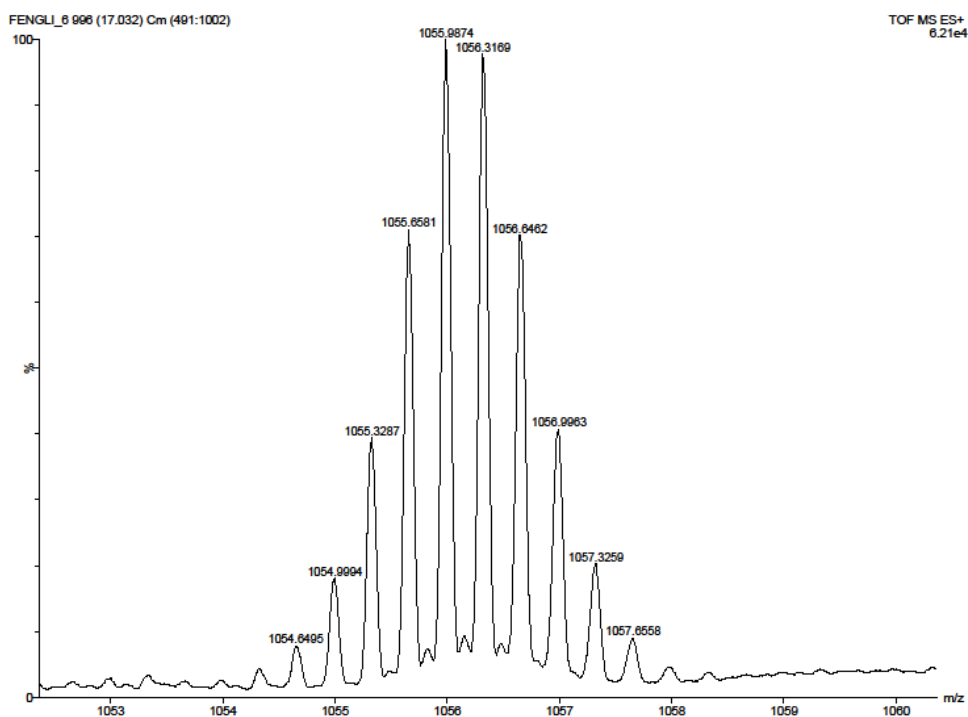
**Figure S4.** Isotope patterns of  $[L+H]^+$



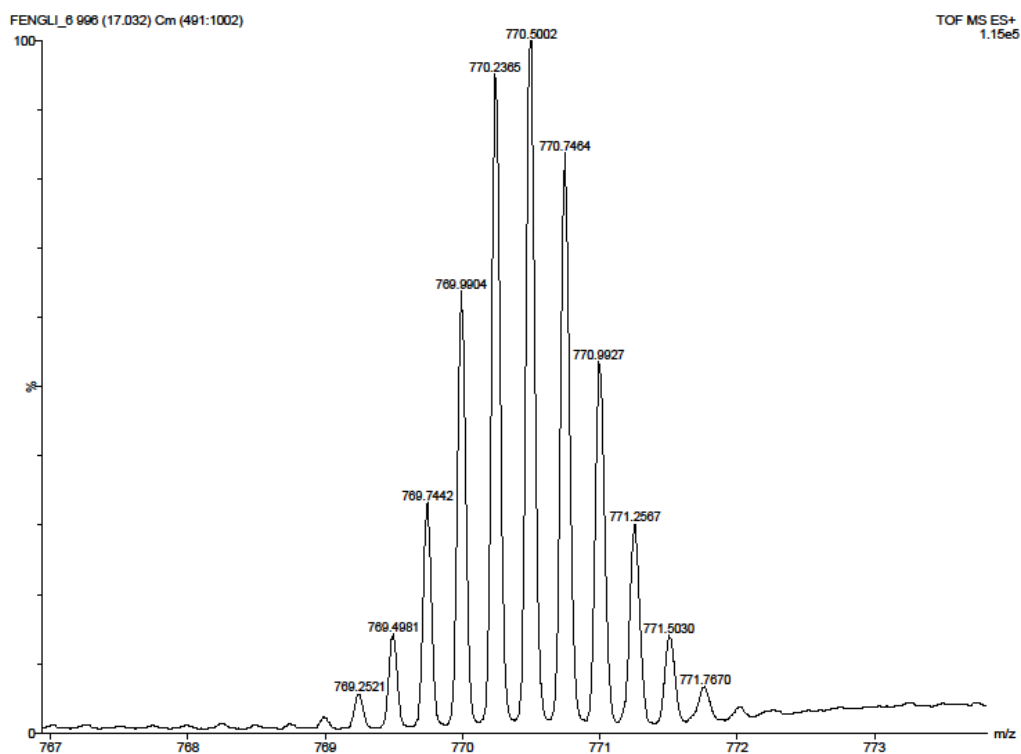
**Figure S5.** High resolution ESI-Mass spectrum of  $\{[Fe_4L_4][BF_4]_7\}^+$  with its isotope patterns.



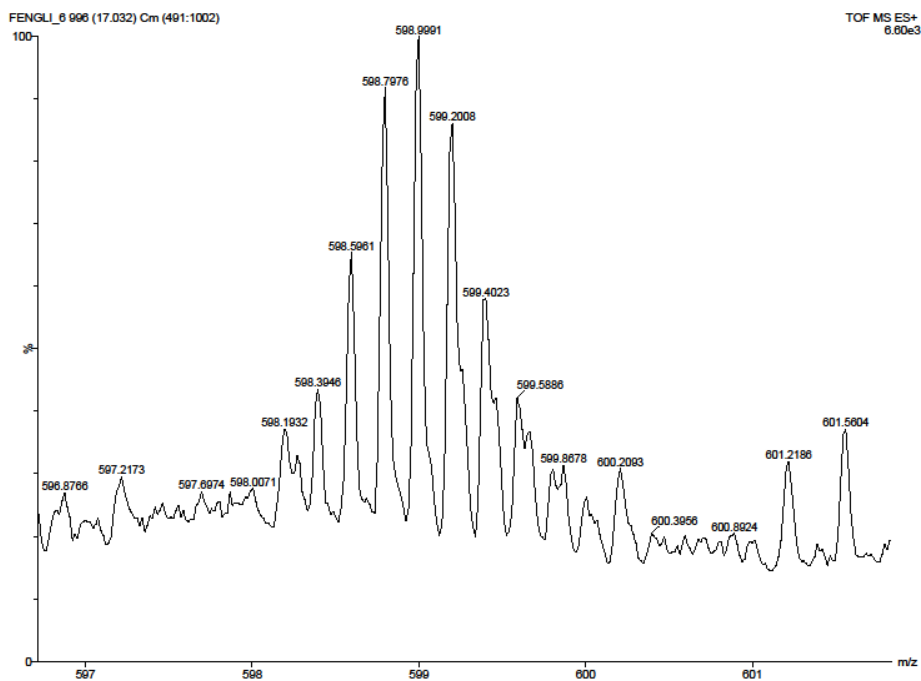
**Figure S6.** High resolution ESI-Mass spectrum of  $\{[\text{Fe}_4\text{L}_4][\text{BF}_4]_6\}^{2+}$  with its isotope patterns.



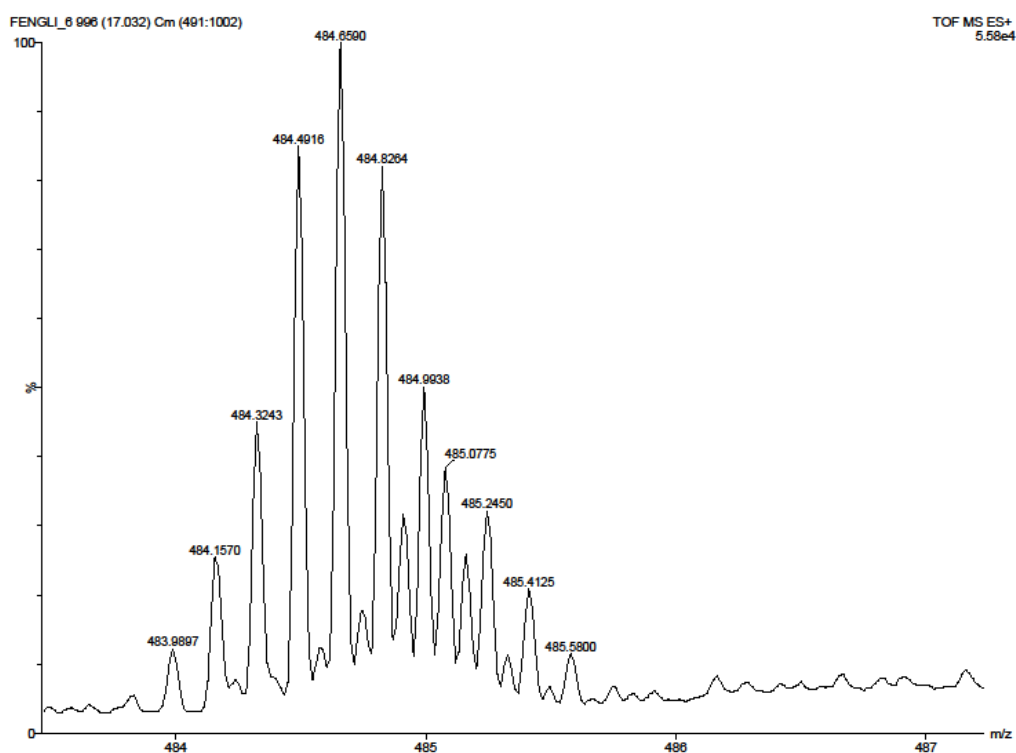
**Figure S7.** High resolution ESI-Mass spectrum of  $\{[\text{Fe}_4\text{L}_4][\text{BF}_4]_5\}^{3+}$  with its isotope patterns.



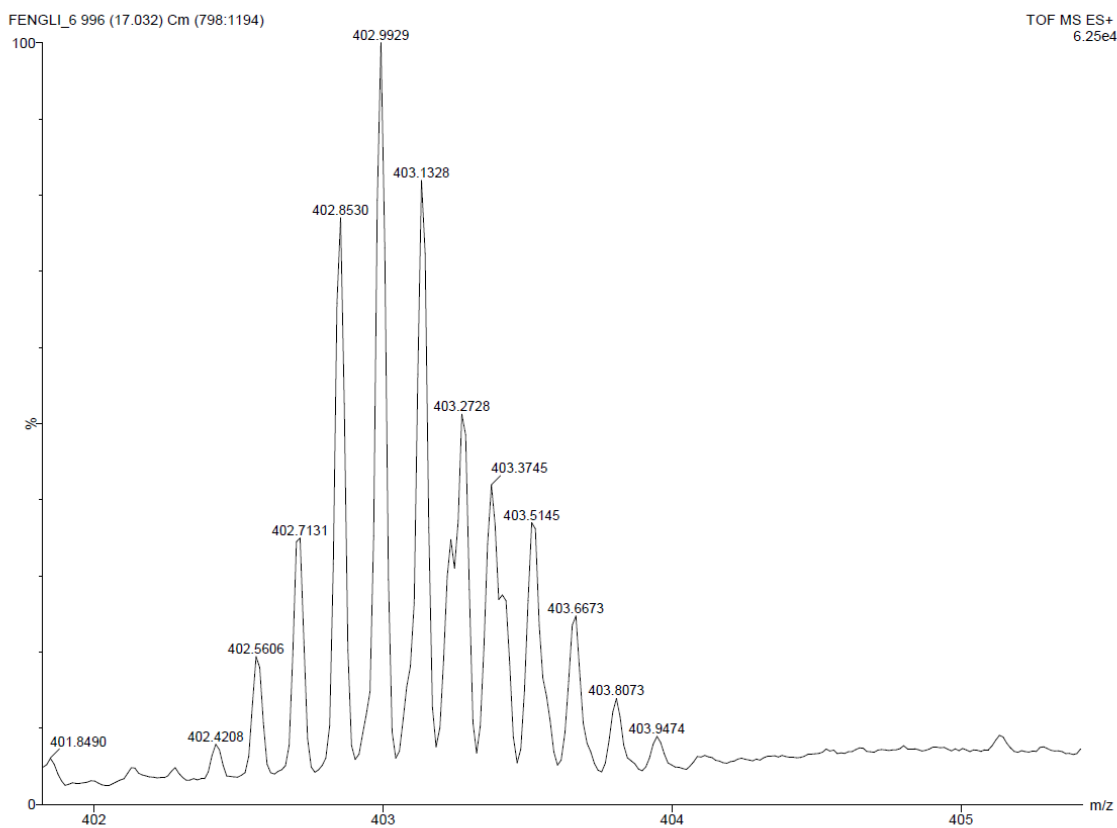
**Figure S8.** High resolution ESI-Mass spectrum of  $\{[Fe_4L_4] [BF_4]_4\}^{4+}$  with its isotope patterns.



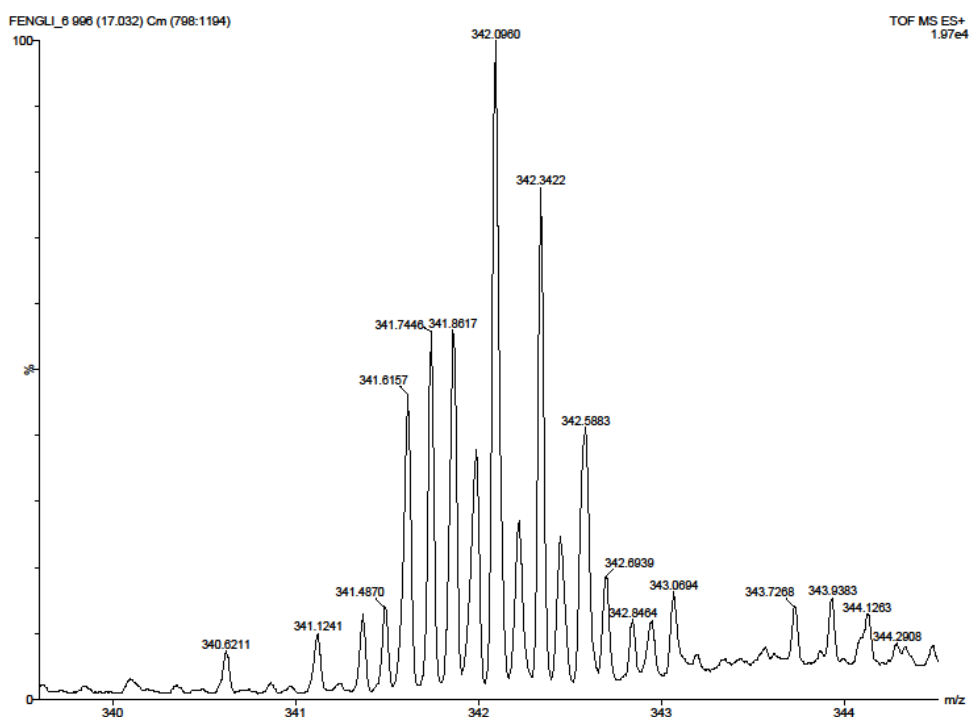
**Figure S9.** High resolution ESI-Mass spectrum of  $\{[Fe_4L_4] [BF_4]_3\}^{5+}$  with its isotope patterns.



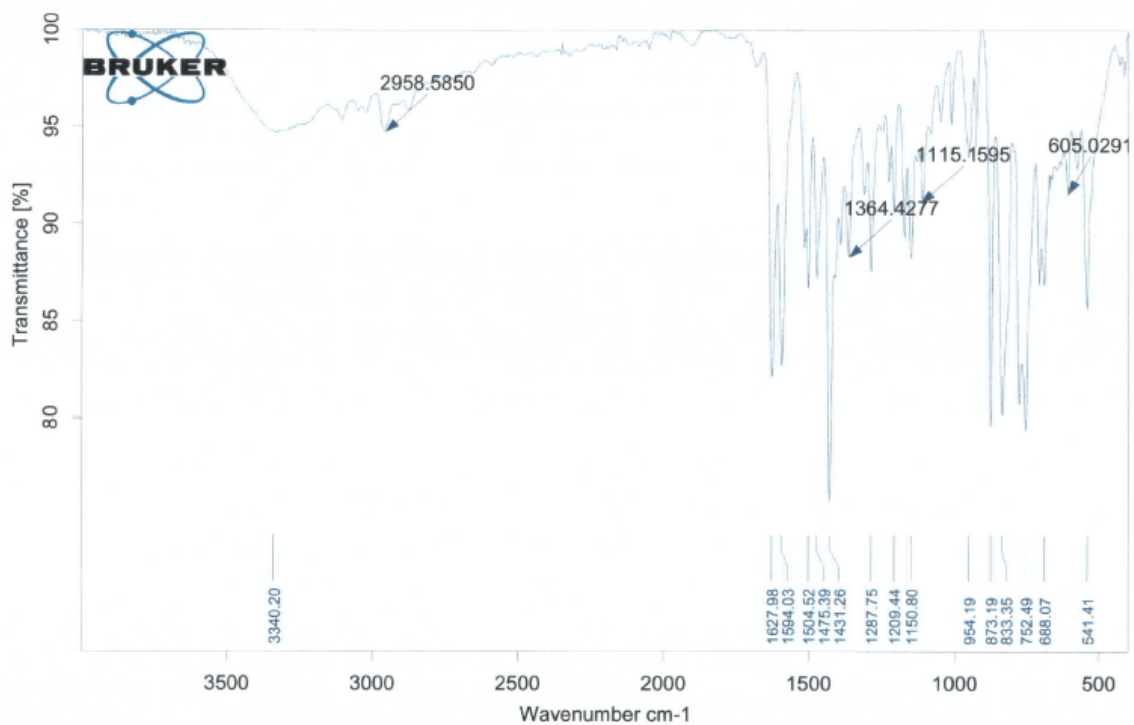
**Figure S10.** High resolution ESI-Mass spectrum of  $\{[\text{Fe}_4\text{L}_4] [\text{BF}_4]_2\}^{6+}$  with its isotope patterns.



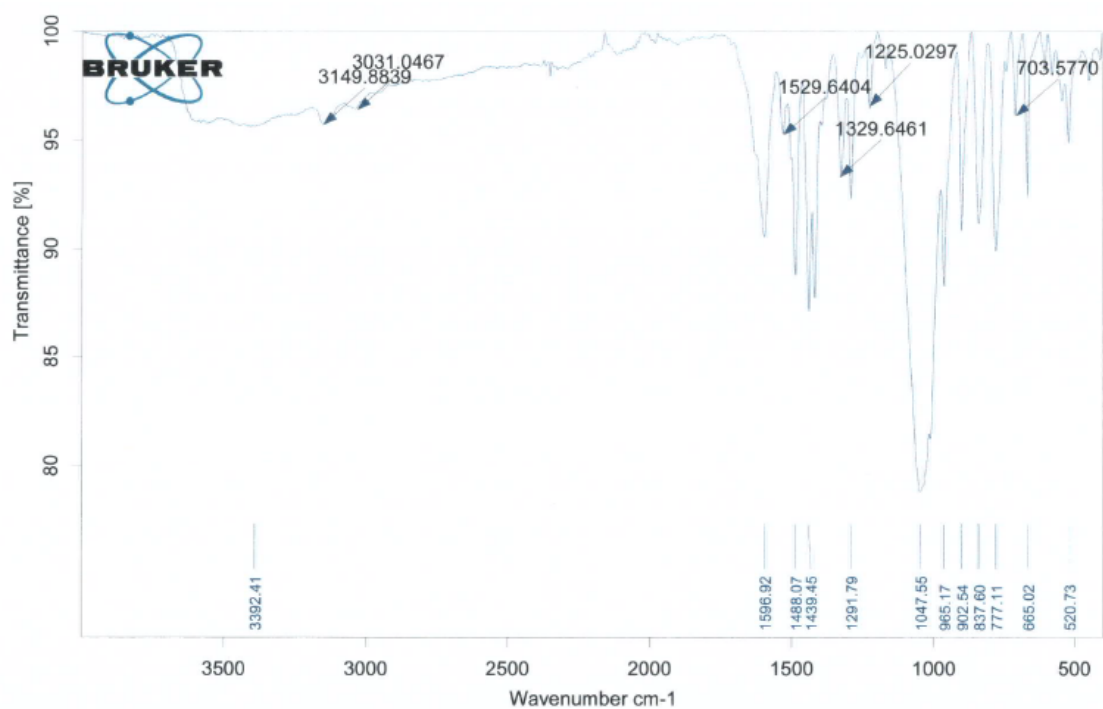
**Figure S11.** High resolution ESI-Mass spectrum of  $\{[\text{Fe}_4\text{L}_4] [\text{BF}_4]\}^{7+}$  with its isotope patterns.



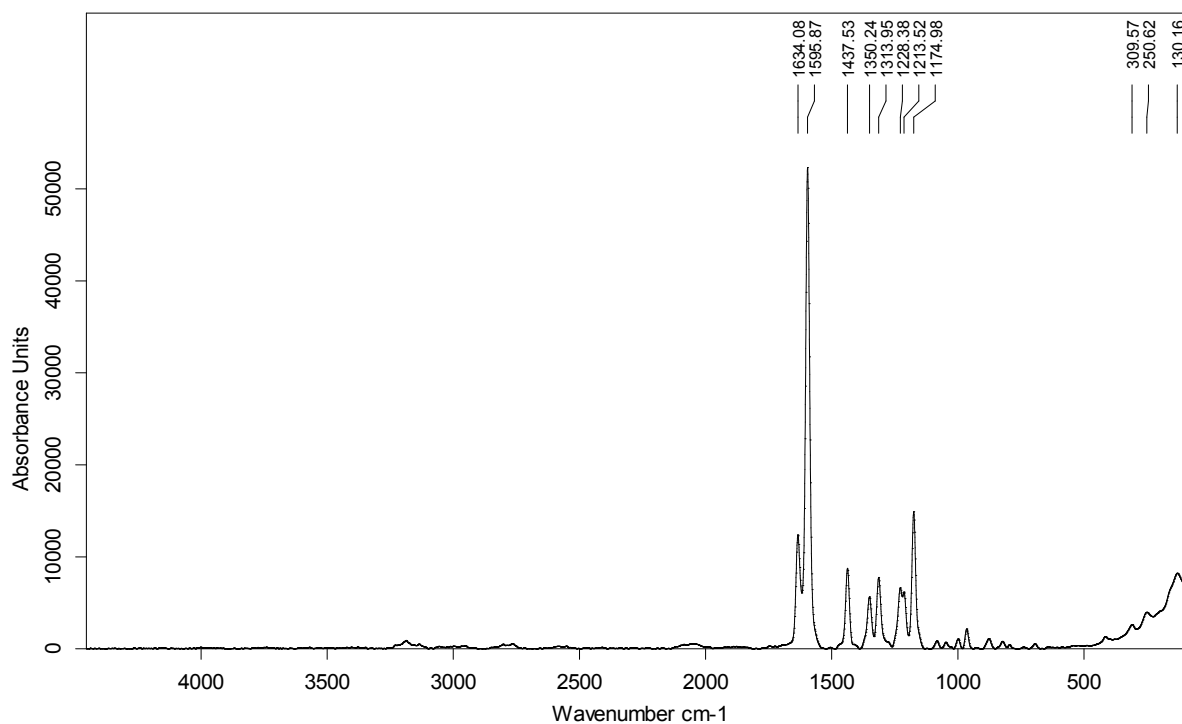
**Figure S12.** High resolution ESI-Mass spectrum of  $[\text{Fe}_4\text{L}_4]^{8+}$  with its isotope patterns.



**Figure S13:** FT-IR spectrum of **L**

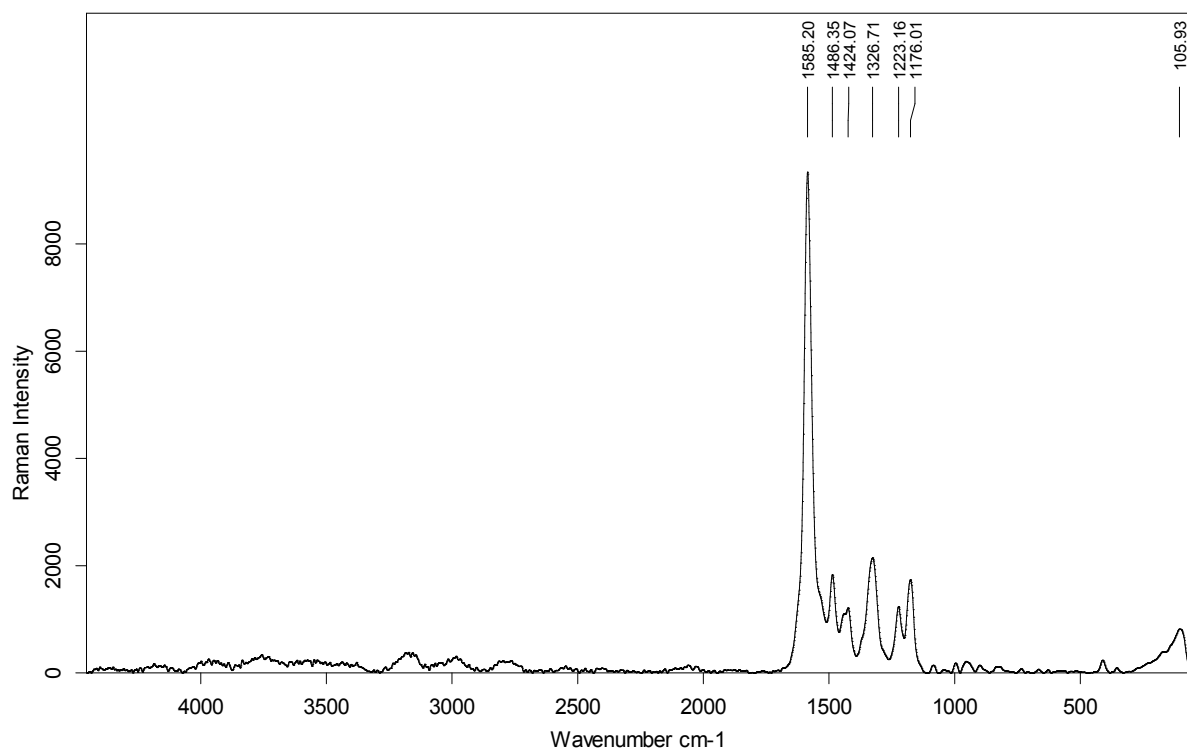


**Figure S14:** FT-IR spectrum of cage 1

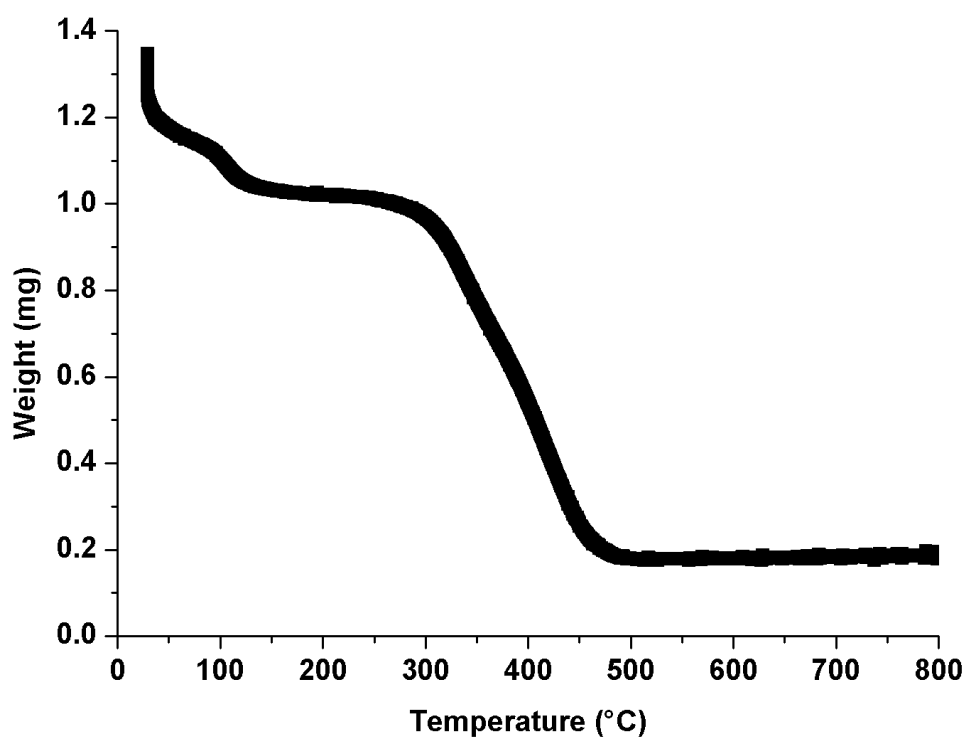


**Figure S15:** Raman Spectrum of L





**Figure S16:** Raman Spectrum of cage 1



**Figure S17:** Thermogravimetric analysis result for cage 1.