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Supporting Information

Regulated stepwise ESDPT mechanism associated with chalcogen substitutions for BDIBD derivatives

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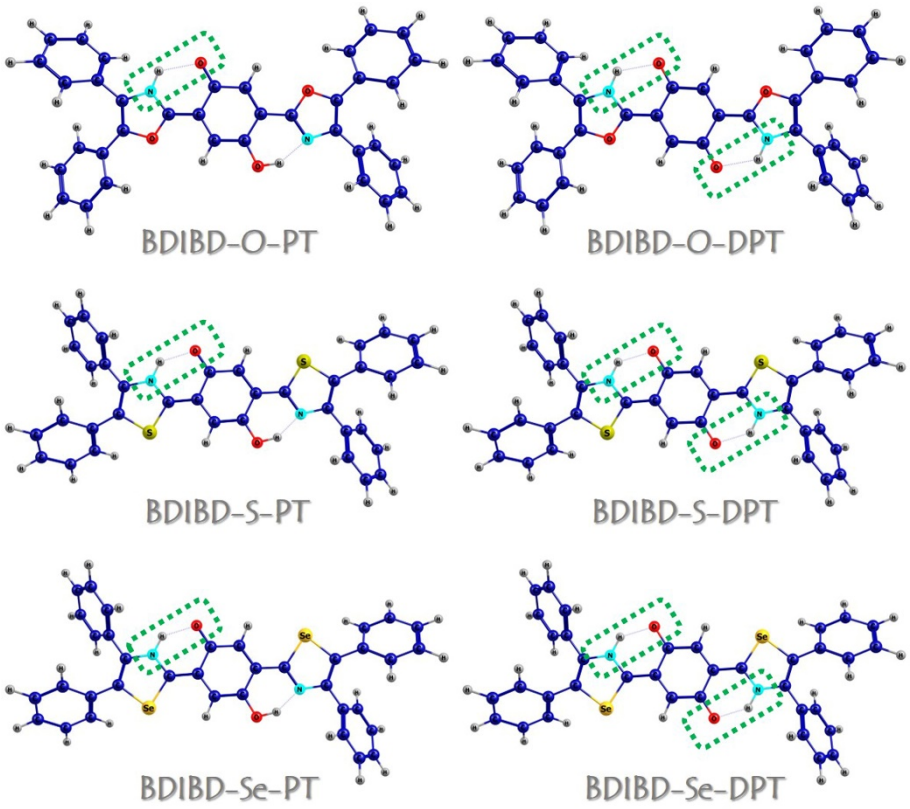

Figure S1. Optimized geometries of single proton-transfer BDIBD-O-PT, BDIBD-S-PT and BDIBD-Se-PT as well as the double proton-transfer BDIBD-O-DPT, BDIBD-S-DPT and BDIBD-Se-DPT fluorophores.

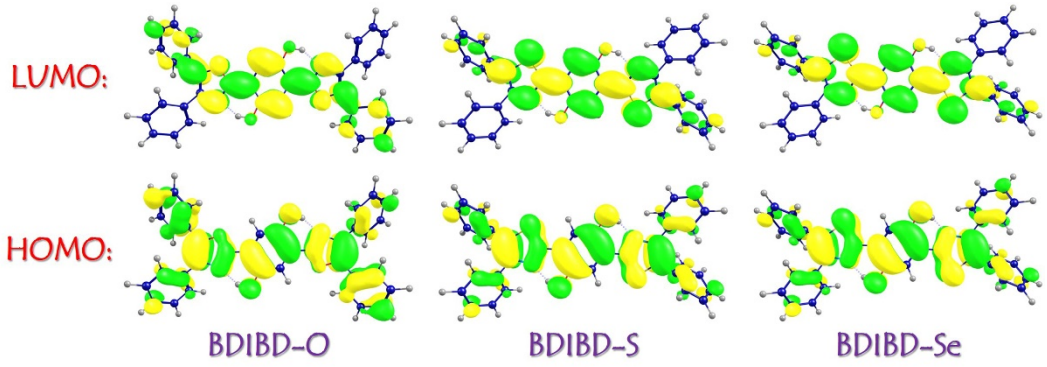

Figure S2. HOMO & LUMO orbitals obtained by CAM-B3LYP functional for BDIBD-O, BDIBD-S and BDIBD-Se compounds.

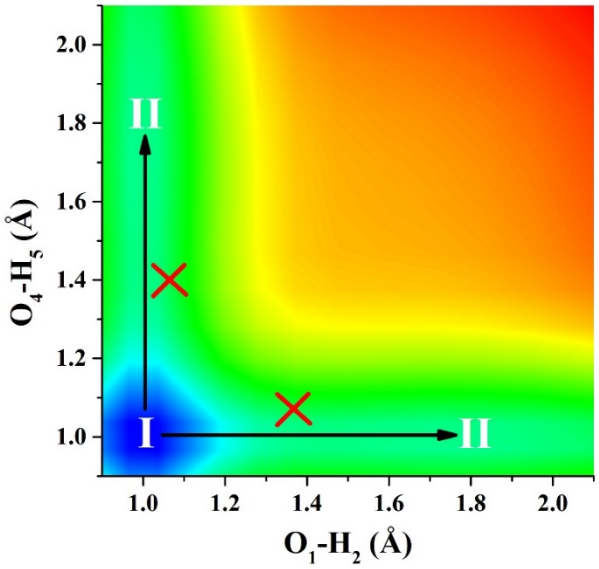

Figure S3. The projection plane of S_0-state PES for BDIBD derivatives. I: S_1-state BDIBD derivatives; II: BDIBD-PT derivatives.

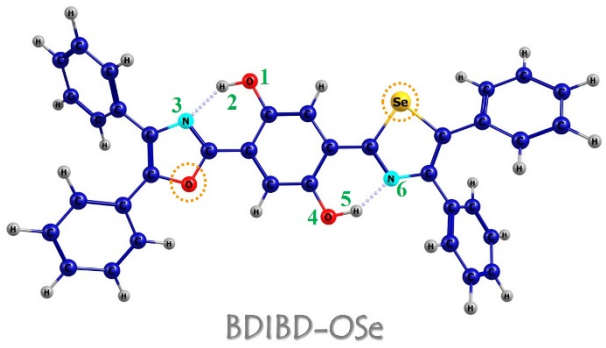

Figure S4. Optimized geometry of BDIBD-OSe fluorophore.

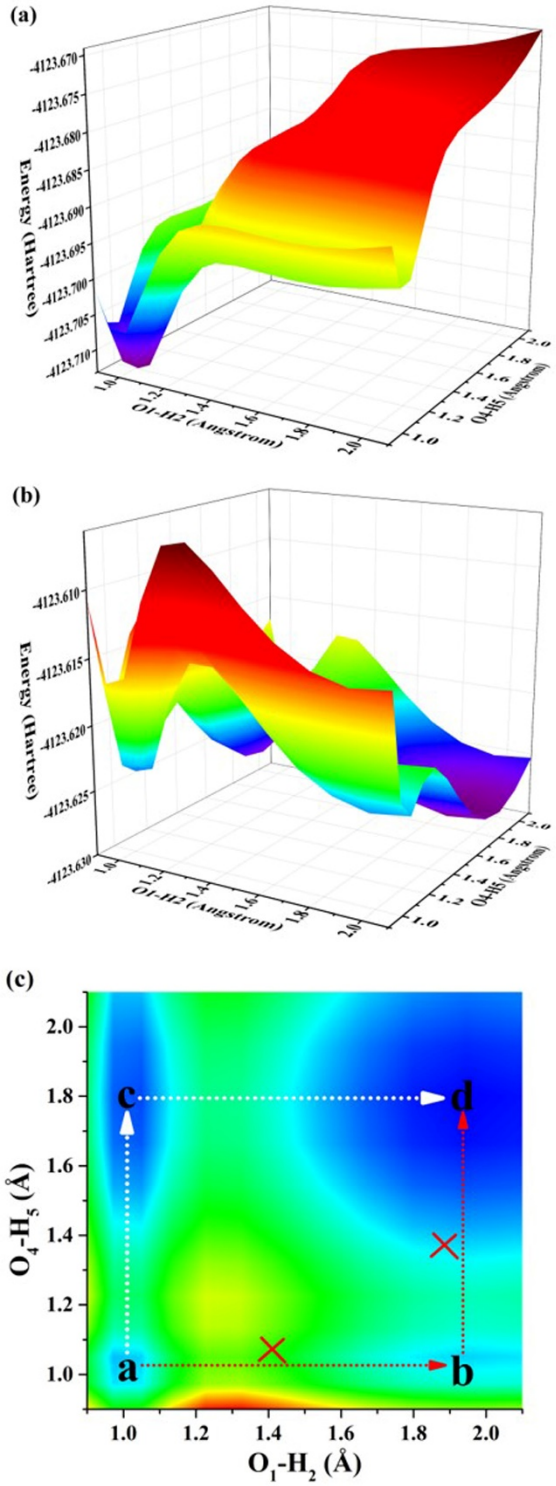

Figure S5. (a) S_0-state PES for BDIBD-OSe, (b) S_1-state PES for BDIBD-OSe. (c) The projection plane of S_1-state PES for BDIBD-OSe. Herein, **a** stands for S_1-state BDIBD-OSe; **b** stands for the S_1-state single proton-transfer tautomer along with O_1-H_2···N_3 hydrogen bond; **c** stands for the S_1-state single proton-transfer tautomer along with O_4-H_5···N_6 hydrogen bond; **d** stands for the S_1-state ESDPT tautomer. The stepwise ESDPT should occur along with **a** → **c** → **d** path.

Table S1. Parameters of bond lengths (Å) and bong angles (Δ°) involved in dual hydrogen bonds for BDIBD-O-PT, BDIBD-S-PT and BDIBD-Se-PT in CH_3CN solvent in both S_0 and S_1 states.

	BDIBD-O-PT		BDIBD-S-PT		BDIBD-Se-PT	
	S_0	S_1	S_0	S_1	S_0	S_1
O_1-H_2	1.7347	1.9783	1.5646	1.8164	1.5684	1.7910
H_2-N_3	1.0420	1.0203	1.0705	1.0297	1.0688	1.0320
O_4-H_5	0.9842	1.0042	0.9894	1.0177	0.9904	1.0208
H_5-N_6	1.7989	1.7029	1.7381	1.6265	1.7309	1.6140
$\Delta(O_1H_2N_3)$	132.56	123.22	142.26	132.52	142.85	134.42
$\Delta(O_4H_5N_6)$	146.10	148.13	147.02	149.56	147.16	149.87

Table S2. Parameters of bond lengths (Å) and bong angles (Δ°) involved in dual hydrogen bonds for BDIBD-O-DPT, BDIBD-S-DPT and BDIBD-Se-DPT in CH_3CN solvent in both S_0 and S_1 states.

	BDIBD-O-DPT		BDIBD-S-DPT		BDIBD-Se-DPT	
	S_0	S_1	S_0	S_1	S_0	S_1
O_1-H_2	0.9867	1.9560	0.9922	1.8062	0.9933	1.7849
H_2-N_3	1.7959	1.0205	1.7315	1.0299	1.7233	1.0319
O_4-H_5	0.9867	1.9560	0.9922	1.8062	0.9933	1.7849
H_5-N_6	1.7959	1.0205	1.7315	1.0299	1.7233	1.0319
$\Delta(O_1H_2N_3)$	145.82	124.07	146.87	132.98	147.02	134.70
$\Delta(O_4H_5N_6)$	145.82	124.07	146.87	132.98	147.02	134.70

Table S3. Simulated BCP parameters involved in the hydrogen bond O_1-$H_2\cdots N_3$ or O_4-$H_5\cdots N_6$ as well as predicted hydrogen bonding energy E_{HB} (kcal/mol) for BDIBD-O, BDIBD-S and BDIBD-Se systems in CH_3CN solvent in S_0 and S_1 states.

	States	ρ(r)	V(r)	G(r)	H(r)	E(HB)
BDIBD-O	S_0	0.041983	-0.037481	0.031860	-0.005621	-8.623
	S_1	0.044600	-0.040682	0.033778	-0.005893	-9.207
BDIBD-S	S_0	0.049915	-0.047067	0.037387	-0.009681	-10.393
	S_1	0.056297	-0.054889	0.041583	-0.013306	-11.816
BDIBD-Se	S_0	0.051167	-0.048515	0.038125	-0.01039	-10.672
	S_1	0.057761	-0.056585	0.042386	-0.014199	-12.143

ρ(r): Density of all electrons.
V(r): Potential energy density.
G(r): Lagrangian kinetic energy.
H(r): Energy density.
E_{HB}: Hydrogen bonding energy based on -223.08*ρ(r)+0.7423.

Table S4. Vertical excitation energies (λ nm), oscillator strength (*f*), transition compositions and percentages for BDIBD-O, BDIBD-S and BDIBD-Se compounds in CH_3CN solvent based on CAM-B3LYP functional.

	Transition	λ	f	Composition	CI (%)
BDIBD-O	$S_0 \rightarrow S_1$	369.79	1.2636	H → L	95.96
	$S_0 \rightarrow S_2$	309.77	0.2753	H-2 → L	91.64
	$S_0 \rightarrow S_3$	299.70	0.0000	H-1 → L	90.87
BDIBD-S	$S_0 \rightarrow S_1$	390.84	1.1655	H → L	96.03
	$S_0 \rightarrow S_2$	322.45	0.3085	H-1 → L	91.28
	$S_0 \rightarrow S_3$	305.43	0.0027	H-2 → L	89.79
BDIBD-Se	$S_0 \rightarrow S_1$	401.82	1.1469	H → L	96.57
	$S_0 \rightarrow S_2$	330.88	0.2304	H-1 → L	91.77
	$S_0 \rightarrow S_3$	316.02	0.0019	H-2 → L	90.35

Table S5. The calculated Mulliken's charge and NPA charge of O_1, H_2, N_3, O_4, H_5 and N_6 atoms for BDIBD-O, BDIBD-S and BDIBD-Se in CH_3CN solvent in both S_0 and S_1 states.

		Mulliken's charge		NPA charge	
	atoms	S_0	S_1	S_0	S_1
BDIBD-O	O_1	-0.300	-0.296	-0.667	-0.666
	H_2	0.308	0.309	0.506	0.506
	N_3	-0.167	-0.168	-0.496	-0.497
	O_4	-0.300	-0.296	-0.667	-0.666
	H_5	0.308	0.309	0.506	0.506
	N_6	-0.167	-0.168	-0.496	-0.497
BDIBD-S	O_1	-0.305	-0.299	-0.672	-0.670
	H_2	0.320	0.322	0.504	0.503
	N_3	-0.135	-0.138	-0.480	-0.482
	O_4	-0.305	-0.299	-0.672	-0.670
	H_5	0.320	0.322	0.504	0.503
	N_6	-0.135	-0.138	-0.480	-0.482
BDIBD-Se	O_1	-0.305	-0.299	-0.672	-0.670
	H_2	0.322	0.324	0.503	0.502
	N_3	-0.146	-0.149	-0.490	-0.493
	O_4	-0.305	-0.299	-0.672	-0.670
	H_5	0.322	0.324	0.503	0.502
	N_6	-0.146	-0.149	-0.490	-0.493

Table S6. The absolute energies (a.u.) of the stable optimized S_1-state A, B as well as C points of respective BDIBD-O, BDIBD-S and BDIBD-Se fluorophores.

	BDIBD-O	BDIBD-S	BDIBD-Se
A	-1797.2890	-2443.2254	-6449.9610
B	-1797.2858	-2443.2277	-6449.9638
C	-1797.2891	-2443.2318	-6449.9687

The coordinates of the searched TS forms in S_1 state

BDIBD-O (TS1):

	X	Y	Z
C	-1.41836300	0.23590400	0.01849900
C	-0.73313900	-1.06663900	0.03188500
C	0.66584400	-1.08499700	0.03163800
C	1.42192300	0.09743500	0.01391700
C	0.72280500	1.36963300	-0.00548800
C	-0.66470600	1.41565500	-0.00192200
H	1.16223600	-2.04531100	0.03811100
H	-1.15112700	2.38152500	-0.01001900
C	-4.95249100	0.74263000	0.01808400
C	-4.84929800	-0.64036500	0.02182000
C	4.91483200	0.69243900	-0.00484000
C	4.88260300	-0.69421100	-0.01695800
C	2.83400600	0.09958000	-0.00888800
C	-2.81865000	0.19415700	0.04613800
N	3.63074700	1.16300900	-0.01739900
N	-3.51786200	-0.94638000	0.06234000
C	6.05082500	1.62015800	0.05796400
C	6.02208900	2.80349100	-0.68975400
C	7.14709900	1.37109400	0.89226400
C	7.07643300	3.70661900	-0.61956900
H	5.17227100	3.00651600	-1.32886600
C	8.19855400	2.27654400	0.96209200
H	7.16904400	0.47072000	1.49234900
C	8.16918300	3.44513200	0.20381100
H	7.04569900	4.61468200	-1.20898100
H	9.03865500	2.07329400	1.61456200
H	8.98999900	4.14940100	0.25850400
C	5.85089100	-1.76102200	-0.08281800
C	7.14923500	-1.54997300	-0.58703600
C	5.49493000	-3.06140800	0.32810200
C	8.05893500	-2.59367600	-0.64916300
H	7.43525800	-0.57101100	-0.94407100
C	6.41265200	-4.09957000	0.25891600
H	4.49960200	-3.24516000	0.70965100
C	7.70082800	-3.87381600	-0.22389100
H	9.05118600	-2.41170100	-1.04339400
H	6.12248100	-5.09038800	0.58647400
H	8.41505500	-4.68582300	-0.27584800
C	-5.86637500	-1.69207800	-0.04486700
C	-5.70154000	-2.86399000	0.70366900

C	-6.97945100	-1.56896300	-0.88517400
C	-6.64244500	-3.88370900	0.62601200
H	-4.84084400	-2.96844100	1.35225900
C	-7.91635000	-2.59125400	-0.96057400
H	-7.10264600	-0.67701100	-1.48517000
C	-7.75339400	-3.74950600	-0.20323200
H	-6.50911900	-4.78246400	1.21499700
H	-8.77123500	-2.48691600	-1.61684700
H	-8.48590200	-4.54470500	-0.26289300
C	-6.02829400	1.69864900	0.06179600
C	-7.30122700	1.35452200	0.55895900
C	-5.80804600	3.02468800	-0.36318700
C	-8.31728900	2.29537600	0.59974800
H	-7.48387900	0.35569200	0.92853600
C	-6.83235300	3.95848800	-0.31484400
H	-4.83476500	3.30956300	-0.73926800
C	-8.09344600	3.60124700	0.16045200
H	-9.28787300	2.01346800	0.98879000
H	-6.64731500	4.97064900	-0.65285300
H	-8.89077400	4.33272000	0.19612600
O	-1.43105600	-2.16587200	0.03762300
H	-2.66544800	-1.82599000	0.04230900
O	1.39277600	2.52609500	-0.02177500
H	2.37534900	2.33596000	-0.01639200
O	3.54547600	-1.06482900	-0.00019600
O	-3.65431600	1.25894900	0.01509700

BDIBD-O (TS2):

	X	Y	Z
C	1.40751300	-0.16180900	-0.00394900
C	0.73173400	-1.46972200	-0.00014600
C	-0.69260700	-1.45980400	0.00770800
C	-1.43410300	-0.28186300	0.01225600
C	-0.74510500	1.00687700	0.00749400
C	0.66009100	1.01913800	-0.00071600
H	-1.19231900	-2.42002800	0.01709200
H	1.15223800	1.98280600	-0.01070300
C	4.88975100	0.67462300	-0.02976500
C	4.97952700	-0.69083200	-0.01691500
C	-4.86524100	0.63025900	0.01474200
C	-4.98354800	-0.74215800	0.02698000
C	-2.84261600	-0.22002100	0.04209100
C	2.81363200	-0.13064800	-0.03297300
N	-3.52365000	0.92699100	0.04617200

N	3.67963500	-1.15795600	-0.04205000
C	-5.87069400	1.69513800	-0.06003300
C	-5.68824100	2.87539400	0.67042800
C	-6.99342500	1.57346200	-0.88693200
C	-6.61921300	3.90455100	0.58775100
H	-4.81958800	2.98044100	1.30836500
C	-7.92217600	2.60339600	-0.96610400
H	-7.13231700	0.67384900	-1.47206200
C	-7.74039300	3.77084500	-0.22737300
H	-6.46977000	4.81027000	1.16226300
H	-8.78527400	2.49785800	-1.61157900
H	-8.46542900	4.57265000	-0.29085000
C	-6.07105200	-1.69313300	0.08176900
C	-7.32814000	-1.34162500	0.60637900
C	-5.87508600	-3.01366000	-0.36311500
C	-8.35604400	-2.27108400	0.65486300
H	-7.49227800	-0.34344900	0.98730800
C	-6.90879500	-3.93878900	-0.30442200
H	-4.91206100	-3.30500800	-0.76059200
C	-8.15616900	-3.57422800	0.19815400
H	-9.31618200	-1.98141400	1.06402600
H	-6.74020200	-4.94915200	-0.65657700
H	-8.96088000	-4.29726500	0.24121600
C	6.11959700	-1.60782500	0.04552000
C	6.13560400	-2.76033000	-0.74841400
C	7.18439100	-1.36094600	0.91960000
C	7.20544500	-3.64497700	-0.67494900
H	5.32021000	-2.95641300	-1.43375900
C	8.25214200	-2.24600800	0.98617800
H	7.16875400	-0.47995800	1.54770300
C	8.26663400	-3.38907900	0.18911800
H	7.21161100	-4.53113300	-1.29688500
H	9.07042000	-2.04781600	1.66687200
H	9.09993400	-4.07821300	0.24416100
C	5.83252100	1.77088000	-0.07435900
C	7.12845500	1.59833000	-0.59033500
C	5.44691400	3.04477300	0.37765300
C	8.01553600	2.66347300	-0.62638700
H	7.43356800	0.63455700	-0.97308100
C	6.34112100	4.10601100	0.33224400
H	4.44984900	3.19427400	0.76970600
C	7.62977500	3.92173500	-0.16376600
H	9.00987700	2.51493700	-1.02876800
H	6.03097200	5.08036800	0.68891800

H	8.32527400	4.75079300	-0.19666800
O	1.39953800	-2.54813800	0.00173000
H	3.31951200	-2.11158300	-0.00014700
O	-1.42574500	2.12019000	0.00470700
H	-2.64294300	1.79982100	0.01568300
O	-3.68613800	-1.27642100	0.02727200
O	3.53218400	1.01230700	-0.02772600

BDIBD-S (TS1):

	X	Y	Z
C	-1.41525900	0.07778600	-0.02618400
C	-0.81398700	-1.24704100	-0.03216600
C	0.57004200	-1.40458900	-0.04046600
C	1.43192300	-0.30755400	-0.04175100
C	0.84413300	1.03861900	-0.02518900
C	-0.54988000	1.17661300	-0.02448600
H	0.95529800	-2.41616600	-0.05035500
H	-0.93917000	2.18647800	-0.01782700
C	-5.24149300	0.83219600	0.00863800
C	-4.96877600	-0.53141600	0.01200800
C	4.94094900	0.49636900	-0.00385400
C	5.29919600	-0.84538800	-0.00119300
C	2.84463400	-0.40440000	-0.05283400
C	-2.83382600	0.19761300	-0.02579400
N	3.60215000	0.70671900	-0.05063400
N	-3.65289200	-0.85717200	-0.02194000
C	5.83155100	1.66838400	0.07895900
C	5.57552000	2.79420200	-0.71209100
C	6.91201500	1.69193300	0.96811400
C	6.39321900	3.91524000	-0.62509500
H	4.74148000	2.78467100	-1.40256900
C	7.72533000	2.81455900	1.05443500
H	7.10861000	0.83158900	1.59383900
C	7.47149900	3.92810500	0.25607800
H	6.18940200	4.77754500	-1.24763700
H	8.55550700	2.82267500	1.74971300
H	8.10794900	4.80160500	0.32355500
C	6.61421300	-1.46919500	-0.05764100
C	7.64965400	-0.90150800	-0.82322800
C	6.87272800	-2.67403700	0.62037500
C	8.89735300	-1.50393200	-0.88389400
H	7.46578700	0.00764500	-1.37870700
C	8.12251600	-3.27515300	0.55106400
H	6.09607700	-3.12877000	1.22339200
C	9.14334900	-2.69235200	-0.19664600

H	9.67912500	-1.05124700	-1.48141100
H	8.30162600	-4.19825300	1.08841600
H	10.11777100	-3.16139400	-0.24903700
C	-5.95400500	-1.62927900	0.09228100
C	-5.78851000	-2.77201800	-0.69848200
C	-7.03709700	-1.56856800	0.97637600
C	-6.69579600	-3.82273000	-0.61882500
H	-4.94958500	-2.82894300	-1.38043900
C	-7.94067400	-2.62108900	1.05721900
H	-7.16642800	-0.69619300	1.60326000
C	-7.77618800	-3.74998200	0.25724800
H	-6.55982800	-4.69795700	-1.24220900
H	-8.77160100	-2.56233600	1.74940500
H	-8.48234300	-4.56869100	0.31973800
C	-6.51209700	1.54463800	-0.05981900
C	-6.69901600	2.76077500	0.62110800
C	-7.57407700	1.05145000	-0.83988000
C	-7.90507600	3.44475200	0.53990200
H	-5.90047100	3.16014300	1.23459900
C	-8.77842500	1.73585900	-0.91287200
H	-7.44466400	0.13337400	-1.39611800
C	-8.95343000	2.93510200	-0.22288700
H	-8.02847400	4.37565900	1.07963500
H	-9.58132300	1.33835900	-1.52168000
H	-9.89370400	3.46843900	-0.28455800
O	-1.56692400	-2.34310700	-0.02868200
H	-2.54026300	-2.05442900	-0.01860800
O	1.61845900	2.08658000	-0.01038900
H	2.76390500	1.65372300	-0.01963800
S	3.83783800	-1.85362700	-0.02504600
S	-3.71877800	1.73013100	-0.00403800

BDIBD-S (TS2):

	X	Y	Z
C	-1.40483900	0.01831300	-0.04709300
C	-0.82747600	-1.33944500	-0.04048500
C	0.59408800	-1.44481500	-0.04945200
C	1.44497900	-0.34714100	-0.05317400
C	0.85405900	0.98760500	-0.05163100
C	-0.54508300	1.11693800	-0.05259000
H	0.99361100	-2.45203000	-0.05055800
H	-0.93149000	2.12905700	-0.05702000

C	-5.25092400	0.81998000	0.00742600
C	-5.02888900	-0.53326300	-0.00085100
C	4.95535100	0.48842800	-0.00788900
C	5.32443900	-0.84263200	0.01647600
C	2.86511100	-0.42769700	-0.05599800
C	-2.81465200	0.17850500	-0.05096600
N	3.60996400	0.68934100	-0.06507100
N	-3.69526400	-0.84664800	-0.04947700
C	5.83557000	1.67096900	0.05818200
C	5.56950200	2.78417100	-0.74705400
C	6.91952800	1.71598100	0.94187800
C	6.37928100	3.91268700	-0.67920400
H	4.73209700	2.75964600	-1.43314700
C	7.72656200	2.84486900	1.00822900
H	7.12497800	0.86582400	1.57870200
C	7.46183700	3.94579000	0.19606100
H	6.16584000	4.76498400	-1.31239500
H	8.56008900	2.86788900	1.69931800
H	8.09240800	4.82462800	0.24854500
C	6.64814900	-1.45896000	-0.02496800
C	7.66744600	-0.91829400	-0.82752100
C	6.92782100	-2.62317800	0.70949000
C	8.92375700	-1.50626500	-0.86994500
H	7.46601600	-0.03776200	-1.42229800
C	8.18476800	-3.21344400	0.65679100
H	6.16118300	-3.05681700	1.34036900
C	9.19118500	-2.65627900	-0.12821400
H	9.69459900	-1.07280500	-1.49545500
H	8.37983600	-4.10739500	1.23641700
H	10.17093200	-3.11559700	-0.16719200
C	-6.01011700	-1.62961700	0.06426600
C	-5.87095100	-2.74601500	-0.76790500
C	-7.07441700	-1.57932900	0.97108200
C	-6.78694400	-3.78990200	-0.69847800
H	-5.05686500	-2.79125300	-1.48107900
C	-7.98759600	-2.62346000	1.03564900
H	-7.18018600	-0.72379600	1.62474600
C	-7.84813100	-3.73036400	0.20055600
H	-6.67351700	-4.64659300	-1.35080200
H	-8.80589000	-2.57643100	1.74317600
H	-8.56161600	-4.54317500	0.25285700
C	-6.50758600	1.56541900	-0.02988300
C	-6.66745800	2.74399000	0.71501300
C	-7.57249700	1.12988400	-0.83501900

C	-7.86098200	3.45401200	0.66906700
H	-5.86137300	3.09457600	1.34818700
C	-8.76489300	1.83882500	-0.87129600
H	-7.45789100	0.23774700	-1.43553200
C	-8.91629800	3.00319200	-0.11973500
H	-7.96820800	4.35771600	1.25602000
H	-9.57540900	1.48822100	-1.49821200
H	-9.84647700	3.55632000	-0.15344200
O	-1.56423100	-2.37282400	-0.02695800
H	-3.27941600	-1.78801000	-0.01767500
O	1.61404800	2.04975700	-0.04849500
H	2.75398500	1.63205800	-0.04909200
S	3.86895200	-1.86733900	-0.00208500
S	-3.70025700	1.68995900	-0.02565700

BDIBD-Se (TS1):

	X	Y	Z
C	1.43262300	-0.28942300	-0.05456400
C	0.83787000	1.05477500	-0.04393200
C	-0.55592500	1.18686300	-0.04406000
C	-1.41943400	0.08678600	-0.04160800
C	-0.81151500	-1.23729900	-0.04681400
C	0.57221000	-1.38799200	-0.05415600
H	-0.94651000	2.19653600	-0.04264600
H	0.96013400	-2.39867600	-0.06397500
C	5.40786600	-0.72600400	0.01723000
C	4.94175300	0.57999300	-0.00512500
C	-4.97550300	-0.60139100	0.00967700
C	-5.36423200	0.73170200	0.02500500
C	-2.83805600	0.20161100	-0.03428800
C	2.84515900	-0.38532200	-0.05797600
N	-3.64417400	-0.85827500	-0.03687500
N	3.59436300	0.72843200	-0.06287700
C	-5.88513100	-1.76671600	0.08251300
C	-5.65650500	-2.88096300	-0.73282400
C	-6.95736200	-1.79484300	0.98119600
C	-6.49147100	-3.99067600	-0.66256100
H	-4.82586100	-2.86953700	-1.42712600
C	-7.78840100	-2.90624000	1.05310400
H	-7.13519500	-0.94488500	1.62666600
C	-7.56174200	-4.00638200	0.22872800
H	-6.30714900	-4.84282200	-1.30524200
H	-8.61129600	-2.91570800	1.75725200

H	-8.21147800	-4.87104500	0.28406700
C	-6.69905800	1.31604600	-0.04019400
C	-7.68897900	0.75822000	-0.87035200
C	-7.02508100	2.47051800	0.69335200
C	-8.95533300	1.32016000	-0.94249900
H	-7.45405200	-0.11388700	-1.46498700
C	-8.29307400	3.03190100	0.61451100
H	-6.28498700	2.91640000	1.34707100
C	-9.26708400	2.45848900	-0.19984200
H	-9.70021500	0.87468900	-1.59063900
H	-8.52281100	3.91646200	1.19582800
H	-10.25553000	2.89632600	-0.26032300
C	5.75808800	1.80909000	0.06821400
C	5.44956700	2.90048800	-0.75174600
C	6.81881800	1.91740400	0.97441700
C	6.19621000	4.07093200	-0.67571800
H	4.63073800	2.82576000	-1.45634000
C	7.56095900	3.08916100	1.05025400
H	7.05589500	1.08365200	1.62174000
C	7.25530900	4.16819800	0.22325800
H	5.95222200	4.90583600	-1.32081900
H	8.37609100	3.16226700	1.75944400
H	7.83637600	5.08008000	0.28228000
C	6.77511100	-1.22637700	-0.03481000
C	7.15877100	-2.36778200	0.69178600
C	7.74081000	-0.60099600	-0.84576300
C	8.45866000	-2.85163500	0.62504400
H	6.43856400	-2.86376500	1.33158000
C	9.03889700	-1.08601100	-0.90510200
H	7.46259800	0.26089000	-1.43644900
C	9.40749800	-2.21203600	-0.16957500
H	8.73294800	-3.72709500	1.20063000
H	9.76460600	-0.59046700	-1.53834000
H	10.42096300	-2.58961800	-0.22052800
O	1.60757600	2.10662300	-0.03382600
H	2.74486400	1.67499500	-0.03962500
O	-1.56039300	-2.33552900	-0.04342700
H	-2.53545100	-2.04470600	-0.03440100
Se	-3.81882100	1.84549600	0.01414300
Se	3.93211500	-1.94217400	-0.00348100

BDIBD-Se (TS2):

	X	Y	Z

C	-1.41191000	0.03289700	-0.05484900
C	-0.82669700	-1.32396300	-0.05040200
C	0.59541800	-1.42331600	-0.05931200
C	1.44489600	-0.32569900	-0.06051600
C	0.84640600	1.00717500	-0.06091400
C	-0.55214400	1.13172000	-0.06235400
H	0.99608200	-2.43021900	-0.06278100
H	-0.93864800	2.14411400	-0.06889800
C	-5.37866700	0.72436200	0.02364300
C	-5.03723900	-0.60147100	0.00075000
C	4.95565200	0.57456800	-0.00702100
C	5.43157300	-0.72002100	0.03148700
C	2.86545400	-0.40519200	-0.05800200
C	-2.82143800	0.19118000	-0.05454400
N	3.60216600	0.71387000	-0.07177400
N	-3.68779200	-0.84442800	-0.05562600
C	5.76127300	1.81309800	0.05259000
C	5.44383500	2.89366100	-0.77803600
C	6.82404700	1.94026400	0.95360500
C	6.18219700	4.07065200	-0.71737700
H	4.62264300	2.80602100	-1.47845900
C	7.55971300	3.11740200	1.01327300
H	7.06910500	1.11522800	1.60922000
C	7.24420300	4.18557800	0.17597700
H	5.92942500	4.89685500	-1.37044200
H	8.37718000	3.20332700	1.71849800
H	7.81913700	5.10209900	0.22297400
C	6.80558100	-1.21362100	-0.01262600
C	7.75790600	-0.61288000	-0.85455800
C	7.20558000	-2.31896300	0.75656200
C	9.06216100	-1.08483000	-0.90250500
H	7.46589100	0.22366300	-1.47485800
C	8.51049900	-2.79331700	0.69966200
H	6.49316600	-2.79684700	1.41860200
C	9.44757400	-2.17665400	-0.12572100
H	9.77878300	-0.60630900	-1.55895400
H	8.79699500	-3.64319200	1.30698300
H	10.46463500	-2.54566700	-0.16863700
C	-5.94143000	-1.76654600	0.05824700
C	-5.74083100	-2.85466100	-0.79836700
C	-6.99311200	-1.80623900	0.97991100
C	-6.58377500	-3.95906700	-0.73818200
H	-4.93633500	-2.83119200	-1.52337000
C	-7.83352800	-2.91043600	1.03556600

H	-7.14648000	-0.97240000	1.65190400
C	-7.63313400	-3.98888600	0.17607700
H	-6.42295900	-4.79311600	-1.40965800
H	-8.64254800	-2.93223100	1.75494200
H	-8.28980800	-4.84867000	0.22121100
C	-6.70300700	1.34189700	-0.01261600
C	-6.99931100	2.46261300	0.77836600
C	-7.70104700	0.83992800	-0.86393300
C	-8.25751100	3.05058000	0.73236600
H	-6.24729800	2.86227500	1.44822900
C	-8.95817600	1.42679200	-0.90164500
H	-7.48299100	-0.00869400	-1.49815500
C	-9.24381500	2.53366100	-0.10386800
H	-8.46898600	3.91050800	1.35571600
H	-9.71481400	1.02578400	-1.56473700
H	-10.22429000	2.99173400	-0.13824700
O	-1.55635600	-2.36167400	-0.03902900
H	-3.24568400	-1.77633800	-0.02978300
O	1.60218100	2.07256900	-0.05972200
H	2.73114600	1.65794000	-0.05961600
Se	3.96225400	-1.95223000	0.01770200
Se	-3.80089200	1.80983200	-0.01076800