10.1071/CH21189
Australian Journal of Chemistry

Supplementary Material

Properties tuning of supramolecular discotics by non-mesogenic triazines and acids

Chunming He[A], *Kunlun Wang*[A,*], *Yue Wang*[A], *Shengang Xu*[A], *Yingliang Liu*[A,*] and *Shaokui Cao*[A,*]

[A]Henan Key Laboratory of Advanced Nylon Materials and Application, School of Materials Science and Engineering, Zhengzhou University, Zhengzhou, Henan Province, China

*Correspondence to: Email: wangkunlun206@zzu.edu.cn; liuylxn@zzu.edu; cncaoshaokui@zzu.edu.cn

Materials

Propyl gallate (98%, aladdin, Shanghai, China), 1-bromododecane (98%, aladdin, Shanghai, China), acetone (99%, Kermel, Tianjin, China), potassium carbonate (K_2CO_3, 98%, Kermel, Tianjin, China), potassium ydroxide (KOH, 98%, Kermel, Tianjin, China), ethanol (EtOH, 98%, Kermel, Tianjin, China), concentrated sulfuric acid (H_2SO_4, 12M, Kermel, Tianjin, China), 7-(bromomethyl)pentadecane (95%, aladdin, Shanghai, China), ammonia solution (28%, Kermel, Tianjin, China), cyanuric chloride (99%, aladdin), dodecylamine (98%, aladdin, Shanghai, China), 1,4-dioxane (99%, Kermel, Tianjin, China), 4-butylaniline (97%, aladdin, Shanghai, China), sodium bicarbonate ($NaHCO_3$, 98%, Kermel, Tianjin, China), methanol (MeOH, 99%, Kermel, Tianjin, China), dichloromethane (DCM, 98%, Kermel, Tianjin, China), sodium chloride (NaCl, 99.5%, Kermel, Tianjin, China), ethyl acetate (EA, 99%, Kermel, Tianjin, China), anhydrous magnesium sulfate ($MgSO_4$, 99.5%, Kermel, Tianjin, China), trichloromethane ($CHCl_3$, 99%, Kermel, Tianjin, China), silica gel (63-200 μm, Haiyang, China).

^{1}H NMR and ^{13}CNMR experimentsfor All Compounds

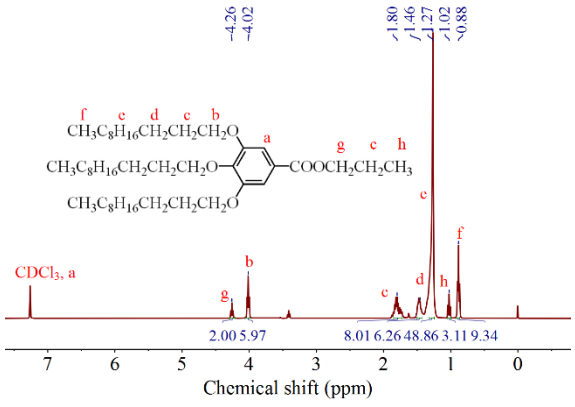

Figure SM1. ^{1}H NMR of compound 1a in $CDCl_3$.

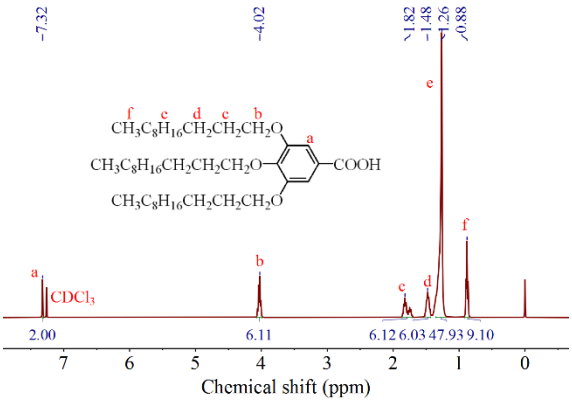

Figure SM2. ^{1}H NMR of compound **A1**in **CDCl$_3$**.

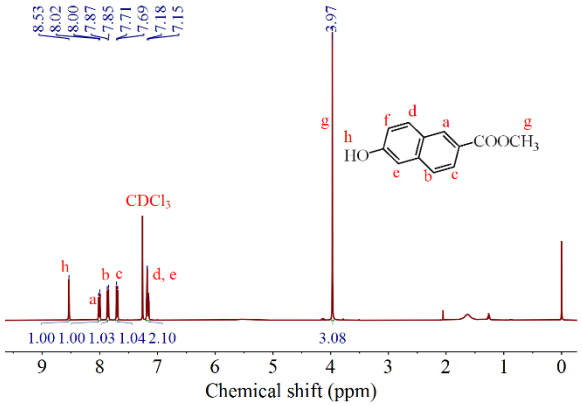

Figure SM3. ^{1}H NMR of compound **2a** in **CDCl$_3$**.

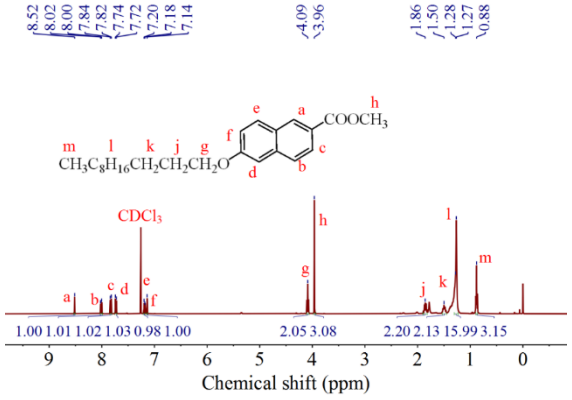

Figure SM4. ^{1}H NMR of compound **2b** in **CDCl$_3$**.

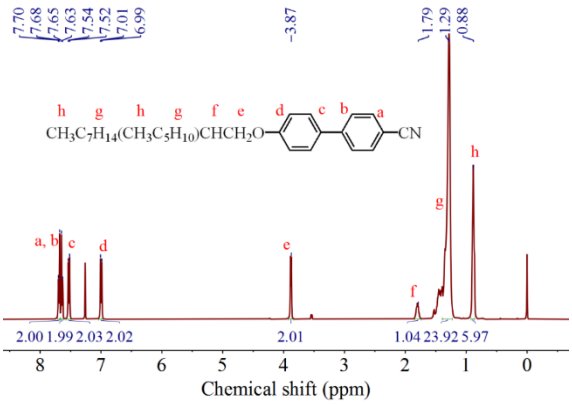

Figure SM5. ^{1}H NMR of compound **3a** in **$CDCl_3$**.

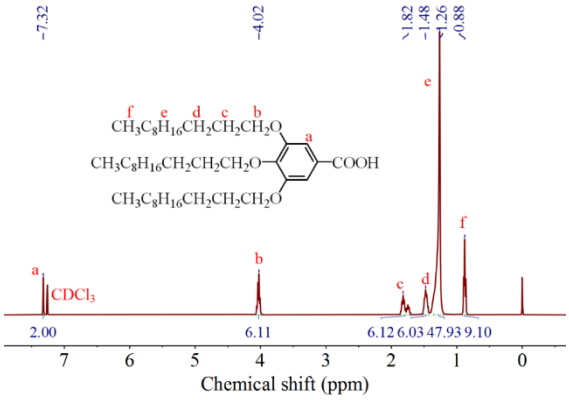

Figure SM6. ^{1}H NMR of compound **A1** in **$CDCl_3$**.

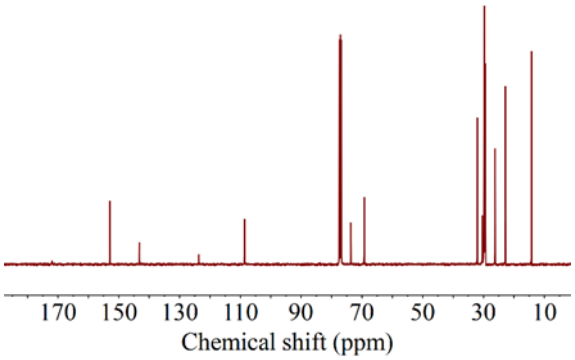

Figure SM7. ^{13}C NMR of A1 in $CDCl_3$.

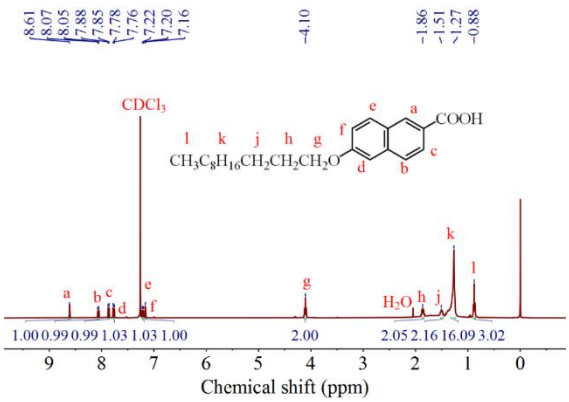

Figure SM8. ^{1}H NMR of compound **A2** in **$CDCl_3$**.

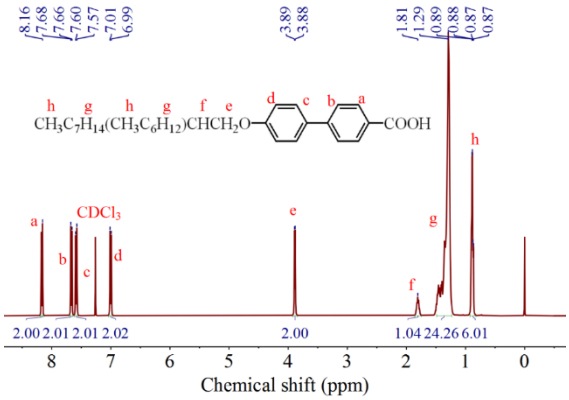

Figure SM9. ^{1}H NMR of compound **A4** in **$CDCl_3$**.

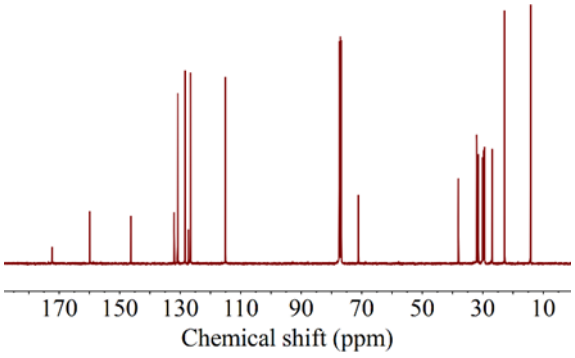

Figure SM10. ^{13}C NMR of A1 in $CDCl_3$.

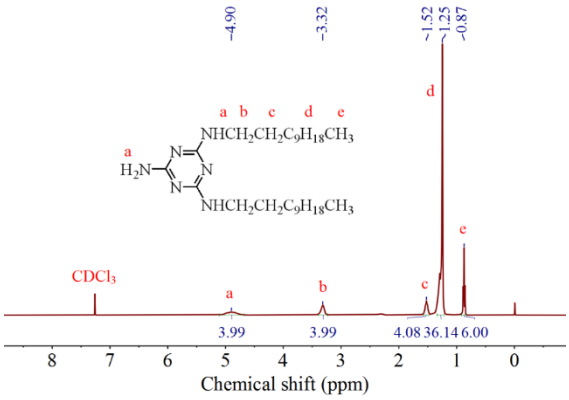

Figure SM11. ^{1}H NMR of compound **T1** in **$CDCl_3$**.

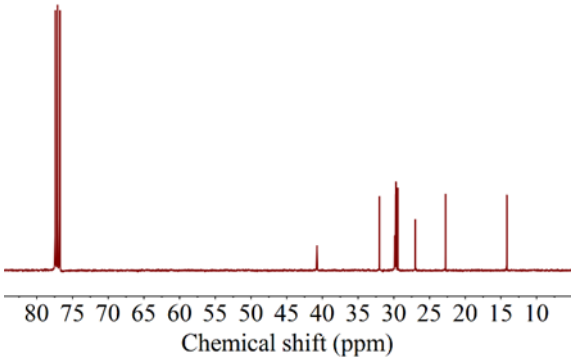

Figure SM12. ^{13}C NMR of compound **T1** in **$CDCl_3$**.

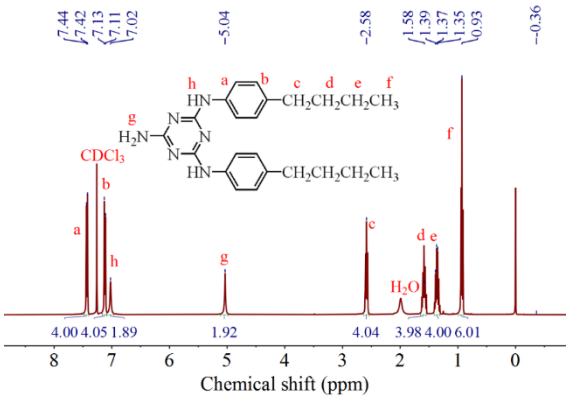

Figure SM13. ^{1}H NMR of compound **T2** in **$CDCl_3$**.

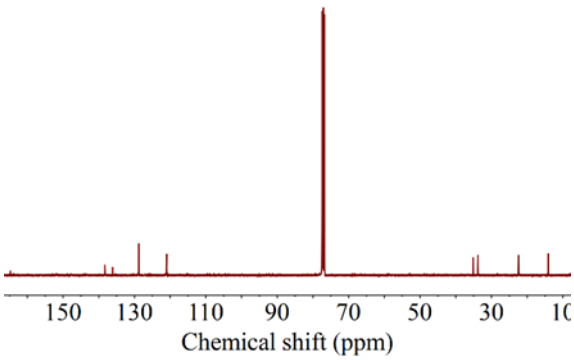

Figure SM14. ^{13}C NMR of compound **T2** in **$CDCl_3$**

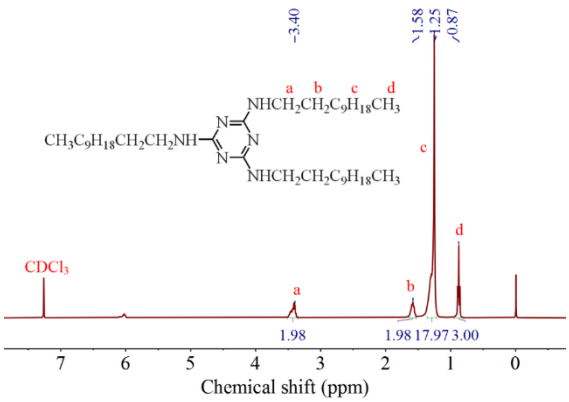

Figure SM15. ^{1}H NMR of compound **T3** in **$CDCl_3$**.

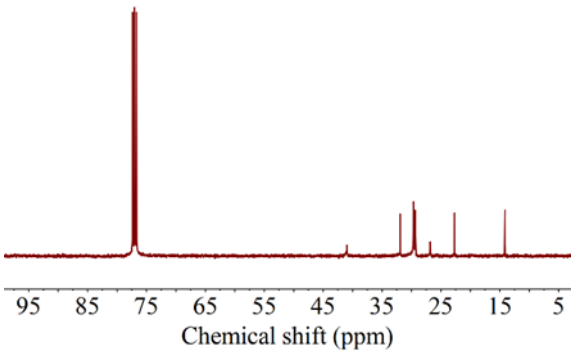

Figure SM16. ^{13}C NMR of **T3** in **$CDCl_3$**.

^{1}H NMR experimentsof the Hydrogen Bonded Complexes

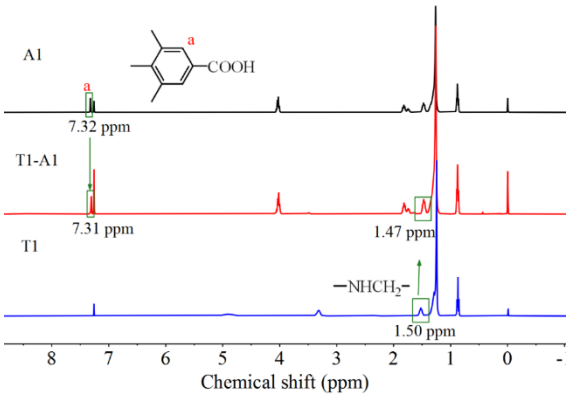

Figure SM17. ^{1}H NMR of complex **T1-A1** in **$CDCl_3$**.

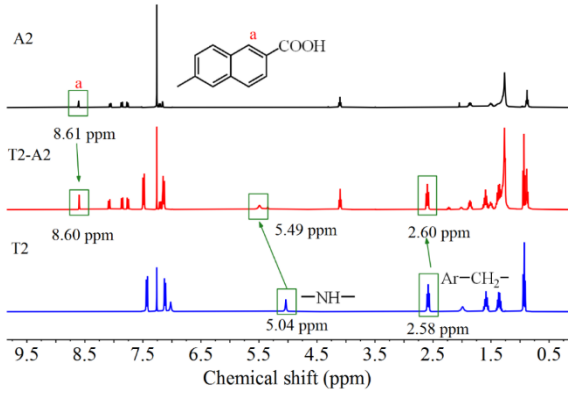

Figure SM18. ^{1}H NMR of complex **T2-A2** in **$CDCl_3$**.

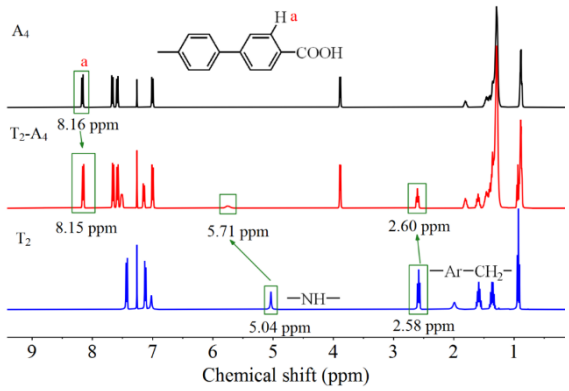

Figure SM19. ^{1}H NMR of complex **T2-A4** in **$CDCl_3$**.

MALDI-TOF-MS experiments

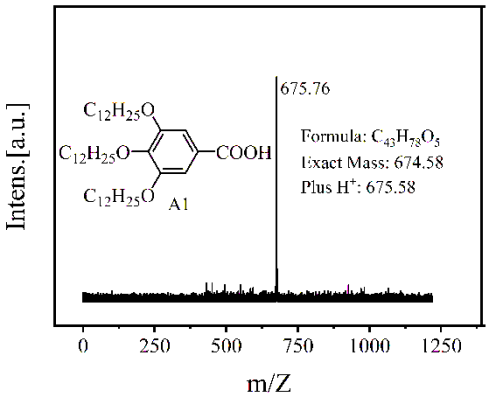

Figure SM20. MALDI-TOF MS spectra of **A1**.

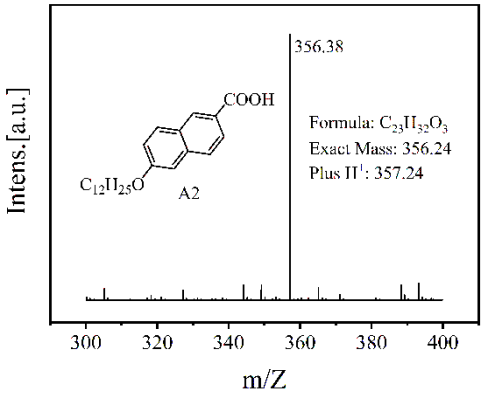

Figure SM21. MALDI-TOF MS spectra of **A2**.

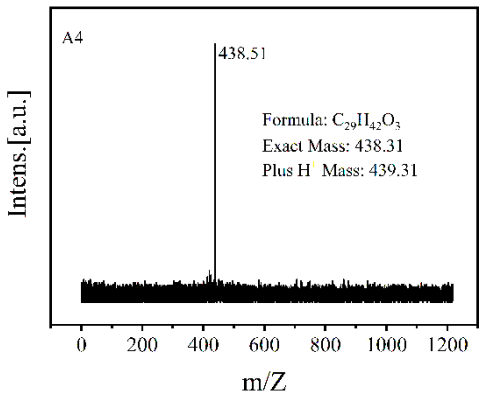

Figure SM22. MALDI-TOF MS spectra of **A4**.

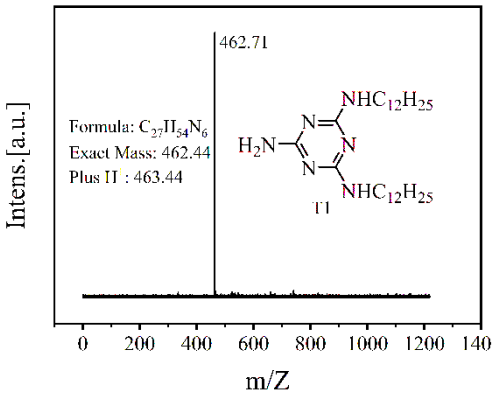

Figure SM23. MALDI-TOF MS spectra of **T1**.

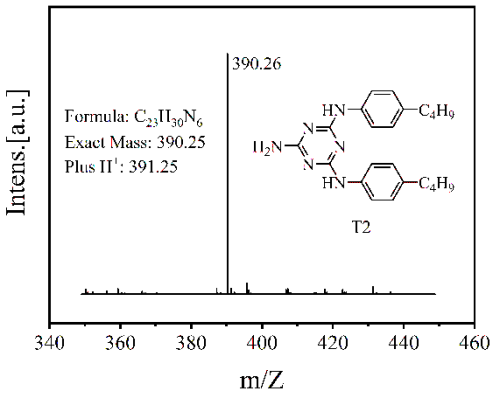

Figure SM24. MALDI-TOF MS spectra of **T2**.

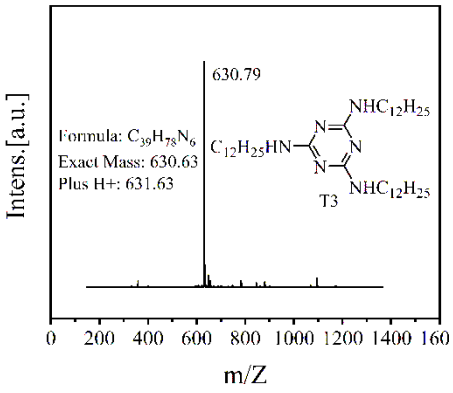

Figure SM25. MALDI-TOF MS spectra of **T3**.

FT-IR experiments

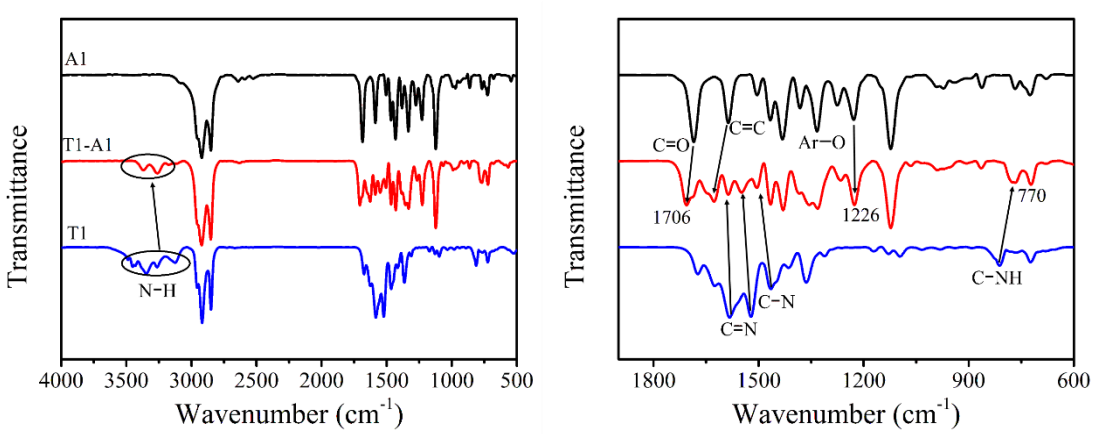

Figure SM26. FT-IR spectra for **A1** (black), complex **T1-A1** (red) and **T1**(blue).

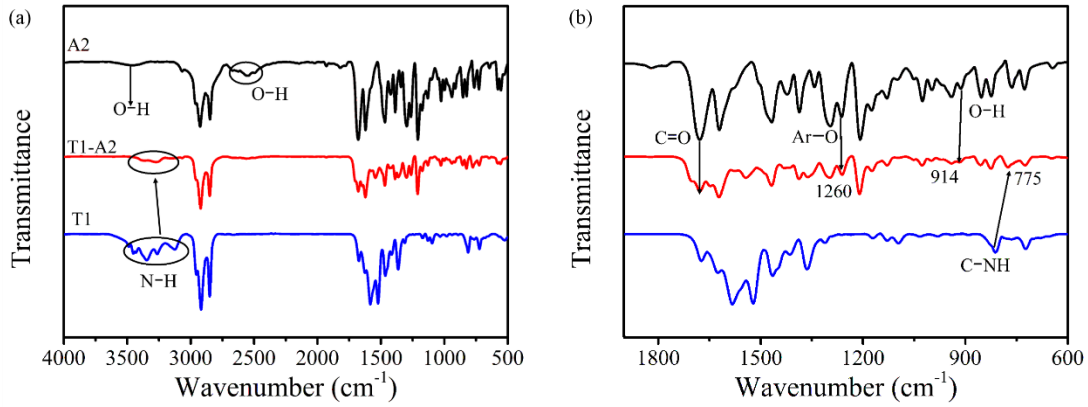

Figure SM27. FT-IR spectra for **A2** (black), complex **T1-A2** (red) and **T1** (blue).

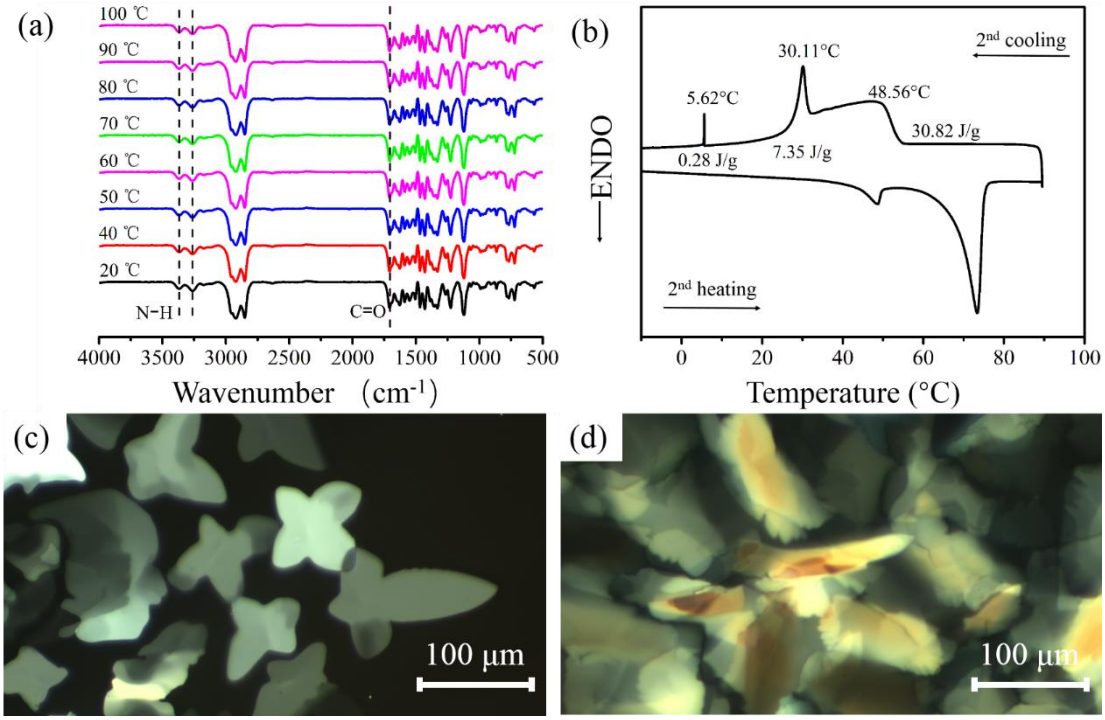

Figure SM28. (a) Variable-temperature of complex **T1-A1**; (b) DSC thermogram of complex **T1-A1**; POM microphotograph of compound **T1-A1**: (c) the third cooling, 56.1°C, 0.1°C/min; (d) the third cooling, 31.5°C, 0.1°C/min.

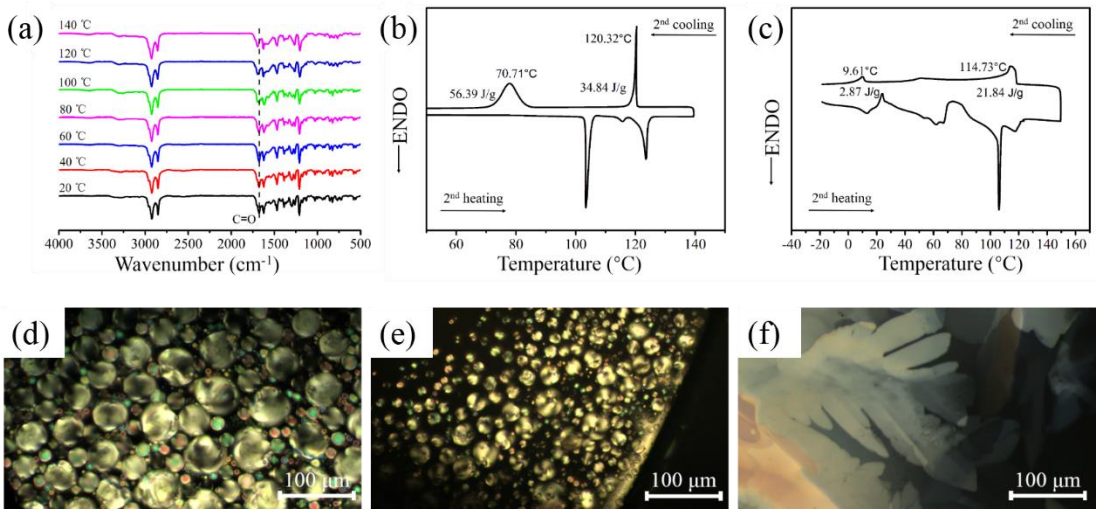

Figure SM29. (a) Variable-temperature of complex **T1-A2**; (b) DSC thermogram of compound **A1**; (c) DSC thermogram of compound **T1-A2**; POM microphotograph of compound **T1-A2**: (d) the third cooling, 121.2°C, 0.1°C/min; (e) the third cooling, 118.6°C, 0.1°C/min; (f) the fourth cooling, 117.9°C, 0.1°C/min.

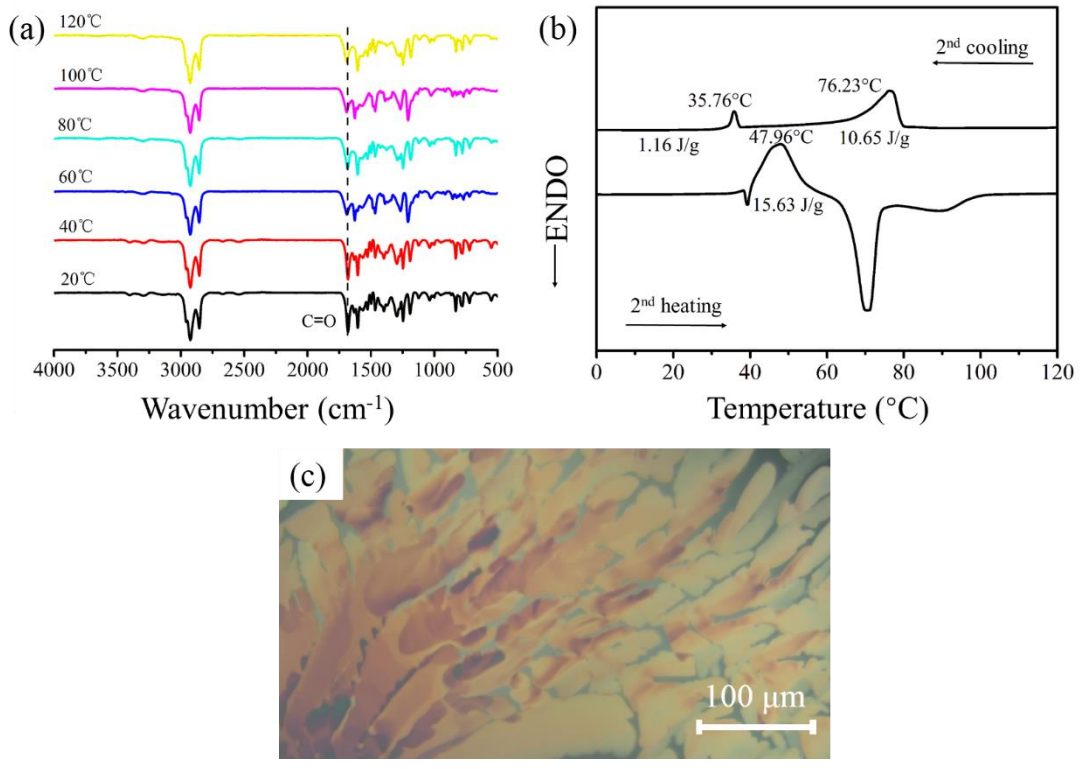

Figure SM30. (a) Variable-temperature of complex **T1-A4**; (b) DSC thermogram of compound **T1-A4**; (c) POM microphotograph of compound **T1-A4** (the third cooling, 79.6°C, 0.1°C/min).

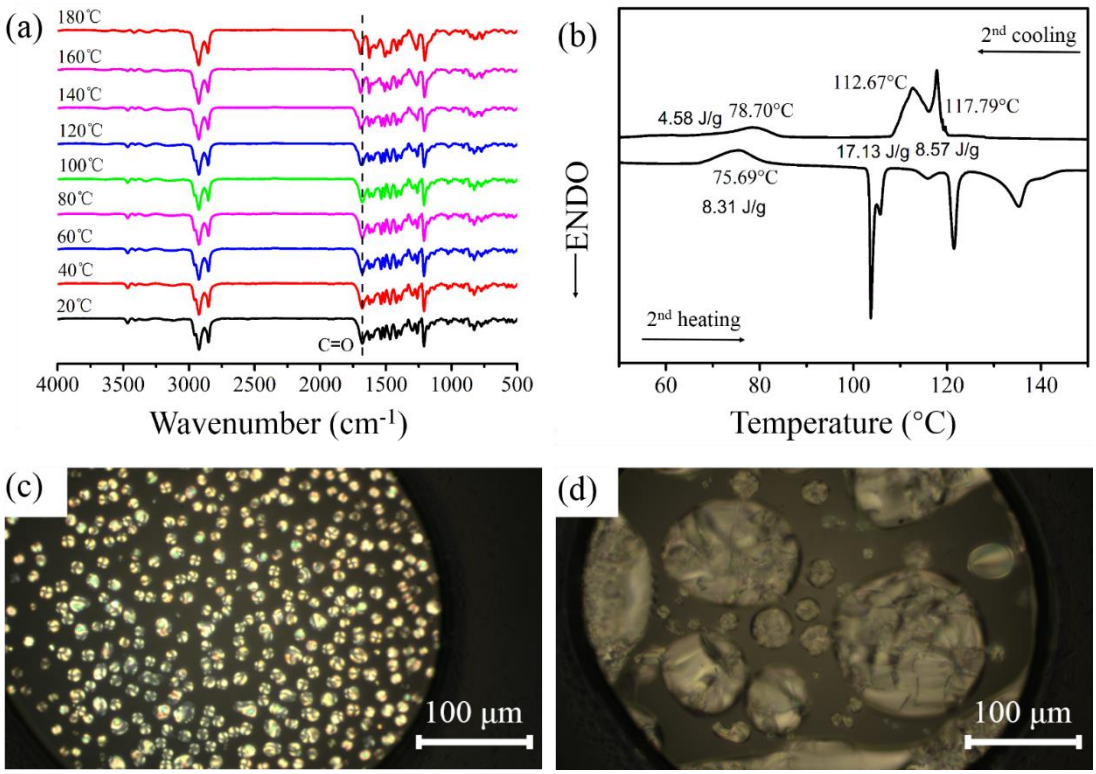

Figure SM31. (a) variable temperature infrared spectrum of **T2-A2**; (b) DSC thermogram of **T2-A2**; POM diagram: (c) **T2-A2** (119.7°C, 0.1°C/min); (d) **T2-A2** (at room temperature).

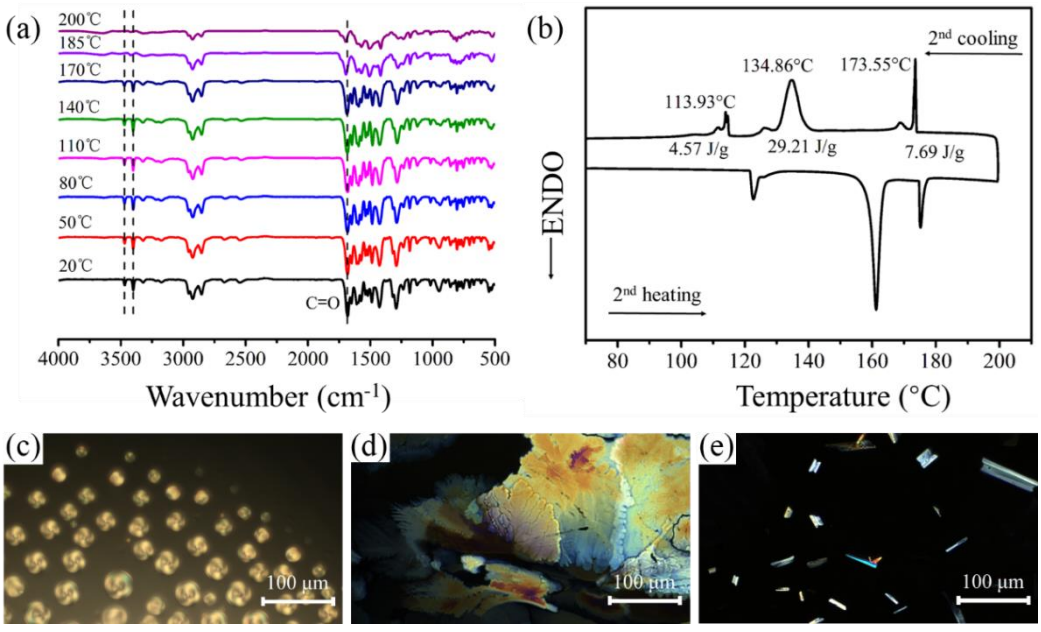

Figure SM32. (a) Variable-temperature of complex **T2-A3**; (b) DSC thermogram of compound **T2-A3**; POM microphotograph of compound **T2-A3**: (c)174.2°C, 0.1°C/min; (d)141.2°C, 0.1°C/min; (e) 115.1°C, 0.1°C/min.

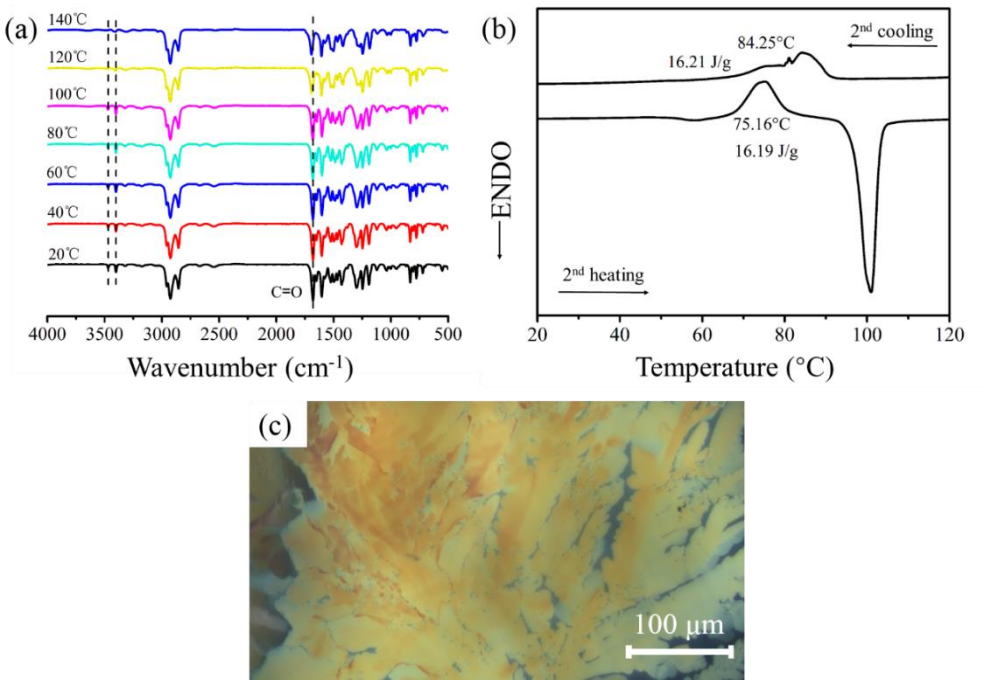

Figure SM33. (a) Variable-temperature of complex **T2-A4**; (b) DSC thermogram of compound **T2-A4**; (c) POM microphotograph of compound **T2-A4**(the third cooling, 92.1°C, 0.1°C/min).

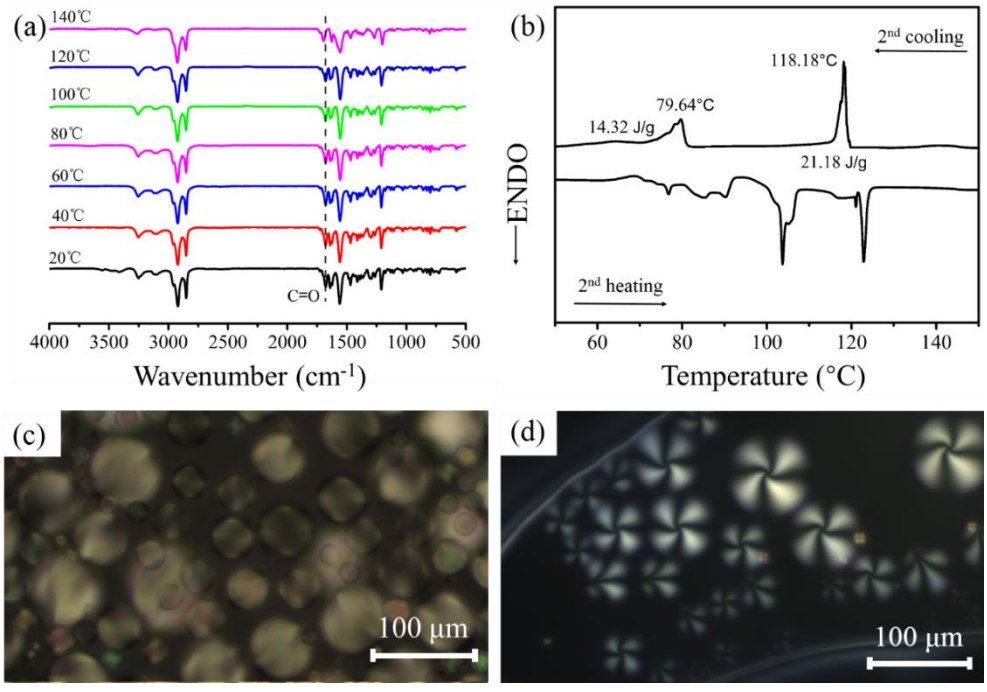

Figure SM34. (a) Variable-temperature of complex **T3-A2**; (b) DSC thermogram of compound **T3-A2**; POM microphotograph of compound **T3-A2**: (c) the third cooling, 174.2°C, 0.1°C/min; (d) the third cooling, 119.7°C, 0.1°C/min; (e) the fourth cooling, 81.3°C, 0.1°C/min.

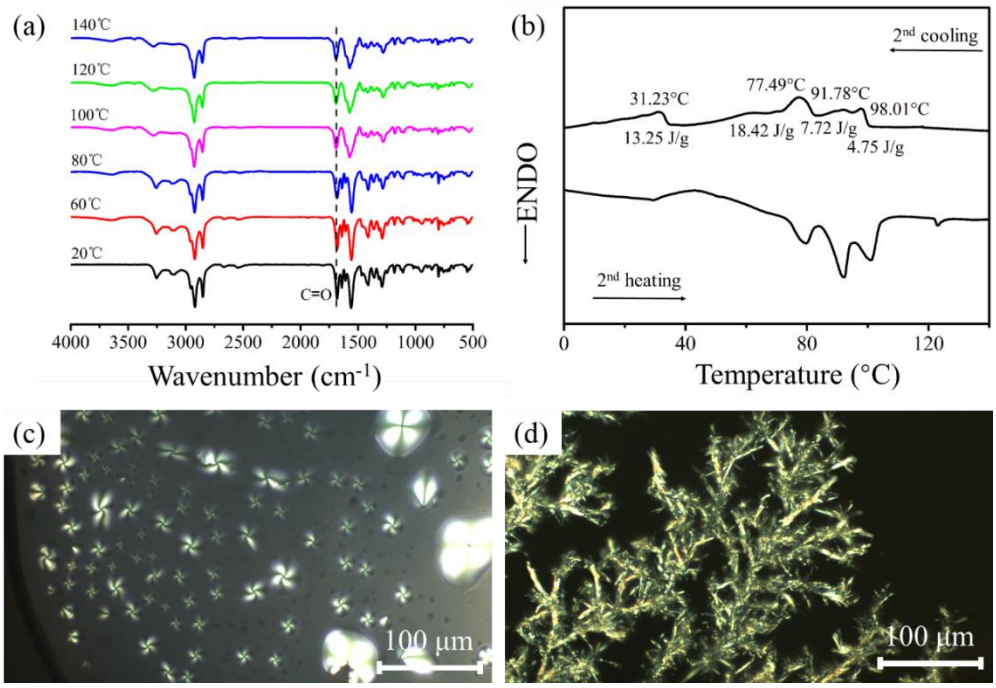

Figure SM35. (a) Variable-temperature of complex **T3-A3**;(b) DSC thermogram of compound **T3-A3**; POM microphotograph of compound **T3-A3**: (c) the third cooling, 174.2°C, 0.1°C/min; (d) the third cooling, 101.4°C, 0.1°C/min; (e) the fourth cooling, 82.3°C, 0.1°C/min.

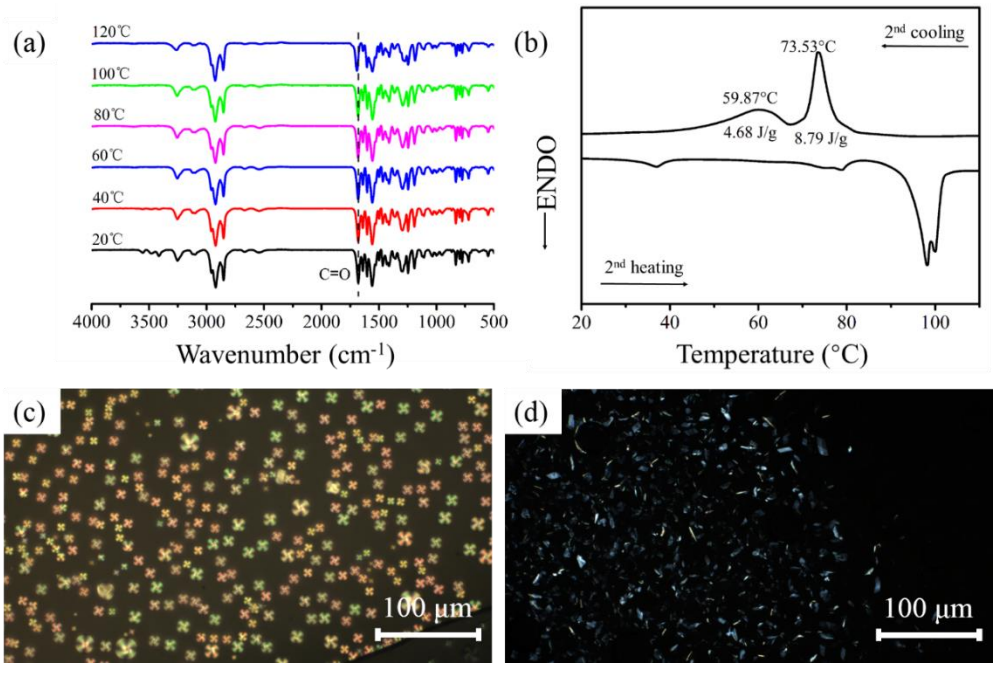

Figure SM36. (a) Variable-temperature of complex **T3-A4**; (b) DSC thermogram of compound **T3-A4**; POM microphotograph of compound **T3-A4**: (c) the third cooling, 174.2°C, 0.1°C/min; (d) the third cooling, 81.4°C, 0.1°C/min; (e) the fourth cooling, 66.1°C, 0.1°C/min.

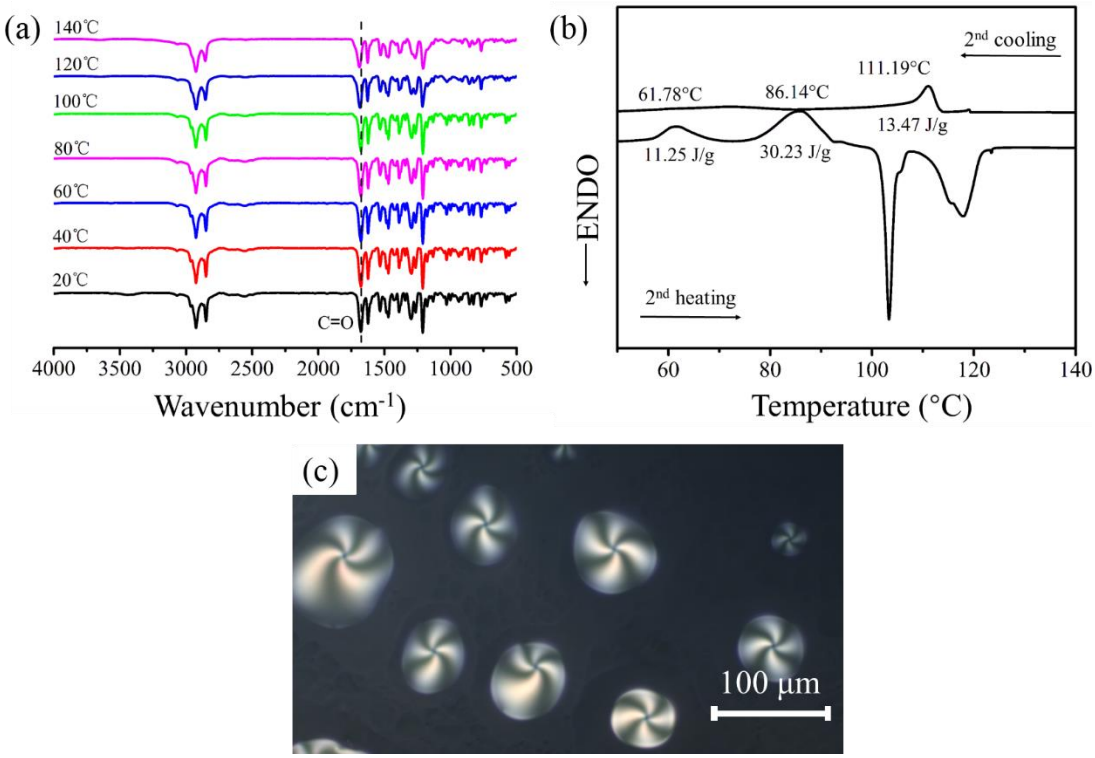

Figure SM37. (a) Variable-temperature of complex **T4-A2**; (b) DSC thermogram of compound **T4-A2**;(c) POM microphotograph of compound **T4-A2:**(the third cooling, 92.1°C, 0.1°C/min).

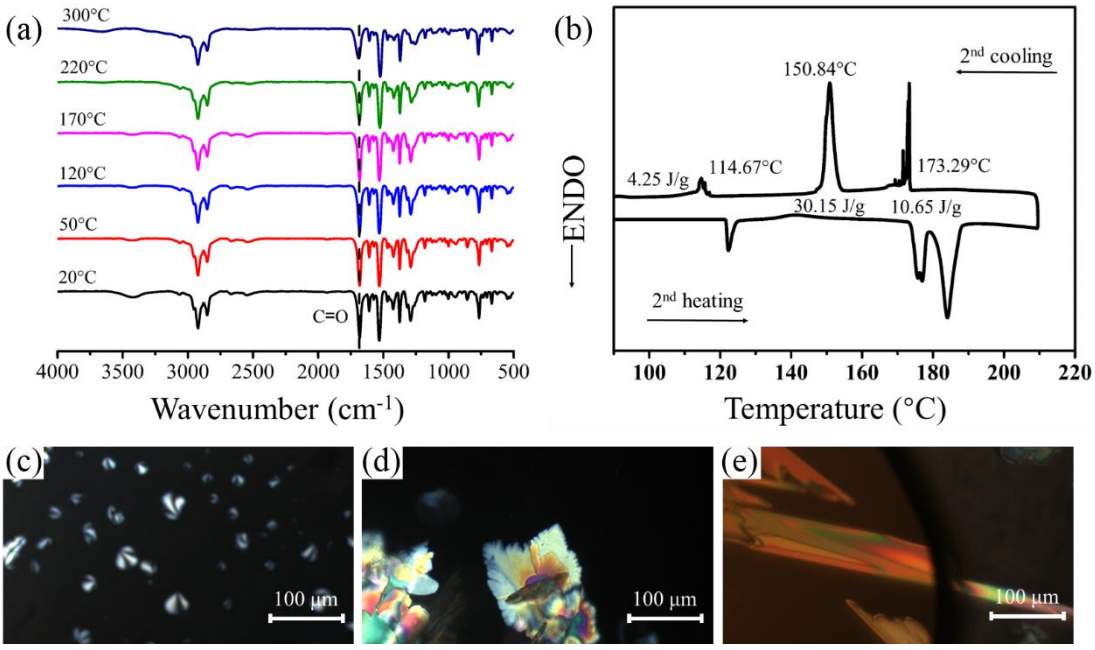

Figure SM38. (a) Variable-temperature of complex **T4-A3**; (b) DSC thermogram of compound **T4-A3**; POM microphotograph of compound **T4-A3**: (c) the third cooling, 174.5°C, 0.1°C/min; (d) the third cooling, 155.1°C, 0.1°C/min; (e) the fourth cooling, 118.4°C, 0.1°C/min.

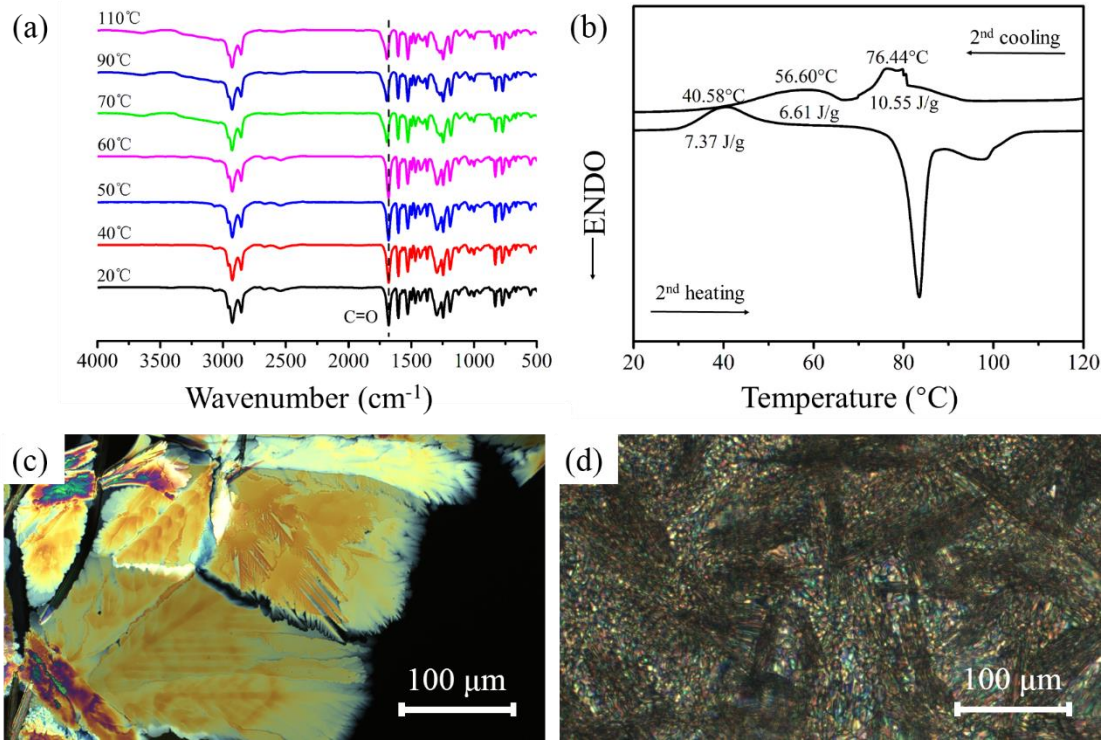

Figure SM39. (a) Variable-temperature of complex **T4-A4**; (b) DSC thermogram of compound **T4-A4**; POM microphotograph of compound **T4-A4**: (c) the third cooling, 92.5°C, 0.1°C/min; (d) the third cooling, 155.1°C, 0.1°C/min; (e) at room temperature, 0.1°C/min.