

Supporting Information

High-barrier polyimide containing carbazole moiety: synthesis, gas barrier properties and molecular simulations

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Table S1

Figures S1-S11

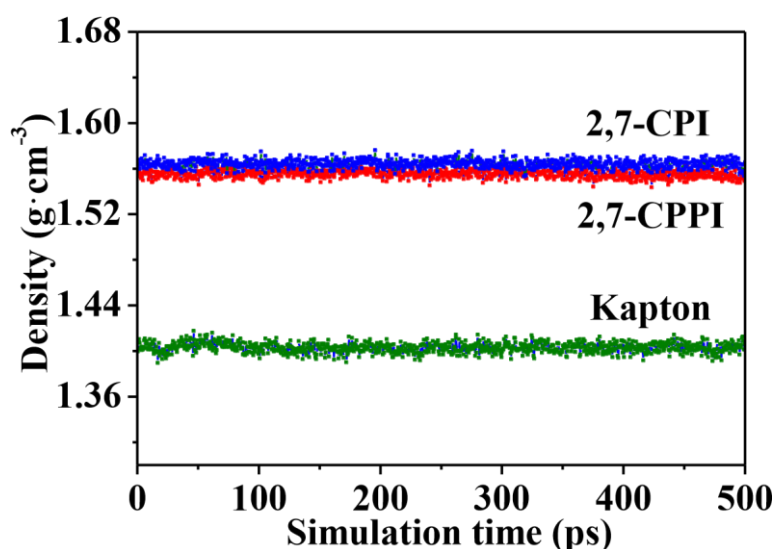


Figure S1 Plots of density versus simulation time in the NPT simulation for Kapton, 2,7-CPPI and 2,7-CPI.

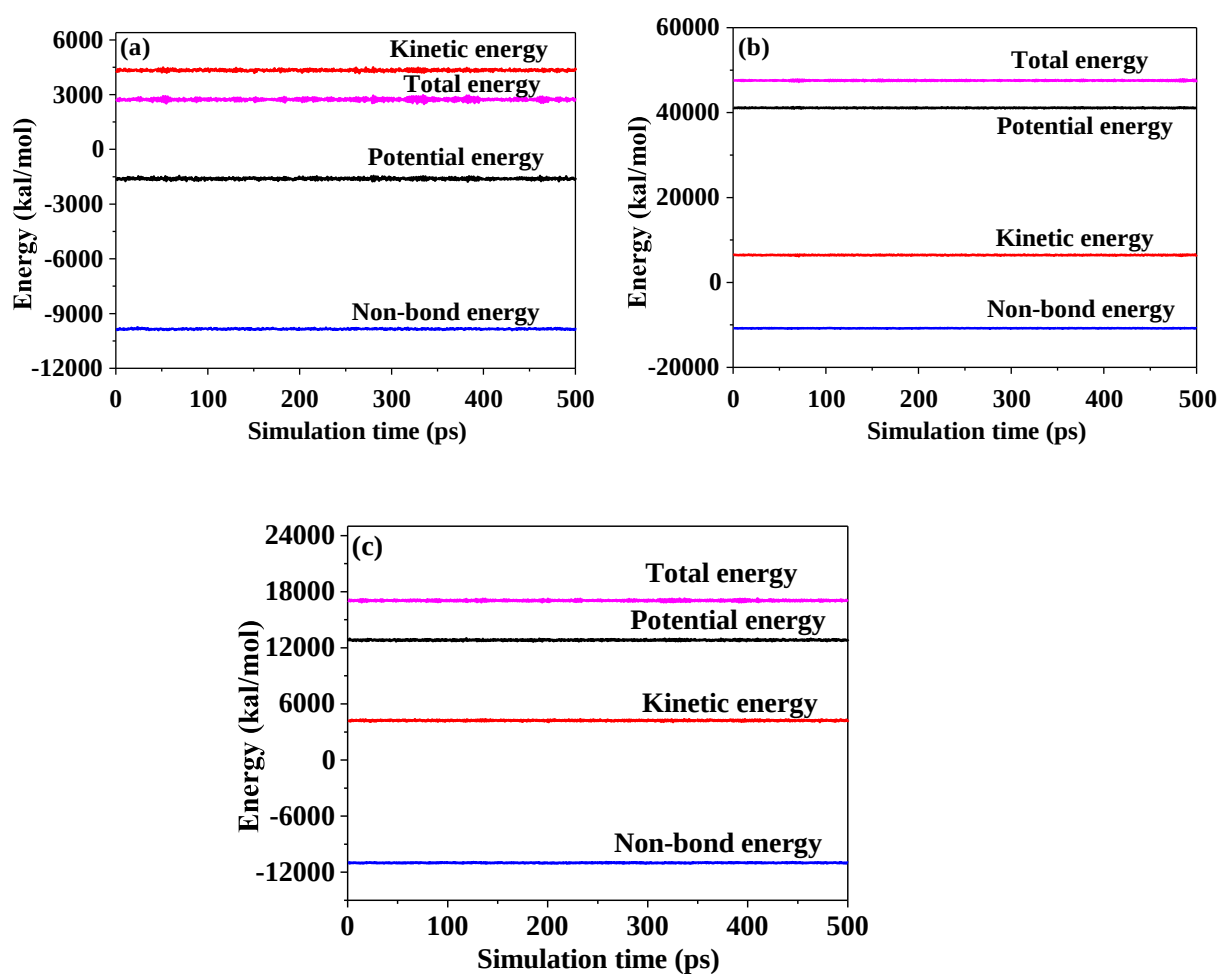


Figure S2 Plots of energy versus simulation time in the NPT simulation for (a) Kapton, (b) 2,7-CPPI and (c) 2,7-CPI.

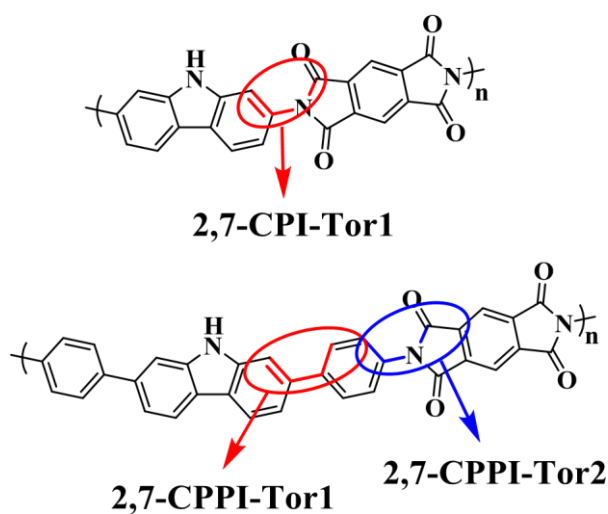


Figure S3 Schematic diagrams of the analyzed atomic segments for the dihedral angle analysis.

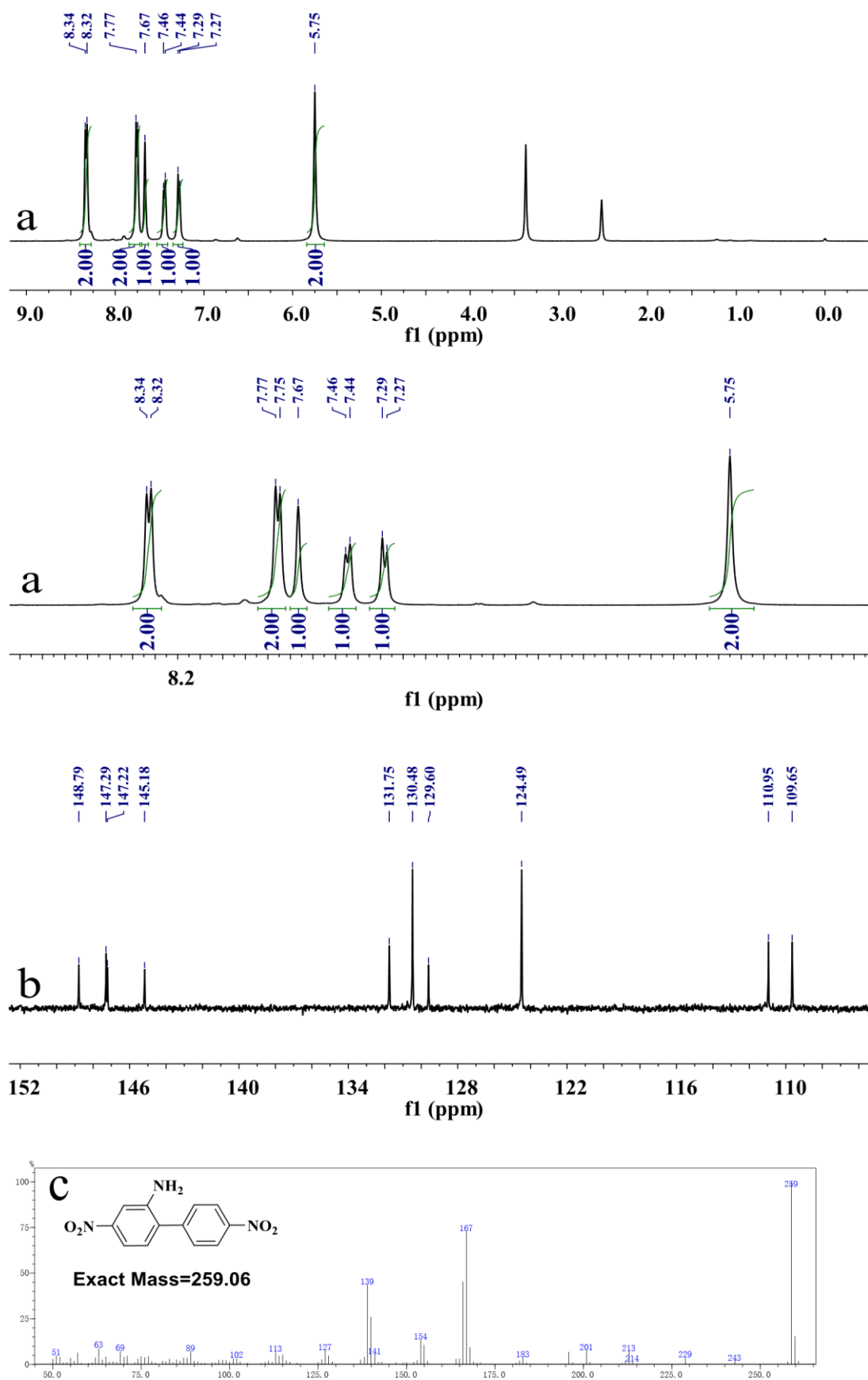


Figure S4 ^1H NMR (a), ^{13}C NMR (b) and MS (c) spectra of DPNA.

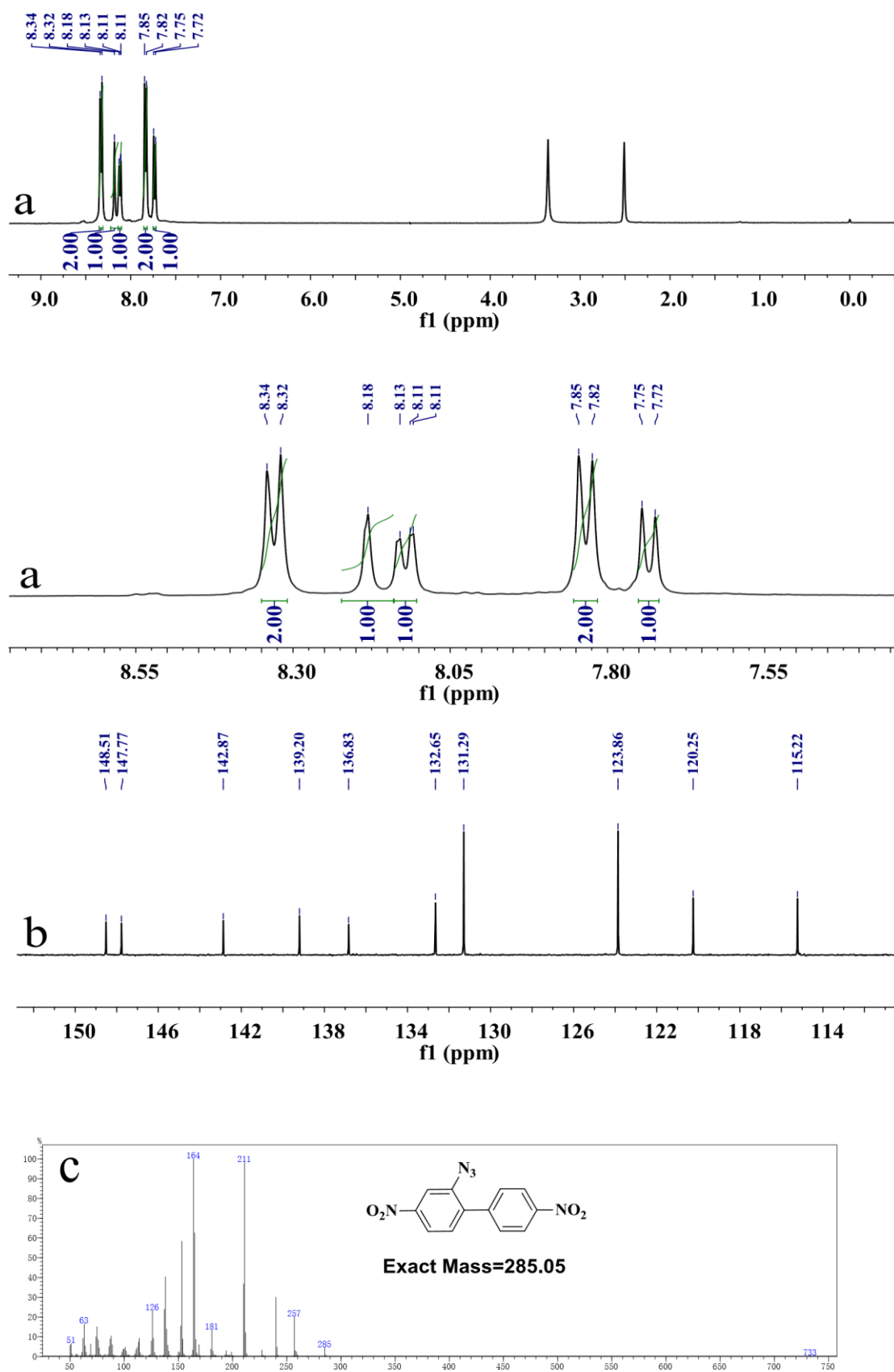


Figure S5 ^1H NMR (a), ^{13}C NMR (b) and MS (c) spectra of DPNN₃.

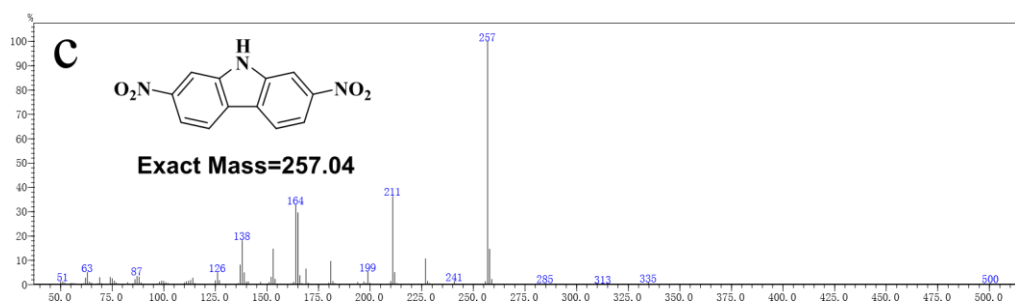
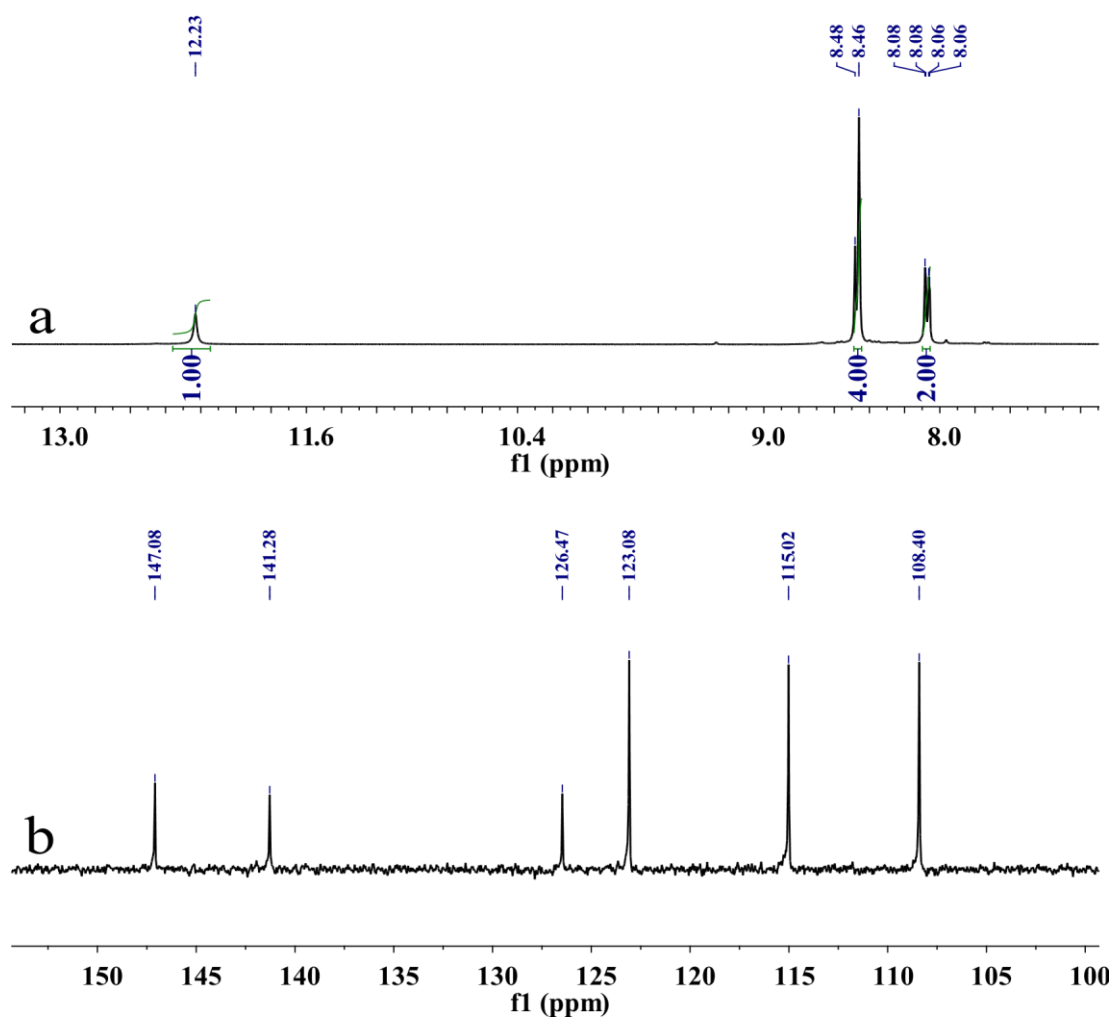


Figure S6 ^1H NMR (a), ^{13}C NMR (b) and MS (c) spectra of 2,7-CDN.

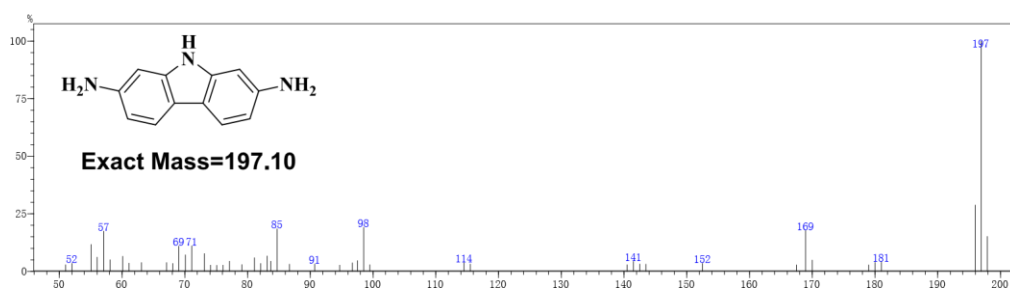


Figure S7 The MS spectrum of 2,7-CDA.

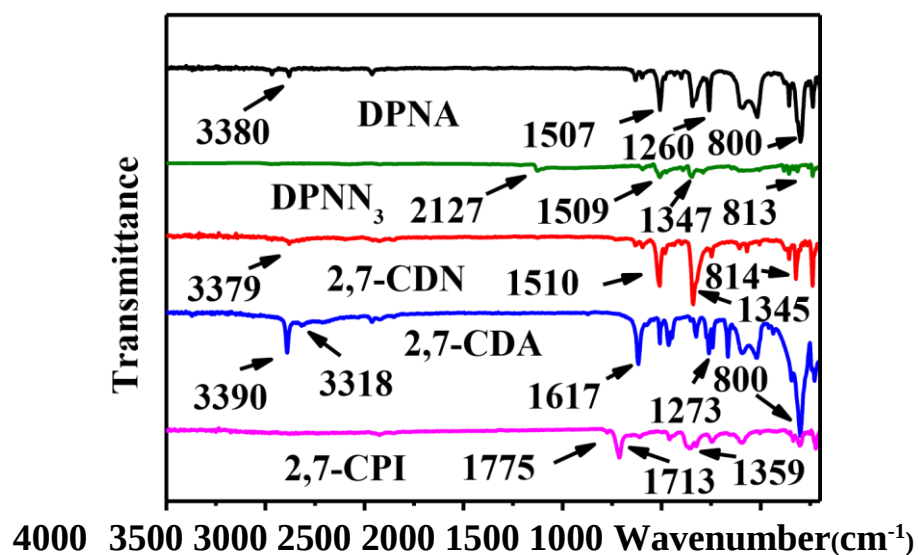


Figure S8 FT-IR spectra of DPNA, DPNN₃, 2,7-CDN, 2,7-CDA and 2,7-CPI.

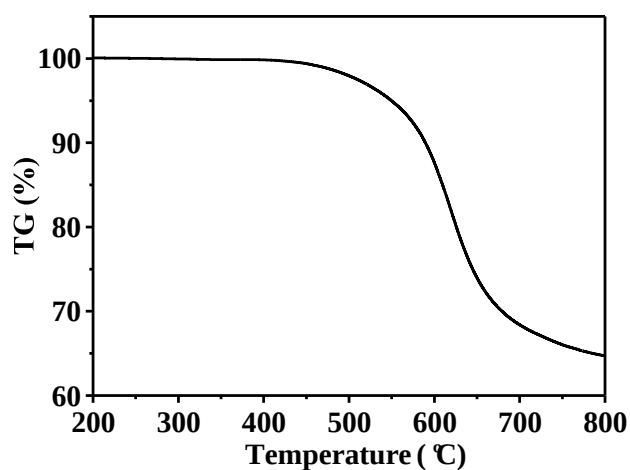


Figure S9 TGA curve of the 2,7-CPI film.



Figure S10 Photo image of the flexible 2,7-CPI film.

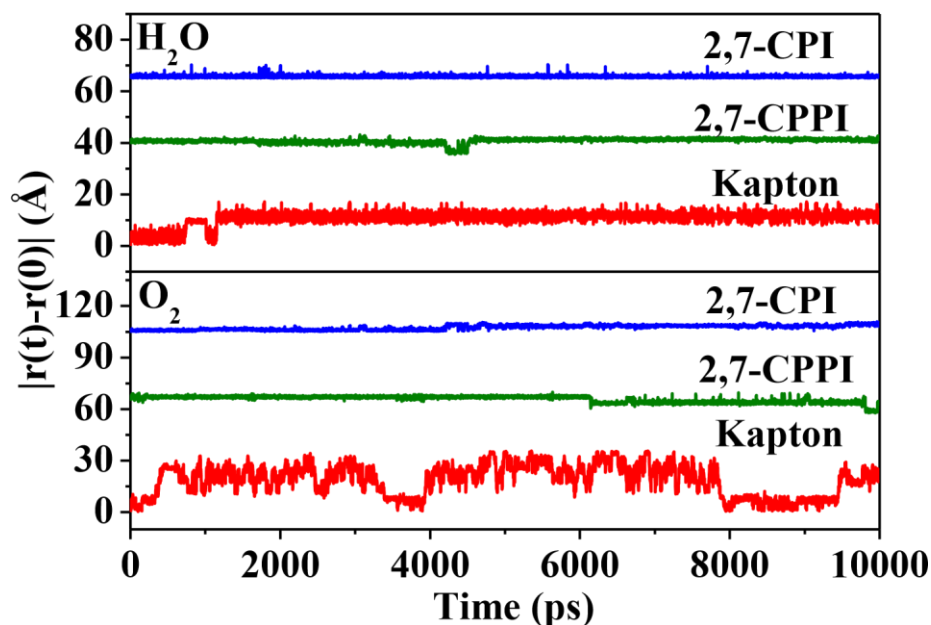


Figure S11 Displacement of O₂ and H₂O from their initial positions in Kapton, 2,7-CPPI and 2,7-CPI.

Table S1 The positron lifetime data of Kapton, 2,7-CPPI and 2,7-CPI films.

PIs	$\tau_1(\text{ns})$	$I_1(\%)$	$\tau_2(\text{ns})$	$I_2(\%)$
Kapton ^a	0.17	13.0	0.38	86.8
2,7-CPPI ^a	0.17	7.4	0.34	92.4
2,7-CPI	0.13	17.3	0.34	82.5

^a The positron lifetime data are obtained from Ref. [1].

References

1. Liu, Y.; Huang, J.; Tan, J.; Zeng, Y.; Liu, J.; Zhang, H.; Pei, Y.; Xiang, X.; Liu, Y. Intrinsic high-barrier polyimide with low free volume derived from a novel diamine monomer containing rigid planar moiety. *Polymer* **2017**, *114*, 289-297.