Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Computational insight into the halogen bonded self-assembly of hexa-coordinated metalloporphyrins

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EXPERIMENTAL SECTION

Materials: Pyrrole, 4-iodobenzaldehyde, 4-chlorobenzoic acid,3-bromobenzoic acid were obtained from TCI chemicals. Solvents likepropionic acid, chloroform, dimethylformamide (DMF), Diethyl ether, hexane were obtainedcommercial sources and purified by standard procedures before use.Free-base porphyrins were prepared following the Adlermethod.[1]Sn(TIPP)$(OH)_2$ were prepared by literature methods.[2]

Physical Measurements.

UV-vis spectra were recorded on a Perkin Elmer UV-Vis-NIR spectrometer. IR spectra were recorded on a Bruker Tensor 27 system spectrophotometer in ATR mode.

General procedure of synthesis of the complexes:

A mixture of *trans*-Dihydroxo[5,10,15,20-tetrakis(4-iodophenyl)porphyrinato]tin(IV) (0.01 mmol) was dissolve in 5 ml of $CHCl_3$ and corresponding halogenated carboxylic acid (0.025 mmol) was dissolve in 0.5 mL of DMF . The resulting solution was heated for 1 h at 70 °Cin bath reactor. After cooling, themixture was left for slow evaporation at ambient conditions dark red solid was precipitated out. Filter the solid and wash with hexane. All the complexes were isolated in morethan 60% yield.

Compound 1.X-rayquality crystals were obtained by slow evaporation of DMF-$CHCl_3$ (1:10) solution of **1** into the diethyl ether. After 7 days fine pink crystal of complex were obtained. Yield (7.9 mg, 78%). FT-IR (KBr, cm^{-1}) 2928, 1656, 1460, 1252, 1052, 796, 754, 672, 524, 462. UV-Vis in $CHCl_3$: λ_{max}/nm (log e) 424(5.48), 554(2.98), 592(2.15).

Compound 2.X-rayquality crystals were obtained diffusion of DMF-$CHCl_3$ (1:10) solution ofcompound **2** into the hexane. After 7 days fine pink crystal of complex were obtained. Yield (7.9 mg, 78%). FT-IR (KBr, cm^{-1}) 2914, 1664, 1466, 1210, 1032, 794, 754, 672, 561, 454. UV-Vis in $CHCl_3$: λ_{max}/nm (log e) 425(5.46), 558(2.92), 598(2.12).

***Computational Details*:**

DFT calculations have been carried out by employing a B3LYP hybrid functional using, Gaussian 09, revision B.05, package.[5] Using the method of Becke's three-parameter hybrid exchange functional,[6] the nonlocal correlation provided by the Lee, Yang, and Parr expression,[7] and Vosko, Wilk, and Nussair 1980 correlation functional (III) for local correction. The basis set was LANL2DZ for the Sn and I and Br -atom and 6-31G* for C, N, O, Cl and F and H-atom. The coordinates are taken directly from the single-crystal X-ray data. Geometry optimization of **Model-I** and **Model-II** were performed in the gas phase by varying different functional and basis set. We have chose CAM-B3LYP, M062X, OPBE, PBE0 as different hybrid functional and varying different basis set from 6-31G* to def2-TZVPP triple-ζvalence pseudopotential basis set to carry out the same calculation. The optimized geometries were confirmed to be the potential energy minima by vibrational frequency calculations at the same level of theory as no imaginary frequencies were found. The ^{1}H and ^{127}I NMR spectra of **Model-I** chemical shifts were calculated from the optimized geometries by GIAO method and suggest the occurrence of the ring current effect in these systems. Molecularelectrostatic potential surfaces were calculated from optimized geometry. $V_{S,max}$and $V_{S,min}$were calculated using the Multiwfn 3.3 program[8] from the optimized geometry of the model complexes.

For interaction energy calculation the primary coordinates for the dimer molecules under study were taken from their respective experimentally determined crystal structures of compound **2**. For simplicity, we have replaced Sn metal with Zn and remove the axial ligands and only consider Type-II halogen bond interaction as observed in X-ray structure of compound 2. Dimer structure was optimized in gas phase. Frequency calculations were

carried out on all of the optimized geometries ensured that there were no imaginary frequencies. Basis set superposition error (BSSE)-corrected interaction energies of fully optimized complexes were calculated at B3LYP/6-31G*(d,p) using the counterpoise method using Gaussian 09. Noncovalent Interaction−Reduced Density Gradient (NCI-RDG) Analysis (NCI-RDG) analysis was performed using the Multiwfn program.[8]

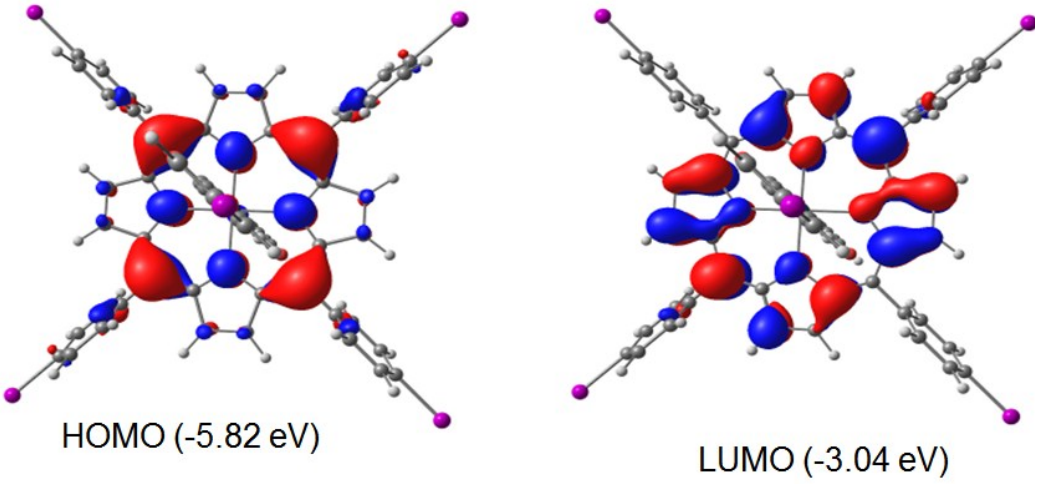

Figure S1. HOMO (*left*) and LUMO (*right*) with its energy (in eV) in the **ModelI**, computational level: B3LYP/6-31G*(d,p)

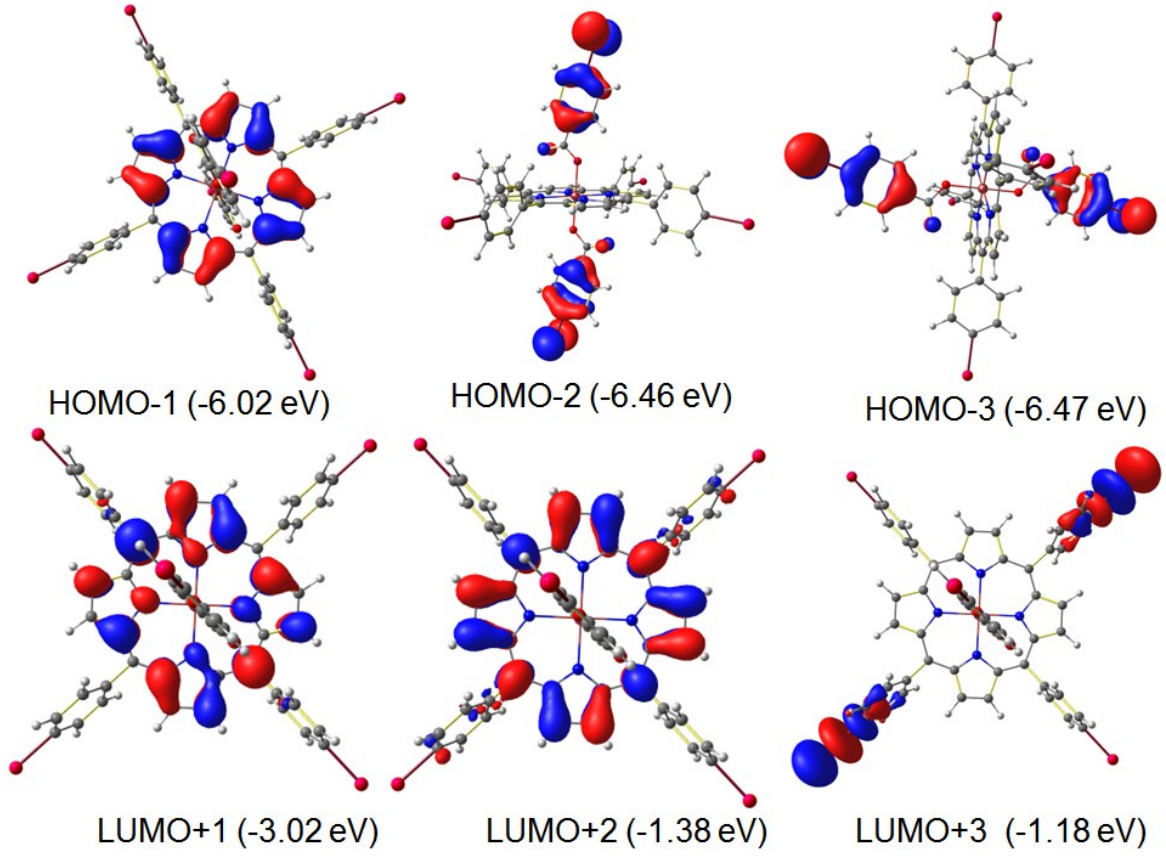

Figure S2. Different HOMO and LUMO label with its energy (in eV) in the **Model I**, computational level: B3LYP/6-31G*(d,p)

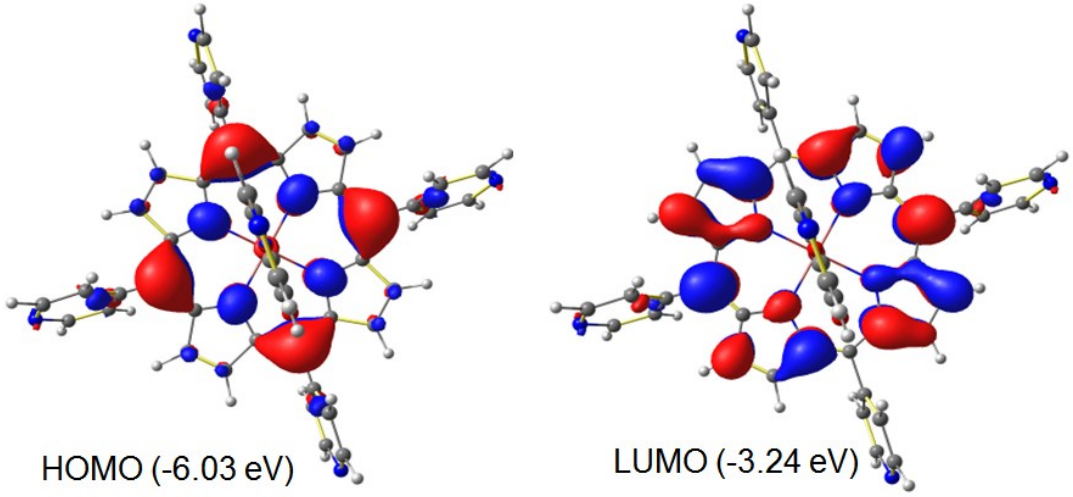

Figure S3. HOMO (*left*) and LUMO (*right*) with its energy (in eV) in the **Model II,** computational level: B3LYP/6-31G*(d,p)

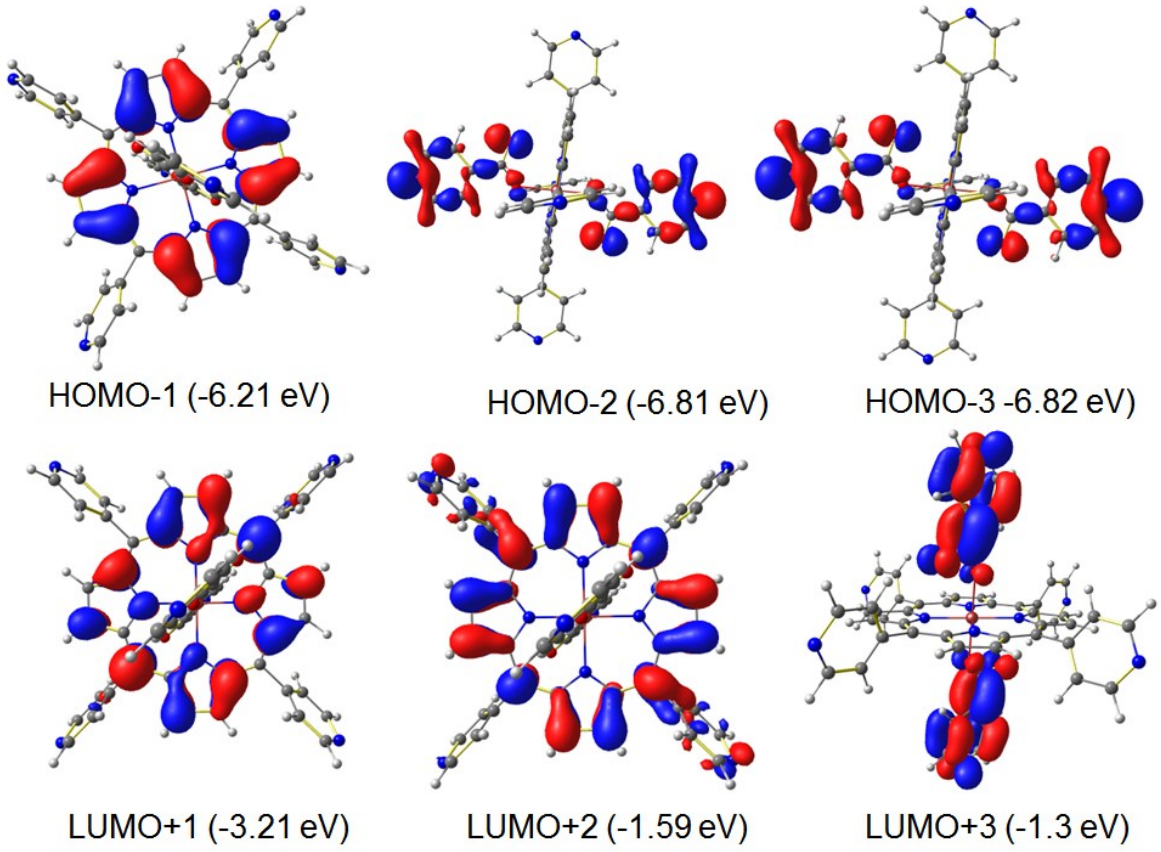

Figure S4. Different HOMO and LUMO label and its energy (in eV) in the **Model II,** computational level: B3LYP/6-31G*(d,p)

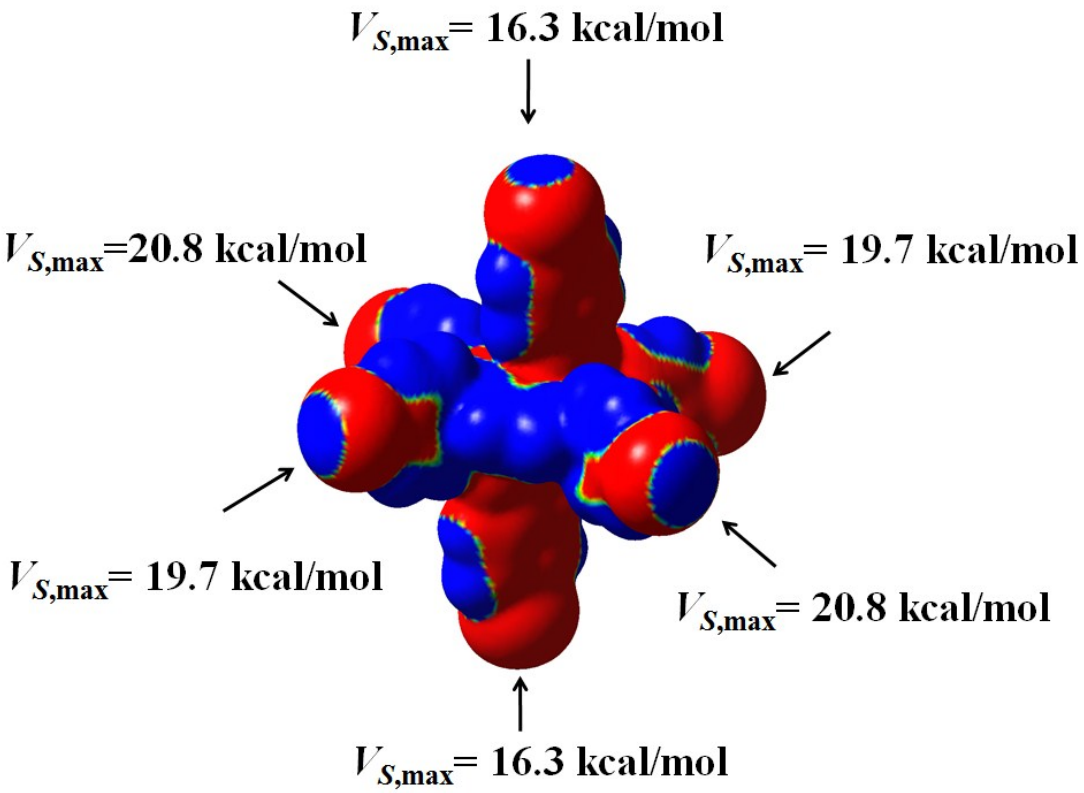

Figure S5. Computed electrostatic potential on the 0.001 au molecular surface of Sn(IV)L_2-5,10,15,20-meso-tetrakis(4-iodophenyl)porphyrin; (L= 4-iodo-benzoate), **ModelI**.Computational level: B3LYP/6-31G*(d,p)

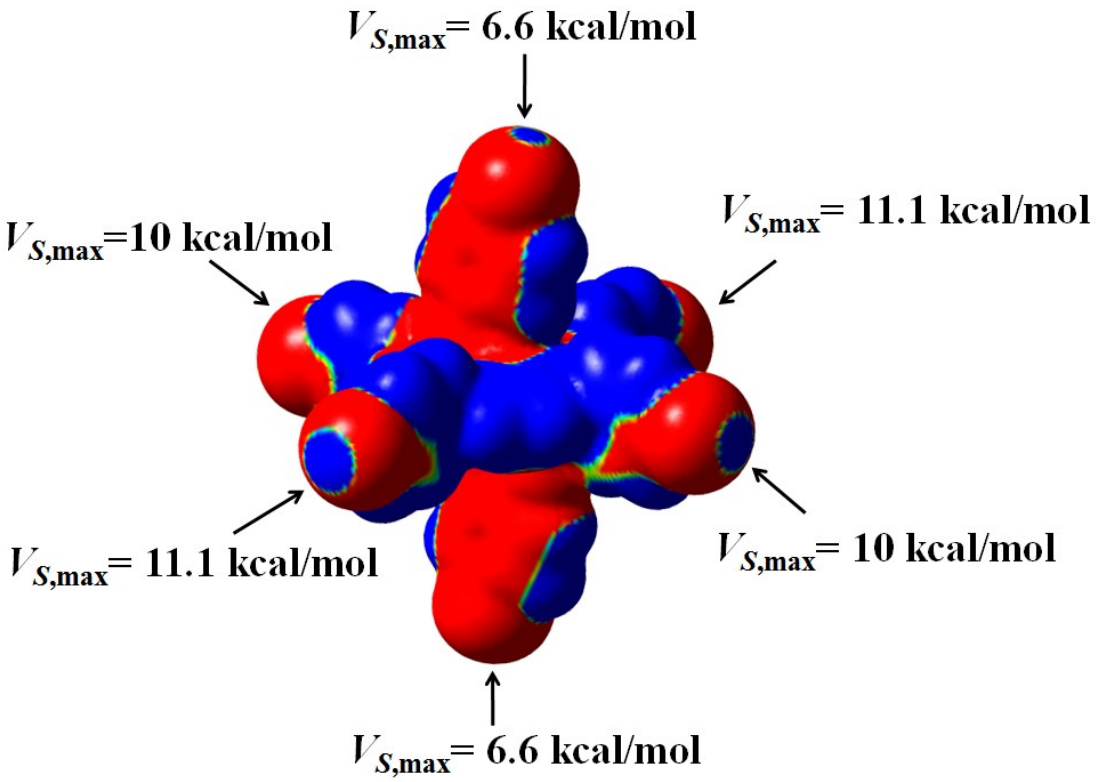

Figure S6. Computed electrostatic potential on the 0.001 au molecular surface of Sn(IV)L_2-5,10,15,20-meso-tetrakis(4-bromophenyl)porphyrin; (L= 4-bromo-benzoate), **ModelI**.Computational level: B3LYP/6-31G*(d,p)

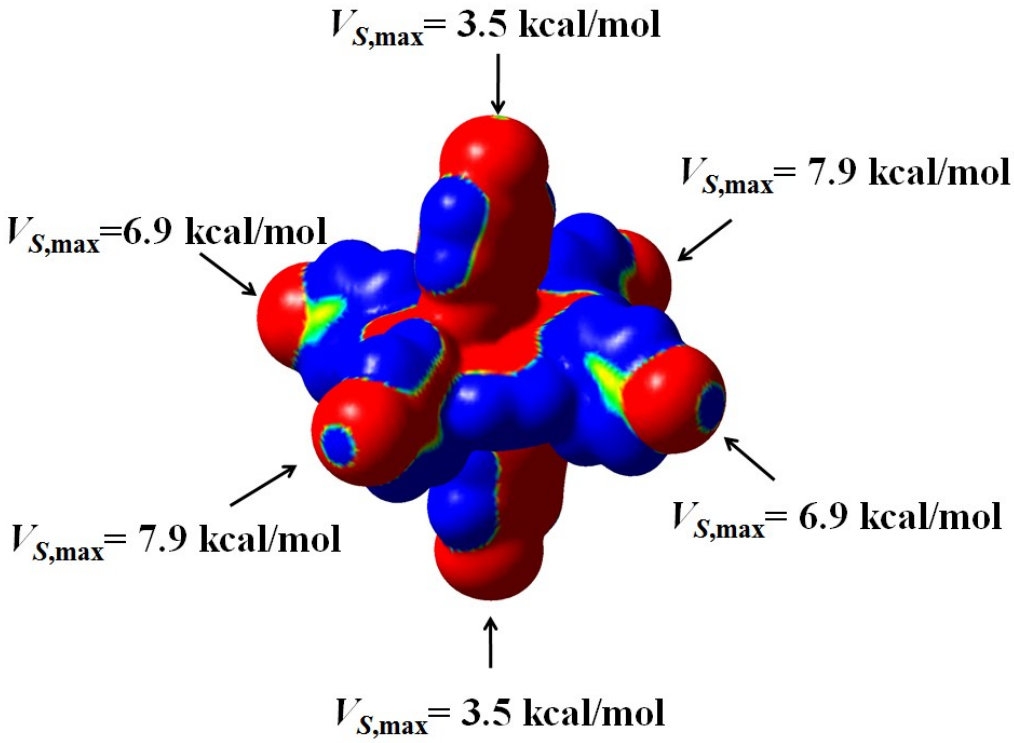

Figure S7. Computed electrostatic potential on the 0.001 au molecular surface of Sn(IV)L_2-5,10,15,20-meso-tetrakis(4-chlorophenyl)porphyrin; (L= 4-chloro-benzoate), **ModelI**.Computational level: B3LYP/6-31G*(d,p)

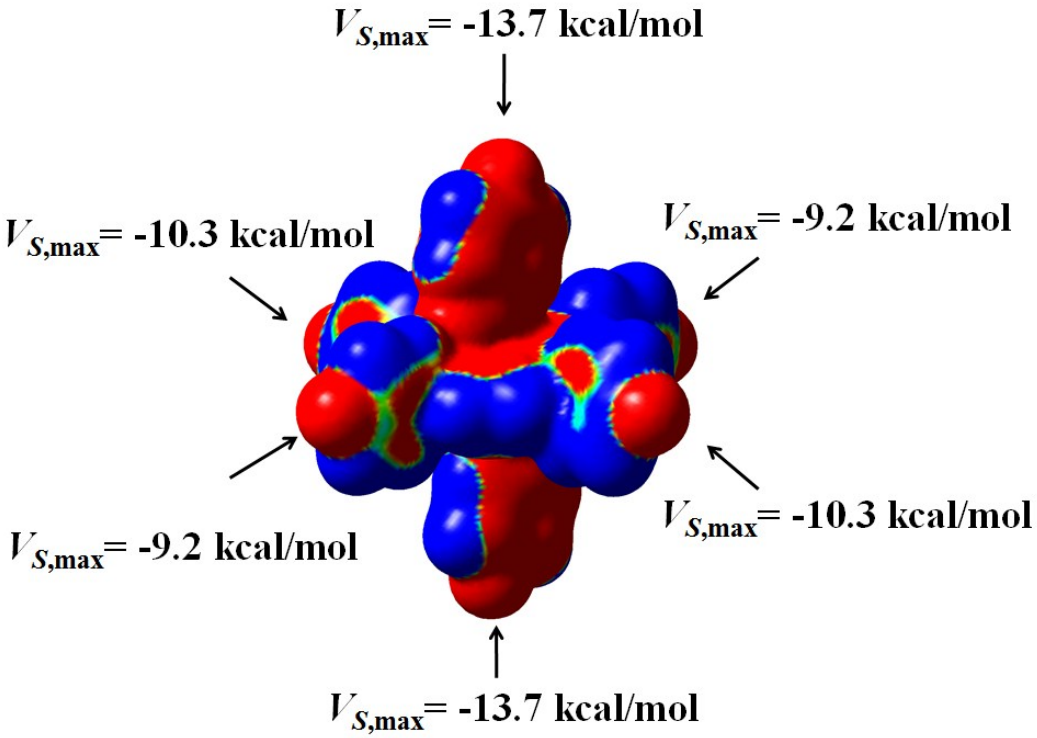

Figure S8. Computed electrostatic potential on the 0.001 au molecular surface of Sn(IV)L_2-5,10,15,20-meso-tetrakis(4-fluorophenyl)porphyrin; (L= 4-fluoro-benzoate), **ModelI**.Computational level: B3LYP/6-31G*(d,p)

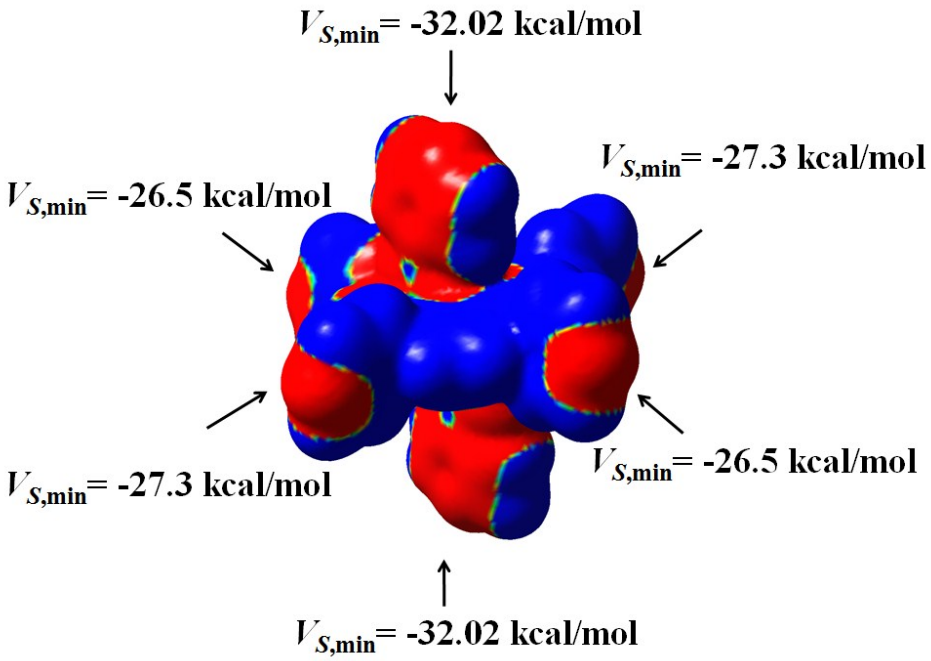

Figure S9. Computed electrostatic potential on the 0.001 au molecular surface of Sn(IV)L_2-5,10,15,20-meso-tetrakis(4-pyridyl)porphyrin; (L= isonicontinate), **ModelII**.Computational level: B3LYP/6-31G*(d,p)

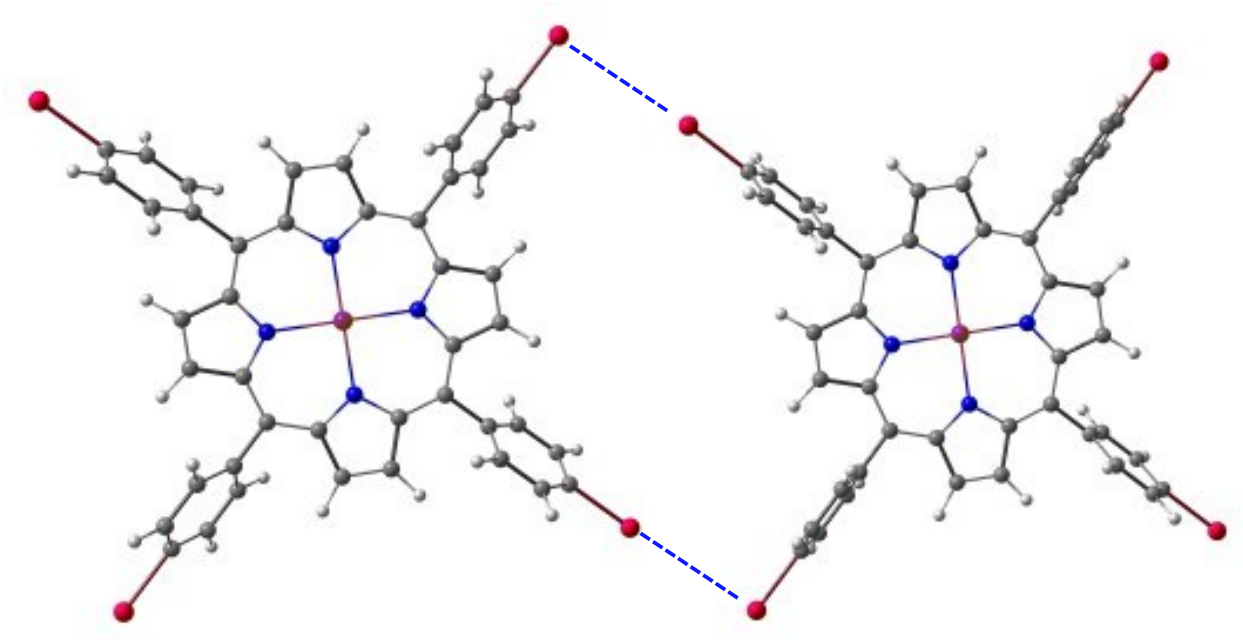

Figure-S10: Optimized geometry of Zn(TIPP) dimer with Type-II halogen bond interaction. Computational level: B3LYP/6-31G*(d,p)

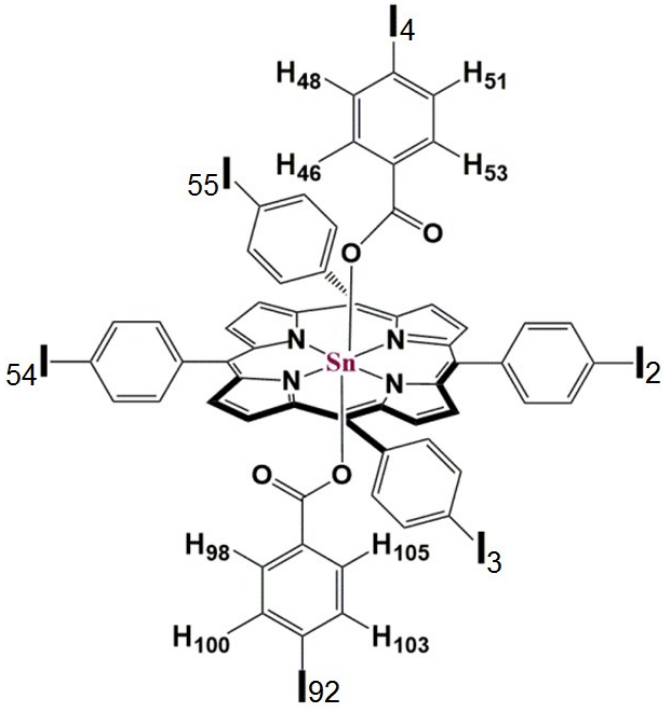

Figure S11. The numbering schemes that are used in the ^{1}H NMR assignment of **Model I**.

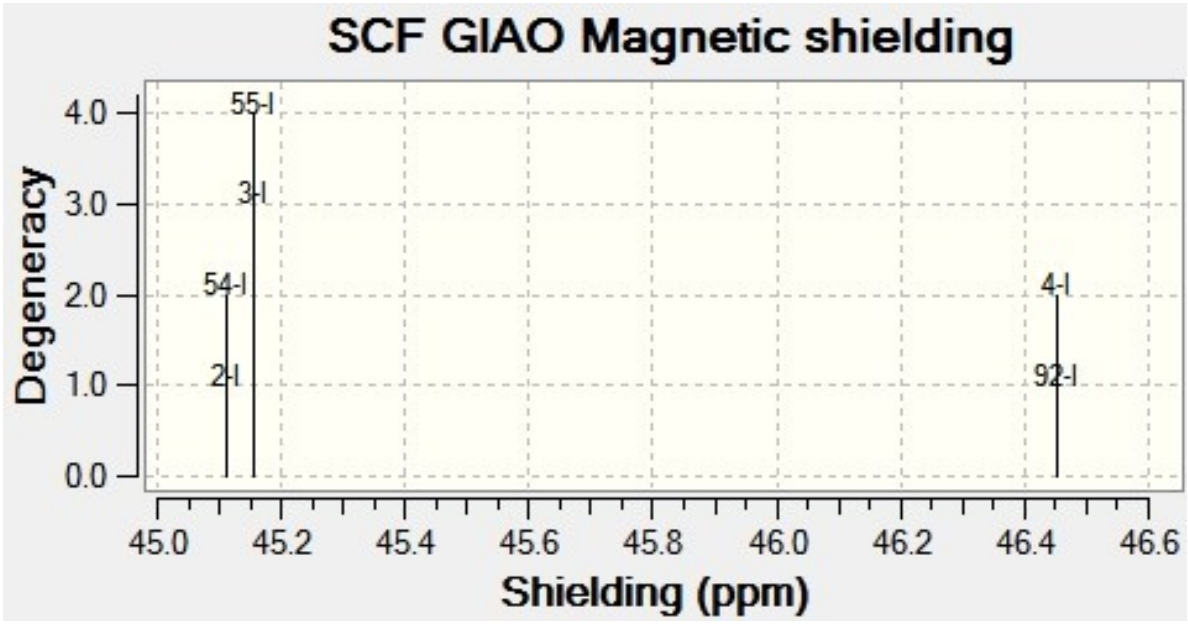

Figure S12. Calculated ^{127}I NMR spectra of **Model1**Chemical shifts were calculated with the B3LYP/6-31G*/LanL2DZ optimized geometries byGIAO method.

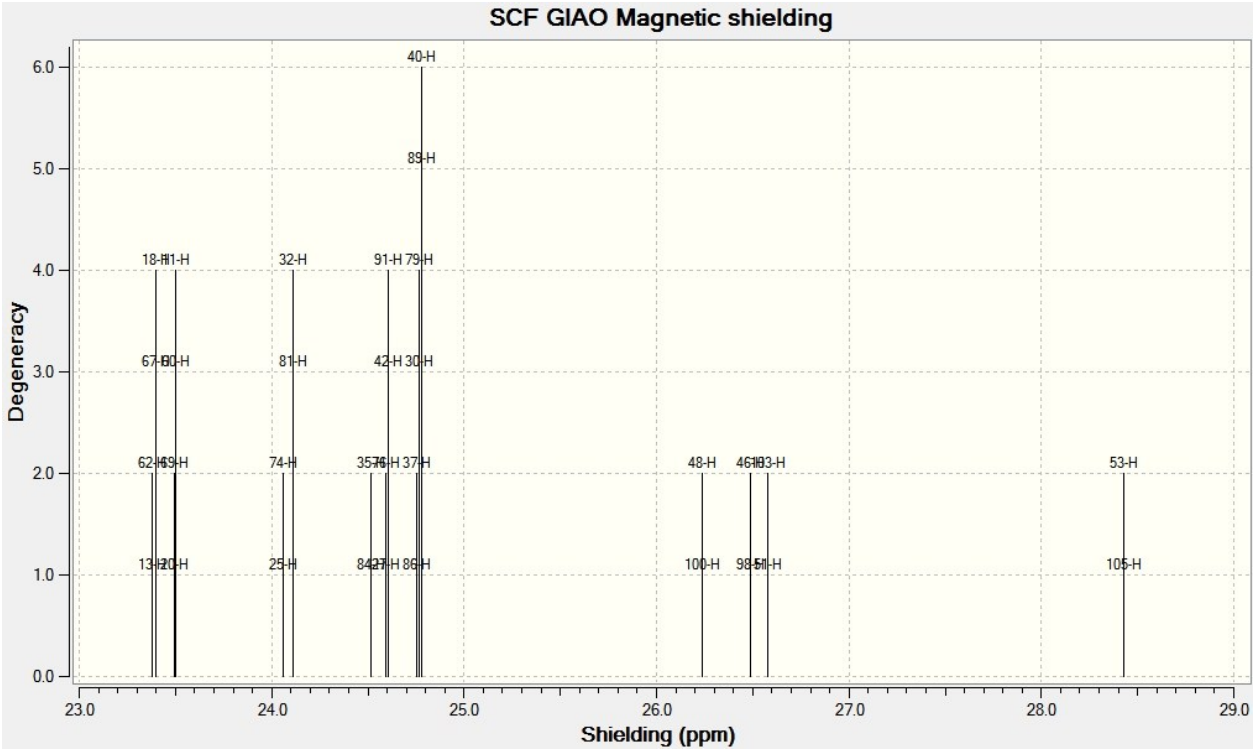

Figure S13. Calculated ^{1}H NMR spectra of **Model I**chemical shifts were calculated with the B3LYP/6-31G*/LanL2DZ optimized geometries byGIAO method.

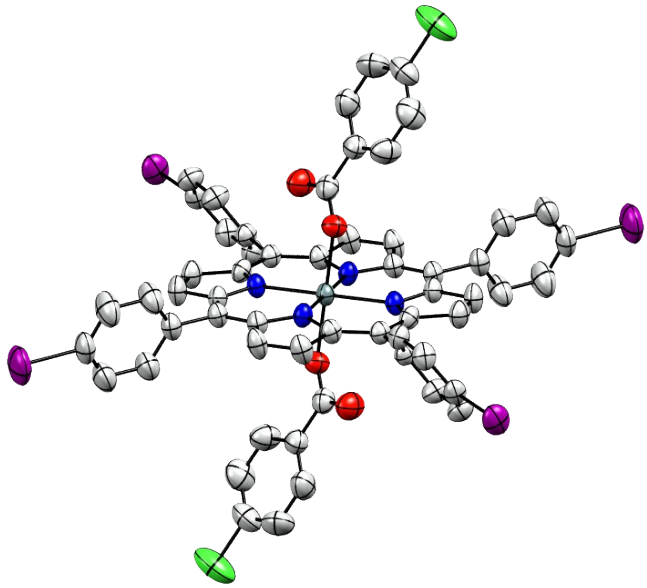

Figure S14. Perspective view of compound **2** showing 50% thermal ellipsoids for all non-hydrogen atoms at 293 K (H-atoms have been omitted for clarity). The atoms C-, N-, I- and Cl-atoms are depicted in gray, blue, purple and green, respectively.

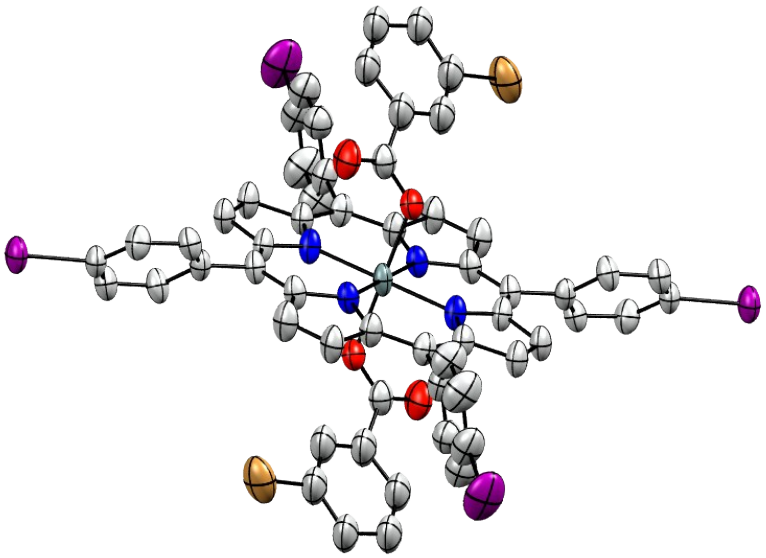

Figure S15. Perspective view of compound **1** showing 50% thermal ellipsoids for all non-hydrogen atoms at 293 K (H-atoms have been omitted for clarity). The atoms C-, N-, I- and Br-atoms are depicted in gray, blue, purple and brown, respectively.

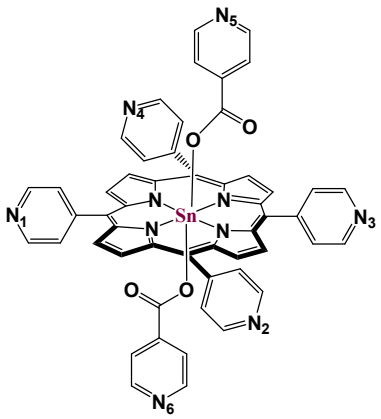

Figure-S16: Model –II for calculation of Vs, min with different functional

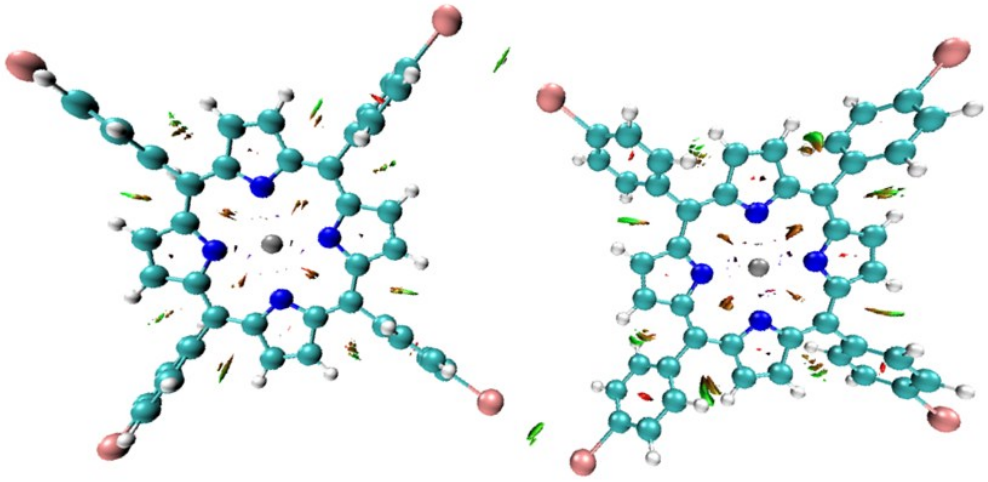

Figure-S17: Gradient isosurfaces (s = 0.4 au) for the homomolecular Zn(TIPP) dimer with Type-II halogen bond interaction. The surfaces are colored on a blue-green-red scale according to values of sign(λ_2)ρ, ranging from -0.02 to 0.02 au. Blue indicates strong attractive interactions, and red indicates strong nonbonded overlap.

Table S1: $V_{s,min}$(kcal mol^{-1}) of nitrogen atom in Model-II in different functional.

	B3LYP (Vs, min)	B3PW91 (Vs, min)	B3P86 (Vs, min)	OPBE (Vs, min)	PBE0 (Vs, min)
N1	-27.6	-27.3	-27.4	-27.5	-27.5
N2	-26.8	-26.5	-26.4	-26.6	-26.6
N3	-27.7	-27.4	-27.6	-27.4	-27.4
N4	-26.6	-26.4	-26.2	-26.3	-26.3
N5	-32.2	-32.1	-31.9	-31.8	-31.8
N6	-32.1	-32.09	-31.9	-31.9	-31.9

Table S2. Negative X•••X interaction energies (Kcal mol^{-1}), E_{int}, with BSSE correction calculated for the dimer model with different functionals.

	Different functional with 6-31G*(d,p) basis set			**B3LYP functional with different basis set**		
	B3LYP	**M06-2X**	**CAM-B3LYP**	**6-311G(d,p)**	**def2-TZVP**	**def2-TZVPP**
Zn(TIPP)-dimer	-0.15	-0.21	-0.18	-0.16	-0.19	-0.2

Coordinates of optimized geometry:

ModelI:Sn(IV)-5,10,15,20-meso-tetrakis(4-iodophenyl)porphyrin [$Sn(L)_2$-TIPP](where L= 4-iodobenzoate moiety)

Sn	-2.06297600	3.77457600	7.34039900
I	-10.03100600	9.24001900	9.45051600
I	-6.19292800	1.16490400	-1.30330800
I	-5.32088500	-3.68638000	11.49847500
N	-2.55569800	5.11125200	8.87576500
N	-3.80416200	4.30176400	6.30536700
O	-2.93394900	2.17090900	8.28787300
O	-4.95705400	2.95287300	8.93837800
C	-1.83417000	5.31865100	10.03084000
C	-2.56745400	6.24808000	10.85508300
H	-2.25340100	6.59286100	11.82910100
C	-3.71164000	6.57679000	10.18806500
H	-4.49750600	7.24012600	10.51809400
C	-3.71017900	5.85817500	8.93889500
C	-4.73191800	5.89683800	7.97039400
C	-4.76126400	5.18059900	6.75767800
C	-5.81494100	5.23972100	5.77621900
H	-6.70242900	5.84969100	5.85862600
C	-5.48121900	4.39200400	4.76028400
H	-6.05125100	4.18109000	3.86770000
C	-4.20942100	3.79623100	5.09014900
C	-3.51684700	2.84421700	4.31139800
C	-5.95259200	6.70063000	8.30611500
C	-6.00349700	8.08641800	8.11259900
H	-5.14121500	8.60547900	7.70285000
C	-7.15340200	8.81263400	8.43438700
H	-7.18008000	9.88525100	8.27585900
C	-8.25765700	8.13985800	8.95531300
C	-8.22886800	6.76047300	9.16047500
H	-9.08895500	6.24295400	9.57078700
C	-7.07487800	6.04605900	8.83441000
H	-7.03143000	4.97257600	8.99677400
C	-4.13681100	2.45251500	3.00464300
C	-4.69441500	1.17778700	2.82891800
H	-4.68309700	0.46973400	3.65280700
C	-5.27661000	0.80735500	1.61516100
H	-5.70902500	-0.18067900	1.50146600
C	-5.29909100	1.72211300	0.56305000
C	-4.74962800	2.99528900	0.70969600
H	-4.76249500	3.70382200	-0.11132000
C	-4.17295500	3.35293100	1.92988500
H	-3.73762400	4.34165800	2.04452600

C	-4.11252800	2.06385500	8.86508100
C	-4.36974300	0.70647800	9.46514400
C	-5.58996200	0.47458100	10.11057800
H	-6.31392900	1.28158000	10.15486000
C	-5.86958800	-0.76406300	10.68624900
H	-6.81753700	-0.93484600	11.18485400
C	-4.91076500	-1.77499200	10.61015700
C	-3.68844900	-1.56872700	9.97082100
H	-2.95097000	-2.36211400	9.91718600
C	-3.42437500	-0.32345300	9.39945600
H	-2.48002100	-0.14121900	8.89853500
I	5.90504400	-1.69087800	5.23027400
I	2.06697100	6.38424100	15.98410900
N	-1.57025900	2.43789500	5.80503600
N	-0.32178800	3.24739400	8.37542700
C	-2.29178600	2.23049700	4.64996000
C	-1.55850400	1.30106600	3.82571700
H	-1.87255800	0.95628500	2.85169900
C	-0.41431900	0.97235600	4.49273500
H	0.37154800	0.30902100	4.16270400
C	-0.41577800	1.69097200	5.74190400
C	0.60596400	1.65231400	6.71040200
C	0.63531400	2.36855800	7.92311600
C	1.68899000	2.30943700	8.90457500
H	2.57647700	1.69946500	8.82216900
C	1.35526700	3.15715300	9.92051000
H	1.92529800	3.36806500	10.81309600
C	0.08346900	3.75292500	9.59064700
C	-0.60910700	4.70493500	10.36940000
C	1.82663600	0.84851900	6.37468100
C	1.87753600	-0.53727100	6.56818700
H	1.01525100	-1.05633100	6.97793100
C	3.02743900	-1.26348800	6.24639800
H	3.05411200	-2.33610700	6.40491900
C	4.13169800	-0.59071400	5.72548000
C	4.10291400	0.78867200	5.52032500
H	4.96300300	1.30619100	5.11001600
C	2.94892600	1.50308900	5.84639100
H	2.90548000	2.57657200	5.68402800
C	0.01085600	5.09663600	11.67615600
C	0.56846200	6.37136200	11.85188100
H	0.55714800	7.07941500	11.02799200
C	1.15065700	6.74179300	13.06563900
H	1.58307400	7.72982600	13.17933400
C	1.17313400	5.82703500	14.11774900
C	0.62366800	4.55386000	13.97110300

H	0.63653400	3.84532700	14.79212000
C	0.04699600	4.19621900	12.75091300
H	-0.38833700	3.20749400	12.63627300
I	1.19509200	11.23560700	3.18257200
O	-1.19199900	5.37824600	6.39293400
O	0.83127000	4.59640300	5.74279800
C	-0.01335900	5.48534300	5.81585900
C	0.24387400	6.84272500	5.21581700
C	1.46420200	7.07469800	4.57061800
H	2.18823800	6.26775100	4.52649700
C	1.74385000	8.31334900	3.99497300
H	2.69188400	8.48419000	3.49654900
C	0.78493800	9.32420900	4.07085400
C	-0.43748900	9.11786900	4.70995500
H	-1.17503600	9.91120300	4.76342800
C	-0.70158300	7.87258800	5.28129700
H	-1.64602100	7.69029700	5.78203700

ModelII:Sn(IV)-5,10,15,20-meso-tetrakis(4-pyridyl)porphyrin [$Sn(L)_2$-TPyP](where L= isonicitinate moiety)

Sn	-0.00064800	-0.00056600	0.00075000
C	-2.05344000	2.18288800	0.65834100
O	-2.90086700	1.76620100	-0.12526400
O	-0.86710800	1.65302200	0.86421300
C	-2.76164500	-0.74713600	-1.95740000
N	-1.70683500	-1.18970800	0.24686800
C	-2.71592000	-1.33328000	-0.67790600
C	-2.05008900	-1.88818000	1.38333700
N	-2.91660000	-4.37055100	5.77548300
C	-1.92592100	-4.19415400	3.58209500
H	-1.56241500	-4.70283500	2.69430200
C	0.72759900	-1.43450700	4.01883500
H	0.45789900	-2.02107300	4.88437700
C	-2.32104700	3.40806100	1.49871000
C	-1.85633500	-2.79813100	3.68236700
C	-1.29430700	-1.96380400	2.57268000
N	-0.61577000	0.50338300	-1.93604900
C	-0.05992900	-1.32365300	2.81527500
C	-3.77709100	5.20269000	2.15434900
C	-3.54356800	4.07341600	1.37086900
H	-4.28460900	3.70354800	0.67071100
C	-1.85334400	0.68003200	-3.84452100
H	-2.66175400	0.53702200	-4.54631800
C	-1.39048200	3.91227400	2.41169200
H	-0.43172200	3.42280000	2.53933800

C	-6.16222500	-0.23931100	-3.53577700
H	-6.95568200	0.50539600	-3.57215400
C	-3.33576100	-2.50320100	1.15923900
H	-3.86888500	-3.10618200	1.87916200
N	-6.37640100	-1.36131900	-4.23560800
C	-4.00781600	-0.97585600	-2.75791800
C	-2.33429900	-2.21376600	4.86294100
H	-2.31459000	-1.13589400	4.99273800
C	-3.74034800	-2.16542100	-0.09919200
H	-4.66102800	-2.44504000	-0.58978400
C	-2.84884600	-3.03666900	5.86607400
H	-3.22886200	-2.59929900	6.78789000
C	-2.45834800	-4.92407800	4.64605000
H	-2.51550600	-6.00978000	4.58729700
C	-1.72566000	5.04961800	3.14742800
C	-4.22389200	-2.15227500	-3.48435300
H	-3.47877400	-2.94237300	-3.49587900
C	-5.41510600	-2.29170300	-4.19998300
H	-5.60356500	-3.19745000	-4.77434600
C	-1.78853000	0.09535000	-2.52896100
C	-5.00918300	0.00339900	-2.78771200
H	-4.88543800	0.92461800	-2.22616700
C	2.76049300	0.74576500	1.95878700
N	1.70556100	1.18851900	-0.24538400
C	2.71467600	1.33204900	0.67937200
C	2.04869900	1.88721600	-1.38175100
N	2.91492700	4.37018800	-5.77359200
C	1.92397400	4.19341500	-3.58035800
H	1.56018300	4.70195000	-2.69259900
C	-0.72874600	1.43316500	-4.01743000
H	-0.45901500	2.01967800	-4.88299900
C	1.85484900	2.79737500	-3.68068700
C	1.29291300	1.96285700	-2.57108800
N	0.61449900	-0.50452100	1.93755200
C	0.05864100	1.32254600	-2.81376100
C	1.85229400	-0.68153500	3.84585000
H	2.66084600	-0.53874300	4.54752800
C	6.16159000	0.23758700	3.53588500
H	6.95524000	-0.50695300	3.57148200
C	3.33430900	2.50234300	-1.15760500
H	3.86731800	3.10552500	-1.87744500
N	6.37565800	1.35908900	4.23656200
C	4.00681200	0.97422300	2.75916600
C	2.33317700	2.21319100	-4.86120000
H	2.31382200	1.13531600	-4.99103000
C	3.73898900	2.16439000	0.10075300

H	4.65965200	2.44402900	0.59136700
C	2.84761100	3.03628700	-5.86423400
H	3.22790200	2.59906700	-6.78600700
C	2.45633200	4.92353800	-4.64421300
H	2.51314100	6.00925700	-4.58541900
C	4.22275600	2.15010200	3.48649900
H	3.47744500	2.94000600	3.49883700
C	5.41412300	2.28926000	4.20193400
H	5.60250300	3.19459400	4.77697200
C	1.78737500	-0.09669400	2.53036900
C	5.00842700	-0.00481200	2.78790800
H	4.88473800	-0.92562700	2.22568600
C	2.05217000	-2.18401200	-0.65712300
O	2.89972900	-1.76738200	0.12637700
O	0.86572600	-1.65426900	-0.86260600
C	2.31975800	-3.40896300	-1.49782200
C	3.77585100	-5.20331400	-2.15411200
C	3.54234600	-4.07425800	-1.37031200
H	4.28345300	-3.70451500	-0.67015800
C	1.38911200	-3.91301300	-2.41081000
H	0.43029700	-3.42357900	-2.53820100
C	1.72428100	-5.05014000	-3.14688600
H	4.71947500	-5.74105000	-2.07475000
H	1.01902600	-5.46483700	-3.86598700
H	-4.72066500	5.74047700	2.07472800
H	-1.02046600	5.46444800	3.86651200
N	2.89199500	-5.69621900	-3.03290400
N	-2.89331000	5.69575600	3.03312700

Coordinates of Zn(II)-5,10,15,20-meso-tetrakis(4-iodophenyl)porphyrin dimer

Zn	-1.982347000	4.106055000	7.515303000
I	-10.150220000	9.485708000	9.140939000
I	1.060292000	6.005846000	16.758466000
N	-0.324468000	3.592458000	8.641443000
N	-2.704148000	5.233888000	9.092733000
C	-6.067512000	6.811812000	8.317170000
C	-4.829838000	6.004136000	8.069520000
C	-3.905401000	5.902202000	9.131126000
C	-0.071179000	3.971895000	9.938756000
C	-8.380720000	8.326759000	8.784029000

C	0.727609000	2.807495000	8.231477000
C	-5.996944000	8.203755000	8.477553000
H	-5.032634000	8.699896000	8.413299000
C	-0.901449000	4.786145000	10.738484000
C	-0.444764000	5.067739000	12.137621000
C	-7.143917000	8.965442000	8.709407000
H	-7.066498000	10.041066000	8.824627000
C	-2.130643000	5.351795000	10.337026000
C	-4.099507000	6.457178000	10.453584000
H	-4.965997000	7.014638000	10.778197000
C	-7.326528000	6.198012000	8.397736000
H	-7.403131000	5.120290000	8.284576000
C	1.193270000	3.408498000	10.360861000
H	1.650754000	3.549694000	11.329143000
C	1.678319000	2.682369000	9.315424000
H	2.595958000	2.113476000	9.282254000
C	-8.482978000	6.945011000	8.630335000
H	-9.445224000	6.448818000	8.694428000
C	-3.008264000	6.118622000	11.195140000
H	-2.823675000	6.349941000	12.234059000
C	-0.052859000	6.359588000	12.519446000
H	-0.074742000	7.161910000	11.787344000
C	0.407800000	5.599309000	14.755814000
C	-0.399726000	4.049166000	13.101424000
H	-0.706638000	3.043168000	12.829524000
C	0.023108000	4.305574000	14.407152000
H	0.044560000	3.503995000	15.137389000
C	0.373650000	6.632481000	13.820634000
H	0.677506000	7.637567000	14.092131000
I	6.182917000	-1.269370000	5.865401000
I	-5.025857000	2.188509000	-1.725642000

N	-3.640214000	4.619582000	6.389376000
N	-1.260253000	2.978637000	5.937965000
C	2.103177000	1.401353000	6.712491000
C	0.865532000	2.208602000	6.960956000
C	-0.058602000	2.311124000	5.898985000
C	-3.894588000	4.238450000	5.092752000
C	4.414366000	-0.111674000	6.236495000
C	-4.692561000	5.404064000	6.799497000
C	2.031381000	0.010671000	6.541893000
H	1.066488000	-0.484930000	6.600477000
C	-3.064295000	3.424459000	4.292725000
C	-3.521992000	3.140295000	2.894473000
C	3.177590000	-0.750523000	6.305026000
H	3.098887000	-1.824852000	6.179728000
C	-1.834133000	2.860547000	4.693804000
C	0.135938000	1.757199000	4.576019000
H	1.002609000	1.200603000	4.250374000
C	3.362947000	2.014538000	6.638919000
H	3.440413000	3.091327000	6.759890000
C	-5.160140000	4.799993000	4.671442000
H	-5.618471000	4.656853000	3.703860000
C	-5.644658000	5.526995000	5.716495000
H	-6.562951000	6.094801000	5.750241000
C	4.518993000	1.268320000	6.401740000
H	5.481784000	1.763928000	6.341848000
C	-0.955970000	2.094983000	3.835166000
H	-1.140951000	1.863688000	2.796348000
C	-3.909769000	1.846646000	2.514444000
H	-3.884503000	1.045306000	3.247562000
C	-4.375128000	2.601894000	0.275554000
C	-3.571857000	4.157460000	1.929418000

H	-3.268568000	5.164999000	2.199866000
C	-3.994750000	3.897249000	0.624476000
H	-4.019983000	4.698280000	-0.106416000
C	-4.336179000	1.571195000	1.213877000
H	-4.636881000	0.564538000	0.944275000
Zn	1.982345000	-4.106057000	-7.515301000
I	-6.183386000	1.268564000	-5.865081000
I	5.025363000	-2.189474000	1.726007000
N	3.640207000	-4.619603000	-6.389375000
N	1.260107000	-2.978892000	-5.937847000
C	-2.103409000	-1.401756000	-6.712306000
C	-0.865695000	-2.208882000	-6.960824000
C	0.058403000	-2.311476000	-5.898828000
C	3.894503000	-4.238617000	-5.092692000
C	-4.414731000	0.111044000	-6.236225000
C	4.692630000	-5.403951000	-6.799557000
C	-2.031720000	-0.011092000	-6.541511000
H	-1.066860000	0.484586000	-6.599976000
C	3.064117000	-3.424793000	-4.292593000
C	3.521738000	-3.140775000	-2.894286000
C	-3.177995000	0.749989000	-6.304600000
H	-3.099375000	1.824306000	-6.179151000
C	1.833926000	-2.860924000	-4.693647000
C	-0.136236000	-1.757747000	-4.575794000
H	-1.002965000	-1.201265000	-4.250110000
C	-3.363140000	-2.015039000	-6.638884000
H	-3.440524000	-3.091817000	-6.760007000
C	5.160084000	-4.800114000	-4.671408000
H	5.618369000	-4.657059000	-3.703792000
C	5.644697000	-5.526946000	-5.716536000
H	6.563036000	-6.094675000	-5.750320000

C	-4.519251000	-1.268936000	-6.401665000
H	-5.482011000	-1.764619000	-6.341894000
C	0.955671000	-2.095539000	-3.834944000
H	1.140592000	-1.864367000	-2.796087000
C	3.909394000	-1.847144000	-2.514073000
H	3.884089000	-1.045709000	-3.247087000
C	4.374739000	-2.602648000	-0.275266000
C	3.571653000	-4.158062000	-1.929364000
H	3.268456000	-5.165590000	-2.199954000
C	3.994478000	-3.897988000	-0.624372000
H	4.019751000	-4.699113000	0.106416000
C	4.335737000	-1.571829000	-1.213456000
H	4.636347000	-0.565183000	-0.943710000
I	10.150690000	-9.484883000	-9.141304000
I	-1.059792000	-6.004904000	-16.758823000
N	0.324473000	-3.592438000	-8.641440000
N	2.704292000	-5.233634000	-9.092847000
C	6.067746000	-6.811402000	-8.317356000
C	4.830000000	-6.003852000	-8.069650000
C	3.905597000	-5.901854000	-9.131278000
C	0.071264000	-3.971726000	-9.938812000
C	8.381088000	-8.326114000	-8.784316000
C	-0.727676000	-2.807600000	-8.231417000
C	5.997291000	-8.203330000	-8.477912000
H	5.033017000	-8.699554000	-8.413754000
C	0.901624000	-4.785815000	-10.738611000
C	0.445014000	-5.067267000	-12.137801000
C	7.144331000	-8.964901000	-8.709818000
H	7.066999000	-10.040516000	-8.825173000
C	2.130843000	-5.351426000	-10.337176000
C	4.099795000	-6.456646000	-10.453800000

H	4.966340000	-7.013997000	-10.778452000
C	7.326718000	-6.197495000	-8.397799000
H	7.403234000	-5.119781000	-8.284504000
C	-1.193206000	-3.408364000	-10.360897000
H	-1.650641000	-3.549468000	-11.329217000
C	-1.678346000	-2.682397000	-9.315390000
H	-2.596023000	-2.113567000	-9.282189000
C	8.483234000	-6.944377000	-8.630448000
H	9.445444000	-6.448103000	-8.694445000
C	3.008553000	-6.118082000	-11.195353000
H	2.824020000	-6.349285000	-12.234308000
C	0.053214000	-6.359095000	-12.519802000
H	0.075123000	-7.161507000	-11.787799000
C	-0.407409000	-5.598570000	-14.756094000
C	0.399945000	-4.048577000	-13.101479000
H	0.706777000	-3.042591000	-12.829443000
C	-0.022819000	-4.304852000	-14.407257000
H	-0.044298000	-3.503184000	-15.137395000
C	-0.373225000	-6.631856000	-13.821041000
H	-0.677000000	-7.636929000	-14.092675000

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