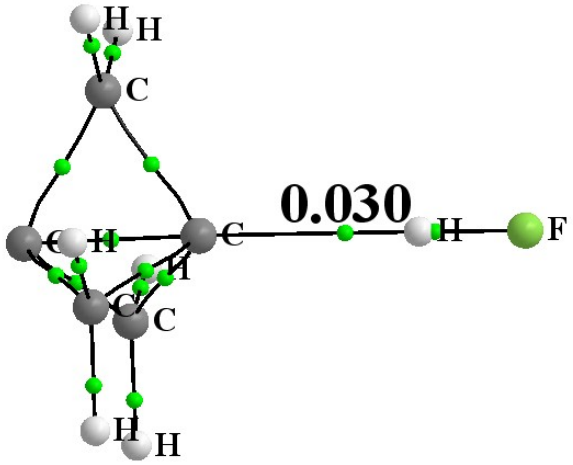
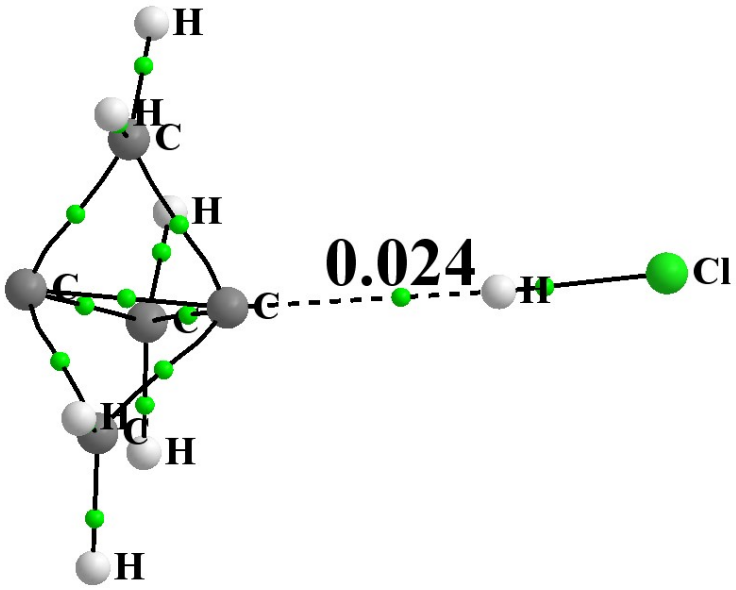
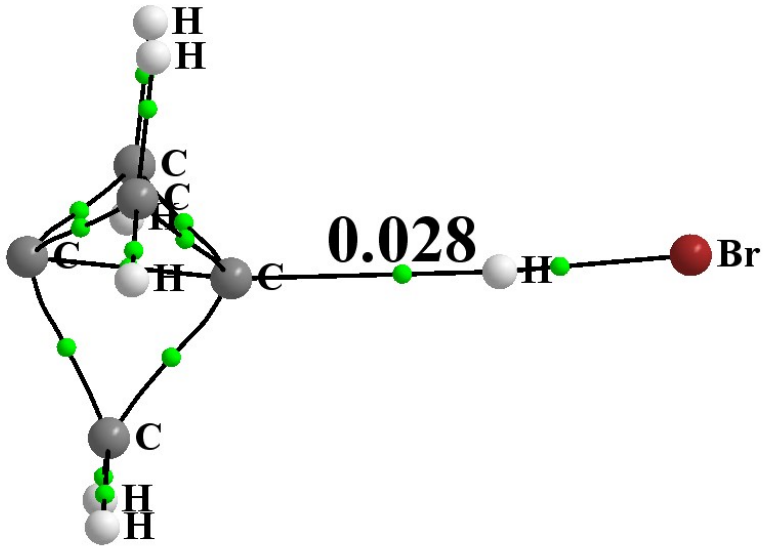
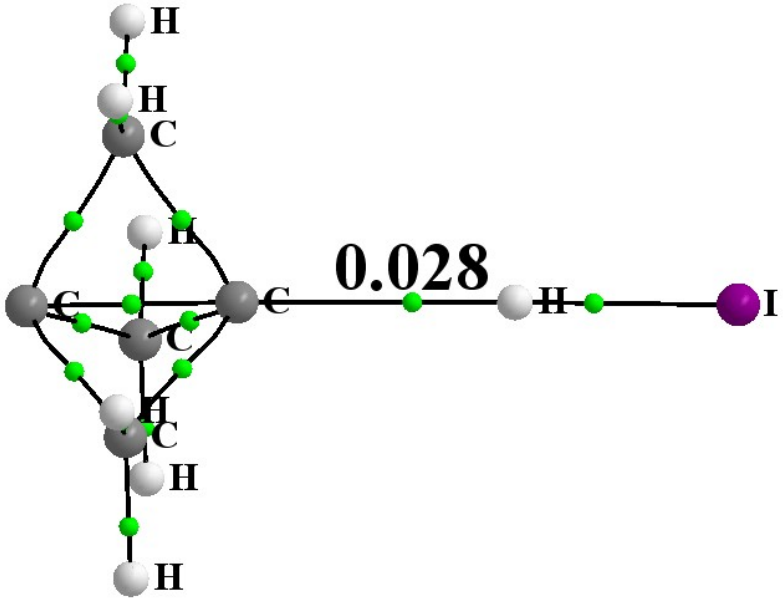
SUPPORTING INFORMATION

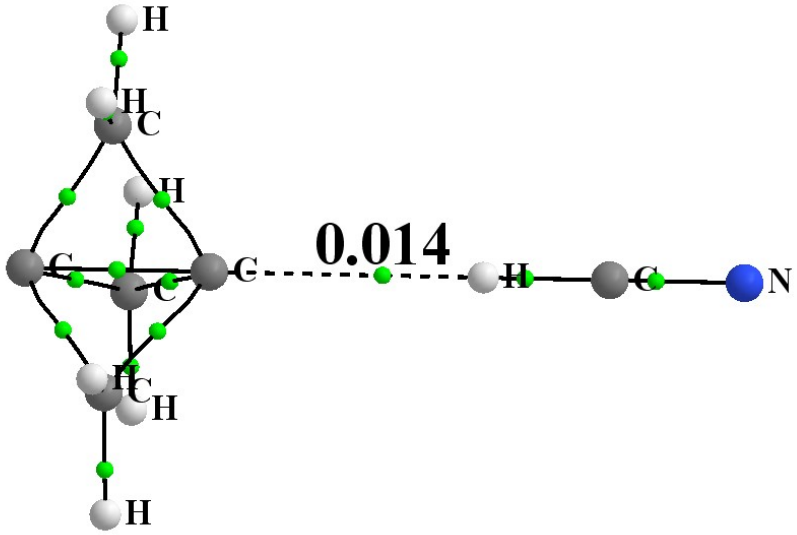
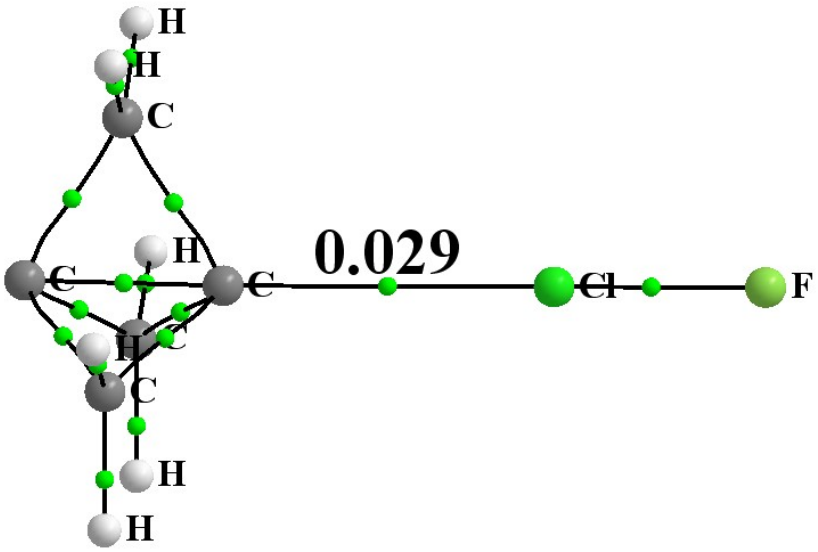
Ability of Strained C Atoms to Act as Electron Donor

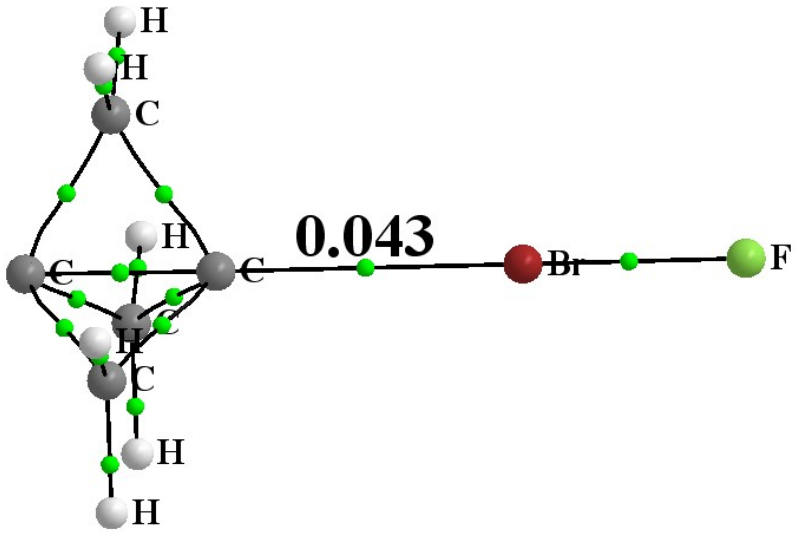
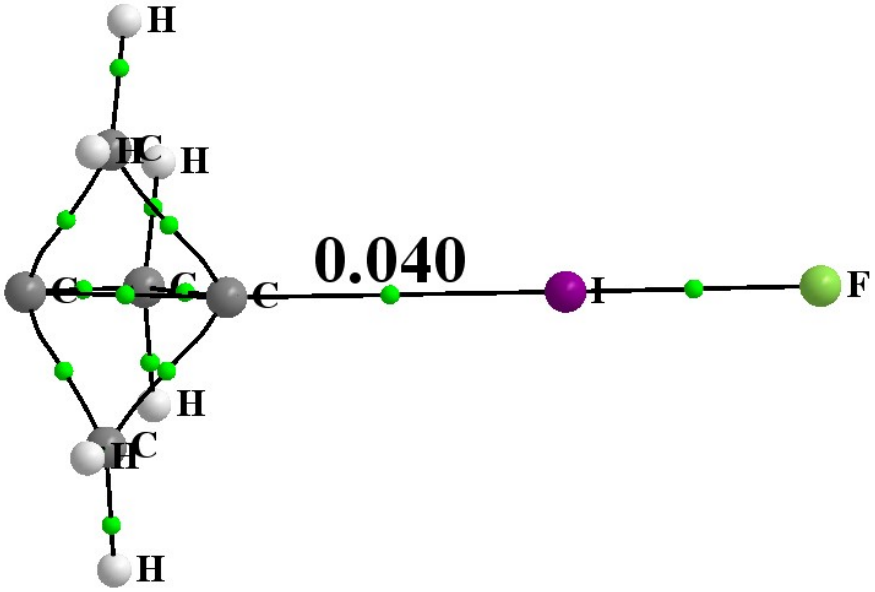
Mariusz Michalczyk Wiktor Zierkiewicz, and Steve Scheiner

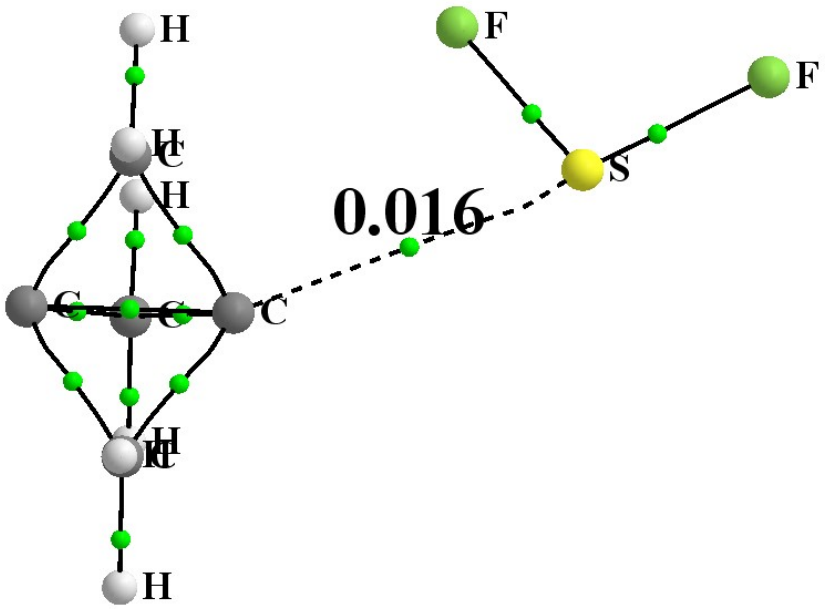
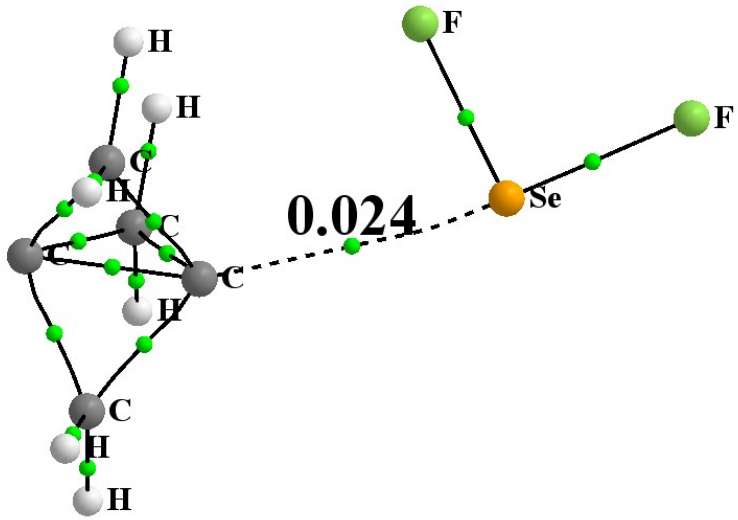
Fig. S1 QTAIM molecular diagrams for fully optimized complexes. The density of the critical point is shown in au.

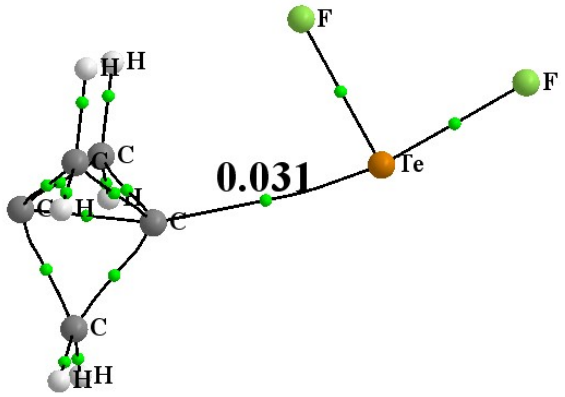
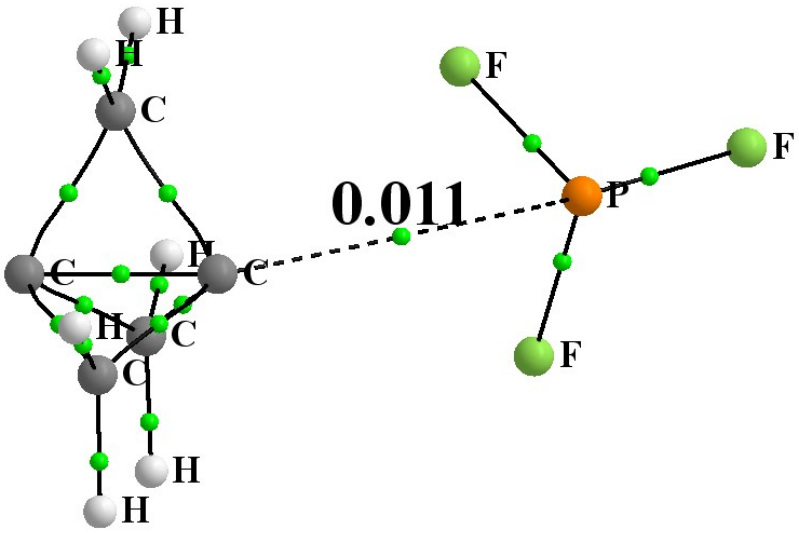
[1.1.1]propellane	
HF	
HCl	

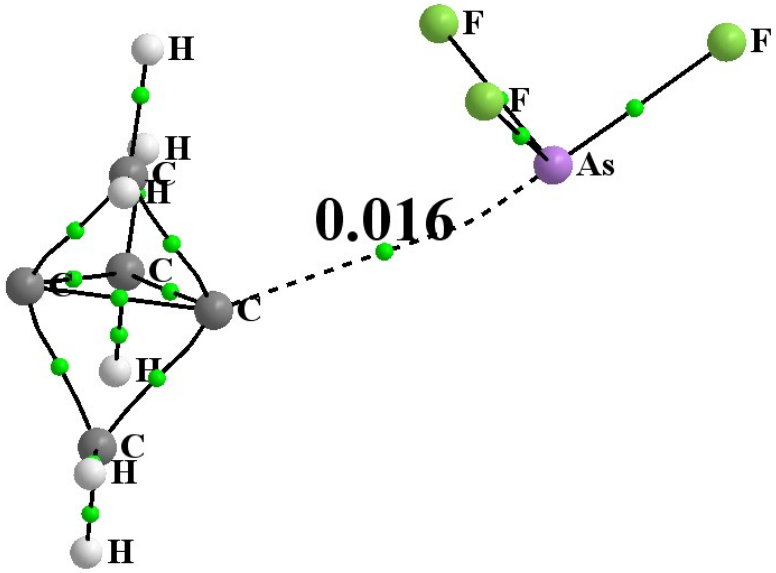
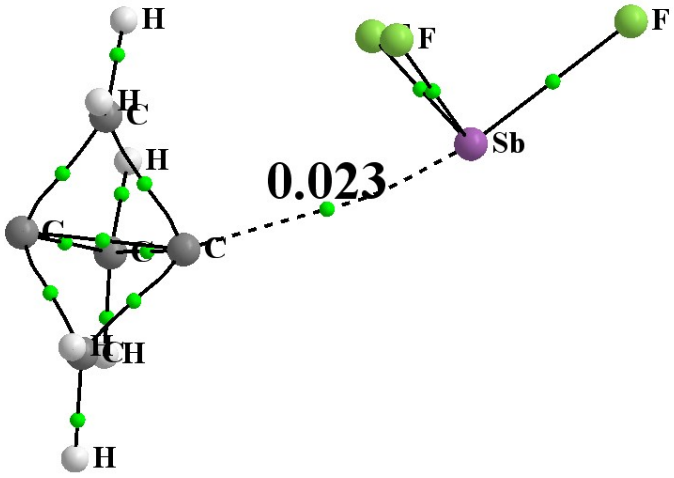
HBr	 H H C C H C H C 0.028 H Br C H H
HI	 H H C H C C 0.028 H I C H C H H

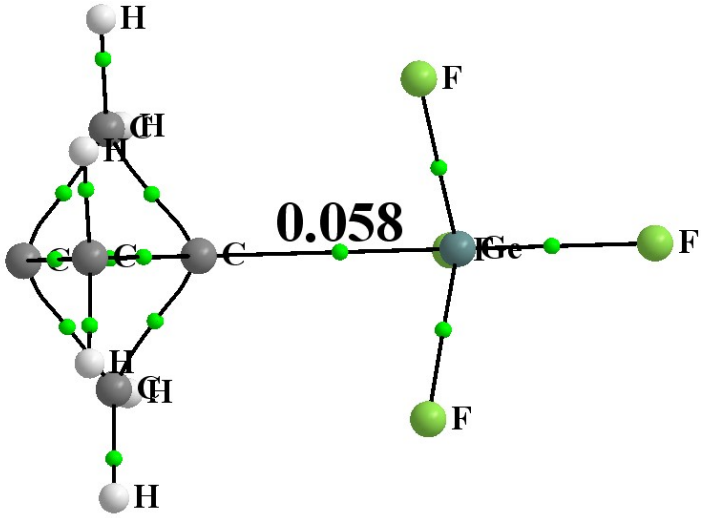
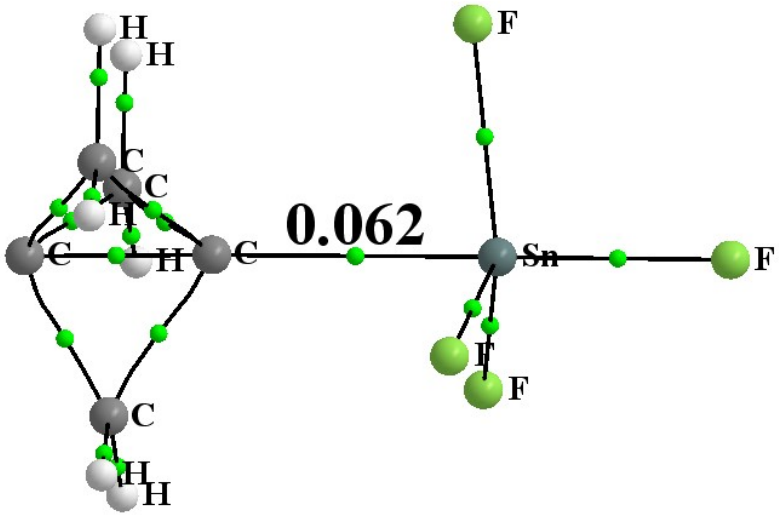
HCN	 H H C H C C C 0.014 H C N H C H H
FCl	 H H C H C C 0.029 Cl F H C C H H

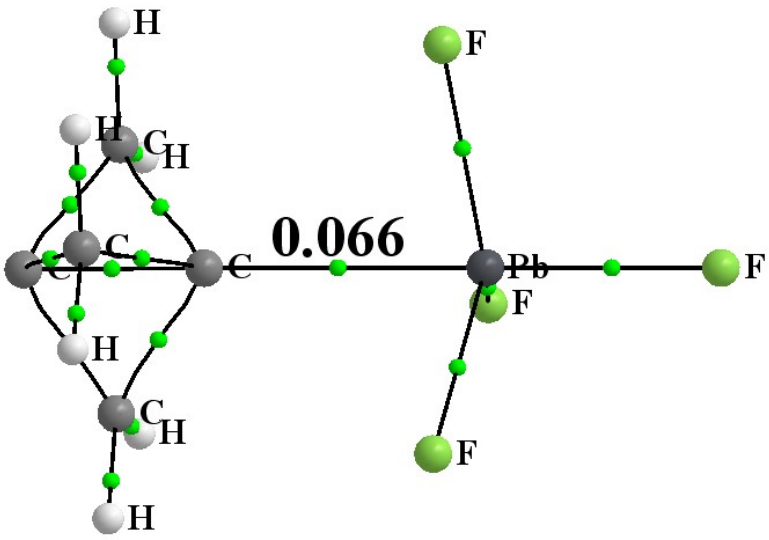
FBr	 H H C H C C 0.043 Br F C H C H H
FI	 H H C H C C 0.040 I F H H C H

SF_2	 H F F S 0.016 C C C H
SeF_2	 H H F F Se 0.024 C C H

TeF_2	 F F Te 0.031 H H C C C H H C C H H
PF_3	 H H C F F 0.011 P C C H H C C F H H

AsF_3	 F F F As 0.016 H H C H C C H C H H
SbF_3	 H H C H F F Sb 0.023 C C C H CH H

GeF_4	 H F 0.058 F F H
SnF_4	 H H F C C 0.062 C Sn F F C H H

PbF_4	

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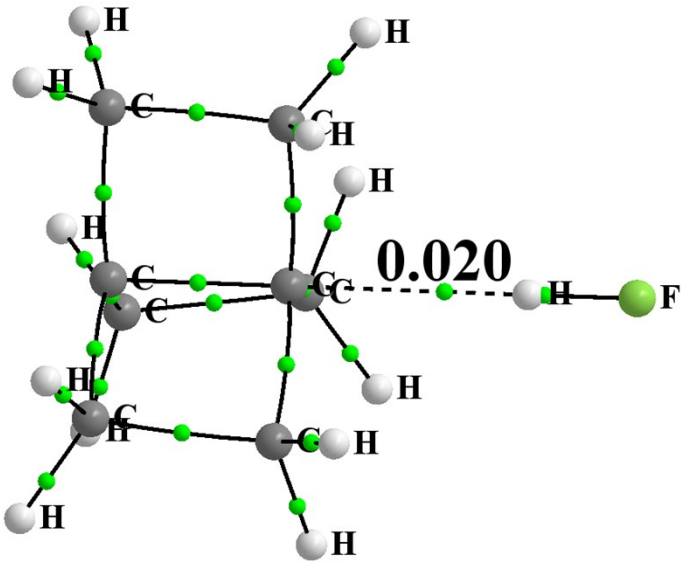
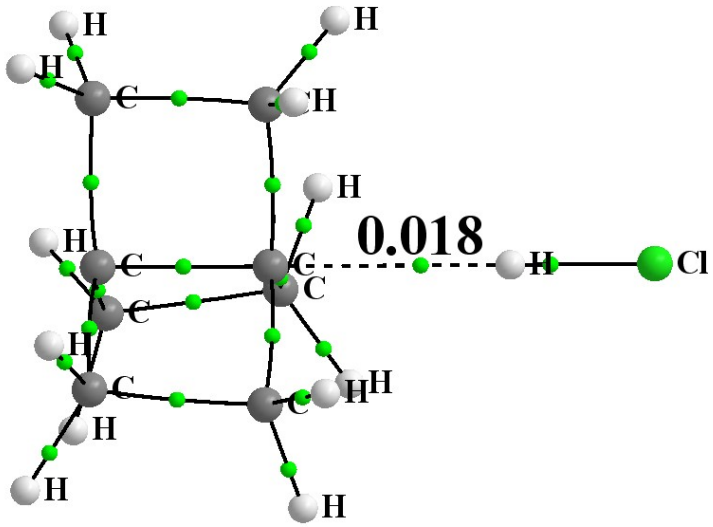
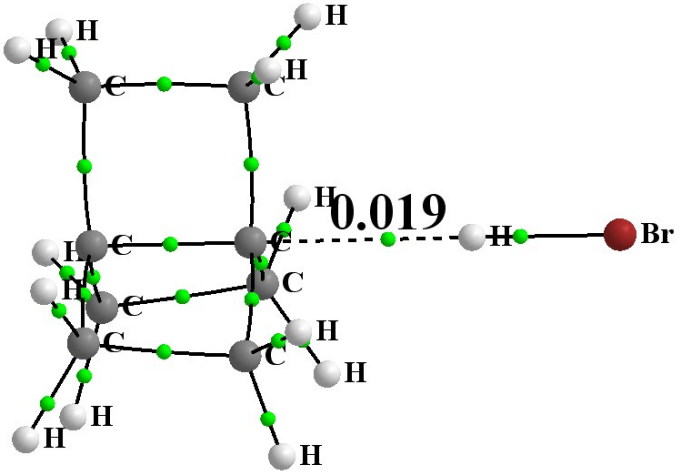
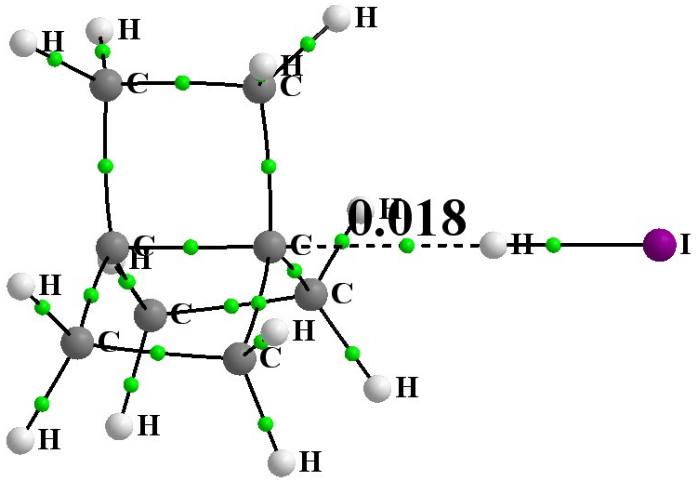
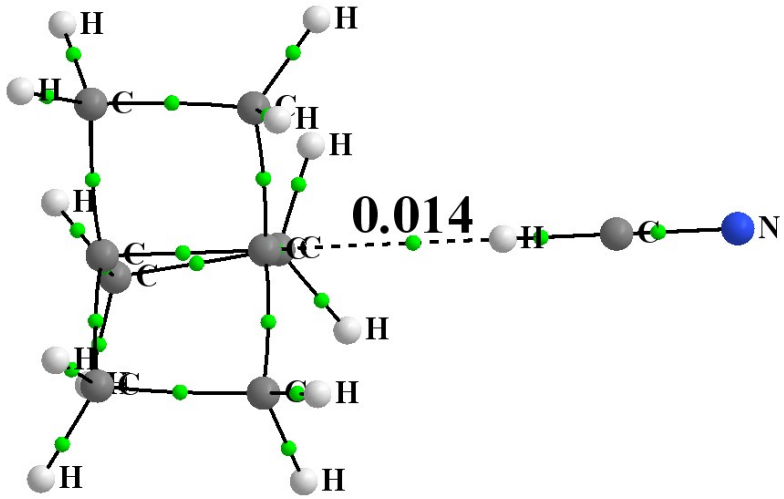
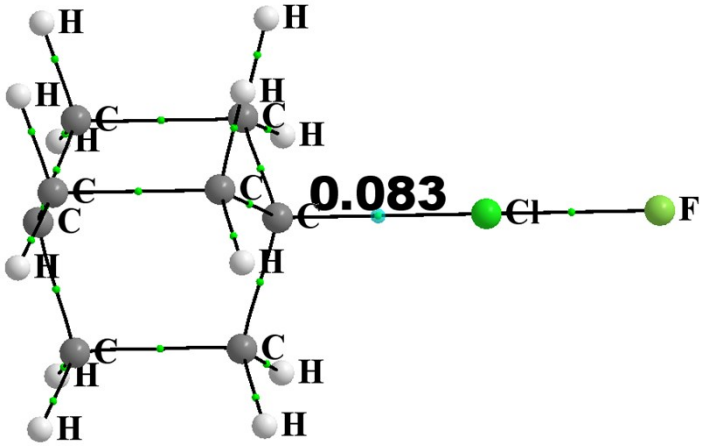
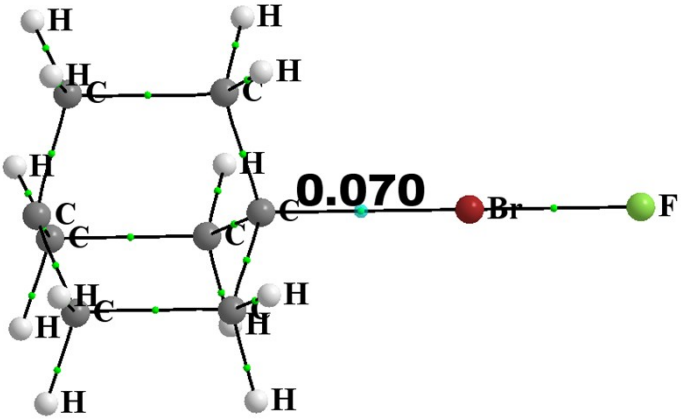
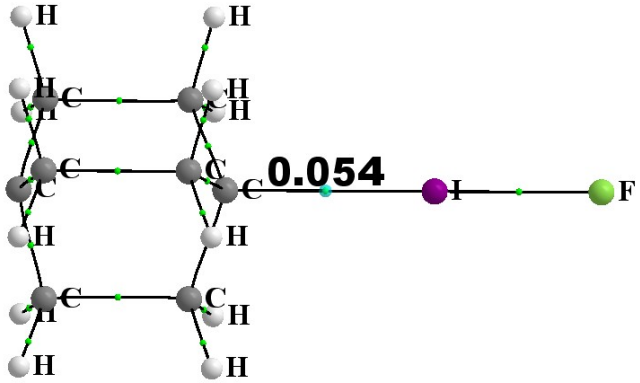
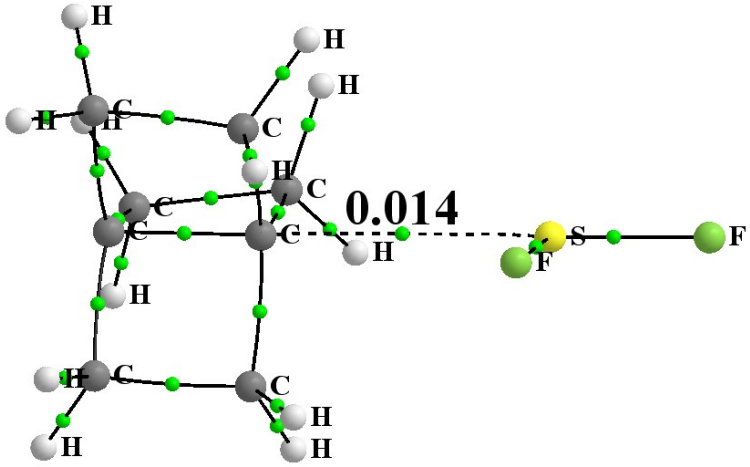
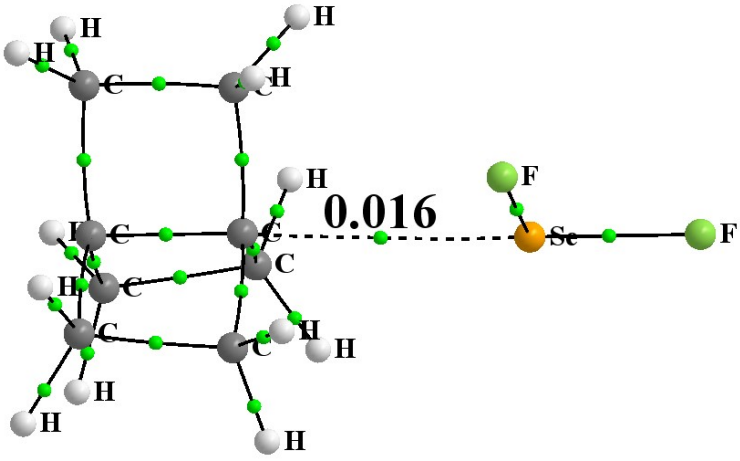
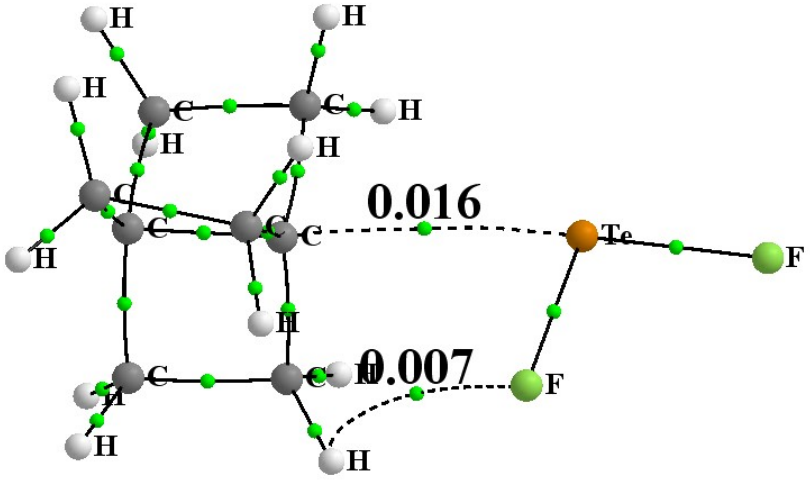
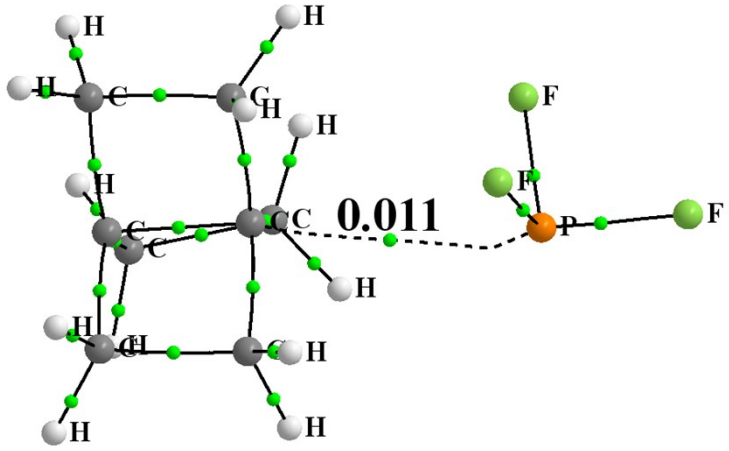
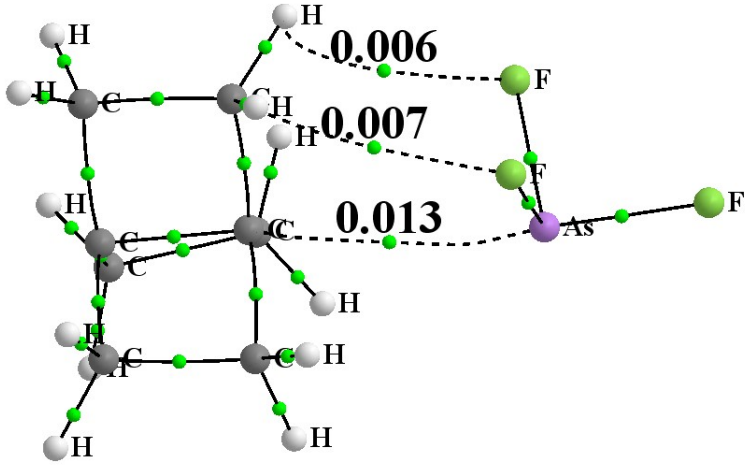
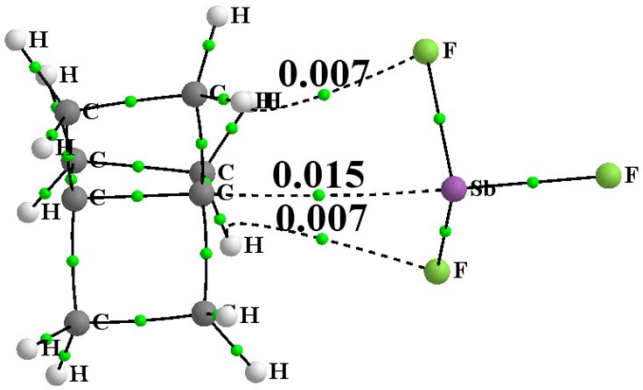
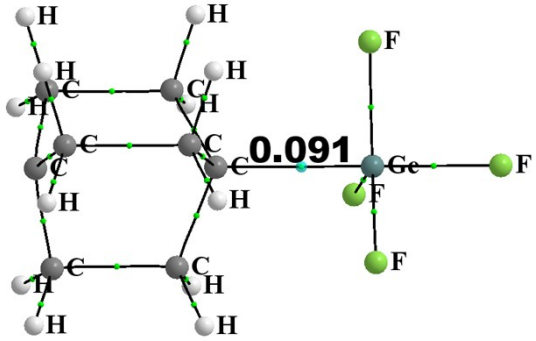
HF	

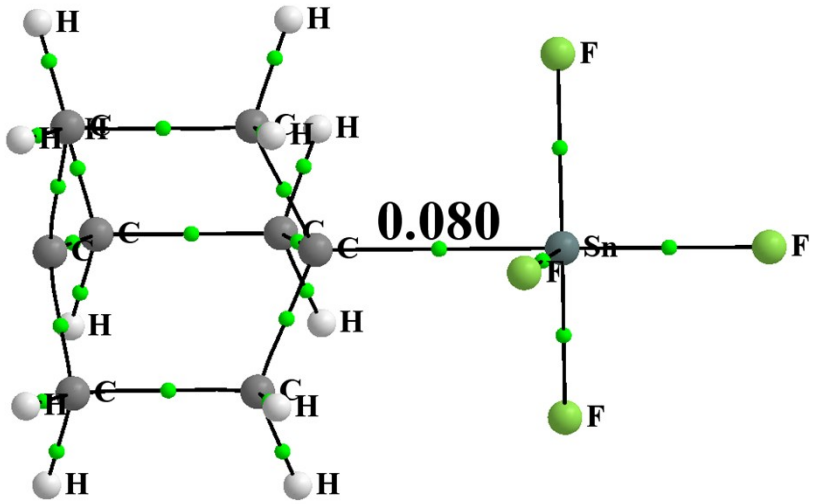
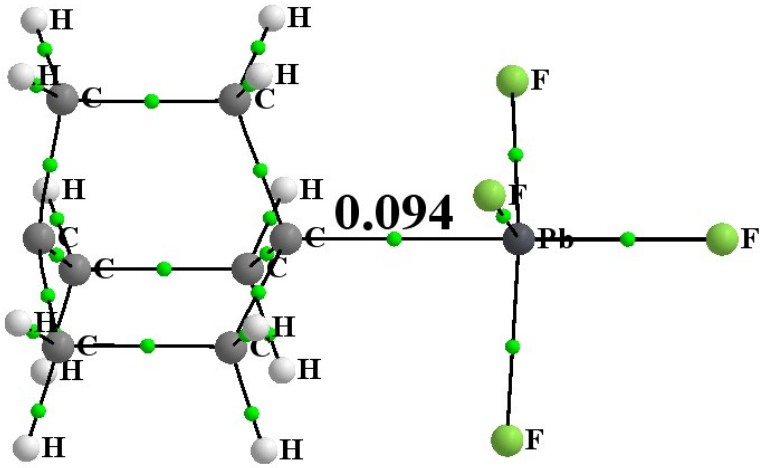
HCl	
HBr	
HI	

HCN	
FCl	
FBr	

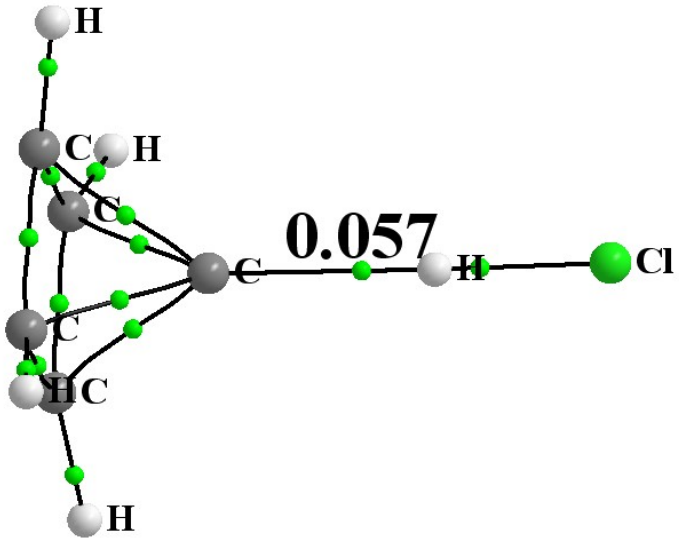
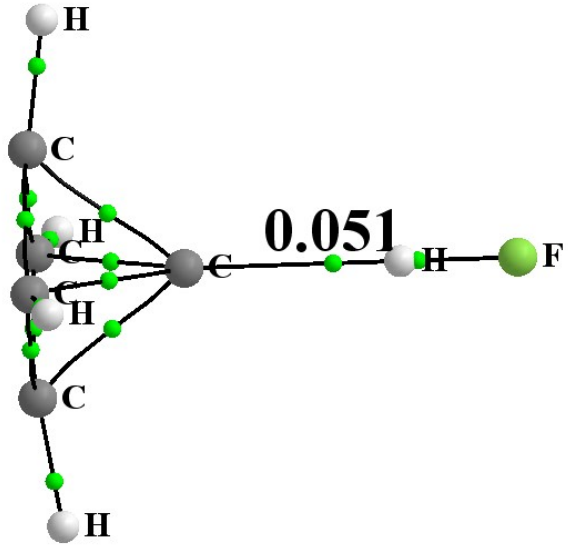
FI	
SF_2	
SeF_2	

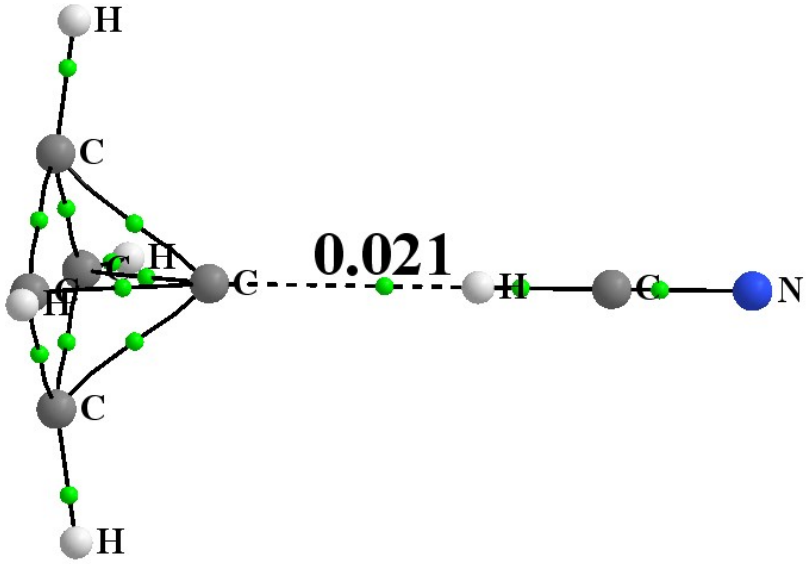
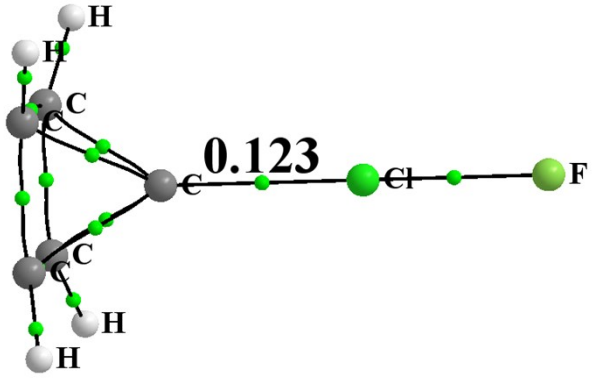
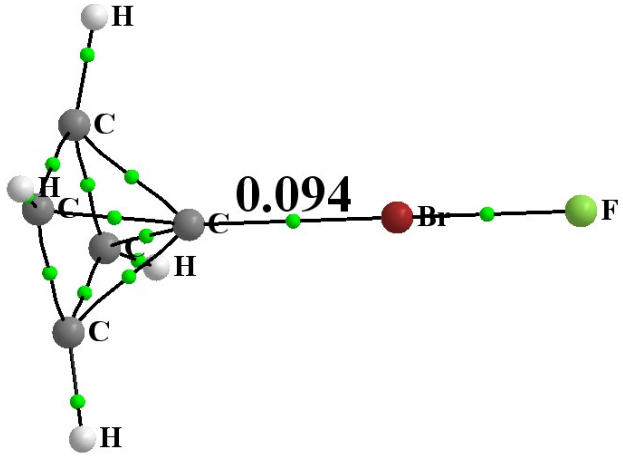
TeF_2	
PF_3	

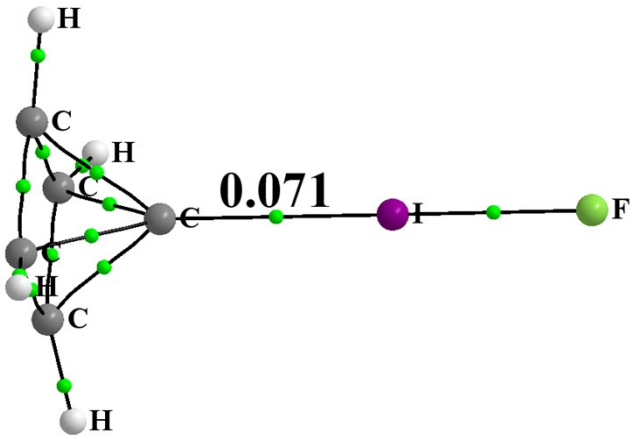
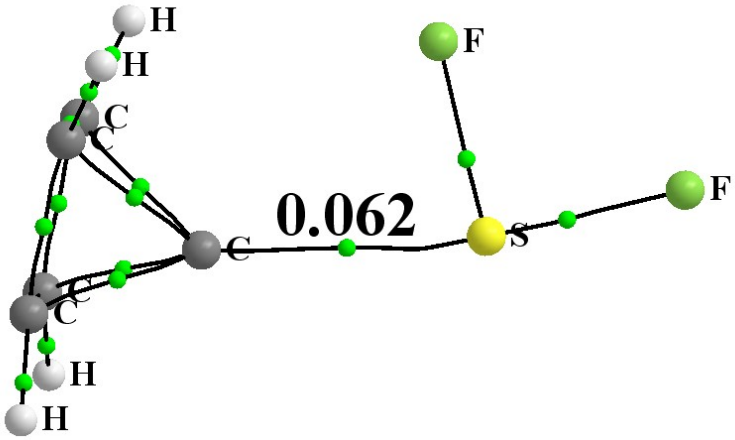
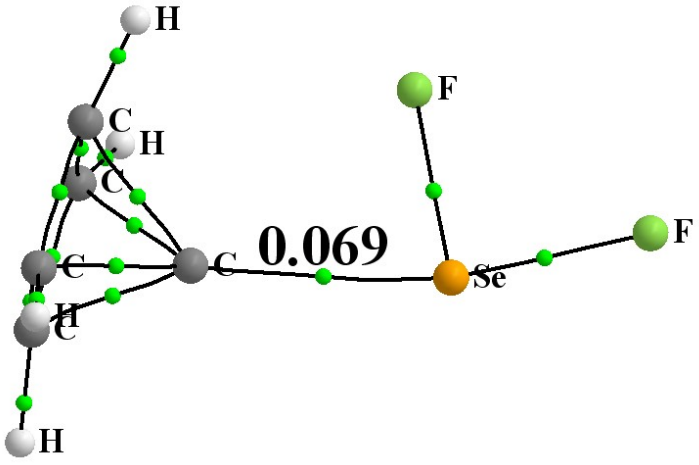
AsF_3	
SbF_3	
GeF_4	

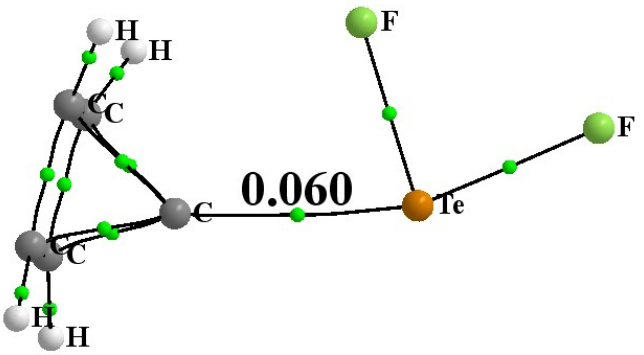
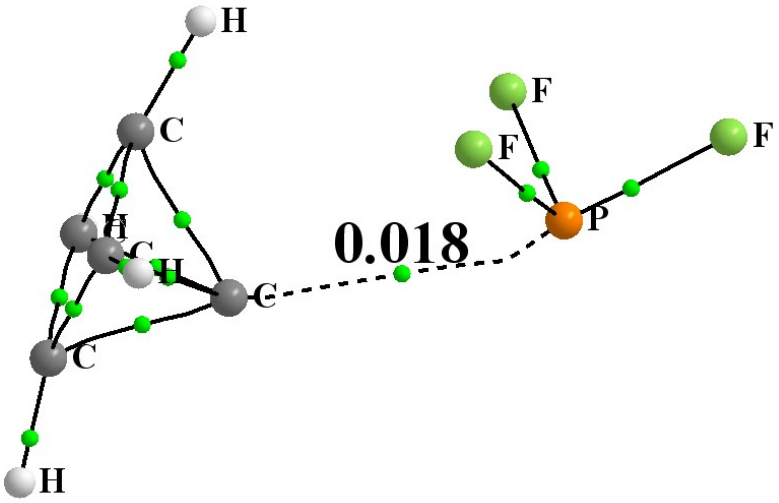
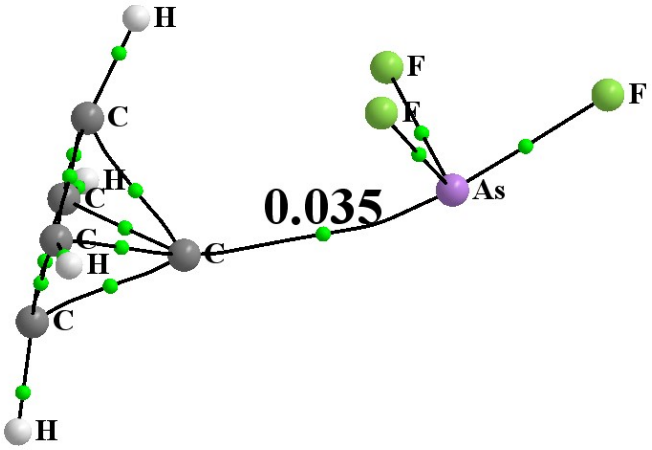
SnF_4	
PbF_4	

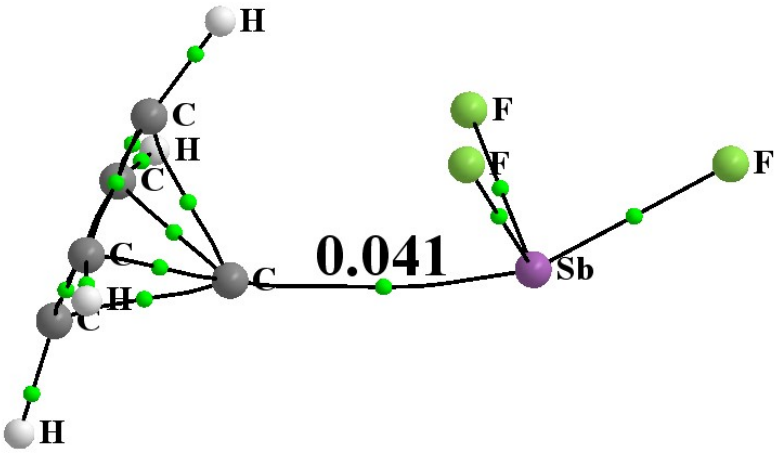
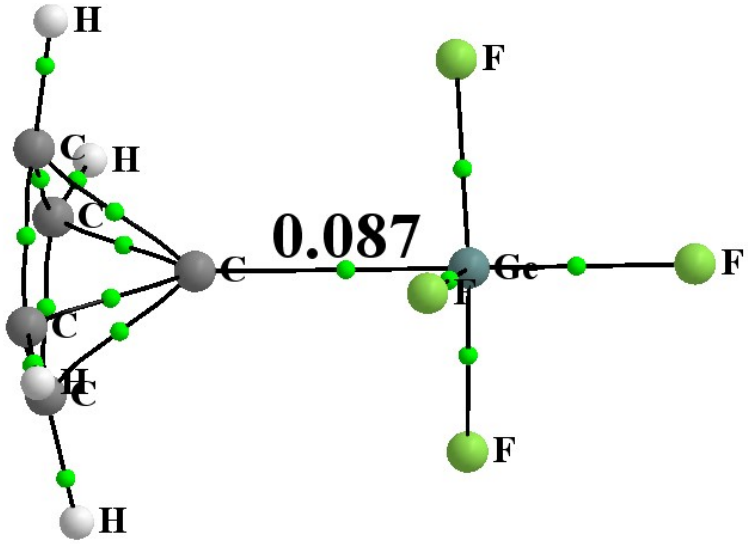
pyramidane	

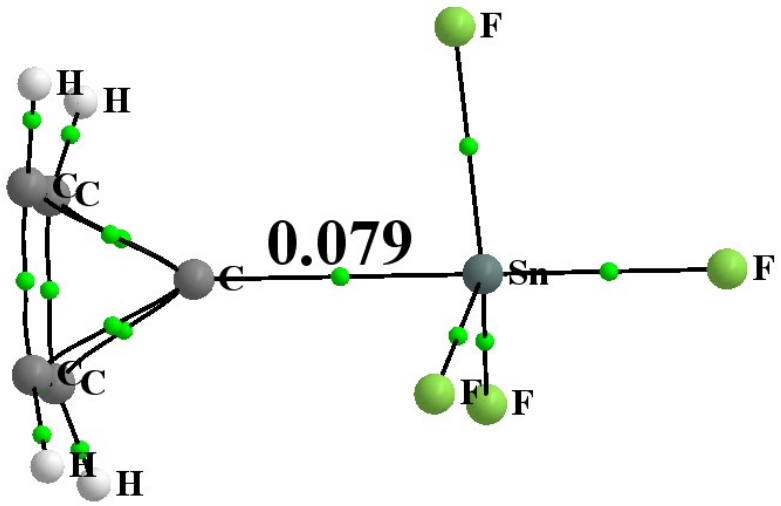
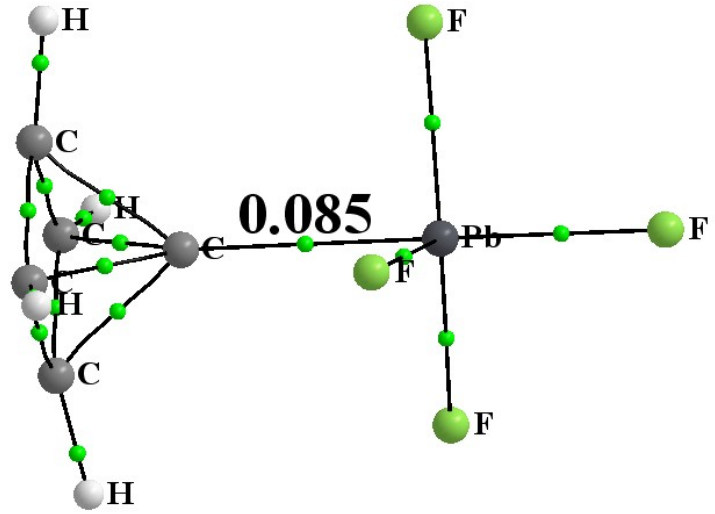
HCl	 H C H C 0.057 C H Cl C HC H
HF	 H C H C 0.051 C H F C H C H

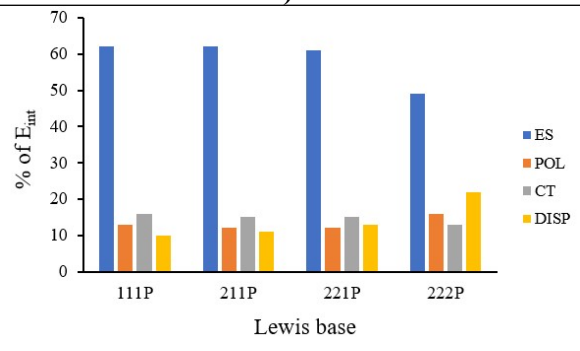
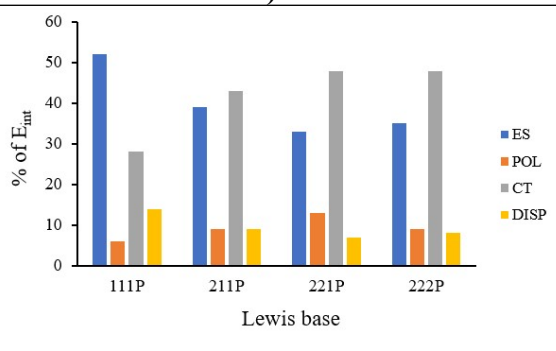
HCN	 H C C H H C 0.021 H C N C H
FCl	 H H C C 0.123 C Cl F C C H H
FBr	 H C H C 0.094 C Br F C H C H

FI	 H C H C 0.071 C I F H C H
SF_2	 H H F C C 0.062 F C S C H H
SeF_2	 H F C H C C 0.069 F C Se H C H

TeF_2	
PF_3	
AsF_3	

SbF_3	 H C H C C H C H C 0.041 F F F Sb
GeF_4	 H C H C C C H C H 0.087 F Ge F F F

SnF_4	
PbF_4	

a) HF	b) ClF
	
c) SF_2	**d) PF_3**

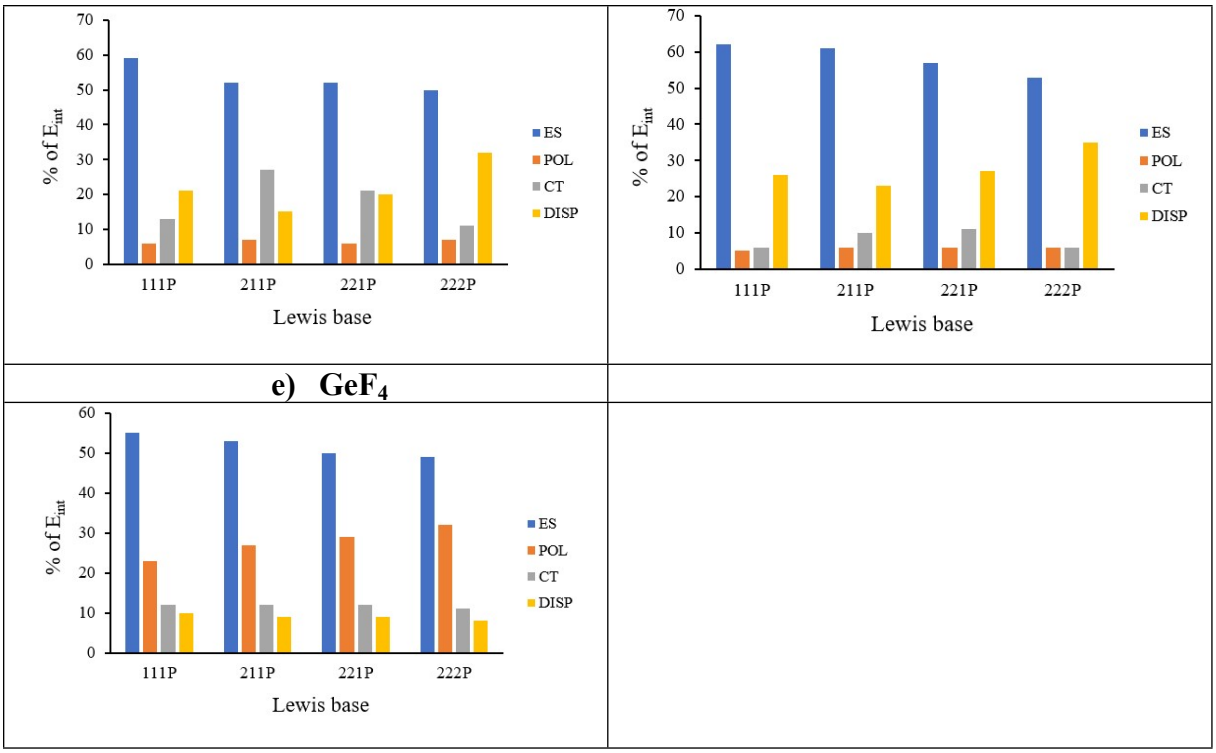


Fig. S2. Percentage contributions of ALMO-EDA decomposition terms of interaction energies for selected dimers. ES= electrostatic term, POL = polarization, CT = charge transfer, DISP = dispersion, Percentage contributions are defined as fraction of sum of attractive elements.

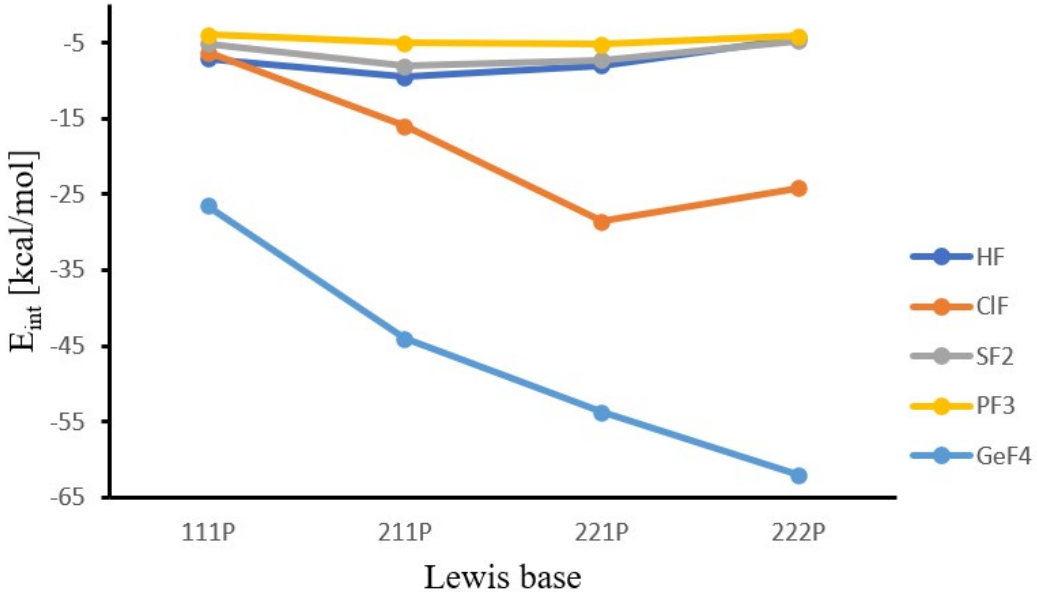


Fig. S3. Comparison of interaction energies for selected dimers.

Table S1.
Singlet-triplet separations (kcal/mol) and T1 diagnostic parameter for monomers and selected complexes

monomer	Triplet - Singlet	T1 value
111P	98.25	0.010
222P	11.50	0.009
pyramidane	75.16	0.010
dimer		
111P···BrF	77.00	0.011
111P···SnF_4	124.40	0.014
222P···BrF	68.43	0.010
222P···SnF_4	58.27	0.019
pyramidane···BrF	113.83	0.012
pyramidane···SnF_4	166.44	0.013

Table S2. Bond dissociation energies of optimized dimers (kcal/mol) calculated at M06-2X/def2-TZVPP level of theory.

Dimer	111P	222P	pyramidane
HF	-5.03	-3.26	-11.41
HCl	-3.27	-2.80	-8.08
HBr	-2.85	-2.29	-10.97
HI	-2.30	-2.36	-15.87
HCN	-1.99	-1.44	-5.39
ClF	-5.48	-13.53	-15.25
BrF	-8.32	-18.30	-20.68
IF	-10.99	-20.71	-23.94
SF_2	-4.19	-3.89	-8.48
SeF_2	-6.84	-5.30	-15.37

TeF_2	-10.32	-6.96	-21.34
PF_3	-3.18	-3.47	-5.40
AsF_3	-6.33	-4.79	-10.58
SbF_3	-9.07	-6.51	-17.21
GeF_4	-8.29	-19.26	-24.81
SnF_4	-21.64	-35.43	-38.10
PbF_4	-22.84	-42.99	-38.91

Table S3. ALMO-EDA decomposition of interaction energies (kcal/mol) for complexes involving 111P. ES= electrostatic term, PAULI = Pauli repulsion, DISP = dispersion, POL = polarization, CT = charge transfer.

	ES	EX	DISP	POL	CT	Total
HF	-13.86	15.35	-2.21	-2.82	-3.51	-7.05
HCl	-10.22	13.02	-2.16	-1.62	-3.44	-4.42
HBr	-10.97	15.95	-2.46	-1.83	-4.86	-4.16
HI	-7.31	14.75	-3.64	-1.59	-5.39	-3.18
HCN	-7.01	6.72	-1.23	-1.06	-1.26	-3.84
FCl	-15.59	23.66	-4.25	-1.70	-8.43	-6.31
FBr	-23.53	38.64	-5.55	-4.62	-14.95	-10.01
FI	-25.68	41.36	-8.11	-6.87	-13.59	-12.89
SF_2	-13.05	16.97	-4.75	-1.32	-2.97	-5.12
SeF_2	-19.70	26.24	-6.05	-3.13	-5.57	-8.22
TeF_2	-22.93	34.37	-8.75	-6.27	-8.89	-12.46
PF_3	-11.07	13.89	-4.60	-0.93	-1.15	-3.87

AsF_3	-17.02	20.71	-5.79	-2.28	-2.33	-6.71
SbF_3	-18.45	25.78	-8.13	-5.02	-4.97	-10.79
GeF_4	-57.93	79.78	-10.86	-24.30	-13.18	-26.48
SnF_4	-55.19	73.01	-9.96	-26.78	-17.06	-35.98
PbF_4	-55.42	77.61	-10.24	-22.29	-23.16	-33.50

Table S4. ALMO-EDA decomposition of interaction energies (kcal/mol) for complexes involving 222P. ES= electrostatic term, PAULI = Pauli repulsion, DISP = dispersion, POL = polarization, CT = charge transfer.

	ES	EX	DISP	POL	CT	Total
HF	-6.96	9.72	-3.09	-2.19	-1.85	-4.37
HCl	-6.04	9.60	-3.62	-1.40	-2.03	-3.49
HBr	-6.08	10.11	-3.86	-1.33	-2.26	-3.41
HI	-3.66	8.23	-4.34	-1.08	-2.22	-3.07
HCN	-4.44	6.41	-2.53	-1.34	-1.13	-3.04
FCl	-39.06	87.22	-8.70	-10.08	-53.59	-24.20
FBr	-38.47	75.00	-8.41	-11.57	-41.73	-25.18
FI	-46.05	75.64	-12.55	-11.53	-29.29	-23.78
SF_2	-10.50	16.07	-6.63	-1.36	-2.32	-4.74
SeF_2	-12.49	18.96	-7.65	-2.36	-2.69	-6.23
TeF_2	-8.21	16.04	-9.16	-3.57	-3.14	-8.05
PF_3	-10.33	15.32	-6.87	-1.14	-1.12	-4.14
AsF_3	-12.66	18.45	-7.65	-2.18	-1.52	-5.56
SbF_3	-8.03	15.29	-8.85	-3.59	-2.38	-7.56

GeF_4	-94.10	129.53	-14.88	-61.00	-21.58	-62.03
SnF_4	-93.81	120.43	-14.16	-44.49	-32.43	-64.46
PbF_4	-112.57	156.09	-15.71	-45.05	-55.68	-72.92

Table S5. ALMO-EDA decomposition of interaction energies (kcal/mol) for complexes involving pyramidane. ES= electrostatic term, PAULI = Pauli repulsion, DISP = dispersion, POL = polarization, CT = charge transfer.

	ES	EX	DISP	POL	CT	Total
HF	-31.67	32.85	-3.24	-5.08	-7.50	-14.64
HCl	-29.07	40.10	-3.66	-6.30	-12.88	-11.81
HBr	-	-	-	-	-	-
HI	-	-	-	-	-	-
HCN	-14.72	12.99	-1.78	-1.71	-2.47	-7.70
FCl	-61.07	139.30	-8.12	-31.28	-66.78	-27.95
FBr	-58.79	108.02	-7.17	-23.67	-46.90	-28.51
FI	-75.76	111.36	-11.63	-20.46	-32.45	-28.94
SF_2	-45.62	73.76	-8.06	-8.84	-25.14	-13.90
SeF_2	-55.32	86.33	-8.45	-16.00	-28.65	-22.09
TeF_2	-68.45	95.54	-12.11	-18.20	-24.16	-27.39
PF_3	-19.67	23.47	-5.71	-2.00	-2.81	-6.72
AsF_3	-37.81	47.24	-7.73	-6.54	-8.67	-13.50
SbF_3	-48.17	61.68	-10.73	-11.72	-12.66	-21.61

GeF_4	-106.74	125.51	-11.19	-41.66	-19.05	-53.13
SnF_4	-102.48	111.44	-9.52	-33.13	-23.02	-56.71
PbF_4	-105.65	125.85	-10.26	-30.91	-32.95	-53.93

Table S6. Percentage contributions of ALMO-EDA decomposition terms of interaction energies for selected complexes involving 111P, 211P, 221P and 222P Lewis bases. ES= electrostatic term, PAULI = Pauli repulsion, DISP = dispersion, POL = polarization, CT = charge transfer.

		%ES	%POL	%CT	%DISP
HF	111P	62	13	16	10
	211P	62	12	15	11
	221P	61	12	15	13
	222P	49	16	13	22
ClF	111P	52	6	28	14
	211P	39	9	43	9
	221P	33	13	48	7
	222P	35	9	48	8
SF_2	111P	59	6	13	21
	211P	52	7	27	15
	221P	52	6	21	20
	222P	50	7	11	32
PF_3	111P	62	5	6	26
	211P	61	6	10	23
	221P	57	6	11	27
	222P	53	6	6	35

GeF_4	111P	55	23	12	10
	211P	53	27	12	9
	221P	50	29	12	9
	222P	49	32	11	8

Table S7. IQA interaction terms (kcal/mol) for σ-hole atom···C interactions.

	111P			222P			pyramidane		
	E_{int}	V_{cl}	V_{xc}	E_{int}	V_{cl}	V_{xc}	E_{int}	V_{cl}	V_{xc}
HF	-43.59	-34.72	-8.87	-28.02	-23.47	-4.54	-62.76	-46.31	-16.46
HCl	-23.65	-13.20	-10.45	-13.70	-7.90	-5.81	-50.91	-24.58	-26.33
HBr	-21.38	-7.87	-13.51	-10.51	-4.07	-6.44	-	-	-
HI	-16.30	-1.51	-14.80	-6.84	-0.91	-5.93	-	-	-
HCN	-14.56	-8.52	-6.04	-9.31	-4.96	-4.35	-24.29	-14.30	-9.98
FCl	-33.95	-9.66	-24.29	-69.61	-1.39	-68.21	-113.61	-6.28	-107.33
FBr	-62.56	-16.44	-46.12	-81.95	-8.22	-73.73	-131.34	-23.6	-107.74
FI	-63.06	-23.67	-39.38	-68.93	-17.08	-51.85	-114.67	-38.59	-76.08
SF_2	-41.38	-29.66	-11.73	-26.01	-19.00	-7.01	-92.47	-41.06	-51.41
SeF_2	-54.11	-35.16	-18.94	-30.95	-22.60	-8.35	-114.38	-53.44	-60.94
TeF_2	-76.53	-49.77	-26.75	-39.01	-29.80	-9.21	-133.51	-76.93	-56.58
PF_3	-54.71	-49.16	-5.56	-34.40	-30.42	-3.99	-76.70	-66.57	-10.13
AsF_3	-63.12	-53.73	-9.39	-38.57	-33.26	-5.31	-102.22	-78.93	-23.29
SbF_3	-86.59	-71.07	-15.52	-48.35	-41.79	-6.56	-132.94	-103.31	-29.63

GeF_4	-184.25	-156.54	-27.70	-223.64	-170.99	-52.65	-249.83	-203.54	-46.29
SnF_4	-228.54	-184.99	-43.55	-192.06	-137.60	-54.46	-267.13	-207.39	-59.74
PbF_4	-157.93	-113.68	-44.25	-146.39	-74.57	-71.82	-185.79	-124.17	-61.62

Table S8. Coordinates of studied systems

monomer				
[1.1.1]propellane	C	-0.40554400	1.22778700	-0.00007000
	C	1.26606100	-0.26266600	-0.00003200
	C	-0.00001000	0.00002300	0.77214100
	H	0.28315400	2.06175200	-0.00010600
	H	-1.45547900	1.48746800	-0.00006700
	H	2.01582200	0.51684400	-0.00006300
	H	1.64401600	-1.27604400	0.00001500
	C	-0.00002500	-0.00004100	-0.77204300
	C	-0.86051800	-0.96511300	0.00001100
	H	-0.56047600	-2.00422200	0.00006200
	H	-1.92707900	-0.78563200	0.00002500
[2.2.2]propellane	C	0.85432500	1.28504300	-0.77409100
	C	-1.54024700	0.09714700	-0.77393500
	C	-0.00009700	-0.00001900	-0.76605100
	H	0.47384800	2.11680100	-1.36735700
	H	1.88844300	1.09857200	-1.06679100
	H	-1.89635300	1.08562600	-1.06707400
	H	-2.07003400	-0.64871600	-1.36686300
	C	-0.00003200	0.00004400	0.76605700
	C	0.68584000	-1.38243100	-0.77390700
	H	0.00771100	-2.18512000	-1.06658700
	H	1.59647700	-1.46856000	-1.36710500
	C	0.66232100	1.39393500	0.77386600
	H	1.57144100	1.49547200	1.36692100
	H	-0.02932600	2.18499300	1.06664200
	C	-1.53832100	-0.12327800	0.77402400
	H	-2.08072700	0.61333000	1.36710800
	H	-1.87751400	-1.11775900	1.06695400
	C	0.87610300	-1.27037400	0.77403700
	H	0.50975300	-2.10846500	1.36728200
	H	1.90693500	-1.06657700	1.06686000
pyramidane	C	-0.02943600	1.01842600	-0.24021100
	C	0.00017100	-0.00001900	1.01815000
	C	-1.01848600	-0.02939400	-0.24050800
	C	1.01842600	0.02938500	-0.24063800
	C	0.02934200	-1.01843800	-0.24021600
	H	-0.06013200	2.08069100	-0.08268100

	H	-2.08057300	-0.06009000	-0.08173300
	H	2.08060300	0.06008200	-0.08250100
	H	0.06004500	-2.08071200	-0.08275100

dimer				
[1.1.1]propellane				
HF	C	-0.40792000	1.24534200	0.09881000
	C	1.26854700	-0.24763000	0.01687300
	C	0.00295100	-0.02088200	0.77747000
	H	0.28321200	2.07609100	0.13077000
	H	-1.45821600	1.50131900	0.11267500
	H	2.01558000	0.53334400	0.04587300
	H	1.64285300	-1.26030300	-0.03985700
	C	-0.00590600	0.05429600	-0.75712600
	C	-0.86457800	-0.95169800	-0.00480900
	H	-0.56147000	-1.98785800	-0.06248600
	H	-1.93010200	-0.76902600	0.00518600
	H	-0.02035500	0.09716800	-2.68812800
	F	-0.02748000	0.10947800	-3.62193500
HCl	C	-0.39335000	1.21556600	-0.00373200
	C	1.28047700	-0.27607800	0.09697900
	C	-0.01220000	0.01094000	0.79884500
	H	0.29716900	2.04763600	-0.01314100
	H	-1.44284900	1.47160700	-0.05143800
	H	2.02811600	0.50506100	0.09261300
	H	1.65565000	-1.28924500	0.14023100
	C	0.03855400	-0.04045600	-0.73861200
	C	-0.84981200	-0.98112600	0.05120400
	H	-0.54809100	-2.01861300	0.09266100
	H	-1.91490200	-0.80002500	0.00678000
	Cl	-0.13497800	0.33865800	-4.08026500
	H	-0.04933900	0.15736900	-2.80130700
HBr	C	-0.38226500	1.22533800	0.00284100
	C	1.28784000	-0.26956900	0.11505900
	C	-0.02232700	0.00413400	0.79055800
	H	0.30867600	2.05670700	0.02815300
	H	-1.43010500	1.48308700	-0.06739700
	H	2.03575100	0.51068700	0.14638000
	H	1.66121000	-1.28383400	0.14708600
	C	0.06798700	-0.01529500	-0.74615300
	C	-0.84098400	-0.97139900	0.00228500
	H	-0.54055100	-2.00974200	0.02929400
	H	-1.90441300	-0.78816100	-0.06688100
	H	-0.06101700	0.12636800	-2.75439300

	Br	-0.23497800	0.29333800	-4.17968000
HI	C	-0.40730900	1.24352200	0.10635400
	C	1.26687400	-0.24746900	0.02447900
	C	0.00310000	-0.02156000	0.79914800
	H	0.28314900	2.07508500	0.13948800
	H	-1.45758000	1.50050800	0.12151100
	H	2.01496900	0.53276300	0.05464100
	H	1.64212900	-1.26014100	-0.03062500
	C	-0.00574500	0.05344500	-0.74011100
	C	-0.86325800	-0.95053300	0.00264800
	H	-0.56101300	-1.98729600	-0.05335700
	H	-1.92921600	-0.76907700	0.01396700
	H	-0.02165500	0.10016300	-2.77245200
	I	-0.03219000	0.11885500	-4.40624800
HCN	C	-0.41028300	1.23925400	0.15405500
	C	1.26454300	-0.25177700	0.06745300
	C	0.00417600	-0.02413400	0.84512500
	H	0.27978400	2.07131400	0.18409000
	H	-1.46041300	1.49630900	0.17646600
	H	2.01274900	0.52852600	0.09450600
	H	1.64057600	-1.26434700	0.01589900
	C	-0.01279400	0.04647700	-0.69278800
	C	-0.86618100	-0.95588400	0.05710900
	H	-0.56435100	-1.99295600	0.00526200
	H	-1.93215500	-0.77527700	0.07625700
	C	0.17601500	0.39401900	-4.06111700
	H	0.10212200	0.27132700	-2.99579300
	N	0.25592600	0.52549200	-5.19366800
FCl	C	-0.40661400	1.23095500	-0.04826700
	C	1.26887800	-0.26223800	-0.04046200
	C	0.00015400	0.00437500	0.74845800
	H	0.28426800	2.06269200	-0.04586500
	H	-1.45709200	1.48703400	-0.04298500
	H	2.01577400	0.51957100	-0.03821200
	H	1.64388500	-1.27630400	-0.02984300
	C	0.00000500	-0.00287200	-0.79071600
	C	-0.86198400	-0.96667800	-0.03692700
	H	-0.55857000	-2.00441200	-0.02617000
	H	-1.92770200	-0.78424100	-0.03167600
	F	-0.02951600	0.12020000	4.95934900
	Cl	-0.01807200	0.07463300	3.31722300
FBr	C	-0.40890000	1.23859900	-0.07976400
	C	1.26843200	-0.25568100	-0.03189000
	C	-0.00667400	0.02840900	0.75865600
	H	0.28321200	2.06910300	-0.08736800

	H	-1.45966700	1.49295800	-0.08278600
	H	2.01388300	0.52730800	-0.03734400
	H	1.64139400	-1.26966600	0.00776900
	C	0.00260000	-0.01186500	-0.77912400
	C	-0.86495900	-0.96089200	-0.02638000
	H	-0.55989500	-1.99731800	0.01356600
	H	-1.93023600	-0.77657800	-0.02698400
	F	-0.01419900	0.06579100	5.03173800
	Br	-0.01157700	0.05254500	3.23381800
FI	C	-0.40620000	1.24125000	-0.00403500
	C	1.27259600	-0.25528800	-0.02018100
	C	-0.00453100	-0.00386700	0.70029200
	H	0.28663400	2.07108400	0.00248800
	H	-1.45690600	1.49509700	-0.02155200
	H	2.01760200	0.52800700	-0.01207200
	H	1.64512400	-1.26978100	-0.04499700
	C	0.00766400	0.02217400	-0.83612400
	C	-0.86279900	-0.96057400	-0.04726600
	H	-0.55722700	-1.99715900	-0.07391700
	H	-1.92766500	-0.77498800	-0.06499100
	F	-0.10135200	0.23724200	-5.36889900
	I	-0.04918200	0.14075800	-3.42373000
SF_2	C	-0.43786600	1.14214100	0.12785200
	C	1.20701500	-0.38222300	0.06699900
	C	-0.17115700	-0.24366000	0.68303200
	H	0.24679000	1.92397600	0.42721900
	H	-1.47388700	1.43362400	0.02234000
	H	1.94640100	0.34888600	0.36432700
	H	1.57142700	-1.38791600	-0.09168600
	C	0.07902400	0.08655000	-0.80062600
	C	-0.89996100	-0.98567800	-0.41262900
	H	-0.60706200	-2.01122400	-0.59119800
	H	-1.95102900	-0.76596800	-0.54073400
	F	0.55261100	0.49889200	5.02956800
	S	0.23644300	0.17255600	3.49690700
	F	1.26869800	1.22555800	2.88546000
SeF_2	C	-0.42578300	1.16227800	0.09941700
	C	1.21661900	-0.36971400	0.06836000
	C	-0.15938600	-0.21076900	0.70391200
	H	0.26364000	1.94730900	0.37789400
	H	-1.46266600	1.45089400	-0.00446100
	H	1.95766200	0.36730400	0.34565300
	H	1.57413400	-1.38194600	-0.06126400
	C	0.07895500	0.07451100	-0.78862700
	C	-0.89922200	-0.98255600	-0.36990700

	H	-0.60962800	-2.01347800	-0.52025700
	H	-1.95051600	-0.76271900	-0.49520000
	F	0.56188800	0.43189400	5.08212600
	Se	0.17194400	0.06150400	3.42129000
	F	1.24980400	1.28100300	2.80789500
TeF_2	C	-0.37543500	1.19008000	-0.13558000
	C	1.28718300	-0.24934400	0.33728500
	C	-0.14393800	-0.01293100	0.70486400
	H	0.27360600	2.04119300	0.01698100
	H	-1.38741400	1.40455900	-0.44976200
	H	1.98509200	0.55747700	0.51351900
	H	1.67441000	-1.25051400	0.46716400
	C	0.26898300	-0.04592700	-0.77409200
	C	-0.75635500	-1.02690600	-0.19051000
	H	-0.42868300	-2.05205800	-0.08708100
	H	-1.77913000	-0.87640200	-0.50690400
	F	-0.55261700	0.12600800	-5.28424600
	F	-1.69655500	0.32635300	-2.86285900
	Te	0.07731000	0.01051500	-3.48031400
PF_3	C	-0.27245200	1.08604700	0.38160000
	C	1.20859700	-0.30877100	-0.56153600
	C	0.41860300	-0.21752300	0.72135000
	H	0.36252700	1.94372000	0.20595500
	H	-1.20770100	1.28819400	0.88621500
	H	1.89337900	0.50007600	-0.77684700
	H	1.52984900	-1.29330700	-0.87313900
	C	-0.26175300	-0.00618200	-0.64598200
	C	-0.71568200	-1.10830500	0.26751300
	H	-0.46222800	-2.12104600	-0.01511500
	H	-1.66638500	-0.98011100	0.76696300
	F	-1.25193700	0.01460000	3.34209500
	F	0.43556500	1.65930400	3.37115800
	P	0.23581800	0.17110500	3.83299900
	F	-0.11189800	0.49754200	5.33363100
AsF_3	C	-0.54719200	1.05671700	0.43975200
	C	1.21315700	-0.28794600	0.07995200
	C	-0.15978100	-0.38785200	0.71945600
	H	0.07815400	1.81786100	0.88621100
	H	-1.60574300	1.27454900	0.40628000
	H	1.89523600	0.43146100	0.51205800
	H	1.65424600	-1.20864300	-0.27714500
	C	0.03189500	0.24308200	-0.67160900
	C	-0.84891600	-0.95991000	-0.49986400
	H	-0.47832500	-1.90345000	-0.87659700
	H	-1.91661800	-0.80702800	-0.57735700

	F	0.16978100	0.31686800	5.33892500
	F	-1.28742200	0.95621800	3.39468600
	F	1.23611400	0.87891600	3.13439400
	As	-0.01674400	-0.15698900	3.69504300
SbF_3	C	-0.59131400	0.97773700	0.73128100
	C	1.22032900	-0.09254700	-0.06117700
	C	0.04571400	-0.41067100	0.85974000
	H	0.00836500	1.80661300	1.08169800
	H	-1.65022400	1.03500000	0.94037200
	H	1.87302100	0.70679900	0.26148200
	H	1.69340700	-0.93227600	-0.55188700
	C	-0.15747200	0.27106000	-0.50247400
	C	-0.80842600	-1.04785800	-0.22152400
	H	-0.40111500	-1.91820700	-0.71753400
	H	-1.87790700	-1.04949800	-0.06234500
	F	1.13160400	0.17065400	5.41900100
	F	-0.90105500	0.63275700	3.67253400
	F	1.74718800	0.96872800	2.90252000
	Sb	0.68235800	-0.40233700	3.66452800
GeF_4	C	-0.37170000	1.27206900	0.12606800
	C	1.29334400	-0.25316600	0.14686300
	C	0.04506900	0.06735800	0.99933900
	H	0.33673800	2.08755300	0.09104500
	H	-1.41911200	1.53548400	0.16745200
	H	2.04418600	0.52347900	0.11231300
	H	1.64670000	-1.27289100	0.20561300
	C	0.00065300	-0.00186400	-0.52400800
	C	-0.85893700	-0.92983800	0.24002500
	H	-0.56041800	-1.96679900	0.30118000
	H	-1.91872300	-0.72242200	0.28431800
	F	0.62023100	-1.46553600	3.09260600
	F	-1.56197000	0.52730600	3.06512100
	F	0.16087100	0.24852100	4.96963400
	F	1.25385600	1.41785100	2.94244500
	Ge	0.11060300	0.17005700	3.25312200
SnF_4	C	-0.40908300	1.23971900	-0.06343000
	C	1.27610800	-0.26245000	0.08982400
	C	-0.01852700	0.06989300	0.87297600
	H	0.29079700	2.06280000	-0.09119400
	H	-1.46097100	1.48741600	-0.07943800
	H	2.01627200	0.52470900	0.06581400
	H	1.63732400	-1.27464300	0.20418900
	C	0.01141900	-0.05223800	-0.64326300
	C	-0.87362100	-0.96866600	0.10217000
	H	-0.56297000	-1.99747600	0.21694600

	H	-1.93654400	-0.77335800	0.09137400
	F	0.53856800	-1.58181800	3.08198600
	F	-1.92299800	0.57995800	2.88425600
	F	-0.12064700	0.33852000	5.07832300
	F	1.18638700	1.62453700	2.89727200
	Sn	-0.07360400	0.22219400	3.18705400
PbF_4	C	-0.73795700	1.10329100	0.06367400
	C	1.30544000	0.13525900	-0.01408300
	C	0.05558600	0.06936400	0.89460400
	H	-0.30167800	2.09093000	0.01446700
	H	-1.81313700	1.04380900	0.15647200
	H	1.79024600	1.09997900	-0.06341100
	H	1.94408700	-0.73626900	0.01436300
	C	-0.03538500	-0.00322200	-0.62331900
	C	-0.54911100	-1.14936500	0.15741700
	H	0.04631400	-2.05076600	0.19136000
	H	-1.61990000	-1.26199800	0.25207200
	F	1.27791600	-1.51554700	2.98378900
	F	-1.79421300	0.02982600	3.12341200
	F	0.32244800	0.21865700	5.22986500
	F	1.07772100	1.91798800	2.88209700
	Pb	0.20215900	0.15409000	3.25398600

dimer				
[2.2.2]propellane				
HF	C	0.39106400	1.37989800	-4.03026900
	C	-1.02253100	-0.88732000	-4.04570100
	C	0.33779400	-0.16144700	-3.99848700
	H	-0.35248000	1.87632700	-4.65213500
	H	1.37636200	1.75977000	-4.29945600
	H	-1.83404600	-0.23654400	-4.37051500
	H	-1.06021700	-1.80496000	-4.63097100
	C	0.29332200	-0.14414300	-2.46575200
	C	1.64666100	-0.97734900	-3.96704200
	H	1.49914200	-2.01840200	-4.25348900
	H	2.47996000	-0.57567300	-4.54177300
	C	0.12483100	1.39657100	-2.49171100
	H	0.82641400	1.96814900	-1.88504600
	H	-0.88675800	1.70726200	-2.23089400
	C	-0.95608800	-1.06117700	-2.49538300
	H	-1.82165700	-0.71468000	-1.93170000
	H	-0.72907700	-2.08053200	-2.18367000
	C	1.71152600	-0.76785800	-2.42098300
	H	1.82369600	-1.66615400	-1.81481300
	H	2.47064300	-0.04901100	-2.11302800
	H	0.22721600	-0.11675500	-0.44227500

	F	0.20260900	-0.10438900	0.48273000
HCl	C	0.38487700	1.38021600	-4.03885000
	C	-1.01972200	-0.89267100	-4.05396200
	C	0.33782900	-0.16139200	-4.01007400
	H	-0.36704900	1.87399900	-4.65286900
	H	1.36547400	1.76586400	-4.31704300
	H	-1.83396400	-0.24886800	-4.38593000
	H	-1.05149200	-1.81503600	-4.63230600
	C	0.29471200	-0.14493000	-2.47644300
	C	1.64988100	-0.97212700	-3.97789400
	H	1.50950500	-2.01192200	-4.27258500
	H	2.48362600	-0.56209000	-4.54622500
	C	0.13165900	1.39400100	-2.49720900
	H	0.84312600	1.96024700	-1.89650900
	H	-0.87544800	1.71049700	-2.22517200
	C	-0.95604400	-1.05610400	-2.50153100
	H	-1.82115700	-0.69940200	-1.94293200
	H	-0.73655800	-2.07455000	-2.18065200
	C	1.70857100	-0.77246600	-2.42944200
	H	1.81286800	-1.67655100	-1.82992800
	H	2.47045000	-0.06037200	-2.11182300
	Cl	0.19384000	-0.09958300	0.93341200
	H	0.22896800	-0.11806500	-0.34994700
HBr	C	0.38078900	1.38068200	-4.04076700
	C	-1.01790700	-0.89566000	-4.05611000
	C	0.33760200	-0.16089500	-4.01110700
	H	-0.37333800	1.87162300	-4.65442800
	H	1.35986600	1.76898300	-4.32064000
	H	-1.83318000	-0.25522800	-4.39206900
	H	-1.04549500	-1.81970800	-4.63204200
	C	0.29222000	-0.14334500	-2.47639700
	C	1.65161600	-0.96813500	-3.97624100
	H	1.51550900	-2.00788000	-4.27316900
	H	2.48555900	-0.55442600	-4.54164400
	C	0.12881400	1.39510500	-2.49886900
	H	0.84136400	1.96136100	-1.89934500
	H	-0.87784700	1.71210300	-2.22562000
	C	-0.95772500	-1.05490600	-2.50314400
	H	-1.82443300	-0.69663200	-1.94790200
	H	-0.73913900	-2.07245800	-2.17863100
	C	1.70578800	-0.77033900	-2.42742500
	H	1.80781800	-1.67557700	-1.82913000
	H	2.46701200	-0.05921000	-2.10592300
	H	0.22515400	-0.11836800	-0.33873700
	Br	0.21963700	-0.11614900	1.08937700
HI	C	0.38154900	1.37990400	-4.04576700

	C	-1.01726600	-0.89629600	-4.06088100
	C	0.33831800	-0.16167800	-4.01651900
	H	-0.37428100	1.87073200	-4.65752600
	H	1.35970800	1.76873300	-4.32827000
	H	-1.83213700	-0.25709600	-4.40033400
	H	-1.04391900	-1.82214000	-4.63407000
	C	0.29215400	-0.14352300	-2.48113800
	C	1.65221100	-0.96893300	-3.97964900
	H	1.51732400	-2.00814700	-4.27911200
	H	2.48732500	-0.55384100	-4.54244200
	C	0.13298900	1.39434000	-2.50309000
	H	0.84922500	1.95796200	-1.90526700
	H	-0.87181500	1.71511200	-2.22695400
	C	-0.95934100	-1.05120600	-2.50708200
	H	-1.82575100	-0.68812100	-1.95430000
	H	-0.74474800	-2.06846700	-2.17868200
	C	1.70301300	-0.77375900	-2.43003800
	H	1.80049000	-1.68061500	-1.83324200
	H	2.46579000	-0.06578000	-2.10491100
	H	0.22111600	-0.11405800	-0.29653700
	I	0.21253000	-0.10944700	1.31576000
HCN	C	0.38374200	1.38022500	-4.07692300
	C	-1.02060300	-0.89329700	-4.08609600
	C	0.33728700	-0.16164400	-4.05033600
	H	-0.37295600	1.87514900	-4.68390200
	H	1.36188700	1.76744700	-4.36109200
	H	-1.83737800	-0.25005700	-4.41256500
	H	-1.05606700	-1.81583900	-4.66371800
	C	0.30328900	-0.14710700	-2.51872700
	C	1.64992600	-0.97201800	-4.02660300
	H	1.50937300	-2.01143100	-4.32212800
	H	2.48098300	-0.56043400	-4.59750100
	C	0.14085600	1.39158000	-2.53293500
	H	0.85794200	1.95880500	-1.93924500
	H	-0.86409800	1.71044500	-2.25541300
	C	-0.94727800	-1.05764100	-2.53346500
	H	-1.81089900	-0.70134200	-1.97192100
	H	-0.72783600	-2.07757500	-2.21687500
	C	1.71713800	-0.77506800	-2.47748900
	H	1.82570400	-1.68253500	-1.88325000
	H	2.48332400	-0.06513900	-2.16470200
	C	0.29955100	-0.10038400	0.79500900
	N	0.28782700	-0.08230700	1.93748600
	H	0.31041500	-0.11727600	-0.27654100
FCl	C	2.10019000	-1.30889400	0.51077400

	C	2.10027900	1.09639600	0.87832800
	C	2.40689600	-0.00025000	0.00039500
	H	2.40016900	-1.47725200	1.54019600
	H	2.39990400	-2.12967900	-0.13308300
	H	2.39967500	0.94930200	1.91119300
	H	2.40097700	2.07181600	0.50929400
	C	-0.06160500	0.00022500	-0.00025300
	C	2.10086600	0.21206100	-1.38834700
	H	2.40100900	1.17993700	-1.77722300
	H	2.40107600	-0.59535300	-2.04866500
	C	0.37801600	-1.30126700	0.50809000
	H	0.08602100	-2.13681200	-0.12217900
	H	0.08611000	-1.48841800	1.53782700
	C	0.37811700	1.09119800	0.87265400
	H	0.08567600	0.96357700	1.91134700
	H	0.08659700	2.07652400	0.51945500
	C	0.37852200	0.21074800	-1.38143200
	H	0.08656100	1.17427900	-1.79015400
	H	0.08685300	-0.58758500	-2.05836100
	F	-3.99969600	-0.00006400	0.00025700
	Cl	-2.21241500	-0.00006200	-0.00018900
FBr	C	2.55734600	0.02633900	1.40367200
	C	2.55654900	1.20303800	-0.72486800
	C	2.86231000	0.00035000	-0.00038400
	H	2.85523200	0.93436100	1.91817600
	H	2.85557100	-0.86185900	1.95152600
	H	2.85432500	2.12168700	-0.22951100
	H	2.85432200	1.19488100	-1.76851900
	C	0.39253000	-0.00026100	0.00020000
	C	2.55732500	-1.22878100	-0.67952300
	H	2.85484200	-1.25921500	-1.72281600
	H	2.85567400	-2.12819100	-0.15037200
	C	0.83031600	0.02600700	1.39700800
	H	0.54199300	-0.85485300	1.96399000
	H	0.54204500	0.92774100	1.93024000
	C	0.82979600	1.19648400	-0.72089800
	H	0.54132400	2.12764700	-0.24107400
	H	0.54116300	1.20774400	-1.76833200
	C	0.83025500	-1.22311800	-0.67554500
	H	0.54172500	-1.27383100	-1.72181100
	H	0.54246500	-2.13582000	-0.16106900
	F	-3.79316400	0.00005600	-0.00055600
	Br	-1.90687900	-0.00003300	0.00018900
FI	C	2.95706300	-0.52981300	-1.29826500
	C	2.95718400	-0.85914300	1.10811100
	C	3.26386100	0.00034000	-0.00001900

	H	3.25036600	-1.56327000	-1.45249500
	H	3.25004200	0.10039400	-2.13182900
	H	3.25043500	-1.89603900	0.97898000
	H	3.25022200	-0.47600200	2.08030200
	C	0.78910300	-0.00021600	0.00001300
	C	2.95676700	1.38960000	0.19011800
	H	3.24963300	1.79639200	1.15269700
	H	3.24963800	2.04002100	-0.62779900
	C	1.21981100	-0.52796100	-1.29267400
	H	0.93754000	0.08909300	-2.14119300
	H	0.93797900	-1.56274200	-1.46645200
	C	1.21990900	-0.85579700	1.10341500
	H	0.93810200	-1.89926700	0.99313500
	H	0.93787200	-0.48909300	2.08645200
	C	1.21937500	1.38325400	0.18926400
	H	0.93727900	1.80944400	1.14800300
	H	0.93727200	2.05106200	-0.61994700
	F	-3.71809700	0.00035900	-0.00004700
	I	-1.72003700	-0.00009000	0.00001500
SF_2	C	0.08375700	1.54449500	-0.75492200
	C	-1.36929700	-0.69629500	-0.66856200
	C	0.00334600	0.00566400	-0.69759900
	H	-0.67993700	2.04556400	-1.34838600
	H	1.06146800	1.90123700	-1.07877200
	H	-2.18340100	-0.03683800	-0.96892800
	H	-1.44913600	-1.62305800	-1.23543000
	C	0.02917800	0.04761600	0.84040000
	C	1.29688900	-0.83247100	-0.71244500
	H	1.12056600	-1.87443200	-0.97891400
	H	2.11150600	-0.45167600	-1.32708100
	C	-0.10793200	1.58779300	0.79394400
	H	0.63374000	2.15232200	1.35900600
	H	-1.09875300	1.92306100	1.09921400
	C	-1.23491600	-0.84344800	0.88024400
	H	-2.06689800	-0.46879600	1.47544900
	H	-1.01346700	-1.86147700	1.20132200
	C	1.43141700	-0.60415000	0.82659300
	H	1.54777500	-1.50182200	1.43557100
	H	2.21930400	0.10089300	1.09377700
	F	0.41046100	0.00293600	5.31357700
	S	0.27102600	0.01795300	3.72683700
	F	-1.07092600	0.86934200	3.66251300
SeF_2	C	0.08365800	1.54438200	-0.75614400
	C	-1.37104400	-0.69372300	-0.66692200
	C	0.00176900	0.00624800	-0.70078300

	H	-0.68201600	2.04680700	-1.34563100
	H	1.06054300	1.89991800	-1.08365500
	H	-2.18598200	-0.03094900	-0.95702200
	H	-1.45561600	-1.61649900	-1.23938200
	C	0.03921800	0.04282000	0.84001000
	C	1.29316600	-0.83338800	-0.73210100
	H	1.11233600	-1.87453100	-0.99822800
	H	2.10187800	-0.45220700	-1.35399700
	C	-0.10103000	1.58466400	0.79255700
	H	0.64065000	2.15181900	1.35491000
	H	-1.09117200	1.91448300	1.10432800
	C	-1.22577300	-0.85095900	0.87876800
	H	-2.05284300	-0.48101400	1.48347500
	H	-1.00065800	-1.87110600	1.19049400
	C	1.44436600	-0.60833000	0.80476700
	H	1.57167900	-1.50909400	1.40815400
	H	2.23377200	0.09817300	1.06367400
	F	0.37040400	0.01859100	5.47067100
	Se	0.30141800	-0.01550400	3.73838300
	F	-1.14295500	0.93381300	3.64108300
TeF_2	C	0.05422700	1.53669100	-0.83395500
	C	-1.35954100	-0.72610400	-0.81823700
	C	-0.00022900	-0.00200800	-0.78298300
	H	-0.69213100	2.02414900	-1.45934900
	H	1.03856900	1.91177600	-1.11373300
	H	-2.17131000	-0.07461400	-1.14052200
	H	-1.40116900	-1.64532200	-1.40079600
	C	-0.03426800	0.02913900	0.76025700
	C	1.30579000	-0.81786600	-0.76133100
	H	1.15472900	-1.86153800	-1.03551200
	H	2.13357200	-0.42112300	-1.34705900
	C	-0.20378600	1.57069000	0.70344200
	H	0.50036600	2.15319400	1.29731600
	H	-1.21306300	1.87815400	0.97344200
	C	-1.28292600	-0.89257700	0.73024300
	H	-2.14385000	-0.54534700	1.29956600
	H	-1.04951300	-1.91049600	1.04327900
	C	1.38711000	-0.59429400	0.78031700
	H	1.50909200	-1.49622200	1.38405300
	H	2.15039800	0.12828400	1.07220400
	F	-0.06875600	0.09486200	5.63077200
	F	-1.55487000	0.86478800	3.46575800
	Te	0.09735400	-0.01722100	3.74405500
PF_3	C	-0.03315300	1.57224900	-0.74105600
	C	-1.33608100	-0.75734900	-0.85627500

	C	-0.01336500	0.03046300	-0.76860900
	H	-0.79142400	2.05700700	-1.35483300
	H	0.93645200	2.00735400	-0.98326400
	H	-2.17498300	-0.13532200	-1.16817700
	H	-1.32433100	-1.65514100	-1.47312800
	C	-0.07641700	-0.00948100	0.76620000
	C	1.33143500	-0.72382400	-0.74673200
	H	1.23742800	-1.75946900	-1.07348800
	H	2.15287300	-0.26289500	-1.29386100
	C	-0.31821900	1.51752200	0.79368700
	H	0.34645600	2.09893100	1.43174300
	H	-1.34697100	1.76830600	1.05159100
	C	-1.27690300	-0.98069700	0.68897200
	H	-2.16589200	-0.69331600	1.25097000
	H	-1.00551800	-1.99935900	0.96856500
	C	1.36495800	-0.56767500	0.80711800
	H	1.50935100	-1.48467500	1.37981200
	H	2.08704600	0.17155600	1.15376200
	F	-0.25471100	-0.35291400	5.40280700
	F	-1.36607500	0.66688500	3.60216800
	P	-0.19568700	-0.35398000	3.83215800
	F	0.98830500	0.66755000	3.69093000
AsF_3	C	0.02353300	1.59009400	-0.63742400
	C	-1.37121100	-0.68590700	-0.71841800
	C	-0.01715300	0.05031000	-0.69701600
	H	-0.75343200	2.11518900	-1.19151500
	H	0.99154200	1.99426600	-0.93321700
	H	-2.20382500	-0.02546300	-0.95936100
	H	-1.43299900	-1.56728700	-1.35536900
	C	0.01738700	-0.02456400	0.83928300
	C	1.29613300	-0.75194000	-0.78326500
	H	1.14224500	-1.77515300	-1.12581000
	H	2.09594300	-0.30671100	-1.37336500
	C	-0.16541100	1.51116000	0.91025100
	H	0.55855500	2.05231600	1.51742900
	H	-1.16550800	1.79055200	1.23951300
	C	-1.22307000	-0.95139200	0.81337100
	H	-2.06411000	-0.64610500	1.43671100
	H	-0.97349100	-1.98764100	1.04737000
	C	1.43868200	-0.63564600	0.76699300
	H	1.58980000	-1.57453800	1.30272700
	H	2.20772000	0.06854500	1.08356400
	F	0.12743600	-0.42090900	5.56858300
	F	-1.18804500	0.69851500	3.73216400
	F	1.34622900	0.70826100	3.67296800
	As	0.08695200	-0.44039100	3.85359300

SbF_3	C	-0.05209400	1.49159200	-0.82369300
	C	-1.19083500	-0.92082500	-0.80913900
	C	0.06881900	-0.03972600	-0.70511800
	H	-1.00790100	1.80818200	-1.24085700
	H	0.74619200	1.99769900	-1.36436600
	H	-1.95846500	-0.58759600	-1.50611300
	H	-0.95739100	-1.96342900	-1.02242800
	C	-0.09147600	0.04366300	0.82517800
	C	1.45496300	-0.69246000	-0.54262600
	H	1.61092800	-1.62897200	-1.07621500
	H	2.26917700	-0.01242000	-0.79210400
	C	0.00473100	1.58962400	0.73240500
	H	0.95314600	1.96524900	1.11519700
	H	-0.80411100	2.15616000	1.19921400
	C	-1.47225100	-0.65368400	0.70259800
	H	-2.30355700	0.03443200	0.86777100
	H	-1.61941900	-1.53768000	1.32465900
	C	1.19409500	-0.80776100	0.99125400
	H	0.97182400	-1.82144500	1.32094600
	H	1.95750500	-0.39447600	1.64809000
	F	-0.11694400	-1.47820100	3.70349200
	F	-0.58272400	0.31917000	5.71641400
	F	1.12119400	0.99720100	3.68402200
	Sb	-0.63920300	0.33124900	3.82739700
GeF_4	C	2.79372100	1.17674600	0.78390400
	C	2.79358400	0.09000800	-1.41113000
	C	3.05244300	-0.00037700	0.00013400
	H	3.11465300	2.10405400	0.32092500
	H	3.11505300	1.10739900	1.81790000
	H	3.11539100	1.01990800	-1.86825700
	H	3.11380800	-0.77486400	-1.98270800
	C	0.61368800	0.00045200	-0.00010900
	C	2.79298300	-1.26761800	0.62747200
	H	3.11413800	-2.12859300	0.05057700
	H	3.11348400	-1.33042300	1.66214800
	C	1.10509400	1.17156600	0.78089100
	H	0.80992000	1.13375600	1.82622700
	H	0.80957300	2.12200500	0.34432700
	C	1.10482700	0.09115300	-1.40491600
	H	0.81008100	1.01564900	-1.89455300
	H	0.80864500	-0.76183900	-2.00983900
	C	1.10440600	-1.26171600	0.62370000
	H	0.80898600	-2.14786000	0.06804400
	H	0.80840500	-1.35886200	1.66495800
	F	-1.42310400	-1.45559800	-0.97615500

	F	-1.42378200	1.57344900	-0.77199700
	F	-3.23873800	-0.00035300	-0.00032400
	F	-1.42380300	-0.11788000	1.74851100
	Ge	-1.50380600	0.00005700	0.00000800
SnF_4	C	-0.19052100	1.43158100	-0.94740400
	C	-1.12832700	-0.82873700	-0.93491600
	C	-0.00571000	0.02870900	-1.19988900
	H	-1.14788600	1.82601900	-1.27138900
	H	0.63567900	2.05953700	-1.26386400
	H	-2.08521000	-0.43222700	-1.25781000
	H	-0.99111000	-1.85994800	-1.24290700
	C	-0.01724600	0.04725000	1.23526600
	C	1.29801500	-0.51087700	-0.92478900
	H	1.43275600	-1.54268400	-1.23193000
	H	2.12272800	0.11839000	-1.24258900
	C	-0.19889300	1.44019700	0.74845300
	H	0.61233900	2.10181100	1.04201100
	H	-1.15660900	1.86821800	1.03410200
	C	-1.13235900	-0.81423100	0.76121100
	H	-2.11124700	-0.43819400	1.04814500
	H	-1.02419300	-1.85324900	1.06268500
	C	1.28671300	-0.49536900	0.77092600
	H	1.45019200	-1.52646200	1.07440800
	H	2.13225200	0.12225000	1.06367600
	F	0.23505300	-1.84650800	3.40083000
	F	-1.81990200	0.79742900	3.35610900
	F	-0.05327600	0.08364400	5.40469700
	F	1.49407100	1.24924500	3.38545300
	Sn	-0.03341500	0.06718700	3.50289100
PbF_4	C	0.06919900	1.40325700	-0.52199900
	C	-1.27659400	-0.65254400	-0.52951100
	C	-0.00436300	-0.01584100	-0.76088100
	H	-0.78987300	1.96192000	-0.87828400
	H	1.00521600	1.85962700	-0.82638400
	H	-2.13087800	-0.08153800	-0.87775700
	H	-1.32277400	-1.68804100	-0.85000800
	C	-0.06050400	0.01051600	1.63794700
	C	1.17618600	-0.78987300	-0.47243600
	H	1.11708600	-1.82751900	-0.78363400
	H	2.10441100	-0.32385300	-0.78589600
	C	0.02037500	1.42138300	1.15596000
	H	0.92901600	1.92051100	1.48341500
	H	-0.85453800	2.00447200	1.43272400
	C	-1.31090000	-0.64213500	1.14752400
	H	-2.20485200	-0.09327200	1.43326500
	H	-1.38648400	-1.68038100	1.46126500

	C	1.14127300	-0.76294400	1.20564600
	H	1.10504700	-1.80043300	1.52847200
	H	2.07032400	-0.29766000	1.52566100
	F	-1.83183800	1.14376000	3.70078900
	F	1.72154700	0.97207500	3.77093400
	F	-0.14606300	0.05393000	5.87355700
	F	-0.20229900	-2.01871900	3.76495700
	Pb	-0.10802000	0.03440600	3.89874600

dimer				
pyramidane				
HF	C	-0.03077900	1.02055700	-0.22182400
	C	-0.00476600	-0.00017400	1.00957100
	C	-1.02171100	-0.02951100	-0.22589300
	C	1.01950500	0.02939200	-0.21776900
	C	0.02812400	-1.02068300	-0.22187200
	H	-0.06215900	2.08221300	-0.05952700
	H	-2.08383700	-0.06020700	-0.06644300
	H	2.08074200	0.06005500	-0.05275500
	H	0.05810200	-2.08238000	-0.05957300
	F	-0.08532300	-0.00395100	3.71792500
	H	-0.05085600	-0.00229100	2.76261200
HCl	C	0.08445600	-1.01356500	0.08404100
	C	-0.02902900	0.04094800	-1.11136900
	C	-1.02781200	-0.09278200	0.12958800
	C	1.00573600	0.09880600	0.10640100
	C	-0.10629600	1.01905600	0.15187100
	H	0.18134100	-2.06561500	-0.11194700
	H	-2.08770600	-0.18698100	-0.02012000
	H	2.06074800	0.20379900	-0.06865300
	H	-0.20776500	2.08109700	0.02322500
	Cl	-0.04587800	0.30066600	-4.19209600
	H	-0.04172800	0.16811700	-2.84351500
HBr	-			
HI	-			
HCN	C	-0.03066200	1.01741000	-0.22679200
	C	0.00189700	-0.03648400	0.98955600
	C	-1.02068300	-0.03132800	-0.25364500
	C	1.01840800	0.02785600	-0.25705200
	C	0.02840600	-1.02088400	-0.28382800
	H	-0.06111300	2.07524300	-0.04115700
	H	-2.08291100	-0.06656100	-0.09603200
	H	2.08138500	0.05438700	-0.10279900
	H	0.05956500	-2.08744700	-0.15774400
	C	0.00886400	-0.12490400	4.25655900

	H	0.00762100	-0.09640500	3.17221200
	N	0.01006100	-0.15437600	5.39998800
FCl	C	-0.03034000	1.02759800	-0.20023800
	C	-0.00515100	0.02168600	1.01442100
	C	-1.02583100	-0.02698900	-0.18722800
	C	1.02429400	0.03226600	-0.18069500
	C	0.02880300	-1.02228200	-0.16769900
	H	-0.06159000	2.09012900	-0.04005000
	H	-2.08632900	-0.05484500	-0.01349100
	H	2.08349600	0.06577700	-0.00018900
	H	0.05879600	-2.07918300	0.02640500
	F	-0.02074800	0.08594000	4.77613300
	Cl	-0.01302800	0.05466600	2.97611400
FBr	C	-0.03088200	1.02541900	-0.23514300
	C	-0.00289600	0.01253900	0.97778800
	C	-1.02427000	-0.02978300	-0.22718300
	C	1.02441000	0.03219000	-0.22278100
	C	0.03104400	-1.02317300	-0.21487300
	H	-0.06339800	2.08713100	-0.07028000
	H	-2.08489400	-0.06017800	-0.05517400
	H	2.08416300	0.06604000	-0.04612800
	H	0.06272800	-2.08173200	-0.03090000
	F	-0.01338300	0.05495700	5.00172800
	Br	-0.00843900	0.03485700	3.11541500
FI	C	0.02326000	-1.03110500	0.13242300
	C	-0.01462900	0.03998100	-1.03261900
	C	-1.02582300	-0.03393800	0.18349500
	C	1.02160500	0.01777800	0.16373800
	C	-0.02761000	1.01481300	0.21485300
	H	0.04786800	-2.08413600	-0.08157200
	H	-2.08819700	-0.05379600	0.02137400
	H	2.08056800	0.05147900	-0.01712400
	H	-0.05580200	2.08146900	0.08529500
	F	-0.06899600	0.23362500	-5.36784800
	I	-0.04281600	0.14175900	-3.36773200
SF_2	C	0.00390700	1.04752200	0.04851800
	C	-0.07300500	-0.08147800	1.17216400
	C	-0.98721400	0.00832700	-0.12159300
	C	1.05077100	0.05408800	0.04827800
	C	0.06511600	-0.99001000	-0.12186900
	H	-0.03628800	2.08593500	0.32383100
	H	-2.05915900	-0.02774900	-0.05731700
	H	2.08968900	0.06847100	0.32429000
	H	0.08530500	-2.06234600	-0.05704700

	F	0.54216700	0.54288500	5.01378100
	S	0.16842200	0.16069900	3.45170800
	F	1.23221400	1.26473200	2.92149200
SeF_2	C	0.01627800	1.06614400	0.07917600
	C	-0.07328000	-0.06344400	1.19478700
	C	-0.97732500	0.03049200	-0.09917000
	C	1.06122700	0.06862200	0.09081600
	C	0.07325100	-0.97418700	-0.08647100
	H	-0.02051700	2.10292200	0.36168100
	H	-2.05001600	-0.00137500	-0.04290000
	H	2.09647500	0.08233000	0.38060300
	H	0.08935200	-2.04682100	-0.02391300
	F	0.54572400	0.73594400	5.11564600
	Se	0.09603600	0.17998600	3.46297900
	F	1.19098200	1.42526000	2.85935900
TeF_2	C	-0.00439400	-1.02475100	0.11203400
	C	0.20652200	-0.18418300	-1.20738300
	C	-1.05434100	-0.09445600	-0.23998700
	C	0.94758500	0.07448100	0.15834800
	C	-0.11148400	0.99722000	-0.19295900
	H	0.08128000	-2.09585100	0.12385900
	H	-2.04563200	-0.19407900	-0.64464100
	H	2.01788500	0.14233800	0.22522300
	H	-0.13966200	2.01361300	-0.54261800
	F	-0.48058000	0.41103400	-5.39780400
	F	-1.33588700	0.98101700	-3.01100600
	Te	0.14564700	-0.08419900	-3.62005200
PF_3	C	-0.10750800	0.94854400	0.38977300
	C	0.23850900	-0.43282300	1.15147000
	C	-1.03443600	-0.13885200	0.20757300
	C	0.95094700	0.14374500	-0.16818300
	C	0.02260700	-0.94846500	-0.35129400
	H	-0.13788600	1.87278200	0.93807900
	H	-2.02998500	-0.33823600	0.55963700
	H	2.01960900	0.24029600	-0.22131500
	H	0.12362200	-1.98854900	-0.60045600
	F	-1.32159800	0.73535800	3.33013200
	F	0.95988700	1.33253200	3.44393300
	P	0.00916300	0.20178800	3.99391200
	F	-0.24286500	0.89025200	5.39757700
AsF_3	C	-0.00420300	0.96060500	0.20682900
	C	-0.00586800	-0.43995700	0.99745300
	C	-1.01118300	-0.00229900	-0.16333900
	C	1.03122600	0.01607300	-0.12922100
	C	0.02486700	-0.95616100	-0.50287700

	H	-0.02172600	1.88233100	0.76056100
	H	-2.07510400	-0.06254000	-0.02445500
	H	2.09036100	-0.02531200	0.04813000
	H	0.03835100	-2.00362400	-0.74114600
	F	0.01281400	0.73154600	5.15678700
	F	-1.27036700	0.98846600	3.04356500
	F	1.29393700	0.95295600	3.03899000
	As	-0.00141400	-0.04714000	3.59868300
SbF_3	C	0.00825400	1.06367300	0.46518300
	C	0.10129500	-0.29968500	1.30403200
	C	-0.97181000	0.04007300	0.18874800
	C	1.06895000	0.15270000	0.11885400
	C	0.09394800	-0.88225000	-0.16206400
	H	-0.02606200	2.00397500	0.98661700
	H	-2.02562000	-0.05889000	0.37405500
	H	2.13400200	0.16855800	0.26370300
	H	0.14605100	-1.93674600	-0.36120700
	F	0.81922400	1.17382100	5.38659800
	F	-0.90425400	1.31455000	3.34997000
	F	1.88796600	1.00295500	2.95425600
	Sb	0.46881200	0.08672800	3.84468200
GeF_4	C	-0.04405100	1.03360100	-0.21317800
	C	0.03199100	0.04999400	1.00273700
	C	-1.01962700	-0.03954600	-0.15998600
	C	1.02973300	0.05654300	-0.20509200
	C	0.05318400	-1.01527400	-0.15187300
	H	-0.08843300	2.09844100	-0.07144600
	H	-2.07330500	-0.08060500	0.05106500
	H	2.09236900	0.11465700	-0.05188800
	H	0.10940400	-2.06602100	0.07030600
	F	0.53767000	-1.54126500	3.01651300
	F	-1.58781500	0.57850900	2.98531200
	F	0.14408300	0.21601200	4.82110300
	F	1.30809100	1.35611700	2.86025800
	Ge	0.09025600	0.13696800	3.09600900
SnF_4	C	-0.04422000	1.05490300	0.01726900
	C	-0.02474300	0.11361800	1.26993100
	C	-1.03568500	-0.00326400	0.07108300
	C	1.01506000	0.06522000	0.09869600
	C	0.02221200	-0.99159900	0.15232900
	H	-0.07810100	2.12510400	0.11589800
	H	-2.09709100	-0.02354100	0.24492400
	H	2.07365000	0.11447200	0.28067300
	H	0.05697300	-2.03549300	0.40977600
	F	0.51234900	-1.58704500	3.43734100

	F	-1.94610800	0.60739500	3.25333600
	F	-0.12624500	0.34205500	5.40463700
	F	1.20094200	1.64490000	3.27618400
	Sn	-0.08071200	0.23667100	3.50947300
PbF_4	C	-0.03657400	1.04851000	0.05199600
	C	0.13509100	0.08237300	1.27111300
	C	-0.99326200	-0.03554900	0.18267500
	C	1.05035500	0.08355100	0.00754000
	C	0.09012200	-0.99996400	0.13829400
	H	-0.08306200	2.11511900	0.18323900
	H	-2.02811100	-0.08657500	0.47400300
	H	2.12105500	0.15356800	0.07710600
	H	0.17517900	-2.04787400	0.36656600
	F	1.18294500	-1.60703900	3.35744400
	F	-1.80005400	0.15325300	3.39071500
	F	0.27614100	0.21228300	5.52603600
	F	1.19832400	1.89600700	3.25637900
	Pb	0.21626300	0.15652100	3.54852500