SUPPORTING INFORMATION

FOR:

Thiophene and Selenophene-Based Heteroacenes: Combined Quantum Chemical DFT, and Spectroscopic Raman and UV-Vis-NIR Study

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Figure S1.– Solid-state ^{13}C-NMR spectrum (125 MHz) of compound **3** recorded in CPMAS mode; δ (ppm): 142.6, 135.3, 133.4, 131.3 and 122.3.

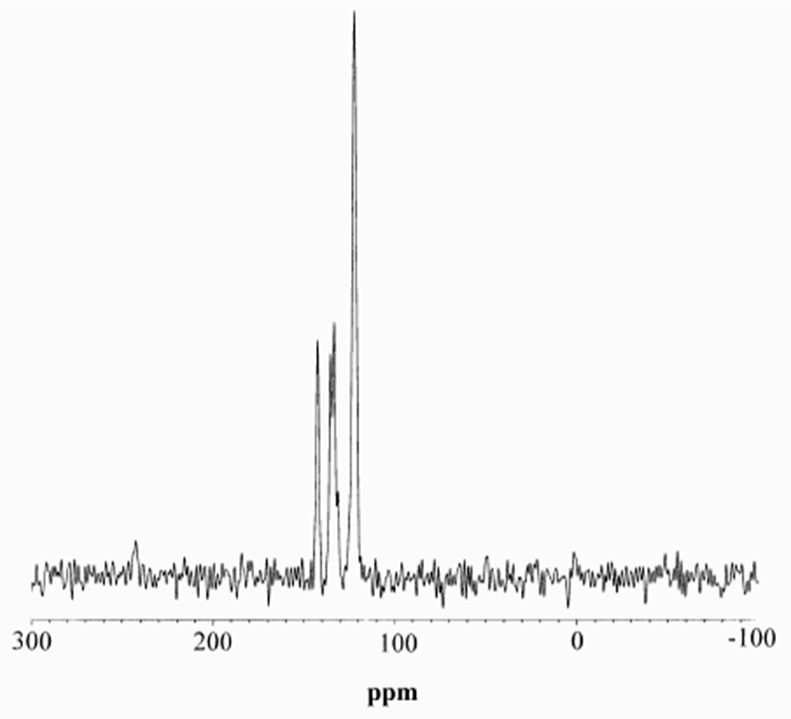

Figure S2.– Solid-state ^{13}C -NMR spectrum (125 MHz) of compound **4** recorded in CPMAS mode; δ (ppm): 141.9, 139.5, 136.1 and 122.3.

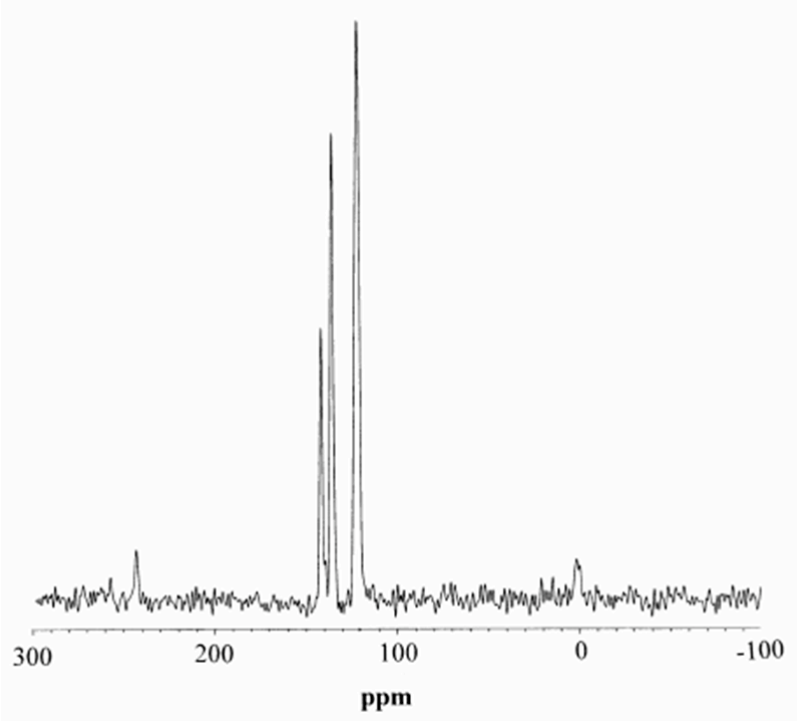

Figure S3.– TGA results for **3** and **4**.

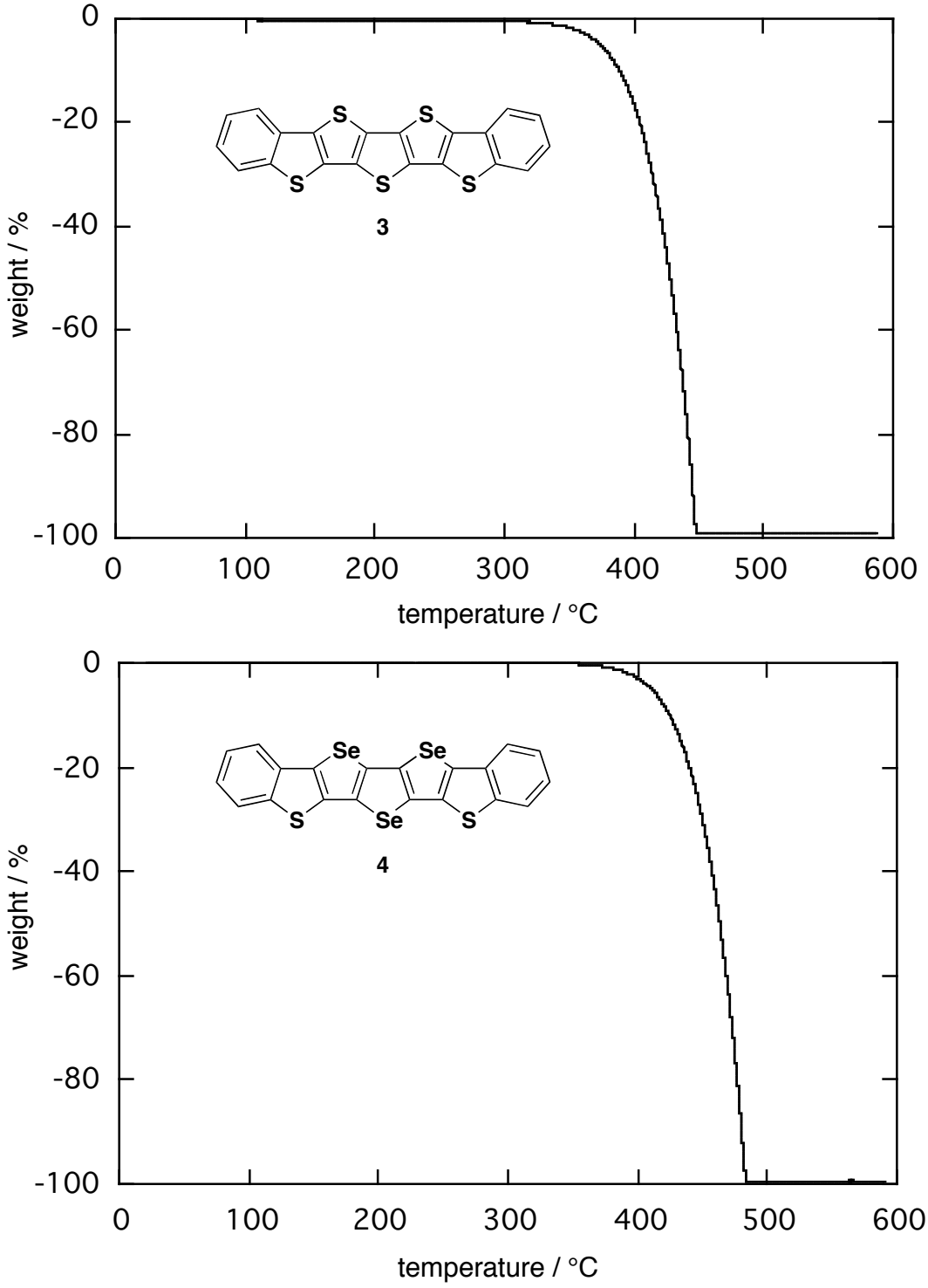

Figure S4.– DSC results for **3** and **4**.

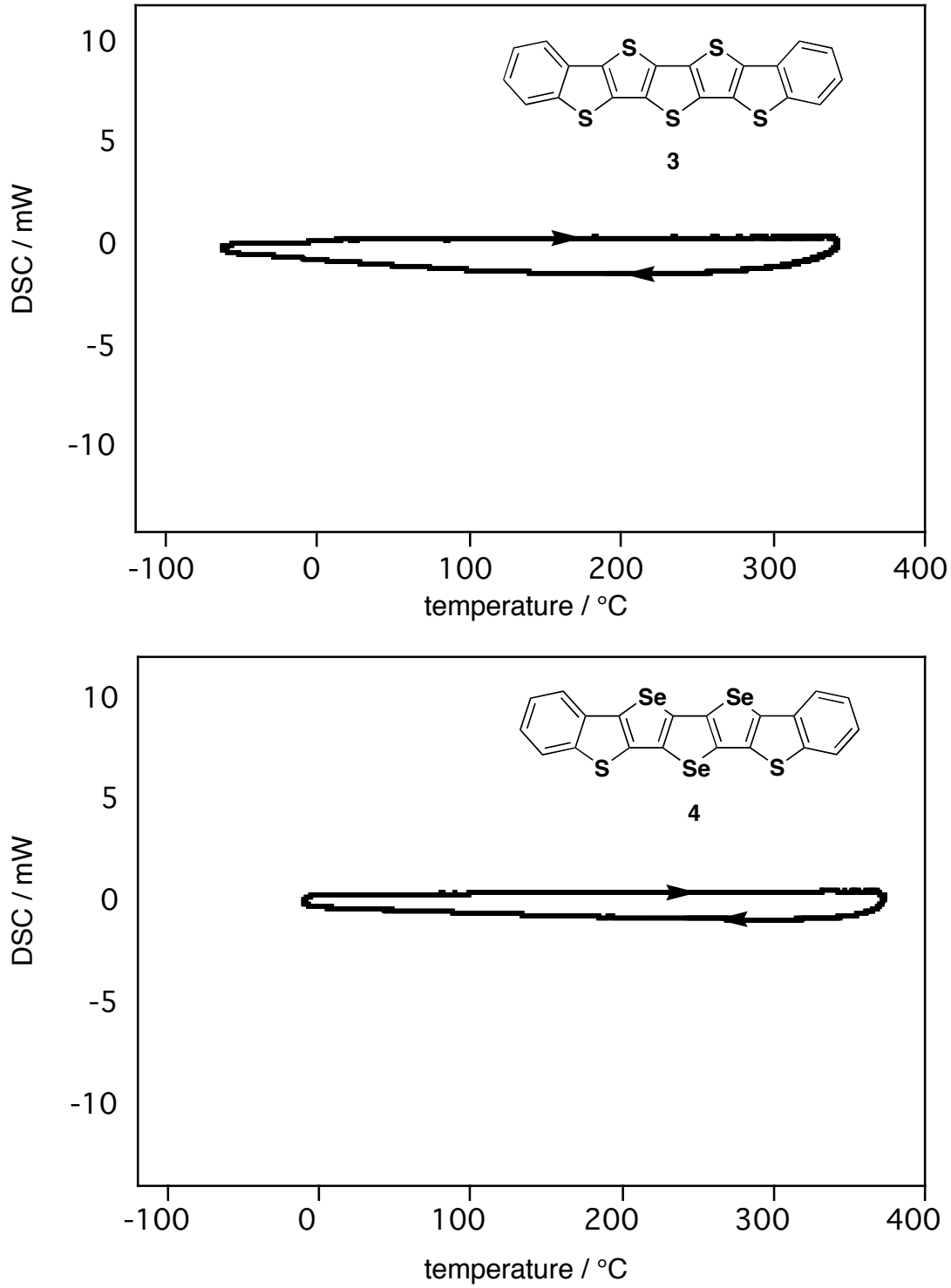

Figure S5.– DFT//B3LYP/6-31G** electronic density contours (0.03 *e*/bohr^3) for selected MOs of theoretical model all-syn P3TP.