Electronic Supplementary Material (ESI) for Nanoscale.

# Electronic Supplementary Materials (ESI) for:

# Effect of chemical structure of polyfluorene on selective extraction of semiconducting single-walled carbon nanotubes

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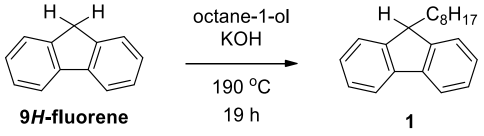
## Table of Contents of Supporting Information

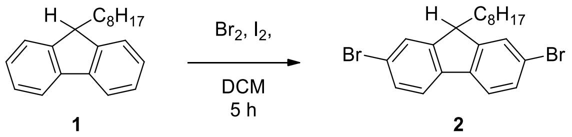
## Synthesis of 9-octyl-9*H*-fluorene (1)



A mixture of 9*H*-fluorene (1.66 g, 10 mmol), potassium hydroxide (KOH) (0.2 g, 5.0 mmol) and octane-1-ol (6.77 g, 52 mmol) was stirred at 190 ºC for 12 h. KOH (0.28 g) was added to the mixture, then stirred at 190 ºC for 12 h, to which KOH (0.14 g) was added, then the mixture was stirred at 190 ºC for 6 h. After cooling to room temperature, excess octane-1-ol was removed from the mixture by distillation to provide a crude product, which was purified by column chromatography using hexane as an eluent to give 9-octyl-9*H*-fluorene (**1**) as a colorless liquid (2.4 g, 86%).

Anal. Calcd. C, 90.37; H, 9.34 for C21H26; Found: C, 90.59; H, 9.41%. $^1$H NMR $\delta_H$ (300 MHz, $CDCl_3$, $Me_4Si$): 0.86 (3H, t, $CH_3$, *J*=6), 1.19-1.25 (12H, m, $CH_2$+$CH_3$), 1.98 (2H, m, $CH_2$), 3.96 (1H, t, *J*=6), 7.39 (4H, m, Ar-H), 7.51 (2H, d, Ar-H, *J*=6), and 7.75 (2H, d, Ar-H, *J*=6).

## Synthesis of 2,7-dibromo-9-octyl-9*H*-fluorene (2)



Bromine (114 μL, 2.1 mmol) was added dropwise over 10 min to a stirred solution of 9-octyl-9*H*-fluorene 1 (332 mg, 1.19 mmol) and iodine (25 mg) in dichloromethane (8.0 mL) at 0 ºC in the dark. The mixture was stirred for 1 h at 0ºC in the dark and then for 3.0 h at room temperature in the dark followed by quenching with an aqueous sodium thiosulfate (20%, 10 mL), from which the aqueous phase was separated, then extraction was carried out with dichloromethane (4 times, each 50mL), then dried over magnesium sulfate and evaporated under reduced pressure to provide a crude product, which was recrystallized from methanol to give 2,7-dibromo-9-octyl-9*H*-fluoerene 2 as a white solid (450 mg, 87%).

Anal. Calcd. C, 57.61; H, 5.52. for $C_{21}H_{24}Br_2$. Found; C, 57.82; H, 5.55%. $^1$H NMR $\delta_H$ (300 MHz, $CDCl_3$, $Me_4Si$) 0.86 (3H, t, $CH_3$, *J*=6), 1.11-1.21 (12H, m, $CH_2$+$CH_3$), 1.93-2.00 (2H, m, $CH_2$), 3.96 (1H, t, *J*=6), 7.49 (2H, m, Ar-H), 7.57 (2H, d, Ar-H, *J*=8), and 7.62 (2H, s, Ar-H).

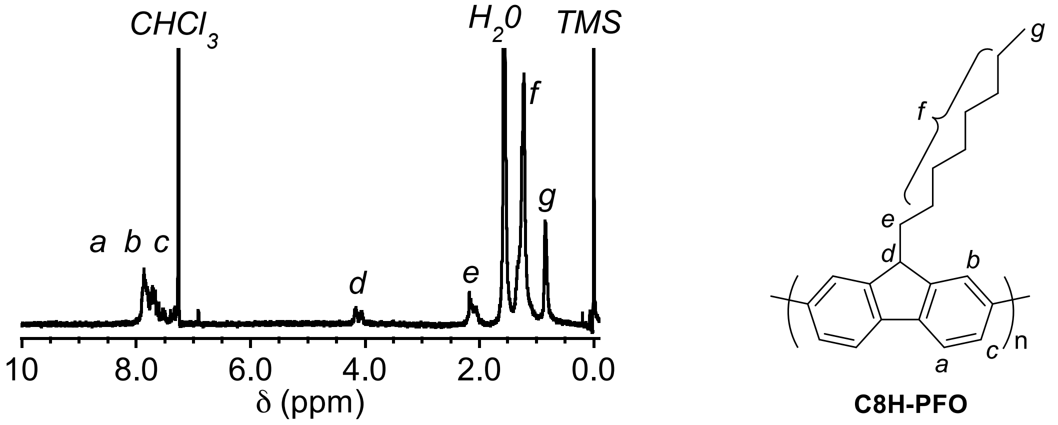


**Fig. S1** $^1$ H NMR spectrum of poly (9-octyl-9*H*-fuluorene-2,7-diyl) (**C8H-PF**).

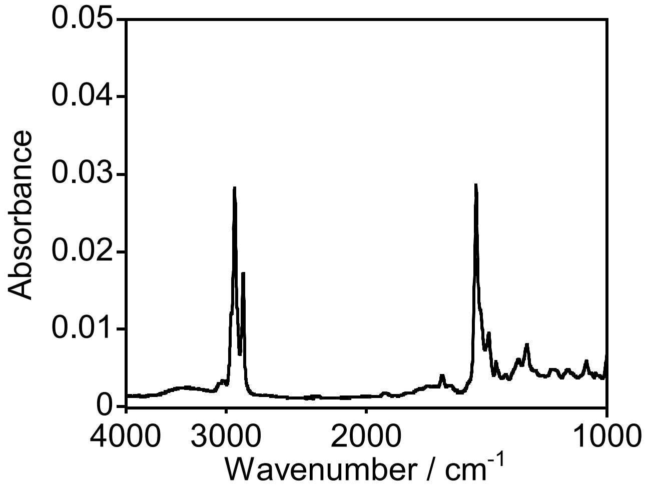


**Fig. S2** FT-IR spectrum of poly (9-octyl-9*H*-fuluorene-2,7-diyl) (**C8H-PF**).

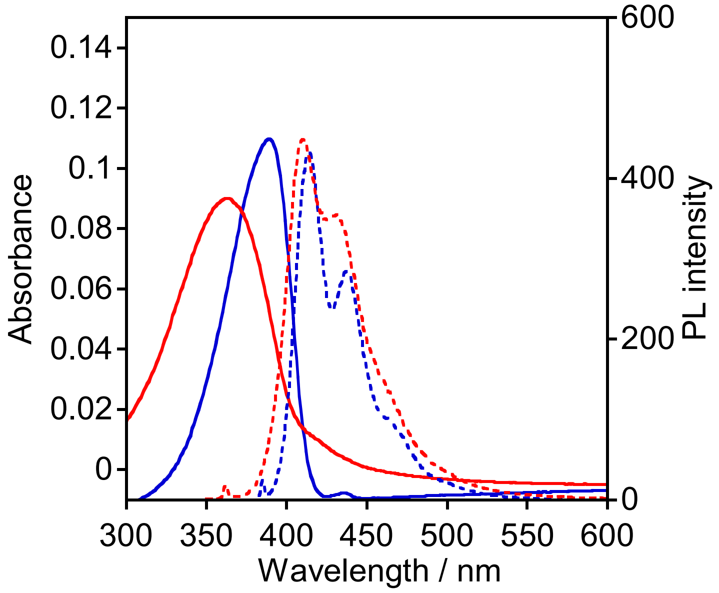


**Fig. S3** UV-vis absorption (solid line) and fluorescence spectra (dotted line) of **C8H-PF** (red) and **2C8-PF** (blue) in toluene for comparison. Excitation wavelengths for the fluorescence spectra were 365 nm and 385 nm for **C8H-PF** and **2C8-PF**, respectively.

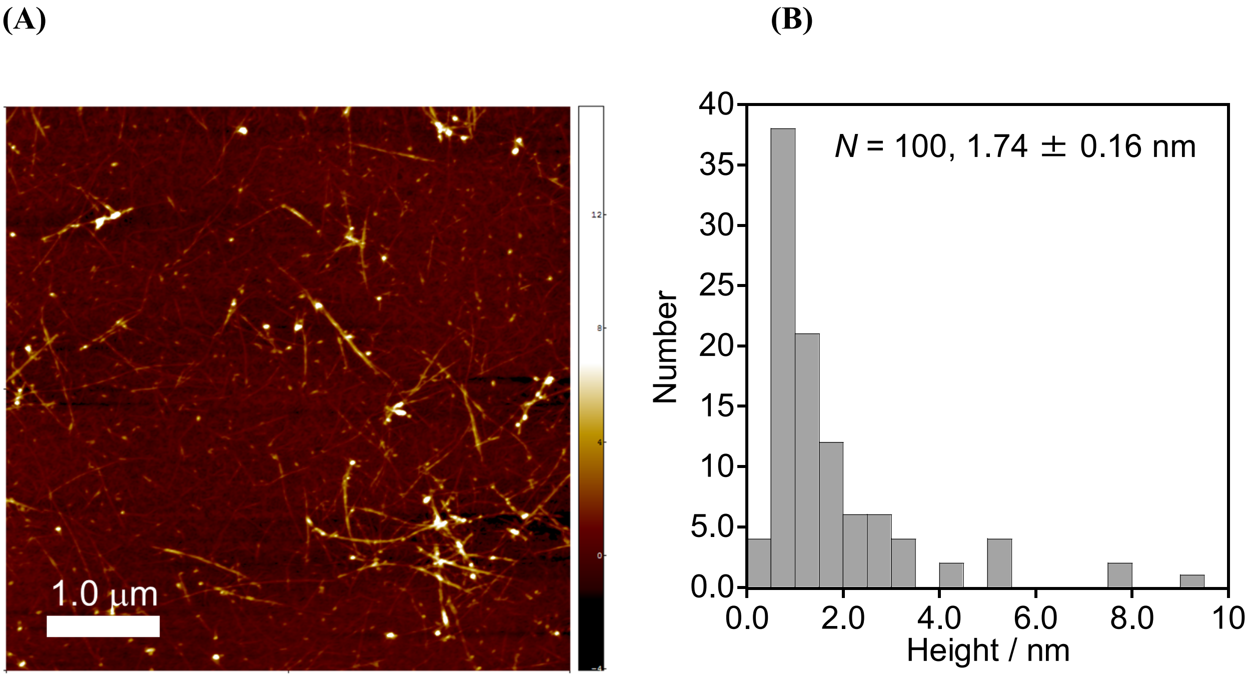


**Fig. S4** AFM image (A) and its height histogram (B) of the **2C8-PF**-SWNTs.

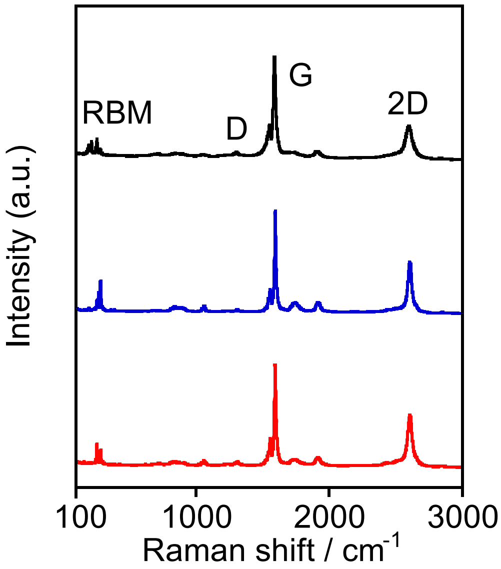


**Fig. S5** Raman spectra excited at 633 nm of the filter cakes of the **C8H-PF**-SWNTs (red) together with SC-SWNTs (black) and 2**C8-PF**-SWNTs (blue) for comparison. Range is 100~3000 cm$^{-1}$.

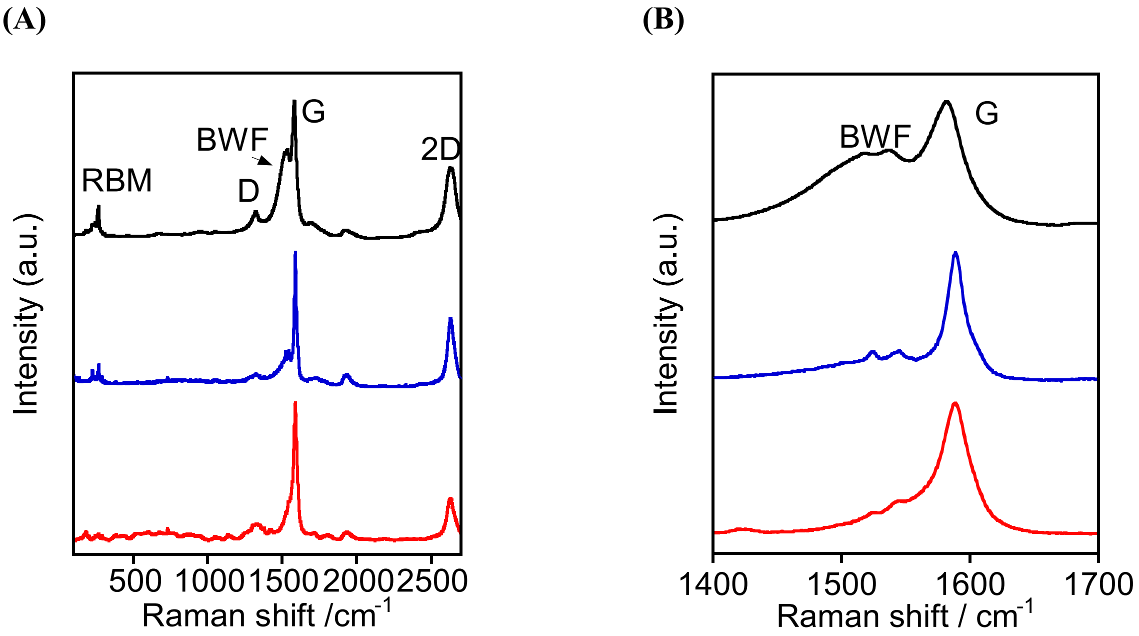


**Fig. S6** Raman spectra excited at 532 nm of the filter cakes of the **C8H-PF**-SWNTs (red) together with SC-SWNTs (black) and the **2C8-PF**-SWNTs (blue) for comparison.

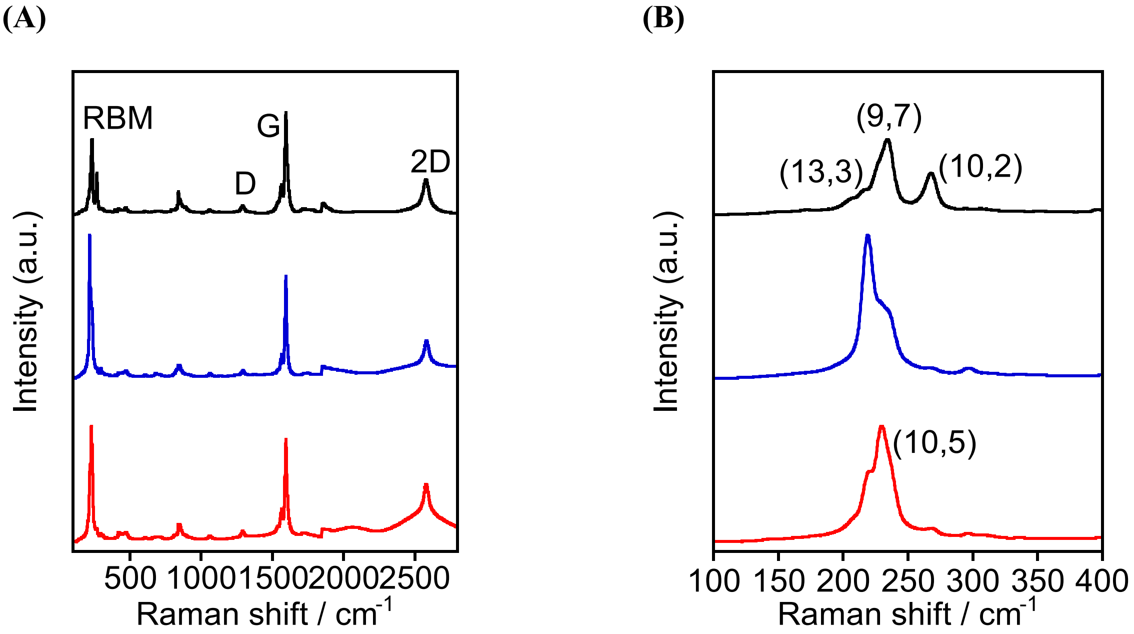


**Fig. S7** Raman spectra excited at 785 nm of the filter cakes of the **C8H-PF**-SWNTs (red) together with the SC-SWNTs (black) and the **2C8-PF**-SWNTs (blue) for comparison.

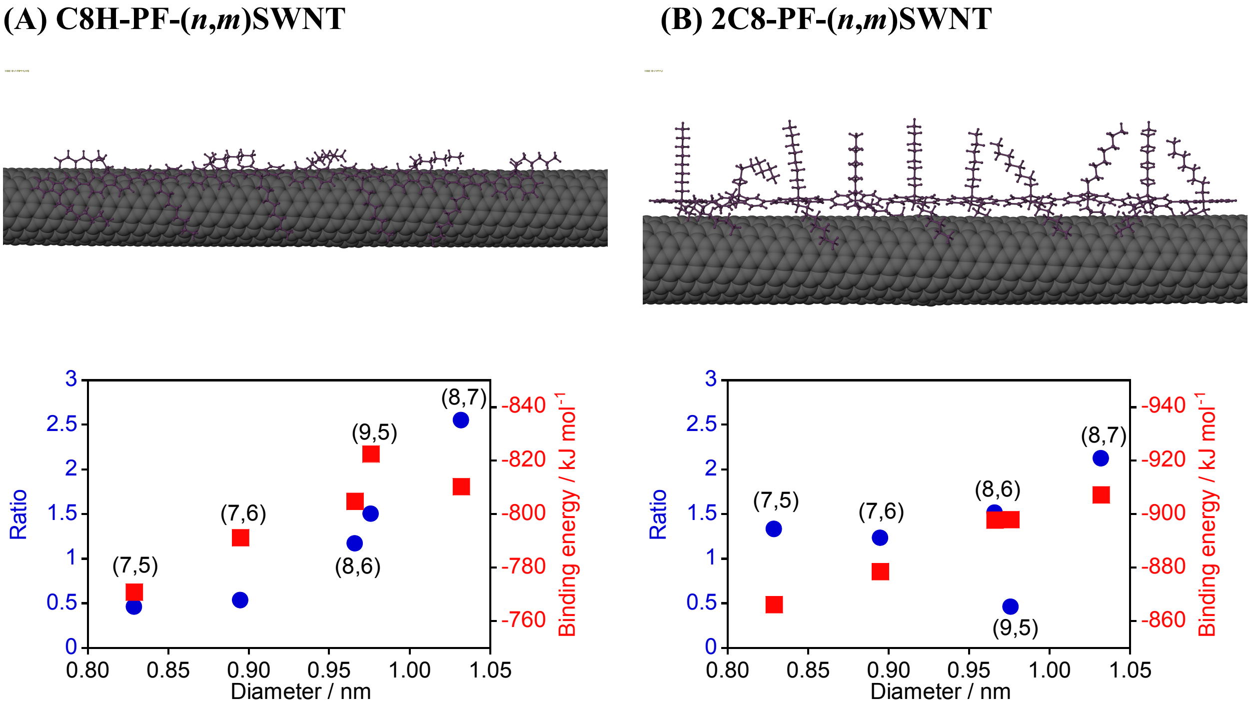


**Fig. S8** Ratios of the calibrated contents of the **C8H-PF**-(*n*,*m*)SWNTs (A) and **2C8-PF**-(*n*,*m*)SWNTs (B) and calibrated contents of the SC-(*n*,*m*)SWNTs and binding energies of the **C8-PF**-(*n*,*m*)SWNTs (A) and **2C8-PF**-(*n*,*m*)SWNTs (B) as a function of diameter of the SWNTs. Upper images were the most stable composite structures of **C8H-PF**-(8,7)SWNT (A) and **2C8-PF**-(8,7)SWNT (B).

**Table S1** Calibrated content of the SWNT species deduced from the PL mappings of the **C8H-PF**-SWNTs, **2C8-PF**-SWNTs and SC-SWNTs

| SWNT | | | PL intensity (a.u.) | | | Calibrated PL intensity (a.u.)[a] | | | Calibrated content / % | | | Ratio[b] | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Chiral index (*n*,*m*) | Diameter / nm | Chiral angle /° | C8H-PF | 2C8-PF | SC | C8H-PF | 2C8-PF | SC | C8H-PF | 2C8-PF | SC | C8H-PF | 2C8-PF |
| (6,5) | 0.757 | 27.02 | 2025 | 505 | 561 | 3022 | 754 | 837 | 2.3 | 0.5 | 4.3 | 0.53 | 0.12 |
| (8,3) | 0.782 | 15.40 | 759 | 324 | 463 | 356 | 152 | 217 | 0.3 | 0.1 | 1.1 | 0.27 | 0.09 |
| (7,5) | 0.829 | 24.54 | 2769 | 10098 | 902 | 3900 | 14223 | 1271 | 3.0 | 8.7 | 6.6 | 0.45 | 1.32 |
| (8,4) | 0.840 | 19.19 | 1589 | 5507 | 552 | 3454 | 11972 | 1200 | 2.6 | 7.3 | 6.2 | 0.42 | 1.18 |
| (10,2) | 0.884 | 9.09 | 1380 | 301 | 690 | 580 | 126 | 290 | 0.4 | 0.1 | 1.5 | 0.27 | 0.07 |
| (7,6) | 0.895 | 27.47 | 4218 | 12211 | 1179 | 8974 | 25981 | 2508 | 6.9 | 15.9 | 12.9 | 0.53 | 1.23 |
| (11,1) | 0.910 | 4.41 | 1797 | 3452 | 242 | 6912 | 13277 | 932 | 5.3 | 8.1 | 4.8 | 1.10 | 1.69 |
| (9,4) | 0.916 | 17.53 | 3118 | 2405 | 1089 | 4455 | 3436 | 1555 | 3.4 | 2.1 | 8.0 | 0.43 | 0.26 |
| (10,3) | 0.936 | 12.79 | 2231 | 3594 | 343 | 7967 | 12836 | 1224 | 6.1 | 7.9 | 6.3 | 0.97 | 1.25 |
| (8,6) | 0.966 | 25.31 | 8204 | 13198 | 1042 | 16744 | 26935 | 2126 | 12.8 | 16.5 | 11.0 | 1.16 | 1.50 |
| (9,5) | 0.976 | 20.66 | 5243 | 2019 | 518 | 18726 | 7211 | 1852 | 14.4 | 4.4 | 9.6 | 1.50 | 0.46 |
| (11,3) | 1.014 | 11.79 | 2607 | 2654 | 577 | 4418 | 4498 | 978 | 3.4 | 2.8 | 5.0 | 0.68 | 0.56 |
| (8,7) | 1.032 | 27.80 | 7758 | 8055 | 452 | 25861 | 26850 | 1505 | 19.8 | 16.5 | 7.8 | 2.54 | 2.12 |
| (10,5) | 1.050 | 19.16 | 3176 | 1015 | 595 | 6758 | 2160 | 1266 | 5.2 | 1.3 | 6.5 | 0.80 | 0.20 |
| (9,7) | 1.103 | 25.88 | 4943 | 3442 | 438 | 18307 | 12748 | 1622 | 14.0 | 7.8 | 8.4 | 1.67 | 0.93 |

[a] calibration factors were used according to the paper Y. Oyama et al., *Carbon*, **2006**, *44*, 873.

[b] ratio of calibrated content of polymer-SWNTs and calibrated content of SC-SWNTs

**Table S2** Assignments of the absorption peaks of the **C8H-PF**-SWNTs and **2C8-PF**-SWNTs to each chiral index of (*n*,*m*)SWNTs

| Chiral index of (*n*,*m*)SWNT | Wavelength / nm | |
|---|---|---|
| | **C8H-PF**-SWNTs | **2C8-PF**-SWNTs |
| (9,7) | 1353 | 1345 |
| (8,7) | 1283 | 1282 |
| (8,6) | 1199 | 1194 |
| (7,6), (8,4) | 1139 | 1135 |
| (10,2) | 1075 | - |
| (7,5) | 1046 | 1044 |
| (6,5) | 994 | - |
| (8,3) | - | 981 |
| (13,2) | 877 | 876 |
| (9,7) | 805 | 799 |
| (8,6), (8,7) | 733 | 727 |
| (9,5), (8,3) | 684 | - |
| (7,5), (7,6) | 657 | 653 |