Supporting Information

1. Materials and General methods

All chemicals and solvents were purified according to the standard procedure.[S1] Tellurium powder and copper nano powder(80−200nm) were purchased from Adamas Reagent Co. Ltd and Shanghai Macklin Biochemical Technology Co. Ltd, respectively. The melting points were determined on a WRS-2 melting point apparatus. The high resolution mass spectral analysis (HRMS) was carried out on Bruker APEX II type mass spectrometer. The ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Advance III 400 MHz (100 MHz for ^{13}C) spectrometer using $CDCl_3$ as solvent. The chemical shifts of ^{1}H and ^{13}C NMR were recorded by using TMS as internal standard. The UV-Vis absorption spectra were measured on a UV-2006 UV-Specterophotometer. Fluorescence excitation and emission were recorded on a RF-5301(pc)s Spectrofluorophotometer. Fluorescence lifetime and steady state were measured on a FLS920 Spectrofluorophotometer. All of the measurements were conducted in CH_2Cl_2 solution (10^{-5} mol L^{-1}) at 20 °C. The single-crystal X-ray diffraction was carried out on a SuperNova (Agilent) diffractometer. The crystal structure was solved by a direct method *SIR*2004[S2] and refined by full-matrix least-square method on F^2 by means of *SHELX*L-97.[S3] The calculated positions of the hydrogen atoms were included in the final refinement.

References

[S1] Purification of Laboratory Chemicals, 5th ed., Wilfres L.F. Armarege, Christina L.L.Chai.

[S2] M. C. Burla, R Caliandro., M. Camalli, B. Carrozzini, G. L. Cascarano, L. de Caro, C. Giacovazzo, G. Polidori, R. Spagna, *J. Appl. Cryst.* **2005**, *38*, 381-388.

[S3] G. M. Sheldrick, *SHELXL-97, A Program for Crystal Structure Refinement*, University of Göttingen, Göttingen, Germany, **1997**.

[S4] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador,

J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, E.01, Gaussian, Inc., Wallingford CT, 2013.

[S5] a) A. D. Becke, J. Chem. Phys. 1993, 98, 5648-5652; b) C. Lee, W. Yang, R. G. Parr, Phys. Rev. *B,* **1988**, 37, 785.

[S6] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.,* **2005**, *7*, 3297

[S7] J. Tomasi, B. Mennucci, R. Cammi, *Chem. Rev*., **2005**, *105*, 2999.

[S8] P. V. R. Schleyer, C. Maerker, A. Dransfeld, H. Jiao, N. J. R. V. E. Hommes, *J. Am. Chem. Soc.,* **1996**, *118*, 6317.

[S9] Z. Chen, C. S. Wannere, C. Corminboeuf, R. Puchta, P. V. R Schleyer, *Chem. Rev.,* **2005**, *105*, 3842.

[S10] F. London, *J. Phys. Radium,* **1937**, *8*, 397.

[S11] H. F. Hameka, *Mol. Phys.,* **1958**, *1*, 203.

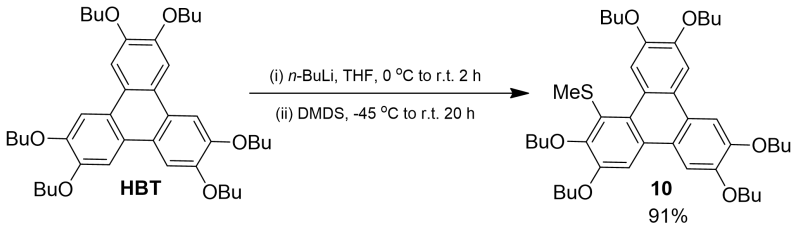
[S12] R. Ditchfield, *Mol. Phys.*, **1974**, *27*, 789.

[S13] K. Wolinski, J. F. Hinton, P. Pulay, *J. Am. Chem. Soc.,* **1990**, *112*, 8251.

[S14] G. A. Andrienko, Chemcraft, Version 1.8 (built 523b); http://www.chemcraftprog.com.

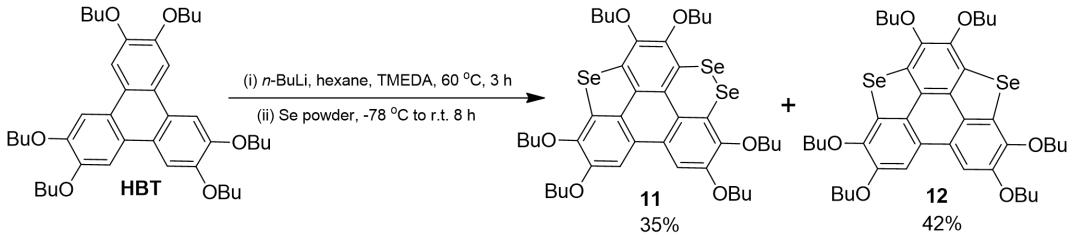
2. Synthesis

2.1 Synthesis of **10** from **HBT**



To a solution of HBT (13.2 g, 0.02 mol) in THF (100 mL) was added 2.4 M hexane solution of *n*-butyllithium (21.2 mL, 0.036 mol) at 0 °C. After the mixture was stirred for 2 h at room temperature, dimethyldisulfide (3.54 mL, 0.04 mol) was added to the solution at -45 °C, and the resulting mixture was stirred for 20 h at room temperature. The mixture was poured into a saturated aqueous ammonium chloride solution (100 mL) and was extracted with ether (30 mL × 3). The combined ethereal extracts were washed with brine (50 mL × 3), dried with $MgSO_4$, and concentrated in vacuo. The crude product was further purified by column chromatography on silica (eluent, CH_2Cl_2: petro ether, 1:4, *v/v*) to afford **10** as a white solid (6.4 g, yield 91%). mp: 72.1-74.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 9.18 (s, 1H), 7.80 (d, J = 6.8 Hz, 4H), 4.29-4.17 (m, 12H), 2.32 (s, 3H), 2.00-1.89 (m, 12H), 1.72-1.55 (m, 12H), 1.09-1.02 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 150.69, 149.84, 149.53, 148.75, 148.12, 147.27, 128.54, 127.37, 124.79, 124.60, 124.12, 123.79, 123.42, 111.38, 108.17, 106.83, 106.66, 105.69, 73.36, 69.61, 69.31, 69.15, 68.75, 68.64, 32.54, 31.47, 31.41, 31.32, 29.74, 20.09, 19.46, 19.42, 19.37, 14.09, 14.04, 14.02, 13.98, 1.18, 1.15, 1.07; HRMS: calculated for $C_{43}H_{62}O_6S$+Na, 729.4159; found, 729.4180.

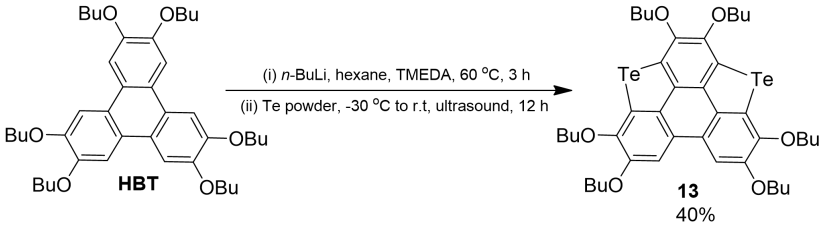
2.2 Synthesis of **11** and **12** from **HBT**



To a hexane (100 mL) solution of HBT (13.2 g, 0.02 mol) was added TMEDA (12 mL, 0.08 mol) and *n*-butyllithium (2.4 M in hexane, 33.4 mL, 0.08 mol) at 60 °C for 3 hours. The resulting solution was cooled to -78 °C and diluted with 80 mL THF. Selenium powder (12.79 g, 0.16 mol) was added in one portion. The resulting mixture was slowly warmed to room temperature and

allowed to stir overnight. The reaction was quenched by adding distilled water and then extracted with CH_2Cl_2 (3 × 60 mL). The organic layers were combined and dried over anhydrous Na_2SO_4, then concentrated under reduced pressure. The crude product was further purified by column chromatography on silica (eluent, CH_2Cl_2: petro ether, 1:4, *v/v*) to afford **11** as orange solid (6.3 g, yield 35%). mp: 93.9-96.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 7.76 (d, *J* = 7.8 Hz, 2H), 4.36-4.24 (m, 12H), 1.98-1.82 (m, 12H), 1.68-1.58 (m, 12H), 1.09-1.02(m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 151.95, 151.68, 147.78, 146.50, 144.99, 144.95, 131.24, 130.04, 129.39, 128.46, 128.20, 126.15, 125.12, 124.93, 119.11, 115.65, 105.74, 104.78, 74.16, 73.15, 73.02, 69.59, 68.39, 32.63, 32.60, 32.54, 31.66, 31.42, 29.76, 19.50, 19.40, 14.12, 14.09, 14.04, 14.00; HRMS: calculated for $C_{42}H_{56}O_6Se_3$+H, 895.1653; found, 895.1647. And **12** as orange solid (7.5 g, 42%). mp: 103.6-105.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 7.83-7.82 (m, 2H), 4.37 (dt, *J* = 13.1 Hz, 6.5 Hz, 8H), 4.28 (t, *J* = 6.3 Hz, 4H), 2.00-1.93 (m, 4H), 1.91-1.84 (m, 8H), 1.70-1.60 (m, 12H), 1.10-1.03 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 151.86, 147.84, 145.21, 132.03, 129.08, 129.01, 125.11, 123.02, 105.57, 73.03, 72.83, 69.76, 32.57, 32.49, 31.73, 19.52, 19.44, 19.41, 14.05; HRMS: calculated for $C_{42}H_{56}O_6Se_2$, 816.2402; found, 816.2393.

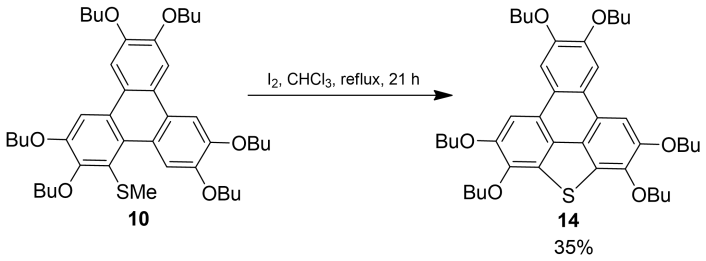
2.3 Synthesis of **13** from **HBT**



To a hexane (100 mL) solution of 2,3,6,7,10,11-hexabutoxytriphenylene HBT (13.2 g, 0.02mol) was added TMEDA (12 mL, 0.08moL) and *n*-butyllithium (2.4 M in hexane, 33.4 mL, 0.08 mol) at 60 °C for 3 h. The resulting solution was cooled to -30 °C and diluted with 80 mL THF. Tellurium powder (25.5 g, 0.2 mol) was added in one portion. The resulting black mixturewas slowly warmed to room temperature and allowed to stir under ultrasound for 12 hours.The reaction was quenched by adding distilled water and then extracted with CH_2Cl_2 (3 × 100mL). The organic layers were combined and dried over anhydrous Na_2SO_4, then concentrated under reduced pressure. The crude product was further purified by column chromatography on silica (eluent, CH_2Cl_2: petro ether, 1:4, *v/v*) to afford **13** as yellow solid (7.48g**,** 40%). mp： 113.4-115.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 7.90 (s, 2H), 4.33-4.28 (m, 12H), 2.00-1.93 (m, 4H), 1.88-1.81 (m, 8H), 1.70-1.57 (m, 12H), 1.05 (dt, *J* = 14.6, 7.4 Hz, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 151.20, 150.85, 149.24, 136.84, 133.85, 127.47, 122.03, 115.40, 106.15, 73.15, 72.82, 69.45, 32.82, 32.78,

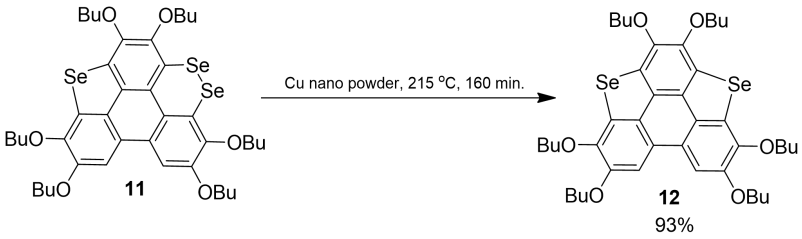
31.71, 19.56, 19.51, 14.02, 14.01, 13.97; HRMS: calculated for $C_{42}H_{56}O_6Te_2$+H, 915.2256; found, 915.2239.

2.4 Synthesis of **14** from **10**



A solution of **10** (6.26 g, 8.8 mmol) and iodine (22.35 g, 88 mmol) in chloroform (200 mL) was refluxed for 21 h. After cooling to room temperature, saturated aqueous sodium hydrogen sulfite solution (200 mL) was added, and the resulting precipitate was collected by filtration and was washed with water and chloroform. The organic layers were combined and dried over anhydrous Na_2SO_4, then concentrated under reduced pressure. The crude product was further purified by column chromatography on silica (eluent, CH_2Cl_2: petro ether, 1:3, *v/v*) to give a sample of **14** as yellow solid (2.1 g, 35%). mp: 122.3-124.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 7.91 (s, 2H), 7.78 (s, 2H), 4.36 (t, *J* = 6.5 Hz, 4H), 4.29 (t, *J* = 6.3 Hz, 8H), 2.01-1.85 (m, 12H), 1.70-1.61 (m, 12H), 1.10-1.03(m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 151.69, 149.18, 142.41, 130.23, 126.44, 124.23, 123.03, 107.52, 104.19, 73.01, 70.15, 69.19, 32.51, 31.77, 31.48, 19.50, 19.42, 19.34, 14.07, 14.03; HRMS: calculated for $C_{42}H_{58}O_6S$+H, 691.4027; found, 691.4025.

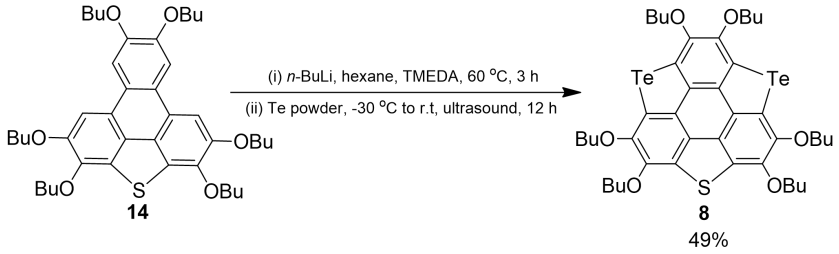
2.5 Synthesis of **12** from **11**



The mixture of **11** (1.79 g, 2 mmol) and copper nanopowder (80-100 nm, 1.28 g, 20 mmol) was slowly heated to 215 °C and kept at this temperature for 2 h 40 min under argon. After cooled down to room temperature, the reaction mixture was washed with CH_2Cl_2. The solution was concentrated and further purified by column chromatography on silica (eluent, CH_2Cl_2: petro ether, 1:4, *v/v*) to give **12** as yellow solid (1.52 g, 93%). mp: 103.6-105.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 7.83-7.82 (m, 2H), 4.37 (dt, *J* = 13.1, 6.5 Hz, 8H), 4.28 (t, *J* = 6.3 Hz, 4H), 2.00-1.93 (m, 4H), 1.91-1.84 (m, 8H), 1.70-1.60 (m, 12H), 1.10-1.03 (m, 18H); ^{13}C NMR (100 MHz,

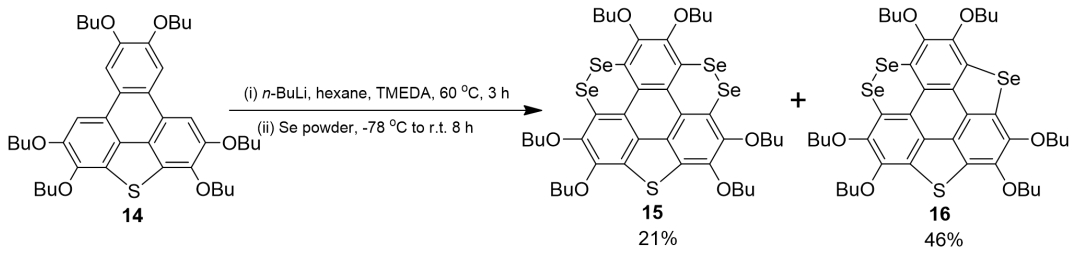
$CDCl_3$): δ(ppm) 151.86, 147.84, 145.21, 132.03, 129.08, 129.01, 125.11, 123.02, 105.57, 73.03, 72.83, 69.76, 32.57, 32.49, 31.73, 19.52, 19.44, 19.41, 14.05; HRMS: calculated for $C_{42}H_{56}O_6Se_2$, 816.2402; found, 816.2393.

2.6 Synthesis of **8** from **14**



To a hexane (50 mL) solution of **13** (2.07 g, 3 mmol) was added TMEDA (2.25 mL, 15mmol) and *n*-butyllithium (2.4 M in hexane, 6.25 mL, 15 mmol) at 60 °C for 3 h. The resulting solution was cooled to -78 °C and diluted with 30 mL THF. Tellurium powder (3.828 g, 30mmol) was added in one portion. The resulting black mixture was slowly warmed to room temperature and allowed to stir under ultrasound for 12 hours. The reaction was quenched by adding distilled water and then extracted with CH_2Cl_2 (3 × 100 mL). The organic layers were combined and dried over anhydrous Na_2SO_4, then concentrated under reduced pressure. The crude product was further purified by column chromatography on silica (eluent, CH_2Cl_2: petro ether, 1:4, *v/v*) to afford **8** as a yellow solid (1.39g, 49%). mp: 79.4 -80.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.51 (t, J = 6.5 Hz, 4H), 4.33 (q, J = 6.3 Hz, 8H), 1.97-1.85 (m, 12H), 1.73-1.59 (m, 12H), 1.07 (td, J = 7.4, 3.7 Hz, 18H); ^{13}C NMR(100 MHz $CDCl_3$): δ(ppm) 152.28, 146.37, 136.49, 132.67, 128.91, 127.28, 118.39, 113.11, 73.04, 72.91, 72.65, 32.64, 32.58, 32.38, 19.58, 19.36, 14.09, 14.03; HRMS: calculated for $C_{42}H_{54}O_6STe_2$, 944.1742; found, 944.1718.

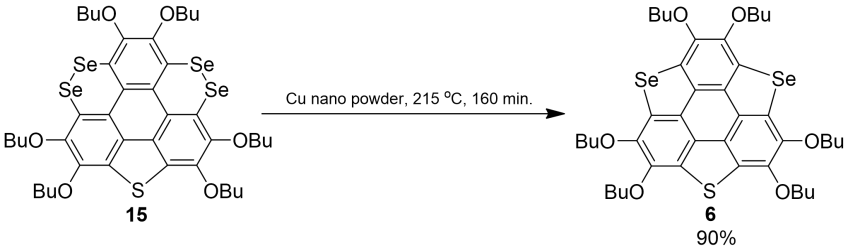
2.7 Synthesis of **15** and **16** from **14**



To a hexane (70 mL) solution of **14** (4.14 g, 6 mmol) was added TMEDA (9 mL, 60 mmol) and *n*-butyllithium (2.4 M in hexane, 25 mL, 60 mmol) at 60 °C for 3 hours. The resulting solution was cooled to -78 °C and diluted with 50 mL THF. Selenium powder (4.8 g, 60 mmol) was added in one portion. The resulting mixture was slowly warmed to room temperature and allowed to stir

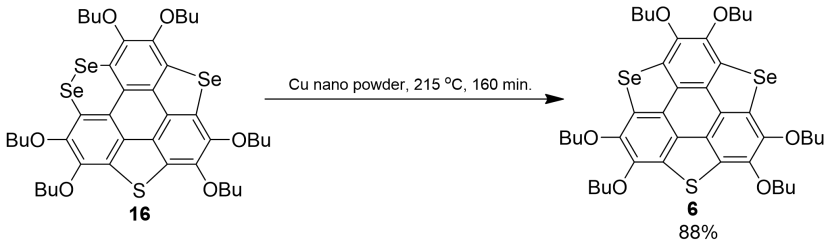
under room temperature for 8 hours. The reaction was quenched by adding distilled water and then extracted with CH_2Cl_2 (3 × 20 mL). The organic layers were combined and dried over anhydrous Na_2SO_4, then concentrated under reduced pressure. The crude product was further purified by column chromatography on silica (eluent, CH_2Cl_2: petro ether, 1:4, *v/v*) to afford **15** as a red solid (1.3 g, yield 21%). mp: 97.1-98.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.38 (t, *J* = 6.5 Hz, 4H), 4.26 (t, *J* = 6.6 Hz, 8H), 1.94-1.84 (m, 12H), 1.67-1.57 (m, 12H), 1.06-1.01 (m, 18H); ^{13}C NMR(100 MHz $CDCl_3$): δ(ppm) 148.59, 147.10, 146.49, 130.03, 129.39, 129.25, 125.18, 119.35, 117.08, 74.29, 73.98, 73.29, 32.55, 32.48, 19.46, 19.44, 19.30, 14.09, 13.99; HRMS: calculated for $C_{42}H_{54}O_6SSe_4$, 1044.0304; found, 1044.0308. And **16** as red solid (2.5 g, 46%). mp: 57.0-59.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.45 (t, *J* = 6.4 Hz, 4H), 4.37 (t, *J* = 6.4 Hz, 4H), 4.27 (t, *J* = 6.6 Hz, 4H), 1.96-1.83 (m, 12H), 1.68-1.59 (m, 12H), 1.07-1.03 (m, 18H); ^{13}C NMR(100 MHz, $CDCl_3$): δ(ppm) 149.32, 148.20, 147.22, 147.06, 146.95, 146.13, 131.68, 130.68, 129.94, 129.59, 127.23, 126.39, 125.79, 124.72, 124.01, 122.72, 115.13, 114.90, 74.26, 74.24, 73.12, 73.05, 72.84, 72.77, 32.62, 32.49, 32.44, 32.40, 32.38, 19.46, 19.40, 19.37, 19.33, 19.29, 14.11, 14.01. HRMS: calculated for $C_{42}H_{54}O_6SSe_3$, 924.1139; found, 924.1135.

2.8 Synthesis of **6** from **15**



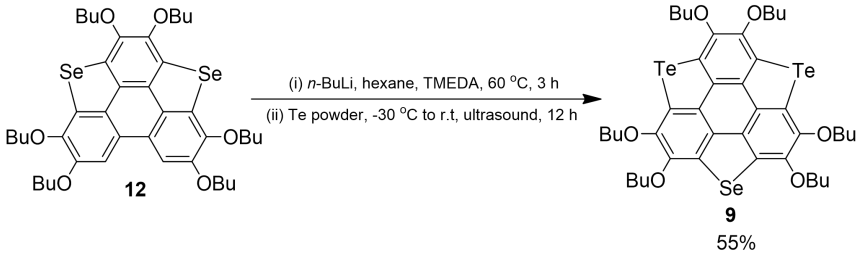
The mixture of **15** (0.3 g, 0.3 mmol) and copper nanopowder (80-100 nm, 0.19 g, 3 mmol) was slowly heated to 215 °C and kept at this temperature for 2 h 40 min under argon. After cooled down to room temperature, the reaction mixture was washed with CH_2Cl_2. The solution was concentrated and further purified by column chromatography on silica (eluent, CH_2Cl_2: petro ether, 1:4, *v/v*) to give **6** as yellow solid (0.23 g, 90%). mp: 103.2-104.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.47 (t, *J* = 6.5 Hz, 4H), 4.39 (td, *J* = 6.4, 1.6 Hz, 8H), 1.96-1.87 (m, 12H), 1.71-1.61 (m, 12H), 1.07 (t, *J* = 7.4 Hz, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 148.29, 146.23, 129.63, 128.14, 127.23, 127.07, 126.35, 124.75, 72.65, 72.62, 72.56, 58.18, 32.38, 32.36, 32.33, 19.41, 19.34, 18.30, 14.02, 14.01; HRMS: calculated for $C_{42}H_{54}O_6SSe_2$, 846.1966; found, 846.1990.

2.9 Synthesis of **6** from **16**



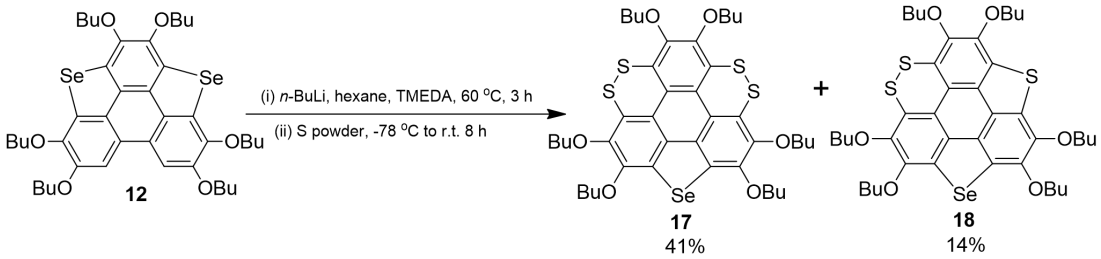
The mixture of **16** (0.93 g, 1 mmol) and copper nanopowder (80-100 nm, 0.64 g, 10 mmol) was slowly heated to 215 °C and kept at this temperature for 2 h 40 min under argon. After cooled down to room temperature, the reaction mixture was washed with CH_2Cl_2. The solution was concentrated and further purified by column chromatography on silica (eluent, CH_2Cl_2: petro ether, 1:4, *v/v*) to give **6** as yellow solid (0.75 g, 88%). mp: 103.2-104.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.47 (t, *J* = 6.5 Hz, 4H), 4.39 (td, *J* = 6.4, 1.6 Hz, 8H), 1.96-1.87 (m, 12H), 1.71-1.61 (m, 12H), 1.07 (t, *J* = 7.4 Hz, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 148.29, 146.23, 129.63, 128.14, 127.23, 127.07, 126.35, 124.75, 72.65, 72.62, 72.56, 58.18, 32.38, 32.36, 32.33, 19.41, 19.34, 18.30, 14.02, 14.01; HRMS: calculated for $C_{42}H_{54}O_6SSe_2$, 846.1966; found, 846.1990.

2.10 Synthesis of 9 from 12



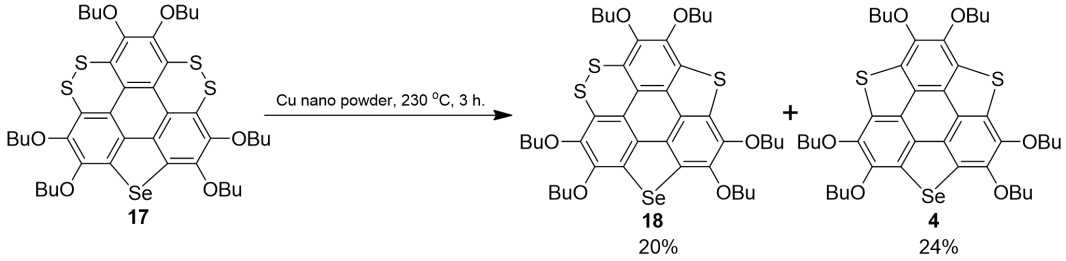
To a hexane (60 mL) solution of **12** (1.63 g, 2 mmol) was added TMEDA (1.19 mL, 8 mmol) and *n*-butyllithium (2.4 M in hexane, 3.3 mL, 8 mmol) at 60 °C for 3 hours. The resulting solution was cooled to -78 °C and diluted with 40 mL THF. Tellurium powder (2.54 g, 20mmol) was added in one portion. The resulting black mixturewas slowly warmed to room temperature and allowed to stir under ultrasound for 12 hours.The reaction was quenched by adding distilled water and then extracted with CH_2Cl_2 (3 × 100 mL). The organic layers were combined and dried over anhydrous Na_2SO_4, then concentrated under reduced pressure. The crude product was further purified by column chromatography on silica (eluent, CH_2Cl_2: petro ether, 1:4, v/v) to afford **9** as a yellow solid (1.09g, 55%), mp: 69.3-70.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.43 (t, *J* = 6.5 Hz, 4H), 4.33 (td, *J* = 6.4 Hz, 1.2 Hz, 8H), 1.94-1.84 (m, 12H), 1.70-1.57 (m, 12H), 1.05 (td, J = 7.4, 1.9 Hz, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 152.28, 152.17, 148.32, 136.53, 134.23, 131.38, 126.74, 117.93, 114.75, 73.09, 72.98, 72.71, 32.68, 32.65, 32.48, 19.61, 19.45, 14.11, 14.07; HRMS: calculated for $C_{42}H_{54}O_6SeTe_2$+H, 993.1265; found, 993.1247.

2.11 Synthesis of **17** and **18** from **12**



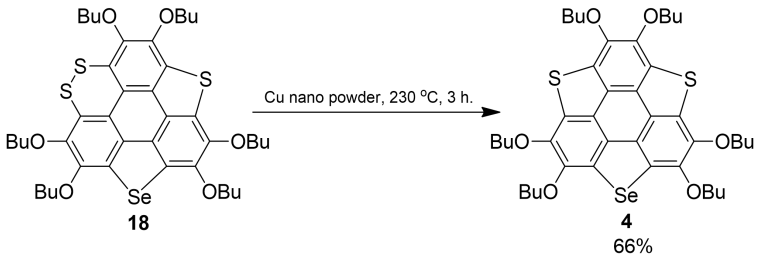
To a hexane (70 mL) solution of **12** (4.9 g, 6 mmol) was added TMEDA (3.6 mL, 24 mmol) and *n*-butyllithium (2.4 M in hexane, 10 mL, 24 mmol) at 60 °C for 3 hours. The resulting solution was cooled to -78 °C and diluted with 30 mL THF. sulfur powder (1.92 g, 60 mmol) was added in one portion. The resulting mixture was slowly warmed to room temperature and allowed to stir under room temperature for 8 hours. The reaction was quenched by adding distilled water and then extracted with CH_2Cl_2 (3 × 20 mL). The organic layers were combined and dried over anhydrous Na_2SO_4, then concentrated under reduced pressure. The crude product was further purified by column chromatography on silica (eluent, CH_2Cl_2: petro ether, 1:4, *v/v*) to afford **17** as a red solid (2.136 g, yield 41%). mp: 64.2-66.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.35 (t, *J* = 6.5 Hz, 4H), 4.23 (t, *J* = 6.6 Hz, 8H), 1.92-1.84 (m, 12H), 1.66-1.56 (m, 12H), 1.03 (td, *J* = 7.3, 1.5 Hz, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 149.22, 148.53, 146.55, 130.60, 129.13, 126.38, 124.54, 123.85, 122.61, 74.59, 74.34, 73.33, 32.54, 32.42, 32.38, 19.39, 19.36, 14.03, 13.99; HRMS: calculated for $C_{42}H_{54}O_6S_4Se$, 862.1963; found, 862.1959. And **18** as red solid (0.7 g, 14%). mp: 61.2-63.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.46 (td, *J* = 6.5, 1.7 Hz, 4H), 4.38 (t, *J* = 6.2 Hz, 4H), 4.24 (td, *J* = 6.5, 1.4 Hz, 4H), 1.94-1.83 (m, 12H), 1.70-1.57 (m, 12H), 1.05 (t, *J* = 7.4 Hz, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 149.97, 148.36, 147.84, 146.66, 146.42, 146.29, 130.59, 129.39, 128.82, 128.49, 126.95, 126.12, 124.95, 122.87, 122.73, 120.89, 120.68, 120.63, 74.61, 72.97, 72.93, 72.75, 72.69, 32.49, 32.44, 32.41, 32.35, 19.39, 19.36, 19.33, 19.28, 14.07, 14.02, 14.00, 13.98; HRMS: calculated for $C_{42}H_{54}O_6S_3Se$, 830.2242; found, 830.2221.

2.12 Synthesis of **4** and **18** from **17**



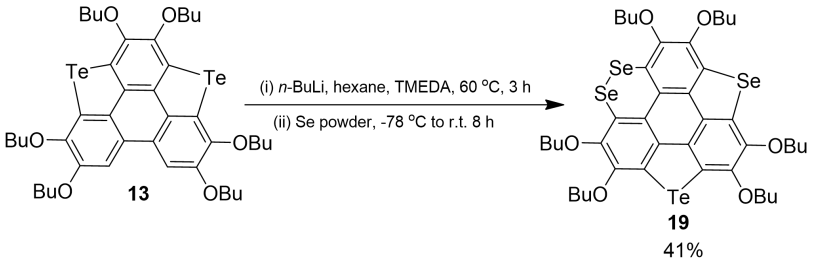
The mixture of **17** (2 g, 2.48 mmol) and copper nanopowder (80-100 nm, 1.59 g, 24.8 mmol) was slowly heated to 215 °C and kept at this temperature for 2 h 40 min under argon. After cooled down to room temperature, the reaction mixture was washed with CH_2Cl_2. The solution was concentrated and further purified by column chromatography on silica (eluent, CH_2Cl_2: petro ether, 1:4, *v/v*) to give **18** as a red soild (0.41 g, 20%). mp: 61.2-63.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm) 4.46 (td, *J* = 6.5 Hz, 1.7 Hz, 4H), 4.38 (t, *J* = 6.2 Hz, 4H), 4.24 (td, *J* = 6.5, 1.4 Hz, 4H), 1.94-1.83 (m, 12H), 1.70-1.57 (m, 12H), 1.05 (t, *J* = 7.4 Hz, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 149.97, 148.36, 147.84, 146.66, 146.42, 146.29, 130.59, 129.39, 128.82, 128.49, 126.95, 126.12, 124.95, 122.87, 122.73, 120.89, 120.68, 120.63, 74.61, 72.97, 72.93, 72.75, 72.69, 32.49, 32.44, 32.41, 32.35, 19.39, 19.36, 19.33, 19.28, 14.07, 14.02, 14.00, 13.98; HRMS: calculated for $C_{42}H_{54}O_6S_3Se$, 830.2242; found, 830.2221. And **4** as yellow solid (0.48g, 24%). mp: 146.2-147.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.45 (t, *J* = 6.5 Hz, 8H), 4.37 (t, *J* = 6.5 Hz, 4H), 1.94-1.86 (m, 12H), 1.69-1.59 (m, 12H), 1.05 (t, *J* = 7.4 Hz, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 148.56, 146.56, 146.51 130.22, 129.58, 129.34, 128.31, 127.92, 127.31, 73.04, 72.95, 32.33, 32.30, 32.29, 19.38, 19.32, 13.99; HRMS: calculated for $C_{42}H_{54}O_6S_2Se$, 798.2522; found,798.2545.

2.13 Synthesis of **4** from **18**



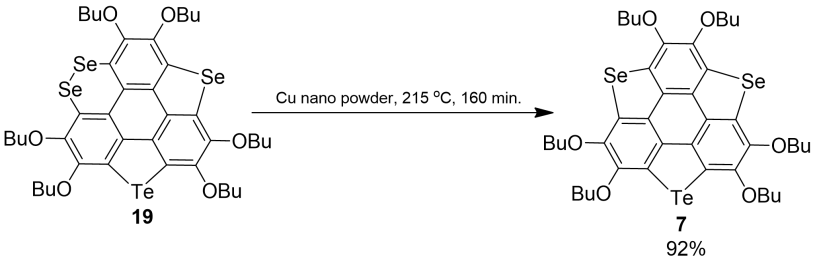
The mixture of **18** (0.3 g, 0.32 mmol) and copper nanopowder (80-100 nm, 0.2 g, 3.2 mmol) was slowly heated to 230 °C and kept at this temperature for 3 h under argon. After cooled down to room temperature, the reaction mixture was washed with CH_2Cl_2. The solution was concentrated and further purified by column chromatography on silica (eluent, CH_2Cl_2: petro ether, 1:4, *v/v*) to give **4** as yellow solid (181 mg, 66%). mp: 146.2-147.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.45 (t, *J* = 6.5 Hz, 8H), 4.37 (t, *J* = 6.5 Hz, 4H), 1.94-1.86 (m, 12H), 1.69-1.59 (m, 12H), 1.05 (t, *J* = 7.4 Hz, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 148.56, 146.56, 146.51 130.22, 129.58, 129.34, 128.31, 127.92, 127.31, 73.04, 72.95, 32.33, 32.30, 32.29, 19.38, 19.32, 13.99; HRMS: calculated for $C_{42}H_{54}O_6S_2Se$, 798.2522; found, 798.2545.

2.14 Synthesis of **19** from **13**



To a hexane (30 mL) solution of **13** (1.83 g, 2 mmol) was added TMEDA (1.2 mL, 8 mmol) and *n*-butyllithium (2.4 M in hexane, 3.33 mL, 8 mmol) at 60 °C for 3 hours. The resulting solution was cooled to -78 °C and diluted with 30 mL THF. Selenium powder (1.6 g, 20 mmol) was added in one portion. The resulting mixture was slowly warmed to room temperature and allowed to stir under room temperature for 8 hours. The reaction was quenched by adding distilled water and then extracted with CH_2Cl_2 (3 × 100 mL). The organic layers were combined and dried over anhydrous Na_2SO_4, then concentrated under reduced pressure. The crude product was further purified by column chromatography on silica (eluent, CH_2Cl_2: petro ether, 1:4, *v/v*) to afford **19** as a yellow solid (0.85 g, yield 41%). mp: 48.9-51.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.38-4.35 (m, 4H), 4.34-4.25 (m, 8H), 1.96-1.80 (m, 12H), 1.67-1.58 (m, 12H), 1.04 (td, *J* = 7.3, 3.5 Hz, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 152.94, 152.01, 148.94, 147.67, 146.97, 146.40, 136.64, 134.43, 131.97, 131.61, 130.51, 128.78, 126.44, 126.42, 122.13, 117.07, 115.99, 113.90, 74.22, 74.09, 73.39, 73.15, 73.07, 73.04, 32.79, 32.73, 32.61, 32.58, 32.56, 32.53, 19.56, 19.54, 19.47, 19.41, 19.38, 14.10, 14.05, 14.01; HRMS: calculated for $C_{42}H_{54}O_6Se_3Te$, 1020.0463; found, 1020.0452.

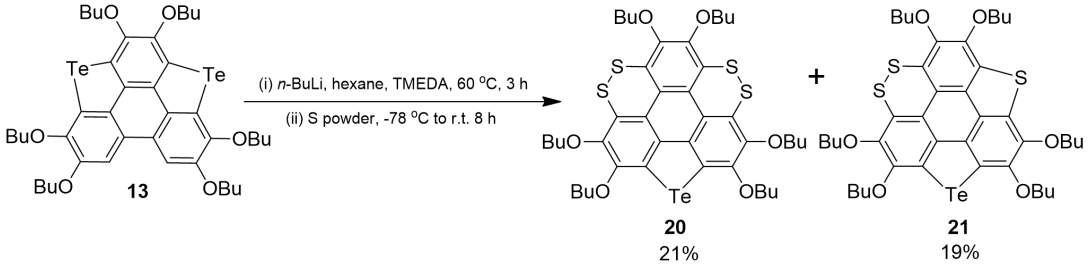
2.15 Synthesis of 7 from 19



The mixture of **19** (0.85 g, 0.83 mmol) and copper nanopowder (80-100 nm, 0.53 g, 8.3 mmol) was slowly heated to 215 °C and kept at this temperature for 2 h 40 min under argon. After cooled down to room temperature, the reaction mixture was washed with CH_2Cl_2. The solution was concentrated and further purified by column chromatography on silica (eluent, CH_2Cl_2: petro ether, 1:4, *v/v*) to give **7** as yellow solid (723 mg, 92%). mp: 85.2-87.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.43 (td, *J* = 6.4, 2.5 Hz, 8H), 4.32 (t, *J* = 6.4 Hz, 4H), 1.95-1.84 (m, 12H), 1.71-1.59 (m, 12H), 1.06 (td, *J* = 7.4, 2.1 Hz, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 152.17, 146.46,

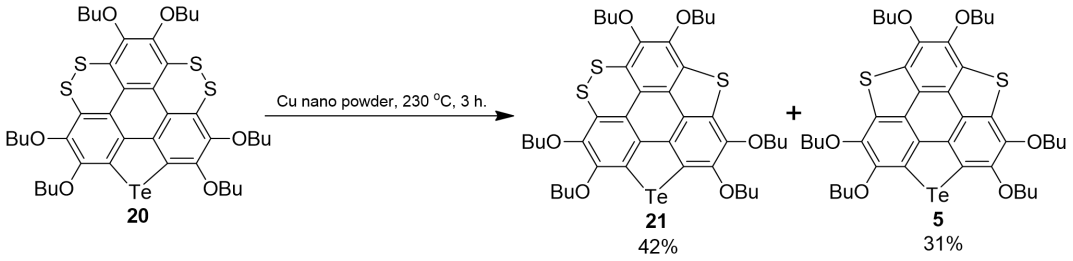
146.37, 133.15, 129.49, 128.96, 125.78, 125.56, 114.87, 72.90, 72.76, 72.54, 32.54, 32.37, 32.33, 19.58, 19.37, 14.11, 14.05; HRMS: calculated for $C_{42}H_{54}O_6Se_2Te$, 941.1331; found, 941.1350.

2.16 Synthesis of **20** and **21** from **13**



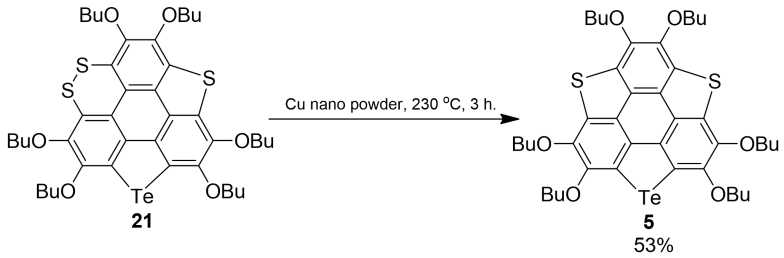
To a hexane (80 mL) solution of **13** (5.5 g, 6 mmol) was added TMEDA (3.6 mL, 24 mmol) and *n*-butyllithium (2.4 M in hexane, 10 mL, 24 mmol) at 60 °C for 3 hours. The resulting solution was cooled to -78 °C and diluted with 40 mL THF. Sulfur powder (1.92 g, 60 mmol) was added in one portion. The resulting mixture was slowly warmed to room temperature and allowed to stir under room temperature for 8 hours. The reaction was quenched by adding distilled water and then extracted with CH_2Cl_2 (3 × 100 mL). The organic layers were combined and dried over anhydrous Na_2SO_4, then concentrated under reduced pressure. The crude product was further purified by column chromatography on silica (eluent, CH_2Cl_2: petro ether, 1:4, *v/v*) to afford **20** as red solid (1.1 g, yield 21%). mp: 70.5-74.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.32 (t, *J* = 6.5 Hz, 4H), 4.21 (dd, *J* = 14.4, 6.7 Hz, 8H), 1.91-1.79 (m, 12H), 1.64-1.53 (m, 12H), 1.03 (td, *J* = 7.4, 2.3 Hz, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 153.12, 148.17, 145.69, 135.49, 126.73, 126.58, 125.25, 123.65, 119.84, 74.44, 74.29, 73.27, 32.78, 32.37, 19.50, 19.38, 19.34, 14.03; HRMS: calculated for $C_{42}H_{54}O_6S_4Te$, 912.1860; found, 912.1853. And **21** as yellow solid (1.0 g, yield 19%). mp: 50.2-53.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.45 (td, *J* = 6.5Hz, 1.1 Hz, 4H), 4.31 (dd, *J* = 12.2, 6.3 Hz, 4H), 4.24 (td, *J* = 6.6, 2.1 Hz, 4H), 1.93-1.79 (m, 12H), 1.69-1.54 (m, 12H), 1.06-1.01 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 153.82, 152.35, 147.62, 146.53, 146.36, 146.08, 135.52, 132.49, 128.85, 128.84, 128.75, 126.93, 125.62, 121.94, 121.37, 121.13, 120.98, 112.50, 74.63, 74.49, 73.34, 73.09, 72.98, 72.87, 32.70, 32.64, 32.47, 32.43, 32.38, 19.50, 19.47, 19.34, 19.28, 19.24, 13.96, 13.88; HRMS: calculated for $C_{42}H_{54}O_6S_3Te$, 880.2139; found, 880.2136.

2.17 Synthesis of **5** and **21** from **20**



The mixture of **20** (0.5 g, 0.54 mmol) and copper nanopowder (80-100 nm, 346 mg, 5.4 mmol) was slowly heated to 230 °C and kept at this temperature for 3 h under argon. After cooled down to room temperature, the reaction mixture was washed with CH_2Cl_2. The solution was concentrated and further purified by column chromatography on silica (eluent, CH_2Cl_2: petro ether, 1:4, *v/v*) to give **21** as yellow solid (200 mg, 42%). mp: 50.2-53.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.45 (td, *J* = 6.5, 1.1 Hz, 4H), 4.31 (dd, *J* = 12.2, 6.3 Hz, 4H), 4.24 (td, *J* = 6.6Hz, 2.1 Hz, 4H), 1.93-1.79 (m, 12H), 1.69-1.54 (m, 12H), 1.06-1.01 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 153.82, 152.35, 147.62, 146.53, 146.36, 146.08, 135.52, 132.49, 128.85, 128.84, 128.75, 126.93, 125.62, 121.94, 121.37, 121.13, 120.98, 112.50, 74.63, 74.49, 73.34, 73.09, 72.98, 72.87, 32.70, 32.64, 32.47, 32.43, 32.38, 19.50, 19.47, 19.34, 19.28, 19.24, 13.96, 13.88; HRMS: calculated for $C_{42}H_{54}O_6S_3Te$, 880.2139; found, 880.2136. And **5** as a yellow solid (142 mg, 31%). mp: 80.1-81.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.48 (td, *J* = 6.4, 4.8 Hz, 8H), 4.30 (t, *J* = 6.4 Hz, 4H), 1.96- 1.84 (m, 12H), 1.71-1.59 (m, 12H), 1.08-1.04 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 152.21, 146.49, 144.41, 133.20, 129.54, 129.03, 125.84, 125.62, 114.92, 72.92, 72.78, 72.56, 32.53, 32.36, 32.32, 19.57, 19.36, 14.09, 14.03; HRMS: calculated for $C_{42}H_{54}O_6S_2Te$, 848.2419; found, 848.2413.

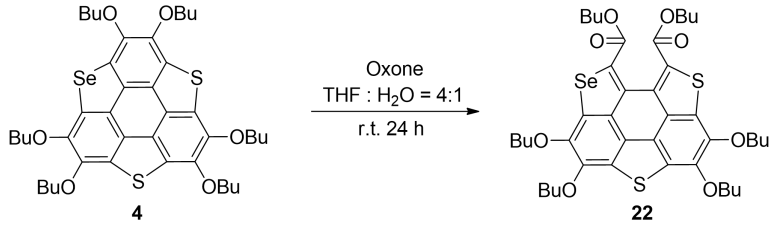
2.18 Synthesis of 5 from 21



The mixture of **21** (0.3 g, 0.34 mmol) and copper nanopowder (80-100 nm, 218 mg, 3.4 mmol) was slowly heated to 230 °C and kept at this temperature for 3 h under argon. After cooled down to room temperature, the reaction mixture was washed with CH_2Cl_2. The solution was concentrated and further purified by column chromatography on silica (eluent, CH_2Cl_2: petro ether, 1:4, *v/v*) to give **5** as yellow solid (153 mg, 53%). mp: 80.1-81.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.48 (td, *J* = 6.4, 4.8 Hz, 8H), 4.30 (t, *J* = 6.4 Hz, 4H), 1.96-1.84 (m, 12H), 1.71-1.59 (m, 12H),

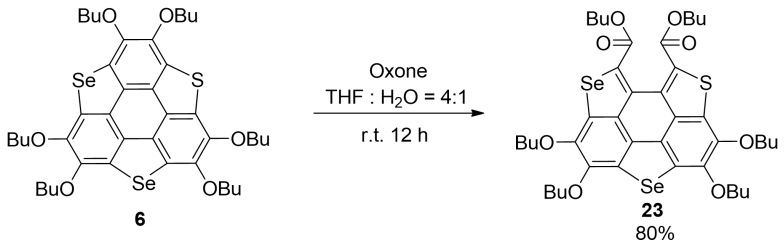
1.08-1.04 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 152.21, 146.49, 146.41, 133.20, 129.54, 129.03, 125.84, 125.62, 114.92, 72.92, 72.78, 72.56, 32.53, 32.36, 32.32, 19.57, 19.36, 14.09, 14.03; HRMS: calculated for $C_{42}H_{54}O_6S_2Te$, 848.2419; found, 848.2413.

2.19 Synthesis of **22** from **4**



Compound **4** (478.9 mg, 0.6 mmol) and Oxone (737.71 mg, 1.2 mmol) were dissolved in the mixed solvent of THF (40 mL) and H_2O (10 mL). The resulting mixture was stirred at room temperature for 24 h. The reaction was quenched by adding distilled water and extracted with CH_2Cl_2 (3 × 15 mL). The organic layers were combined and dried over anhydrous Na_2SO_4, then concentrated under reduced pressure. The crude product was further purified by column chromatography on silica-gel (eluent, CH_2Cl_2: petro ether, 1:2, v/v) to afford **22** as red powder (344.5 mg, yield 69%). mp: 67.0-68.4 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.51-4.26 (m, 12H), 1.93 -1.83 (m, 8H), 1.81-1.76 (m, 4H), 1.68-1.56 (m, 8H), 1.54-1.45(m, 4H), 1.06-0.98 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 164.81, 163.69, 163.62, 149.53, 147.71, 147.69, 146.40, 144.50, 144.41, 136.74, 133.30, 133.23, 132.91, 131.99, 131.89, 131.49, 131.30, 130.83, 129.93, 129.54, 128.87, 128.62, 128.29, 126.40, 126.38, 126.30, 125.65, 73.70, 73.66, 72.73, 72.57, 65.53, 32.53, 32.45, 32.43, 32.33, 32.27, 30.69, 30.68, 19.39, 19.33, 19.30, 19.29, 19.26, 13.96, 13.94, 13.90, 13.81; IR (KBr Pellent) 1709.6 (C=O) cm^{-1}; HRMS: calculated for $C_{42}H_{54}O_8S_2Se$+H, 831.2498; found, 831.2505.

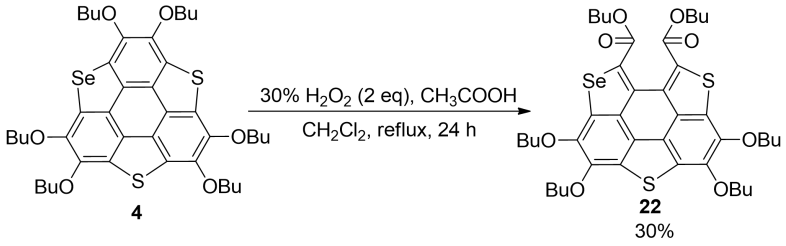
2.20 Synthesis of **23** from **6**



Compound **6** (151.5 mg, 0.18 mmol) and Oxone (221.3 mg, 0.36 mmol) were dissolved in the mixed solvent of THF (16 mL) and H_2O (4 mL). The resulting mixture was stirred at room temperature for 24 h. The reaction was quenched by adding distilled water and extracted with CH_2Cl_2 (3 × 15 mL). The organic layers were combined and dried over anhydrous Na_2SO_4, then

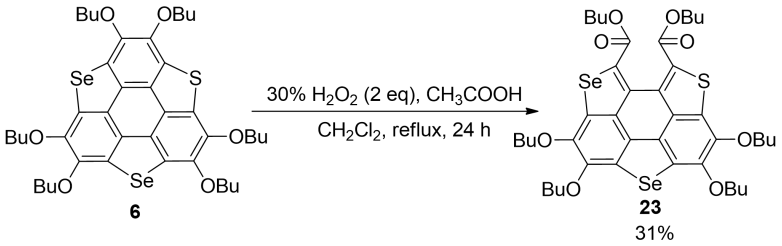
concentrated under reduced pressure. The crude product was further purified by column chromatography on silica-gel (eluent, CH_2Cl_2: petro ether, 1:2, v/v) to afford **23** as red powder (126.3 mg, yield 80%). mp: 63.2-65.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.49-4.26 (m, 12H), 1.93 -1.83 (m, 8H), 1.81-1.75 (m, 4H), 1.68-1.56 (m, 8H), 1.54-1.45 (m, 4H), 1.06-0.98 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 163.94, 163.87, 162.76, 148.24, 146.40, 145.51, 145.40, 143.49, 136.42, 135.01, 133.94, 132.29, , 131.87, 131.57, 131.43, 130.55, 129.79, 129.48, 128.59, 127.90, 127.33, 126.05, 125.26, 125.13, 72.62, 72.56, 71.81, 71.64, 64.46, 31.51, 31.49, 31.41, 31.32, 31.25, 29.65, 18.35, 18.29, 18.25, 18.22, 12.92, 12.89, 12.78; IR (KBr Pellent) 1708.9 (C=O) cm^{-1}; HRMS: calculated for $C_{42}H_{54}O_8SSe_2$+H, 879.1943; found, 879.1945.

2.21 Synthesis of 22 from 4



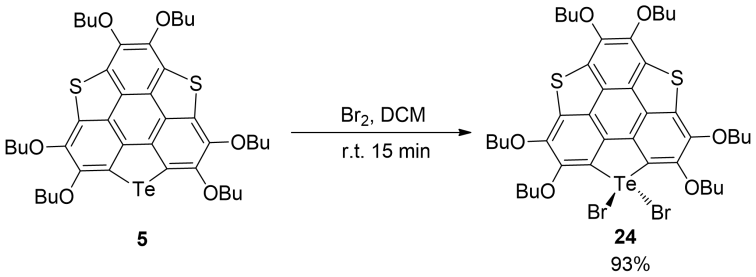
Compound **4** (120 mg, 0.15 mmol) and hydrogen peroxide (H_2O_2 aqueous 30%, 9.2 μL) were dissolved in the mixed solvent of dichloromethane (CH_2Cl_2, 10 mL) and glacial acetic acid (AcOH, 2 mL). The resulting mixture was stirred at 60 °C for 12 h. The reaction mixture was then diluted by adding distilled water (20 ml) and then extracted with CH_2Cl_2 (3 × 15 mL). The organic layers were combined and dried over anhydrous Na_2SO_4, then concentrated under reduced pressure. The crude product was further purified by column chromatography on silica (eluent, CH_2Cl_2: petro ether, 1:2, v/v) to afford compound **22** as red powder (37.3 mg, yield 30%). mp: 67.0-68.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.51-4.26 (m, 12H), 1.93-1.83 (m, 8H), 1.81-1.76 (m, 4H), 1.68-1.56 (m, 8H), 1.54-1.45(m, 4H), 1.06-0.98 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 164.81, 163.69, 163.62, 149.53, 147.71, 147.69, 146.40, 144.50, 144.41, 136.74, 133.30, 133.23, 132.91, 131.99, 131.89, 131.49, 131.30, 130.83, 129.93, 129.54, 128.87, 128.62, 128.29, 126.40, 126.38, 126.30, 125.65, 73.70, 73.66, 72.73, 72.57, 65.53, 32.53, 32.45, 32.43, 32.33, 32.27, 30.69, 30.68, 19.39, 19.33, 19.30, 19.29, 19.26, 13.96, 13.94, 13.90, 13.81; IR (KBr Pellent) 1709.6 (C=O) cm^{-1}; HRMS: calculated for $C_{42}H_{54}O_8S_2Se$+H, 831.2498; found, 831.2505.

2.22 Synthesis of 23 from 6



Compound **6** (253.8 mg, 0.3 mmol) and hydrogen peroxide (H_2O_2 aqueous 30%, 61.3 μL) were dissolved in the mixed solvent of dichloromethane (CH_2Cl_2, 10 mL) and glacial acetic acid (AcOH, 2 mL). The resulting mixture was stirred at 60 °C for 12h. The reaction mixture was then diluted by adding distilled water (20 ml) and then extracted with CH_2Cl_2 (3 × 15 mL). The organic layers were combined and dried over anhydrous Na_2SO_4, then concentrated under reduced pressure. The crude product was further purified by column chromatography on silica (eluent, CH_2Cl_2: petro ether, 1:2, v/v) to afford compound **23** as red power (81.6 mg, yield 31%). mp: 63.2-65.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.49-4.26 (m, 12H), 1.93-1.83 (m, 8H), 1.81-1.75 (m, 4H), 1.68-1.56 (m, 8H), 1.54-1.45 (m, 4H), 1.06-0.98 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 163.94, 163.87, 162.76, 148.24, 146.40, 145.51, 145.40, 143.49, 136.42, 135.01, 133.94, 132.29, , 131.87, 131.57, 131.43, 130.55, 129.79, 129.48, 128.59, 127.90, 127.33, 126.05, 125.26, 125.13, 72.62, 72.56, 71.81, 71.64, 64.46, 31.51, 31.49, 31.41, 31.32, 31.25, 29.65, 18.35, 18.29, 18.25, 18.22, 12.92, 12.89, 12.78; IR (KBr Pellent) 1708.9 (C=O) cm^{-1}; HRMS: calculated for $C_{42}H_{54}O_8SSe_2$+H, 879.1943; found, 879.1945.

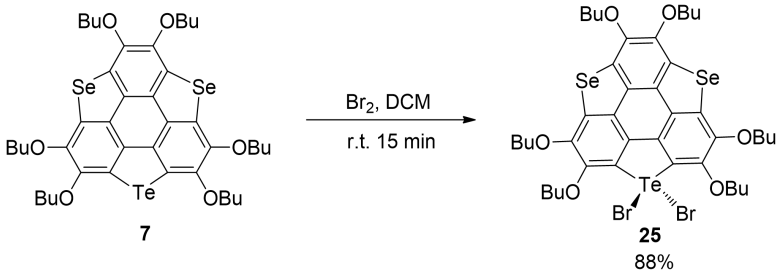
3.23 Synthesis of **24** from **5**



Compound **5** (28.32 mg, 0.033 mmol) was dissolved in CH_2Cl_2 (5 mL), and a solution of bromine (5.27 mg, 0.033 mmol) was added slowly. After stirred at room temperature for 15 min, and The solution was concentrated. The residue was dissolved in *n*-hexane (20 mL) .The resulting kept in a refrigerator for 2 hours (-20 °C) to give red precipitate. The precipitate was collected by suction, washed with n-hexane, and dried in air to give **24** as red solid (30.9 mg, 93% yield). mp: 149.5-151.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.56 (t, J = 6.3 Hz, 4H), 4.52-4.46 (m, 8H), 2.05-1.88 (m, 12H), 1.73-1.60 (m, 12H), 1.11-1.04 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm)

150.94, 147.43, 147.09, 134.63, 132.69, 129.81, 128.94, 125.69, 125.25, 73.04, 73.00, 72.96, 32.21, 32.17, 32.06, 19.38, 19.26, 19.25, 13.90.

3.24 Synthesis of **25** from **7**



Compound **7** (29.6 mg, 0.031 mmol) was dissolved in CH_2Cl_2 (5 mL), and a solution of bromine (5.27 mg, 0.031 mmol) was added slowly. After stirred at room temperature for 15 min, and The solution was concentrated. The residue was dissolved in *n*-hexane (20 mL) .The resulting kept in a refrigerator for 2 hours (-20 °C) to give red precipitate. The precipitate was collected by suction, washed with *n*-hexane, and dried in air to give **25** as red solid (30.1 mg, 88% yield). mp: 183.6 - 185.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ(ppm) 4.58 (t, J = 6.0 Hz, 4H), 4.46-4.39 (m, 8H), 2.05-1.98 (m, 4H), 1.95-1.86 (m, 8H), 1.73-1.59 (m, 12H), 1.11-1.04 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ(ppm) 150.75, 149.32, 149.26, 133.43, 133.29, 131.52, 128.93, 128.21, 124.64, 73.15, 72.88, 72.82, 32.31, 32.28, 32.18, 19.39, 19.34, 19.32, 13.92.

3. Thermogravimetric Analyses

Thermogravimetric analyses (TGA) were conducted on 1090B type thermal analyzer (Dupont Engineering Polymers).

Table S1. Thermal stability of compounds **4-9**.

Comp	**4**	**5**	**6**	**7**	**8**	**9**
T_d / ºC	321	317	317	315	334	319

T_d : degradation temperature.

Table S2. Thermal stability of compounds **22-25**.

Comp	**22**	**23**	**24**	**25**
T_d / ºC	297	310	214	217

T_d : degradation temperature.

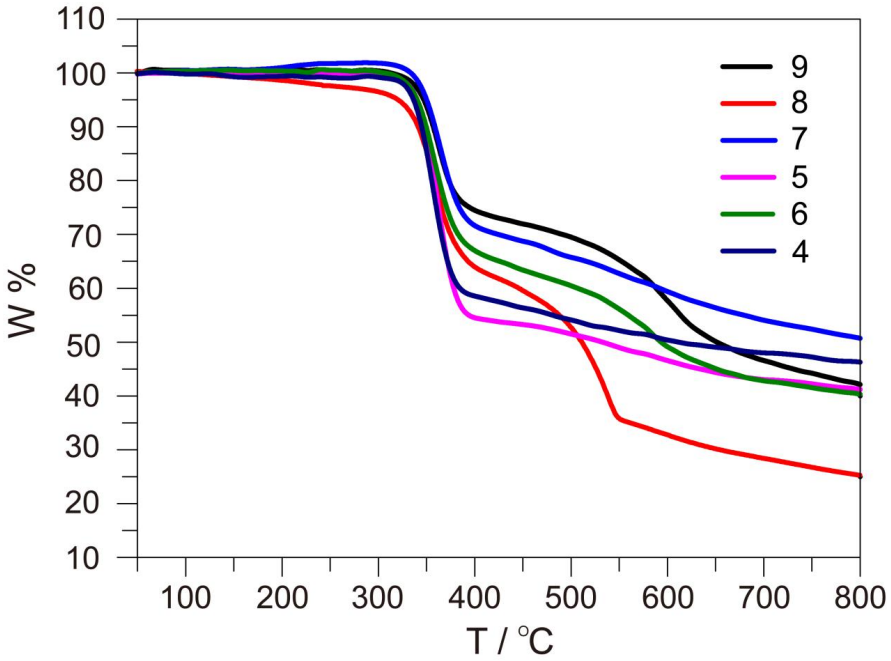


Figure S1. Thermogravimetric analyses of compounds **4-9**.

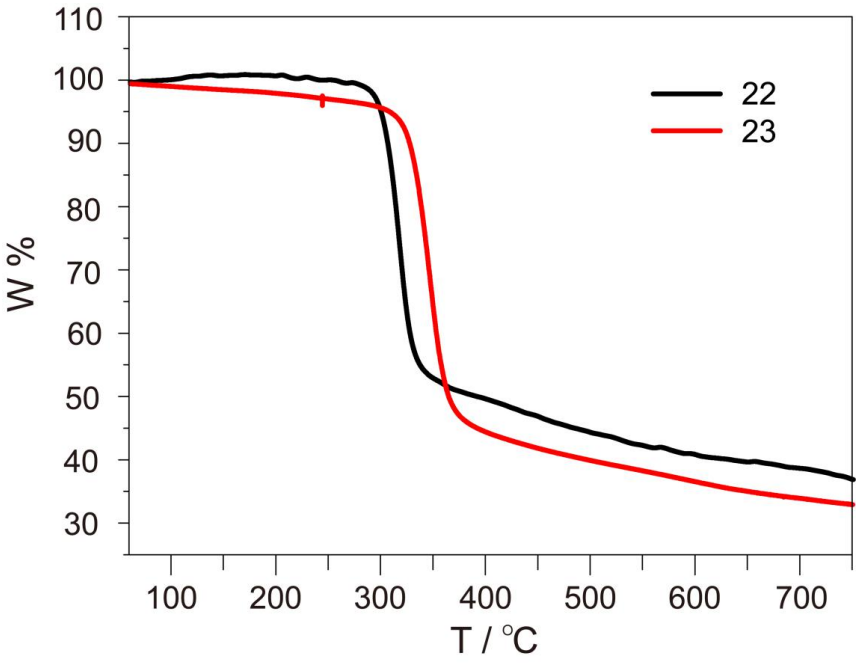


Figure S2. Thermogravimetric analyses of compounds **22** and **23**.

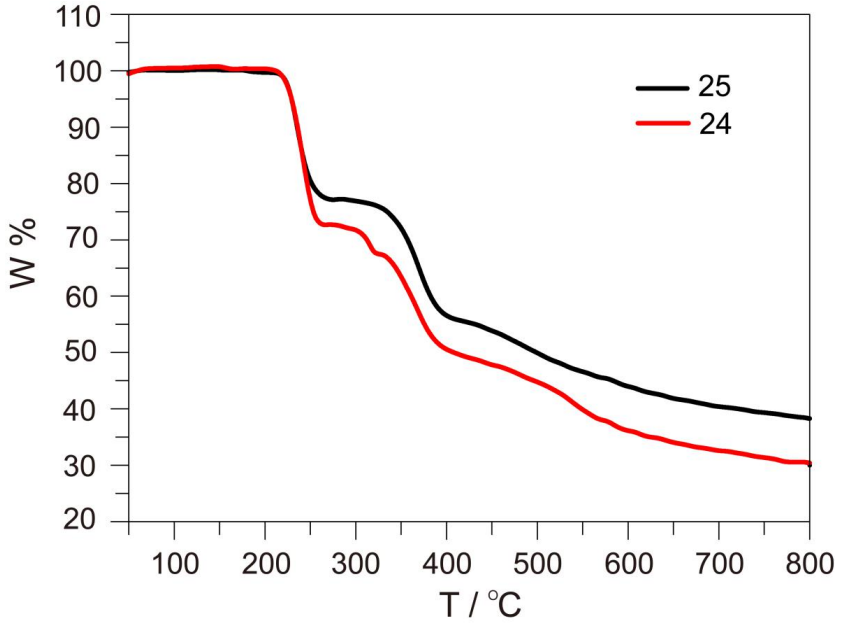


Figure S3. Thermogravimetric analyses of compounds **24** and **25**.

4. Crystal structural data

The single crystals of **4** (pale yellow needle)**, 6** (pale yellow needle)**, 9** (pale yellow needle) and **22** (red needle) were obtained by slow evaporation of its CH_2Cl_2-CH_3CN (1 : 1, v/v), CH_2Cl_2, CH_2Cl_2-ethanol (1 : 1, v/v) and ethyl acetate-ethanol (1 : 1, v/v) solution at room temperature, respectively. The Selected crystallographic data for **4**, **6**, **9**, and **22** are summarized in **Table S3**.

Table S3. Selected crystallographic data for **4**, **6**, **9**, and **22**.

	4	**6**	**9**	**22**
CCDC number	1867769	1867770	1867771	1867772
Empirical formula	$C_{42}H_{54}O_6S_2Se$	$C_{42}H_{54}O_6SSe_2$	$C_{42}H_{54}O_6SeTe_2$	$C_{42}H_{54}O_8S_2Se$
Formula weight	797.93	844.83	989.01	829.93
Temperature[K]	173(1)	174(2)	174(2)	290(1)
λ [Å]	0.71037 (Mo-Kα)	0.71037 (Mo-Kα)	0.71037 (Mo-Kα)	1.54184 (Cu-Kα)
Crystal size [mm^3]	0.31×0.11×0.09	0.35×0.10×0.08	0.32×0.14×0.09	0.36×0.12×0.08
Crystal system	triclinic	triclinic	triclinic	monoclinic
space group	*P*-1	*P*-1	*P*-1	$P2_1/n$
a [Å]	14.2625(6)	14.2879(4)	12.1441(8)	17.4194(2)
b [Å]	18.0213(12)	18.0394(7)	16.8305(9)	8.20520(10)
c [Å]	31.3062(19)	31.4094(8)	20.8669(13)	28.3968(4)
α [°]	86.466(5)	86.414(2)	98.844(5)	90
β [°]	83.674(5)	83.365(2)	91.448(5)	90.1660(10)
γ [°]	83.298(5)	83.373(2)	102.981(5)	90
V [$Å^3$]	7933.2(8)	7977.7(4)	4098.7(4)	4058.73(9)
Z	8	8	4	4
d_{calc} [g cm^{-3}]	1.336	1.407	1.603	1.358
μ [mm^{-1}]	1.098	1.952	2.356	2.630
2θmax [°]	57.14	57.352	57.266	139.576
Data / restraints / parameters	35946/13/1861	36108/2/1861	18324/0/926	7448/6/513
GooF	0.978	1.024	1.050	1.954
R [$I > 2\sigma(I)$]	0.1279	0.0737	0.1224	0.1451
wR_2	0.2179	0.1493	0.2831	0.4154

5. UV-Vis Spectra

The UV-Vis spectra of the compounds so far obtained were measured in their dichloromethane (CH_2Cl_2) solution (c = 1.0 × 10^{-5} mol L^{-1}) at 20 °C on a UV-2600 UV-Vis spectrometer (Shimadzu). **Table S4** summarizes the absorption spectra data of the compounds **22-25**.

Table S4. UV-Vis spectra of compounds **22-25** in CH_2Cl_2 solution.

Comp.	λ_{max}/nm	log ε	λ_{max}/nm	log ε	λ_{max}/nm	log ε	λ_{max}/nm	log ε
22	276	4.25	327	4.38	423	3.85	477	3.89
23	278	4.44	329	4.56	430	4.07	482	4.12
24	255	4.53	299	4.86	449	3.47		
25	255	4.64	300	4.92	437	3.49		

6. Fluorescence

Fluorescence excitation and emission spectra were recorded with an RF-5301(pc)s Spectrofluorophotometer, fluorescence lifetime and steady state were measured on FLS920 Spectrofluorophotometer. Measurement conditions: solvent, CH_2Cl_2; concentration, 10^{-5} mol L^{-1}; temperature, 20 °C.

Table S5. The emission and excitation properties of compounds **4, 5, 6, 7, 22** and **23** in CH_2Cl_2 solution. [a]

compounds	λ_{ex} / nm	λ_{em} / nm	Stocks shift / nm	Φ_F / %	τ_1 / ns
4	297	415	118		
5	289	400	111		
6	314	411	97		
7	283	404	121		
22	328	630	302	16.00	10.73
23	329	630	301	9.87	8.09

[a] λ_{ex}: excitation wavelength; λ_{em}: maximum emission wavelength; Φ_F: fluorescence quantum yield; τ_1 fluorescence lifetime

7. Electrochemical properties

The redox potentials were obtained by cyclic voltammetry (CV) method on a RST 5000 electrochemical analyzer with glassy carbon discs as the working electrode, Pt wire as the counter electrode, and SCE electrode as the reference electrode. Measurement conditions: solvent, CH_2Cl_2; concentration, 1×10^{-4} mol L^{-1}; supporting electrolyte, $(n\text{-Bu})_4NPF_6$ (0.1 M); scan speed, 50 mV s^{-1}; temperature, 20 °C.

Table S6. The first oxidation potential of compounds **4**, **5**, **6**, **7**, **8**, **9**, **22**, **23**, **24** and **25**.

Comp.	**4**	**5**	**6**	**7**	**8**	**9**	**22**	**23**	**24**	**25**
E_{ox}^1 / **V**	0.96	0.93	0.93	0.92	0.90	0.90	0.94	0.95	0.60	0.61

[a] E_{ox}^1 : The first oxidation potential.

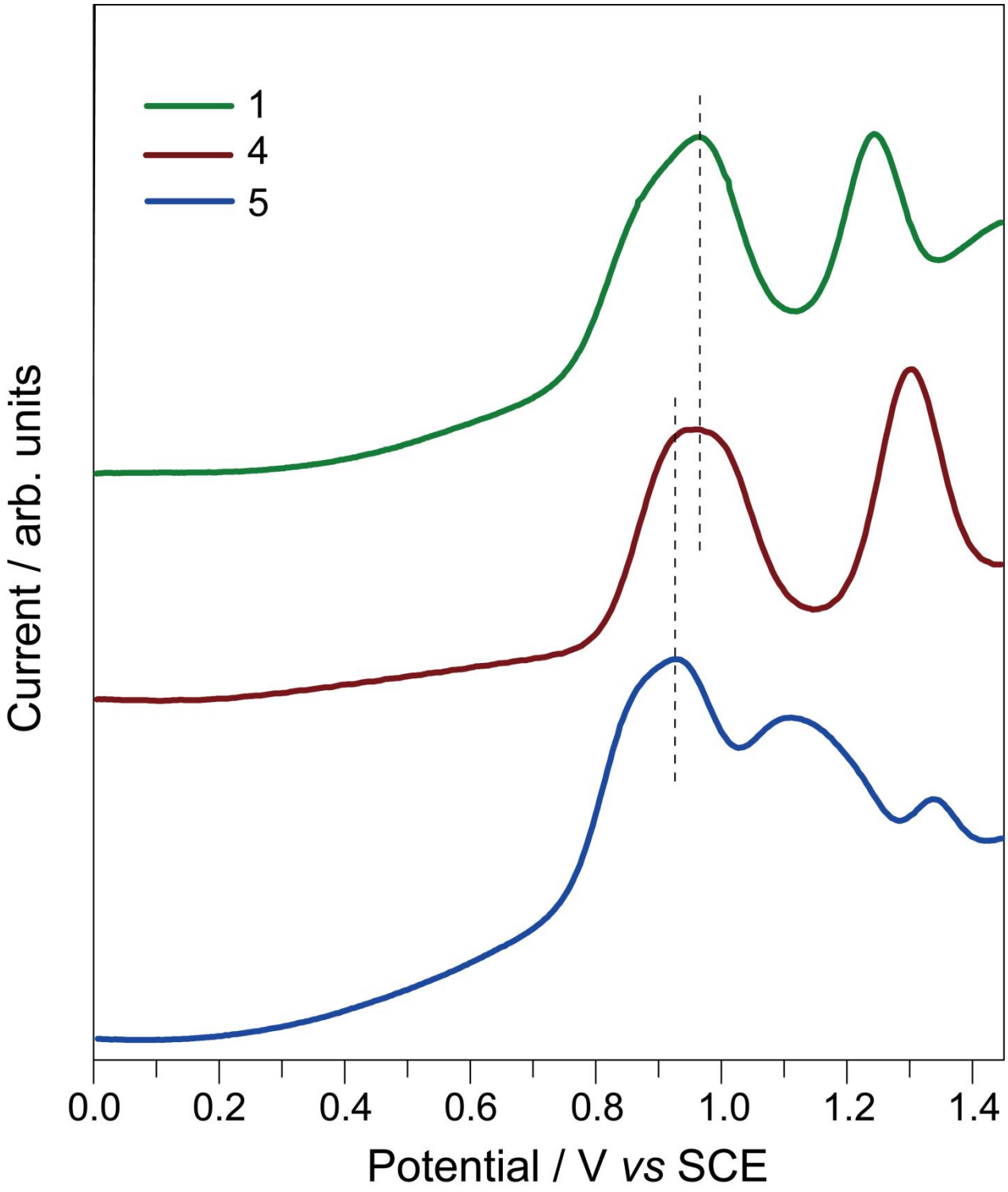


Fig. S4 Differential pulse voltammetry (DPV) analyses for compounds **1, 4,** and **5**

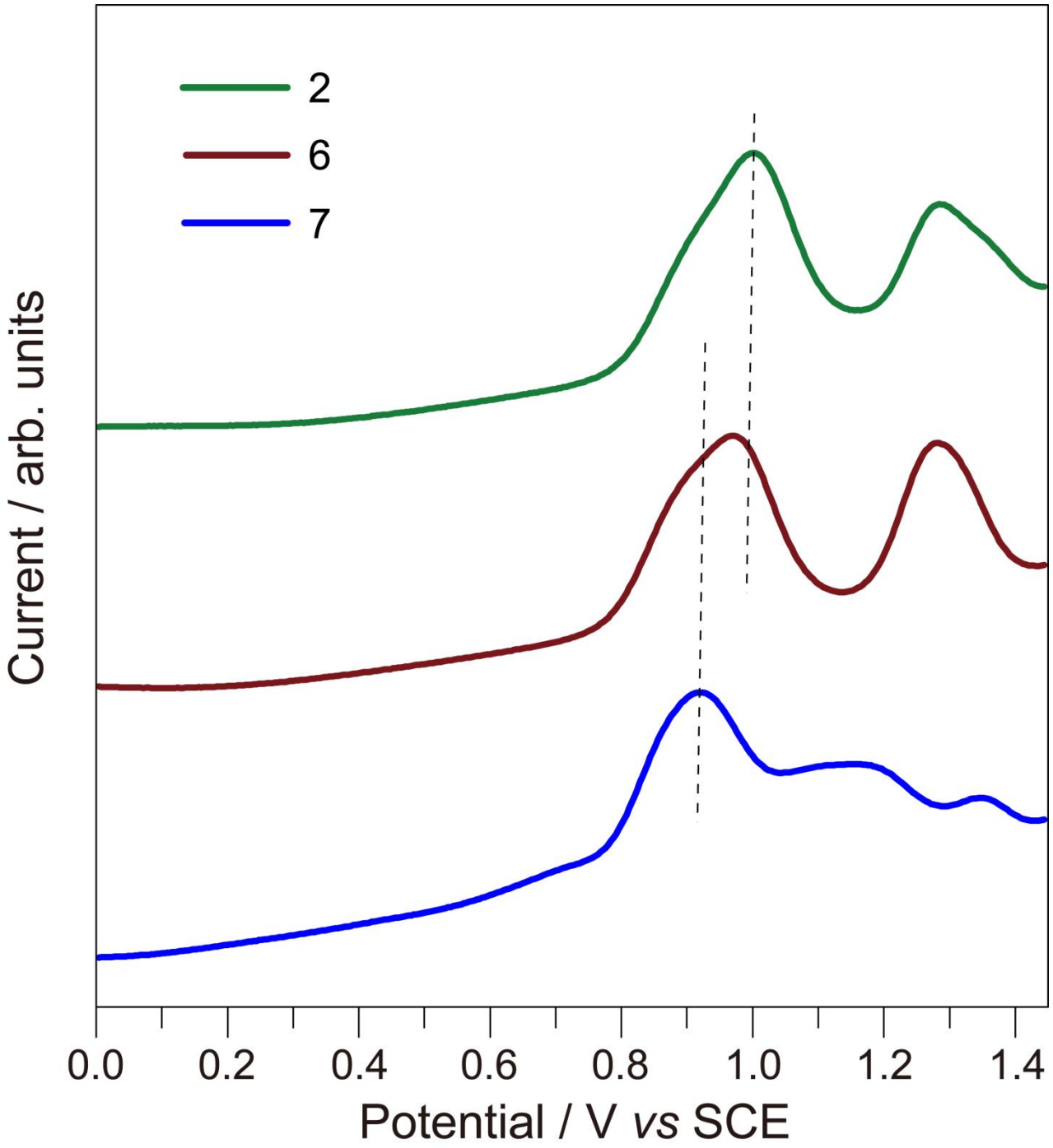


Fig. S5 Differential pulse voltammetry (DPV) analyses for compounds **2**, **6,** and **7**.

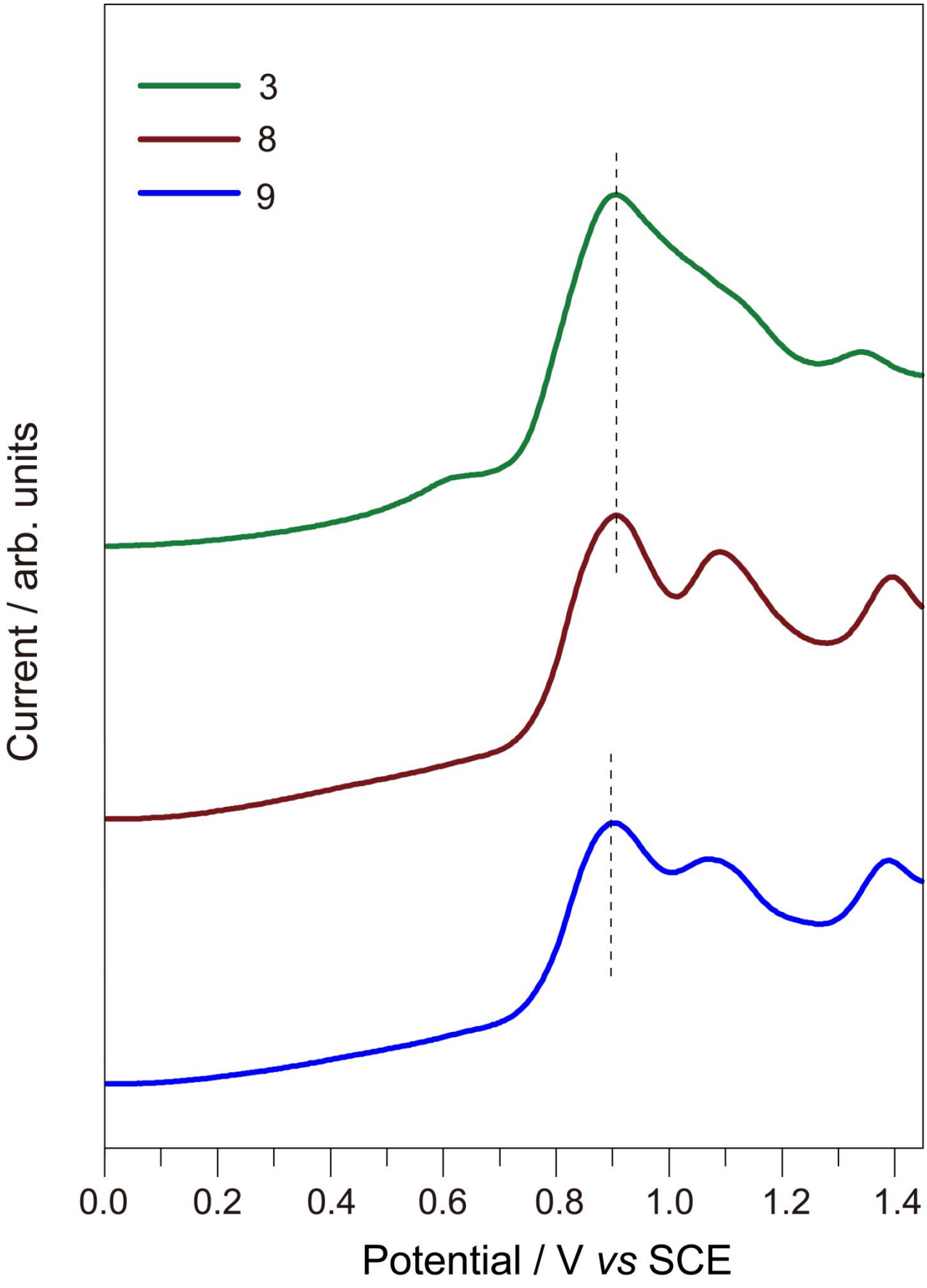


Fig. S6 Differential pulse voltammetry (DPV) analyses for compounds **3, 8** and **9**

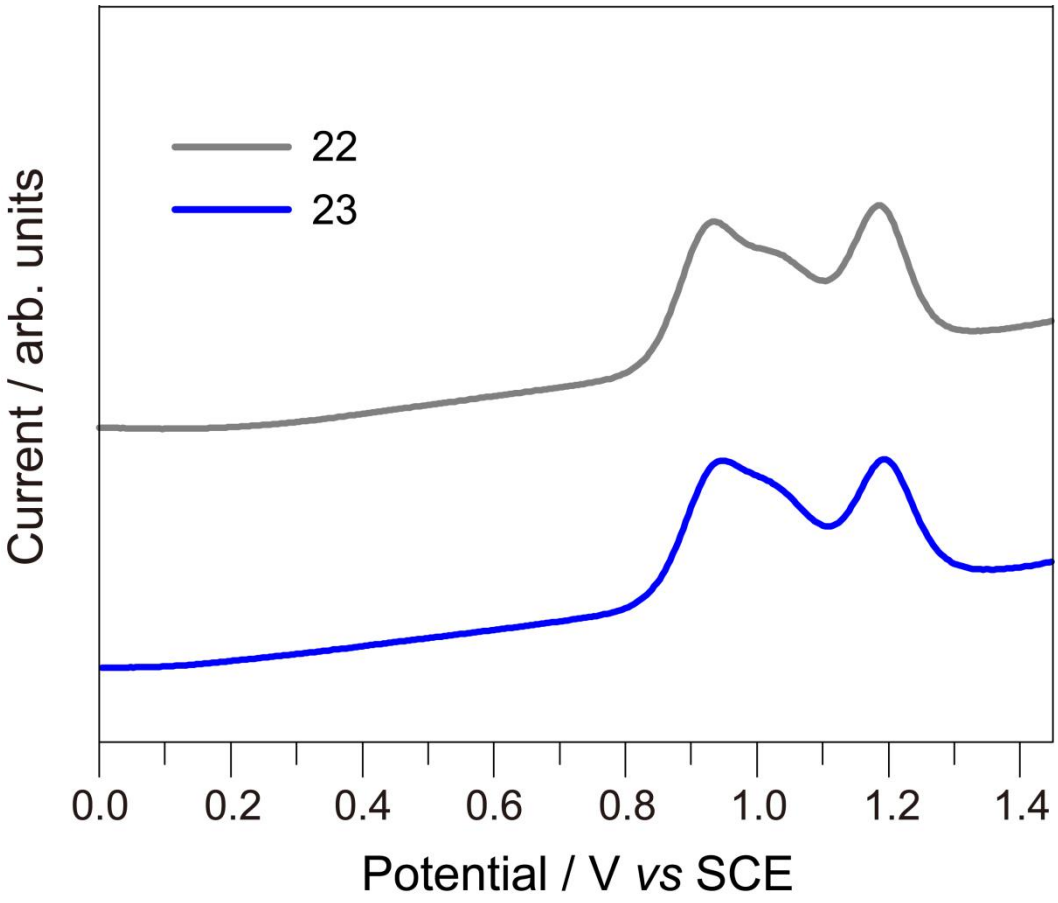


Fig. S7 Differential pulse voltammetry (DPV) analyses for compounds **22** and **23**,

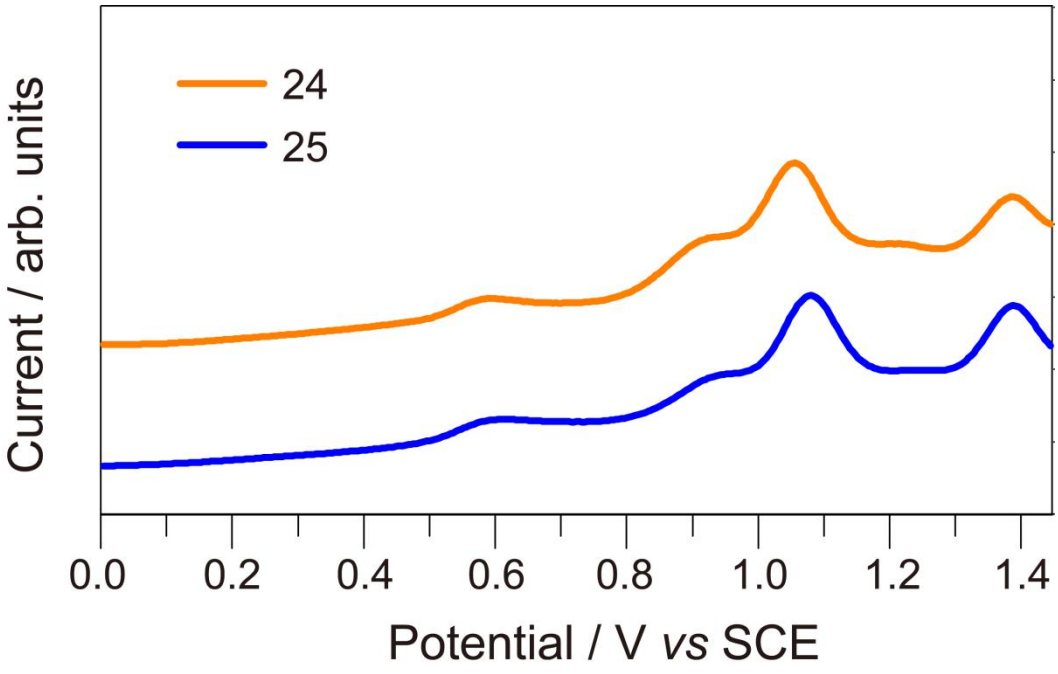


Fig. S8 Differential pulse voltammetry (DPV) analyses for compounds **24** and **25**.

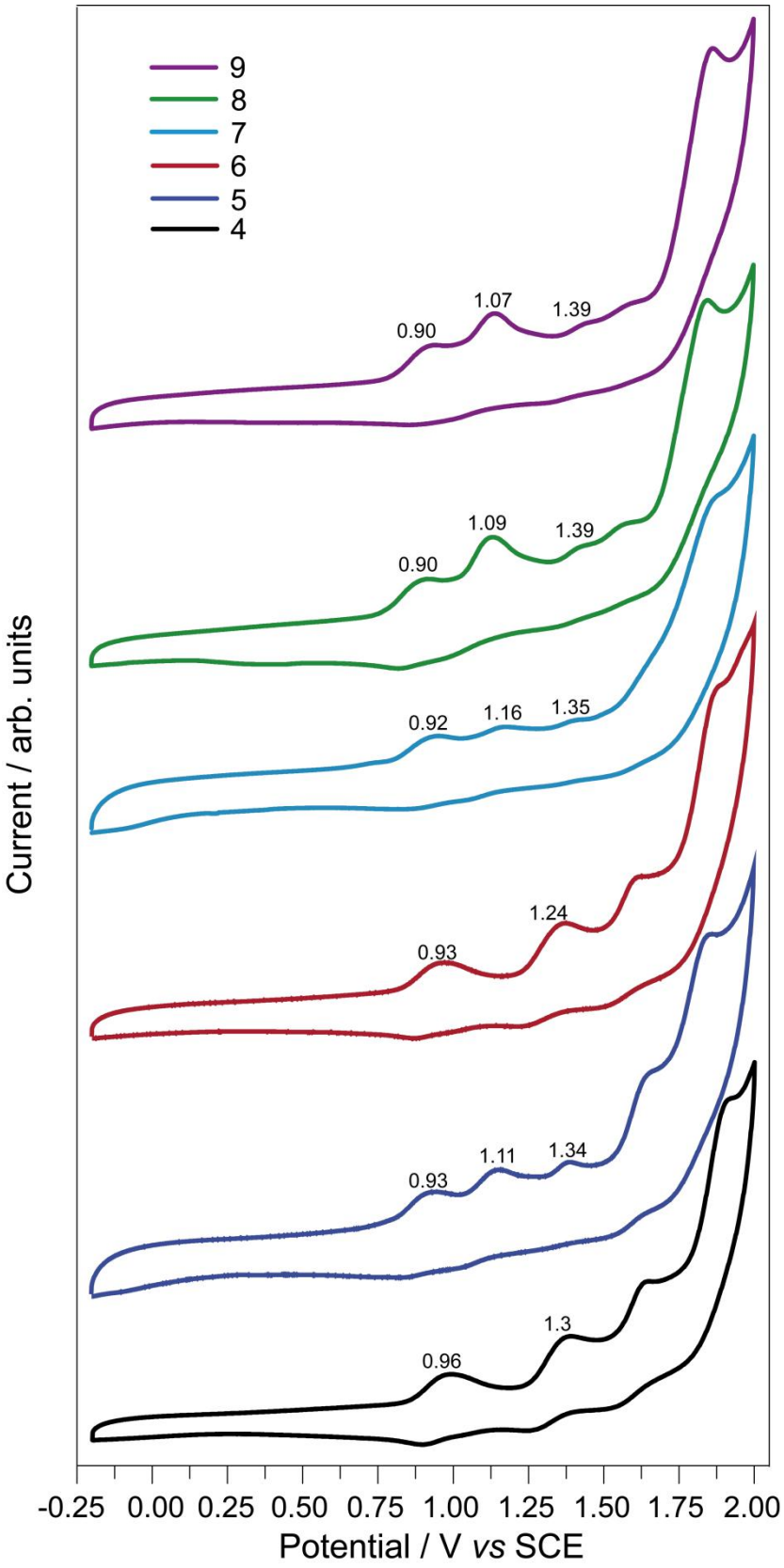


Fig S9. Cyclic voltammogram of **4-9.**

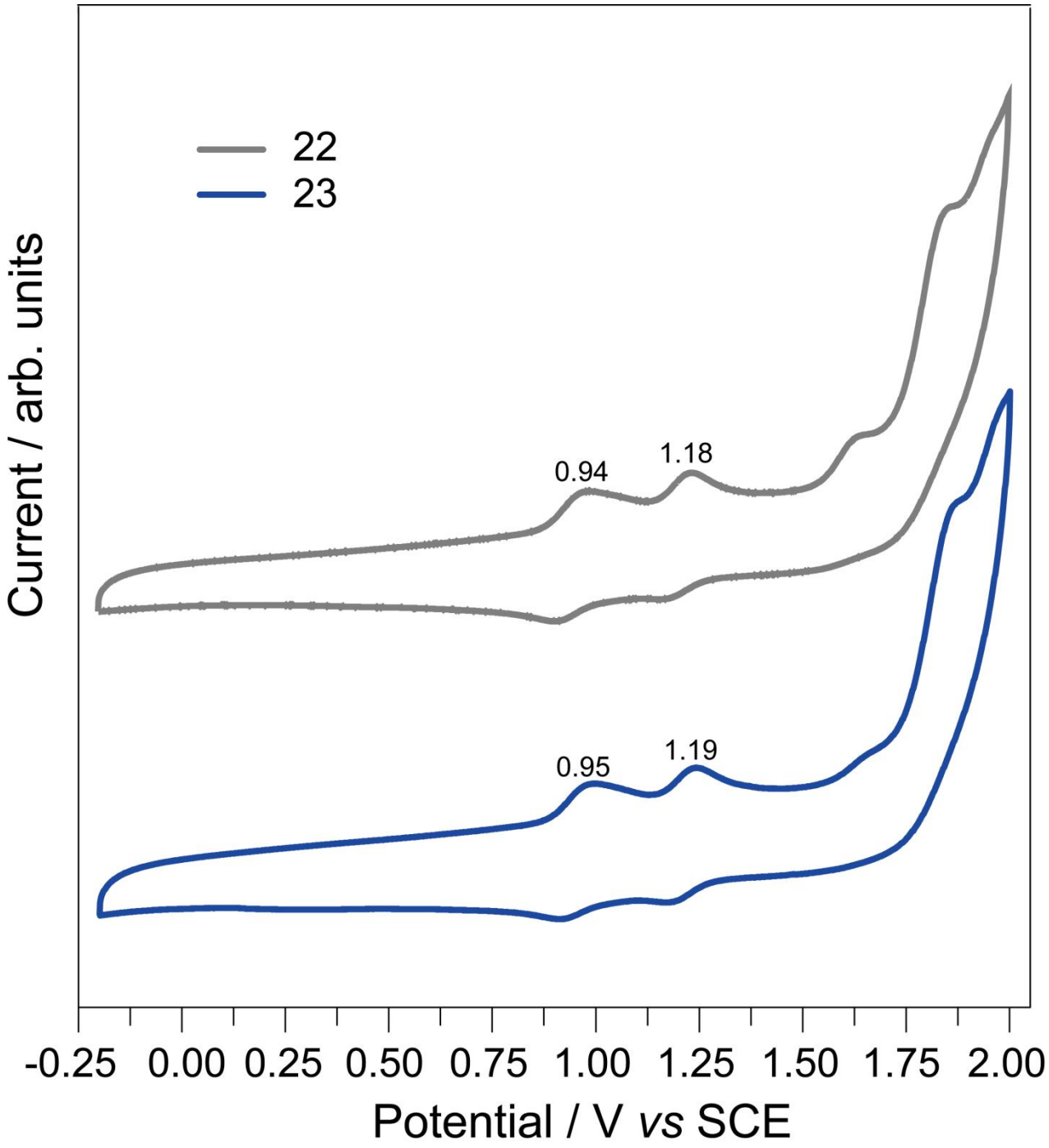


Fig S10. Cyclic voltammogram of **22** and **23.**

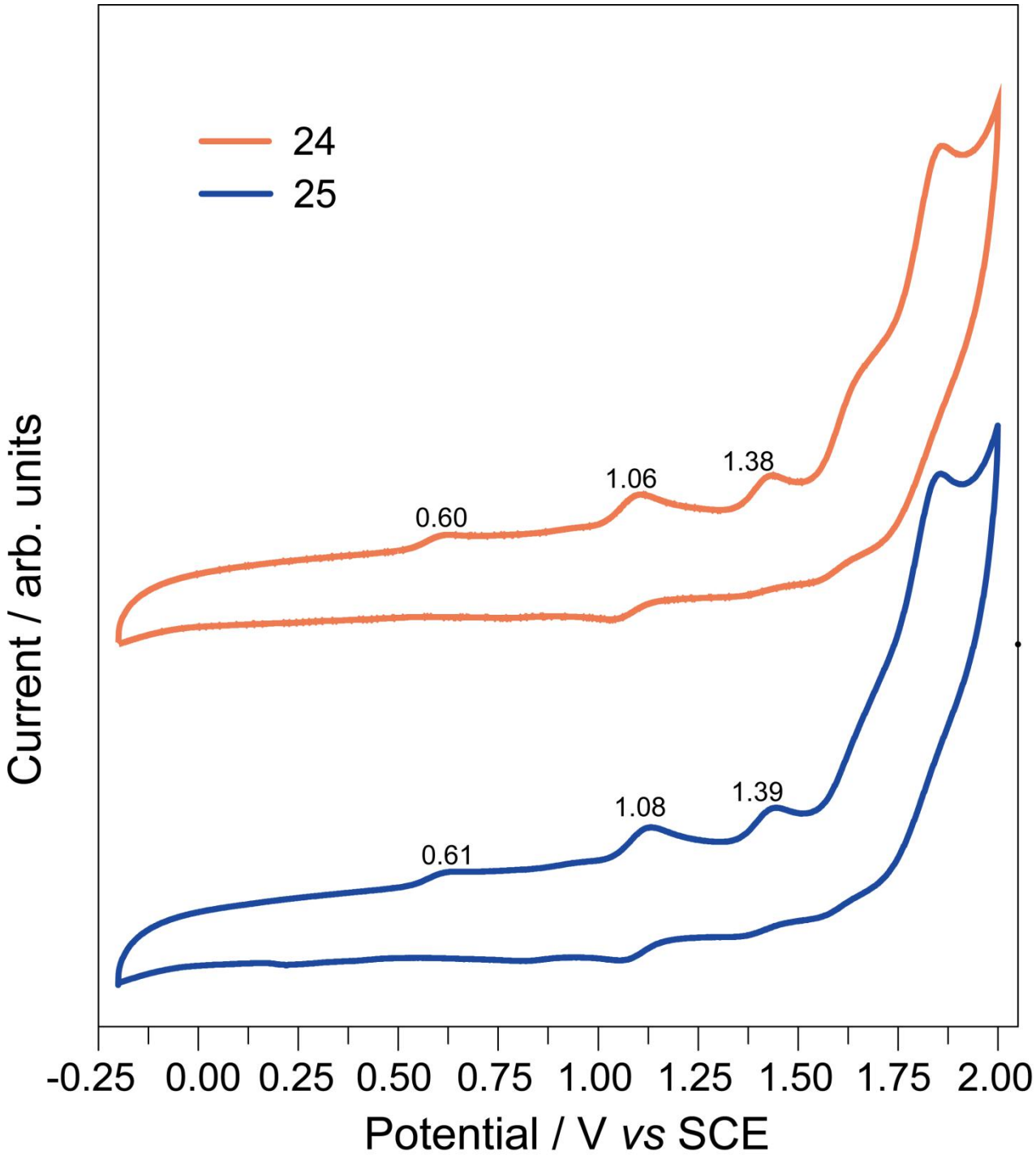
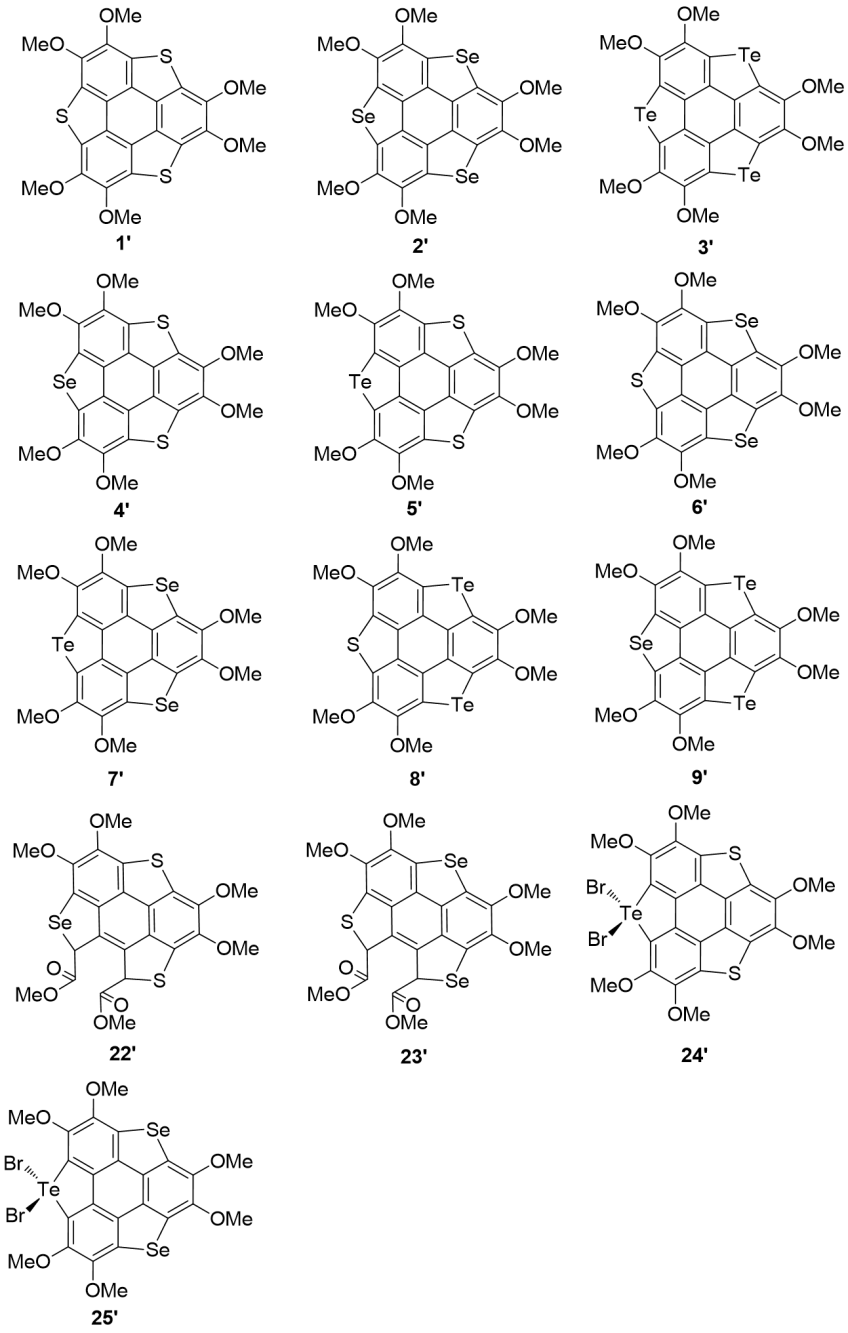


Fig S11. Cyclic voltammogram of **24** and **25.**

6 Theoretical Calculation

All the calculations were performed with Gaussian 09 software package.[S4] Geometry optimizations were carried out using B3LYP[S5]/Def2SVP[S6]/IEFPCM(dichloromethane) [S7] method. For metal-ligand complexes, we use the XRD single crystal structures as initial structures for optimization. Molecular orbital energies were calculated at B3LYP/Def2-TZVP[S10]/IEFPCM(dichloromethane) level of theory using optimized structures, and aromaticity of each ring is measured by nucleus independent chemical shift (NICS)[S8] [S9], which was computed using the gauge invariant atomic orbital (GIAO)[S10-S13] approach at the GIAO-B3LYP/Def2-TZVP/IEFPCM(chloroform) level with optimized structures. The optimized structures and molecular orbitals are displayed using Chemcraft.[S14] During the structure optimization and frontier orbital calculation, the butyl groups on **1, 2, 3, 4, 5, 6, 7, 8, 9, 22, 23, 24, and 25** were replaced by methyl groups to give the corresponding **1', 2', 3', 4'**, **5'**, **6', 7', 8', 9', 22', 23', 24', and 25'** (**Scheme S1**), because they have almost no contribution on the HOMO and LUMO orbitals and the geometry of the conjugated framework.



Scheme S1. The chemical structures of compounds **1', 2', 3', 4'**, **5'**, **6', 7', 8', 9', 22', 23', 24',** and **25'.**

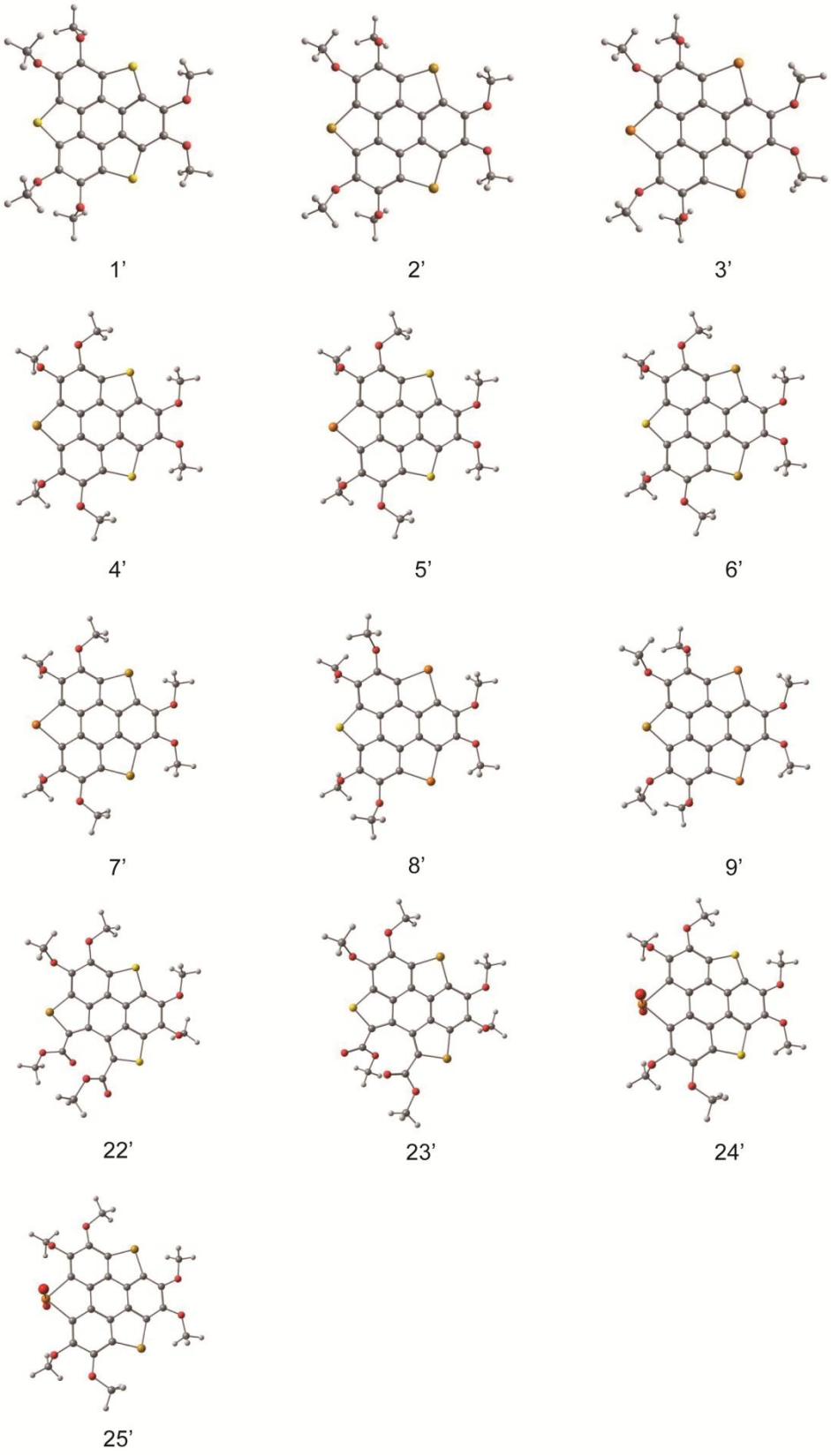


Fig S12. Optimized structures of **1’, 2’, 3’, 4’**, **5’**, **6’, 7’, 8’, 9’, 22’, 23’, 24’,** and **25’.**

Table S7. The calculated energy level for the frontier orbitals for compound **1', 2', 3', 4'**, **5'**, **6', 7', 8', 9', 22', 23', 24',** and **25'.**

compounds	Energy levels / eV				
	HOMO-1	HOMO	LUMO	LUMO+1	E_g[a]
1'	-5.64	-5.37	-1.49	-1.40	3.88
2'	-5.58	-5.31	-1.39	-1.36	3.92
3'	-5.42	-5.26	-1.36	-1.34	3.90
4'	-5.33	-5.28	-1.32	-1.21	3.94
5'	-5.27	-5.25	-1.28	-1.22	3.97
6'	-5.33	-5.25	-1.36	-1.16	3.89
7'	-5.25	-5.22	-1.28	-1.20	3.94
8'	-5.44	-5.24	-1.39	-1.34	3.95
9'	-5.44	-5.27	-1.37	-1.33	3.90
22'	-5.94	-5.47	-2.81	-1.21	2.66
23'	-5.88	-5.46	-2.81	-1.25	2.65
24'	-5.67	-5.50	-2.82	-2.12	2.68
25'	-5.65	-5.46	-2.82	-2.07	2.64

[a]$Eg = E_{LUMO} - E_{HOMO}$

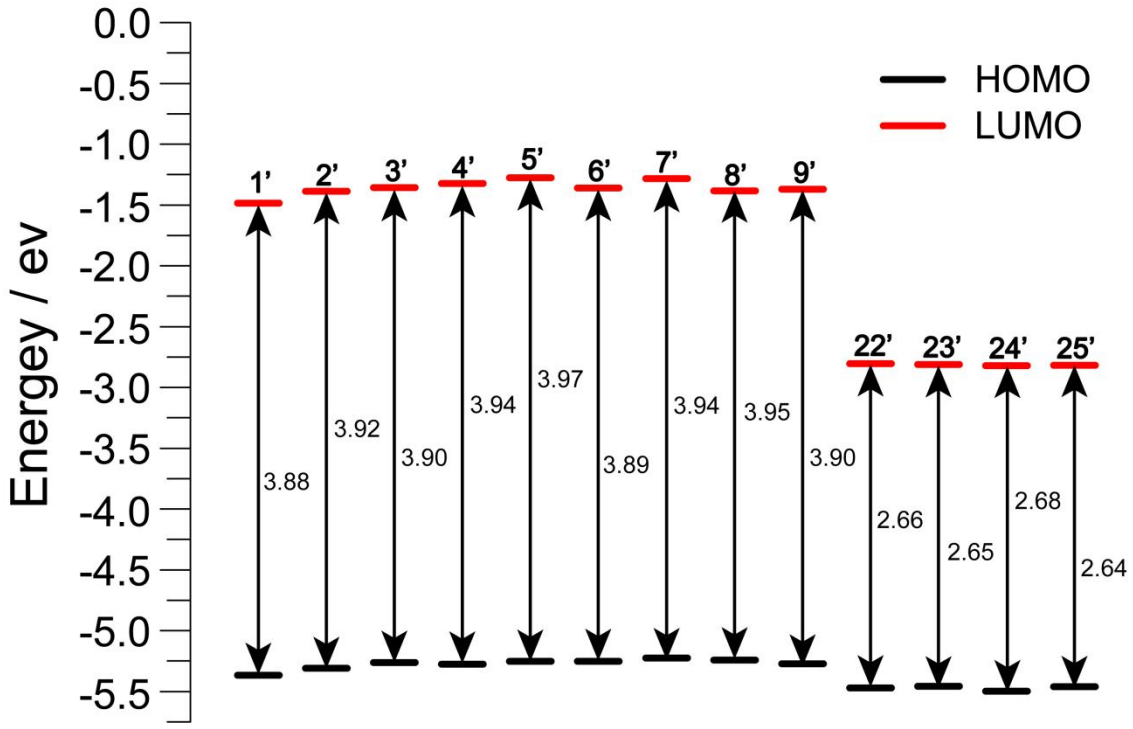


Fig S13. Schematic plot of HOMO–LUMO levels of compounds **1', 2', 3', 4'**, **5'**, **6', 7', 8', 9', 22', 23', 24',** and **25'.**

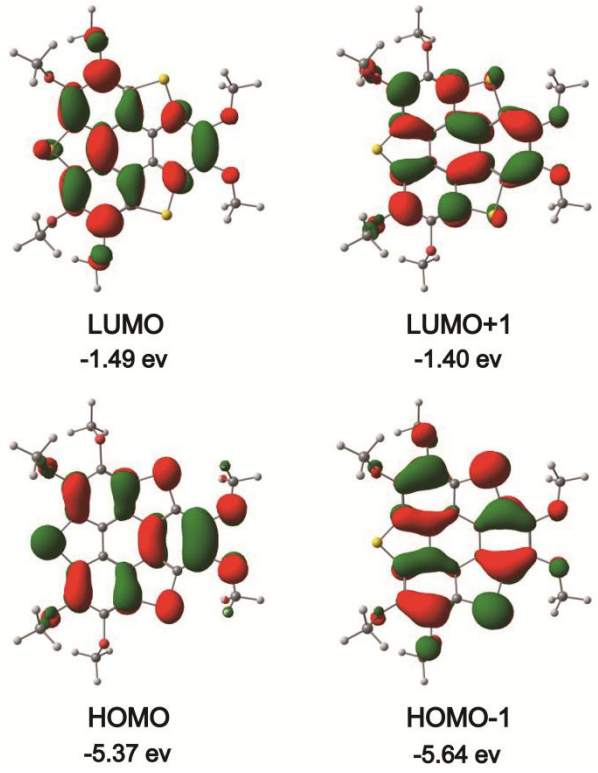


Fig S14. Calculated molecular orbitals of compound **1'**.

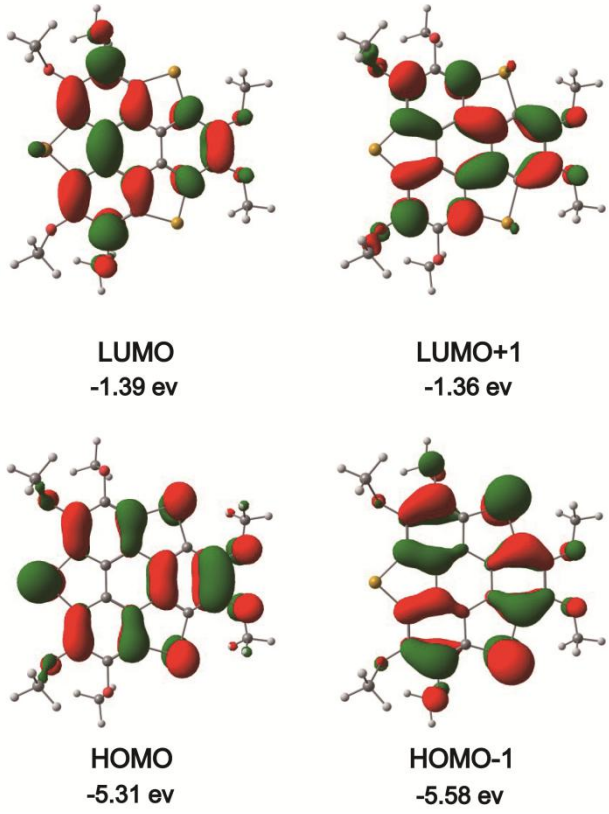


Fig S15. Calculated molecular orbitals of compound **2'**.

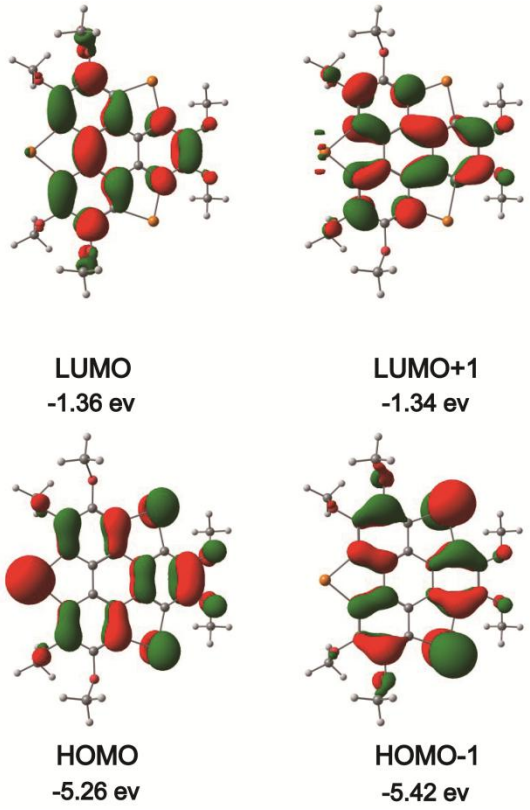


Fig S16. Calculated molecular orbitals of compound **3'**.

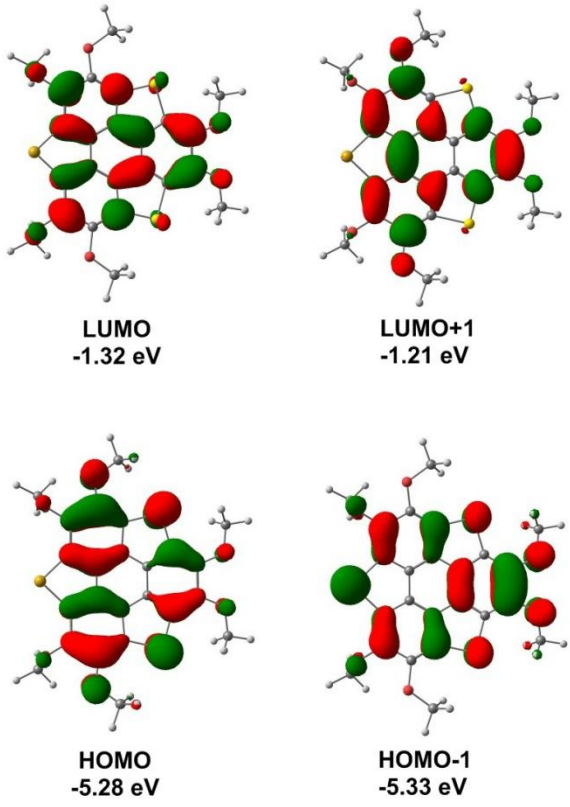


Fig S17. Calculated molecular orbitals of compound **4'**.

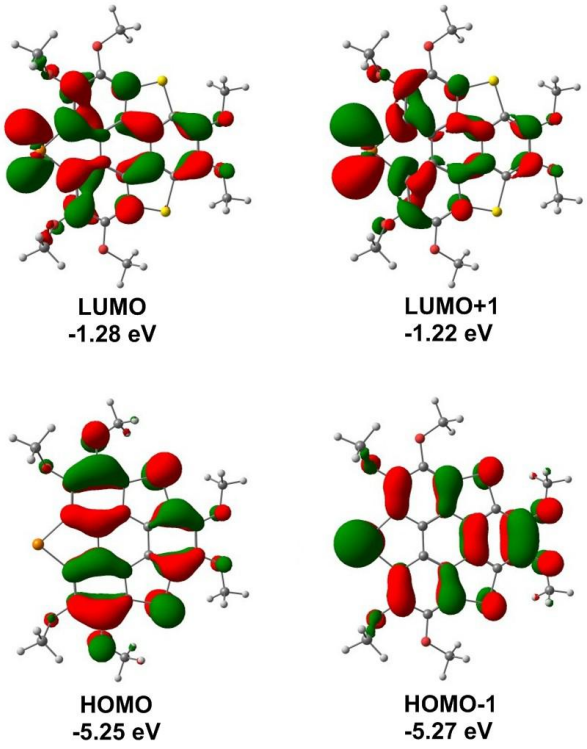


Fig S18. Calculated molecular orbitals of compound **5'**.

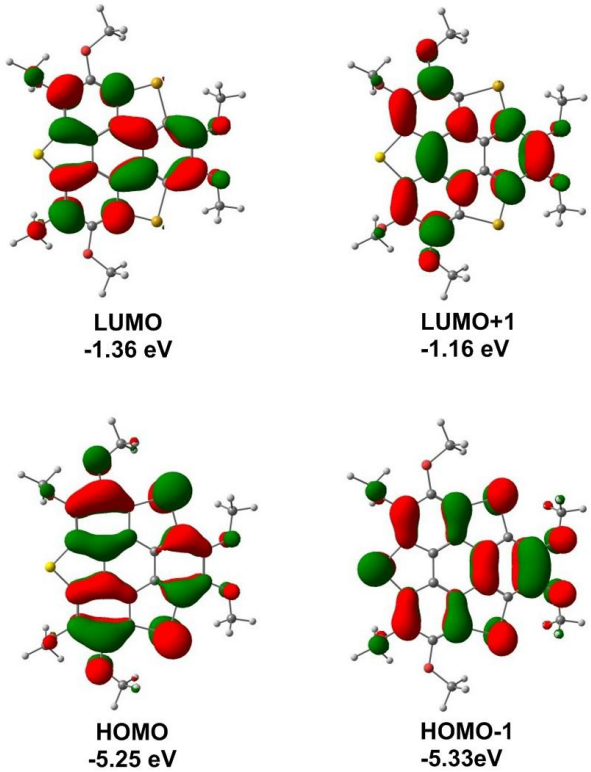


Fig S19. Calculated molecular orbitals of compound **6'**.

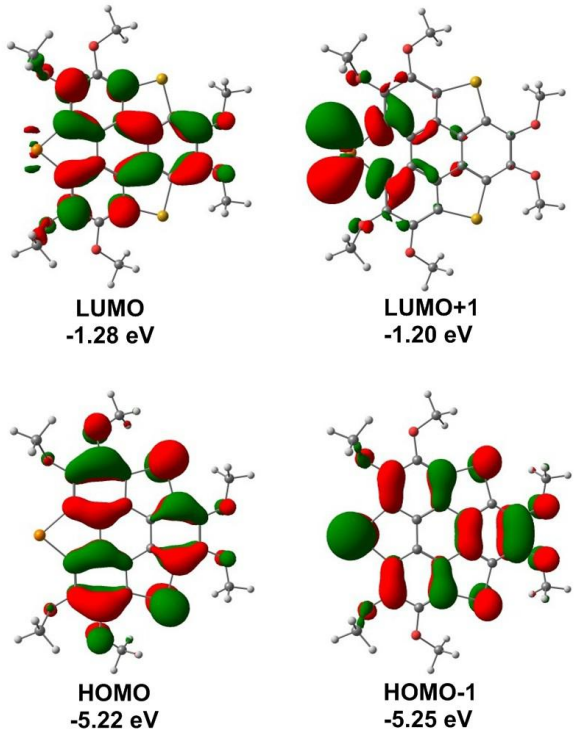


Fig S20. Calculated molecular orbitals of compound **7'**

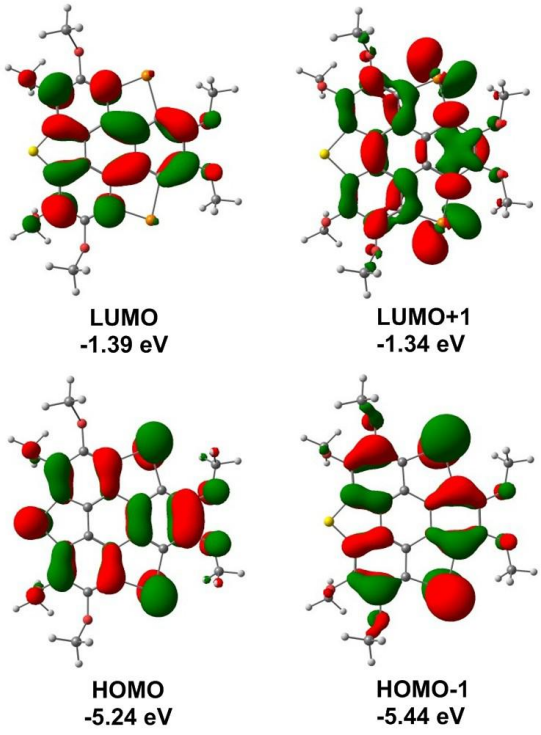


Fig S21. Calculated molecular orbitals of compound **8'**

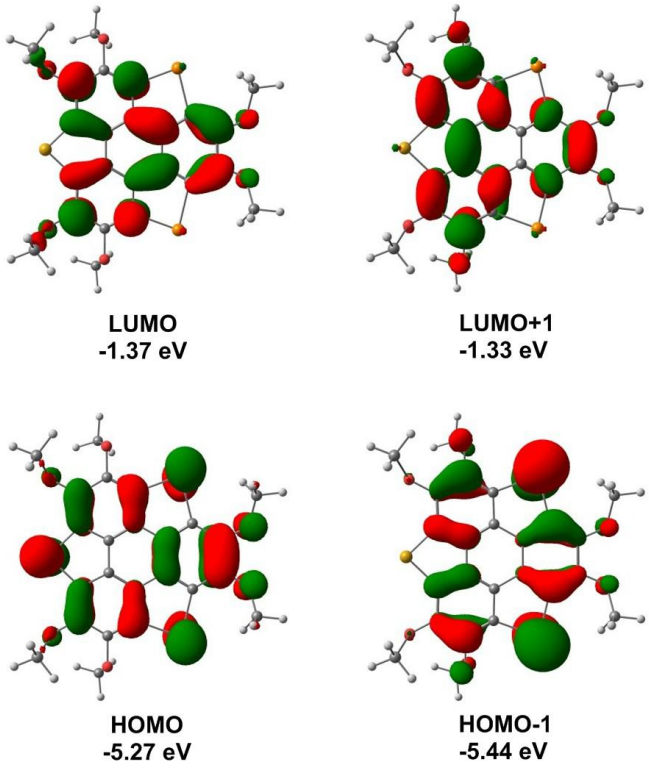


Fig S22. Calculated molecular orbitals of compound **9'**

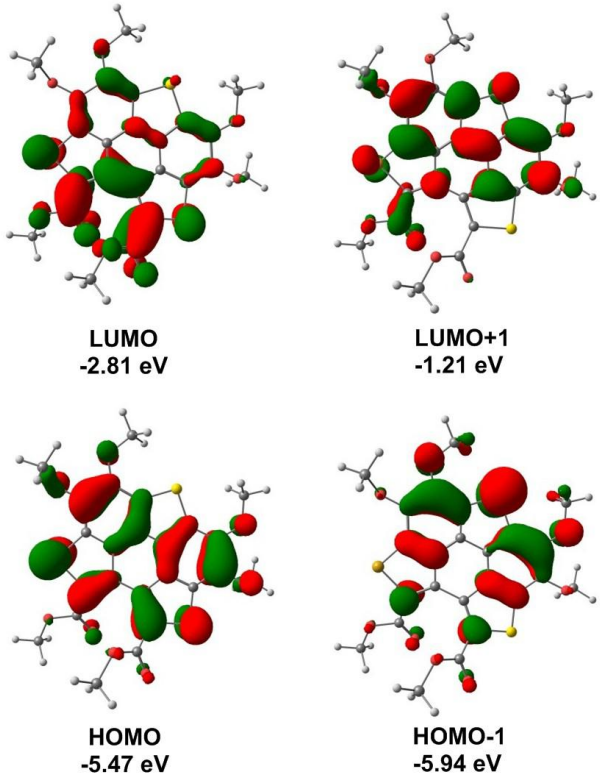


Fig S23. Calculated molecular orbitals of compound **22'**

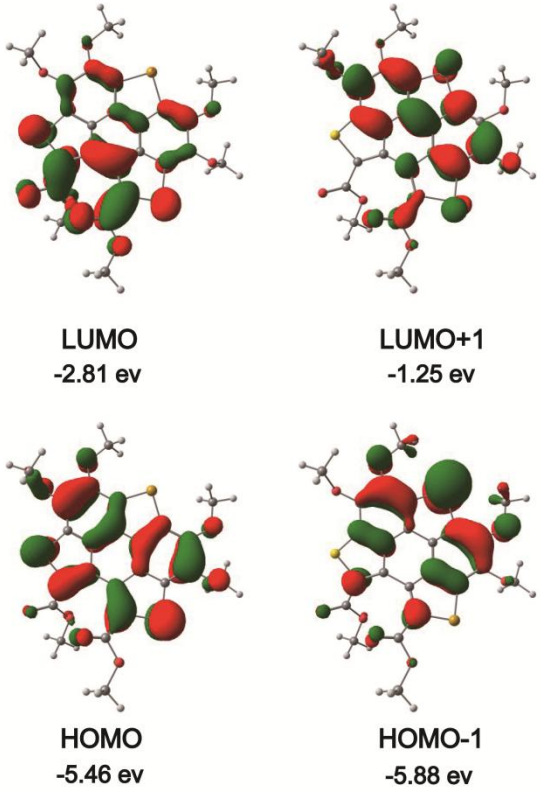


Fig S24. Calculated molecular orbitals of compound **23'**

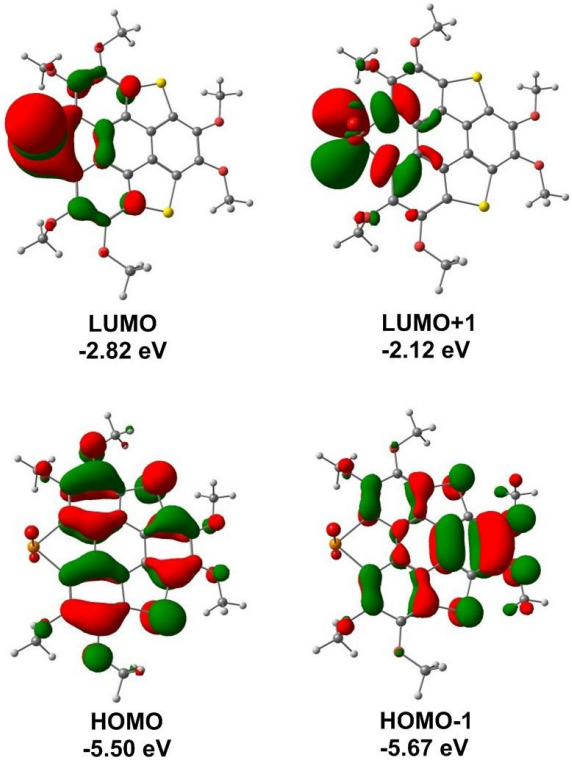


Fig S25. Calculated molecular orbitals of compound **24'**

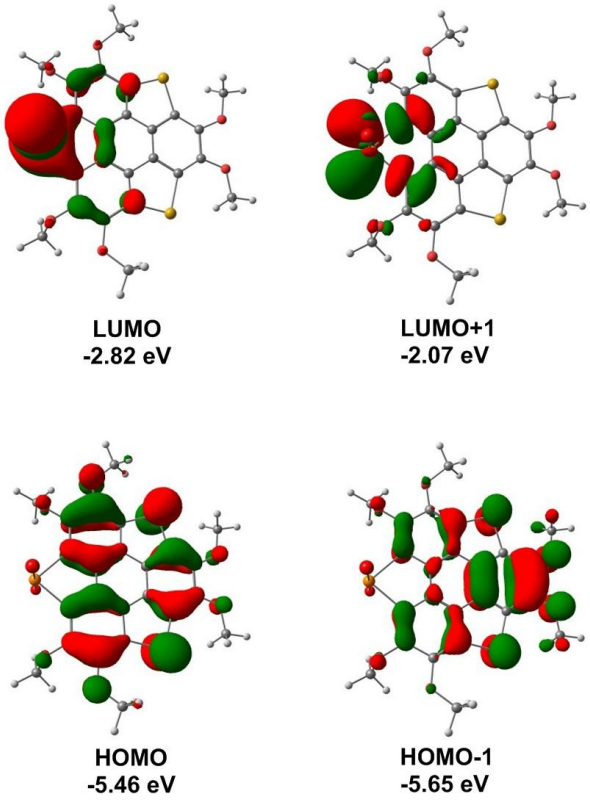
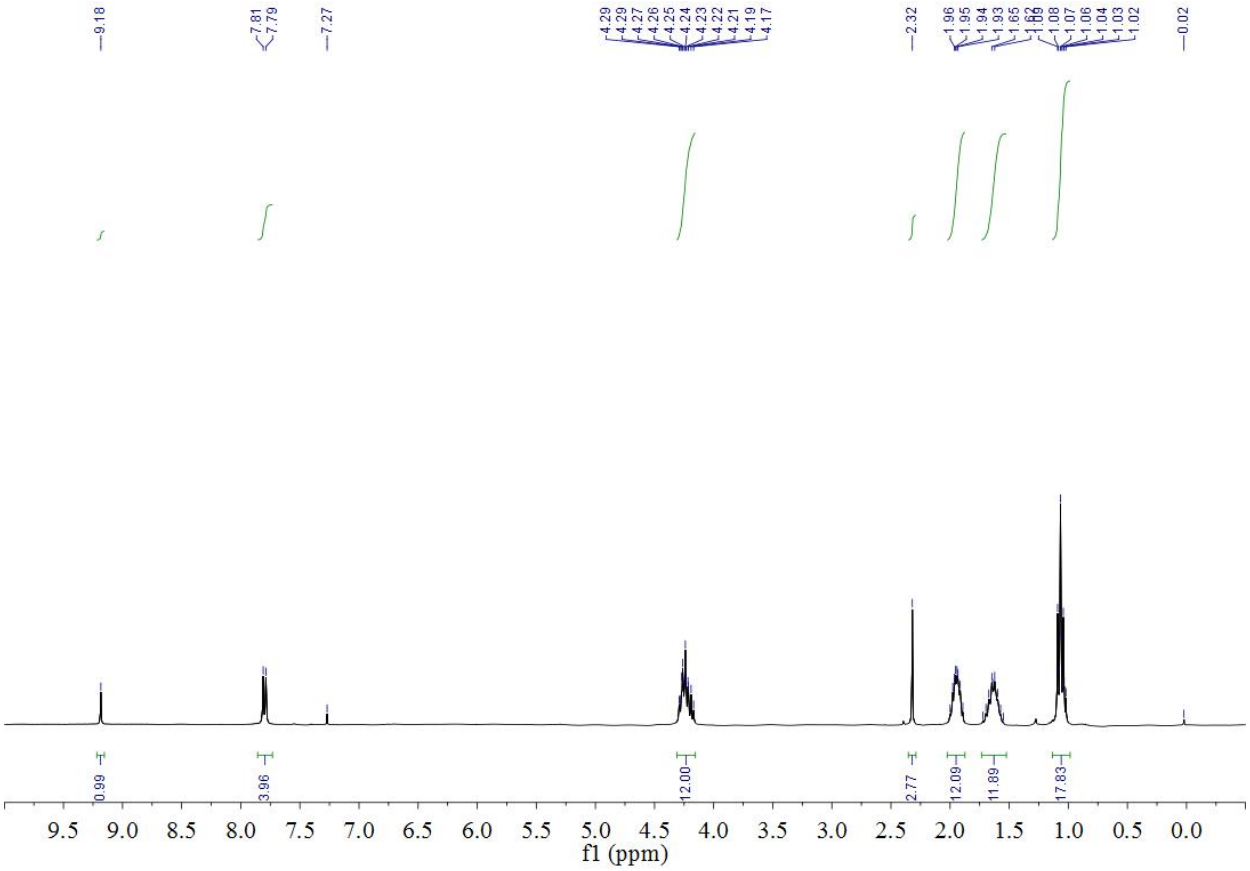
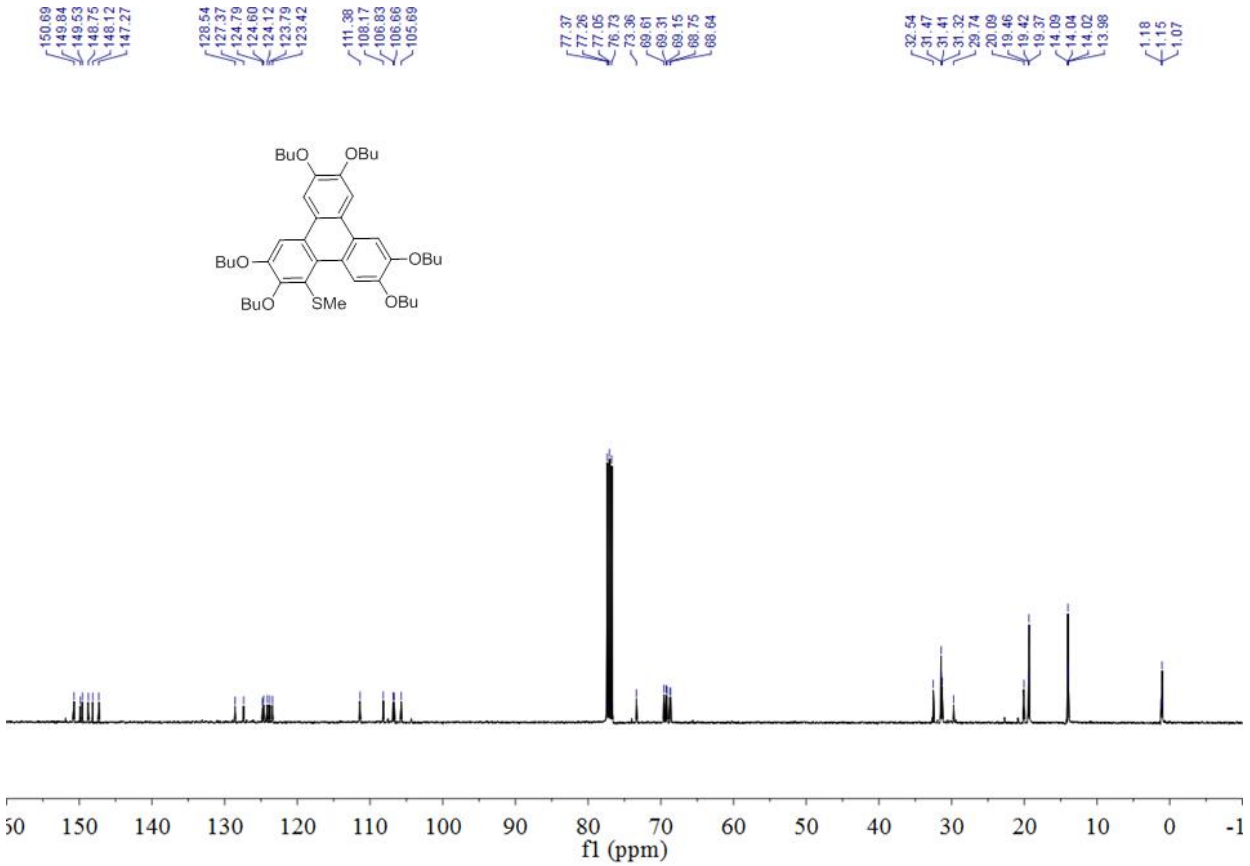
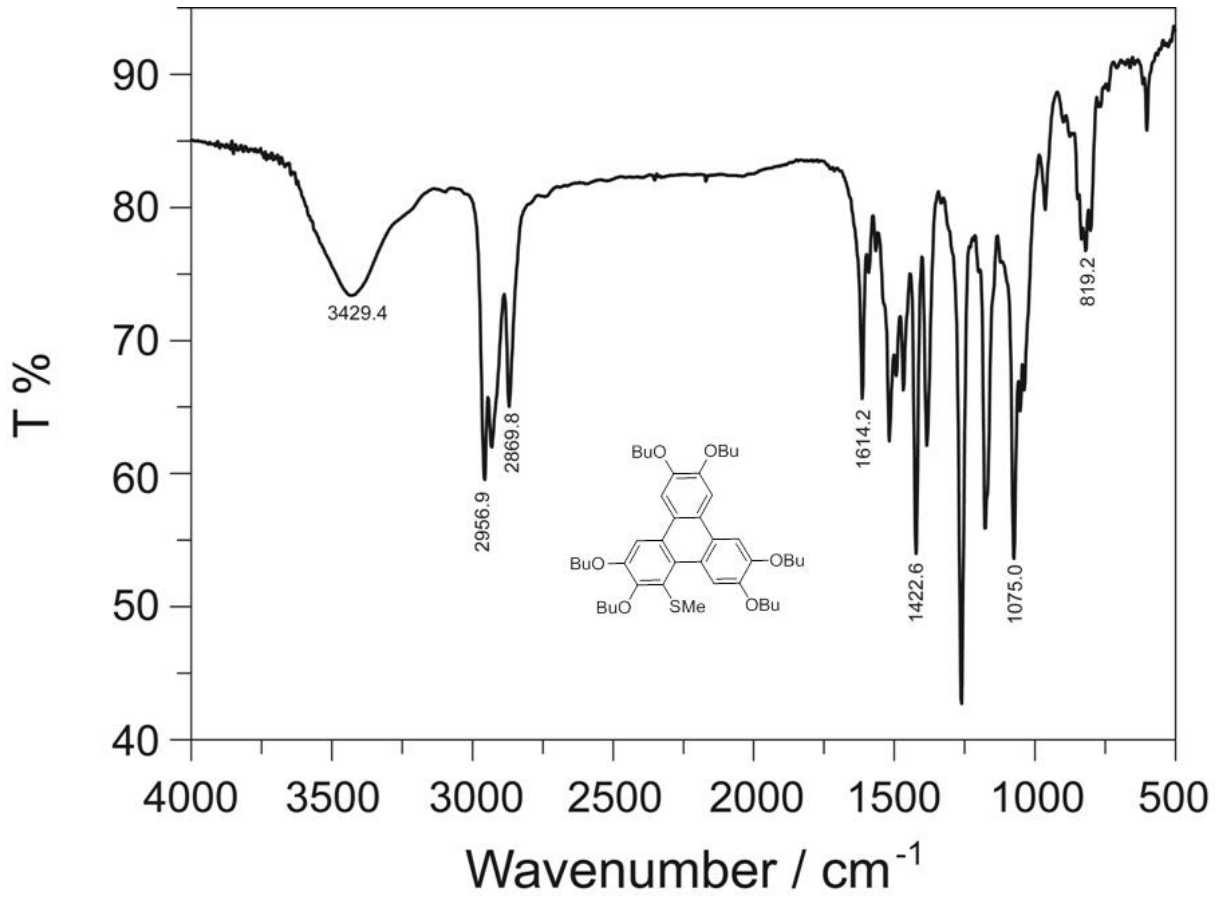


Fig S26. Calculated molecular orbitals of compound **25'**

7. ^{1}H NMR, ^{13}C NMR and IR Spectra of products






T %
Wavenumber / cm-1
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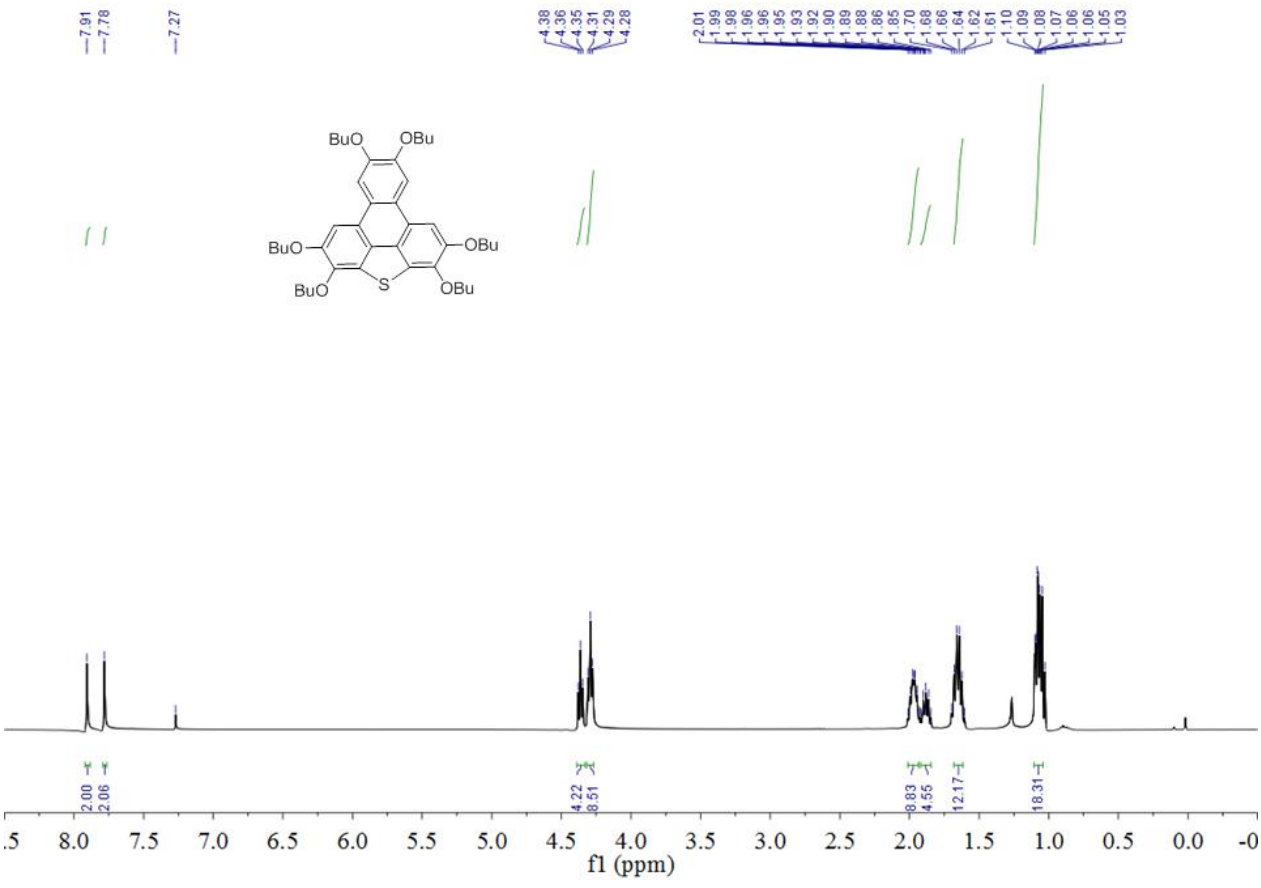
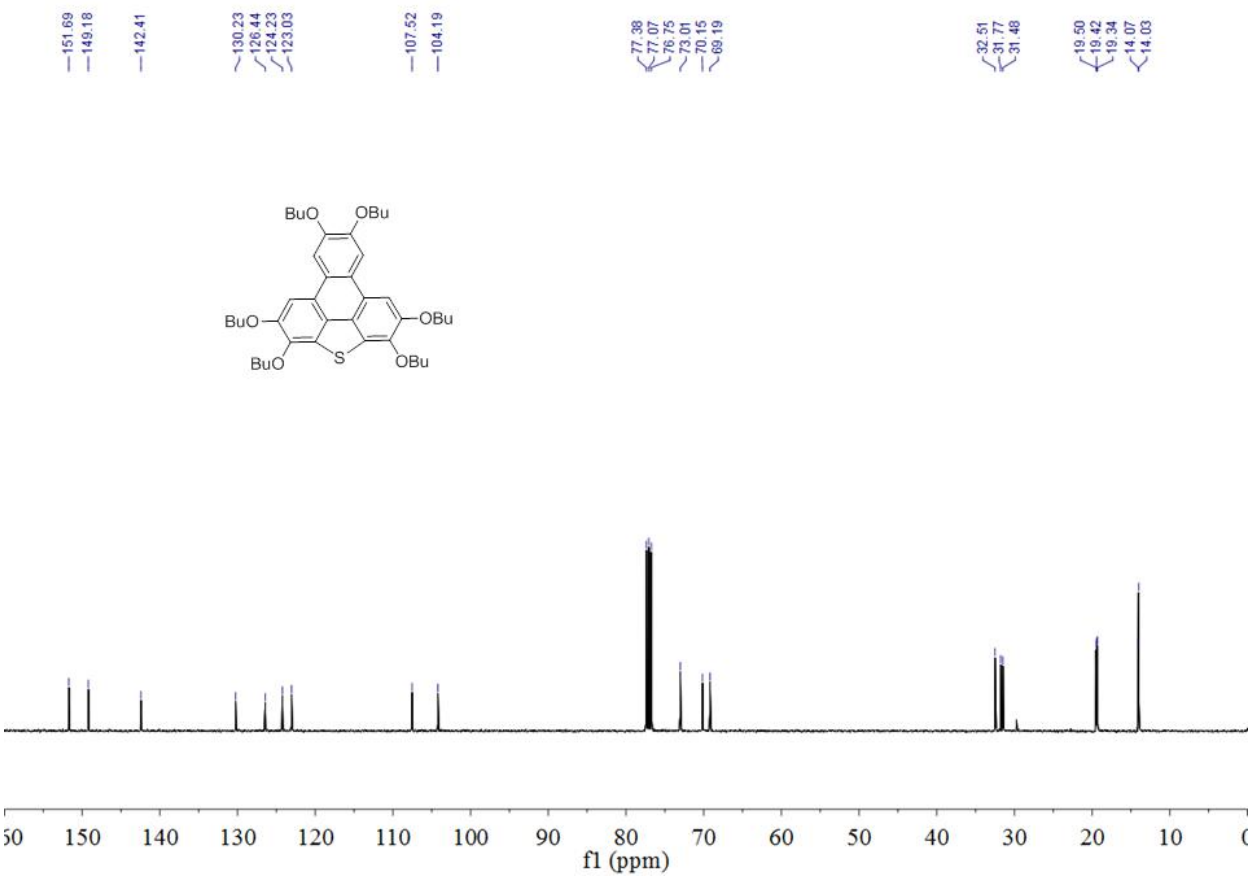
2869.8
1614.2
1422.6
1075.0
819.2
BuO
OBu
SMe


f1 (ppm)
BuO
OBu
S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149.18
142.41
130.23
126.44
124.23
123.03
107.52
104.19
77.38
77.07
76.75
73.01
70.15
69.19
32.51
31.77
31.48
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14.03
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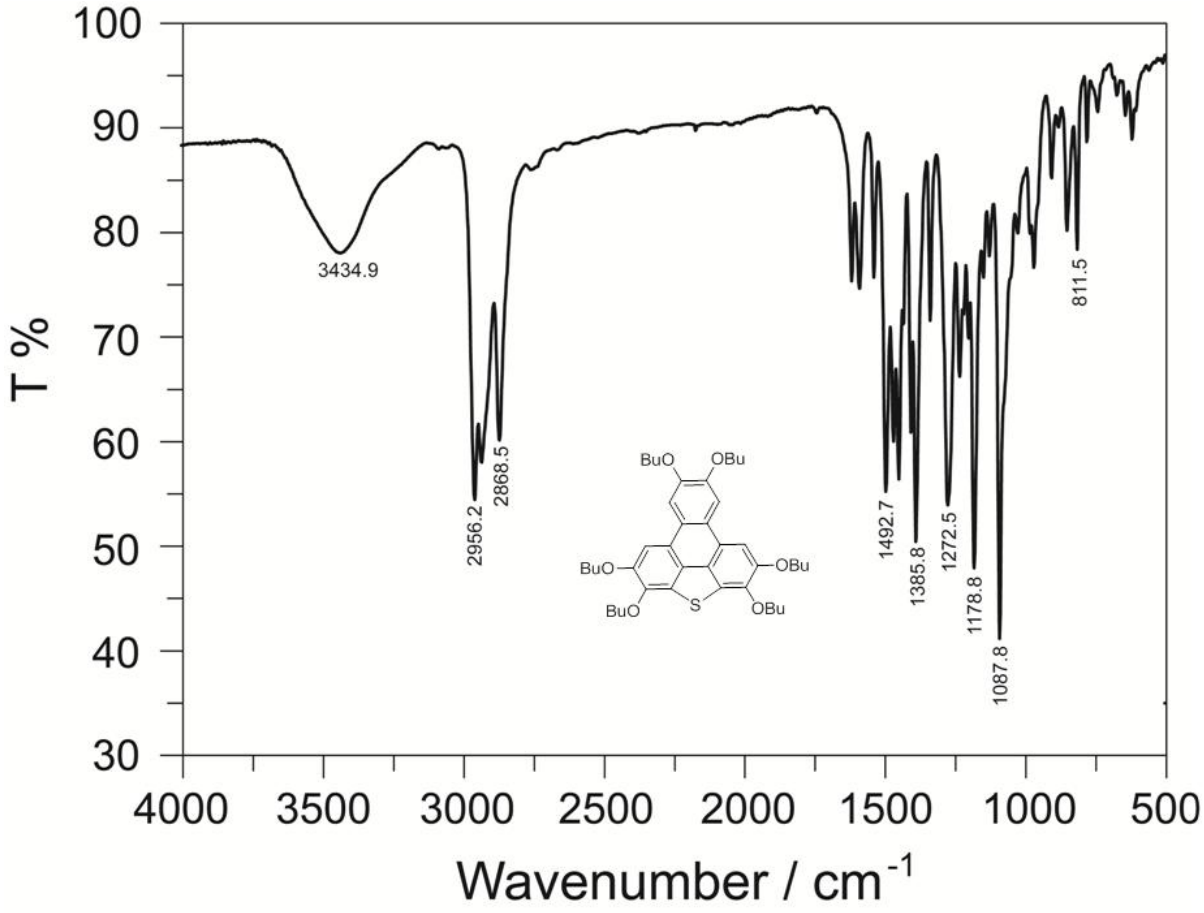
OBu
BuO
OBu
BuO
S
OBu
f1 (ppm)


T %
Wavenumber / cm-1
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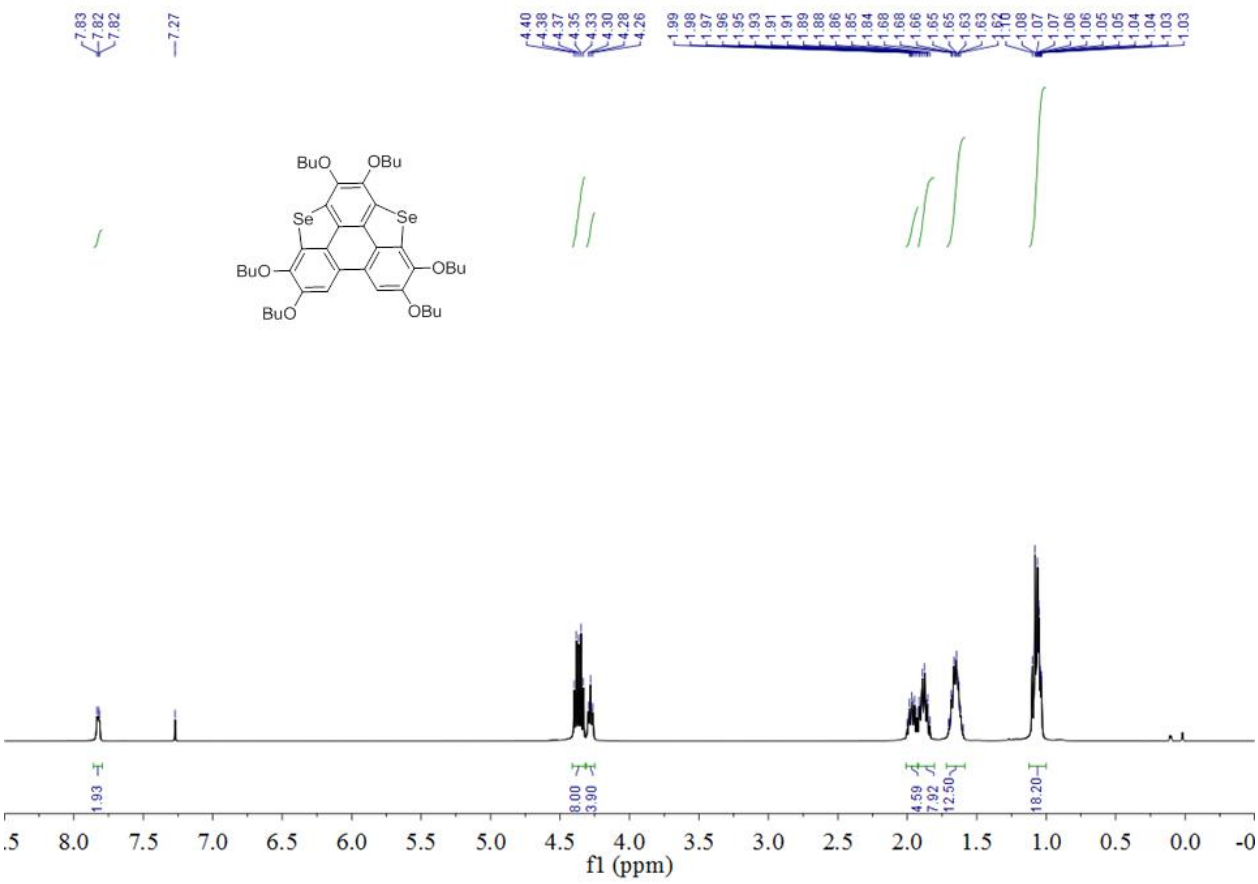
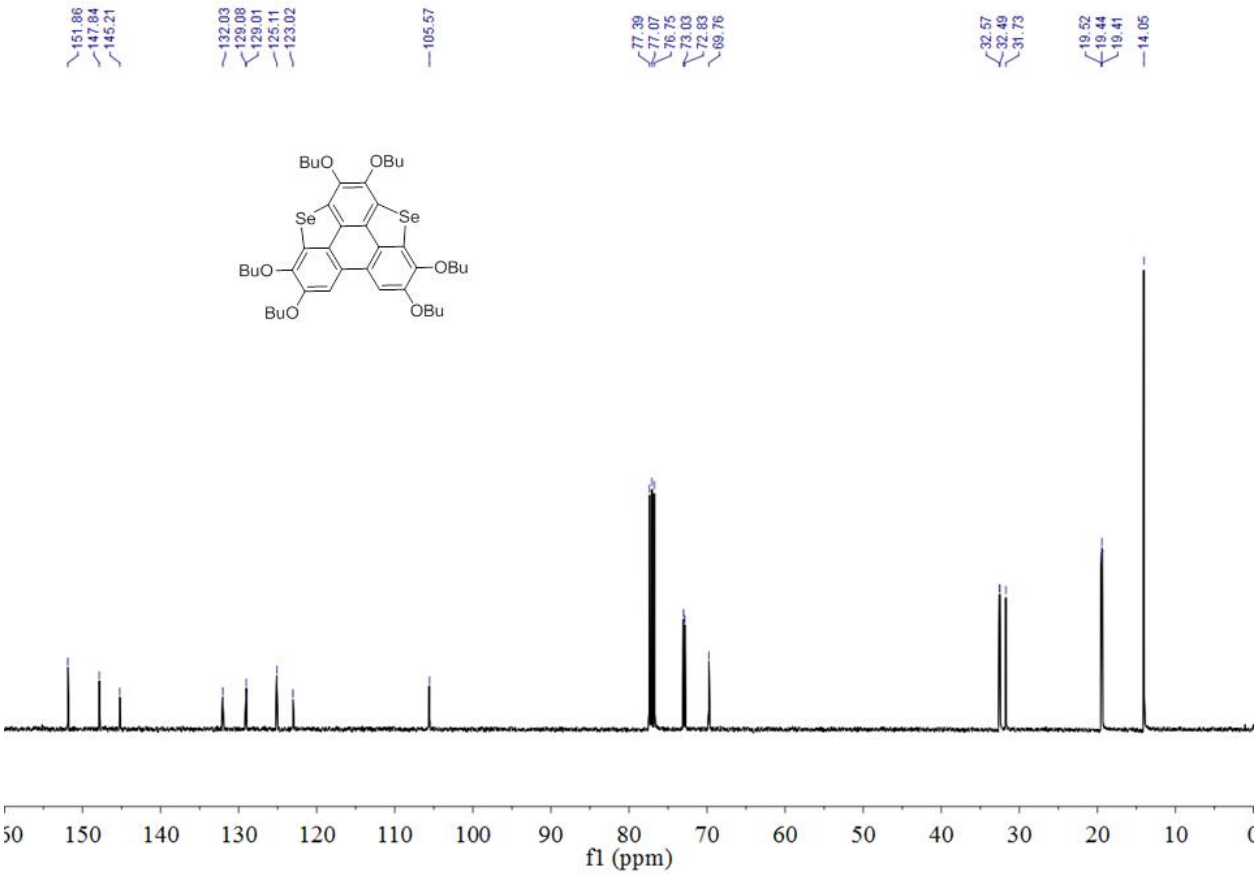
2868.5
1492.7
1385.8
1272.5
1178.8
1087.8
811.5
BuO
OBu
BuO
OBu
BuO
S
OBu


7.83
7.82
7.82
7.27
4.40
4.38
4.37
4.35
4.33
4.30
4.28
4.26
1.99
1.98
1.97
1.96
1.95
1.93
1.91
1.91
1.89
1.88
1.86
1.85
1.84
1.68
1.68
1.66
1.65
1.65
1.63
1.63
1.62
1.61
1.08
1.07
1.07
1.06
1.06
1.05
1.05
1.04
1.04
1.03
1.03
BuO
OBu
Se
Se
BuO
OBu
BuO
OBu
1.93
8.00
3.90
4.59
7.92
12.50
18.20
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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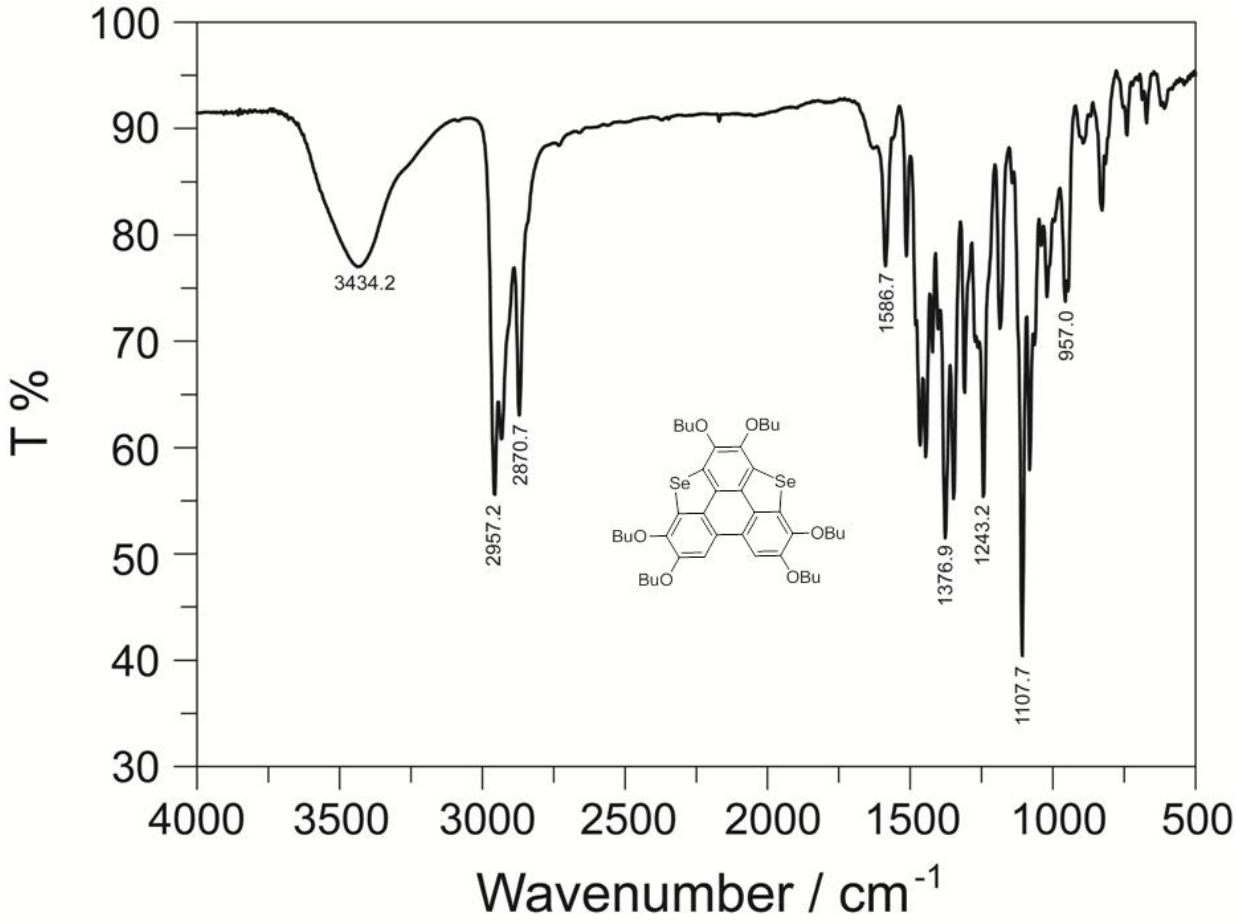
147.84
145.21
132.03
129.08
129.01
125.11
123.02
105.57
77.39
77.07
76.75
73.03
72.83
69.76
32.57
32.49
31.73
19.52
19.44
19.41
14.05
BuO
OBu
Se
Se
BuO
OBu
BuO
OBu
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


T %
Wavenumber / cm-1
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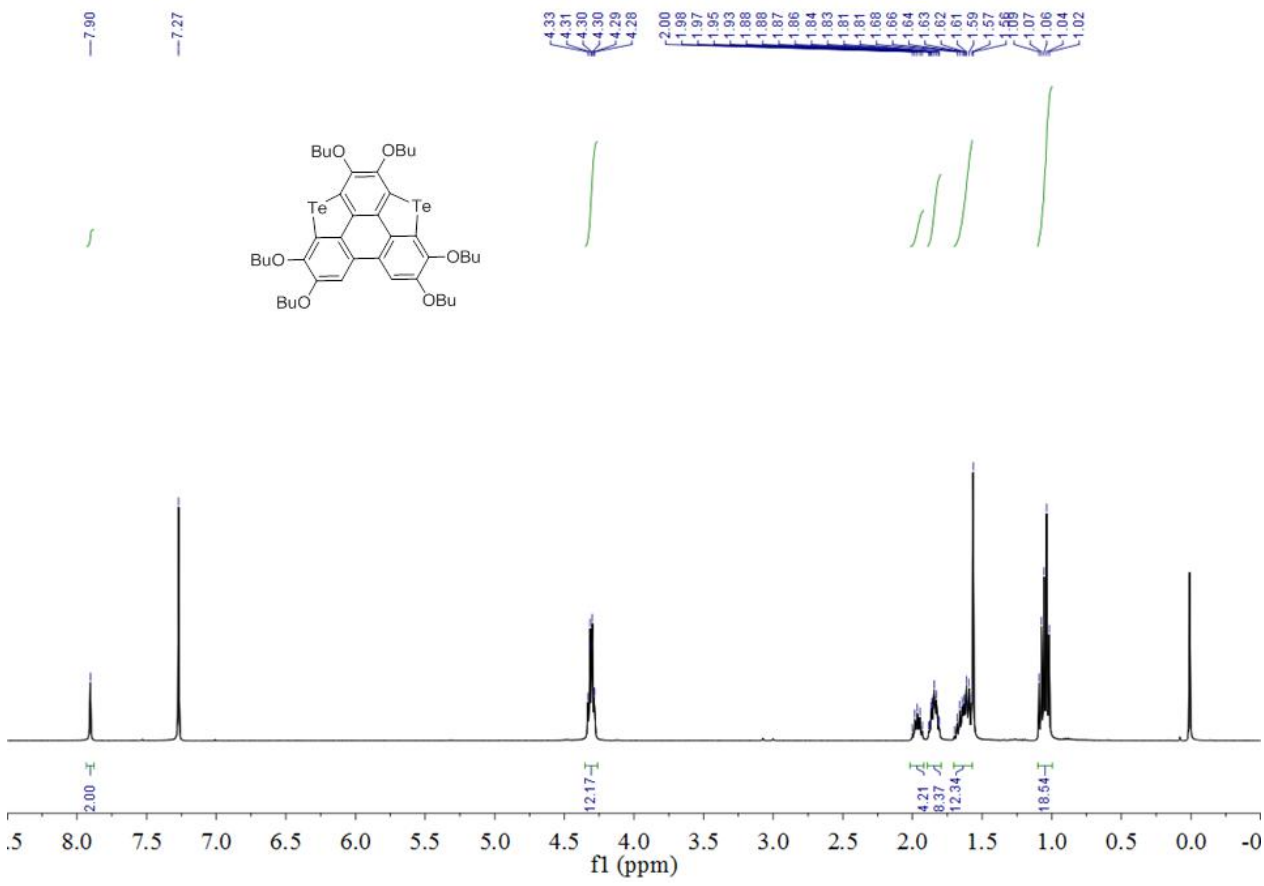
2870.7
1586.7
1376.9
1243.2
1107.7
957.0
BuO
OBu
Se
Se
BuO
OBu
BuO
OBu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4.30
4.29
4.28
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1.98
1.97
1.95
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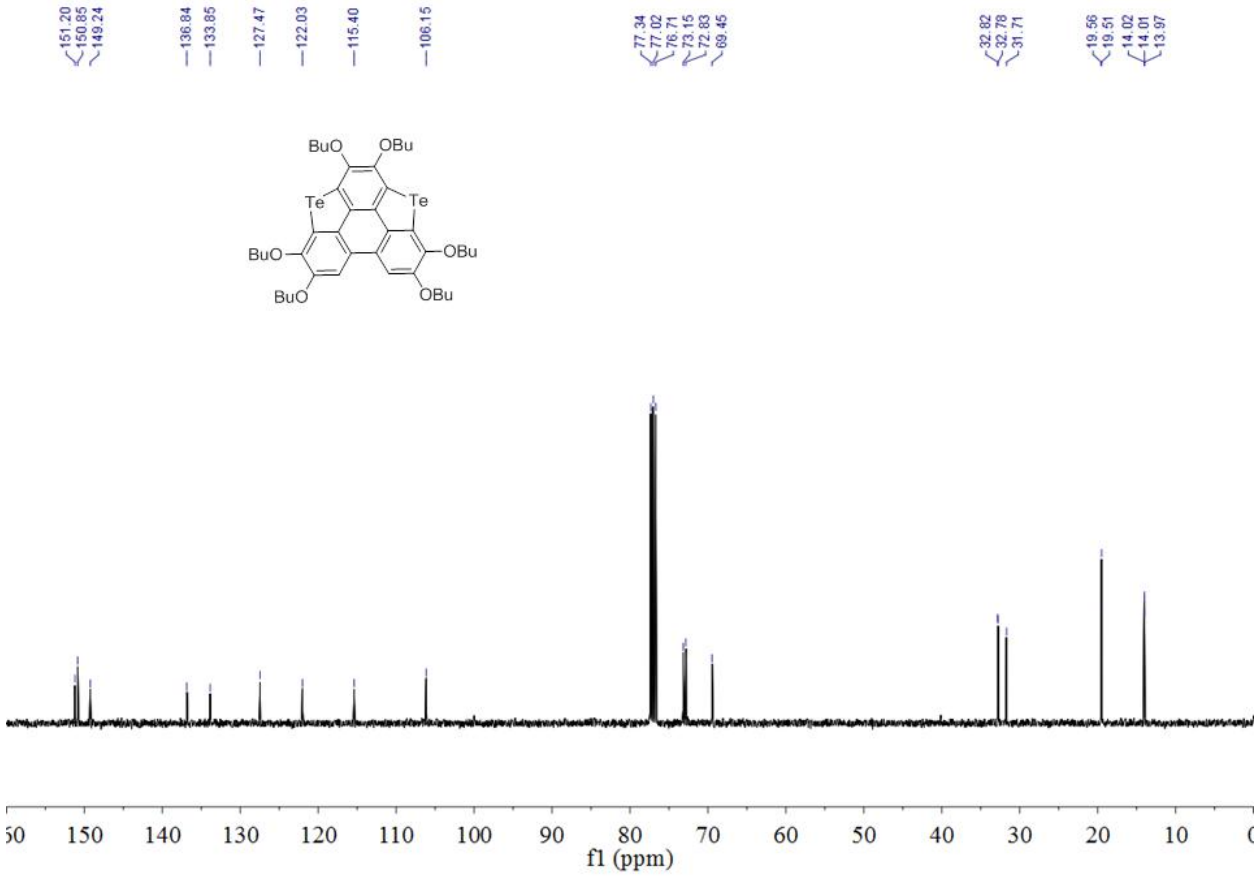
1.88
1.88
1.87
1.86
1.84
1.83
1.81
1.81
1.68
1.66
1.64
1.63
1.62
1.61
1.59
1.57
1.07
1.06
1.04
1.02
BuO
OBu
Te
Te
BuO
OBu
BuO
OBu
2.00
12.17
4.21
8.37
12.34
18.54
f1 (ppm)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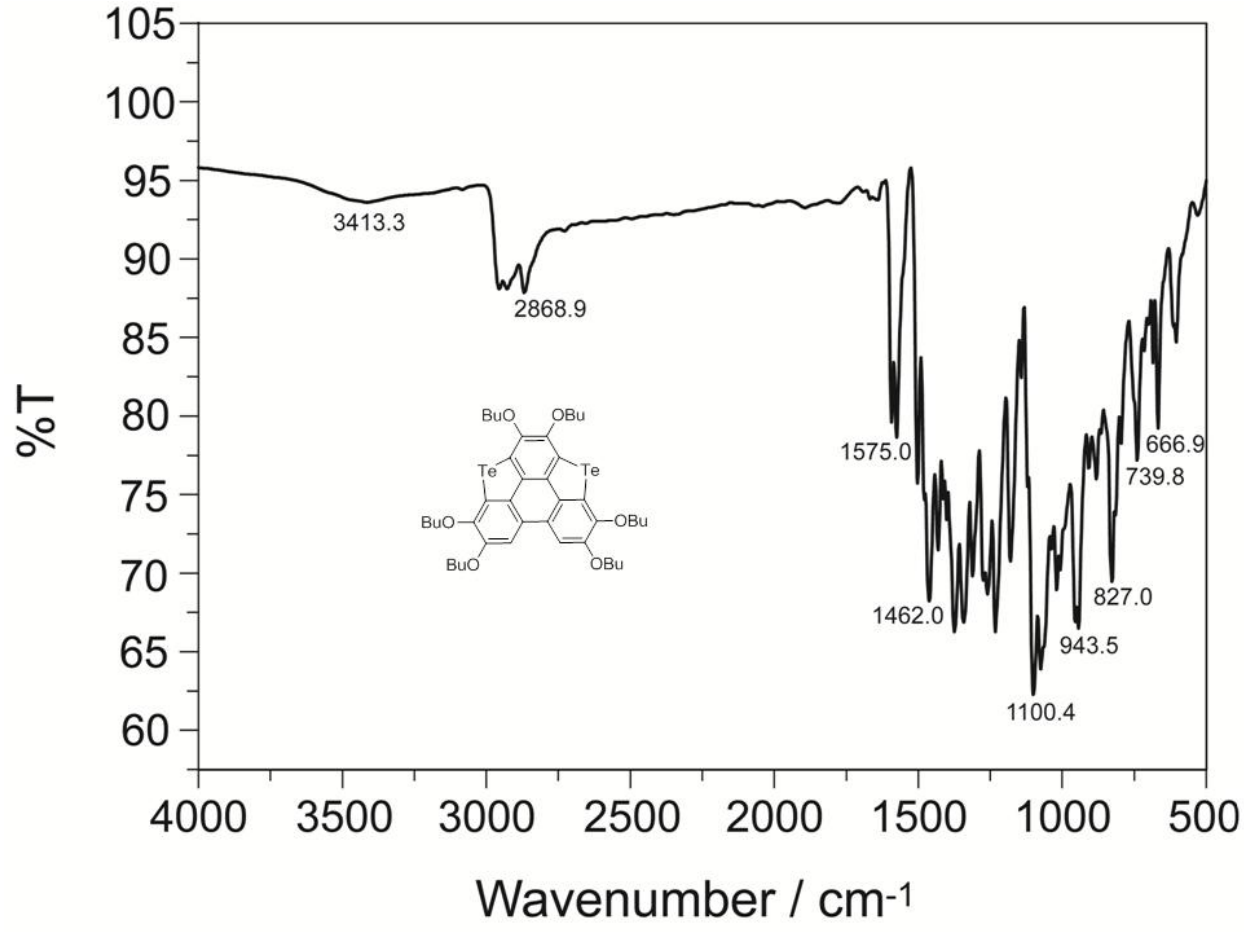
127.47
122.03
115.40
106.15
77.34
77.02
76.71
73.15
72.83
69.45
32.82
32.78
31.71
19.56
19.51
14.02
14.01
13.97
BuO
OBu
Te
Te
BuO
OBu
BuO
OBu
f1 (ppm)


%T
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1462.0
1100.4
943.5
827.0
739.8
666.9
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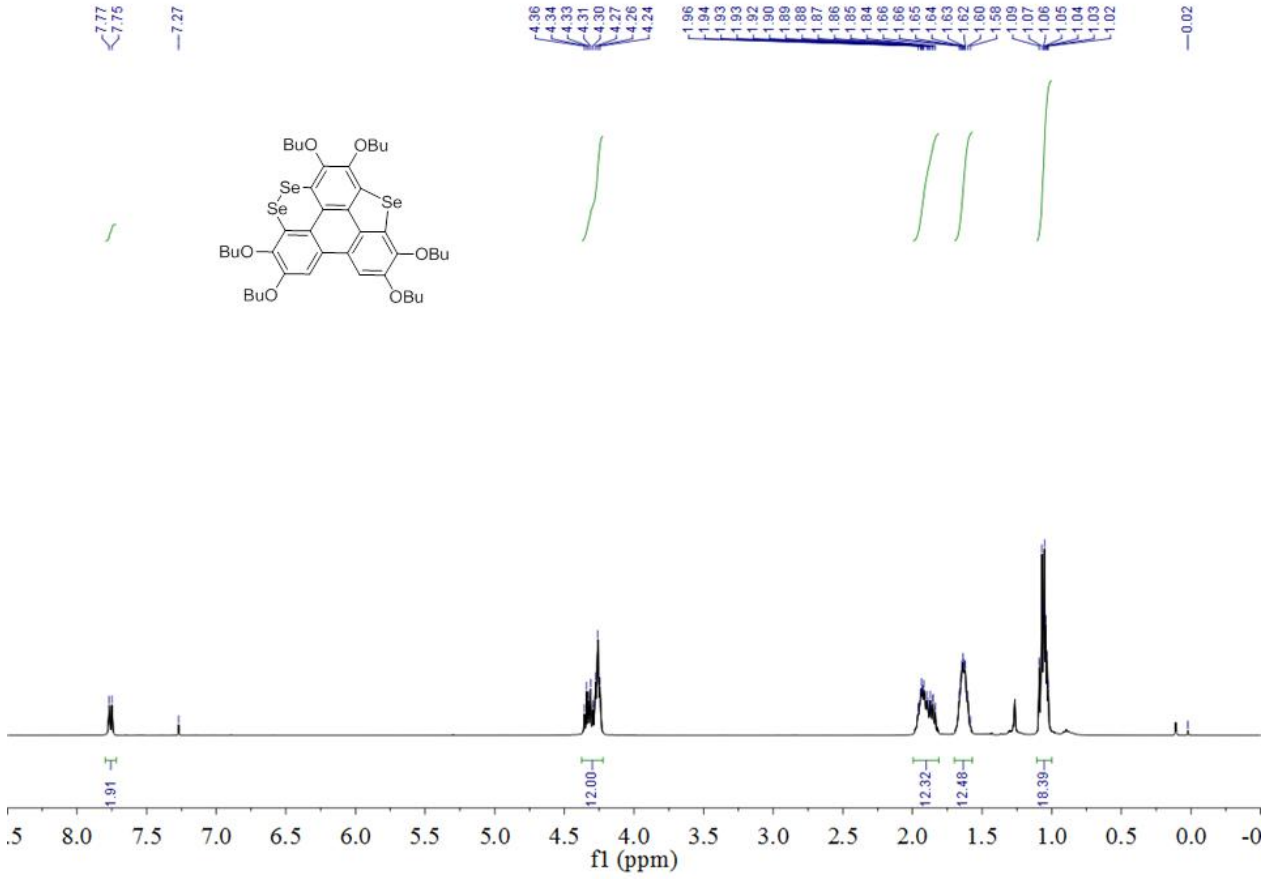
OBu
Te
Te
BuO
OBu
BuO
OBu
Wavenumber / cm-1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4.31
4.30
4.27
4.26
4.24
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1.93
1.93
1.92
1.90
1.89
1.88
1.87
1.86
1.85
1.84
1.66
1.66
1.65
1.64
1.63
1.62
1.60
1.58
1.09
1.07
1.06
1.05
1.04
1.03
1.02
0.02
BuO
OBu
Se
Se
Se
BuO
OBu
BuO
OBu
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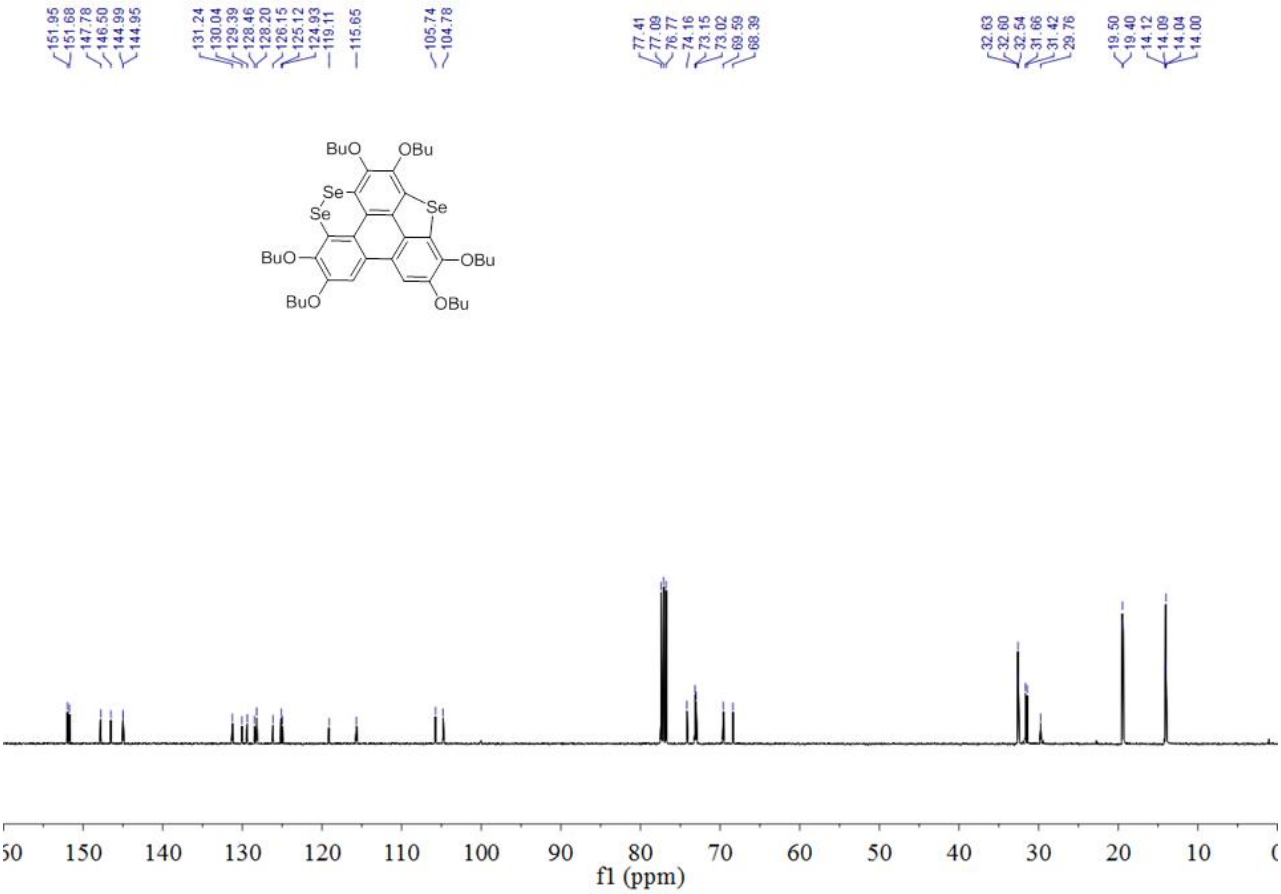
12.00
12.32
12.48
18.39
f1 (ppm)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144.95
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130.04
129.39
128.46
128.20
126.15
125.12
124.93
119.11
115.65
105.74
104.78
77.41
77.09
76.77
74.16
73.15
73.02
69.59
68.39
32.63
32.60
32.54
31.66
31.42
29.76
19.50
19.40
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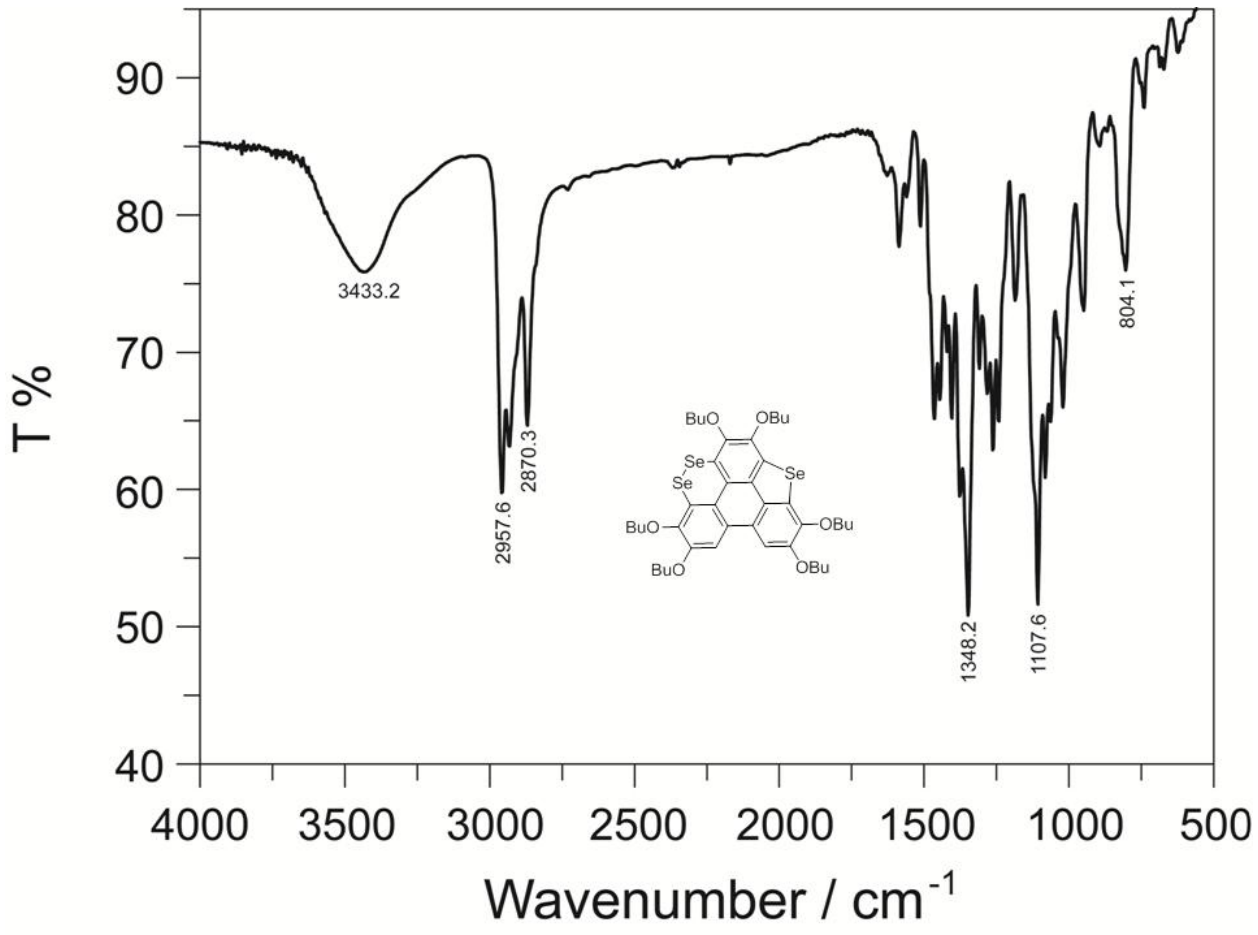
14.09
14.04
14.00
BuO
OBu
Se
Se
Se
BuO
OBu
BuO
OBu
f1 (ppm)


T %
Wavenumber / cm-1
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2870.3
1348.2
1107.6
804.1
BuO
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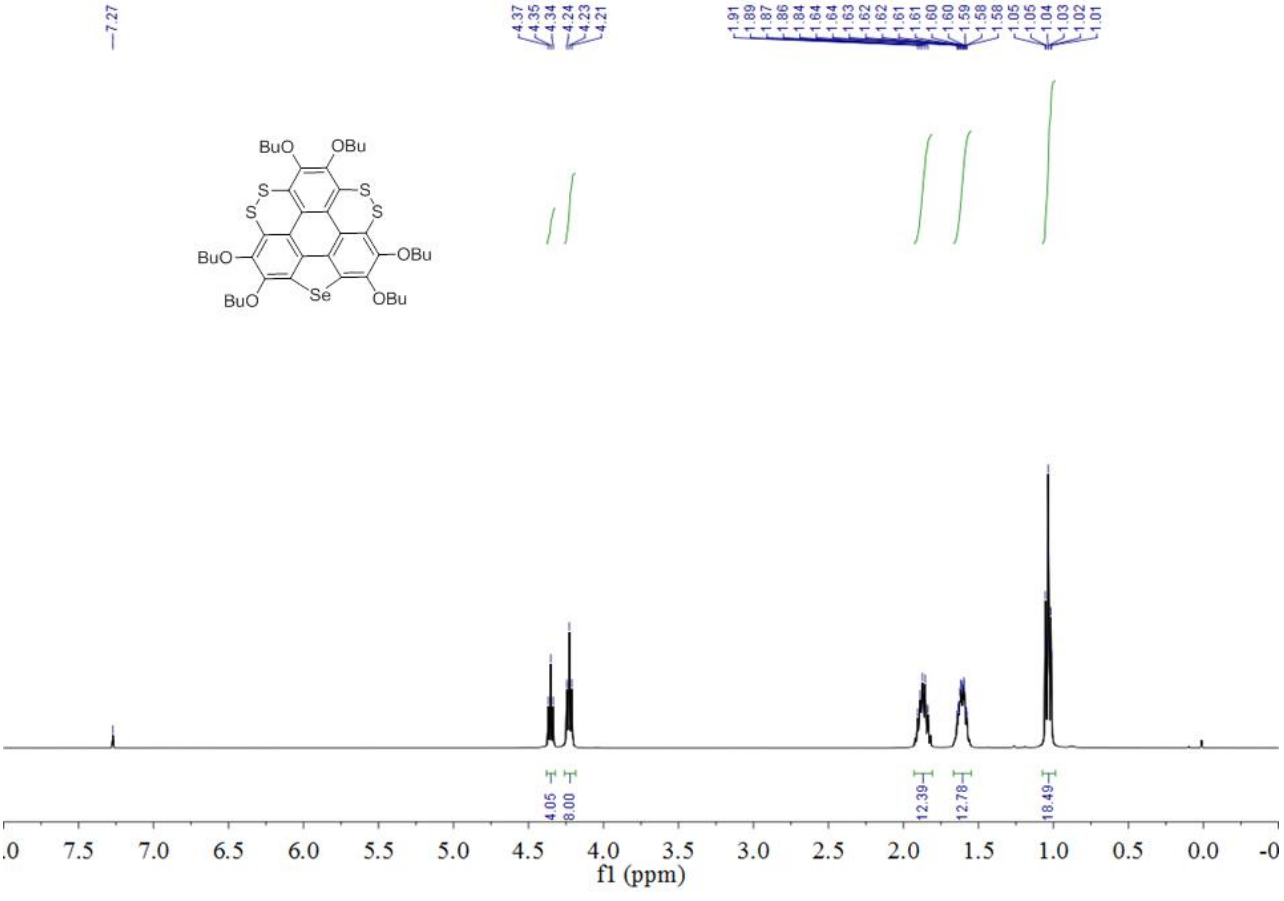
Se
Se
Se
BuO
OBu
BuO
OBu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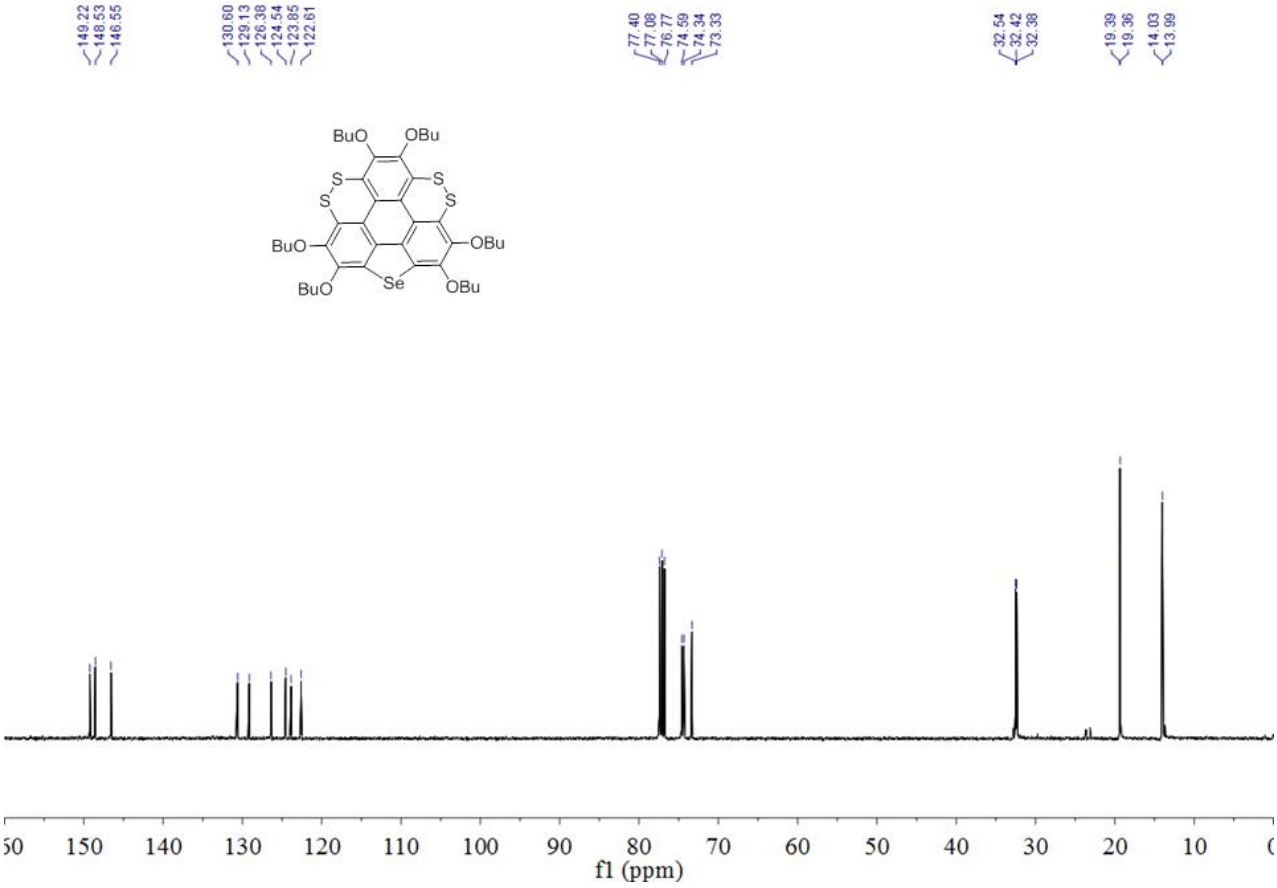
4.37
4.35
4.34
4.24
4.23
4.21
1.91
1.89
1.87
1.86
1.84
1.64
1.63
1.62
1.61
1.60
1.59
1.58
1.05
1.04
1.03
1.02
1.01
BuO
OBu
S
S
S
S
BuO
OBu
BuO
Se
OBu
4.05
8.00
12.39
12.78
18.49
f1 (ppm)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130.60
129.13
126.38
124.54
123.65
122.61
77.40
77.08
76.77
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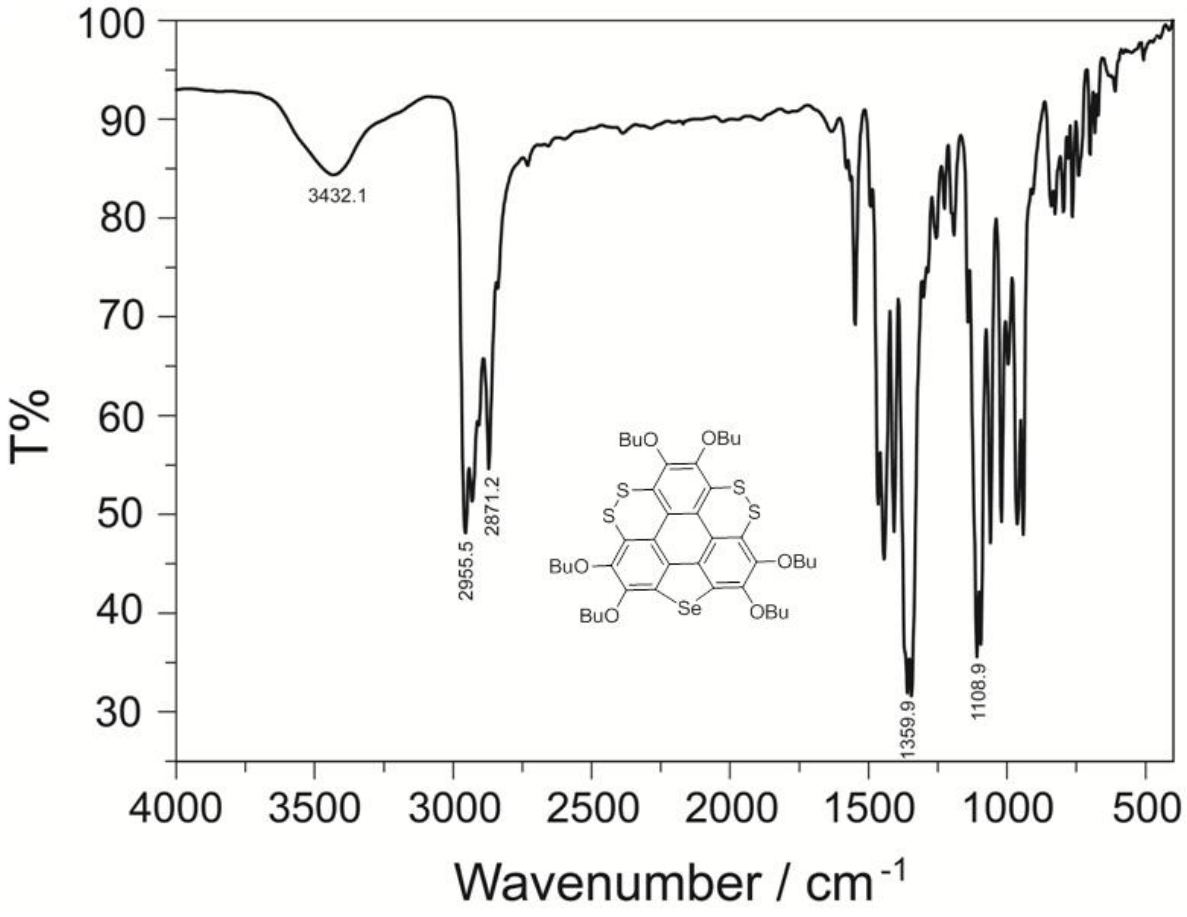
74.34
73.33
32.54
32.42
32.38
19.39
19.36
14.03
13.99
BuO
OBu
S
S
S
S
BuO
OBu
BuO
Se
OBu
f1 (ppm)


T%
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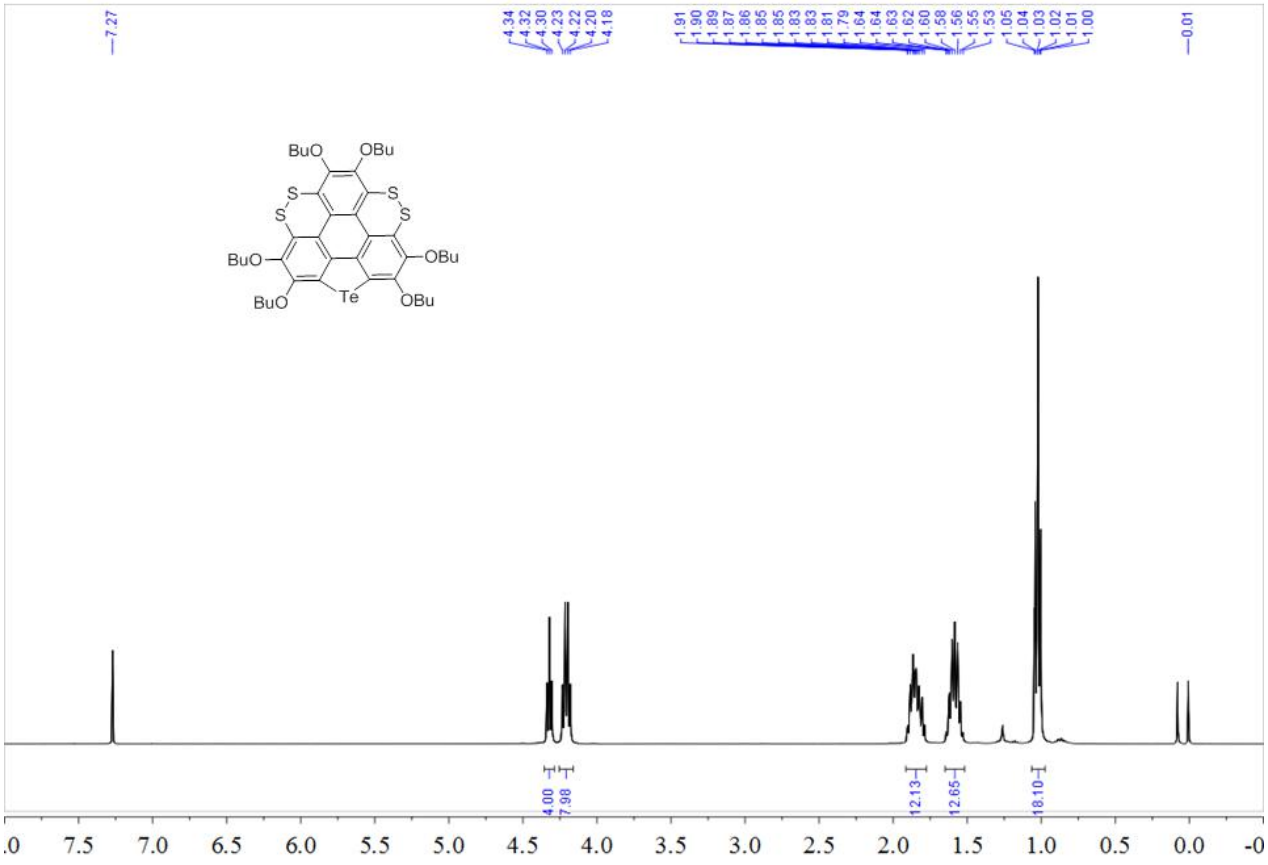
2955.5
2871.2
1359.9
1108.9
Wavenumber / cm-1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4.34
4.32
4.30
4.23
4.22
4.20
4.18
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1.90
1.89
1.87
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1.85
1.85
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1.81
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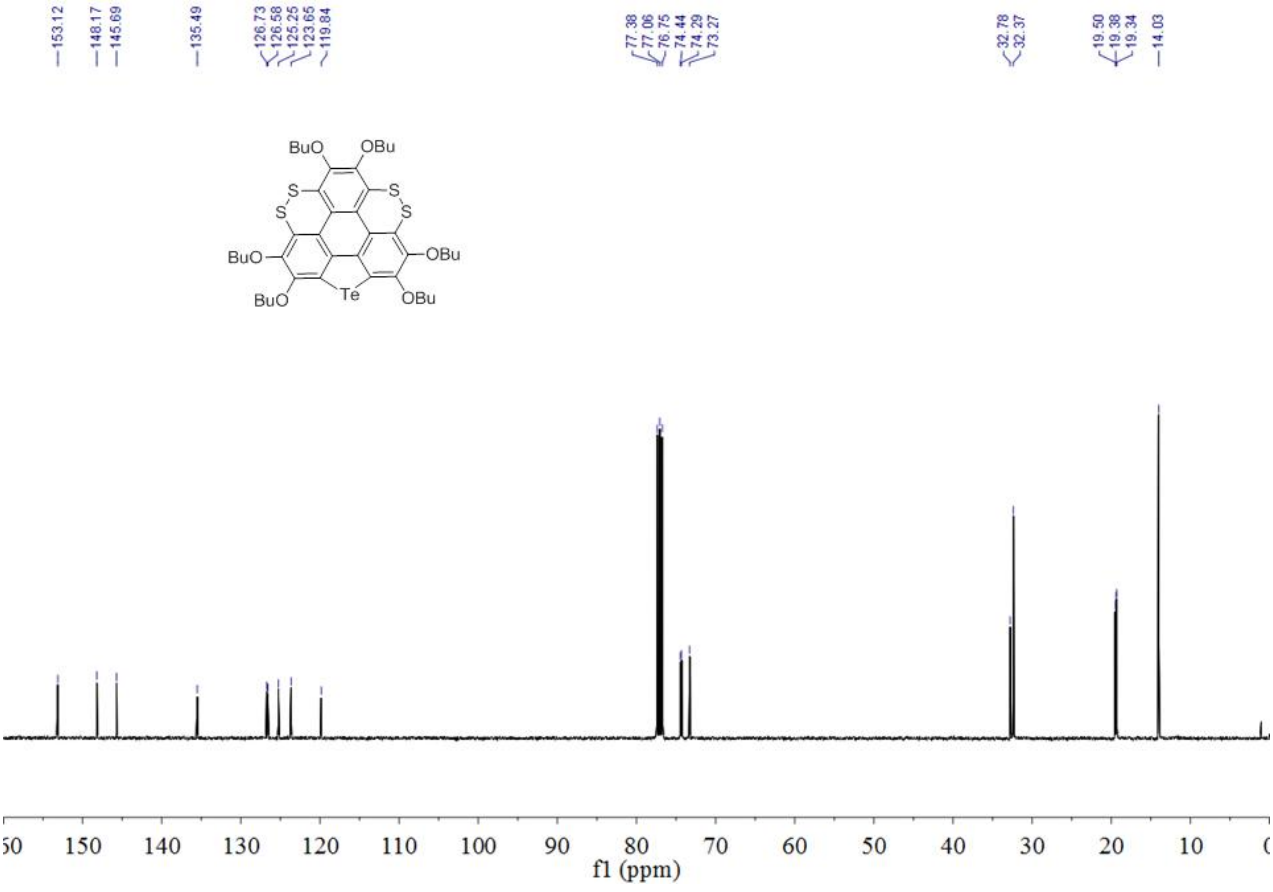
1.64
1.63
1.62
1.60
1.58
1.56
1.55
1.53
1.05
1.04
1.03
1.02
1.01
1.00
0.01
BuO
OBu
S
S
S
S
BuO
OBu
BuO
Te
OBu
4.00
7.98
12.13
12.65
18.10
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0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135.49
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126.58
125.25
123.65
119.84
77.38
77.06
76.75
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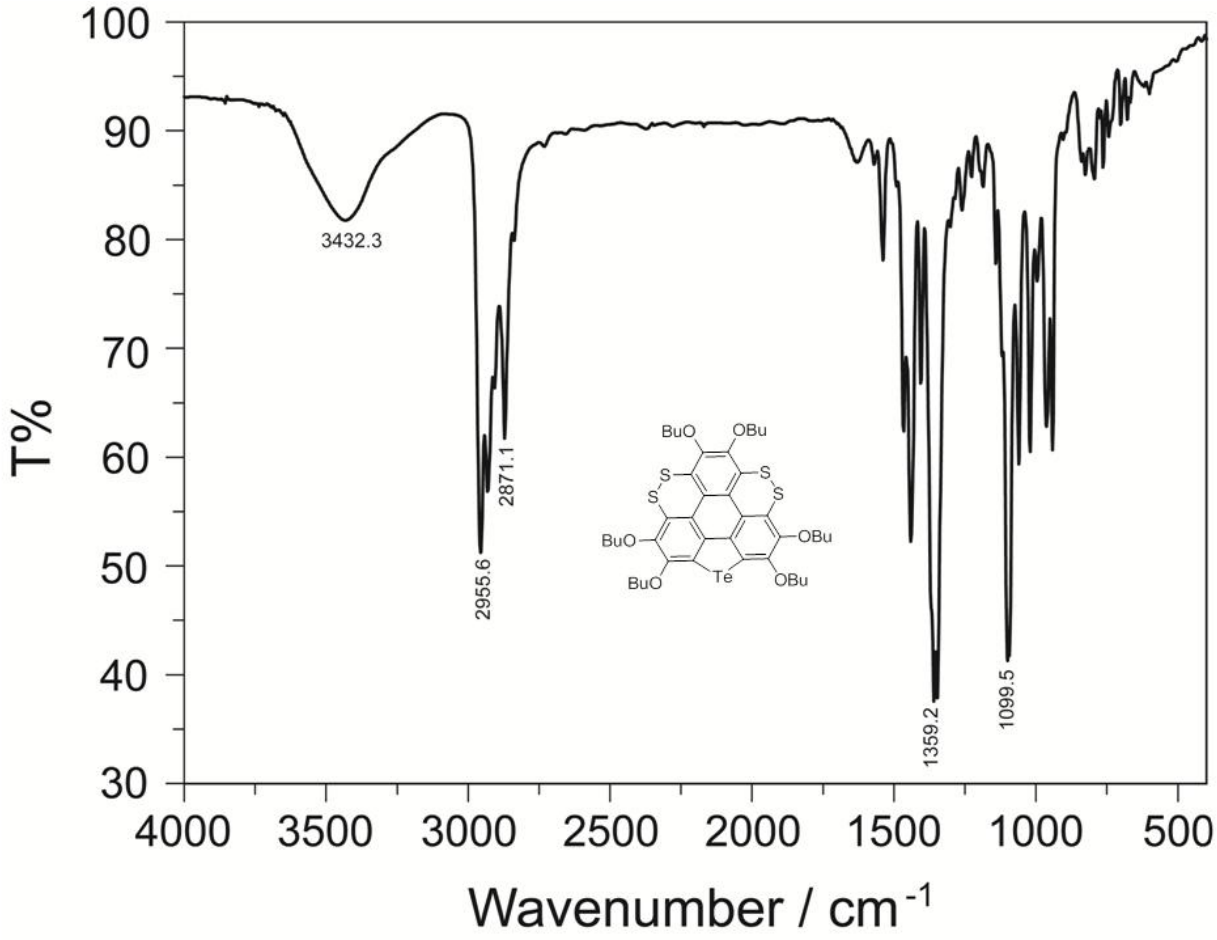
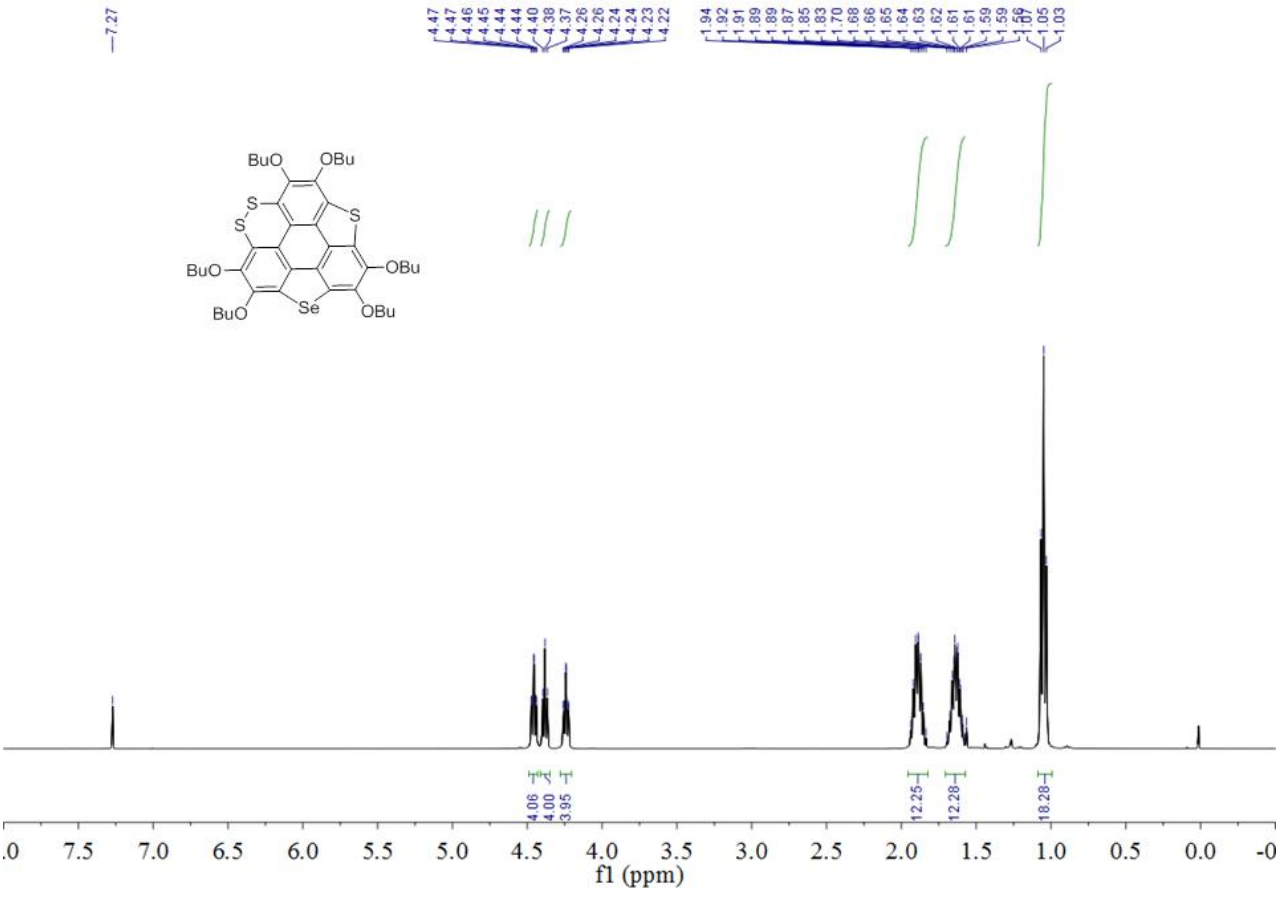
74.29
73.27
32.78
32.37
19.50
19.38
19.34
14.03
BuO
OBu
S
S
S
S
BuO
OBu
BuO
Te
OBu
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


100
90
80
70
60
50
40
30
T%
3432.3
2955.6
2871.1
1359.2
1099.5
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber / cm-1
BuO
OBu
S
Te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4.44
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4.38
4.37
4.26
4.24
4.23
4.22
1.94
1.92
1.91
1.89
1.87
1.85
1.83
1.70
1.68
1.66
1.65
1.64
1.63
1.62
1.61
1.59
1.05
1.03
BuO
OBu
S
Se
4.06
4.00
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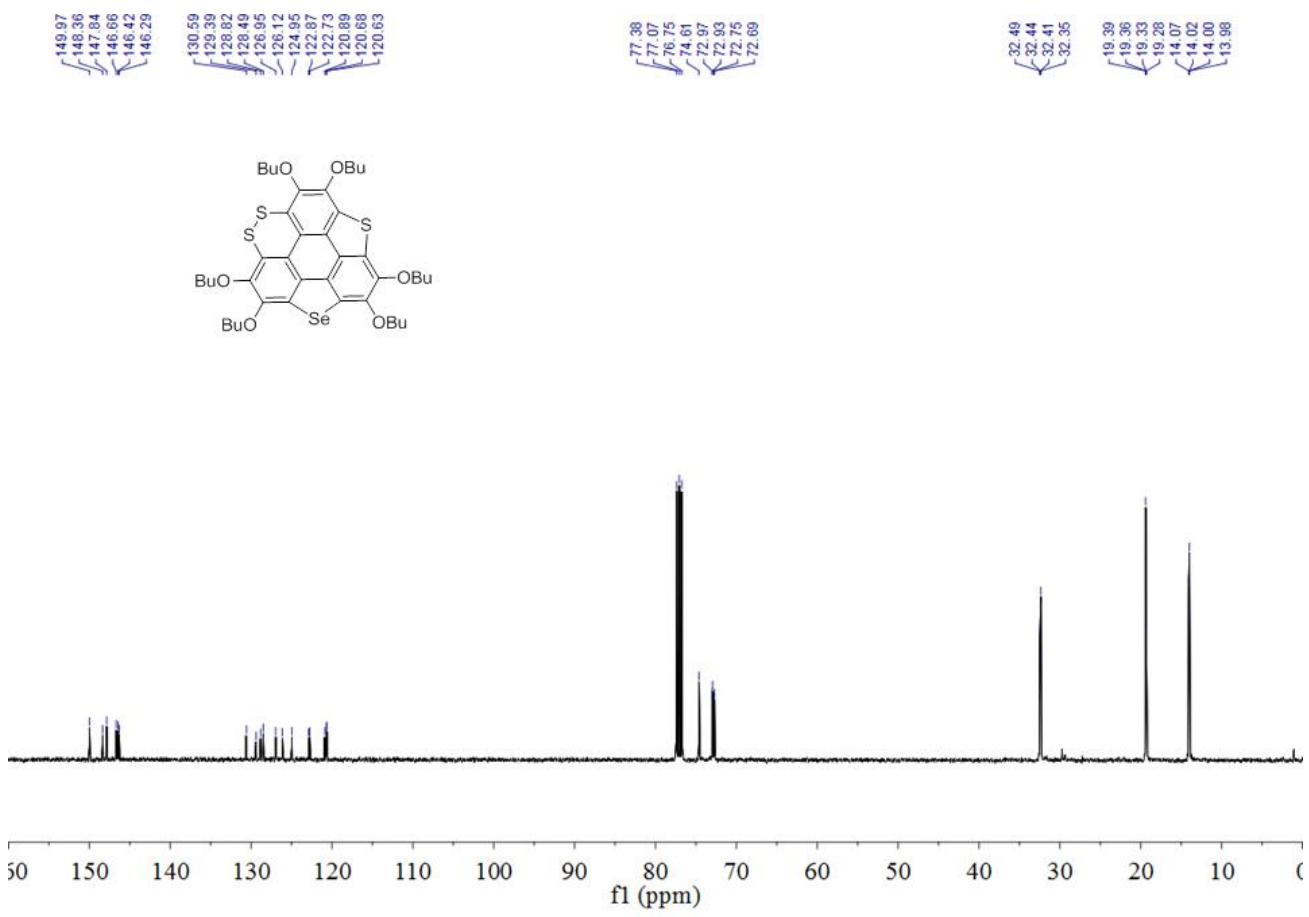
12.25
12.28
18.28
f1 (ppm)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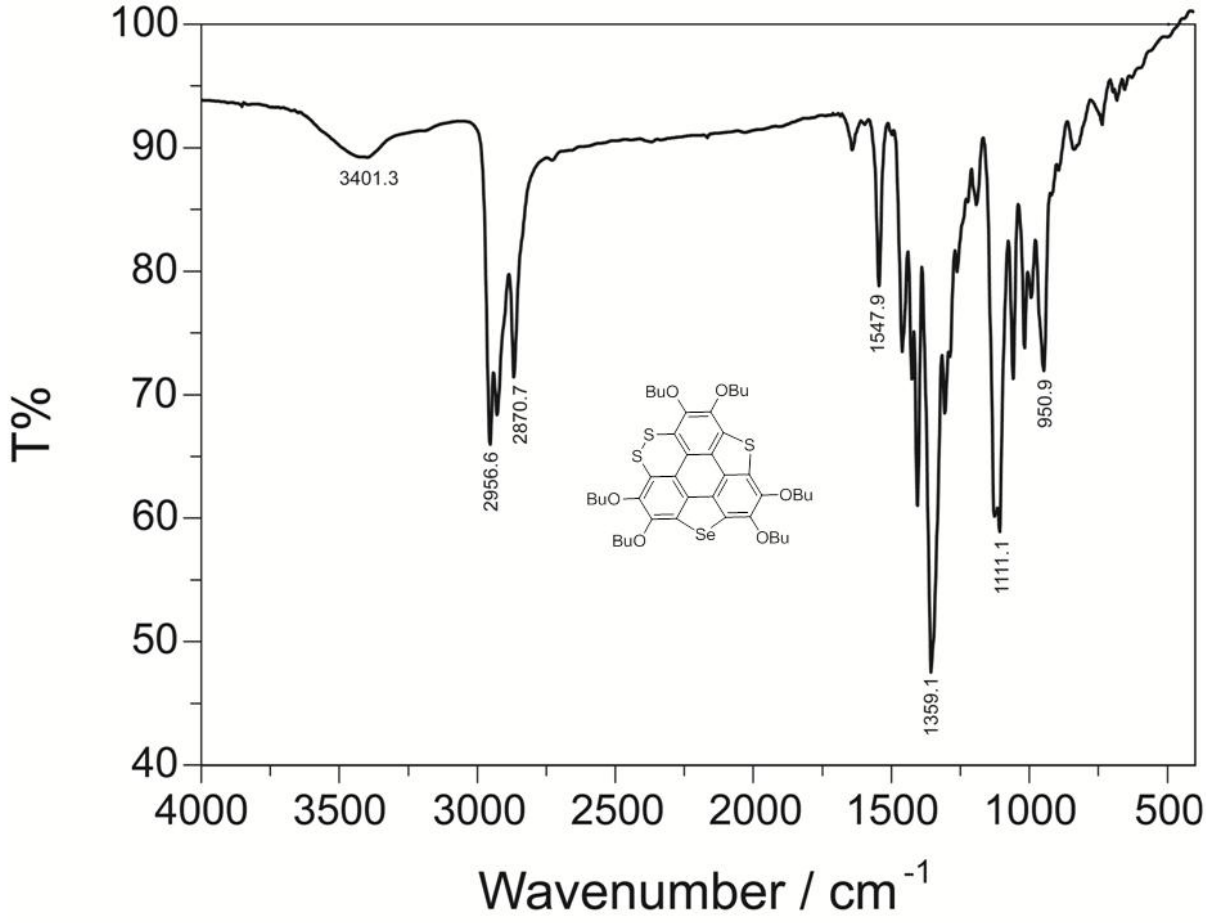
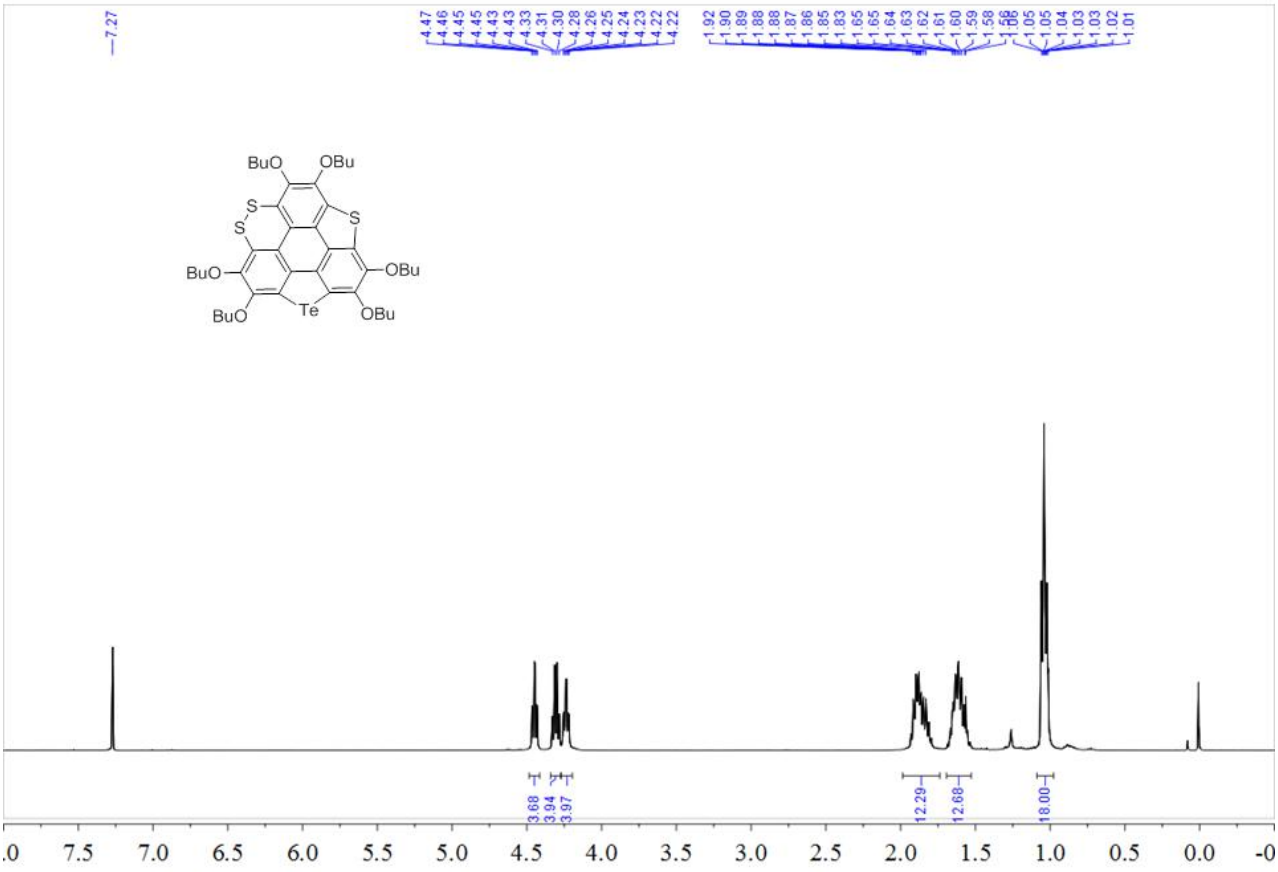
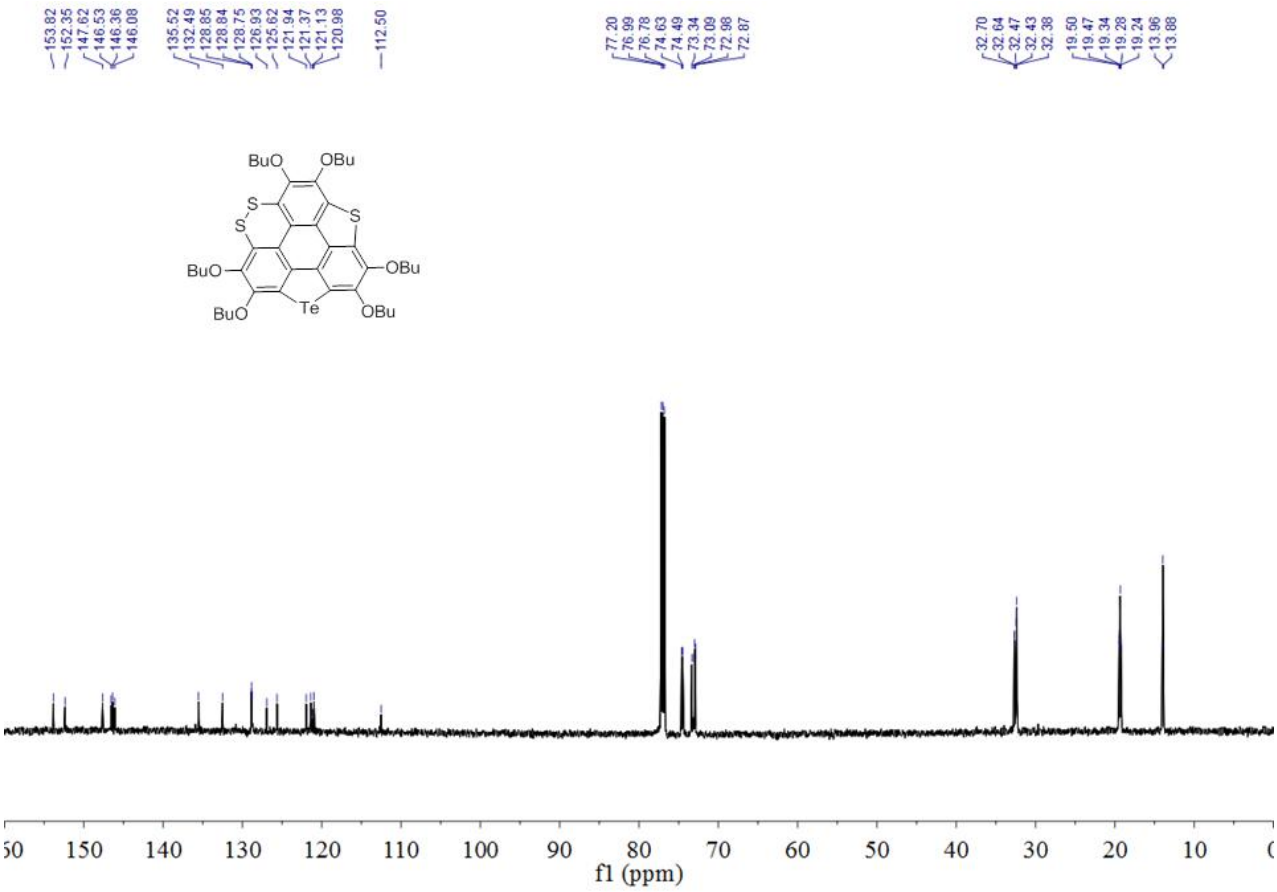
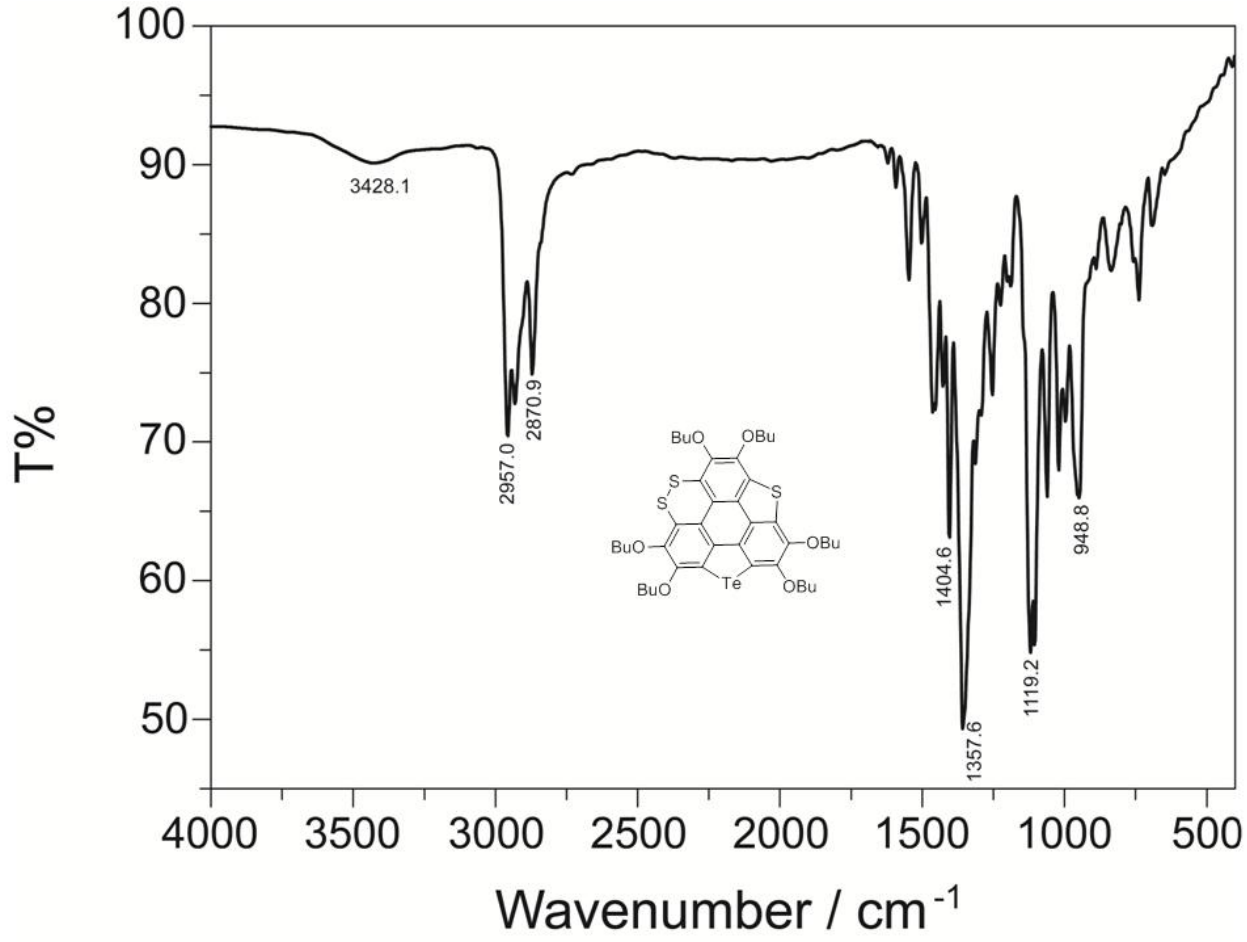
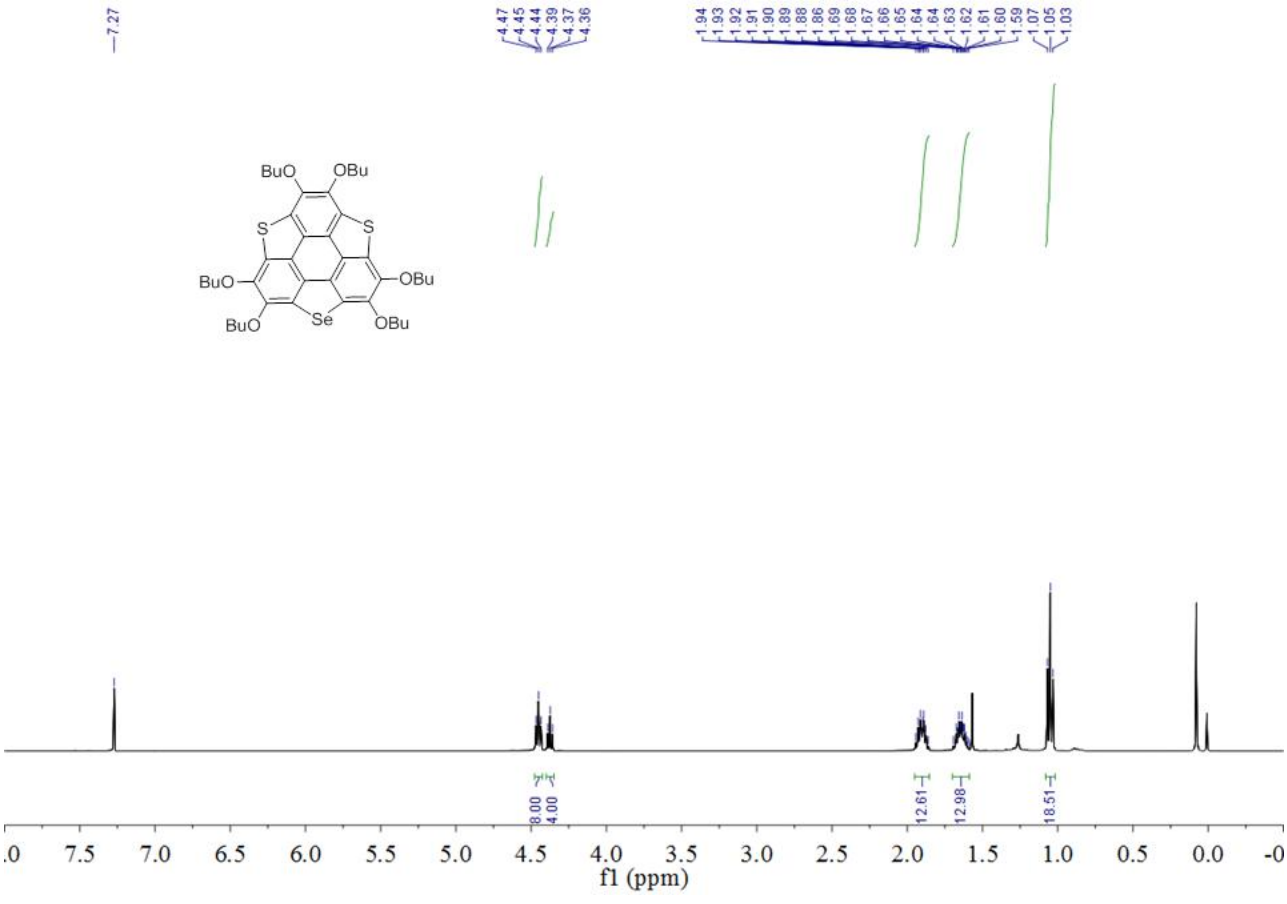
146.29
130.59
129.39
128.82
128.49
126.95
126.12
124.95
122.87
122.73
120.89
120.68
120.63
77.38
77.07
76.75
74.61
72.97
72.93
72.75
72.69
32.49
32.44
32.41
32.35
19.39
19.36
19.33
19.28
14.07
14.02
14.00
13.98
BuO
OBu
S
S
S
BuO
OBu
BuO
Se
OBu
f1 (ppm)

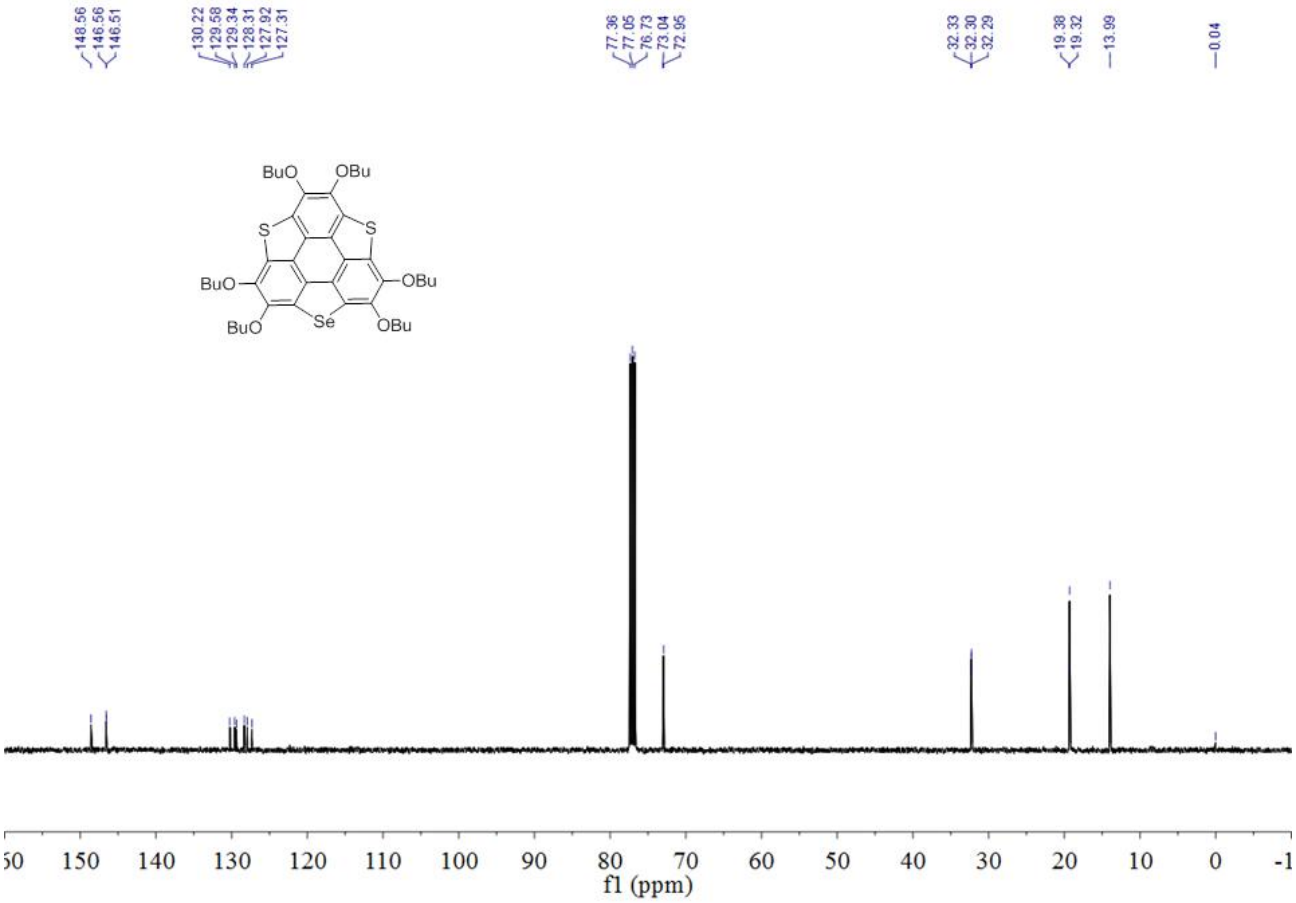

T%
100
90
80
70
60
50
40
3401.3
2956.6
2870.7
1547.9
1359.1
1111.1
950.9
BuO
OBu
S
S
S
BuO
OBu
BuO
Se
OBu
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber / cm-1

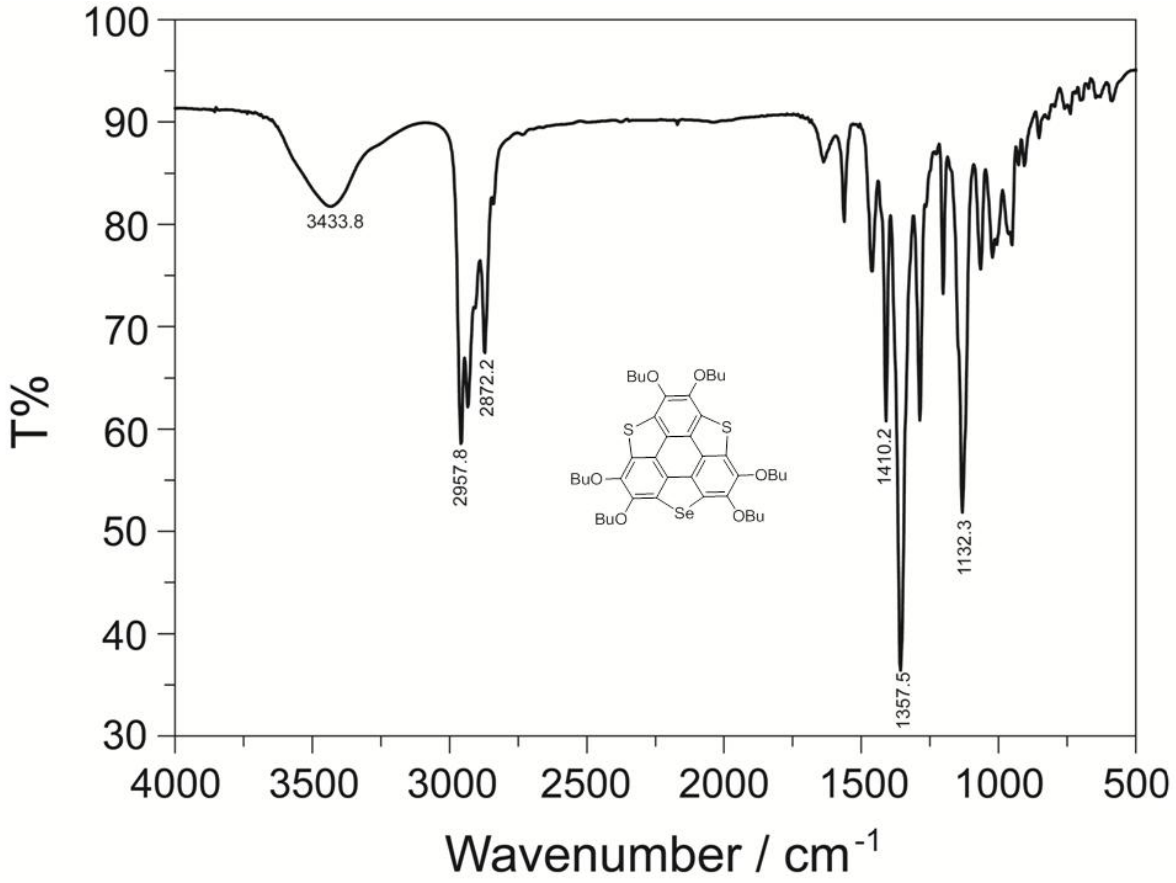

7.27
4.47
4.46
4.45
4.45
4.43
4.43
4.33
4.31
4.30
4.28
4.26
4.25
4.24
4.23
4.22
4.22
1.92
1.90
1.89
1.88
1.88
1.87
1.86
1.85
1.83
1.65
1.65
1.64
1.63
1.62
1.61
1.60
1.59
1.58
1.56
1.06
1.05
1.05
1.04
1.03
1.03
1.02
1.01
BuO
OBu
S
S
S
BuO
OBu
BuO
Te
OBu
3.68
3.94
3.97
12.29
12.68
18.00
.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0

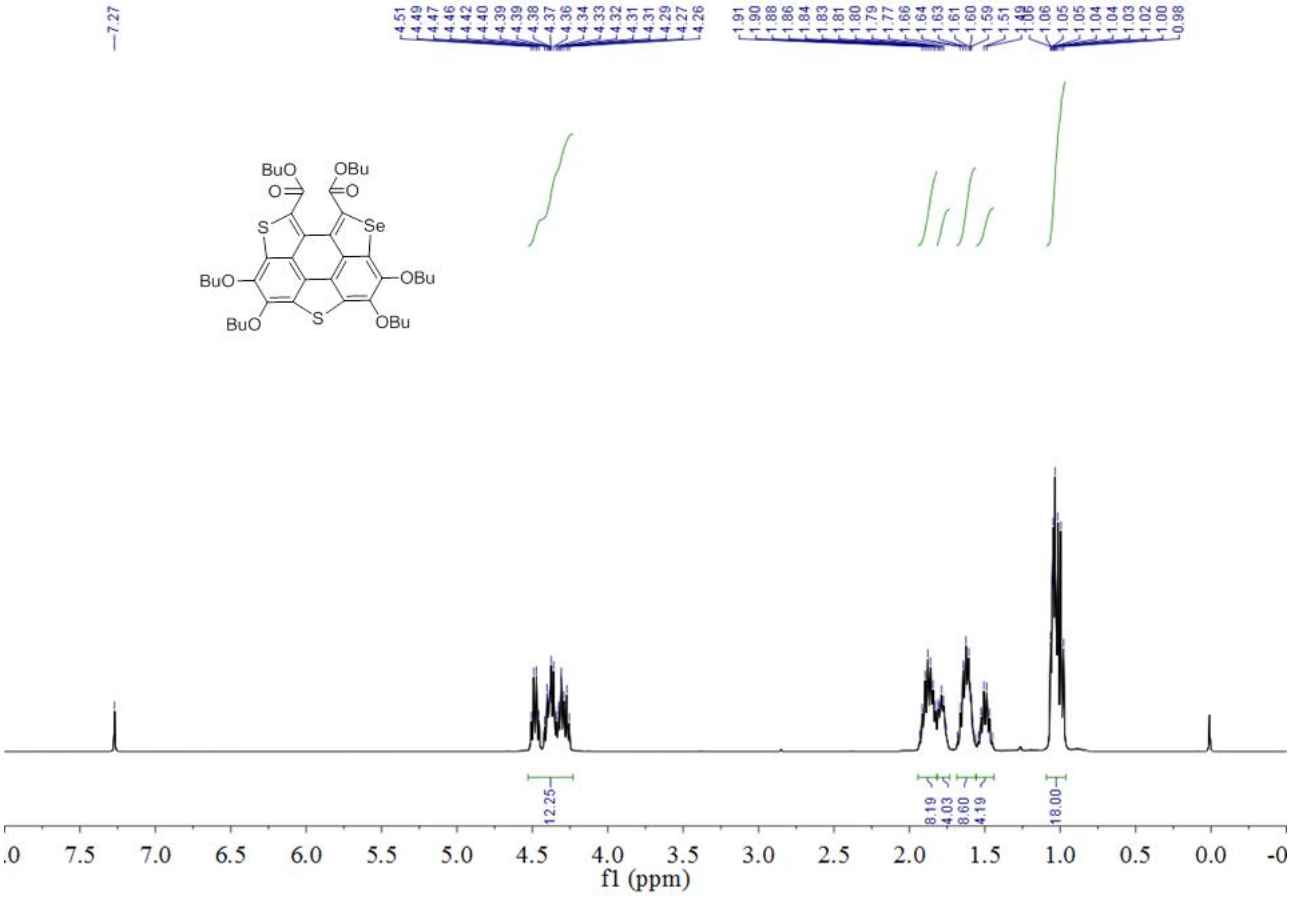

153.82
152.35
147.62
146.53
146.36
146.08
135.52
132.49
128.85
128.84
128.75
126.93
125.62
121.94
121.37
121.13
120.98
112.50
77.20
76.99
76.78
74.63
74.49
73.34
73.09
72.98
72.87
32.70
32.64
32.47
32.43
32.38
19.50
19.47
19.34
19.28
19.24
13.96
13.88
BuO
OBu
S
S
S
BuO
OBu
BuO
Te
OBu
50
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

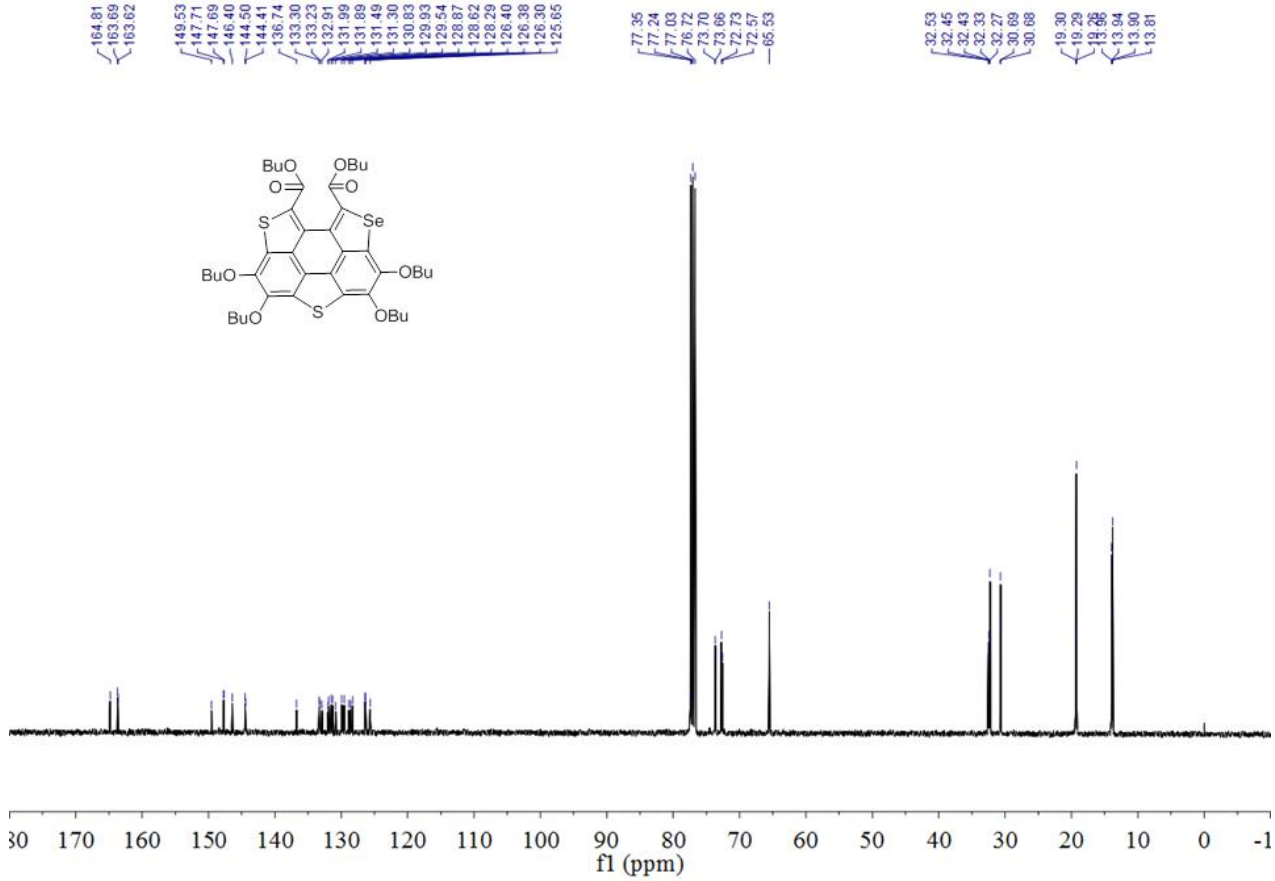

100
90
80
70
60
50
T%
3428.1
2957.0
2870.9
1404.6
1357.6
1119.2
948.8
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber / cm-1
BuO
OBu
S
Te

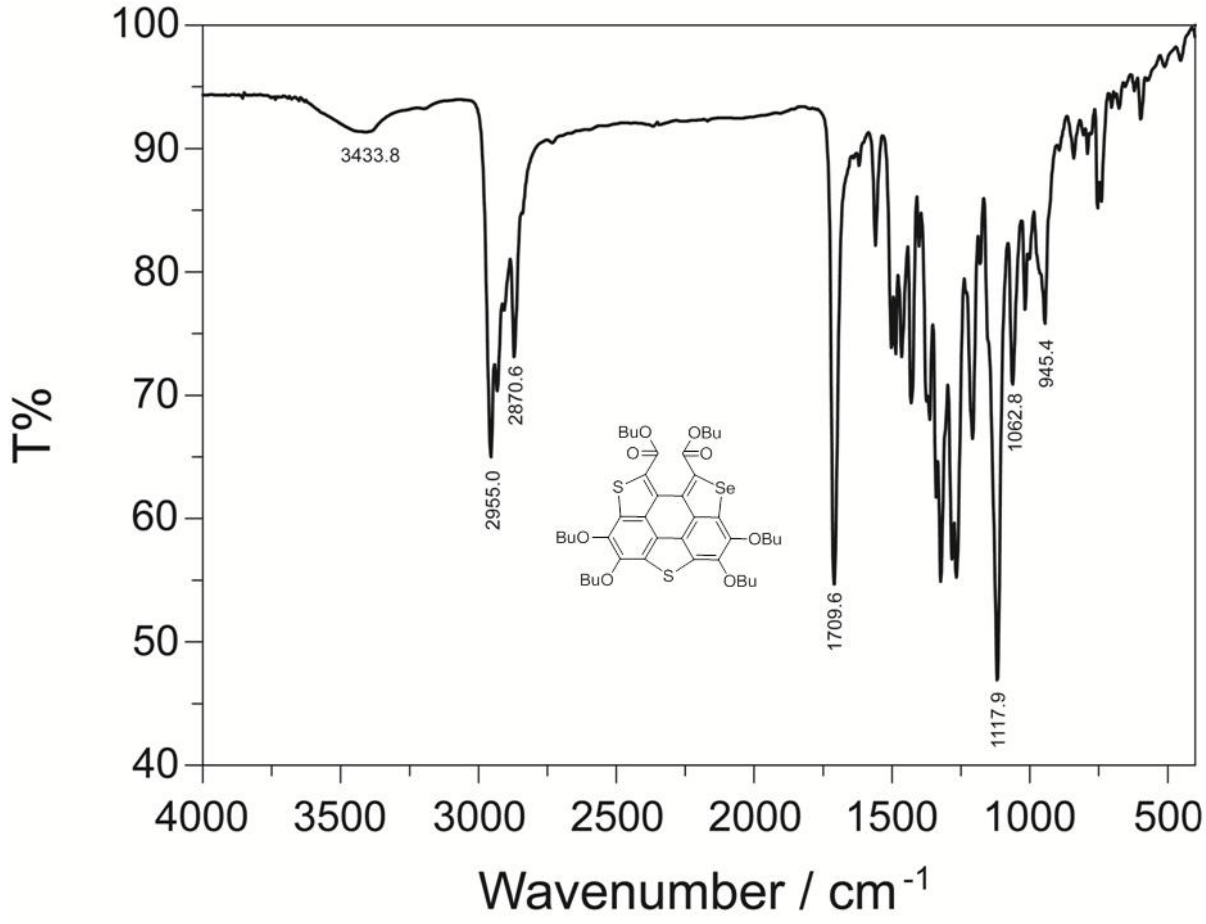

7.27
4.47
4.45
4.44
4.39
4.37
4.36
1.94
1.93
1.92
1.91
1.90
1.89
1.88
1.86
1.69
1.68
1.67
1.66
1.65
1.64
1.64
1.63
1.62
1.61
1.60
1.59
1.07
1.05
1.03
BuO
OBu
S
Se
8.00
4.00
12.61
12.98
18.51
f1 (ppm)

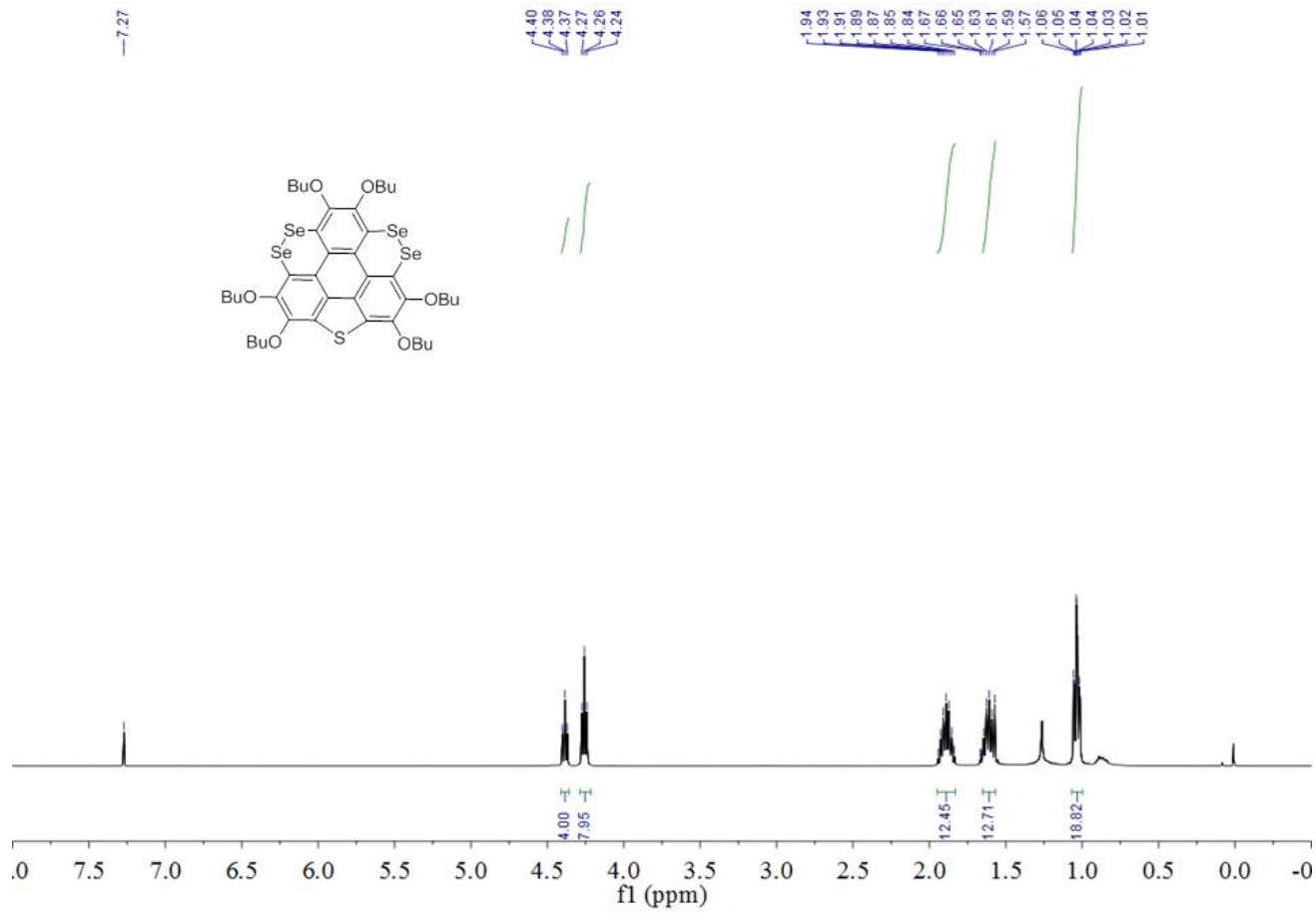

148.56
146.56
146.51
130.22
129.58
129.34
128.31
127.92
127.31
77.36
77.05
76.73
73.04
72.95
32.33
32.30
32.29
19.38
19.32
13.99
0.04
BuO
OBu
S
S
BuO
OBu
BuO
Se
OBu
f1 (ppm)

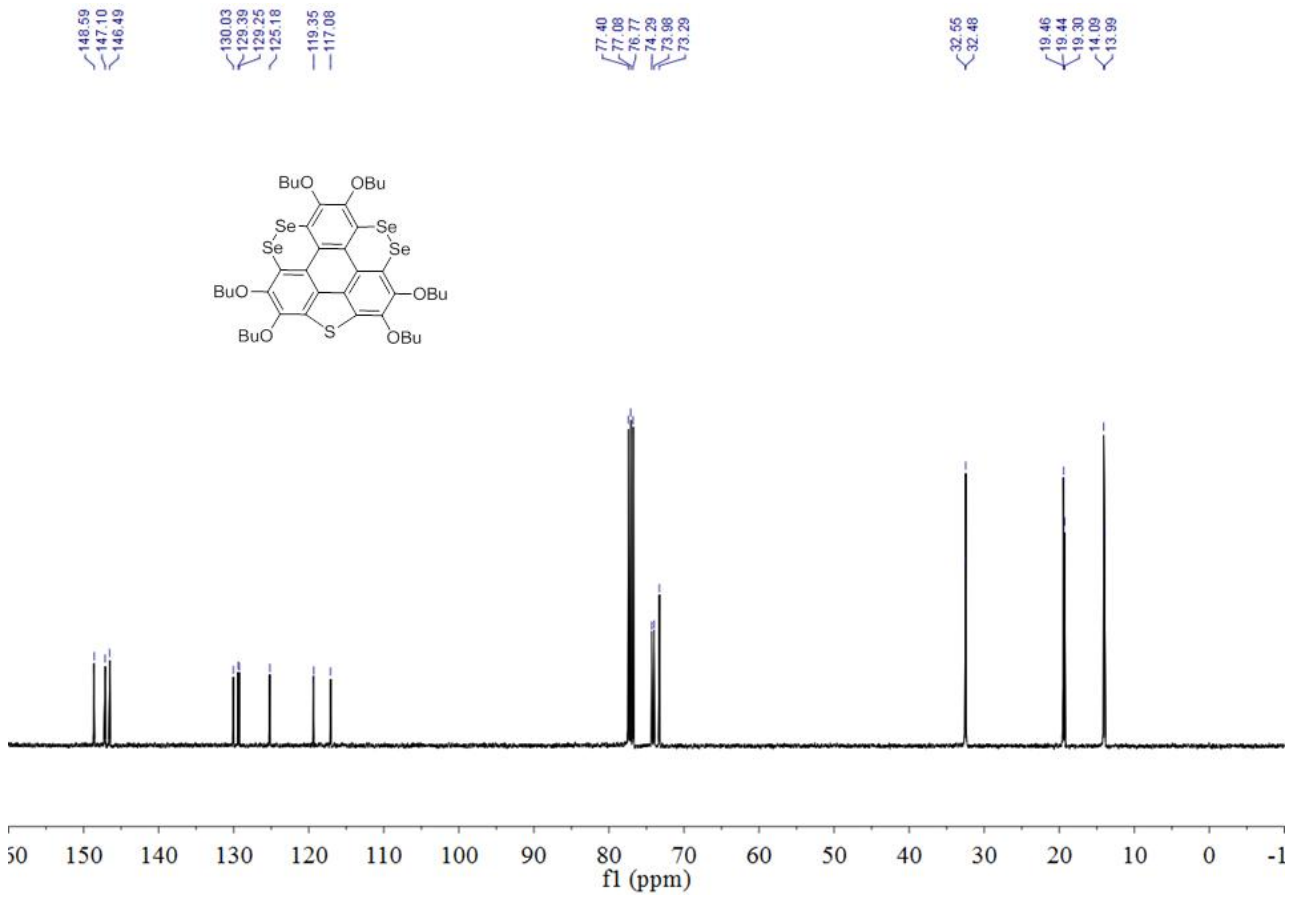

T%
100
90
80
70
60
50
40
30
3433.8
2957.8
2872.2
1410.2
1357.5
1132.3
BuO
OBu
S
S
BuO
OBu
BuO
Se
OBu
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber / cm-1

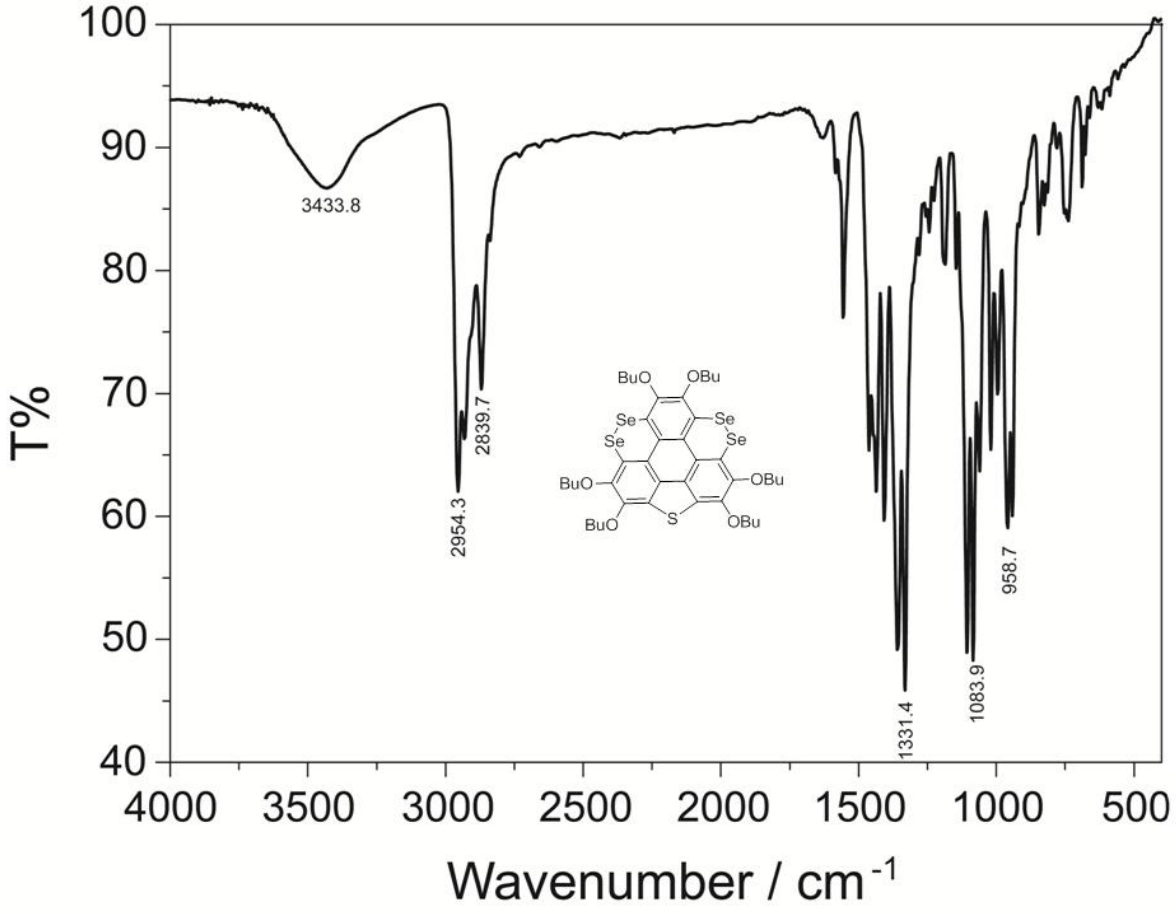

BuO
OBu
O
O
S
Se
BuO
OBu
BuO
S
OBu
12.25
8.19
4.03
8.60
4.19
18.00
f1 (ppm)

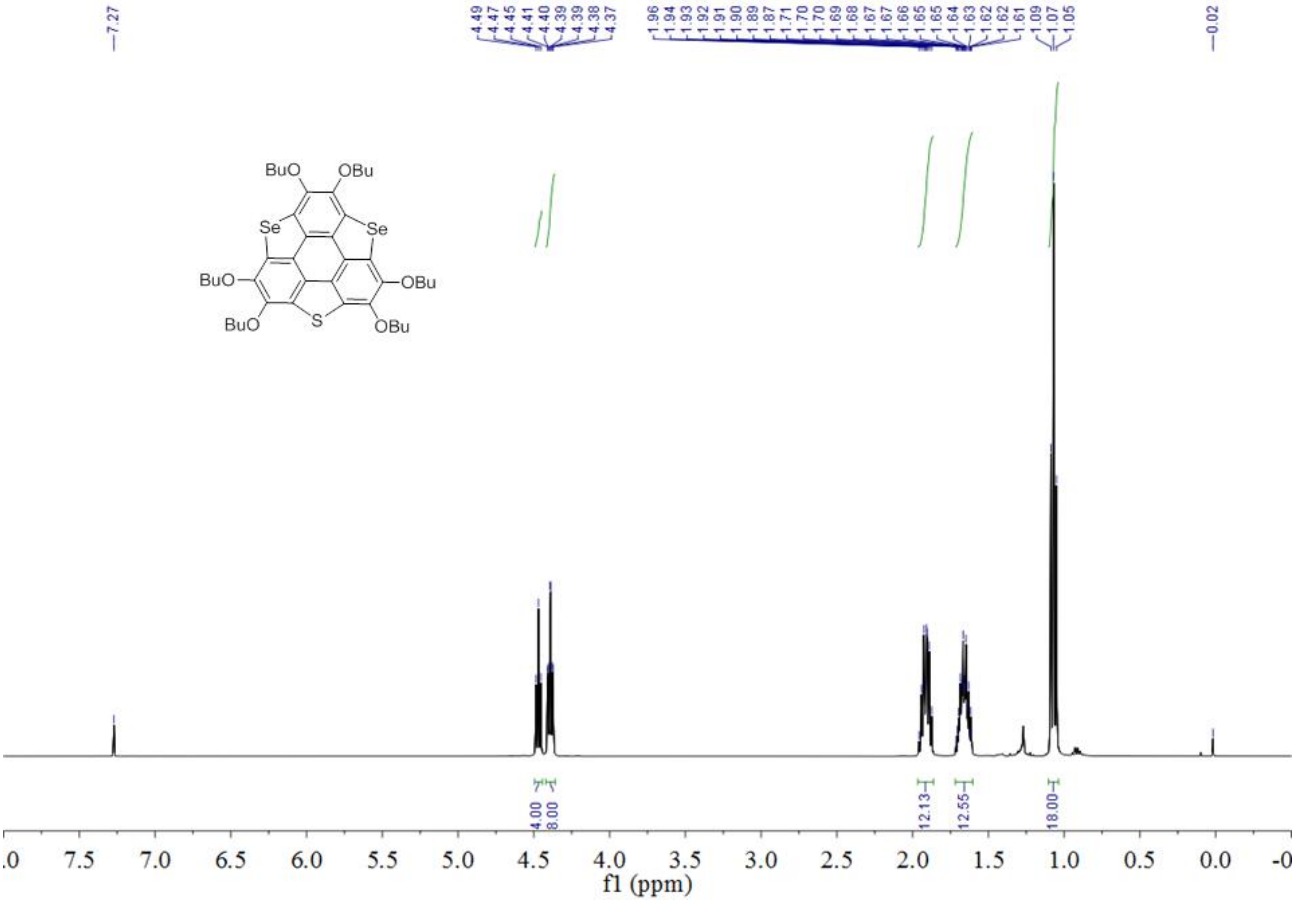

BuO
OBu
O
O
S
Se
BuO
OBu
BuO
S
OBu
f1 (ppm)

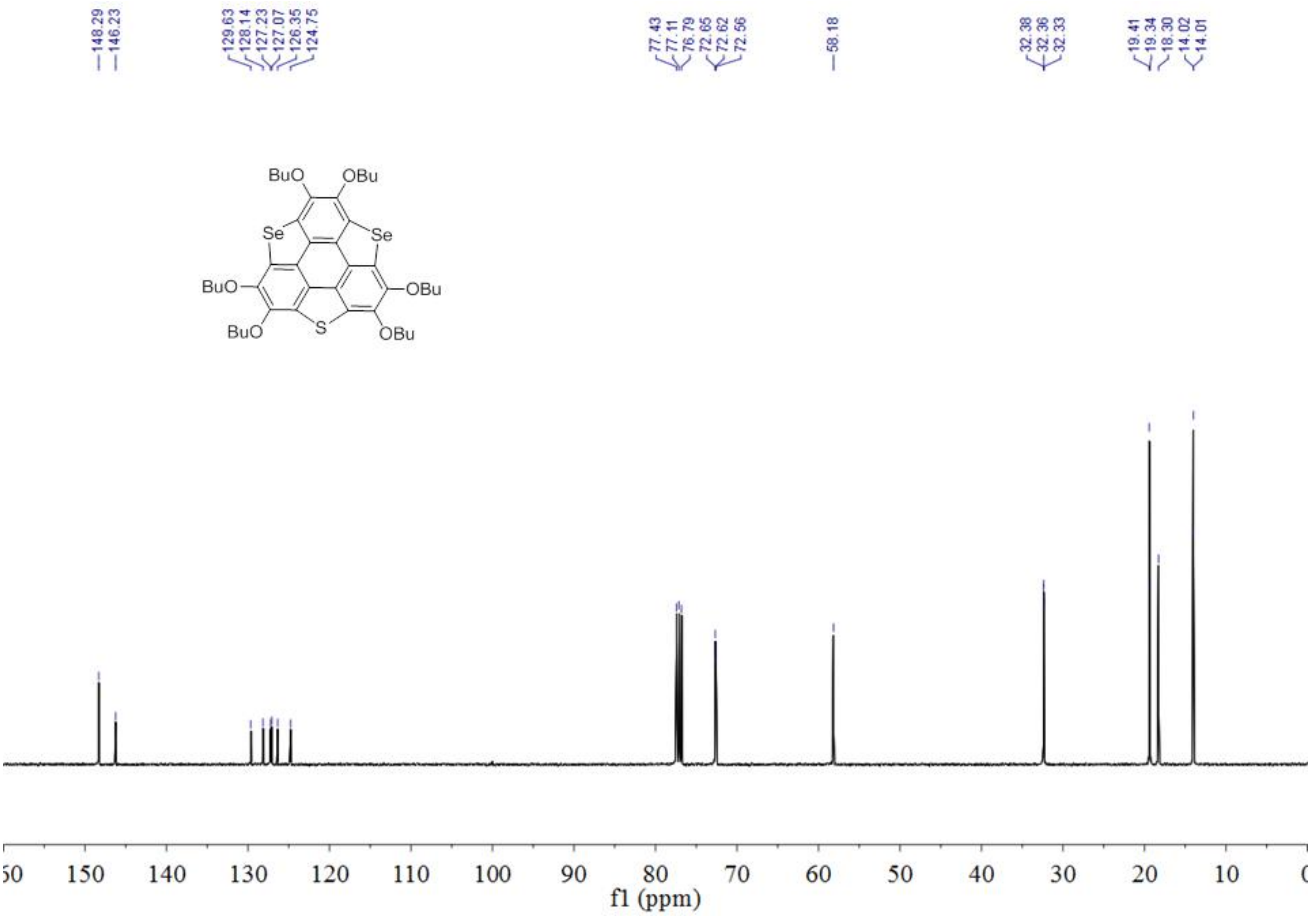

T%
Wavenumber / cm-1
3433.8
2955.0
2870.6
1709.6
1117.9
1062.8
945.4
BuO
OBu
S
Se

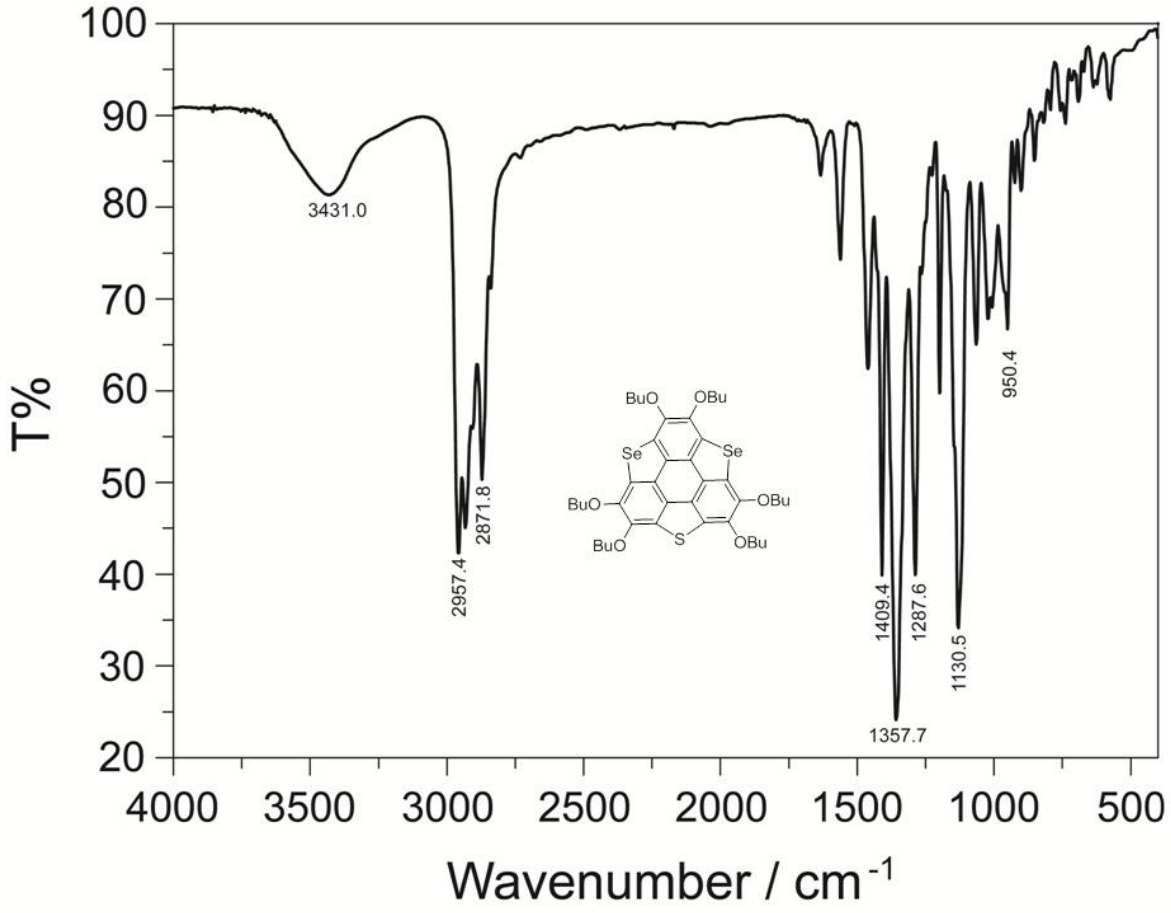

7.27
4.40
4.38
4.37
4.27
4.26
4.24
1.94
1.93
1.91
1.89
1.87
1.85
1.84
1.67
1.66
1.65
1.63
1.61
1.59
1.57
1.06
1.05
1.04
1.04
1.03
1.02
1.01
BuO
OBu
Se
S
4.00
7.95
12.45
12.71
18.82
f1 (ppm)

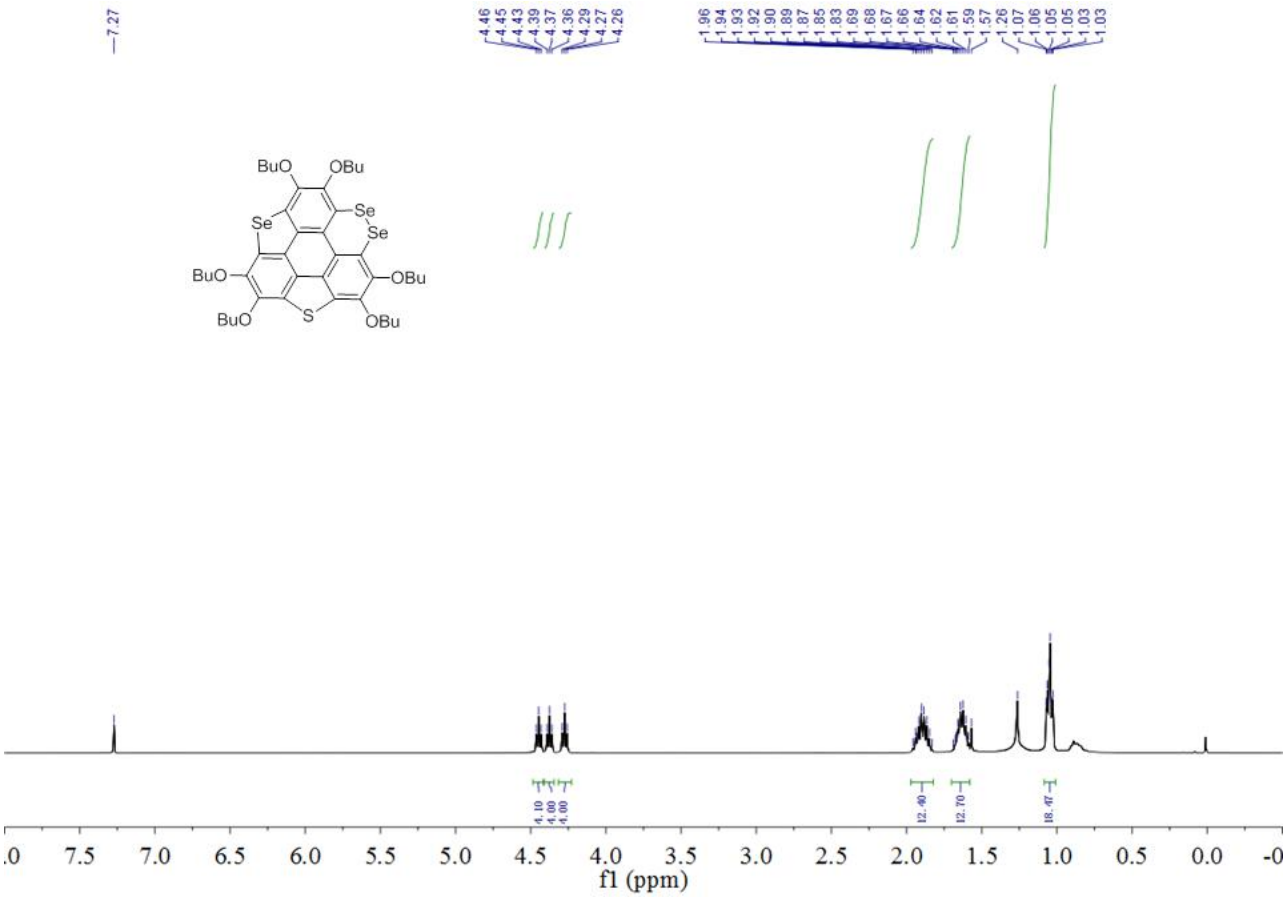

148.59
147.10
146.49
130.03
129.39
129.25
125.18
119.35
117.08
77.40
77.08
76.77
74.29
73.98
73.29
32.55
32.48
19.46
19.44
19.30
14.09
13.99
BuO
OBu
Se
Se
Se
Se
BuO
OBu
BuO
S
OBu
f1 (ppm)

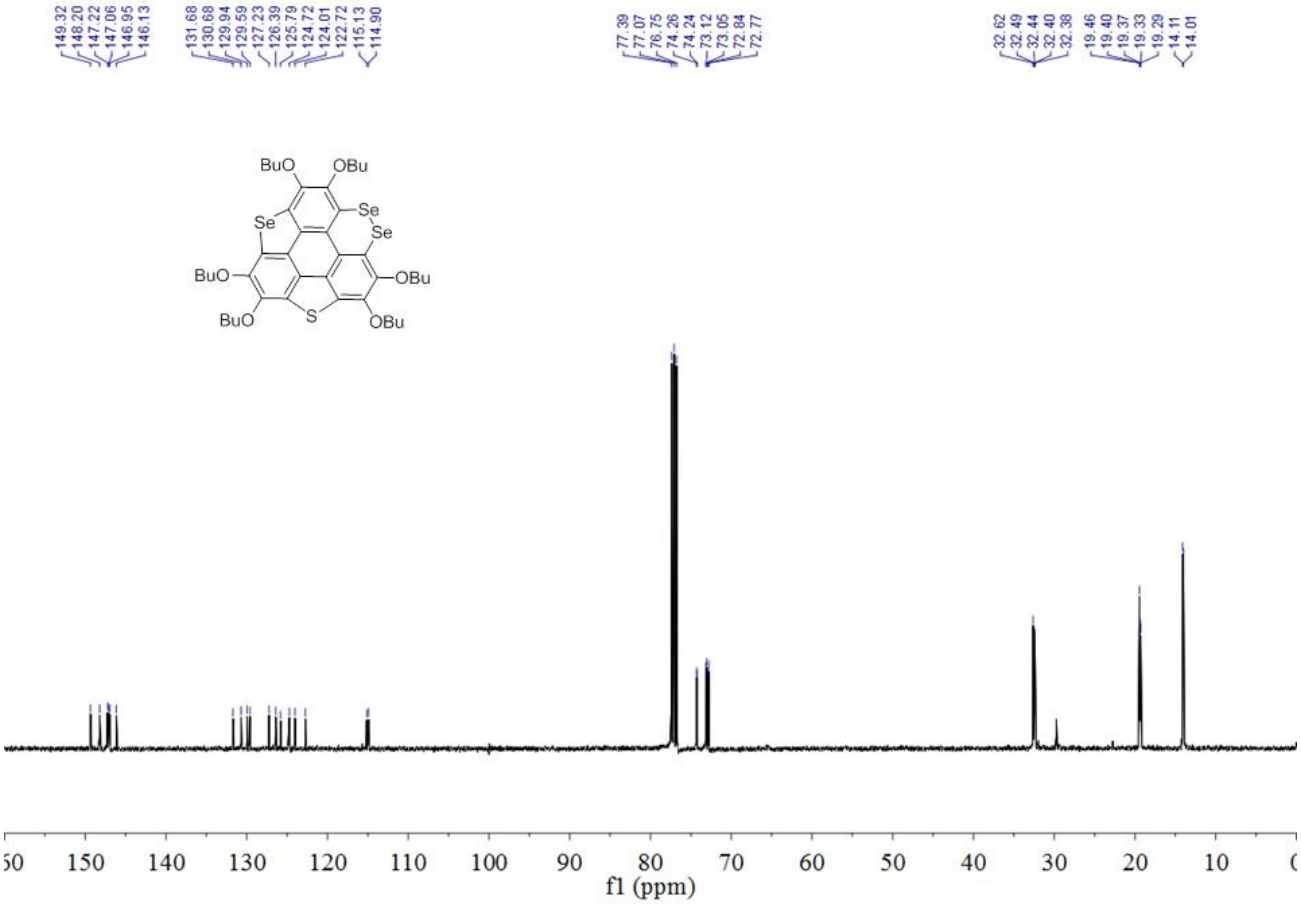

T%
3433.8
2954.3
2839.7
1331.4
1083.9
958.7
BuO
OBu
Se
Se
Se
Se
BuO
OBu
BuO
S
OBu
Wavenumber / cm-1

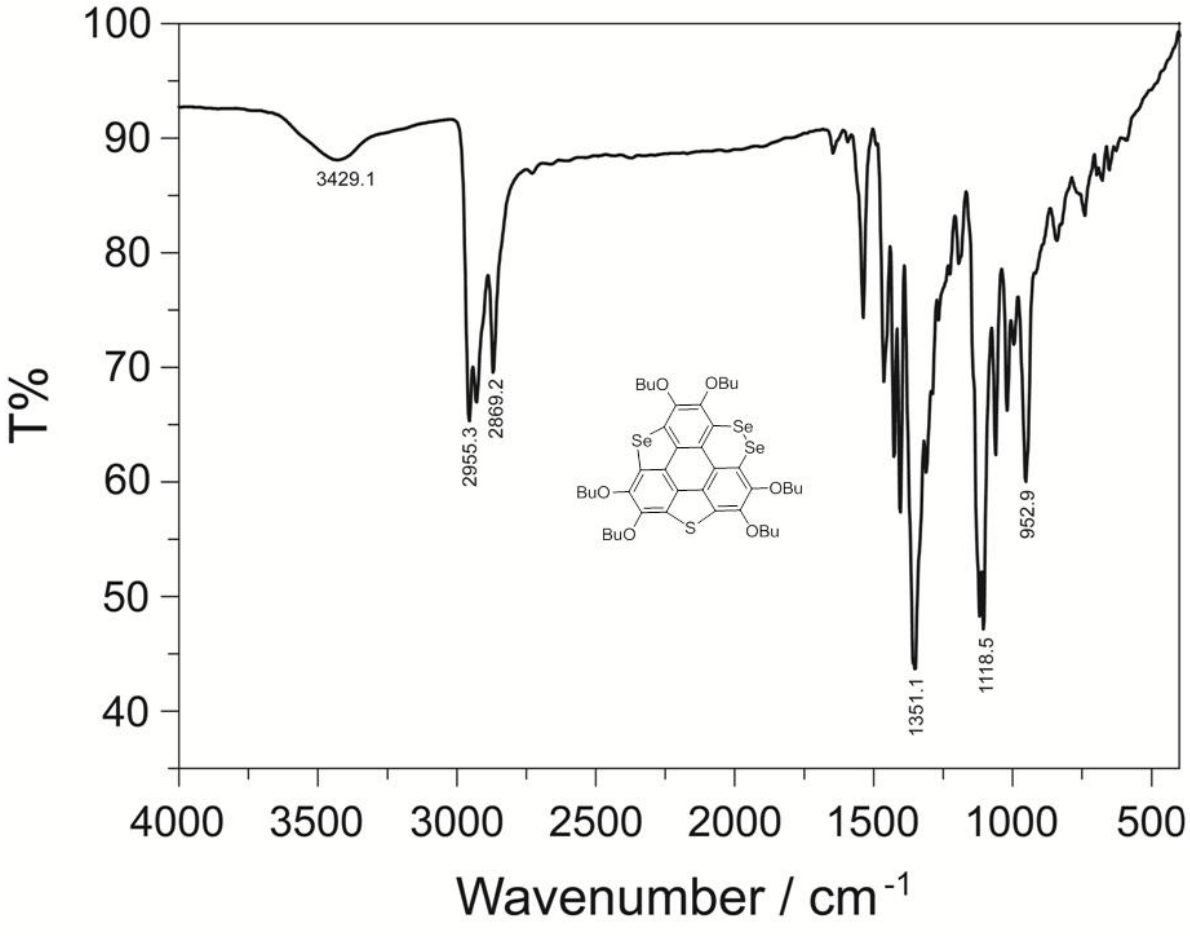

7.27
4.49
4.47
4.45
4.41
4.40
4.39
4.39
4.38
4.37
1.96
1.94
1.93
1.92
1.91
1.90
1.89
1.87
1.71
1.70
1.70
1.69
1.68
1.67
1.67
1.66
1.65
1.65
1.64
1.63
1.62
1.62
1.61
1.09
1.07
1.05
0.02
BuO
OBu
Se
Se
BuO
OBu
BuO
S
OBu
4.00
8.00
12.13
12.55
18.00
f1 (ppm)

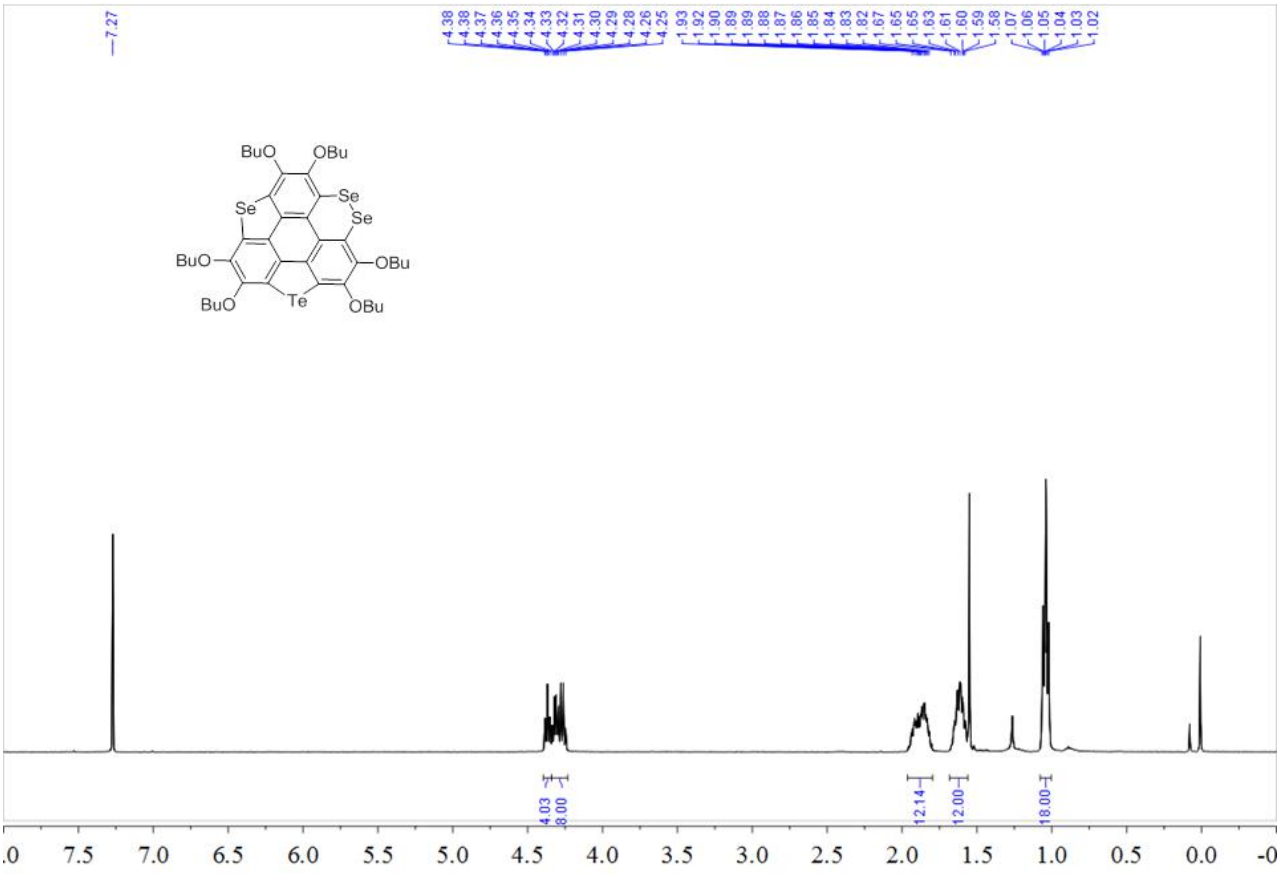

148.29
146.23
129.63
128.14
127.23
127.07
126.35
124.75
77.43
77.11
76.79
72.65
72.62
72.56
58.18
32.38
32.36
32.33
19.41
19.34
18.30
14.02
14.01
BuO
OBu
Se
Se
BuO
OBu
BuO
S
OBu
f1 (ppm)

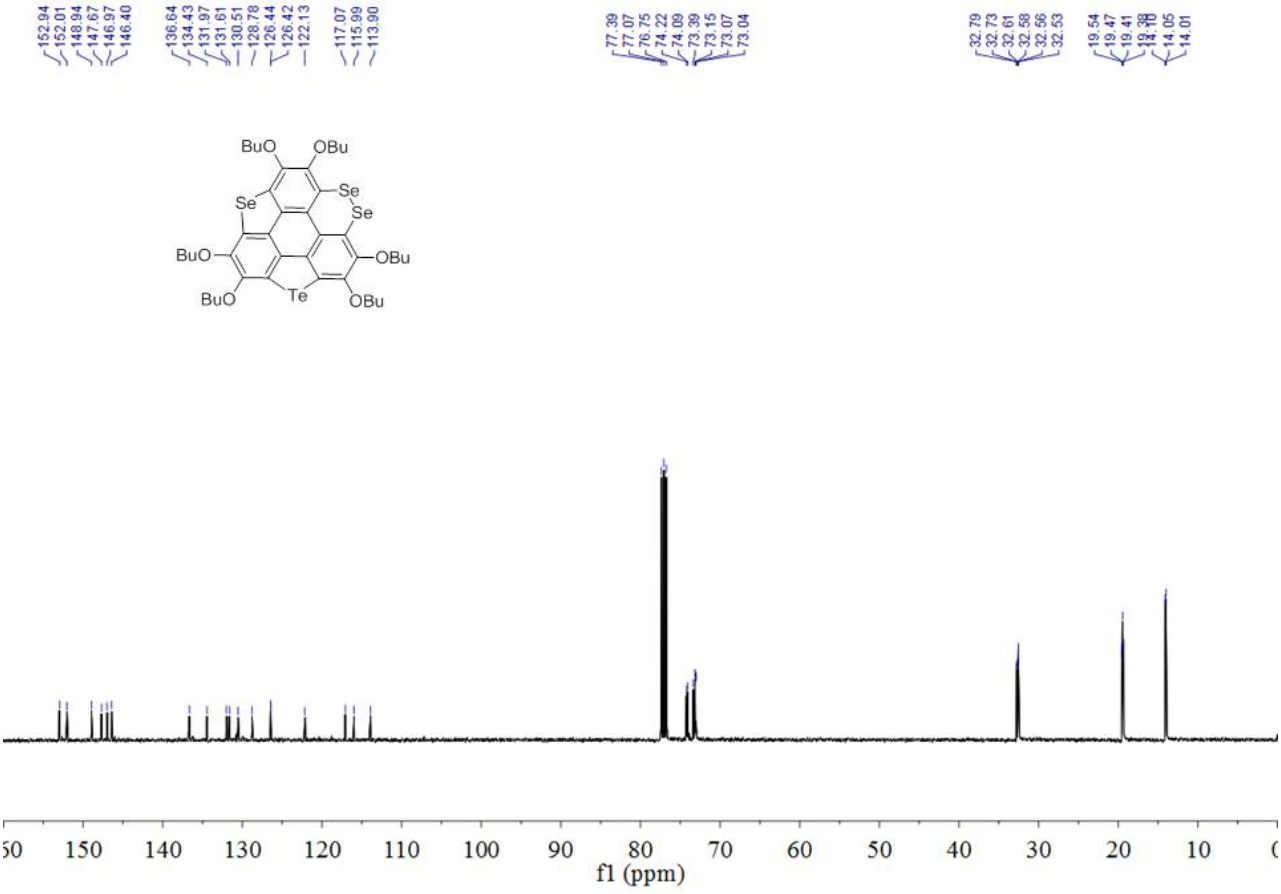

T%
Wavenumber / cm-1
3431.0
2957.4
2871.8
1409.4
1357.7
1287.6
1130.5
950.4
BuO
OBu
Se
Se
BuO
OBu
BuO
S
OBu

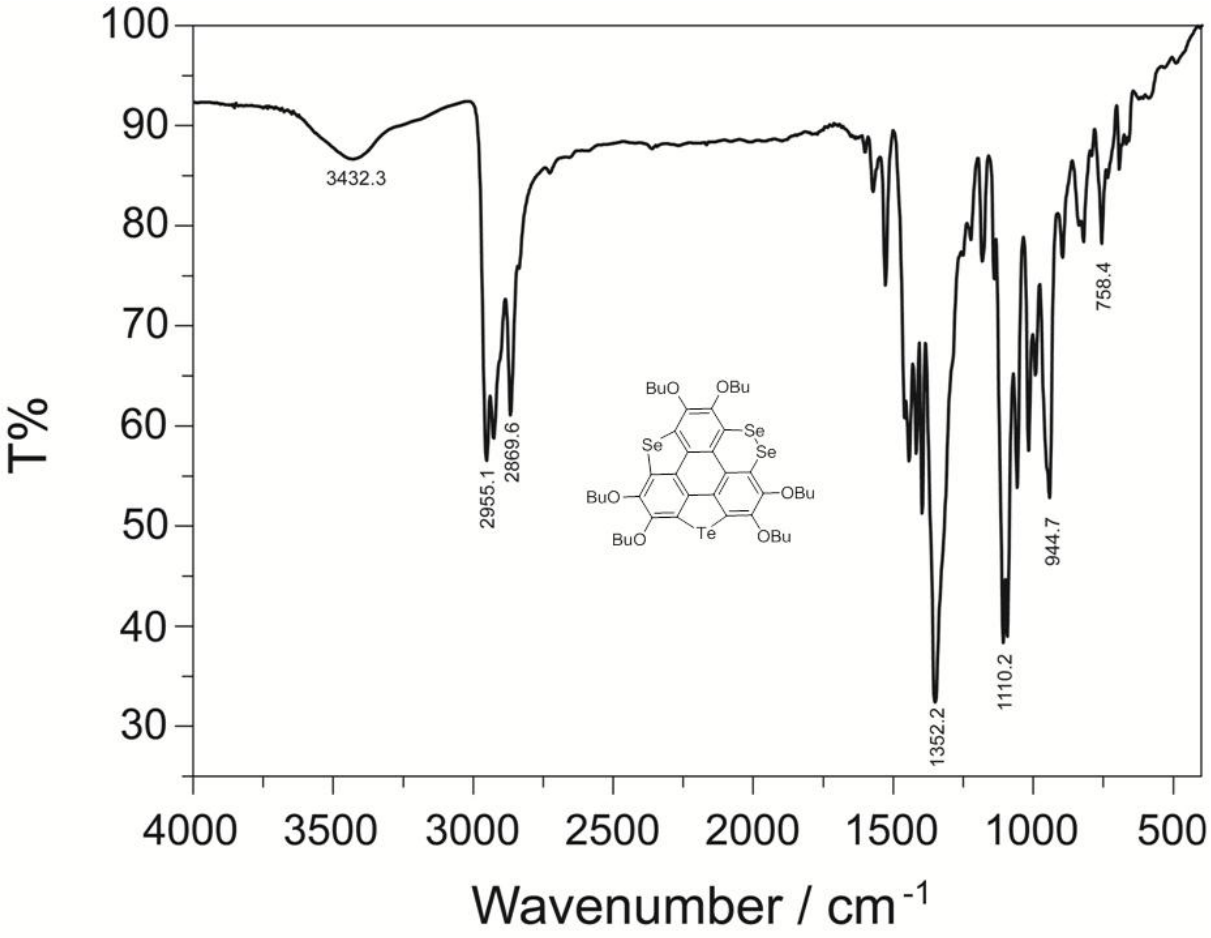

7.27
4.46
4.45
4.43
4.39
4.37
4.36
4.29
4.27
4.26
1.96
1.94
1.93
1.92
1.90
1.89
1.87
1.85
1.83
1.69
1.68
1.67
1.66
1.64
1.62
1.61
1.59
1.57
1.26
1.07
1.06
1.05
1.05
1.03
1.03
BuO
OBu
Se
Se
Se
BuO
OBu
BuO
S
OBu
4.10
4.00
4.00
12.40
12.70
18.47
f1 (ppm)

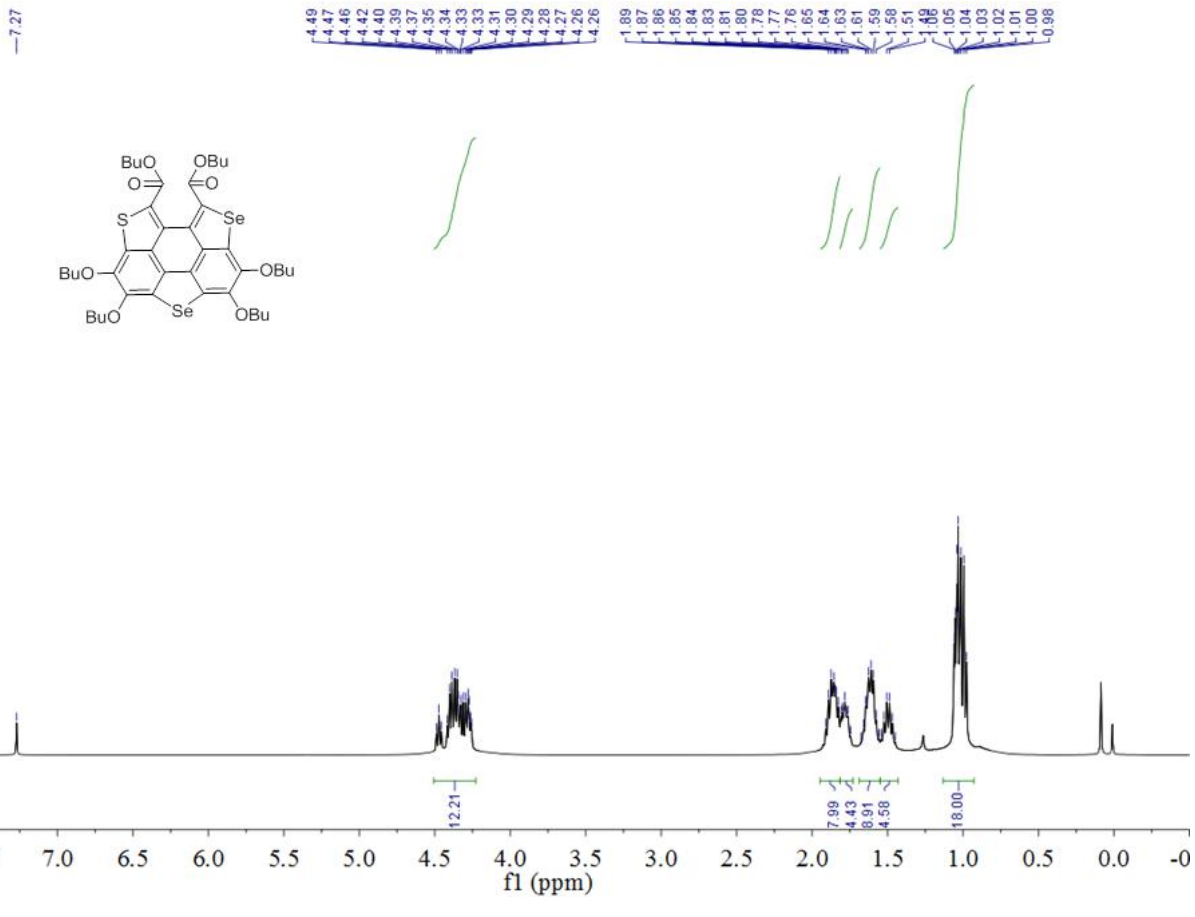

149.32
148.20
147.22
147.06
146.95
146.13
131.68
130.68
129.94
129.59
127.23
126.39
125.79
124.72
124.01
122.72
115.13
114.90
77.39
77.07
76.75
74.26
74.24
73.12
73.05
72.84
72.77
32.62
32.49
32.44
32.40
32.38
19.46
19.40
19.37
19.33
19.29
14.11
14.01
BuO
OBu
Se
Se
Se
BuO
OBu
BuO
S
OBu
f1 (ppm)

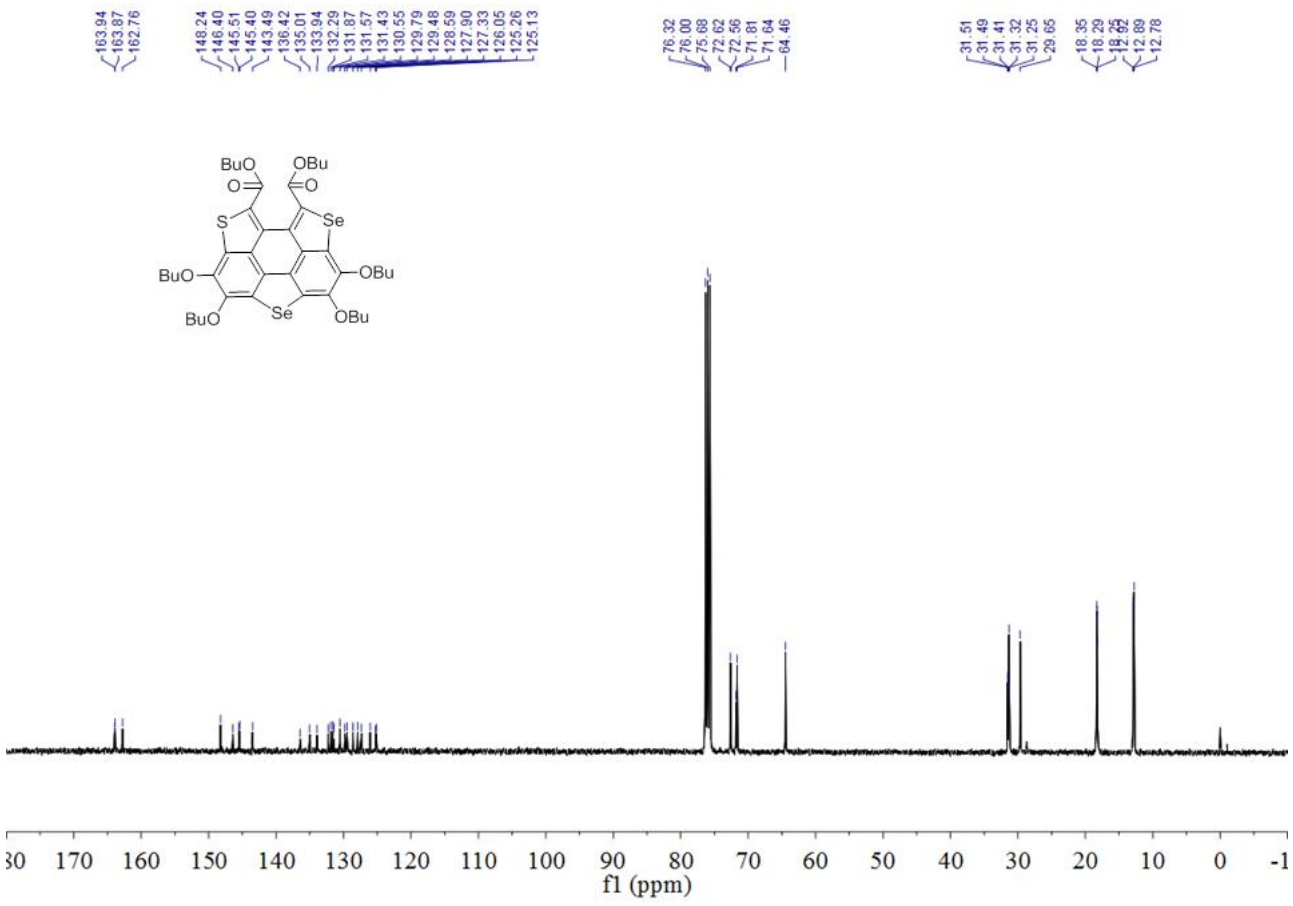

100
90
80
70
60
50
40
T%
3429.1
2955.3
2869.2
1351.1
1118.5
952.9
BuO
OBu
Se
Se
Se
BuO
OBu
BuO
S
OBu
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber / cm -1

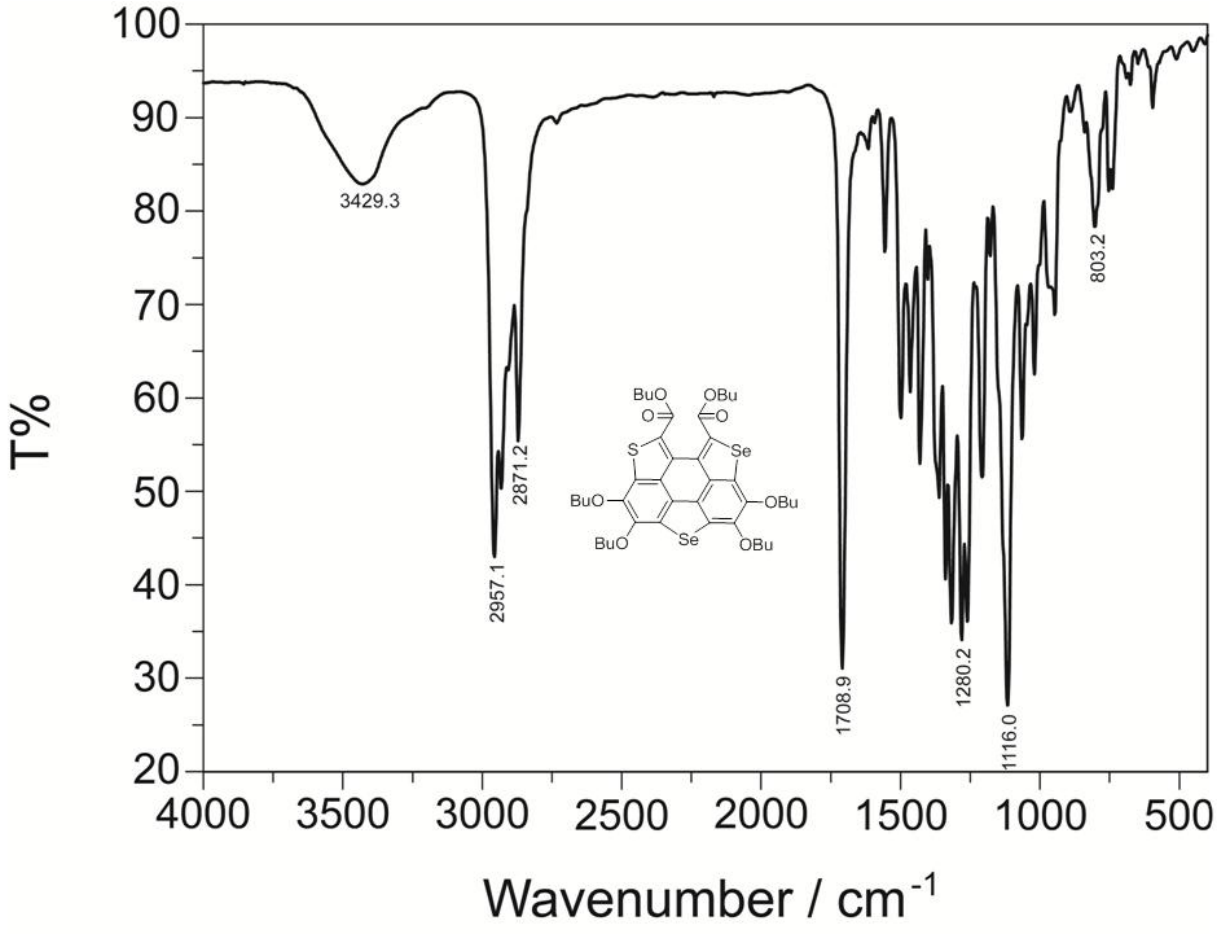

7.27
4.38
4.38
4.37
4.36
4.35
4.34
4.33
4.32
4.31
4.30
4.29
4.28
4.26
4.25
1.93
1.92
1.90
1.89
1.89
1.88
1.87
1.86
1.85
1.84
1.83
1.82
1.67
1.65
1.65
1.63
1.61
1.60
1.59
1.58
1.07
1.06
1.05
1.04
1.03
1.02
BuO
OBu
Se
Se
Se
BuO
OBu
BuO
Te
OBu
4.03
8.00
12.14
12.00
18.00
.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0

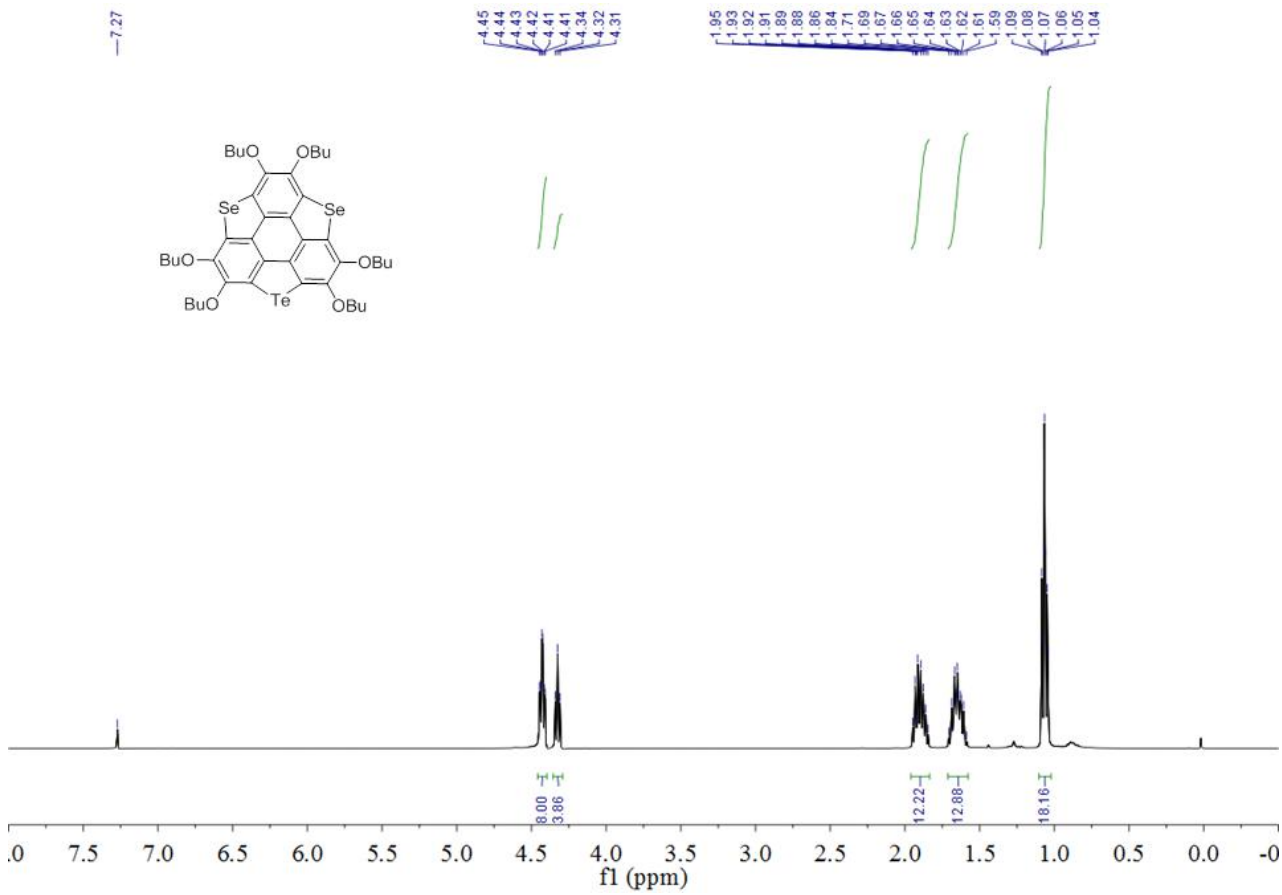

152.94
152.01
148.94
147.67
146.97
146.40
136.64
134.43
131.97
131.61
130.51
128.78
126.44
126.42
122.13
117.07
115.99
113.90
77.39
77.07
76.75
74.22
74.09
73.39
73.15
73.07
73.04
32.79
32.73
32.61
32.58
32.56
32.53
19.54
19.47
19.41
19.38
14.10
14.05
14.01
BuO
OBu
Se
Se
Se
BuO
OBu
BuO
Te
OBu
50
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

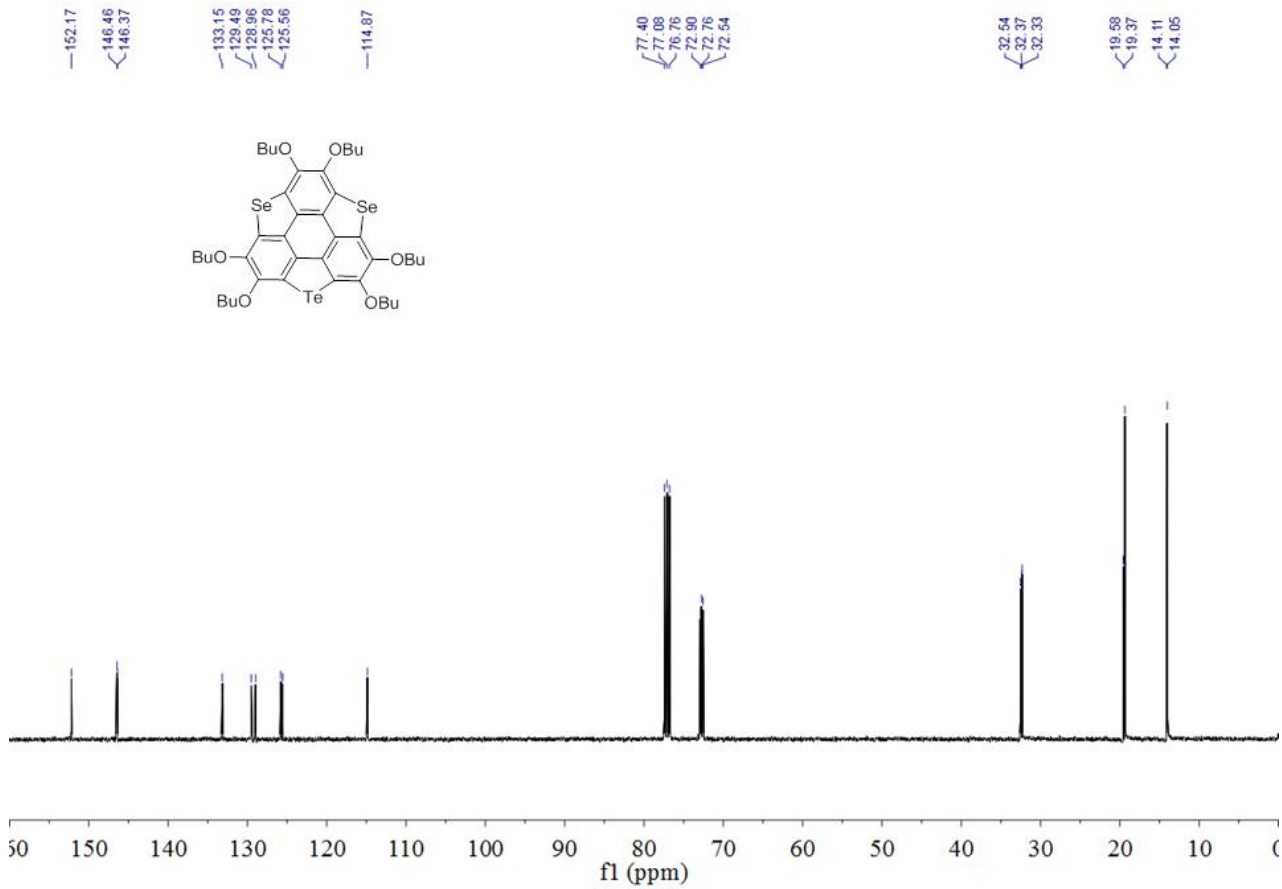

T%
Wavenumber / cm-1
3432.3
2955.1
2869.6
1352.2
1110.2
944.7
758.4
BuO
OBu
Se
Te

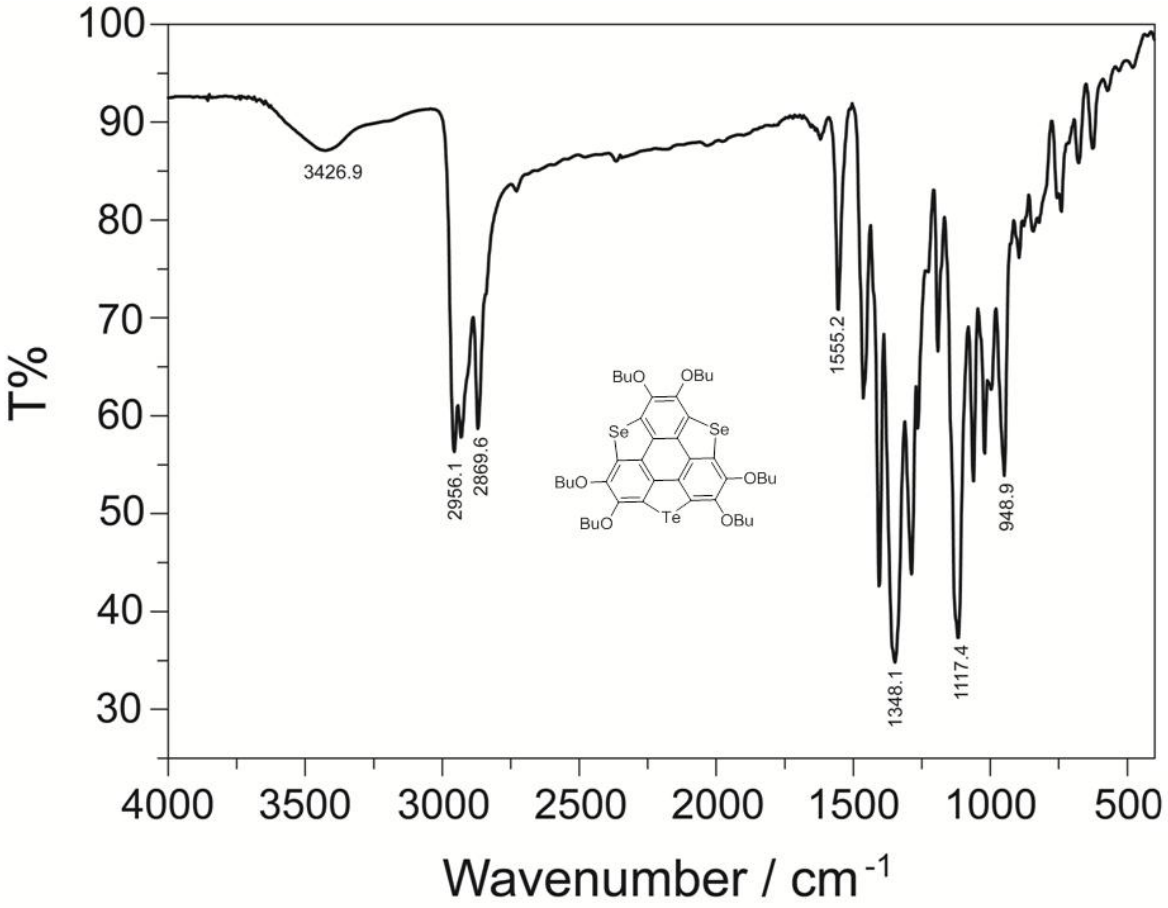

7.27
BuO
OBu
S
Se
f1 (ppm)

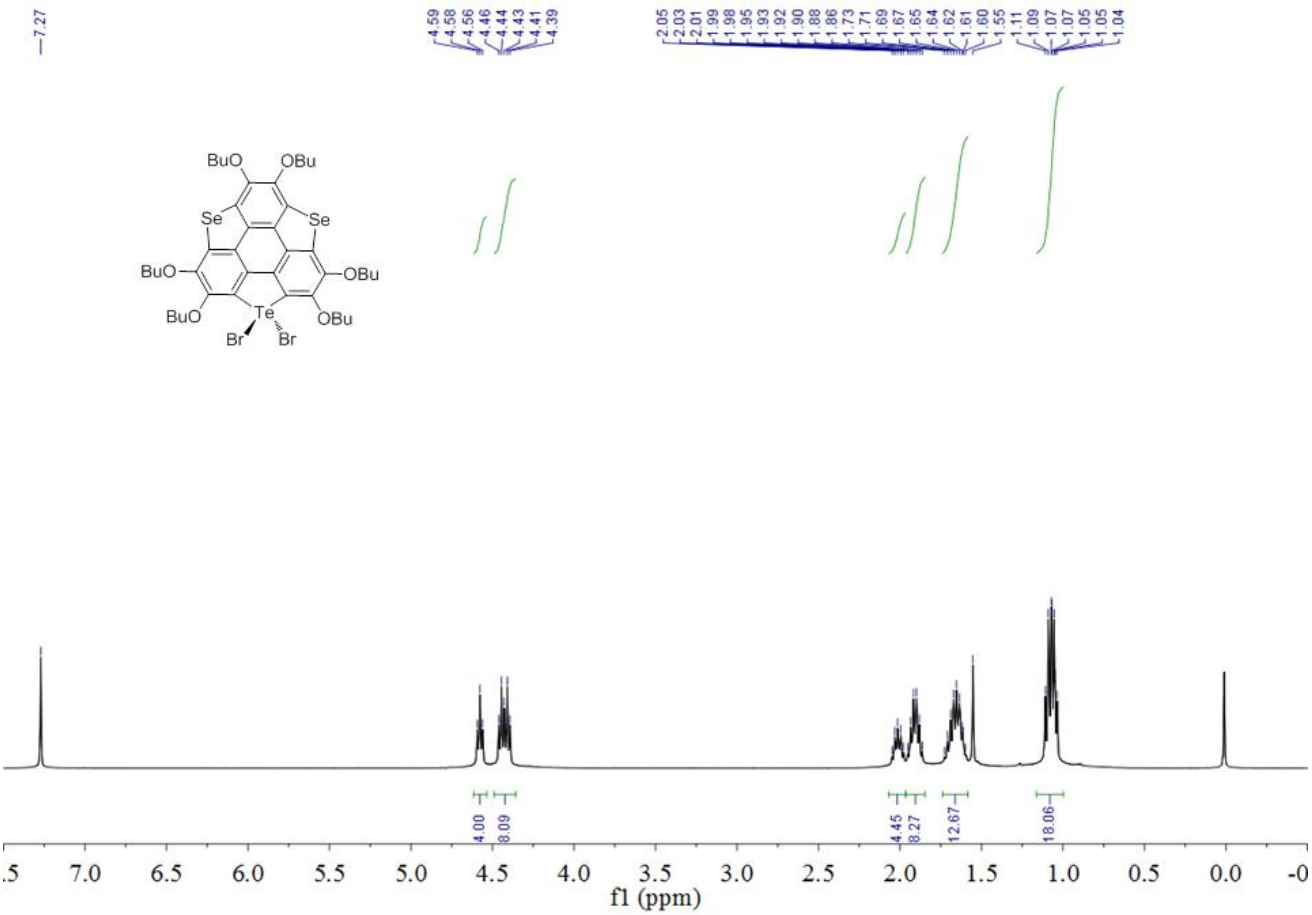

163.94
163.87
162.76
148.24
146.40
145.51
145.40
143.49
136.42
135.01
133.94
132.29
131.87
131.57
131.43
130.55
129.79
129.48
128.59
127.90
127.33
126.05
125.26
125.13
76.32
76.00
75.68
72.62
72.56
71.81
71.64
64.46
31.51
31.49
31.41
31.32
31.25
29.65
18.35
18.29
12.92
12.89
12.78
BuO
OBu
S
Se
BuO
OBu
BuO
Se
OBu
f1 (ppm)

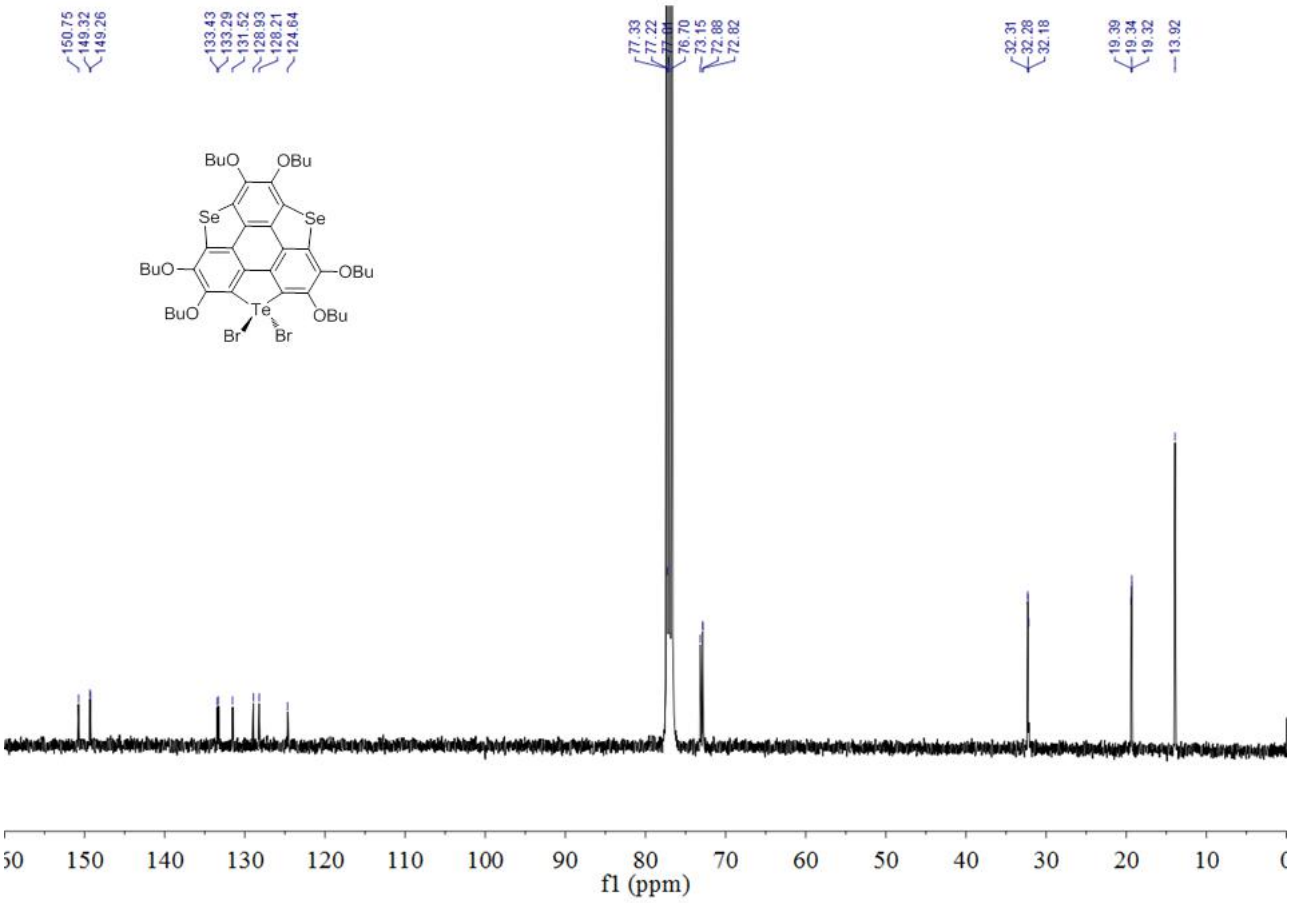

T%
Wavenumber / cm-1
3429.3
2957.1
2871.2
1708.9
1280.2
1116.0
803.2
BuO
OBu
S
Se
BuO
OBu
BuO
Se
OBu

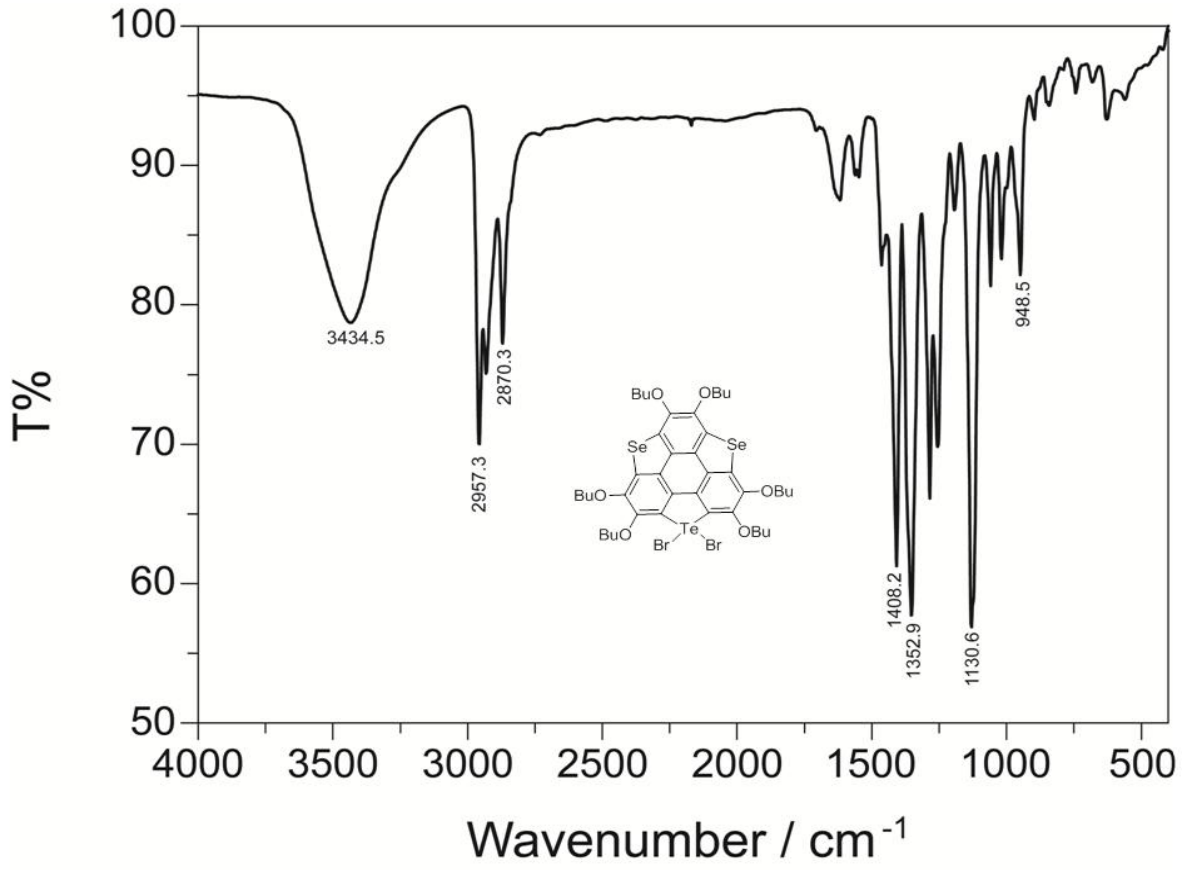

7.27
4.45
4.44
4.43
4.42
4.41
4.41
4.34
4.32
4.31
1.95
1.93
1.92
1.91
1.89
1.88
1.86
1.84
1.71
1.69
1.67
1.66
1.65
1.64
1.63
1.62
1.61
1.59
1.09
1.08
1.07
1.06
1.05
1.04
BuO
OBu
Se
Se
BuO
OBu
BuO
Te
OBu
8.00
3.86
12.22
12.88
18.16
f1 (ppm)

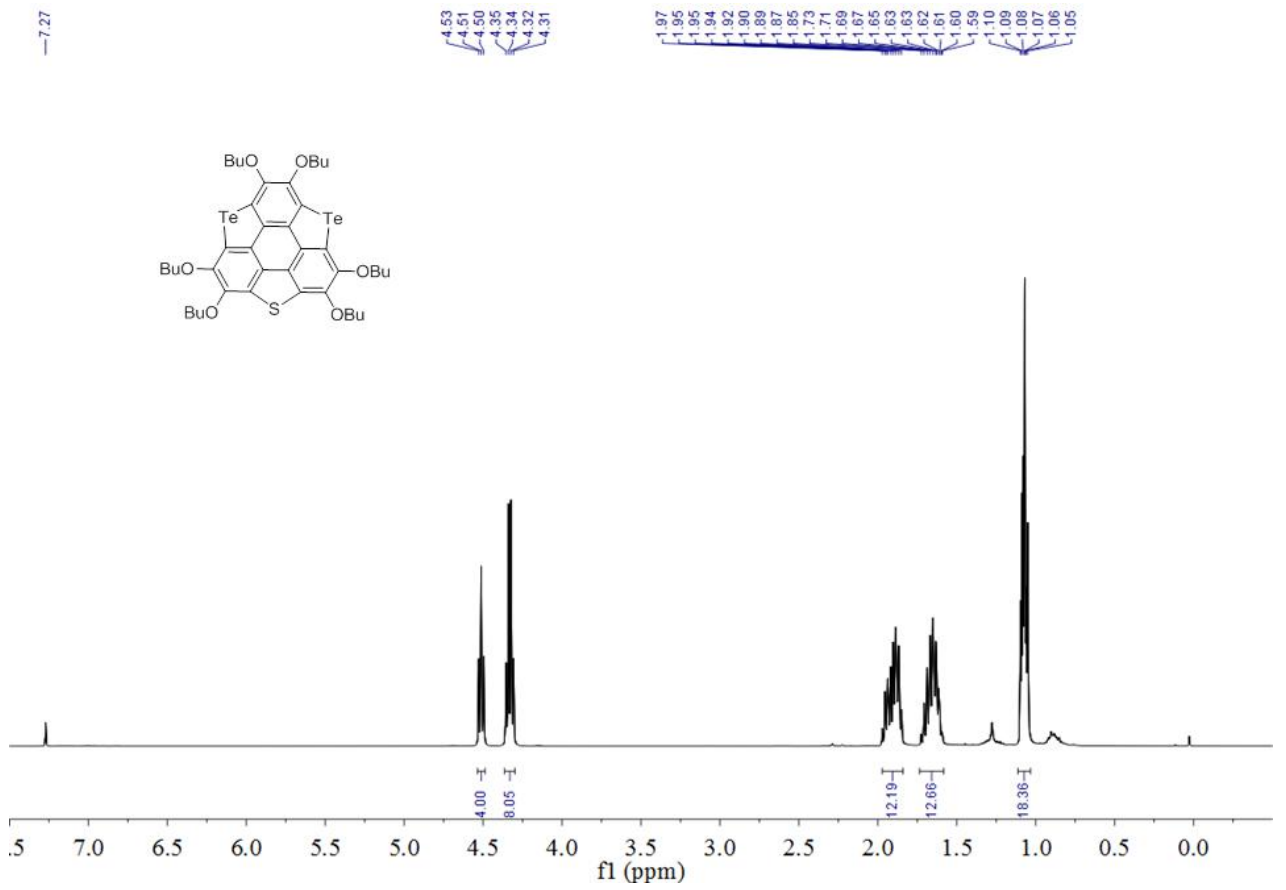

152.17
146.46
146.37
133.15
129.49
128.96
125.78
125.56
114.87
77.40
77.08
76.76
72.90
72.76
72.54
32.54
32.37
32.33
19.58
19.37
14.11
14.05
BuO
OBu
Se
Se
BuO
OBu
BuO
Te
OBu
f1 (ppm)

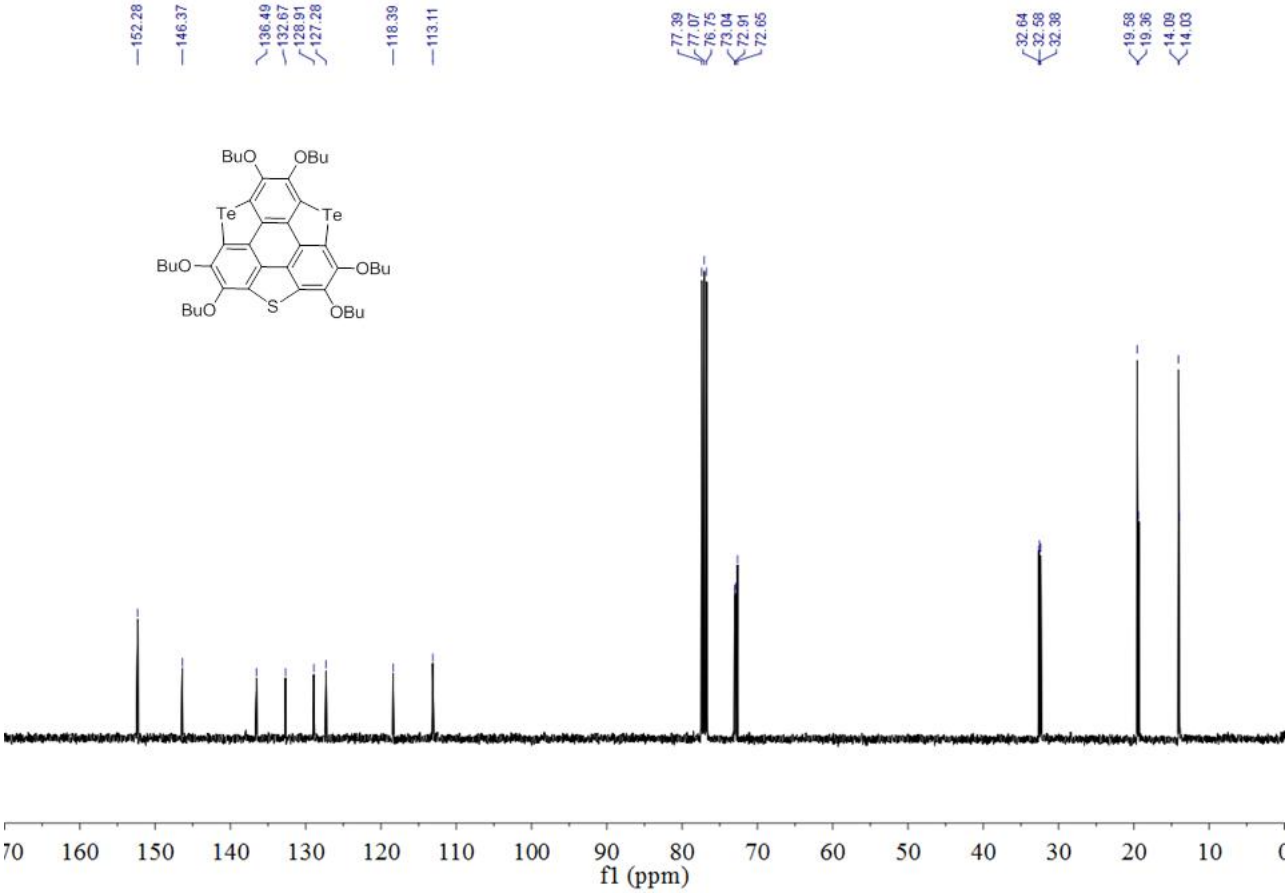

T%
Wavenumber / cm-1
3426.9
2956.1
2869.6
1555.2
1348.1
1117.4
948.9
BuO
OBu
Se
Te

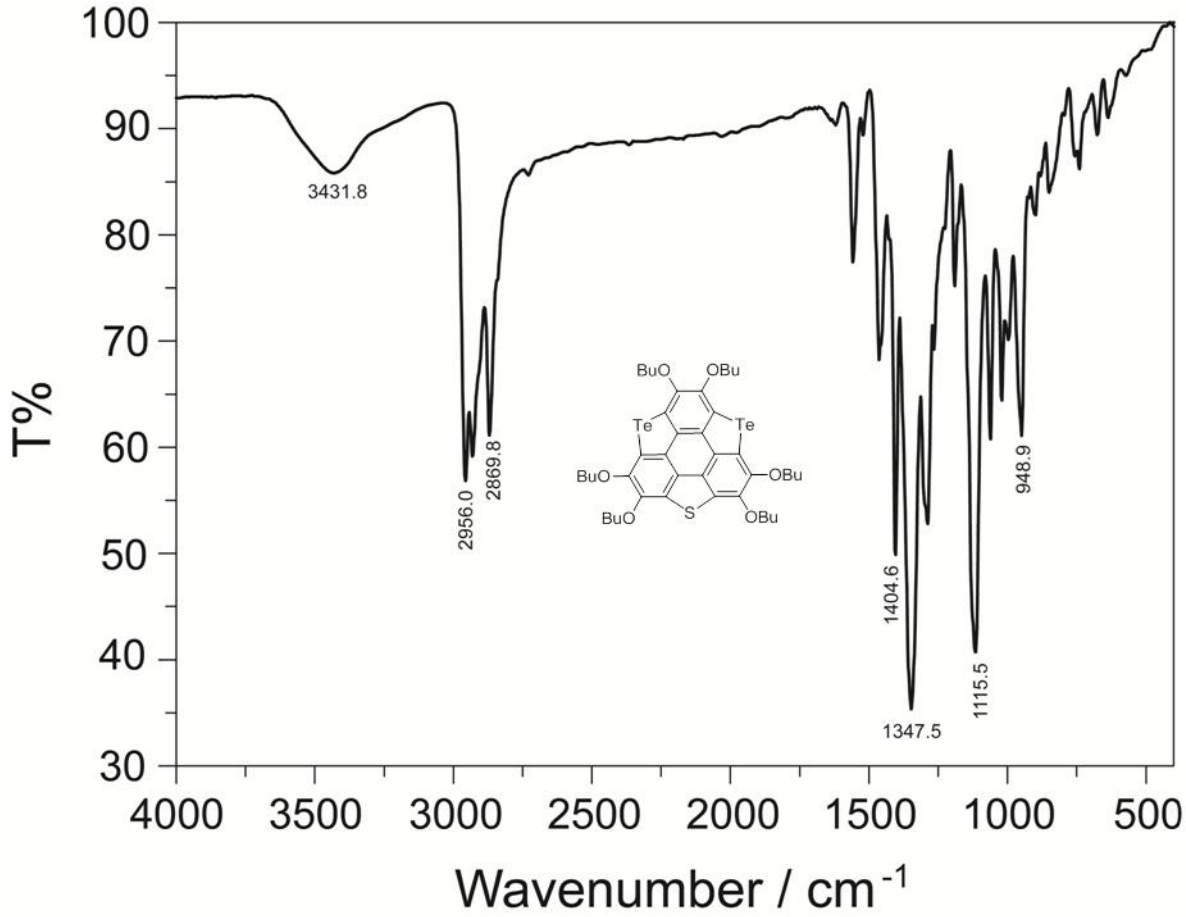

7.27
4.59
4.58
4.56
4.46
4.44
4.43
4.41
4.39
2.05
2.03
2.01
1.99
1.98
1.95
1.93
1.92
1.90
1.88
1.86
1.73
1.71
1.69
1.67
1.65
1.64
1.62
1.61
1.60
1.55
1.11
1.09
1.07
1.07
1.05
1.05
1.04
BuO
OBu
Se
Te
Br
4.00
8.09
4.45
8.27
12.67
18.06
f1 (ppm)

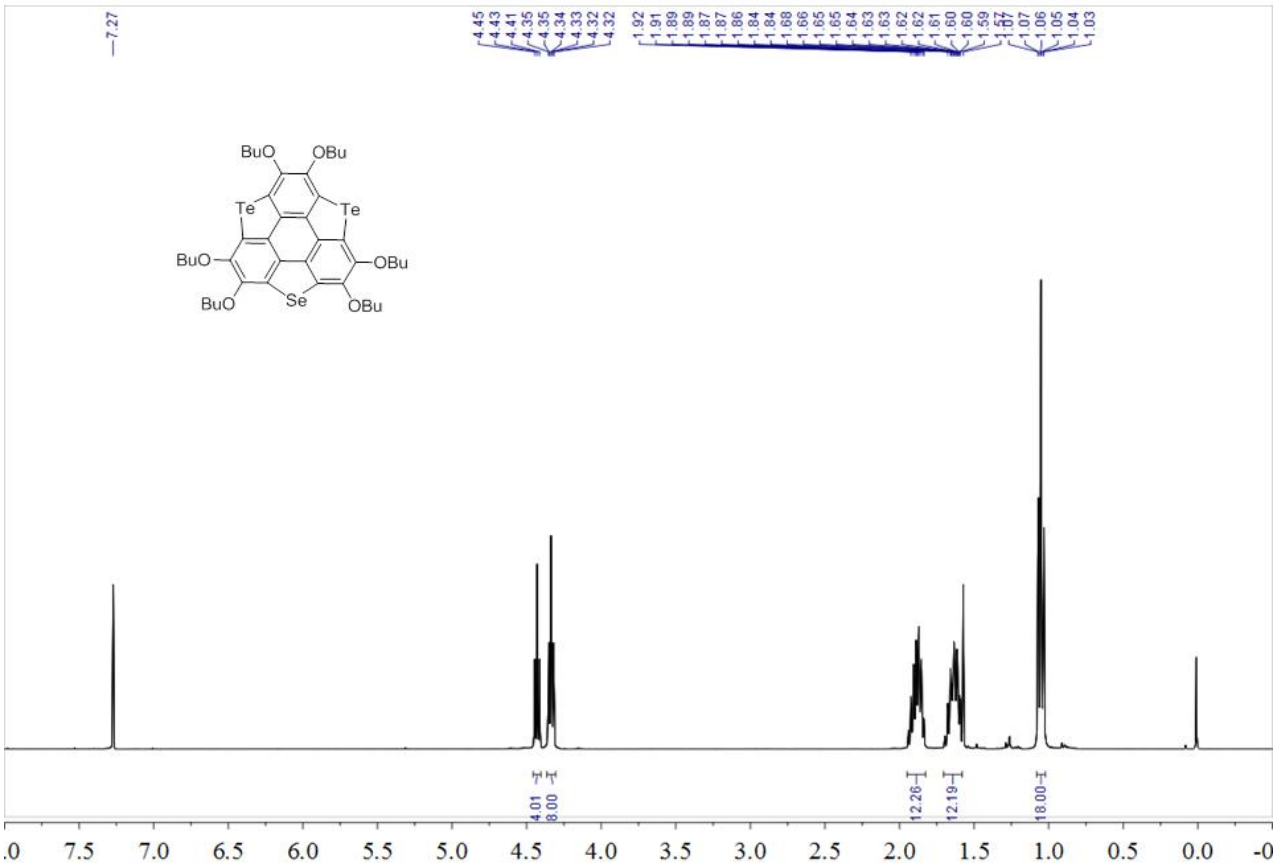

150.75
149.32
149.26
133.43
133.29
131.52
128.93
128.21
124.64
77.33
77.22
77.01
76.70
73.15
72.88
72.82
32.31
32.28
32.18
19.39
19.34
19.32
13.92
BuO
OBu
Se
Se
BuO
OBu
BuO
Te
OBu
Br
Br
f1 (ppm)

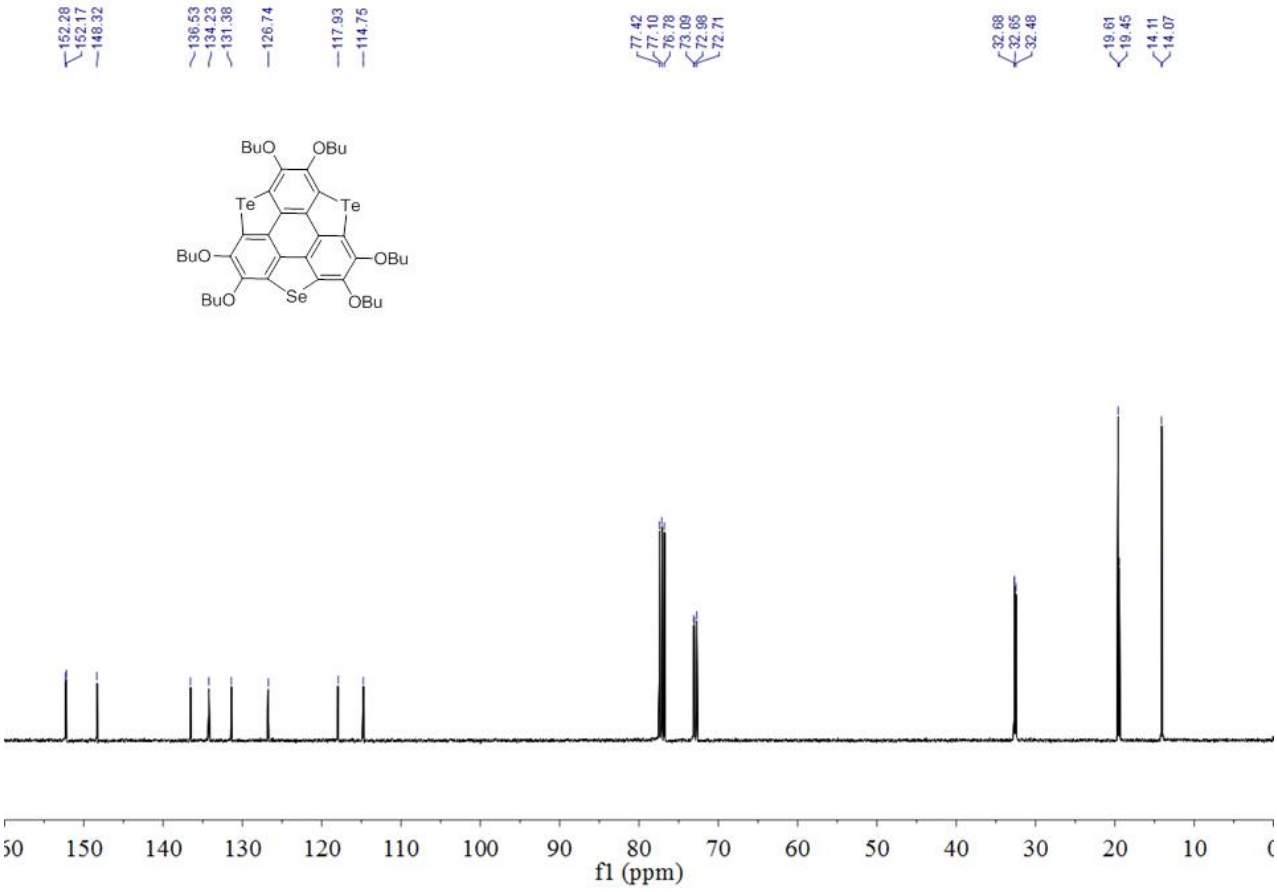

T%
3434.5
2957.3
2870.3
1408.2
1352.9
1130.6
948.5
Wavenumber / cm -1

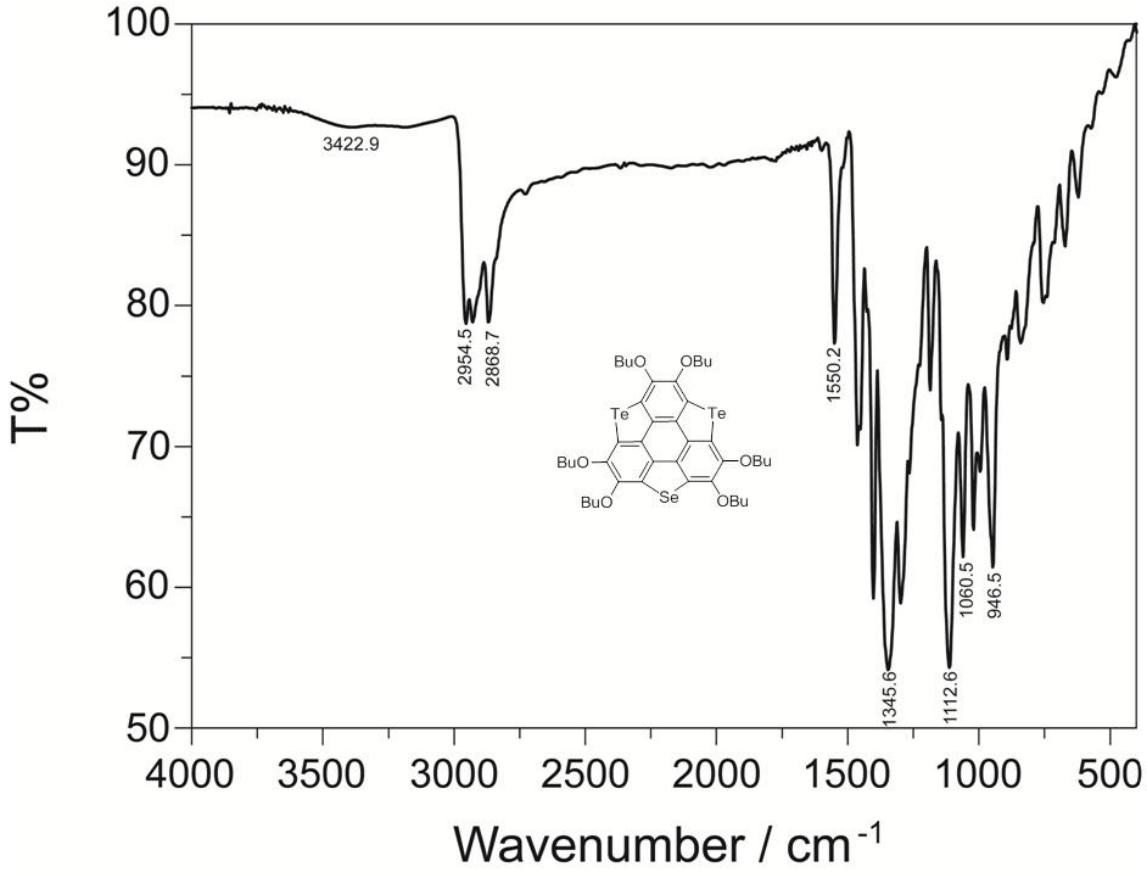

7.27
4.53
4.51
4.50
4.35
4.34
4.32
4.31
1.97
1.95
1.95
1.94
1.92
1.90
1.89
1.87
1.85
1.73
1.71
1.69
1.67
1.65
1.63
1.63
1.62
1.61
1.60
1.59
1.10
1.09
1.08
1.07
1.06
1.05
BuO
OBu
Te
Te
BuO
OBu
BuO
S
OBu
4.00
8.05
12.19
12.66
18.36
f1 (ppm)

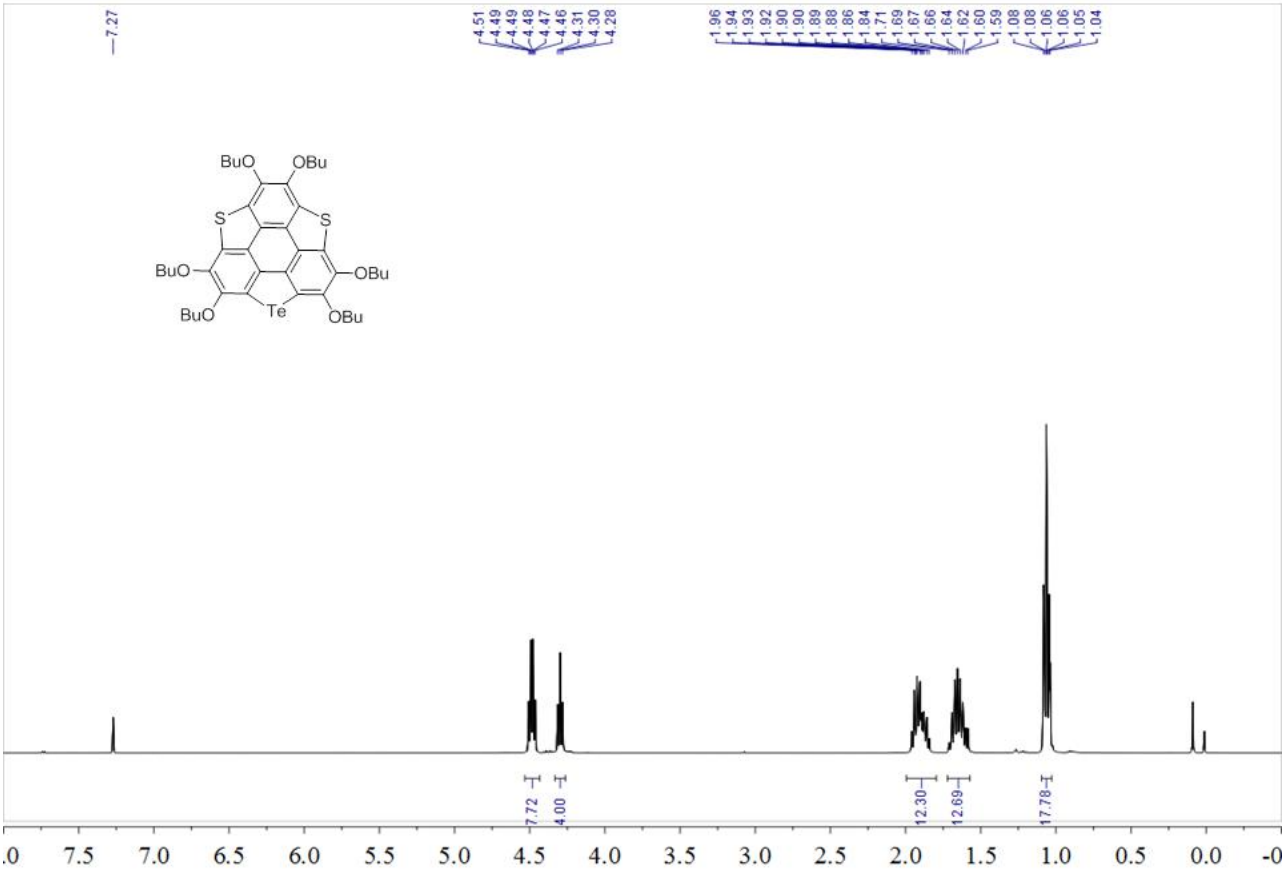

152.28
146.37
136.49
132.67
128.91
127.28
118.39
113.11
77.39
77.07
76.75
73.04
72.91
72.65
32.64
32.58
32.38
19.58
19.36
14.09
14.03
BuO
OBu
Te
Te
BuO
OBu
BuO
S
OBu
f1 (ppm)

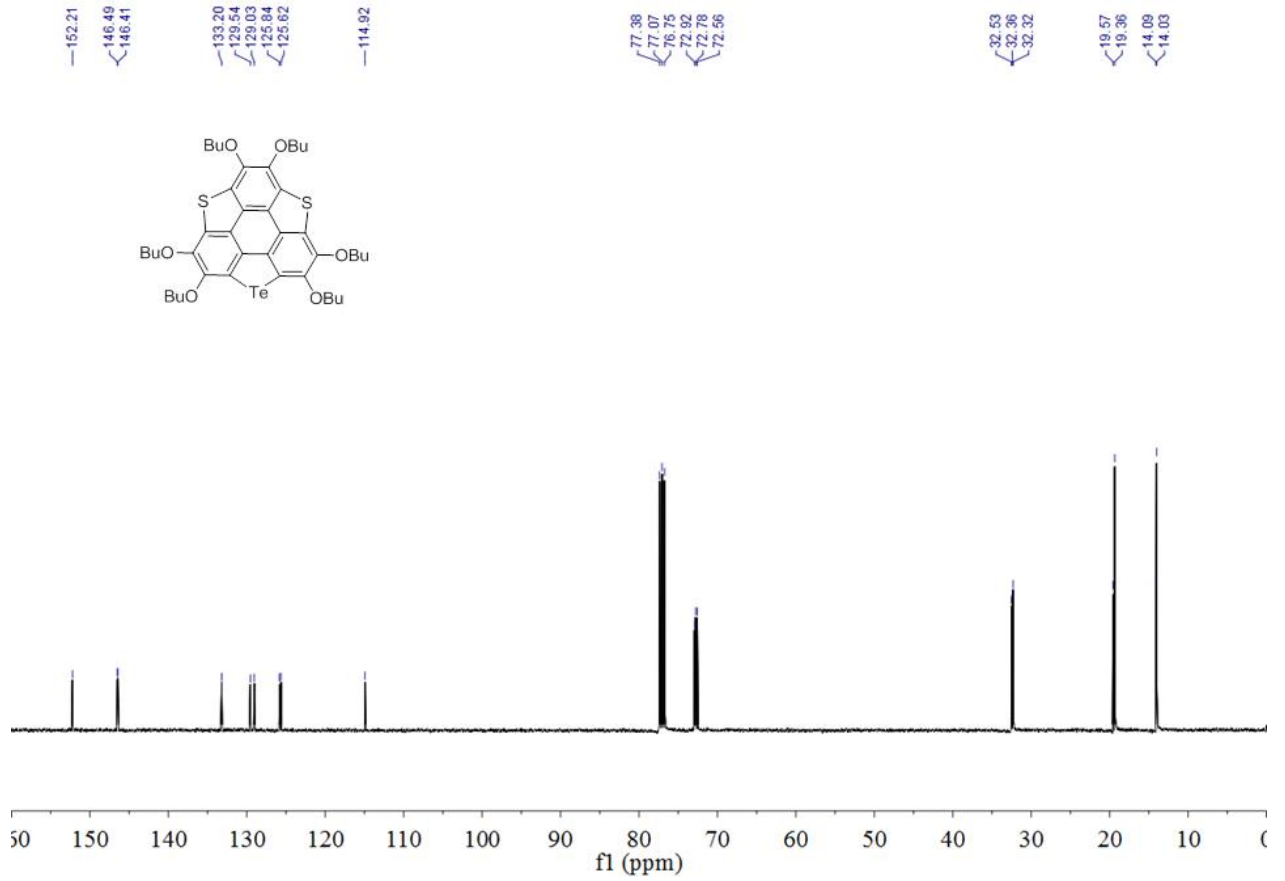

T%
Wavenumber / cm-1
3431.8
2956.0
2869.8
1404.6
1347.5
1115.5
948.9
BuO
OBu
Te
Te
BuO
OBu
BuO
S
OBu

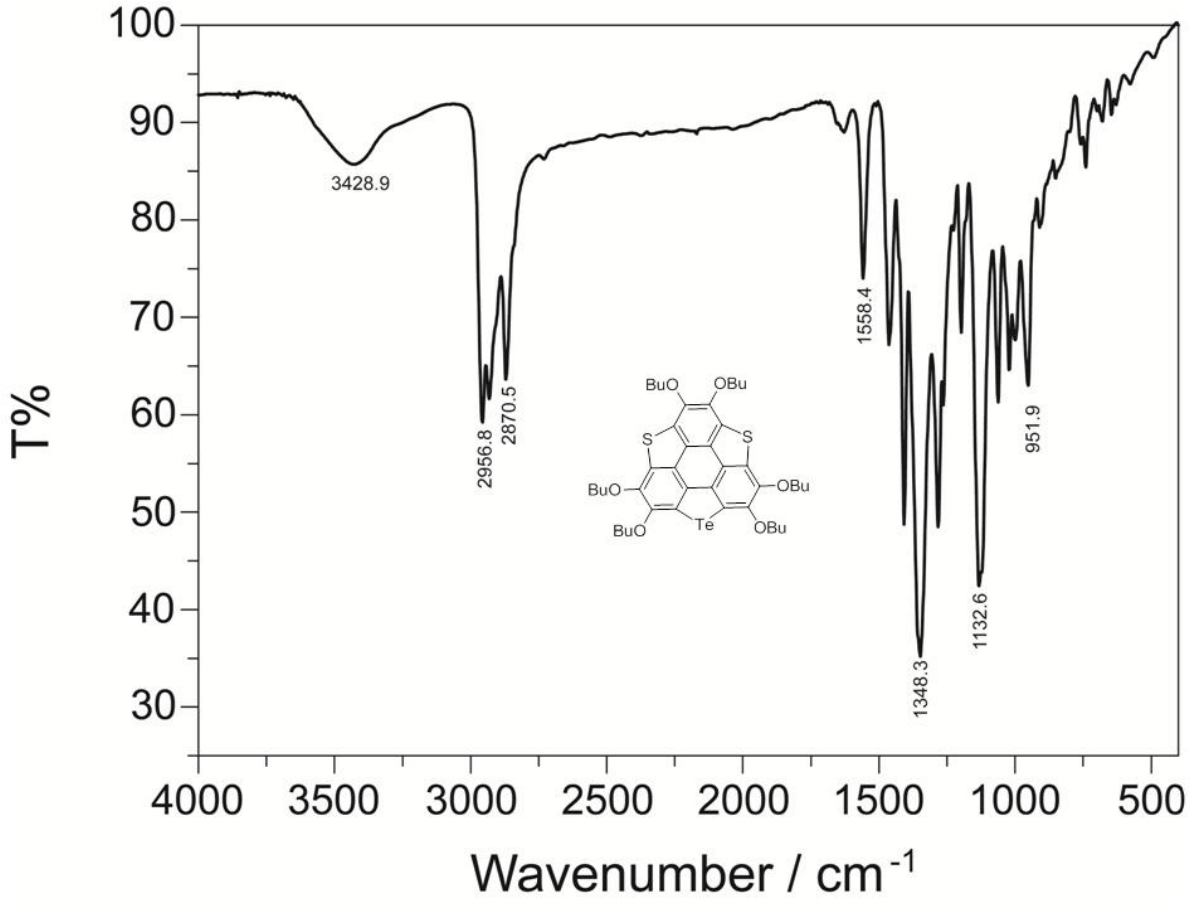

7.27
BuO
OBu
Te
Te
BuO
OBu
BuO
Se
OBu
4.01
8.00
12.26
12.19
18.00

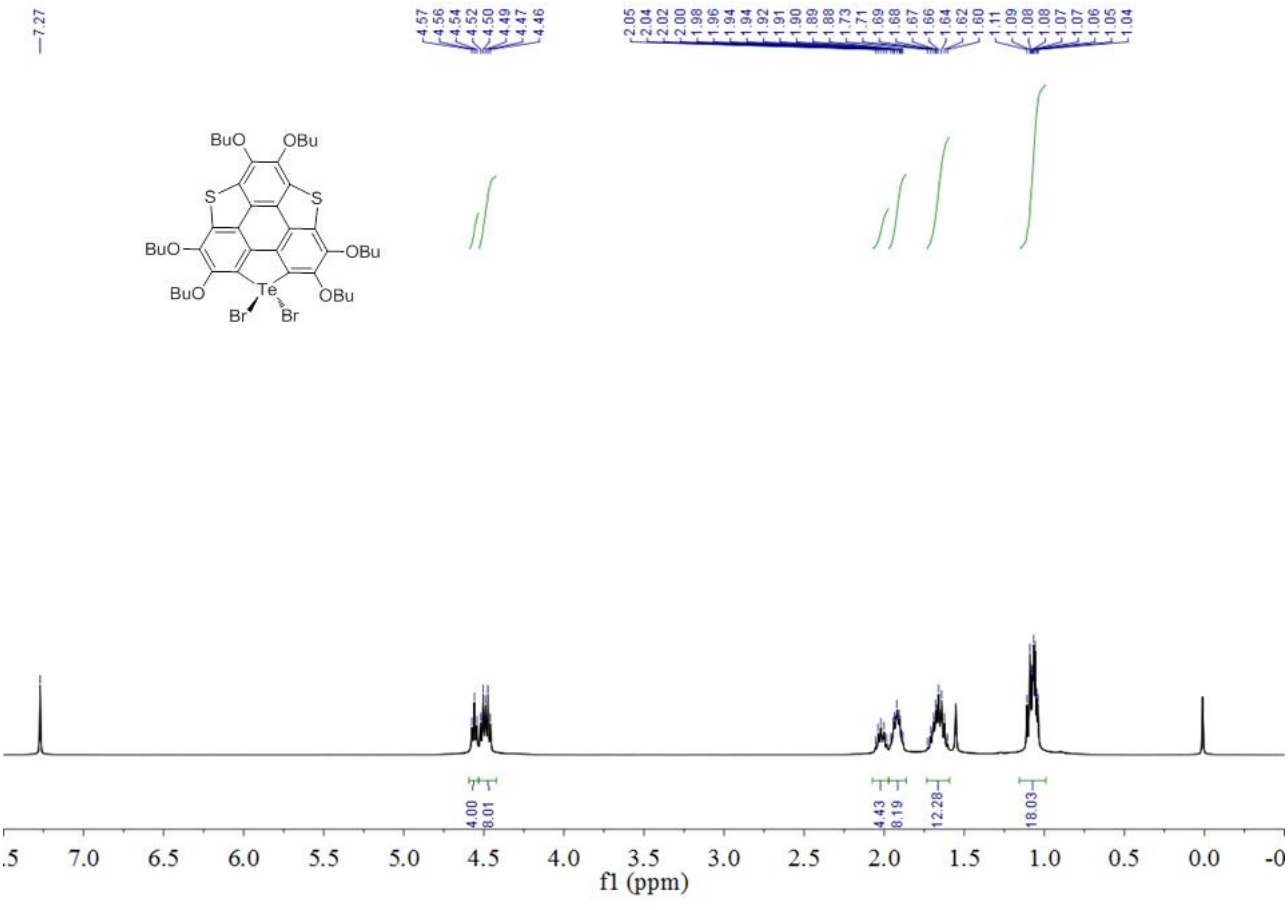

152.28
152.17
148.32
136.53
134.23
131.38
126.74
117.93
114.75
77.42
77.10
76.78
73.09
72.98
72.71
32.68
32.65
32.48
19.61
19.45
14.11
14.07
BuO
OBu
Te
Te
BuO
OBu
BuO
Se
OBu
f1 (ppm)

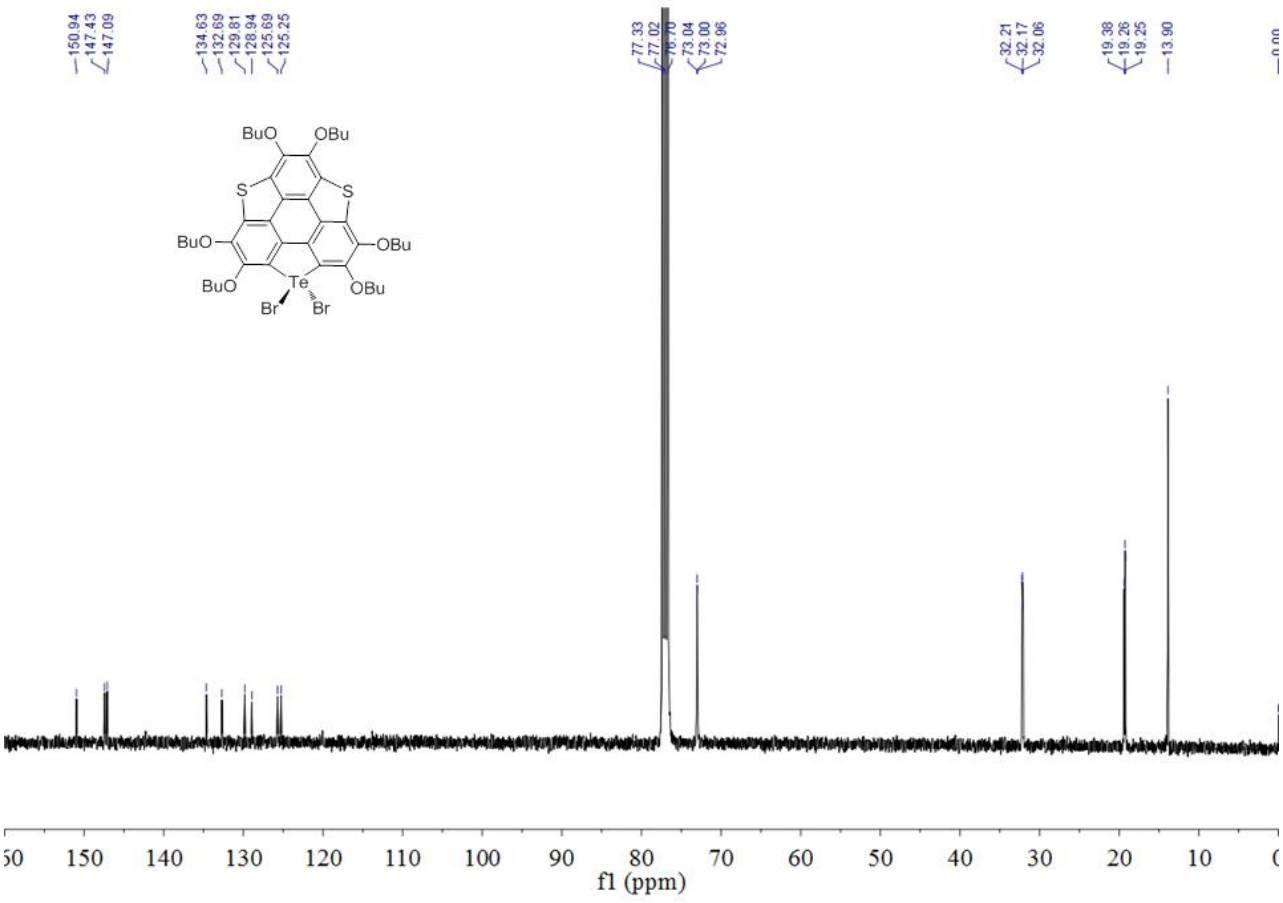

T%
3422.9
2954.5
2868.7
1550.2
1345.6
1112.6
1060.5
946.5
Wavenumber / cm-1

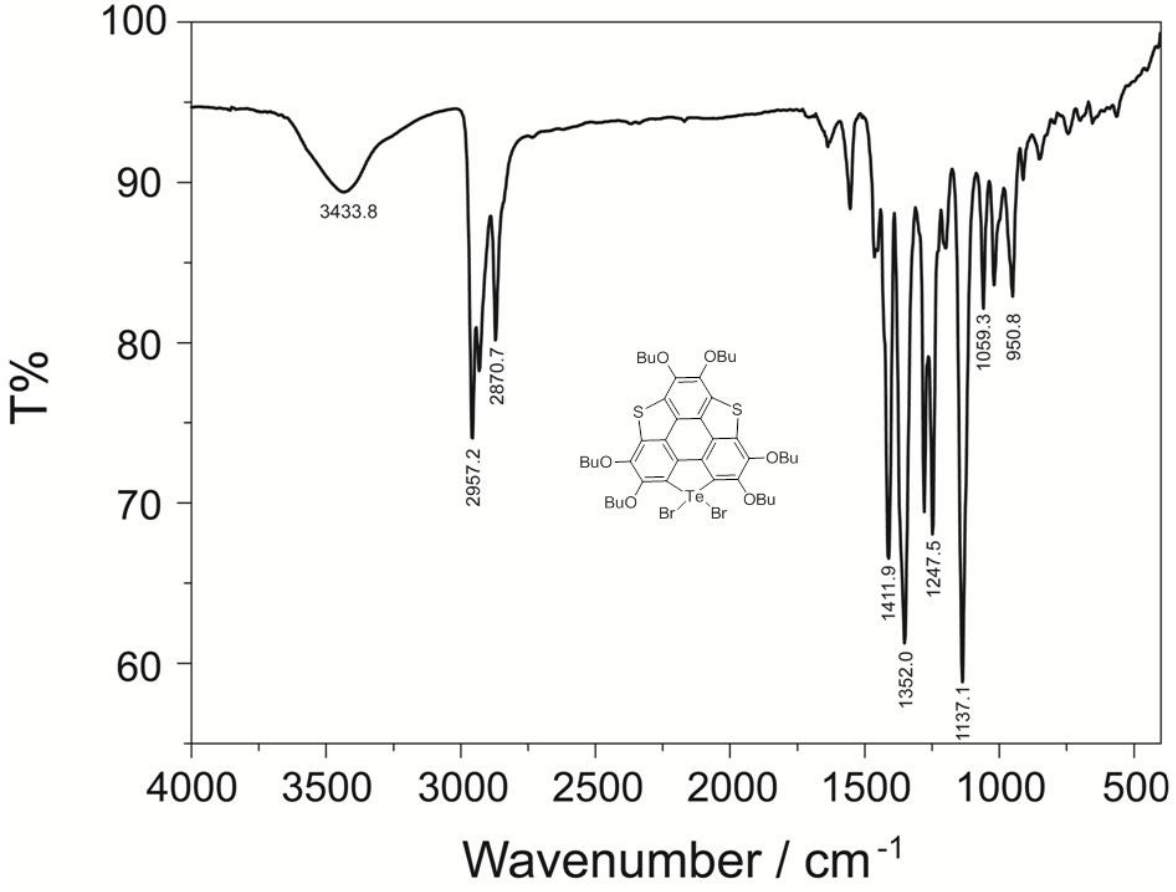

7.27
4.51
4.49
4.49
4.48
4.47
4.46
4.31
4.30
4.28
1.96
1.94
1.93
1.92
1.90
1.90
1.89
1.88
1.86
1.84
1.71
1.69
1.67
1.66
1.64
1.62
1.60
1.59
1.08
1.08
1.06
1.06
1.05
1.04
BuO
OBu
S
S
BuO
OBu
BuO
Te
OBu
7.72
4.00
12.30
12.69
17.78
.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0


152.21
146.49
146.41
133.20
129.54
129.03
125.84
125.62
114.92
77.38
77.07
76.75
72.92
72.78
72.56
32.53
32.36
32.32
19.57
19.36
14.09
14.03
BuO
OBu
S
S
BuO
OBu
BuO
Te
OBu
50
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


T%
Wavenumber / cm-1
3428.9
2956.8
2870.5
1558.4
1348.3
1132.6
951.9
BuO
OBu
S
Te
Br


7.27
4.57
4.56
4.54
4.52
4.50
4.49
4.47
4.46
2.05
2.04
2.02
2.00
1.98
1.96
1.94
1.92
1.91
1.90
1.89
1.88
1.73
1.71
1.69
1.68
1.67
1.66
1.64
1.62
1.60
1.11
1.09
1.08
1.08
1.07
1.07
1.06
1.05
1.04
BuO
OBu
S
Te
Br
4.00
8.01
4.43
8.19
12.28
18.03
f1 (ppm)


150.94
147.43
147.09
134.63
132.69
129.81
128.94
125.69
125.25
77.33
77.02
76.70
73.04
73.00
72.96
32.21
32.17
32.06
19.38
19.26
19.25
13.90
BuO
OBu
S
S
BuO
OBu
BuO
OBu
Te
Br
Br
f1 (ppm)


T%
100
90
80
70
60
3433.8
2957.2
2870.7
1411.9
1352.0
1247.5
1137.1
1059.3
950.8
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber / cm-1
BuO
OBu
S
S
BuO
OBu
BuO
OBu
Te
Br
Br

9. Cartesian Coordinate

1’

C	2.39016300	-0.16557200	1.45304400
C	1.28682100	-0.56914800	0.69558600
C	1.28682100	-0.56914800	-0.69558600
C	2.39016300	-0.16557200	-1.45304400
C	3.56735800	0.14170100	-0.72810200
C	3.56735800	0.14170100	0.72810200
C	0.05838800	-0.63476200	1.39761700
C	-1.14679200	-0.71265100	0.70648100
C	-1.14679200	-0.71265100	-0.70648100
C	0.05838800	-0.63476200	-1.39761700
C	0.11493000	-0.28335600	2.74298800
C	-1.11552900	-0.07432700	3.40915000
C	-2.36114700	-0.12611500	2.68378200
C	-2.37186400	-0.41515100	1.30057000
C	-2.37186400	-0.41515100	-1.30057000
C	-2.36114700	-0.12611500	-2.68378200
C	-1.11552900	-0.07432700	-3.40915000
C	0.11493000	-0.28335600	-2.74298800
S	1.83225400	0.04510300	3.17926300
S	1.83225400	0.04510300	-3.17926300
O	-1.12196400	0.29339000	4.72399400
C	-1.59462800	-0.68889700	5.64923400
O	-3.53029900	0.14701300	3.33504600
C	-3.76529000	1.51808400	3.67174600
O	-3.53029900	0.14701300	-3.33504600
C	-3.76529000	1.51808400	-3.67174600
O	-1.12196400	0.29339000	-4.72399400
C	-1.59462800	-0.68889700	-5.64923400
O	4.75248300	0.51280600	1.26315700

C	4.98489100	0.33239500	2.64985100
O	4.75248300	0.51280600	-1.26315700
C	4.98489100	0.33239500	-2.64985100
H	-2.64351900	-0.95588600	5.44640300
H	-0.96943200	-1.59704200	5.60781200
H	-2.99606700	1.89732400	4.36167800
H	-3.78775700	2.14418700	2.76389400
H	-3.78775700	2.14418700	-2.76389400
H	-2.99606700	1.89732400	-4.36167800
H	-0.96943200	-1.59704200	-5.60781200
H	-2.64351900	-0.95588600	-5.44640300
H	4.39522800	1.03749800	3.25900000
H	4.76299900	-0.70148800	2.96349300
H	4.76299900	-0.70148800	-2.96349300
H	4.39522800	1.03749800	-3.25900000
H	-1.51744400	-0.24234600	6.64964400
H	-4.74815200	1.55688800	4.16022900
H	-4.74815200	1.55688800	-4.16022900
H	-1.51744400	-0.24234600	-6.64964400
H	6.05101400	0.53642000	-2.81553400
H	6.05101400	0.53642000	2.81553400
S	-3.61856300	-0.24451200	0.00000000

2’

C	2.45134000	-0.05254100	1.45157600
C	1.27018200	-0.03199000	0.69718800
C	1.27018200	-0.03199000	-0.69718800
C	2.45134000	-0.05254100	-1.45157600
C	3.66250900	-0.07685700	-0.72893000
C	3.66250900	-0.07685700	0.72893000
C	0.03580100	-0.00293000	1.39979300
C	-1.17247000	0.03028000	0.70691800
C	-1.17247000	0.03028000	-0.70691800
C	0.03580100	-0.00293000	-1.39979300
C	0.07035500	0.00464300	2.79261500
C	-1.15557700	0.03759900	3.48502500
C	-2.40401800	0.04161900	2.76324400
C	-2.40753300	0.04801300	1.35523800
C	-2.40753300	0.04801300	-1.35523800
C	-2.40401800	0.04161900	-2.76324400
C	-1.15557700	0.03759900	-3.48502500
C	0.07035500	0.00464300	-2.79261500
Se	1.92409000	-0.03356400	3.35184900
Se	1.92409000	-0.03356400	-3.35184900
O	-1.15768500	0.02723600	4.85220600
C	-1.56055600	1.24026800	5.49481700
O	-3.58715300	0.07783300	3.44665800
C	-3.95406000	-1.11622800	4.14366400
O	-3.58715300	0.07783300	-3.44665800
C	-3.95406000	-1.11622800	-4.14366400
O	-1.15768500	0.02723600	-4.85220600
C	-1.56055600	1.24026800	-5.49481700
O	4.91006900	-0.10004800	-1.25140300
C	5.09898100	-0.13858400	-2.65338100

O	4.91006900	-0.10004800	1.25140300
C	5.09898100	-0.13858400	2.65338100
H	-0.89960800	2.07417800	5.20375200
H	-2.60275000	1.49644600	5.24971200
H	-4.04532000	-1.96429000	3.44400700
H	-3.22068400	-1.36423600	4.92631500
H	-3.22068400	-1.36423600	-4.92631500
H	-4.04532000	-1.96429000	-3.44400700
H	-2.60275000	1.49644600	-5.24971200
H	-0.89960800	2.07417800	-5.20375200
H	4.65139600	-1.04247300	-3.09972100
H	4.69353300	0.76219500	-3.14422000
H	4.69353300	0.76219500	3.14422000
H	4.65139600	-1.04247300	3.09972100
H	6.18392700	-0.16713400	2.81907500
H	6.18392700	-0.16713400	-2.81907500
H	-1.46942900	1.06811900	-6.57567400
H	-4.93182600	-0.92257900	-4.60482200
H	-4.93182600	-0.92257900	4.60482200
H	-1.46942900	1.06811900	6.57567400
Se	-3.80646200	0.07418000	0.00000000

3’

C	1.43264300	2.49546000	-0.01294300
C	0.70437400	1.28501800	-0.02273400
C	-0.70434300	1.28503400	-0.02273400
C	-1.43258400	2.49549200	-0.01294100
C	-0.72165500	3.70461300	-0.01076100
C	0.72174000	3.70459800	-0.01076400
C	1.41450500	0.03365800	-0.00734400
C	0.71505700	-1.18620200	-0.00101600
C	-0.71508400	-1.18618500	-0.00101600
C	-1.41450400	0.03369100	-0.00734400
C	2.81652900	0.02643100	0.02971800
C	3.51703900	-1.18571900	0.05292000
C	2.80168000	-2.42310400	0.01220300
C	1.40185500	-2.41137900	0.00301500
C	-1.40191100	-2.41134600	0.00301500
C	-2.80173700	-2.42303800	0.01220300
C	-3.51706600	-1.18563700	0.05292000
C	-2.81652800	0.02649800	0.02971900
O	4.88603900	-1.15984400	0.07658200
C	5.51065700	-1.65269000	1.26574700
O	3.46206900	-3.62217200	0.02430700
C	4.22086400	-3.93977200	-1.14598200
O	-3.46215300	-3.62209100	0.02430700
C	-4.22097900	-3.93966100	-1.14597000
O	-4.88606500	-1.15972900	0.07658400
C	-5.51069100	-1.65258600	1.26574000
O	-1.26314600	4.94870700	0.02140500
C	-2.53919300	5.20053000	-0.53338600
O	1.26325400	4.94868100	0.02139400
C	2.53933200	5.20046900	-0.53334000

H	5.18151400	-1.07566500	2.14641400
H	5.28794900	-2.71887500	1.42475700
H	3.56973500	-3.97159200	-2.03588900
H	5.02922300	-3.21098200	-1.31149400
H	-5.02937400	-3.21089500	-1.31141500
H	-3.56988300	-3.97140800	-2.03590300
H	-5.28806300	-2.71879600	1.42469100
H	-5.18148100	-1.07563300	2.14642800
H	-2.64852500	4.74346000	-1.53070700
H	-3.35788900	4.85785000	0.12479500
H	3.35798900	4.85776400	0.12487800
H	2.64869600	4.74340000	-1.53065700
H	2.62783500	6.29147600	-0.62888400
H	-2.62766100	6.29153900	-0.62893900
H	-6.59229700	-1.51908000	1.13021000
H	-4.65291500	-4.93553100	-0.97930200
H	4.65284700	-4.93561500	-0.97928000
H	6.59226900	-1.51927600	1.13018300
Te	-3.54587100	2.02493700	0.05385300
Te	3.54592000	2.02485300	0.05384700
Te	-0.00004800	-4.02970500	0.00402900

4’

C	-0.11564500	2.57003300	-1.45396800
C	-0.25446700	1.40819300	-0.69363900
C	-0.25446700	1.40819300	0.69363900
C	-0.11564500	2.57003300	1.45396800
C	-0.02791300	3.78250800	0.72908400
C	-0.02791300	3.78250800	-0.72908400
C	-0.22022800	0.18688400	-1.40336900
C	-0.19228500	-1.01598500	-0.70749400
C	-0.19228500	-1.01598500	0.70749400
C	-0.22022800	0.18688400	1.40336900
C	-0.05249900	0.28318900	-2.78692500
C	0.11062100	-0.94290700	-3.48388700
C	0.13179400	-2.19975300	-2.75747200
C	0.00077000	-2.23188500	-1.35904500
C	0.00077000	-2.23188500	1.35904500
C	0.13179400	-2.19975300	2.75747200
C	0.11062100	-0.94290700	3.48388700
C	-0.05249900	0.28318900	2.78692500
S	0.01749200	2.05976300	-3.19771800
S	0.01749200	2.05976300	3.19771800
Se	0.16884600	-3.62216600	0.00000000
O	0.37469100	-3.35503100	-3.44320200
C	-0.70319700	-3.87981300	-4.21717300
O	0.37469100	-3.35503100	3.44320200
C	-0.70319700	-3.87981300	4.21717300
O	0.29435700	-1.08797600	4.81748800
C	0.25065500	0.04714600	5.66629700
O	0.09118100	5.02142900	1.25976600
C	-0.05490400	5.20401800	2.65693900
O	0.09118100	5.02142900	-1.25976600

C	-0.05490400	5.20401800	-2.65693900
O	0.29435700	-1.08797600	-4.81748800
C	0.25065500	0.04714600	-5.66629700
H	-1.58574300	-4.07575800	-3.58369900
H	-0.98349700	-3.19553500	-5.03299900
H	-0.98349700	-3.19553500	5.03299900
H	-1.58574300	-4.07575800	3.58369900
H	1.07745800	0.74368500	5.45151100
H	-0.71314700	0.57638300	5.58248600
H	-1.02108100	4.81199500	3.01650100
H	0.76807300	4.73129500	3.21857800
H	0.76807300	4.73129500	-3.21857800
H	-1.02108100	4.81199500	-3.01650100
H	-0.71314700	0.57638300	-5.58248600
H	1.07745800	0.74368500	-5.45151100
H	-0.02184800	6.28709300	-2.83412600
H	-0.02184800	6.28709300	2.83412600
H	0.36274600	-0.32729000	6.69204500
H	-0.35127200	-4.82840500	4.64537100
H	-0.35127200	-4.82840500	-4.64537100
H	0.36274600	-0.32729000	-6.69204500

5’

C	-0.02741900	2.81286700	1.45228600
C	-0.01546500	1.64260600	0.69191800
C	-0.01546500	1.64260600	-0.69191800
C	-0.02741900	2.81286700	-1.45228600
C	-0.04929900	4.02829900	-0.72888800
C	-0.04929900	4.02829900	0.72888800
C	0.02022000	0.42151300	1.40037800
C	0.05121500	-0.79402300	0.71415700
C	0.05121500	-0.79402300	-0.71415700
C	0.02022000	0.42151300	-1.40037800
C	0.04135600	0.53989200	2.79512500
C	0.09563900	-0.66739000	3.53308100
C	0.10986400	-1.93298500	2.82945200
C	0.09262200	-1.99470200	1.42939700
C	0.09262200	-1.99470200	-1.42939700
C	0.10986400	-1.93298500	-2.82945200
C	0.09563900	-0.66739000	-3.53308100
C	0.04135600	0.53989200	-2.79512500
S	0.00436900	2.31532600	3.20025200
S	0.00436900	2.31532600	-3.20025200
Te	0.15658500	-3.61189200	0.00000000
O	-0.06730900	5.27409900	1.25721200
C	-0.12318500	5.44398900	2.66208000
O	-0.06730900	5.27409900	-1.25721200
C	-0.12318500	5.44398900	-2.66208000
O	0.14651200	-0.78965900	-4.88066900
C	0.24709200	0.36419000	-5.69880700
O	0.20761800	-3.09157200	-3.54926200
C	-0.95737400	-3.50937100	-4.25966400
O	0.20761800	-3.09157200	3.54926200

C	-0.95737400	-3.50937100	4.25966400
O	0.14651200	-0.78965900	4.88066900
C	0.24709200	0.36419000	5.69880700
H	-1.03079000	4.98660500	3.09024500
H	0.77002900	5.02861800	3.15788700
H	0.77002900	5.02861800	-3.15788700
H	-1.03079000	4.98660500	-3.09024500
H	-0.64135300	1.00988000	-5.60096300
H	1.15561600	0.94353700	-5.46691100
H	-1.81120100	-3.64602200	-3.57334900
H	-1.23125700	-2.78807200	-5.04471300
H	-1.23125700	-2.78807200	5.04471300
H	-1.81120100	-3.64602200	3.57334900
H	1.15561600	0.94353700	5.46691100
H	-0.64135300	1.00988000	5.60096300
H	-0.15408500	6.52649200	2.84288100
H	-0.15408500	6.52649200	-2.84288100
H	0.30917600	0.00545400	-6.73439600
H	-0.71341800	-4.47478800	-4.72400900
H	-0.71341800	-4.47478800	4.72400900
H	0.30917600	0.00545400	6.73439600

6’

C	2.15481700	0.03062400	1.44663000
C	0.96934200	-0.00253200	0.69977700
C	0.96934200	-0.00253200	-0.69977700
C	2.15481700	0.03062400	-1.44663000
C	3.36658200	0.07045500	-0.72767000
C	3.36658200	0.07045500	0.72767000
C	-0.25950900	-0.05113000	1.41626000
C	-1.44781200	-0.09286600	0.70199400
C	-1.44781200	-0.09286600	-0.70199400
C	-0.25950900	-0.05113000	-1.41626000
C	-0.24571900	-0.06950000	2.81471300
C	-1.50557700	-0.13238600	3.46449000
C	-2.74004700	-0.16850000	2.70184600
C	-2.70461500	-0.14887600	1.29906700
C	-2.70461500	-0.14887600	-1.29906700
C	-2.74004700	-0.16850000	-2.70184600
C	-1.50557700	-0.13238600	-3.46449000
C	-0.24571900	-0.06950000	-2.81471300
O	4.61377800	0.10710700	1.25216600
C	4.80057300	0.17040900	2.65319100
O	4.61377800	0.10710700	-1.25216600
C	4.80057300	0.17040900	-2.65319100
O	-1.71108300	-0.17203100	-4.80424300
C	-0.61366000	-0.27953700	-5.69265900
O	-3.92955400	-0.27901800	-3.35961000
C	-4.41958300	0.89793500	-4.00149000
O	-3.92955400	-0.27901800	3.35961000
C	-4.41958300	0.89793500	4.00149000
O	-1.71108300	-0.17203100	4.80424300
C	-0.61366000	-0.27953700	5.69265900

H	4.34058400	1.07531000	3.08471400
H	4.40738300	-0.72804600	3.15824500
H	4.40738300	-0.72804600	-3.15824500
H	4.34058400	1.07531000	-3.08471400
H	0.04064500	0.60741100	-5.64173900
H	-0.02541400	-1.19169200	-5.49870300
H	-4.55549300	1.71692600	-3.27397500
H	-3.74297500	1.22974300	-4.80420300
H	-3.74297500	1.22974300	4.80420300
H	-4.55549300	1.71692600	3.27397500
H	-0.02541400	-1.19169200	5.49870300
H	0.04064500	0.60741100	5.64173900
H	5.88484200	0.21580400	2.81993500
H	5.88484200	0.21580400	-2.81993500
H	-1.03673600	-0.34118600	-6.70374500
H	-5.39513500	0.63753000	-4.43440900
H	-5.39513500	0.63753000	4.43440900
H	-1.03673600	-0.34118600	6.70374500
Se	1.64261700	-0.00441800	-3.34347100
Se	1.64261700	-0.00441800	3.34347100
S	-3.96007200	-0.20807700	0.00000000

7’

C	-0.02008100	2.60481300	1.43833500
C	0.00726600	1.41247600	0.69827400
C	0.00726600	1.41247600	-0.69827400
C	-0.02008100	2.60481300	-1.43833500
C	-0.05218200	3.81840000	-0.72543500
C	-0.05218200	3.81840000	0.72543500
C	0.04291900	0.18042600	1.41417000
C	0.06887900	-1.03214800	0.71441900
C	0.06887900	-1.03214800	-0.71441900
C	0.04291900	0.18042600	-1.41417000
C	0.05564400	0.23937300	2.81825800
C	0.09682400	-0.97903600	3.53145300
C	0.10331000	-2.22730500	2.80858100
C	0.09306800	-2.24706200	1.41210600
C	0.09306800	-2.24706200	-1.41210600
C	0.10331000	-2.22730500	-2.80858100
C	0.09682400	-0.97903600	-3.53145300
C	0.05564400	0.23937300	-2.81825800
Te	0.14072900	-3.86503000	0.00000000
O	-0.07904500	5.06598800	1.25156200
C	-0.18027600	5.26047200	2.64904600
O	-0.07904500	5.06598800	-1.25156200
C	-0.18027600	5.26047200	-2.64904600
O	0.13500000	-1.13033700	-4.87854700
C	0.33732000	-0.01636000	-5.72960500
O	0.18566300	-3.40803600	-3.49306000
C	-0.97628300	-3.82351800	-4.21048100
O	0.18566300	-3.40803600	3.49306000
C	-0.97628300	-3.82351800	4.21048100
O	0.13500000	-1.13033700	4.87854700

C	0.33732000	-0.01636000	5.72960500
H	-1.09933900	4.80850100	3.05822600
H	0.70160700	4.86662900	3.18203300
H	0.70160700	4.86662900	-3.18203300
H	-1.09933900	4.80850100	-3.05822600
H	-0.51290400	0.68574800	-5.69356000
H	1.27300300	0.51315400	-5.48648700
H	-1.84440100	-3.91836700	-3.53521600
H	-1.21991700	-3.12308100	-5.02354400
H	-1.21991700	-3.12308100	5.02354400
H	-1.84440100	-3.91836700	3.53521600
H	1.27300300	0.51315400	5.48648700
H	-0.51290400	0.68574800	5.69356000
H	-0.22375600	6.34606700	2.80812200
H	-0.22375600	6.34606700	-2.80812200
H	0.41180000	-0.41539200	-6.74965300
H	-0.74574800	-4.80927700	-4.63736100
H	-0.74574800	-4.80927700	4.63736100
H	0.41180000	-0.41539200	6.74965300
Se	0.00615600	2.12272600	-3.32914800
Se	0.00615600	2.12272600	3.32914800

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C	0.04314100	-2.08737900	1.44142000
C	-0.00297100	-0.88214900	0.70634600
C	-0.00297100	-0.88214900	-0.70634600
C	0.04314100	-2.08737900	-1.44142000
C	0.08562900	-3.29353100	-0.72537500
C	0.08562900	-3.29353100	0.72537500
C	-0.04035000	0.36651600	1.41847200
C	-0.08541000	1.56135500	0.70278200
C	-0.08541000	1.56135500	-0.70278200
C	-0.04035000	0.36651600	-1.41847200
C	-0.02896200	0.42551900	2.81550300
C	-0.05507500	1.67989900	3.45124100
C	-0.06871900	2.90061700	2.69309600
C	-0.09286900	2.82913100	1.28960900
C	-0.09286900	2.82913100	-1.28960900
C	-0.06871900	2.90061700	-2.69309600
C	-0.05507500	1.67989900	-3.45124100
C	-0.02896200	0.42551900	-2.81550300
O	0.13735600	-4.54448000	1.24324400
C	0.03715300	-4.77419000	2.63309700
O	0.13735600	-4.54448000	-1.24324400
C	0.03715300	-4.77419000	-2.63309700
O	-0.02025000	1.72667800	-4.82004700
C	-1.20968800	2.18232600	-5.47062400
O	-0.08838400	4.11290600	-3.32159300
C	1.12034800	4.50403100	-3.97888300
O	-0.08838400	4.11290600	3.32159300
C	1.12034800	4.50403100	3.97888300
O	-0.02025000	1.72667800	4.82004700
C	-1.20968800	2.18232600	5.47062400

H	0.89492800	-4.35040600	3.18338000
H	-0.90908500	-4.38575000	3.04605000
H	-0.90908500	-4.38575000	-3.04605000
H	0.89492800	-4.35040600	-3.18338000
H	-2.06681900	1.53638800	-5.21500200
H	-1.44267900	3.22322100	-5.19859100
H	1.95318700	4.56805200	-3.25828400
H	1.38486000	3.79945700	-4.78247600
H	1.38486000	3.79945700	4.78247600
H	1.95318700	4.56805200	3.25828400
H	-1.44267900	3.22322100	5.19859100
H	-2.06681900	1.53638800	5.21500200
H	0.05237200	-5.86400100	2.76774400
H	0.05237200	-5.86400100	-2.76774400
H	-1.02064200	2.11921500	-6.55073300
H	0.93715300	5.49835500	-4.40769200
H	0.93715300	5.49835500	4.40769200
H	-1.02064200	2.11921500	6.55073300
S	-0.11133100	4.08264700	0.00000000
Te	0.05123500	-1.56998900	3.56372900
Te	0.05123500	-1.56998900	-3.56372900

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C	-0.02293400	2.29262900	1.43759200
C	-0.02220900	1.08478400	0.70550300
C	-0.02220900	1.08478400	-0.70550300
C	-0.02293400	2.29262900	-1.43759200
C	-0.03032400	3.50055700	-0.72368000
C	-0.03032400	3.50055700	0.72368000
C	-0.00302500	-0.16511800	1.41683800
C	0.01082600	-1.37074200	0.70776500
C	0.01082600	-1.37074200	-0.70776500
C	-0.00302500	-0.16511800	-1.41683800
C	0.02512800	-0.20155300	2.81618400
C	0.04871300	-1.43819500	3.48019300
C	0.02204500	-2.66668900	2.74058100
C	0.01875700	-2.61985100	1.33861300
C	0.01875700	-2.61985100	-1.33861300
C	0.02204500	-2.66668900	-2.74058100
C	0.04871300	-1.43819500	-3.48019300
C	0.02512800	-0.20155300	-2.81618400
O	-0.01676700	4.74886300	1.25306200
C	-0.41112100	4.98173600	2.58988600
O	-0.01676700	4.74886300	-1.25306200
C	-0.41112100	4.98173600	-2.58988600
O	0.05846800	-1.45287300	-4.84978000
C	1.25231100	-1.93725900	-5.47171900
O	0.03893800	-3.87457000	-3.38018700
C	-1.14385700	-4.22360400	-4.10534900
O	0.03893800	-3.87457000	3.38018700
C	-1.14385700	-4.22360400	4.10534900
O	0.05846800	-1.45287300	4.84978000
C	1.25231100	-1.93725900	5.47171900

H	-1.38932000	4.52458000	2.81311100
H	0.34421700	4.62775300	3.31405000
H	0.34421700	4.62775300	-3.31405000
H	-1.38932000	4.52458000	-2.81311100
H	2.12312900	-1.33124700	-5.16928400
H	1.43709500	-2.99268500	-5.21953200
H	-2.01683300	-4.26169000	-3.43201600
H	-1.34095900	-3.50881900	-4.91912900
H	-1.34095900	-3.50881900	4.91912900
H	-2.01683300	-4.26169000	3.43201600
H	1.43709500	-2.99268500	5.21953200
H	2.12312900	-1.33124700	5.16928400
H	-0.49537300	6.07110700	2.70315400
H	-0.49537300	6.07110700	-2.70315400
H	1.10339500	-1.83922700	-6.55541700
H	-0.96984400	-5.22241200	-4.52744200
H	-0.96984400	-5.22241200	4.52744200
H	1.10339500	-1.83922700	6.55541700
Se	0.02637800	-4.01675900	0.00000000
Te	0.03163600	1.79665400	3.55568700
Te	0.03163600	1.79665400	-3.55568700

22’

C	3.10112500	0.01486700	-0.00821200
C	1.71315700	-0.10691700	-0.00687200
C	1.02265600	-1.31113300	-0.01327400
C	1.76407300	-2.49299600	0.01322200
C	3.17662200	-2.44323600	-0.00555500
C	3.86353300	-1.19181100	-0.01515000
C	0.98810000	1.09746500	0.04876800
C	-0.40618600	1.06188600	0.02865800
C	-1.18517100	-0.16352700	-0.05233800
C	-0.41651300	-1.43088400	0.05013300
C	1.76582000	2.25575300	0.06045900
C	1.08156000	3.50561500	0.05007600
C	-0.34569900	3.50098600	0.01266000
C	-1.07087000	2.29240000	-0.01814700
C	-2.53041200	0.11996200	-0.26154300
C	-3.60861800	-0.77139400	-0.71478200
C	-1.98888000	-3.47634800	0.58209700
C	-0.74014700	-2.77399000	0.20812100
S	3.50268300	1.77089400	0.03508500
S	0.67158100	-3.84935700	0.14342300
Se	-2.92088500	1.99947200	-0.22878200
O	-1.03800600	4.67438000	-0.07973900
C	-1.08099600	5.49743700	1.08732300
O	-4.80964200	-0.16212700	-0.63892000
C	-5.93548700	-0.87337000	-1.16059800
O	-2.76574100	-2.73974600	1.38604500
C	-3.98836600	-3.34747400	1.81531000
O	3.87609300	-3.61208200	0.05779100
C	4.54676400	-4.02749000	-1.13344200
O	5.21035400	-1.29344500	-0.00897600

C	6.02584600	-0.13219100	0.02067300
O	1.64087200	4.73314600	0.04574800
C	3.05194100	4.89273500	0.04959200
H	-1.49349400	4.94204400	1.94711400
H	-0.08263600	5.88225700	1.34464300
H	-5.76869800	-1.15028700	-2.21179800
H	-6.12244100	-1.78692300	-0.57685400
H	-4.60533600	-3.62537900	0.94881900
H	-3.78424500	-4.24824100	2.41271700
H	3.83406300	-4.13965600	-1.96849200
H	5.33643100	-3.31547300	-1.41817100
H	5.86405900	0.49785400	-0.86909100
H	5.85269400	0.45755100	0.93526600
H	3.50590000	4.44783600	0.94989500
H	3.50787700	4.45934300	-0.85494800
H	7.06484300	-0.48563700	0.01933000
H	4.99933200	-5.00392100	-0.91386000
H	-4.50256000	-2.59575700	2.42565400
H	-6.79045400	-0.19225200	-1.07712200
H	-1.74562700	6.33960800	0.85157500
H	3.23841800	5.97413600	0.05654000
O	-2.22442400	-4.62932400	0.28723300
O	-3.46567300	-1.89102700	-1.16191000

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C	2.86728400	-0.60024400	-0.02663000
C	1.47834800	-0.44684200	-0.01729000
C	0.59062500	-1.52204100	-0.01346600
C	1.11211300	-2.81833500	0.01791900
C	2.50543500	-3.03057700	-0.00993000
C	3.39952700	-1.92169800	-0.03282200
C	0.95014000	0.86927100	0.03516800
C	-0.44004400	1.04515500	0.01382200
C	-1.40429800	-0.04120900	-0.06046300
C	-0.84920100	-1.40857300	0.05512900
C	1.86660300	1.92599100	0.04859500
C	1.36407700	3.25658800	0.04134100
C	-0.04588700	3.45673900	0.00214200
C	-0.92411500	2.35919200	-0.03477400
C	-2.69159100	0.43947200	-0.27412600
C	-3.89078000	-0.27916000	-0.73040000
C	-2.74066900	-3.15204100	0.62194300
C	-1.39514500	-2.67513800	0.22946300
S	-0.18860500	-3.97158300	0.16749900
Se	-2.79490500	2.35277700	-0.24765100
O	-0.57261400	4.71324100	-0.08534500
C	-0.49379000	5.53480900	1.08088300
O	-4.98301200	0.51058900	-0.67033400
C	-6.20186300	-0.02002400	-1.19770400
O	-3.38024000	-2.28155900	1.41333000
C	-4.68462400	-2.66934100	1.85653400
O	2.97806700	-4.30717700	0.06078000
C	3.56506700	-4.84656600	-1.12514600
O	4.70697500	-2.26695300	-0.03435900
C	5.72910000	-1.28497600	-0.02169700

O	2.08867500	4.39646800	0.03162400
C	3.49962900	4.37773800	0.17492900
H	-0.96960000	5.03966900	1.94470800
H	0.54949600	5.78186300	1.32864500
H	-6.07295900	-0.32516600	-2.24642600
H	-6.53312800	-0.89006600	-0.61161400
H	-5.34377300	-2.85388500	0.99609800
H	-4.63087700	-3.58199000	2.46813200
H	2.84851500	-4.82542500	-1.96406000
H	4.47644800	-4.29789000	-1.40710100
H	5.68579100	-0.64175700	-0.91618300
H	5.68718200	-0.66901500	0.89150900
H	3.80445600	3.88722000	1.11371900
H	3.98756200	3.89049800	-0.68519600
H	6.68105700	-1.83112000	-0.03056900
H	3.82346100	-5.88999600	-0.89958100
H	-5.06278800	-1.83263200	2.45561900
H	-6.94102700	0.78627300	-1.12408200
H	-1.04139700	6.45851300	0.84984900
H	3.81954100	5.42713200	0.20544100
O	-3.16554900	-4.25589600	0.35198500
O	-3.92237100	-1.41138500	-1.16773800
Se	3.65533500	1.17208500	0.01091700

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C	0.00279900	3.50515900	1.45315900
C	0.06091800	2.33801300	0.69173700
C	0.06091800	2.33801300	-0.69173700
C	0.00279900	3.50515900	-1.45315900
C	-0.04789500	4.71944900	-0.73037800
C	-0.04789500	4.71944900	0.73037800
C	0.08728900	1.11781600	1.39922600
C	0.11771800	-0.09413500	0.71456700
C	0.11771800	-0.09413500	-0.71456700
C	0.08728900	1.11781600	-1.39922600
C	0.05150800	1.23203700	2.79702800
C	0.05509300	0.02770000	3.53859000
C	0.06701000	-1.24560500	2.83571200
C	0.10067000	-1.28350100	1.43983500
C	0.10067000	-1.28350100	-1.43983500
C	0.06701000	-1.24560500	-2.83571200
C	0.05509300	0.02770000	-3.53859000
C	0.05150800	1.23203700	-2.79702800
S	-0.01005100	3.00298800	3.20221300
S	-0.01005100	3.00298800	-3.20221300
Te	0.11901100	-2.90678300	0.00000000
O	-0.10519000	5.96155200	1.25618600
C	-0.10636000	6.13488900	2.66288400
O	-0.10519000	5.96155200	-1.25618600
C	-0.10636000	6.13488900	-2.66288400
O	0.05113200	-0.09750100	-4.88185900
C	0.17726800	1.04907500	-5.71098900
O	0.10103100	-2.40412400	-3.54389900
C	-1.09547000	-2.79019500	-4.23116600
O	0.10103100	-2.40412400	3.54389900

C	-1.09547000	-2.79019500	4.23116600
O	0.05113200	-0.09750100	4.88185900
C	0.17726800	1.04907500	5.71098900
H	-0.99033700	5.66732900	3.12756800
H	0.81251000	5.73246100	3.12072900
H	0.81251000	5.73246100	-3.12072900
H	-0.99033700	5.66732900	-3.12756800
H	-0.68919800	1.72169800	-5.60373200
H	1.10826100	1.59699700	-5.49435600
H	-1.92361200	-2.92628000	-3.51583600
H	-1.37681300	-2.04798200	-4.99223000
H	-1.37681300	-2.04798200	4.99223000
H	-1.92361200	-2.92628000	3.51583600
H	1.10826100	1.59699700	5.49435600
H	-0.68919800	1.72169800	5.60373200
H	-0.14517400	7.21722700	2.84156200
H	-0.14517400	7.21722700	-2.84156200
H	0.21196200	0.67981900	-6.74374600
H	-0.87525500	-3.74883800	-4.71889000
H	-0.87525500	-3.74883800	4.71889000
H	0.21196200	0.67981900	6.74374600
Br	-2.63572900	-2.94609700	0.00000000
Br	2.84916400	-2.90004500	0.00000000

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C	-0.02264900	3.28134500	1.43953800
C	0.01637700	2.09121500	0.69816800
C	0.01637700	2.09121500	-0.69816800
C	-0.02264900	3.28134500	-1.43953800
C	-0.05934300	4.49442500	-0.72676000
C	-0.05934300	4.49442500	0.72676000
C	0.04635200	0.86020500	1.41300700
C	0.07675100	-0.34805700	0.71476900
C	0.07675100	-0.34805700	-0.71476900
C	0.04635200	0.86020500	-1.41300700
C	0.03568400	0.91498100	2.82079900
C	0.05649900	-0.30037100	3.53671400
C	0.06565000	-1.55614600	2.81373600
C	0.07972300	-1.55180800	1.42182600
C	0.07972300	-1.55180800	-1.42182600
C	0.06565000	-1.55614600	-2.81373600
C	0.05649900	-0.30037100	-3.53671400
C	0.03568400	0.91498100	-2.82079900
Te	0.11824600	-3.17411700	0.00000000
O	-0.09931600	5.73944600	1.25012300
C	-0.10200800	5.93841700	2.65155500
O	-0.09931600	5.73944600	-1.25012300
C	-0.10200800	5.93841700	-2.65155500
O	0.07327700	-0.45512100	-4.87880000
C	0.26931900	0.65453800	-5.74101700
O	0.12348700	-2.73527000	-3.48492900
C	-1.04511900	-3.14386600	-4.20686000
O	0.12348700	-2.73527000	3.48492900
C	-1.04511900	-3.14386600	4.20686000
O	0.07327700	-0.45512100	4.87880000

C	0.26931900	0.65453800	5.74101700
H	-0.99358000	5.49335900	3.12435000
H	0.81352300	5.54129700	3.12098100
H	0.81352300	5.54129700	-3.12098100
H	-0.99358000	5.49335900	-3.12435000
H	-0.57856300	1.35810900	-5.69637000
H	1.21109200	1.17852700	-5.51198600
H	-1.89892800	-3.26486300	-3.51965100
H	-1.29949700	-2.42300200	-4.99698200
H	-1.29949700	-2.42300200	4.99698200
H	-1.89892800	-3.26486300	3.51965100
H	1.21109200	1.17852700	5.51198600
H	-0.57856300	1.35810900	5.69637000
H	-0.13088800	7.02444100	2.80927400
H	-0.13088800	7.02444100	-2.80927400
H	0.32810700	0.24705200	-6.75830000
H	-0.80313200	-4.11413800	-4.65993900
H	-0.80313200	-4.11413800	4.65993900
H	0.32810700	0.24705200	6.75830000
Br	-2.63819700	-3.25734700	0.00000000
Br	2.85122200	-3.13988800	0.00000000
Se	-0.02157300	2.79518100	-3.33127500
Se	-0.02157300	2.79518100	3.33127500