*Supporting Information for*

# Aggregate emission behaviors and reversible mechanofluorochromic properties of α-cyanostilbene functionalized indolo[3,2-*b*]carbazole derivatives

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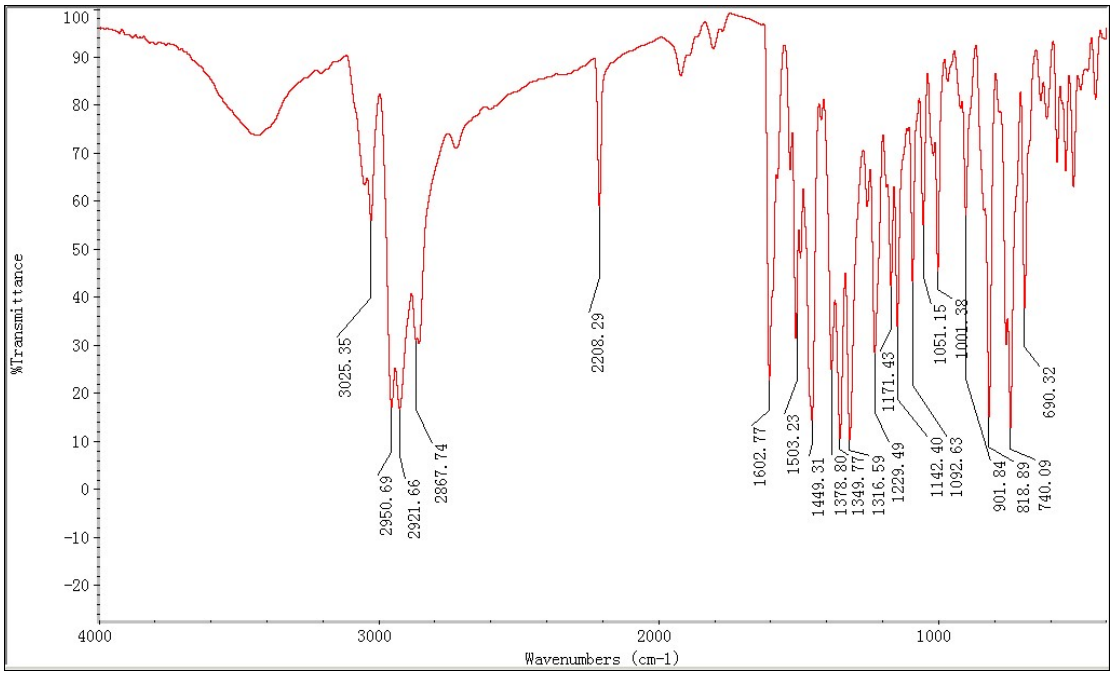


Fig. S1 FT-IR spectrum of **ICZH**.

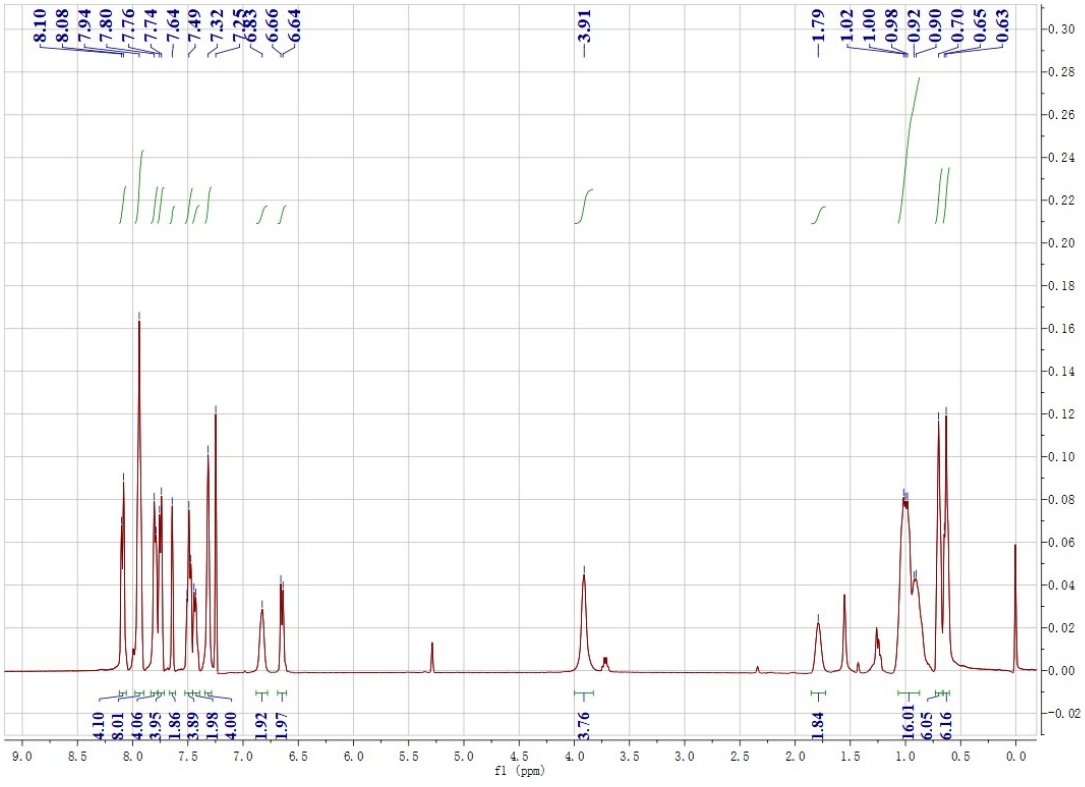


Fig. S2 $^{1}$H NMR spectrum of **ICZH** in $CDCl_3$.

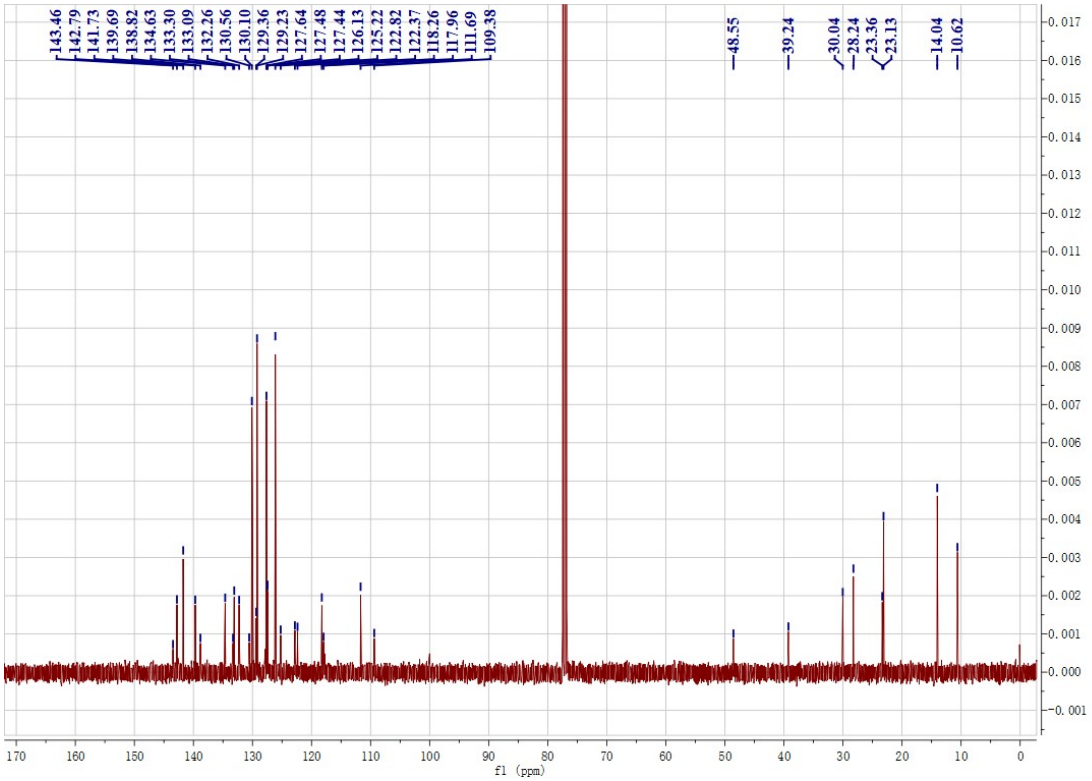


Fig. S3 $^{13}C$ NMR spectrum of **ICZH** in $CDCl_3$.

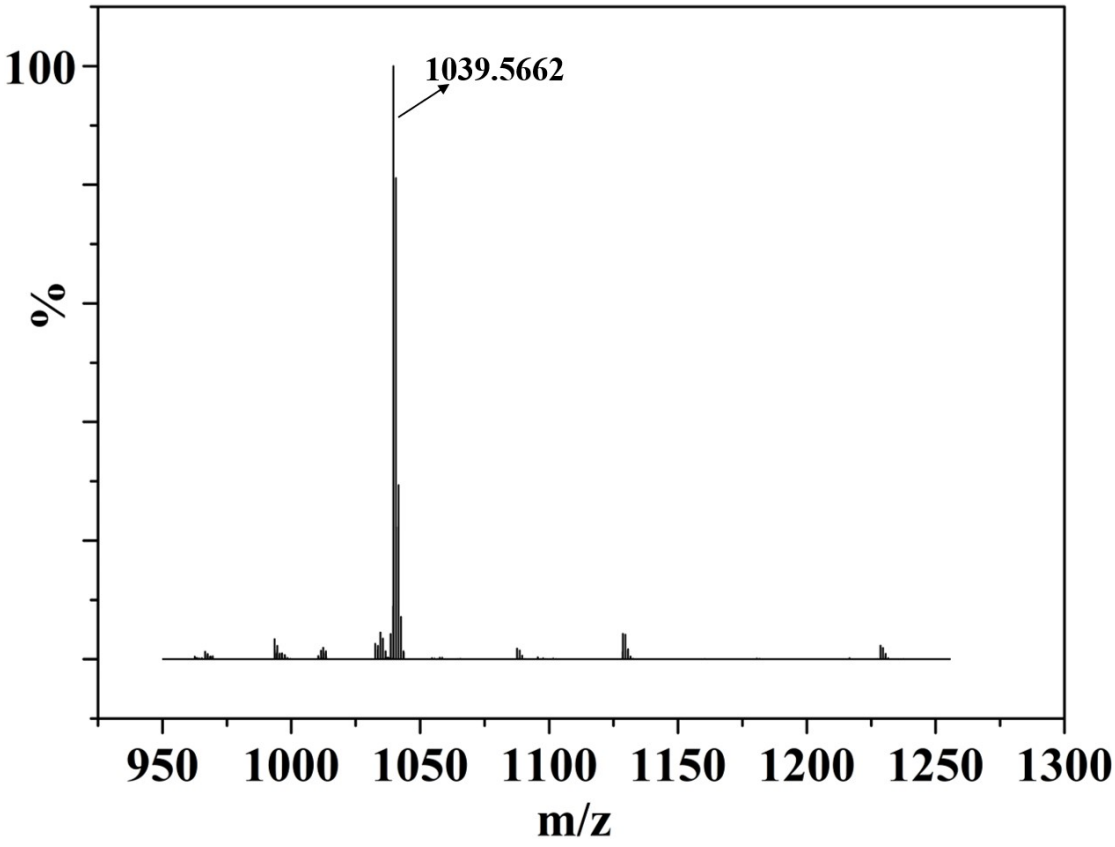


Fig. S4 HP-MS spectrum of **ICZH**.

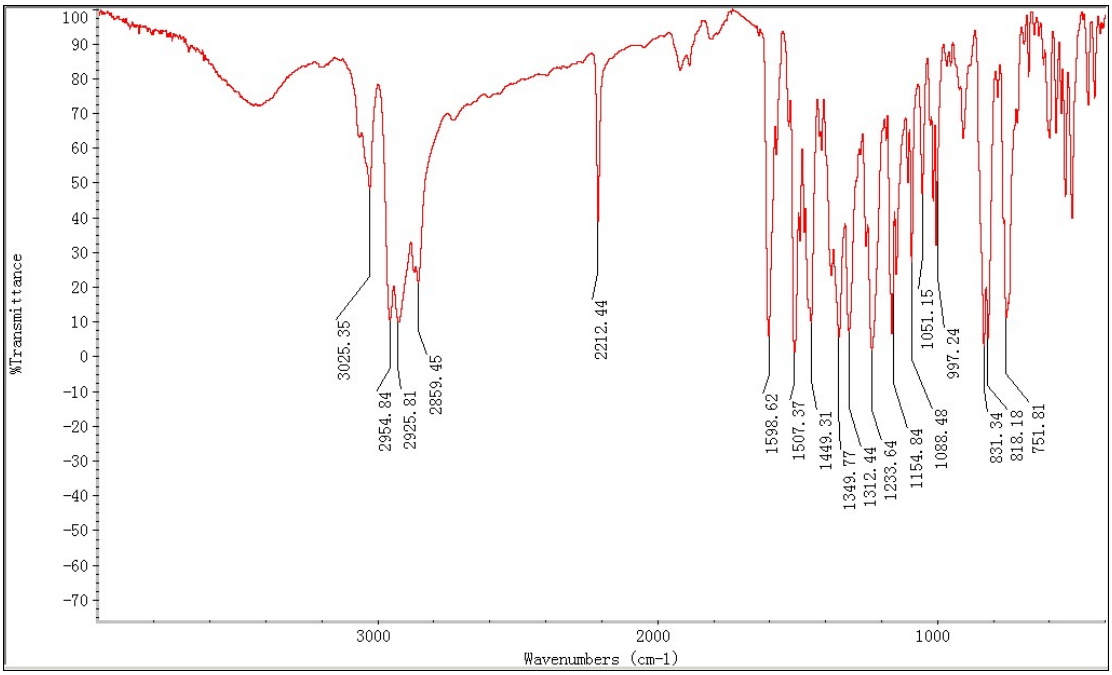


Fig. S5 FT-IR spectrum of **ICZF**.

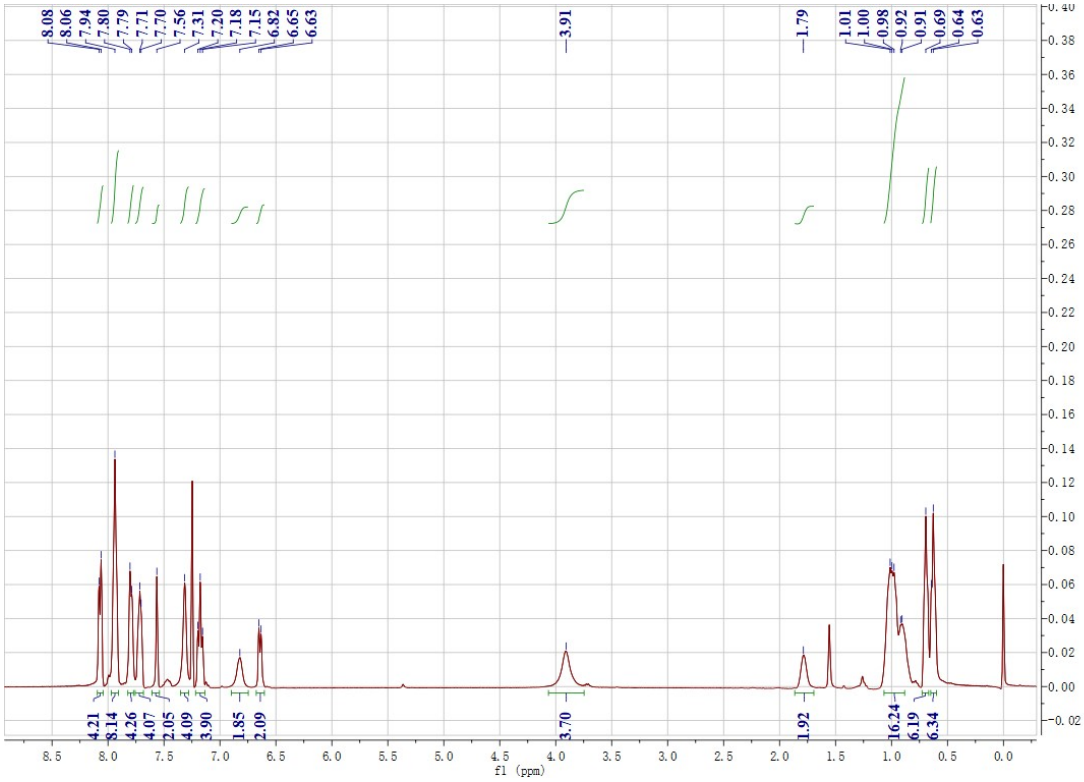


Fig. S6 $^{1}$H NMR spectrum of **ICZF** in $CDCl_3$.

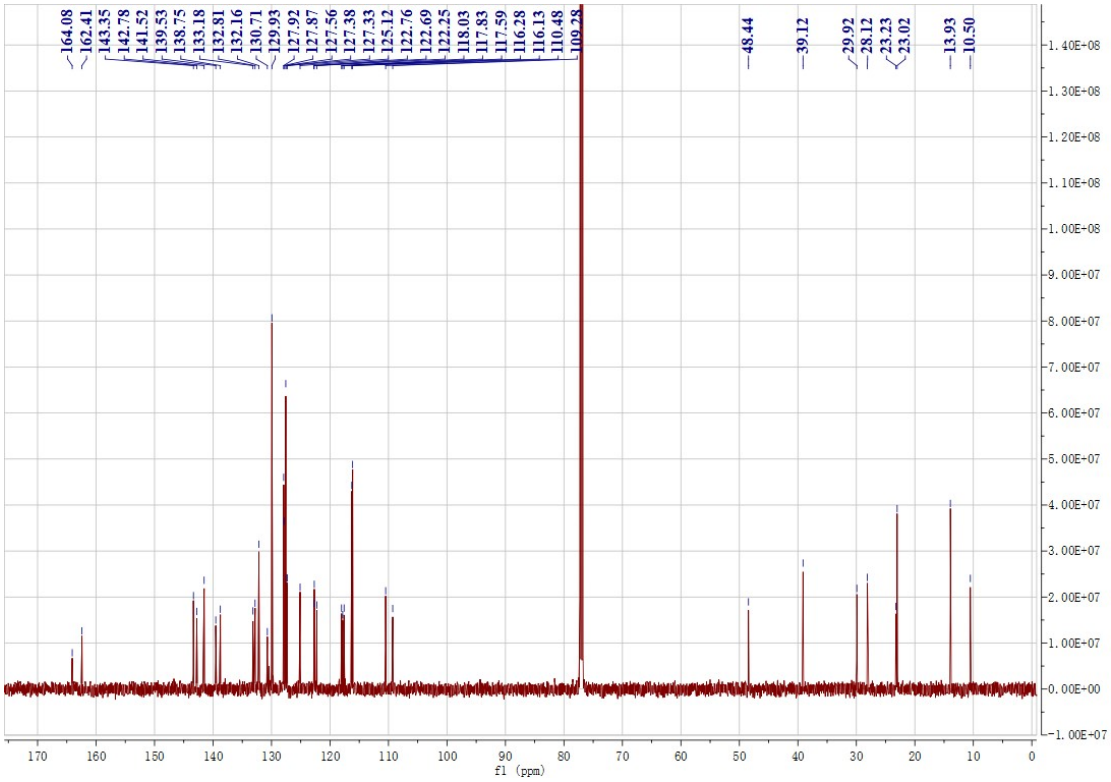


Fig. S7 $^{13}C$ NMR spectrum of **ICZF** in $CDCl_3$.

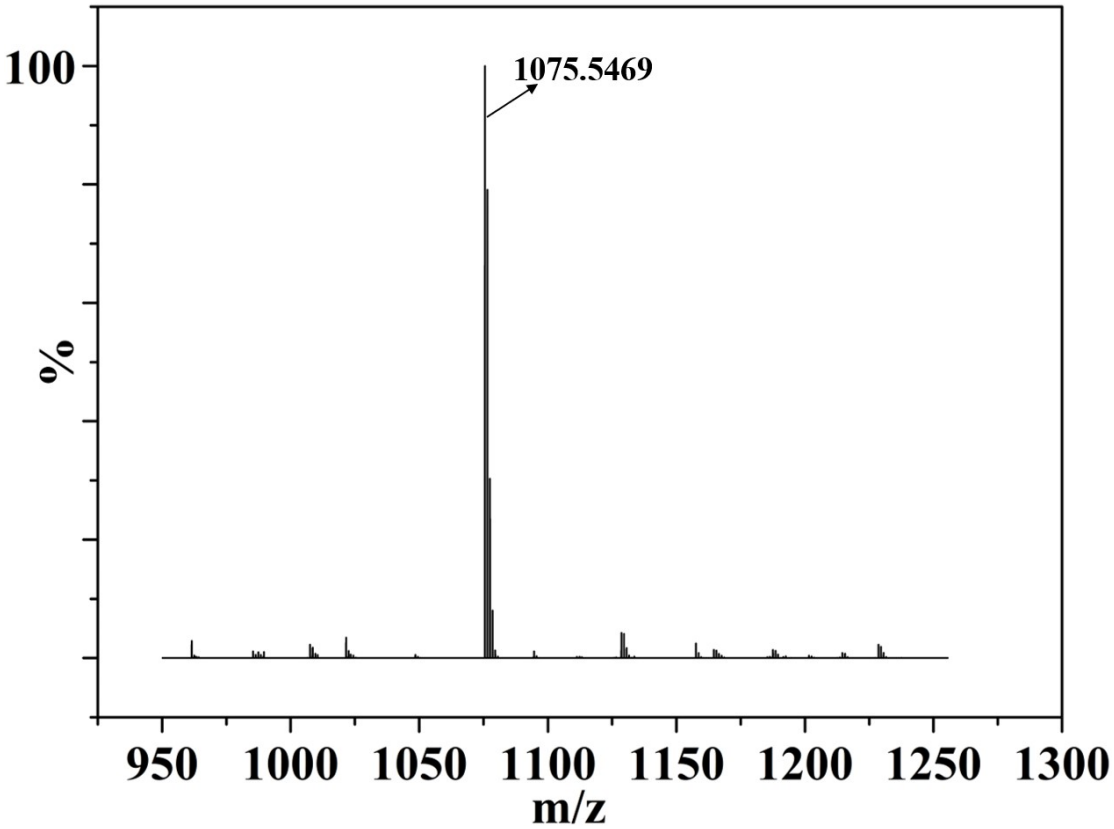


Fig. S8 HP-MS spectrum of **ICZF**.

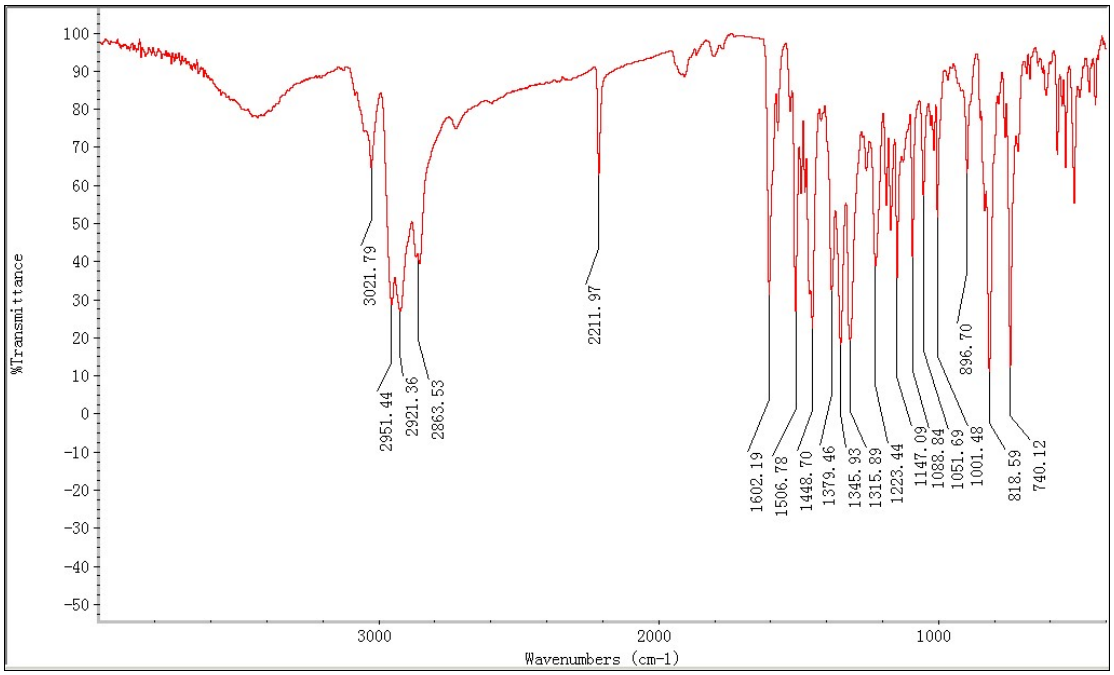


Fig. S9 FT-IR spectrum of **ICZCH$_3$**.

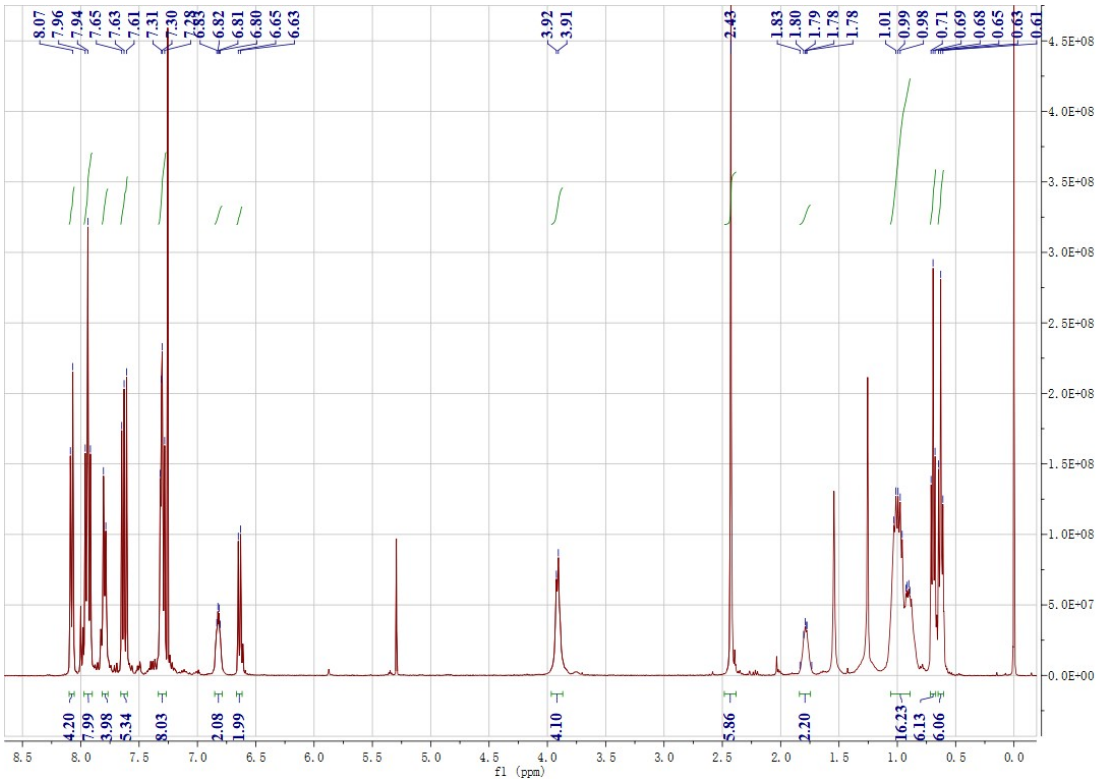


Fig. S10 $^1$H NMR spectrum of **ICZCH$_3$** in $CDCl_3$.

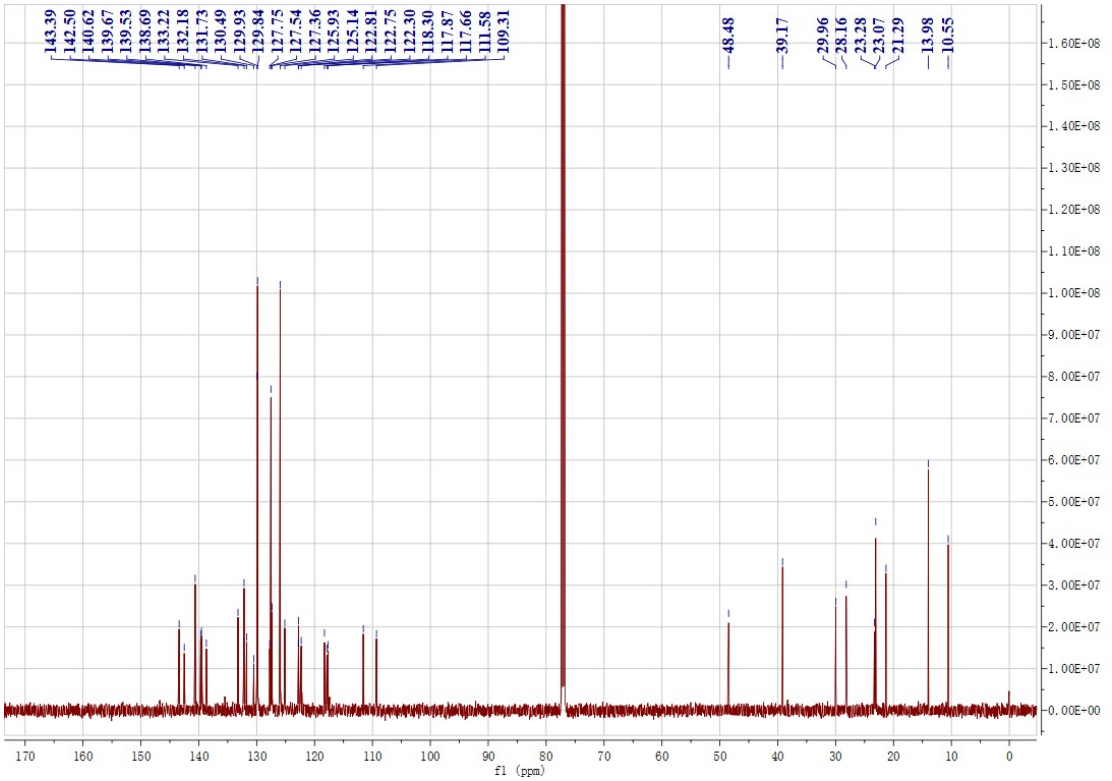


Fig. S11 $^{13}C$ NMR spectrum of **ICZCH$_3$** in $CDCl_3$.

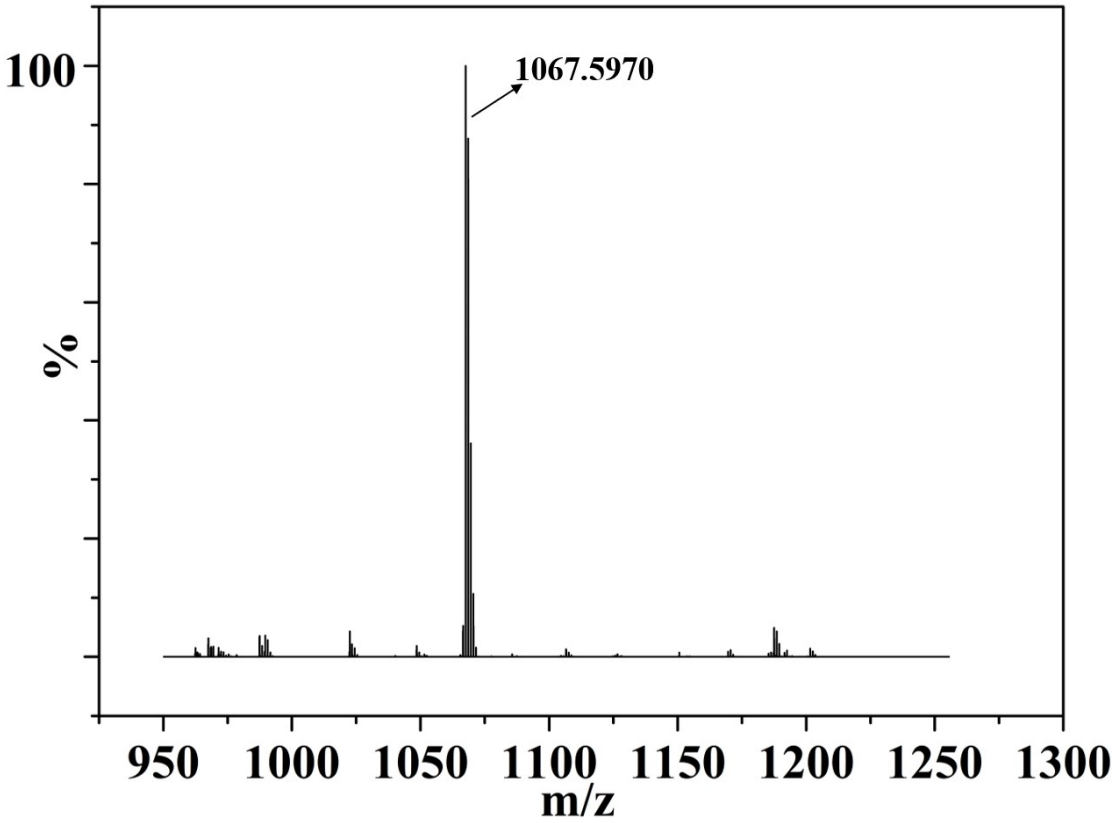


Fig. S12 HP-MS spectrum of **ICZCH$_3$**.

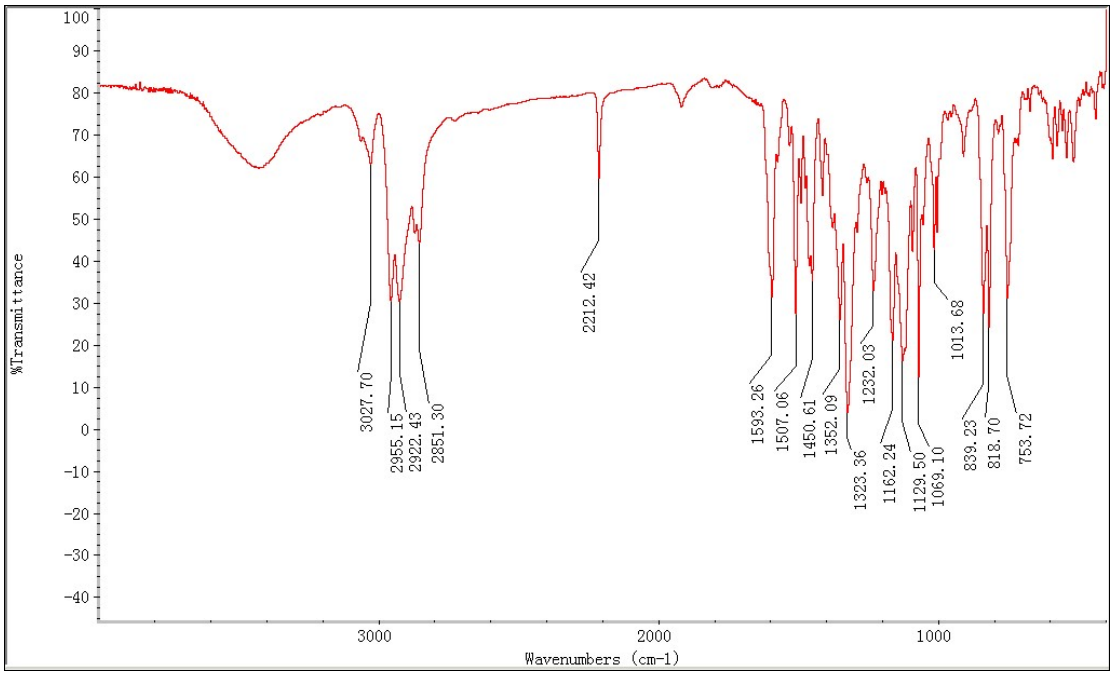


Fig. S13 FT-IR spectrum of **ICZCF$_3$**.

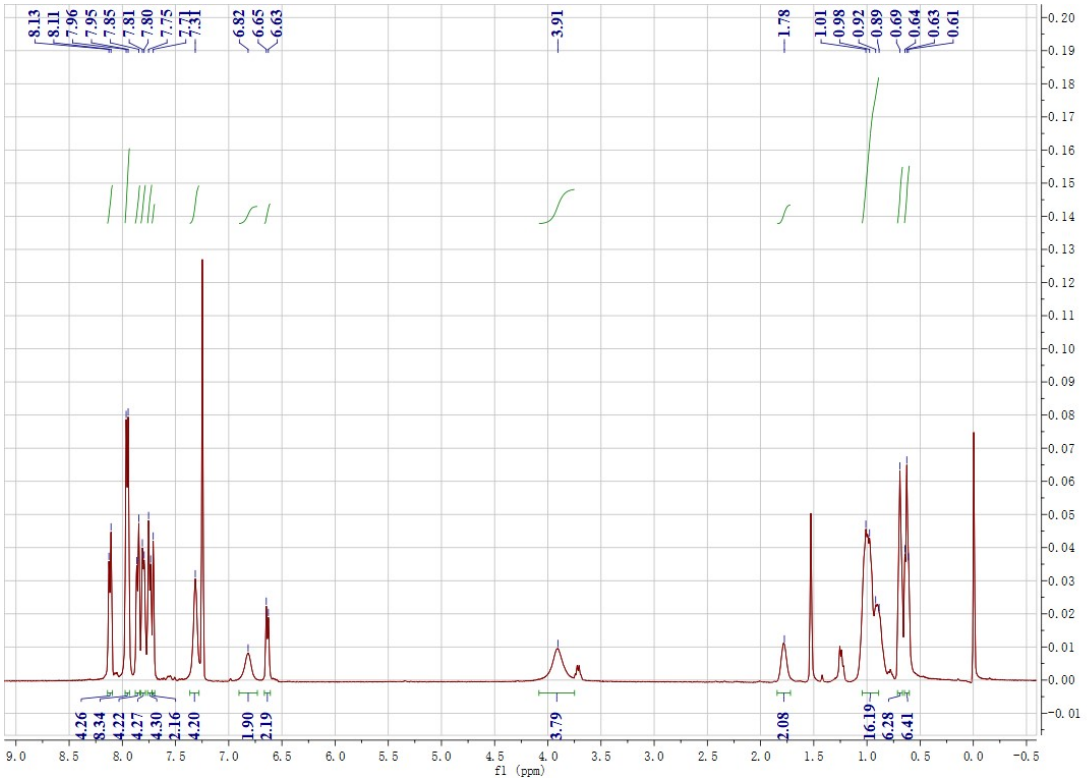


Fig. S14 $^1$H NMR spectrum of **ICZCF$_3$** in $CDCl_3$.

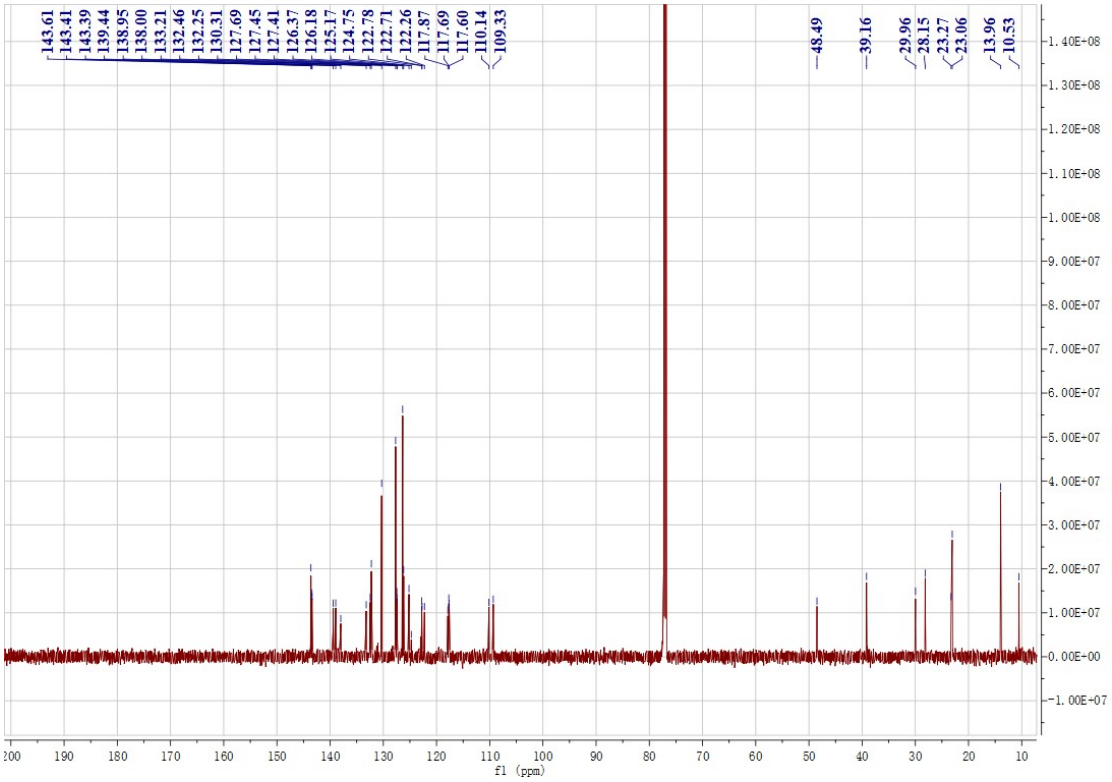


Fig. S15 $^{13}C$ NMR spectrum of **ICZCF$_3$** in $CDCl_3$.

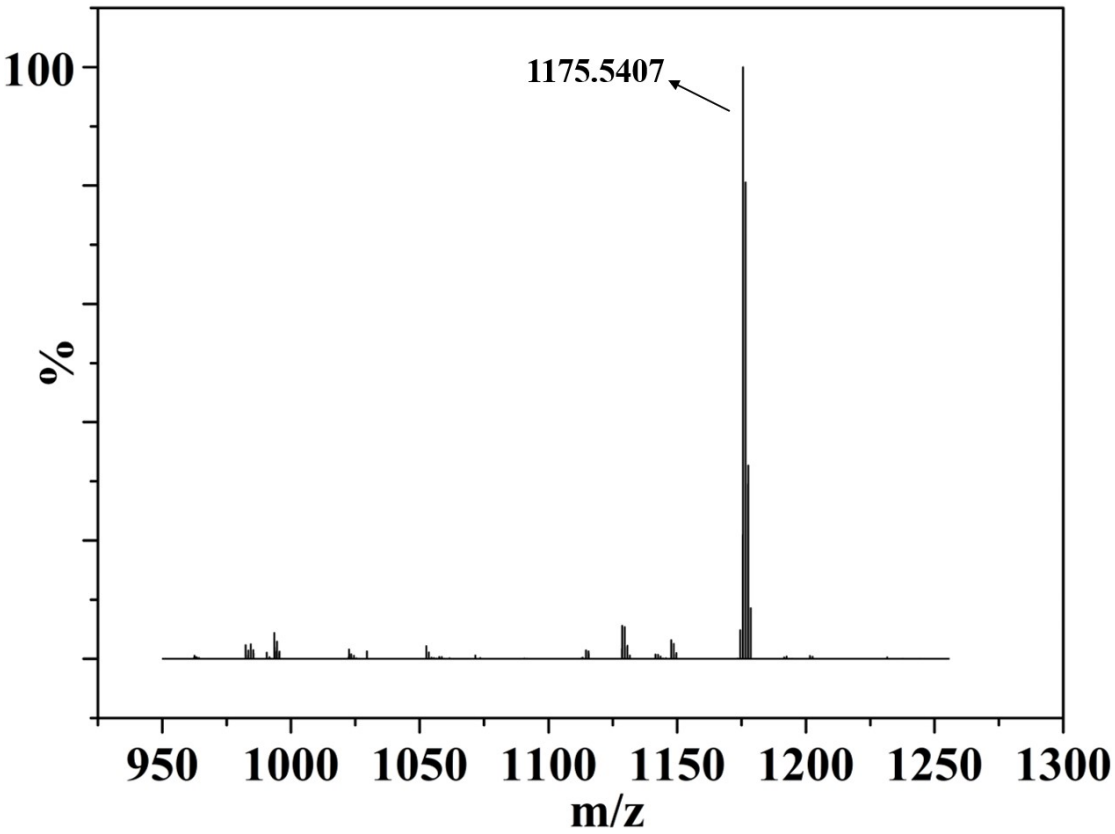


Fig. S16 HP-MS spectrum of **ICZCF$_3$**.

Table S1 Summary of crystallographic data for compound **ICZCF$_3$**

| Identification | **ICZCF$_3$** | *Data/restraints/parameters* | 6759/6/400 |
|---|---|---|---|
| Wavelength (Å) | 1.54178 | Final R indices [I>2σ(I)] | $R_1$ = 0.2572<br>$wR_2$ = 0.5680 |
| Crystal system | triclinic | | |
| Space group | pī | Empirical formula | $C_{78}H_{68}F_6N_4$ |
| *a* (Å) | 10.0055(2) | Formula weight | 1175.36 |
| *b* (Å) | 13.0597(3) | *F(000)* | 618 |
| *c* (Å) | 14.2217(3) | *Volume* | 1696.84(6) |
| *a* (°) | 101.9360(10) | *Z*, Calculated density | 2, 1.150 g/cm$^3$ |
| *β* (°) | 104.1170(10) | *Goodness-of-fit on* $F^2$ | 2.705 |
| *γ* (°) | 101.9760(10) | Largest diff. peak and hole | 3.883 and -0.629 e.A$^{-3}$ |
| Reflections collected / unique | 14629/6759 [R(int) = 0.0342] | *θ* range for data collection | 3.33 to 74.47 ° |
| Limiting indices | -12 ≤ h ≤ 11<br>-16 ≤ k ≤ 15<br>-17 ≤ l ≤ 17 | R indices (all data) | $R_1$ = 0.2756<br>$wR_2$ = 0.5934 |

Table S2 Selected Bond distance (Å), bond angle (°) and torsion angle (°) for compound **ICZ-CF$_3$**

| Bond distance (Å) | | bond angle (°) | | torsion angle °) | |
|---|---|---|---|---|---|
| F3-C1 | 1.326(9) | C31-N2-C24 | 108.0(4) | F2-C1-C2-C5 | -121.24 |
| N2-C32 | 1.463(6) | C31-N2-C32 | 123.0(5) | F2-C1-C2-C3 | 58.02 |
| N2-C31 | 1.385(7) | C15-C14-C17 | 121.7(5) | C1-C2-C3-C4 | 179.08 |
| N2-C24 | 1.403(7) | C13-C14-C17 | 119.9(5) | N1-C9-C8-C7 | 2.23 |
| N1-C9 | 1.161(8) | C5-C2-C1 | 122.3(6) | C10-C8-C7-C6 | 169.46 |
| C22-C21 | 1.382(7) | F2-C1-F3 | 105.7(7) | C11-C10-C8-C9 | -7.76 |
| C22-C17 | 1.407(8) | F2-C1-C2 | 114.4(6) | C13-C14-C17-C22 | -142.14 |
| C23-C20 | 1.500(6) | C6-C7-C8 | 120.9(5) | C21-C20-C23-C24 | 92.17 |
| C14-C17 | 1.478(7) | N2-C32-C33 | 115.5(5) | C23-C24-N2-C32 | 2.70 |
| C11-C10 | 1.464(7) | C34-C33-36 | 108.4(14) | C33-C32-N2-C31 | 92.63 |
| C8-C7 | 1.483(7) | C27-C26-C25 | 135.4(5) | C20-C23-C25-C26 | 1.82 |
| C31-C26 | 1.417(7) | C31-C26-C25 | 106.1(5) | C32-C33-C34-C35 | 162.91 |
| C29-C28 | 1.374(9) | C32-C33-C36 | 105.3(8) | C33-C36-C37-C38 | 152.68 |
| C29-C30 | 1.383(8) | C24-C25-C26 | 106.9(4) | F1-C1-C2-C3-C5 | -114.94 |

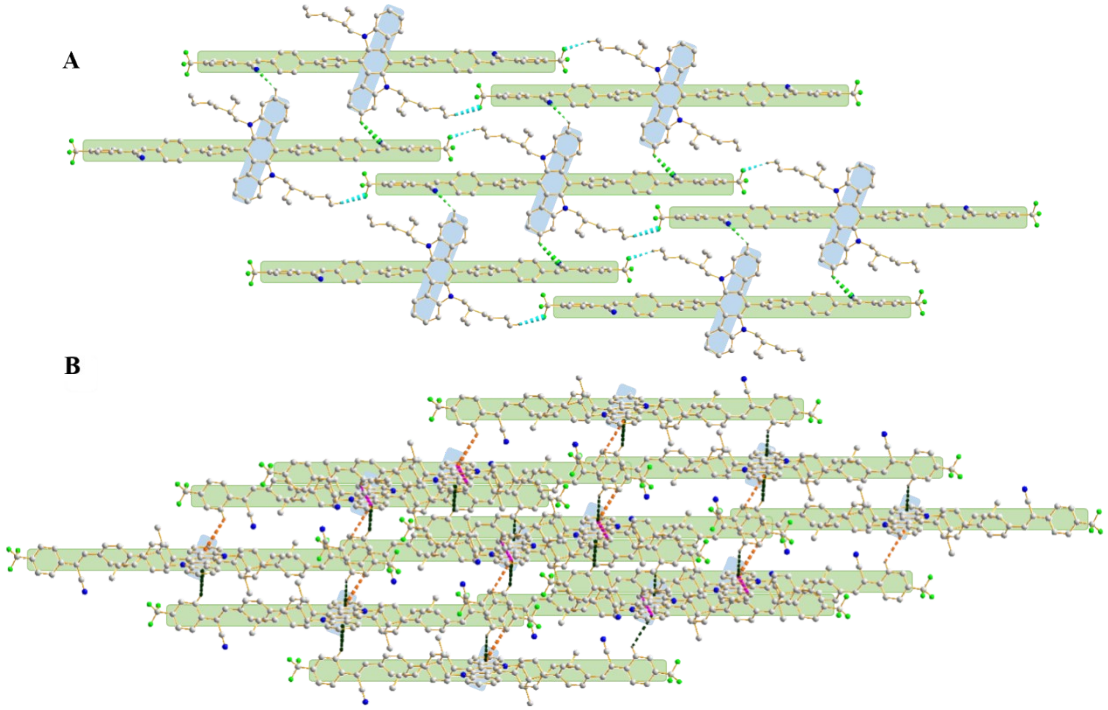


Fig. S17 (A) The molecular packing by hydrogen bond interaction and (B) C-H···πinteraction (hydrogen atoms are omitted for the sake of clarity).

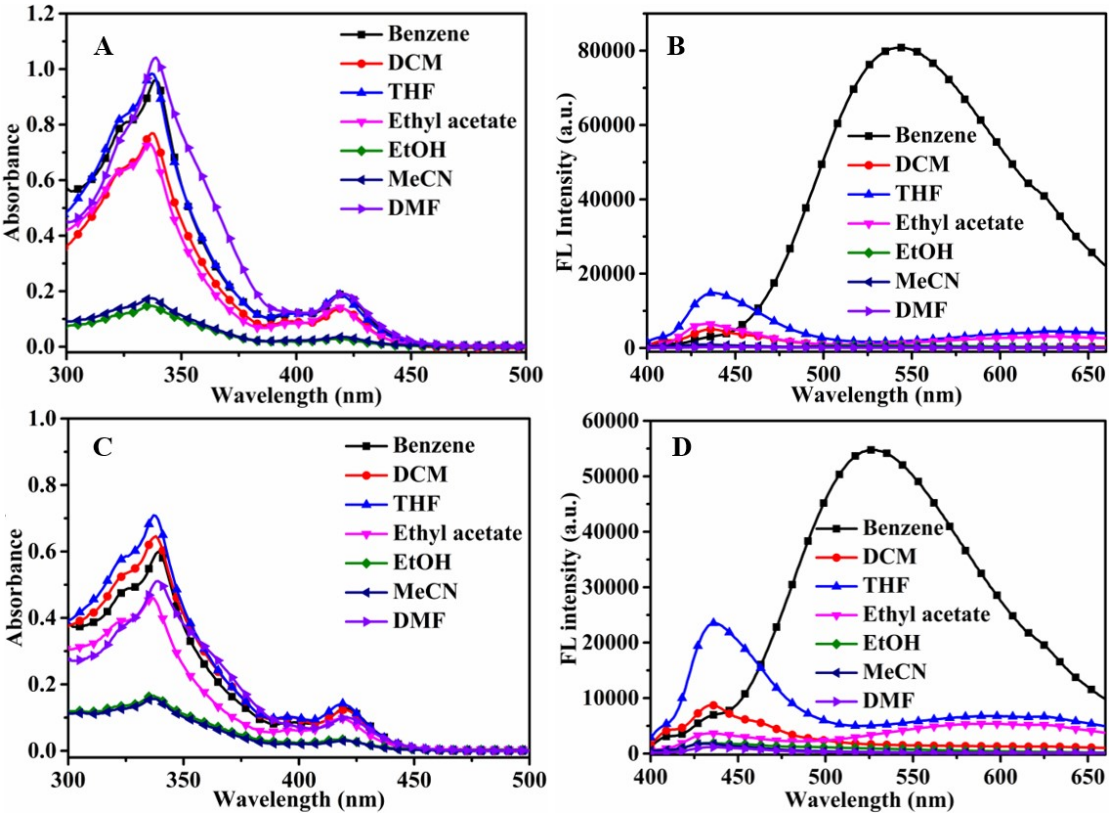


Fig. S18 (A, C) The UV-vis spectra and (B, D) fluorescence spectra of compounds **ICZH** and **ICZCH$_3$** in different solvents, respectively.

**Table S3** Photophysical properties of compounds **ICZ-H, ICZ-F, ICZ-CH3 and ICZ-$CF_3$** in different polar solvents.

| Compounds | Solvents | λ[a] max | λ[b] max | ε ($\times 10^4$)[c] | Δν [d] | Φ[e] |
|---|---|---|---|---|---|---|
| | Benzene | 339 | 544 | 9.58 | 11116 | |
| | DCM | 338 | 436 | 7.68 | 6650 | |
| | THF | 337 | 437 | 9.85 | 6790 | |
| **ICZH** | Ethyl acetate | 336 | 434 | 7.28 | 6720 | 17.53% |
| | EtOH | 336 | / | 1.44 | / | |
| | MeCN | 336 | 433 | 1.80 | 6667 | |
| | DMF | 339 | / | 10.42 | / | |
| | Benzene | 339 | 541 | 7.90 | 11014 | |
| | DCM | 338 | 436 | 9.03 | 6650 | pristine: |
| | THF | 337 | 438 | 10.38 | 6843 | 8.31% |
| **ICZF** | Ethyl acetate | 336 | 438 | 9.64 | 6931 | |
| | EtOH | 334 | 451 | 1.40 | 7767 | ground: |
| | MeCN | 337 | 436 | 2.02 | 6738 | 11.73% |
| | DMF | 338 | 443 | 7.08 | 7012 | |
| | Benzene | 339 | 526 | 5.98 | 10487 | |
| | DCM | 337 | 434 | 6.44 | 6632 | |
| | THF | 338 | 436 | 7.07 | 6650 | |
| **ICZ$CH_3$** | Ethyl acetate | 336 | 433 | 4.57 | 6667 | 17.10% |
| | EtOH | 336 | 432 | 1.66 | 6614 | |
| | MeCN | 337 | 432 | 1.56 | 6525 | |
| | DMF | 338 | 432 | 5.08 | 6438 | |
| | Benzene | 338 | 581 | 1.56 | 12374 | |
| | DCM | 338 | 436 | 3.21 | 6650 | pristine: |
| | THF | 337 | 436 | 1.87 | 6738 | 5.80% |
| **ICZ$CF_3$** | Ethyl acetate | 337 | 428 | 2.26 | 6309 | |
| | EtOH | 336 | 431 | 1.57 | 6560 | ground: |
| | MeCN | 337 | 432 | 2.39 | 6525 | 5.08% |
| | DMF | 337 | 437 | 1.56 | 6790 | |

[a] Peak position of the longest absorption band. [b] Peak position of fluorescence emission, excited at the absorption maximum. [c] Molar absorptivity (L/cm/mol). [d] Stokes' shift in $cm^{-1}$. [e] Quantum yields in the solid state.

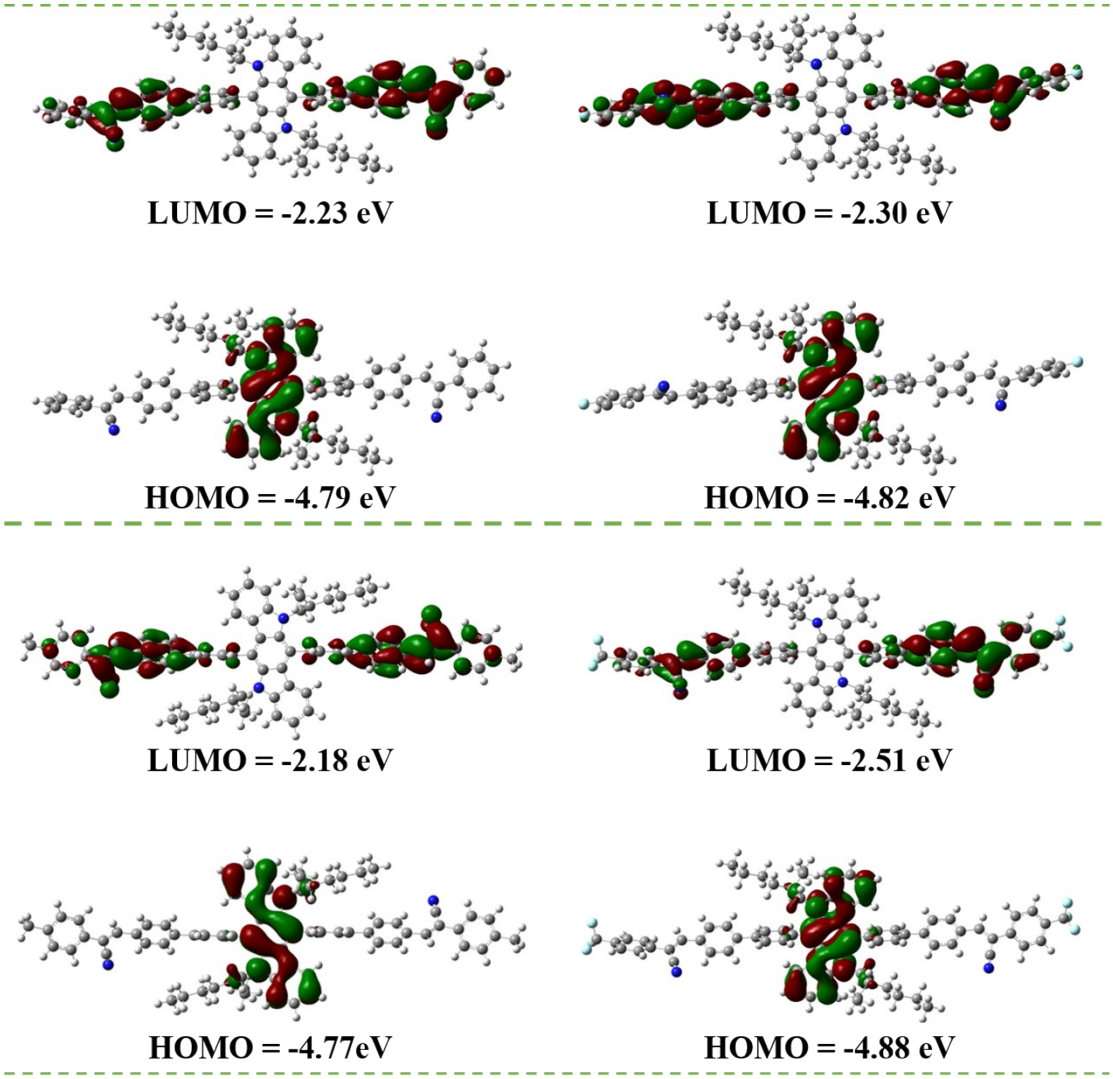


Fig. S19 Optimized molecular structure and molecular orbital amplitude plots of the HOMO and LUMO levels and electron cloud distribution of **ICZH, ICZF, ICZCH$_3$** and **ICZCF$_3$** calculated using the B3LYP/6-31G* basis set.

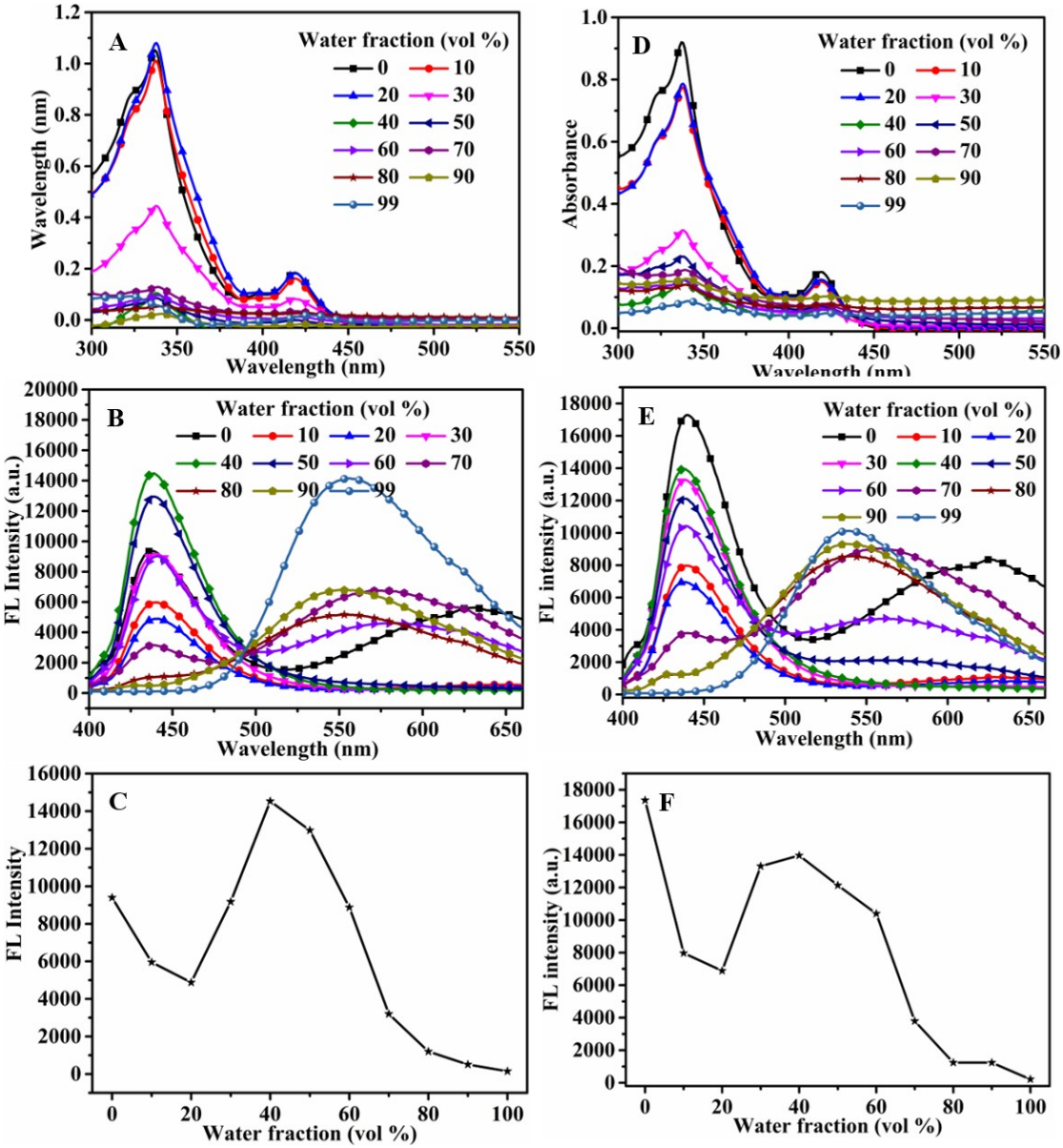


Fig. S20 (A, D) The UV-vis absorption and (B, E) fluorescence spectra of compounds **ICZH** and **ICZCH$_3$** in THF-water mixtures with different water volume fractions; (C, F) the effect of water volume fractions on the emission intensity of 440 nm.

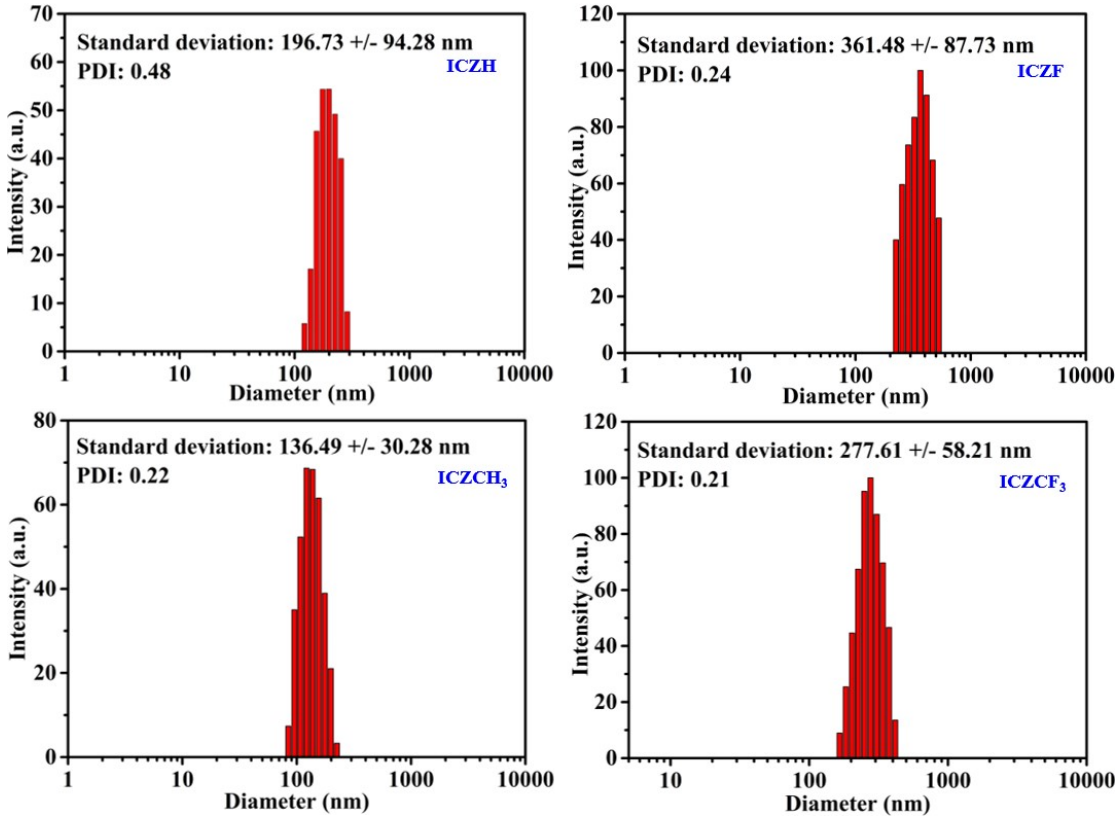


Fig. S21 Size distributions of **ICZH**, **ICZF**, **ICZCH$_3$** and **ICZCF$_3$** in THF-$H_2O$ mixtures ($f_w$ = 50%).

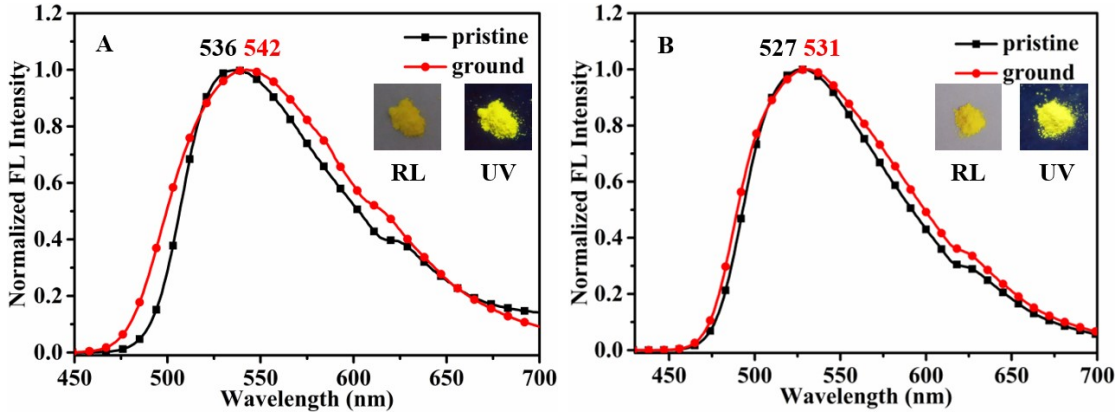


Fig. S22 Emission spectra of compound **ICZH** (A) and **ICZCH$_3$** (B) of pristine and ground samples. Inset: Photographs under room light and 365 nm light.

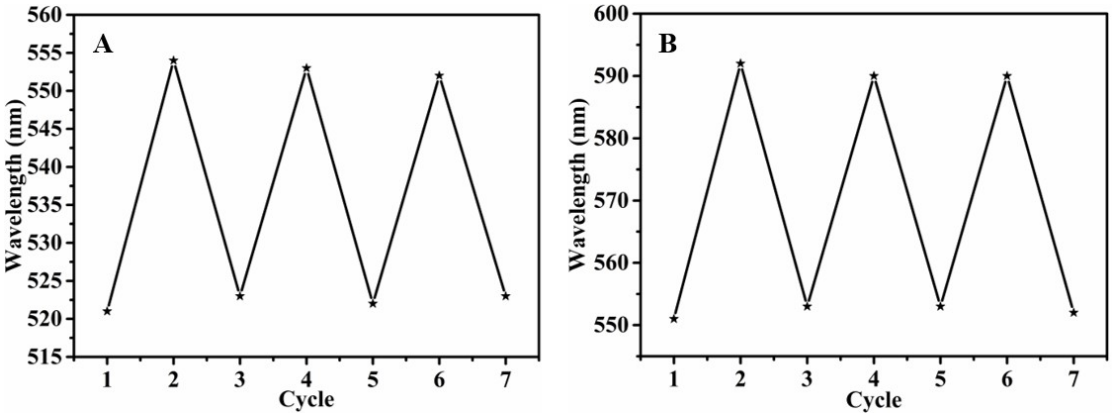


Fig S23 Repeated switching of compounds **ICZF** (A) and **ICZCF$_3$** (B) by ground-fumed cycles.

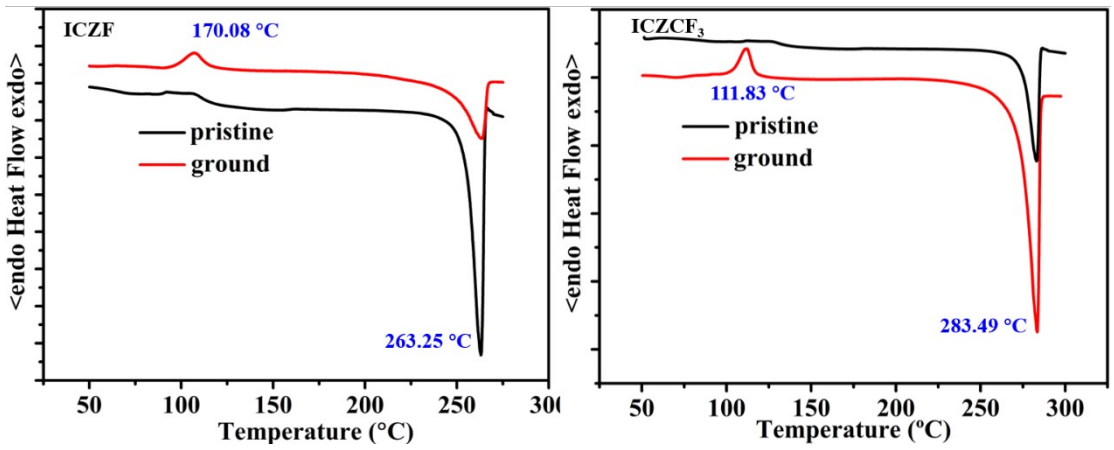


Fig. S24 DSC curve of compounds **ICZF** (A) and **ICZCF$_3$** (B) in the pristine and ground powders. (Scan rate: 10 °C min$^{-1}$).