Electronic Supporting Information

Ferrocene and ferrocenium inclusion compounds with cucurbiturils: A study of metal atom dynamics probed by Mössbauer spectroscopy

Clara I. R. Magalhães,^a Ana C. Gomes,^a André D. Lopes,^b Isabel S. Gonçalves,^a Martyn Pillinger,^{*a} Eunyoung Jin,^c Ikjin Kim,^d Young Ho Ko,^e Kimoon Kim,^{c,d,e} Israel Nowik^f and Rolfe H. Herber^{*f}

- a Department of Chemistry, CICECO Aveiro Institute of Materials, Campus
 Universitário de Santiago, University of Aveiro, 3810-193 Aveiro, Portugal. E-mail:
 mpillinger@ua.pt.
- b Faculty of Science and Technology, CIQA, University of the Algarve, Campus de Gambelas, 8005-136 Faro, Portugal
- c Department of Chemistry, Pohang University of Science and Technology (POSTECH), Pohang, 790-784, Korea.
- d Division of Advanced Materials Science, Pohang University of Science and Technology (POSTECH), Pohang, 790-784, Korea
- e Center for Self-assembly and Complexity (CSC), Institute for Basic Science (IBS), Pohang, 790-784, Korea
- f Racah Institute of Physics, The Hebrew University of Jerusalem, 91904 Jerusalem, Israel. E-mail: rolfe.herber@mail.huji.ac.il



Fig. S1. 1 H-NMR (850 MHz, D₂O) spectra of 1:1 complexes (a) 4 and (b) 5.



Fig. S2. MALDI-TOF mass spectrum of CB7·ferrocenium complex 6a.



Fig. S3. ²³Na NMR spectrum (132 MHz, D₂O) of 1:1 inclusion complex 5.



Fig. S4. ^{31}P NMR spectrum (203 MHz, D2O) of 1:1 inclusion complex 6a.



Fig. S5. Powder XRD patterns of (a) $FcPF_6$, (b) CB7, (c) inclusion compound **6b**, (d) CB8 and (e) inclusion compound **7**.



Fig. S6. Representative SEM images of the inclusion compounds (a) 6b and (b) 7.



Fig. S7. TGA (**A**) and DTG (**B**) profiles for $FcPF_6$ (- · - ·), CB7 (- - -), inclusion compound **6b** (-----), CB8 (- · - · ·) and inclusion compound **7** (-----).



Fig. S8. FTIR spectra (KBr) of (a) FcPF₆, (b) CB7, (c) inclusion compound **6b**, (d) CB8 and (e) inclusion compound **7**.