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Supporting Information

Tuning carbonyl interactions in dibenzochalcogenophenes

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1. Materials and Methods

Chemicals were purchased from the following: *Sigma Aldrich*, *ABCR*, *TCI, Fisher Scientific* and *Carl Roth*. The substances were used without further purification. Anhydrous THF was dried over sodium and distilled. DCM was dried over calcium chloride. Diethyl ether was freshly distilled before usage.

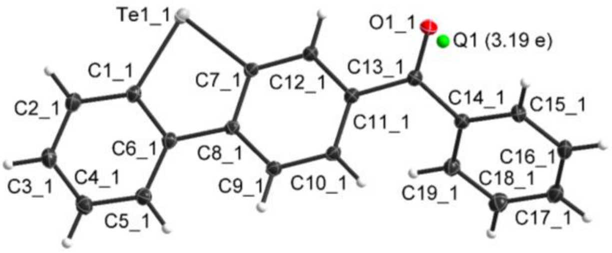
Sensitive reactions were examined using known Schlenk techniques under Ar atmosphere. Dry DMF and DMSO were commercially available dried over mole sieve (3 Å) from *Acros Organics*. For thin-layer chromatography (TLC), the silica plates used were *Polygram SIL G/UV*$_{254}$ from *Macherey-Nagel*. Spot visualization was performed using 254 and 365 nm or specific stains. Flash-chromatography was carried out by using silica gel *MN 60 M* (0.04 – 0.063 mm) from *Macherey-Nagel.* Purity (>99%) of the final compounds (**4a-c**, **12b-c**) was determined using high-performance liquid chromatography (HPLC, column: Nucleodur 100-5, normal phase, 90:10 *n*-hexane : ethyl acetate, *Waters HPLC*, UV detection at 270 and 365 nm). For the tellurium compounds (**4c**, **12c**), the solvents had to be degassed with argon to minimize oxidation by contact with column material. HPLC chromatogram of **12a** was measured on a semipreparative HPLC (column: VP250/10 Nucleodur 100-5, normal phase, 85:15 *n*-hexane : ethyl acetate, *Jasco* HPLC, UV detection at 270 nm *via* photodiode array detector). NMR spectra were measured on a *Bruker AVNEO400* (^{1}H: 400 MHz, ^{11}B: 128 MHz, ^{13}C: 101 MHz, ^{19}F: 376 MHz, ^{77}Se: 76 MHz, ^{125}Te: 126 MHz) and *AVHD600* (^{1}H: 600 MHz, ^{13}C: 151 MHz, ^{77}Se: 114 MHz, ^{125}Te: 189 MHz) spectrometer. The measurements were performed at room temperature, ^{13}C-NMR spectra were recorded with proton decoupling. Spectra are given with frequency, solvent, and temperature. Abbreviation of the multiplicity is given by: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), td (triplet of doublet), br (broad). Chemical shifts are given in parts per million (ppm). Coupling constants *J* are given in Hertz (Hz). The protonated residue of the used solvent acts as an internal standard. High-resolution mass spectra were measured using *Bruker maXis 4G* with electrospray- (ESI) or atmospheric pressure chemical ionization (APCI). GC-MS analysis was performed using *Agilent 5873N MSD* with electron ionization (EI). FT-IR spectra were measured using a *Jasco FT/IR-4600* spectrometer. Solutions in freshly distilled 2-methyltetrahydrofuran (MTHF, >98%) with a concentration of 10 µM were freshly prepared and measured in quartz glass cuvettes (10 x 4 mm, 1.4 ml). UV/Vis spectra were recorded with a *Jasco V-550* spectrophotometer.

X-ray diffraction

All single crystals of the final compounds (**4a-c**, **12a-c**) were obtained by slow evaporation from DCM layered with *n*-hexane. Diaryliodonium salts (**7**, **10**) were crystallized by evaporation with acetone. The crystal of 3-bromodibenzo[*b,d*]selenophene (**16b**) was received from chloroform.

The crystals were mounted on nylon loops in inert oil. The single crystal structures were collected on a *Bruker AXS D8 Venture Photon II* (monochromated Cu$_{K\alpha}$ radiation, K_α = 1.54178 Å, microfocus source) diffractometer at 100(2) K. For **12c** and **7**, a *Bruker AXS D8 Kappa* diffractometer with *APEX2* detector (monochromated Mo$_{K\alpha}$ radiation, K_α = 0.71073 Å) diffractometer was used at 100(2) K. The structures were solved using Direct Methods (SHELXS-2013)[1] and refined anisotropically by full-matrix least-squares on F^2 (SHELXL-2017)[2,3]. Absorption corrections were performed semi-empirically from equivalent reflections on basis of multi-scans and numerical form indexed faces in case of **4c** and **12c** (*Bruker AXS APEX3*). Hydrogen atoms were refined using a riding model.

In **12c**, Q1 modelled as alternate position of O1_1 led to n. p. d. displacement parameters and an occupancy close to 0. Fixing the occupancies at 0.5 led to both positions joining at one point with unrealistic displacement parameters for both positions. The long C–O bond length also supports the idea that Q1 is not an alternate position of O1_1. EADP and SADI/DFIX restraints (sigma 0.01) and free occupancies can fix this, but SHELXL assesses these restraints as "non agreeable" and the conformation of the second orientation remains unlikely. The most likely explanation is a full body disorder of residue 1 and Q1 being the alternate position of Te1_1. An attempt to refine this accordingly led to a reduction of the negative residual density at Te1_1, however, since no other atoms of the proposed orientation can be identified, we prefer to leave Q1 unmodelled.

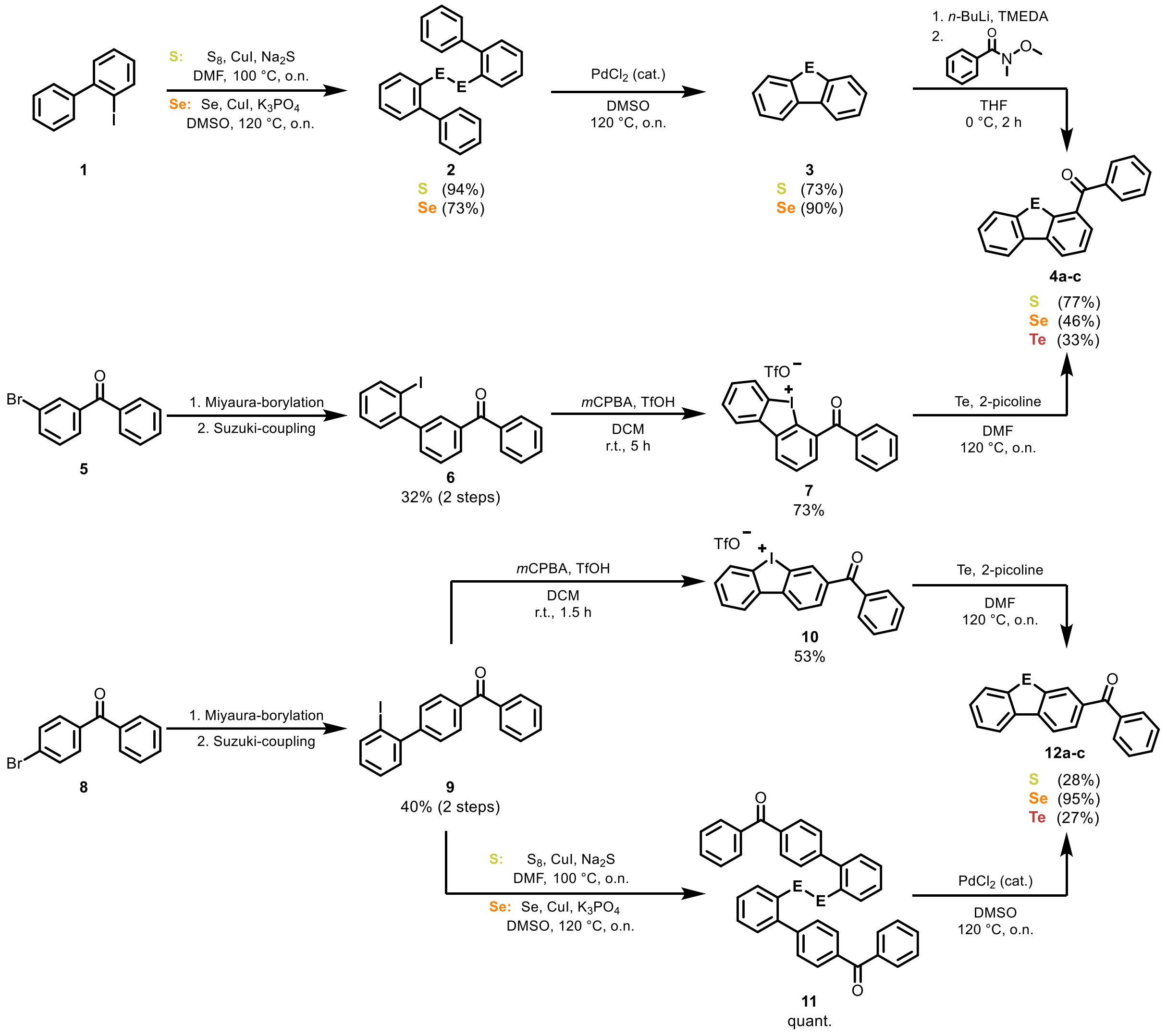


Data sets for compounds **4b** and **10** were collected with a *Bruker D8 Venture Photon III* (Cu) diffractometer. Programs used: data collection: *APEX4* Version 2021.4-0[4]; cell refinement: *SAINT* Version 8.40B; data reduction *SAINT* Version 8.40B; absorption correction: *SADABS* Version 2016/2; structure solution: *SHELXT*-Version 2018-3[5]; structure refinement *SHELXL*-Version 2018-3[2] and graphics, *XP*[6]. *R*-values are given for observed reflections, and wR^2 values are given for all reflections.

Exceptions and special features: For compound **10** a badly disordered acetone molecule was found in the asymmetrical unit and could not be satisfactorily refined. The program SQUEEZE[7] was therefore used to mathematically remove the solvent's effect. The quoted formula and derived parameters do not include the squeezed solvent molecule.

2. Synthetic procedures

Overview of synthesis of target compounds



General Procedure A (GPA)

GPA1[8,9]

The corresponding iodobiphenyl (2 eq.), freshly ground elemental chalcogen (S_8: 2 eq.; Se: 6 eq.), a base (S: Na_2S (2 eq.); Se: K_3PO_4 (6 eq.)) and CuI (0.2 eq.) were dissolved in dry solvent (S: DMF; Se: DMSO) in a flame-dried pressure tube under argon atmosphere. The suspension was stirred at 120 °C overnight. The mixture was diluted with H_2O, extracted three times with ethyl acetate and dried over $MgSO_4$. The product was used without any further purification.

GPA2[8]

The disulfide/diselenide (0.5 eq.) and $PdCl_2$ (5mol%) were dissolved in dry DMSO in a flame-dried pressure tube under an argon atmosphere. The mixture was stirred at 120 °C overnight and afterwards diluted with H_2O. The aqueous phase was extracted three times with ethyl acetate, and the organic layers were combined, dried over $MgSO_4$, filtered and concentrated. The product was isolated by column chromatography (eluent: cyclohexane).

General Procedure B (GPB)

Cyclic diaryliodonium salts were synthesized using the procedure reported by Jiang *et al*.[10] A solution of *m*CPBA (70%, 1.5 eq.) in DCM was combined with the corresponding iodobiphenyl (1 eq.) under stirring. Trifluoromethanesulfonic acid (3 eq.) was added dropwise, the mixture was stirred for 1 h at room temperature. With the addition of Et_2O, the product was precipitated, isolated by filtration, and washed with Et_2O. The cyclic diaryliodonium salts were air-stable but could not be dried *in vacuo* due to decomposition. Therefore, residues of solvents, especially water, could not be fully removed.

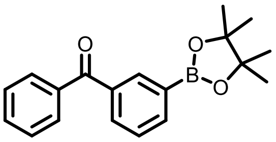
General Procedure C (GPC)

With an adaptation of the literature[11] in a flame-dried Schlenk tube, the dibenzochalcogenophene (1 eq.) was dissolved in dry THF with TMEDA (1.1 eq.) at 0 °C under argon. *n*-Butyllithium (2.5 M in hexane, 1.5 eq.) was added dropwise. A colour change to orange/red indicated the lithiation, the mixture was stirred at 0 °C, and afterwards, *N*-methoxy-*N*-methylbenzamide (1.5 eq.) was added dropwise. After slowly warming the reaction to room temperature, the mixture was stirred overnight. The reaction was stopped with the addition of saturated NH_4Cl solution, and the aqueous phase was extracted three times using ethyl acetate. The combined organic layers were dried over $MgSO_4$, filtered and concentrated. Column chromatography yielded the product.

General Procedure D (GPD)

The synthesis of the dibenzotellurophenes was performed according to the literature.[10] In a flame-dried pressure tube, the cyclic diaryliodonium salt (1 eq.) and freshly ground elemental tellurium (3 eq.) were dissolved in 2-picoline (35 eq.) and dry DMF under argon. The suspension was heated at 120 °C overnight. After the reaction was completed, the product was isolated by flash-column chromatography.

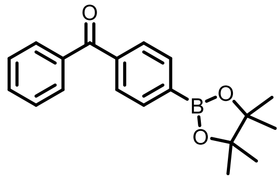
Phenyl[3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolane-2-yl)phenyl]methanone (5.1)



The synthesis was adapted according to the literature.[12] In a flame-dried Schlenk flask, 3-bromobenzophenone (**5**, 2.51 g, 9.61 mmol, 1 eq.), potassium acetate (2.82 g, 28.7 mmol, 3 eq.) and bis(pinacolato)diboron (2.98 g, 11.7 mmol, 1.2 eq.) were suspended in 75 ml dry 1,4-dioxane. The suspension was degassed with argon for 30 min. Thereafter [1,1′-bis(diphenylphosphino)ferrocene]dichloropalladium(II) (434 mg, 0.59 mmol, 6 mol%) was added and the reaction was refluxed at 110 °C for 24 h. After completion, the mixture was diluted with 70 ml H_2O and the aqueous phase was extracted five times using 100 ml DCM. The combined organic layers were dried over $MgSO_4$, filtered and concentrated. The product was afforded by column chromatography (*n*-pentane/DCM 1:1 → 0:1) (**5.1**, white solid, 1.94 g, 6.30 mmol, 65.8%).

M($C_{19}H_{21}BO_3$): 308.18 g/mol. **M.p.:** 98 °C. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ [ppm] = 8.22 (s, 1H), 8.02 (dt, $^3J_{HH}$ = 7.4, $^4J_{HH}$ = 1.2 Hz, 1H), 7.89 – 7.78 (m, 3H), 7.62 – 7.56 (m, $^3J_{HH}$ = 6.9, $^4J_{HH}$ = 1.3 Hz, 1H), 7.52 – 7.46 (m, 3H), 1.35 (s, 12H). **^{11}B-NMR (128 MHz, $CDCl_3$, 298 K):** δ [ppm] = 22.40. **^{13}C-NMR (101 MHz, $CDCl_3$, 298 K):** δ [ppm] = 197.09, 138.75, 137.78, 137.31, 136.18, 132.79, 132.56, 130.26, 128.45, 127.80, 84.26, 25.01. **HR-MS (ESI, 70 eV, DCM): m/z:** $[C_{19}H_{21}BO_3 + H]^+$ 309.1661, calculated: $[M + H]^+$ 309.1660. $[C_{19}H_{21}BO_3 + Na]^+$ 331.1483, calculated: $[M + Na]^+$ 331.1479. Spectroscopic data is in agreement with the literature.[13]

Phenyl[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolane-2-yl)phenyl]methanone (8.1)

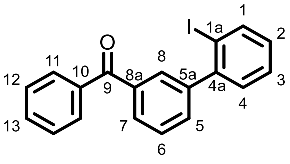


Analogue to the synthesis of compound **5**[12], 4-bromobenzophenone (**8**, 3.08 g, 11.8 mmol, 1 eq.), potassium acetate (3.43 g, 34.5 mmol, 3 eq.) and bis(pinacolato)diboron (3.72 g, 14.7 mmol, 1.2 eq.) in 90 ml dry 1,4-dioxane were suspended and degassed. After the addition of [1,1′-bis(diphenylphosphine)ferrocene]dichloropalladium(II) (520 mg, 0.71 mmol, 6 mol%), the reaction was refluxed at 110 °C for 24 h. After purification, the product was isolated (**8.1**, white solid, 2.65 g, 8.60 mmol, 74.9%).

M($C_{19}H_{21}BO_3$): 308.18 g/mol. **M.p.:** 122 °C. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ [ppm] = 7.92 (d, $^3J_{HH}$ = 8.2 Hz, 2H), 7.83 – 7.75 (m, 4H), 7.63 – 7.56 (m, 1H), 7.52 – 7.44 (m, 2H), 1.37 (s, 12H). **^{11}B-NMR (128 MHz, $CDCl_3$, 298 K):** δ [ppm] = 30.50. **^{13}C-NMR (101 MHz, $CDCl_3$, 298 K):** δ [ppm] = 197.09, 139.91, 137.65, 134.70, 132.67, 130.26, 129.16, 128.44, 84.35, 25.03. **HR-MS (ESI, 70 eV, DCM): m/z:** $[C_{19}H_{21}BO_3 + H]^+$ 309.1667, calculated: $[M + H]^+$ 309.1660.

$[C_{19}H_{21}BO_3 + Na]^+$ 331.1484, calculated: $[M + Na]^+$ 331.1479. Spectroscopic data is in agreement with the literature.[14]

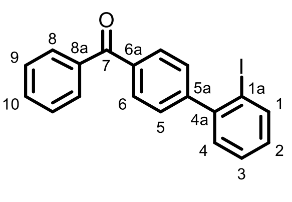
(2′-Iodo-[1,1′-biphenyl]-3-yl)-phenylmethanone (6)



The synthesis was adapted according to the literature.[12] In a flame-dried Schlenk flask, 1,2-diiodobenzene (2.15 g, 0.85 ml, 6.50 mmol, 2 eq.), sodium carbonate (1.39 g, 13.1 mmol, 4 eq.) and the pinacolboronic ester **5.1** (1.03 g, 2.15 mmol, 1 eq.) were diluted in 23 ml toluene, 6.5 ml ethanol and 3.25 ml water. Under stirring, the mixture was degassed with argon for 30 min. Thereafter, Palladium-tetrakis(triphenylphosphine) (112 mg, 0.097 mmol, 3 mol%) was added, and the reaction mixture was refluxed at 80 °C for 28 h. Afterwards, the mixture was diluted with 100 ml H_2O and the aqueous phase was extracted five times with 100 ml ethyl acetate. The combined organic layers were dried over $MgSO_4$, filtered and concentrated. Column chromatography (cyclohexane/ethyl acetate 19:1) yielded the product (**6**, orange oil, 613 mg, 1.60 mmol, 49.1%).

M($C_{19}H_{13}IO$): 384.22 g/mol. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ [ppm] = 7.96 (dd, $^3J_{HH}$ = 8.0, $^4J_{HH}$ = 1.1 Hz, 1H, C_1-*H*), 7.90 – 7.85 (m, 3H, C_7-*H*, C_{11}-*H*), 7.77 – 7.74 (dt, $^4J_{HH}$ = 1.7, 1.0 Hz, 1H, C_8-*H*), 7.62 – 7.55 (m, 3H, C_5-*H*, C_6-*H*, C_{13}-*H*), 7.52 – 7.46 (m, 2H, C_{12}-*H*), 7.40 (td, $^3J_{HH}$ = 7.5, $^4J_{HH}$ = 1.2 Hz, 1H, C_3-*H*), 7.32 (dd, $^3J_{HH}$ = 7.6, $^4J_{HH}$ = 1.7 Hz, 1H, C_4-*H*), 7.06 (ddd, $^3J_{HH}$ = 7.9, 7.4, $^4J_{HH}$ = 1.8 Hz, 1H, C_2-*H*). **^{13}C-NMR (101 MHz, $CDCl_3$, 298 K):** δ [ppm] = 196.63 (C_9), 145.71 (C_{4a}), 144.35 (C_{5a}), 139.71 (C_1), 137.61 (C_{7a}/C_{10}), 137.53 (C_{7a}/C_{10}), 133.37 (C_5), 132.67 (C_{13}), 131.09 (C_8), 130.31 (C_{11}), 130.24 (C_4), 129.41 (C_2/C_7), 129.38 (C_2/C_7), 128.49 (C_{12}), 128.43 (C_3), 128.32 (C_6), 98.54 (C_{1a}). **HR-MS (ESI, 70 eV, DCM): m/z:** $[C_{19}H_{13}IO + H]^+$ 385.0084, calculated: $[M + H]^+$ 385.0084. $[C_{19}H_{13}IO + Na]^+$ 406.9507, calculated: $[M + Na]^+$ 406.9503. $[(C_{19}H_{13}IO)_2 + Na]^+$ 790.9907, calculated: $[M_2 + Na]^+$ 790.9914. **IR:** $\tilde{\nu}$ [cm^{-1}] = 3055, 2922, 2851, 1953, 1918, 1811, 1735, 1655, 1596, 1556, 1485, 1445, 1431, 1317, 1267, 1239, 1178, 1115, 1092, 1026, 1011, 999, 947, 927, 912, 865, 818, 781, 756, 718, 701, 644, 616, 602.

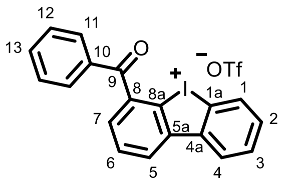
(2′-Iodo-[1,1′-biphenyl]-4-yl)phenylmethanone (9)



The synthesis was prepared analogue to the synthesis of compound **6**.[12] 1,2-Diiodobenzene (1.64 g, 0.65 ml, 4.97 mmol, 1.5 eq.), sodium carbonate (1.83 g, 17.3 mmol, 5 eq.) and the pinacolboronic ester **8.1** (1.03 g, 3.33 mmol, 1 eq.) were dissolved in 25 ml toluene, 12 ml ethanol and 3.25 ml H_2O and degassed. After the addition of Palladium-tetrakis(triphenylphosphine) (112 mg, 0.097 mmol, 3 mol%), the suspension was refluxed at 95 °C for 63 h. After purification, the product was isolated (**9**, orange oil, 670 mg, 1.74 mmol, 53.7%).

M($C_{19}H_{13}IO$): 384.22 g/mol. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ [ppm] = 7.99 (dd, $^3J_{HH}$ = 8.0, $^4J_{HH}$ = 1.1 Hz, 1H, C_1-*H*), 7.90 – 7.84 (m, 4H, C_6-*H*, C_8-*H*), 7.64 – 7.59 (m, 1H, C_{10}-*H*), 7.54 – 7.49 (m, 2H, C_9-*H*), 7.49 – 7.45 (m, 2H, C_5-*H*), 7.43 (td, $^3J_{HH}$ = 7.5, $^4J_{HH}$ = 1.2 Hz, 1H, C_3-*H*), 7.33 (dd, $^3J_{HH}$ = 7.6, $^4J_{HH}$ = 1.7 Hz, 1H, C_4-*H*), 7.11 – 7.05 (m, 1H, C_2-*H*). **^{13}C-NMR (101 MHz, $CDCl_3$, 298 K):** δ [ppm] = 196.51 (C_7), 148.25 (C_{5a}), 145.73 (C_{4a}), 139.86 (C_1), 137.75 (C_{8a}), 136.76 (C_{6a}), 132.60 (C_{10}), 130.20 (C_6/C_8), 130.08 (C_4), 130.02 (C_6/C_8), 129.48 (C_2, C_5), 128.48 (C_9), 128.42 (C_3), 97.97 (C_{1a}). **HR-MS (ESI, 70 eV, DCM): m/z:** $[C_{19}H_{13}IO + H]^+$ 385.0085, calculated: $[M + H]^+$ 385.0084. $[C_{19}H_{13}IO + Na]^+$ 406.9506, calculated: $[M + Na]^+$ 406.9503. $[(C_{19}H_{13}IO)_2 + Na]^+$ 790.9911, calculated: $[M_2 + Na]^+$ 790.9914. **IR:** $\tilde{\nu}$ [cm^{-1}] = 3060, 2959, 2923, 2852, 2360, 1732, 1655, 1596, 1577, 1508, 1459, 1419, 1396, 1260, 1177, 1092, 1074, 1014, 997, 939, 923, 867, 848, 795, 762, 742, 694, 682, 647, 626.

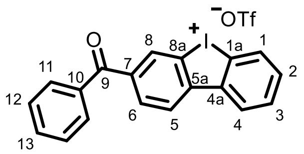
4-Benzoyldibenzo[*b,d*]iodol-5-ium-trifluoromethanesulfonate (7)



According to **GPB**, *m*CPBA (433 mg, 1.76 mmol) in 3.2 ml DCM and the iodobiphenyl (**6**, 355 mg, 0.924 mmol) in 3.75 ml DCM were combined. After the addition of trifluoromethanesulfonic acid (428 mg, 0.25 ml, 2.85 mmol), the reaction was stirred for 5 h. After precipitation with Et_2O, the product was isolated by filtration (**7**, white solid, 356 mg, 0.669 mmol, 73.4%).

M($C_{19}H_{12}IO\cdot F_3CSO_3$): 532.27 g/mol. **M.p.:** 222-224 °C. **^{1}H-NMR (400 MHz, acetone-d_6, 298 K):** δ [ppm] = 8.96 (dd, $^3J_{HH}$ = 7.8, $^4J_{HH}$ = 0.8 Hz, 1H, C_5-*H*), 8.68 (dd, $^3J_{HH}$ = 7.9, $^4J_{HH}$ = 1.2 Hz, 1H, C_4-*H*), 8.54 (dd, $^3J_{HH}$ = 7.6, $^4J_{HH}$ = 0.9 Hz, 1H, C_7-*H*), 8.48 (d, $^3J_{HH}$ = 7.8 Hz, 1H, C_1-*H*), 8.29 (t, $^3J_{HH}$ = 7.7 Hz, 1H, C_6-*H*), 8.04 – 7.97 (m, 3H, C_3-*H*, C_{11}-*H*), 7.89 – 7.82 (m, 2H, C_2-*H*, C_{13}-*H*), 7.73 (t, $^3J_{HH}$ = 7.7 Hz, 2H, C_{12}-*H*). **^{13}C-NMR (101 MHz, acetone-d_6, 298 K):** δ [ppm] = 194.99 (C_9), 144.75 (C_{5a}), 140.40 (C_{4a}), 136.44 (C_7), 135.72 (C_{10}), 134.87 (C_{13}), 133.39 (C_6), 132.95 (C_5), 132.91 (C_2), 132.85 (C_8), 132.16 (C_3), 132.12 (C_1), 131.30 (C_{11}), 130.00 (C_{12}), 128.38 (C_4), 123.18 (C_{1a}), 122.24 (d, $^1J_{CF}$ = 321.6 Hz, CF_3), 118.90 (C_{8a}). **^{19}F-NMR (376 MHz, acetone-d_6, 298 K):** δ [ppm] = -78.88 (CF_3). **HR-MS (ESI, 70 eV, acetone): m/z:** $[C_{19}H_{12}IO]^+$ 382.9928, calculated: $[M]^+$ 382.9927. **IR:** $\tilde{\nu}$ [cm^{-1}] = 2359, 2313, 2159, 1748, 1733, 1716, 1698, 1635, 1577, 1558, 1522, 1508, 1489, 1437, 1396, 1320, 1277, 1259, 1237, 1222, 1159, 1025, 957, 818, 759, 735, 720, 698, 656, 632.

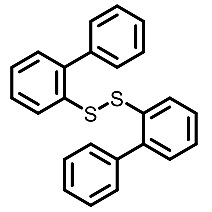
3-Benzoyldibenzo[*b,d*]iodol-5-ium-trifluoromethanesulfonate (10)



Based on **GPB**, the iodobiphenyl (**9**, 107 mg, 0.278 mmol) in 1 ml DCM was combined with *m*CPBA (133 mg, 0.541 mmol) in 1 ml DCM under stirring. After adding trifluoromethanesulfonic acid (128 mg, 75 µL, 0.85 mmol) and stirring for 1.5 h, the product was isolated by precipitation and filtration (**10**, white solid, 72.8 mg, 0.137 mmol, 52.6%).

M($C_{19}H_{12}IO\cdot F_3CSO_3$): 532.27 g/mol. **M.p.:** 195-197 °C. **^{1}H-NMR (400 MHz, acetone-d$_6$, 298 K):** δ [ppm] = 8.75 (d, $^4J_{HH}$ = 1.5 Hz, 1H, C_8-*H*), 8.68 (d, $^3J_{HH}$ = 8.2 Hz, 1H, C_5-*H*), 8.64 (dd, $^3J_{HH}$ = 7.9, $^4J_{HH}$ = 1.4 Hz, 1H, C_4-*H*), 8.44 (dd, $^3J_{HH}$ = 8.4, $^4J_{HH}$ = 0.8 Hz, 1H, C_1-*H*), 8.30 (dd, $^3J_{HH}$ = 8.2, $^4J_{HH}$ = 1.5 Hz, 1H, C_6-*H*), 8.03 – 7.98 (m, 1H, C_3-*H*), 7.91 – 7.84 (m, 3H, C_{11}-*H*, C_2-*H*), 7.77 – 7.71 (m, 1H, C_{13}-*H*), 7.65 – 7.59 (m, 2H, C_{12}-*H*). **^{13}C-NMR (101 MHz, acetone-d$_6$, 298 K):** δ [ppm] = 194.24 (C_9), 146.54 (C_{5a}), 142.35 (C_{4a}), 140.57 (C_7), 137.57 (C_{10}), 134.07 (C_{13}), 133.39 (C_8), 133.34 (C_2), 133.09 (C_6), 132.37 (C_3), 132.19 (C_1), 130.80 (C_{11}), 129.65 (C_{12}), 129.10 (C_4), 128.04 (C_5), 122.99 (C_{1a}), 122.02 (d, $^1J_{CF}$ = 321.1 Hz, CF_3), 122.02 (C_{8a}). **^{19}F-NMR (376 MHz, acetone-d$_6$, 298 K):** δ [ppm] = -78.93 (CF_3). **HR-MS (ESI, 70 eV, acetone): m/z:** $[C_{19}H_{12}IO]^+$ 382.9913, calculated: $[M]^+$ 382.9927. **IR:** $\tilde{\nu}$ [cm^{-1}] = 2170, 2037, 2026, 2006, 1958, 1657, 1592, 1448, 1383, 1287, 1261, 1222, 1158, 1025, 988, 913, 840, 796, 771, 732, 700, 671, 651, 635.

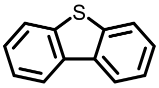
Bis([1,1′-biphenyl]-2-yl)disulfide (2a)



The synthesis was performed following **GPA1**.[8,9] 2-Iodo-1,1′-biphenyl (**1**, 1.50 g, 0.95 ml, 5.35 mmol), sulphur (268 mg, 5.35 mmol), $Na_2S\cdot 9\,H_2O$ (1.29 g, 5.36 mmol) and CuI (102 mg, 0.54 mmol) were dispersed in 10 ml dry DMF and brought to reaction at 100 °C overnight. After extraction and column chromatography (cyclohexane), the product was isolated (**2a**, yellow oil, 945 mg, 2.55 mmol, 95.2%).

M($C_{24}H_{18}S_2$): 370.53 g/mol. **^{1}H-NMR (400 MHz, CDCl$_3$, 298 K):** δ [ppm] = 7.59 (d, $^3J_{HH}$ = 6.1 Hz, 2H), 7.46 – 7.37 (m, 10H), 7.29 – 7.20 (m, 6H). **^{13}C-NMR (101 MHz, CDCl$_3$, 298 K):** δ [ppm] = 141.52, 139.93, 135.11, 130.31, 129.56, 128.31, 128.27, 127.91, 127.16, 126.59. **HR-MS (APCI, 70 eV, DCM): m/z:** $[C_{24}H_{18}S_2 + H]^+$ 371.0925, calculated: $[M + H]^+$ 371.0923. Spectroscopic data is in agreement with the literature.[8]

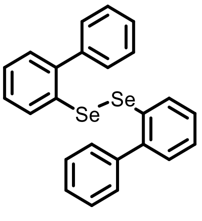
Dibenzo[*b,d*]thiophene (3a)



According to **GPA2**, the disulfide **2a** (300 mg, 0.81 mmol) and $PdCl_2$ (5mol%) were dissolved in 2 ml dry DMSO under an argon atmosphere and brought to reaction at 120 °C overnight. After column chromatography (cyclohexane), the product was isolated (**3a**, white solid, 217 mg, 1.18 mmol, 72.8%).

M($C_{12}H_8S$): 184.26 g/mol. **M.p.:** 98 °C. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ [ppm] = 8.20 – 8.14 (m, 2H), 7.90 – 7.83 (m, 2H), 7.50 – 7.43 (m, 4H). **^{13}C-NMR (101 MHz, $CDCl_3$, 298 K):** δ [ppm] = 139.56, 135.68, 126.84, 124.49, 122.95, 121.71. **MS (GC): m/z:** $[C_{12}H_8S]^+$ 184, calculated: $[M]^+$ 184. Spectroscopic data is in agreement with the literature.[15]

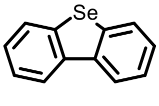
Bis([1,1′-biphenyl]-2-yl)diselenide (2b)



Following **GPA1**[8,9]**,** 2-iodo-1,1′-biphenyl (**1**, 429 mg, 0.27 ml, 1.53 mmol), selenium (712 mg, 9.02 mmol), K_3PO_4 (1.96 g, 8.57 mmol) and CuI (5.44 mg, 0.29 mmol) were dissolved in 3 ml dry DMSO and brought to reaction at 120 °C overnight. After column chromatography (cyclohexane), the product was isolated (**2b**, orange oil, 243 mg, 0.52 mmol, 73.2%).

M($C_{24}H_{18}Se_2$): 464.35 g/mol. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ [ppm] = 7.71 – 7.66 (m, 2H), 7.48 – 7.40 (m, 10H), 7.25 – 7.19 (m, 6H). **^{13}C-NMR (101 MHz, $CDCl_3$, 298 K):** δ [ppm] = 142.50, 141.25, 130.74, 129.91, 129.77, 129.25, 128.69, 128.53, 128.16, 127.09. **^{77}Se-NMR (76 MHz, $CDCl_3$, 298 K):** δ [ppm] = 410.11. **HR-MS (APCI, 70 eV, DCM): m/z:** $[C_{24}H_{18}Se_2 + H]^+$ 465.9741, calculated: $[M + H]^+$ 465.9738.

Dibenzo[*b,d*]selenophene (3b)

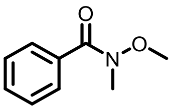


Following **GPA2**[8]**,** the diselenide **2b** (186 mg, 0.401 mmol) and $PdCl_2$ (5mol%) were dissolved in 1 ml dry DMSO in a flame-dried pressure tube under an argon atmosphere. The mixture was stirred at 120 °C overnight and after column chromatography (cyclohexane), the product was isolated (**3b**, white solid, 166 mg, 0.72 mmol, 89.6%)

M($C_{12}H_8Se$): 231.17 g/mol. **M.p.:** 63 °C. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ [ppm] = 8.14 (dd, $^3J_{HH}$ = 7.8, $^4J_{HH}$ = 1.3 Hz, 2H), 7.91 – 7.87 (m, 2H), 7.47 (td, $^3J_{HH}$ = 7.6, $^4J_{HH}$ = 1.2 Hz, 2H), 7.39 (td, $^3J_{HH}$ = 7.6, $^4J_{HH}$ = 1.4 Hz, 2H). **^{13}C-NMR (101 MHz, $CDCl_3$, 298 K):** δ [ppm] = 139.43, 138.41, 127.00, 126.22, 124.98, 122.99. **^{77}Se-NMR (76 MHz, $CDCl_3$, 298 K):** δ [ppm] = 450.49. **HR-MS (APCI, 70 eV, DCM):**

m/z: [$C_{12}H_8Se$ + H]$^+$ 232.9824, calculated: [M + H]$^+$ 232.9864. Spectroscopic data is in agreement with the literature.[8,16]

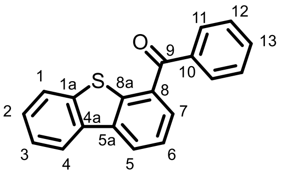
N-methoxy-*N*-methylbenzamide



The synthesis was performed as described in the literature.[17] The product was isolated by extraction (colourless oil, 3.42 g, 18.7 mmol, 99.3%).

M($C_9H_{11}NO_2$): 165.19 g/mol. **^{1}H-NMR (400 MHz, CDCl$_3$, 298 K):** δ [ppm] = 7.56 – 7.51 (m, 2H), 7.34 – 7.23 (m, 3H), 3.42 (s, 3H), 3.22 (s, 3H). **^{13}C-NMR (101 MHz, CDCl$_3$, 298 K):** δ [ppm] = 170.09, 134.26, 130.68, 128.26, 128.13, 61.16. **HR-MS (ESI, 70 eV, acetone): m/z:** [$C_9H_{11}NO_2$ + H]$^+$ 166.0868, calculated: [M + H]$^+$ 166.0863. [$C_9H_{11}NO_2$ + Na]$^+$ 188.0687, calculated: [M + Na]$^+$ 188.0682. [($C_9H_{11}NO_2$)$_2$ + H]$^+$ 353.1475, calculated: [M$_2$ + H]$^+$ 353.1472. Spectroscopic data agrees with the literature.[18]

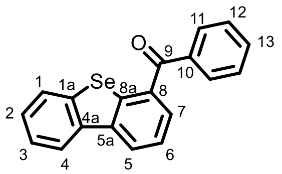
4-Benzoyldibenzo[*b,d*]thiophene (4a)



Following **GPC**, dibenzothiophene (**3a**, 50.2 mg, 0.272 mmol, 1 eq.) with TMEDA (34.7 mg, 50 µL, 0.298 mmol, 1.1 eq.) was dissolved in 1 ml THF at 0 °C. *n*-Butyllithium (27.2 mg, 0.17 ml, 2.5 M in hexane, 0.425 mmol, 1.5 eq.) was added. After stirring for 1 h at 0 °C, *N*-methoxy-*N*-methylbenzamide (76.5 mg, 0.07 ml, 0.463 mmol, 1.7 eq.) were added and stirred overnight at room temperature. Column chromatography (cyclohexane/ethyl acetate 19:1) yielded the product as a colourless crystalline solid (**4a**, 60.6 mg, 0.210 mmol, 77.5%).

M($C_{19}H_{12}OS$): 288.36 g/mol. **M.p.:** 156-158 °C. **^{1}H-NMR (600 MHz, acetone-d$_6$, 298 K):** δ [ppm] = 8.67 (dd, $^3J_{HH}$ = 7.8, $^4J_{HH}$ = 1.0 Hz, 1H, C_5-*H*), 8.46 – 8.42 (m, 1H, C_4-*H*), 8.10 – 8.07 (m, 1H, C_1-*H*), 7.99 (dd, $^3J_{HH}$ = 7.5, $^3J_{HH}$ = 1.0 Hz, 1H, C_7-*H*), 7.85 – 7.81 (m, 2H, C_{11}-*H*), 7.73 – 7.68 (m, 2H, C_{13}-*H*), 7.64 – 7.55 (m, 4H, C_2-*H*, C_3-*H*, C_6-*H*, C_{12}-*H*). **^{13}C-NMR (151 MHz, acetone-d$_6$, 298 K):** δ [ppm] = 196.18 (C_9), 142.58 (C_{1a}), 141.05 ($C_{8a)}$, 139.26 (C_{10}), 138.39 (C_{5a}), 135.09 (C_{4a}), 132.94 (C_{13}), 132.71 (C_7), 131.24 (C_8), 130.37 (C_{12}), 129.45 (C_{11}), 128.47 (C_2), 127.19 (C_5), 125.82 (C_3), 125.29 (C_6), 123.70 (C_1), 122.82 (C_4). **HR-MS (ESI, 70 eV, DCM): m/z:** [$C_{19}H_{12}OS$ + H]$^+$ 286.0689, calculated: [M + H]$^+$ 286.0682. [$C_{19}H_{12}OS$ + Na]$^+$ 311.0509, calculated: [M + Na]$^+$ 311.0501. [($C_{19}H_{12}OS$)$_2$ + H]$^+$ 599.1119, calculated: [M$_2$ + H]$^+$ 599.1110. **IR:** $\tilde{\nu}$ [cm-^{1}] = 3048, 3019, 2943, 1716, 1697, 1652, 1599, 1551, 1542, 1508, 1497, 1489, 1454, 1418, 1396, 1335, 1314, 1281, 1254, 1206, 1167, 1096, 1048, 1000, 959, 941, 918, 847, 794, 779, 751, 730, 698, 664, 633, 605. Spectroscopic data agrees with the literature.[19]

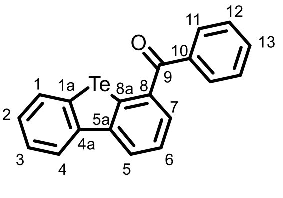
4-Benzoyldibenzo[*b,d*]selenophene (4b)



Following **GPC**, dibenzoselenophene (**3b**, 31.6 mg, 0.137 mmol, 1 eq.) with TMEDA (16.6 mg, 30 µL, 0.143 mmol, 1.1 eq.) was dissolved in 1 ml THF at 0 °C. *n*-Butyllithium (12.8 mg, 0.08 ml, 2.5 M in hexane, 0.20 mmol, 1.5 eq.) was added. After stirring for 1.5 h at 0 °C, *N*-methoxy-*N*-methylbenzamide (32.8 mg, 0.03 ml, 0.198 mmol, 1.5 eq.) was added and stirred overnight at room temperature. Column chromatography (cyclohexane/DCM 1:1) yielded the product (**4b**, light orange solid, 20.1 mg, 0.0599 mmol, 46.2%).

M($C_{19}H_{12}OSe$): 335.28 g/mol. **M.p.:** 141-142 °C. **^{1}H-NMR (600 MHz, acetone-d$_6$, 298 K):** δ [ppm] = 8.65 (d, $^3J_{HH}$ = 7.7 Hz, 1H, C_5-*H*), 8.42 (d, $^3J_{HH}$ = 7.8 Hz, 1H, C_4-*H*), 8.15 (d, $^3J_{HH}$ = 7.7 Hz, 1H, C_1-*H*), 8.01 (d, $^3J_{HH}$ = 7.5 Hz, 1H, C_7-*H*), 7.83 (d, $^3J_{HH}$ = 7.2 Hz, 2H, C_{11}-*H*), 7.74 (t, $^3J_{HH}$ = 7.6 Hz, 1H, C_6-*H*), 7.70 (t, $^3J_{HH}$ = 7.4 Hz, 1H, C_{13}-*H*), 7.63 (t, $^3J_{HH}$ = 7.6 Hz, 2H, C_{12}-*H*), 7.57 (t, $^3J_{HH}$ = 7.3 Hz, 1H, C_3-*H*), 7.53 (t, $^3J_{HH}$ = 7.2 Hz, 1H, C_2-*H*). **^{13}C-NMR (151 MHz, acetone-d$_6$, 298 K):** δ [ppm] = 196.39 (C_9), 143.15 (C_{1a}), 141.86 (C_{8a}), 141.26 (C_{5a}), 139.26 (C_{10}), 137.75 (C_{4a}), 133.20 (C_7), 132.97 (C_8), 132.81 (C_{13}), 130.31 (C_{11}), 129.46 (C_{12}), 128.49 (C_2), 128.31 (C_5), 126.91 (C_1), 126.12 (C_3), 126.00 (C_6), 124.01 (C_4). **^{77}Se-NMR (114 MHz, acetone-d$_6$, 298 K):** δ [ppm] = 509.02. **HR-MS (ESI, 70 eV, DCM): m/z:** $[C_{19}H_{12}OSe + H]^+$ 337.0126, calculated: $[M + H]^+$ 337.0127. $[C_{19}H_{12}OSe + Na]^+$ 358.9946, calculated: $[M + Na]^+$ 358.9946. $[(C_{19}H_{12}OSe)_2 + Na]^+$ 695.0000, calculated: $[M_2 + Na]^+$ 694.9999. **IR:** $\tilde{\nu}$ [cm^{-1}] = 3046, 2958, 2922, 2852, 2175, 2134, 2023, 1958, 1937, 1869, 1793, 1771, 1716, 1698, 1685, 1671, 1636, 1596, 1523, 1475, 1440, 1395, 1273, 1259, 1177, 1090, 1074, 1017, 957, 919, 865, 798, 789, 752, 729, 697, 651, 628.

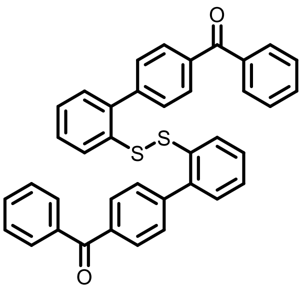
4-Benzoyldibenzo[*b,d*]tellurophene (4c)



Following **GPD**, the iodonium salt **7** (304 mg, 0.570 mmol, 1 eq.) with tellurium (233 mg, 1.82 mmol, 3.2 eq.) was dissolved in 2-picoline (1.89 g, 2 ml, 20.3 mmol, 35.5 eq.) and 5.5 ml dry DMF. The suspension was stirred under argon at 120 °C for 30 h. After the reaction was completed, the crude product was concentrated. After double column chromatography (cyclohexane/ethyl acetate 19:1; cyclohexane/DCM 4:1), the product was isolated (**4c**, yellow solid, 71.2 mg, 0.185 mmol, 32.9%).

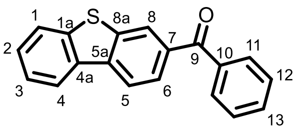
M($C_{19}H_{12}OTe$): 383.90 g/mol. **M.p.:** 175-178 °C. **^{1}H-NMR (600 MHz, acetone-d$_6$, 298 K):** δ [ppm] = 8.63 (dd, $^3J_{HH}$ = 7.6 Hz, 1H, C_5-*H*), 8.41 (d, $^3J_{HH}$ = 7.9 Hz, 1H, C_4-*H*), 8.21 (d, $^3J_{HH}$ = 7.6 Hz, 1H, C_1-*H*), 8.09 (d, $^3J_{HH}$ = 7.5 Hz, 1H, C_7-*H*), 7.86 – 7.82 (m, 2H, C_{11}-*H*), 7.78 (t, $^3J_{HH}$ = 7.6 Hz, 1H, C_6-*H*), 7.71 (t, $^3J_{HH}$ = 7.5 Hz, 1H, C_{13}-*H*), 7.64 (t, $^3J_{HH}$ = 7.6 Hz, 2H, C_{12}-*H*), 7.57 – 7.51 (m, 1H, C_3-*H*), 7.42 (ps-dd, $^3J_{HH}$ = 7.4, $^4J_{HH}$ = 1.2 Hz, 1H, C_2-*H*). **^{13}C-NMR (151 MHz, acetone-d$_6$, 298 K):** δ [ppm] = 196.55 (C_9), 146.73 (C_{5a}), 143.15 (C_{4a}), 139.08 (C_{10}), 136.18 (C_8), 135.45 (C_{1a}), 133.96 (C_{8a}), 133.73 (C_7), 133.10 (C_1), 132.73 (C_{13}), 130.30 (C_{11}), 129.44 (C_5, C_{12}), 128.21 (C_2), 126.85 (C_6), 126.56 (C_3), 125.47 (C_4). **^{125}Te-NMR (189 MHz, acetone-d$_6$, 298 K):** δ [ppm] = 717.98. **HR-MS (ESI, 70 eV, DCM): m/z:** $[C_{19}H_{12}OTe + H]^+$ 387.0021, calculated: $[M + H]^+$ 387.0024. $[C_{19}H_{12}OTe + Na]^+$ 408.9842, calculated: $[M + Na]^+$ 408.9844. $[(C_{19}H_{12}OTe)_2 + Na]^+$ 790.9762, calculated: $[M_2 + Na]^+$ 790.9768. **IR:** $\tilde{\nu}$ [cm^{-1}] = 2954, 2921, 2850, 1935, 1883, 1868, 1829, 1793, 1771, 1748, 1716, 1698, 1654, 1595, 1508, 1489, 1438, 1393, 1316, 1270, 1251, 1205, 1177, 1101, 1038, 1015, 999, 957, 863, 815, 785, 753, 732, 722, 697, 648, 626.

3-Benzoyldibenzo[*b,d*]thiophene (12a)



Following **GPA**[8,9], iodobiphenyl **9** (501 mg, 1.30 mmol), sulphur (81.4 mg, 2.54 mmol), $Na_2S \cdot 9H_2O$ (481 mg, 2.00 mmol) and CuI (52.3 mg, 0.27 mmol) were suspended in 2.5 ml dry DMF under argon atmosphere and brought to reaction at 100 °C overnight. After extraction with ethyl acetate, the product was yielded by concentration and was used without further purification (**11a**, yellow oil, 344 mg, 0.59 mmol, quant.).

M($C_{38}H_{26}O_2S_2$): 578.74 g/mol. **HR-MS (ESI, 70 eV, DCM): m/z:** $[C_{38}H_{26}O_2S_2 + H]^+$ 579.1467, calculated: $[M + H]^+$ 579.1447. $[C_{38}H_{26}O_2S_2 + Na]^+$ 601.1287, calculated: $[M + Na]^+$ 601.1266.

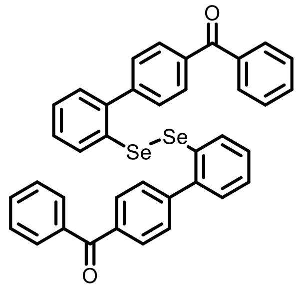


According to **GPA2**[8], disulfide **11a** (180 mg, 0.31 mmol) and $PdCl_2$ (5mol%) were dissolved in 1 ml dry DMSO under an argon atmosphere and stirred at 120 °C overnight. After column chromatography (cyclohexane/ethyl acetate 9:1), the product was isolated (**12a**, white solid, 51.0 mg, 0.177 mmol, 28%).

M($C_{19}H_{12}OS$): 288.36 g/mol. **M.p.:** 129-131 °C. **^{1}H-NMR (600 MHz, acetone-d$_6$, 298 K):** δ [ppm] = 8.49 (d, $^3J_{HH}$ = 8.2 Hz, 1H), 8.46 (d, $^3J_{HH}$ = 7.3 Hz, 1H), 8.41 (d, $^4J_{HH}$ = 0.9 Hz, 1H), 8.06 (d, $^3J_{HH}$ = 7.5 Hz, 1H), 7.93 (dd, $^3J_{HH}$ = 8.2, $^4J_{HH}$ = 1.4 Hz, 1H), 7.89 – 7.85 (m, 2H), 7.70 (t, $^3J_{HH}$ = 7.4 Hz, 1H), 7.65 – 7.56 (m, 4H). **^{13}C-NMR (151 MHz, acetone-d$_6$, 298 K):** δ [ppm] = 196.12, 141.83, 140.12, 139.64, 138.86, 137.08, 135.65, 133.41, 130.76, 129.44, 129.06, 127.04, 126.02, 125.92, 124.04, 123.69, 122.62. **HR-MS (ESI, 70 eV, DCM): m/z:** $[C_{19}H_{12}OS + H]^+$ 289.0681, calculated: $[M + H]^+$ 289.0682. $[C_{19}H_{12}OS + Na]^+$ 311.0502, calculated: $[M + Na]^+$ 311.0501. $[(C_{19}H_{12}OS)_2 + Na]^+$ 599.1004, calculated: $[M_2 + Na]^+$ 599.1110.

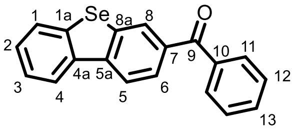
IR: $\tilde{\nu}$ [cm^{-1}] = 3019, 2922, 2359, 2344, 2187, 2175, 2160, 2010, 2001, 1988, 1748, 1716, 1698, 1685, 1636, 1542, 1522, 1507, 1497, 1418, 1338, 1018, 900, 859, 814, 735, 716, 688, 658, 628, 606.

3-Benzoyldibenzo[*b,d*]selenophene (12b)



Following **GPA**[8,9], iodobiphenyl **9** (254 mg, 0.66 mmol), selenium (312 mg, 3.96 mmol), K_3PO_4 (1.12 g, 5.26 mmol) and CuI (24.8 mg, 0.13 mmol) were suspended in 2 ml dry DMSO under argon atmosphere and brought to reaction at 120 °C overnight. After extraction with ethyl acetate, the product was yielded by concentration and was used without further purification (**11b**, orange oil, 235 mg, 0.35 mmol, quant.).

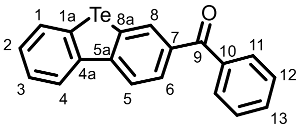
M($C_{38}H_{26}O_2Se_2$): 672.57 g/mol. **^{77}Se-NMR (76 MHz, acetone-d$_6$, 298 K):** δ [ppm] = 422.81. **HR-MS (ESI, 70 eV, DCM): m/z:** [$C_{38}H_{26}O_2Se_2$ + Na]$^+$ 675.0342, calculated: [M + Na]$^+$ 675.0344. [($C_{38}H_{26}O_2Se_2$)$_2$ + Na]$^+$ 1369.0432, calculated: [M$_2$ + Na]$^+$ 1369.0461.



According to **GPA2**[8], diselenide **11b** (51.0 mg, 0.076 mmol) and $PdCl_2$ (5mol%) were dissolved in 1 ml dry DMSO under an argon atmosphere and stirred at 120 °C overnight. After column chromatography (cyclohexane/ethyl acetate 19:1), the product was isolated (**12b**, light orange solid, 48.5 mg, 0.145 mmol, 95.4%).

M($C_{19}H_{12}OSe$): 335.28 g/mol. **M.p.:** 153-155 °C. **^{1}H-NMR (600 MHz, acetone-d$_6$, 298 K):** δ [ppm] = 8.49 (d, $^4J_{HH}$ = 0.6 Hz, 1H, C$_8$-*H*), 8.45 (d, $^3J_{HH}$ = 8.2 Hz, 1H, C$_5$-*H*), 8.42 (d, $^3J_{HH}$ = 7.8 Hz, 1H, C$_4$-*H*), 8.13 (d, $^3J_{HH}$ = 7.8 Hz, 1H, C$_1$-*H*), 7.93 (dd, $^3J_{HH}$ = 8.2, $^4J_{HH}$ = 1.3 Hz, 1H, C$_6$-*H*), 7.86 (d, $^3J_{HH}$ = 7.3 Hz, 2H, C$_{11}$-*H*), 7.69 (t, $^3J_{HH}$ = 7.4 Hz, 1H, C$_{13}$-*H*), 7.59 (m, 3H, C$_{12}$-*H,* C$_3$-*H*), 7.54 (dd, $^3J_{HH}$ = 7.6, $^4J_{HH}$ = 0.9 Hz, 1H, C$_2$-*H*). **^{13}C-NMR (151 MHz, acetone-d$_6$, 298 K):** δ [ppm] = 196.00 (*C*$_9$), 142.48 (*C*$_{5a}$), 141.90 (*C*$_{1a}$), 140.09 (*C*$_7$/*C*$_8$), 138.81 (*C*$_{10}$), 138.25 (*C*$_{4a}$), 136.84 (*C*$_7$/*C*$_8$), 133.28 (*C*$_{13}$), 130.64 (*C*$_{11}$), 129.33 (*C*$_{12}$), 129.13 (*C*$_8$), 128.94 (*C*$_2$), 127.37 (*C*$_6$), 127.31 (*C*$_1$), 126.24 (*C*$_3$), 124.82 (*C*$_4$), 123.63 (*C*$_5$). **^{77}Se-NMR (114 MHz, acetone-d$_6$, 298 K):** δ [ppm] = 461.81. **HR-MS (ESI, 70 eV, DCM): m/z:** [$C_{19}H_{12}OSe$ + H]$^+$ 337.0125, calculated: [M + H]$^+$ 337.0127. [$C_{19}H_{12}OSe$ + Na]$^+$ 358.9946, calculated: [M + Na]$^+$ 358.9946. **IR:** $\tilde{\nu}$ [cm^{-1}] = 3048, 2922, 2851, 2384, 2341, 2301, 2220, 2192, 2135, 2076, 2036, 1997, 1935, 1871, 1790, 1699, 1649, 1591, 1489, 1383, 1304, 1280, 1254, 1228, 1178, 1076, 1046, 1000, 958, 897, 845, 761, 725, 699, 686, 664, 617. Spectroscopic data is in agreement with the literature.[20]

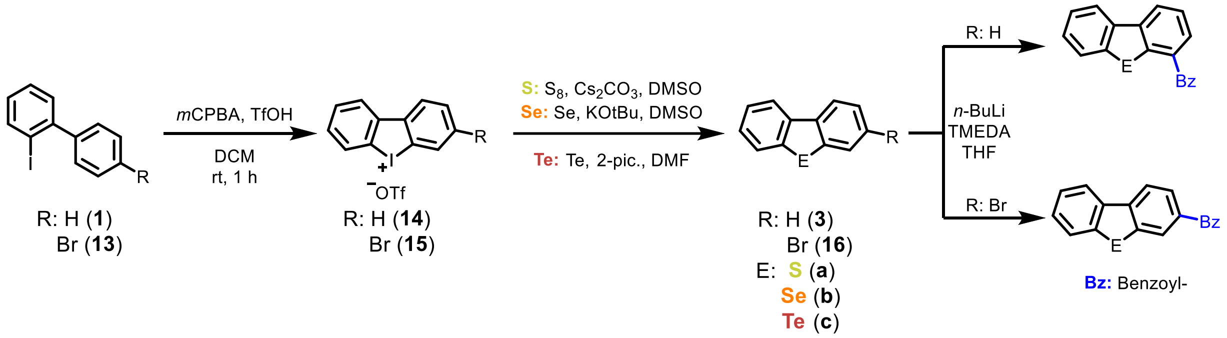
3-Benzoyldibenzo[*b,d*]tellurophene (12c)



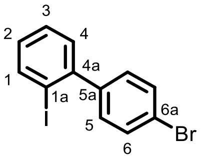
Following **GPD**, the iodonium salt **10** (254 mg, 0.486 mmol, 1 eq.) with tellurium (187 mg, 1.46 mmol, 3 eq.) was dissolved in 2-picoline (1.51 g, 1.60 ml, 16.2 mmol, 33 eq.) and 3.5 ml dry DMF. The suspension was stirred under argon at 120 °C for 30 h. After complete reaction, the crude product was concentrated. After column chromatography (cyclohexane/ethyl acetate 19:1), the product was isolated (**12c**, yellow solid, 49.6 mg, 0.129 mmol, 27.0%).

M($C_{19}H_{12}OTe$): 383.90 g/mol. **M.p.:** 141-143 °C. **^{1}H-NMR (600 MHz, acetone-d$_6$, 298 K):** δ [ppm] = 8.54 (d, $^4J_{HH}$ = 1.3 Hz, 1H, C$_8$-*H*), 8.42 – 8.36 (m, 2H, C$_5$-*H*, C$_4$-*H*), 8.18 (d, $^3J_{HH}$ = 7.8 Hz, 1H, C$_1$-*H*), 7.90 (dd, $^3J_{HH}$ = 8.3, $^4J_{HH}$ = 1.3 Hz, 1H, C$_6$-*H*), 7.85 (d, $^3J_{HH}$ = 7.3 Hz, 2H, C$_{11}$-*H*), 7.68 (t, $^3J_{HH}$ = 7.4 Hz, 1H, C$_{13}$-*H*), 7.58 (t, $^3J_{HH}$ = 7.7 Hz, 2H, C$_{12}$-*H*), 7.54 (t, $^3J_{HH}$ = 7.6 Hz, 1H, C$_3$-*H*), 7.41 (t, $^3J_{HH}$ = 7.4 Hz, 1H, C$_2$-*H*). **^{13}C-NMR (151 MHz, acetone-d$_6$, 298 K):** δ [ppm] = 196.15 (C_9), 148.52 (C_{5a}), 144.07 (C_7/C_{8a}), 139.03 (C_{10}), 136.36 (C_7/C_{8a}), 135.73 (C_8), 133.88 (C_1), 133.26 (C_{13}), 132.37 (C_{1a}), 130.68 (C_{11}), 130.32 (C_{4a}), 129.38 (C_{12}), 128.63 (C_2), 128.05 (C_6), 126.87 (C_3), 126.49 (C_4), 125.17 (C_5). **^{125}Te-NMR (189 MHz, acetone-d$_6$, 298 K):** δ [ppm] = 681.22. **HR-MS (ESI, 70 eV, DCM): m/z:** [$C_{19}H_{12}OTe$ + H]$^+$ 387.0020, calculated: [M + H]$^+$ 387.0024. [$C_{19}H_{12}OTe$ + Na]$^+$ 408.9843, calculated: [M + Na]$^+$ 408.9844. [($C_{19}H_{12}OTe$)$_2$ + Na]$^+$ 790.9763, calculated: [M$_2$ + Na]$^+$ 790.9768. **IR:** $\tilde{\nu}$ [cm^{-1}] = 3043, 2920, 2851, 1644, 1631, 1595, 1575, 1467, 1428, 1378, 1314, 1302, 1275, 1254, 1231, 1177, 1152, 1073, 1037, 998, 951, 906, 843, 825, 796, 778, 767, 759, 723, 696, 674, 654, 633.

Unsuccessful synthetic pathways



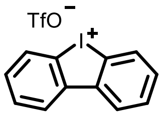
4’-Bromo-2-iodo-1,1’-biphenyl (13)



Synthesis was performed by adaptation of the literature.[21] In a dried Schlenk flask, 1,2-diiodobenzene (3.03 g, 1.20 ml, 9.18 mmol, 1 eq.), 4-bromophenylboronic acid (2.21 g, 11.0 mmol, 1.2 eq.)and potassium carbonate (5.13 g, 37.1 mmol, 4 eq.) were dissolved in 12 ml H_2O and 9.4 ml 1,2-dimethoxyethane. The suspension was degassed with argon for 30 min. After the addition of tetrakis(triphenylphosphine)-palladium(0) (245 mg, 0.212 mmol, 2 mol%), the reaction mixture was refluxed overnight. Afterwards, the suspension was diluted with H_2O and extracted four times with 100 ml ethyl acetate. Combined organic layers were dried over $MgSO_4$ and purified by column chromatography (cyclohexane) yielding the product (**13**, colourless oil, 1.43 g, 3.99 mmol, 43.5%).

M($C_{12}H_8BrI$): 359.00 g/mol. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ [ppm] = 7.95 (dd, $^3J_{HH}$ = 8.0, $^4J_{HH}$ = 1.0 Hz, 1H, C_1-*H*), 7.58 – 7.54 (m, 2H, C_6-*H*), 7.39 (td, $^3J_{HH}$ = 7.5, $^4J_{HH}$ = 1.2 Hz, 1H, C_3-*H*), 7.29 – 7.25 (m, 1H, C_4-*H*), 7.24 – 7.20 (m, 2H, C_5-*H*), 7.0 (td, $^3J_{HH}$ = 7.7, $^4J_{HH}$ = 1.7 Hz, 1H, C_2-*H*). **^{13}C-NMR (101 MHz, $CDCl_3$, 298 K):** δ [ppm] = 145.54 (C_{4a}), 143.12 (C_{5a}), 139.77 (C_1), 131.31 (C_6), 131.12 (C_5), 130.07 (C_4), 129.25 (C_2), 128.39 (C_3), 122.10 (C_{6a}), 98.39 (C_{1a}). **MS (GC): m/z:** $[C_{12}H_8BrI]^+$ 357.90, calculated: $[M]^+$ 357.88. **IR**: $\tilde{\nu}$ [cm^{-1}] = 3046, 3024, 2920, 2850, 1992, 1923, 1896, 1845, 1802, 1781, 1772, 1762, 1698, 1647, 1625, 1495, 1456, 1389, 1291, 1246, 1177, 1070, 1012, 997, 960, 942, 865, 822, 750, 722, 660.

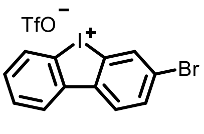
Dibenzo[*b,d*]-iodol-5-ium-trifluoromethane sulfonate (14)



Synthesis was performed according to literature[10] using 2-iodobiphenyl (**1**, 2.57 g, 1.65 ml, 9.19 mmol) in 35 ml DCM, *m*CPBA (70%, 3.38 g, 13.7 mmol, 1.5 eq.) in 30 ml DCM and trifluoromethanesulfonic acid (4.10 g, 2.40 ml, 27.35 mmol, 3 eq.). The product was isolated by precipitation (**14**, white solid, 3.82 g, 8.91 mmol, 99.8%).

M($C_{12}H_8I{\cdot}CF_3O_3S$): 428.17 g/mol. **m.p.:** 245-246 °C. **^{1}H-NMR (400 MHz, DMSO-d$_6$, 298 K):** δ [ppm] = 8.50 (dd, $^3J_{HH}$ = 7.9, $^4J_{HH}$ = 1.2 Hz, 2H, H_{Ar}), 8.22 (d, $^3J_{HH}$ = 7.6 Hz, 2H, H_{Ar}), 7.90 – 7.83 (m, 2H, H_{Ar}), 7.76 – 7.69 (m, 2H, H_{Ar}). **^{13}C-NMR (101 MHz, DMSO-d$_6$, 298 K):** δ [ppm] = 141.79, 131.17, 130.79, 130.64, 127.07, 121.66, 120.71 (d, $^1J_{\mathrm{CF}}$ = 322.5 Hz). **^{19}F-NMR (376 MHz, DMSO-d$_6$, 298 K):** δ [ppm] = -77.75 (CF_3). Spectroscopic data is in agreement with the literature.[10]

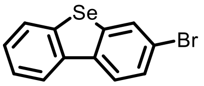
3-Bromodibenzo[*b,d*]-iodol-5-ium-trifluoromethane sulfonate (15)



Synthesis was performed according to literature[10] using 4’-bromo-2-iodobiphenyl (**13**, 1.00 g, 0.54 ml, 2.80 mmol) in 16 ml DCM, *m*CPBA (70%, 1.11 g, 4.51 mmol, 1.6 eq.) in 10 ml DCM and trifluoromethanesulfonic acid (1.28 g, 0.75 ml, 8.55 mmol, 3 eq.). The product was isolated by precipitation (**15**, white solid, 1.40 g, 2.76 mmol, 99.1%).

M($C_{12}H_8BrI{\cdot}CF_3O_3S$): 507.06 g/mol. **m.p.:** 302-304 °C. **^{1}H-NMR (400 MHz, acetone-d$_6$, 298 K):** δ [ppm] = 8.53 (d, $^4J_{HH}$ = 1.8 Hz, 1H), 8.50 (dd, $^3J_{HH}$ = 7.9, $^4J_{HH}$ = 1.4 Hz, 1H), 8.42 (d, $^3J_{HH}$ = 8.5 Hz, 1H), 8.37 (dd, $^3J_{HH}$ = 8.4, $^4J_{HH}$ = 0.7 Hz, 1H), 8.09 (dd, $^3J_{HH}$ = 8.5, $^4J_{HH}$ = 1.8 Hz, 1H), 7.97 – 7.92 (m, 1H), 7.84 – 7.78 (m, 1H). **^{13}C-NMR (101 MHz, acetone-d$_6$, 298 K):** δ [ppm] = 142.62, 142.30, 135.37, 134.15, 132.70, 132.20, 131.87, 129.19, 128.38, 124.29, 122.32, 122.23, 121.90 (d, $^1J_{\mathrm{CF}}$ = 320.6 Hz). **^{19}F-NMR (376 MHz, acetone-d$_6$, 298 K):** δ [ppm] = -78.95 (CF_3). **HR-MS (ESI, 70 eV, acetone): m/z:** [$C_{12}H_8BrI$]$^+$ 356.8772, calculated: [M]$^+$ 356.8770. Spectroscopic data is in agreement with the literature.[10]

3-Bromodibenzo[*b,d*]selenophene (16b)

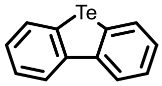


Synthesis was performed under adaptation of the literature.[15] In a dried pressure tube, iodonium salt **15** (403 mg, 0.795 mmol, 1 eq.), sodium *tert*-butanolate (419 mg, 3.73 mmol, 4.7 eq.) and freshly ground selenium (217 mg, 2.75 mmol, 3.5 eq.) were dissolved in 8 ml dry DMSO under argon. The reaction was stirred overnight at 80 °C. After conversion, the suspension was diluted with 20 ml H_2O and extracted three times with 20 ml ethyl acetate. The combined organic layers were dried over $MgSO_4$, concentrated and purified by column chromatography (cyclohexane) yielding the product (**16b**, light brownish solid, 46.6 mg, 0.150 mmol, 19.1%). The product was contaminated and could not be further purified.

M($C_{12}H_7BrSe$): 310.06 g/mol. **^{1}H-NMR (400 MHz, CDCl$_3$, 298 K):** δ [ppm] = 8.11 – 8.08 (m, 1H), 8.02 (d, $^4J_{HH}$ = 1.8 Hz, 1H), 7.97 (d, $^3J_{HH}$ = 8.4 Hz, 1H), 7.87 (dt, $^3J_{HH}$ = 7.7, $^4J_{HH}$ = 0.8 Hz, 1H), 7.57 (dd, $^3J_{HH}$ = 8.4, $^4J_{HH}$ = 1.8 Hz, 1H), 7.51 – 7.39 (m, 2H). **^{77}Se-NMR (76 MHz, CDCl$_3$, 298 K):** δ [ppm] = 462.00.

HR-MS (APCI, 70 eV, DCM): m/z: $[C_{12}H_7BrSe + H]^+$ 310.8953, calculated: $[M + H]^+$ 310.8966. Spectroscopic data is in agreement with the literature.[15]

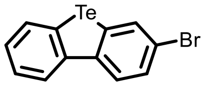
Dibenzo[*b,d*]tellurophene (3c)



Synthesis was performed according to the literature.[10] Iodonium salt **14** (508 mg, 1.19 mmol, 1 eq.), freshly ground tellurium (427 mg, 3.34 mmol, 2.8 eq.) and 2-picoline (3.77 g, 4 ml, 40.5 mmol, 30 eq.) were brought to reaction in 8 ml dry DMF. After concentration, column chromatography (cyclohexane/ethyl acetate 19:1) yielded the product **3c** (yellow solid, 256 mg, 0.917 mmol, 78.5%).

M($C_{12}H_8Te$): 279.80 g/mol. **m.p.:** 96 °C. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ [ppm] = 8.11 (dd, $^3J_{HH}$ = 8.1, $^4J_{HH}$ = 1.2 Hz), 7.89 (dd, $^3J_{HH}$ = 7.7, $^4J_{HH}$ = 1.1 Hz, 1H), 7.46 (ddd, $^3J_{HH}$ = 8.2, 7.1, $^4J_{HH}$ = 1.2 Hz, 1H), 7.30 (td, $^3J_{HH}$ = 7.5, $^4J_{HH}$ = 1.3 Hz, 1H). **^{13}C-NMR (101 MHz, $CDCl_3$, 298 K):** δ [ppm] = 144.14, 132.74, 128.77, 127.02, 125.84, 124.76. **^{125}Te-NMR (126 MHz, $CDCl_3$, 298 K):** δ [ppm] = 653.16. **HR-MS (APCI, 70 eV, DCM): m/z:** $[C_{12}H_8Te + H]^+$ 282.9674, calculated: $[M + H]^+$ 282.9761. Spectroscopic data is in agreement with the literature.[10]

3-Bromodibenzo[*b,d*]tellurophene (16c)



The synthesis was performed according to the literature[10] using iodonium salt **15** (279 mg, 0.55 mmol, 1 eq.), freshly ground tellurium (176 mg, 1.38 mmol, 2.5 eq.) and 2-picoline (1.57 g, 2 ml, 20.3 mmol, 37 eq.) in 4 ml dry DMSO. Extraction and column chromatography (cyclohexane) yielded the product **16c** (yellow solid, 81.6 mg, 0.228 mmol, 46.1%).

M($C_{12}H_7BrTe$): 358.69 g/mol. **m.p.:** 126-130°C. **^{1}H-NMR (400 MHz, $CDCl_3$, 298 K):** δ [ppm] = 8.06 (dd, $^3J_{HH}$ = 8.1, $^4J_{HH}$ = 1.2 Hz, 1H), 8.00 (d, $^4J_{HH}$ = 1.9 Hz, 1H), 7.93 (d, $^3J_{HH}$ = 8.5 Hz, 1H), 7.87 (dd, $^3J_{HH}$ = 7.8, $^4J_{HH}$ = 1.2 Hz, 1H), 7.56 (dd, $^3J_{HH}$ = 8.5, $^4J_{HH}$ = 1.9 Hz, 1H), 7.46 (ddd, $^3J_{HH}$ = 8.1, 7.2, $^4J_{HH}$ = 1.2 Hz, 1H), 7.33 (td, $^3J_{HH}$ = 7.5, $^4J_{HH}$ = 1.3 Hz, 1H). **^{13}C-NMR (101 MHz, $CDCl_3$, 298 K):** δ [ppm] = 143.12, 142.99, 134.88, 132.65, 130.44, 129.21, 128.83, 127.39, 126.08, 125.72, 124.85, 120.89. **^{125}Te-NMR (126 MHz, $CDCl_3$, 298 K**): δ [ppm] = 681.79. **HR-MS (APCI, 70 eV, DCM): m/z:** $[C_{12}H_7BrTe + H]^+$ 360.8816, calculated: $[M + H]^+$ 360.8848. Spectroscopic data is in agreement with the literature.[10]

3. NMR-Spectra

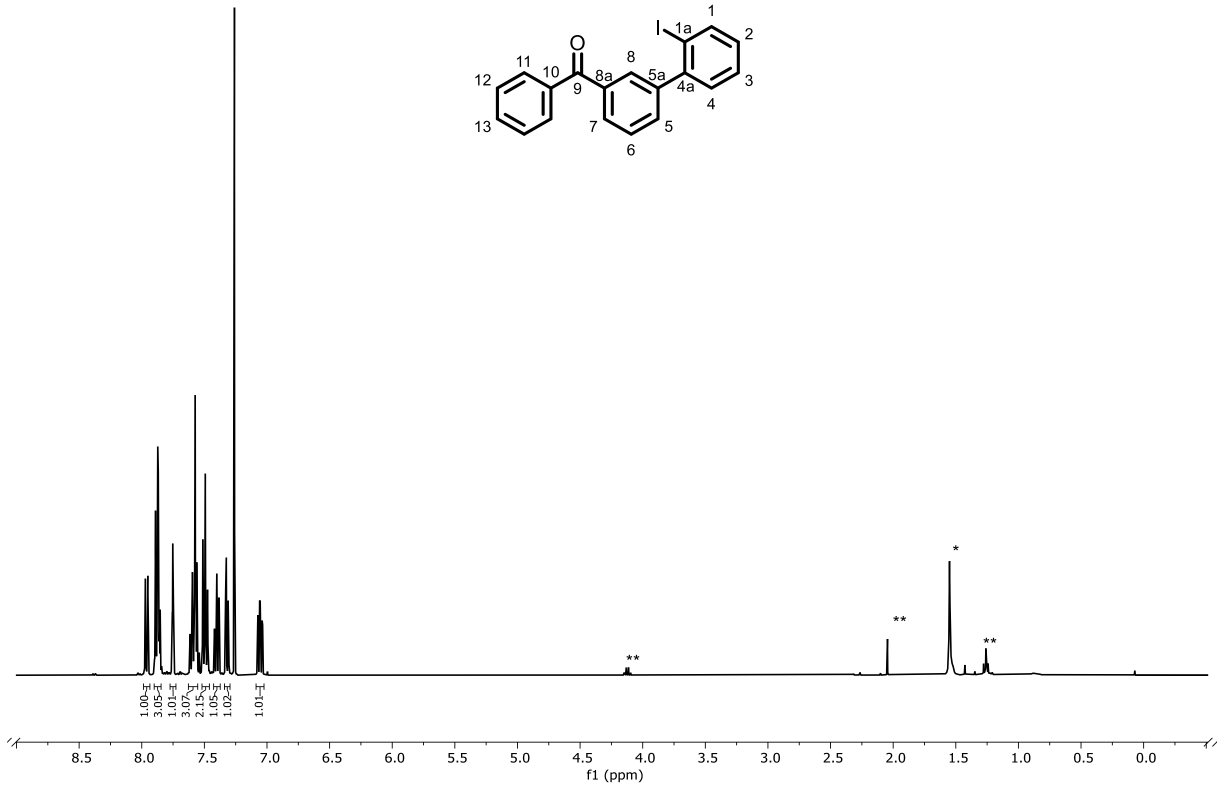


Figure S1: ^{1}H-NMR (400 MHz, $CDCl_3$, 298 K) of compound **6** (*water, **ethyl acetate).

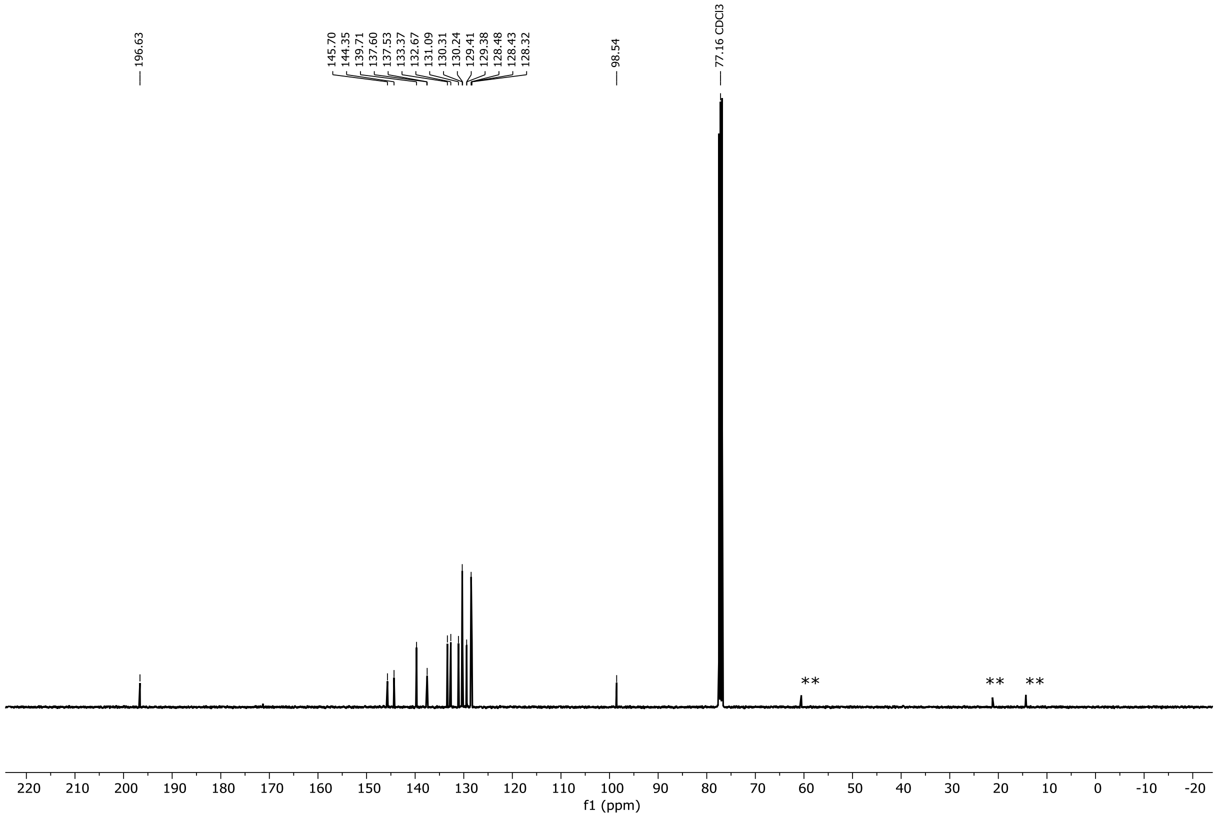


Figure S2: ^{13}C-NMR spectrum (101 MHz, $CDCl_3$, 298 K) of compound **6** (**ethyl acetate).

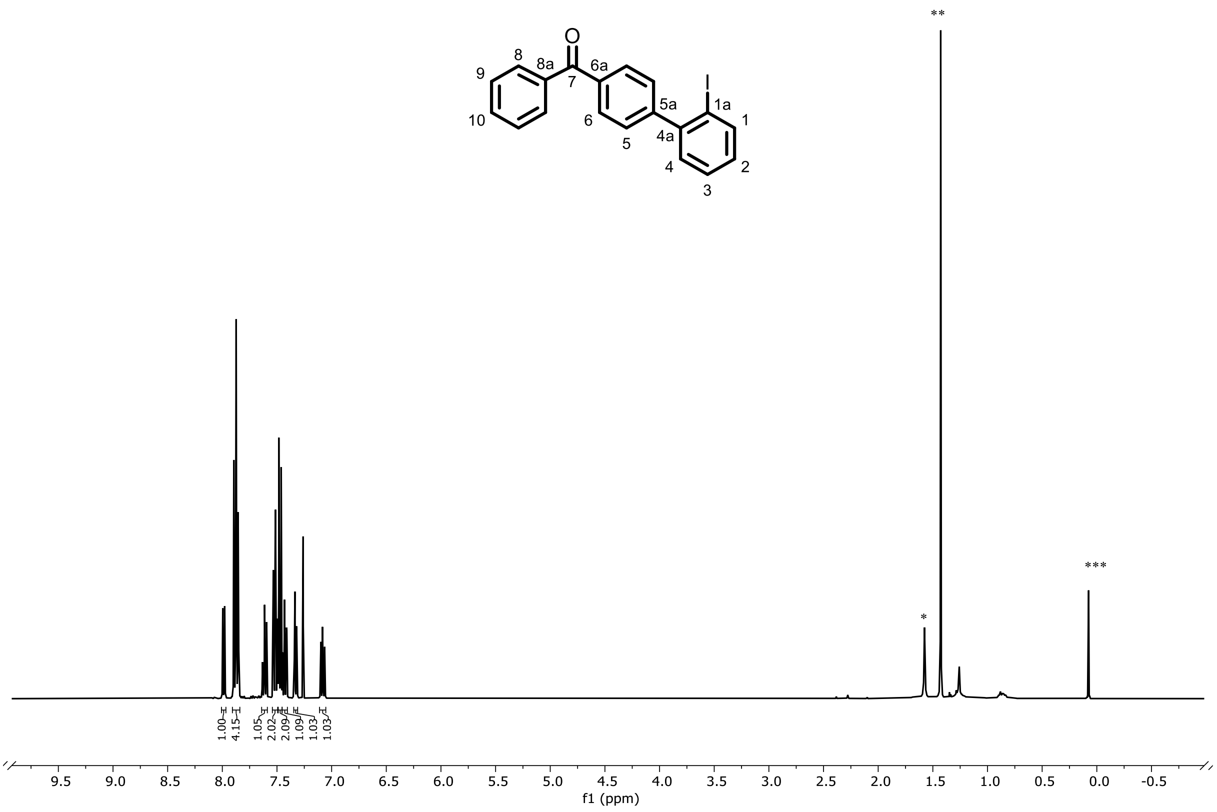


Figure S3: ^{1}H-NMR (400 MHz, $CDCl_3$, 298 K) of compound **9** (*water, **cyclohexane, ***grease).

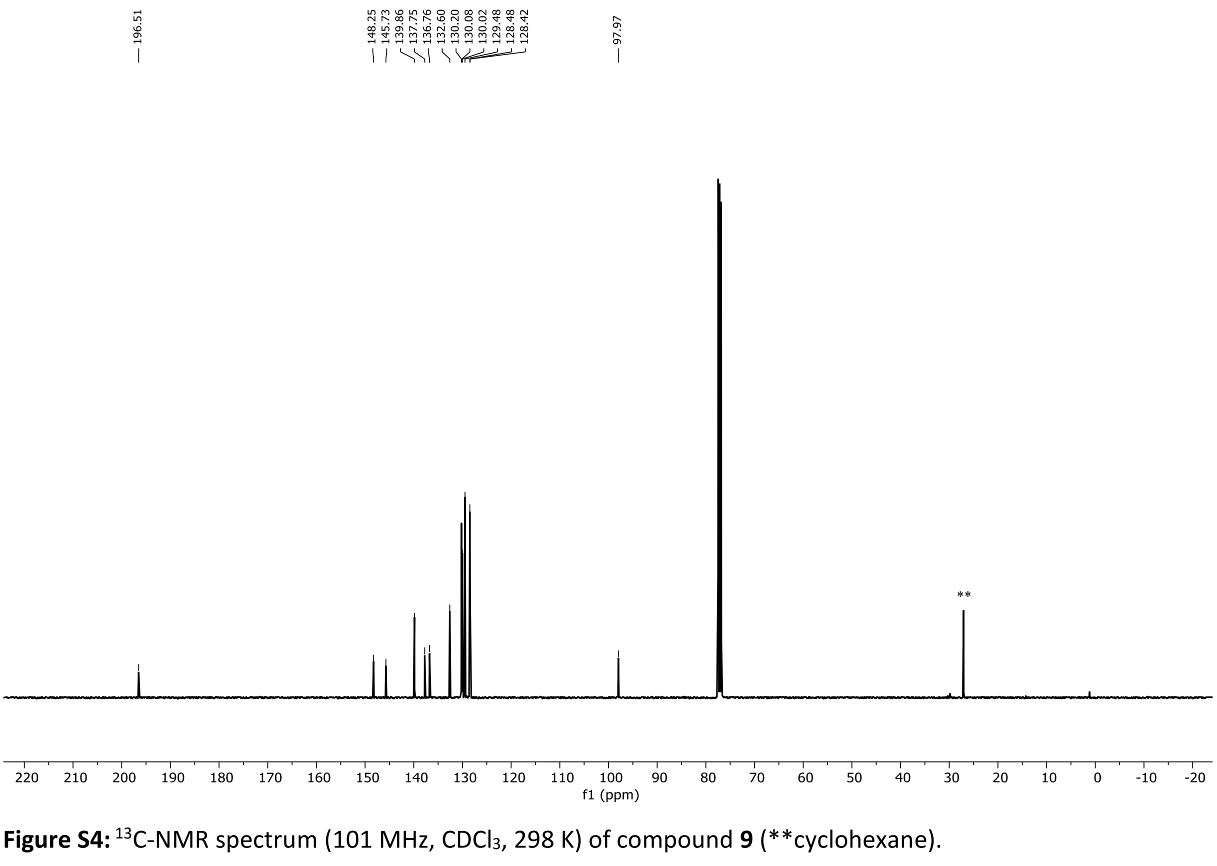


Figure S4: ^{13}C-NMR spectrum (101 MHz, $CDCl_3$, 298 K) of compound **9** (**cyclohexane).

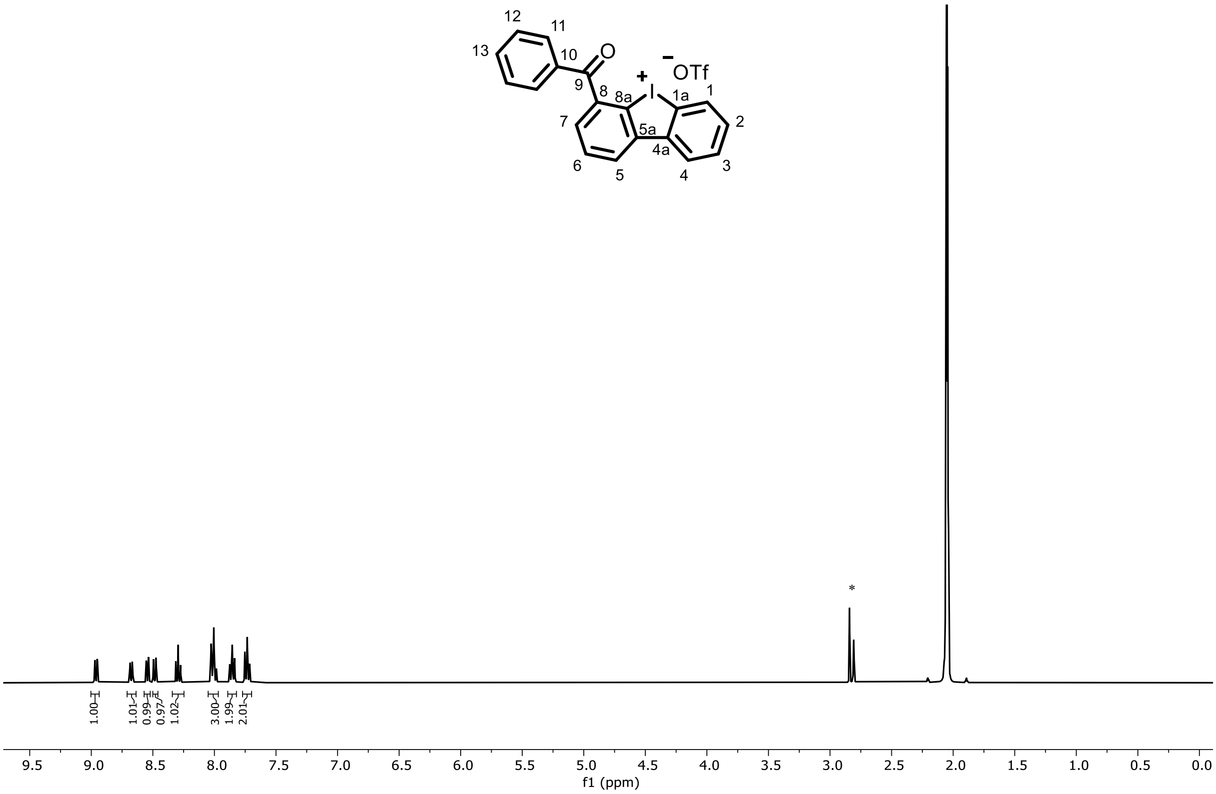


Figure S5: ^{1}H-NMR (400 MHz, acetone-d$_6$, 298 K) of compound **7** (*water/HDO).

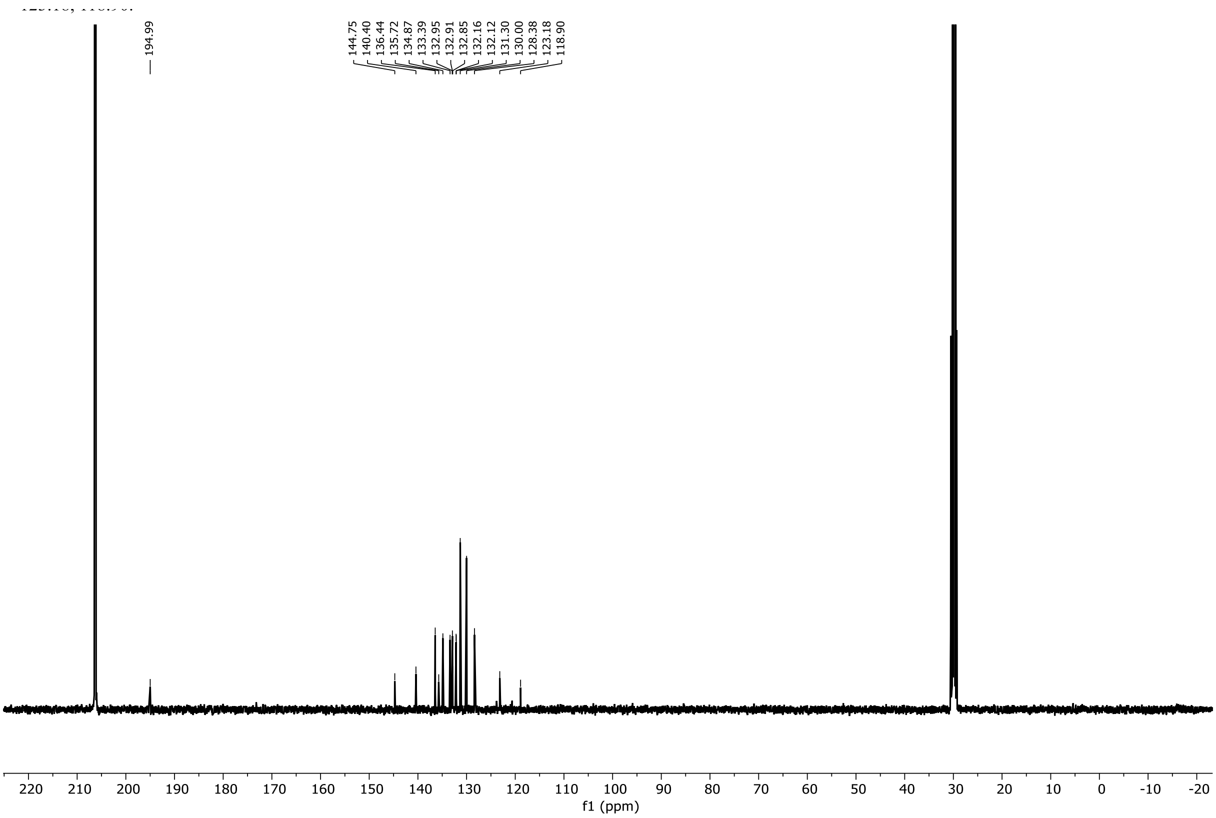


Figure S6: ^{13}C-NMR (101 MHz, acetone-d$_6$, 298 K) of compound **7**.

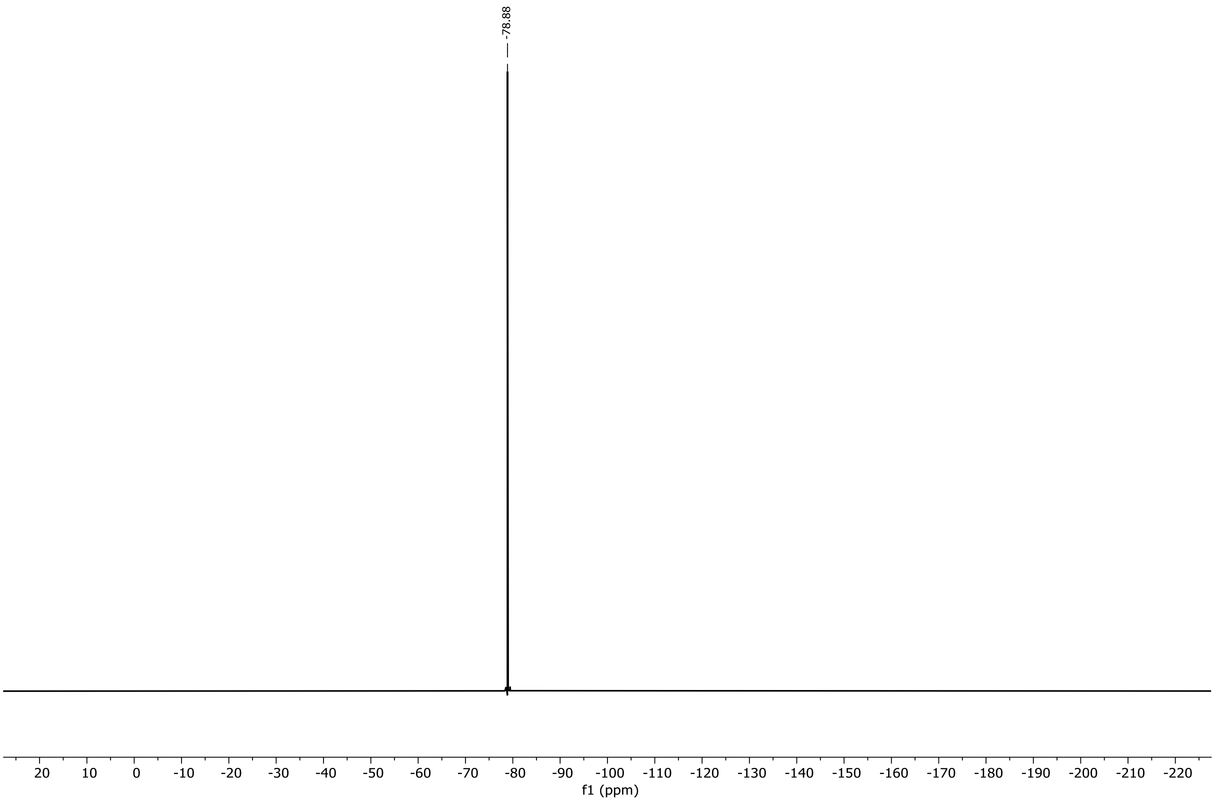


Figure S7: ^{19}F-NMR spectrum (376 MHz, acetone-d$_6$, 298 K) of compound **7**.

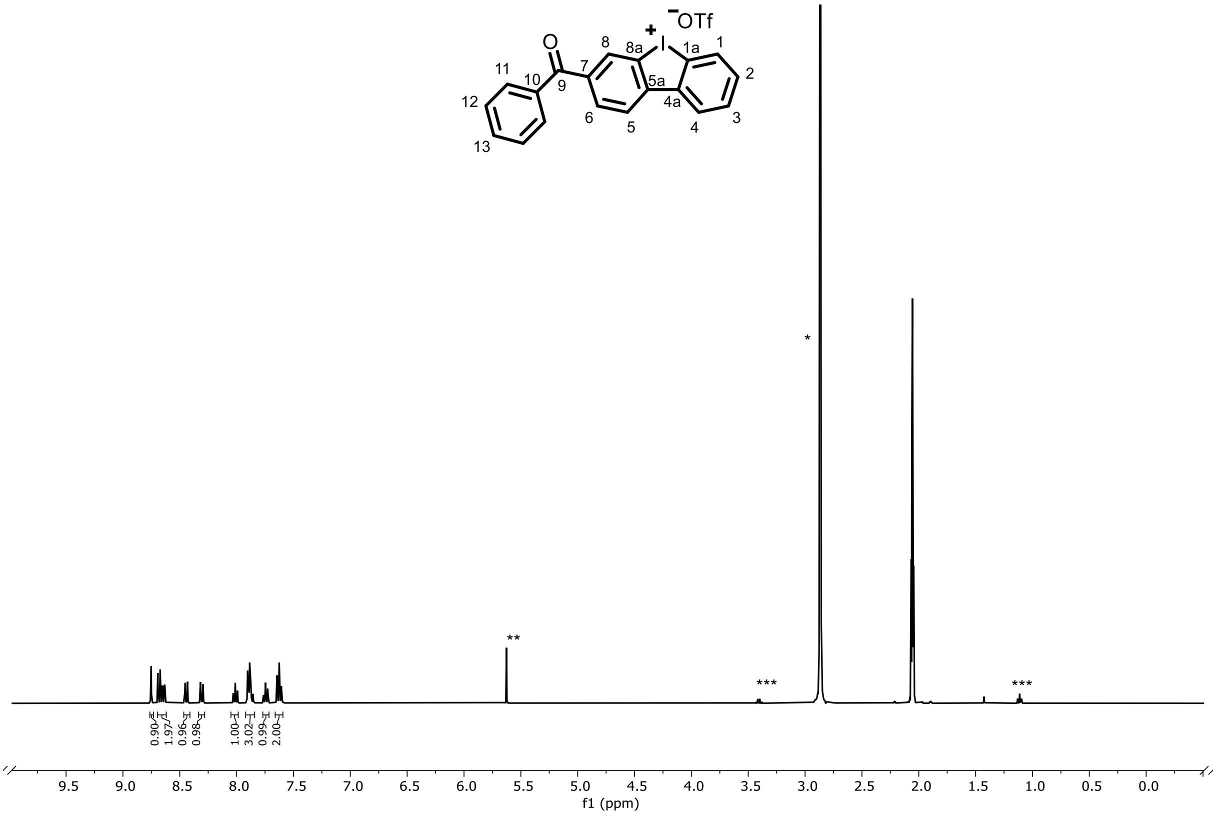


Figure S8: ^{1}H-NMR (400 MHz, acetone-d$_6$, 298 K) of compound **10** (*water/HDO, **DCM, ***Et$_2$O).

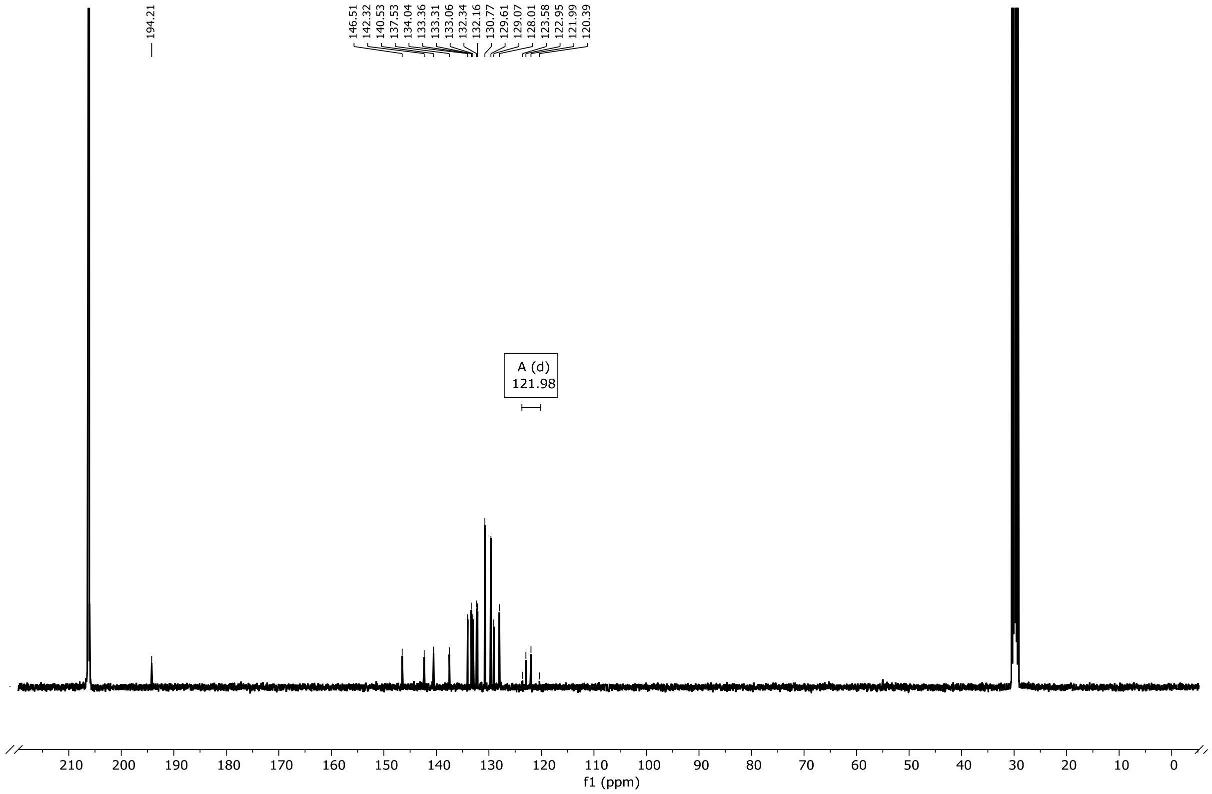


Figure S9: ^{13}C-NMR (101 MHz, acetone-d$_6$, 298 K) of compound **10**.

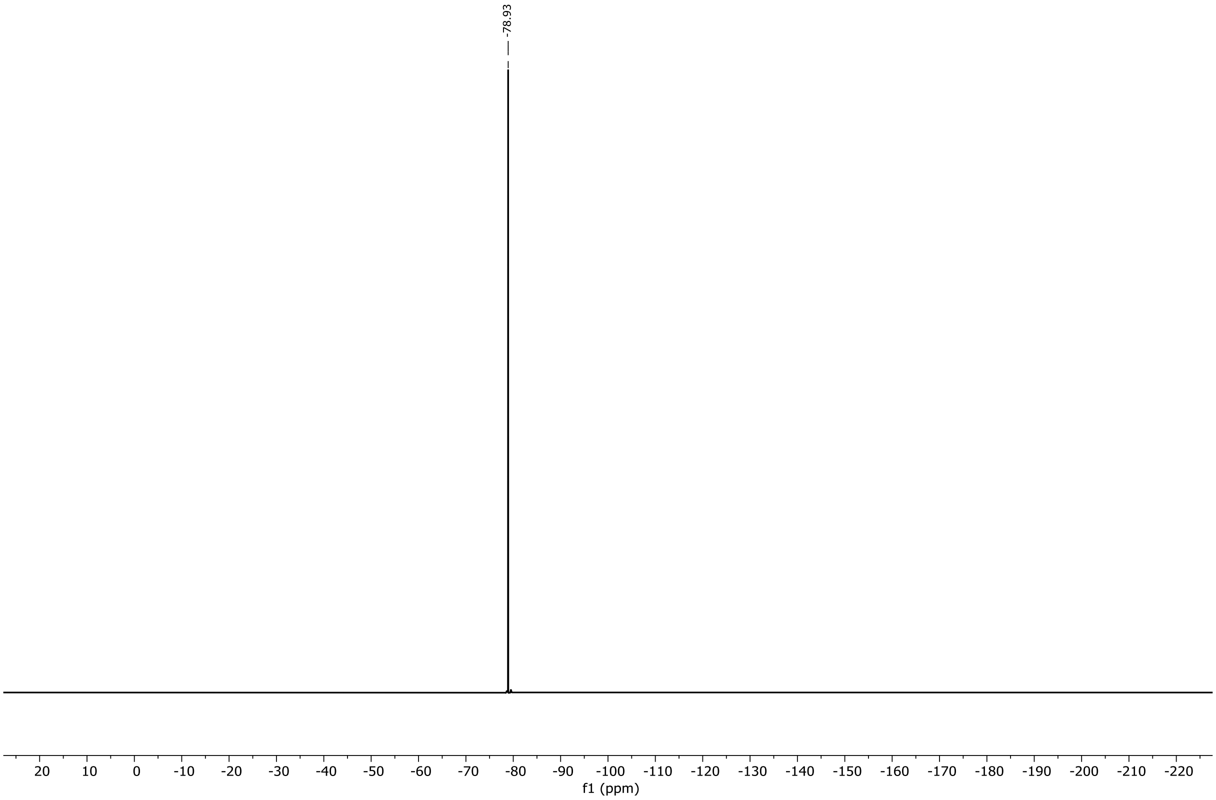


Figure S10: ^{19}F-NMR spectrum (376 MHz, acetone-d$_6$, 298 K) of compound **10**.

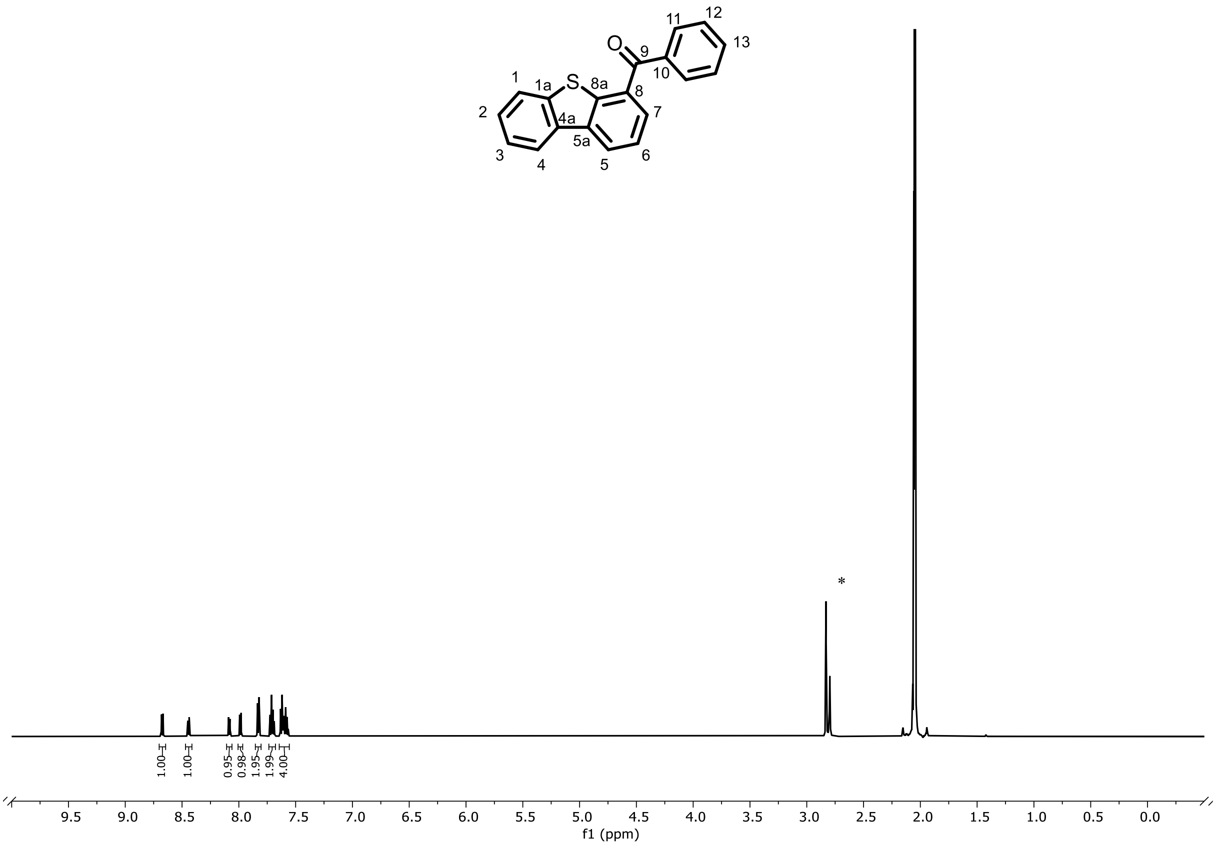


Figure S11: ^{1}H-NMR (600 MHz, acetone-d$_6$, 298 K) of compound **4a** (*water/HDO).

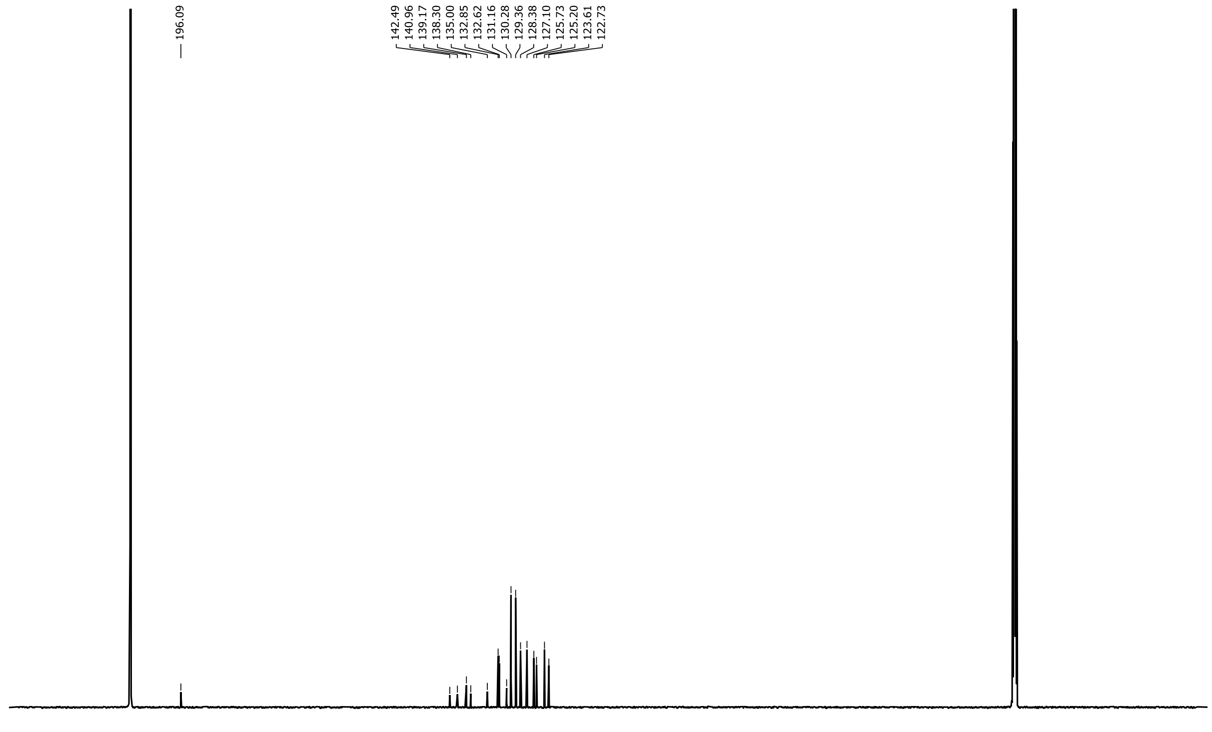


Figure S12: ^{13}C-NMR spectrum (151 MHz, acetone-d$_6$, 298 K) of compound **4a** (*water/HDO).

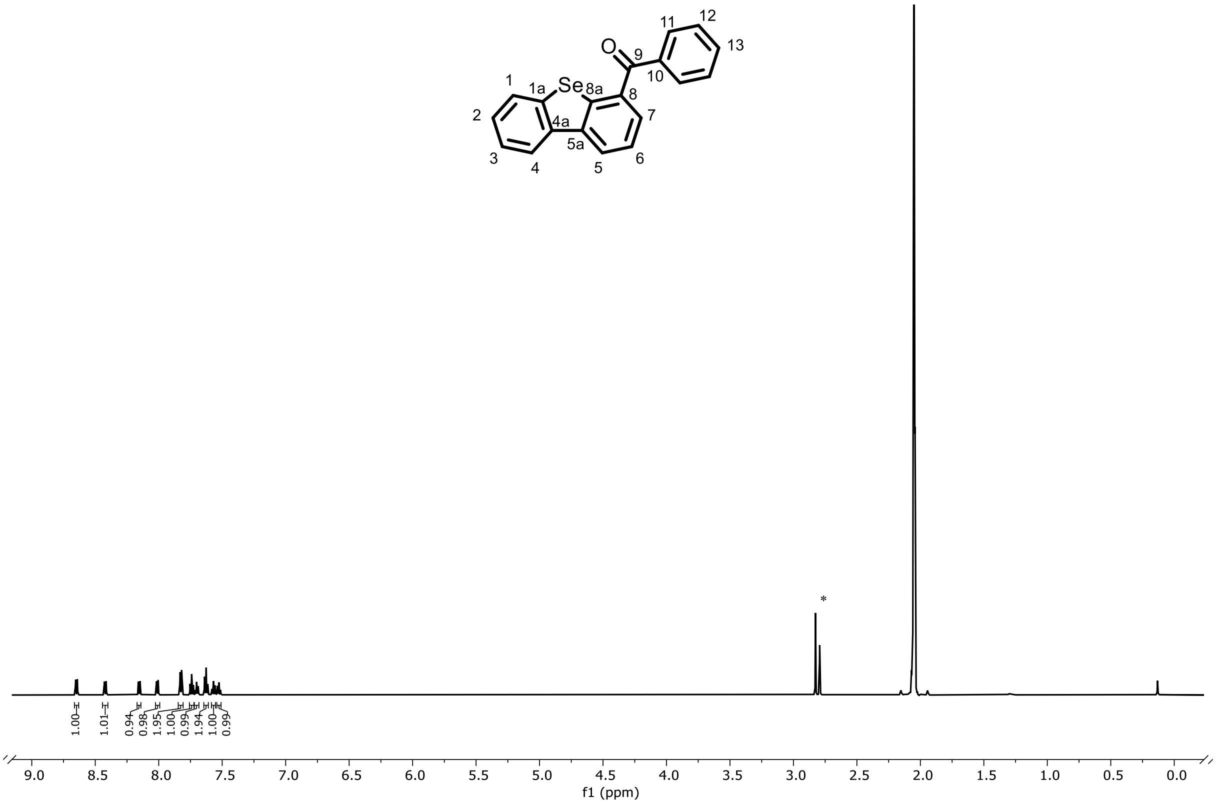


Figure S13: ^{1}H-NMR (600 MHz, acetone-d$_6$, 298 K) of compound **4b** (*water/HDO).

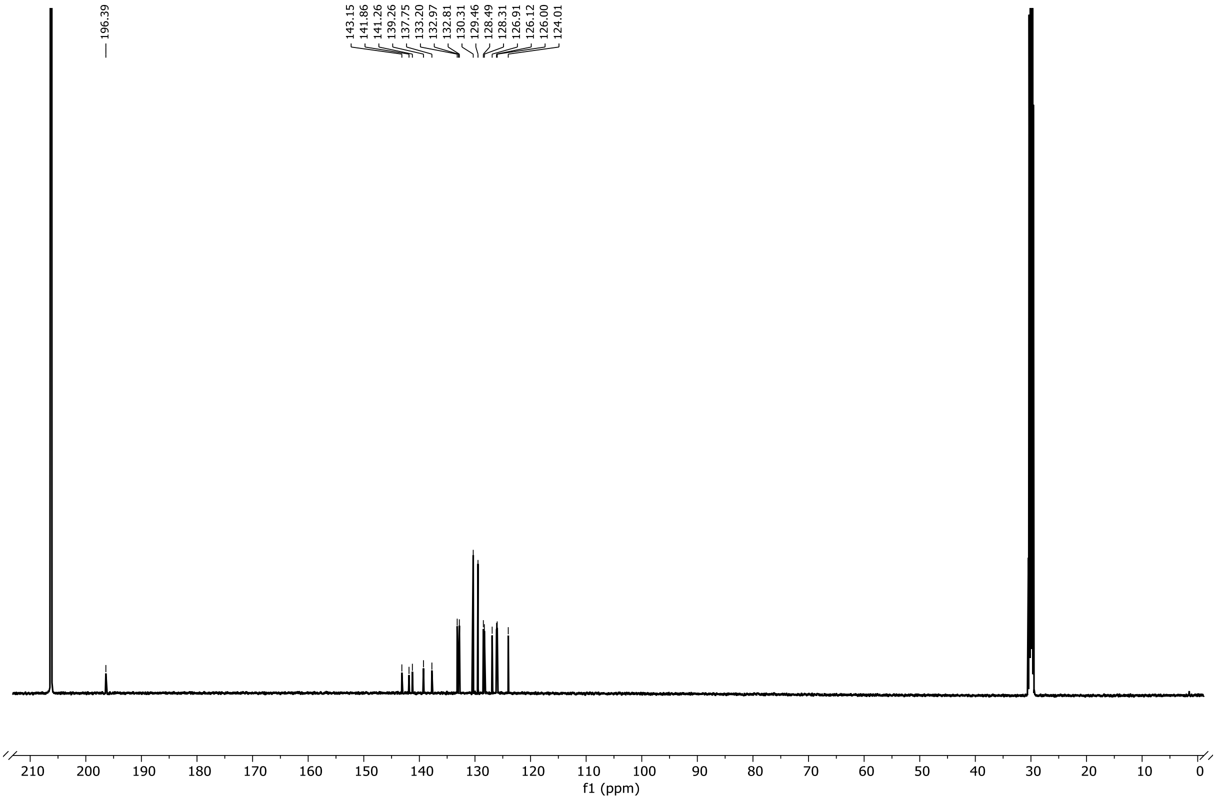


Figure S14: ^{13}C-NMR (151 MHz, acetone-d$_6$, 298 K) of compound **4b**.

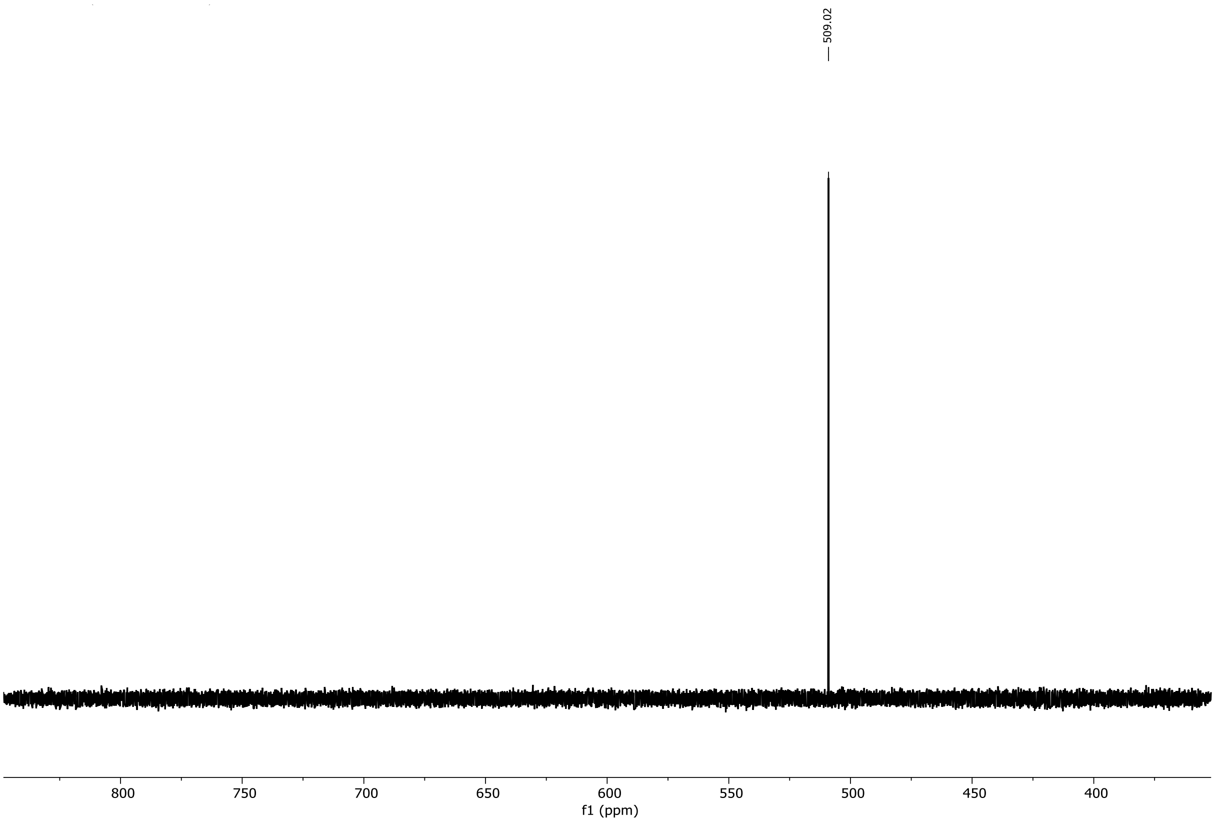


Figure S15: ^{77}Se-NMR spectrum (114 MHz, acetone-d$_6$, 298 K) of compound **4b**.

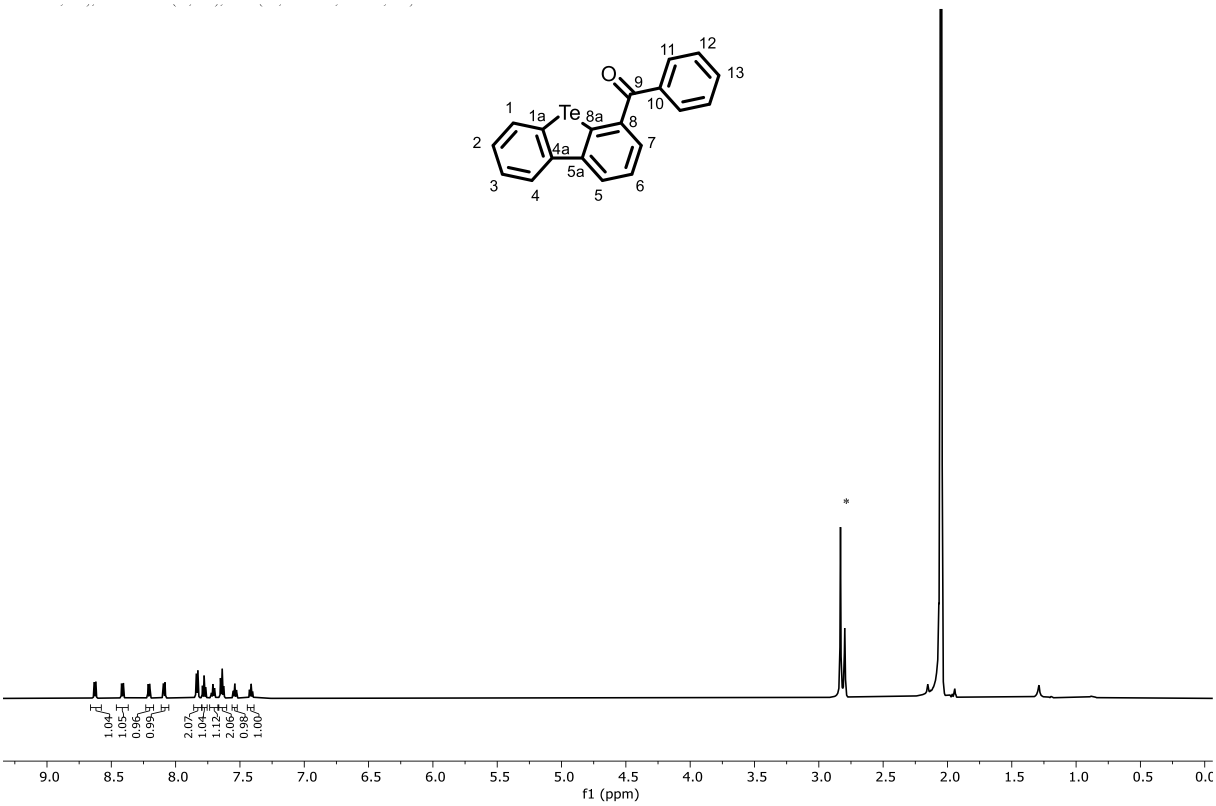


Figure S16: ^{1}H-NMR (600 MHz, acetone-d$_6$, 298 K) of compound **4c** (*water/HDO).

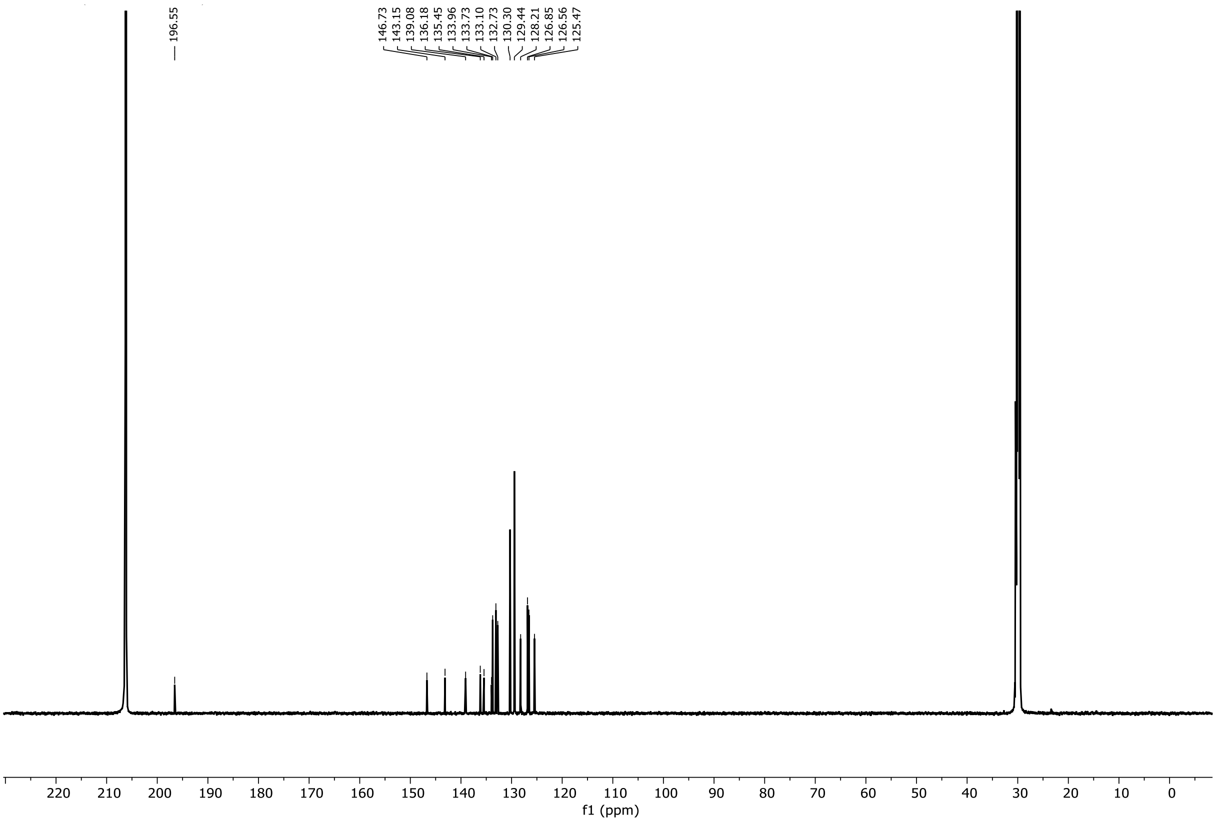


Figure S17: ^{13}C-NMR (151 MHz, acetone-d$_6$, 298 K) of compound **4c**.

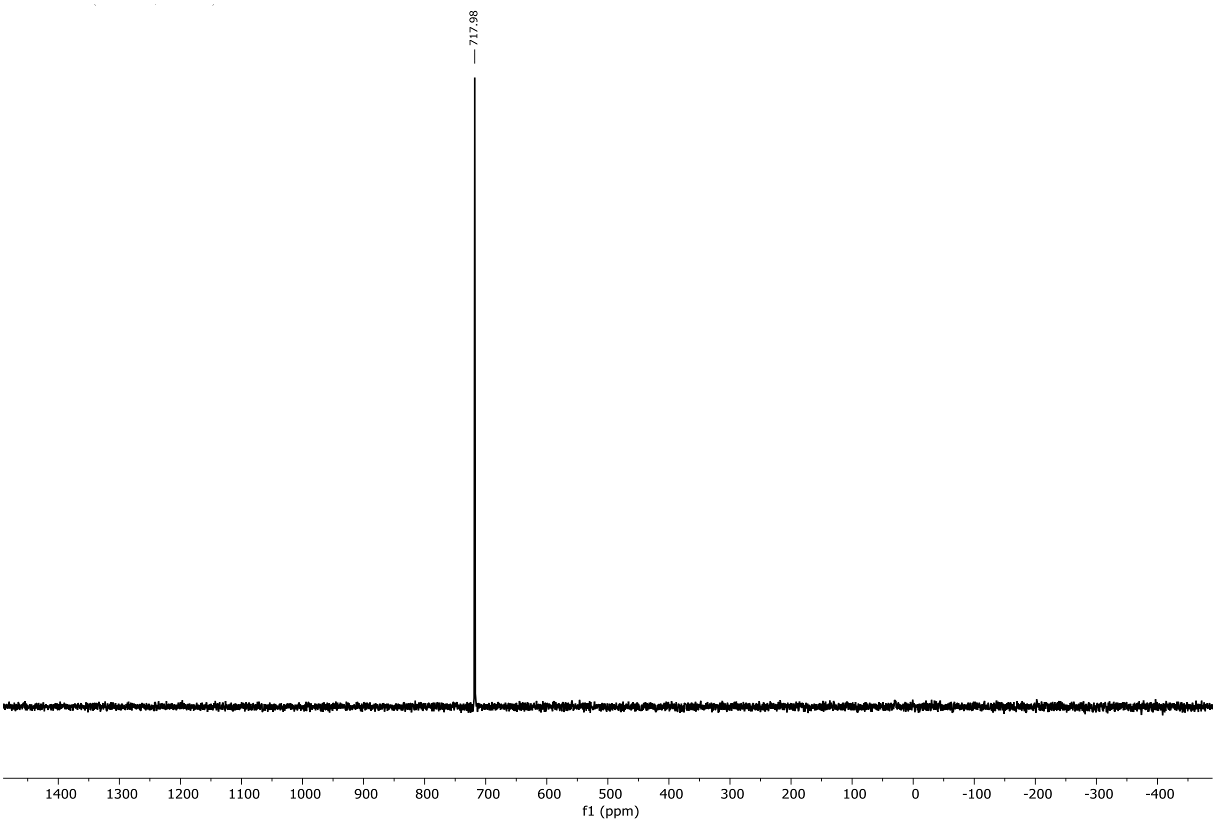


Figure S18: ^{125}Te-NMR spectrum (186 MHz, acetone-d$_6$, 298 K) of compound **4c**.

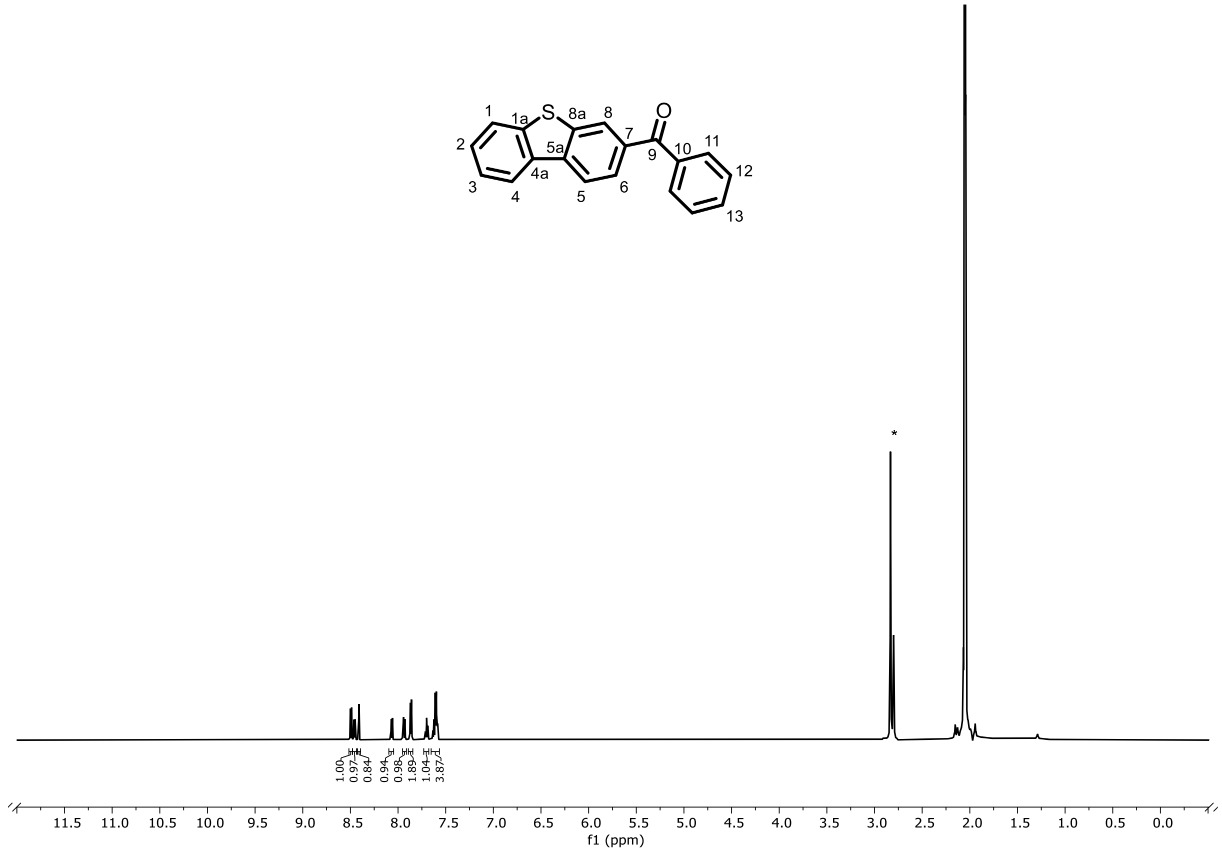


Figure S19: ^{1}H-NMR (600 MHz, acetone-d$_6$, 298 K) of compound **12a** (*water/HDO).

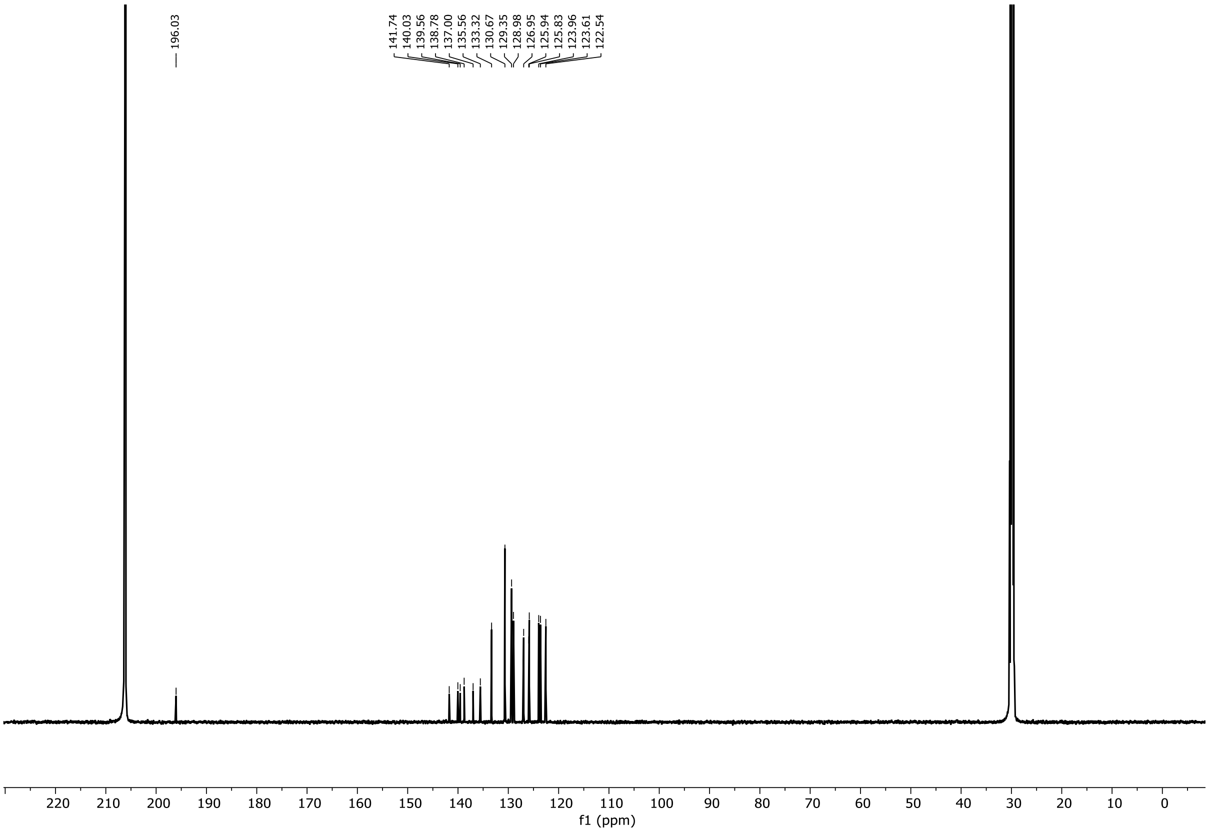


Figure S20: ^{13}C-NMR (bottom, 151 MHz, acetone-d$_6$, 298 K) of compound **12a**.

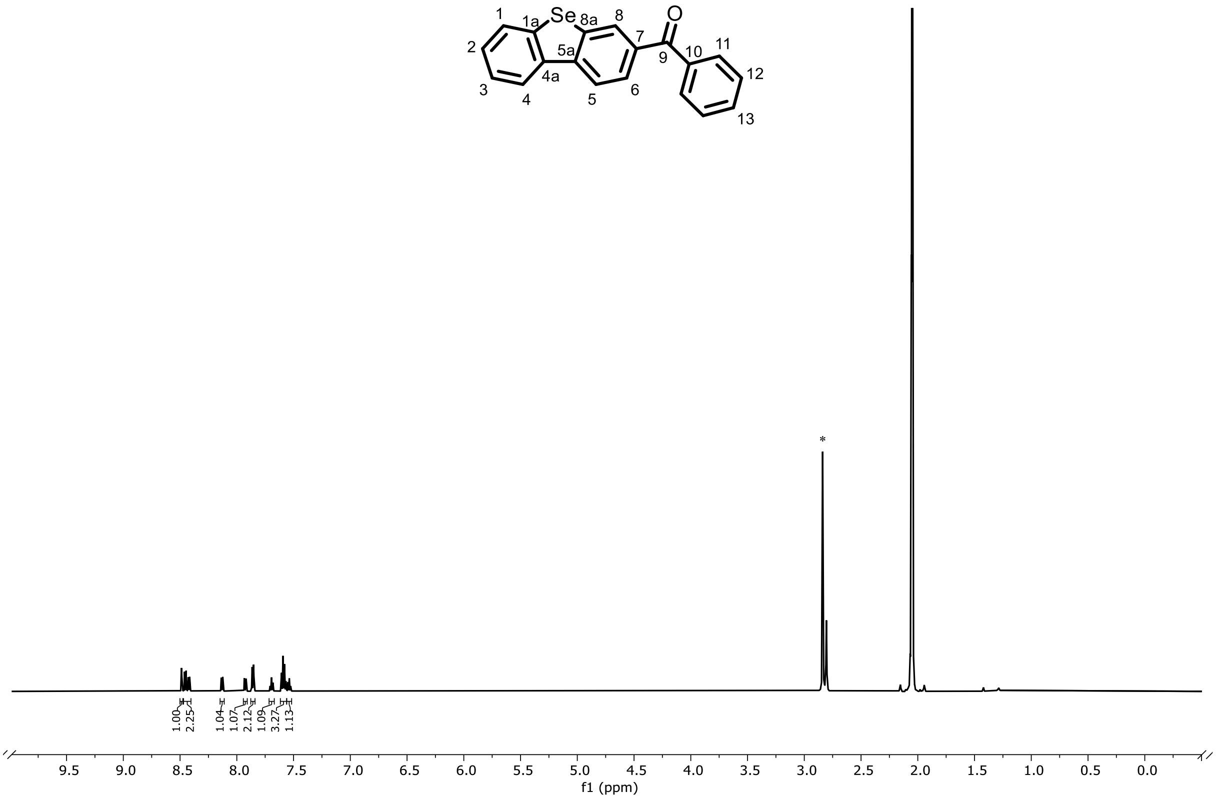


Figure S21: ^{1}H-NMR (600 MHz, acetone-d$_6$, 298 K) of compound **12b** (*water/HDO).

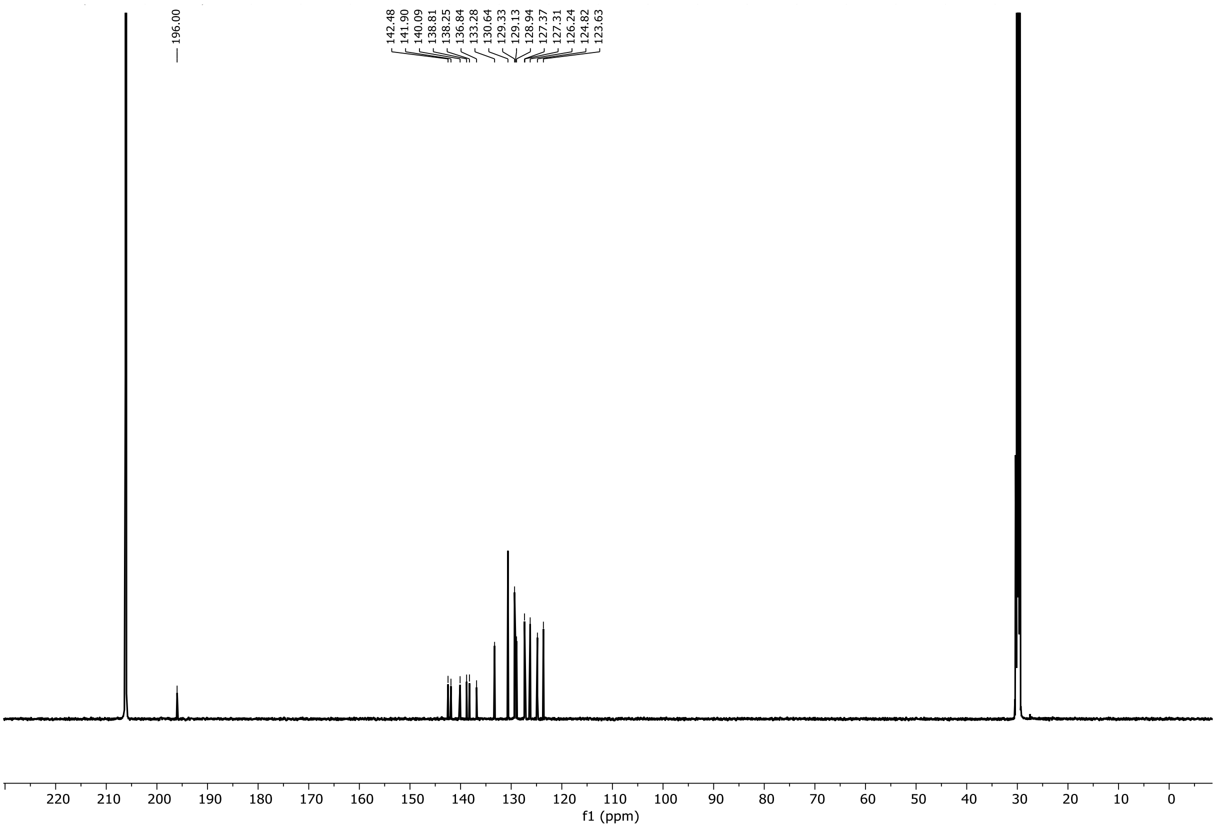


Figure S22: ^{13}C-NMR (151 MHz, acetone-d$_6$, 298 K) of compound **12b**.

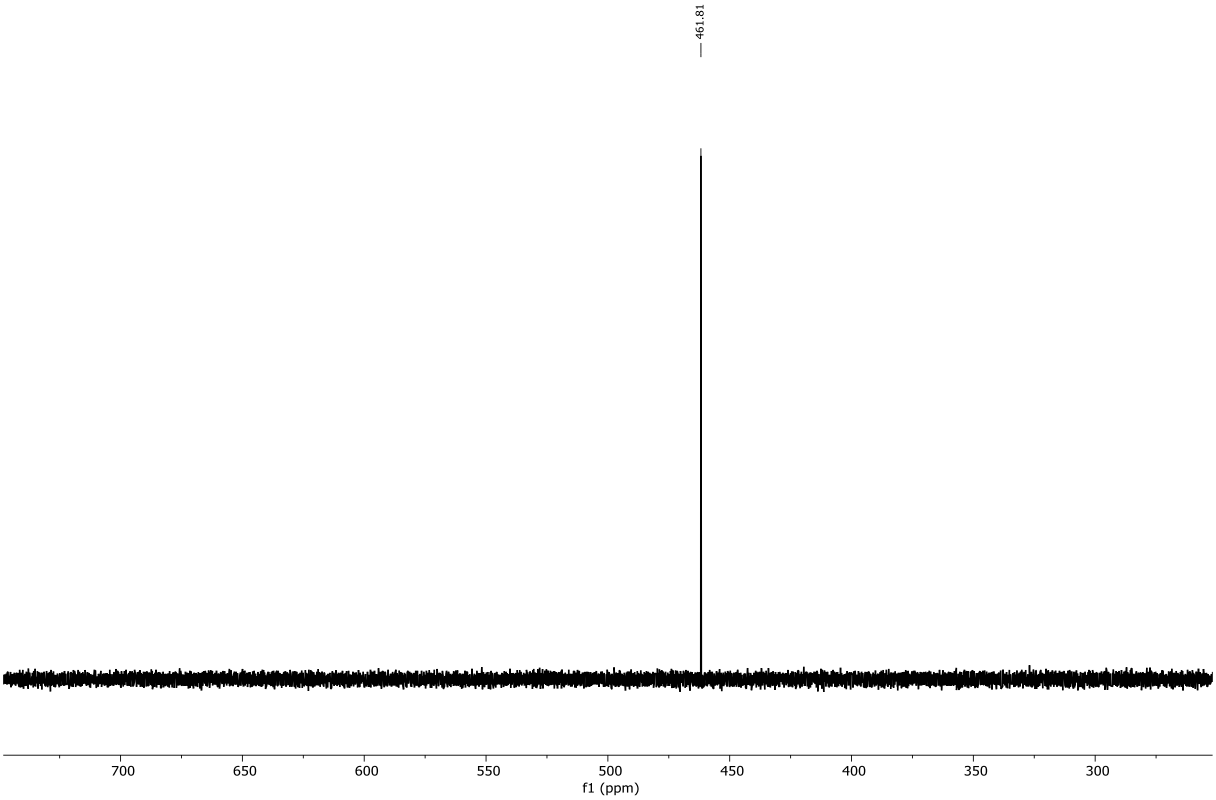


Figure S23: ^{77}Se-NMR spectrum (114 MHz, acetone-d$_6$, 298 K) of compound **12b**.

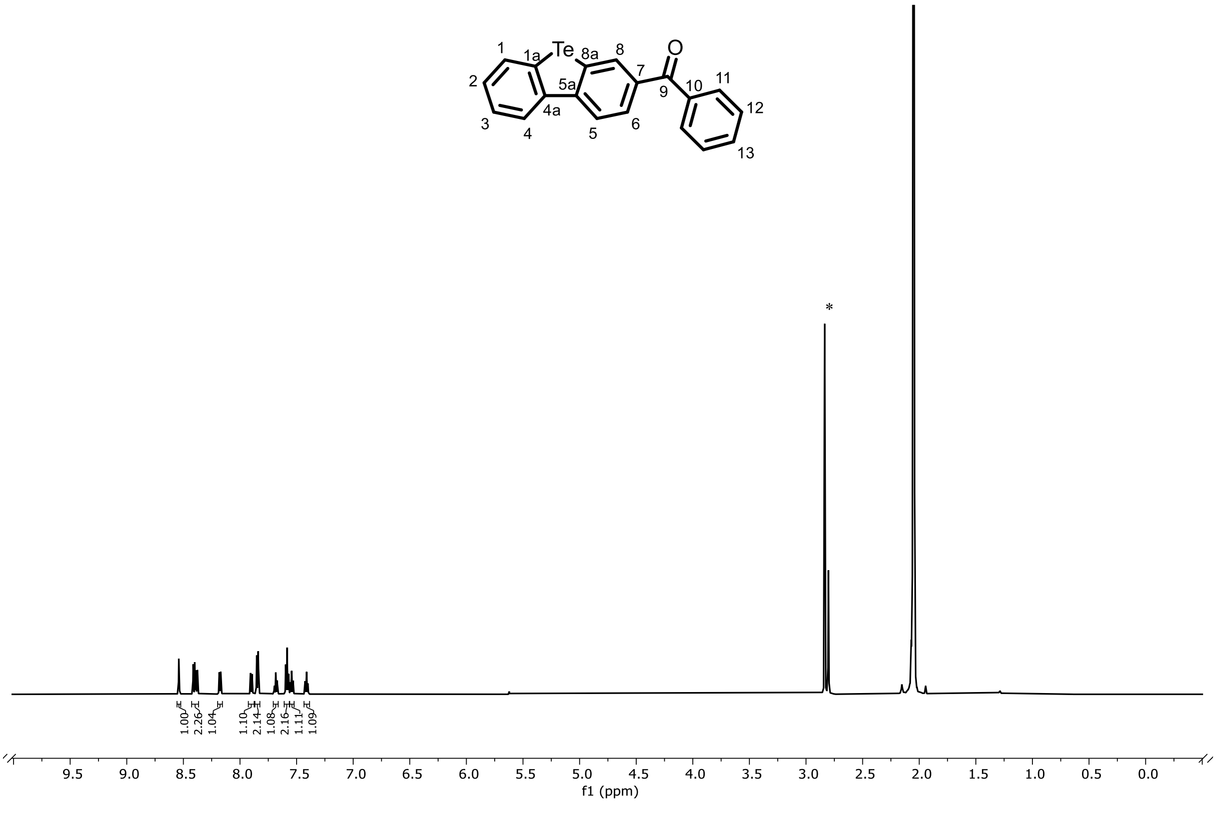


Figure S24: ^{1}H-NMR (600 MHz, acetone-d$_6$, 298 K) of compound **12c** (*water/HDO).

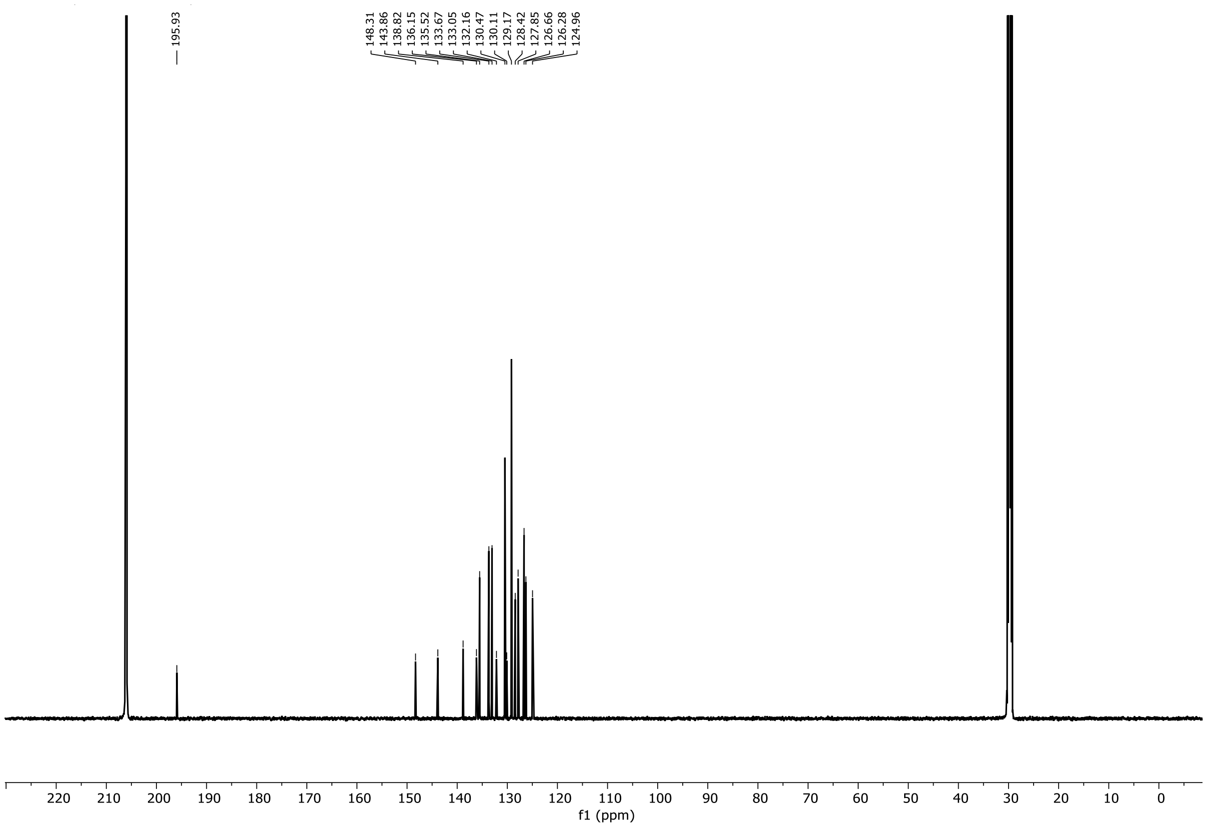


Figure S25: ^{13}C-NMR (151 MHz, acetone-d$_6$, 298 K) of compound **12c**.

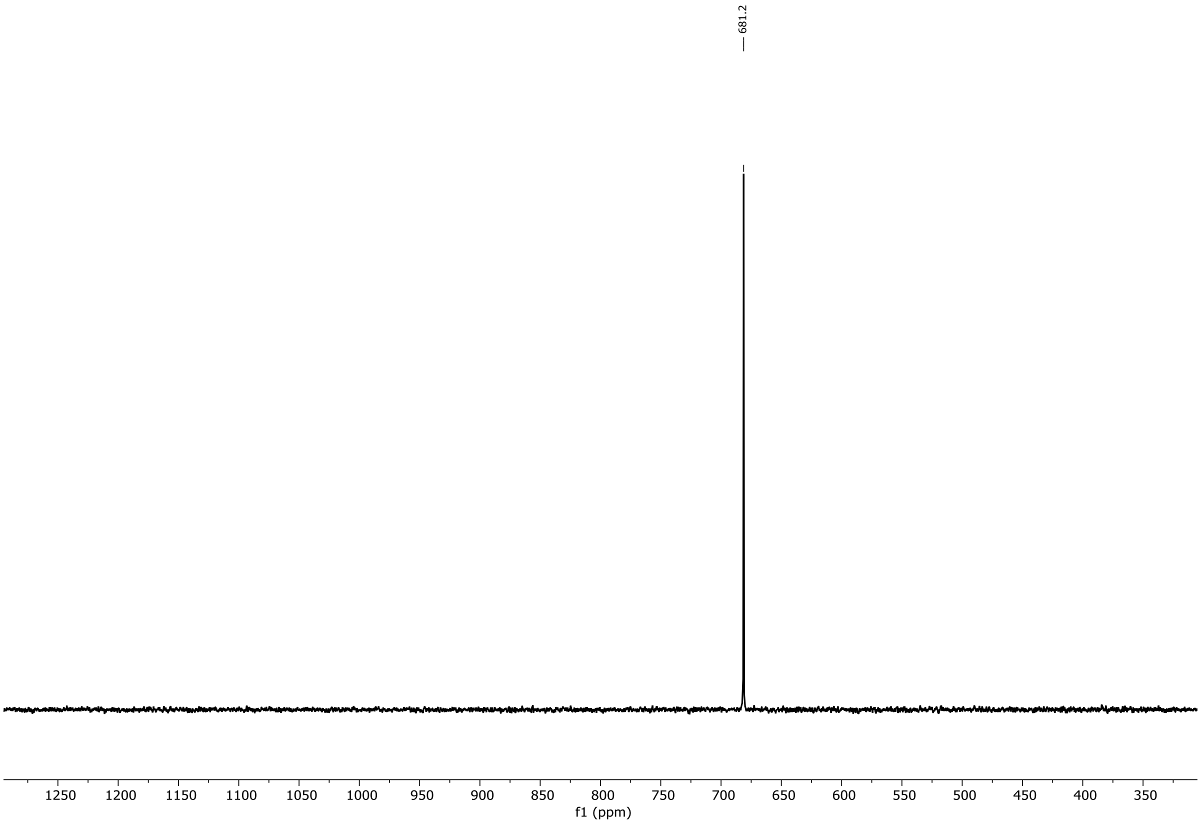
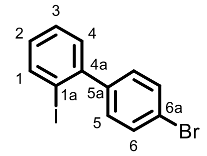


Figure S26: ^{125}Te-NMR spectrum (186 MHz, acetone-d$_6$, 298 K) of compound **12c**.



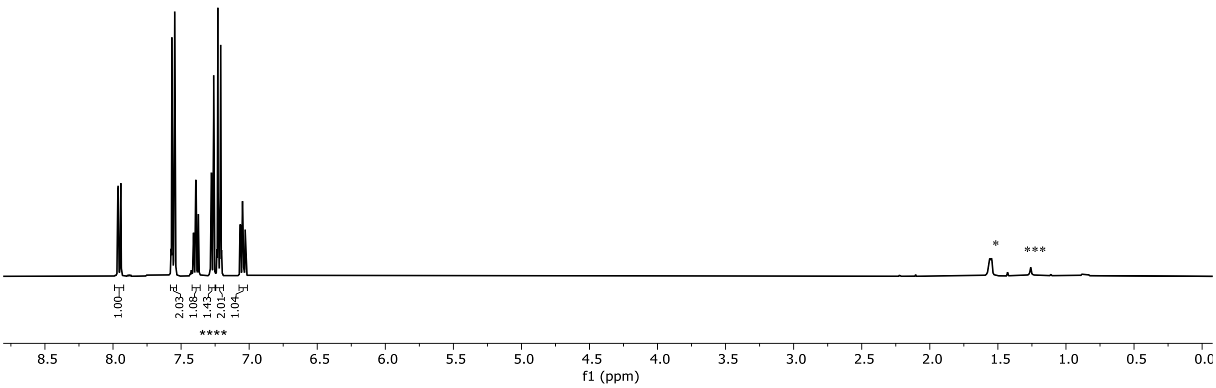


Figure S27: ^{1}H-NMR (400 MHz, $CDCl_3$, 298 K) of compound **13** (*water, ***grease, ****integral of signal at 7.29 – 7.25 ppm is not fitting due to overlap with $CHCl_3$ residue signal).

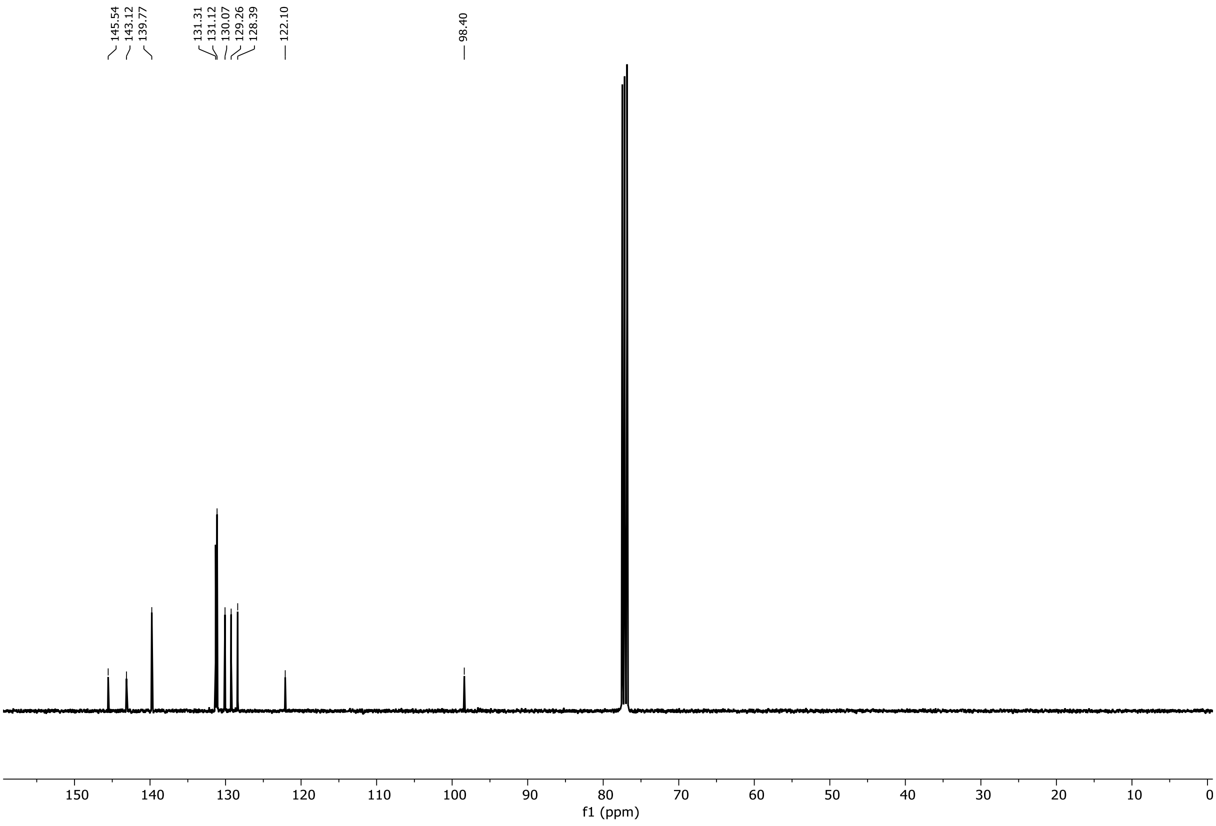


Figure S28: ^{13}C-NMR (101 MHz, $CDCl_3$, 298 K) of compound **13**.

4. HPLC Chromatograms

Table S1: Purities of the final compounds (**4a-c**, **12a-c**) by HPLC.

4a	**4b**	**4c**	**12a**	**12b**	**12c**
99%	100%	100%	100%	100%	99%

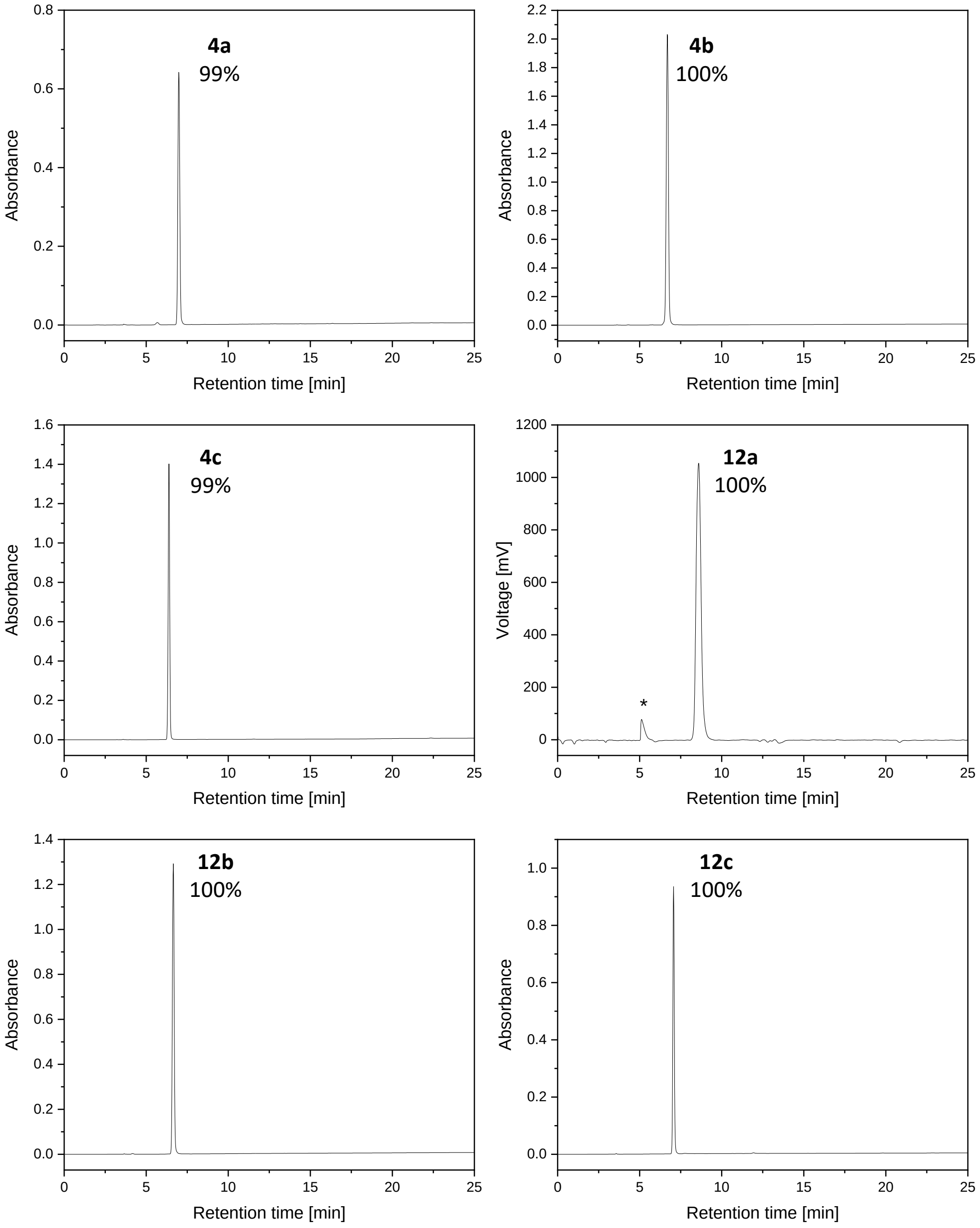


Figure S29: HPLC chromatograms of compounds **4a-c** and **12a-c** with determined purity (detection wavelength: 270 nm, *ethyl acetate injection peak).

5. UV/Vis Spectra

Table S2: Absorption bands of the compounds **4a-c** & **12a-c** in 10 µM solution in 2-methyltetrahydrofuran in nm.

4a	4b	4c	12a	12b	12c
357	370	414	344	350	379

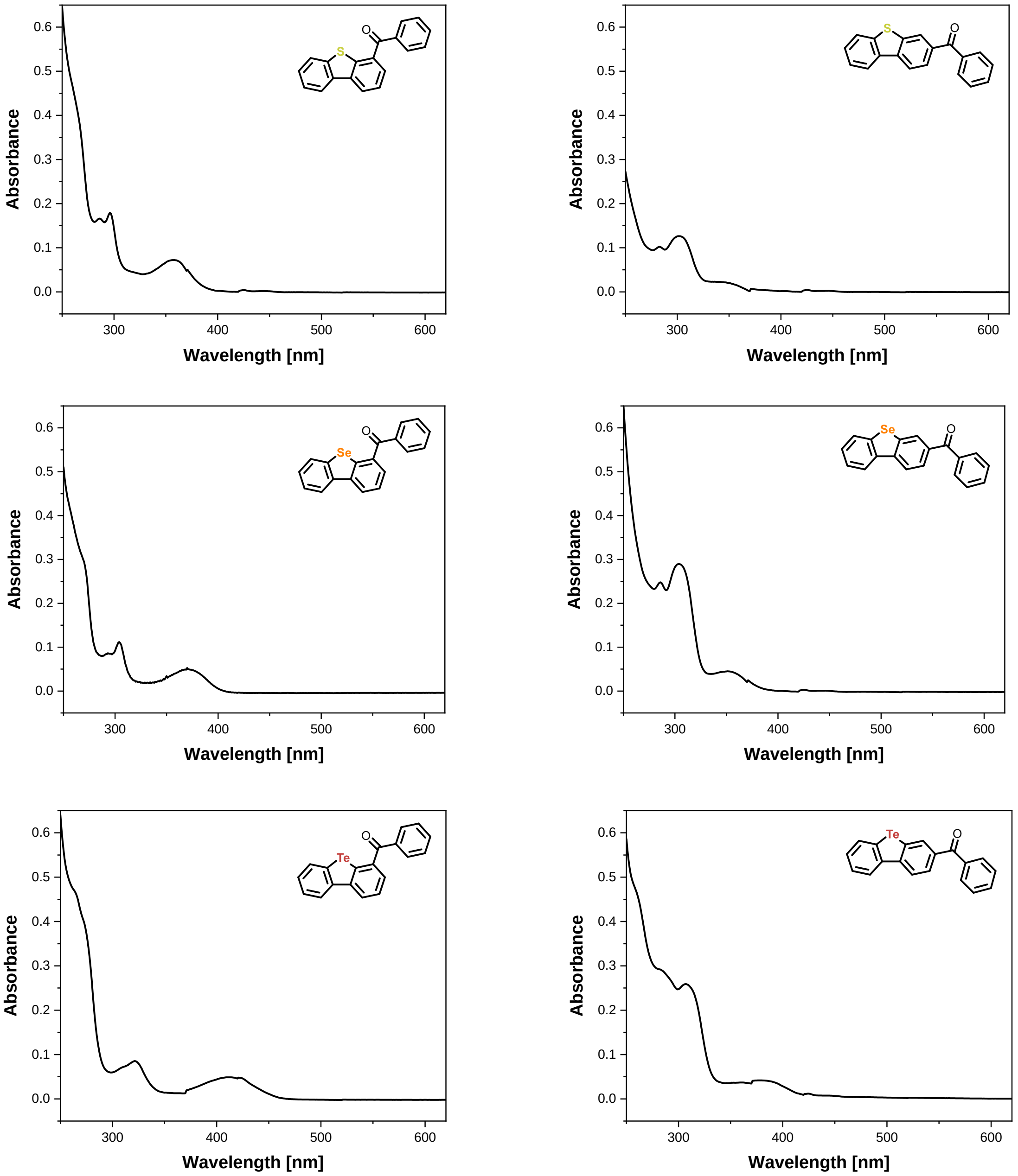


Figure S30: UV/Vis-spectra of the final compounds **4a-c** (left) and **12a-c** (right) (10 µM, 2-methyltetrahydrofuran).

6. *X-ray diffractometric analysis of single crystals*

Table S3: Crystallographic data of BzDBE. CCDC-xxxxxx (given in the table) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Identification code	**4a**	**4b**	**4c**	**12a**	**12b**	**12c**
Name in CIF file	lh_056_1m	dan10580	lh_076_2m	lh_058_3m	lh_066_1m	lh_061_5m
CCDC number	2403909	2389700	2403910	2403912	2403913	2403914
Empirical formula	$C_{19}H_{12}OS$	$C_{19}H_{12}OSe$	$C_{19}H_{12}OTe$	$C_{19}H_{12}OS$	$C_{19}H_{12}OSe$	$C_{19}H_{12}OTe$
M [g·mol^{-1}]	288.35	335.25	383.89	288.35	335.25	383.89
Crystal size [mm]	0.270 × 0.139 × 0.071	0.047 x 0.050 x 0.245	0.384 × 0.246 × 0.046	0.228 × 0.123 × 0.033	0.298 × 0.183 × 0.041	0.249 × 0.214 × 0.116
T [K]	100(2)	101(2)	100(2)	100(2)	100(2)	100(2)
a	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/n$	$C2/c$	$P2_1/n$	$P2_1/n$	$P2_1/c$
a [Å]	4.7662(3)	4.81200(10)	19.670(2)	3.9473(2)	3.9799(4)	10.6483(11)
b [Å]	19.7037(11)	19.7752(5)	8.7121(9)	29.7393(16)	29.881(3)	20.468(2)
c [Å]	14.7618(8)	14.9145(4)	16.4513(17)	11.4521(6)	11.4398(11)	13.8551(13)
α [°]	90	90	90	90	90	90
β [°]	96.564(3)	98.5190(10)	91.509(2)	91.572(3)	92.136(2)	110.162(3)
γ [°]	90	90	90	90	90	90
V [Å^3]	1377.22(14)	1403.58(6)	2818.2(5)	1343.86(12)	1359.5(2)	2834.7(5)
Z	4	4	8	4	4	8
D_{calc} [g·cm^{-3}]	1.391	1.586	1.810	1.425	1.638	1.799
$\mu(MK_\alpha$ [mm^{-1}])	2.030 (Cu)	3.568 (Cu)	16.612 (Cu)	2.081 (Cu)	3.684 (Cu)	2.094 (Mo)
Transmissions	0.75/0.51	0.8500/0.4750	0.15/0.01	0.75/0.57	0.75/0.49	0.63/0.52
$F(000)$	600	672	1488	600	672	1488
Index ranges	$-5 \le h \le 6$	$-5 \le h \le 5$	$-24 \le h \le 24$	$-4 \le h \le 3$	$-5 \le h \le 5$	$-17 \le h \le 17$
	$-24 \le k \le 24$	$-23 \le k \le 23$	$-11 \le k \le 10$	$-37 \le k \le 37$	$-38 \le k \le 37$	$-34 \le k \le 34$
	$-17 \le l \le 18$	$-17 \le l \le 17$	$-18 \le l \le 20$	$-14 \le l \le 14$	$-13 \le l \le 14$	$-23 \le l \le 22$
θ_{max} [°]	80.311	66.67	79.758	80.243	79.447	36.377
Reflections collected	22425	21306	43827	47736	45438	70437
Independent reflections	2814	2470	3043	2900	2932	13772
R_{int}	0.0819	0.0371	0.0574	0.0807	0.0442	0.0198
Refined parameters	190	190	190	190	190	380
R_1 [$I > 2\sigma(I)$]	0.0511	0.0224	0.0271	0.0377	0.0268	0.0245
wR_2 [all data]	0.1400	0.0575	0.0778	0.0986	0.0745	0.0600
GooF	1.058	1.051	1.092	1.055	1.061	1.156
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	0.423/-0.479	0.354/-0.393	1.005/-0.552	0.402/-0.397	0.582/-0.621	3.193/-0.681

Table S4: Crystallographic data of **7**, **10** and **16b**. CCDC-xxxxxx (given in the table) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Identification code	**7**	**10**	**16b**
Name in CIF file	lh_075_2m	dan10578	lh_032_2m
CCDC number	2403911	2389699	2403915
Empirical formula	$C_{19}H_{12}OSe$	$C_{23}H_{18}F_3IO_5S$	$C_{12}H_7BrSe$
M [g·mol^{-1}]	532.26	590.33	310.05
Crystal size [mm]	0.377 × 0.268 × 0.086	0.079 x 0.085 x 0.234	0.296 × 0.081 × 0.046
T [K]	100(2)	102(2)	100(2)
a	monoclinic	monoclinic	monoclinic
Space group	$P2_1/c$	$C2/c$	$P2_1/c$
a [Å]	10.160(5)	32.0840(11)	17.2909(14)
b [Å]	15.349(7)	6.2079(2)	4.0044(3)
c [Å]	13.056(6)	21.7596(7)	14.8721(12)
α [°]	90	90	90
β [°]	109.40(2)	106.7090(10)	105.3747(19)
γ [°]	90	90	90
V [Å^3]	1920.4(16)	4151.0(2)	992.89(14)
Z	4	8	4
D_{calc} [g·cm^{-3}]	1.841	1.889	2.074
$\mu(MK_\alpha$ [mm^{-1}])	1.830 (Mo)	13.638 (Cu)	9.420 (Cu)
Transmissions	0.75/0.53	0.4120/0.1430	0.75/0.33
F(000)	1040	2336	592
Index ranges	$-15 \le h \le 15$	$-38 \le h \le 38$	$-21 \le h \le 22$
	$-23 \le k \le 23$	$-7 \le k \le 7$	$-4 \le k \le 5$
	$-20 \le l \le 20$	$-25 \le l \le 25$	$-19 \le l \le 18$
θ_{max} [°]	33.333	66.77	80.217
Reflections collected	137648	33596	32849
Independent reflections	7402	3666	2133
R_{int}	0.0755	0.0490	0.0505
Refined parameters	262	262	127
R_1 [$I > 2\sigma(I)$]	0.0335	0.0284	0.0276
wR_2 [all data]	0.0955	0.0759	0.0913
GooF	1.150	1.063	1.086
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	0.992/-1.378	0.704/-0.766	0.855/-1.133

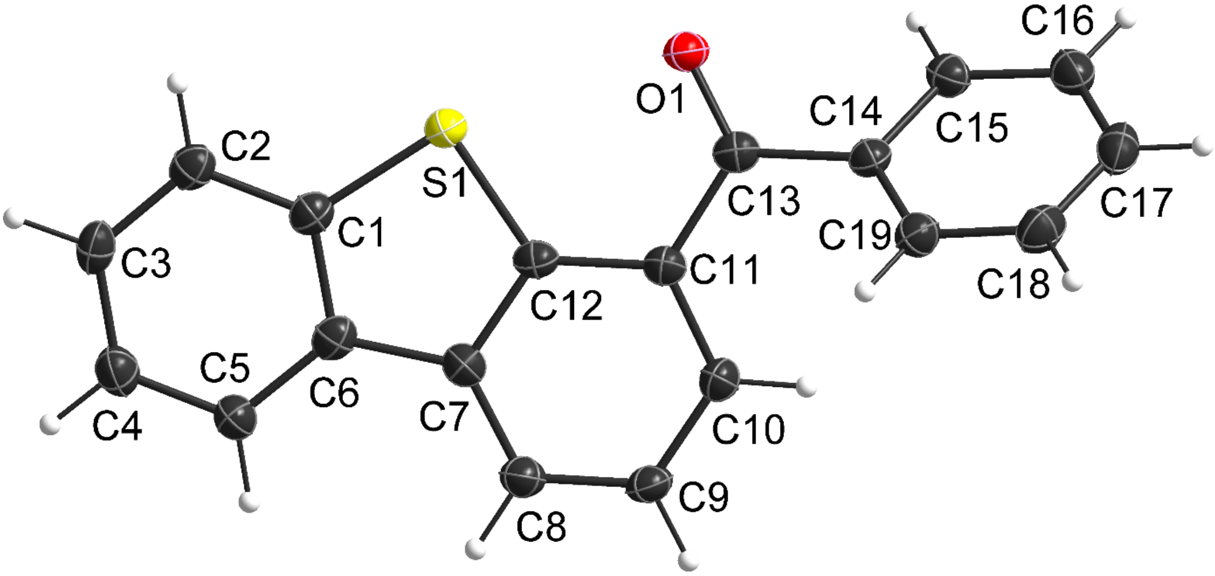


Figure S31: Asymmetric unit of the crystal structure of **4a** (CCDC 2403909). Displacement ellipsoids are shown at 50% probability.

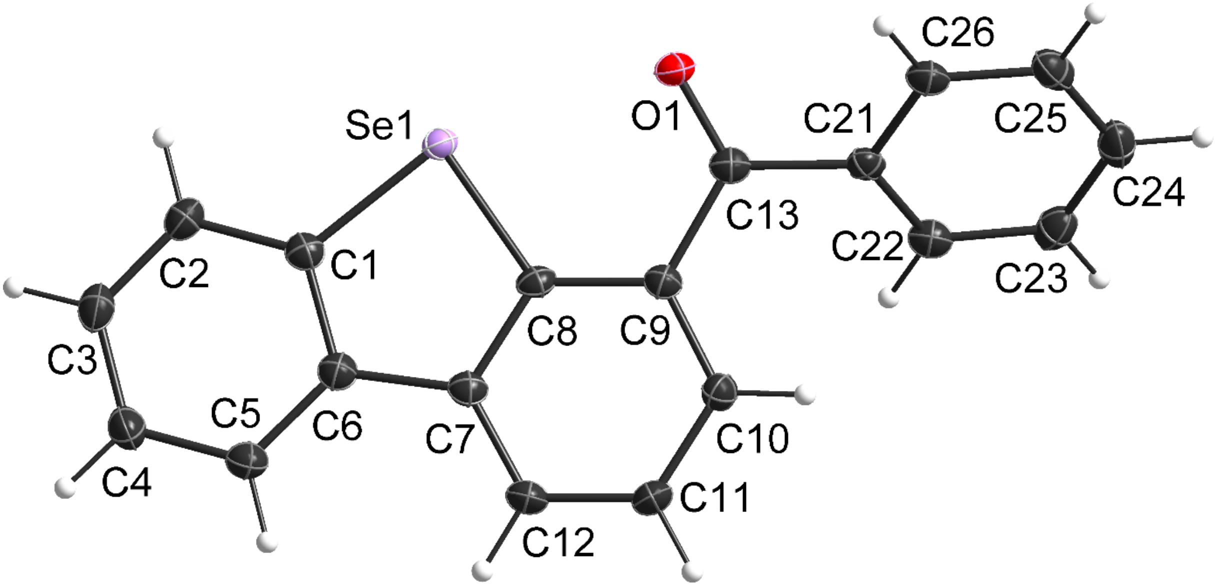


Figure S32: Asymmetric unit of the crystal structure of **4b** (CCDC 2389700). Displacement ellipsoids are shown at 50% probability.

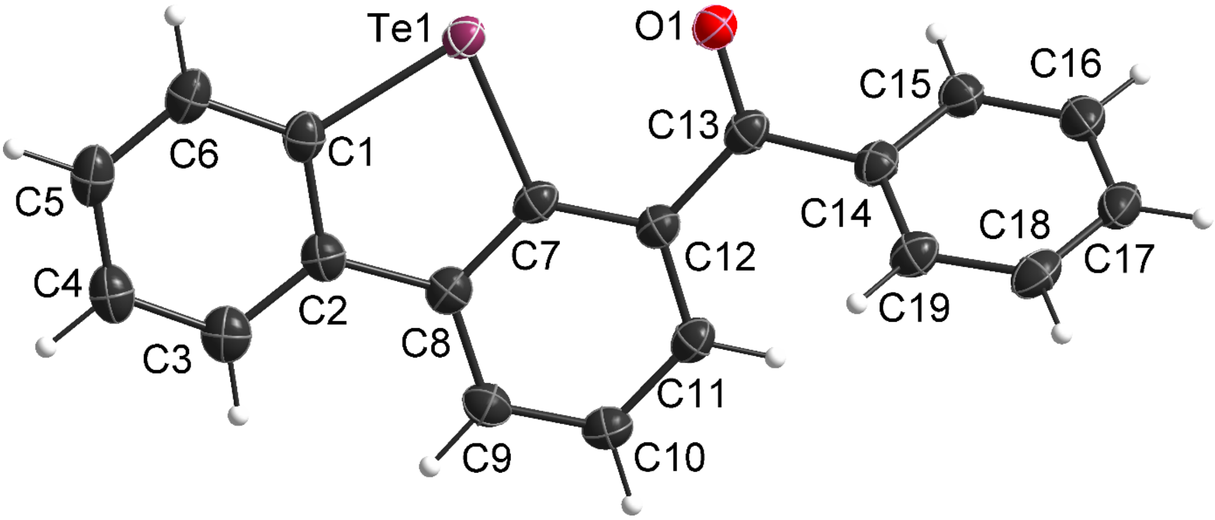


Figure S33: Asymmetric unit of the crystal structure of **4c** (CCDC 2403910). Displacement ellipsoids are shown at 50% probability.

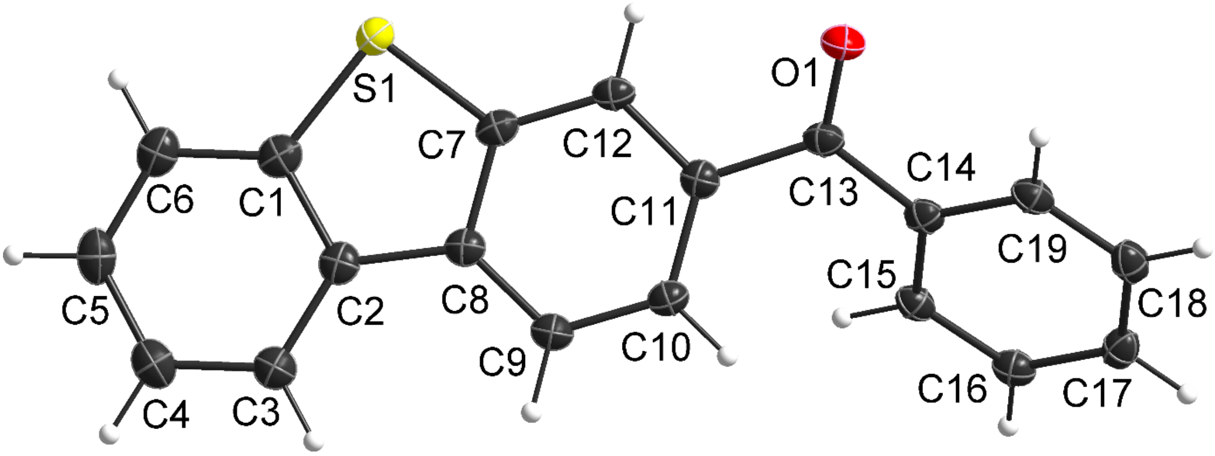


Figure S34: Asymmetric unit of the crystal structure of **12a** (CCDC 2403912). Displacement ellipsoids are shown at 50% probability.

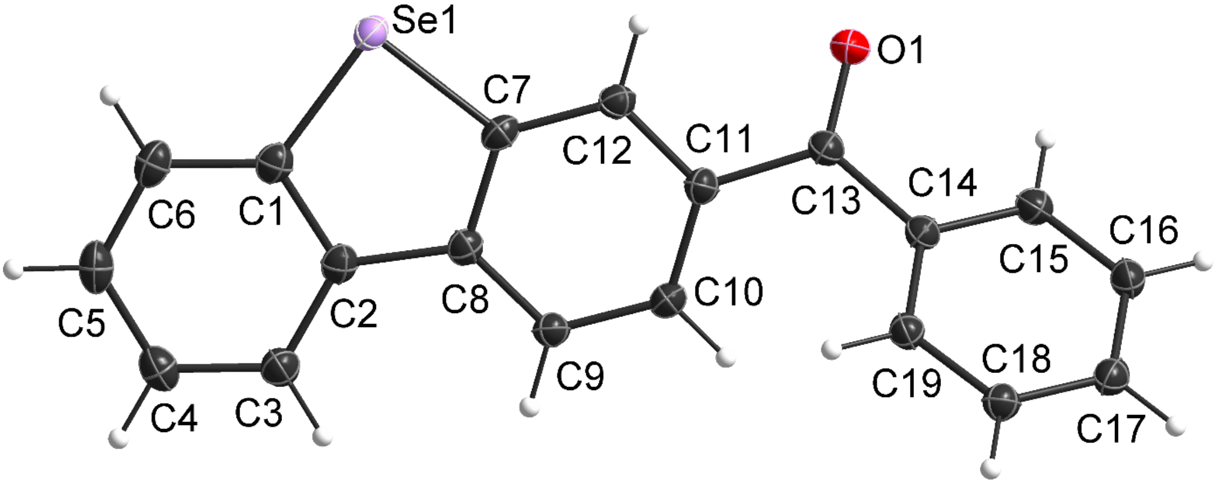


Figure S35: Asymmetric unit of the crystal structure of **12b** (CCDC 2403913). Displacement ellipsoids are shown at 50% probability.

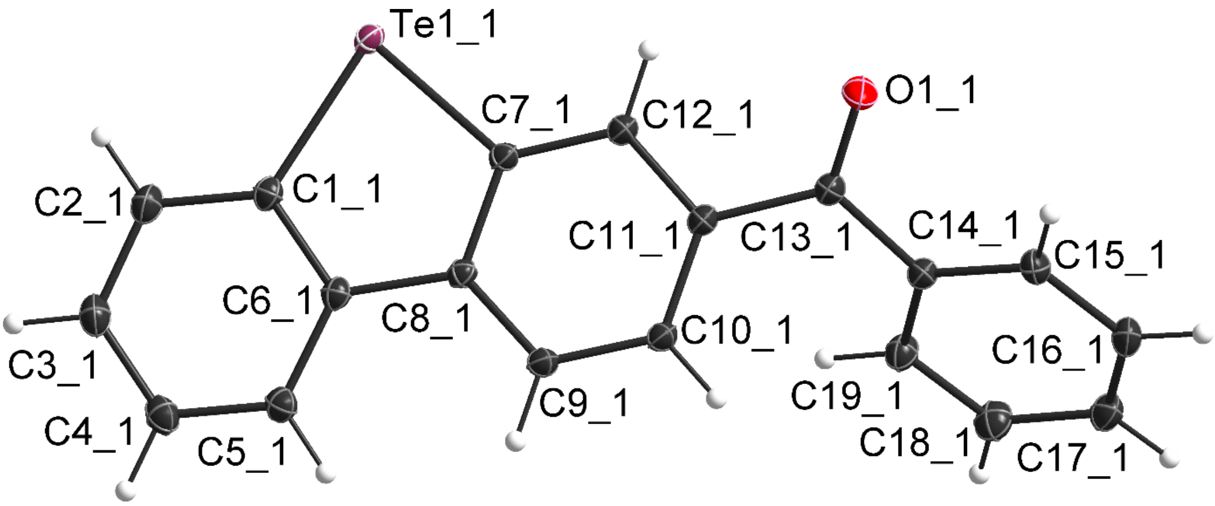


Figure S36: Molecular geometry of the crystal structure of **12c** (CCDC 2403914). For better display, only one residue of the asymmetric unit is shown. Displacement ellipsoids are shown at 50% probability.

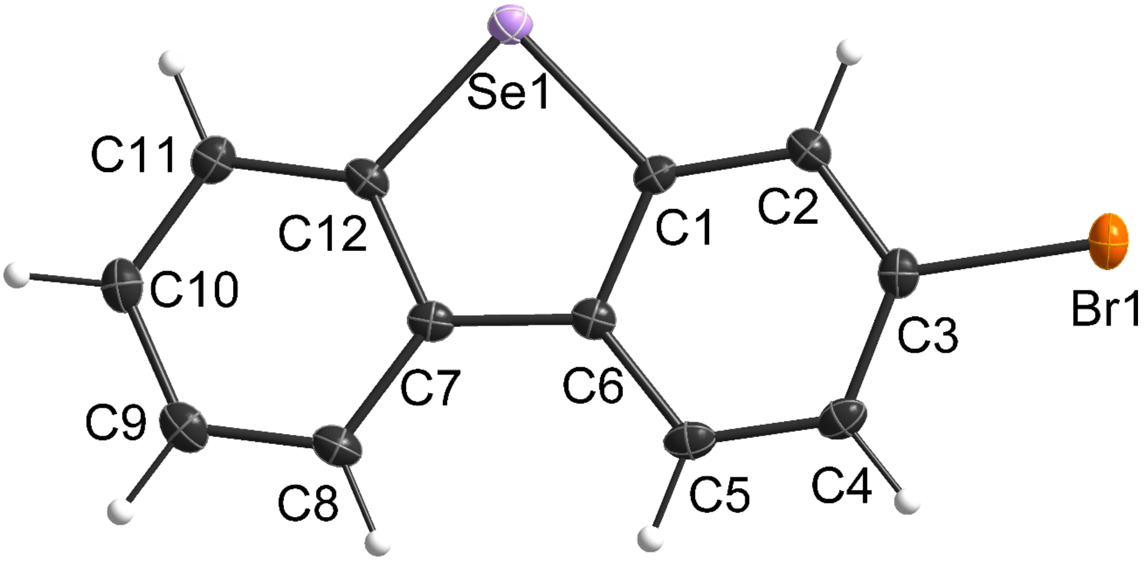


Figure S37: Asymmetric unit of the crystal structure of **16b** (CCDC 2403915). Displacement ellipsoids are shown at 50% probability.

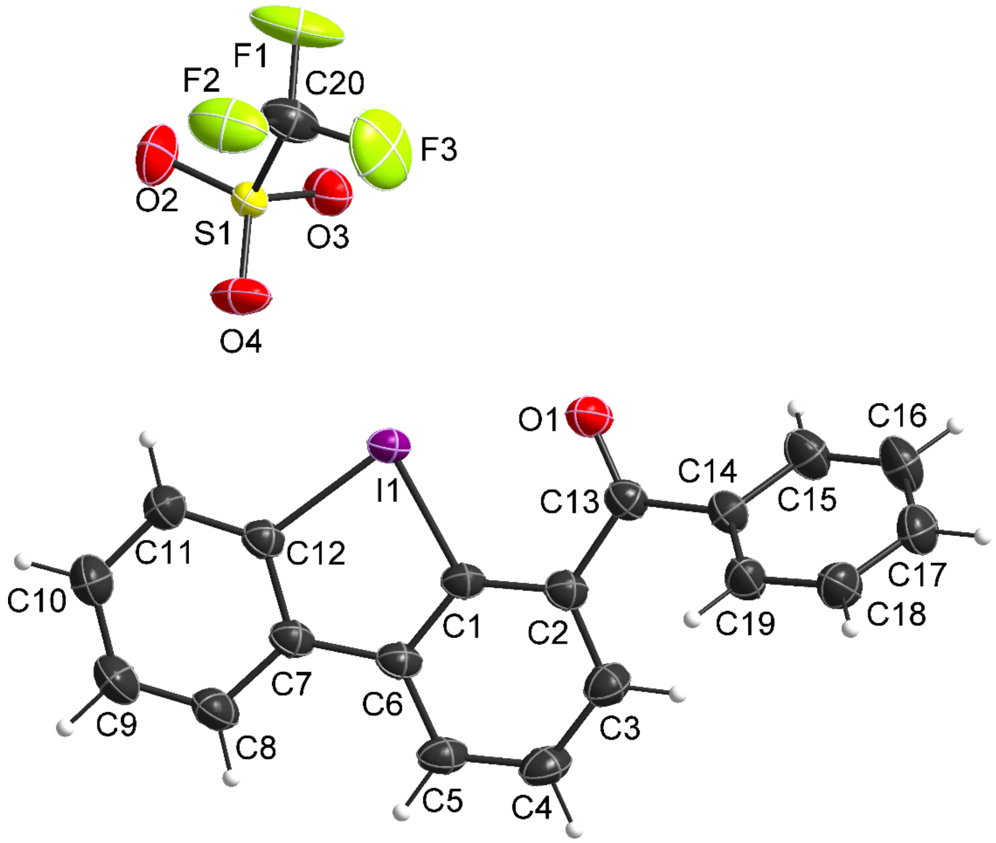


Figure S38: Asymmetric unit of the crystal structure of **7** (CCDC 2403911). Displacement ellipsoids are shown at 50% probability.

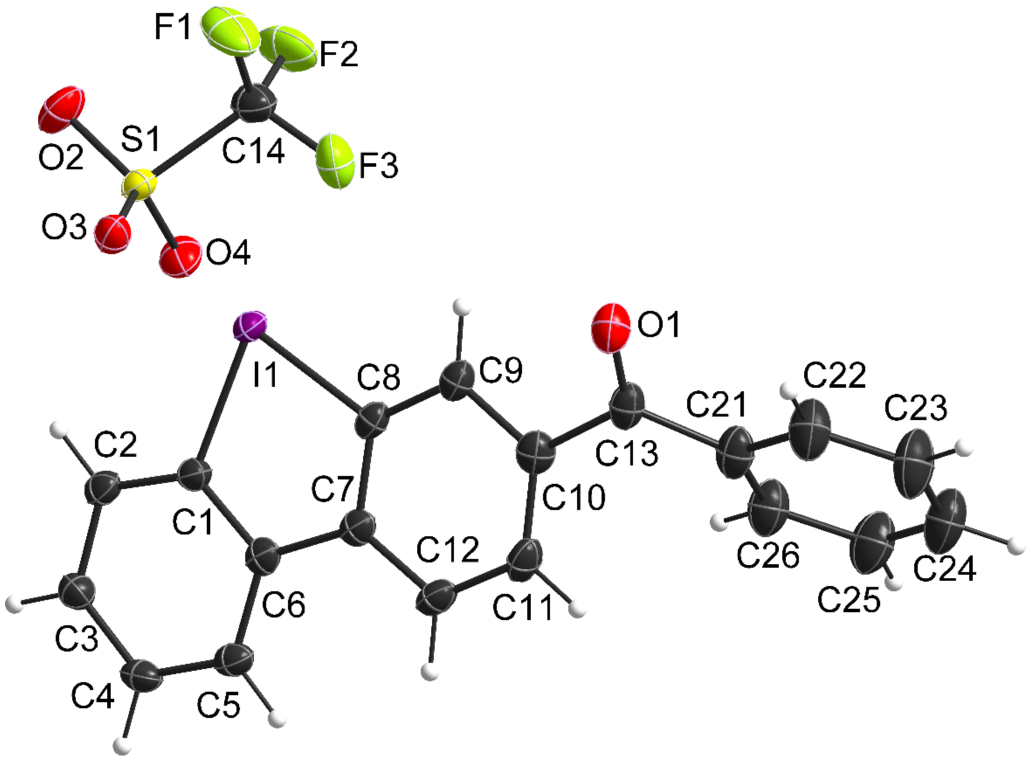


Figure S39: Asymmetric unit of the crystal structure of **10** (CCDC 2389699). Displacement ellipsoids are shown at 50% probability.

7. Molecular packing analysis in the crystal lattice

Selected contacts (between atoms X and Y) were determined using ShelXL-2017.[1–3] The standard deviation is indicated behind the value in brackets. Z describes the atom next to the contact atom, which was used to measure angles. If there were two equivalent binding partners (Z, Z’), both angles were measured. For interactions with π systems, centroids (M) were used. The angles were determined using planes, which include all atoms in the ring. Additionally, the average distance between every atom in the ring and the contact atom/ring was calculated. By the distance between the two moieties and the distance between the plane and the contact moiety, the horizontal shift was measured. The indication of the atoms is equal to the atom numbers in the CIF files.

In order to analyse the interaction between the molecules in the solid state, the quantum theory of atoms in molecules (QTAIM)[22] and the interacting quantum atoms (IQA)[23] analyses were used. The geometries were obtained from the X-ray data (single point calculations) (for full information see chapter 10).

Table S5: Selected contacts from the crystal structure of **4a**. M means the centre of the aromatic ring. a describes the horizontal shift between the ring centre and the contact moiety. Interaction energies were obtained *via* IQA from single point calculations.

X···Y	**X-Y [Å]**	**<(ZXY) [°]**	**<(Z’XY) [°]**	**<(XYZ) [°]**	**<(XYZ’) [°]**	**$E_{X\cdots Y}$ [kcal/mol]**
S1···O1	2.7434(19)	163.58(10)	73.39(10)	98.98(16)		-15.7
S1···O1_$3	3.718(2)	98.31(10)	118.75(9)	71.85(15)		-2.1
S1···H9_$1	2.97	105	155	144		-3.0
S1···C11_$3	3.594(3)	75.23(10)	89.82(10)	90.66(16)	100.70(16)	-2.3
O1···H5_$2	2.54	132		127		-3.5
O1···H8_$2	2.43	111		140		-4.2
O1···C15_$3	3.249(3)	119.71(18)	96.38(18)	91.70(16)		-2.1
O1···H15_$3	2.77	112		107		-1.9
	M-X [Å]	**<(MX)**	**øM-X [Å]**	**a [Å]**		
CT1···CT3_$3	3.61	0.69(17)	3.86	1.06		
CT2···CT3_$3	3.66	0.91(17)	3.91	1.22		

Symmetry operations used: $1 -1/2+x, 1/2-y, -1/2+z; $2 1/2+x, 1/2-y, 1/2+z; $3 -1+x, +y, +z.

Table S6: Selected contacts from the crystal structure of **4b**. M means the centre of the aromatic ring. a describes the horizontal shift between the ring centre and the contact moiety. Interaction energies were obtained *via* IQA from single point calculations.

X···Y	**X-Y [Å]**	**<(ZXY) [°]**	**<(Z'XY) [°]**	**<(XYZ) [°]**	**$E_{X\cdots Y}$ [kcal/mol]**
Se1···O1	2.7418(13)	158.09(6)	71.64(6)	102.25(11)	-18.6
Se1···O1_$3	3.7430(13)	98.37(6)	116.57(6)	72.41(10)	-2.6
Se1···C13_$3	3.5693(18)	95.84(6)	97.56(6)	37.31(2)	-2.1
Se1···H11_$1	2.97	103	161	146	-3.7
O1···H5_$2	2.55	149		167	-3.3
O1···H12_$2	2.51	138		171	-3.4
O1···H26_$3	2.80	110		109	-1.7
	M-X [Å]	**<(MX)**	**øM-X [Å]**	**a [Å]**	
CT1···CT3_$3	3.64	0.76(12)	3.89	1.09	
CT2···CT3_$3	3.69	1.13(12)	3.93	1.23	

Symmetry operations used: $1 -1/2+x, 1/2-y, 1/2+z; $2 1/2+x, 1/2-y, 1/2+z; $3 -1+x, +y, +z.

Table S7: Selected contacts from the crystal structure of **4c**. M means the centre of the aromatic ring. a describes the horizontal shift between the ring centre and the contact moiety. Interaction energies were obtained *via* IQA from single point calculations.

X···Y	**X-Y [Å]**	**<(ZXY) [°]**	**<(Z'XY) [°]**	**<(XYZ) [°]**	**$E_{X\cdots Y}$ [kcal/mol]**
Te1···O1	2.8081(19)	149.76(8)	46.73(6)	105.04(16)	-22.5
Te1···Te1_$3	4.4338(5)	97.13(7)	61.74(7)	-	-2.2
Te1···H5_$1	3.28	83	146	140	-3.2
Te1···H16_$2	3.28	130	99	156	-3.6
Te1···H19_$3	3.25	77	146	134	-2.8
O1···H3_$4	2.78	156		167	-1.8
O1···H9_$4	2.83	118		170	-1.9
O1···C15_$2	3.276(4)	130.09(18)		141.75(19)	-1.3
O1···H15_$2	2.42	127		150	-4.4
C18···C18_$5	3.349(6)	87.97(19)			-
	M-X [Å]	**<(MXY)**	**øM-X [Å]**	**a [Å]**	
CT1···H18_$6	2.98	154	3.28	0.85	
CT2···C7_$3	3.62	78	3.92	1.03	
CT2···C8_$3	3.65	80	3.88	0.37	
CT3···C1_$3	3.53	86	3.80	0.17	
	M-M [Å]	**<(MM)**	**øM-C_x [Å]**	**a [Å]**	
CT3···CT3_$7	3.71	0	3.94	1.40	

Symmetry operations used: $1 1/2-x, -1/2+y, 1/2-z; $2 -x, -y, -z; $3 -x, +y, 1/2-z; $4 +x, -1+y, +z; $5 -1/2-x, 1/2-y, -z; $6 1/2+x, 1/2+y, +z; $7 -x, -1+y, 1/2-z.

Table S8: Selected contacts from the crystal structure of **12a**. M means the centre of the aromatic ring. a describes the horizontal shift between the ring centre and the contact moiety. Interaction energies were obtained *via* IQA from single point calculations.

X···Y	**X-Y [Å]**	**<(ZXY) [°]**	**<(Z'XY) [°]**	**<(XYZ) [°]**	**$E_{X\cdots Y}$ [kcal/mol]**
S1···C2_$1	3.6774(17)	72.07(6)	92.19(6)	85.05(10)	-1.5
S1···C8_$1	3.6034(17)	88.39(6)	75.56(6)	83.27(10)	-2.0
O1···H9_$2	2.65	116		118	-2.6
O1···C10_$2	3.0991(19)	144.28(13)		157.30(13)	-1.6
O1···H10_$2	2.42	148		128	-4.0
O1···H15_$3	2.60	140		156	-3.1
C12···H16_$3	2.80	117		152	-1.6
	M-X [Å]	**<(MXY)**	**øM-X [Å]**	**a [Å]**	
CT2···H16_$3	3.85	163	4.01	3.01	
CT3···H16_$3	3.63	130	3.82	2.71	
	M-M [Å]	**<(MM)**	**øM-C_x [Å]**	**a [Å]**	
CT1···CT1_$1	3.95	0	4.16	1.84	
CT2···CT2_$1	3.95	0	4.14	1.84	
CT3···CT3_$1	3.95	0	4.16	1.88	
CT4···CT4_$1	3.95	0	4.16	1.75	

Symmetry operations used: $1 -1+x, +y, +z; $2 -1/2+x, 1/2-y, 1/2+z; $3 1/2+x, 1/2-y, 1/2+z.

Table S9: Selected contacts from the crystal structure of **12b**. M means the centre of the aromatic ring. a describes the horizontal shift between the ring centre and the contact moiety. Interaction energies were obtained *via* IQA from single point calculations.

X···Y	**X-Y [Å]**	**<(ZXY) [°]**	**<(Z’XY) [°]**	**<(XYZ) [°]**	**<(XYZ’) [°]**	**$E_{X\cdots Y}$ [kcal/mol]**
Se1···Se1_$1	3.9799(4)	109.09(50)	110.20(5)	70.91(5)	69.80(5)	-4.1
Se1···C2_$1	3.6954(17)	72.23(6)	89.30(5)	83.73(10)		-2.0
Se1···C8_$1	3.6650(16)	88.05(6)	73.35(6)	83.34(9)		-2.2
Se1···H17_$2	3.22	150	122	113		-2.1
O1···H9_$2	2.62	117		119		-2.8
O1···C10_$2	3.1104(19)	144.41(12)		158.35(12)		-1.6
O1···H10_$2	2.45	147		127		-3.8
O1···H19_$3	2.62	138		157		-2.9
C12···H18_$3	2.80	119		151		-1.6
	M-X [Å]	**<(MXY)**	**øM-X [Å]**	**a [Å]**		
CT3···H18_$3	3.62	159	3.81	2.71		
	M-M [Å]	**<(MM)**	**øM-C_x [Å]**	**a [Å]**		
CT1···CT1_$1	3.98	0	4.19	1.86		
CT2···CT2_$1	3.98	0	4.18	1.86		
CT3···CT3_$1	3.98	0	4.19	1.92		
CT4···CT4_$1	3.98	0	4.20	1.74		

Symmetry operations used: $1 -1+x, +y, +z; $2 -1/2+x, 1/2-y, 1/2+z; $3 1/2+x, 1/2-y, 1/2+z.

Table S10: Selected contacts from the crystal structure of **12c**. M means the centre of the aromatic ring. a describes the horizontal shift between the ring centre and the contact moiety. Interaction energies were obtained *via* IQA from single point calculations.

X···Y	X-Y [Å]	<(ZXY) [°]	<(Z'XY) [°]	<(XYZ) [°]	<(XYZ') [°]	$E_{X\cdots Y}$ [kcal/mol]
Te1_1···Te1_2	4.1037(3)	74.04(4)	66.39(4)	101.87(4)	110.01(4)	-7.6
Te1_1···O1_2_$1	3.3439(11)	158.73(4)	80.14(4)	128.12(9)		-7.3
Te1_2···O1_1_$1	3.2371(12)	158.32(4)	80.71(4)	135.42(10)		-9.0
Te1_1···H15_2_$1	3.31	152	125	116		-2.6
Te1_2···H18_1_$2	3.31	126	68	149		-2.6
O1_1···C12_2_$1	3.1900(19)	134.18(11)		144.93(9)		-1.4
O1_1···H12_2_$1	2.40	124		140		-4.5
O1_2···H5_2_$3	2.69	91		162		-2.3
O1_2···H9_2_$3	2.50	124		151		-3.6
O1_2···C12_1_$1	3.2135(18)	130.98(9)		142.56(10)		-1.3
O1_2···H12_1_$1	2.41	122		142		-4.5
O1_2···H17_1_$2	2.82	136		159		-1.9
	M-X [Å]	**<(MXY)**	**øM-X [Å]**	**a [Å]**		
CT1_2···C5_1	3.44	89	3.72	0.20		
CT1_2···H18_2_$1	2.67	164	3.01	0.19		
CT2_1···Te1_2	3.67	82/91	3.93	0.41		
CT2_1···C4_1_$1	3.42	84	3.71	0.56		
CT2_2···H17_2_$1	2.75	151	3.10	0.26		
	M-M [Å]	**<(MM)**	**øM-C_x [Å]**	**a [Å]**		
CT1_1···CT1_1_$4	3.89	0	4.10	1.80		
CT1_1···CT1_2	3.85	6.91(7)	4.08	1.78		
CT2_1···CT1_1_$4	3.77	2.74(6)	4.00	1.53		
CT2_1···CT2_2	3.95	5.84(5)	4.19	1.88		
CT3_1···CT3_2	3.94	4.64(7)	4.17	1.85		
CT4_1···CT4_1_$4	4.28	0	4.47	2.53		

Symmetry operations used: $1 1-x, 1-y, 1-z; $2 -1+x, +y, +z; $3 +x, 1/2-y, 1/2+z; $4 1-x, 1-y, -z.

Visualization of interactions and packing patterns was carried out using Mercury 4.0.[24] All displacement ellipsoids are shown at 50% probability. Specific interactions are highlighted by certain colours for clarity (chalcogen (black), hydrogen bonding (red), π-π stacking (green), CH···π interaction (blue)).

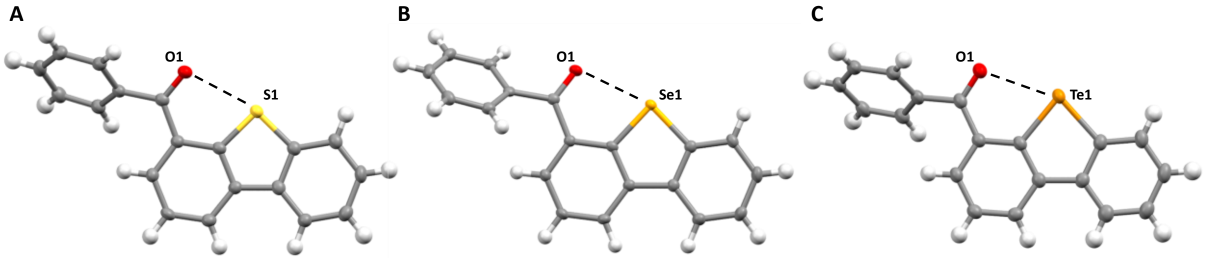


Figure S40: Intramolecular E···O interaction found in the 4-BzDBE crystal structures (S (A, **4a**), Se (B, **4b**), Te (C, **4c**)).

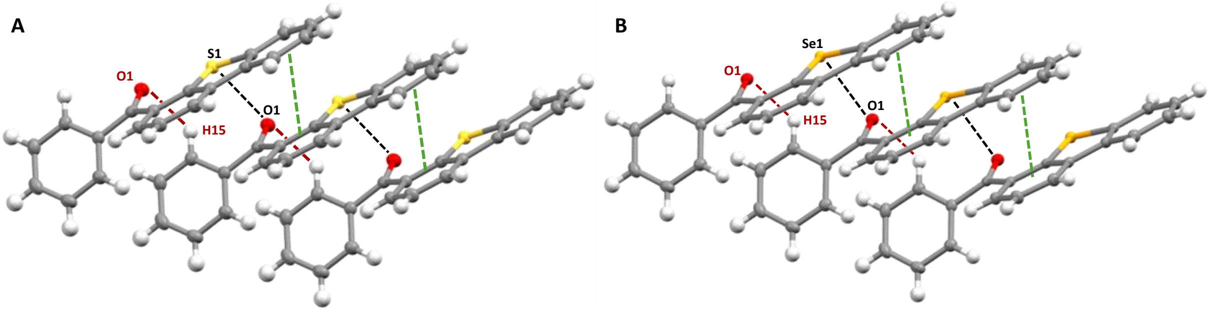


Figure S41: First interaction motif for compounds **4a** & **4b** determined by π-π stacking (green), hydrogen bonding (red) and chalcogen interaction (black) (A: S, B: Se).

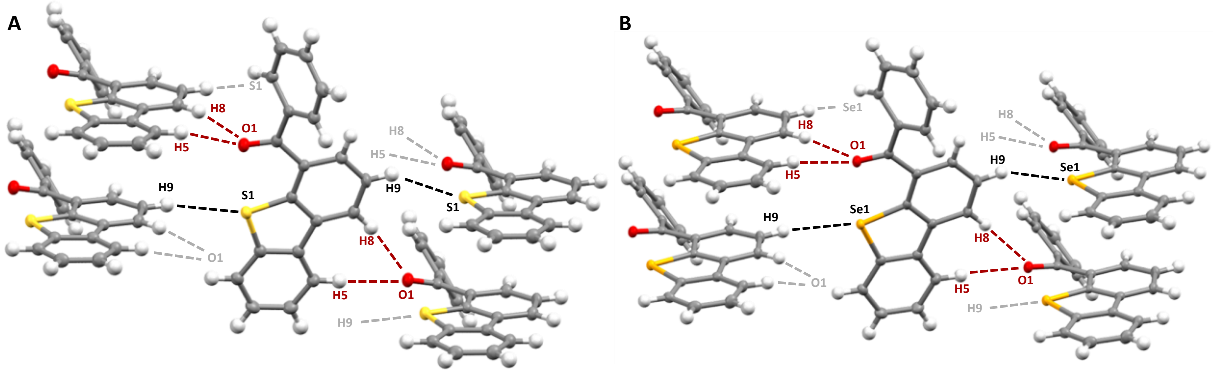


Figure S42: Second interaction motif for compounds **4a** & **4b** determined by hydrogen bonding (red) and chalcogen hydrogen interaction (black) (A: S, B: Se).

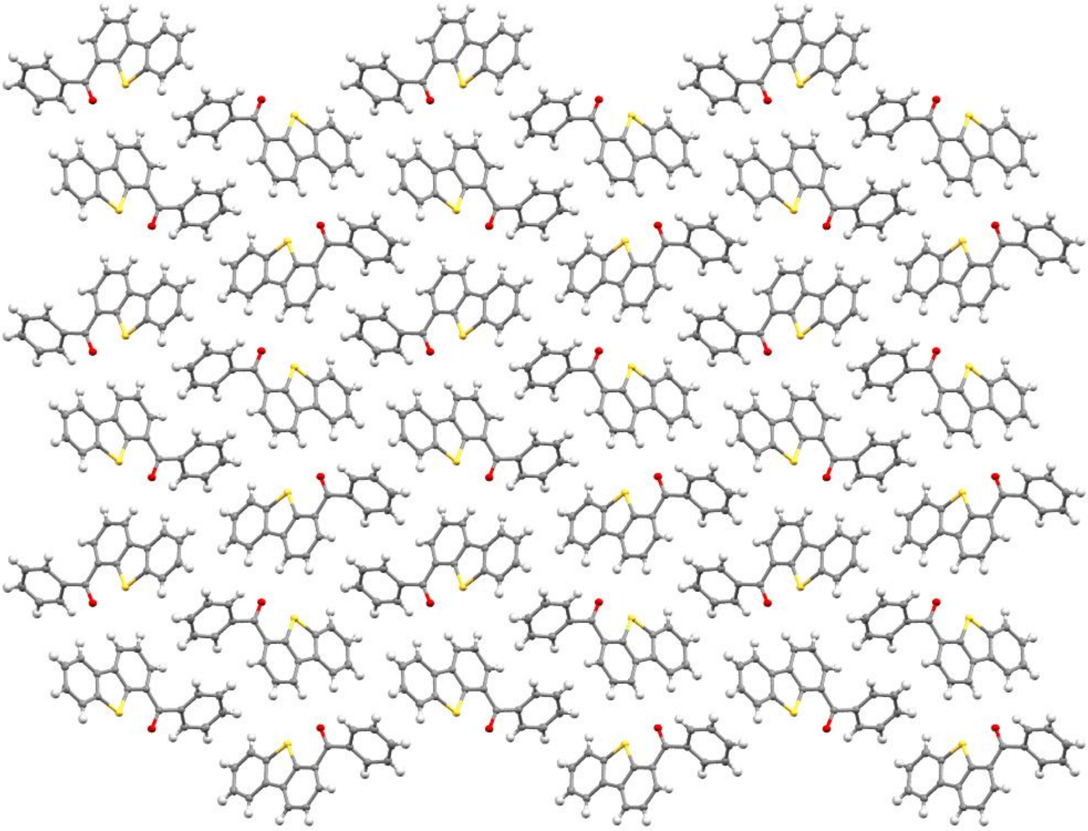


Figure S43: Cutout of the full packing of **4a** parallel to a.

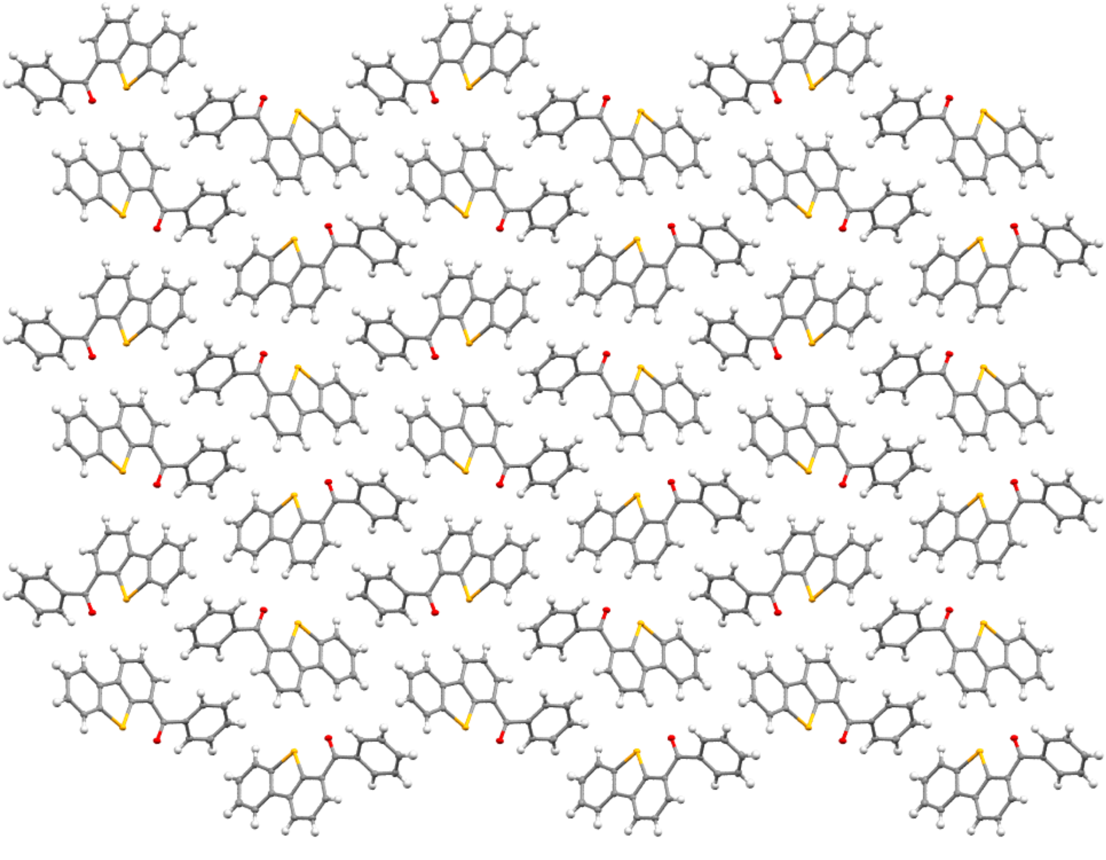


Figure S44: Cutout of the full packing of **4b** parallel to a.

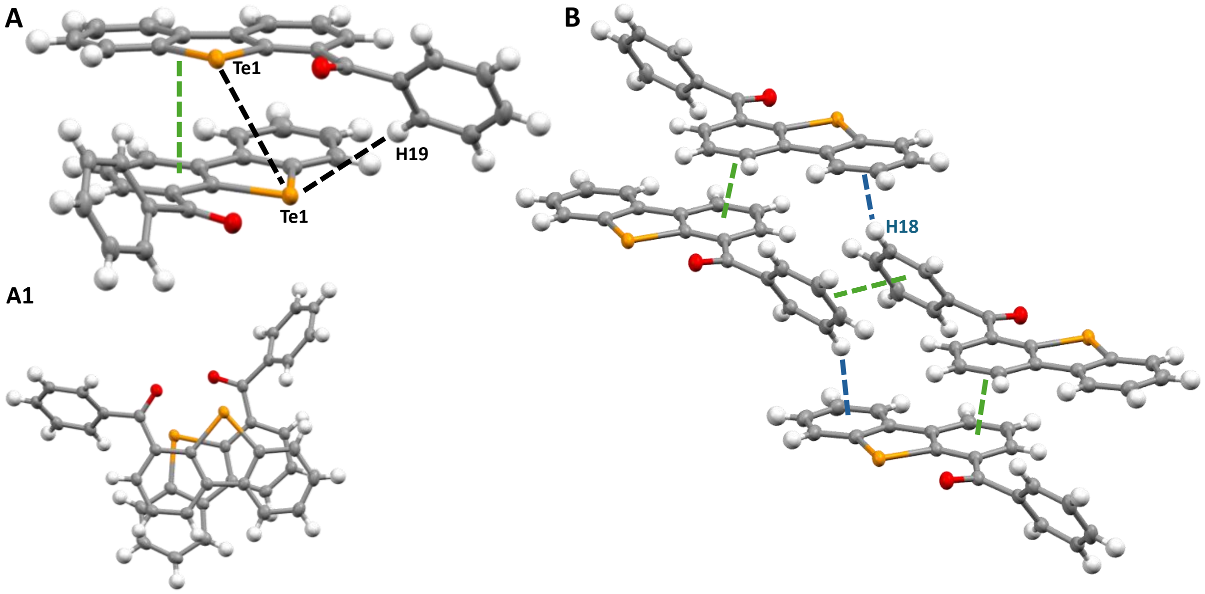


Figure S45: First packing motif of **4c** showing twisted π-π interactions (green) with additional Te···H contact (black) (A, A1). The second packing motif between these stacked dimers is determined by π-π stacking and CH···π interaction (blue) (B).

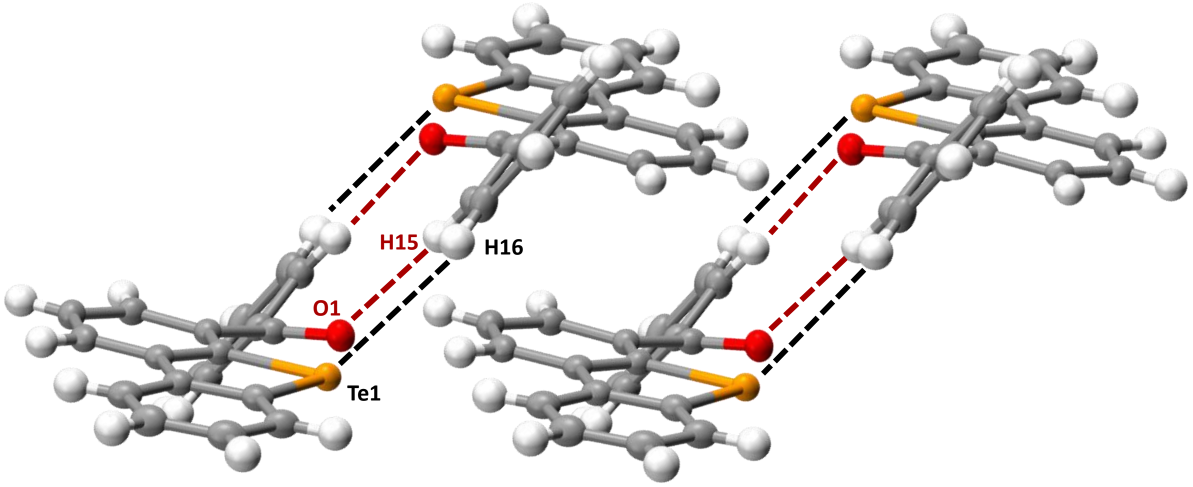


Figure S46: Interaction motif between the layers of double strands of **4c** by hydrogen bonding (red) accompanied by Te···H interaction (black).

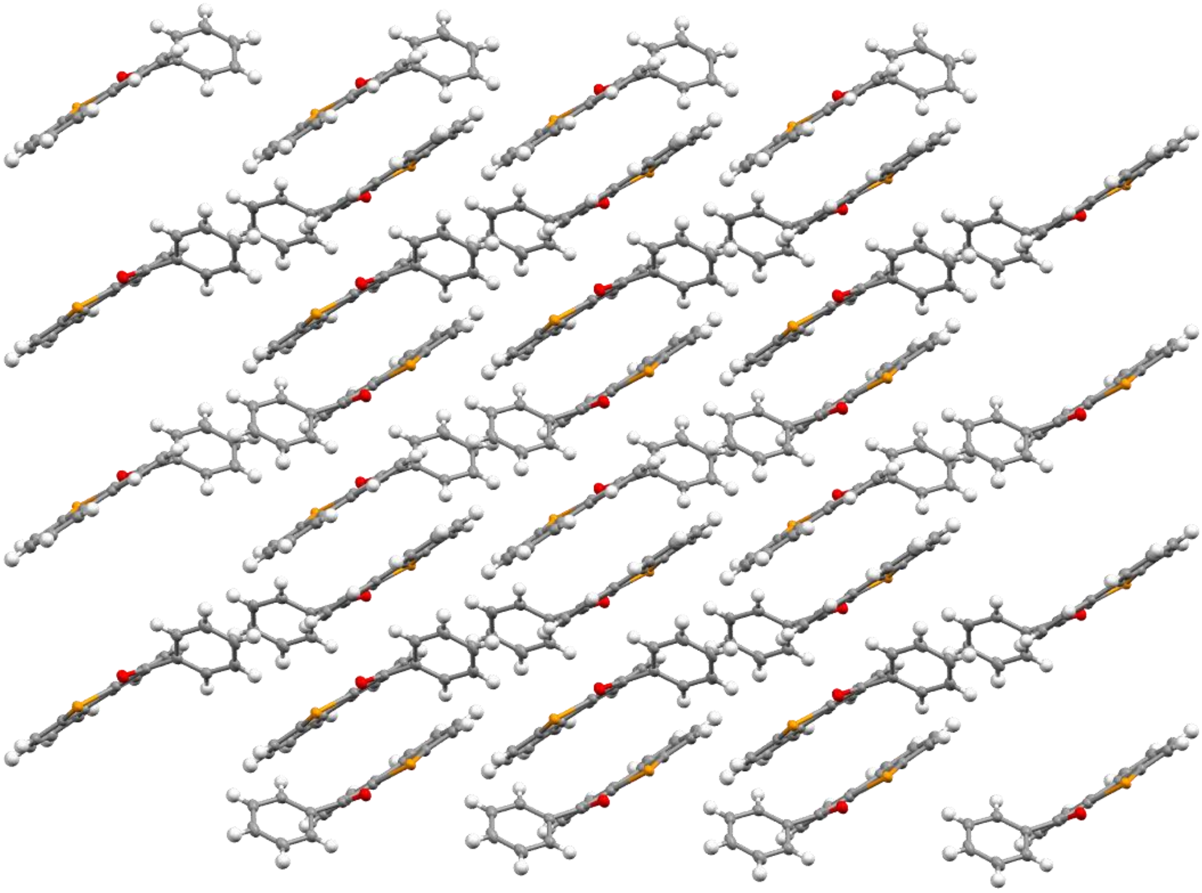


Figure S47: Cutout of the full packing of **4c** parallel to b.

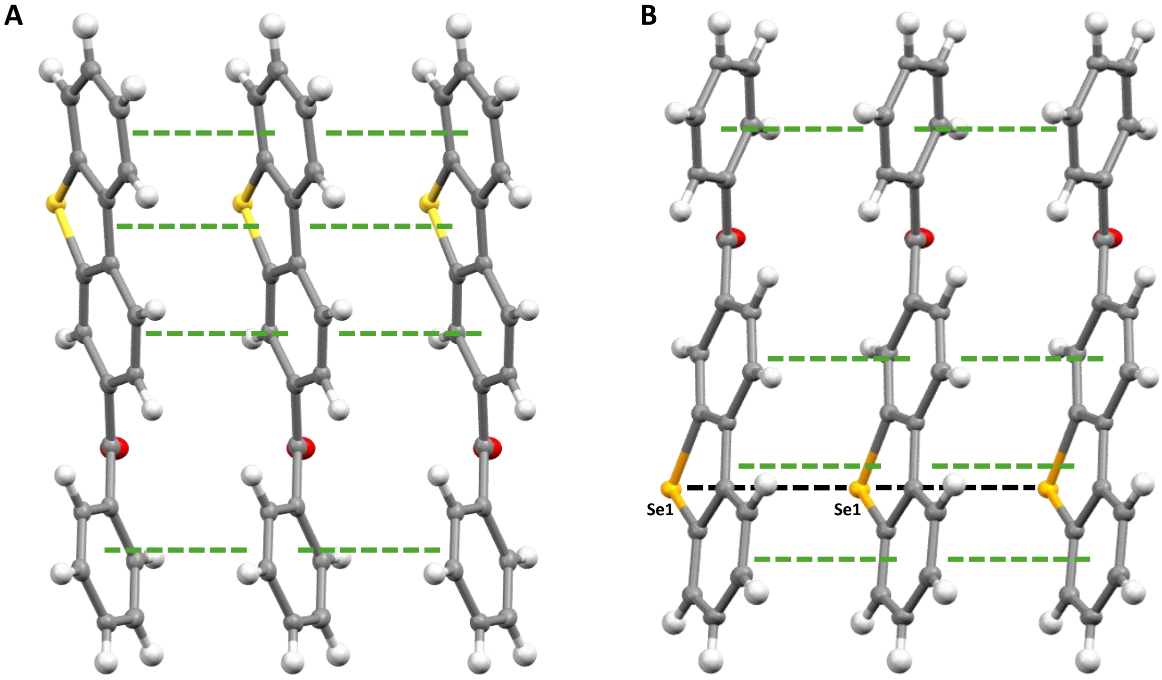


Figure S48: π-π stacking in the crystal packing of **12a** & **12b** (A: S, B: Se).

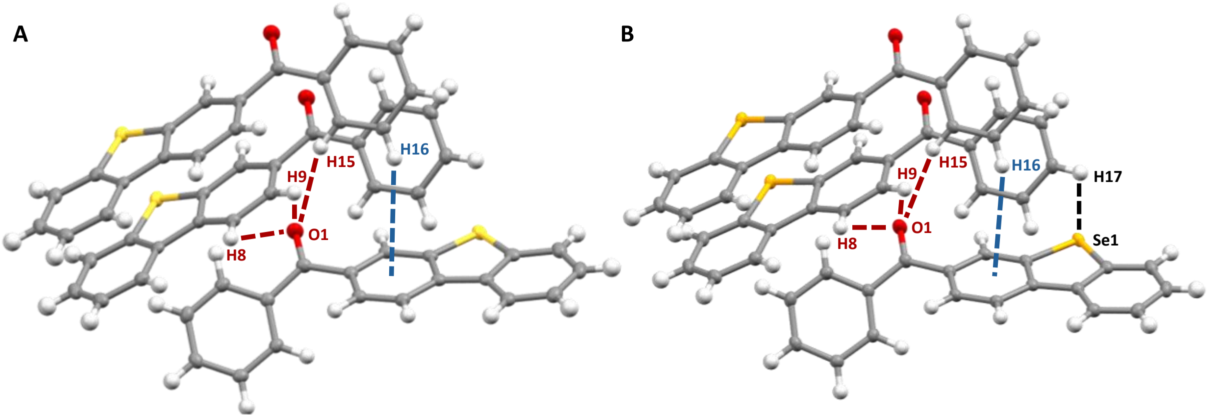


Figure S49: Hydrogen bonding (red) accompanied by weak CH···π interaction (blue) and chalcogen-participating interaction (black) in packing of **12a** & **12b** (A: S, B: Se).

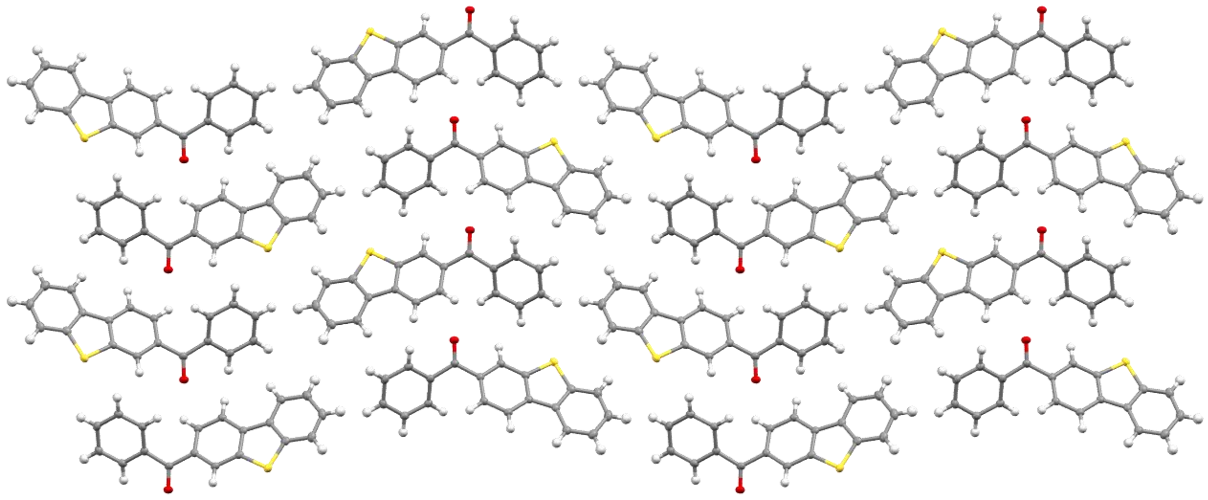


Figure S50: Cutout of the full packing of **12a** parallel to a.

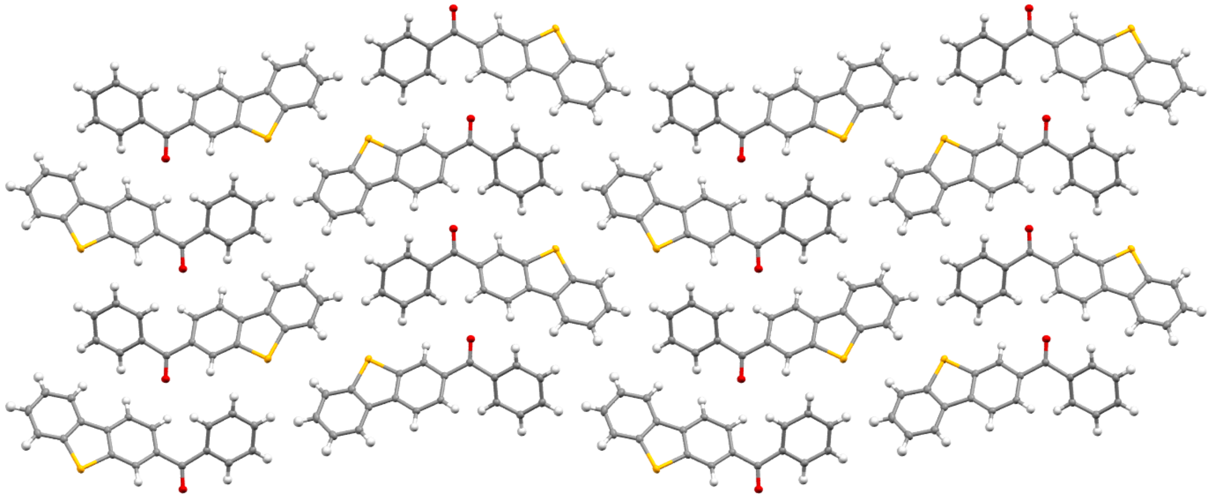


Figure S51: Cutout of the full packing of **12b** parallel to a.

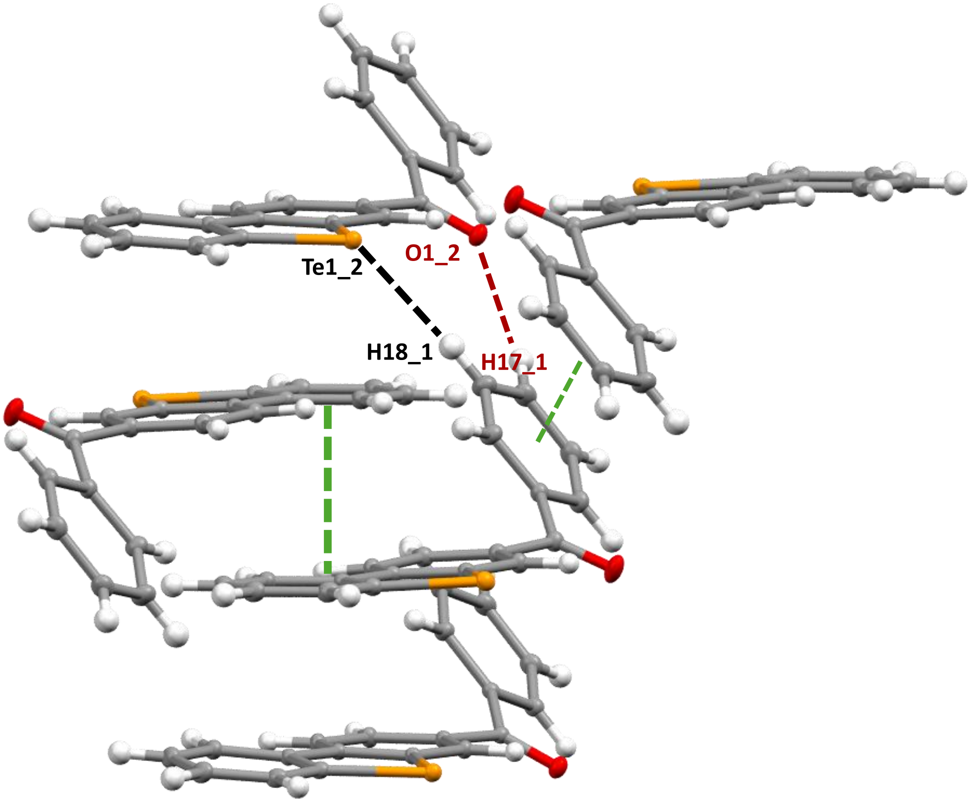


Figure S52: Interaction of residue 1 (**12c_1**) with other main dimer moieties via π-π stacking (green), chalcogen interaction (black) and hydrogen bonding (red).

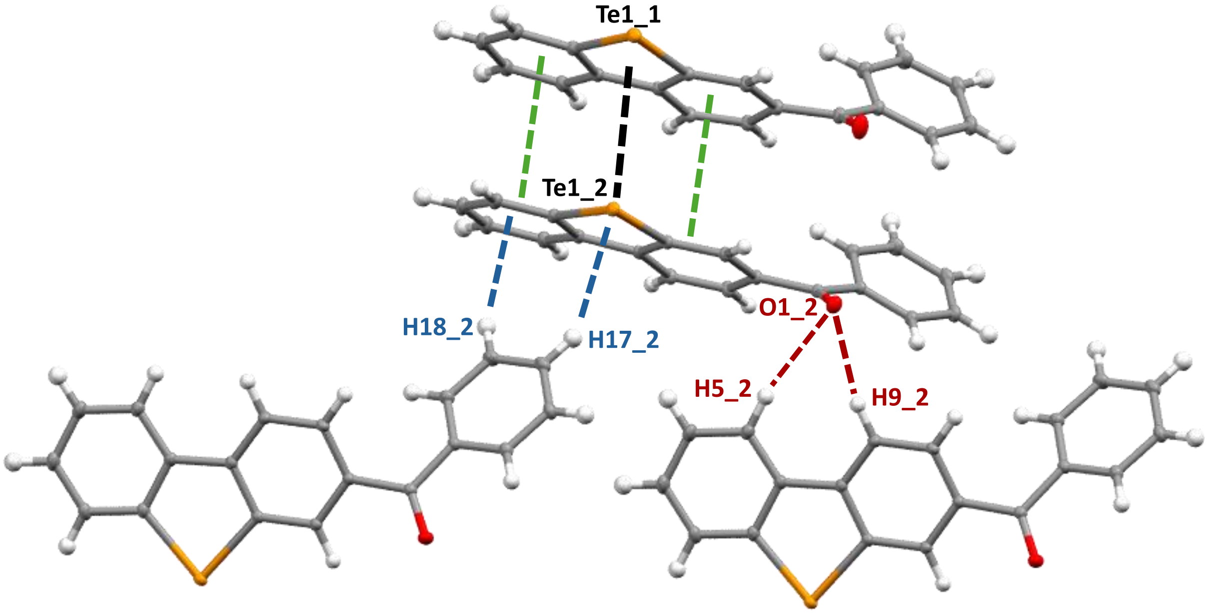


Figure S53: Interaction of residue 2 (**12c_2**) with other main dimer moieties via CH···π (blue) and O···H (red) interactions. The two molecules of the asymmetric unit interact by π-π (green) and Te (black) participating contacts.

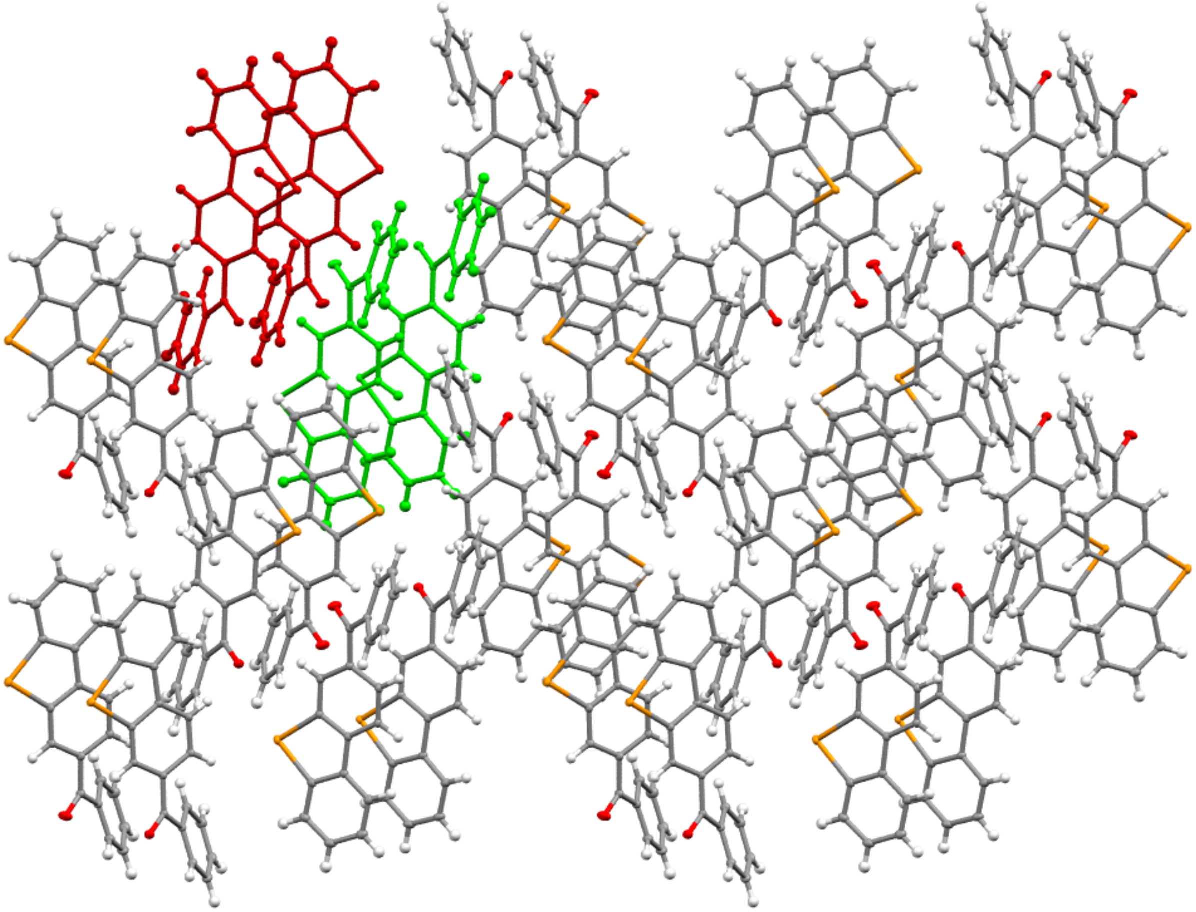


Figure S54: Cutout of packing of **12c** parallel to a. Red and green molecules are shown to clarify the repeating dimer moiety in the packing.

8. Hirshfeld surface analyses

All final compound crystal structures were analysed using CrystalExplorer17.[25] The Hirshfeld (HS) surfaces were performed in high quality. The surfaces with the value of d_{norm} are shown below. Additionally, we investigated the Fingerprint plots (FPP) to quantify the occurring interactions in the packing. Reciprocal contacts are included. Due to two independent molecules in the asymmetric unit, we obtained two different HS surfaces and FPP as well for **12c**.

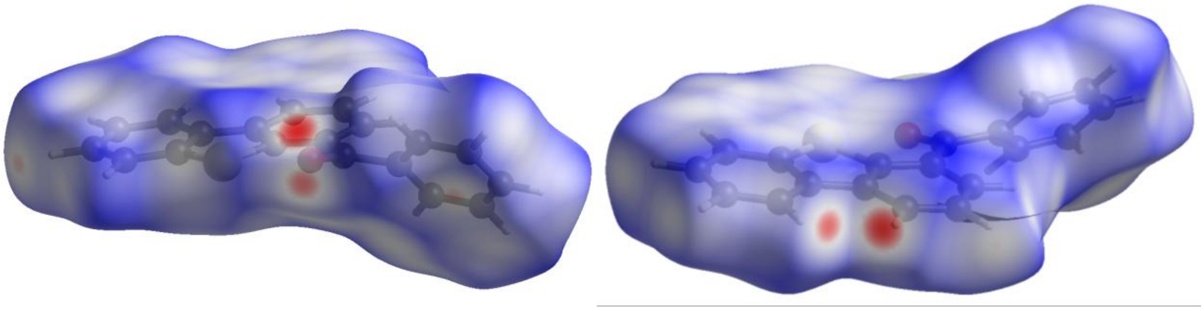


Figure S55: Hirshfeld surface of **4a** mapped with d_{norm} (front (left), back (right), quality: high).

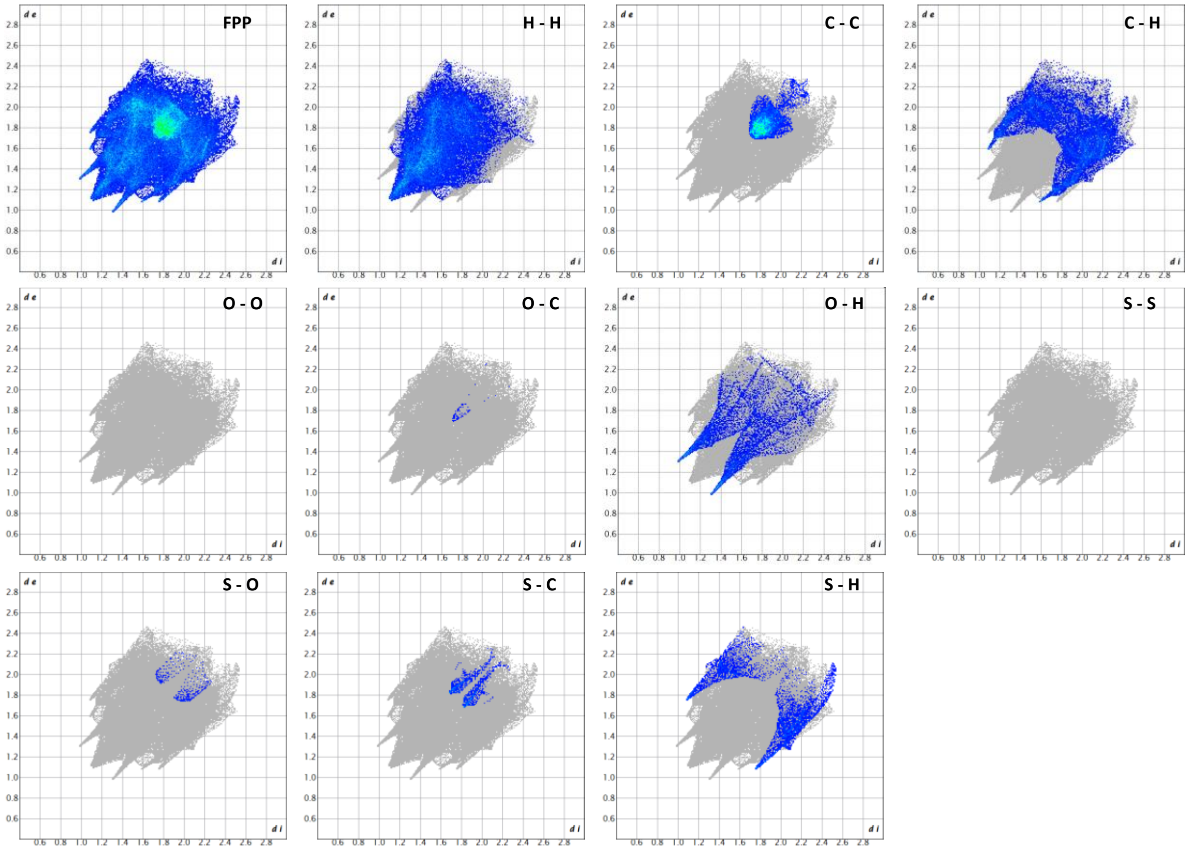


Figure S56: Fingerprint plot for **4a** resolved into the contacts of all elements contained. Reciprocal contacts are included.

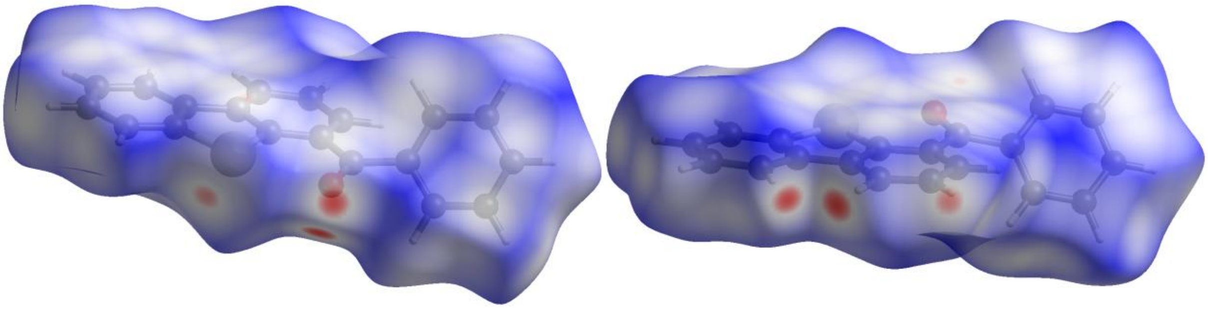


Figure S57: Hirshfeld surface of **4b** mapped with d_{norm} (front (left), back (right), quality: high).

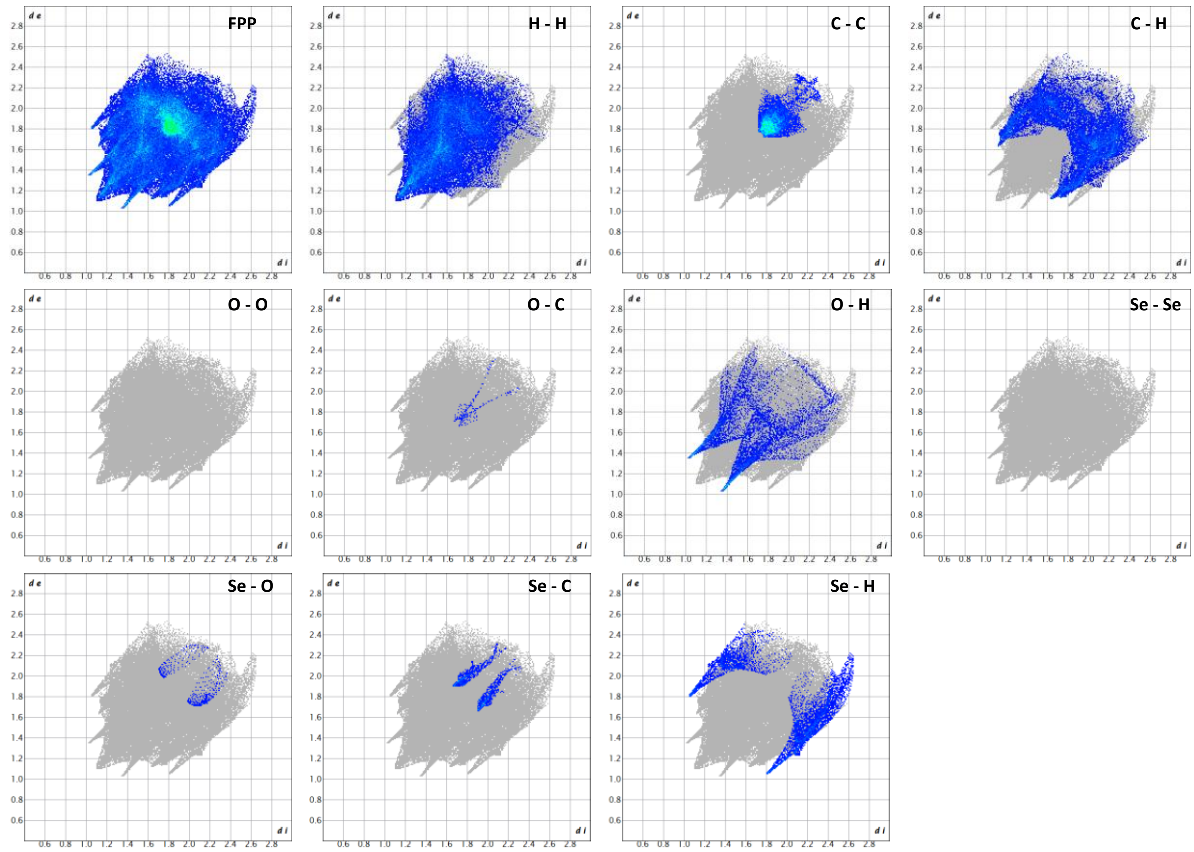


Figure S58: Fingerprint plot for **4b** resolved into the contacts of all elements contained. Reciprocal contacts are included.

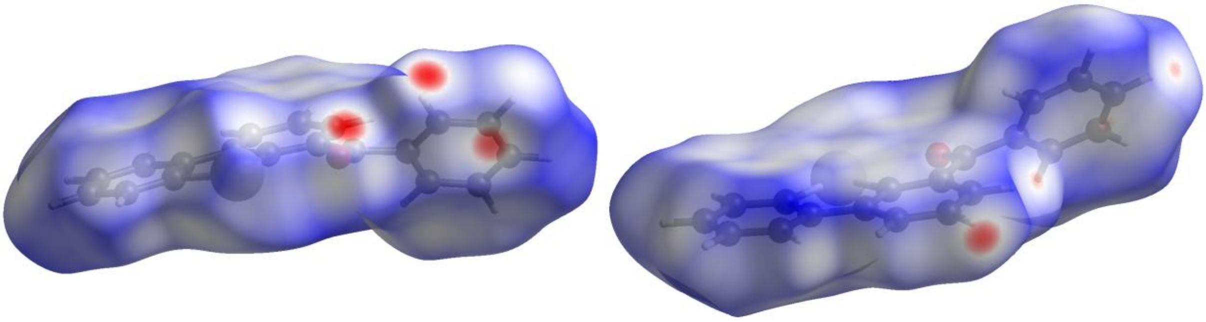


Figure S59: Hirshfeld surface of **4c** mapped with d_{norm} (front (left), back (right), quality: high).

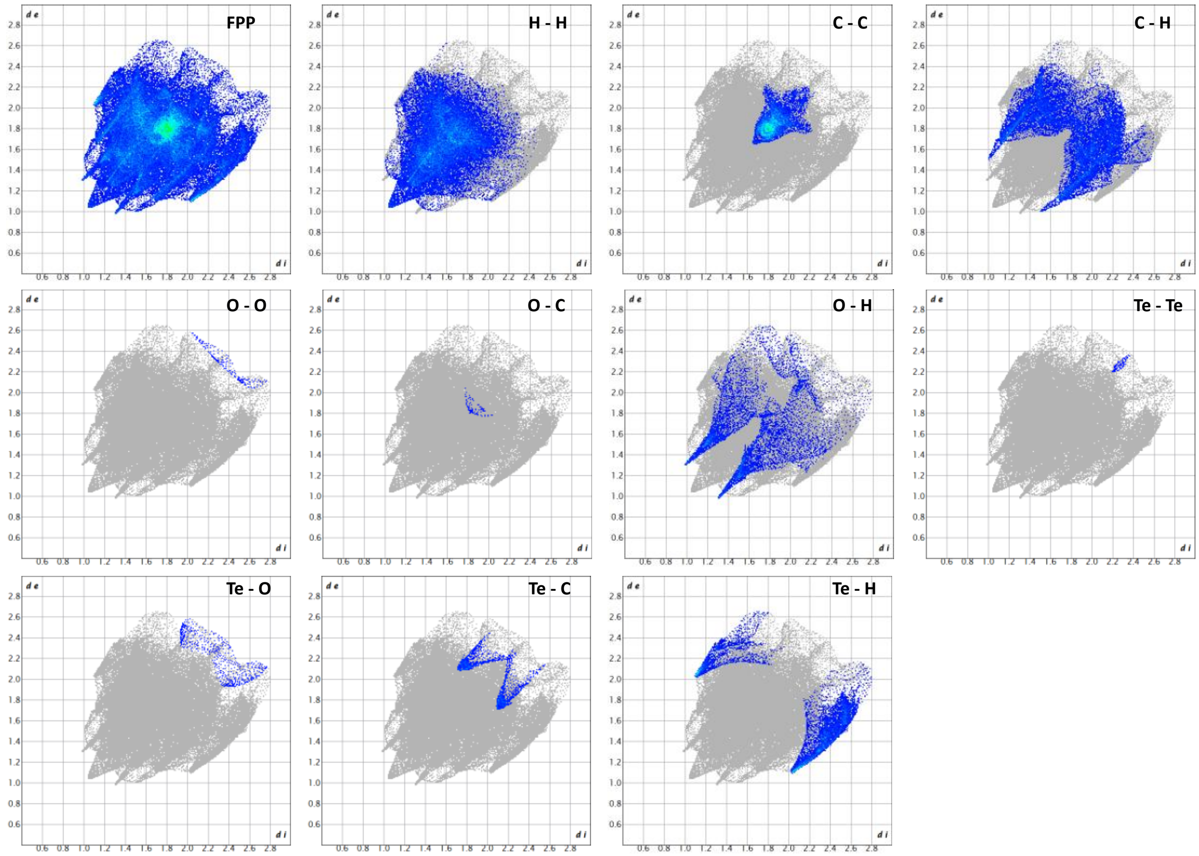


Figure S60: Fingerprint plot for **4c** resolved into the contacts of all elements contained. Reciprocal contacts are included.

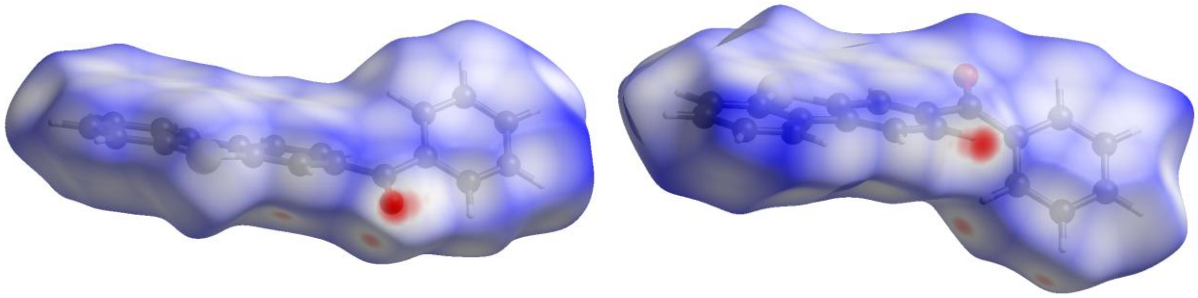


Figure S61: Hirshfeld surface of **12a** mapped with d_{norm} (front (left), back (right), quality: high).

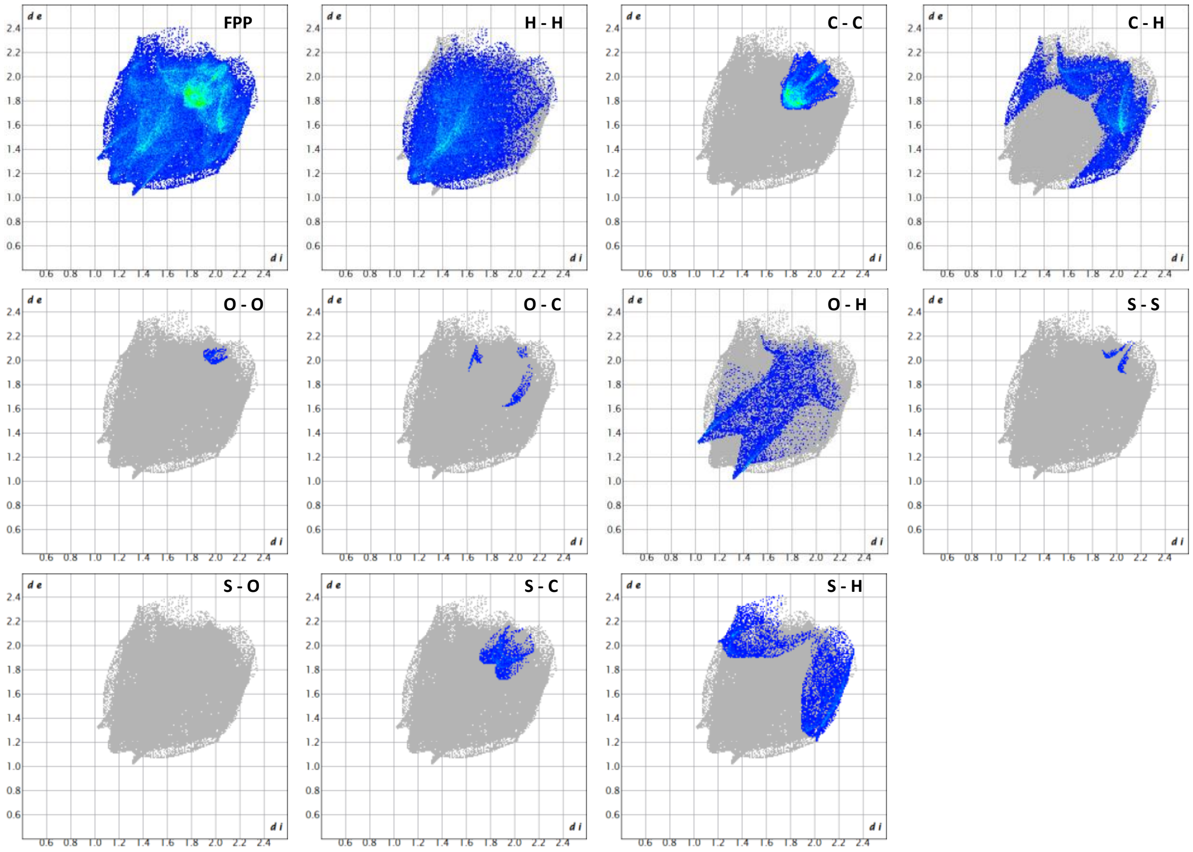


Figure S62: Fingerprint plot for **12a** resolved into the contacts of all elements contained. Reciprocal contacts are included.

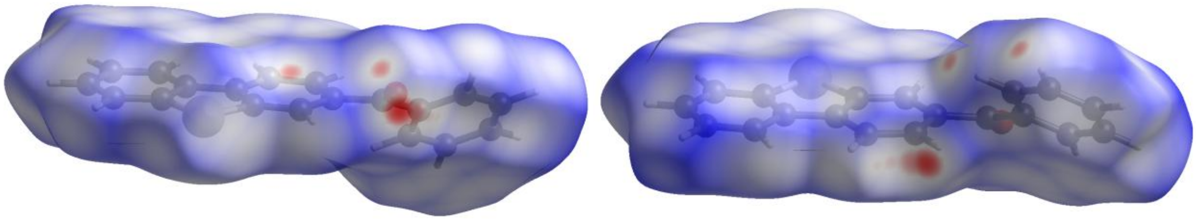


Figure S63: Hirshfeld surface of **12b** mapped with d_{norm} (front (left), back (right), quality: high).

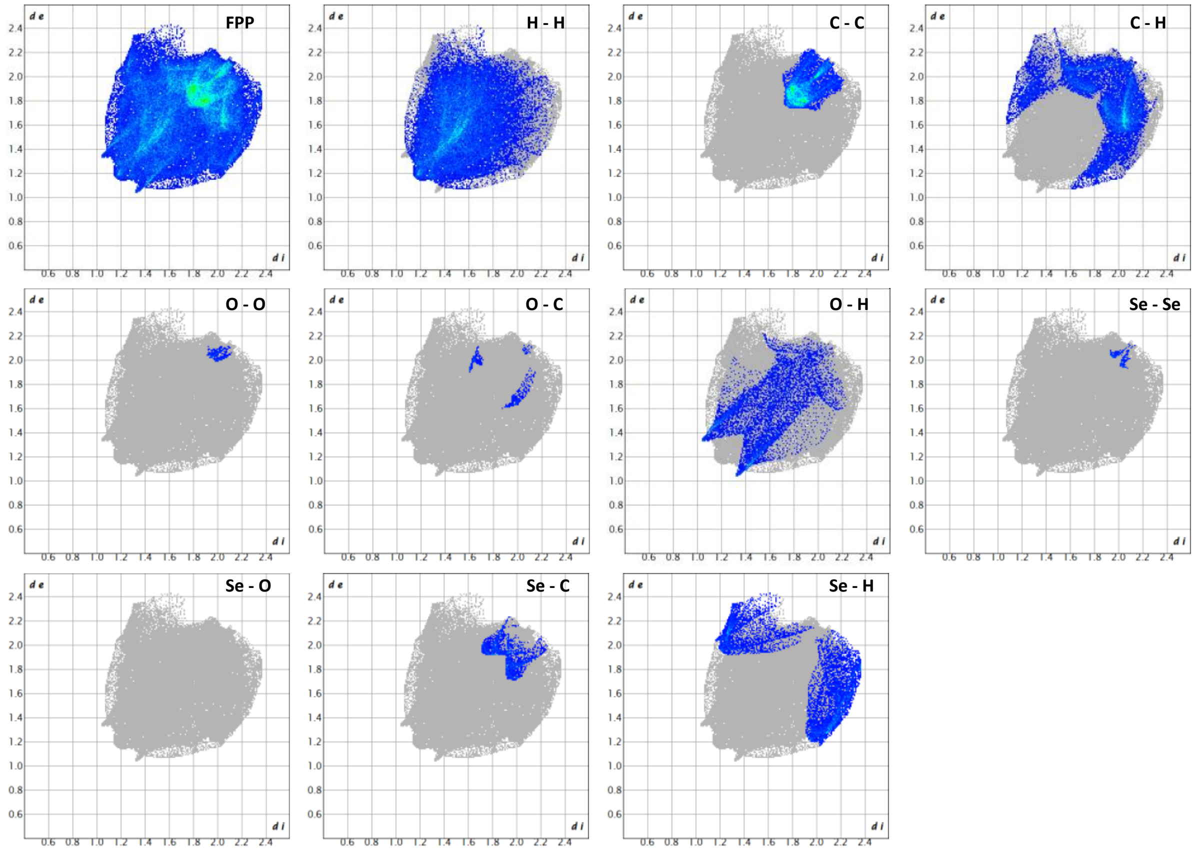


Figure S64: Fingerprint plot for **12b** resolved into the contacts of all elements contained. Reciprocal contacts are included.

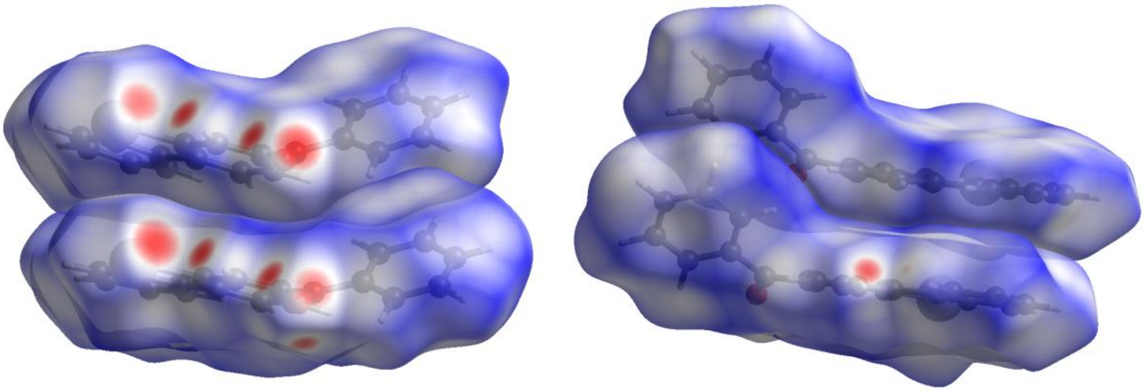


Figure S65: Hirshfeld surface of **12c** mapped with d_{norm} (front (left), back (right), quality: high; upper molecule: residue 1). Due to two molecules in the asymmetric unit, two different Hirshfeld surfaces were obtained.

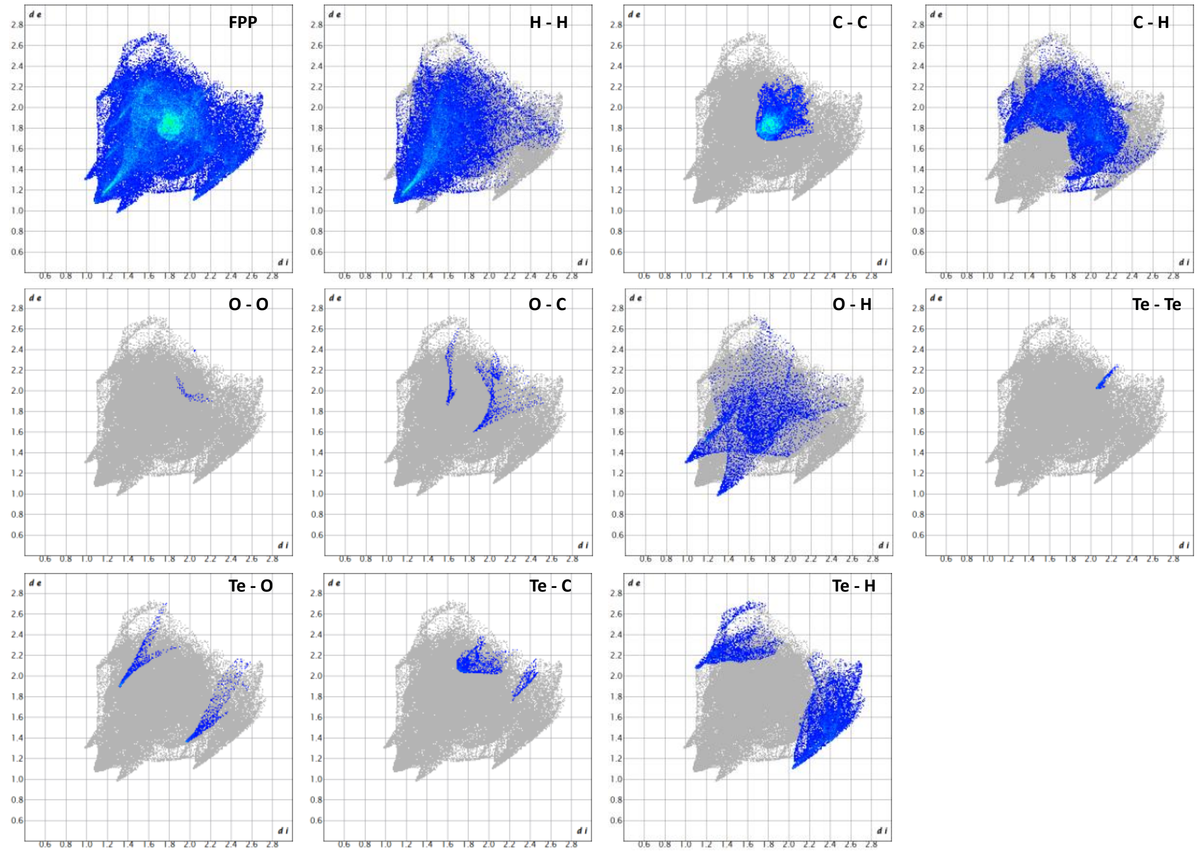


Figure S66: Fingerprint plot for **12c_1** resolved into the contacts of all elements contained. Reciprocal contacts are included.

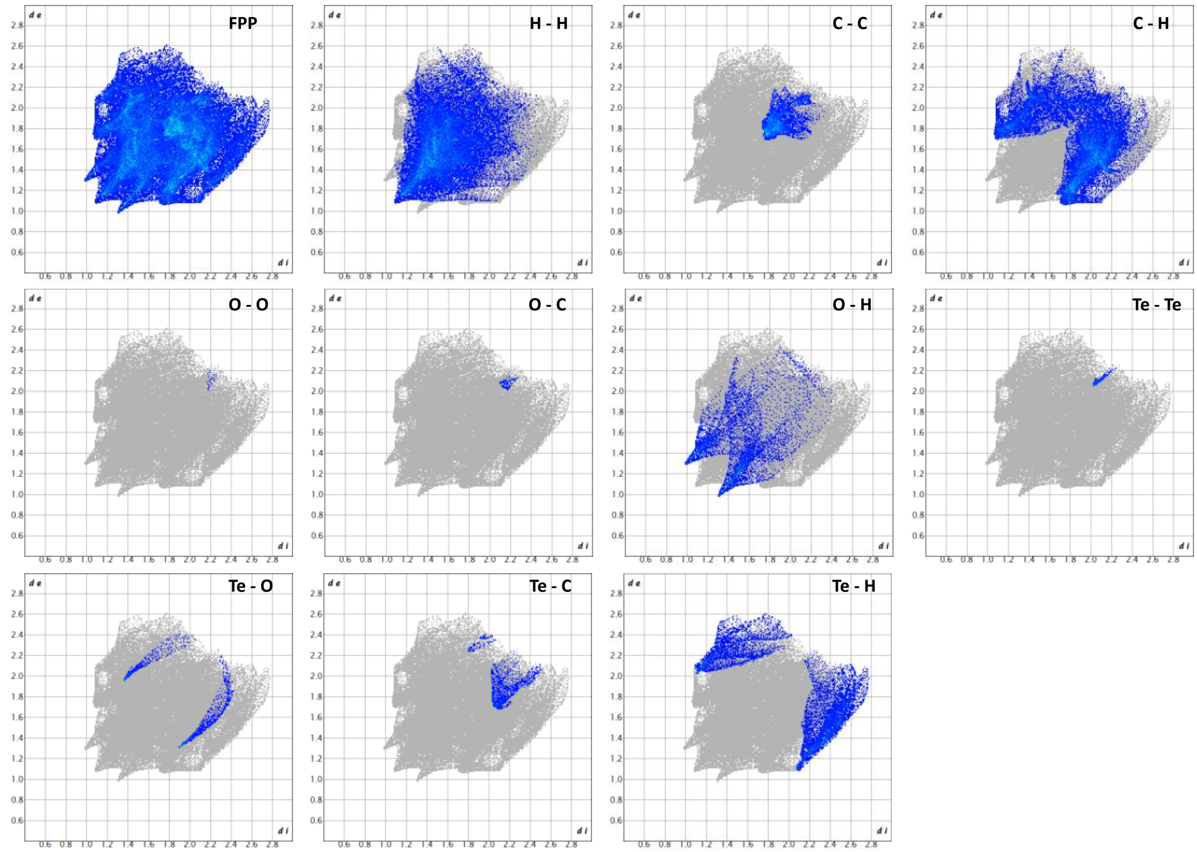


Figure S67: Fingerprint plot for **12c_2** resolved into the contacts of all elements contained. Reciprocal contacts are included.

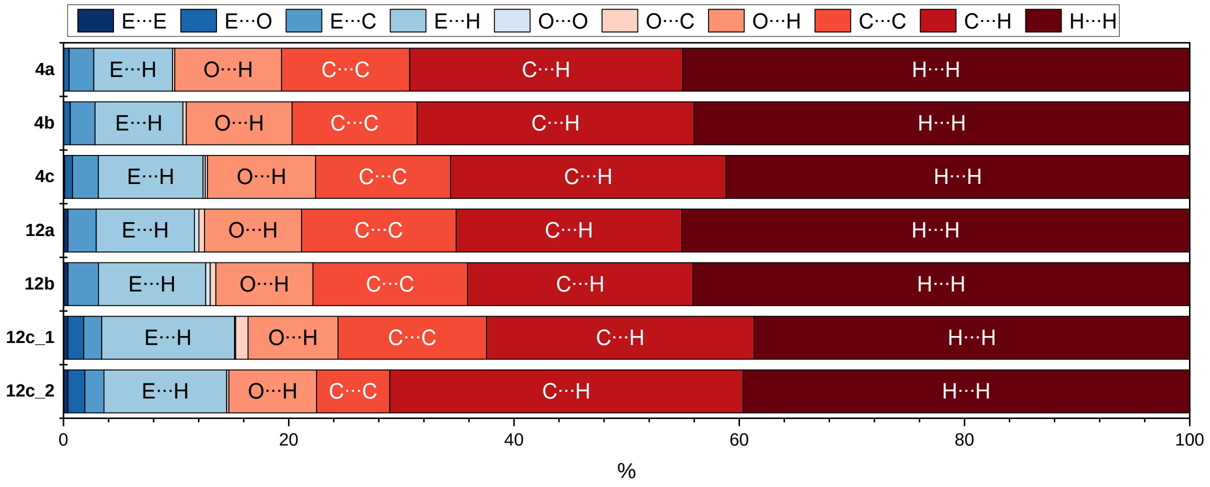


Figure S68: Histogram with all interactions found by Hirshfeld analysis in the crystal structures of BzDBE (**4a-c**, **12a-c**). Reciprocal contacts were summarized as one.

Table S11: Summary of percentages of interactions by Hirshfeld analysis for **4a-c** compounds.

4a

Inside atom	*Outside atom*				**sum**
	E	**O**	**C**	**H**	
E	0.0	0.2	1.1	2.5	3.8
O	0.3	0.0	0.1	4.2	4.6
C	1.1	0.1	11.4	9.9	22.5
H	4.5	5.3	14.4	45.1	69.3
sum	5.9	5.6	27.0	61.7	

4b

Inside atom	*Outside atom*				**sum**
	E	**O**	**C**	**H**	
E	0.0	0.2	1.1	2.5	3.8
O	0.4	0.0	0.2	4.2	4.8
C	1.1	0.1	11.1	10.1	22.4
H	5.3	5.2	14.5	44.0	69.0
sum	6.8	5.5	26.9	60.8	

4c

Inside atom	*Outside atom*				**sum**
	E	**O**	**C**	**H**	
E	0.1	0.3	1.1	2.4	3.9
O	0.4	0.2	0.1	4.1	4.8
C	1.2	0.1	12.0	10.6	23.9
H	6.9	5.5	13.9	41.2	67.5
sum	8.6	6.1	27.1	58.3	

Table S12: Summary of percentages of interactions by Hirshfeld analysis for **12a-c** compounds.

12a

Inside atom	*Outside atom*				**sum**
	E	**O**	**C**	**H**	
E	0.4	0.0	1.2	3.0	4.6
O	0.0	0.4	0.3	4.0	4.7
C	1.3	0.2	13.7	7.4	22.6
H	5.7	4.6	12.6	45.0	67.9
sum	7.4	5.2	27.8	59.4	

12b

Inside atom	*Outside atom*				**sum**
	E	**O**	**C**	**H**	
E	0.4	0.0	1.3	3.1	4.8
O	0.0	0.4	0.3	4.0	4.7
C	1.4	0.2	13.7	7.5	22.8
H	6.4	4.6	12.5	44.0	67.5
sum	8.2	5.2	27.8	58.6	

12c_1

Inside atom	*Outside atom*				**sum**
	E	**O**	**C**	**H**	
E	0.4	0.7	1.3	3.0	5.4
O	0.7	0.1	0.7	3.9	5.4
C	0.3	0.4	13.2	12.3	26.2
H	8.8	4.1	11.5	38.7	63.1
sum	10.2	5.3	26.7	57.9	

12c_2

Inside atom	*Outside atom*				**sum**
	E	**O**	**C**	**H**	
E	0.4	0.5	0.1	3.5	4.5
O	1.0	0.0	0.2	3.3	4.5
C	1.6	0.0	6.5	10.7	18.8
H	7.4	4.5	20.7	39.7	72.3
sum	10.4	5.0	27.5	57.2	

Table S13: Percentages of interactions for BzDBE compounds determined by Hirshfeld analysis. Reciprocal contacts are summarized.

	4a	**4b**	**4c**	**12a**	**12b**	**12c_1**	**12c_2**
E-E	0.0	0.0	0.1	0.4	0.4	0.4	0.4
E-O	0.5	0.6	0.7	0.0	0.0	1.4	1.5
E-C	2.2	2.2	2.3	2.5	2.7	1.6	1.7
E-H	7.0	7.8	9.3	8.7	9.5	11.8	10.9
O-O	0.0	0.0	0.2	0.4	0.4	0.1	0.0
O-C	0.2	0.3	0.2	0.5	0.5	1.1	0.2
O-H	9.5	9.4	9.6	8.6	8.6	8.0	7.8
C-C	11.4	11.1	12.0	13.7	13.7	13.2	6.5
C-H	24.3	24.6	24.5	20.0	20.0	23.8	31.4
H-H	45.1	44.0	41.2	45.0	44.0	38.7	39.7

9. *Electrostatic potential surfaces (ESP)*

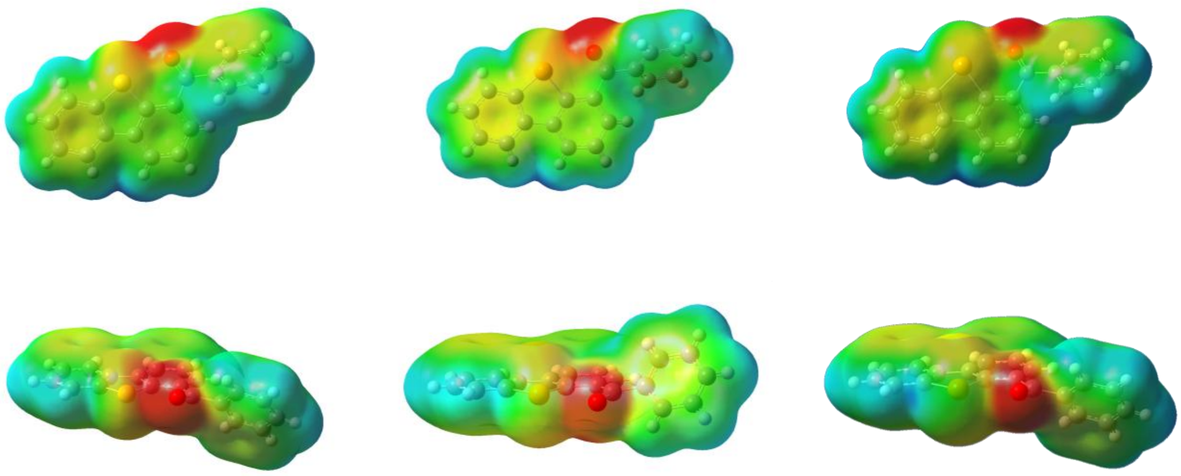


Figure S69: Generated (B3LYP/TZVP (S, Se); B3LYP/aug-cc-pVTZ-pp (Te)) molecular electrostatic potentials on the 0.001 au electron density isosurface of **4a-c** (S – Te, left-right) compounds. Colouring between -0.045 (red) and 0.045 (blue).

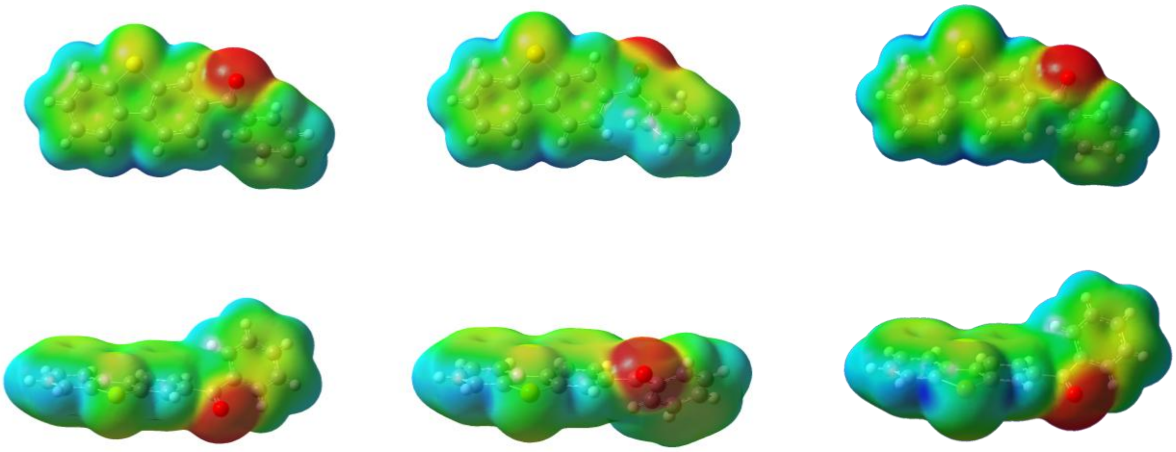
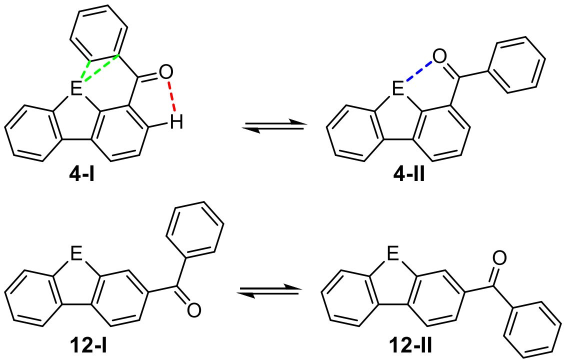


Figure S70: Generated (B3LYP-GD3BJ/TZVP (S, Se); B3LYP-GD3BJ/aug-cc-pVTZ-PP (Te))[26–28] molecular electrostatic potentials on the 0.001 au electron density isosurface of **12a-c** (S – Te, left-right) compounds. Colouring between -0.045 (red) and 0.045 (blue).

10. Quantum chemical calculations

All calculations were performed by using the programs Gaussian 16[26] and the Amsterdam Modeling Suite (AMS; Amsterdam Density Functional (ADF)).[29] The geometrical parameters were optimized by means of B3LYP[30] with additional dispersion correction with Becke-Johnson damping.[28] The basis sets applied were def2-TZVP[31] for the light elements (H, C, O, S and Se) and aug-cc-pVTZ-PP[32] for tellurium. This method is abbreviated in the following as B3LYP-D3BJ/def2-TZVP, aug-cc-pVTZ-PP. For the monomers (**4-I**, **4-II**, **12-I** and **12-II**) no symmetry restriction was applied. Frequency calculations were carried out to verify the nature of the stationary point. It turned out that all monomeric structures have none. For the geometry optimisation of the dimer structures **12·12,** the C_i point group was used as symmetry restriction. Frequency analysis of the C_i-symmetric structures of **12·12** shows an imaginary frequency for all systems. If the C_i restriction is cancelled in a subsequent geometry optimisation calculation, a minimum containing chalcogen bonds is only obtained for the tellurium compound **12c·12c**.

The bond energy analysis calculations[33] were performed by means of the density functional B3LYP-D3BJ and the basis set TZ2P.[34] To treat relativistic effects, the zeroth order regular approximation (ZORA)[35] to the Dirac equation was used for the bond energy analysis. In order to analyse the interaction between the molecules in the solid state, the quantum theory of atoms in molecules (QTAIM)[22] and the interacting quantum atoms (IQA)[23] analyses were used.



		ΔE	$E_{E\cdots O}$	$E_{O\cdots H}$	$E_{E\cdots C}$
d	E = O	+1.1	-4.3	-2.8	-5.9
a	S	-1.2	-15.2	-2.6	-8.9
b	Se	-2.0	-18.3	-2.7	-10.2
c	Te	-4.0	-26.3	-2.7	-13.1

		ΔE
d	E = O	-0.1
a	S	+0.1
b	Se	+0.1
c	Te	+0.1

Figure S71: Energy differences ΔE between the isomers **4-I/II** and **12-I/II** calculated by means of B3LYP-D3BJ/def2-TZVP, aug-cc-pVTZ-PP as well as the covalent parts of the interaction energy between the atoms of the E···O, O···H and E···C bonds in the isomers **4-I** (O···H and E···C) and **4-II** (E···O) calculated by an interacting quantum atoms analysis (IQA, B3LYP-D3BJ/TZ2P). The energies are given in kcal/mol.

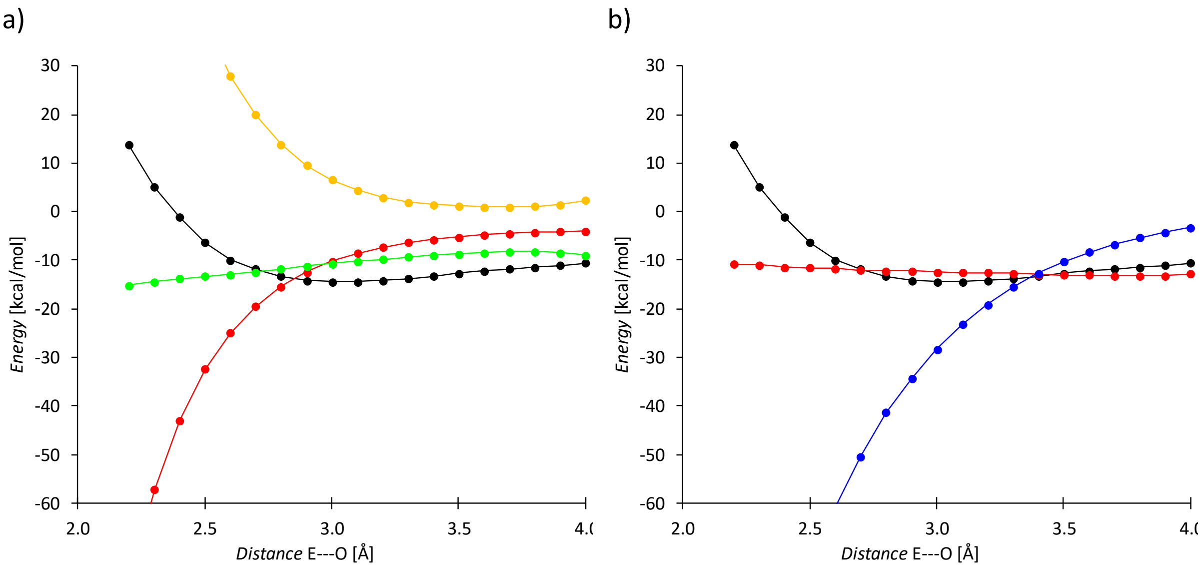


Figure S72: a) The energy terms ΔE_0 (total steric interaction, yellow), ΔE_{oi} (total orbital interactions, red), ΔE_{Disp} (dispersion energy, green) and ΔE_{total} (total bonding energy, black) of the dimers **4c·4c** (E = Te) as functions of chalcogen–oxygen distance ($d_{E\cdots O}$) calculated by an energy decomposition analysis (EDA, B3LYP-D3BJ/TZ2P). b) The sum of the covalent parts of the interaction energy between the atoms of the E···O (blue) and H···O (red) bonds of the dimers **4c·4c** (E = Te) as functions of chalcogen–oxygen distance ($d_{E\cdots O}$) calculated by an interacting quantum atoms analysis (IQA, B3LYP-D3BJ/TZ2P) as well as ΔE_{total} (total bonding energy, black) calculated by an energy decomposition analysis (EDA, B3LYP-D3BJ/TZ2P). The geometries of the dimer **4c·4c** stem from calculations (B3LYP-D3BJ/def2-TZVP, aug-cc-pVTZ-PP) with symmetry restriction (C_i).

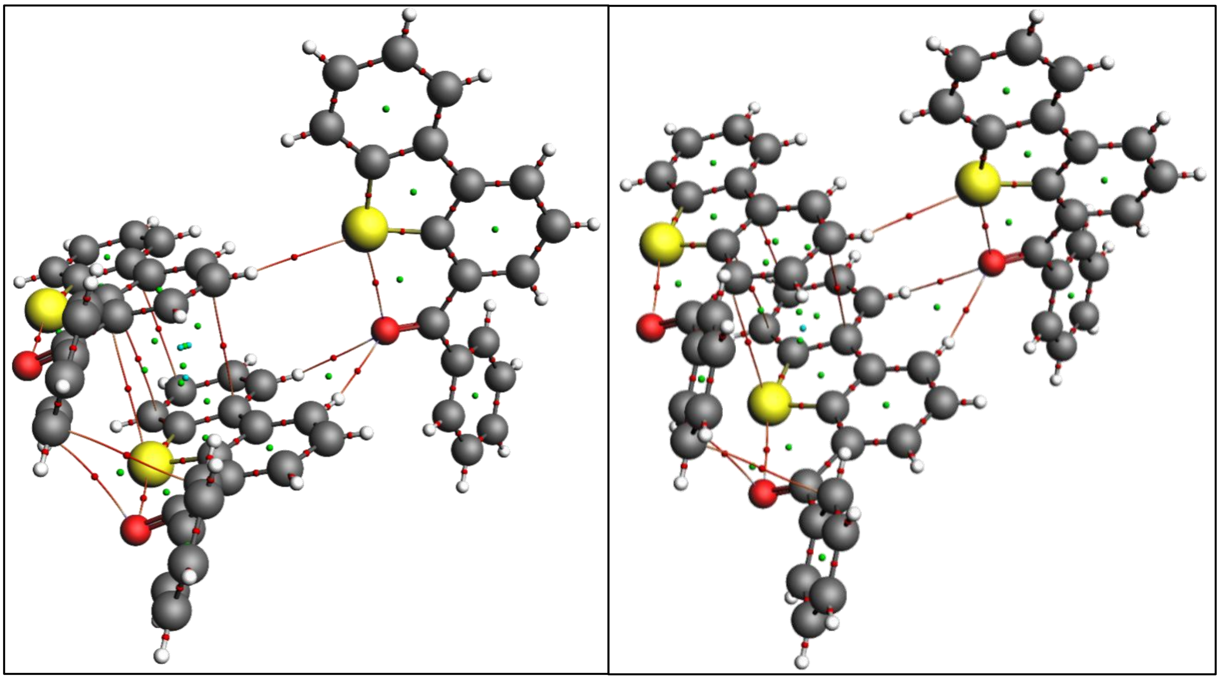


Figure S73: Selected motif from the solid-state structure of **4a** showing bond (red dots), ring (green dots) and cage (blue dots) critical points using QTAIM (B3LYP-D3BJ/def2-TZVP).

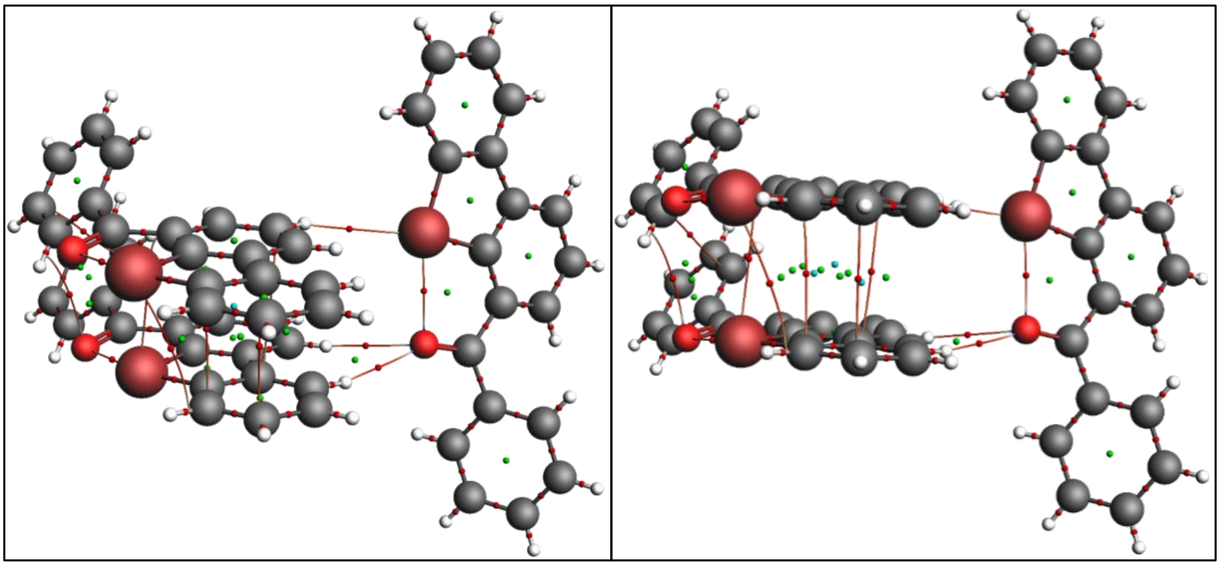


Figure S74: Selected motif from the solid-state structure of **4b** showing bond (red dots), ring (green dots) and cage (blue dots) critical points using QTAIM (B3LYP-D3BJ/def2-TZVP).

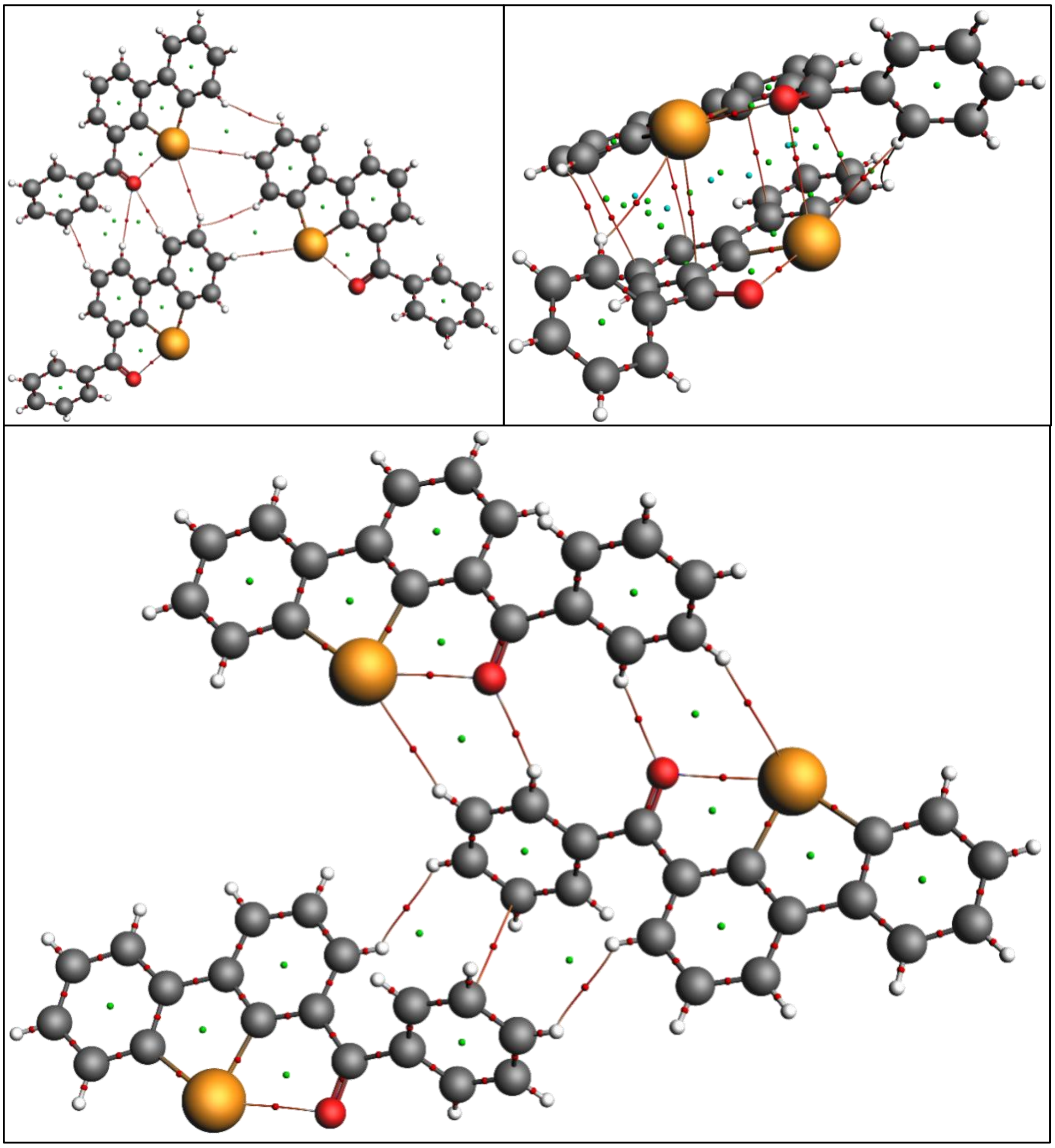


Figure S75: Selected motifs from the solid-state structure of **4c** showing bond (red dots), ring (green dots) and cage (blue dots) critical points using QTAIM (B3LYP-D3BJ/ aug-cc-pVTZ-PP).

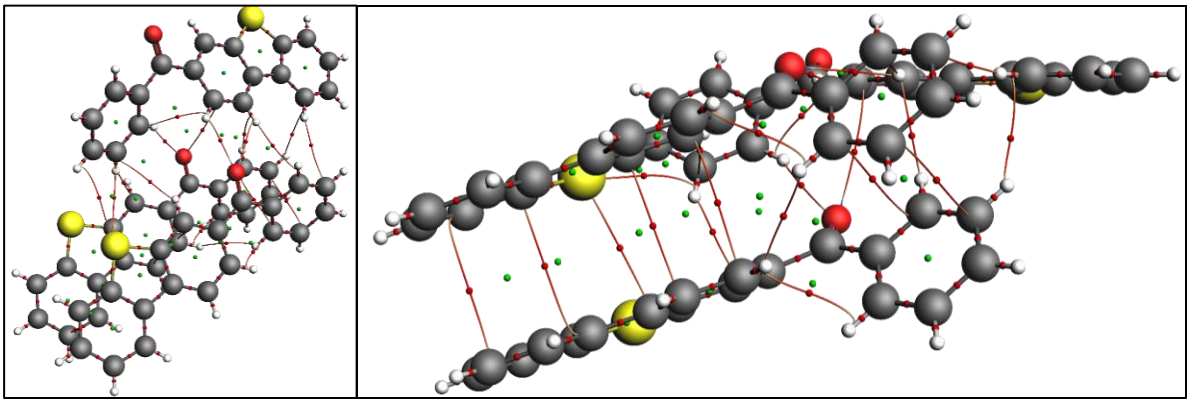


Figure S76: Selected motif from the solid-state structure of **12a** showing bond (red dots), ring (green dots) and cage (blue dots) critical points using QTAIM (B3LYP-D3BJ/def2-TZVP).

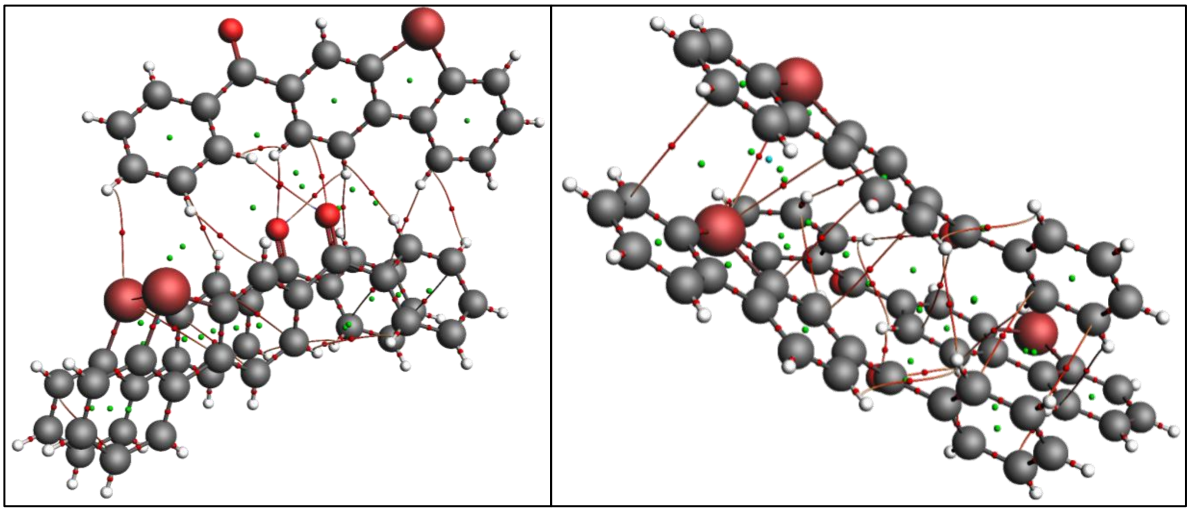


Figure S77: Selected motif from the solid-state structure of **12b** showing bond (red dots), ring (green dots) and cage (blue dots) critical points using QTAIM (B3LYP-D3BJ/def2-TZVP).

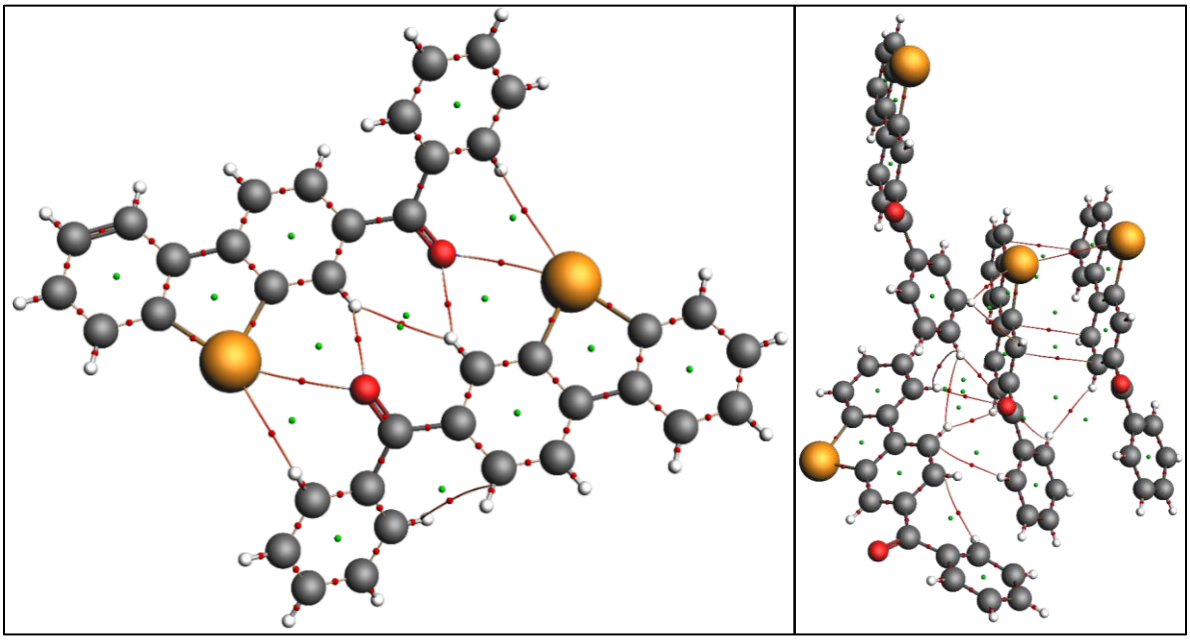


Figure S78: Selected motif from the solid-state structure of **12c** showing bond (red dots), ring (green dots) and cage (blue dots) critical points using QTAIM (B3LYP-D3BJ/ aug-cc-pVTZ-PP).

Cartesian coordinates and absolute energies for all calculated compounds

Cartesian coordinates of the optimized geometry structure of **4a-I** at B3LYP-D3BJ/def2-TZVP (E = -1205.096891 au; number of imaginary frequencies = 0):

C	-4.15092400	-2.28450800	-0.28070900
C	-4.77118400	-1.11081300	0.15982200
C	-4.03561100	0.04709400	0.34470600
C	-2.66201000	0.04366800	0.09005300
C	-2.05425000	-1.14569100	-0.35289500
C	-2.78992900	-2.31213900	-0.53969000
C	-1.70730500	1.12636000	0.20742900
C	-0.39698900	0.72479500	-0.13506500
S	-0.33185200	-0.96473400	-0.60852600
C	-1.94146200	2.44960200	0.58207500
C	-0.89897500	3.36134300	0.58532800
C	0.38217500	2.96390200	0.21180900
C	0.65960900	1.64435300	-0.13613500
H	-4.73887100	-3.18190900	-0.42182700
H	-5.83501600	-1.10917000	0.35658500
H	-4.52240600	0.95205300	0.68486000
H	-2.31042200	-3.22021400	-0.88032000
H	-2.94008200	2.76285000	0.85796700
H	-1.08031500	4.38966700	0.86775800
H	1.19281100	3.67911600	0.18288200
C	2.05556000	1.31158200	-0.56461800
O	2.66450500	2.07271000	-1.29161100
C	2.68956100	0.05960000	-0.06427000
C	3.68743500	-0.54472400	-0.83165400
C	2.35215300	-0.48177000	1.17703100
C	4.32150300	-1.68810300	-0.37350400
H	3.94900900	-0.10322300	-1.78355100
C	3.00646900	-1.61178700	1.64623600
H	1.58543800	-0.01095700	1.77705000
C	3.98351100	-2.22103400	0.86784000
H	5.08305600	-2.16346600	-0.97783500
H	2.75007500	-2.02059700	2.61471000
H	4.48429000	-3.11047500	1.22829100

Cartesian coordinates of the optimized geometry structure of **4a-II** at B3LYP-D3BJ/def2-TZVP (E = -1205.099391 au; number of imaginary frequencies = 0):

C	5.37018600	-0.95607100	0.36246600
C	5.41849600	0.43667600	0.23777600
C	4.25662500	1.16714300	0.05889500
C	3.02697800	0.50629200	0.00416900
C	2.99302000	-0.89456900	0.13239200
C	4.16129600	-1.63097600	0.30948600
C	1.69896000	1.05407200	-0.17323800
C	0.70370100	0.05215500	-0.16108900
S	1.37010300	-1.55073000	0.01622300
C	1.32626000	2.38582600	-0.35191700
C	-0.00959200	2.71628800	-0.51499400
C	-0.98795900	1.72723800	-0.46982400
C	-0.65708500	0.38463200	-0.27461300
H	6.28707300	-1.51368500	0.50222000
H	6.37250100	0.94515300	0.28150900
H	4.30108100	2.24456200	-0.03706100
H	4.12574000	-2.70830300	0.40481400
H	2.08363600	3.15900700	-0.37218600
H	-0.29684000	3.74667400	-0.67536000
H	-2.02396700	1.99916600	-0.60654800
C	-1.67461500	-0.69256300	-0.23799000
O	-1.33767800	-1.85636500	-0.39267900
C	-3.11392800	-0.36627900	-0.00624500
C	-4.07676100	-1.09629700	-0.70557700
C	-3.52324400	0.57398000	0.94078400

C	-5.42601000	-0.86518700	-0.48724100
H	-3.74961900	-1.84308300	-1.41617400
C	-4.87542200	0.78578800	1.17676900
H	-2.78519200	1.11961800	1.51240700
C	-5.82795200	0.07587600	0.45582200
H	-6.16618900	-1.42354000	-1.04547000
H	-5.18469000	1.50351300	1.92541300
H	-6.88148500	0.24938500	0.63333100

Cartesian coordinates of the optimized geometry structure of **4b-I** at B3LYP-D3BJ/def2-TZVP (E = -3208.459612 au; number of imaginary frequencies = 0):

C	-4.29602700	-2.05210400	-0.10770700
C	-4.82790400	-0.82030200	0.28116600
C	-4.00916300	0.28856500	0.40929200
C	-2.63920500	0.18345000	0.15017500
C	-2.12390500	-1.06425900	-0.23975500
C	-2.94059000	-2.18143500	-0.36952100
C	-1.64471500	1.24110500	0.22748800
C	-0.33009200	0.83615600	-0.08327300
Se	-0.24648500	-1.01703200	-0.52434600
C	-1.87966100	2.57905500	0.55080800
C	-0.84201400	3.49622500	0.53057800
C	0.44155500	3.09197400	0.17974900
C	0.72006200	1.75912000	-0.11601700
H	-4.94455100	-2.91278700	-0.20639100
H	-5.88724300	-0.73225600	0.48262300
H	-4.43182600	1.23842400	0.70996400
H	-2.52942300	-3.13607400	-0.67028600
H	-2.88054200	2.90192700	0.80585300
H	-1.03179100	4.53291700	0.77435800
H	1.25047800	3.80767000	0.12504100
C	2.11504500	1.41589800	-0.53915400
O	2.72122200	2.15391300	-1.29136200
C	2.75032400	0.17703100	-0.00781900
C	3.71416100	-0.47400300	-0.78062900
C	2.44717900	-0.30515800	1.26648000
C	4.34749200	-1.60600100	-0.29419500
H	3.94966200	-0.07802200	-1.75902400
C	3.10374900	-1.42198600	1.76366300
H	1.70483600	0.20112800	1.86833500
C	4.04520800	-2.07878600	0.98045700
H	5.08144600	-2.11869200	-0.90210700
H	2.87453700	-1.78472800	2.75691600
H	4.54614600	-2.95897700	1.36267600

Cartesian coordinates of the optimized geometry structure of **4b-II** at B3LYP-D3BJ/def2-TZVP (E = -3208.463548 au; number of imaginary frequencies = 0):

C	5.33914600	-0.51950800	0.31378700
C	5.27085600	0.87042400	0.18787800
C	4.04856700	1.50030400	0.02841100
C	2.87235000	0.74538000	-0.00627800
C	2.95740200	-0.65175400	0.12312600
C	4.18457400	-1.28660000	0.28070900
C	1.51353600	1.23697300	-0.16464200
C	0.52617200	0.23222100	-0.14380800
Se	1.25335600	-1.50412000	0.02538000
C	1.11749000	2.56375800	-0.33754100
C	-0.22372200	2.88181000	-0.48921200
C	-1.19131700	1.88496800	-0.43751800
C	-0.83669700	0.54687800	-0.24365800
H	6.29978300	-1.00221500	0.43860200
H	6.17922000	1.45764500	0.21520500
H	4.00613600	2.57768600	-0.06807200
H	4.24089300	-2.36315600	0.37767500

H	1.86295800	3.34799900	-0.36494600
H	-0.52066700	3.90991700	-0.64681000
H	-2.23129800	2.14440900	-0.56772400
C	-1.83295400	-0.54753300	-0.18934800
O	-1.46948600	-1.71079400	-0.29603600
C	-3.28303100	-0.24878600	0.00146700
C	-4.21297400	-1.00492900	-0.71441700
C	-3.73473000	0.69233200	0.92817400
C	-5.57167000	-0.79805900	-0.53324600
H	-3.85386100	-1.75220700	-1.40886600
C	-5.09643700	0.87952500	1.12721500
H	-3.02248100	1.25696900	1.51385800
C	-6.01608000	0.14416300	0.38927200
H	-6.28605400	-1.37655600	-1.10439100
H	-5.43873700	1.59796300	1.86062300
H	-7.07699900	0.29856400	0.53798000

Cartesian coordinates of the optimized geometry structure of **4c-I** at B3LYP-D3BJ/def2-TZVP,aug-cc-pVTZ-PP (E = -1074.977415 au; number of imaginary frequencies = 0):

C	-4.47504100	-1.79294500	0.03346800
C	-4.90875300	-0.50721100	0.35764800
C	-4.00455800	0.53812200	0.43082100
C	-2.64311900	0.32486900	0.18218600
C	-2.22590500	-0.97867500	-0.14170200
C	-3.13193900	-2.03106000	-0.21542500
C	-1.61054100	1.36010800	0.22070000
C	-0.28284500	0.96305100	-0.04566600
Te	-0.14920200	-1.10694900	-0.43333600
C	-1.85951300	2.71175700	0.47956700
C	-0.83773600	3.64552900	0.43451200
C	0.45443700	3.24856900	0.11581000
C	0.74804800	1.90567800	-0.11329600
H	-5.18586000	-2.60704600	-0.02468100
H	-5.95732000	-0.32433400	0.55208400
H	-4.35945600	1.52870400	0.68208400
H	-2.79811800	-3.02994400	-0.46533800
H	-2.86609200	3.03723800	0.70504900
H	-1.05016600	4.68810000	0.63013200
H	1.25368900	3.97231000	0.03208100
C	2.14602600	1.56483900	-0.52555300
O	2.75109900	2.28551900	-1.29480600
C	2.78831100	0.33874000	0.03074100
C	3.70139100	-0.36735900	-0.75568600
C	2.54350100	-0.07331900	1.34225300
C	4.34024100	-1.48546000	-0.24464400
H	3.89323500	-0.02546200	-1.76361600
C	3.21149600	-1.17265400	1.86364100
H	1.83788800	0.47466000	1.95184800
C	4.09902800	-1.88591100	1.06755900
H	5.03254400	-2.04239800	-0.86233000
H	3.02841900	-1.48036500	2.88453500
H	4.60579900	-2.75429700	1.46847300

Cartesian coordinates of the optimized geometry structure of **4c-II** at B3LYP-D3BJ/def2-TZVP,aug-cc-pVTZ-PP (E = -1074.984679 au; number of imaginary frequencies = 0):

C	5.33024300	-0.06268700	0.24218500
C	5.13719900	1.31430600	0.12685600
C	3.85946100	1.83111700	-0.00173100
C	2.74728100	0.98148500	-0.01682600
C	2.95555300	-0.40576600	0.10211500
C	4.24135300	-0.92184800	0.22892700
C	1.35775000	1.42112600	-0.14694200
C	0.37089900	0.41795900	-0.11576500
Te	1.14770100	-1.50891500	0.03311300

C	0.94242900	2.74462800	-0.30845700
C	-0.40357200	3.05850400	-0.44390700
C	-1.36716000	2.06110500	-0.38746600
C	-0.99249500	0.72600200	-0.19975200
H	6.33119800	-0.46241100	0.34309000
H	5.98871600	1.98195500	0.13807000
H	3.72631300	2.90163400	-0.08905800
H	4.39859300	-1.98955200	0.31880200
H	1.67678700	3.53852600	-0.34407800
H	-0.70306100	4.08694800	-0.59502800
H	-2.40933600	2.31508300	-0.51045600
C	-1.96442600	-0.38409200	-0.13174100
O	-1.57060100	-1.54705700	-0.18597200
C	-3.42477300	-0.12432000	0.00827800
C	-4.31191300	-0.91417700	-0.72578800
C	-3.92966600	0.81865000	0.90551200
C	-5.68040700	-0.73811000	-0.59249500
H	-3.91288700	-1.66179100	-1.39765800
C	-5.30126600	0.97500500	1.05625900
H	-3.25112500	1.40729000	1.50717000
C	-6.17786400	0.20657000	0.29983800
H	-6.36109200	-1.34254300	-1.17769300
H	-5.68496600	1.69523000	1.76702400
H	-7.24652100	0.33694500	0.41112300

Cartesian coordinates of the optimized geometry structure of **12a-I** at B3LYP-D3BJ/def2-TZVP (E = -1205.098304 au; number of imaginary frequencies = 0):

C	-5.66626000	-0.77710300	0.07101500
C	-5.51291300	0.56976100	0.41777200
C	-4.25704500	1.14913900	0.44817300
C	-3.13180900	0.38339800	0.13014500
C	-3.30470300	-0.97228100	-0.21742000
C	-4.56702000	-1.55743800	-0.24853900
C	-1.74097200	0.77724200	0.09656300
C	-0.89868600	-0.29126200	-0.27041200
S	-1.78841800	-1.76776600	-0.58391200
C	-1.16730500	2.02578800	0.36160100
C	0.19798900	2.19078400	0.25919700
C	1.03267600	1.11378800	-0.08567400
C	0.47860300	-0.13472500	-0.35553100
C	2.49619300	1.37393800	-0.22387600
O	2.89590100	2.48460400	-0.52408400
C	3.46901500	0.26265700	0.00621800
C	3.24499700	-0.74485100	0.94662500
C	4.20871200	-1.71922900	1.17209400
C	5.39450700	-1.70582100	0.44778400
C	5.62521300	-0.70330200	-0.49003600
C	4.67408300	0.28246500	-0.69957600
H	-6.65495100	-1.21645200	0.05139500
H	-6.38462200	1.16136500	0.66364600
H	-4.14388400	2.19141700	0.71706900
H	-4.68805600	-2.59847500	-0.51682000
H	-1.79547000	2.86157200	0.64134700
H	0.65536400	3.15322300	0.43981700
H	1.10824200	-0.96258100	-0.64864000
H	2.32812300	-0.75310900	1.51951100
H	4.03414000	-2.48746600	1.91408000
H	6.14071600	-2.47148100	0.61694100
H	6.55001300	-0.68971000	-1.05206500
H	4.84621600	1.08142200	-1.40774800

Cartesian coordinates of the optimized geometry structure of **12a-II** at B3LYP-D3BJ/def2-TZVP (E = -1205.098112 au; number of imaginary frequencies = 0):

C	-5.77602700	-0.78401600	0.09578900

C	-5.05957400	-1.91936900	-0.29814300
C	-3.68330500	-1.87052800	-0.43068300
C	-3.00292600	-0.67804000	-0.16933100
C	-3.74040200	0.45663400	0.22682300
C	-5.12492300	0.40988900	0.36070100
C	-1.58535700	-0.40199000	-0.24359200
C	-1.28845400	0.93568700	0.09741700
S	-2.72307700	1.85357700	0.50917300
C	-0.53643400	-1.25324800	-0.59788100
C	0.76444600	-0.78561800	-0.58920400
C	1.04897900	0.54669500	-0.24675900
C	0.01134200	1.41494400	0.08422100
C	2.43358500	1.10439400	-0.29325400
O	2.61324800	2.28340000	-0.54113700
C	3.59923400	0.20679500	-0.03101700
C	3.53173400	-0.86188000	0.86481900
C	4.66098100	-1.62580000	1.12969700
C	5.86008600	-1.34087400	0.48784400
C	5.93458500	-0.27640500	-0.40613000
C	4.81447600	0.50107000	-0.65339300
H	-6.85225200	-0.83699300	0.19519700
H	-5.58752700	-2.84168500	-0.50049600
H	-3.13375500	-2.75166100	-0.73596500
H	-5.68124800	1.28645800	0.66479600
H	-0.74112600	-2.27735200	-0.88166700
H	1.57051600	-1.44588600	-0.87471300
H	0.24266100	2.44442600	0.32023000
H	2.60285400	-1.08121200	1.37274600
H	4.60482400	-2.44209100	1.83805600
H	6.73715100	-1.94313200	0.68721800
H	6.86892700	-0.05134500	-0.90379900
H	4.85994600	1.34598800	-1.32681300

Cartesian coordinates of the optimized geometry structure of **12b-I** at B3LYP-D3BJ/def2-TZVP (E = -3208.460247 au; number of imaginary frequencies = 0):

C	-5.55312700	-0.22878500	0.25418400
C	-5.26615700	1.11716200	0.49647700
C	-3.96062600	1.57376500	0.45740300
C	-2.91501900	0.68876600	0.17425200
C	-3.22569100	-0.66309100	-0.06687100
C	-4.53528600	-1.12660400	-0.02874500
C	-1.49974700	0.99901200	0.09419500
C	-0.68113400	-0.10559900	-0.20488600
Se	-1.68054900	-1.70608400	-0.43317600
C	-0.89115700	2.24786700	0.27114900
C	0.47669700	2.37819900	0.15175100
C	1.28504700	1.26412700	-0.12367800
C	0.69674000	0.01456700	-0.30683600
C	2.75345100	1.47821700	-0.28472800
O	3.17864600	2.55575800	-0.66107700
C	3.69932000	0.36093900	0.01722300
C	3.45348600	-0.57482900	1.02395200
C	4.39310100	-1.55606000	1.31263700
C	5.57598500	-1.62180900	0.58645800
C	5.82827400	-0.69112700	-0.41753900
C	4.90164400	0.30227400	-0.69109200
H	-6.57762500	-0.57574600	0.28697100
H	-6.07060500	1.80642600	0.71594100
H	-3.74717000	2.61773200	0.64636800
H	-4.76015100	-2.16813300	-0.21627200
H	-1.49678200	3.11562200	0.49758100
H	0.95375800	3.34126100	0.26638000
H	1.30714500	-0.84409000	-0.54742000
H	2.53883600	-0.52120900	1.59798300
H	4.20204100	-2.26773200	2.10524600
H	6.30326800	-2.39307800	0.80527300

H	6.75088800	-0.73919000	-0.98126900
H	5.09108500	1.04695900	-1.45202800

Cartesian coordinates of the optimized geometry structure of **12b-II** at B3LYP-D3BJ/def2-TZVP (E = -3208.460059 au; number of imaginary frequencies = 0):

C	5.40977100	1.41215400	0.01916200
C	4.56521100	2.48305000	-0.28500100
C	3.19897300	2.29031200	-0.38854400
C	2.65160700	1.01866500	-0.18921100
C	3.51950100	-0.04679700	0.11673000
C	4.89250300	0.14191500	0.22161600
C	1.25125800	0.64457700	-0.26081300
C	1.00218500	-0.72080000	-0.01264000
Se	2.59591100	-1.69025600	0.35150200
C	0.16407300	1.47506700	-0.54691700
C	-1.12018300	0.96335600	-0.56173500
C	-1.35369300	-0.39711100	-0.31054800
C	-0.27807300	-1.24396700	-0.04889200
C	-2.71625000	-1.00330500	-0.38403600
O	-2.85334400	-2.16957200	-0.70789700
C	-3.91246700	-0.16999300	-0.05565200
C	-3.87751600	0.83849800	0.90917500
C	-5.03215400	1.54029400	1.23043000
C	-6.22485900	1.25399700	0.57735000
C	-6.26693200	0.24925300	-0.38521200
C	-5.12076800	-0.46755900	-0.68980600
H	6.47701300	1.57306100	0.09782200
H	4.98286300	3.46882400	-0.44062800
H	2.55191700	3.12511200	-0.62460800
H	5.54880800	-0.68541600	0.45676800
H	0.32626200	2.52336400	-0.76067600
H	-1.95061800	1.61389900	-0.79511200
H	-0.47092900	-2.29486600	0.11714500
H	-2.95351900	1.05796500	1.42585700
H	-5.00074600	2.30916100	1.99142400
H	-7.12201700	1.80841600	0.82113500
H	-7.19617300	0.02297000	-0.89179300
H	-5.14018400	-1.26685200	-1.41795600

Cartesian coordinates of the optimized geometry structure of **12c-I** at B3LYP-D3BJ/def2-TZVP,aug-cc-pVTZ-PP (E = -1074.976368 au; number of imaginary frequencies = 0):

C	-5.44213400	0.38342500	0.37257700
C	-5.00176800	1.69862000	0.52621300
C	-3.65455900	1.99976800	0.43518000
C	-2.71164600	0.99379600	0.18794700
C	-3.17787000	-0.32710700	0.03632400
C	-4.53094100	-0.63255800	0.12732100
C	-1.27248400	1.20530600	0.07399400
C	-0.47679400	0.06947900	-0.16993700
Te	-1.61867400	-1.68809400	-0.32736900
C	-0.62682000	2.44580900	0.18130100
C	0.74258800	2.54363900	0.05222500
C	1.52576800	1.40136200	-0.16505100
C	0.90313000	0.16034900	-0.28055200
C	2.99796900	1.57067100	-0.33961200
O	3.44874400	2.61616600	-0.77252400
C	3.91646100	0.44713200	0.01883000
C	3.64934700	-0.42865500	1.07302200
C	4.56416400	-1.41767000	1.41070400
C	5.74290100	-1.55155100	0.68707200
C	6.01631300	-0.68081800	-0.36406500
C	5.11483500	0.32084300	-0.68721900
H	-6.49707700	0.15277600	0.44460500
H	-5.71667600	2.48780800	0.71763800

H	-3.32863600	3.02404400	0.55713800
H	-4.87656200	-1.65115400	0.00879000
H	-1.20744400	3.34029200	0.36277900
H	1.23751800	3.50252800	0.11545800
H	1.49639000	-0.72130100	-0.47758600
H	2.73791100	-0.32163400	1.64471100
H	4.35718200	-2.08206400	2.23954400
H	6.45069900	-2.32901800	0.94446800
H	6.93582300	-0.78180900	-0.92587000
H	5.32121900	1.02006500	-1.48595800

Cartesian coordinates of the optimized geometry structure of **12c-II** at B3LYP-D3BJ/def2-TZVP,aug-cc-pVTZ-PP (E = -1074.976174 au; number of imaginary frequencies = 0):

C	5.33024300	-0.06268700	0.24218500
C	5.13719900	1.31430600	0.12685600
C	3.85946100	1.83111700	-0.00173100
C	2.74728100	0.98148500	-0.01682600
C	2.95555300	-0.40576600	0.10211500
C	4.24135300	-0.92184800	0.22892700
C	1.35775000	1.42112600	-0.14694200
C	0.37089900	0.41795900	-0.11576500
Te	1.14770100	-1.50891500	0.03311300
C	0.94242900	2.74462800	-0.30845700
C	-0.40357200	3.05850400	-0.44390700
C	-1.36716000	2.06110500	-0.38746600
C	-0.99249500	0.72600200	-0.19975200
H	6.33119800	-0.46241100	0.34309000
H	5.98871600	1.98195500	0.13807000
H	3.72631300	2.90163400	-0.08905800
H	4.39859300	-1.98955200	0.31880200
H	1.67678700	3.53852600	-0.34407800
H	-0.70306100	4.08694800	-0.59502800
H	-2.40933600	2.31508300	-0.51045600
C	-1.96442600	-0.38409200	-0.13174100
O	-1.57060100	-1.54705700	-0.18597200
C	-3.42477300	-0.12432000	0.00827800
C	-4.31191300	-0.91417700	-0.72578800
C	-3.92966600	0.81865000	0.90551200
C	-5.68040700	-0.73811000	-0.59249500
H	-3.91288700	-1.66179100	-1.39765800
C	-5.30126600	0.97500500	1.05625900
H	-3.25112500	1.40729000	1.50717000
C	-6.17786400	0.20657000	0.29983800
H	-6.36109200	-1.34254300	-1.17769300
H	-5.68496600	1.69523000	1.76702400
H	-7.24652100	0.33694500	0.41112300

Cartesian coordinates of the optimized geometry structure of **12a·12a** at B3LYP-D3BJ/def2-TZVP (C_i symmetry restriction; E = -2410.208827 au; number of imaginary frequencies = 1):

S	0.44880300	0.97994500	-3.85817400
O	-0.75496800	-1.82832500	0.66786400
C	0.21351400	0.43946500	-5.50595000
C	0.36006900	1.21699900	-6.65201200
H	0.64501100	2.25830300	-6.57946100
C	0.13391800	0.63135600	-7.88679500
H	0.24451000	1.22361000	-8.78582000
C	-0.23547200	-0.71492800	-7.98513600
H	-0.40765700	-1.15310900	-8.95923400
C	-0.38181600	-1.48695800	-6.84655400
H	-0.66809000	-2.52782300	-6.92725200
C	-0.15900900	-0.91854900	-5.58922100

C	0.04948600	-0.61520400	-3.24934200
C	-0.25421600	-1.52870600	-4.28245900
C	-0.59706700	-2.84019100	-3.94200500
H	-0.84996700	-3.55291900	-4.71627400
C	-0.61821100	-3.22553400	-2.61509900
H	-0.89770500	-4.23703100	-2.35699000
C	-0.31775300	-2.30568100	-1.59519700
C	0.00931600	-0.99018800	-1.91587200
H	0.23741600	-0.27722300	-1.13848300
C	-0.41061100	-2.66438800	-0.15302900
C	-0.07823900	-4.04787300	0.29666200
C	-0.67000800	-4.52083000	1.47077200
H	-1.37095300	-3.88160700	1.98966300
C	-0.35689200	-5.78059700	1.95439600
H	-0.82953100	-6.14603400	2.85688600
C	0.57105200	-6.57308000	1.28399900
H	0.82149500	-7.55443500	1.66613600
C	1.18150300	-6.10118400	0.12834800
H	1.91581900	-6.70850800	-0.38462100
C	0.85297600	-4.84691400	-0.36938700
H	1.33828900	-4.47743100	-1.26176000
S	-0.44880300	-0.97994500	3.85817400
O	0.75496800	1.82832500	-0.66786400
C	-0.21351400	-0.43946500	5.50595000
C	-0.36006900	-1.21699900	6.65201200
H	-0.64501100	-2.25830300	6.57946100
C	-0.13391800	-0.63135600	7.88679500
H	-0.24451000	-1.22361000	8.78582000
C	0.23547200	0.71492800	7.98513600
H	0.40765700	1.15310900	8.95923400
C	0.38181600	1.48695800	6.84655400
H	0.66809000	2.52782300	6.92725200
C	0.15900900	0.91854900	5.58922100
C	-0.04948600	0.61520400	3.24934200
C	0.25421600	1.52870600	4.28245900
C	0.59706700	2.84019100	3.94200500
H	0.84996700	3.55291900	4.71627400
C	0.61821100	3.22553400	2.61509900
H	0.89770500	4.23703100	2.35699000
C	0.31775300	2.30568100	1.59519700
C	-0.00931600	0.99018800	1.91587200
H	-0.23741600	0.27722300	1.13848300
C	0.41061100	2.66438800	0.15302900
C	0.07823900	4.04787300	-0.29666200
C	0.67000800	4.52083000	-1.47077200
H	1.37095300	3.88160700	-1.98966300
C	0.35689200	5.78059700	-1.95439600
H	0.82953100	6.14603400	-2.85688600
C	-0.57105200	6.57308000	-1.28399900
H	-0.82149500	7.55443500	-1.66613600
C	-1.18150300	6.10118400	-0.12834800
H	-1.91581900	6.70850800	0.38462100
C	-0.85297600	4.84691400	0.36938700
H	-1.33828900	4.47743100	1.26176000

Cartesian coordinates of the optimized geometry structure of **12a·12a** at B3LYP-D3BJ/def2-TZVP (no symmetry restriction; E = -2410.220047 au; number of imaginary frequencies = 0):

S	-3.42382700	-0.87624500	0.93670300
O	1.67248600	-0.72084100	2.85528000
C	-4.11272400	-2.04531900	-0.16751400
C	-5.44067800	-2.09849500	-0.58175000
H	-6.16101300	-1.37653700	-0.22061100
C	-5.82038500	-3.09477500	-1.46651500
H	-6.84911700	-3.14956300	-1.79790100
C	-4.89052100	-4.02952000	-1.93508300

H	-5.20775800	-4.80037500	-2.62476600
C	-3.57080800	-3.97497500	-1.52267200
H	-2.85528200	-4.70028200	-1.88834800
C	-3.16296800	-2.97907200	-0.63098400
C	-1.84250000	-1.61822900	0.79090300
C	-1.85027100	-2.73042600	-0.07795700
C	-0.65635300	-3.42358900	-0.29011500
H	-0.64237300	-4.30009100	-0.92491800
C	0.50834400	-2.98655000	0.31084100
H	1.42547800	-3.53325700	0.14989500
C	0.51021600	-1.85847600	1.14994200
C	-0.68276500	-1.19088800	1.41681900
H	-0.68431000	-0.34755500	2.09165300
C	1.74627500	-1.35051200	1.81442000
C	3.08099700	-1.60440300	1.19073500
C	4.19724700	-1.64501300	2.02961200
H	4.04751900	-1.51662600	3.09265100
C	5.46427400	-1.83754300	1.50380800
H	6.32185800	-1.87905700	2.16296400
C	5.63423000	-1.97248700	0.12864500
H	6.62506500	-2.11121400	-0.28449200
C	4.53401000	-1.90900900	-0.71502200
H	4.66599500	-1.97289300	-1.78614300
C	3.26317400	-1.72779500	-0.18769400
H	2.41640800	-1.64550400	-0.85247400
S	3.38054900	1.99622700	1.00984700
O	-1.95170200	1.83385100	2.30852100
C	4.08069500	1.57357700	-0.53472500
C	5.43918100	1.48830400	-0.82209600
H	6.17820000	1.69269900	-0.05937200
C	5.82485600	1.12419600	-2.10105600
H	6.87788900	1.05189900	-2.33973000
C	4.87058600	0.84413000	-3.08539300
H	5.19323800	0.56099300	-4.07858800
C	3.51965900	0.92940600	-2.79835800
H	2.78505400	0.71252900	-3.56337200
C	3.10544600	1.29700800	-1.51563900
C	1.76485900	1.83493000	0.35973300
C	1.76406100	1.44651200	-0.99760400
C	0.53889400	1.26949900	-1.64679600
H	0.51339600	0.93930500	-2.67716600
C	-0.64071300	1.52617300	-0.97497400
H	-1.58726300	1.38391900	-1.47655800
C	-0.62622400	1.93367300	0.36898900
C	0.58205000	2.05856100	1.04773600
H	0.57809000	2.32480900	2.09532800
C	-1.88253600	2.17109200	1.13824400
C	-3.04156000	2.83179600	0.47131200
C	-4.31506900	2.64012400	1.01383600
H	-4.41534500	2.00111400	1.87955400
C	-5.41770600	3.25788000	0.44833800
H	-6.40233800	3.09551100	0.86741800
C	-5.25928500	4.09228000	-0.65547500
H	-6.12080000	4.57886500	-1.09464000
C	-3.99411200	4.30679900	-1.18761900
H	-3.86607800	4.96802400	-2.03469900
C	-2.88936500	3.67530000	-0.63066400
H	-1.90541300	3.85453200	-1.04012900

Cartesian coordinates of the optimized geometry structure of **12b·12b** at B3LYP-D3BJ/def2-TZVP (C_i symmetry restriction; E = -6416.935857 au; number of imaginary frequencies = 1):

Se	0.40932000	0.96546600	-3.86440300
O	-0.70701200	-1.83140200	0.81578700
C	0.13386300	0.18107000	-5.57349800
C	0.22822500	0.83406600	-6.79809400

H	0.47967100	1.88561100	-6.84477700
C	-0.00451400	0.11800400	-7.96185900
H	0.06693400	0.61648000	-8.91991700
C	-0.33013700	-1.24026400	-7.90753100
H	-0.50933400	-1.78696600	-8.82383700
C	-0.42468100	-1.88830100	-6.68883500
H	-0.67761300	-2.94018400	-6.65458300
C	-0.19414000	-1.18684600	-5.50067100
C	0.03074400	-0.75523200	-3.14778900
C	-0.25320600	-1.70768600	-4.14831400
C	-0.56009100	-3.01437900	-3.75402600
H	-0.79812900	-3.76140300	-4.49993000
C	-0.56887000	-3.35664200	-2.41508500
H	-0.82451700	-4.36530500	-2.12342900
C	-0.28761700	-2.39611800	-1.42991200
C	0.00736500	-1.08617200	-1.80483200
H	0.22424200	-0.34278400	-1.05400900
C	-0.37059100	-2.69963600	0.02394900
C	-0.04268400	-4.06602900	0.52396000
C	-0.65422100	-4.50459600	1.70118100
H	-1.37029800	-3.85522100	2.18559400
C	-0.34447100	-5.74684400	2.23031100
H	-0.83272300	-6.08618400	3.13464200
C	0.59985200	-6.55491800	1.60296200
H	0.84798300	-7.52216500	2.02083200
C	1.22898200	-6.11701600	0.44389500
H	1.97543000	-6.73650400	-0.03591000
C	0.90344900	-4.88129700	-0.09994700
H	1.40247700	-4.53782100	-0.99520800
Se	-0.40932000	-0.96546600	3.86440300
O	0.70701200	1.83140200	-0.81578700
C	-0.13386300	-0.18107000	5.57349800
C	-0.22822500	-0.83406600	6.79809400
H	-0.47967100	-1.88561100	6.84477700
C	0.00451400	-0.11800400	7.96185900
H	-0.06693400	-0.61648000	8.91991700
C	0.33013700	1.24026400	7.90753100
H	0.50933400	1.78696600	8.82383700
C	0.42468100	1.88830100	6.68883500
H	0.67761300	2.94018400	6.65458300
C	0.19414000	1.18684600	5.50067100
C	-0.03074400	0.75523200	3.14778900
C	0.25320600	1.70768600	4.14831400
C	0.56009100	3.01437900	3.75402600
H	0.79812900	3.76140300	4.49993000
C	0.56887000	3.35664200	2.41508500
H	0.82451700	4.36530500	2.12342900
C	0.28761700	2.39611800	1.42991200
C	-0.00736500	1.08617200	1.80483200
H	-0.22424200	0.34278400	1.05400900
C	0.37059100	2.69963600	-0.02394900
C	0.04268400	4.06602900	-0.52396000
C	0.65422100	4.50459600	-1.70118100
H	1.37029800	3.85522100	-2.18559400
C	0.34447100	5.74684400	-2.23031100
H	0.83272300	6.08618400	-3.13464200
C	-0.59985200	6.55491800	-1.60296200
H	-0.84798300	7.52216500	-2.02083200
C	-1.22898200	6.11701600	-0.44389500
H	-1.97543000	6.73650400	0.03591000
C	-0.90344900	4.88129700	0.09994700
H	-1.40247700	4.53782100	0.99520800

Cartesian coordinates of the optimized geometry structure of **12b·12b** at B3LYP-D3BJ/def2-TZVP (no symmetry restriction; E = -6416.945157 au; number of imaginary frequencies = 0):

Se	3.62874200	-0.58697400	-0.84750800
O	-1.58849300	-0.78666800	-2.79206100
C	4.34265400	-1.93999400	0.27752900
C	5.65134800	-2.01305400	0.74109300
H	6.37757700	-1.25915900	0.46711200
C	6.01344300	-3.07002600	1.56197100
H	7.02930800	-3.13849300	1.92886600
C	5.07818100	-4.04573700	1.91733200
H	5.37461500	-4.86583700	2.55777400
C	3.77628400	-3.96962700	1.45433400
H	3.05806800	-4.72953200	1.73395200
C	3.38617700	-2.91310000	0.62488000
C	1.97846800	-1.52526200	-0.74403000
C	2.07071900	-2.68029200	0.05832000
C	0.92552600	-3.46464100	0.22323600
H	0.97181500	-4.37405900	0.80796900
C	-0.26856200	-3.08222400	-0.35706400
H	-1.14343700	-3.70216600	-0.22868700
C	-0.35088100	-1.91529100	-1.13357800
C	0.79342500	-1.14983500	-1.35135800
H	0.73454400	-0.27286500	-1.97927700
C	-1.61746400	-1.46995500	-1.78317900
C	-2.92995600	-1.85560500	-1.18124700
C	-4.03495900	-1.96232200	-2.02874900
H	-3.89167800	-1.79142400	-3.08670200
C	-5.28487200	-2.26953000	-1.51672100
H	-6.13351300	-2.36134100	-2.18234400
C	-5.45003100	-2.45286500	-0.14646800
H	-6.42884800	-2.67971900	0.25627200
C	-4.36195400	-2.32653900	0.70601100
H	-4.49336300	-2.42826100	1.77433600
C	-3.10685200	-2.03336500	0.19173400
H	-2.27127500	-1.90414800	0.86337500
Se	-3.65395800	1.74190800	-0.91948400
O	1.83997300	1.98006900	-2.12699500
C	-4.24634600	1.15429000	0.78293700
C	-5.56572000	0.92892600	1.15563300
H	-6.37325200	1.09573300	0.45561800
C	-5.83081000	0.47319400	2.43689200
H	-6.85415400	0.29222400	2.73900000
C	-4.78816100	0.24140300	3.33840800
H	-5.00951100	-0.11562500	4.33554600
C	-3.47535700	0.46929700	2.96450700
H	-2.67357100	0.28878200	3.66892100
C	-3.18206900	0.93191700	1.67790200
C	-1.89579200	1.66239800	-0.21295000
C	-1.87191800	1.21847900	1.12446200
C	-0.63418900	1.11144500	1.76786200
H	-0.58291300	0.74249100	2.78387800
C	0.52494400	1.48778800	1.11695000
H	1.47774900	1.40095200	1.61975100
C	0.48223600	1.94506700	-0.20832300
C	-0.73284800	2.00063900	-0.88495600
H	-0.74716400	2.30755300	-1.92134300
C	1.71692700	2.31437200	-0.95962500
C	2.78258900	3.10515700	-0.27992900
C	4.06514200	3.10478800	-0.83561800
H	4.24205100	2.51466300	-1.72360300
C	5.08015900	3.84679700	-0.25633300
H	6.07322800	3.83271600	-0.68645800
C	4.82232700	4.61470600	0.87675100
H	5.61516300	5.19786600	1.32749300
C	3.54543100	4.63907600	1.42320500
H	3.33859900	5.24797800	2.29358600
C	2.52956200	3.88448600	0.85054600
H	1.53465100	3.91692700	1.27090600

Cartesian coordinates of the optimized geometry structure of **12c·12c** at B3LYP-D3BJ/def2-TZVP,aug-cc-pVTZ-PP (C_i symmetry restriction; E = -2149.974898 au; number of imaginary frequencies = 1):

Te	0.38937300	1.18964200	-3.84094600
O	-0.72825900	-1.83901400	0.87083200
C	0.05314700	0.17384900	-5.65589300
C	0.10816000	0.72617400	-6.93228800
H	0.34042700	1.77496700	-7.06749100
C	-0.13591800	-0.07297200	-8.03839600
H	-0.09309300	0.35525700	-9.03169500
C	-0.43597900	-1.42652300	-7.87426300
H	-0.62544200	-2.04662900	-8.74052600
C	-0.49241800	-1.97833700	-6.60717800
H	-0.72615300	-3.02883100	-6.49463400
C	-0.25008600	-1.19095900	-5.47398300
C	-0.01127600	-0.73119800	-3.08363500
C	-0.28863500	-1.67279100	-4.09821900
C	-0.58709200	-2.98592800	-3.71020100
H	-0.81895200	-3.72911500	-4.46119600
C	-0.60212700	-3.34788500	-2.37699300
H	-0.85621700	-4.36169300	-2.10223600
C	-0.33189900	-2.39886000	-1.37926000
C	-0.03925400	-1.08564500	-1.74738700
H	0.17401400	-0.35165000	-0.98753500
C	-0.42598400	-2.71311000	0.06741800
C	-0.15738200	-4.09565300	0.55394500
C	-0.83983200	-4.54811900	1.68587300
H	-1.57486900	-3.90070900	2.14397600
C	-0.58172500	-5.80764900	2.20217300
H	-1.12538600	-6.15772000	3.06999800
C	0.38068900	-6.61919100	1.60815300
H	0.58909600	-7.59957900	2.01684200
C	1.07765500	-6.16895800	0.49329600
H	1.83674600	-6.79248300	0.03935400
C	0.80338500	-4.91632100	-0.03962900
H	1.35295000	-4.56330400	-0.90108300
Te	-0.38937300	-1.18964200	3.84094600
O	0.72825900	1.83901400	-0.87083200
C	-0.05314700	-0.17384900	5.65589300
C	-0.10816000	-0.72617400	6.93228800
H	-0.34042700	-1.77496700	7.06749100
C	0.13591800	0.07297200	8.03839600
H	0.09309300	-0.35525700	9.03169500
C	0.43597900	1.42652300	7.87426300
H	0.62544200	2.04662900	8.74052600
C	0.49241800	1.97833700	6.60717800
H	0.72615300	3.02883100	6.49463400
C	0.25008600	1.19095900	5.47398300
C	0.01127600	0.73119800	3.08363500
C	0.28863500	1.67279100	4.09821900
C	0.58709200	2.98592800	3.71020100
H	0.81895200	3.72911500	4.46119600
C	0.60212700	3.34788500	2.37699300
H	0.85621700	4.36169300	2.10223600
C	0.33189900	2.39886000	1.37926000
C	0.03925400	1.08564500	1.74738700
H	-0.17401400	0.35165000	0.98753500
C	0.42598400	2.71311000	-0.06741800
C	0.15738200	4.09565300	-0.55394500
C	0.83983200	4.54811900	-1.68587300
H	1.57486900	3.90070900	-2.14397600
C	0.58172500	5.80764900	-2.20217300
H	1.12538600	6.15772000	-3.06999800
C	-0.38068900	6.61919100	-1.60815300
H	-0.58909600	7.59957900	-2.01684200
C	-1.07765500	6.16895800	-0.49329600
H	-1.83674600	6.79248300	-0.03935400

C	-0.80338500	4.91632100	0.03962900
H	-1.35295000	4.56330400	0.90108300

Cartesian coordinates of the optimized geometry structure of **12c·12c** at B3LYP-D3BJ/def2-TZVP,aug-cc-pVTZ-PP (no symmetry restriction; E = -2149.975165 au; number of imaginary frequencies = 0):

Te	-4.03265100	0.66041300	-0.07109500
O	0.95655500	-1.57892300	1.58325000
C	-5.55180900	-0.72781900	-0.51459700
C	-6.87362500	-0.43071900	-0.83320300
H	-7.21153900	0.59698600	-0.87408300
C	-7.76366100	-1.45939800	-1.10016700
H	-8.79204800	-1.23007300	-1.34841000
C	-7.33735000	-2.78784700	-1.04959800
H	-8.03574800	-3.58741400	-1.25871200
C	-6.02450100	-3.08613400	-0.73257000
H	-5.70767900	-4.12011100	-0.69684500
C	-5.10599200	-2.06430300	-0.45857200
C	-2.92840600	-1.11731200	0.12688000
C	-3.70449000	-2.27143200	-0.11390100
C	-3.07599300	-3.51884700	0.00145700
H	-3.64480400	-4.42489000	-0.15852000
C	-1.73622200	-3.61207000	0.32394200
H	-1.27816700	-4.58575500	0.42214600
C	-0.97731800	-2.45465800	0.55847900
C	-1.59142400	-1.20531200	0.46705700
H	-1.01870200	-0.31105500	0.65124700
C	0.44898900	-2.50261700	0.95737600
C	1.28991700	-3.67708600	0.58790700
C	2.28988600	-4.08432300	1.47375300
H	2.38553400	-3.57269200	2.42176500
C	3.14220600	-5.12386400	1.13754700
H	3.90503200	-5.44418800	1.83524500
C	3.02240800	-5.74848500	-0.10053400
H	3.69518600	-6.55298900	-0.36842100
C	2.04203500	-5.33603000	-0.99499200
H	1.95793400	-5.80949400	-1.96443100
C	1.17005600	-4.31230500	-0.64870000
H	0.41540300	-3.98441500	-1.34999800
Te	3.75606700	-0.75579300	0.57241900
O	-1.28818800	1.95804200	0.49337000
C	5.31122700	0.21564800	-0.46301600
C	6.58566400	-0.29105000	-0.70024500
H	6.86427100	-1.27088800	-0.33361500
C	7.50447800	0.46578700	-1.41052000
H	8.49672400	0.07409300	-1.59459500
C	7.15364900	1.73020300	-1.88743900
H	7.87423700	2.31757500	-2.44113500
C	5.88732000	2.23551100	-1.65460100
H	5.62938500	3.21710700	-2.02976000
C	4.94130400	1.48979200	-0.93901200
C	2.77263600	1.04327700	0.10322900
C	3.58307200	1.92869300	-0.64114400
C	3.02504100	3.14930700	-1.04183000
H	3.61165800	3.84251500	-1.62954000
C	1.72660200	3.48050500	-0.70727500
H	1.31112800	4.41767300	-1.04849200
C	0.93357700	2.59397800	0.03729000
C	1.46992600	1.36932100	0.43758800
H	0.86538500	0.68457500	1.01244200
C	-0.49181600	2.87509800	0.34150300
C	-0.96526000	4.28510300	0.45235900
C	-2.27090300	4.58295300	0.05591500
H	-2.88376300	3.79268600	-0.35513200
C	-2.76425400	5.87166500	0.18146600
H	-3.77138500	6.09862000	-0.14324600

C	-1.96738600	6.87135400	0.73215600
H	-2.35600100	7.87590000	0.83939900
C	-0.67466500	6.57826500	1.14964600
H	-0.05890700	7.35023100	1.59240300
C	-0.17008700	5.29310600	1.00070500
H	0.83329400	5.06508600	1.33246100

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