

Supporting Information

Novel carbazole-based donor-isoindolo[2,1-a]benzimidazol-11-one acceptor polymers for ternary flash memory and light-emitting

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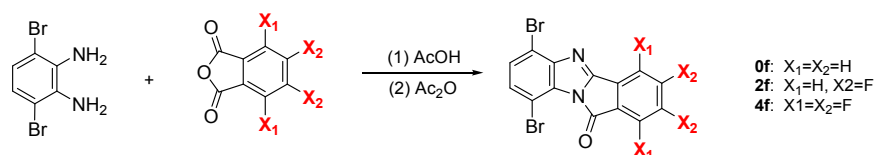
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1. Synthesis of monomer **0f**, **2f** and **4f**

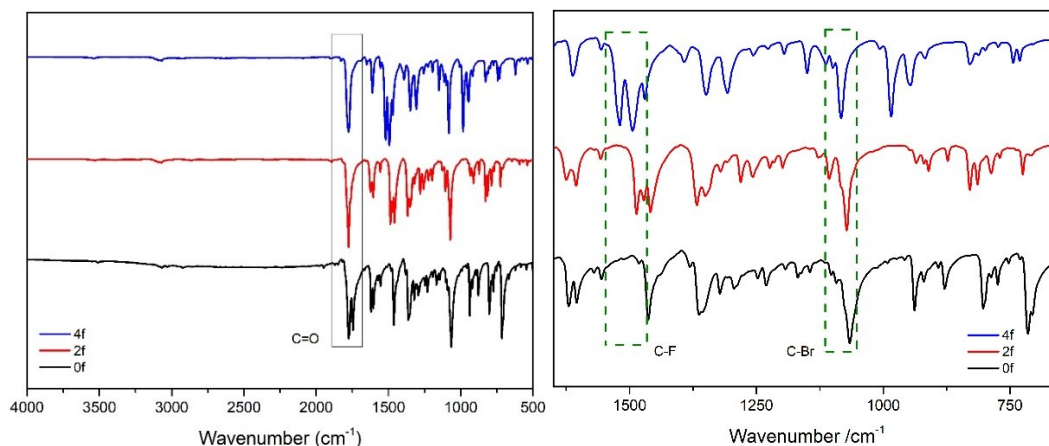


A mixture of 3,6-dibromo-1,2-phenylenediamine (1.33 g, 5 mmol) and phthalic anhydride (0.74 g, 5 mmol) were stirred in glacial acetic acid under nitrogen at 120 °C for 3 hours. The precipitation was washed with water and methanol, dried under vacuum and refluxed in 2 mL of acetic anhydride under nitrogen for 6 h. The crude production was purified by column chromatography (silica gel, dichloromethane / petroleum ether = 2:1, v: v). The yellow monomer **0f** was obtained with yield of 1.36 g (72%).

A mixture of 3,6-dibromo-1,2-phenylenediamine (1.33 g, 5 mmol) and 4,5-difluorophthalic anhydride (0.92 g, 5 mmol) were stirred in glacial acetic acid under nitrogen at 120 °C for 2 hours. The precipitation was washed with water and methanol, dried under vacuum and refluxed in 2 mL of acetic anhydride under nitrogen for 6 h. The crude production was purified by column chromatography (silica gel, dichloromethane / petroleum ether = 2:1, v: v) and afforded 1.58 g (76%) of yellow solid monomer **2f**.

A mixture of 3,6-dibromo-1,2-phenylenediamine (1.33 g, 5 mmol) and 4,5-difluorophthalic anhydride (0.92 g, 5 mmol) were stirred in glacial acetic acid under nitrogen at 120 °C for 2 hours. The precipitation was washed with water and methanol, dried under vacuum and refluxed in 2 mL of acetic anhydride under nitrogen for 6 h. The crude production was purified by column chromatography (silica gel, dichloromethane / petroleum ether = 2:1, v: v) and afforded 1.47 g (65%) of yellow solid monomer **4f**.

2. FT-IR and ¹H-NMR of monomer 0f, 2f and 4f



In the case of IR spectrum, monomers exhibited similar characteristic bands around 1770 cm^{-1} (C=O stretching), 1600 cm^{-1} (C=C and C=N stretching). Note that the stretching vibrations of carbonyl groups in condensed cyclic γ -lactams would move to above 1760 cm^{-1} in their IR spectra. ^[1] The C-X bonds don't usually possess a constant vibrational frequency nor do they always have unique absorption band features, which may lead to the difficulty of locating and recognizing their absorption. ^[2] Since the C-F stretching could exhibit two or more bands of polyfluorinated aliphatic hydrocarbons with a broad range of 1400-1000 cm^{-1} , ^[2] and compared with the non-fluorinated monomer 0f and with three polymers which possess no C-Br bond, the aromatic C-Br and C-F stretching bands of three monomers were assumed to be as follows:

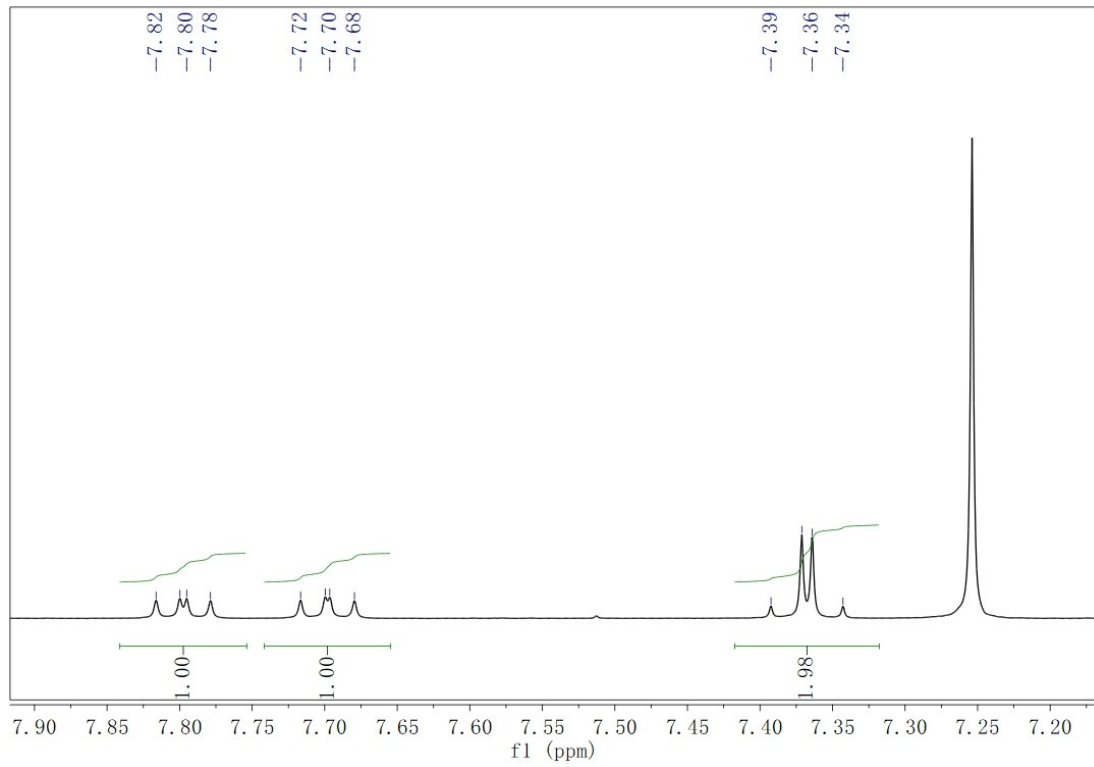
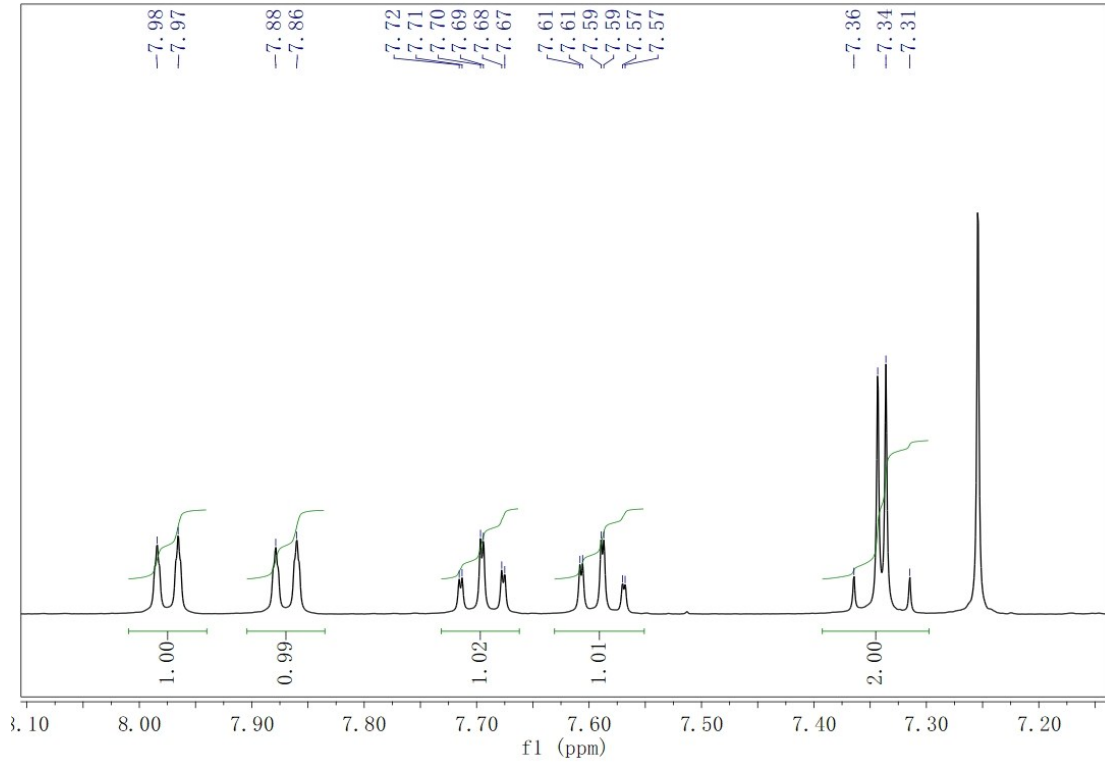
0f: 1066 cm^{-1} (C-Br)

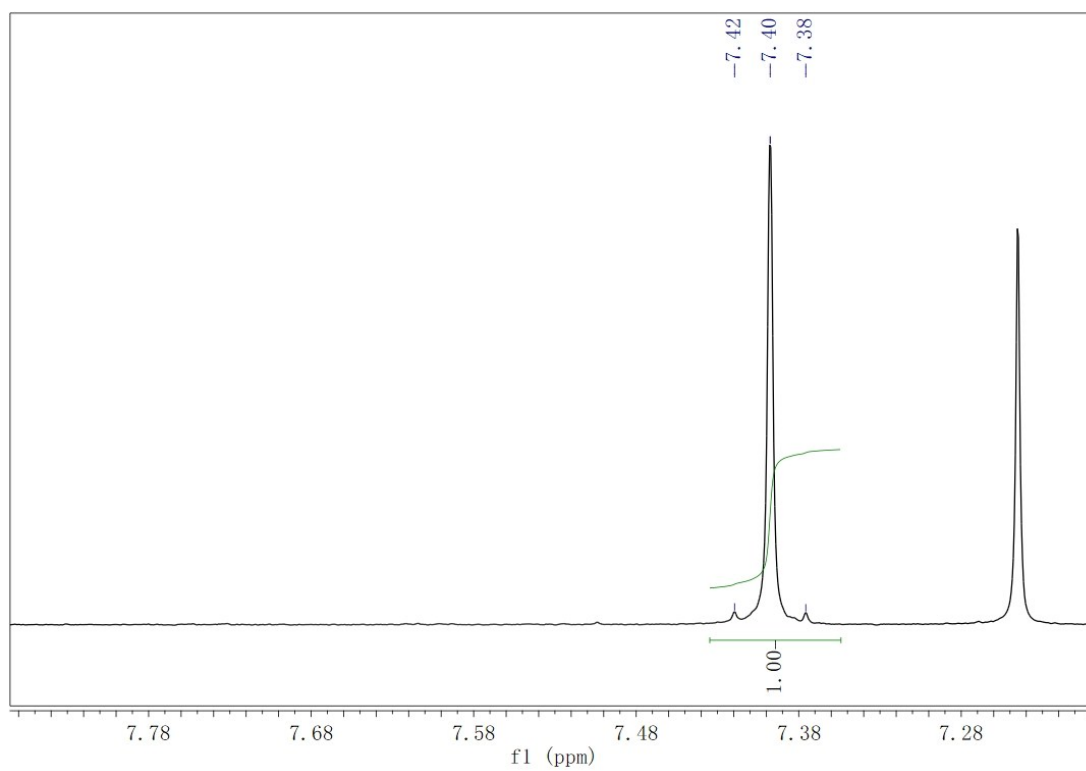
2f: 1072 cm^{-1} (C-Br); 1472 cm^{-1} and 1486 cm^{-1} (C-F)

4f: 1083 cm^{-1} (C-Br); 1494 cm^{-1} and 1519 cm^{-1} (C-F)

¹ E. V. Gromachevskaya, A. V. Finko, A. V. Butin, K. S. Pushkareva, V. D. Strelkov, L. I. Isakova, G. D. Krapivin, *Chem. Heterocycl. Compd.* **2013**, *49*, 1331-1344.

² The Sadtler Handbook of Infrared Spectra, in: Sadtler Spectral Handbooks, Bio-Rad Laboratories, Inc., Informatics Division.





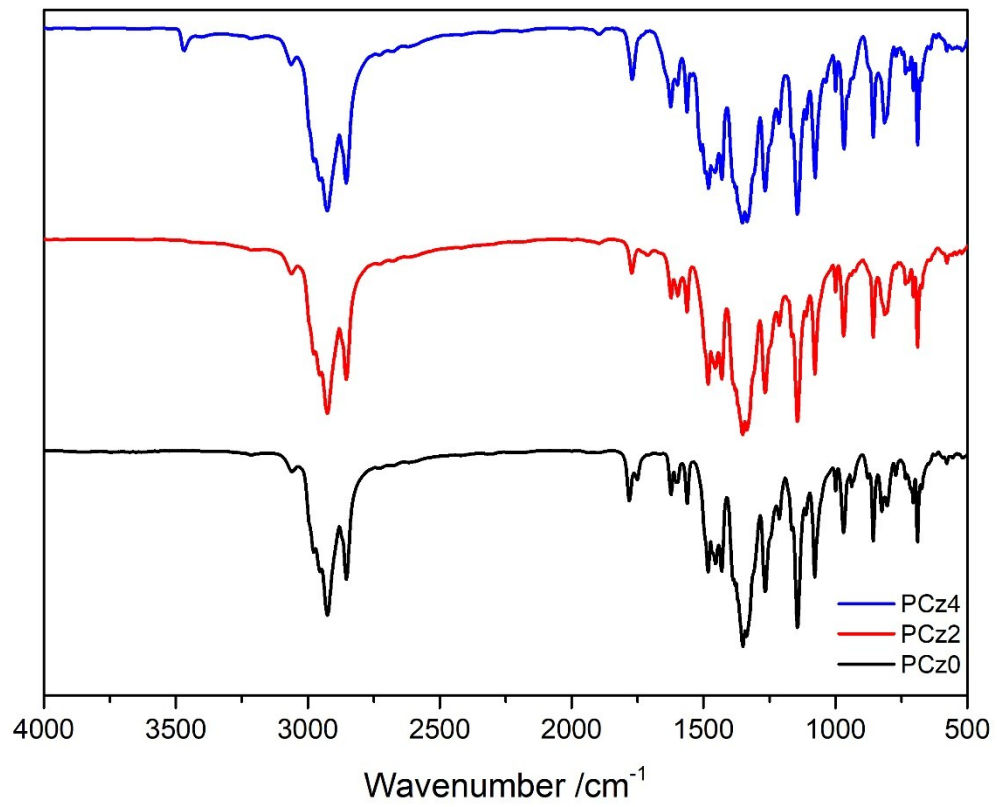
¹H-NMR (400 MHz, CDCl₃), δ (ppm):

0f: 7.97 (d, 1 H), 7.87 (d, 1 H), 7.70 (td, 1 H), 7.59 (td, 1 H), 7.39–7.30 (m, 2 H).

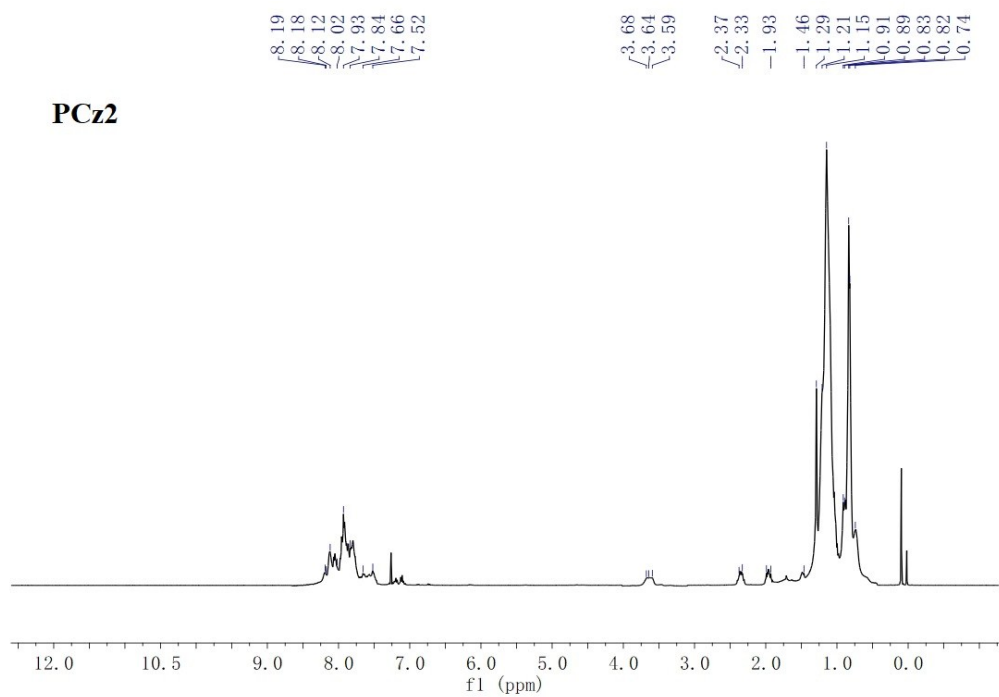
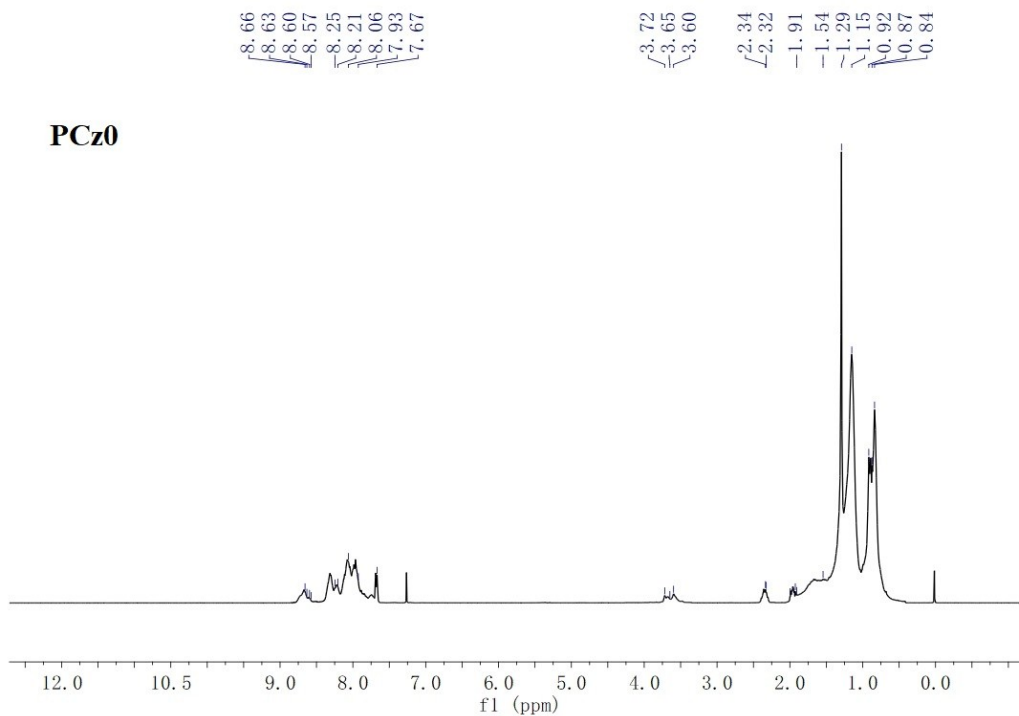
2f: 7.80 (dd, 1 H), 7.70 (dd, 1 H), 7.42–7.39 (m, 2 H).

4f: 7.40 (m, 1 H)

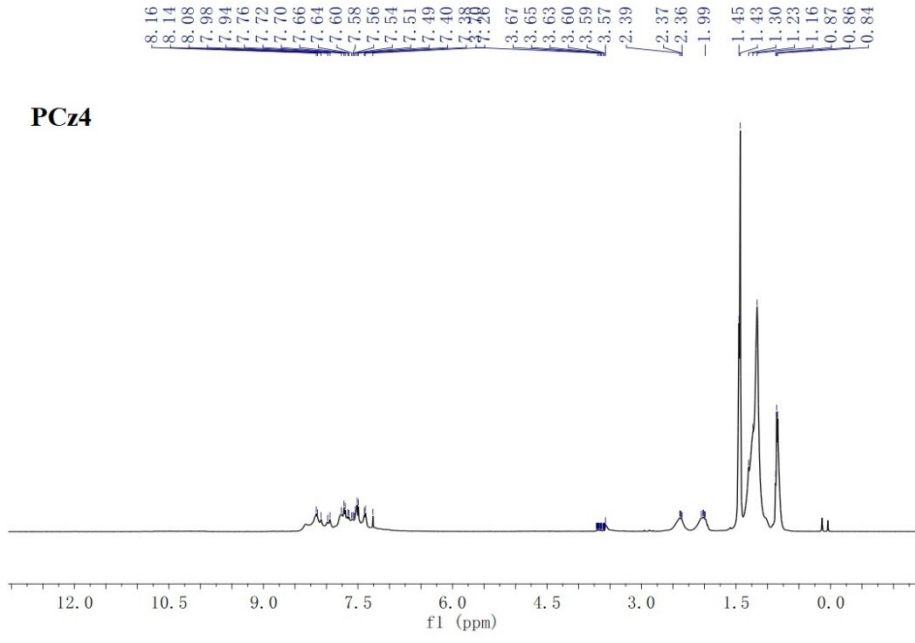
3. FT-IR of polymer PCz0, PCz2 and PCz4



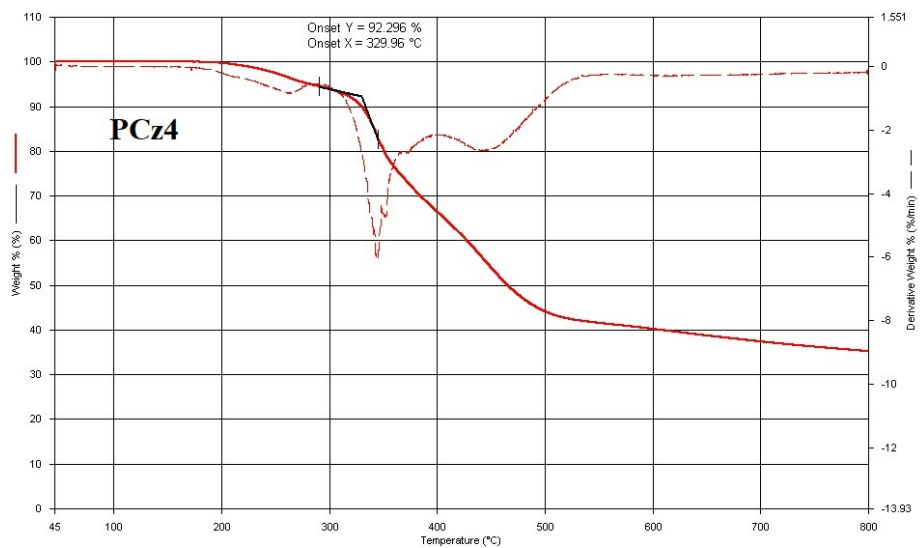
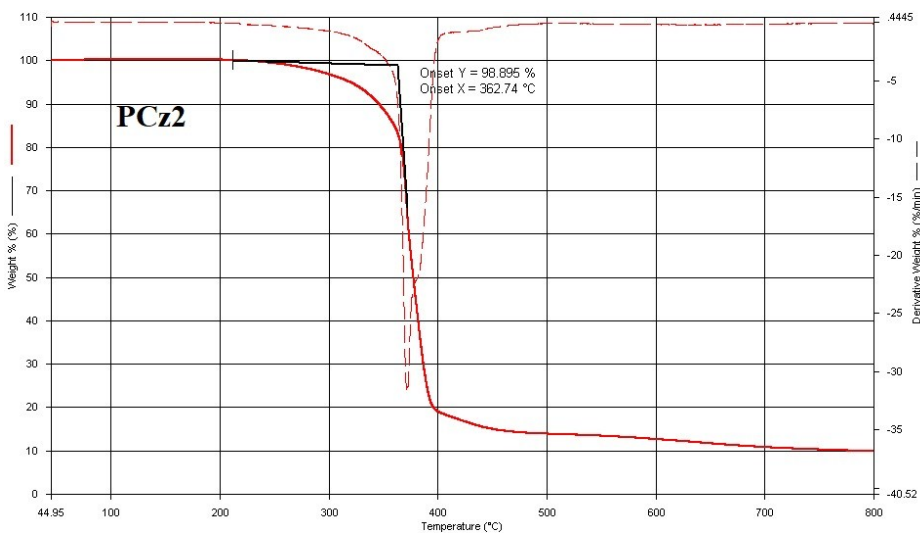
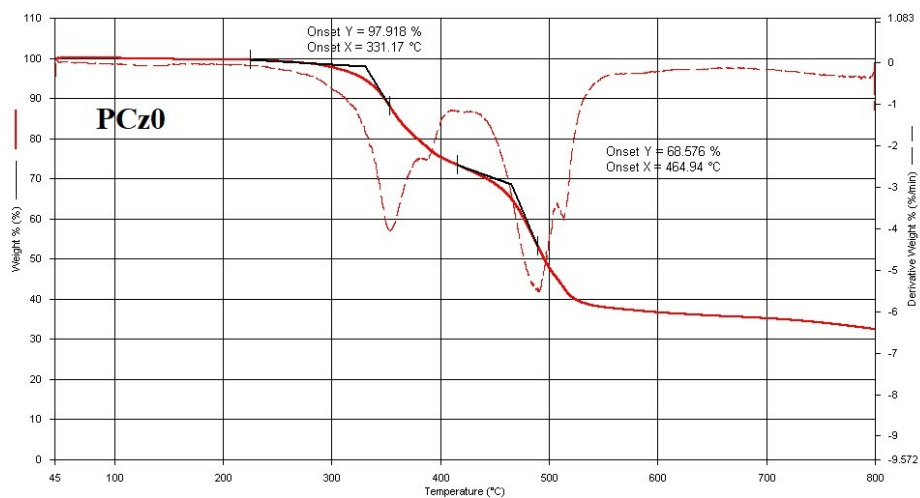
4. ^1H -NMR of polymer PCz0, PCz2 and PCz4



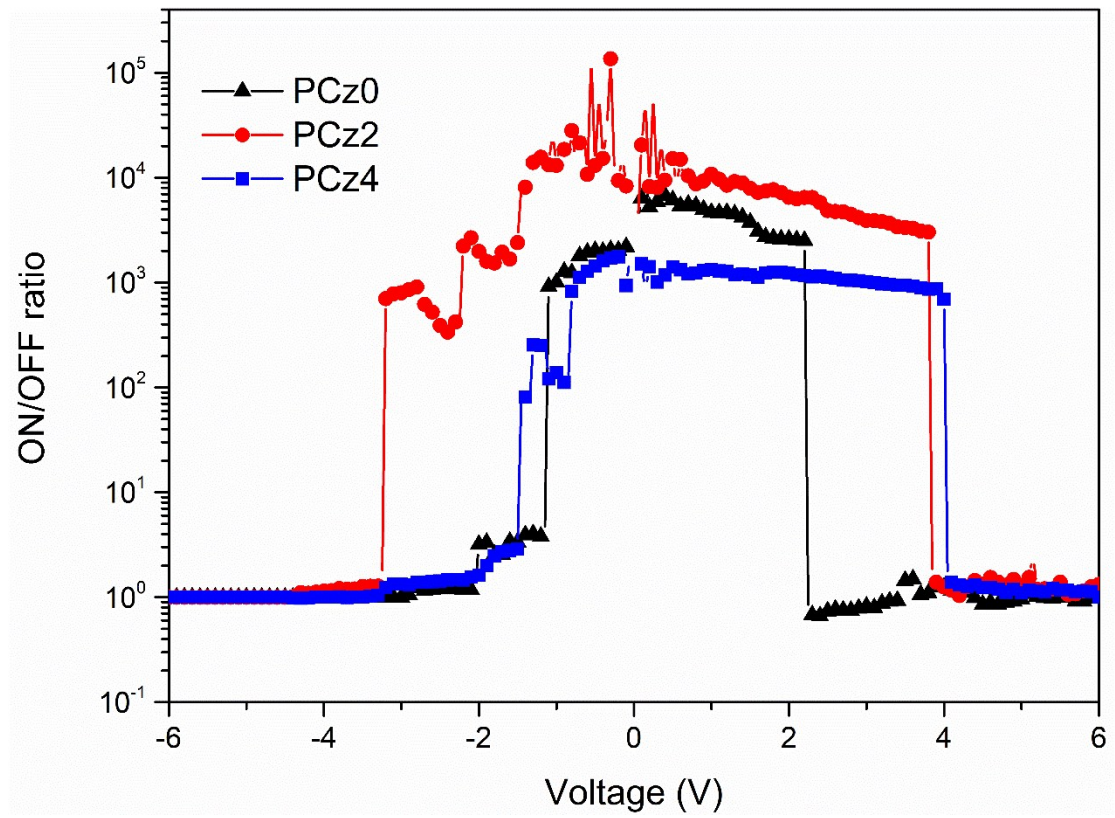
PCz4



5. Thermal gravimetric analyses of polymer PCz0, PCz2 and PCz4



6. The ON/OFF current ratio of three memory devices



7. Illustration of molecular orbitals and the corresponding energy levels based on optimized repeated unit of PCz2 and PCz4.

