

Electronic Supplementary Information

Pentamethylcyclopentadienyl molybdenum(V) complexes derived from iodoanilines: synthesis, structure, and ROP of ϵ -caprolactone.

Tian Xing,^a Mark R. J. Elsegood,^b Sophie H. Dale^b and Carl Redshaw^{a*}

^a *Plastics Collaboratory, Department of Chemistry, The University of Hull, Cottingham Rd, Hull, HU6 7RX, U.K.*

^b *Chemistry Department, Loughborough University, Loughborough, Leicestershire, LE11 3TU, U.K.*

Contents

Figure S1. Alternative views of **1**.

Figure S2. Views of the molecular structure of $[2\text{-I-NH}_3\text{C}_6\text{H}_4]^+\text{Cl}^-$.

Figure S3. Packing of complex **2**·MeCN.

Figure S4. Packing views of **3**.

Figure S5. Different views of $[3\text{-I-NH}_3\text{C}_6\text{H}_4]^+\text{Cl}^-$.

Figure S6. Different views of the packing of **4**.

Figure S7. Packing of complex **5**.

Figure S8. Alternative view and packing of **6**·MeCN

Figure S9. Packing of complex **7**.

Figure S10. Packing of aniline complex **8**.

Figure S11. ^1H NMR spectrum (CDCl_3 , 400 MHz, 298 K) of the PCL synthesized with **3**/BnOH at 130 °C under N_2 (entry 7, Table 1).

Figure S12. Mass spectrum of the PCL synthesized with **2**/BnOH (entry 2, Table 1).

Figure S13. Mass spectrum of the PCL synthesized with **2**/BnOH (entry 2, Table 2).

Figure S14. Mass spectrum of the PCL synthesized with **2**/BnOH (entry 5, Table 3).

Figure S15. Kinetics for **8** *versus* **2**.

Figure S1. Alternative views of **1**.

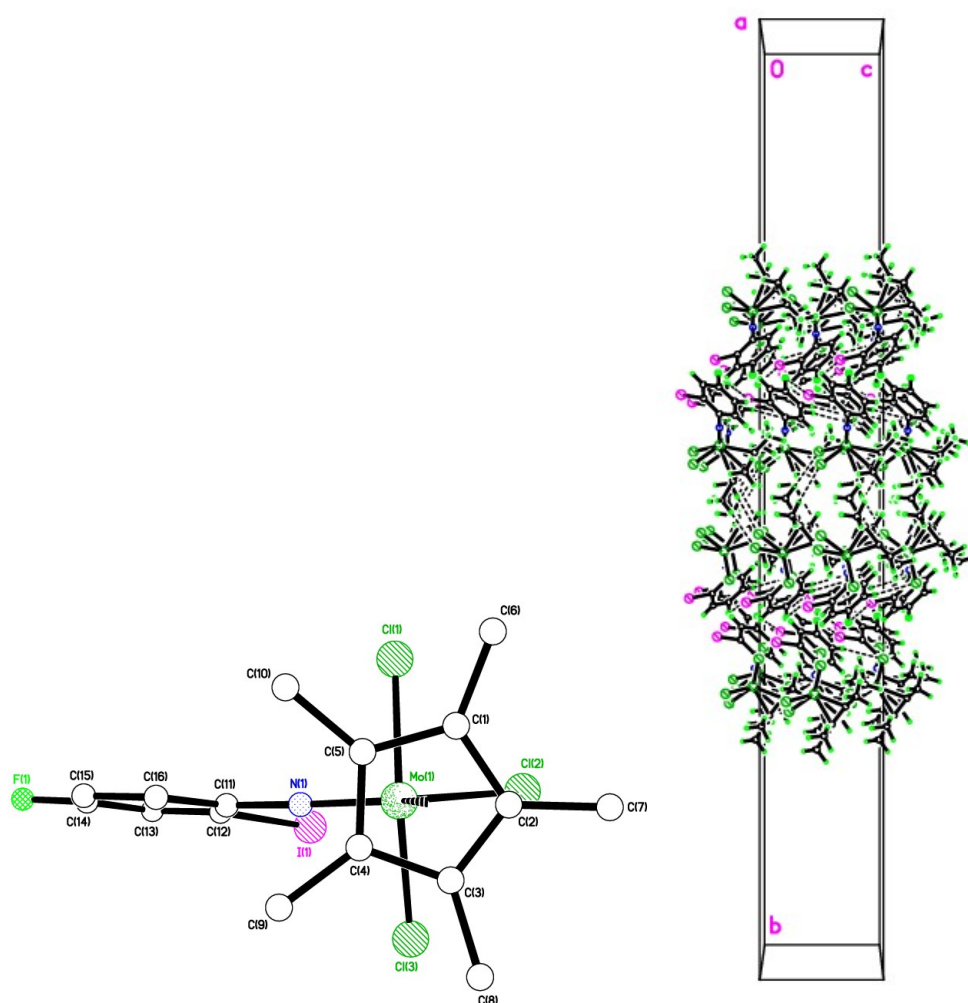
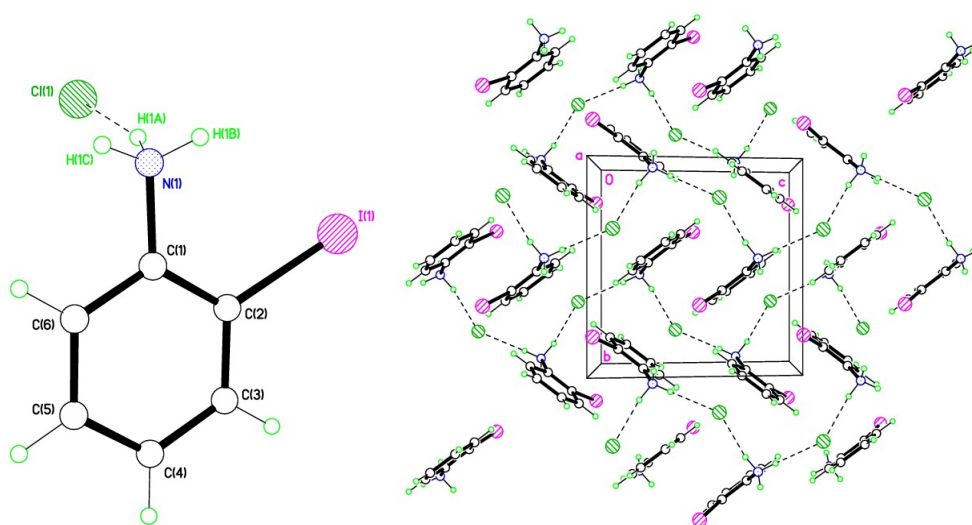


Figure S2. Views of the molecular structure of $[2\text{-I-NH}_3\text{C}_6\text{H}_4]^+\text{Cl}^-$.



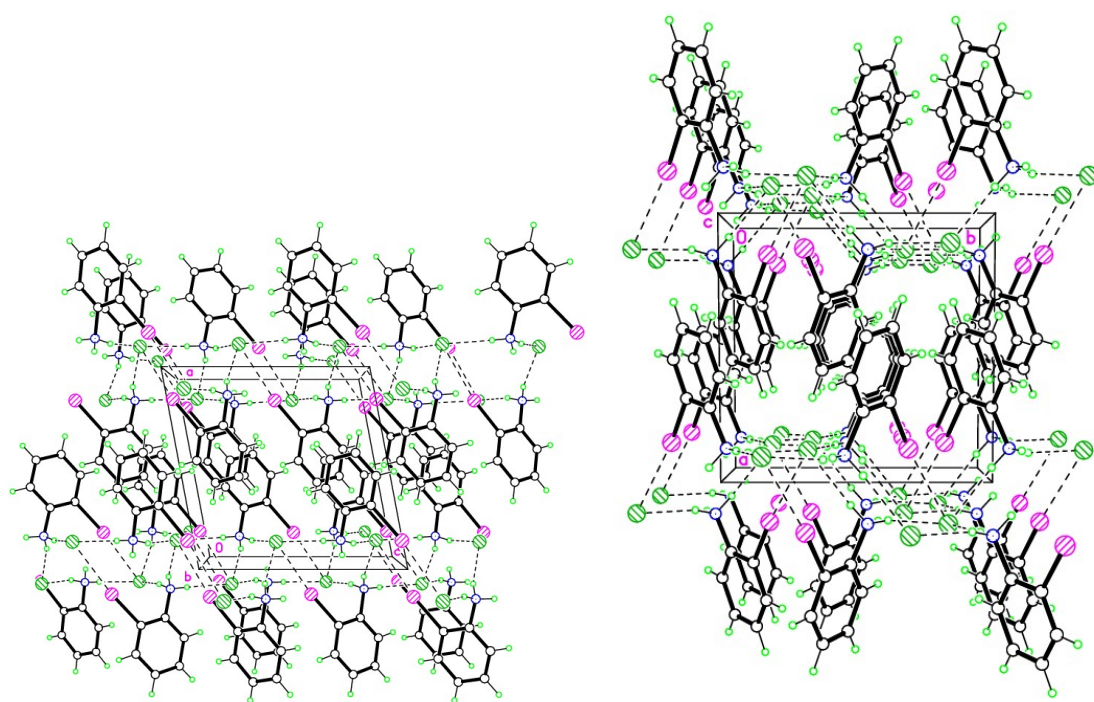


Figure S3. Packing of complex 2·MeCN.

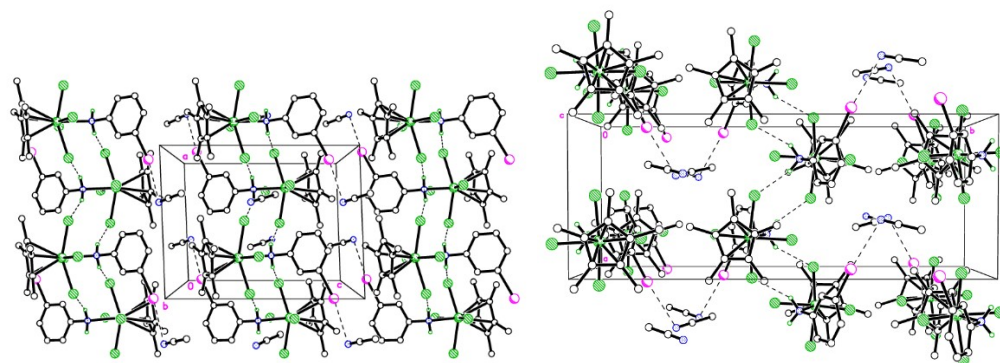


Figure S4. Packing views of **3**.

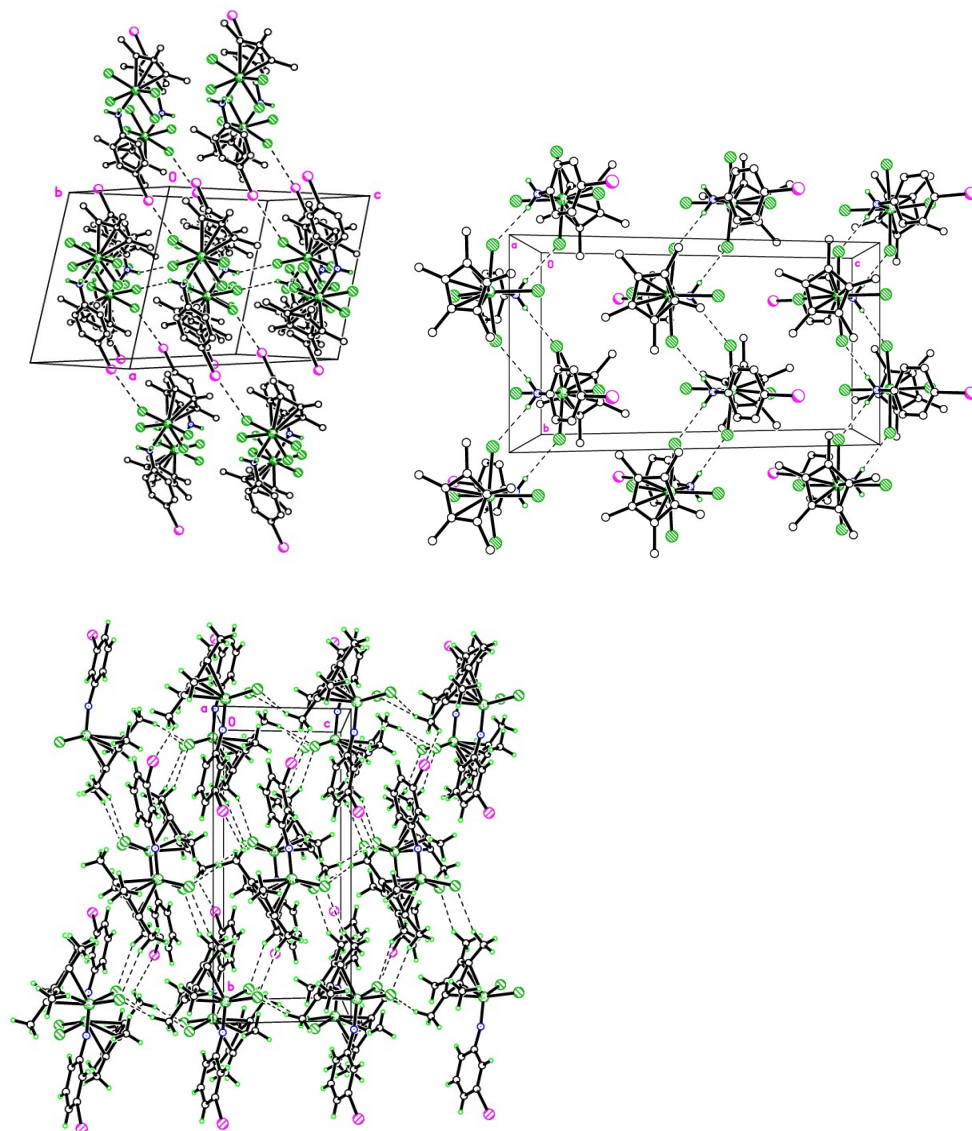


Figure S5. Different views of $[3\text{-I-NH}_3\text{C}_6\text{H}_4]^+\text{Cl}^-$.

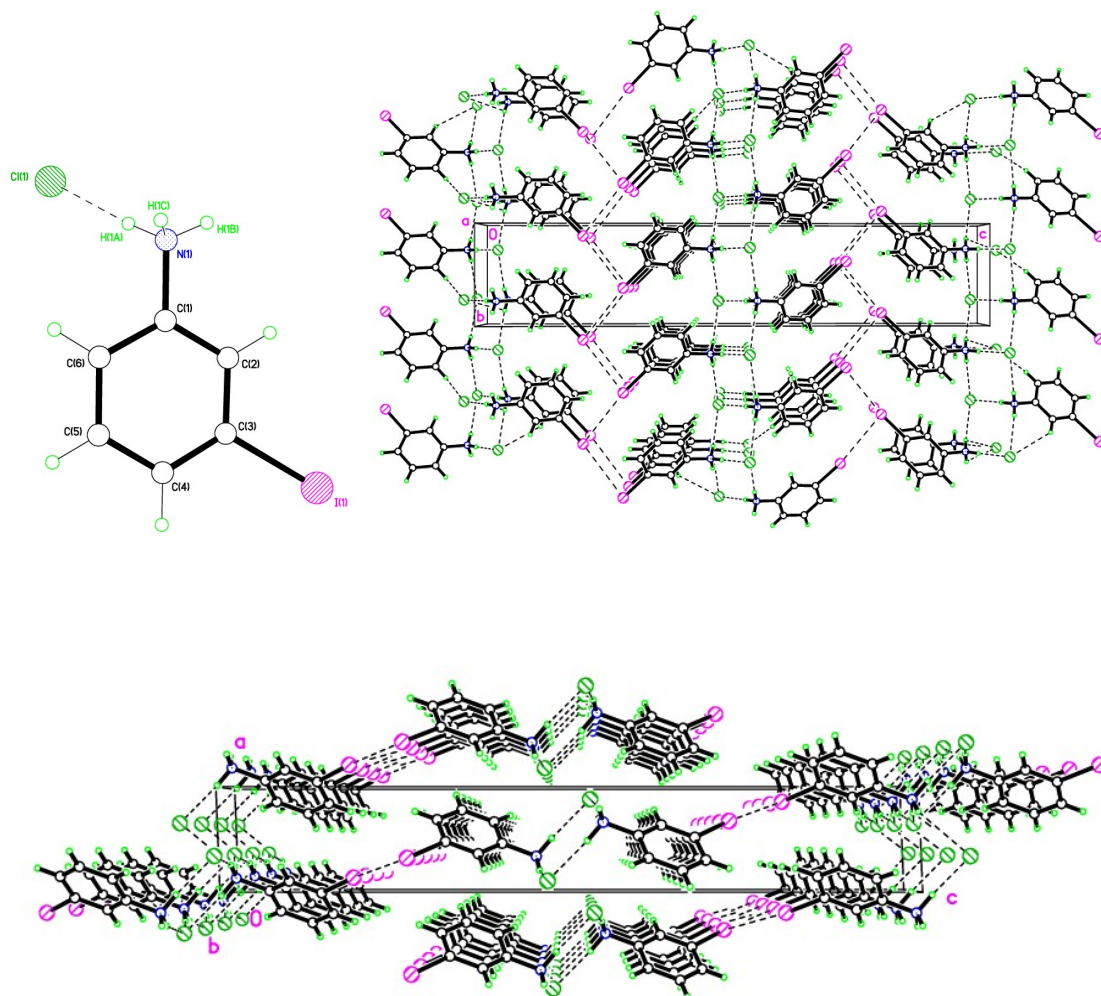


Figure S6. Different views of the packing of 4.

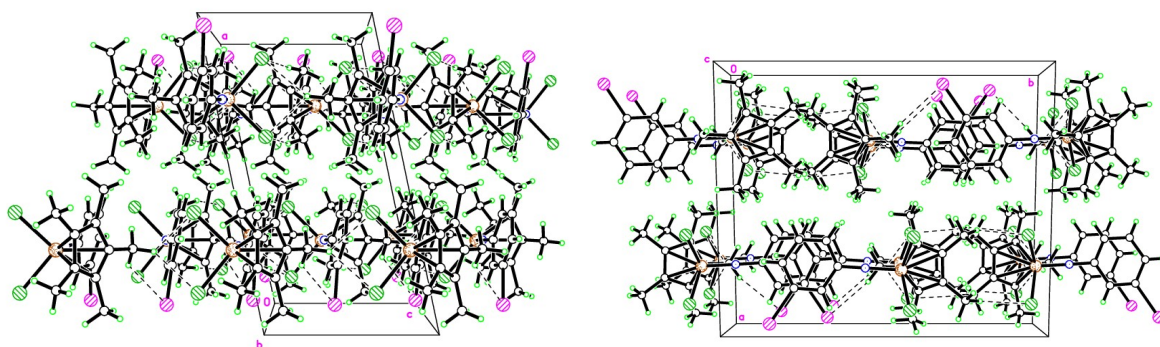


Figure S7. Packing of complex 5.

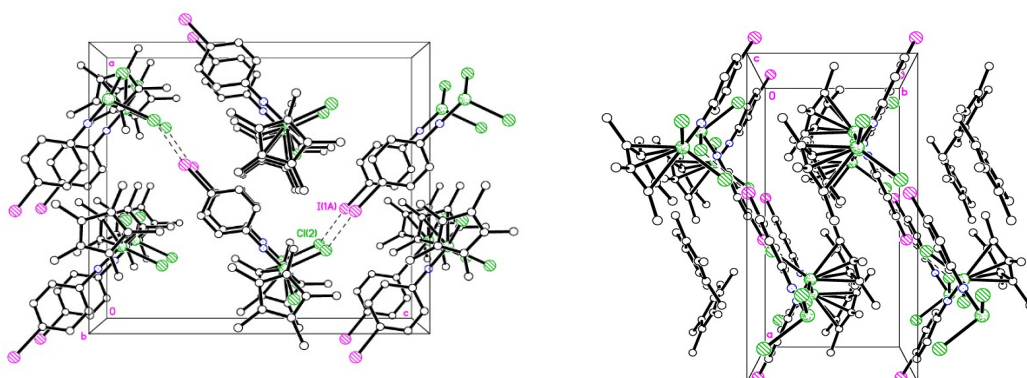
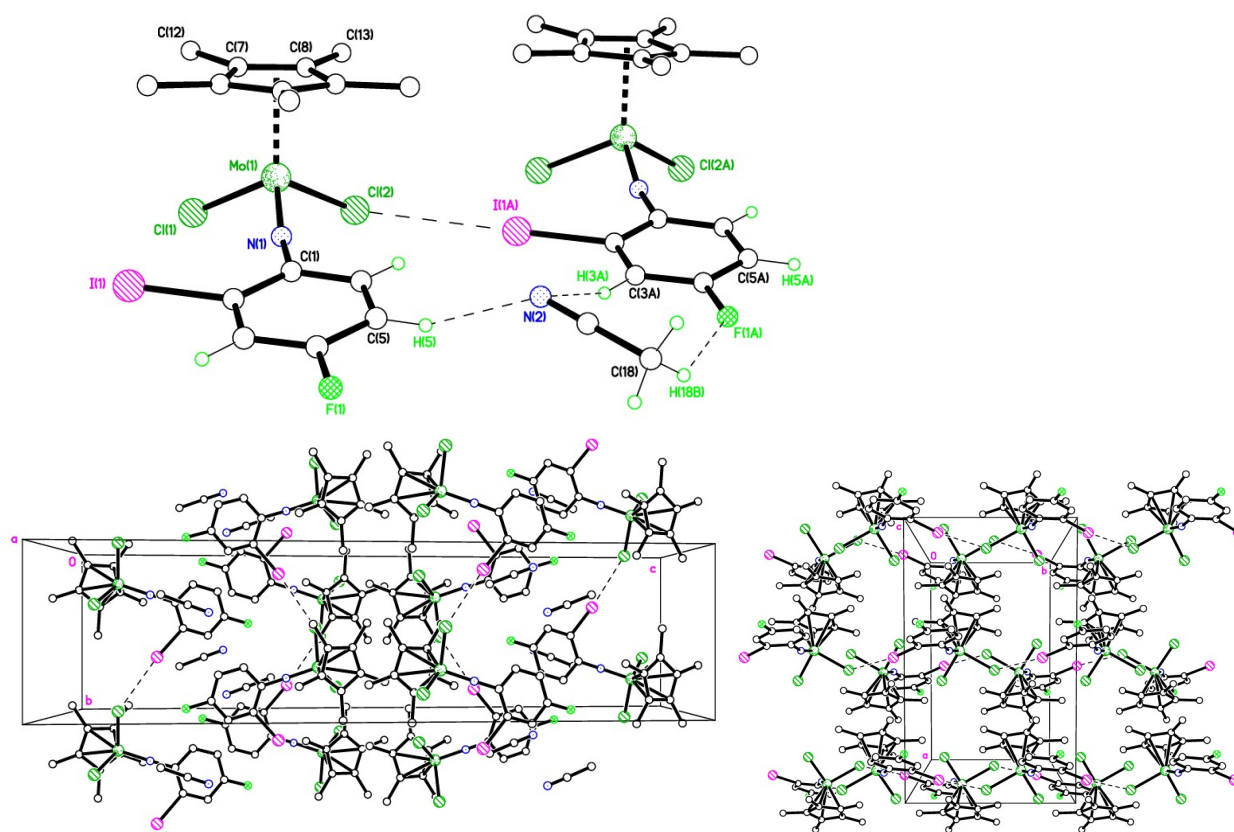


Figure S8. Alternative view and packing of 6·MeCN



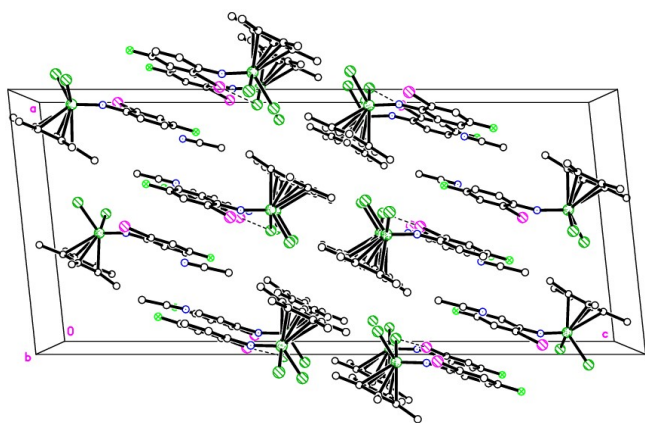


Figure S9. Packing of complex 7.

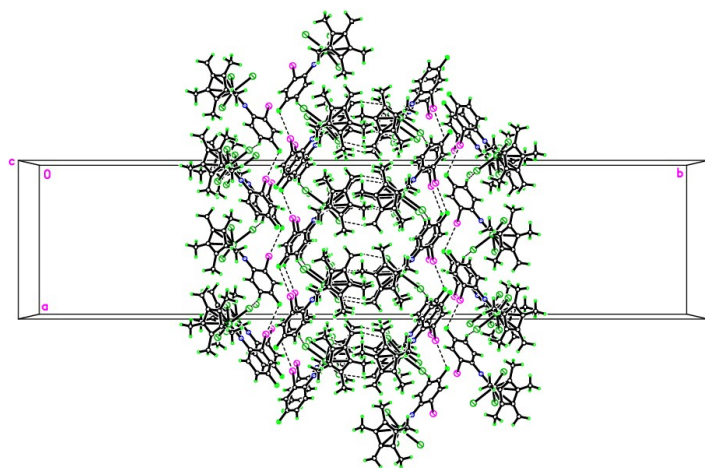


Figure S10. Packing of aniline complex 8.

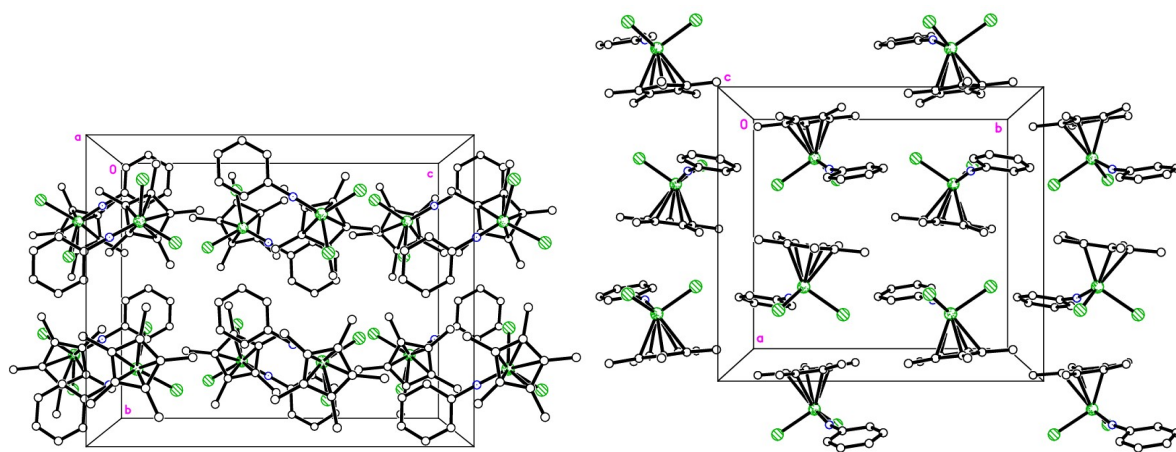


Figure S11. ^1H NMR spectrum (CDCl_3 , 400 MHz, 298 K) of the PCL synthesized with **3**/BnOH at 130 °C under N_2 (entry 7, Table 1).

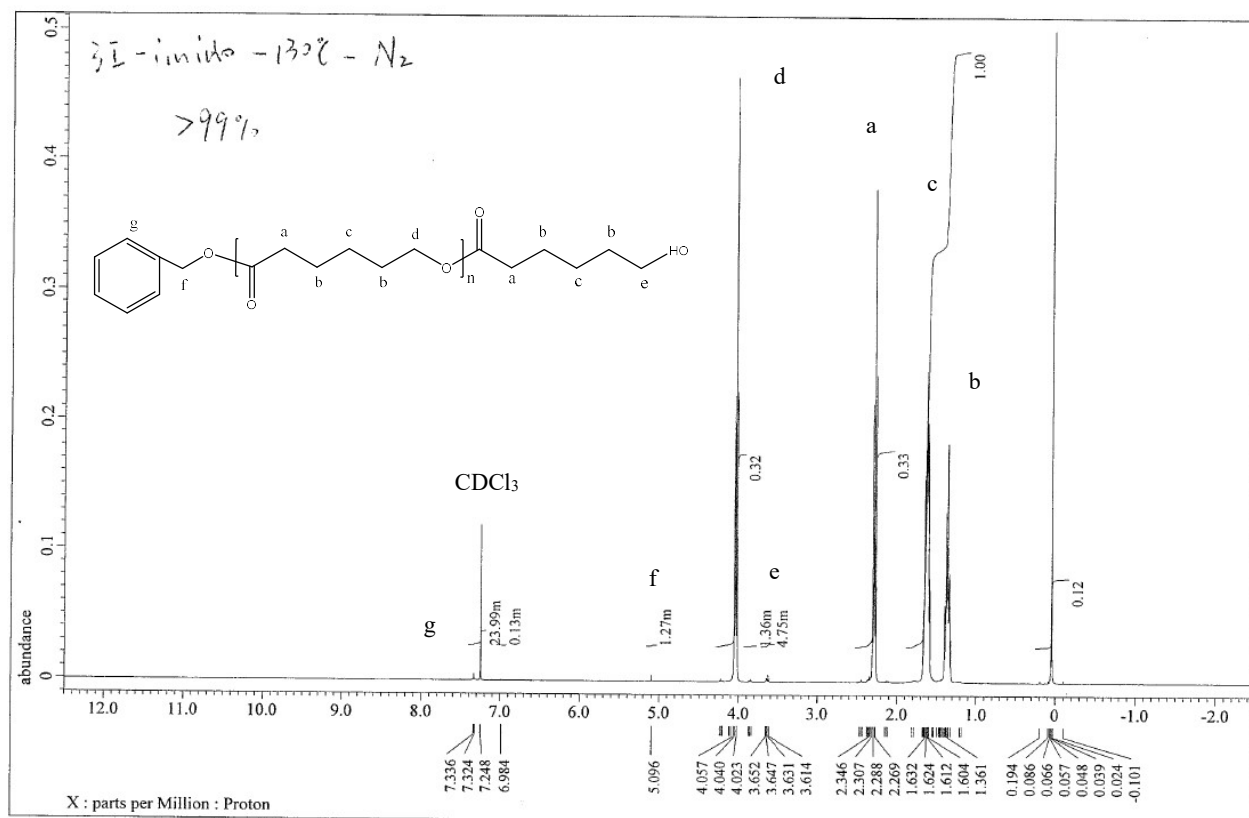


Figure S12. Mass spectrum of the PCL synthesized with 2/BnOH (entry 2, Table 1).

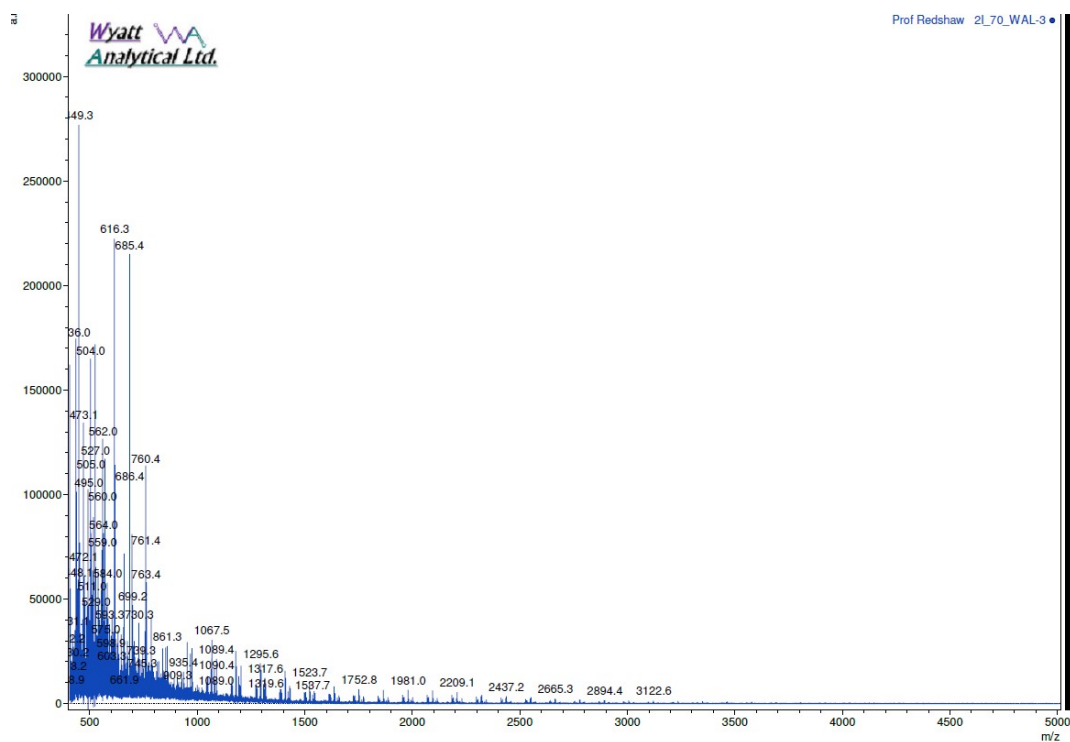


Figure S13. Mass spectrum of the PCL synthesized with **2**/BnOH (entry 2, Table 2).

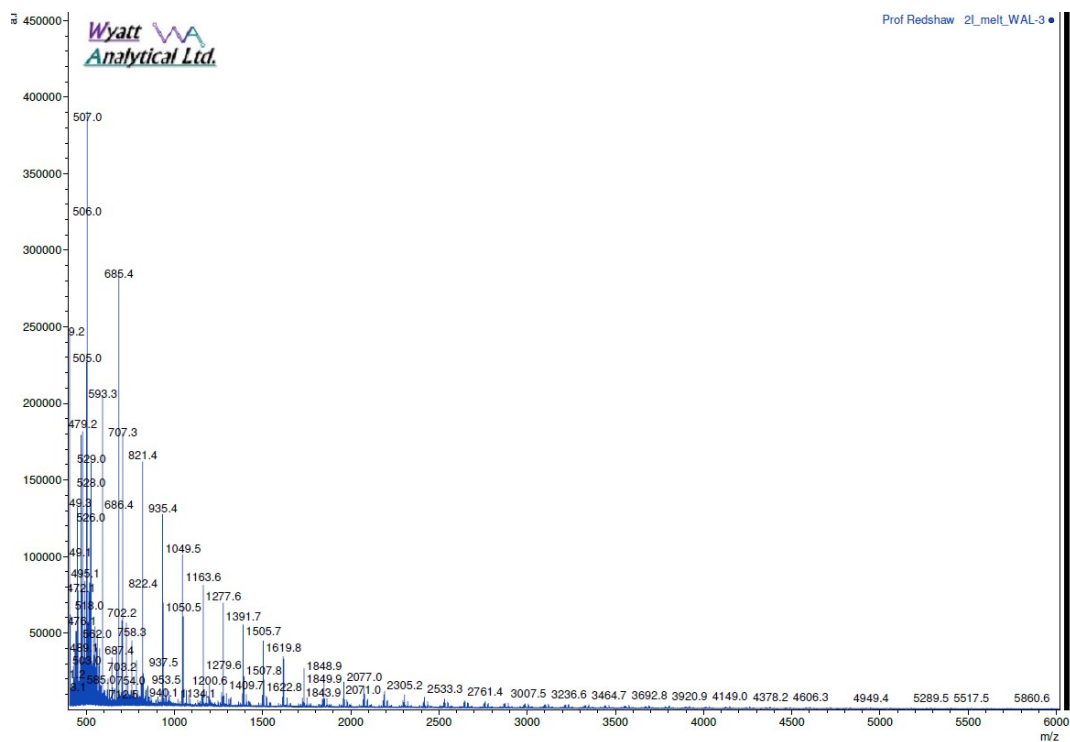


Figure S14. Mass spectrum of the PCL synthesized with **2**/BnOH (entry 5, Table 3).

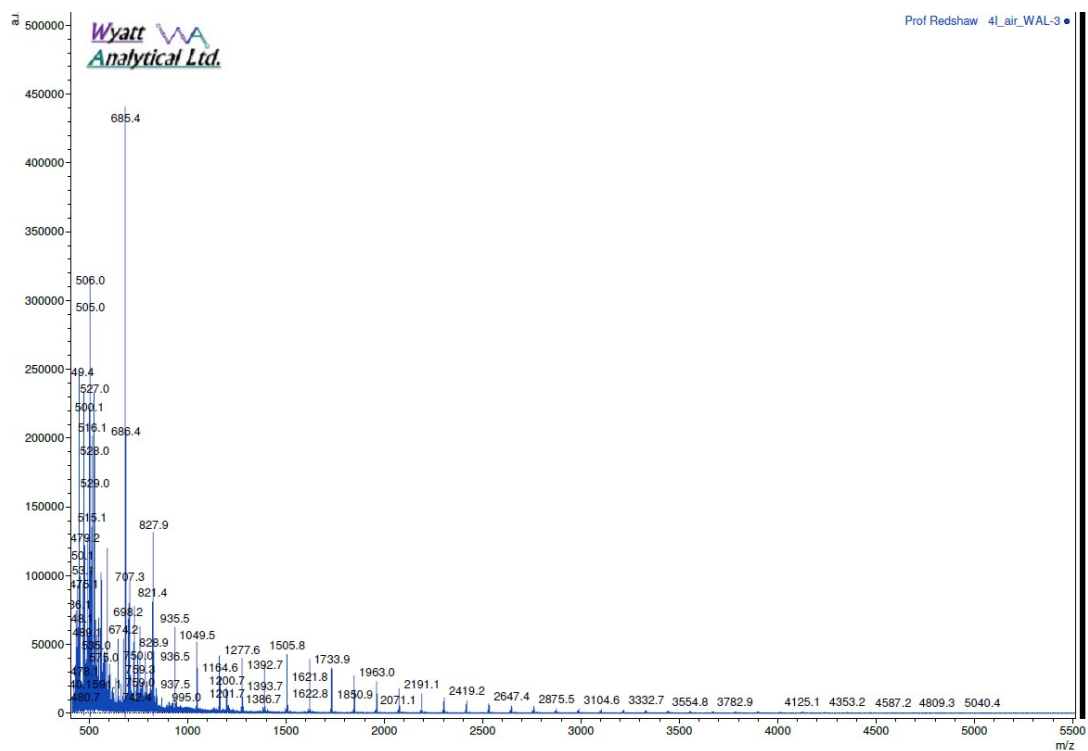


Figure S15. Kinetics for **8** versus **2**.

