Electronic Supplementary Information

Unveiling the Influence of Oxidation State and Heavy Atom Effects in Chalcogen Group on Boron Centered D(X)BNA Core: A Computational Study on RTP Versus TADF

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CONTENT CAPTIONS

Table S1. Calculated bond lengths (in Å) and dihedral angles (in º) between the core and the donor units obtained from B3LYP/6-31+G* level of theory.

Molecules	C-X	C-X´	B-C	C-B-C-C	C-N	C-N-C-C
1	1.374	1.365	1.523	3.41	1.421	121.16
2	1.771	1.770	1.545	25.15	1.421	121.05
3	1.910	1.913	1.554	30.69	1.421	121.29
4	2.117	2.127	1.568	36.26	1.421	120.87
5	1.822	1.824	1.559	31.55	1.418	123.80
6	1.805	1.806	1.569	31.64	1.417	124.94
7	1.963	1.969	1.568	36.91	1.418	124.10
8	1.374	1.365	1.524	1.01	1.436	90.20
9	1.770	1.770	1.545	25.16	1.436	90.25
10	1.910	1.913	1.554	30.69	1.436	90.45
11	2.117	2.127	1.568	36.24	1.436	90.03
12	1.822	1.824	1.559	31.50	1.435	90.72
13	1.805	1.806	1.569	31.63	1.434	90.52
14	1.964	1.969	1.568	36.86	1.435	90.62

Table S2. Calculated MPP and SDP values of the core units (in Å).

Core Units	MPP	SDP
DOBNA (O)	0.000	0.000
DTBNA (S)	0.443	1.647
DSBNA (Se)	0.572	2.241
DTeBNA (Te)	0.707	2.864
DTBNA-DO (SO)	0.665	2.368
DTBNA-TO (SO_2)	0.921	4.651
DSBNA-DO (SeO)	0.780	2.776

Table S3. Calculated HOMO, LUMO, H-L gaps, vertical singlet (S_1) and triplet (T_1) energies, vertical singlet-triplet energy differences (ΔE_{ST}) of core and donor units at the B3LYP/PBE0/ M06//6-31+G* level of theory. (All values are in eV)

Units	B3LYP			B3LYP			PBE0			M06		
	HOMO	**LUMO**	**H-L Gap**	**S_1**	**T_1**	**ΔE_{ST}**	**S_1**	**T_1**	**ΔE_{ST}**	**S_1**	**T_1**	**ΔE_{ST}**
DOBNA	-5.92	-2.00	3.91	3.37	2.87	0.50	3.48	2.93	0.55	3.49	2.99	0.50
DTBNA	-5.67	-2.18	3.49	2.92	2.51	0.41	3.05	2.56	0.49	3.04	2.62	0.42
DSBNA	-5.60	-2.26	3.34	2.78	2.40	0.38	2.88	2.46	0.42	2.89	2.50	0.39
DTeBNA	-5.45	-2.29	3.16	2.55	2.28	0.27	2.63	2.32	0.31	2.66	2.38	0.28
DTBNA-DO	-6.59	-3.05	3.55	2.85	2.68	0.17	3.00	2.76	0.24	3.07	2.80	0.27
DTBNA-TO	-7.73	-3.47	4.26	3.56	2.90	0.66	3.69	2.84	0.85	3.68	2.85	0.83
DSBNA-DO	-6.59	-3.08	3.51	2.82	2.72	0.10	2.97	2.84	0.13	2.99	2.87	0.12
P-CBZ	-5.64	-1.01	4.62	3.98	3.15	0.83	4.09	3.04	1.05	4.02	3.01	1.01
P-DMAC	-5.13	-0.81	4.32	3.53	3.17	0.36	3.69	3.08	0.61	3.70	3.09	0.61

Table S4. The calculated HOMO and LUMO molecular orbital contribution (%) of newly designed molecules using the B3LYP/6-31+G* level of theory.

Molecules	Orbital	Energy (eV)	CBZ (%)	Phenyl (%)	Core (%)
1	HOMO	-5.65	85.82	10.98	-
	LUMO	-2.18	-	10.80	88.09
2	HOMO	-5.65	78.17	10.45	11.39
	LUMO	-2.32	-	8.31	90.83
3	HOMO	-5.63	50.73	7.49	41.77
	LUMO	-2.40	-	7.41	91.83
4	HOMO	-5.51	-	-	97.70
	LUMO	-2.42	-	6.90	92.39
5	HOMO	-5.76	86.63	11.15	-
	LUMO	-3.10	-	5.08	94.34
6	HOMO	-5.82	86.84	11.09	-
	LUMO	-3.48		-	95.56
7	HOMO	-5.76	86.65	11.17	-
	LUMO	-3.13	-	5.01	94.41
8	HOMO	-5.17	96.26	-	-
	LUMO	-2.18	-	10.96	88.39
9	HOMO	-5.18	96.27	-	-
	LUMO	-2.33	-	8.43	91.07
10	HOMO	-5.18	96.29	-	-
	LUMO	-2.40	-	5.04	94.67
11	HOMO	-5.17	96.32	-	-
	LUMO	-2.42	-	-	95.89
12	HOMO	-5.25	96.27	-	-
	LUMO	-3.11	-	7.51	92.06
13	HOMO	-5.30	97.73		-

	LUMO	-3.50	-	4.97	94.75
14	HOMO	-5.26	96.26		-
	LUMO	-3.14	-	7.03	92.55

Table S5. Calculated vertical excited state energies of the molecules with different solvents (Toluene, and Dichloromethane) using M06/6-31+G* level of theory. (All the values are in eV)

	Toluene			**Dichloromethane**		
Molecules	S_1	T_1	ΔE_{ST}	S_1	T_1	ΔE_{ST}
1	3.35	2.85	0.50	3.37	2.86	0.51
2	2.96	2.57	0.38	2.97	2.58	0.39
3	2.82	2.47	0.34	2.83	2.49	0.35
4	2.60	2.36	0.24	2.61	2.36	0.24
5	2.72	2.50	0.22	2.79	2.53	0.26
6	2.39	2.27	0.13	2.43	2.29	0.14
7	2.70	2.50	0.20	2.78	2.53	0.25
8	3.00	2.90	0.11	3.05	2.90	0.14
9	2.91	2.58	0.34	2.95	2.58	0.37
10	2.82	2.48	0.34	2.83	2.49	0.35
11	2.60	2.35	0.25	2.60	2.36	0.24
12	2.29	2.29	0.00	2.38	2.38	0.00
13	1.94	1.94	0.00	2.00	2.00	0.00
14	2.27	2.27	0.00	2.37	2.37	0.00

Table S6. The calculated vertical singlet (S_1) and triplet (T_1) energies, configuration interaction (CI), and overlap extents (I_S, and I_T in %) of newly designed systems at M06/6-31+G* level of theory.

Molecules	State	Energy	CI	ΔE_{ST}	I_S	I_T
1	S_1	3.36	H → L 62.1%, H-1→ L 31.8%	0.52	36.86	50.92
	T_1	2.84	H → L 25.2%, H-3 → L 19.8%, H-1 → L 19.0%, H → L+1 7.8%, H-3 → L+1 5.7%			
2	S_1	2.98	H → L 51.3%, H-1 → L 46.0%	0.42	48.09	48.37
	T_1	2.56	H → L 49.5%, H-1 → L 41.0%			
3	S_1	2.83	H -> L 97.3%	0.37	47.31	47.52
	T_1	2.46	H → L 58.4%, H-4 → L 14.6%, H-3 → L 8.6%			
4	S_1	2.61	H → L 98.7%	0.27	48.39	48.39
	T_1	2.34	H → L 80.7%, H-2 → L 10.9%			
5	S_1	2.68	H → L 68.4%, H-1 → L 29.4%	0.20	18.08	29.96
	T_1	2.48	H → L 66.4%, H-1 → L 25.5%			
6	S_1	2.38	H → L 97.8%	0.13	16.67	22.45
	T_1	2.25	H → L 64.6%, H-4 → L 15.0%			
7	S_1	2.65	H → L 97.8%	0.19	17.78	27.36
	T_1	2.46	H → L 93.6%			
8	S_1	2.94	H → L 90.6%, H → L+1 7.9%	0.05	06.80	63.14
	T_1	2.89	H-1 → L 49.6%, H-2 → L 21.7%, H-2 → L+1 8.5%			
9	S_1	2.86	H → L 92.8%, H → L+1 5.7%	0.29	05.96	57.24
	T_1	2.57	H-1 → L 91.4%			
10	S_1	2.79	H → L 98.2%	0.33	05.51	54.13
	T_1	2.46	H → L 98.1%			
11	S_1	2.69	H → L 99.0%	0.37	47.75	47.75
	T_1	2.32	H → L 99.0%			
12	S_1	2.21	H-1 → L 92.4%	0.00	04.23	04.23
	T_1	2.21	H-1 → L 92.4%			
13	S_1	1.89	H → L 98.3%	0.00	03.76	03.76
	T_1	1.89	H → L 98.2%			

14	S_1	2.17	H-1 → L 98.2%	0.00	04.18	04.18
	T_1	2.17	H-1 → L 93.9%			

Table S7. Calculated SOC constants between the selected states at M06/def2-SVP level of theory for S_0 geometry. (All the values in cm^{-1})

	S_0-Geometry		
Molecules	$\langle S_1\|\hat{H_{SO}}\|T_1\rangle$	$\langle T_1\|\hat{H_{SO}}\|S_0\rangle$	$\langle S_1\|\hat{H_{SO}}\|T_2\rangle$
1	0.192	0.314	0.045
2	0.311	2.003	0.481
3	2.184	12.376	4.616
4	7.315	69.152	15.635
5	0.283	0.558	0.962
6	0.186	0.766	0.293
7	0.186	1.469	3.254
8	0.383	0.520	0.301
9	0.485	2.138	0.428
10	2.248	12.526	4.073
11	7.667	69.406	16.043
12	0.280	0.621	0.303
13	0.238	0.402	0.398
14	0.347	1.858	0.430

Table S8. Calculated SOC constants between the selected states at M06/def2-SVP level of theory for S_1 geometry. (All the values in cm^{-1})

	S_1-Geometry		
Molecules	$\langle S_1\|\hat{H_{SO}}\|T_1\rangle$	$\langle T_1\|\hat{H_{SO}}\|S_0\rangle$	$\langle S_1\|\hat{H_{SO}}\|T_2\rangle$
1	0.372	0.411	0.092
2	0.426	1.295	0.494
3	2.162	7.466	4.594
4	8.296	75.436	20.983
5	0.265	0.970	0.400
6	0.070	0.489	0.361
7	0.304	1.134	1.687
8	0.272	0.878	0.462
9	0.385	1.869	0.531
10	2.224	13.643	6.099
11	11.519	67.349	21.512
12	0.261	0.553	0.308
13	0.142	0.390	0.434
14	0.312	0.555	0.162

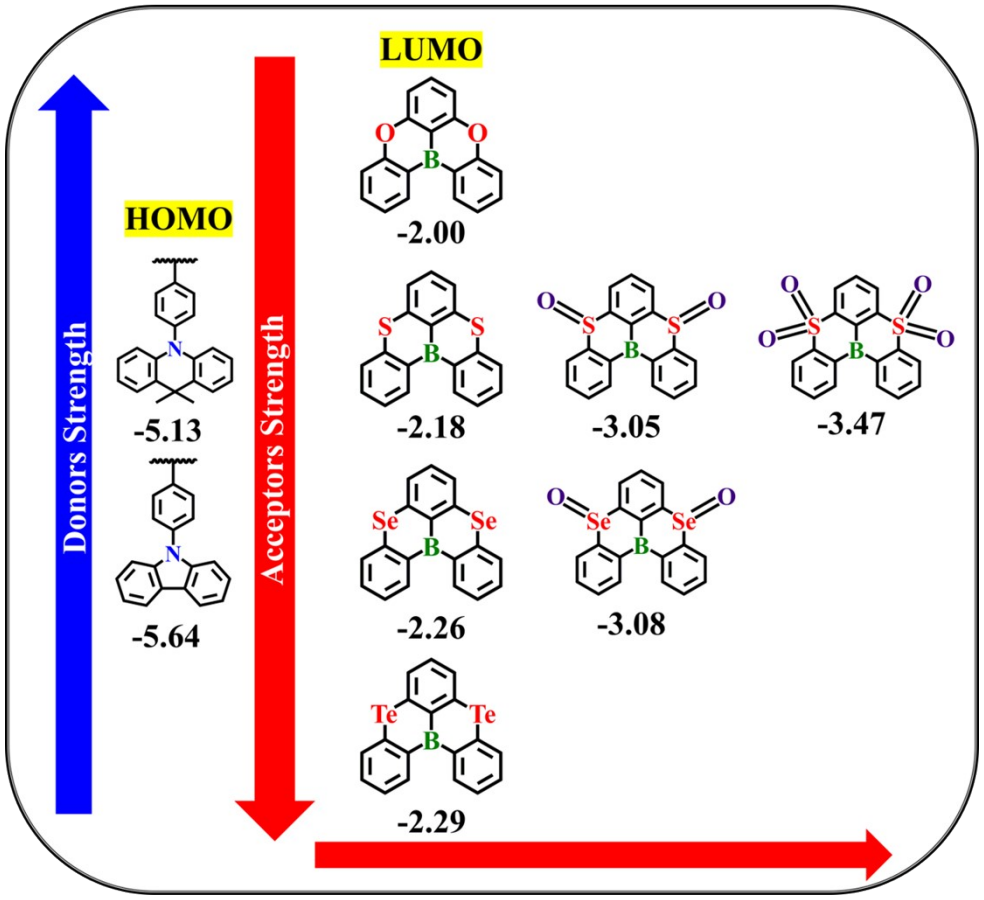

Figure S1. Chemical structures of the donor and core units, along with their HOMO and LUMO energies (all values in eV), were analyzed to assess their donor and acceptor strengths.

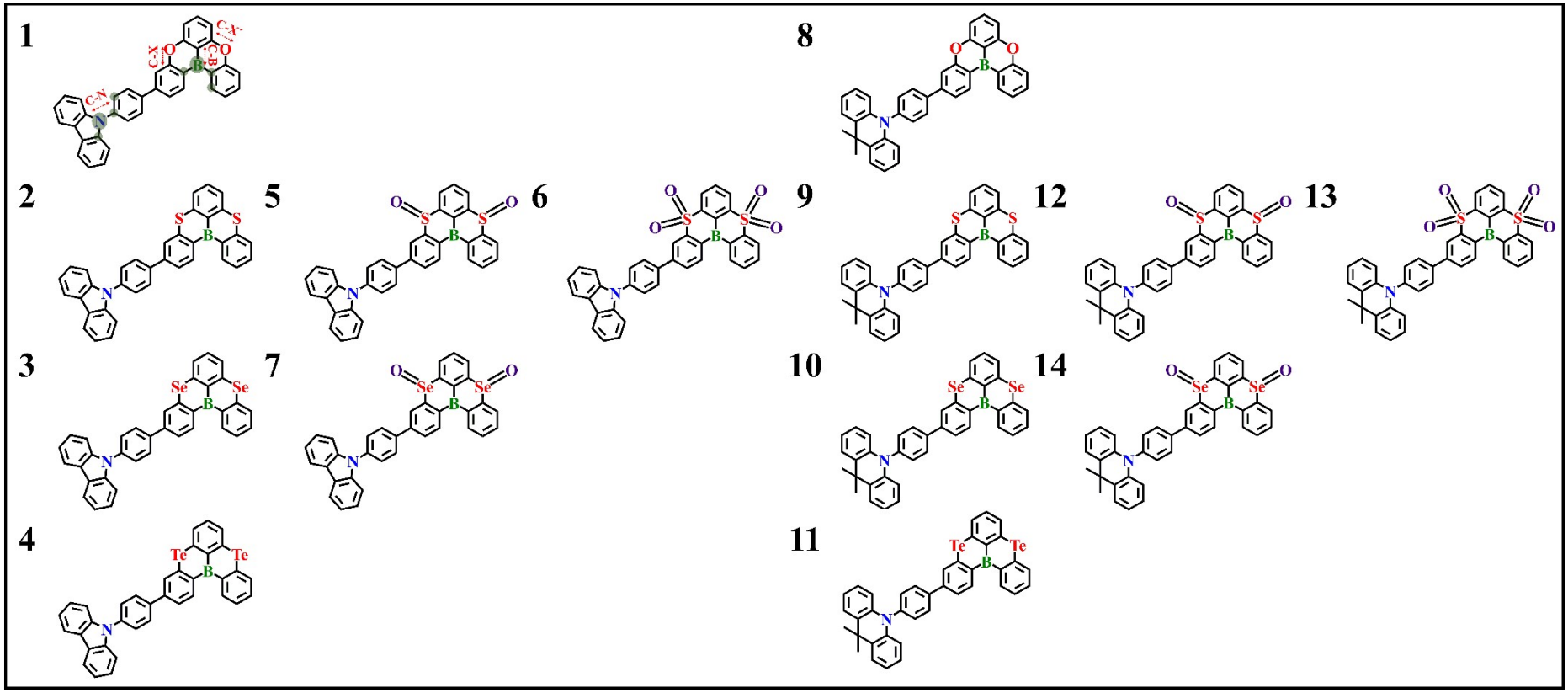

Figure S2. Chemical structures of newly proposed molecules.

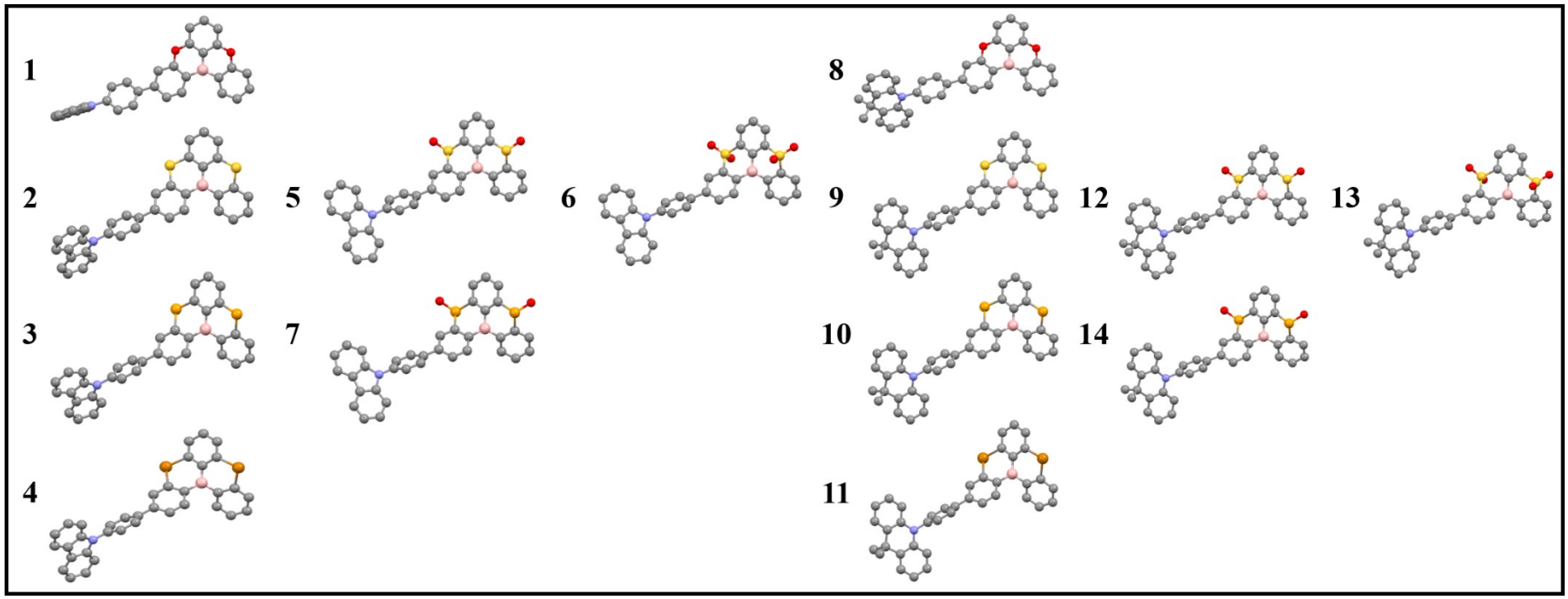

Figure S3. Optimized geometries (S_0 geometry) of newly proposed molecules as obtained at B3LYP/6-31+G* level of theory. The hydrogen atoms are omitted here for clarity.

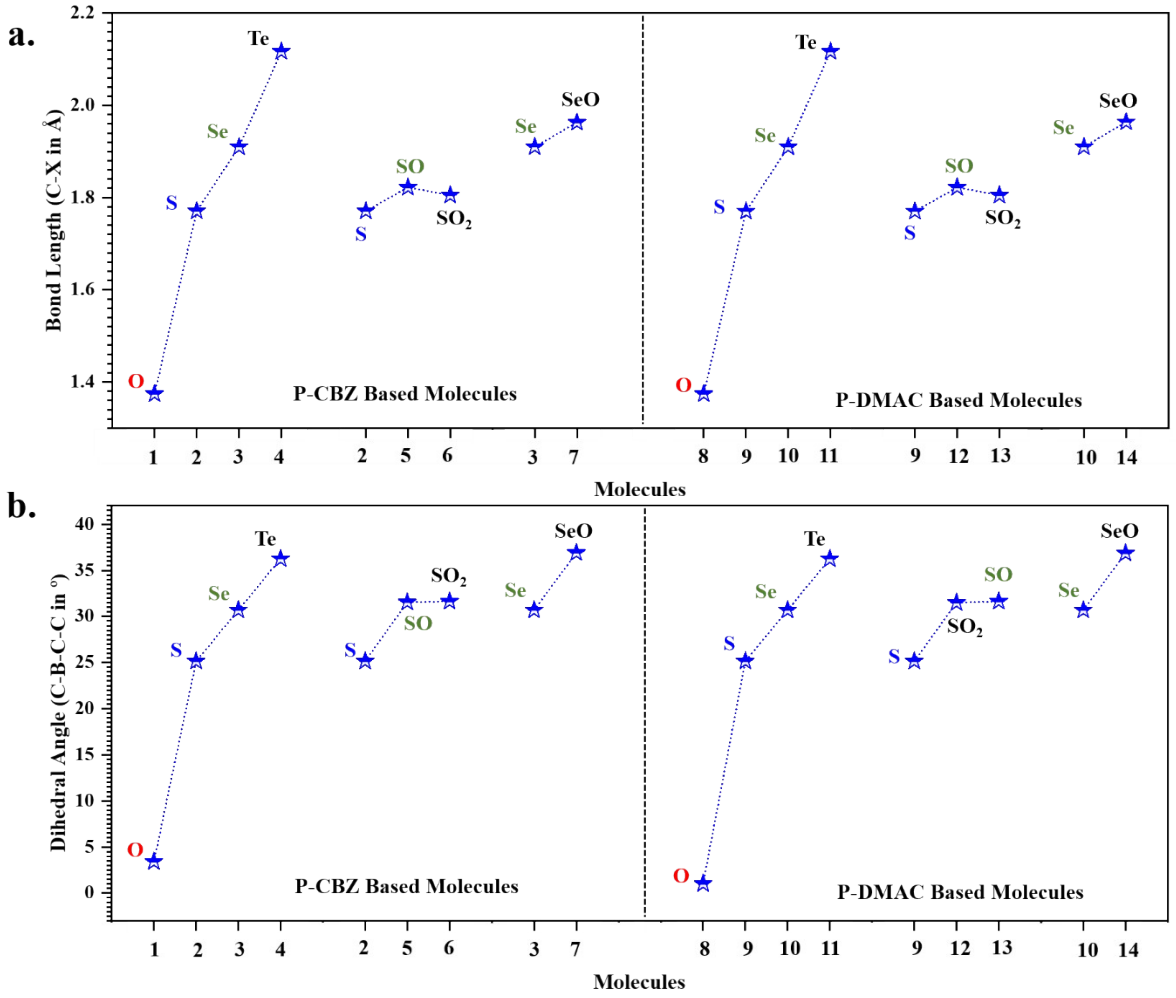

Figure S4. Evolution of C-X bond length (figure a) and C-B-C-C dihedral angles (figure b) for the newly proposed molecules with heavy atom and oxidation effects.

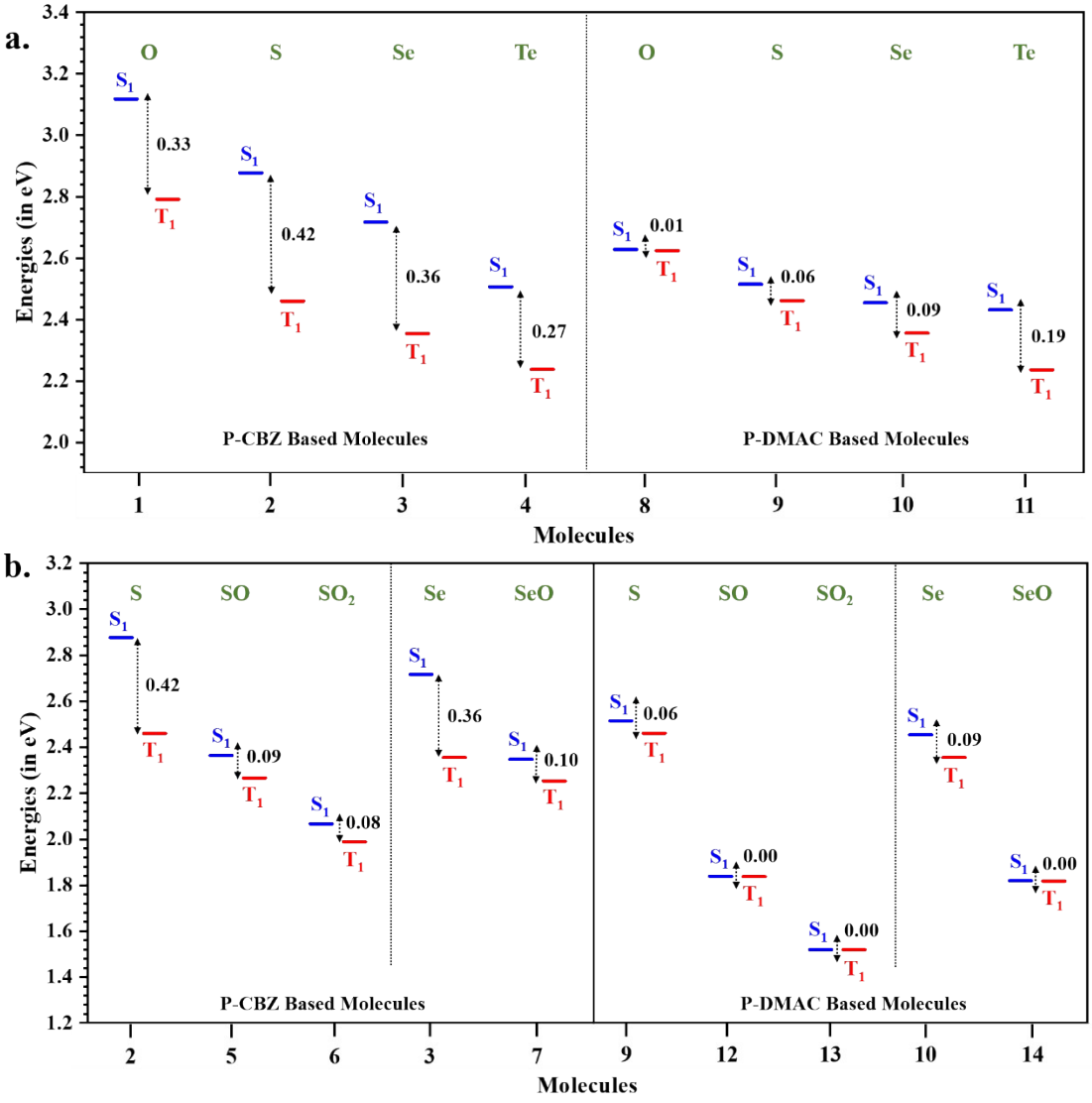

Figure S5. Evolution of vertical singlet (S_1), triplet (T_1), and ΔE_{ST} energies of newly designed molecules obtained at B3LYP functional with 6-31+G* basis set (Figures a and b represent the heavy and oxidation effect evolutions, respectively).

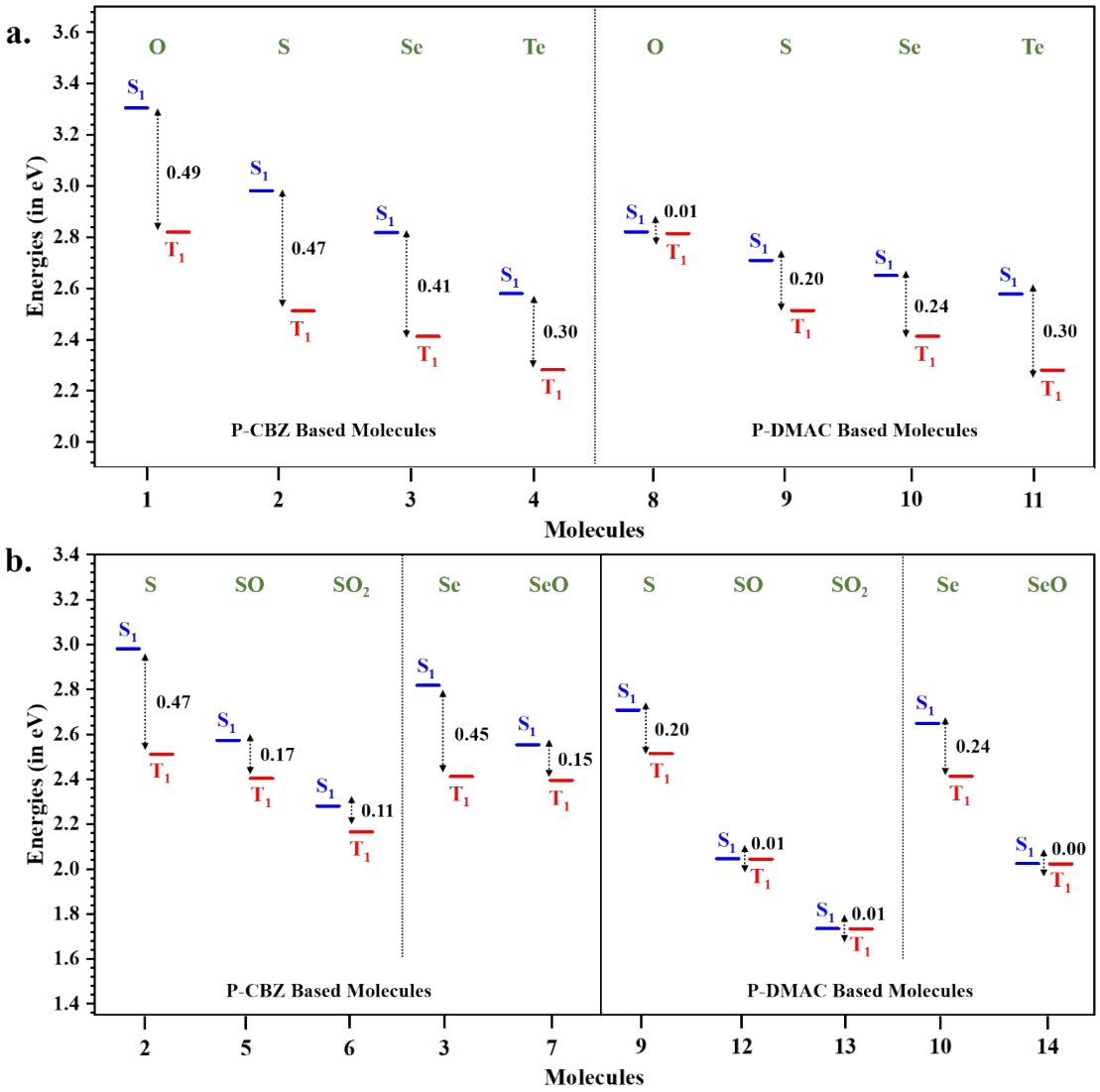

Figure S6. Evolution of vertical singlet (S_1), triplet (T_1), and ΔE_{ST} energies of newly designed molecules obtained at PBE0 functional with 6-31+G* basis set (Figures a and b represent the heavy and oxidation effect evolutions, respectively).

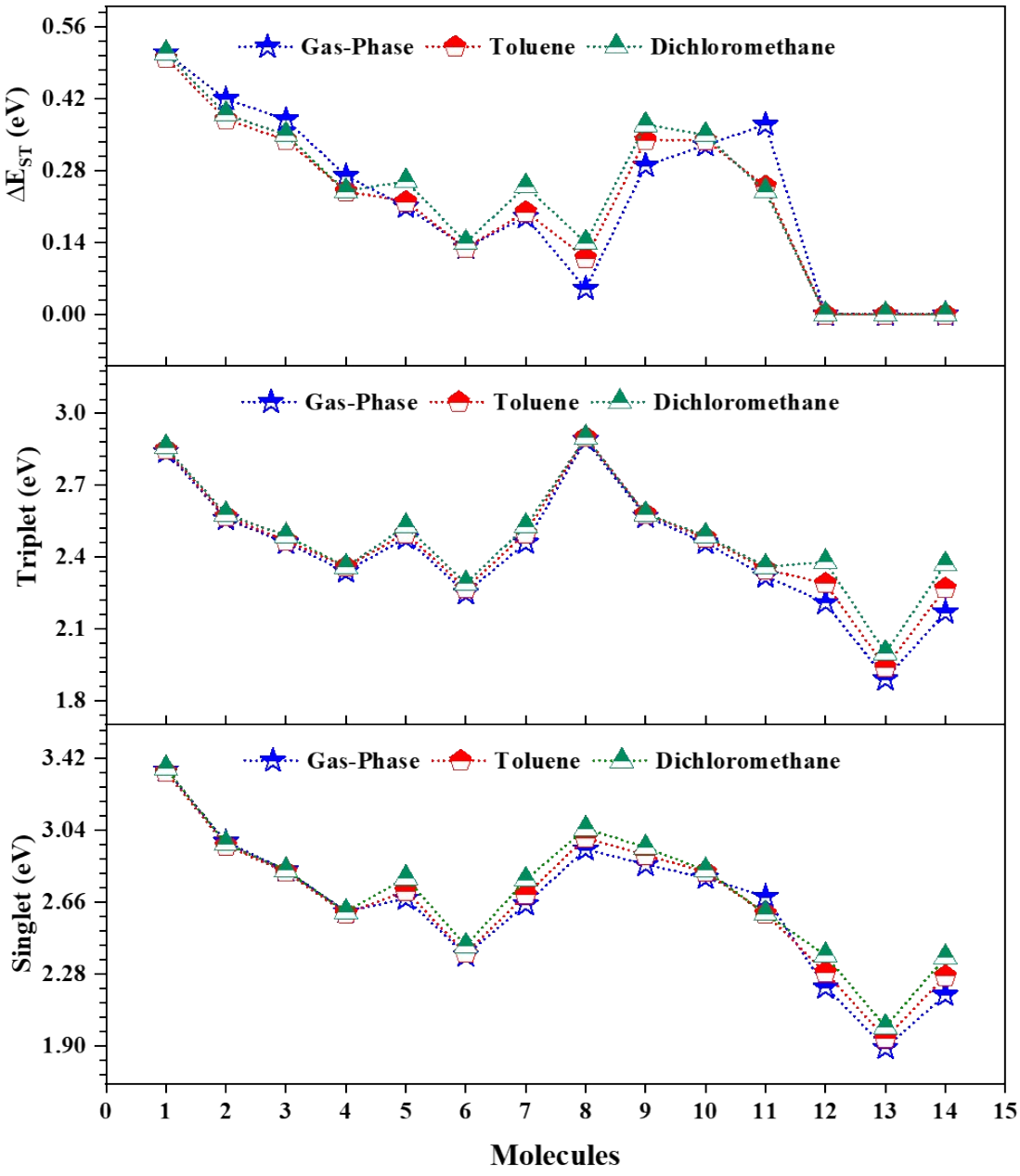

Figure S7. Comparison of vertical singlet (S_1), triplet (T_1), and ΔE_{ST} energies of the molecules using different solvent models with gas-phase medium obtained at the M06/6-31+G* level of theory.

Cartesian coordinates of optimized structures obtained from B3LYP/6-31+G* level of theory. (All the cartesian coordinates are in Å)

Molecule-1

Atoms	x	y	z
C	6.00494200	1.33463700	-0.29135000
C	5.82866300	2.71826500	-0.54303500
C	7.34913100	0.89174900	-0.24426600
C	6.89291500	3.58656900	-0.74665800
H	4.82405200	3.12436900	-0.56840100
C	8.43850700	1.75059600	-0.45329900
C	8.20774300	3.09513600	-0.70636500
H	6.70919100	4.64090000	-0.93493100
H	9.44385500	1.34299100	-0.40680400
C	3.34559700	0.35338900	-0.09471500
C	2.54529900	1.47236800	-0.43249400
C	2.62207800	-0.81674500	0.23794900
C	1.15959200	1.43976600	-0.42784500
H	3.02886800	2.40167800	-0.71039700
C	1.22263900	-0.86800000	0.25514000
C	0.46886800	0.25912800	-0.07454800
H	0.60037000	2.33861500	-0.67154900
H	0.74581000	-1.81266200	0.49766800
C	5.42949300	-1.11582900	0.26453800
C	4.56653500	-2.18931600	0.55702600
C	6.81072300	-1.38846900	0.28426700
C	5.03578400	-3.46823700	0.85614500
C	7.32044400	-2.65441300	0.57487100
C	6.41721900	-3.68202000	0.85932800
H	4.33475100	-4.26680400	1.07601600
H	8.39277600	-2.82045900	0.57848500
H	6.79865900	-4.67345600	1.08904300
H	9.04834600	3.76533200	-0.86680300
C	-1.01532700	0.21396100	-0.05982700
C	-1.71045600	-0.50402400	0.92940800
C	-1.77035200	0.88862900	-1.03557600
C	-3.10328100	-0.55568000	0.94031500
H	-1.15542600	-1.01944900	1.70836400
C	-3.16373500	0.85393700	-1.02267900
H	-1.26249600	1.43742000	-1.82381100
C	-3.84090800	0.12712700	-0.03521600
H	-3.62439900	-1.12482000	1.70466500
H	-3.73210400	1.38978300	-1.77736100
C	-6.07517700	-0.38812100	-1.05950300
C	-6.08445600	0.50635400	1.02763700
C	-5.71128300	-0.93887900	-2.29288500
C	-7.43468400	-0.26699400	-0.67035700
C	-5.73356300	1.07820500	2.25517400
C	-7.44062400	0.30416000	0.66112300
C	-6.73462300	-1.35354700	-3.14565600

H	-4.66961600	-1.04695700	-2.57884200
C	-8.44321700	-0.69124700	-1.54557600
C	-6.76547900	1.43141200	3.12512100
H	-4.69555100	1.24791100	2.52401700
C	-8.45794000	0.66782300	1.55327500
C	-8.08849300	-1.22938200	-2.78136200
H	-6.47739800	-1.78397600	-4.11006600
H	-9.48950200	-0.60534800	-1.26259700
C	-8.11541300	1.22664900	2.78330700
H	-6.51836200	1.87652600	4.08550000
H	-9.50180200	0.51945400	1.28773700
H	-8.86181000	-1.56085000	-3.46897400
H	-8.89556900	1.51154600	3.48394400
N	-5.26153300	0.08358300	-0.02277800
B	4.89539000	0.27342900	-0.05919200
O	3.21164500	-2.01419900	0.56272100
O	7.71937700	-0.40676600	0.01128400

Molecule-2

Atoms	**x**	**y**	**z**
C	5.42184700	1.51853600	-0.31317900
C	4.88949400	2.81927200	-0.12829900
C	6.77116200	1.45066600	-0.73957500
C	5.61540700	3.97230800	-0.40405700
H	3.88128600	2.91742700	0.26236600
C	7.50487600	2.60992700	-1.04947300
C	6.92539400	3.86337100	-0.89042600
H	5.17067500	4.95057400	-0.24179400
H	8.53549200	2.52538300	-1.38557600
C	3.04104300	0.20023600	-0.03177900
C	2.27337100	1.10527900	-0.80536000
C	2.30281400	-0.78314200	0.67062400
C	0.88619200	1.08305400	-0.83457600
H	2.79143600	1.84307300	-1.41021600
C	0.89925400	-0.79633400	0.66975700
C	0.16958100	0.13953500	-0.07043700
H	0.34896000	1.81633400	-1.42972200
H	0.37307600	-1.57976000	1.20932800
C	5.35595900	-1.07006600	0.33601200
C	4.73233400	-2.14291000	1.03005000
C	6.71658700	-1.26468800	-0.02753700
C	5.41907400	-3.32164500	1.34764900
C	7.40346600	-2.44871700	0.27208100
C	6.75029100	-3.46769200	0.96195800
H	4.91156700	-4.12506800	1.87470000
H	8.44506100	-2.56390100	-0.01541300
H	7.28326000	-4.38429300	1.20131200
H	7.50287300	4.75561800	-1.11910200
C	-1.31502300	0.11612100	-0.07207900

C	-2.03728400	-0.15903500	1.10271600
C	-2.04372500	0.36980300	-1.24779800
C	-3.43082200	-0.18891200	1.10423000
H	-1.50304400	-0.33950400	2.03154800
C	-3.43745900	0.35668800	-1.25089000
H	-1.51484400	0.56725300	-2.17608900
C	-4.14183300	0.07301200	-0.07380100
H	-3.97299600	-0.41487800	2.01784200
H	-3.98526200	0.56606200	-2.16510700
C	-6.36881900	-0.77394100	-0.86736400
C	-6.39429500	0.85480100	0.71479600
C	-5.99584500	-1.76070300	-1.78615800
C	-7.73174100	-0.49841200	-0.58308400
C	-6.05231200	1.85156800	1.63484600
C	-7.74801600	0.54124700	0.42585800
C	-7.01317200	-2.46118900	-2.43481500
H	-4.95202800	-1.98140600	-1.98680300
C	-8.73408500	-1.21648900	-1.24851300
C	-7.09108000	2.52327300	2.27998700
H	-5.01575400	2.10113100	1.83928400
C	-8.77234400	1.23087800	1.08786900
C	-8.37004400	-2.19249200	-2.17450800
H	-6.74884500	-3.23231100	-3.15384800
H	-9.78289300	-1.01760000	-1.04209400
C	-8.43898500	2.21668400	2.01505300
H	-6.85094400	3.30131500	3.00006300
H	-9.81445000	1.00260300	0.87794900
H	-9.13848000	-2.75515000	-2.69758800
H	-9.22468600	2.75746700	2.53555500
N	-5.56293500	0.05185200	-0.07484100
B	4.59795600	0.23222400	-0.00568900
S	3.06136400	-2.07503500	1.61421200
S	7.65386900	-0.07082800	-0.93877000

Molecule-3

Atoms	**x**	**y**	**z**
C	4.74665800	1.71850900	-0.09932400
C	4.17037000	2.92370300	0.37312400
C	6.04830200	1.81565600	-0.64173100
C	4.82446500	4.14873900	0.28234200
H	3.18709300	2.88592000	0.83321500
C	6.71134500	3.04610600	-0.75195100
C	6.09715400	4.21045400	-0.29838200
H	4.35117000	5.05033600	0.66223000
H	7.71385000	3.09255100	-1.17013300
C	2.43400600	0.30662800	0.03939700
C	1.67860700	1.24018900	-0.71091100
C	1.68967400	-0.69837300	0.69688800
C	0.29097900	1.20813100	-0.76931400

H	2.20440600	2.01351500	-1.26350900
C	0.29137300	-0.73142100	0.65805200
C	-0.43214600	0.22725000	-0.06296300
H	-0.24094400	1.96427800	-1.34029200
H	-0.24253300	-1.53513900	1.15856500
C	4.80374600	-0.95478200	0.22538700
C	4.27344200	-2.08258400	0.90425800
C	6.11740700	-1.10063300	-0.29150200
C	4.99770300	-3.26861000	1.05925000
C	6.84839600	-2.28431000	-0.14443800
C	6.28480800	-3.36432000	0.53236500
H	4.55750800	-4.11932000	1.57235800
H	7.85773500	-2.36031300	-0.53977600
H	6.85076500	-4.28509300	0.64932200
H	6.62061400	5.16017300	-0.37648900
C	-1.91567300	0.19411400	-0.09148600
C	-2.65435700	-0.12032800	1.06313000
C	-2.62696400	0.48168900	-1.26992500
C	-4.04753700	-0.15750900	1.04162900
H	-2.13341400	-0.32672500	1.99411200
C	-4.02030300	0.46056800	-1.29561600
H	-2.08406700	0.71113200	-2.18269500
C	-4.74133700	0.13698700	-0.13900800
H	-4.60277200	-0.41416600	1.93914300
H	-4.55497900	0.69574200	-2.21132500
C	-6.95047000	-0.69560300	-0.99513200
C	-7.01042000	0.87837900	0.64065800
C	-6.55732900	-1.64837000	-1.94099800
C	-8.31926200	-0.43873100	-0.72190400
C	-6.68892600	1.84582200	1.59862300
C	-8.35752600	0.56602600	0.32122500
C	-7.56020500	-2.33306800	-2.62788300
H	-5.50922700	-1.85561700	-2.13344800
C	-9.30681100	-1.14021500	-1.42602700
C	-7.74169200	2.48838900	2.25071000
H	-5.65726300	2.09530200	1.82652300
C	-9.39623300	1.22607200	0.99092500
C	-8.92255700	-2.08197200	-2.37891500
H	-7.28005800	-3.07775600	-3.36846400
H	-10.35986500	-0.95513200	-1.22858600
C	-9.08339500	2.18206700	1.95571700
H	-7.51756700	3.24324500	3.00003300
H	-10.43352600	0.99821000	0.75799300
H	-9.67936000	-2.63148700	-2.93206100
H	-9.88039400	2.69969800	2.48254100
N	-6.16199600	0.10807000	-0.16326400
B	3.99294600	0.36027500	0.05458900
Se	2.53915100	-2.07327200	1.71527700
Se	6.99468200	0.28400400	-1.27754100

Molecule-4

Atoms	x	y	z
C	-4.18768200	1.79149600	-0.34873200
C	-3.57065400	2.75080600	-1.19102000
C	-5.41370700	2.17066300	0.24680300
C	-4.11923100	4.01156900	-1.41467800
H	-2.63832600	2.48912600	-1.68361800
C	-5.95821500	3.44759900	0.05026800
C	-5.31247600	4.36679800	-0.77729000
H	-3.61833900	4.71517800	-2.07455700
H	-6.89997700	3.72253800	0.51962300
C	-1.95235400	0.30439600	-0.19801500
C	-1.21891900	1.33989600	0.43265900
C	-1.18823500	-0.76513700	-0.71972300
C	0.16836600	1.32959300	0.52374600
H	-1.76154400	2.17835600	0.86023400
C	0.20954200	-0.76918700	-0.65709400
C	0.91297400	0.27651000	-0.03840300
H	0.68116400	2.15982100	1.00192800
H	0.76734600	-1.61759100	-1.04597100
C	-4.38678100	-0.91667600	-0.06311000
C	-3.96397500	-2.16835300	-0.59104900
C	-5.64580900	-0.91343300	0.59963200
C	-4.74489800	-3.32422900	-0.47690200
C	-6.41580100	-2.07463000	0.73516300
C	-5.96754900	-3.27723500	0.19129100
H	-4.39410300	-4.26979300	-0.88288400
H	-7.37822000	-2.04261900	1.23984600
H	-6.57023100	-4.17717700	0.28821000
H	-5.75001300	5.34957400	-0.93599900
C	2.39555400	0.25679600	0.03622200
C	3.17196400	-0.19660300	-1.04553100
C	3.06888400	0.69273100	1.19184700
C	4.56411900	-0.22224800	-0.97584500
H	2.68206500	-0.52082500	-1.95962200
C	4.46104000	0.68403000	1.26370500
H	2.49661000	1.03075000	2.05130100
C	5.21940800	0.22227900	0.17989000
H	5.14837100	-0.58603100	-1.81610300
H	4.96571900	1.03473300	2.15927800
C	7.40275900	-0.48719100	1.19824300
C	7.51000900	0.88127500	-0.61091900
C	6.98210000	-1.32270800	2.23880200
C	8.77909300	-0.25446600	0.93998100
C	7.21581400	1.72468000	-1.68789900
C	8.84752900	0.61935000	-0.21385000
C	7.96478400	-1.91303800	3.03449800
H	5.92899300	-1.51282900	2.42127700
C	9.74592200	-0.85944600	1.75433100

C	8.28695000	2.29321900	-2.37838100
H	6.19110500	1.93696500	-1.97668700
C	9.90511700	1.20276700	-0.92452900
C	9.33398900	-1.68343900	2.80069600
H	7.66343300	-2.56569100	3.84979500
H	10.80417800	-0.69140600	1.57007000
C	9.61989800	2.03455100	-2.00635700
H	8.08443800	2.95142900	-3.21936300
H	10.93520600	1.01228300	-0.63344200
H	10.07426700	-2.15725300	3.43956900
H	10.43150800	2.49183800	-2.56569100
N	6.63892600	0.20581000	0.25178600
B	-3.51794100	0.38068700	-0.20253400
Te	-6.45530300	0.82973300	1.51184000
Te	-2.14169000	-2.40268300	-1.66468100

Molecule-5

Atoms	**x**	**y**	**z**
C	-5.23866300	-1.62789900	0.29524700
C	-4.94967100	-2.73986400	1.11568400
C	-6.52743500	-1.59051500	-0.28253600
C	-5.89219100	-3.74324300	1.34740200
H	-3.98087100	-2.79734100	1.60510600
C	-7.47733500	-2.58763300	-0.07701400
C	-7.15656400	-3.66445500	0.75585400
H	-5.64464000	-4.58142200	1.99333900
H	-8.45592200	-2.50556400	-0.54170000
C	-2.73546700	-0.45271700	0.31994900
C	-1.97153500	-1.56768500	-0.08732700
C	-1.99899900	0.70002200	0.67196500
C	-0.58074300	-1.52567800	-0.14680600
H	-2.48336700	-2.47851900	-0.38708000
C	-0.61244300	0.75973400	0.62996100
C	0.12680300	-0.35963000	0.20158900
H	-0.03405200	-2.41403500	-0.45040400
H	-0.11654100	1.69303100	0.88147400
C	-4.93116400	0.98812600	-0.06801200
C	-4.31627700	2.18607800	0.34419000
C	-6.16607000	1.12252800	-0.73077800
C	-4.88375200	3.43988300	0.12455000
C	-6.75923800	2.35990900	-0.97636900
C	-6.11070600	3.51977200	-0.54163400
H	-4.36464300	4.33463500	0.45603700
H	-7.71816300	2.40878200	-1.48432500
S	-6.94875600	-0.32348300	-1.52076200
S	-2.83810300	2.13766700	1.41167400
H	-6.56352200	4.49095100	-0.72287400
H	-7.89673800	-4.43788200	0.94408400
O	-2.00399300	3.38180400	1.16556800

O	-8.45340900	-0.12541800	-1.53859400
C	1.60628800	-0.30543100	0.12015000
C	2.35890400	0.42227600	1.05991300
C	2.30230500	-0.97895300	-0.90023000
C	3.74948800	0.46558200	0.99324500
H	1.85514000	0.93084400	1.87706700
C	3.69157900	-0.92345100	-0.98514100
H	1.74955200	-1.51820200	-1.66452000
C	4.42806900	-0.20419800	-0.03403300
H	4.31594000	1.00440600	1.74685800
H	4.20993600	-1.41950300	-1.80030300
C	6.70399800	-1.25861600	-0.13220100
C	6.61951900	1.01228700	-0.17757400
C	6.40168300	-2.62190900	-0.04999900
C	8.04364700	-0.79790300	-0.21171200
C	6.21212700	2.34972200	-0.22200900
C	7.98959000	0.64973600	-0.24173900
C	7.46479300	-3.52539400	-0.06917300
H	5.37719600	-2.97092900	0.03292600
C	9.09311700	-1.72575300	-0.22929000
C	7.20339700	3.32745000	-0.31153400
H	5.16229500	2.62414300	-0.19486800
C	8.96551200	1.65092300	-0.33146400
C	8.79849100	-3.08639300	-0.16233400
H	7.25493500	-4.59011700	-0.00754200
H	10.12486600	-1.38831500	-0.28978600
C	8.56776200	2.98628800	-0.36150500
H	6.91162300	4.37385800	-0.34624700
H	10.01955400	1.38911700	-0.38146100
H	9.60392000	-3.81557000	-0.17638900
H	9.31524900	3.77191900	-0.42956300
N	5.84351200	-0.15301400	-0.11158300
B	-4.28205400	-0.40583500	0.19103200

Molecule-6

Atoms	**x**	**y**	**z**
C	-4.95446800	-1.64701200	0.44171100
C	-4.59498500	-2.69349500	1.31392200
C	-6.25554000	-1.70653600	-0.10443200
C	-5.47951800	-3.73459700	1.61057200
H	-3.61892900	-2.67360700	1.79068600
C	-7.15061600	-2.73435100	0.17027200
C	-6.75298200	-3.75765400	1.03881700
H	-5.17598700	-4.52318300	2.29380800
H	-8.14104600	-2.72855400	-0.27436500
C	-2.48851500	-0.42793600	0.28602000
C	-1.73052200	-1.55816500	-0.07985200
C	-1.74595400	0.73887100	0.57117400
C	-0.33829100	-1.52126400	-0.14520600

H	-2.24462800	-2.47947700	-0.33937100
C	-0.36187900	0.79840300	0.51644500
C	0.37512900	-0.34673900	0.15166700
H	0.20384600	-2.42361500	-0.41334900
H	0.14095900	1.73906700	0.71803600
C	-4.73671300	0.96707300	-0.09436700
C	-4.14305500	2.19960700	0.22804300
C	-5.99253000	1.04018600	-0.72115700
C	-4.74263600	3.42719700	-0.04697000
C	-6.62909500	2.24612700	-1.00910400
C	-5.99481700	3.44382700	-0.66777900
H	-4.23571500	4.35048100	0.21615700
H	-7.60365700	2.24490600	-1.48756300
S	-6.75516900	-0.47991600	-1.32829800
S	-2.60551600	2.20670400	1.17396000
O	-1.83029300	3.40423600	0.80431500
O	-2.95278400	1.97349400	2.58910200
O	-6.10031600	-0.82166400	-2.60582100
O	-8.21956600	-0.32313500	-1.28085900
C	1.85437400	-0.30225000	0.07768000
C	2.60280500	0.46243700	0.99112500
C	2.55390500	-1.02249200	-0.90781500
C	3.99381700	0.49705600	0.93258500
H	2.09602300	1.00516600	1.78425400
C	3.94360700	-0.97550200	-0.98528700
H	2.00443000	-1.59136700	-1.65281000
C	4.67695800	-0.21865600	-0.06058700
H	4.55693100	1.06373900	1.66787800
H	4.46498600	-1.50695800	-1.77567400
C	6.94761400	-1.28650800	-0.12053500
C	6.87446500	0.98408200	-0.22084400
C	6.63922600	-2.64595400	-0.00494500
C	8.28944600	-0.83379000	-0.20449100
C	6.47477900	2.32209300	-0.30134500
C	8.24264600	0.61300600	-0.26975000
C	7.69855600	-3.55412000	0.00370700
H	5.61328200	-2.98924300	0.08302100
C	9.33508300	-1.76594100	-0.19366300
C	7.47179200	3.29207200	-0.41041100
H	5.42657400	2.60343500	-0.28720400
C	9.22450500	1.60621300	-0.37972900
C	9.03440000	-3.12324400	-0.09430000
H	7.48372700	-4.61598200	0.09143900
H	10.36847900	-1.43424700	-0.25713100
C	8.83435300	2.94255800	-0.44488700
H	7.18579200	4.33875500	-0.47295100
H	10.27723000	1.33742500	-0.41836400
H	9.83674400	-3.85585700	-0.08621400
H	9.58646500	3.72218000	-0.52877400
N	6.09188100	-0.17608000	-0.13063200

H	-7.44342800	-4.56368500	1.27178400
H	-6.47678200	4.39227500	-0.88689800
B	-4.04118400	-0.40375400	0.21916300

Molecule-7

Atoms	**x**	**y**	**z**
C	-4.66148200	-1.67785700	0.60201300
C	-4.35062000	-2.57388000	1.64843400
C	-5.92020100	-1.83875100	-0.01141700
C	-5.25641100	-3.55469600	2.05921400
H	-3.39633600	-2.48045700	2.16086400
C	-6.83348600	-2.81195600	0.37509900
C	-6.50046200	-3.66767300	1.43163600
H	-4.99639000	-4.22427100	2.87486000
H	-7.79949700	-2.87923200	-0.11895800
C	-2.19977000	-0.46832000	0.42635000
C	-1.45117900	-1.60795500	0.05892300
C	-1.45189900	0.69355900	0.70322700
C	-0.06116000	-1.57361700	-0.03115900
H	-1.97230900	-2.53370600	-0.17242900
C	-0.06884600	0.74777300	0.63229900
C	0.65809900	-0.39465400	0.24132000
H	0.47678100	-2.47880000	-0.29881300
H	0.43788700	1.69018900	0.82402700
C	-4.44015200	0.89116100	-0.12864800
C	-3.91462300	2.15077300	0.21317700
C	-5.62410500	0.90872400	-0.88870900
C	-4.51606600	3.34958600	-0.15902800
C	-6.25265900	2.08587800	-1.28468200
C	-5.69262000	3.31280500	-0.91437400
H	-4.05864500	4.29651700	0.11546900
H	-7.17813000	2.04380500	-1.85309100
H	-6.17321000	4.24043200	-1.21423900
H	-7.21262100	-4.41975100	1.76150200
O	-1.47928200	3.60211600	0.92744200
O	-8.02634300	-0.59588600	-1.60115800
C	2.13583300	-0.35477900	0.13338200
C	2.90775800	0.40971100	1.02712200
C	2.81108300	-1.08008900	-0.86513700
C	4.29732500	0.43938400	0.93742900
H	2.42021200	0.95907300	1.82752400
C	4.19908800	-1.03868100	-0.97385300
H	2.24261800	-1.64973500	-1.59512000
C	4.95522400	-0.28186500	-0.06830400
H	4.87910800	1.00798600	1.65667600
H	4.70125200	-1.57528800	-1.77328500
C	7.22206200	-1.35616700	-0.15882600
C	7.15177200	0.91159700	-0.29813300
C	6.91245500	-2.71260500	-0.01407400

C	8.56309600	-0.90885400	-0.27999000
C	6.75254300	2.24889200	-0.39256500
C	8.51805800	0.53663100	-0.36983300
C	7.96926600	-3.62367800	-0.01283500
H	5.88736400	-3.05061500	0.10074700
C	9.60612400	-1.84405200	-0.27583300
C	7.74863800	3.21462800	-0.54004200
H	5.70521800	2.53213500	-0.36002400
C	9.49896100	1.52587100	-0.51835000
C	9.30396400	-3.19854800	-0.14673300
H	7.75362400	-4.68333500	0.09715700
H	10.63883400	-1.51678500	-0.36763300
C	9.10964900	2.86166000	-0.59825700
H	7.46320500	4.26070800	-0.61439800
H	10.55020900	1.25439000	-0.57504700
H	10.10433200	-3.93339800	-0.14350200
H	9.86105100	3.63818700	-0.71215800
N	6.36928800	-0.24436500	-0.17013400
B	-3.75031700	-0.44795100	0.30768300
Se	-2.36641000	2.27511000	1.42260800
Se	-6.36519400	-0.77267800	-1.59704700

Molecule-8

Atoms	**x**	**y**	**z**
C	6.60583300	1.28119500	-0.49246300
C	6.42610300	2.59704000	-0.98741500
C	7.95193400	0.86606200	-0.34557000
C	7.48862700	3.42951200	-1.31336600
H	5.41985000	2.97779900	-1.11697500
C	9.03964900	1.68993900	-0.67059200
C	8.80545700	2.96915300	-1.15410200
H	7.30178800	4.43179300	-1.68923600
H	10.04662500	1.30713000	-0.53461000
C	3.94785600	0.34210700	-0.13225500
C	3.14475400	1.41890200	-0.58167300
C	3.22673300	-0.78459800	0.33076100
C	1.75902400	1.38468500	-0.57150800
H	3.62519900	2.31876600	-0.94723000
C	1.82746700	-0.83743000	0.35194400
C	1.07138500	0.24558600	-0.09763600
H	1.19758700	2.25281700	-0.90481200
H	1.35241400	-1.75024100	0.69782600
C	6.03552100	-1.06091100	0.42250800
C	5.17458700	-2.09388900	0.84014400
C	7.41791300	-1.31452200	0.50786400
C	5.64649700	-3.31603800	1.31854200
C	7.93049100	-2.52360700	0.97919000
C	7.02893800	-3.51282700	1.38041800
H	4.94681700	-4.08469600	1.63011300

H	9.00364200	-2.67669800	1.02772500
H	7.41253700	-4.46004000	1.75031200
H	9.64509000	3.61162000	-1.40669700
C	-0.41325900	0.19886300	-0.07856600
C	-1.10628200	-0.41247200	0.98176200
C	-1.16700000	0.76652200	-1.12165900
C	-2.50021100	-0.45570500	0.99924500
H	-0.55010700	-0.83576200	1.81368100
C	-2.56096600	0.72308300	-1.10724100
H	-0.65801600	1.22371500	-1.96571600
C	-3.23580400	0.11196900	-0.04585000
H	-3.02639900	-0.92179400	1.82787700
H	-3.13395200	1.15579100	-1.92283000
C	-5.38204400	1.12357500	0.57570400
C	-5.33267100	-1.02333500	-0.62153000
C	-4.67943800	2.19868300	1.16041800
C	-6.79337800	1.11835600	0.60510200
C	-6.74247000	-1.09519000	-0.62901300
C	-4.58145300	-2.05954600	-1.21588100
C	-5.35496800	3.25393600	1.76492600
H	-3.59626800	2.20662400	1.14119100
C	-7.44077300	2.19853900	1.22237000
C	-7.63216100	-0.01166000	-0.00589300
C	-7.33934700	-2.20986600	-1.23578300
H	-3.49928100	-2.00865000	-1.21281500
C	-5.20758400	-3.15100700	-1.80917700
C	-6.74991400	3.26223200	1.80059100
H	-4.78464800	4.06714300	2.20684700
H	-8.52672500	2.20971000	1.25297500
C	-6.60039600	-3.23518700	-1.82375500
H	-8.42341900	-2.28018200	-1.25006100
H	-4.60057000	-3.93282600	-2.25877300
H	-7.29235900	4.07887800	2.26874700
H	-7.10458400	-4.08084400	-2.28308400
N	-4.67091400	0.06922400	-0.02881900
C	-8.55731400	0.58026100	-1.10585400
H	-7.96432300	1.03858800	-1.90476200
H	-9.18627700	-0.19711600	-1.55285600
H	-9.22101300	1.34732600	-0.69251000
C	-8.50866800	-0.65195500	1.10678700
H	-9.13603900	-1.45365900	0.70261400
H	-7.88081700	-1.07745700	1.89715900
H	-9.17215700	0.09069600	1.56278600
B	5.49832400	0.26652000	-0.09804200
O	3.81860500	-1.93481200	0.79349500
O	8.32566800	-0.36997700	0.12476800

Molecule-9

Atoms	**x**	**y**	**z**

C	6.01683700	1.54465500	-0.15879500
C	5.48513200	2.81979300	0.15872800
C	7.36585200	1.52049200	-0.59098400
C	6.21126900	3.99479300	0.00196900
H	4.47742600	2.87778600	0.55857000
C	8.09962300	2.70521700	-0.78138400
C	7.52076300	3.93594600	-0.49422500
H	5.76699100	4.95133800	0.26421000
H	9.12990900	2.65527200	-1.12534000
C	3.63588900	0.20478500	-0.01050500
C	2.86752000	1.18384600	-0.68713600
C	2.89849700	-0.84486000	0.58932900
C	1.48021100	1.16455700	-0.71693200
H	3.38489700	1.97915600	-1.21472900
C	1.49486300	-0.85768500	0.58901900
C	0.76473500	0.14826400	-0.05177600
H	0.94213100	1.95403600	-1.23432400
H	0.96901100	-1.69142100	1.04738600
C	5.95105100	-1.09641100	0.22333000
C	5.32806800	-2.23420600	0.80554700
C	7.31132700	-1.25314100	-0.15952300
C	6.01497900	-3.43914500	1.00093600
C	7.99828100	-2.46155800	0.01736800
C	7.34569100	-3.54534300	0.60080300
H	5.50792300	-4.29188900	1.44428500
H	9.03953600	-2.54696700	-0.28152800
H	7.87874600	-4.48156700	0.74514800
H	8.09836400	4.84675600	-0.63084100
C	-0.72038800	0.12448900	-0.05414700
C	-1.43935500	-0.26633200	1.08990300
C	-1.44881300	0.49258900	-1.19979900
C	-2.83389500	-0.28889100	1.08971300
H	-0.90280600	-0.53014500	1.99728300
C	-2.84331900	0.46924200	-1.20289900
H	-0.91974600	0.77436700	-2.10600500
C	-3.54404600	0.07840200	-0.05754400
H	-3.38019800	-0.58327900	1.98169000
H	-3.39682700	0.74558200	-2.09621900
C	-5.68611700	1.21200400	0.32062100
C	-5.64645700	-1.12557100	-0.44064700
C	-4.97858100	2.37401700	0.69544000
C	-7.09768400	1.22435300	0.33210600
C	-7.05673400	-1.18588400	-0.45196500
C	-4.89977200	-2.26226200	-0.81703100
C	-5.64945400	3.53205700	1.07520400
H	-3.89524700	2.36898400	0.68909300
C	-7.74026400	2.40896400	0.72026100
C	-7.94164300	0.00406700	-0.05847600
C	-7.65867900	-2.39130700	-0.84127800
H	-3.81723700	-2.22044800	-0.81083800

C	-5.53084600	-3.44203900	-1.19808100
C	-7.04453600	3.55874300	1.09046800
H	-5.07546400	4.41072800	1.35866300
H	-8.82629200	2.43481900	0.73457800
C	-6.92421400	-3.51621100	-1.21303300
H	-8.74319200	-2.45432500	-0.85498700
H	-4.92728300	-4.30028400	-1.48262600
H	-7.58340300	4.45506800	1.38465400
H	-7.43226400	-4.43010800	-1.50798100
N	-4.97966700	0.05470900	-0.05926900
C	-8.85171900	0.37976200	-1.26133700
H	-8.24760300	0.67112500	-2.12742100
H	-9.48396800	-0.46444500	-1.55669700
H	-9.51194600	1.21693100	-1.01049800
C	-8.83345300	-0.40333200	1.14776100
H	-9.46463600	-1.26326600	0.89916800
H	-8.21622300	-0.67333500	2.01151600
H	-9.49380200	0.41822300	1.44558200
B	5.19299300	0.23391800	0.01679600
S	3.65783700	-2.22609100	1.39552400
S	8.24792500	0.02719000	-0.94533200

Molecule-10

Atoms	**x**	**y**	**z**
C	5.32007800	1.72348900	0.04782500
C	4.74539500	2.88181500	0.62730900
C	6.61961400	1.86883000	-0.48881700
C	5.39934600	4.11017900	0.64361700
H	3.76376800	2.80297500	1.08571800
C	7.28247000	3.10429700	-0.49137600
C	6.66990200	4.22356800	0.06603200
H	4.92752200	4.97432100	1.10387500
H	8.28352800	3.18796900	-0.90721800
C	3.00813500	0.30396300	0.07065000
C	2.24986700	1.29912800	-0.59242900
C	2.26674100	-0.75480800	0.64118400
C	0.86194600	1.27155100	-0.64799900
H	2.77347900	2.11786300	-1.07760400
C	0.86818400	-0.78411300	0.60661900
C	0.14218200	0.23260500	-0.02665400
H	0.32734800	2.07342000	-1.14989500
H	0.33599400	-1.62795900	1.03814800
C	5.37865600	-0.96791900	0.13512300
C	4.85106400	-2.15147500	0.71391000
C	6.69013500	-1.06704300	-0.39816600
C	5.57567300	-3.34650300	0.75976100
C	7.42148500	-2.25898500	-0.35974800
C	6.86037700	-3.39493800	0.22067200
H	5.13749800	-4.23948900	1.19718300

H	8.42912200	-2.29950500	-0.76454200
H	7.42650700	-4.32244700	0.25280400
H	7.19320300	5.17657100	0.07091600
C	-1.34188500	0.19974900	-0.05410600
C	-2.07542200	-0.21019700	1.07393900
C	-2.05446400	0.58076900	-1.20530100
C	-3.46960100	-0.23969200	1.05239100
H	-1.55073800	-0.48390400	1.98532500
C	-3.44860500	0.54977600	-1.22986900
H	-1.51259200	0.87833200	-2.09886800
C	-4.16413000	0.13936400	-0.10062700
H	-4.02795200	-0.54889600	1.93180900
H	-3.99030600	0.83567700	-2.12740800
C	-6.31762800	1.25768500	0.25655100
C	-6.25377500	-1.07255100	-0.52537800
C	-5.62205500	2.42044200	0.65091200
C	-7.72924400	1.26155600	0.24947100
C	-7.66337500	-1.14127600	-0.55550000
C	-5.49523900	-2.20099000	-0.90294800
C	-6.30482800	3.57108700	1.03191600
H	-4.53872000	2.42178100	0.65894800
C	-8.38400200	2.43888900	0.63942300
C	-8.56057300	0.03943500	-0.16195400
C	-8.25281500	-2.34656700	-0.96388100
H	-4.41315000	-2.15258000	-0.88273400
C	-6.11408600	-3.38079400	-1.30346600
C	-7.70012700	3.58942700	1.02886500
H	-5.73994700	4.45058600	1.33070000
H	-9.47025900	2.45818100	0.63975200
C	-7.50666600	-3.46335400	-1.33684700
H	-9.33665700	-2.41610900	-0.99194700
H	-5.50163200	-4.23251400	-1.58861000
H	-8.24820500	4.47992800	1.32372000
H	-8.00520500	-4.37747200	-1.64694800
N	-5.59932800	0.10801400	-0.12410800
C	-9.45900100	0.42003200	-1.37198300
H	-8.84677500	0.72299000	-2.22833600
H	-10.08231900	-0.42547300	-1.68220200
H	-10.12757000	1.25065700	-1.12150400
C	-9.46366000	-0.38448100	1.03011500
H	-10.08616400	-1.24627300	0.76651700
H	-8.85474600	-0.65817100	1.89860200
H	-10.13277400	0.43014400	1.32742700
B	4.56725300	0.35669800	0.08417900
Se	3.12022700	-2.21450400	1.52987500
Se	7.56348900	0.39974300	-1.26138000

Molecule-11

Atoms	**x**	**y**	**z**

C	4.73428500	1.78640100	0.38266100
C	4.11936500	2.72349500	1.25109200
C	5.95525600	2.18370500	-0.21144800
C	4.66538600	3.98042900	1.50115900
H	3.19102600	2.44715800	1.74321000
C	6.49694500	3.45739700	0.01189200
C	5.85339900	4.35463500	0.86492500
H	4.16635900	4.66654500	2.18058500
H	7.43485000	3.74655900	-0.45661700
C	2.50266400	0.29616600	0.21008200
C	1.76216600	1.34400200	-0.39114000
C	1.74534600	-0.78791600	0.71109300
C	0.37428100	1.33121000	-0.47371300
H	2.29938700	2.19408600	-0.80223600
C	0.34716300	-0.79514000	0.65702700
C	-0.36318500	0.26266300	0.06783300
H	-0.14432000	2.17064500	-0.92899200
H	-0.20568700	-1.65404600	1.02951000
C	4.93999500	-0.91334600	0.03120700
C	4.52441300	-2.17847600	0.53215400
C	6.19503100	-0.89027200	-0.63867200
C	5.30833500	-3.32874100	0.38615900
C	6.96781300	-2.04541900	-0.80625800
C	6.52671400	-3.26194700	-0.28811500
H	4.96311900	-4.28474800	0.77194300
H	7.92699800	-1.99835900	-1.31587900
H	7.13165700	-4.15735100	-0.40985500
H	6.28878800	5.33484100	1.04411100
C	-1.84668200	0.24020300	0.00283000
C	-2.61248200	-0.24187700	1.08023300
C	-2.52758500	0.70211100	-1.13861000
C	-4.00604000	-0.26181300	1.02008000
H	-2.11421400	-0.57974800	1.98485500
C	-3.92096800	0.68240400	-1.20154300
H	-1.96096800	1.05598700	-1.99548400
C	-4.66832300	0.20023300	-0.12194700
H	-4.58868900	-0.62727400	1.86132300
H	-4.43721400	1.03250300	-2.09129600
C	-6.82564300	1.30201900	0.26302700
C	-6.75140200	-0.96152100	-0.69428900
C	-6.13557700	2.42510600	0.76774200
C	-8.23659800	1.31766700	0.21454000
C	-8.16001100	-1.01619800	-0.77213200
C	-5.98814700	-2.06479800	-1.13288500
C	-6.82323600	3.54800300	1.21771400
H	-5.05298300	2.41751200	0.80743300
C	-8.89644600	2.46617300	0.67630900
C	-9.06187900	0.13913600	-0.31841500
C	-8.74396500	-2.18228800	-1.28882500
H	-4.90696200	-2.02725900	-1.07572400

C	-6.60149300	-3.20601200	-1.64051400
C	-8.21805800	3.57748200	1.17513100
H	-6.26273900	4.39703300	1.60088400
H	-9.98205900	2.49419500	0.64550800
C	-7.99319100	-3.27408200	-1.72278400
H	-9.82679800	-2.24030100	-1.35527000
H	-5.98567800	-4.03890000	-1.97044200
H	-8.76976100	4.44649500	1.52257800
H	-8.48735400	-4.15781400	-2.11660700
N	-6.10258300	0.18003100	-0.18534300
C	-9.91489800	0.62119800	-1.52543100
H	-9.27088400	0.98409100	-2.33391500
H	-10.53243100	-0.19195700	-1.92200300
H	-10.58618300	1.43620200	-1.23397400
C	-10.00897800	-0.36715800	0.80560200
H	-10.62861800	-1.19935900	0.45442000
H	-9.43258600	-0.71395000	1.67025200
H	-10.68191300	0.42856700	1.14294000
B	4.06810200	0.37747500	0.20686400
Te	2.70963500	-2.44424300	1.61102500
Te	6.99326500	0.87659000	-1.51430900

Molecule-12

Atoms	**x**	**y**	**z**
C	5.81902900	1.65710600	-0.13663500
C	5.52690500	2.94338400	0.36660200
C	7.10732900	1.47452700	-0.68732500
C	6.46612300	3.97543300	0.32730100
H	4.55843700	3.12324800	0.82606300
C	8.05386100	2.49376400	-0.75021800
C	7.73015500	3.74925300	-0.22571000
H	6.21629500	4.95213500	0.73311200
H	9.03222200	2.29669700	-1.17948600
C	3.31984200	0.52157600	0.19899500
C	2.55221700	1.49016500	-0.48273500
C	2.58816700	-0.50148700	0.84144200
C	1.16124400	1.43069000	-0.52546900
H	3.06083700	2.29217400	-1.01139400
C	1.20136300	-0.57261600	0.82125200
C	0.45889500	0.39470200	0.11788100
H	0.61058600	2.20657200	-1.04996000
H	0.70764000	-1.40789500	1.31004900
C	5.52014400	-0.96426500	0.19342000
C	4.90988000	-2.01535000	0.90466400
C	6.75486300	-1.26268400	-0.41387900
C	5.48152200	-3.28134000	1.01786200
C	7.35206000	-2.51946500	-0.32999700

C	6.70798300	-3.52813900	0.39297200
H	4.96600400	-4.06051300	1.57199800
H	8.31063900	-2.69591200	-0.80951700
H	7.16397700	-4.51160700	0.46998000
H	8.46782400	4.54729700	-0.24671500
C	-1.02218900	0.31840900	0.05796500
C	-1.76955700	-0.11613100	1.16777000
C	-1.71760800	0.67798900	-1.11094000
C	-3.16117400	-0.18341400	1.11313800
H	-1.26129900	-0.38131100	2.09060700
C	-3.10893700	0.60720000	-1.16851100
H	-1.16504200	0.98785800	-1.99365000
C	-3.83905300	0.17770900	-0.05563800
H	-3.73059000	-0.51105600	1.97847100
H	-3.63698400	0.87602600	-2.07921800
C	-6.02915400	1.23822500	0.24554600
C	-5.88314600	-1.09144000	-0.53108800
C	-5.37548600	2.41875900	0.65815300
C	-7.43955600	1.20506900	0.19858000
C	-7.28888100	-1.19602200	-0.60056700
C	-5.08516700	-2.19993800	-0.88468000
C	-6.09845200	3.55161000	1.01807300
H	-4.29320100	2.44856000	0.69781600
C	-8.13535300	2.36528600	0.56815300
C	-8.22698500	-0.03861100	-0.23405300
C	-7.83524000	-2.41664100	-1.02321500
H	-4.00559700	-2.12498600	-0.83286400
C	-5.66175000	-3.39602500	-1.29989200
C	-7.49299900	3.53356000	0.97513700
H	-5.56545400	4.44559300	1.33203600
H	-9.22128600	2.35626800	0.53763600
C	-7.05017400	-3.51413100	-1.37268400
H	-8.91567800	-2.51431700	-1.08151500
H	-5.01971500	-4.23231100	-1.56458700
H	-8.07224500	4.40960300	1.25313000
H	-7.51598100	-4.44134500	-1.69445100
N	-5.27106800	0.10695800	-0.11333700
C	-9.10086200	0.31771500	-1.46914500
H	-8.47325000	0.63606100	-2.30862100
H	-9.69292300	-0.54400000	-1.79540100
H	-9.79771000	1.13063900	-1.23841200
C	-9.15150600	-0.48477100	0.93317600
H	-9.74411100	-1.36239600	0.65355200
H	-8.56017200	-0.74224800	1.81857900
H	-9.84932900	0.31255900	1.21064700
B	4.86683000	0.44712800	0.08266400
S	3.43335400	-1.69553800	1.92681500
S	7.53164600	-0.06956700	-1.55421500
O	2.60303700	-2.96316800	2.01392100

Molecule-13

Atoms	x	y	z
C	5.52493600	1.71218300	-0.03624000
C	5.16390800	2.96030100	0.50863300
C	6.82443300	1.61938000	-0.58155200
C	6.04569800	4.04505600	0.49851600
H	4.18910400	3.07242800	0.97506100
C	7.71658600	2.68530500	-0.60924800
C	7.31763400	3.91004800	-0.06099400
H	5.74117300	4.99287900	0.93405200
H	8.70585700	2.55764800	-1.03788600
C	3.06241300	0.49170300	0.16357600
C	2.30032600	1.47145300	-0.50309400
C	2.32521600	-0.55010800	0.76758400
C	0.90785100	1.41322600	-0.55180100
H	2.81072700	2.28386500	-1.01290800
C	0.94092600	-0.62638200	0.73626200
C	0.20034600	0.36775600	0.06591200
H	0.36118800	2.20092900	-1.06250600
H	0.44087100	-1.47258600	1.19711900
C	5.31501400	-0.94796600	0.18209400
C	4.72647400	-2.04181100	0.83980100
C	6.56944800	-1.19069000	-0.40332400
C	5.32961800	-3.29567100	0.91837000
C	7.20944700	-2.42727600	-0.34332600
C	6.58016800	-3.48263600	0.32270800
H	4.82666700	-4.10921200	1.43204700
H	8.18281100	-2.55786700	-0.80615700
H	7.06485100	-4.45319100	0.37698200
H	8.00589700	4.75084500	-0.06571700
C	-1.28077100	0.30077300	0.01168200
C	-2.02327400	-0.15239200	1.11725500
C	-1.97950700	0.68885900	-1.14599000
C	-3.41551300	-0.21049700	1.06892600
H	-1.51159200	-0.43683600	2.03256800
C	-3.37137700	0.62667300	-1.19677500
H	-1.43017200	1.01351300	-2.02544400
C	-4.09757700	0.17821700	-0.08860100
H	-3.98211000	-0.55176200	1.93075200
H	-3.90314200	0.91695300	-2.09860800
C	-6.27945100	1.24349600	0.25056900
C	-6.15082800	-1.06886100	-0.58118700
C	-5.61672400	2.41050600	0.68615300
C	-7.69013500	1.21850800	0.21190100
C	-7.55746400	-1.16415900	-0.64388200
C	-5.36114800	-2.17299200	-0.96548400
C	-6.33126700	3.53836200	1.07736000
H	-4.53404900	2.43410500	0.71956500

C	-8.37729600	2.37332000	0.61321600
C	-8.48689800	-0.01050400	-0.24496300
C	-8.11308600	-2.37170400	-1.09122600
H	-4.28082900	-2.10521100	-0.91917100
C	-5.94685200	-3.35607200	-1.40466100
C	-7.72607300	3.52834000	1.04324900
H	-5.79153900	4.42192700	1.40873100
H	-9.46340800	2.37068500	0.58973100
C	-7.33627800	-3.46494600	-1.47113500
H	-9.19436100	-2.46223200	-1.14487600
H	-5.31119700	-4.18937300	-1.69306800
H	-8.29884300	4.40052600	1.34562800
H	-7.80921200	-4.38186100	-1.81140600
N	-5.52978200	0.11659600	-0.13969100
C	-9.36560300	0.37919100	-1.46649000
H	-8.74097500	0.71371700	-2.30188700
H	-9.96415600	-0.47151000	-1.80936100
H	-10.05674700	1.19014300	-1.21298000
C	-9.40719900	-0.47882500	0.91688200
H	-10.00629600	-1.34639200	0.62027400
H	-8.81239200	-0.76013500	1.79265200
H	-10.09902400	0.31552100	1.21690700
B	4.61570000	0.45401300	0.10136600
S	3.19211100	-1.78640500	1.75597500
S	7.32483400	0.10035400	-1.41493000
O	3.54337100	-1.16236400	3.04619500
O	8.78986800	-0.03297400	-1.33131000
O	2.42020800	-3.04147900	1.74185800

Molecule-14

Atoms	**x**	**y**	**z**
C	5.21516000	1.78908400	0.12646500
C	4.90151600	2.93289800	0.89319200
C	6.47119100	1.78480800	-0.51305600
C	5.80235500	3.99288900	1.01993600
H	3.94917800	2.97651300	1.41579500
C	7.37934700	2.83113000	-0.40788600
C	7.04392600	3.93863300	0.37976900
H	5.54039900	4.85655900	1.62545900
H	8.34349100	2.76768000	-0.90608500
C	2.75992600	0.56498700	0.29460800
C	2.00423900	1.55925900	-0.36425600
C	2.02009100	-0.48208400	0.87919600
C	0.61394700	1.49538100	-0.43521100
H	2.51947100	2.38995200	-0.84024100
C	0.63678000	-0.55928600	0.83276300
C	-0.09679500	0.43134800	0.15037800
H	0.06937900	2.29058300	-0.93676000
H	0.13486700	-1.41570000	1.27600300

C	5.00682600	-0.88283300	0.11617900
C	4.48980400	-2.00578900	0.78794100
C	6.18888900	-1.09895800	-0.61581000
C	5.09750600	-3.25751100	0.75088500
C	6.82329400	-2.33616200	-0.68189200
C	6.27164400	-3.42022700	0.00852300
H	4.64672700	-4.09735800	1.27310900
H	7.74699700	-2.44451500	-1.24437000
H	6.75697400	-4.39193400	-0.03166200
H	7.75225300	4.75562700	0.49107400
C	-1.57631600	0.35816600	0.06462200
C	-2.34010200	-0.11338800	1.14777000
C	-2.25379700	0.75988200	-1.10099200
C	-3.73082900	-0.17605300	1.07068200
H	-1.84555500	-0.41148800	2.06799000
C	-3.64419200	0.69374400	-1.18107500
H	-1.68773200	1.09957000	-1.96399800
C	-4.39095400	0.22684100	-0.09460800
H	-4.31332800	-0.53279400	1.91554500
H	-4.15870300	0.99527700	-2.08927700
C	-6.58391600	1.27922600	0.21296000
C	-6.42900800	-1.02064800	-0.64659800
C	-5.93513300	2.44203000	0.68000800
C	-7.99340300	1.25094600	0.14184300
C	-7.83350900	-1.11910700	-0.74362500
C	-5.62717600	-2.11787300	-1.02561300
C	-6.66204200	3.56198200	1.07100700
H	-4.85356400	2.46804800	0.73789800
C	-8.69324800	2.39785100	0.54390300
C	-8.77551600	0.02685600	-0.35202600
C	-8.37485800	-2.32221000	-1.21956300
H	-4.54852500	-2.04790300	-0.95222400
C	-6.19882200	-3.29672900	-1.49359100
C	-8.05574100	3.54847200	1.00521700
H	-6.13281000	4.44240200	1.42688200
H	-9.77853800	2.39248700	0.49529300
C	-7.58599200	-3.40840200	-1.59478900
H	-9.45430600	-2.41484400	-1.30013100
H	-5.55394900	-4.12472200	-1.77675500
H	-8.63805600	4.41460800	1.30683600
H	-8.04796500	-4.32217200	-1.95787600
N	-5.82191700	0.16066000	-0.17592800
C	-9.62414900	0.43211700	-1.58966200
H	-8.97942900	0.77985800	-2.40414100
H	-10.21165000	-0.41495900	-1.95962700
H	-10.32343500	1.23798200	-1.34211000
C	-9.72388900	-0.45972000	0.77935100
H	-10.31340100	-1.32408900	0.45539600
H	-9.15076300	-0.75242100	1.66578300
H	-10.42493300	0.32889800	1.07308200

B	4.31071900	0.52091900	0.17866900
O	2.06534800	-3.22250300	1.87794400
O	8.58071500	0.16924500	-1.71653500
Se	2.94619200	-1.80720800	1.99371700
Se	6.91868800	0.33269000	-1.75417800