Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.


# Cyano-containing Tetraphenylethene Isomers: Similar Bright Mechanoluminescence, but Diverse Recoverable Processes

*Yuqing Jiang†[a], Xiaoyong Chang†[b], Weiwei Xie[a], Guangxi Huang*[a] and Bing Shi Li*[a]*

*[a]Key Laboratory of New Lithium-Ion Battery and Mesoporous Material, College of Chemistry and Environmental Engineering, Shenzhen University, 1066 Xueyuan Avenue, Nanshan, Shenzhen 518055, China. E-mail: phbingsl@szu.edu.cn; Fax: +86-755-26536141; Tel: +86-755-26558094*

*[b]Department of Chemistry, Southern University of Science and Technology, 1088 Xueyuan Avenue, Nanshan, Shenzhen, 518055, China*

[†] Y. Q. Jiang and X. Y. Chang contributed equally to this work.

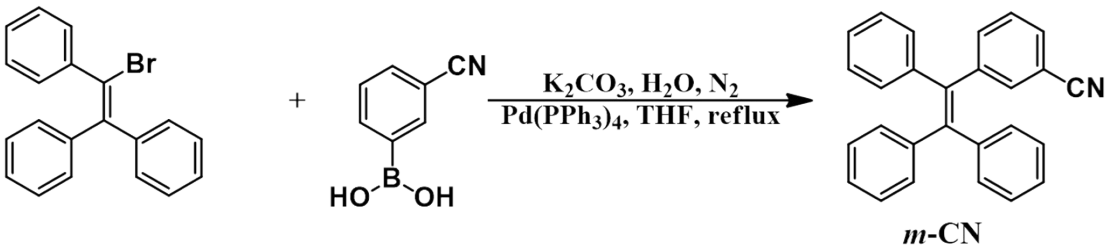
**Materials**

$Pd(PPh_3)_4$, 4-cyanophenylboronic acid, 3-cyanophenylboronic acid, bromotriphenylethylene and other chemicals were all purchased from Energy Chemical Company. $K_2CO_3$ and solvents were all purchased from Xilong Chemical Co., Ltd.. All the chemicals were used as received without further purification. Compound ***p*-CN** (4-(1,2,2-triphenylvinyl)benzonitrile) was prepared according to previous paper.[1]

**Instruments and methods**

$^1H$ and $^{13}C$ NMR spectra were recorded on a VNMRS 500 NMR spectrometer (Varian, USA). High resolution mass spectra (HR-MS) were recorded using an Autoflex III mass spectrometer (MALDI-TOF-MS, Bruker, Germany). Element analysis was performed using a vario EL cube elemental analyzer (Elementar, Germany). UV-Vis spectra were recorded using a UV-2600 spectrometer (Shimadzu, Japan). Absolute quantum efficiency was measured on an integrating sphere (C11347-11, Hamamatsu, Japan). The fluorescence quantum yield ($\Phi_f$) in solution was measured by a relative method using quinine in 0.1 M $H_2SO_4$ ($\Phi_f$ = 54.6%) as a standard. Fluorescence lifetime was measured on a compact fluorescence lifetime spectrometer (C11367-11, Hamamatsu, Japan). DSC measurements were carried out on a NETZSCH DSC 200F3 instrument at a heating rate and a cooling rate of 10 $^oC\ min^{-1}$ in nitrogen. TGA analysis was performed on a NETZSCH SA409PC thermogravimeter. Powder X-ray diffraction (PXRD) patterns were carried out in the reflection mode at room temperature using a 2.2 kW Empyrean X-ray Diffraction System (PANalytical, Netherland). The ML spectra were collected from a spectrometer4 of Acton SP2750 with a liquid-nitrogen-cooled CCD (SPEC-10, Princeton) as a power detector. The theoretical ground-state geometry and electronic structure of molecule was optimized using the density functional theory (DFT) with B3LYP hybrid functional at the basis set level of 6-31+G(d). All the theoretical calculations were performed using Gaussian 03 package.[2]

Scheme S1. Synthetic route of compound ***m*-CN**.



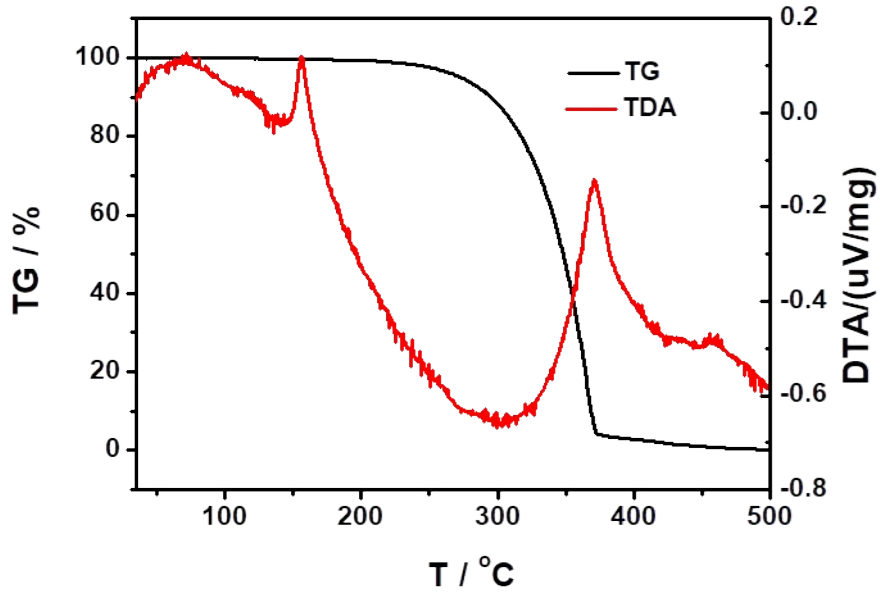




Figure S1. TG and DTA curves of ***p*-CN**.

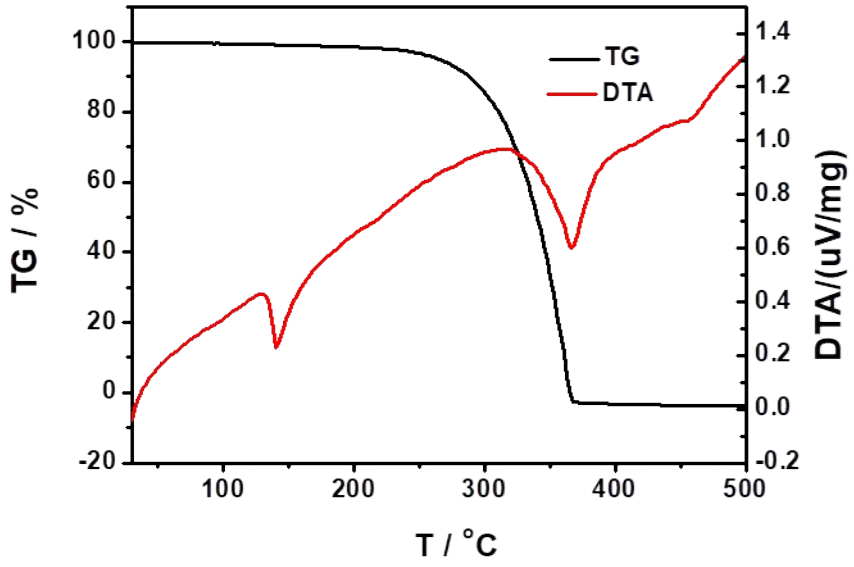



Figure S2. TG and DTA curves of ***m*-CN**.

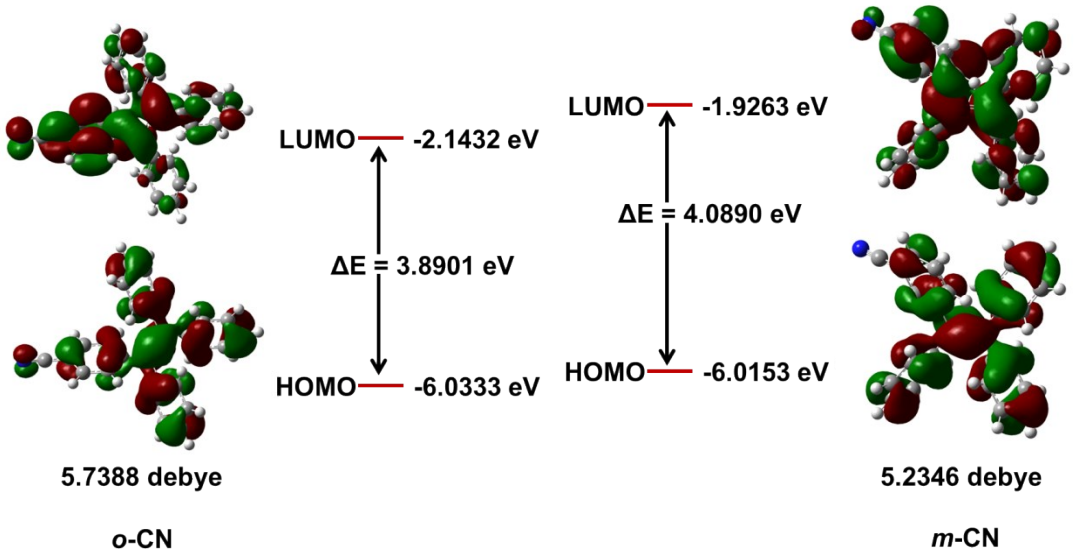



Figure S3. The HOMO and LUMO orbital distribution of ***p*-CN** and ***m*-CN** calculated by B3LYP/6-31+G(d).

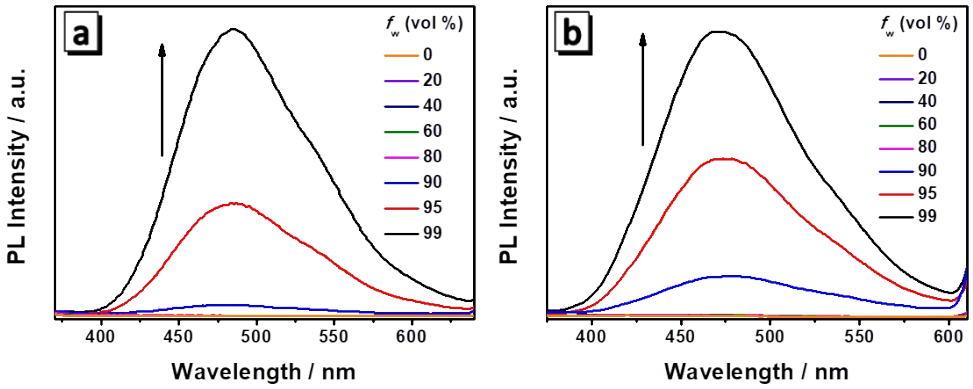



Figure S4. The fluorescence spectra of (a) ***p*-CN** and (b) ***m*-CN** in THF/water mixtures with different water fractions ($f_w$), concentration: 10 μM.

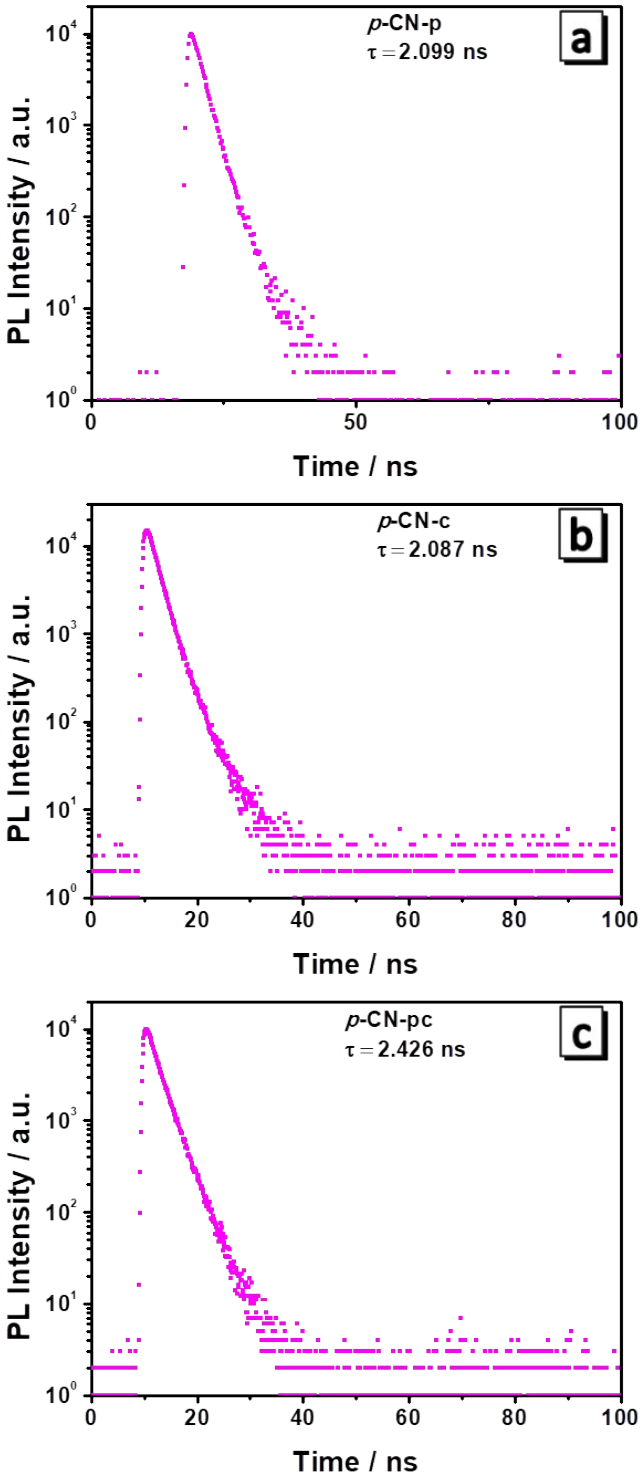



Figure S5. Fluorescence decay curves of (a) ***p*-CN-p**, (b) ***p*-CN-c** and (c) ***p*-CN-pc**.

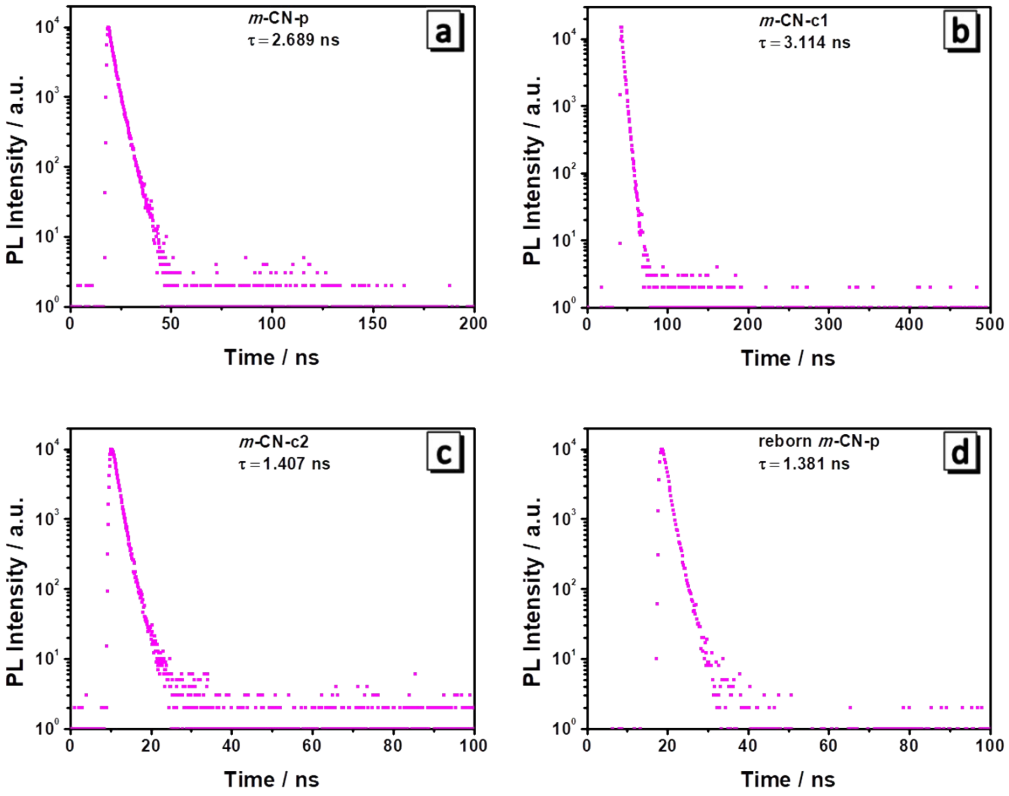



Figure S6. Fluorescence decay curves of (a) ***m*-CN-p**, (b) ***m*-CN-c1**, (c) ***m*-CN-c2** and (d) reborn ***m*-CN-p**.

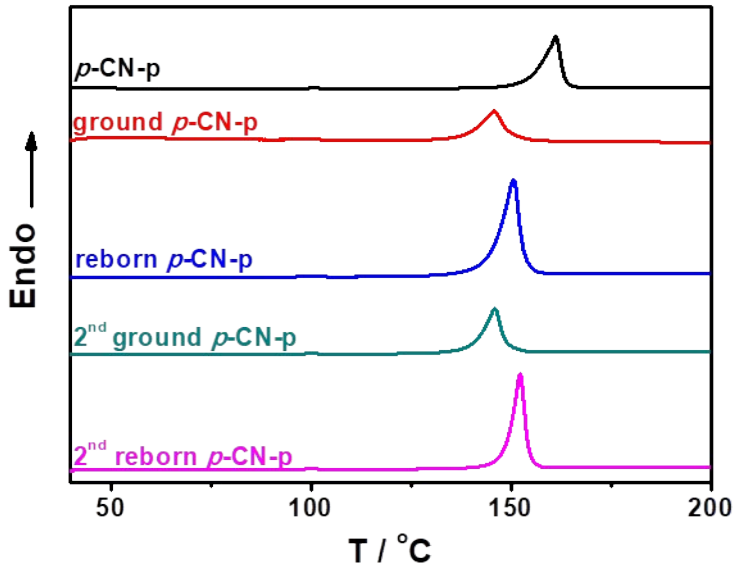



Figure S7. DSC curves of different states of ***p*-CN** during reborn process.

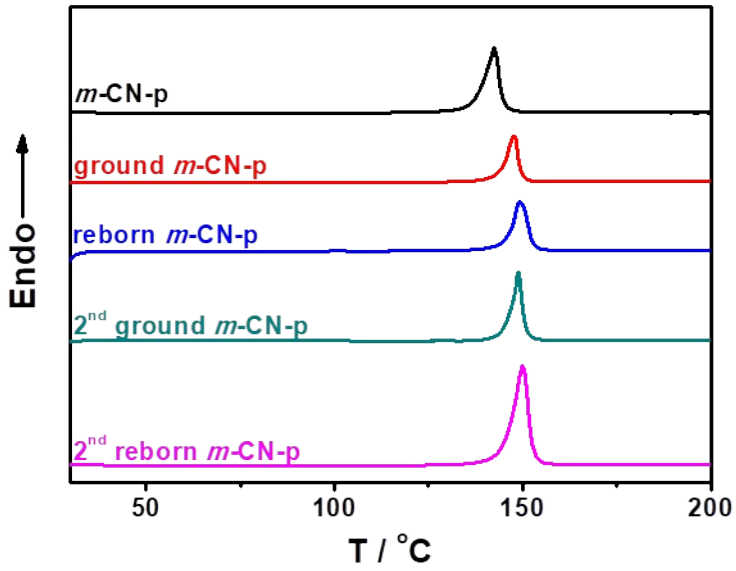



Figure S8. DSC curves of different states of ***m*-CN** during reborn process.

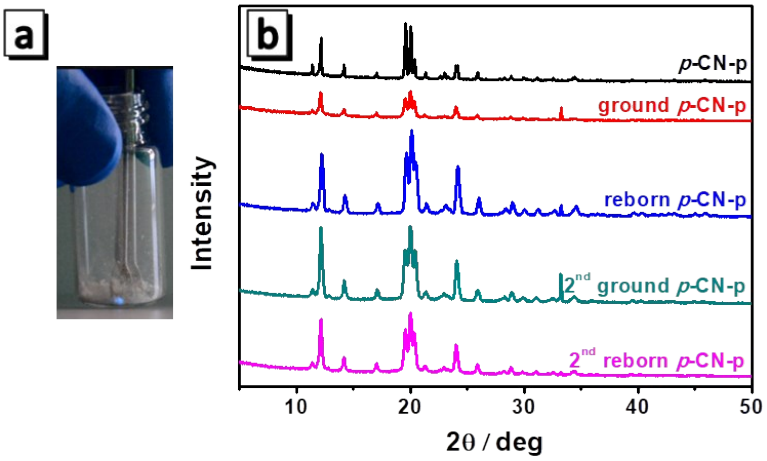



Figure S9. (a) ML image of reborn ***p*-CN-p** under daylight at room temperature. (b) PXRD patterns of ***p*-CN** during recycling process.

Table S1. Single crystal data of ***p*-CN-c**, ***m*-CN-c1** and ***m*-CN-c2**

| | ***p*-CN-c** | ***m*-CN-c1** | ***m*-CN-c2** |
|---|---|---|---|
| CCDC Number | 1904512 | 1917322 | 1904513 |
| Formula | $C_{27}H_{19}N$ | $C_{27}H_{19}N$ | $C_{27}H_{19}N$ |
| Formula Weight /g•mol$^{-1}$ | 357.43 | 357.43 | 357.43 |
| Crystal system | trigonal | tetragonal | monoclinic |
| Space group | $P3_1$ | P4/ncc | $P2_1$ |
| T/K | 150 | 130 | 288 |
| Z | 3 | 4 | 2 |
| a/Å | 9.1128(3) | 13.91783(16) | 10.5183(7) |
| b/Å | 9.1128(3) | 13.91783(16) | 9.3996(6) |
| c/Å | 21.2477(5) | 10.4029(2) | 10.5184(7) |
| α/° | 90 | 90 | 90 |
| β/° | 90 | 90 | 100.09 |
| γ/° | 120 | 90 | 90 |
| V/Å$^3$ | 1528.08(11) | 2015.11(6) | 1023.85(12) |
| $\rho_c$/g•cm$^{-3}$ | 1.165 | 1.178 | 1.159 |
| μ/mm$^{-1}$ | 0.513 | 0.519 | 0.510 |
| F(000) | 564 | 752 | 376 |
| Reflections collected | 4680 | 9168 | 3016 |
| Independent reflections | 2721 | 1034 | 2210 |
| $R_{int}$ | 0.0288 | 0.0253 | 0.0827 |
| $R_1(I > 2\sigma(I))$ | 0.0414 | 0.0593 | 0.1131 |
| $wR_2$ | 0.1117 | 0.2121 | 0.2970 |

| | | | |
|---|---|---|---|
| GOOF | 1.037 | 1.154 | 1.092 |

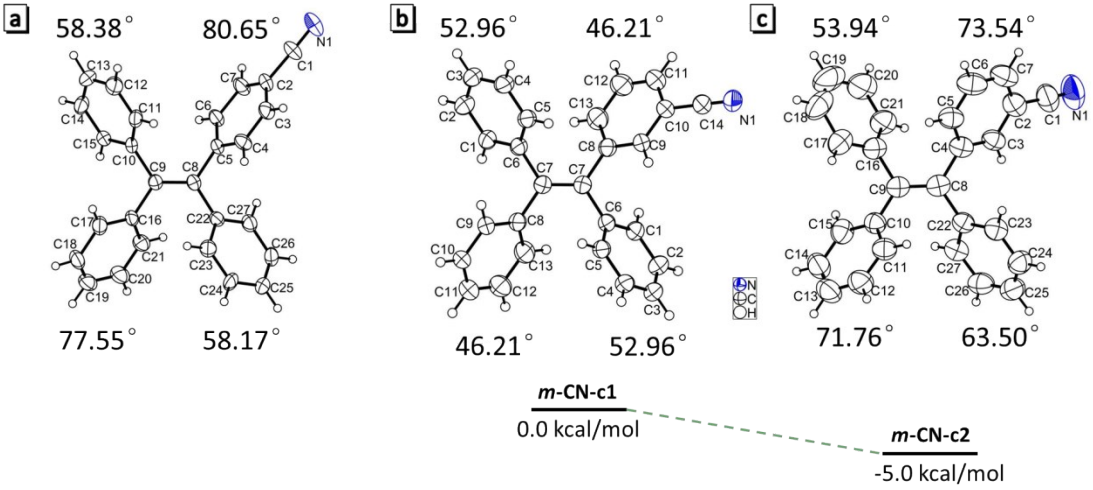



Figure S10. The molecular conformations with labels of carbon/nitrogen atoms and dihedral angles (between the phenyl ring and central ethene group) of (a) ***p*-CN-c**, (b) ***m*-CN-c1** and (c) ***m*-CN-c2**. Ellipsoids represent the 50% probability level. Hydrogen atoms are shown as spheres of arbitrary radii. Bottoms are the calculated single molecule thermal stablization energies of ***m*-CN-c1** and ***m*-CN-c2** based on the crystal data.

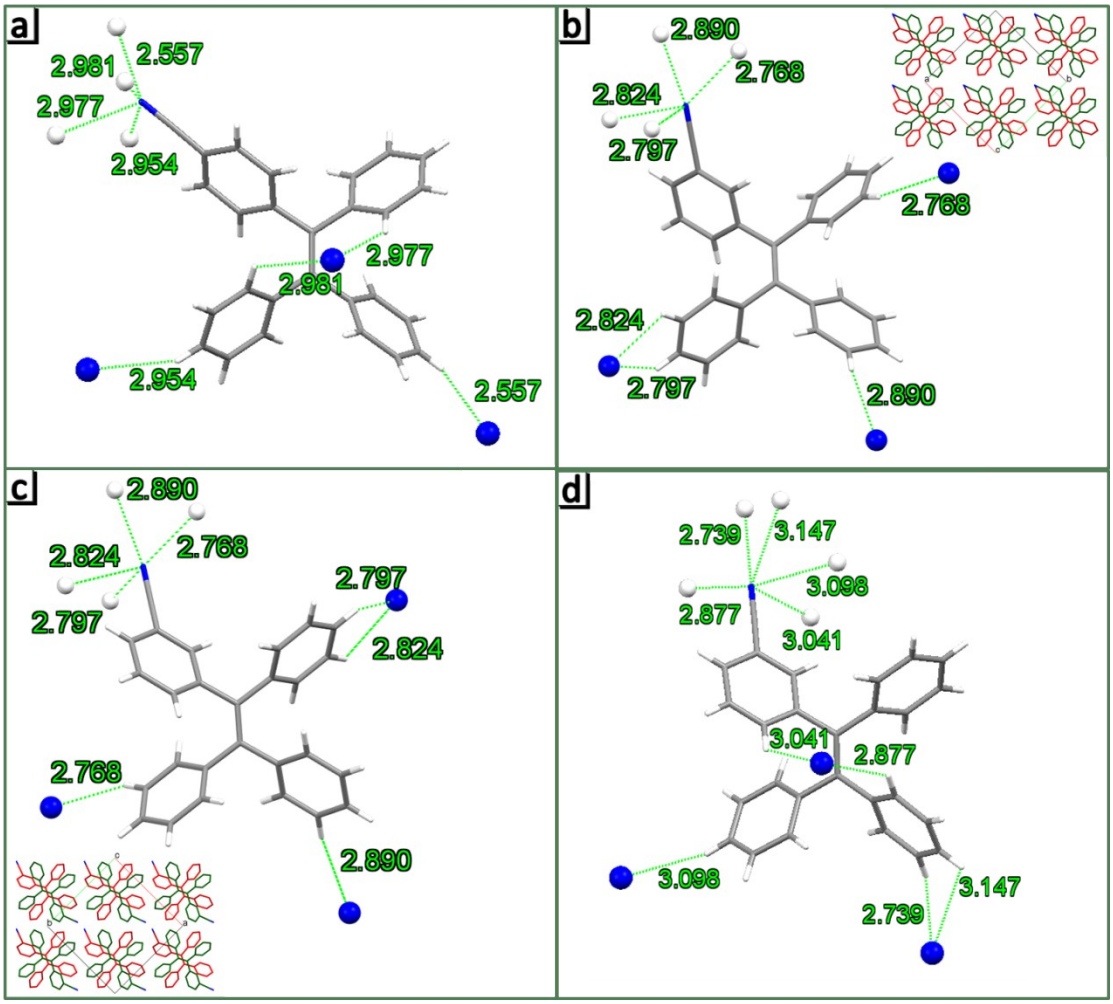



Figure S11. The detailed intermolecular interactions in crystal (a) ***p*-CN-c**, (b, c) ***m*-CN-c1** and (d) ***m*-CN-c2**.

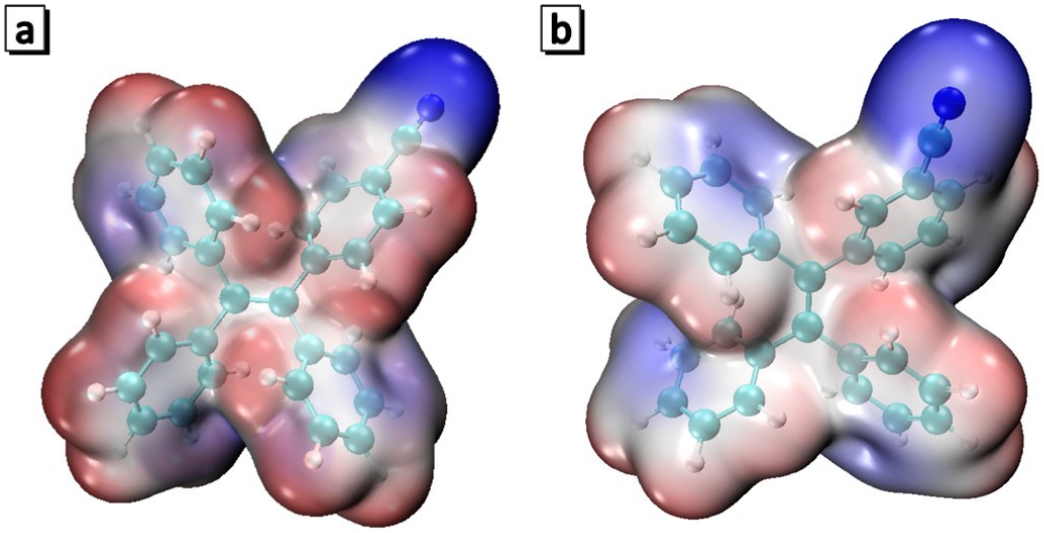



Figure S12. Electrostatic potential of (a) ***p*-CN** and (b) ***m*-CN** at 0.001 a.u. isosurface of electron density at B3lyp/6-31G(d) level.

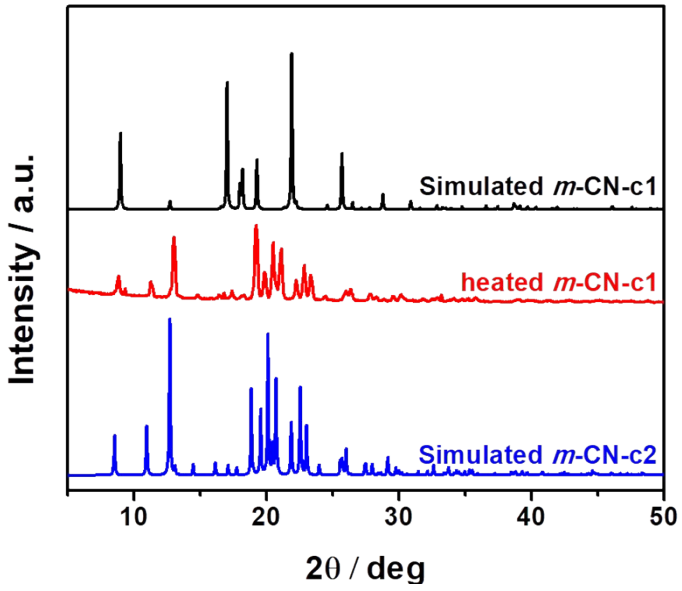



Figure S13. PXRD patterns of ***m*-CN-c1**, heated ***m*-CN-c1** and ***m*-CN-c2**.

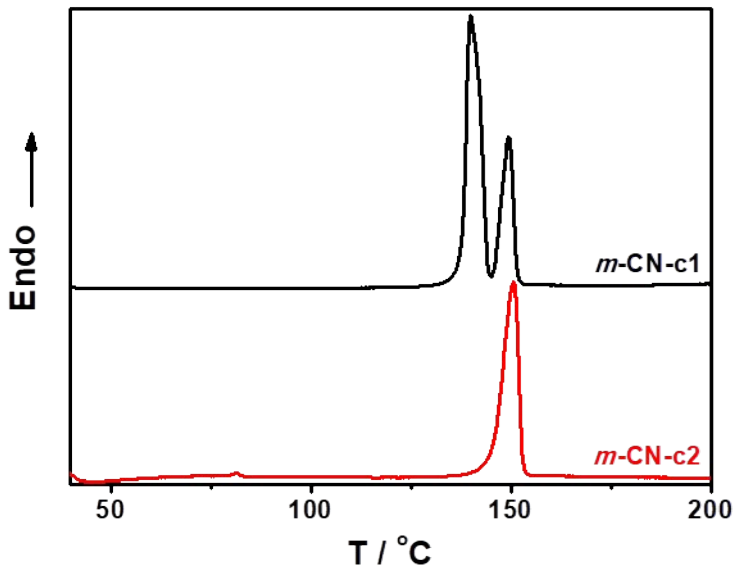



Figure S14. DSC curves of single crystal ***m*-CN-c1** and ***m*-CN-c2**. Heating rate: 5 $^{o}$C/min.

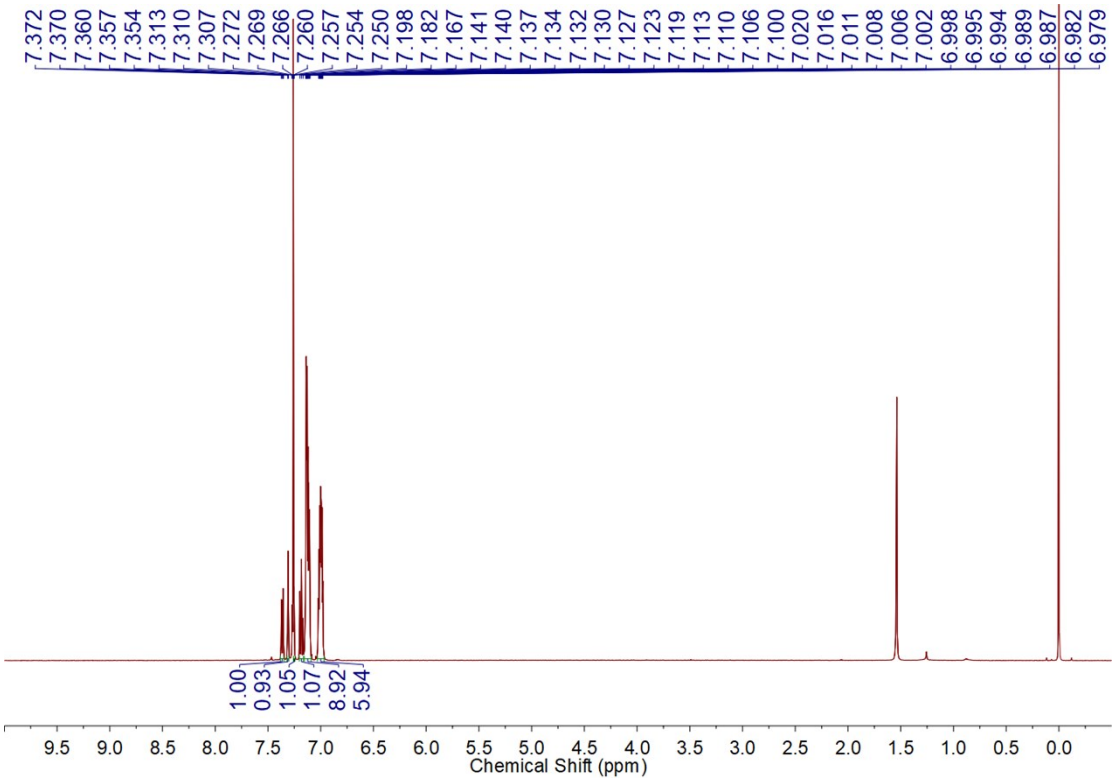



Figure S15. $^{1}$H NMR of compound ***m*-CN**.

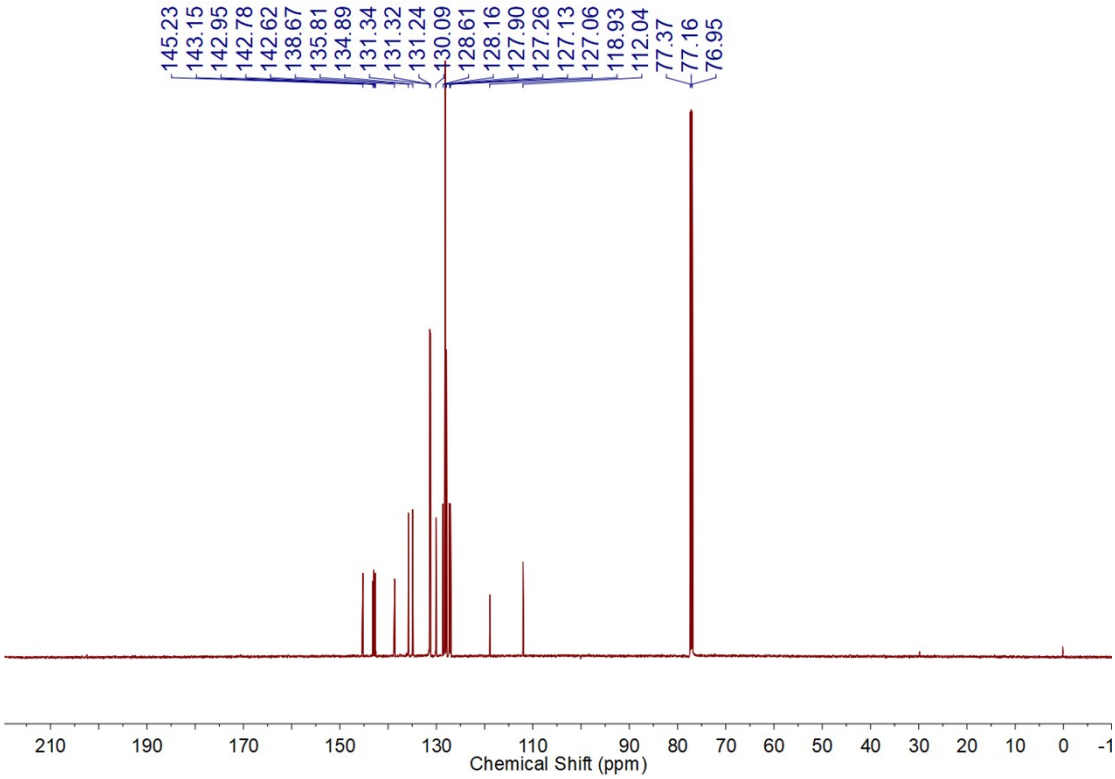



Figure S16. $^{13}C$ NMR of compound ***m*-CN**.

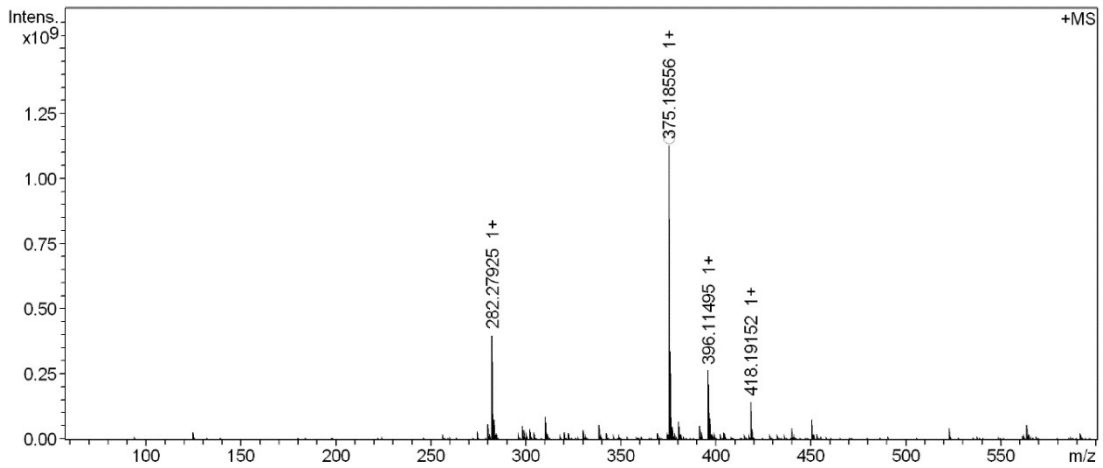



Figure S17. HRMS of compound ***m*-CN**.

## References

1. M. Ouyang et al., ***Wuli Huaxue Xuebao*** 2012, **28**(12), 2944-2952.

2. Gaussian 03, Revision E.01, M. J. Frisch et al., Gaussian, Inc., Wallingford CT, 2009.