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 Nowikf 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, D$_2$O) spectra of 1:1 complexes (a) 4 and (b) 5.

Fig. S2. MALDI-TOF mass spectrum of CB7-ferrocenium complex 6a.
**Fig. S3.** $^{23}$Na NMR spectrum (132 MHz, D$_2$O) of 1:1 inclusion complex 5.

**Fig. S4.** $^{31}$P NMR spectrum (203 MHz, D$_2$O) of 1:1 inclusion complex 6a.
Fig. S5. Powder XRD patterns of (a) FcPF₆, (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) FcPF$_6$, (b) CB7, (c) inclusion compound 6b, (d) CB8 and (e) inclusion compound 7.