Homo and Hetero-Halogen Interaction Based Molecular Associations in Wheel-Axle Topology Derived Sn(IV)-Porphyrin Complexes: An Experimental and Theoretical Analysis.

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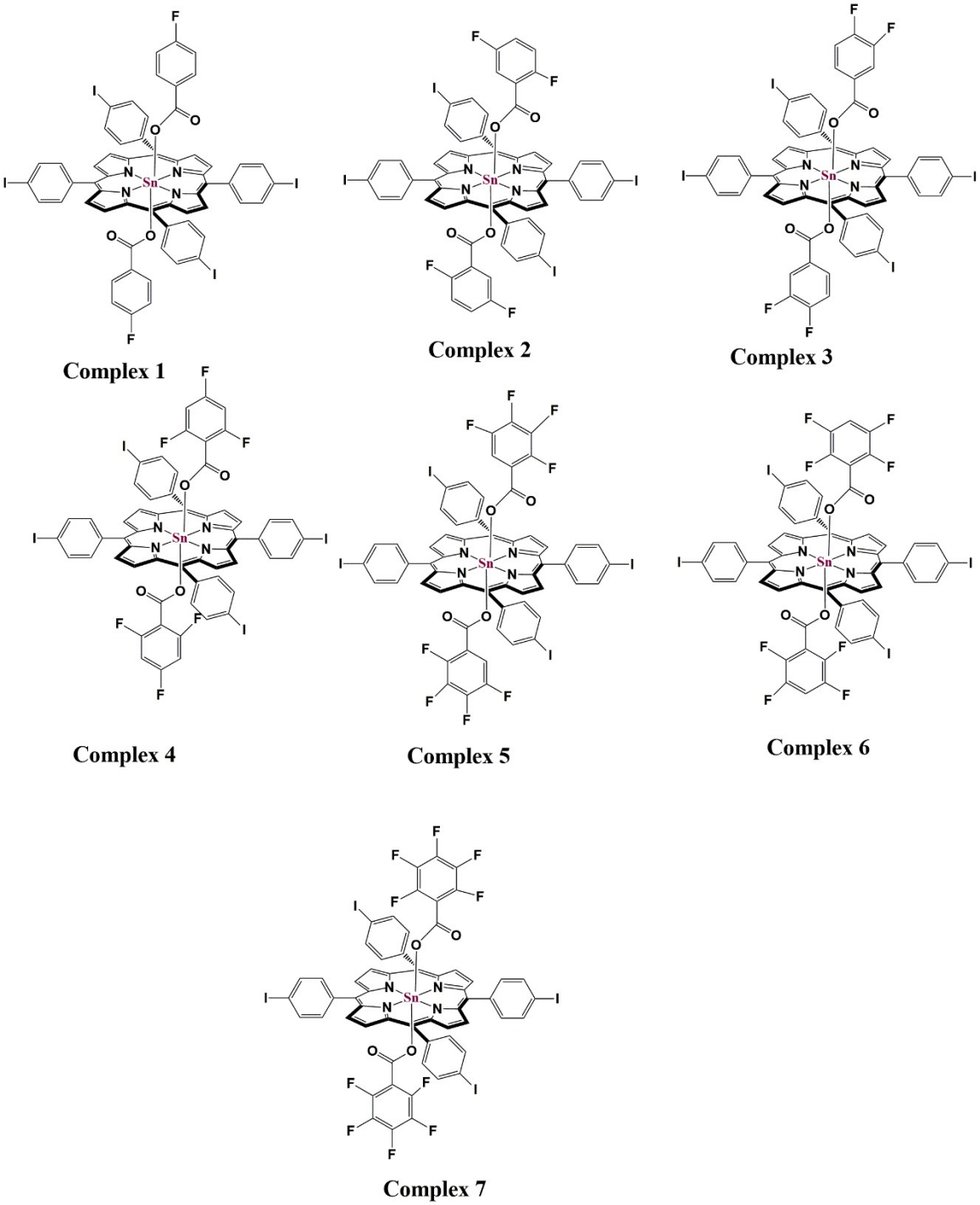
EXPERIMENTAL SECTION

Materials: Pyrrole, 4-iodobenzaldehyde, 4-flouorobenzoic acid, 2,5- diflouorobenzoic acid, 3,4-difluorobenzoic acid, 2,4,6-trifluorobenzoic acid, 2,3,4,5-tetrafluorobenzoic acid, 2,3,4,6-tetrafluorobenzoic acid, 2,3,4,5,6-pentafluorobenzoic acid were obtained from TCI chemicals. Solvents like propionic acid, chloroform ($CHCl_3$), dichloromethane (CH_2Cl_2), methanol, acetone, dimethylformamide (DMF), and hexane were obtained commercial sources and purified by standard procedures before use. Free-base porphyrins were prepared following the Adler method.[1] $Sn(TIPP)(OH)_2$ were prepared by literature methods.[2]

Physical Measurements.

UV-vis spectra were recorded on a Perkin Elmer UV-Vis spectrometer. IR spectra were recorded on a Bruker Tensor 27 system spectrophotometer in ATR mode. Time-resolved fluorescence decays were collected with a commercial time-correlated single-photon counting (TCSPC) setup (Life Spec II, Edinburgh Instruments). The steady state fluorescence spectra of all the samples were recorded using Perkin Elmer LS 55 fluorescence spectrometer. The samples were prepared in dry dichloromethane and the concentration was adjusted so that the absorbance was less than 0.1. Absorption correction was done to normalize the data. Powder X-ray Diffraction (PXRD) was measured by a XEUSS SAXS/WAXS system by Xenocs, operated at 50 kV and 0.60 mA. The X-ray radiation was collimated with FOX2D mirror and two pairs of scatter-less slits from Xenocs.

The data were collected in the transmission mode geometry using Cu Kα radiation (wavelength λ = 1.54 Å).



Scheme S1: Schematic illustration of the Sn(IV)-5,10,15,20-*meso*-tetrakis(4-iodophenyl)porphyrin scaffolds used in this study. Axial ligands (L) 4-fluoro benzoic acid (**1**), 2,5-difluoro benzoic acid (**2**), 3,4-

difluoro benzoic acid (**3**), 2,4,6-trifluoro benzoic acid (**4)**, 2,3,4,5-tetrafluoro benzoic acid (**5**), 2,3,5,6-tetrafluoro benzoic acid (**6**), 2,3,4,5,6-pentafluoro benzoic acid (**7**).

Synthesis of Complex-1

Trans-dihydroxo[5,10,15,20-tetrakis(4-iodophenyl)porphyrinato]tin(IV) (0.01 mmol, 12.8 mg) was dissolved in 5 ml of $CHCl_3$ in a vial. 3.5 mg of 4-fluorobenzoic acid (0.025 mmol) dissolved in 0.5 ml DMF and added to the vial. The resulting solution was heated for 1 h at 70 °C in bath reactor. After cooling, the mixture was left for slow evaporation at ambient conditions, dark red solid was precipitated out. Filtered the solid and washed with hexane. Yield (11.6 mg, 76%). X-ray quality crystals were obtained by slow diffusion of CH_2Cl_2 solution of **1** into the cyclohexane. After 7 days, pink crystals of the complex were obtained. FT-IR (KBr, cm^{-1}) 1720, 1448, 1227, 1038, 765, 751, 668, 565, 442. UV-Vis in DCM: λmax/nm (log e) 428(5.48), 552(2.98), 592(2.15).

Synthesis of Complex-2

Trans-dihydroxo[5,10,15,20-tetrakis(4-iodophenyl)porphyrinato]tin(IV) (0.01 mmol, 12.8 mg) was dissolved in 5 ml of $CHCl_3$ in a vial. 3.9 mg of 2,5-difluorobenzoic acid (0.025 mmol) dissolved in 0.5 ml DMF and added to the vial. The resulting solution was heated for 1 h at 70 °C in bath reactor. After cooling, the mixture was left for slow evaporation at ambient conditions, dark red solid was precipitated out. Yield (11.6 mg, 74%). X-ray quality crystals were obtained slow evaporation of $CHCl_3$ solution of compound **2**. After 7 days, pink crystals of complex were obtained. FT-IR (KBr, cm^{-1}) 1727, 1452, 1257, 1041, 775, 768, 662, 545, 436. UV-Vis in DCM: λmax/nm (log e) 427(5.46), 552(2.92), 592(2.12).

Synthesis of Complex-3

Trans-dihydroxo[5,10,15,20-tetrakis(4-iodophenyl)porphyrinato]tin(IV) (0.01 mmol, 12.8 mg) was dissolved in 5 ml of $CHCl_3$ in a vial. 3.9 mg of 3,4-difluorobenzoic acid (0.025 mmol) dissolved in 0.5 ml DMF and added to the vial. The resulting solution was heated for 1 h at 70 °C in bath reactor. After cooling, the mixture was left for slow evaporation at ambient conditions, dark red solid was precipitated out. Yield (11.6 mg, 74%). X-ray quality crystals were obtained slow diffusion of $CHCl_3$ solution of compound **3** into the cyclohexane. After 10 days, pink crystals of complex were obtained. FT-IR (KBr, cm^{-1}) 1732, 1432, 1242, 1025, 782, 758, 654, 536, 428. UV-Vis in DCM: λmax/nm (log e) 427(5.38), 554(2.98), 594(2.16).

Synthesis of Complex-4

Trans-dihydroxo[5,10,15,20-tetrakis(4-iodophenyl)porphyrinato]tin(IV) (0.01 mmol, 12.8 mg) was dissolved in 5 ml of $CHCl_3$ in a vial. 4.4 mg of 2,4,6-trifluorobenzoic acid (0.025 mmol) dissolved in 0.5 ml DMF and added to the vial. The resulting solution was heated for 1 h at 70 °C in bath reactor. After cooling, the mixture was left for slow evaporation at ambient conditions, dark red solid was precipitated out Yield (12 mg, 75%). X-ray quality crystals were obtained slow diffusion of CH_2Cl_2 solution of compound **4** into the cyclohexane. After 8-9 days, pink crystals of complex were obtained. FT-IR (KBr, cm^{-1}) 1727, 1428, 1198, 1040, 778, 752, 654, 569, 436. UV-Vis in DCM: λmax/nm (log e) 426(5.36), 554(2.68), 584(2.22).

Synthesis of Complex-5

Trans-dihydroxo[5,10,15,20-tetrakis(4-iodophenyl)porphyrinato]tin(IV) (0.01 mmol, 12.8 mg) was dissolved in 5 ml of $CHCl_3$ in a vial. 4.8 mg of 2,3,4,5-tetrafluorobenzoic acid (0.025 mmol) dissolved in 0.5 ml DMF and added to the vial. The resulting solution was heated for 1 h at 70 °C in bath reactor. After cooling, the mixture was left for slow evaporation at ambient conditions, dark red solid was precipitated out Yield (12.7 mg, 78%). X-ray quality crystals were obtained slow evaporation of $CHCl_3$ solution of compound **5**. After 7-8 days, pink crystals of complex were obtained. FT-IR (KBr, cm^{-1}) 1738, 1434, 1212, 1042, 781, 756, 648, 584, 448. UV-Vis in DCM: λmax/nm (log e) 425(5.38), 553(2.78), 598(2.24).

Synthesis of Complex-6

Trans-dihydroxo[5,10,15,20-tetrakis(4-iodophenyl)porphyrinato]tin(IV) (0.01 mmol, 12.8 mg) was dissolved in 5 ml of $CHCl_3$ in a vial. 4.8 mg of 2,3,5,6-tetrafluorobenzoic acid (0.025 mmol) dissolved in 0.5 ml DMF and added to the vial. The resulting solution was heated for 1 h at 70 °C in bath reactor. After cooling, the mixture was left for slow evaporation at ambient conditions, dark red solid was precipitated out Yield (11.7 mg, 72%). X-ray quality crystals were obtained slow diffusion of $CHCl_3$ solution of compound **6** into the cyclohexane. After 8-10 days, pink crystals of complex were obtained. FT-IR (KBr, cm^{-1}) 17636, 1435, 1223, 1107, 782, 754, 642, 572, 442. UV-Vis in DCM: λmax/nm (log e) 424(5.38), 555(2.88), 598(2.46).

Synthesis of Complex-7

Trans-dihydroxo[5,10,15,20-tetrakis(4-iodophenyl)porphyrinato]tin(IV) (0.01 mmol, 12.8 mg) was dissolved in 5 ml of $CHCl_3$ in a vial. 5.3 mg of 2,3,4,5,6-pentafluorobenzoic acid (0.025 mmol) dissolved in 0.5 ml DMF and added to the vial. The resulting solution was heated for 1 h at 70 °C in bath reactor. After cooling, the mixture was left for slow evaporation at ambient conditions, dark red solid was precipitated out Yield (12.5 mg, 75%). X-ray quality crystals were obtained slow evaporation of $CHCl_3$ solution of compound **7**. After 10-12 days, pink crystals of complex were obtained. FT-IR (KBr, cm^{-1}) 1742, 1448, 1224, 1048, 796, 764, 684, 576, 458. UV-Vis in DCM: λmax/nm (log e) 424(5.46), 556(2.78), 598(2.25).

X-ray Structure Determination:

Single-crystal X-ray diffraction data for complexes 1–7 were collected with a "SuperNova diffractometer" equipped with a HyPix3000 detector from Rigaku Oxford Diffraction. Data collection and reduction were performed with an inbuilt program suite (CrysAlisPro 1.171.39.33c (Rigaku OD, 2017)), and an absorption correction (multiscan method) was also done. Structures were solved by the direct method using SHELXS-97 and were refined on F^2 using the full-matrix least-squares technique using the SHELXL-2018/3[3] program package on the WINGX platform.[4] All non-hydrogen atoms were refined anisotropically except those of disordered solvent molecules, which were refined isotopically. Hydrogen atoms were fixed at their stereo-chemical positions and were riding with their respective non-hydrogen atoms with SHELXL default parameters. CCDC deposition numbers 2215489 (compound 1), 2215490 (compound 2), 2215488 (compound 3), 2215493 (compound 4), 2215491 (compound 5), 2215492 (compound 6) and 2215487 (compound 7) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif or by emailing data_request@ccdc.cam.ac.uk or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, U.K.; fax: +44 1223 336033.

Table S1. Crystal data and data collection parameters

	Compound 1	Compound 2	Compound 3	Compound 4
CCDC No	2215489	2215490	2215488	2215493
T, K	293(2)	293(2)	293(2)	293(2)

Formula	C64 H44 F2 I4 N4 O4 Sn	C59 H31 Cl3 F4 I4 N4 O4 Sn	C65 H43 Cl3 F4 I4 N4 O4 Sn	C64 H40 F6 I4 N4 O4 Sn
Formula weight	1597.32	1668.52	1752.67	1669.29
Colour and Habit	Dark pink	Dark pink	Dark pink	Dark pink
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	$C2/c$
a, Å	14.2789(3)	12.5134(4)	12.5356(3)	21.2268(7)
b, Å	16.8821(4)	39.2235(8)	40.7661(8)	15.2917(5)
c, Å	12.1517(3)	12.3836(3)	12.4757(3)	18.6929(5)
α, deg	90	90	90	90
β, deg	96.370(2)	103.376(3)	102.912(2)	94.748(3)
γ, deg	90	90	90	90
V, Å^3	2911.18(12)	5913.2(3)	6214.2(2)	6046.8(3)
Radiation (λ, Å)	Mo Kα (0.71073)	Mo Kα (0.71073)	Mo Kα (0.71073)	Mo Kα (0.71073)
Z	2	4	4	4
d_{calcd}, g•cm^{-3}	1.822	1.874	1.73	1.834
μ, mm^{-1}	2.618	2.718	2.591	2.534
F(000)	1536	3176	3368	3200
No. of unique data	5112	9634	10049	5312
No. of params. refined	355	725	760	373
GOF on F^2	1.059	1.070	1.022	1.073
$R1^a$ [$I > 2\sigma(I)$]	0.0450	0.0554	0.0569	0.0542
$R1^a$ (all data)	0.0559	0.0656	0.0682	0.0655
wR2b (all data)	0.1390	0.1791	0.1658	0.1709

	Compound 5	Compound 6	Compound 7
CCDC No	2215491	2215492	2215487
T, K	293(2)	293(2)	293(2)

Formula	C58 H26 F8 I4 N4 O4 Sn	C70 H50 F8 I4 N4 O4 Sn	C58 H24 F10 I4 N4 O4 Sn
Formula weight	1621.12	1789.43	1657.10
Colour and Habit	Dark pink	Dark pink	Dark pink
Crystal system	Monoclinic	Monoclinic	Triclinic

Space group	$P2_1/c$	$C\,c$	$P\text{-}1$
a, Å	10.6659(1)	15.5029(3)	8.1405(2)
b, Å	24.8734(4)	19.5370(4)	12.0603(3)
c, Å	30.8319(4)	22.8054(4)	14.9740(4)
α, deg	90	90	70.718(2)
β, deg	92.536(1)	102.773(2)	85.026(2)
γ, deg	90	90	83.285(2)
V, Å^3	8171.61(19)	6736.4(2)	1376.30(6)
Radiation (λ, Å)	Mo Kα (0.71073)	Mo Kα (0.71073)	Mo Kα (0.71073)
Z	6	4	1
d_{calcd}, g•cm^{-3}	1.977	1.764	1.999
μ, mm^{-1}	2.815	2.285	2.793
F(000)	4608	3456	784
No. of unique data	14364	9459	4835
No. of params. refined	1069	815	367
GOF on F2	1.078	1.045	1.086
$R1^a$ [I> 2σ(I)]	0.0648	0.0349	0.0424
$R1^a$ (all data)	0.0844	0.0400	0.0496
$wR2^b$ (all data)	0.2147	0.1019	0.1057

Table S2. Intermolecular weak interactions (other than halogen bond interactions) in compounds **1**-7

Compound	(X···Y/π)	D(X··· Y) (Å)	Nature of interaction	Interacting partner
1	C28-H28···C21	2.857 (6)	C-H···π	wheel-axle
	C8-H8···C28	2.803(7)	C-H···π	wheel-axle
	C13-H13···C5	2.816(5)	C-H···π	wheel-wheel
	C13···C23	3.275(9)	π···π	wheel-axle
	C25···C25	3.337(9)	π···π	axle-axle
	C30-H30A···F1	2.595(6)	HB	axle-solvent
	C7-H7···O2	2.661(5)	HB	wheel-axle
	C34-H34A···I2	2.926(1)	HB	wheel-solvent
2	C29-H29···C5	3.697(11)	C-H···π	wheel-wheel
	C29-H29···C6	3.538(11)	C-H···π	wheel-wheel
	C56-H56···C12	2.772(7)	C-H···π	wheel-axle
	C56-H56···C13	2.726(7)	C-H···π	wheel-axle
	C25-H25···C9	2.781(7)	C-H···π	wheel-wheel

	C31-H31···C13	2.781(7)	C-H···π	wheel-wheel
	C8-H8···F1	2.496(9)	HB	wheel-axle
	C59-H59A···O4	2.374(8)	HB	axle-solvent
3	C23-H23···C1	2.773(7)	C-H···π	Wheel-wheel
	C23-H23···C20	2.788(7)	C-H···π	Wheel-wheel
	C25-H25···C8	2.764(8)	C-H···π	Wheel-wheel
	C18-H18···F2	2.515(10)	HB	Wheel-axle
	C62-H62B···F3	2.374(12)	HB	Wheel-axle
	C59-H59···O2	2.218(8)	HB	Axle-solvent
	C50-H50···O4	2.648(6)	HB	Axle-axle
	C60-H60B···Cl3	2.917(8)	HB	Solvent-solvent
4	C33-H33A···I2	3.159(6)	HB	Wheel-solvent
	C19-H19···O1	2.565(4)	HB	Axle-wheel
	C34-H34A···F1	2.633(5)	HB	Axle-solvent
5A	C43-H43···C25	2.845(13)	C-H···π	Wheel-wheel
	C37-H37···C1	2.871(7)	C-H···π	Wheel-wheel
	C51-H51···C30	2.861(8)	C-H···π	Wheel-axle
	C7-H7···I4	3.071(1)	HB	Wheel-wheel
	C67-H67···I4	3.003(8)	HB	Wheel-wheel
	C29-H29···O2	2.557(9)	HB	Wheel-axle
5B	C41-H41···C67	2.878 (8)	C-H···π	Wheel-wheel
	C40-H40···F61	2.581(6)	HB	Wheel-axle
	C63-H63···F62	2.516(9)	HB	Wheel-axle
	C26-H26···F63	2.643(7)	HB	Wheel-axle
	C35-H35···F64	2.644(7)	HB	Wheel-axle
6	C35-H35···C7	2.771(8)	C-H···π	Wheel-wheel
	C25-H25···C17	2.848(9)	C-H···π	Wheel-wheel
	C60-H60A··C24	2.841(9)	C-H···π	Wheel-solvent
	C2-H2···F2	2.381(8)	HB	Wheel-axle
	C63-H63A···F1	2.589(6)	HB	Axle-solvent
	C12-H12···F6	2.631(7)	HB	Wheel-axle
7	C22-H22···C5	2.852(5)	C-H···π	Wheel-wheel
	C22-H22···C6	2.776(4)	C-H···π	Wheel-wheel
	C8-H8···C24	2.766(4)	C-H···π	Wheel-wheel
	C7-H7···C29	2.838(5)	C-H···π	Wheel-wheel

Table S3. Homo and hetero-halogen bond interactions in compound **1-7**.

Compound	D(X···Y/π)	θ1(C−X···Y)/ θ2(Y···X−C)	D(X···Y) (Å)	Type of interactions	Nature of Interaction	Interacting partner
1	I1···I2	167.3/105.5	3.817(1)	Type II	XB	Wheel-wheel
2	I2···I4	164.3/108.9	3.831(2)	Type II	XB	Wheel-wheel
	F2···Cl2	168.4/107.9	3.208(14)	Type-II	XB	Axle-solvent
5A	I2···F8	161.5/121.7	3.317(9)	Type II	XB	Wheel-axle
	I4···F4	156.4/152.4	3.421(17)	Type-I	XB	Wheel-axle

5B	I62···F64	154.6/101.4	3.336(11)	Type-II	XB	Wheel-axle
6	I1···F8	143.8/104.4	3.265(6)	Type II	XB	Wheel-axle
	I3···F4	148.8/101.4	3.229(5)	Type-II	XB	Wheel-axle
7	I2···I2	133.9/133.9	3.886(1)	Type I	XB	Wheel-wheel

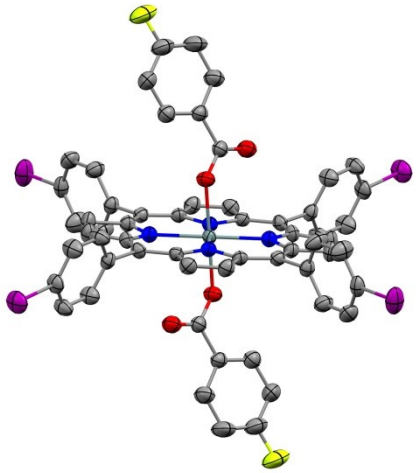


Figure S1. Perspective view of compound **1** showing 40% thermal ellipsoids for all non-hydrogen atoms at 293 K (H-atoms have been omitted for clarity).

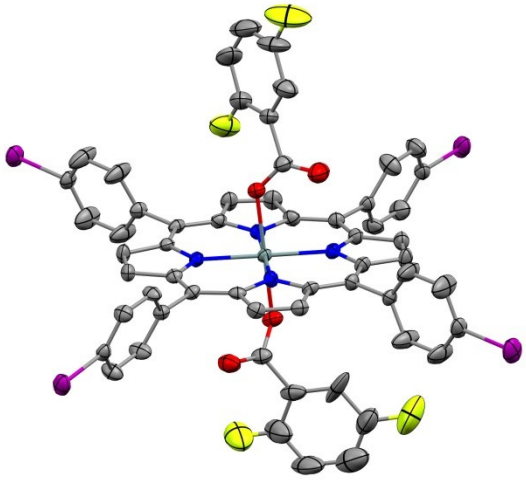


Figure S2. Perspective view of compound **2** showing 40% thermal ellipsoids for all non-hydrogen atoms at 293 K (H-atoms have been omitted for clarity).

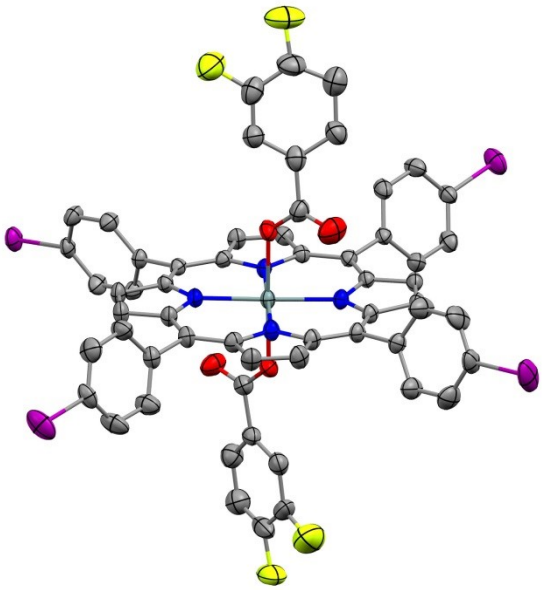


Figure S3. Perspective view of compound **3** showing 40% thermal ellipsoids for all non-hydrogen atoms at 293 K (H-atoms have been omitted for clarity).

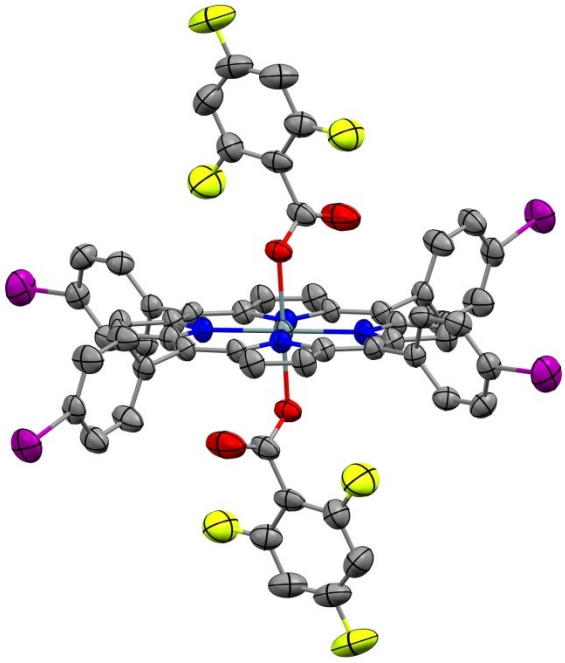


Figure S4. Perspective view of compound **4** showing 40% thermal ellipsoids for all non-hydrogen atoms at 293 K (H-atoms have been omitted for clarity).

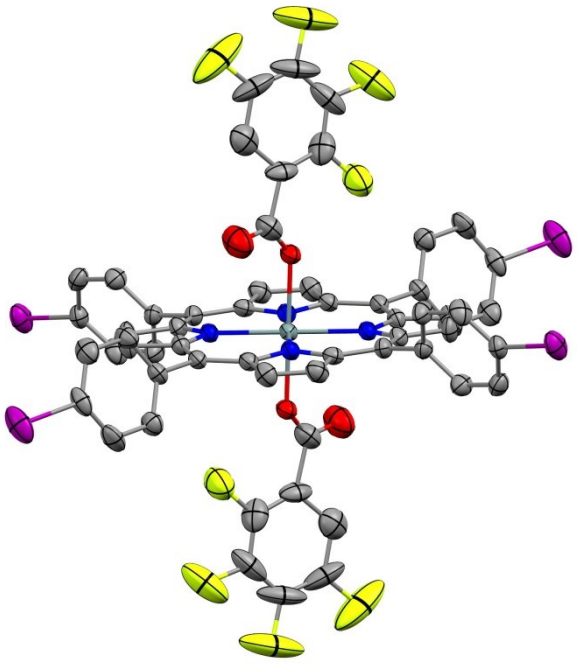


Figure S5. Perspective view of compound **5** showing 40% thermal ellipsoids for all non-hydrogen atoms at 293 K (H-atoms have been omitted for clarity).

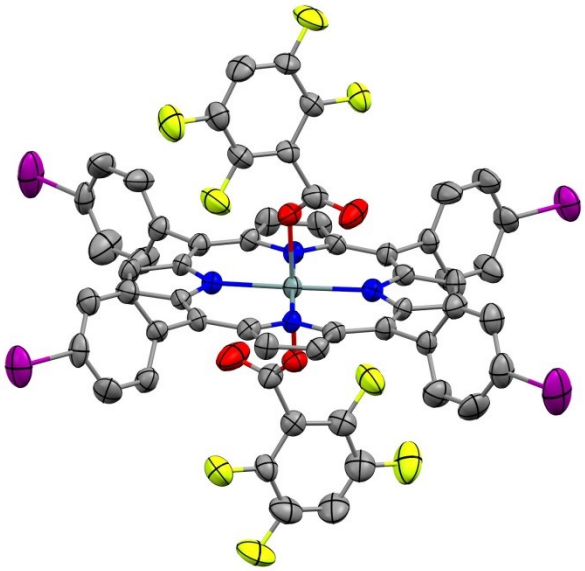


Figure S6. Perspective view of compound **6** showing 40% thermal ellipsoids for all non-hydrogen atoms at 293 K (H-atoms have been omitted for clarity).

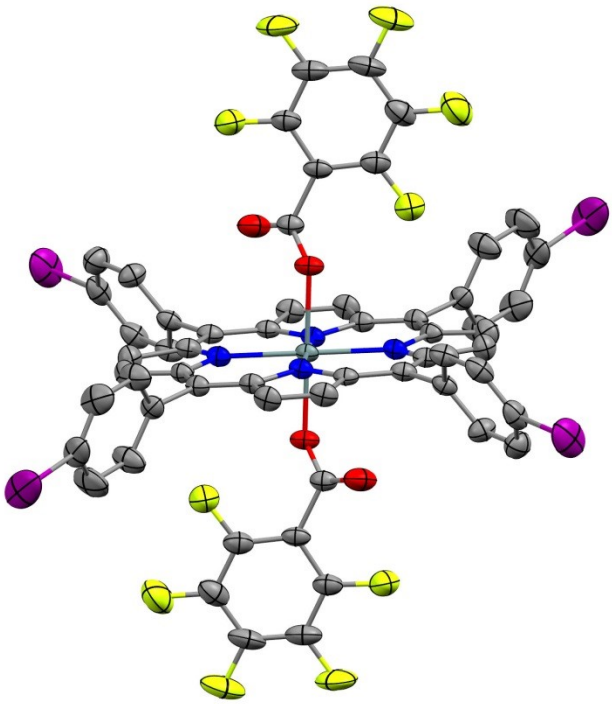


Figure S7. Perspective view of compound **7** showing 40% thermal ellipsoids for all non-hydrogen atoms at 293 K (H-atoms have been omitted for clarity).

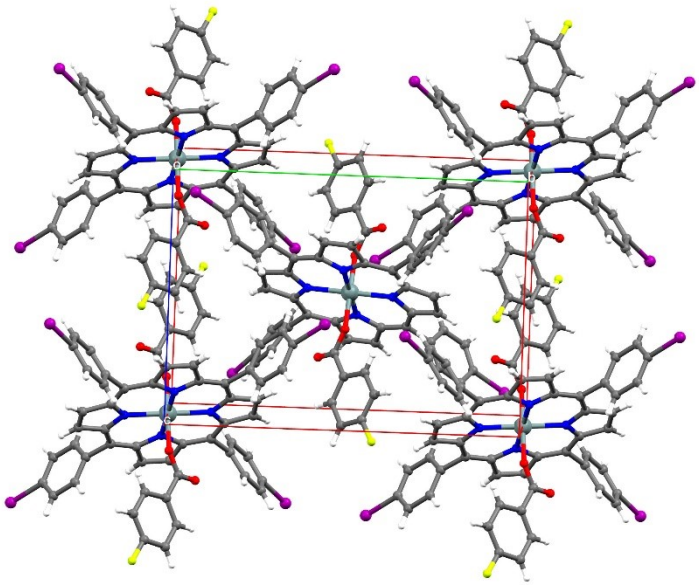


Figure S8. Packing diagram of compound **1** in the crystal lattice viewed along the a-axis

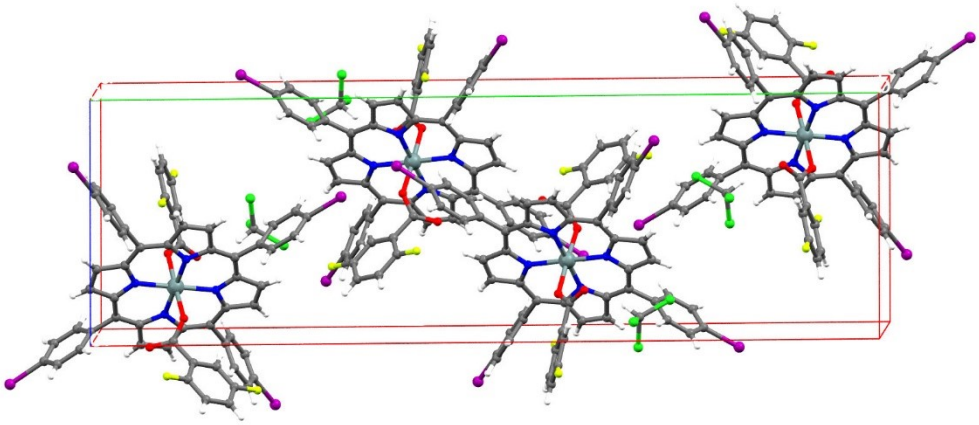


Figure S9. Packing diagram of compound **2** in the crystal lattice viewed along the a-axis

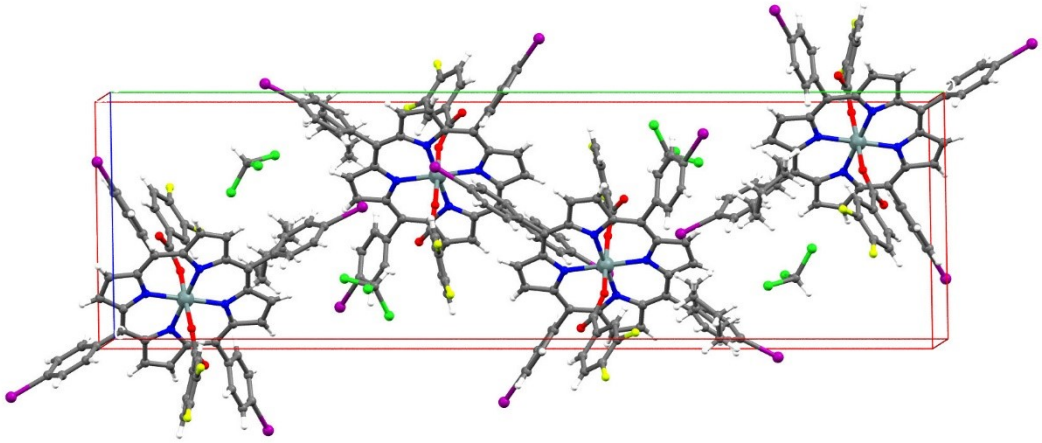


Figure S10. Packing diagram of compound **3** in the crystal lattice viewed along the a-axis

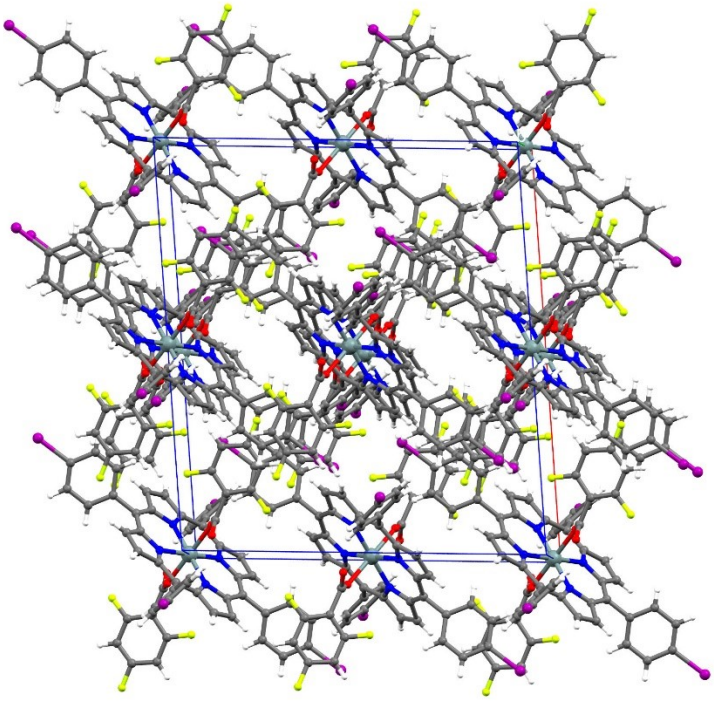


Figure S11. Packing diagram of compound **4** in the crystal lattice viewed along the a-axis

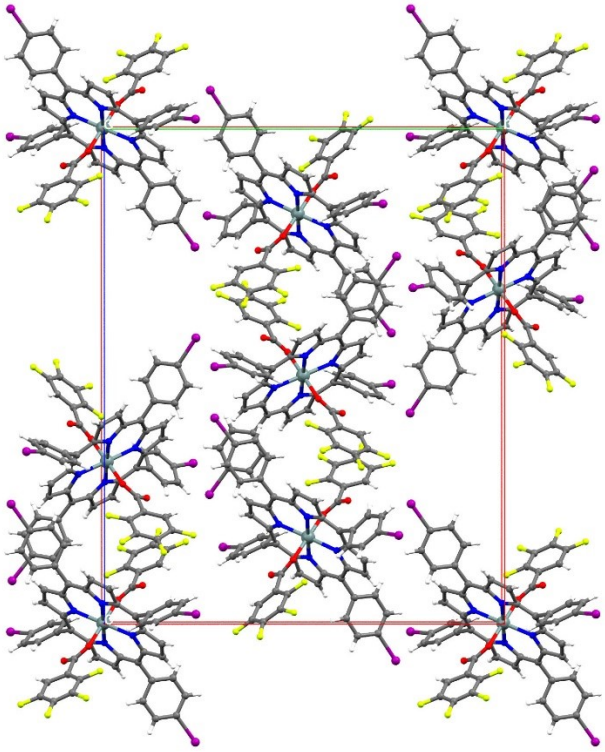


Figure S12. Packing diagram of compound **5** in the crystal lattice viewed along the a-axis

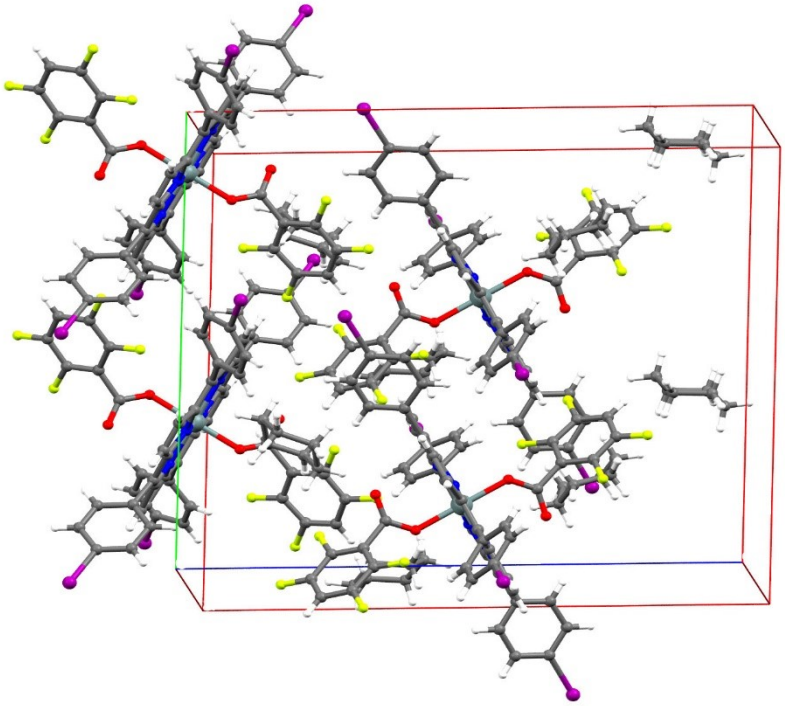


Figure S13. Packing diagram of compound **6** in the crystal lattice viewed along the a-axis

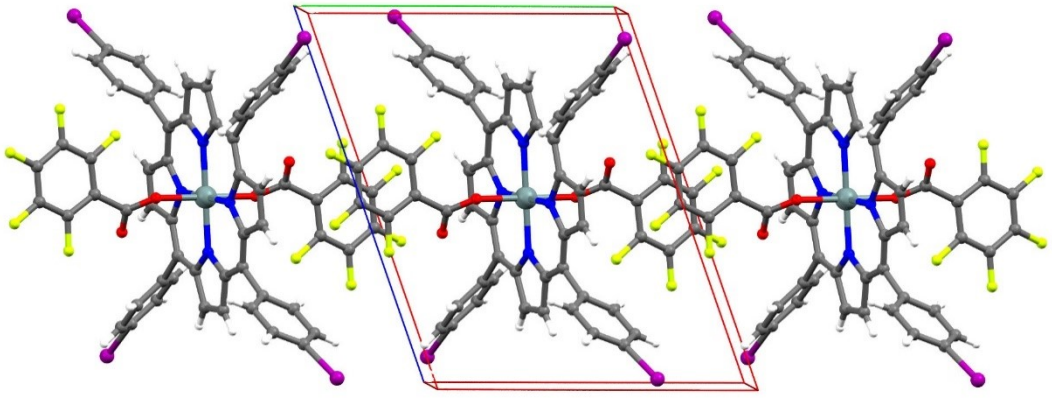


Figure S14. Packing diagram of compound **7** in the crystal lattice viewed along the a-axis

PXRD Analysis:

The bulk purity of the sample was determined by PXRD analysis. Figure S1 depicts comparative experimental and simulated powder X-ray diffraction (PXRD) pattern of compound **2** and **3**. Both experimental and simulated PXRD showed distinctly similar pattern that confirms the bulk purity of the complex.

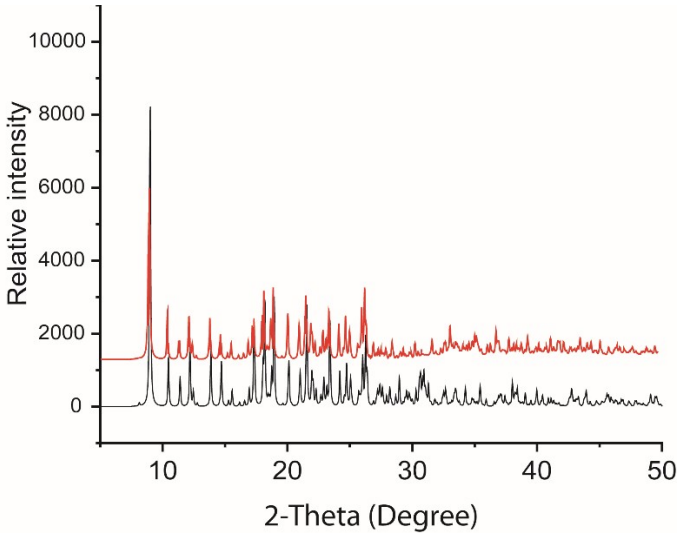


Figure S15. Overlapped experimental (red) and simulated (black) PXRD pattern of compound **1.** Simulated spectra (black) obtained from single crystal structure (Mercury software).

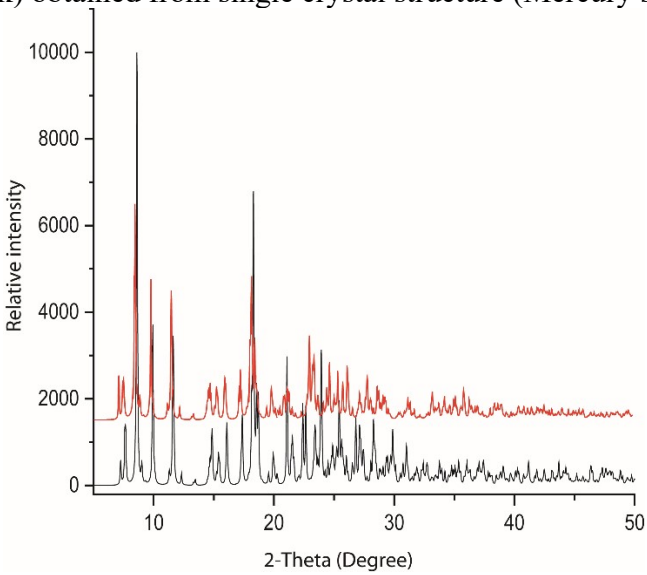


Figure S16. Overlapped experimental (red) and simulated (black) PXRD pattern of compound **2.** Simulated spectra (black) obtained from single crystal structure (Mercury software).

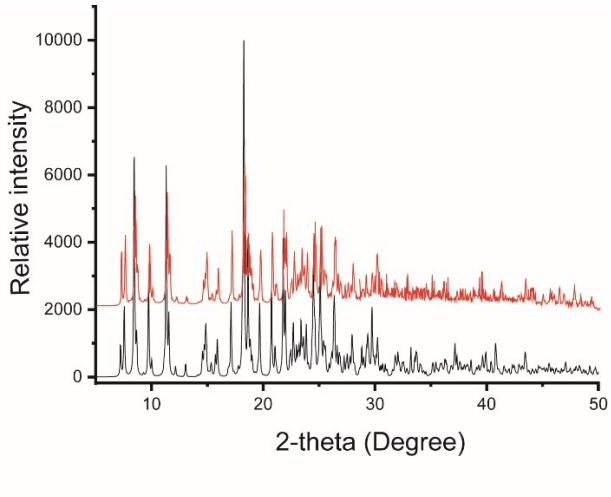


Figure S17. Overlapped experimental (red) and simulated (black) PXRD pattern of compound **3.** Simulated spectra (black) obtained from single crystal structure (Mercury software).

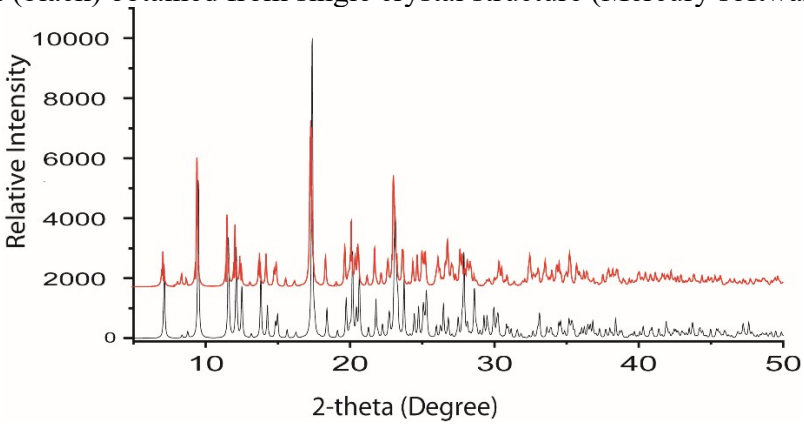


Figure S18. Overlapped experimental (red) and simulated (black) PXRD pattern of compound **4.** Simulated spectra (black) obtained from single crystal structure (Mercury software).

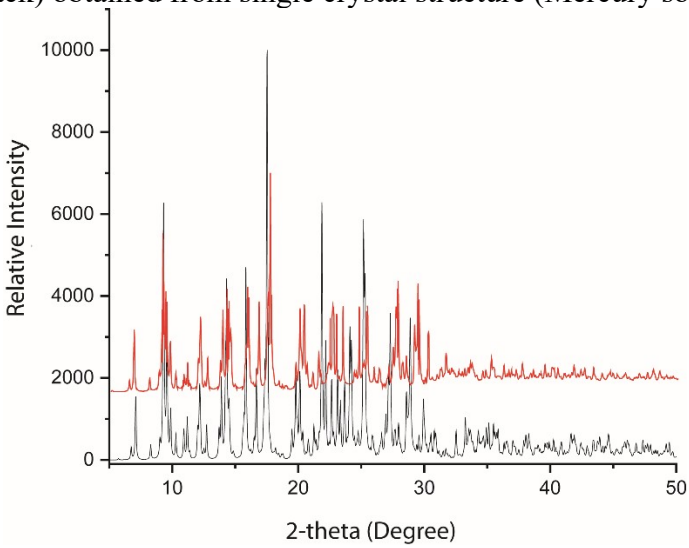


Figure S19. Overlapped experimental (red) and simulated (black) PXRD pattern of compound **5.** Simulated spectra (black) obtained from single crystal structure (Mercury software).

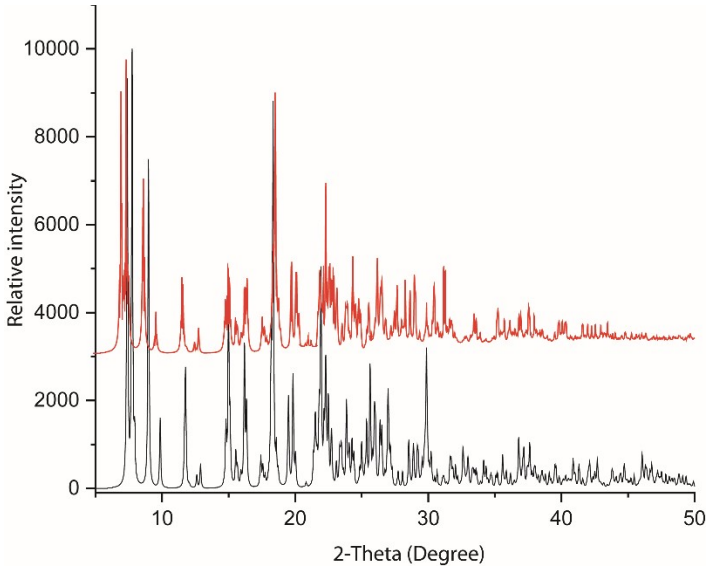


Figure S20. Overlapped experimental (red) and simulated (black) PXRD pattern of compound **6.** Simulated spectra (black) obtained from single crystal structure (Mercury software).

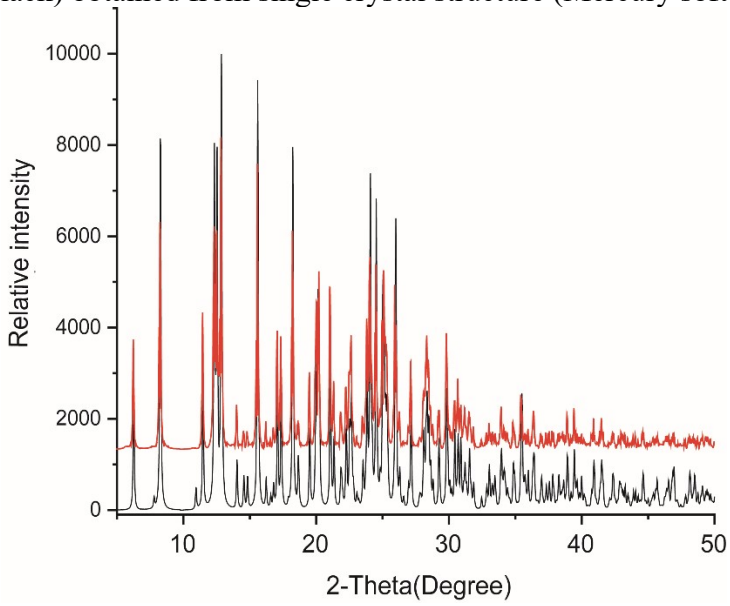


Figure S21. Overlapped experimental (red) and simulated (black) PXRD pattern of compound **7.** Simulated spectra (black) obtained from single crystal structure (Mercury software).

Quantum chemical calculations.

We carried out DFT based geometry optimization on the monomeric and dimeric forms of compound **1, 2, 4, 6** and **7**, starting from the coordinates extracted from X-ray structure. Specifically, we carried out unrestrained geometry optimizations in the gas phase, at the B3LYP level,[5,6] which was combined with the 6-31G* basis set for light atoms (C, N, O, H and F) and a 19-electron effective core potential and associated double-zeta basis set (designated as LAN2DZ)

for heavy atoms (Sn and I). The optimized structures were further verified as minima using vibrational frequency calculations. The interaction energy of the fully-optimized dimer was calculated at the B3LYP level using the extended 6-311+G(d,p)[7] basis set for lighter atoms and a combination of LANL2DZ basis set and pseudopotential for heavier atoms. The counterpoise method was used to correct the interaction energy for basis set superposition error. All calculations were performed using Gaussian 09.[8]

In a previous reported study[9] where intramolecular hydrogen bonding has been studied through AIM analysis with electron density values ranging from 0.129 – 0.217 eÅ^{-3} and laplacian of electron density ranges from 1.53 – 0.424 eÅ^{-5}. In the present study the hetero-halogen bonds have ρ value of 0.029 eÅ^{-3} and $\nabla^2\rho$ value of 0.597 eÅ^{-5} and the homo-halogen bonds have ρ value between 0.045 – 0.057 eÅ^{-3} and $\nabla^2\rho$ value between 0.460 – 0.597 eÅ^{-5}. Unit conversions: For electron density, 1 a.u. = 6.7 eÅ^{-3} For laplacian of electron density, 1 a.u. = 24.1 eÅ^{-5}

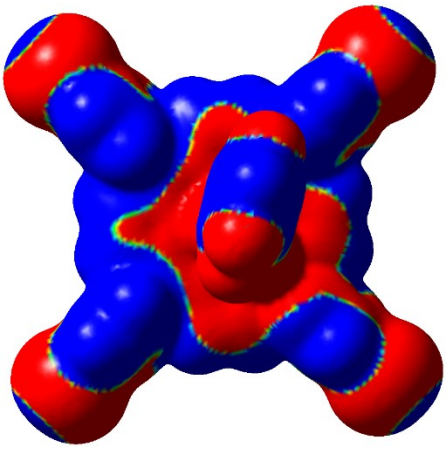


Figure S22. The electrostatic potential surfaces of the monomeric form of compound **6**. The theoretical charge density modeling drawn at surface value of 0.001 electrons/bohr3 Blue, red and green colors represent electropositive, electronegative and neutral regions, respectively.

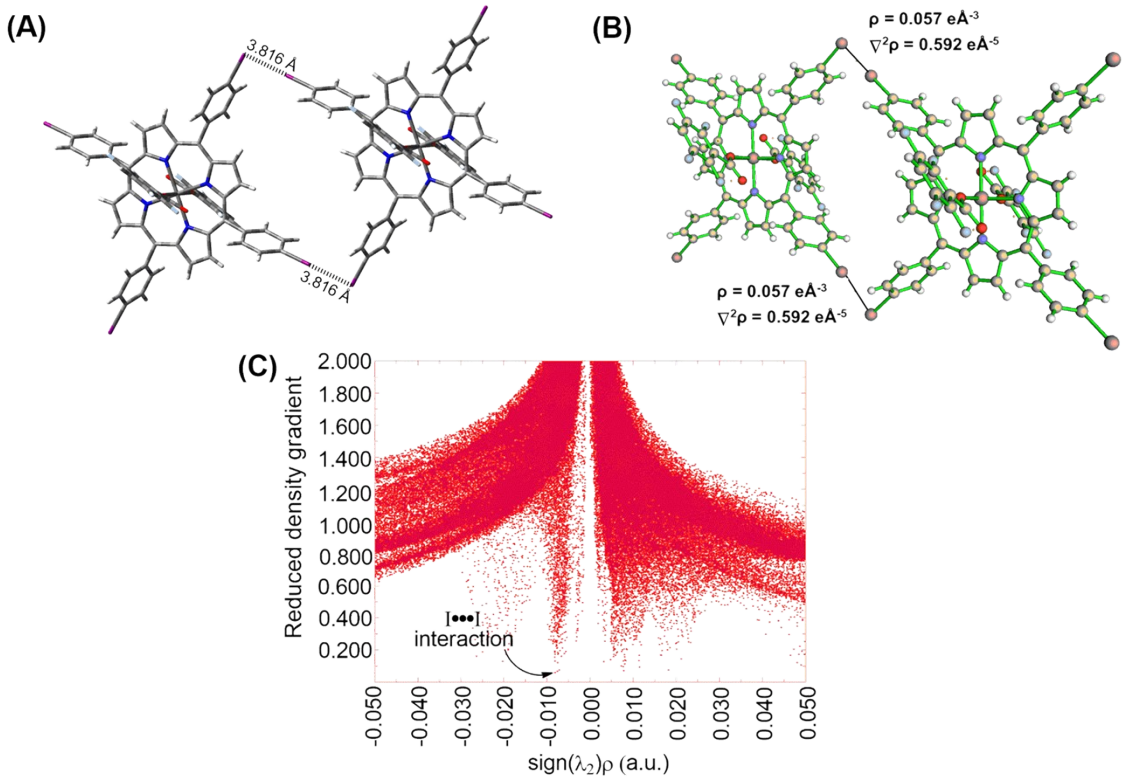


Figure S23. (A) Optimized structure of the dimeric form of compound **6**, depicting homo-halogen bonding (red). (B) Bond critical paths and bond critical points associated with hetero-halogen bonding. (C) NCI plot of reduced density gradient (S) and sign(λ_2)ρ(r) for dimer of compound **6**.

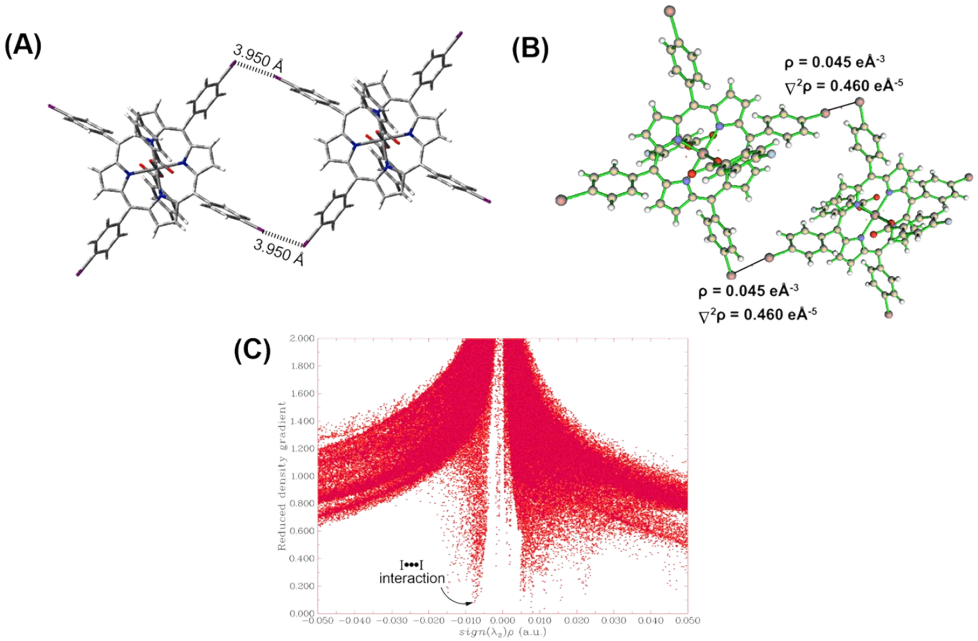


Figure S24 (A) Optimized structure of the dimeric model compound **1**, depicting homo-halogen bonding (dashed black). (B) Bond critical paths and bond critical points associated with homo-halogen bonding. (C) NCI plot of reduced density gradient (S) and sign(λ2)ρ(r) for dimer of compound **1**.

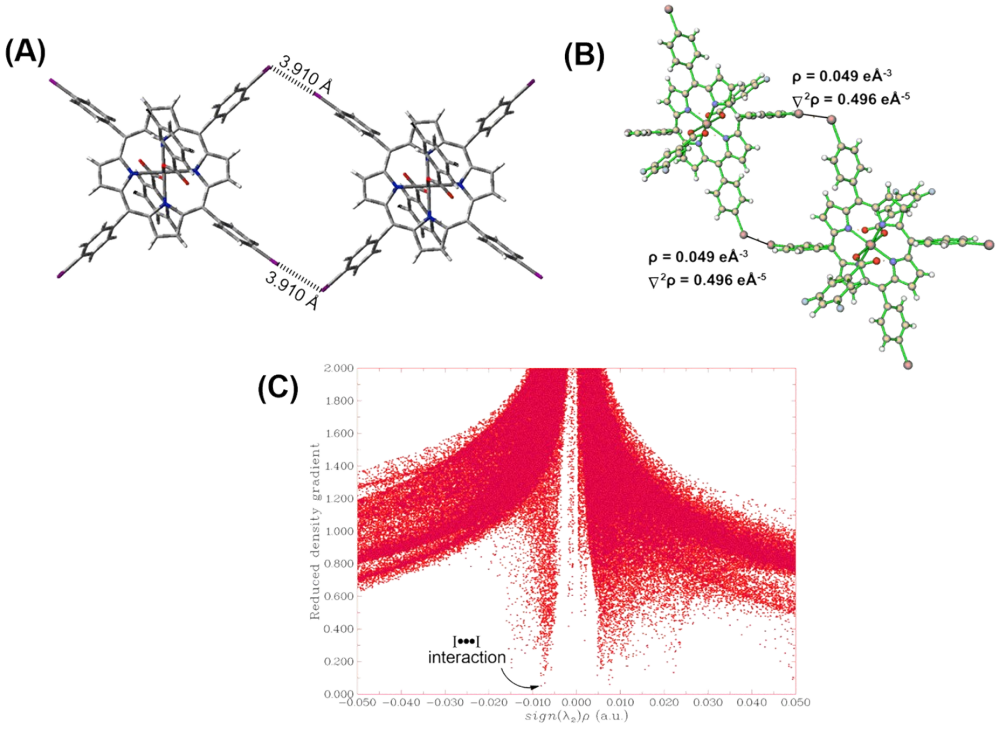


Figure S25 (A) Optimized structure of the dimeric model compound **2**, depicting homo-halogen bonding (dashed black). (B) Bond critical paths and bond critical points associated with homo-halogen bonding. (C) NCI plot of reduced density gradient (S) and sign(λ2)ρ(r) for dimer of compound **2**.

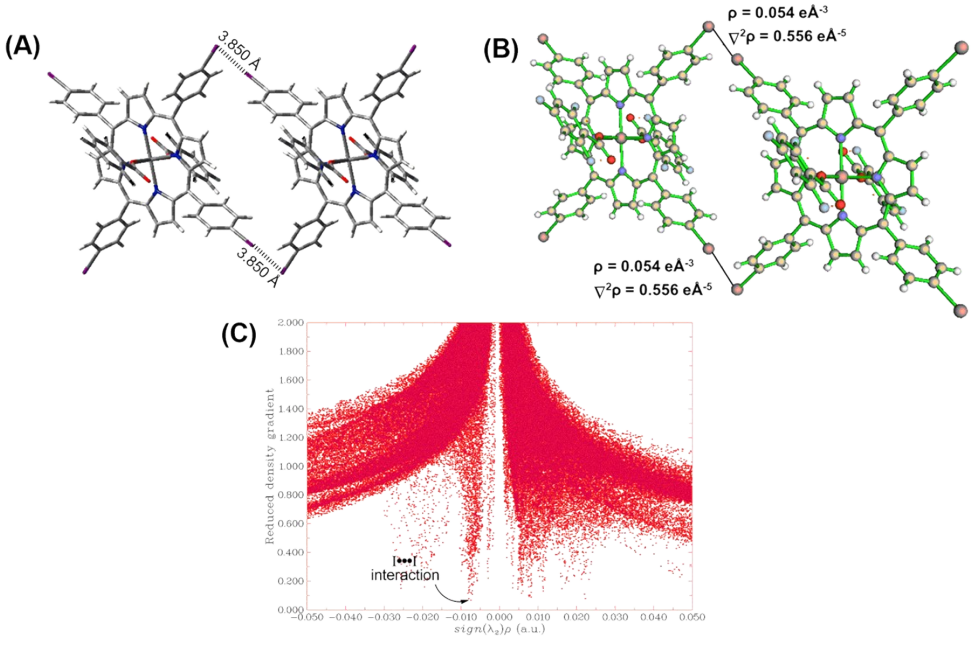


Figure S26(A) Optimized structure of the dimeric model compound **4**, depicting homo-halogen bonding (dashed black). (B) Bond critical paths and bond critical points associated with homo-halogen bonding. (C) NCI plot of reduced density gradient (S) and sign(λ2)ρ(r) for dimer of compound **4**.

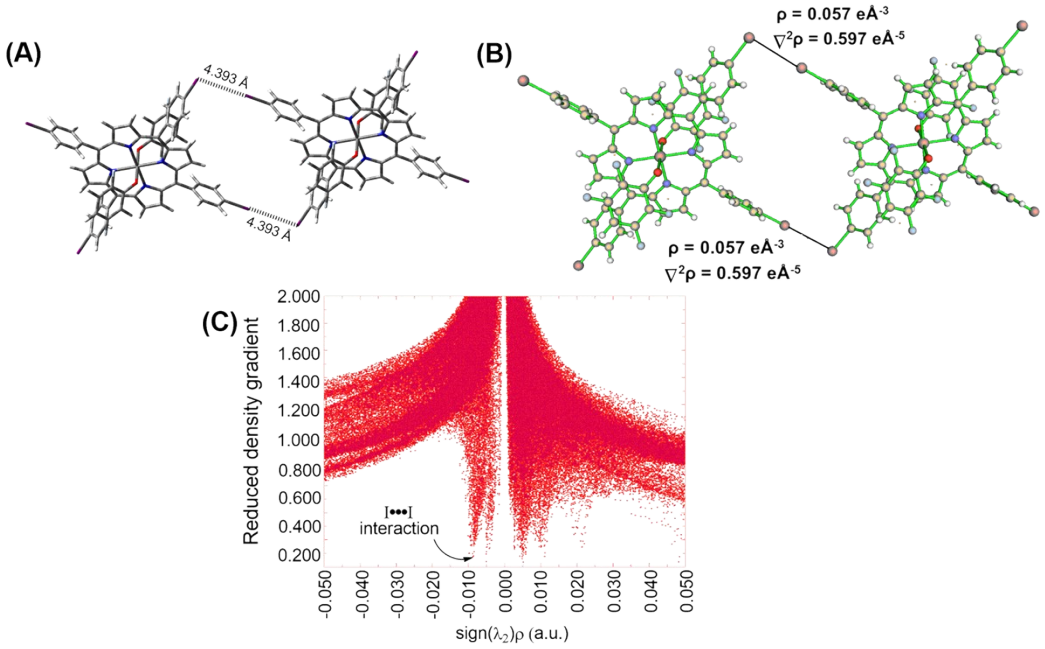


Figure S27 (A) Optimized structure of the dimeric model compound **7**, depicting homo-halogen bonding (dashed black). (B) Bond critical paths and bond critical points associated with homo-halogen bonding. (C) NCI plot of reduced density gradient (S) and sign(λ2)ρ(r) for dimer of compound **7**.

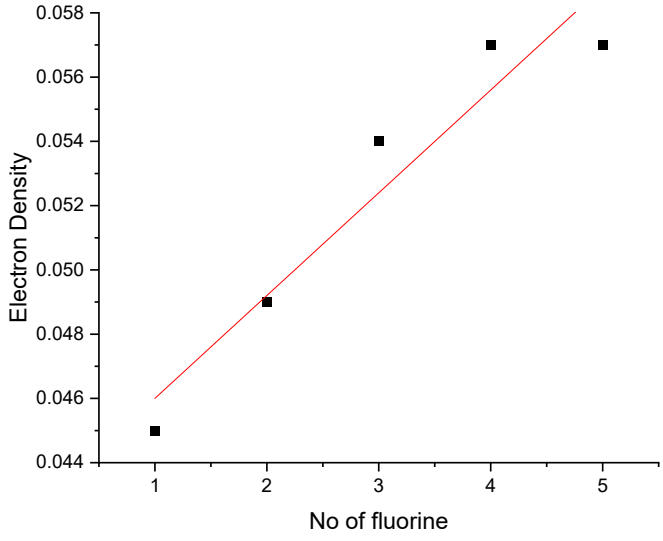


Figure S28. Plot of electron density (ρ^{XBCP}) halogen-bond critical point (XBCP)with increasing number of fluorine atom.

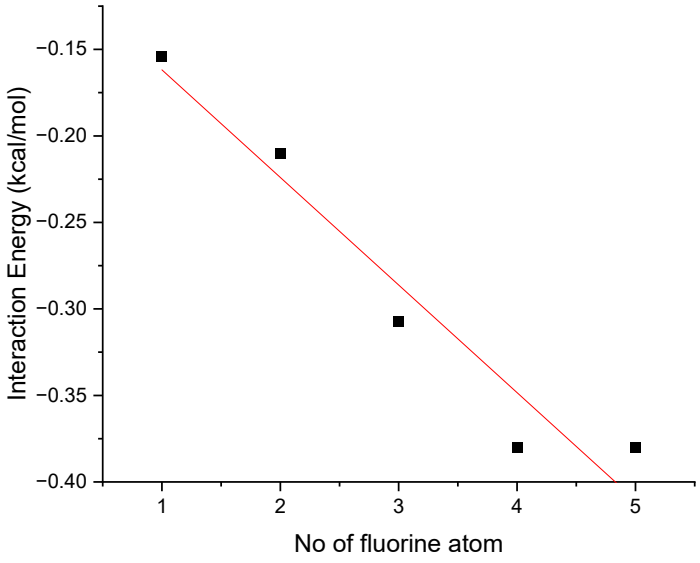


Figure S29. Plot of interaction energy (kcal/mol) with increasing number of fluorine atom.

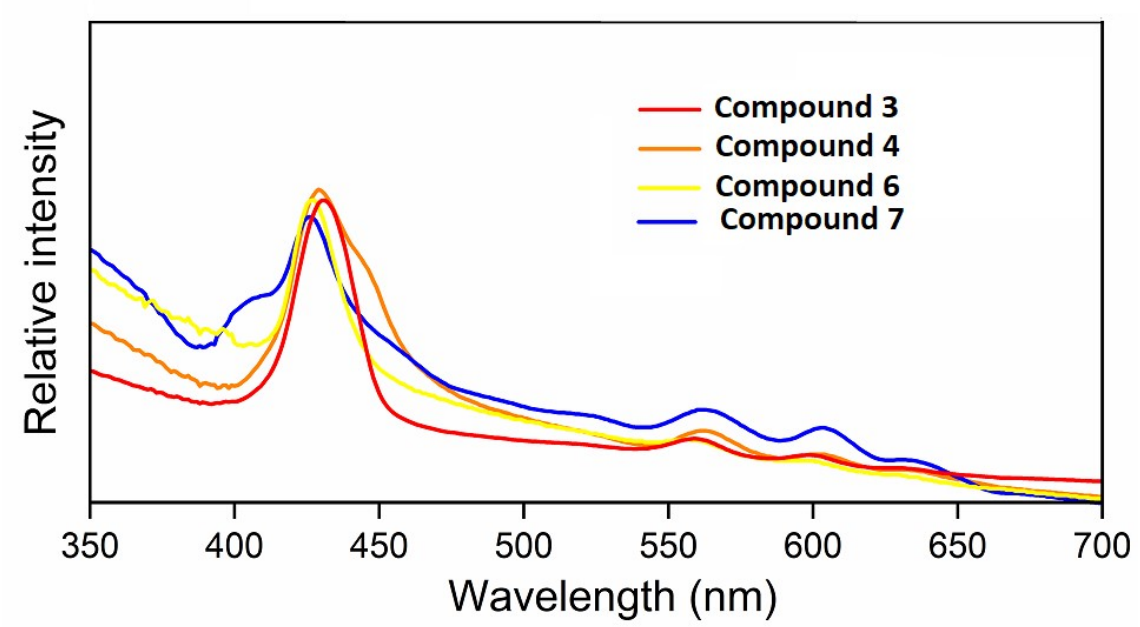


Figure S30. Solid state UV-vis spectra of compound 3, 4 6 and 7 at room temperature.

Coordinates of optimize geometry.

Coordinates of monomer of compound 6

Sn	5.243789000	12.367312000	11.205930000
F	2.684471000	9.553593000	9.221139000
F	1.839528000	7.519791000	7.751006000
F	4.769819000	8.787743000	4.316988000
F	5.474896000	10.975887000	5.727070000
F	7.774965000	15.260351000	13.313492000
F	8.490234000	17.262893000	14.972675000
F	5.698791000	15.498702000	18.286591000
F	4.998671000	13.500067000	16.656322000
I	9.959488000	4.845371000	15.346547000
I	13.791966000	16.586522000	8.786994000
I	0.602620000	19.825561000	6.848019000
I	-3.333286000	8.117037000	13.485638000
N	5.856824000	14.088131000	10.217538000
N	3.258485000	12.958892000	11.031561000
N	4.634843000	10.608591000	12.168078000
N	7.234808000	11.771043000	11.367400000
O	5.070098000	11.235729000	9.447998000
O	4.212098000	12.615041000	7.953399000
O	5.411989000	13.488345000	12.979877000
O	6.359100000	12.046514000	14.423321000
C	7.148372000	14.461287000	9.970663000
C	7.163018000	15.735100000	9.270069000
H	7.903874000	16.205941000	8.963143000
C	5.856567000	16.084812000	9.165537000
H	5.547424000	16.872153000	8.778542000
C	5.016412000	15.064981000	9.732683000
C	3.589326000	15.043490000	9.770493000
C	2.824706000	14.068594000	10.353209000
C	1.397634000	14.027566000	10.302054000

H	0.843003000	14.662518000	9.910612000
C	1.005777000	12.913957000	10.915907000
H	0.126281000	12.626763000	11.013768000
C	2.178997000	12.224301000	11.402986000
C	2.168699000	10.946581000	12.050201000
C	3.314961000	10.260832000	12.430523000
C	3.356818000	9.045631000	13.162253000
H	2.617121000	8.586512000	13.491421000
C	4.645396000	8.658798000	13.304596000
H	4.945463000	7.887087000	13.731624000
C	5.465562000	9.659093000	12.675174000
C	6.877348000	9.631741000	12.581762000
C	7.697349000	10.620313000	12.014615000
C	9.124398000	10.657434000	11.970133000
H	9.687954000	9.993175000	12.294852000
C	9.526792000	11.786672000	11.391866000
H	10.405594000	12.066051000	11.262867000
C	8.334487000	12.493911000	11.002647000
C	8.281576000	13.759909000	10.326519000
C	2.901766000	16.190312000	9.083245000
C	2.834438000	16.260645000	7.684283000
H	3.234107000	15.594433000	7.172738000
C	2.212985000	17.257032000	7.081550000
H	2.192748000	17.290245000	6.151874000
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C	1.677956000	18.210438000	9.154416000
H	1.314447000	18.898140000	9.663736000
C	2.279759000	17.176930000	9.754924000
H	2.267944000	17.137856000	10.682376000
C	0.874353000	10.340934000	12.350455000
C	0.516095000	9.147223000	11.776636000

H	1.099218000	8.742807000	11.173903000
C	-0.681163000	8.523993000	12.065769000
H	-0.907862000	7.730791000	11.636517000
C	-1.519433000	9.063214000	12.966532000
C	-1.235830000	10.280369000	13.589281000
H	-1.830346000	10.673063000	14.187566000
C	-0.025816000	10.872341000	13.271234000
H	0.199295000	11.669450000	13.693814000
C	7.572004000	8.518132000	13.244545000
C	7.813182000	7.365449000	12.577314000
H	7.584853000	7.314653000	11.676551000
C	8.378282000	6.275284000	13.175598000
H	8.436181000	5.464499000	12.721880000
C	8.867267000	6.398368000	14.478923000
C	8.654272000	7.541282000	15.103897000
H	8.941399000	7.619430000	15.984642000
C	8.029870000	8.619724000	14.527854000
H	7.921970000	9.410973000	15.003812000
C	9.630273000	14.418306000	9.950646000
C	10.274131000	14.047103000	8.847490000
H	9.911373000	13.388706000	8.300360000
C	11.497442000	14.644935000	8.504977000
H	11.947306000	14.394862000	7.730989000
C	12.007976000	15.586619000	9.323448000
C	11.347720000	15.979312000	10.451069000
H	11.718808000	16.624033000	11.009320000
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H	9.639053000	15.696026000	11.505295000
C	4.509305000	11.548321000	8.331497000
C	4.129071000	10.337027000	7.526371000
C	3.161378000	9.407065000	8.020122000

C	2.759087000	8.371605000	7.243910000
C	3.283827000	8.119577000	6.002859000
H	3.014313000	7.386940000	5.495763000
C	4.226942000	9.000696000	5.549142000
C	4.604089000	10.110397000	6.265304000
C	6.021081000	13.154262000	14.047447000
C	6.368127000	14.353834000	14.923744000
C	7.233525000	15.344360000	14.525629000
C	7.645141000	16.342700000	15.397479000
C	7.140592000	16.438432000	16.645201000
H	7.418776000	17.114412000	17.223469000
C	6.171401000	15.477211000	17.056661000
C	5.850507000	14.439797000	16.235966000

Coordinates for dimer model ((hetero-halogen interactions) compound 6

Sn	5.243789000	12.367312000	11.205930000
F	2.684471000	9.553593000	9.221139000
F	1.839528000	7.519791000	7.751006000
F	4.769819000	8.787743000	4.316988000
F	5.474896000	10.975887000	5.727070000
F	7.774965000	15.260351000	13.313492000
F	8.490234000	17.262893000	14.972675000
F	5.698791000	15.498702000	18.286591000
F	4.998671000	13.500067000	16.656322000
I	9.959488000	4.845371000	15.346547000
I	13.791966000	16.586522000	8.786994000
I	0.602620000	19.825561000	6.848019000
I	-3.333286000	8.117037000	13.485638000
N	5.856824000	14.088131000	10.217538000
N	3.258485000	12.958892000	11.031561000
N	4.634843000	10.608591000	12.168078000

N	7.234808000	11.771043000	11.367400000
O	5.070098000	11.235729000	9.447998000
O	4.212098000	12.615041000	7.953399000
O	5.411989000	13.488345000	12.979877000
O	6.359100000	12.046514000	14.423321000
C	7.148372000	14.461287000	9.970663000
C	7.163018000	15.735100000	9.270069000
H	7.903874000	16.205941000	8.963143000
C	5.856567000	16.084812000	9.165537000
H	5.547424000	16.872153000	8.778542000
C	5.016412000	15.064981000	9.732683000
C	3.589326000	15.043490000	9.770493000
C	2.824706000	14.068594000	10.353209000
C	1.397634000	14.027566000	10.302054000
H	0.843003000	14.662518000	9.910612000
C	1.005777000	12.913957000	10.915907000
H	0.126281000	12.626763000	11.013768000
C	2.178997000	12.224301000	11.402986000
C	2.168699000	10.946581000	12.050201000
C	3.314961000	10.260832000	12.430523000
C	3.356818000	9.045631000	13.162253000
H	2.617121000	8.586512000	13.491421000
C	4.645396000	8.658798000	13.304596000
H	4.945463000	7.887087000	13.731624000
C	5.465562000	9.659093000	12.675174000
C	6.877348000	9.631741000	12.581762000
C	7.697349000	10.620313000	12.014615000
C	9.124398000	10.657434000	11.970133000
H	9.687954000	9.993175000	12.294852000
C	9.526792000	11.786672000	11.391866000
H	10.405594000	12.066051000	11.262867000

C	8.334487000	12.493911000	11.002647000
C	8.281576000	13.759909000	10.326519000
C	2.901766000	16.190312000	9.083245000
C	2.834438000	16.260645000	7.684283000
H	3.234107000	15.594433000	7.172738000
C	2.212985000	17.257032000	7.081550000
H	2.192748000	17.290245000	6.151874000
C	1.600581000	18.247558000	7.806608000
C	1.677956000	18.210438000	9.154416000
H	1.314447000	18.898140000	9.663736000
C	2.279759000	17.176930000	9.754924000
H	2.267944000	17.137856000	10.682376000
C	0.874353000	10.340934000	12.350455000
C	0.516095000	9.147223000	11.776636000
H	1.099218000	8.742807000	11.173903000
C	-0.681163000	8.523993000	12.065769000
H	-0.907862000	7.730791000	11.636517000
C	-1.519433000	9.063214000	12.966532000
C	-1.235830000	10.280369000	13.589281000
H	-1.830346000	10.673063000	14.187566000
C	-0.025816000	10.872341000	13.271234000
H	0.199295000	11.669450000	13.693814000
C	7.572004000	8.518132000	13.244545000
C	7.813182000	7.365449000	12.577314000
H	7.584853000	7.314653000	11.676551000
C	8.378282000	6.275284000	13.175598000
H	8.436181000	5.464499000	12.721880000
C	8.867267000	6.398368000	14.478923000
C	8.654272000	7.541282000	15.103897000
H	8.941399000	7.619430000	15.984642000
C	8.029870000	8.619724000	14.527854000

H	7.921970000	9.410973000	15.003812000
C	9.630273000	14.418306000	9.950646000
C	10.274131000	14.047103000	8.847490000
H	9.911373000	13.388706000	8.300360000
C	11.497442000	14.644935000	8.504977000
H	11.947306000	14.394862000	7.730989000
C	12.007976000	15.586619000	9.323448000
C	11.347720000	15.979312000	10.451069000
H	11.718808000	16.624033000	11.009320000
C	10.119065000	15.410786000	10.762444000
H	9.639053000	15.696026000	11.505295000
C	4.509305000	11.548321000	8.331497000
C	4.129071000	10.337027000	7.526371000
C	3.161378000	9.407065000	8.020122000
C	2.759087000	8.371605000	7.243910000
C	3.283827000	8.119577000	6.002859000
H	3.014313000	7.386940000	5.495763000
C	4.226942000	9.000696000	5.549142000
C	4.604089000	10.110397000	6.265304000
C	6.021081000	13.154262000	14.047447000
C	6.368127000	14.353834000	14.923744000
C	7.233525000	15.344360000	14.525629000
C	7.645141000	16.342700000	15.397479000
C	7.140592000	16.438432000	16.645201000
H	7.418776000	17.114412000	17.223469000
C	6.171401000	15.477211000	17.056661000
C	5.850507000	14.439797000	16.235966000
Sn	-2.507661000	22.135812000	11.205930000
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F	-2.981631000	18.556243000	4.316988000

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F	-2.052659000	25.267202000	18.286591000
F	-2.752779000	23.268567000	16.656322000
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I	6.040516000	26.355022000	8.786994000
I	-7.148830000	29.594061000	6.848019000
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N	-3.116607000	20.377091000	12.168078000
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O	-3.539352000	22.383541000	7.953399000
O	-2.339461000	23.256845000	12.979877000
O	-1.392350000	21.815014000	14.423321000
C	-0.603078000	24.229787000	9.970663000
C	-0.588432000	25.503600000	9.270069000
H	0.152424000	25.974441000	8.963143000
C	-1.894883000	25.853312000	9.165537000
H	-2.204026000	26.640653000	8.778542000
C	-2.735038000	24.833481000	9.732683000
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C	-4.926744000	23.837094000	10.353209000
C	-6.353816000	23.796066000	10.302054000
H	-6.908447000	24.431018000	9.910612000
C	-6.745673000	22.682457000	10.915907000
H	-7.625169000	22.395263000	11.013768000
C	-5.572453000	21.992801000	11.402986000
C	-5.582751000	20.715081000	12.050201000

C	-4.436489000	20.029332000	12.430523000
C	-4.394632000	18.814131000	13.162253000
H	-5.134329000	18.355012000	13.491421000
C	-3.106054000	18.427298000	13.304596000
H	-2.805987000	17.655587000	13.731624000
C	-2.285888000	19.427593000	12.675174000
C	-0.874102000	19.400241000	12.581762000
C	-0.054101000	20.388813000	12.014615000
C	1.372948000	20.425933000	11.970133000
H	1.936504000	19.761675000	12.294852000
C	1.775342000	21.555172000	11.391866000
H	2.654144000	21.834551000	11.262867000
C	0.583037000	22.262411000	11.002647000
C	0.530126000	23.528409000	10.326519000
C	-4.849684000	25.958812000	9.083245000
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H	-4.517343000	25.362933000	7.172738000
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H	-5.558702000	27.058745000	6.151874000
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H	-8.659312000	17.499291000	11.636517000
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C	-8.987280000	20.048869000	13.589281000

H	-9.581796000	20.441563000	14.187566000
C	-7.777266000	20.640840000	13.271234000
H	-7.552155000	21.437950000	13.693814000
C	-0.179446000	18.286632000	13.244545000
C	0.061732000	17.133949000	12.577314000
H	-0.166597000	17.083153000	11.676551000
C	0.626832000	16.043784000	13.175598000
H	0.684731000	15.232999000	12.721880000
C	1.115817000	16.166867000	14.478923000
C	0.902822000	17.309782000	15.103897000
H	1.189949000	17.387930000	15.984642000
C	0.278420000	18.388224000	14.527854000
H	0.170520000	19.179473000	15.003812000
C	1.878823000	24.186806000	9.950646000
C	2.522681000	23.815603000	8.847490000
H	2.159923000	23.157206000	8.300360000
C	3.745992000	24.413435000	8.504977000
H	4.195856000	24.163362000	7.730989000
C	4.256526000	25.355119000	9.323448000
C	3.596270000	25.747812000	10.451069000
H	3.967358000	26.392533000	11.009320000
C	2.367615000	25.179286000	10.762444000
H	1.887603000	25.464526000	11.505295000
C	-3.242145000	21.316821000	8.331497000
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C	-4.590072000	19.175566000	8.020122000
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C	-4.467623000	17.888077000	6.002859000
H	-4.737137000	17.155440000	5.495763000
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C	-3.147361000	19.878898000	6.265304000

C	-1.730369000	22.922762000	14.047447000
C	-1.383323000	24.122334000	14.923744000
C	-0.517925000	25.112860000	14.525629000
C	-0.106309000	26.111200000	15.397479000
C	-0.610858000	26.206932000	16.645201000
H	-0.332674000	26.882912000	17.223469000
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Coordinates for dimer model of compound 1

Sn	6.430375390	8.472659900	5.991171320
I	2.111875390	1.069459900	1.165271320
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N	6.847475390	6.421459900	5.875271320
O	7.649475390	8.619459900	4.318571320
O	6.541675390	9.883959900	2.858471320
C	3.878675390	9.158059900	4.393471320
C	2.926175390	8.558659900	3.511871320
H	2.231175390	9.000359900	3.078871320
C	3.204975390	7.252059900	3.418871320
H	2.732075390	6.627259900	2.918271320
C	4.353475390	6.990359900	4.220771320
C	5.012275390	5.771459900	4.356071320
C	6.178875390	5.516559900	5.110771320
C	6.870775390	4.258859900	5.206271320
H	6.642575390	3.467759900	4.775371320
C	7.915375390	4.447959900	6.043171320
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C	7.926375390	5.805259900	6.456171320
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H	5.662875390	4.506859900	2.098671320
C	4.241375390	3.127759900	1.719671320
H	4.584875390	2.831659900	0.907471320
C	3.098475390	2.575659900	2.236571320
C	2.600075390	3.021359900	3.414071320
H	1.821475390	2.646259900	3.758171320
C	3.247375390	4.037659900	4.113271320
H	2.901675390	4.330259900	4.925171320
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C	1.671475390	11.452259900	4.364471320
H	1.379975390	10.947459900	5.089371320
C	0.759875390	12.233959900	3.654371320
H	-0.132424610	12.267959900	3.913971320
C	1.192075390	12.951459900	2.571071320
C	2.516575390	12.939659900	2.205171320
H	2.806675390	13.442059900	1.478471320
C	3.412475390	12.174859900	2.928571320
H	4.310375390	12.167859900	2.685871320
C	7.432675390	9.102359900	3.139871320
C	8.373175390	8.584059900	2.108571320
C	8.365175390	9.115859900	0.836871320
C	9.223475390	8.627959900	-0.161828680
C	10.071675390	7.635259900	0.195571320
C	10.130975390	7.081559900	1.429871320
C	9.284875390	7.577859900	2.395971320
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I	13.041375390	2.877859900	10.541471320
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C	9.934675390	8.386559900	8.470571320
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C	9.655875390	9.693159900	8.563571320
H	10.128775390	10.317959900	9.064071320
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C	7.848575390	11.173759900	7.626371320
C	6.681975390	11.428659900	6.871571320
C	5.990075390	12.686359900	6.776171320
H	6.218275390	13.477459900	7.207071320
C	4.945475390	12.497259900	5.939271320
H	4.334875390	13.149359900	5.678871320
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H	11.480875390	5.997759900	6.893071320
C	12.100975390	4.711259900	8.328071320
H	12.993275390	4.677259900	8.068471320
C	11.668775390	3.993759900	9.411371320
C	10.344275390	4.005559900	9.777271320
H	10.054175390	3.503159900	10.503971320

C	9.448375390	4.770359900	9.053871320
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O	5.211375390	8.325759900	7.663871320
O	6.319175390	7.061259900	9.123871320
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C	4.487675390	8.361159900	9.873871320
C	4.495675390	7.829359900	11.145571320
C	3.637375390	8.317259900	12.144271320
C	2.789075390	9.309959900	11.786771320
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C	16.879224610	9.094940100	16.564428680
C	15.926724610	8.495540100	15.682828680
H	15.231724610	8.937240100	15.249828680
C	16.205524610	7.188940100	15.589828680
H	15.732624610	6.564140100	15.089228680
C	17.353924610	6.927240100	16.391728680
C	18.012824610	5.708340100	16.526928680
C	19.179424610	5.453440100	17.281728680
C	19.871324610	4.195740100	17.377128680
H	19.643124610	3.404640100	16.946328680
C	20.915824610	4.384840100	18.214028680
H	21.526524610	3.732740100	18.474428680
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C	16.979624610	10.462340100	16.867528680
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H	18.663424610	4.443740100	14.269528680
C	17.241924610	3.064640100	13.890628680
H	17.585424610	2.768540100	13.078428680
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H	15.902224610	4.267140100	17.096128680
C	15.993324610	11.358840100	16.173128680
C	14.672024610	11.389140100	16.535428680
H	14.380524610	10.884340100	17.260328680
C	13.760424610	12.170840100	15.825328680
H	12.868024610	12.204840100	16.084928680
C	14.192624610	12.888340100	14.742028680
C	15.517124610	12.876540100	14.376128680
H	15.807224610	13.378940100	13.649328680
C	16.413024610	12.111740100	15.099528680
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C	20.433224610	9.039240100	15.310828680
C	21.373724610	8.520940100	14.279528680
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C	23.131524610	7.018440100	13.600828680
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H	19.218724610	13.414340100	19.378028680
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C	17.935024610	11.076840100	17.697228680
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C	20.983024610	12.743140100	21.718728680
H	20.198524610	12.375240100	22.054728680
C	21.619924610	13.754340100	22.433628680
H	21.276524610	14.050440100	23.245928680
C	22.762824610	14.306440100	21.916828680
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C	22.868624610	5.460140100	20.151128680
C	24.189824610	5.429840100	19.788828680
H	24.481424610	5.934640100	19.063928680
C	25.101524610	4.648140100	20.499028680
H	25.993824610	4.614140100	20.239428680
C	24.669324610	3.930640100	21.582228680

C	23.344824610	3.942440100	21.948228680
H	23.054724610	3.440040100	22.674928680
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H	21.550924610	4.714240100	21.467428680
O	18.211824610	8.262640100	19.834728680
O	19.319724610	6.998140100	21.294828680
C	18.428724610	7.779740100	21.013428680
C	17.488224610	8.298040100	22.044828680
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C	15.730424610	9.800540100	22.723528680
C	16.576524610	9.304240100	21.757328680
F	10.887147260	7.123375080	-0.750726490
F	1.973603510	9.821844710	12.733069140
H	3.653939600	7.925240330	13.139734170
H	2.047389980	10.658684630	10.335662710
H	9.206911180	9.019979470	-1.157291520
H	10.813475670	6.286517840	1.646669600
H	22.207460400	8.956859670	11.013565830
H	23.814024900	6.223398050	13.817626950
H	16.654488820	7.862120530	25.310691520
H	15.047870960	10.595510300	22.506634940
F	23.887696490	7.060255290	11.420230860
F	14.974152740	9.758724920	24.904026490
H	9.332422590	7.180328540	3.388245510
H	7.693174670	9.916003170	0.606467790
H	5.167676100	7.029216630	11.375974850
H	3.528428190	9.764891260	8.594197120
H	22.332976540	7.117169070	15.559186760
H	20.693723900	9.852883370	12.777425150

H	18.168209780	6.966115360	23.546941910
H	16.528972690	9.701811130	20.765070610

Coordinates for dimer model of compound 2

Sn	6.440861710	8.463183850	6.005321990
I	2.122361710	1.059983850	1.179421990
I	-0.170038290	14.057883850	1.455121990
N	4.742561710	8.160983850	4.833921990
N	6.857961710	6.411983850	5.889421990
O	7.659961710	8.609983850	4.332721990
O	6.552161710	9.874483850	2.872621990
C	3.889161710	9.148583850	4.407621990
C	2.936661710	8.549183850	3.526021990
H	2.241661710	8.990883850	3.093021990
C	3.215461710	7.242583850	3.433021990
H	2.742561710	6.617783850	2.932421990
C	4.363961710	6.980883850	4.234921990
C	5.022761710	5.761983850	4.370221990
C	6.189361710	5.507083850	5.124921990
C	6.881261710	4.249383850	5.220421990
H	6.653061710	3.458283850	4.789521990
C	7.925861710	4.438483850	6.057321990
H	8.536461710	3.786383850	6.317721990
C	7.936861710	5.795783850	6.470321990
C	3.989561710	10.515983850	4.710721990
C	4.385061710	4.595483850	3.635921990
C	4.888861710	4.129483850	2.448821990
H	5.673361710	4.497383850	2.112821990
C	4.251861710	3.118283850	1.733821990
H	4.595361710	2.822183850	0.921621990
C	3.108961710	2.566183850	2.250721990
C	2.610561710	3.011883850	3.428221990

H	1.831961710	2.636783850	3.772321990
C	3.257861710	4.028183850	4.127421990
H	2.912161710	4.320783850	4.939321990
C	3.003261710	11.412483850	4.016321990
C	1.681961710	11.442783850	4.378621990
H	1.390461710	10.937983850	5.103521990
C	0.770361710	12.224483850	3.668521990
H	-0.121938290	12.258483850	3.928121990
C	1.202561710	12.941983850	2.585221990
C	2.527061710	12.930183850	2.219321990
H	2.817161710	13.432583850	1.492621990
C	3.422961710	12.165383850	2.942721990
H	4.320861710	12.158383850	2.700021990
C	7.443161710	9.092883850	3.154021990
C	8.383661710	8.574583850	2.122721990
C	8.375661710	9.106383850	0.851021990
C	9.233961710	8.618483850	-0.147678010
C	10.082161710	7.625783850	0.209721990
C	10.141461710	7.072083850	1.444021990
C	9.295361710	7.568383850	2.410121990
I	10.759361710	15.866283850	10.831321990
I	13.051861710	2.868383850	10.555621990
N	8.139261710	8.765283850	7.176821990
N	6.023861710	10.514283850	6.121321990
C	8.992661710	7.777683850	7.603121990
C	9.945161710	8.377083850	8.484721990
H	10.640161710	7.935383850	8.917621990
C	9.666361710	9.683683850	8.577721990
H	10.139261710	10.308483850	9.078221990
C	8.517861710	9.945383850	7.775821990
C	7.859061710	11.164283850	7.640521990

C	6.692461710	11.419183850	6.885721990
C	6.000561710	12.676883850	6.790321990
H	6.228761710	13.467983850	7.221221990
C	4.955961710	12.487783850	5.953421990
H	4.345361710	13.139883850	5.693021990
C	4.944961710	11.130483850	5.540421990
C	8.892261710	6.410283850	7.300021990
C	8.496661710	12.330783850	8.374821990
C	7.992961710	12.796783850	9.561921990
H	7.208461710	12.428883850	9.897921990
C	8.629961710	13.807983850	10.276921990
H	8.286461710	14.104083850	11.089121990
C	9.772861710	14.360083850	9.760021990
C	10.271261710	13.914383850	8.582521990
H	11.049861710	14.289483850	8.238421990
C	9.623961710	12.898083850	7.883321990
H	9.969661710	12.605483850	7.071321990
C	9.878561710	5.513783850	7.994421990
C	11.199761710	5.483483850	7.632121990
H	11.491361710	5.988283850	6.907221990
C	12.111461710	4.701783850	8.342221990
H	13.003761710	4.667783850	8.082621990
C	11.679261710	3.984283850	9.425521990
C	10.354761710	3.996083850	9.791421990
H	10.064661710	3.493683850	10.518121990
C	9.458861710	4.760883850	9.068021990
H	8.560861710	4.767883850	9.310721990
O	5.221861710	8.316283850	7.678021990
O	6.329661710	7.051783850	9.138021990
C	5.438661710	7.833383850	8.856621990
C	4.498161710	8.351683850	9.888021990

C	4.506161710	7.819883850	11.159721990
C	3.647861710	8.307783850	12.158421990
C	2.799561710	9.300483850	11.800921990
C	2.740361710	9.854183850	10.566721990
C	3.586461710	9.357883850	9.600621990
Sn	19.420438290	8.419016150	18.147978010
I	15.101938290	1.015816150	13.322078010
I	12.809538290	14.013716150	13.597778010
N	17.722138290	8.116816150	16.976578010
N	19.837538290	6.367816150	18.032078010
O	20.639538290	8.565816150	16.475378010
O	19.531738290	9.830316150	15.015278010
C	16.868738290	9.104416150	16.550278010
C	15.916238290	8.505016150	15.668678010
H	15.221238290	8.946716150	15.235678010
C	16.195038290	7.198416150	15.575678010
H	15.722138290	6.573616150	15.075078010
C	17.343438290	6.936716150	16.377578010
C	18.002338290	5.717816150	16.512778010
C	19.168938290	5.462916150	17.267578010
C	19.860838290	4.205216150	17.362978010
H	19.632638290	3.414116150	16.932178010
C	20.905338290	4.394316150	18.199878010
H	21.516038290	3.742216150	18.460278010
C	20.916438290	5.751616150	18.612978010
C	16.969138290	10.471816150	16.853378010
C	17.364638290	4.551316150	15.778578010
C	17.868438290	4.085316150	14.591378010
H	18.652938290	4.453216150	14.255378010
C	17.231438290	3.074116150	13.876478010
H	17.574938290	2.778016150	13.064278010

C	16.088538290	2.522016150	14.393378010
C	15.590138290	2.967716150	15.570878010
H	14.811538290	2.592616150	15.914978010
C	16.237438290	3.984016150	16.270078010
H	15.891738290	4.276616150	17.081978010
C	15.982838290	11.368316150	16.158978010
C	14.661538290	11.398616150	16.521278010
H	14.370038290	10.893816150	17.246178010
C	13.749938290	12.180316150	15.811178010
H	12.857538290	12.214316150	16.070778010
C	14.182138290	12.897816150	14.727878010
C	15.506638290	12.886016150	14.361978010
H	15.796738290	13.388416150	13.635178010
C	16.402538290	12.121216150	15.085378010
H	17.300438290	12.114216150	14.842678010
C	20.422738290	9.048716150	15.296678010
C	21.363238290	8.530416150	14.265378010
C	21.355238290	9.062216150	12.993678010
C	22.213538290	8.574316150	11.994878010
C	23.061738290	7.581616150	12.352378010
C	23.121038290	7.027916150	13.586678010
C	22.274938290	7.524216150	14.552778010
I	23.738938290	15.822116150	22.973978010
I	26.031338290	2.824216150	22.698278010
N	21.118838290	8.721116150	19.319478010
N	19.003438290	10.470116150	18.263978010
C	21.972238290	7.733516150	19.745778010
C	22.924738290	8.332916150	20.627378010
H	23.619738290	7.891216150	21.060278010
C	22.645938290	9.639516150	20.720278010
H	23.118838290	10.264316150	21.220878010

C	21.497438290	9.901216150	19.918478010
C	20.838538290	11.120116150	19.783178010
C	19.672038290	11.375016150	19.028378010
C	18.980138290	12.632716150	18.932978010
H	19.208238290	13.423816150	19.363878010
C	17.935538290	12.443616150	18.096078010
H	17.324938290	13.095716150	17.835678010
C	17.924538290	11.086316150	17.683078010
C	21.871838290	6.366116150	19.442578010
C	21.476238290	12.286616150	20.517478010
C	20.972538290	12.752616150	21.704578010
H	20.188038290	12.384716150	22.040578010
C	21.609438290	13.763816150	22.419478010
H	21.266038290	14.059916150	23.231778010
C	22.752338290	14.315916150	21.902678010
C	23.250838290	13.870216150	20.725178010
H	24.029438290	14.245316150	20.380978010
C	22.603438290	12.853916150	20.025878010
H	22.949138290	12.561316150	19.213978010
C	22.858138290	5.469616150	20.136978010
C	24.179338290	5.439316150	19.774678010
H	24.470938290	5.944116150	19.049778010
C	25.091038290	4.657616150	20.484878010
H	25.983338290	4.623616150	20.225278010
C	24.658838290	3.940116150	21.568078010
C	23.334338290	3.951916150	21.934078010
H	23.044238290	3.449516150	22.660778010
C	22.438338290	4.716716150	21.210678010
H	21.540438290	4.723716150	21.453278010
O	18.201338290	8.272116150	19.820578010
O	19.309238290	7.007616150	21.280678010

C	18.418238290	7.789216150	20.999278010
C	17.477738290	8.307516150	22.030678010
C	17.485738290	7.775716150	23.302278010
C	16.627438290	8.263616150	24.301078010
C	15.779138290	9.256316150	23.943578010
C	15.719938290	9.810016150	22.709378010
C	16.566038290	9.313716150	21.743178010
F	3.668760480	7.813179720	13.414379790
F	1.879281990	10.857252440	10.293052240
F	11.002560200	6.068993400	1.717552520
F	9.213062940	9.113087980	-1.403635810
F	16.648337060	7.769012020	25.557035810
F	14.858772460	10.813015930	22.435727030
F	23.982136780	6.024825700	13.860208540
F	22.192639520	9.068920280	10.738920210
H	10.728498680	7.220067740	-0.540306650
H	2.153224740	9.706199960	12.550950630
H	15.132801320	9.662032260	24.693606650
H	23.708075260	7.175900040	11.602349370
H	9.342908910	7.170852490	3.402396180
H	7.703660990	9.906527120	0.620618460
H	5.178162430	7.019740580	11.390125520
H	3.538914520	9.755415210	8.608347790
H	20.683237570	9.862359420	12.763274480
H	22.322490220	7.126645120	15.545036090
H	18.157723450	6.975591410	23.532791240
H	16.518486360	9.711287180	20.750919940

Coordinates for dimer model of compound 4

Sn	6.456591200	8.448969780	6.026547990
I	2.138091200	1.045769780	1.200647990
I	-0.154308800	14.043669780	1.476347990

N	4.758291200	8.146769780	4.855147990
N	6.873691200	6.397769780	5.910647990
O	7.675691200	8.595769780	4.353947990
O	6.567891200	9.860269780	2.893847990
C	3.904891200	9.134369780	4.428847990
C	2.952391200	8.534969780	3.547247990
H	2.257391200	8.976669780	3.114247990
C	3.231191200	7.228369780	3.454247990
H	2.758291200	6.603569780	2.953647990
C	4.379691200	6.966669780	4.256147990
C	5.038491200	5.747769780	4.391447990
C	6.205091200	5.492869780	5.146147990
C	6.896991200	4.235169780	5.241647990
H	6.668791200	3.444069780	4.810747990
C	7.941591200	4.424269780	6.078547990
H	8.552191200	3.772169780	6.338947990
C	7.952591200	5.781569780	6.491547990
C	4.005291200	10.501769780	4.731947990
C	4.400791200	4.581269780	3.657147990
C	4.904591200	4.115269780	2.470047990
H	5.689091200	4.483169780	2.134047990
C	4.267591200	3.104069780	1.755047990
H	4.611091200	2.807969780	0.942847990
C	3.124691200	2.551969780	2.271947990
C	2.626291200	2.997669780	3.449447990
H	1.847691200	2.622569780	3.793547990
C	3.273591200	4.013969780	4.148647990
H	2.927891200	4.306569780	4.960547990
C	3.018991200	11.398269780	4.037547990
C	1.697691200	11.428569780	4.399847990
H	1.406191200	10.923769780	5.124747990

C	0.786091200	12.210269780	3.689747990
H	-0.106208800	12.244269780	3.949347990
C	1.218291200	12.927769780	2.606447990
C	2.542791200	12.915969780	2.240547990
H	2.832891200	13.418369780	1.513847990
C	3.438691200	12.151169780	2.963947990
H	4.336591200	12.144169780	2.721247990
C	7.458891200	9.078669780	3.175247990
C	8.399391200	8.560369780	2.143947990
C	8.391391200	9.092169780	0.872247990
C	9.249691200	8.604269780	-0.126452010
C	10.097891200	7.611569780	0.230947990
C	10.157191200	7.057869780	1.465247990
C	9.311091200	7.554169780	2.431347990
I	10.775091200	15.852069780	10.852547990
I	13.067591200	2.854169780	10.576847990
N	8.154991200	8.751069780	7.198047990
N	6.039591200	10.500069780	6.142547990
C	9.008391200	7.763469780	7.624347990
C	9.960891200	8.362869780	8.505947990
H	10.655891200	7.921169780	8.938847990
C	9.682091200	9.669469780	8.598947990
H	10.154991200	10.294269780	9.099447990
C	8.533591200	9.931169780	7.797047990
C	7.874791200	11.150069780	7.661747990
C	6.708191200	11.404969780	6.906947990
C	6.016291200	12.662669780	6.811547990
H	6.244491200	13.453769780	7.242447990
C	4.971691200	12.473569780	5.974647990
H	4.361091200	13.125669780	5.714247990
C	4.960691200	11.116269780	5.561647990

C	8.907991200	6.396069780	7.321247990
C	8.512391200	12.316569780	8.396047990
C	8.008691200	12.782569780	9.583147990
H	7.224191200	12.414669780	9.919147990
C	8.645691200	13.793769780	10.298147990
H	8.302191200	14.089869780	11.110347990
C	9.788591200	14.345869780	9.781247990
C	10.286991200	13.900169780	8.603747990
H	11.065591200	14.275269780	8.259647990
C	9.639691200	12.883869780	7.904547990
H	9.985391200	12.591269780	7.092547990
C	9.894291200	5.499569780	8.015647990
C	11.215491200	5.469269780	7.653347990
H	11.507091200	5.974069780	6.928447990
C	12.127191200	4.687569780	8.363447990
H	13.019491200	4.653569780	8.103847990
C	11.694991200	3.970069780	9.446747990
C	10.370491200	3.981869780	9.812647990
H	10.080391200	3.479469780	10.539347990
C	9.474591200	4.746669780	9.089247990
H	8.576591200	4.753669780	9.331947990
O	5.237591200	8.302069780	7.699247990
O	6.345391200	7.037569780	9.159247990
C	5.454391200	7.819169780	8.877847990
C	4.513891200	8.337469780	9.909247990
C	4.521891200	7.805669780	11.180947990
C	3.663591200	8.293569780	12.179647990
C	2.815291200	9.286269780	11.822147990
C	2.756091200	9.839969780	10.587947990
C	3.602191200	9.343669780	9.621847990
Sn	19.404708800	8.433230220	18.126752010

I	15.086208800	1.030030220	13.300852010
I	12.793808800	14.027930220	13.576552010
N	17.706408800	8.131030220	16.955352010
N	19.821808800	6.382030220	18.010852010
O	20.623808800	8.580030220	16.454152010
O	19.516008800	9.844530220	14.994052010
C	16.853008800	9.118630220	16.529052010
C	15.900508800	8.519230220	15.647452010
H	15.205508800	8.960930220	15.214452010
C	16.179308800	7.212630220	15.554452010
H	15.706408800	6.587830220	15.053852010
C	17.327708800	6.950930220	16.356352010
C	17.986608800	5.732030220	16.491552010
C	19.153208800	5.477130220	17.246352010
C	19.845108800	4.219430220	17.341752010
H	19.616908800	3.428330220	16.910952010
C	20.889608800	4.408530220	18.178652010
H	21.500308800	3.756430220	18.439052010
C	20.900708800	5.765830220	18.591752010
C	16.953408800	10.486030220	16.832152010
C	17.348908800	4.565530220	15.757352010
C	17.852708800	4.099530220	14.570152010
H	18.637208800	4.467430220	14.234152010
C	17.215708800	3.088330220	13.855252010
H	17.559208800	2.792230220	13.043052010
C	16.072808800	2.536230220	14.372152010
C	15.574408800	2.981930220	15.549652010
H	14.795808800	2.606830220	15.893752010
C	16.221708800	3.998230220	16.248852010
H	15.876008800	4.290830220	17.060752010
C	15.967108800	11.382530220	16.137752010

C	14.645808800	11.412830220	16.500052010
H	14.354308800	10.908030220	17.224952010
C	13.734208800	12.194530220	15.789952010
H	12.841808800	12.228530220	16.049552010
C	14.166408800	12.912030220	14.706652010
C	15.490908800	12.900230220	14.340752010
H	15.781008800	13.402630220	13.613952010
C	16.386808800	12.135430220	15.064152010
H	17.284708800	12.128430220	14.821452010
C	20.407008800	9.062930220	15.275452010
C	21.347508800	8.544630220	14.244152010
C	21.339508800	9.076430220	12.972452010
C	22.197808800	8.588530220	11.973652010
C	23.046008800	7.595830220	12.331152010
C	23.105308800	7.042130220	13.565452010
C	22.259208800	7.538430220	14.531552010
I	23.723208800	15.836330220	22.952752010
I	26.015608800	2.838430220	22.677052010
N	21.103108800	8.735330220	19.298252010
N	18.987708800	10.484330220	18.242752010
C	21.956508800	7.747730220	19.724552010
C	22.909008800	8.347130220	20.606152010
H	23.604008800	7.905430220	21.039052010
C	22.630208800	9.653730220	20.699052010
H	23.103108800	10.278530220	21.199652010
C	21.481708800	9.915430220	19.897252010
C	20.822808800	11.134330220	19.761952010
C	19.656308800	11.389230220	19.007152010
C	18.964408800	12.646930220	18.911752010
H	19.192508800	13.438030220	19.342652010
C	17.919808800	12.457830220	18.074852010

H	17.309208800	13.109930220	17.814452010
C	17.908808800	11.100530220	17.661852010
C	21.856108800	6.380330220	19.421352010
C	21.460508800	12.300830220	20.496252010
C	20.956808800	12.766830220	21.683352010
H	20.172308800	12.398930220	22.019352010
C	21.593708800	13.778030220	22.398252010
H	21.250308800	14.074130220	23.210552010
C	22.736608800	14.330130220	21.881452010
C	23.235108800	13.884430220	20.703952010
H	24.013708800	14.259530220	20.359752010
C	22.587708800	12.868130220	20.004652010
H	22.933408800	12.575530220	19.192752010
C	22.842408800	5.483830220	20.115752010
C	24.163608800	5.453530220	19.753452010
H	24.455208800	5.958330220	19.028552010
C	25.075308800	4.671830220	20.463652010
H	25.967608800	4.637830220	20.204052010
C	24.643108800	3.954330220	21.546852010
C	23.318608800	3.966130220	21.912852010
H	23.028508800	3.463730220	22.639552010
C	22.422608800	4.730930220	21.189452010
H	21.524708800	4.737930220	21.432052010
O	18.185608800	8.286330220	19.799352010
O	19.293508800	7.021830220	21.259452010
C	18.402508800	7.803430220	20.978052010
C	17.462008800	8.321730220	22.009452010
C	17.470008800	7.789930220	23.281052010
C	16.611708800	8.277830220	24.279852010
C	15.763408800	9.270530220	23.922352010
C	15.704208800	9.824230220	22.688152010

C	16.550308800	9.327930220	21.721952010
F	9.371080660	7.052611520	3.683282730
F	7.543539820	10.101696330	0.581551950
F	10.913363070	7.099684960	-0.715349820
F	5.369742570	6.796143220	11.471644040
F	3.542201750	9.845228030	8.369913260
F	1.999819320	9.798154590	12.768445810
H	3.680155410	7.901550210	13.175110840
H	2.073605790	10.634994510	10.371039380
H	9.233126990	8.996289350	-1.121914850
H	10.839691480	6.262827720	1.682046270
H	22.181244590	8.980549790	10.978189160
H	23.787809090	6.247088170	13.782250280
H	16.628273010	7.885810650	25.275314850
H	15.021655150	10.619200420	22.471258270
F	20.491657430	10.085956780	12.681755960
F	22.319204230	7.036821920	15.783466400
F	23.861480680	7.083945410	11.384854190
F	16.490313380	9.829538540	20.470037610
F	18.317840550	6.780427050	23.571886450
F	14.947936930	9.782415040	24.868649820

Coordinates for dimer model of compound 6

Sn	6.46530000	8.44110000	6.03830000
I	2.14680000	1.03790000	1.21240000
I	-0.14560000	14.03580000	1.48810000
N	4.76700000	8.13890000	4.86690000
N	6.88240000	6.38990000	5.92240000
O	7.68440000	8.58790000	4.36570000
O	6.57660000	9.85240000	2.90560000
C	3.91360000	9.12650000	4.44060000
C	2.96110000	8.52710000	3.55900000

H	2.26610000	8.96880000	3.12600000
C	3.23990000	7.22050000	3.46600000
H	2.76700000	6.59570000	2.96540000
C	4.38840000	6.95880000	4.26790000
C	5.04720000	5.73990000	4.40320000
C	6.21380000	5.48500000	5.15790000
C	6.90570000	4.22730000	5.25340000
H	6.67750000	3.43620000	4.82250000
C	7.95030000	4.41640000	6.09030000
H	8.56090000	3.76430000	6.35070000
C	7.96130000	5.77370000	6.50330000
C	4.01400000	10.49390000	4.74370000
C	4.40950000	4.57340000	3.66890000
C	4.91330000	4.10740000	2.48180000
H	5.69780000	4.47530000	2.14580000
C	4.27630000	3.09620000	1.76680000
H	4.61980000	2.80010000	0.95460000
C	3.13340000	2.54410000	2.28370000
C	2.63500000	2.98980000	3.46120000
H	1.85640000	2.61470000	3.80530000
C	3.28230000	4.00610000	4.16040000
H	2.93660000	4.29870000	4.97230000
C	3.02770000	11.39040000	4.04930000
C	1.70640000	11.42070000	4.41160000
H	1.41490000	10.91590000	5.13650000
C	0.79480000	12.20240000	3.70150000
H	-0.09750000	12.23640000	3.96110000
C	1.22700000	12.91990000	2.61820000
C	2.55150000	12.90810000	2.25230000
H	2.84160000	13.41050000	1.52560000
C	3.44740000	12.14330000	2.97570000

H	4.34530000	12.13630000	2.73300000
C	7.46760000	9.07080000	3.18700000
C	8.40810000	8.55250000	2.15570000
C	8.40010000	9.08430000	0.88400000
C	9.25840000	8.59640000	-0.11470000
C	10.10660000	7.60370000	0.24270000
C	10.16590000	7.05000000	1.47700000
C	9.31980000	7.54630000	2.44310000
I	10.78380000	15.84420000	10.86430000
I	13.07630000	2.84630000	10.58860000
N	8.16370000	8.74320000	7.20980000
N	6.04830000	10.49220000	6.15430000
C	9.01710000	7.75560000	7.63610000
C	9.96960000	8.35500000	8.51770000
H	10.66460000	7.91330000	8.95060000
C	9.69080000	9.66160000	8.61070000
H	10.16370000	10.28640000	9.11120000
C	8.54230000	9.92330000	7.80880000
C	7.88350000	11.14220000	7.67350000
C	6.71690000	11.39710000	6.91870000
C	6.02500000	12.65480000	6.82330000
H	6.25320000	13.44590000	7.25420000
C	4.98040000	12.46570000	5.98640000
H	4.36980000	13.11780000	5.72600000
C	4.96940000	11.10840000	5.57340000
C	8.91670000	6.38820000	7.33300000
C	8.52110000	12.30870000	8.40780000
C	8.01740000	12.77470000	9.59490000
H	7.23290000	12.40680000	9.93090000
C	8.65440000	13.78590000	10.30990000
H	8.31090000	14.08200000	11.12210000

C	9.79730000	14.33800000	9.79300000
C	10.29570000	13.89230000	8.61550000
H	11.07430000	14.26740000	8.27140000
C	9.64840000	12.87600000	7.91630000
H	9.99410000	12.58340000	7.10430000
C	9.90300000	5.49170000	8.02740000
C	11.22420000	5.46140000	7.66510000
H	11.51580000	5.96620000	6.94020000
C	12.13590000	4.67970000	8.37520000
H	13.02820000	4.64570000	8.11560000
C	11.70370000	3.96220000	9.45850000
C	10.37920000	3.97400000	9.82440000
H	10.08910000	3.47160000	10.55110000
C	9.48330000	4.73880000	9.10100000
H	8.58530000	4.74580000	9.34370000
O	5.24630000	8.29420000	7.71100000
O	6.35410000	7.02970000	9.17100000
C	5.46310000	7.81130000	8.88960000
C	4.52260000	8.32960000	9.92100000
C	4.53060000	7.79780000	11.19270000
C	3.67230000	8.28570000	12.19140000
C	2.82400000	9.27840000	11.83390000
C	2.76480000	9.83210000	10.59970000
C	3.61090000	9.33580000	9.63360000
Sn	19.39600000	8.44110000	18.11500000
I	15.07750000	1.03790000	13.28910000
I	12.78510000	14.03580000	13.56480000
N	17.69770000	8.13890000	16.94360000
N	19.81310000	6.38990000	17.99910000
O	20.61510000	8.58790000	16.44240000
O	19.50730000	9.85240000	14.98230000

C	16.84430000	9.12650000	16.51730000
C	15.89180000	8.52710000	15.63570000
H	15.19680000	8.96880000	15.20270000
C	16.17060000	7.22050000	15.54270000
H	15.69770000	6.59570000	15.04210000
C	17.31900000	6.95880000	16.34460000
C	17.97790000	5.73990000	16.47980000
C	19.14450000	5.48500000	17.23460000
C	19.83640000	4.22730000	17.33000000
H	19.60820000	3.43620000	16.89920000
C	20.88090000	4.41640000	18.16690000
H	21.49160000	3.76430000	18.42730000
C	20.89200000	5.77370000	18.58000000
C	16.94470000	10.49390000	16.82040000
C	17.34020000	4.57340000	15.74560000
C	17.84400000	4.10740000	14.55840000
H	18.62850000	4.47530000	14.22240000
C	17.20700000	3.09620000	13.84350000
H	17.55050000	2.80010000	13.03130000
C	16.06410000	2.54410000	14.36040000
C	15.56570000	2.98980000	15.53790000
H	14.78710000	2.61470000	15.88200000
C	16.21300000	4.00610000	16.23710000
H	15.86730000	4.29870000	17.04900000
C	15.95840000	11.39040000	16.12600000
C	14.63710000	11.42070000	16.48830000
H	14.34560000	10.91590000	17.21320000
C	13.72550000	12.20240000	15.77820000
H	12.83310000	12.23640000	16.03780000
C	14.15770000	12.91990000	14.69490000
C	15.48220000	12.90810000	14.32900000

H	15.77230000	13.41050000	13.60220000
C	16.37810000	12.14330000	15.05240000
H	17.27600000	12.13630000	14.80970000
C	20.39830000	9.07080000	15.26370000
C	21.33880000	8.55250000	14.23240000
C	21.33080000	9.08430000	12.96070000
C	22.18910000	8.59640000	11.96190000
C	23.03730000	7.60370000	12.31940000
C	23.09660000	7.05000000	13.55370000
C	22.25050000	7.54630000	14.51980000
I	23.71450000	15.84420000	22.94100000
I	26.00690000	2.84630000	22.66530000
N	21.09440000	8.74320000	19.28650000
N	18.97900000	10.49220000	18.23100000
C	21.94780000	7.75560000	19.71280000
C	22.90030000	8.35500000	20.59440000
H	23.59530000	7.91330000	21.02730000
C	22.62150000	9.66160000	20.68730000
H	23.09440000	10.28640000	21.18790000
C	21.47300000	9.92330000	19.88550000
C	20.81410000	11.14220000	19.75020000
C	19.64760000	11.39710000	18.99540000
C	18.95570000	12.65480000	18.90000000
H	19.18380000	13.44590000	19.33090000
C	17.91110000	12.46570000	18.06310000
H	17.30050000	13.11780000	17.80270000
C	17.90010000	11.10840000	17.65010000
C	21.84740000	6.38820000	19.40960000
C	21.45180000	12.30870000	20.48450000
C	20.94810000	12.77470000	21.67160000
H	20.16360000	12.40680000	22.00760000

C	21.58500000	13.78590000	22.38650000
H	21.24160000	14.08200000	23.19880000
C	22.72790000	14.33800000	21.86970000
C	23.22640000	13.89230000	20.69220000
H	24.00500000	14.26740000	20.34800000
C	22.57900000	12.87600000	19.99290000
H	22.92470000	12.58340000	19.18100000
C	22.83370000	5.49170000	20.10400000
C	24.15490000	5.46140000	19.74170000
H	24.44650000	5.96620000	19.01680000
C	25.06660000	4.67970000	20.45190000
H	25.95890000	4.64570000	20.19230000
C	24.63440000	3.96220000	21.53510000
C	23.30990000	3.97400000	21.90110000
H	23.01980000	3.47160000	22.62780000
C	22.41390000	4.73880000	21.17770000
H	21.51600000	4.74580000	21.42030000
O	18.17690000	8.29420000	19.78760000
O	19.28480000	7.02970000	21.24770000
C	18.39380000	7.81130000	20.96630000
C	17.45330000	8.32960000	21.99770000
C	17.46130000	7.79780000	23.26930000
C	16.60300000	8.28570000	24.26810000
C	15.75470000	9.27840000	23.91060000
C	15.69550000	9.83210000	22.67640000
C	16.54160000	9.33580000	21.71020000
F	5.37845137	6.78827345	11.48339604
F	3.69319877	7.79109587	13.44735780
F	1.90372028	10.83516859	10.32603025
F	3.55091055	9.83735826	8.38166527
F	9.37978945	7.04474174	3.69503473

F	11.02699849	6.04690955	1.75053053
F	9.23750123	9.09100413	-1.37065780
F	7.55224863	10.09382655	0.59330396
F	18.30913174	6.78829682	23.56013444
F	16.62389877	7.79109587	25.52405780
F	14.83433417	10.83509978	22.40274902
F	16.48160457	9.83740831	20.45828560
F	23.95769849	6.04690955	13.82723053
F	22.31049543	7.04469169	15.77171440
F	20.48294863	10.09382655	12.67000396
F	22.16820123	9.09100413	10.70594220
H	10.75293697	7.19798389	-0.50732864
H	2.17766303	9.68411611	12.58392864
H	15.10836303	9.68411611	24.66062864
H	23.68363697	7.19798389	11.56937136

Coordinates for dimer model of compound 7

Sn	6.439084090	8.464790210	6.002923200
I	2.120584090	1.061590210	1.177023200
I	-0.171815910	14.059490210	1.452723200
N	4.740784090	8.162590210	4.831523200
N	6.856184090	6.413590210	5.887023200
O	7.658184090	8.611590210	4.330323200
O	6.550384090	9.876090210	2.870223200
F	10.908784090	7.107390210	-0.753976800
C	3.887384090	9.150190210	4.405223200
C	2.934884090	8.550790210	3.523623200
H	2.239884090	8.992490210	3.090623200
C	3.213684090	7.244190210	3.430623200
H	2.740784090	6.619390210	2.930023200
C	4.362184090	6.982490210	4.232523200
C	5.020984090	5.763590210	4.367823200

C	6.187584090	5.508690210	5.122523200
C	6.879484090	4.250990210	5.218023200
H	6.651284090	3.459890210	4.787123200
C	7.924084090	4.440090210	6.054923200
H	8.534684090	3.787990210	6.315323200
C	7.935084090	5.797390210	6.467923200
C	3.987784090	10.517590210	4.708323200
C	4.383284090	4.597090210	3.633523200
C	4.887084090	4.131090210	2.446423200
H	5.671584090	4.498990210	2.110423200
C	4.250084090	3.119890210	1.731423200
H	4.593584090	2.823790210	0.919223200
C	3.107184090	2.567790210	2.248323200
C	2.608784090	3.013490210	3.425823200
H	1.830184090	2.638390210	3.769923200
C	3.256084090	4.029790210	4.125023200
H	2.910384090	4.322390210	4.936923200
C	3.001484090	11.414090210	4.013923200
C	1.680184090	11.444390210	4.376223200
H	1.388684090	10.939590210	5.101123200
C	0.768584090	12.226090210	3.666123200
H	-0.123715910	12.260090210	3.925723200
C	1.200784090	12.943590210	2.582823200
C	2.525284090	12.931790210	2.216923200
H	2.815384090	13.434190210	1.490223200
C	3.421184090	12.166990210	2.940323200
H	4.319084090	12.159990210	2.697623200
C	7.441384090	9.094490210	3.151623200
C	8.381884090	8.576190210	2.120323200
C	8.373884090	9.107990210	0.848623200
C	9.232184090	8.620090210	-0.150076800

C	10.080384090	7.627390210	0.207323200
C	10.139684090	7.073690210	1.441623200
C	9.293584090	7.569990210	2.407723200
I	10.757584090	15.867890210	10.828923200
I	13.050084090	2.869990210	10.553223200
N	8.137484090	8.766890210	7.174423200
N	6.022084090	10.515890210	6.118923200
C	8.990884090	7.779290210	7.600723200
C	9.943384090	8.378690210	8.482323200
H	10.638384090	7.936990210	8.915223200
C	9.664584090	9.685290210	8.575323200
H	10.137484090	10.310090210	9.075823200
C	8.516084090	9.946990210	7.773423200
C	7.857284090	11.165890210	7.638123200
C	6.690684090	11.420790210	6.883323200
C	5.998784090	12.678490210	6.787923200
H	6.226984090	13.469590210	7.218823200
C	4.954184090	12.489390210	5.951023200
H	4.343584090	13.141490210	5.690623200
C	4.943184090	11.132090210	5.538023200
C	8.890484090	6.411890210	7.297623200
C	8.494884090	12.332390210	8.372423200
C	7.991184090	12.798390210	9.559523200
H	7.206684090	12.430490210	9.895523200
C	8.628184090	13.809590210	10.274523200
H	8.284684090	14.105690210	11.086723200
C	9.771084090	14.361690210	9.757623200
C	10.269484090	13.915990210	8.580123200
H	11.048084090	14.291090210	8.236023200
C	9.622184090	12.899690210	7.880923200
H	9.967884090	12.607090210	7.068923200

C	9.876784090	5.515390210	7.992023200
C	11.197984090	5.485090210	7.629723200
H	11.489584090	5.989890210	6.904823200
C	12.109684090	4.703390210	8.339823200
H	13.001984090	4.669390210	8.080223200
C	11.677484090	3.985890210	9.423123200
C	10.352984090	3.997690210	9.789023200
H	10.062884090	3.495290210	10.515723200
C	9.457084090	4.762490210	9.065623200
H	8.559084090	4.769490210	9.308323200
O	5.220084090	8.317890210	7.675623200
O	6.327884090	7.053390210	9.135623200
F	1.969384090	9.822090210	12.759823200
C	5.436884090	7.834990210	8.854223200
C	4.496384090	8.353290210	9.885623200
C	4.504384090	7.821490210	11.157323200
C	3.646084090	8.309390210	12.156023200
C	2.797784090	9.302090210	11.798523200
C	2.738584090	9.855790210	10.564323200
C	3.584684090	9.359490210	9.598223200
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N	-6.022084090	6.366209790	-6.118923200
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H	-2.740784090	10.262709790	-2.930023200
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C	-6.187584090	11.373409790	-5.122523200
C	-6.879484090	12.631109790	-5.218023200
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C	-2.525284090	3.950309790	-2.216923200
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F	-9.211285320	7.767405660	1.406034600
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F	-11.000782580	10.811500240	-1.715153730
F	-3.524694640	7.021051530	-8.346288470
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F	9.353573540	7.068431950	3.659657930
F	11.000782580	6.070599760	1.715153730
F	7.526032720	10.117516760	0.557927160
F	9.211285320	9.114694340	-1.406034600
F	5.352235460	6.811963660	11.448019240
F	3.666982860	7.814786080	13.411981000
F	1.877504370	10.858858800	10.290653450
F	3.524694640	9.861048470	8.346288470

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