Electronic Supplementary Information

A study of the interaction between inverted cucurbit[7]uril and symmetric viologens

Zhongzheng Gao,[a] Dong Bai,[a] Lixia Chen,[a] Zhu Tao,[a] Xin Xiao*[a], Timothy J. Prior[b] and Carl Redshaw [b*]

[a] Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang 550025, China

[b] Department of Chemistry, University of Hull, Hull HU6 7RX, U.K.

Contents

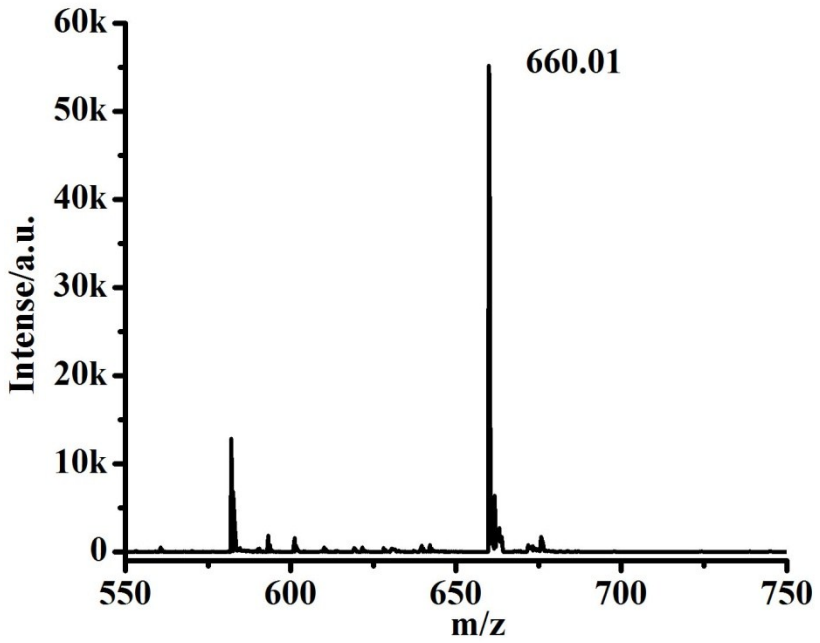


Figure S1. Mass spectrum for the *i*Q[7]- BPY^{2+}system.

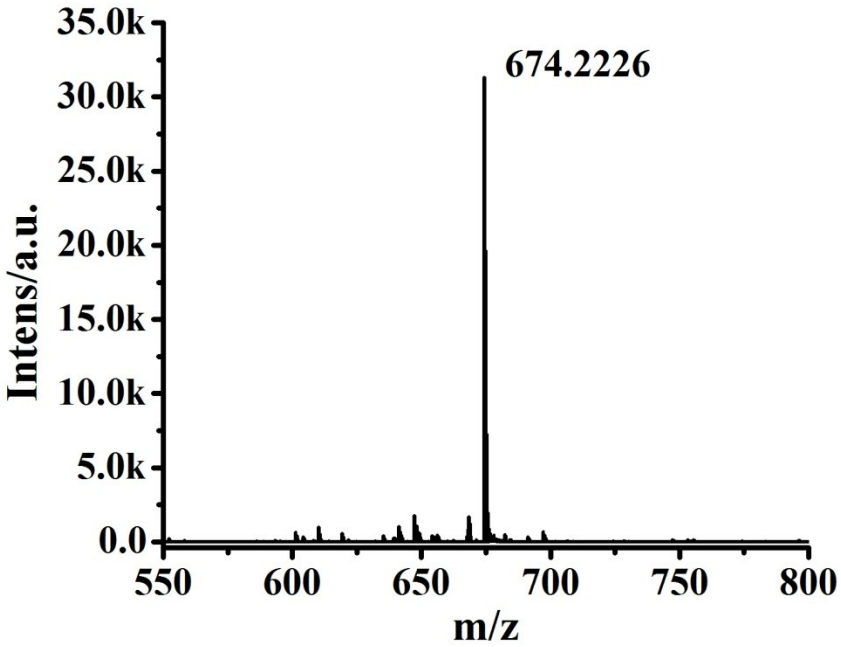


Figure S2. Mass spectrum for the *i*Q[7]- MV^{2+} system.

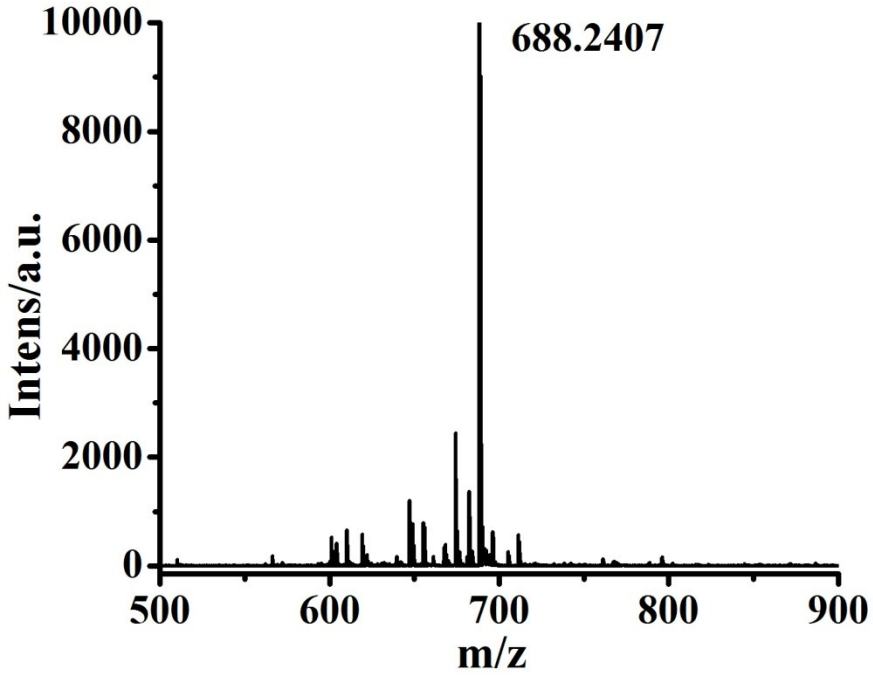


Figure S3. Mass spectrum for the *i*Q[7]-EV^{2+} system.

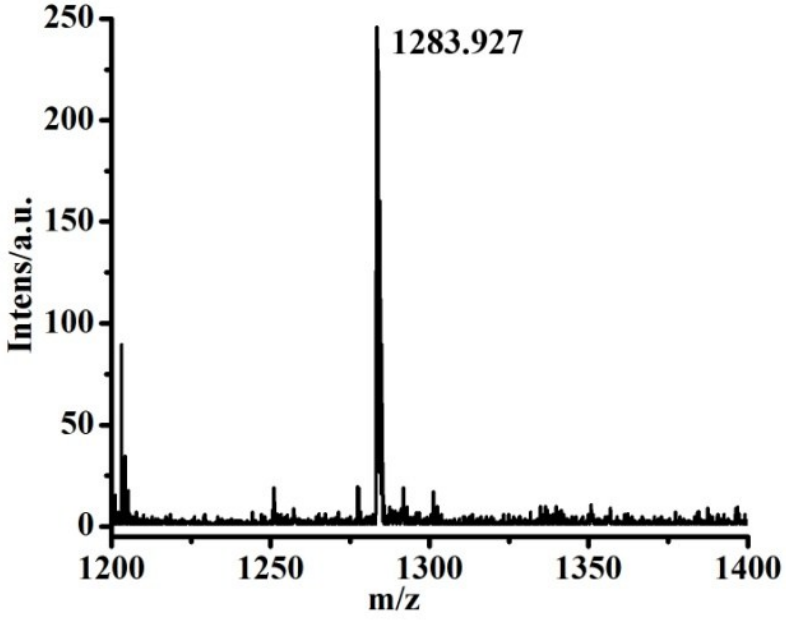


Figure S4. Mass spectrum for the *i*Q[7]- PV^{2+} system.

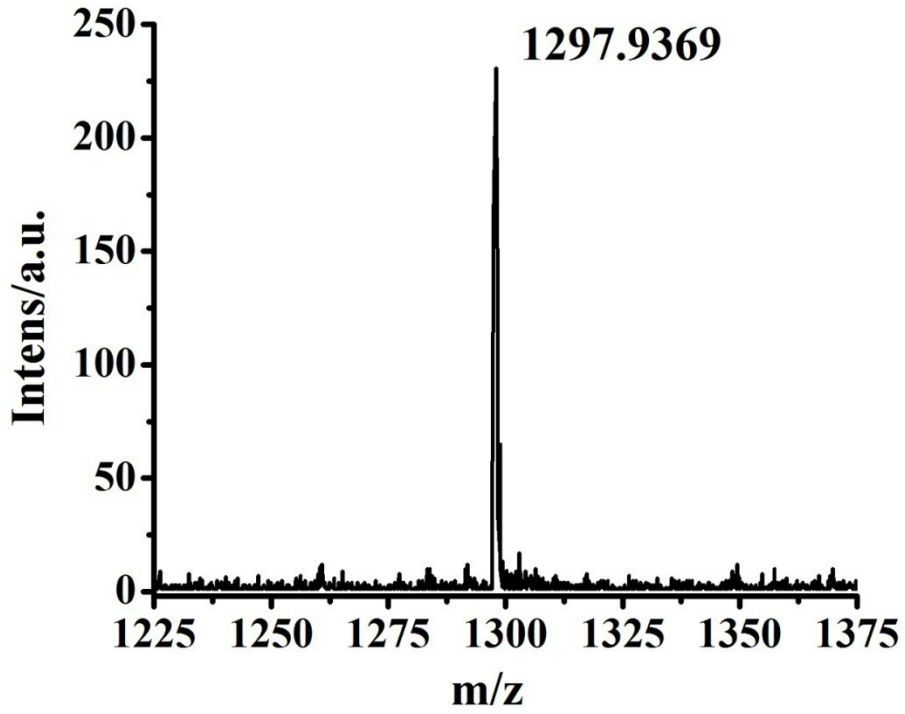


Figure S5. Mass spectrum for the *i*Q[7]- BV^{2+} system.

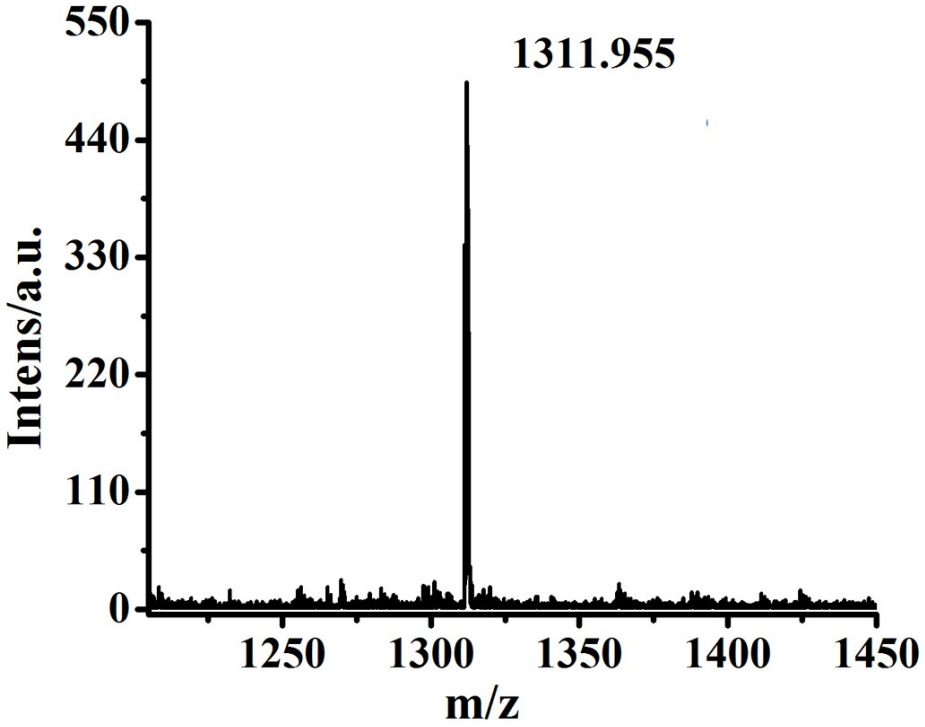


Figure S6. Mass spectrum for the *i*Q[7]- FV^{2+} system.

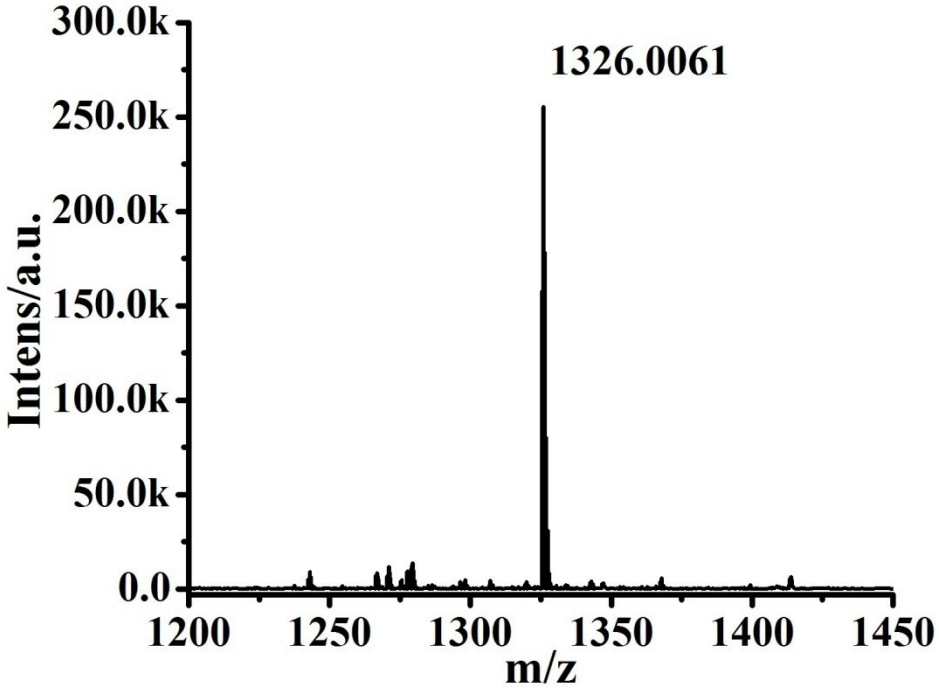


Figure S7. Mass spectrum for the *i*Q[7]- HV^{2+}system.

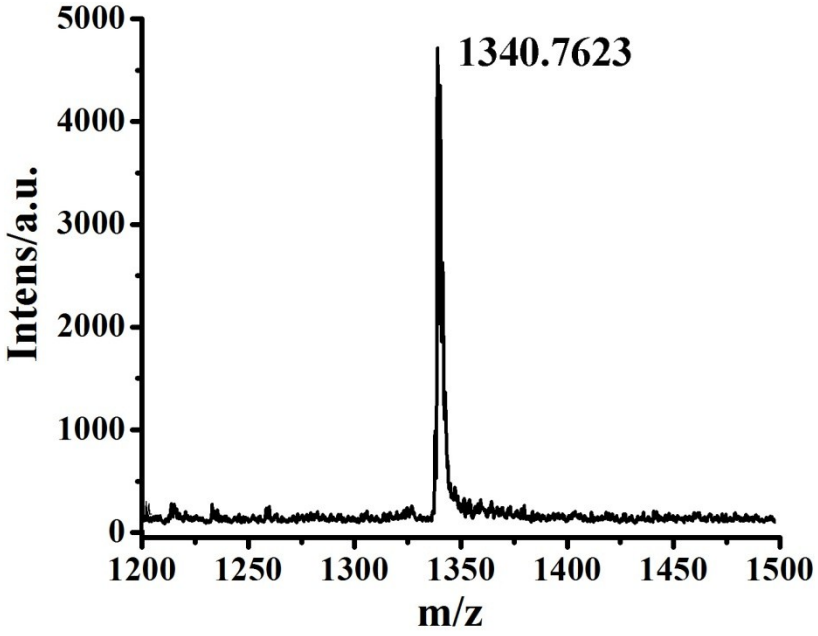


Figure S8. Mass spectrum for the *i*Q[7]- SV^{2+}system.

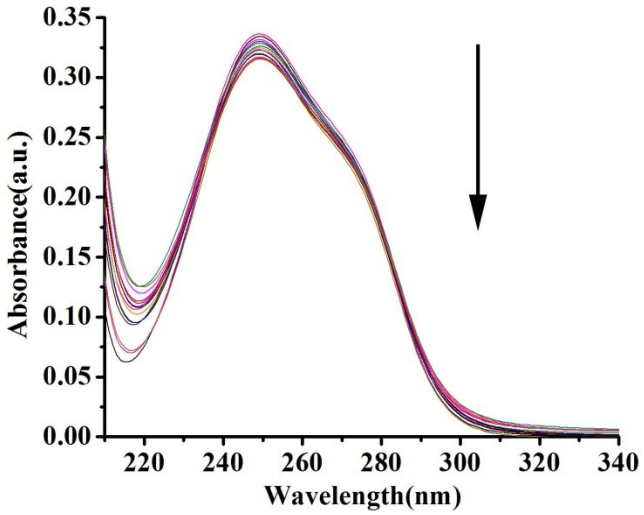


Figure S9. UV spectrum of BPY^{2+} (2×10^{-5} mol L^{-1}) upon addition of increasing amounts (0, 0.1, 0.2, 0.3, 0.4, 05, 0.6, 0.7, 0.8, 0.9, 1.0, 1.2, 1.4, 1.6 equiv.) of *i*Q[7], with an excitation of 247 nm.

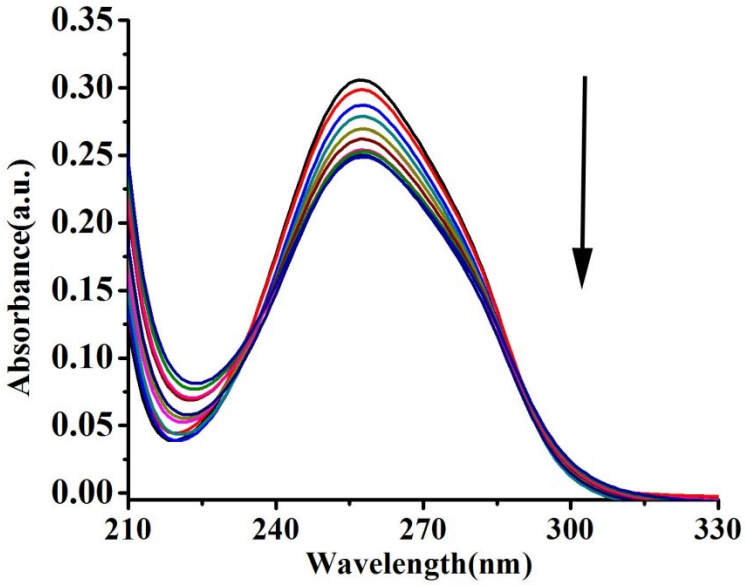


Figure S10. UV spectrum of MV^{2+} (2×10^{-5} mol L^{-1}) upon addition of increasing amounts (0, 0.2, 0.4, 0.6, 0.8, 1.0, 1.2, 1.4, 1.6, 1.8, 2.0 equiv.) of *i*Q[7], with an excitation of 257 nm.

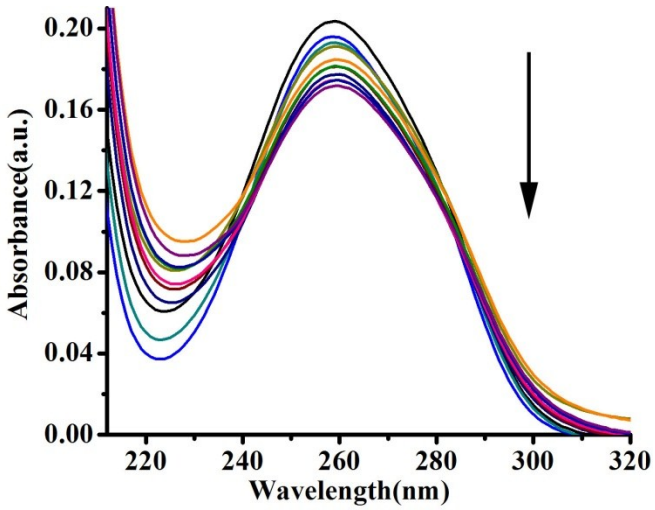


Figure S11. UV spectrum of EV^{2+} (2×10^{-5} mol L^{-1}) upon addition of increasing amounts (0, 0.2, 0.4, 0.6, 0.8, 1.0, 1.2, 1.4, 1.6, 1.8, 2.0 equiv.) of *i*Q[7], with an excitation of 259 nm.

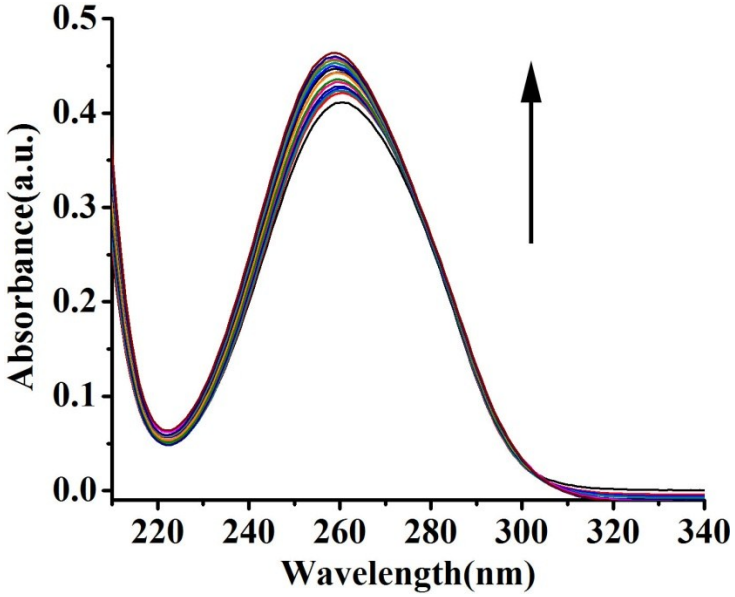


Figure S12. UV spectrum of PV^{2+} (2×10^{-5} mol L^{-1}) upon addition of increasing amounts (0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.2, 1.4, 1.6, 1.8, 2.0 equiv.) of *i*Q[7], with an excitation of 259 nm.

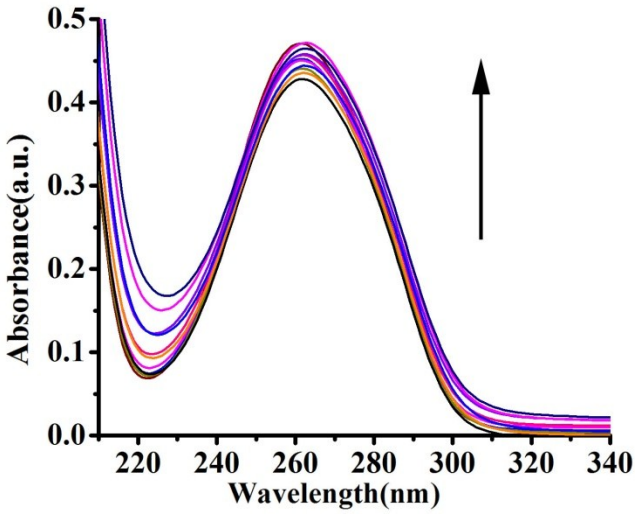


Figure S13. UV spectrum of BV^{2+} (2×10^{-5} mol L^{-1}) upon addition of increasing amounts (0, 0.2, 0.4, 0.6, 0.8, 1.0, 1.2, 1.4, 1.6, 1.8, 2.0 equiv.) of *i*Q[7], with an excitation of 262 nm.

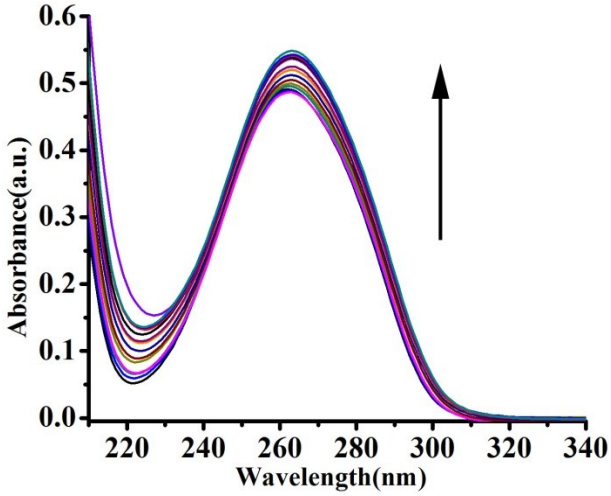


Figure S14. UV spectrum of FV^{2+} (2×10^{-5} mol L^{-1}) upon addition of increasing amounts (0, 0.2, 0.4, 0.6, 0.8, 1.0, 1.2, 1.4, 1.6, 1.8, 2.0, 2.2, 2.4, 2.6 equiv.) of *i*Q[7], with an excitation of 261 nm.

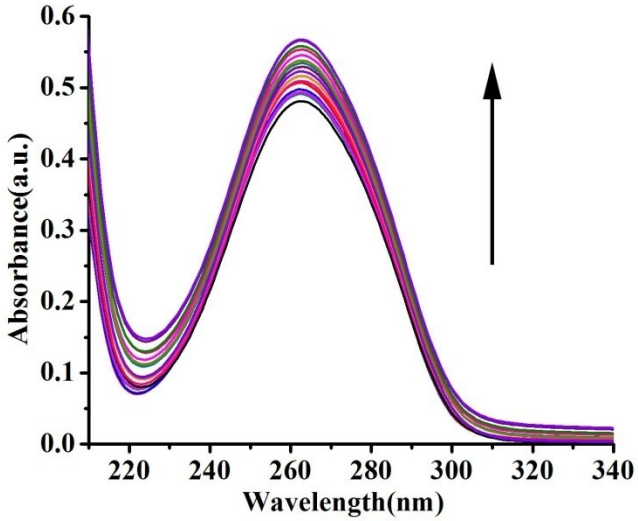


Figure S15. UV spectrum of HV^{2+} (2×10^{-5} mol L^{-1}) upon addition of increasing amounts (0, 0.2, 0.4, 0.6, 0.8, 1.0, 1.2, 1.4, 1.6, 1.8, 2.0, 2.2, 2.4, 2.6 equiv.) of *i*Q[7], with an excitation of 262 nm.

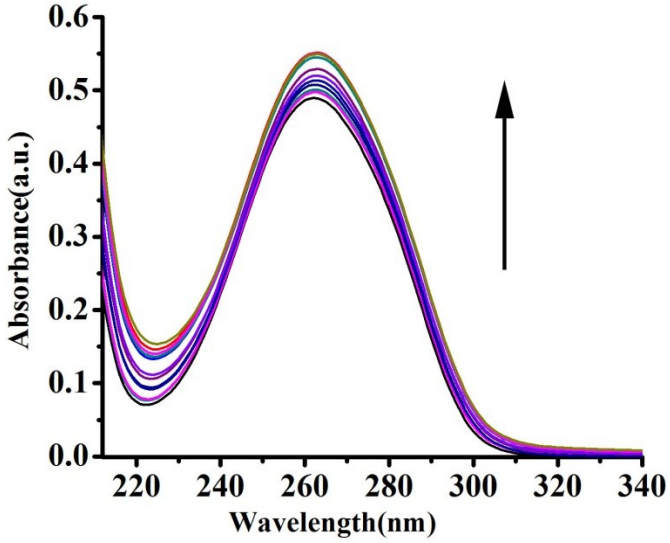
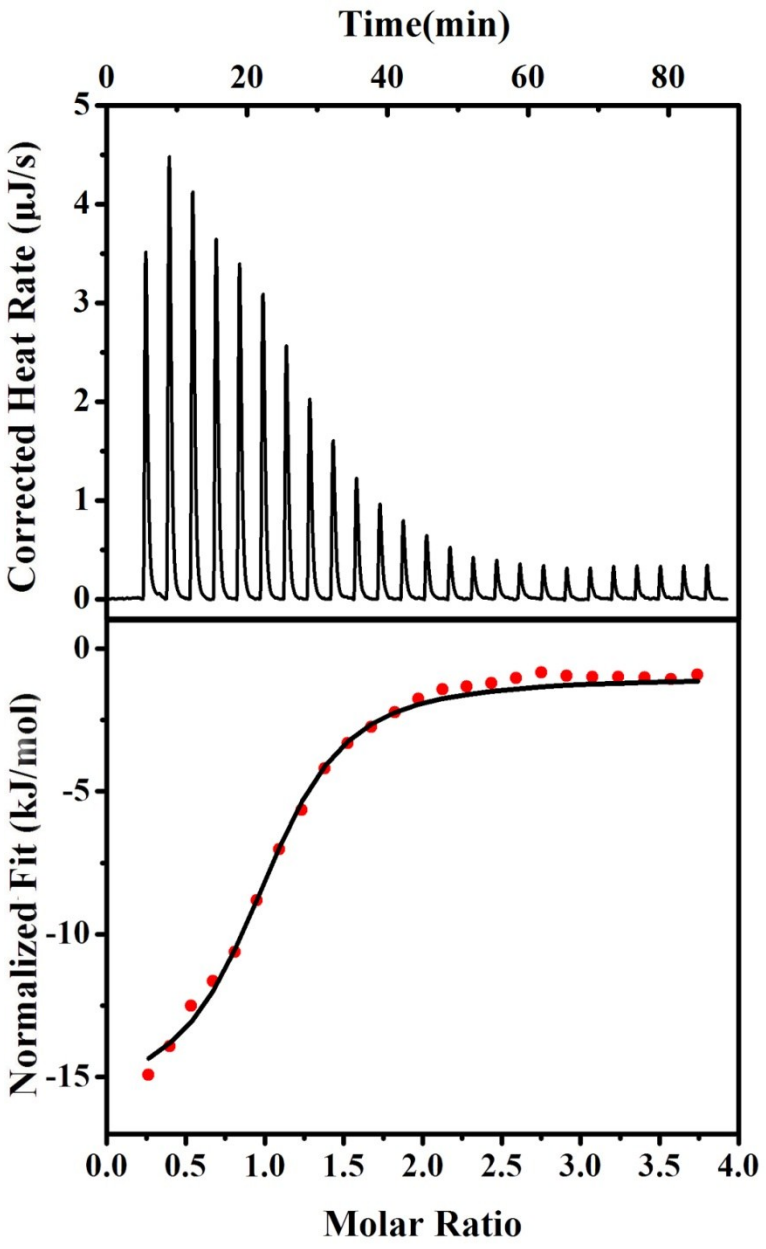
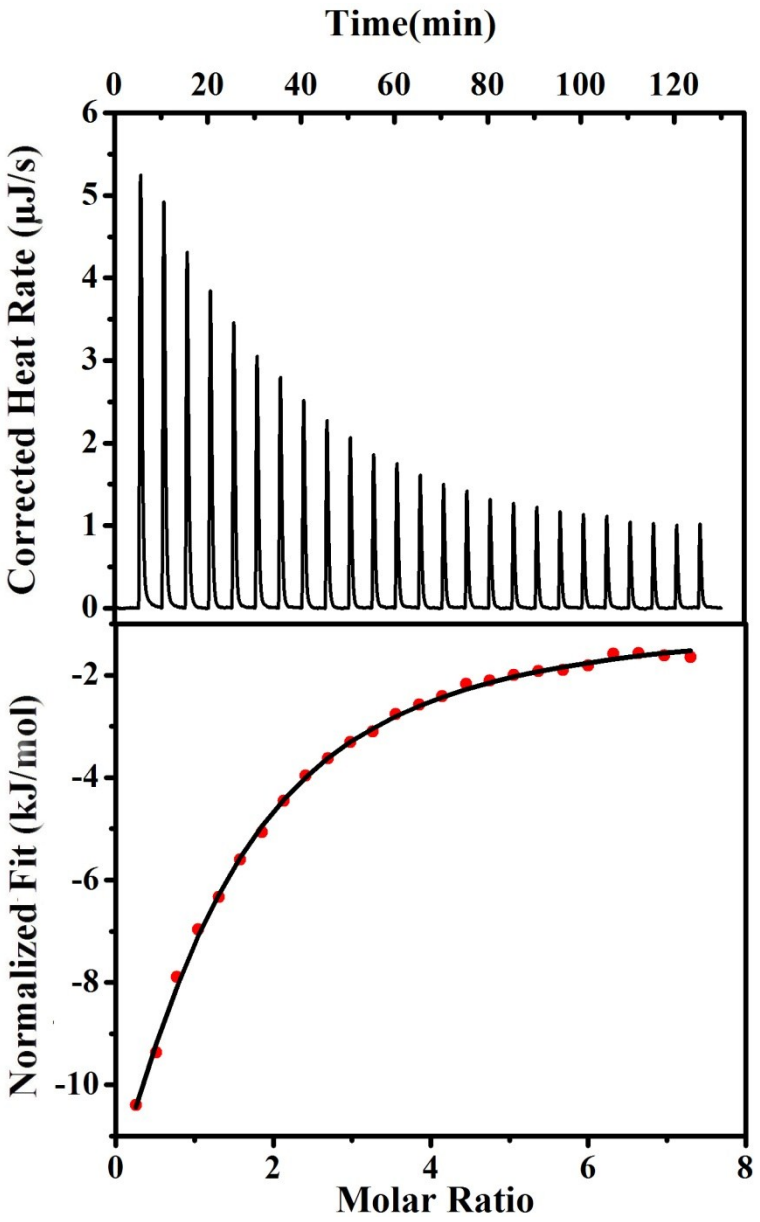


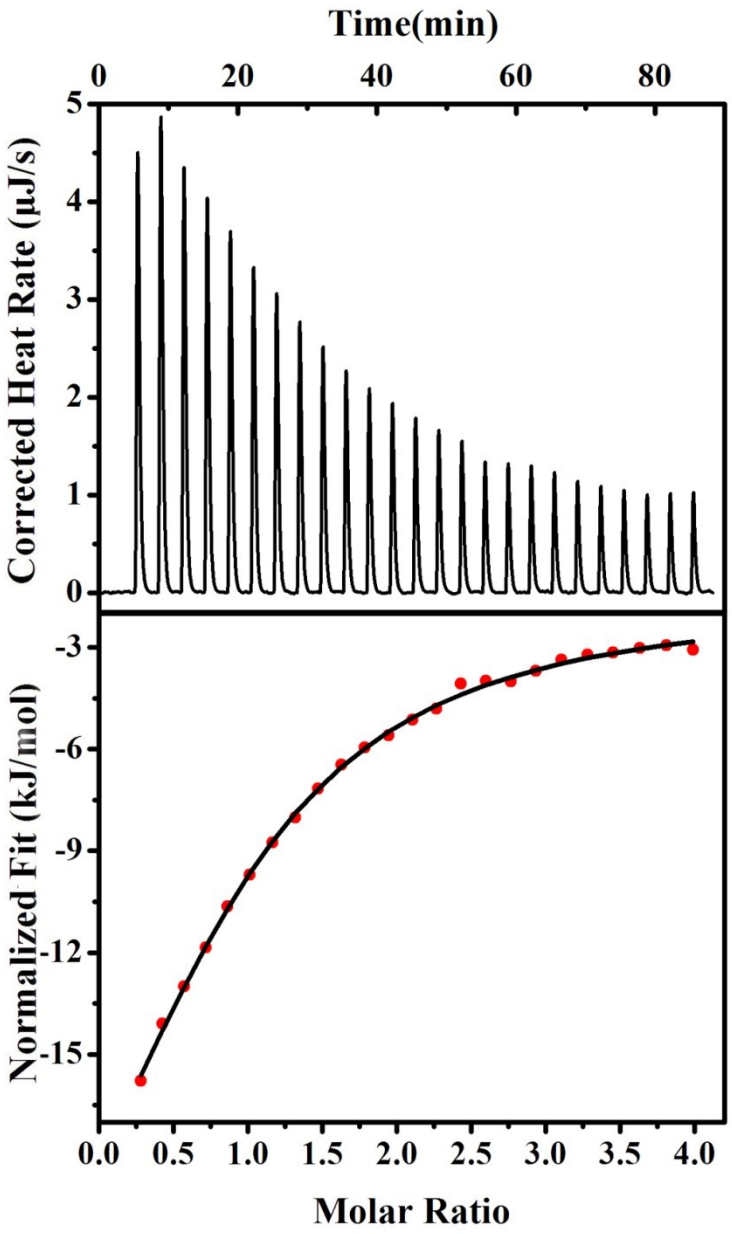
Figure S16. UV spectrum of SV^{2+} (2×10^{-5} mol L^{-1}) upon addition of increasing amounts (0, 0.2, 0.4, 0.6, 0.8, 1.0, 1.2, 1.4, 1.8, 2.2, 2.6, 3.0 equiv.) of *i*Q[7], with an excitation of 261 nm.



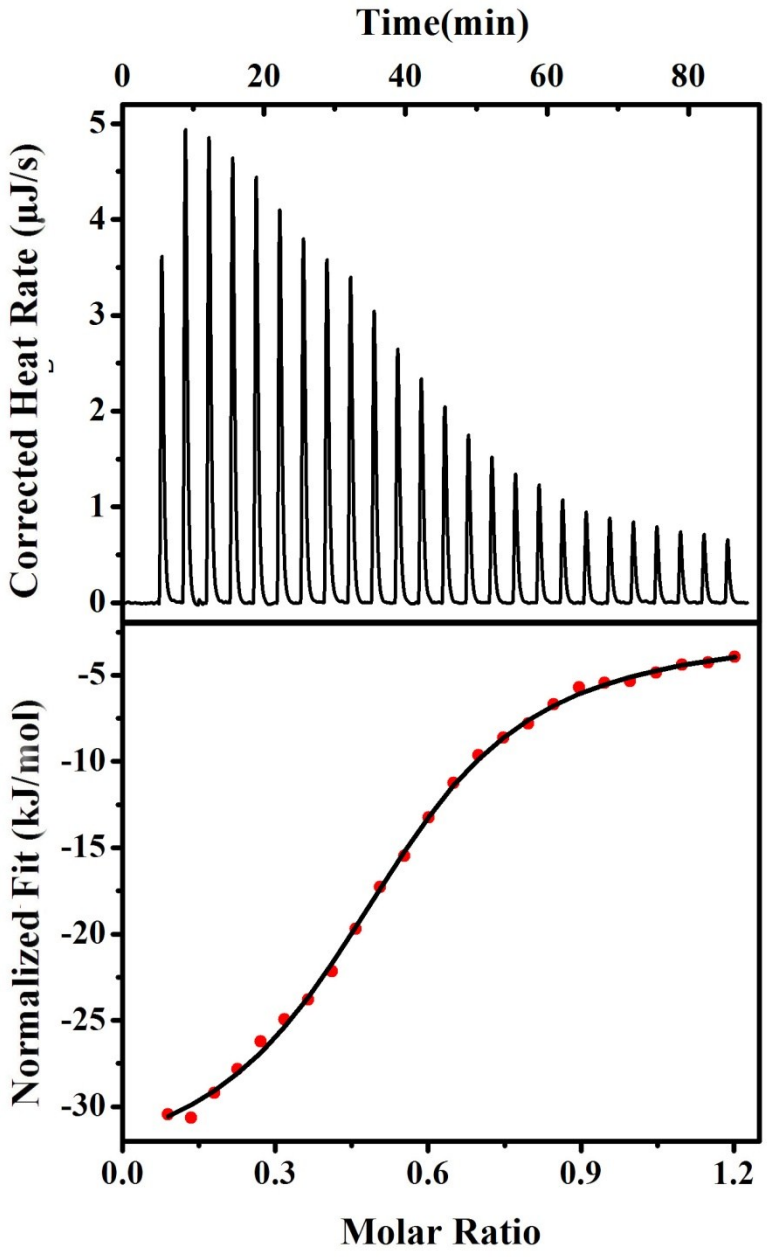
Figures S17. Isothermal Titration Calorimetry for the *i*Q[7]-BPY^{2+}system.



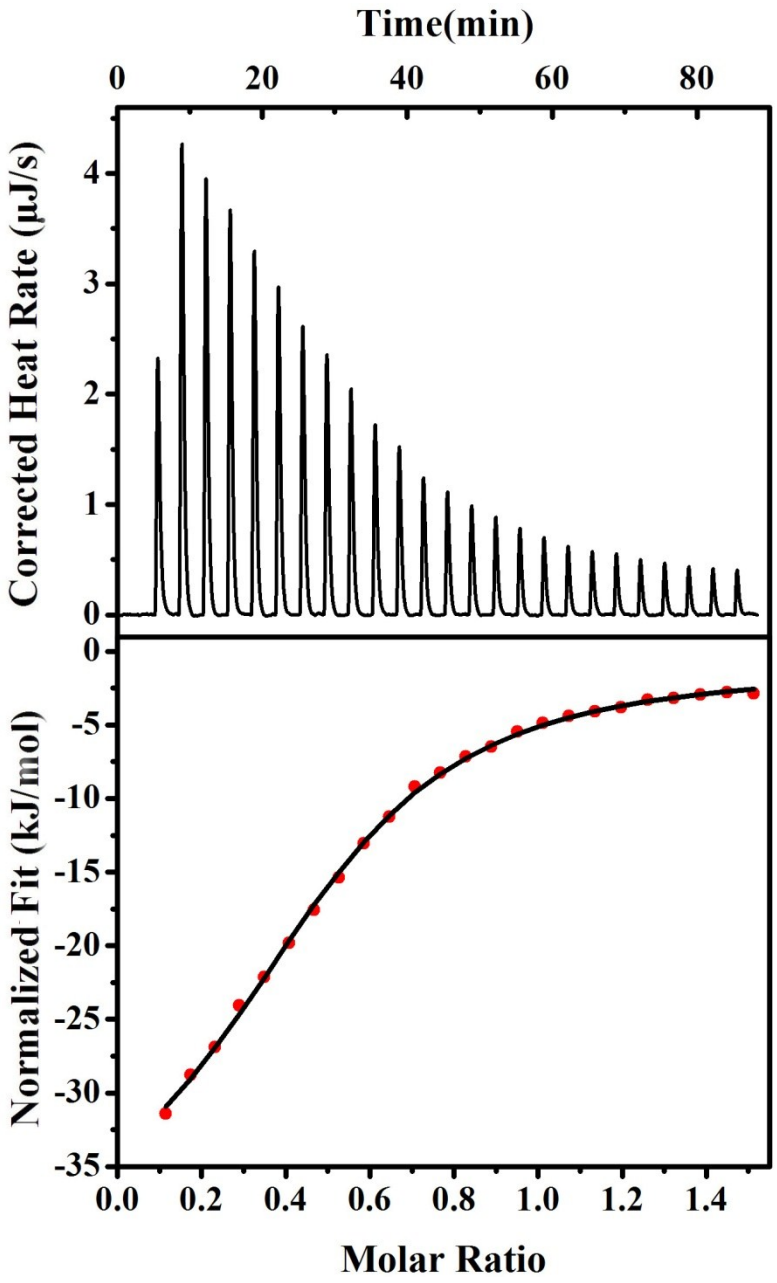
Figures S18. Isothermal Titration Calorimetry for the *i*Q[7]- MV^{2+} system.



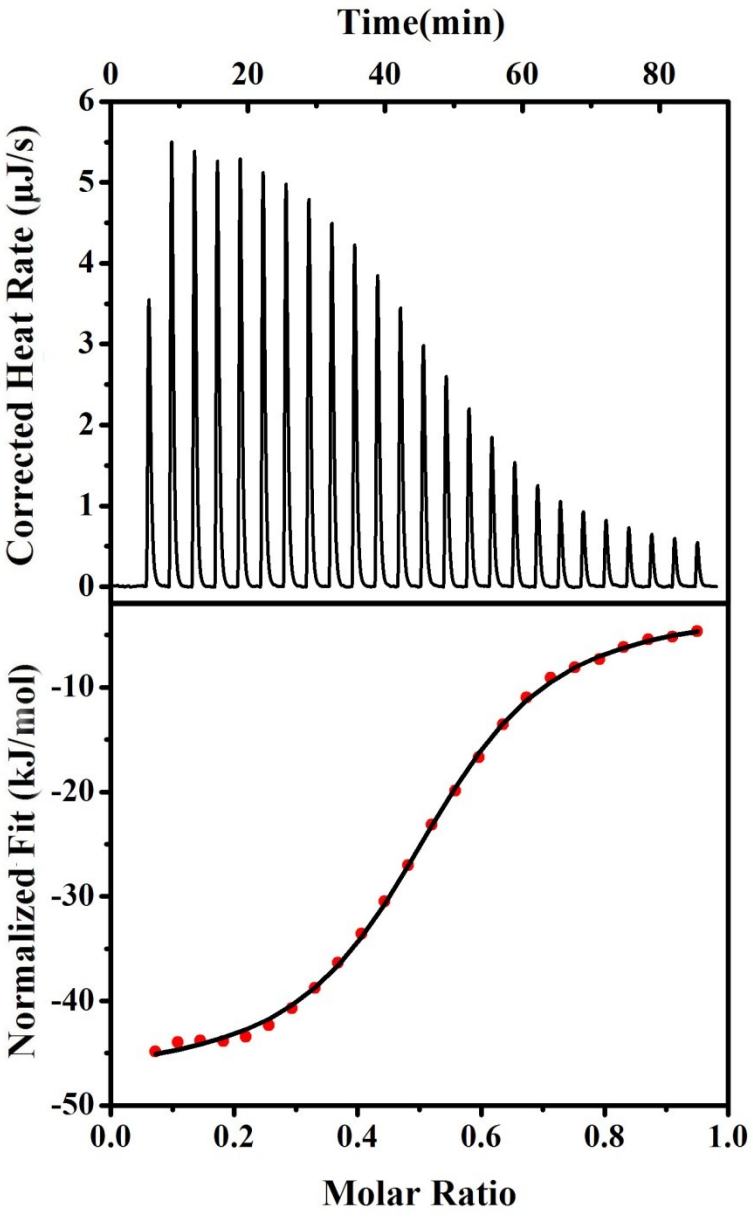
Figures S19. Isothermal Titration Calorimetry for the *i*Q[7]- EV^{2+} system.



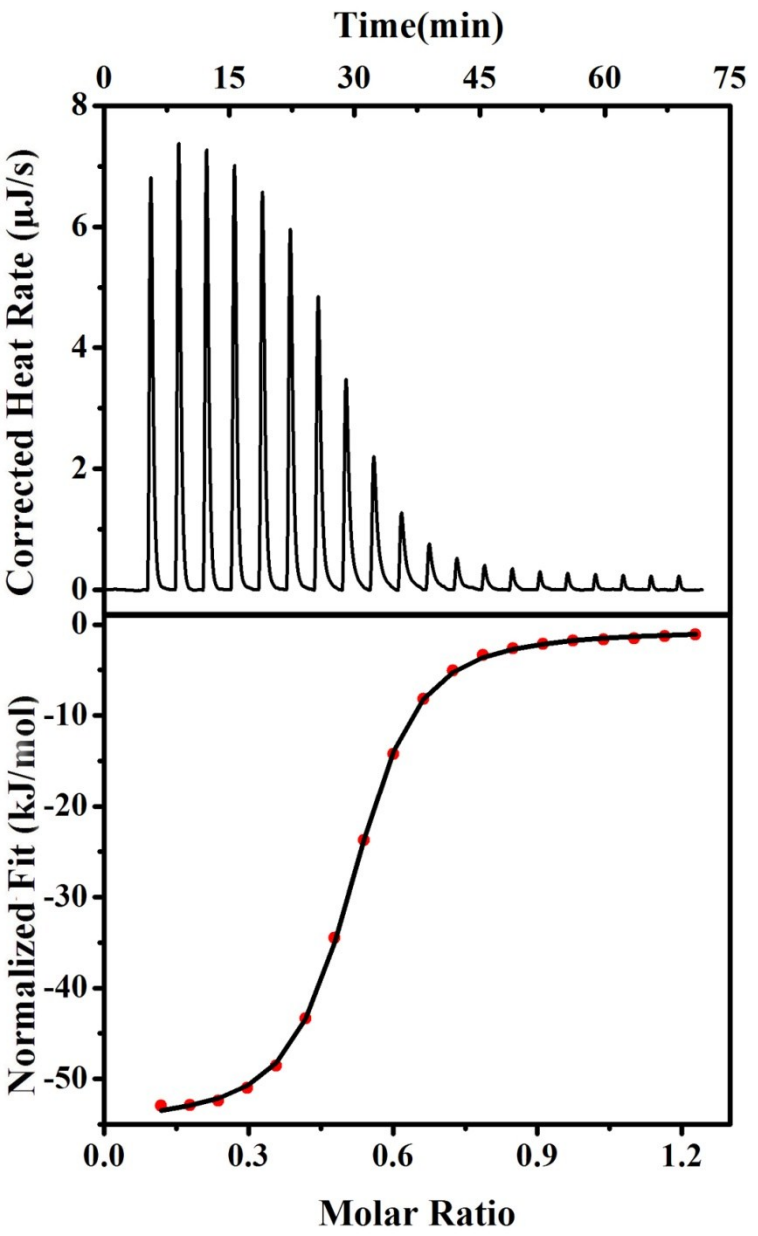
Figures S20. Isothermal Titration Calorimetry for the *i*Q[7]- PV^{2+} system.



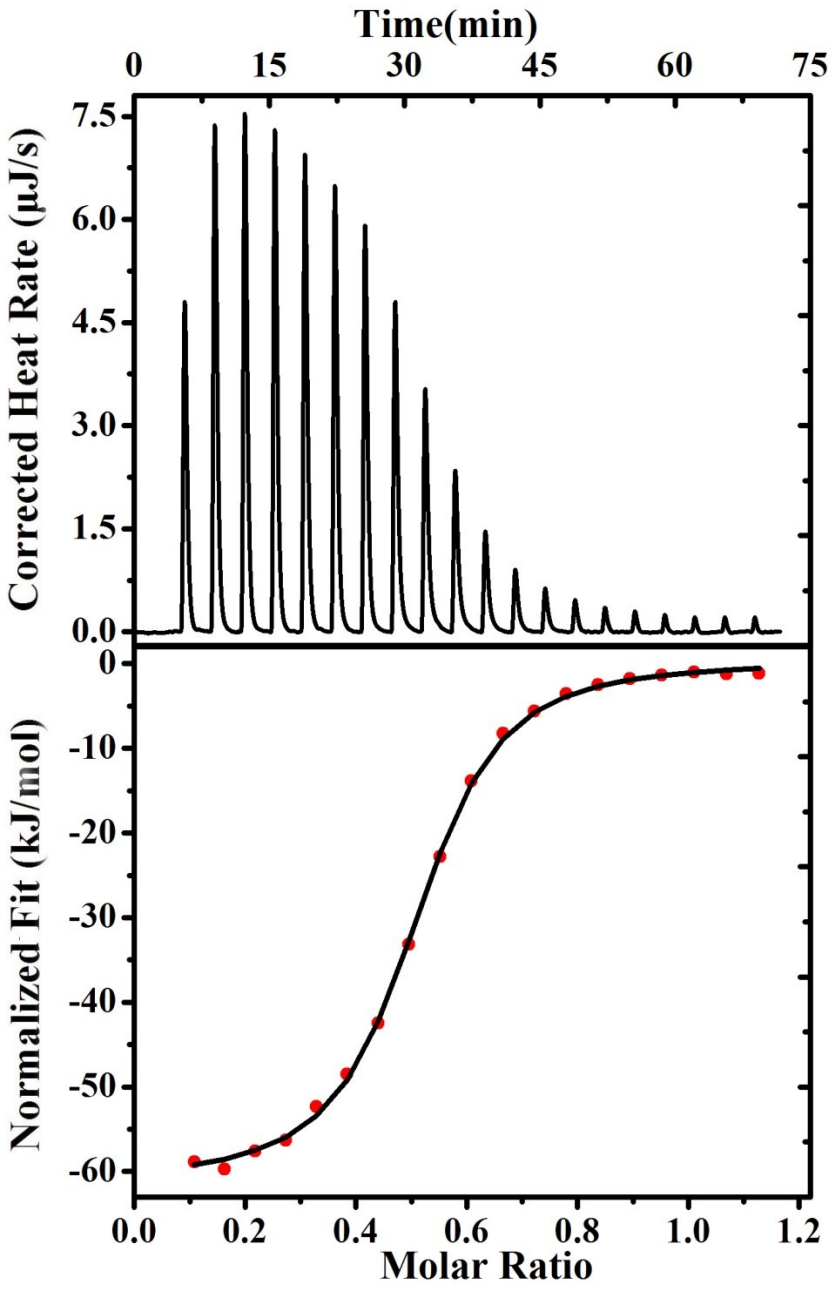
Figures S21. Isothermal Titration Calorimetry for the *i*Q[7]- BV^{2+} system.



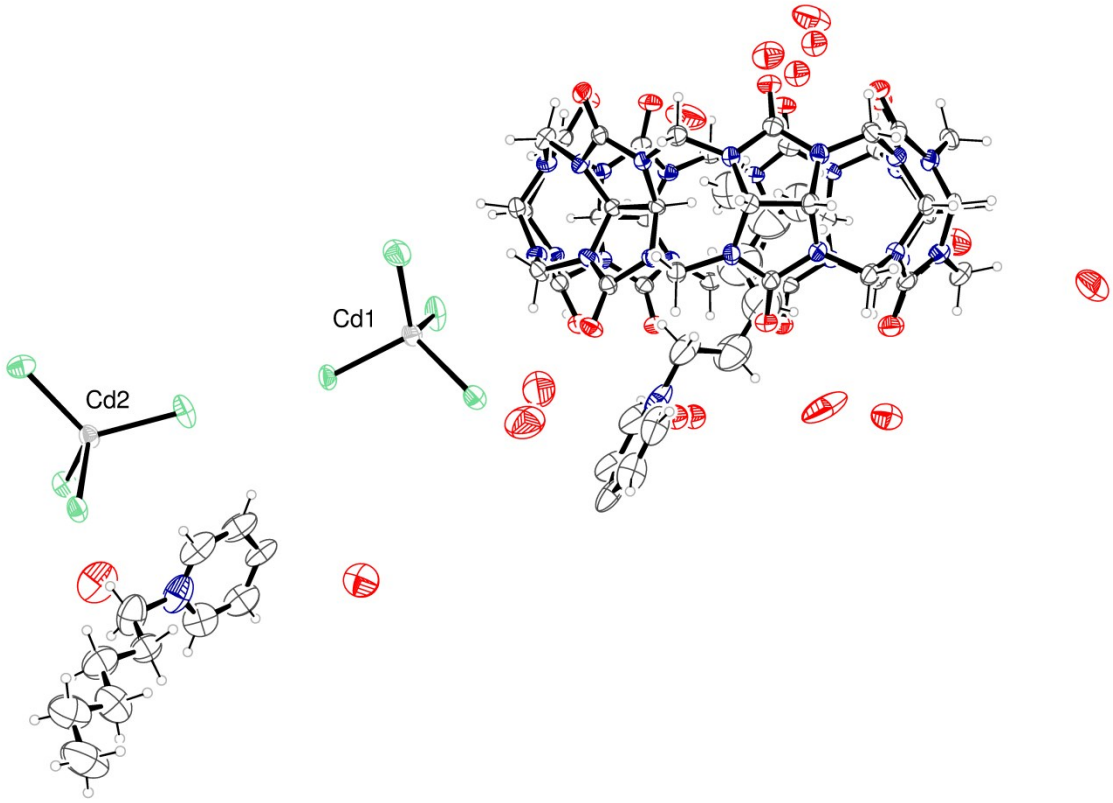
Figures S22. Isothermal Titration Calorimetry for the *i*Q[7]- FV^{2+}system.



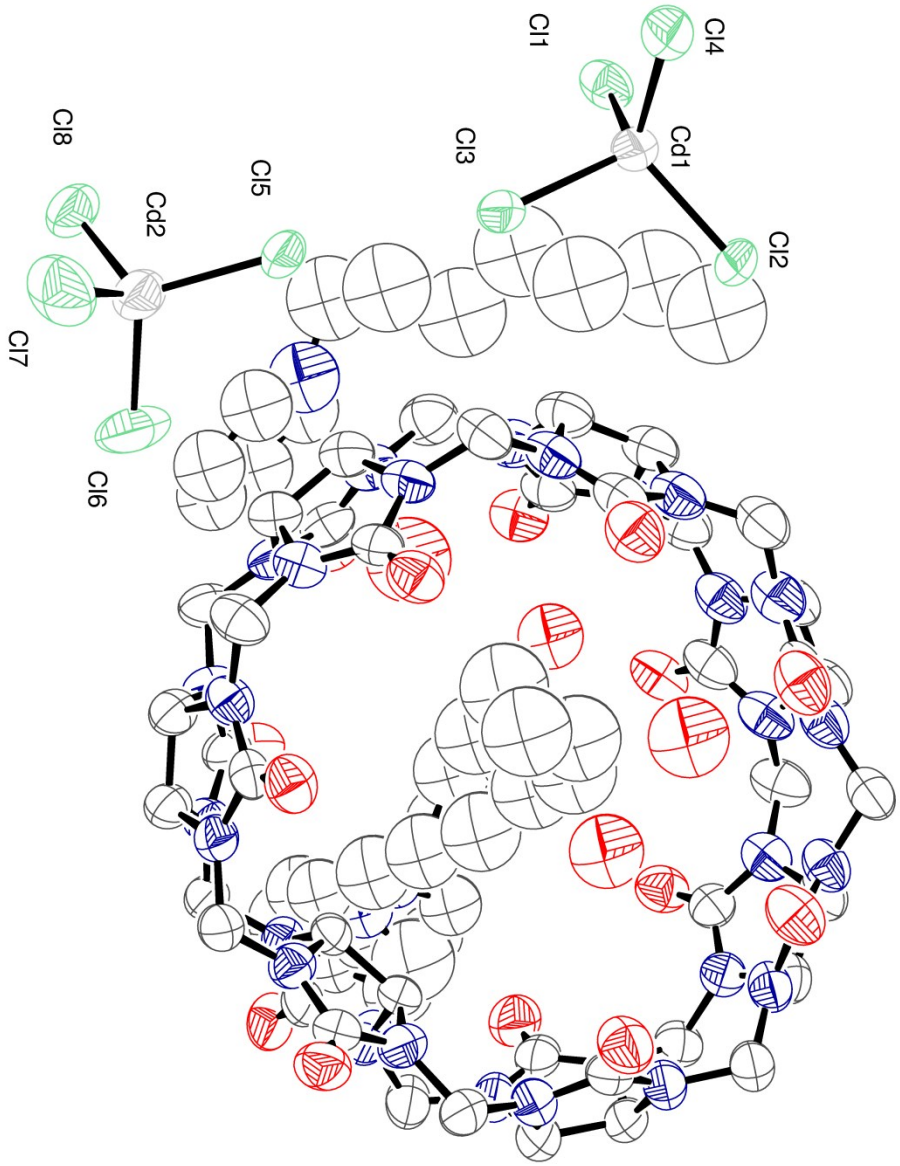
Figures S23. Isothermal Titration Calorimetry for the *i*Q[7]- HV^{2+} system.



Figures S24. Isothermal Titration Calorimetry for the *i*Q[7]- SV^{2+}system.



Figures S25. ORTEP of asymmetric unit of *i*Q[7]- HV^{2+} system with atoms drawn as 30% probability ellipsoids.



Figures S26. ORTEP of asymmetric unit of *i*Q[7]- SV^{2+} system.