Electronic Supplementary Information

Base-iodine-promoted metal-catalyst-free reactions of [60]fullerene with β-keto esters for selective formation of [60]fullerene derivatives

Han-Lin Yang^a, Li-Jun Xu^{b,c}, Wen-Zhong Li^a, Tao Sun^d, Bao-Rong Duan^a, Si Chen^{*,a} and Xiang Gao^b

^aCollege of Chemistry and Chemical Engineering, Yantai University 30 Qingquan Road, Yantai, Shandong 264005, China

^bState Key Laboratory of Electroanalytical Chemistry, Changchun Institute of Applied Chemistry,

Chinese Academy of Sciences, 5625 Renmin Street, Changchun, Jilin 130022, China

^cUniversity of Science and Technology of China, Hefei, Anhui 230026, China

^dSchool of Materials Science and Engineering, Nanyang Technological University, Singapore 639798, Singapore

* E-mail: sichen@ytu.edu.cn; chemchensi@163.com

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Figure S1. UV-visible spectrum of compound 2a in toluene.



Figure S2. MALDI-TOF MS of compound 2a



Figure S3. ¹H NMR spectrum (600 MHz) of compound **2a** recorded in CS₂ with DMSO-*d*₆ as the external lock. The resonances at 2.5 ppm and 3.3 ppm are due to the DMSO solvent and H_2O in DMSO respectively.



Figure S4. ¹³C NMR spectrum (151 MHz) of compound **2a** recorded in CS₂ with DMSO- d_6 as the external lock.



Figure S5. UV-visible spectrum of compound 3a in toluene.



Figure S6. MALDI-TOF MS of compound 3a



Figure S7. ¹H NMR spectrum (600 MHz) of compound **3a** recorded in CS₂ with DMSO-*d*₆ as the external lock. The resonances at 2.5 ppm and 3.3 ppm are due to the DMSO solvent and H_2O in DMSO respectively.



Figure S8. ¹³C NMR spectrum (151 MHz) of compound **3a** recorded in CS₂ with DMSO- d_6 as the external lock.



Figure S9. UV-visible spectrum of compound 2b in toluene.



Figure S10. MALDI-TOF MS of compound 2b



Figure S11. ¹H NMR spectrum (600 MHz) of compound **2b** recorded in CS₂ with DMSO- d_6 as the external lock. The resonances at 2.5 ppm and 3.3 ppm are due to the DMSO solvent and H₂O in DMSO respectively.



Figure S12. ¹³C NMR spectrum (151 MHz) of compound **2b** recorded in CS₂ with DMSO-*d*₆ as the external lock.



Figure S13. UV-visible spectrum of compound 3b in toluene.



Figure S14. MALDI-TOF MS of compound 3b



Figure S15. ¹H NMR spectrum (600 MHz) of compound **3b** recorded in CS₂ with DMSO- d_6 as the external lock. The resonances at 2.5 ppm and 3.3 ppm are due to the DMSO solvent and H₂O in DMSO respectively. The peaks labeled with asterisks belong to toluene residue in the sample.



Figure S16. ¹³C NMR spectrum (151 MHz) of compound **3b** recorded in CS₂ with DMSO-*d*₆ as the external lock. The peaks labeled with asterisks belong to toluene residue in the sample.



Figure S17. UV-visible spectrum of compound 2c in toluene.



Figure S18. MALDI-TOF MS of compound 2c



Figure S19. ¹H NMR spectrum (500 MHz) of compound **2c** recorded in CS_2 -CDCl₃ (v/v=2:1). The resonance at 7.26 ppm is due to the CHCl₃ solvent.



Figure S20. ¹³C NMR spectrum (151 MHz) of compound **2c** recorded in CS₂-CDCl₃ (v/v=2:1).



Figure S21. UV-visible spectrum of compound 3c in toluene.



Figure S22. MALDI-TOF MS of compound 3c



Figure S23. ¹H NMR spectrum (600 MHz) of compound **3c** recorded in CS_2 -CDCl₃ (v/v=2:1). The resonance at 7.26 ppm is due to the CHCl₃ solvent.



Figure S24. ¹³C NMR spectrum (151 MHz) of compound **3c** recorded in CS_2 -CDCl₃ (v/v=2:1).



Figure S25. UV-visible spectrum of compound 2d in toluene.



Figure S26. MALDI-TOF MS of compound 2d



Figure S27. ¹H NMR spectrum (600 MHz) of compound **2d** recorded in CS_2 -CDCl₃ (v/v=2:1). The resonance at 7.26 ppm is due to the CHCl₃ solvent.



Figure S28. ¹³C NMR spectrum (151 MHz) of compound **2d** recorded in CS₂-CDCl₃ (v/v=2:1).



Figure S29. UV-visible spectrum of compound 3d in toluene.



Figure S30. MALDI-TOF MS of compound 3d



Figure S31. ¹H NMR spectrum (600 MHz) of compound **3d** recorded in CS_2 -CDCl₃ (v/v=2:1). The resonance at 7.26 ppm is due to the CHCl₃ solvent.



Figure S32. ¹³C NMR spectrum (151 MHz) of compound **3d** recorded in CS_2 -CDCl₃ (v/v=2:1).



Figure S33. UV-visible spectrum of compound 2e in toluene.



Figure S34. MALDI-TOF MS of compound 2e



Figure S35. ¹H NMR spectrum (600 MHz) of compound **2e** recorded in CS₂-CDCl₃ (v/v=2:1).



Figure S36. ¹³C NMR spectrum (151 MHz) of compound **2e** recorded in CS_2 -CDCl₃ (v/v=2:1).



Figure S37. UV-visible spectrum of compound 3e in toluene.



Figure S38. MALDI-TOF MS of compound 3e



Figure S39. ¹H NMR spectrum (600 MHz) of compound **3e** recorded in CS_2 -CDCl₃ (v/v=2:1).



Figure S40. ¹³C NMR spectrum (151 MHz) of compound **3e** recorded in CS₂-CDCl₃ (v/v=2:1). The peaks labeled with asterisks belong to toluene residue in the sample.



Figure S41. UV-visible spectrum of compound 2f in toluene.



Figure S42. MALDI-TOF MS of compound 2f



Figure S43. ¹H NMR spectrum (600 MHz) of compound **2f** recorded in CS₂-CDCl₃ (v/v=2:1). The resonance at 7.26 ppm is due to the CHCl₃ solvent.



Figure S44. ¹³C NMR spectrum (151 MHz) of compound **2f** recorded in CS₂-CDCl₃ (v/v=2:1).



Figure S45. UV-visible spectrum of compound 3f in toluene.



Figure S46. MALDI-TOF MS of compound 3f



Figure S47. ¹H NMR spectrum (600 MHz) of compound **3f** recorded in CS_2 -CDCl₃ (v/v=2:1). The resonance at 7.26 ppm is due to the CHCl₃ solvent.



Figure S48. ¹³C NMR spectrum (151 MHz) of compound **3f** recorded in CS₂-CDCl₃ (v/v=2:1). The peaks labeled with asterisks belong to toluene residue in the sample.