SUPPORTING INFORMATION

Tetrel-Substituted Pyramidanes as Electron Donor in Noncovalent Bonds

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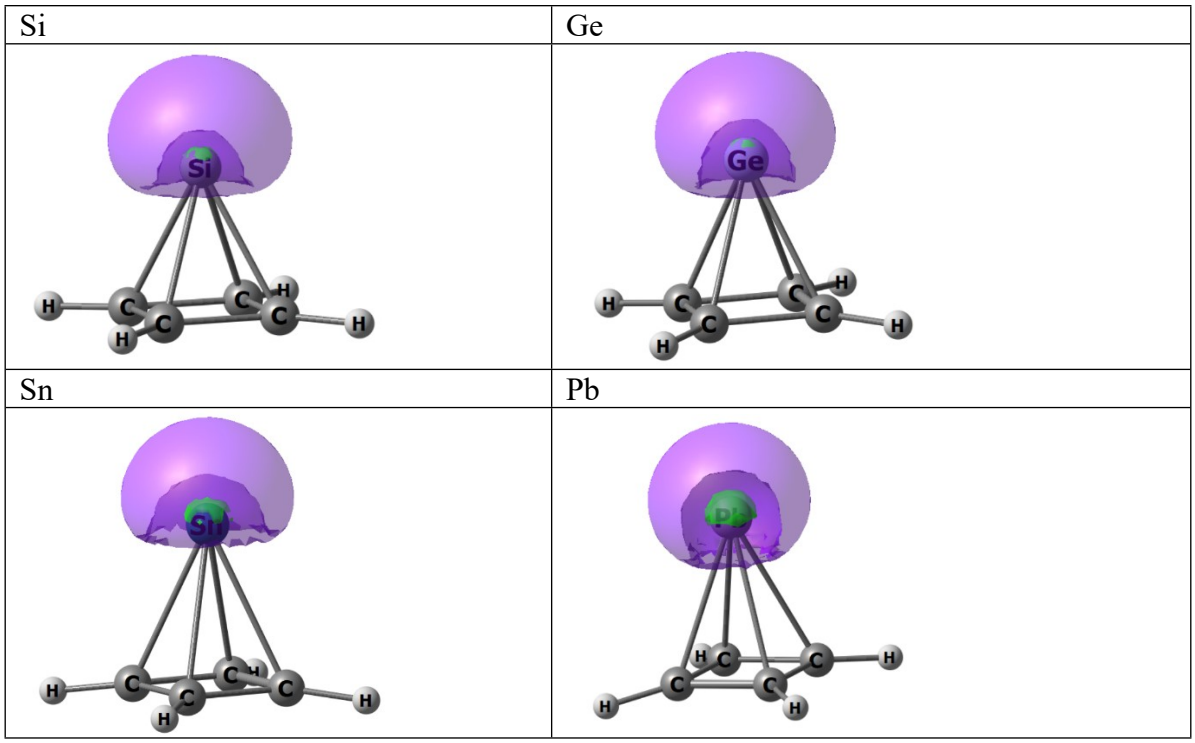


Fig S1. NBO orbital corresponding to T lone pair; isosurface= 0.1 au

Table S1. MEP maxima $V_{s,max}$ (kcal/mol) on the 0.001 au electron isodensity surface for Lewis acids.

	$V_{s,max}$
HF	69.8
HCl	45.2
HBr	38.8
FCl	42.0
FBr	50.4
FI	60.8
$Fe(CO)_4$	18.4
$Ru(CO)_4$	18.1
$Os(CO)_4$	16.3

Table S2. Deformation energies of optimized apical dimers (kcal/mol)

	$Si(C_4H_4)$		$Ge(C_4H_4)$		$Sn(C_4H_4)$	
Dimer	M062X	CCSD(T)	M062X	CCSD(T)	M062X	CCSD(T)
HF	0.15	0.28	0.34	0.13	0.36	0.06
HCl	0.05	0.16	0.33	0.06	0.34	0.02
HBr	0.06	0.16	0.35	0.05	0.38	0.02
FCl	5.03	3.01	0.21	-0.09	0.19	-0.14
FBr	4.19	3.08	0.66	0.42	0.23	0.03
FI	2.46	2.23	0.94	0.76	2.04	1.67
$Fe(CO)_4$	4.24	-1.46	3.53	-1.72	5.62	0.11
$Ru(CO)_4$	4.24	2.97	2.77	1.6	4.07	2.77
$Os(CO)_4$	5.58	5.02	4.37	4.11	8.64	8.84

Table S3. Binding energies of apical dimers (kcal/mol) corrected for BSSE

	$Si(C_4H_4)$		$Ge(C_4H_4)$		$Sn(C_4H_4)$	
Dimer	M062X	CCSD(T)	M062X	CCSD(T)	M062X	CCSD(T)
HF	-3.18	-2.65	-2.03	-1.73	-1.03	-0.44
HCl	-1.88	-1.81	-1.01	-1.28	-0.34	-0.51
HBr	-1.67	-1.70	-0.83	-1.26	-0.23	-0.59
FCl	-5.10	-2.82	-3.15	-1.76	-2.53	-0.83
FBr	-9.72	-6.95	-5.32	-3.53	-4.27	-2.15
FI	-11.82	-9.36	-7.35	-5.39	-6.28	-3.77
$Fe(CO)_4$	-25.92	-41.30	-17.32	-30.02	-14.48	-26.01
$Ru(CO)_4$	-25.17	-31.65	-15.44	-22.03	-13.53	-19.52
$Os(CO)_4$	-32.46	-34.64	-20.65	-23.89	-18.44	-20.65

Table S4. Deformation energies of optimized basal dimers (kcal/mol)

	$Si(C_4H_4)$		$Ge(C_4H_4)$		$Sn(C_4H_4)$		$Pb(C_4H_4)$	
Dimer	M062X	CCSD(T)	M062X	CCSD(T)	M062X	CCSD(T)	M062X	CCSD(T)
HF	0.05	-0.04	0.05	-0.06	0.07	-0.02	0.08	-0.01
HCl	0.02	-0.04	0.02	-0.05	0.04	0	0.04	1.20
HBr	0.04	-0.03	0.05	-0.02	0.06	-0.01	0.06	0.01
FCl	0.12	-0.19	0.14	-0.19	0.37	-0.07	0.56	0.01
FBr	0.17	-0.09	0.19	-0.08	0.82	0.33	2.42	1.47
FI	0.23	0.02	0.27	0.04	1.24	0.76	2.64	1.89
$Fe(CO)_4$	2.83	-1.54	2.83	-1.58	4.07	-0.66	4.55	-0.24
$Ru(CO)_4$	1.34	0.95	1.36	0.94	1.88	1.43	2.21	1.78
$Os(CO)_4$	2.07	2.78	2.14	2.8	4.72	4.72	6.28	6.02

Table S5. Binding energies of optimized basal dimers (kcal/mol) corrected for BSSE

	$Si(C_4H_4)$		$Ge(C_4H_4)$		$Sn(C_4H_4)$		$Pb(C_4H_4)$	
Dimer	M062X	CCSD(T)	M062X	CCSD(T)	M062X	CCSD(T)	M062X	CCSD(T)
HF	-5.13	-3.77	-4.97	-3.70	-5.63	-3.93	-6.16	-4.23
HCl	-3.96	-3.24	-3.86	-3.20	-4.43	-3.31	-4.87	-3.58
HBr	-3.73	-3.21	-3.65	-3.12	-4.25	-3.36	-4.66	-3.56
FCl	-4.38	-2.77	-4.39	-2.81	-5.14	-3.11	-5.73	-3.44
FBr	-5.99	-4.27	-6.04	-4.36	-7.16	-4.97	-8.13	-5.41
FI	-7.66	-5.59	-7.71	-5.73	-9.12	-6.66	-10.39	-7.35
$Fe(CO)_4$	-9.81	-15.18	-9.83	-15.40	-11.41	-17.56	-12.48	-18.72
$Ru(CO)_4$	-7.31	-7.61	-7.41	-7.89	-8.56	-8.99	-9.46	-9.79
$Os(CO)_4$	-7.65	-6.82	-7.79	-7.23	-9.45	-9.86	-11.03	-11.73

Table S6. AIM parameters (au) for the basal dyads.

	$Si(C_4H_4)$			$Ge(C_4H_4)$			$Sn(C_4H_4)$			$Pb(C_4H_4)$		
	ρ	V	H	ρ	V	H	ρ	V	H	ρ	V	H
HF	0.013	-0.011	0.001	0.013	-0.011	0.001	0.015	-0.012	0.000	0.016	-0.012	0.000
HCl	0.012	-0.008	0.001	0.012	-0.008	0.001	0.014	-0.009	0.001	0.014	-0.009	0.001
HBr	0.011	-0.008	-0.001	0.013	-0.008	0.001	0.014	-0.009	0.001	0.014	-0.009	0.001
FCl	0.016	-0.010	0.002	0.016	-0.011	0.002	0.019	-0.013	0.002	0.021	-0.014	0.001
FBr	0.017	-0.011	0.001	0.017	-0.011	0.001	0.023	-0.015	0.000	0.035	-0.023	-0.002
FI	0.017	-0.011	-0.001	0.017	-0.011	0.000	0.024	-0.016	-0.001	0.033	-0.022	-0.003
$Fe(CO)_4$	0.025	-0.025	-0.002	0.025	-0.024	-0.002	0.029	-0.029	-0.003	0.031	-0.031	-0.003
$Ru(CO)_4$	0.020	-0.016	-0.001	0.020	-0.016	-0.001	0.022	-0.018	+0.001	0.023	-0.019	-0.002
$Os(CO)_4$	0.022	-0.017	-0.001	0.023	-0.017	-0.001	0.038	-0.030	-0.005	0.045	-0.037	-0.007

Table S7. Changes in internal bond lengths (Å) and charge on T (e) due to complexation for basal complexes.

$Si(C_4H_4)$	ΔR(C-C)	ΔR(C-Si)	Δq_{Si}
HF	+0.003	-0.002	0.066
HCl	+0.003	-0.001	0.059
HBr	+0.002	0.000	0.058
FCl	0.000	-0.001	0.050
FBr	+0.001	-0.001	0.066
FI	0.000	-0.002	0.083
$Fe(CO)_4$	+0.003	+0.001	0.111
$Ru(CO)_4$	+0.002	+0.002	0.088
$Os(CO)_4$	+0.002	+0.001	0.101

$Ge(C_4H_4)$	ΔR(C-C)	ΔR(C-Ge)	Δq_{Ge}
HF	+0.002	-0.001	0.071
HCl	-0.002	-0.001	0.062
HBr	-0.001	0.000	0.061
FCl	-0.001	0.000	0.054
FBr	-0.001	0.000	0.072
FI	+0.001	+0.002	0.091
$Fe(CO)_4$	+0.002	+0.003[a]	0.118
$Ru(CO)_4$	+0.002	+0.003[a]	0.093
$Os(CO)_4$	+0.002	+0.004[a]	0.109

$Sn(C_4H_4)$	ΔR(C-C)	ΔR(C-Sn)	Δq_{Sn}
HF	+0.001	-0.001	0.086
HCl	+0.001	-0.001	0.076
HBr	+0.001	0.000	0.077
FCl	-0.001	+0.003	0.076
FBr	+0.003	-0.005	0.107
FI	+0.004[a]	+0.007[a]	0.135
$Fe(CO)_4$	+0.008	+0.014	0.153
$Ru(CO)_4$	+0.004	+0.007	0.120
$Os(CO)_4$	+0.005	+0.011	0.163

$Pb(C_4H_4)$	ΔR(C-C)	ΔR(C-Pb)	Δq_{Pb}
HF	+0.002	+0.001	0.087
HCl	+0.001	0.000	0.079
HBr	+0.001	-0.001	0.079

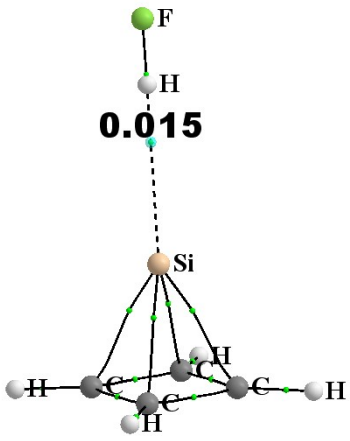
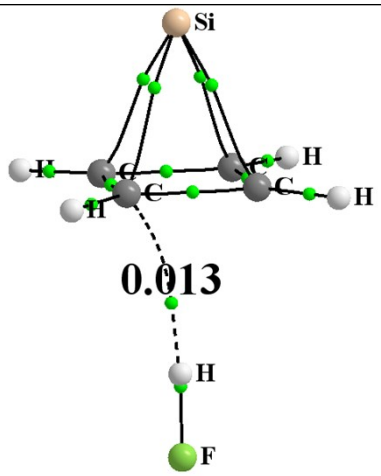
FCl	+0.004	+0.005	0.082
FBr	+0.011	+0.007	0.139
FI	+0.014[a]	+0.009[a]	0.163
$Fe(CO)_4$	+0.007[a]	+0.016[a]	0.156
$Ru(CO)_4$	+0.004[a]	+0.006[a]	0.126
$Os(CO)_4$	+0.006[a]	+0.014[a]	0.180

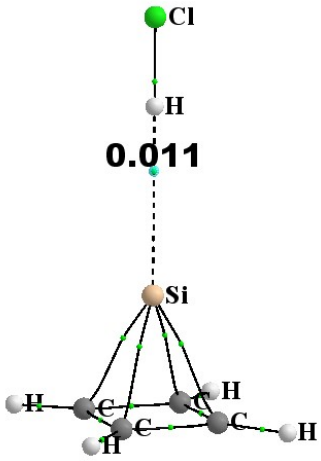
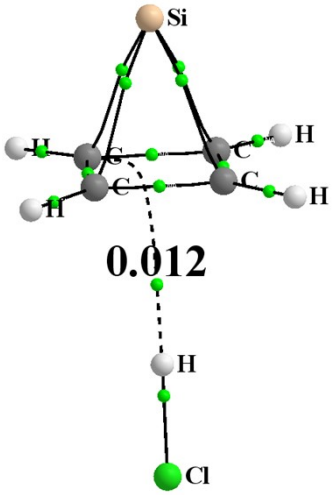
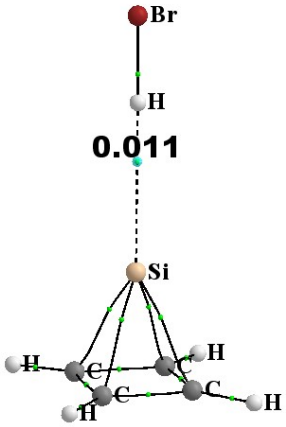
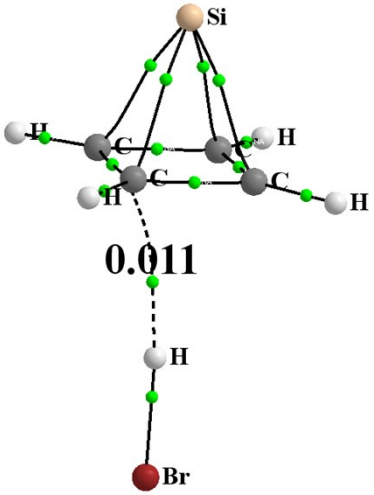
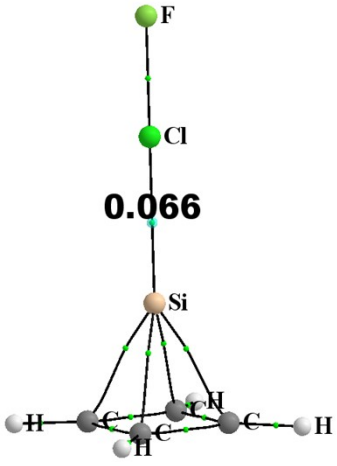
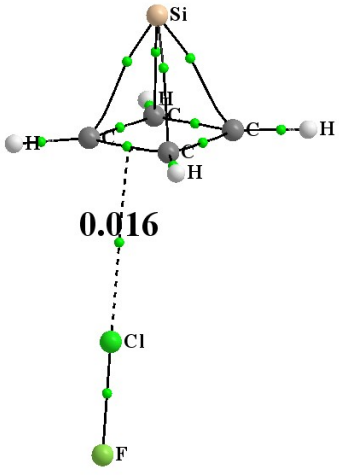
[a]average value

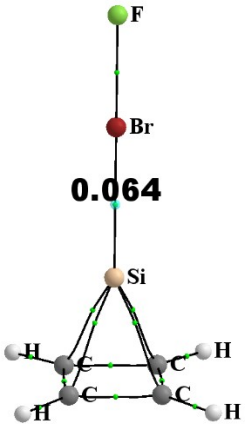
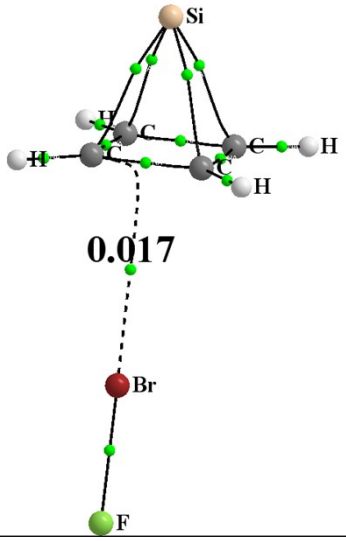
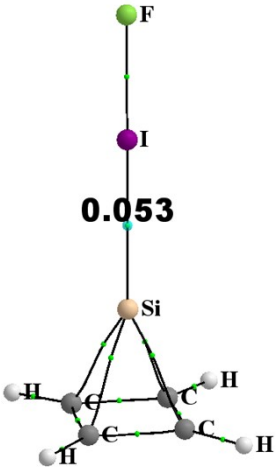
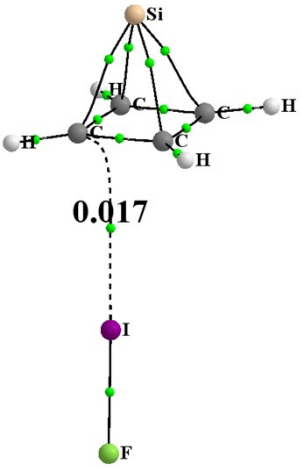
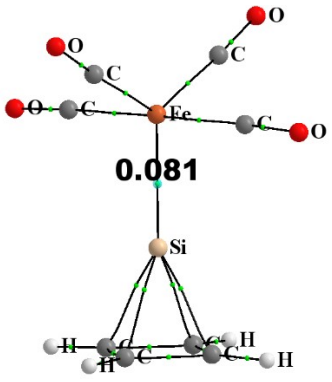
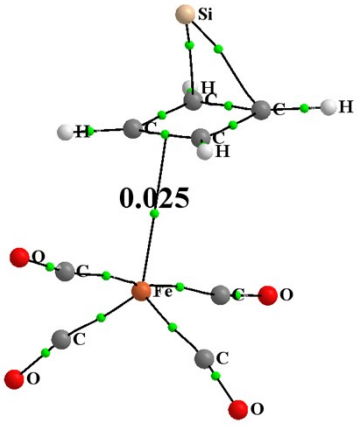
Table S8. Percentage contributions of ALMO-EDA decomposition terms of interaction energies for basal dimers. ES= electrostatic term, POL = polarization, CT = charge transfer, DISP = dispersion, Percentage contributions are defined as fraction of sum of attractive elements.

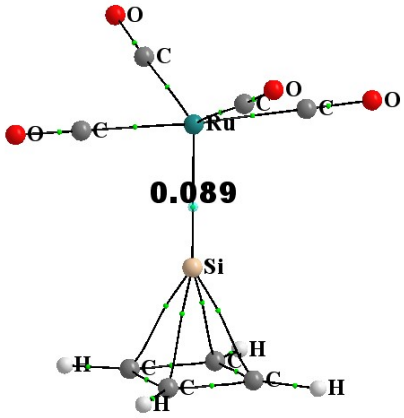
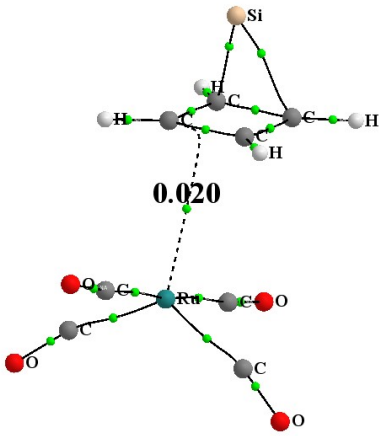
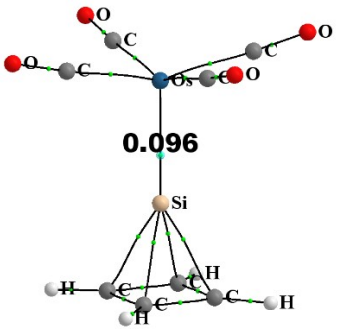
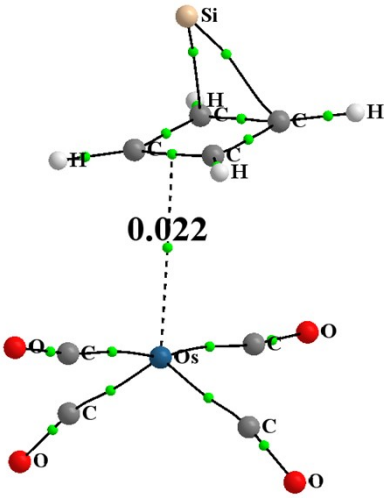
	$Si(C_4H_4)$				$Ge(C_4H_4)$				$Sn(C_4H_4)$				$Pb(C_4H_4)$			
	ES	POL	CT	DISP	ES	POL	CT	DISP	ES	POL	CT	DISP	ES	POL	CT	DISP
HF	56	13	10	21	55	13	10	21	41	18	14	27	43	18	13	26
HCl	53	10	11	25	52	10	12	25	37	13	16	34	39	13	15	33
HBr	52	9	12	26	51	9	13	26	37	12	16	35	38	12	16	34
FCl	51	5	21	22	50	5	22	22	37	7	29	28	38	7	30	26
FBr	50	7	21	22	49	7	22	21	39	9	28	24	41	9	32	18
FI	39	11	21	29	39	11	22	28	40	12	25	23	42	11	28	19
$Fe(CO)_4$	56	9	13	21	56	9	13	21	47	11	17	24	48	12	17	23
$Ru(CO)_4$	44	9	16	32	44	9	16	32	45	9	17	29	46	9	17	28
$Os(CO)_4$	43	8	22	27	43	8	23	27	44	12	24	20	45	13	25	17

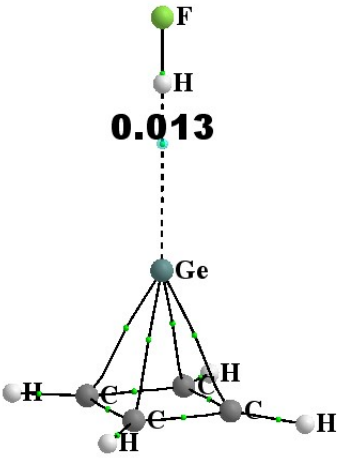
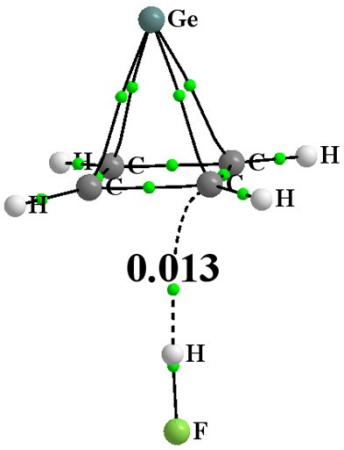
Fig. S2 QTAIM molecular diagrams of fully optimized complexes, apical on left and basal on right. The density of the bond critical point is shown in au.

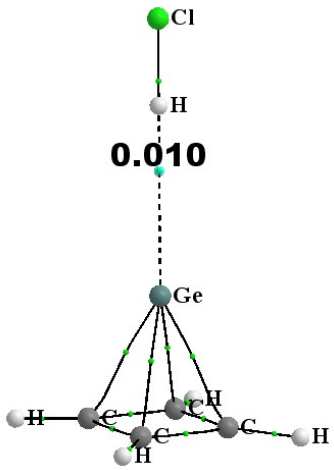
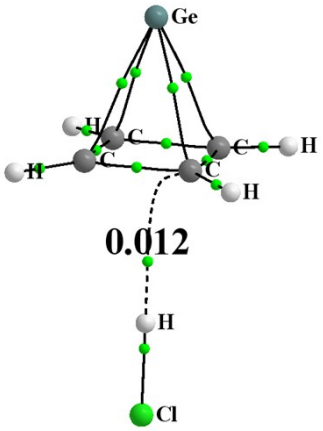
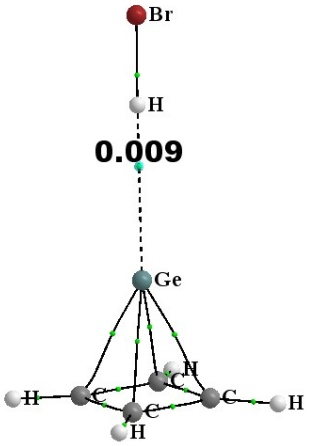
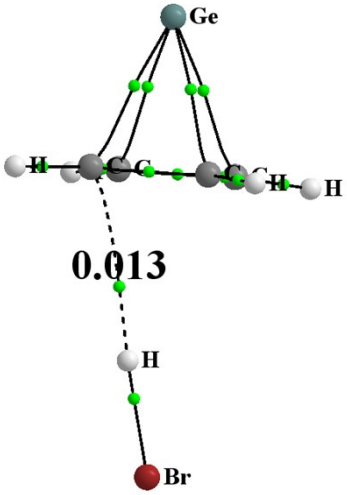
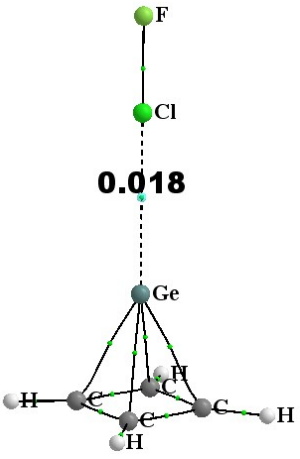
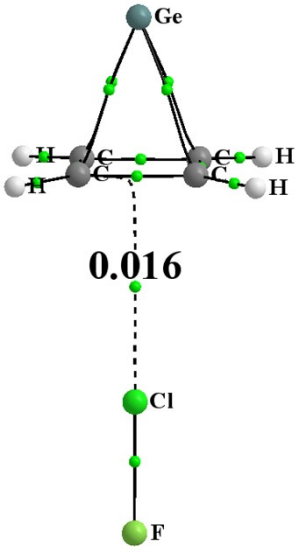
$Si[C_4H_4]$	Apical	Basal
HF		

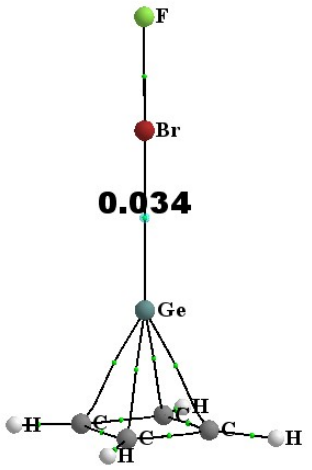
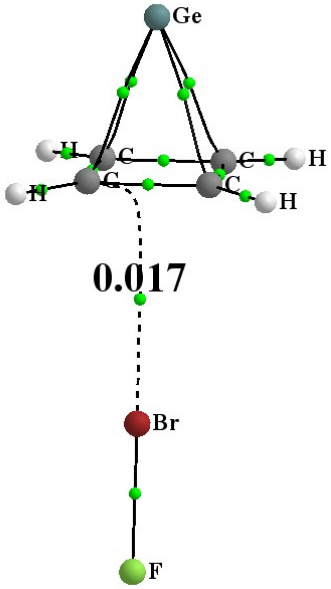
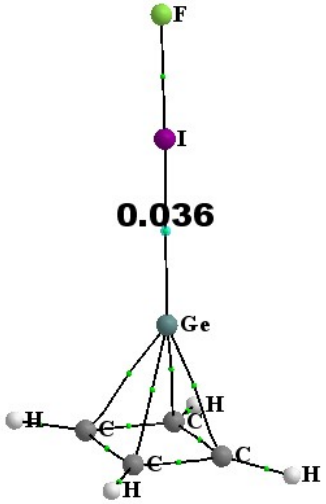
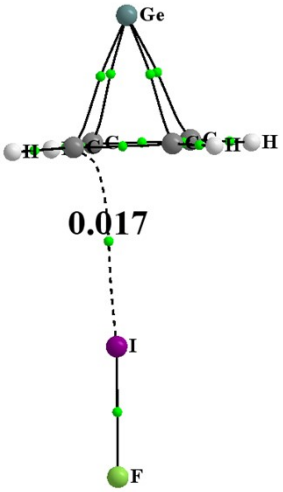
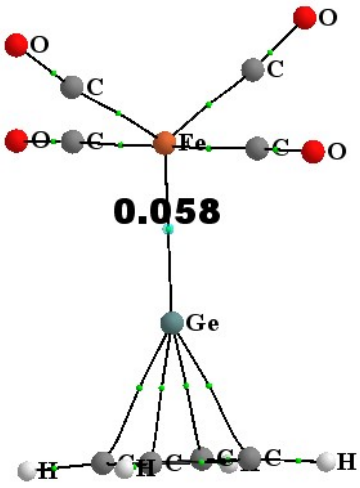
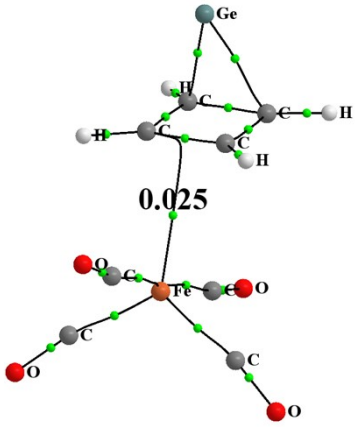
HCl	 Cl H 0.011 Si H C C H C C H H	 Si H C C H C C H H 0.012 H Cl
HBr	 Br H 0.011 Si H C C H C C H H	 Si H C C H C C H H 0.011 H Br
FCl	 F Cl 0.066 Si H C C H C C H H	 Si H C C H C C H H 0.016 Cl F

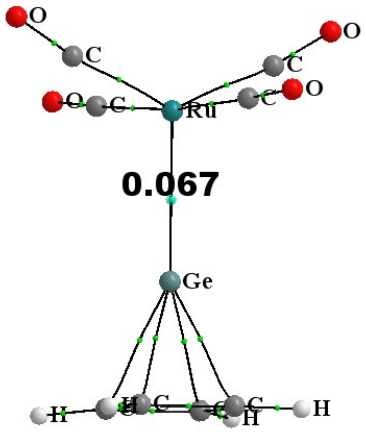
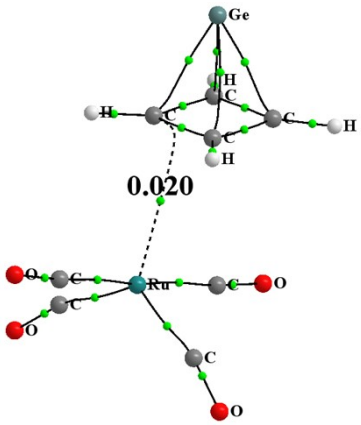
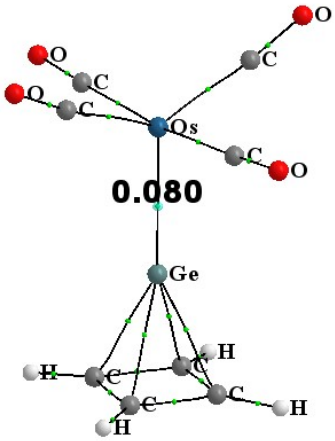
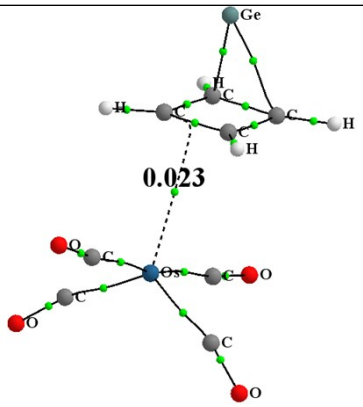
FBr	 F Br 0.064 Si H C C H H C C H	 Si H C C H H C C H 0.017 Br F
FI	 F I 0.053 Si H C C H C C H H	 Si H C C H H C C H 0.017 I F
$Fe(CO)_4$	 O O C C O C Fe C O 0.081 Si H C C H H C C H	 Si H C C H H C C H 0.025 O C Fe C O C O C O

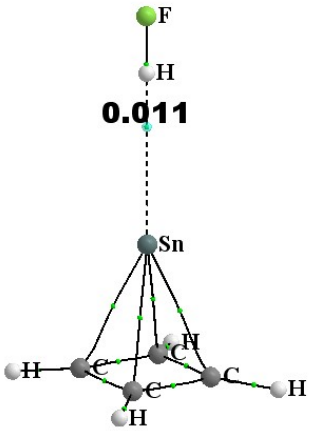
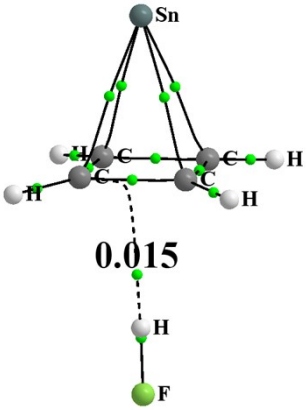
$Ru(CO)_4$		
$Os(CO)_4$		

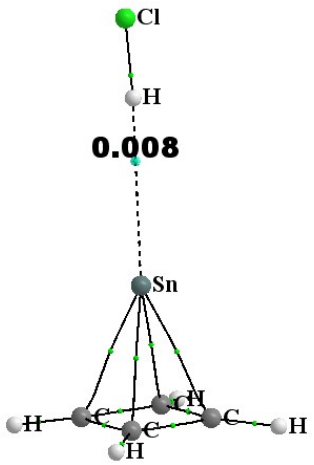
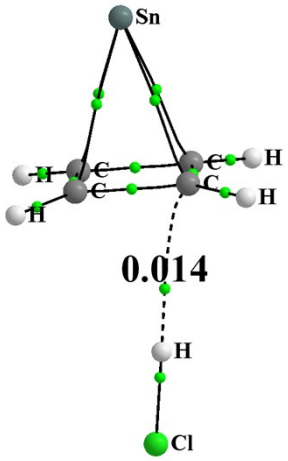
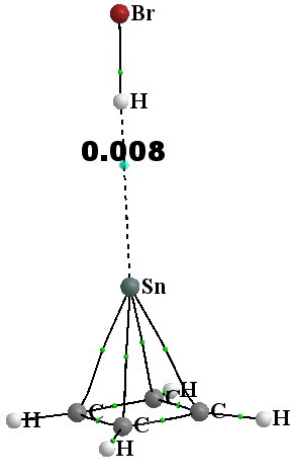
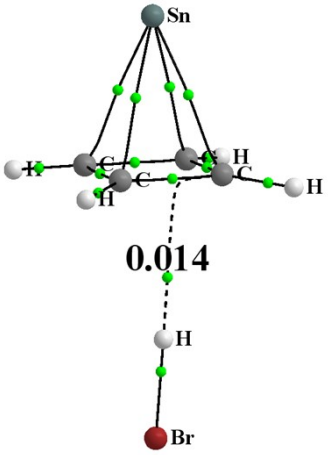
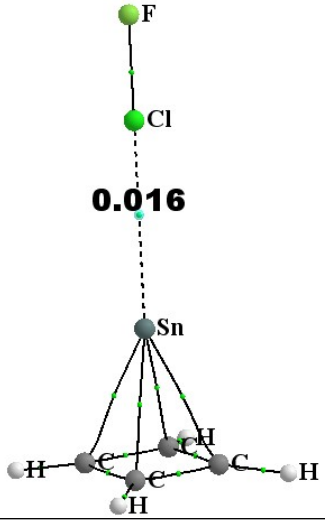
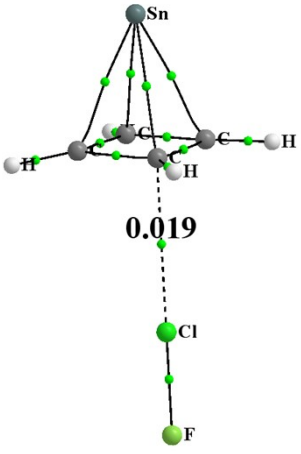
$Ge[C_4H_4]$	Apical	Basal
HF		

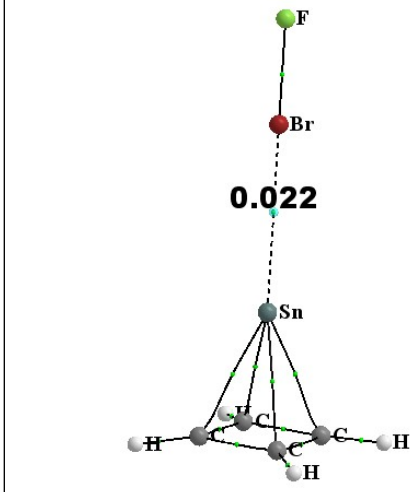
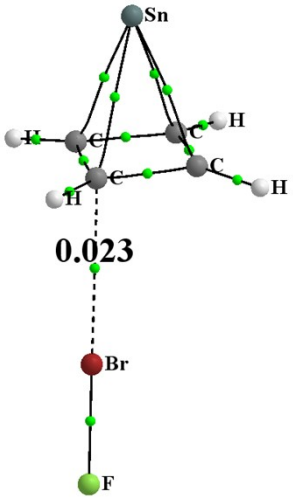
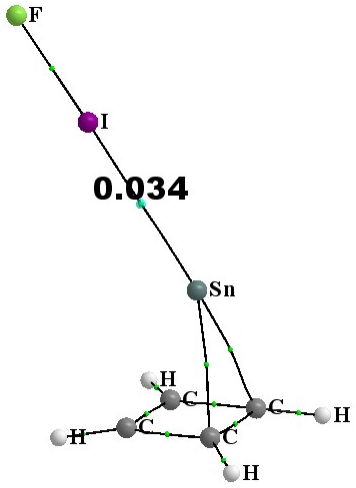
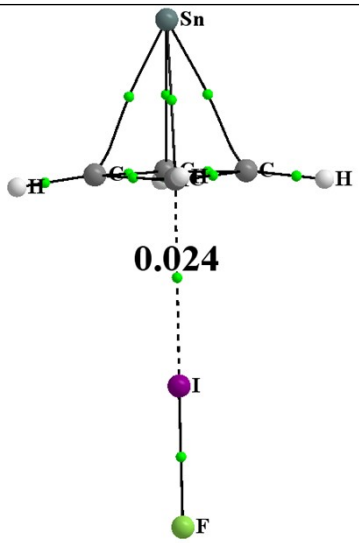
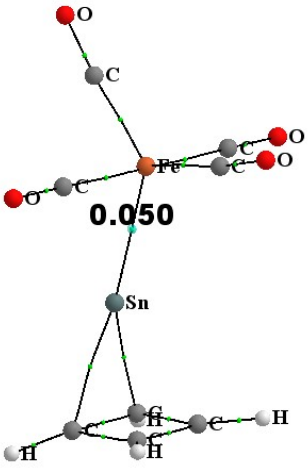
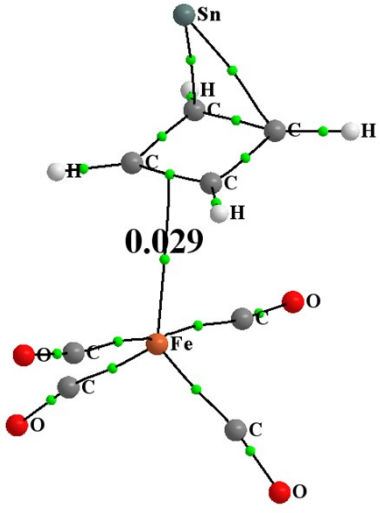
HCl	 Cl H 0.010 Ge H C C H C C H H	 Ge H C C H H C C H 0.012 H Cl
HBr	 Br H 0.009 Ge H C C H C C H H	 Ge H C C C C H H 0.013 H Br
FCl	 F Cl 0.018 Ge H C C H C C H H	 Ge H C C H H C C H 0.016 Cl F

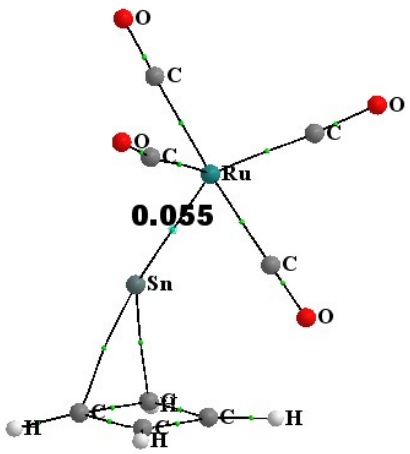
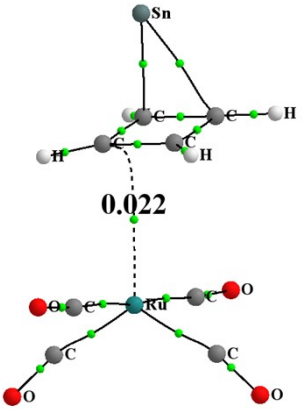
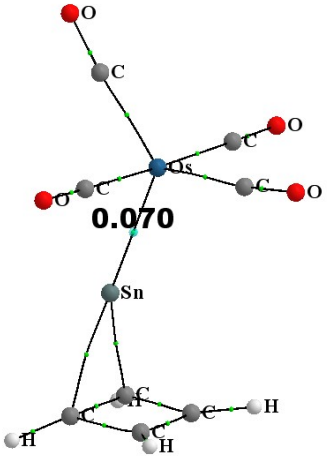
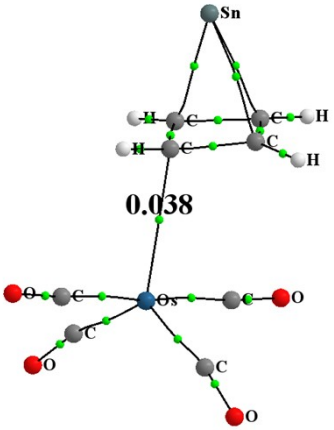
FBr	 F Br 0.034 Ge H C C C C H H H	 Ge H C C H C C H H 0.017 Br F
FI	 F I 0.036 Ge H C C C H H	 Ge H C C H 0.017 I F
$Fe(CO)_4$	 O O C C O C Fe C O 0.058 Ge H C C C C H H	 Ge H C C H C C H 0.025 O C Fe C O C O C O

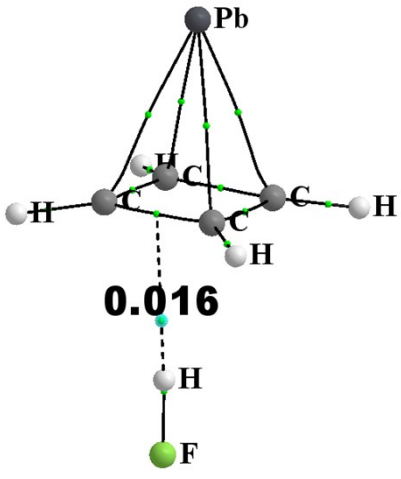
$Ru(CO)_4$		
$Os(CO)_4$		

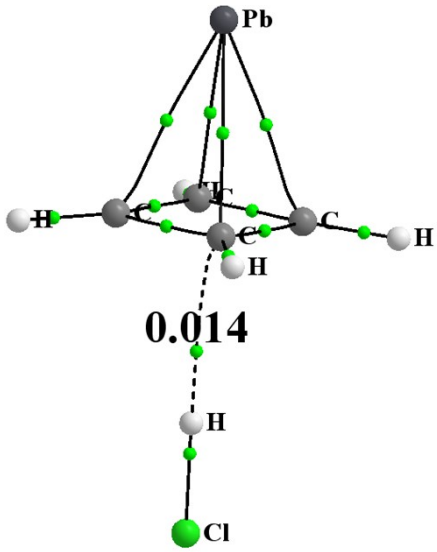
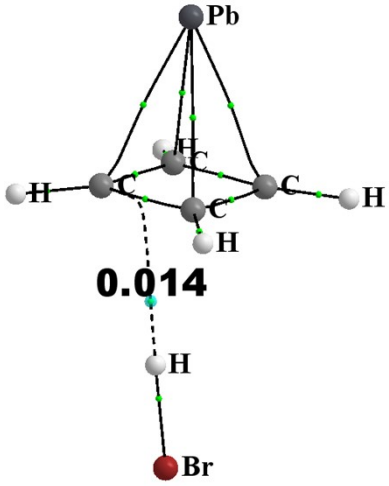
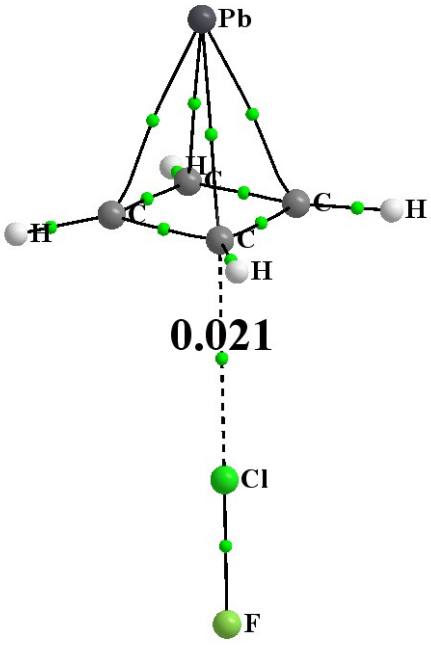
$Sn[C_4H_4]$	Apical	Basal
HF		

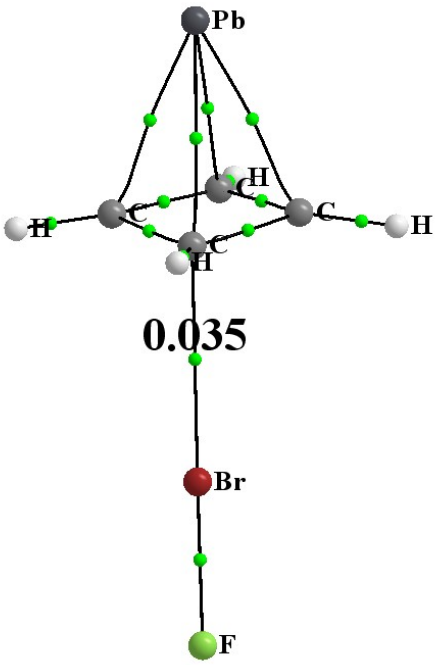
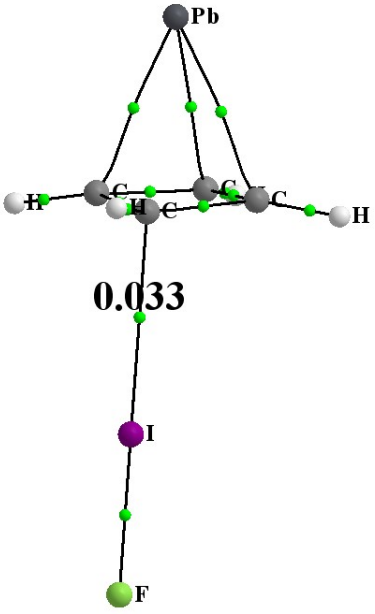
HCl	 Cl H 0.008 Sn H C C C H H H H	 Sn H C C C H H 0.014 H Cl
HBr	 Br H 0.008 Sn H C C C H H H	 Sn H C C C H H 0.014 H Br
FCl	 F Cl 0.016 Sn H C C C H H H	 Sn C C H H 0.019 Cl F

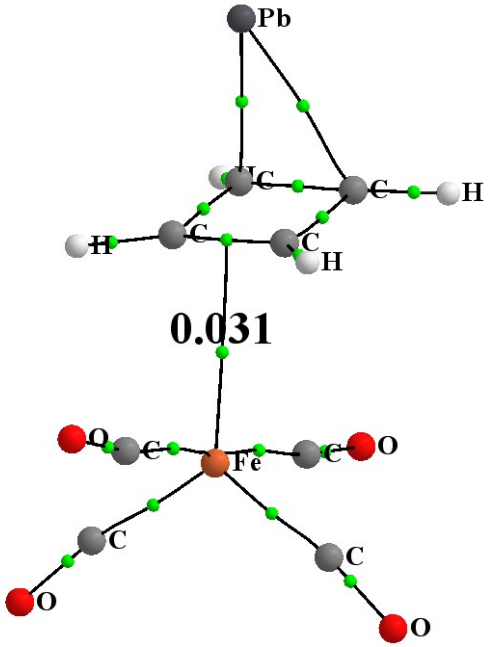
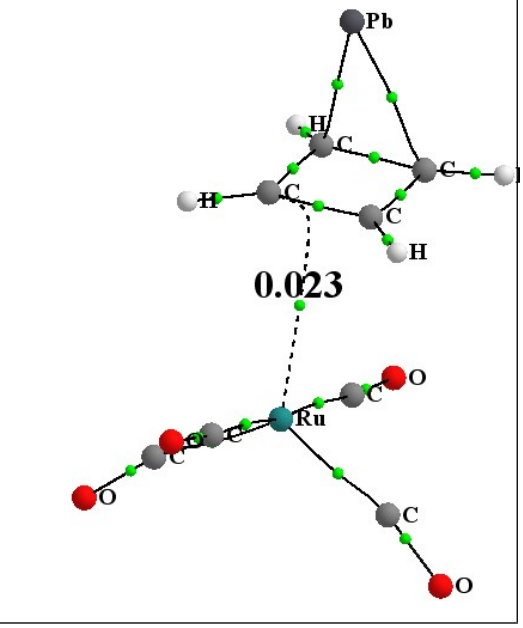
FBr	 F Br 0.022 Sn C C C C H H H H	 Sn H C C C C H H H 0.023 Br F
FI	 F I 0.034 Sn H C C C C H H H	 Sn C C C H H 0.024 I F
$Fe(CO)_4$	 O C C O Fe C C O O C 0.050 Sn C H C C H H H	 Sn H C C H C C H 0.029 O C O C Fe C O C O

$Ru(CO)_4$		
$Os(CO)_4$		

$Pb[C_4H_4]$	Basal
HF	

HCl	 Pb H C C C H H 0.014 H Cl
HBr	 Pb H C C C H H 0.014 H Br
FCl	 Pb H C C C H H 0.021 Cl F

FBr	 Pb H C C H C H H 0.035 Br F
FI	 Pb C C C H H C H 0.033 I F

$Fe(CO)_4$	 Pb C C H H C C H 0.031 O C Fe C O C C O O
$Ru(CO)_4$	 Pb H C C H C C H 0.023 O C Ru C O C O O

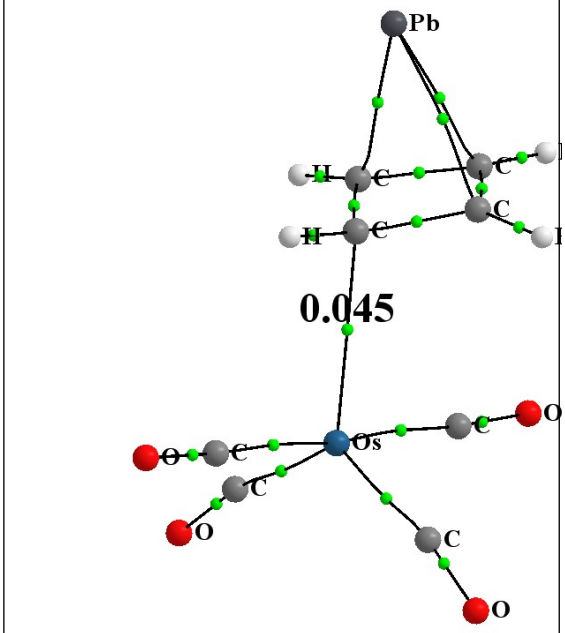
Os(CO)$_4$	

Table S11. Coordinates of monomers and dyads

monomers				
Si[C_4H_4]	C	-0.02965000	1.02568500	-0.20600500
	C	-1.02570800	-0.02962000	-0.20606100
	C	1.02566400	0.02960900	-0.20624400
	C	0.02957900	-1.02570100	-0.20601100
	H	-0.06067900	2.10002300	-0.24783500
	H	-2.10007300	-0.06064400	-0.24718300
	H	2.10000500	0.06063300	-0.24792100
	H	0.06059900	-2.10003600	-0.24789500
	Si	0.00022300	-0.00001800	1.54206500
Ge[C_4H_4]	C	-0.02966800	1.02684100	-0.20623400
	C	-1.02682800	-0.02964000	-0.20626400
	C	1.02678400	0.02962800	-0.20646700
	C	0.02960300	-1.02685700	-0.20624100
	H	-0.06067200	2.09959100	-0.27850600
	H	-2.09961300	-0.06063800	-0.27794000
	H	2.09953400	0.06062600	-0.27864800
	H	0.06059300	-2.09960400	-0.27856100
	Ge	0.00022700	-0.00001800	1.66577100
Sn[C_4H_4]	C	-0.02969500	1.02820800	-0.20708400
	C	-1.02821800	-0.02968000	-0.20715900
	C	1.02819200	0.02966600	-0.20735100
	C	0.02965200	-1.02822600	-0.20708500
	H	-0.06058000	2.09657000	-0.33362000
	H	-2.09666400	-0.06055300	-0.33294800
	H	2.09657300	0.06054100	-0.33367100
	H	0.06051200	-2.09658200	-0.33367500
	Sn	0.00018900	-0.00001400	1.88950400

$Pb[C_4H_4]$	C	-0.02967700	1.02756500	-0.21312600
	C	-1.02759900	-0.02966300	-0.21312800
	C	1.02756800	0.02964900	-0.21334600
	C	0.02963400	-1.02758200	-0.21313000
	H	-0.06052100	2.09448200	-0.35297700
	H	-2.09459700	-0.06049400	-0.35237700
	H	2.09450300	0.06048000	-0.35306500
	H	0.06045000	-2.09449400	-0.35302700
	Pb	0.00019900	-0.00001400	1.99108700

$Si[C_4H_4]$	Apical				Basal			
	C	-0.02697100	1.02707700	-0.42023500	C	0.04149400	-1.02721900	0.24466200
	C	-1.02400500	-0.02952200	-0.42771500	C	-1.03380000	-0.04918400	0.20901200
	C	1.02986700	0.02977400	-0.41290100	C	1.01912900	0.04908600	0.29015800
	C	0.03232800	-1.02683500	-0.42039200	C	-0.05724600	1.02728300	0.25446200
	H	-0.05765300	2.10139100	-0.46335100	H	0.09180900	-2.10116900	0.27911300
HF	H	-2.09806200	-0.06054000	-0.47693000	H	-2.10822900	-0.10070100	0.20649200
	H	2.10438300	0.06080700	-0.45003700	H	2.09046700	0.10031100	0.37228000
	H	0.06369900	-2.10112400	-0.46364300	H	-0.11022600	2.10071100	0.29958300
	F	-0.09878400	-0.00453900	4.75774600	F	-0.09719600	-0.01310800	3.31336200
	H	-0.06981200	-0.00315900	3.83271500	H	-0.05157500	-0.00516200	2.38941400
	Si	-0.00794800	-0.00030900	1.30919400	Si	0.06241500	0.01217200	-1.49408500
	C	0.08741800	-1.02904600	0.27837000	C	0.06193900	-0.96769000	0.25673000
	C	-1.03046900	-0.10425700	0.34288900	C	-1.01402700	0.00635700	0.18012800
	C	1.01451300	0.08663600	0.34823100	C	1.03856400	0.10843200	0.21207200
	C	-0.10345900	1.01150500	0.41277200	C	-0.03805200	1.08164300	0.13544200
	H	0.18734900	-2.09964200	0.25031400	H	0.11338900	-2.03737100	0.35874200
HCl	H	-2.10041000	-0.20715900	0.38264000	H	-2.08828100	-0.04445900	0.20376300
	H	2.08474200	0.18381800	0.39404000	H	2.11141500	0.16432000	0.26781700
	H	-0.20304000	2.07643100	0.52655000	H	-0.09126200	2.15579800	0.11320200
	H	-0.05555900	0.24439400	-4.10193600	Cl	-0.06114200	0.27381000	3.74308900
	Cl	-0.08130400	0.29415400	-5.38443000	H	0.00342200	0.15220700	2.46732600
	Si	-0.01397300	0.10501800	-1.38652100	Si	0.04507700	-0.04502600	-1.54685900
	C	0.08699800	-1.03539600	0.33124100	C	0.04958100	-1.02356500	0.17384900
	C	-1.03128800	-0.10963700	0.37438100	C	-1.02560800	-0.04625400	0.14252800
	C	1.01326100	0.08301800	0.35080100	C	1.02601100	0.05207400	0.20947100
	C	-0.10486300	1.00839800	0.39389200	C	-0.04894300	1.02913800	0.17812800
	H	0.18808100	-2.10617600	0.34265200	H	0.09993000	-2.09743800	0.21237600
HBr	H	-2.10059800	-0.21163400	0.43001300	H	-2.10016000	-0.09777000	0.14429200
	H	2.08382400	0.18276000	0.38074000	H	2.09757200	0.10330300	0.28852500
	H	-0.20468300	2.07680200	0.46810500	H	-0.10183000	2.10274100	0.22035400
	H	-0.05467900	0.23377000	-4.10856500	Br	-0.10450600	-0.01810600	3.89593200
	Br	-0.05608100	0.40376200	-5.52686900	H	-0.10270400	-0.01990600	2.46870000
	Si	-0.03416600	0.03618500	-1.37347100	Si	0.05769900	0.00880300	-1.56970100
FCl	C	-0.02997900	1.03014800	-0.32957600	C	0.92313000	-0.10299600	0.35246300
	C	-1.03011900	-0.02935100	-0.31646400	C	-0.07688200	-1.10004300	0.02057000
	C	1.02963300	0.03022600	-0.30957500	C	-0.10807600	0.93021600	0.33343000
	C	0.02947800	-1.02934700	-0.29644800	C	-1.10106100	-0.07375900	0.00174500
	H	-0.06081800	2.10367300	-0.38986500	H	1.97832300	-0.12256100	0.56186400
	H	-2.10430300	-0.06123500	-0.36296300	H	-0.07060900	-2.16930900	-0.09462900
	H	2.10415100	0.06048700	-0.34895000	H	-0.13003900	1.98908400	0.52304700
	H	0.06065800	-2.10426100	-0.32208400	H	-2.16795800	-0.06828500	-0.13375800
	F	-0.02318000	0.09770500	5.51067600	F	0.20895600	0.29301800	4.78747200
	Cl	-0.01645800	0.06916000	3.77941200	Cl	0.30762900	0.36005900	3.16391900
	Si	-0.00669100	0.02755700	1.38931900	Si	0.21077100	0.18284100	-1.52365300
FBr	C	-0.03080500	1.03028400	-0.35191300	C	0.91128300	-0.11752600	0.35094200
	C	-1.03001100	-0.03119900	-0.34386500	C	-0.07694500	-1.10658000	-0.03470300
	C	1.03073800	0.03119400	-0.33922800	C	-0.12530600	0.91476300	0.33554300
	C	0.03153700	-1.03036500	-0.33117900	C	-1.10423600	-0.08323400	-0.05137400
	H	-0.06318600	2.10414600	-0.40539100	H	1.96328900	-0.13960900	0.57655300
	H	-2.10423400	-0.06424400	-0.38908200	H	-0.06500200	-2.17276100	-0.17496400
	H	2.10518900	0.06320800	-0.37955400	H	-0.15364700	1.97128500	0.53856500
	H	0.06416100	-2.10507900	-0.36324800	H	-2.16784600	-0.07779400	-0.21022300
	F	-0.01486900	0.06092600	5.69846700	F	0.24589500	0.33619800	4.98073200
	Br	-0.01036700	0.04265600	3.84249700	Br	0.30169000	0.37424900	3.21556800
	Si	-0.00397000	0.01674000	1.35496600	Si	0.24500700	0.21927800	-1.53416900
FI	C	0.02237200	-1.04370400	0.24475700	C	0.92701400	-0.11389000	0.30294300

	C	-1.03084200	-0.03761300	0.30073000	C	-0.07523700	-1.10029200	-0.05310400
	C	1.02989000	0.00915000	0.27978000	C	-0.10464600	0.92577500	0.29739100
	C	-0.02341900	1.01512000	0.33566700	C	-1.09659900	-0.07088500	-0.06183300
	H	0.04661700	-2.11910100	0.24122900	H	1.98541800	-0.13859300	0.49712700
	H	-2.10490000	-0.06375200	0.35390000	H	-0.07365900	-2.16872200	-0.17535700
	H	2.10484600	0.03171300	0.31213100	H	-0.12065900	1.98765700	0.47354700
	H	-0.04691300	2.08685800	0.42502500	H	-2.16382200	-0.06180600	-0.19369900
	F	-0.07815200	0.26432300	-6.06558600	F	0.17984600	0.27653900	5.19650200
	I	-0.05104300	0.17551800	-4.08814300	I	0.29344100	0.37619400	3.28225700
	Si	-0.01902800	0.05941700	-1.40520700	Si	0.22308500	0.20629000	-1.57330600
$Fe(CO)_4$	Fe	9.77136000	-0.23505700	8.04915200	Fe	9.53428200	-0.07229900	8.09957300
	Si	11.09225000	0.05577500	6.31126300	Si	12.16100100	0.72385300	4.57142800
	O	7.81732200	1.60744800	6.74608600	O	7.74568200	2.09516800	7.02787300
	O	7.82658100	-2.45504900	7.93203900	O	7.35027900	-2.02507600	8.14975100
	O	11.84687800	-2.04999200	9.19339300	O	11.60142300	-2.15926400	8.79500500
	O	10.07388800	1.62194200	10.32608800	O	9.79855600	1.25556800	10.69819900
	C	12.48482300	1.14158900	5.39138500	C	12.60047300	0.04046700	6.40151100
	C	11.37643000	0.82309900	4.49957800	C	11.86006700	-0.95113300	5.62594000
	C	11.74511800	-0.58551800	4.54233400	C	10.66778200	-0.12239800	5.70342800
	C	12.84938500	-0.26798400	5.43923700	C	11.40891600	0.86995400	6.47989100
	C	8.54693300	0.90751700	7.25306700	C	8.40275000	1.27818200	7.44798900
	C	8.58311800	-1.60959100	7.95034900	C	8.21453100	-1.29384900	8.02909700
	C	11.05044900	-1.36525100	8.77373300	C	10.81912600	-1.38473900	8.55163600
	C	9.97925600	0.92278000	9.43742800	C	9.77706700	0.79922100	9.65540900
	H	10.63461600	1.39873200	3.97422000	H	12.06318900	-1.95003600	5.28365200
	H	12.89085800	2.04670700	5.80666300	H	13.57190600	0.07040200	6.86156400
	H	13.64424400	-0.83218500	5.89481400	H	11.21350600	1.86433000	6.84417200
	H	11.37967300	-1.48187900	4.07374200	H	9.69138100	-0.17364100	5.25216600
$Ru(CO)_4$	Ru	9.74268300	-0.23863700	8.08228500	Ru	9.42757100	-0.05648100	8.18160500
	Si	11.11653300	0.05914900	6.27897000	Si	12.34139800	0.65501800	4.47196800
	O	7.43147000	1.78289100	8.11125500	O	7.39334300	2.08181600	7.33035500
	O	7.95385400	-2.19976900	6.53318600	O	7.27808800	-2.17033400	8.07710200
	O	10.67749900	-2.56012500	9.86137600	O	11.58488200	-2.16448900	8.87495700
	O	11.40105100	1.69372900	9.80311100	O	9.87000100	1.38364800	10.79462700
	C	12.15470900	1.29515700	5.11422300	C	12.66630800	0.02084800	6.35623300
	C	11.31913000	0.39963000	4.32847600	C	11.92255900	-0.96821500	5.58856000
	C	12.12912300	-0.73452800	4.76012700	C	10.77266500	-0.08102900	5.55712600
	C	12.96465400	0.16104900	5.54555400	C	11.51813800	0.91009000	6.32549000
	C	8.29323500	1.04463000	8.08211100	C	8.13409800	1.29199500	7.65486500
	C	8.60993700	-1.47832400	7.10656000	C	8.11623700	-1.40562400	7.96871500
	C	10.34853100	-1.70560900	9.19046300	C	10.78619500	-1.40249900	8.64293600
	C	10.78813400	0.98196200	9.17270200	C	9.81756700	0.92595900	9.75208800
	H	10.48482400	0.52776500	3.66189900	H	12.10654700	-1.98030000	5.27482000
	H	12.19323100	2.35887600	5.26872900	H	13.62539700	0.03933400	6.84246700
	H	13.84623500	0.04319100	6.15034100	H	11.32372300	1.90755300	6.68149700
	H	12.13834900	-1.78795400	4.54320600	H	9.79720100	-0.12258000	5.10287200
$Os(CO)_4$	Os	9.74284500	-0.23944100	8.08195600	Os	9.43241800	-0.07692200	8.20608800
	Si	11.12240300	0.05887300	6.27363500	Si	12.30956800	0.67360500	4.47406200
	O	7.64607100	1.99051800	7.69060900	O	7.49749600	2.10325400	7.18827600
	O	7.66075600	-2.21403400	6.94479100	O	7.26001000	-2.17948600	8.14836600
	O	11.04212400	-2.64151100	9.51878100	O	11.64194400	-2.15734400	8.83176700
	O	11.08928700	1.57580600	10.18409300	O	9.82648300	1.35540900	10.83964800
	C	12.14059500	1.29822000	5.10463700	C	12.65377100	0.03990300	6.35186600
	C	11.31847500	0.38045100	4.32529200	C	11.91840300	-0.95716400	5.58516000
	C	12.14409500	-0.73635100	4.76967000	C	10.75403700	-0.08869100	5.56770400
	C	12.96610000	0.18152600	5.54897800	C	11.49187500	0.91189900	6.33686800
	C	8.42874800	1.17726000	7.81446000	C	8.18751300	1.29885000	7.58667800
	C	8.43726300	-1.48796200	7.34279500	C	8.10485700	-1.41795700	8.03327700
	C	10.58124900	-1.75879800	8.97314500	C	10.81726100	-1.40958100	8.63590000
	C	10.61013000	0.91420800	9.39589800	C	9.78411200	0.89468900	9.79422400
	H	10.48341000	0.48928900	3.65624400	H	12.11219100	-1.96814600	5.27396600
	H	12.16206300	2.36384200	5.24890200	H	13.61226700	0.06599600	6.83878200
	H	13.84813600	0.08296100	6.15653400	H	11.29468100	1.91307800	6.68154400
	H	12.16943100	-1.79177300	4.56415400	H	9.78303100	-0.13668200	5.10410600

$Ge[C_4H_4]$	Apical				Basal			
	C	-0.02638200	1.02817500	-0.45634300	C	0.03818500	-1.02991900	0.24185400
	C	-1.02447300	-0.02951500	-0.46331200	C	-1.03813500	-0.05081300	0.20301000
	C	1.03153300	0.02981900	-0.44953800	C	1.01657900	0.04745600	0.29511800
HF	C	0.03295500	-1.02787900	-0.45650400	C	-0.06083700	1.02677800	0.25617000
	H	-0.05689000	2.10088300	-0.52920700	H	0.08667600	-2.10274100	0.30423900
	H	-2.09677300	-0.06049200	-0.54194900	H	-2.11236000	-0.10268700	0.22526300
	H	2.10458500	0.06082900	-0.51674100	H	2.08475400	0.09809600	0.41236500

	H	0.06443400	-2.10055100	-0.52949500	H	-0.11563800	2.09832600	0.33361800
	F	-0.10127400	-0.00463800	4.91711700	F	08096700	-0.00536600	3.31773100
	H	-0.07349700	-0.00333800	3.99411600	H	-0.04408100	-0.00184600	2.39354000
	Ge	-0.00717600	-0.00027400	1.39630800	Ge	0.07286600	0.01573600	-1.61845400
	C	0.06016200	-1.01206300	0.38257100	C	0.04920400	-0.91813600	0.29765400
	C	-1.05617800	-0.08111800	0.35037100	C	-1.02482300	0.05463000	0.16450700
	C	0.99004800	0.10473800	0.42795300	C	1.02982600	0.15481100	0.21463400
	C	-0.12621600	1.03544200	0.39687300	C	-0.04513700	1.12600600	0.08182300
	H	0.15543700	-2.08162400	0.44540300	H	0.09623100	-1.97803200	0.47626600
HCl	H	-2.12672100	-0.17962700	0.38452400	H	-2.09870600	0.01030400	0.20961000
	H	2.05513700	0.20130400	0.54291900	H	2.09983100	0.21459600	0.30902400
	H	-0.22676700	2.10335400	0.47698300	H	-0.09667300	2.19974900	0.04229600
	Cl	0.10315200	0.16379500	-5.54532200	Cl	-0.09432900	0.48245300	3.72086700
	H	0.08219000	0.12177700	-4.26479700	H	-0.00289700	0.25225700	2.46206100
	Ge	0.03582300	0.03036900	-1.46925300	Ge	0.05811400	-0.09022000	-1.66998900
	C	0.08731900	-1.03803400	0.35202000	C	0.06539100	-1.02996000	0.17286800
	C	-1.03201200	-0.11178200	0.41201100	C	-1.00719600	-0.04995700	0.17271400
	C	1.01478800	0.08104000	0.39215100	C	1.04756000	0.04451900	0.19142700
	C	-0.10433000	1.00652900	0.45211000	C	-0.02944600	1.02513500	0.18859500
	H	0.18844100	-2.10865000	0.37420200	H	0.11304900	-2.10271500	0.23712500
HBr	H	-2.09929800	-0.21619000	0.49534700	H	-2.07944900	-0.10013000	0.24134900
	H	2.08423500	0.17810800	0.45394300	H	2.12032600	0.09329100	0.26010700
	H	-0.20335900	2.07051600	0.57504100	H	-0.08083400	2.09675300	0.26815300
	H	-0.05684700	0.30643000	-4.28039000	Br	-0.07171500	-0.04393000	3.86168400
	Br	-0.05799200	0.32392600	-5.70602300	H	0.28855500	0.04096000	2.4831800
	Ge	-0.03513900	0.06995900	-1.45749100	Ge	0.0	0.01325200	-1.68955700
FCl	C	-0.02935200	1.02598600	-0.47240700	C	0.88712900	0.32539300	0.35990300
	C	-1.02763700	-0.03150300	-0.45885800	C	-0.05036500	-0.79474200	0.36372200
	C	1.02825000	0.02793400	-0.45185700	C	-0.19338100	1.22275700	-0.00996700
	C	0.02995900	-1.02963300	-0.43831300	C	-1.12527400	0.10923300	-0.00584000
	H	-0.06006400	2.09744600	-0.56190900	H	1.92882100	0.44761500	0.60032400
	H	-2.10011800	-0.06376200	-0.53444800	H	0.01332300	-1.84038000	0.60949000
	H	2.10129100	0.05778400	-0.52014700	H	-0.28559700	2.28812900	-0.12457000
	H	0.06122700	-2.10342900	-0.49268100	H	-2.19063600	0.01173800	-0.11611800
	F	-0.02512200	0.10593900	6.08313100	F	0.18933100	-0.01861100	4.79829500
	Cl	-0.01922700	0.07955700	4.45226700	Cl	0.30679000	-0.12080000	3.17727300
	Ge	-0.00683600	0.02844500	1.39870400	Ge	0.24174100	-0.09396300	-1.63394400
FBr	C	-0.03058900	1.02877700	-0.43728000	C	0.91047800	-0.11879200	0.35309700
	C	-1.02911800	-0.03189800	-0.42798500	C	-0.07597600	-1.11051500	-0.03722300
	C	1.03021100	0.03043200	-0.42256700	C	-0.12861500	0.91165000	0.34029700
	C	0.03167400	-1.03041800	-0.41327000	C	-1.10686600	-0.08779500	-0.05181400
	H	-0.06278700	2.10042800	-0.52335700	H	1.95717400	-0.14385300	0.60227800
	H	-2.10143300	-0.06540000	-0.50475800	H	-0.06844900	-2.18023500	-0.14777700
	H	2.10297700	0.06190600	-0.49371200	H	-0.16422200	1.96271100	0.56935400
	H	0.06438300	-2.10372300	-0.47512300	H	-2.17486300	-0.08942600	-0.17816300
	F	-0.01455700	0.06006100	6.03525900	F	0.25242600	0.34606700	4.98081600
	Br	-0.01174200	0.04844600	4.24272000	Br	0.30777000	0.38625900	3.21483500
	Ge	-0.00483600	0.01965600	1.41254100	Ge	0.26532600	0.24219500	-1.65323100
FI	C	0.02692200	-1.04947000	0.33964600	C	0.93110700	-0.12237900	0.29949500
	C	-1.02411000	-0.04095200	0.31102300	C	-0.07652200	-1.10525000	-0.05770200
	C	1.03541900	0.00769000	0.38855700	C	-0.09752500	0.92060800	0.30666800
	C	-0.02219800	1.01143800	0.35949300	C	-1.09634000	-0.07138800	-0.05657900
	H	0.04870600	-2.12194400	0.41705300	H	1.98513800	-0.15681500	0.51502300
	H	-2.09951800	-0.06630800	0.32479000	H	-0.08430500	-2.17646800	-0.15247200
	H	2.10215100	0.03227700	0.52295600	H	-0.11263900	1.97857600	0.50615400
	H	-0.05078900	2.08443600	0.43033300	H	-2.16766000	-0.06412900	-0.14978300
	F	-0.19535800	0.34165400	-6.30822000	F	0.17256000	0.28821700	5.19502500
	I	-0.06429700	0.19079000	-4.37261700	I	0.28408700	0.39849400	3.28046400
	Ge	0.09249900	-0.01168100	-1.47873200	Ge	0.23628200	0.22879900	-1.69382500
	Fe	9.68957600	-0.23385700	8.15620400	Fe	9.53174300	-0.07964900	8.10264100
	Ge	11.12769700	0.11938800	6.27266800	Ge	12.20630800	0.77547100	4.46268200
	O	7.86404400	1.91089800	7.12507600	O	7.75063200	2.09182800	7.02623900
	O	7.50056300	-2.19629400	8.00175200	O	7.34787400	-2.03210200	8.15601800
	O	11.56269700	-2.36783600	9.12125800	O	11.60421400	-2.16397800	8.78656100
	O	10.09448600	1.27921700	10.64940900	O	9.80102500	1.24363200	10.70300000
$Fe(CO)_4$	C	12.39894200	1.27264900	5.07810400	C	12.59906500	0.04864300	6.40480900
	C	11.42162900	0.57155500	4.24398900	C	11.86070200	-0.94700200	5.63087300
	C	12.05827500	-0.69593000	4.56251700	C	10.66637000	-0.11569200	5.70144400
	C	13.03249800	-0.00148900	5.39666000	C	11.40496000	0.87964400	6.47506700
	C	8.55164400	1.10366000	7.51387100	C	8.40276800	1.27295100	7.45031300
	C	8.35977200	-1.45324600	8.00345100	C	8.21215400	-1.30120900	8.03325400
	C	10.85659200	-1.56427900	8.75870000	C	10.81921500	-1.39055800	8.54776900
	C	9.98648400	0.72576500	9.66334000	C	9.77798500	0.78954300	9.65923900

	H	10.62991600	0.87927400	3.58401900	H	12.05510800	-1.95893100	5.32317800
	H	12.62989300	2.30495600	5.27141600	H	13.55632300	0.06518700	6.89456400
	H	13.91525600	-0.29481800	5.93689700	H	11.20168400	1.86644300	6.85527800
	H	11.91321600	-1.71652900	4.25524100	H	9.68378700	-0.17951200	5.26535200
$Ru(CO)_4$	Ru	9.66138800	-0.25367000	8.18509500	Ru	9.42812200	-0.05779800	8.18047400
	Ge	11.14664600	0.06770800	6.21291000	Ge	12.39856600	0.69636100	4.37113900
	O	7.66110400	1.91735600	7.32010100	O	7.39789600	2.08026300	7.31645600
	O	7.44919500	-2.31882900	7.78373600	O	7.27962600	-2.17226000	8.06962500
	O	11.39342100	-2.48321300	9.40511400	O	11.57981200	-2.16637100	8.88437900
	O	10.37000500	1.48564100	10.59216900	O	9.86413900	1.38437900	10.79368400
	C	12.41124300	1.28603500	5.05297900	C	12.66559900	0.01540400	6.36333500
	C	11.45590900	0.58333800	4.20090400	C	11.91643200	-0.96990100	5.59327300
	C	12.11561200	-0.68043000	4.50449200	C	10.77168600	-0.07265100	5.55766400
	C	13.06895400	0.02350100	5.35679200	C	11.52210300	0.91400900	6.32746500
	C	8.40456400	1.12282800	7.62619300	C	8.13676500	1.29093100	7.64620500
	C	8.29480300	-1.56397800	7.86349400	C	8.11787400	-1.40725100	7.96388300
	C	10.76594100	-1.66295200	8.94548800	C	10.78304800	-1.40351500	8.64812300
	C	10.16297800	0.86939400	9.66023200	C	9.81432600	0.92614400	9.75124700
	H	10.66604600	0.88619900	3.53665100	H	12.08237600	-1.99404400	5.30984100
	H	12.60568000	2.31827400	5.28422600	H	13.60913700	0.01402200	6.87956900
	H	13.95058700	-0.26038100	5.90376800	H	11.32525800	1.90386900	6.70297900
	H	12.00910400	-1.69373600	4.16022800	H	9.78915400	-0.11688000	5.11894300
$Os(CO)_4$	Os	9.67475800	-0.23923400	8.17297400	Os	9.43159200	-0.07501000	8.20153200
	Ge	11.14478600	0.12442300	6.24933900	Ge	12.36677300	0.71018200	4.37508200
	O	7.63258400	1.92270000	7.33162000	O	7.50605100	2.10627100	7.16671600
	O	7.51174000	-2.35017800	7.65681300	O	7.25581800	-2.17433700	8.14459000
	O	11.43144100	-2.47237400	9.38810400	O	11.63335700	-2.15758400	8.84320000
	O	10.39005000	1.50785700	10.58915000	O	9.82036300	1.36553600	10.83151700
	C	12.40975400	1.27816200	5.06820100	C	12.65463400	0.03062300	6.36167600
	C	11.43432500	0.57720200	4.22774500	C	11.91473200	-0.96378800	5.59304100
	C	12.07486100	-0.69085800	4.54199900	C	10.75415600	-0.08626900	5.57183600
	C	13.04642200	0.00056600	5.38117700	C	11.49620700	0.91080300	6.34161400
	C	8.39107500	1.13495200	7.62461300	C	8.19202100	1.30168700	7.57161100
	C	8.33590600	-1.57556800	7.78848000	C	8.10221100	-1.41445700	8.02950200
	C	10.79961300	-1.65259800	8.92926400	C	10.81101400	-1.40861700	8.64146700
	C	10.17313800	0.88649300	9.65992800	C	9.78005700	0.90124000	9.78752500
	H	10.64381900	0.88640200	3.56717000	H	12.09110300	-1.98725600	5.31368900
	H	12.64482800	2.31006900	5.25810700	H	13.59789400	0.03769200	6.87826600
	H	13.92810700	-0.29322500	5.92275400	H	11.29713400	1.90556800	6.70352800
	H	11.92597600	-1.71170700	4.23713200	H	9.77680200	-0.13757300	5.12189100

$Sn[C_4H_4]$	Apical				Basal			
	C	-0.02536300	1.02967900	-0.52840500	C	0.06288200	-1.14652900	0.24478900
	C	-1.02475900	-0.02949700	-0.53713700	C	-0.99668700	-0.14821200	0.23835800
	C	1.03412700	0.02989800	-0.51991000	C	1.06372600	-0.08733300	0.27336300
	C	0.03403700	-1.02928300	-0.52864100	C	0.00107000	0.91402400	0.26701700
	H	-0.05525000	2.09781700	-0.65625900	H	0.09173500	-2.21527500	0.36751900
HF	H	-2.09204100	-0.06034400	-0.67185100	H	-2.06607500	-0.18231000	0.35399100
	H	2.10300500	0.06080500	-0.64104700	H	2.13248200	-0.05809300	0.39998500
	H	0.06590300	-2.09734700	-0.65664200	H	-0.03404400	1.98348500	0.38610400
	F	-0.10295300	-0.00472600	5.23921300	F	0.17049900	0.05837800	3.31065800
	H	-0.07955400	-0.00359500	4.31700300	H	0.22810900	0.11578900	2.38815300
	Sn	-0.01011000	-0.00038800	1.54812900	Sn	0.06534600	-0.09600300	-1.83988300
	C	0.08846400	-1.04285000	0.42360700	C	0.08647700	-0.91514100	0.29906200
	C	-1.03270000	-0.11445800	0.46663500	C	-0.98286100	0.07072700	0.23895800
	C	1.01715000	0.07776300	0.46296200	C	1.07566200	0.14772100	0.19962100
	C	-0.10346700	1.00533800	0.50597100	C	0.00615500	1.13711700	0.14144400
	H	0.18880500	-2.11068400	0.51189600	H	0.13063100	-1.96678100	0.52295700
HCl	H	-2.09578900	-0.21925200	0.59719700	H	-2.04991900	0.03831600	0.37738500
	H	2.08199700	0.17267100	0.58675400	H	2.14511100	0.19610300	0.30970600
	H	-0.20247800	2.06404100	0.67210700	H	-0.03468000	2.21310900	0.15375900
	Cl	-0.10231800	0.39304000	-5.86662300	Cl	0.08731300	0.42913600	3.69903400
	H	-0.03303300	0.26717500	-4.59479100	H	-0.00438000	0.63715500	2.43408700
	Sn	-0.02056400	0.06076200	-1.61829000	Sn	0.01563500	-0.05854200	-1.87036200
	C	0.08815400	-1.02653000	0.33508500	C	0.10532100	-0.99701100	0.22586700
	C	-1.03183300	-0.10749500	0.46839700	C	-0.96875200	-0.01553000	0.21941100
	C	1.01797000	0.08352200	0.47916600	C	1.08890800	0.07628900	0.18542500
	C	-0.10257300	1.00443600	0.61275600	C	0.01200400	1.06033900	0.17878100
	H	0.18819000	-2.09781800	0.31008700	H	0.15476100	-2.06050600	0.38336700
HBr	H	-2.09507500	-0.22375000	0.58755500	H	-2.03330200	-0.06108200	0.37079900
	H	2.08282700	0.16502100	0.61187400	H	2.16045700	0.12553500	0.27776800
	H	-0.20047300	2.03979200	0.88939300	H	-0.03598600	2.13240700	0.26537900
	H	-0.06866300	0.30842400	-4.61231600	Br	0.14612800	0.14951700	3.85690700
	Br	-0.07088300	0.13937700	-6.02668000	H	0.33976800	0.34311200	2.45419400

	Sn	-0.02183600	0.27687400	-1.59239700	Sn	0.02493800	-0.01995100	-1.89384500
FCl	C	-0.02915000	1.02639700	-0.54036300	C	0.89260500	0.02338400	0.41469400
	C	-1.02895100	-0.03288700	-0.52871400	C	-0.09456000	-1.02613700	0.18718800
	C	1.03013300	0.02664200	-0.52143000	C	-0.13225000	1.03474200	0.17744200
	C	0.03026200	-1.03253800	-0.50973100	C	-1.11797800	-0.01511900	-0.01998400
	H	-0.05954500	2.09250600	-0.68395200	H	1.94055900	0.04346800	0.66575600
	H	-2.09665300	-0.06570600	-0.65935400	H	-0.10619000	-2.09323400	0.32571700
	H	2.09877400	0.05569500	-0.64507700	H	-0.18392100	2.10176200	0.30709200
	H	0.06162700	-2.10255000	-0.62039000	H	-2.19182200	-0.03446400	-0.08788300
	F	-0.02656600	0.11302400	6.39334900	F	0.19937100	0.04305800	4.75166000
	Cl	-0.02024500	0.08569500	4.76552800	Cl	0.45677600	0.03794100	3.13725700
	Sn	-0.00731400	0.02848600	1.55361700	Sn	0.31159300	0.00286600	-1.86647200
FBr	C	-0.03027500	1.02771600	-0.53955200	C	0.87408500	0.02637800	0.43272000
	C	-1.02940600	-0.03310900	-0.52836300	C	-0.10100300	-1.02768500	0.16408600
	C	1.03104700	0.02913200	-0.52249000	C	-0.14726600	1.03467800	0.15577900
	C	0.03187900	-1.03258200	-0.51124500	C	-1.12151500	-0.01994400	-0.06555500
	H	-0.06215500	2.09429400	-0.67932700	H	1.93027300	0.04988000	0.65182600
	H	-2.09700300	-0.06720700	-0.65939100	H	-0.11437200	-2.09481800	0.30211700
	H	2.09942300	0.05968000	-0.64791000	H	-0.20901100	2.10030300	0.29224100
	H	0.06458300	-2.10185800	-0.62800600	H	-2.19432100	-0.04565400	-0.14824300
	F	-0.01543600	0.06529000	6.46887700	F	0.22487500	0.04699700	4.92171400
	Br	-0.01298800	0.05494300	4.69572800	Br	0.47947900	0.03892300	3.16122400
	Sn	-0.00548700	0.02196700	1.54414800	Sn	0.35295800	0.00921000	-1.87544100
FI	C	0.00576400	-1.06151600	0.51037500	C	0.85675200	0.01717400	0.43328800
	C	-0.98496100	-0.05897600	0.15881000	C	-0.11555400	-1.03180000	0.12306200
	C	1.04188300	0.02111900	0.53577700	C	-0.15270500	1.03206500	0.12584600
	C	0.00552900	0.97544700	0.18331200	C	-1.12377100	-0.01703700	-0.12521000
	H	-0.04176500	-2.04663700	0.94007600	H	1.91725400	0.03539800	0.63668600
	H	-2.04372200	-0.08917700	-0.03985300	H	-0.14089700	-2.09887200	0.25990000
	H	2.01424500	0.10057400	0.98914900	H	-0.21466300	2.09774900	0.26222500
	H	-0.00574100	2.03891300	0.00910800	H	-2.19472600	-0.03604800	-0.23107000
	F	-0.58806900	0.76474900	-6.28749700	F	0.25363800	0.05778000	5.16100800
	I	-0.12384100	0.24960900	-4.46318700	I	0.48548500	0.05091000	3.24093600
	Sn	0.57010400	-0.51617600	-1.60178500	Sn	0.40337000	0.01094900	-1.89420200
$Fe(CO)_4$	Fe	9.37844800	-0.13880300	8.61815400	Fe	9.55629100	-0.07265700	8.07754800
	Sn	10.62359400	0.55626800	6.47581200	Sn	12.33803800	0.81152800	4.28775800
	O	7.30003300	-1.50374000	6.94011400	O	7.76326400	2.09162200	7.01292100
	O	10.03682900	-2.69777800	9.90968800	O	7.37435500	-2.02800700	8.13029900
	O	11.48079900	1.24336100	10.25174700	O	11.61368700	-2.16029800	8.78839200
	O	7.30289900	1.55630500	9.83209300	O	9.81616500	1.24870200	10.68020000
	C	12.33293100	1.19047200	5.19384700	C	12.57873600	0.04903600	6.42889100
	C	11.31523200	0.46055900	4.35864700	C	11.83270900	-0.95403900	5.64719400
	C	11.85657000	-0.79475100	4.87478700	C	10.63909400	-0.11190300	5.72885100
	C	12.81492300	-0.10766500	5.66118200	C	11.37309900	0.87465300	6.49747600
	C	8.08539600	-0.98737900	7.56682800	C	8.42050100	1.27440400	7.43367200
	C	9.82655600	-1.72285100	9.36658900	C	8.23753800	-1.29398700	8.01394900
	C	10.69138400	0.72502700	9.63177900	C	10.83532000	-1.38394300	8.53675700
	C	8.11176600	0.94938400	9.31416600	C	9.79193900	0.79171700	9.63715700
	H	10.79157200	0.72797700	3.45744200	H	11.98372500	-2.00320200	5.46034200
	H	12.79001400	2.15962500	5.09525500	H	13.47637400	0.00299500	7.02098900
	H	13.56680300	-0.41059200	6.37259500	H	11.18107200	1.87961500	6.83899900
	H	11.58497700	-1.83077700	4.74815300	H	9.67000900	-0.15152700	5.25688700
$Ru(CO)_4$	Ru	9.26397800	-0.40622700	8.43248700	Ru	9.44061100	-0.05749800	8.16355800
	Sn	10.21997800	0.11141000	5.96988800	Sn	12.49958200	0.76040600	4.19400300
	O	6.30313000	-0.55764900	7.59111600	O	7.41725400	2.07563100	7.27777400
	O	9.13329500	-3.35050800	9.20676100	O	7.28512200	-2.16511000	8.09404200
	O	12.12363800	-0.31055700	9.55011500	O	11.59807500	-2.15656500	8.87644700
	O	8.59594600	2.03626700	10.12702400	O	9.85007100	1.38258600	10.78095000
	C	11.69619400	1.26108300	4.71377700	C	12.66140900	0.00553700	6.36931900
	C	11.86979100	-0.21905700	4.47149000	C	11.89385500	-0.97258600	5.59322600
	C	12.59895600	-0.29694300	5.72042500	C	10.75411400	-0.06277300	5.58475500
	C	12.43446700	1.10473100	5.94964000	C	11.51707800	0.90878600	6.35279700
	C	7.39363000	-0.49885100	7.88307200	C	8.15328600	1.28702700	7.61742500
	C	9.20743400	-2.27755300	8.83843100	C	8.12601200	-1.40417500	7.97359600
	C	11.07295300	-0.34454600	9.13221300	C	10.79755700	-1.39791400	8.63838000
	C	8.86222700	1.17927400	9.42909000	C	9.80975400	0.92420900	9.73740000
	H	11.84244900	-0.82304200	3.58150700	H	12.01542000	-2.02102800	5.38350800
	H	11.49922300	2.09171700	4.05891200	H	13.56485100	-0.04642300	6.95169500
	H	12.71712700	1.77891600	6.74239500	H	11.32969900	1.89713200	6.74008700
	H	13.05631100	-1.10382400	6.27053600	H	9.76816900	-0.09253100	5.14931800
$Os(CO)_4$	Os	9.36375100	-0.12245100	8.61881500	Os	9.37796100	-0.10808700	8.08571200
	Sn	10.57582900	0.65898300	6.43890800	Sn	12.44505000	0.75864000	4.21072400
	O	7.16237700	-1.57277500	7.00525700	O	6.98476900	1.46780500	6.93435600

	O	10.25529900	-2.82940100	9.72651000	O	7.69588400	-2.62433400	8.19486500
	O	11.48277500	1.24213000	10.40768400	O	11.86887900	-1.64518100	9.09260800
	O	7.23156800	1.74327900	9.78289500	O	9.41696900	1.68849200	10.52369800
	C	12.33164200	1.18759900	5.21448900	C	12.67737500	-0.41460300	6.20669100
	C	11.30281700	0.43783100	4.36765000	C	11.42797700	-0.82122000	5.58523200
	C	11.87659000	-0.80385200	4.88198800	C	10.82586100	0.46258800	5.96287100
	C	12.82133500	-0.11576200	5.65968100	C	12.11740500	0.89150400	6.51170100
	C	7.97298500	-1.03604000	7.58581100	C	7.85773200	0.88741900	7.36464900
	C	9.96536500	-1.82837700	9.26654300	C	8.36552000	-1.71092900	8.02994400
	C	10.71104700	0.74796100	9.74251700	C	10.94870600	-1.08827800	8.74069800
	C	8.03397900	1.09486100	9.30010800	C	9.48607600	1.09728100	9.54615200
	H	10.83772100	0.69431900	3.43112300	H	11.03449400	-1.75942800	5.23385400
	H	12.81840100	2.13509300	5.05787700	H	13.55350700	-0.94644800	6.53780900
	H	13.55209900	-0.41722300	6.39473900	H	12.43602900	1.72220500	7.11747400
	H	11.59514800	-1.84153400	4.78628300	H	9.96172300	1.00728700	5.59924400

$Pb[C_4H_4]$	Basal			
HF	C	0.05759700	-1.14929300	0.24234100
	C	-1.00009700	-0.15039300	0.24127900
	C	1.05864600	-0.09211900	0.28045500
	C	-0.00195100	0.90946200	0.27939700
	H	0.08469700	-2.21751600	0.37214500
	H	-2.06827500	-0.18433400	0.36984300
	H	2.12646300	-0.06523100	0.41791700
	H	-0.03638500	1.97721400	0.41566900
	F	0.19887300	0.06207200	3.31467500
	H	0.25280600	0.11805900	2.39120400
	Pb	0.06466900	-0.08500300	-1.94137100
HCl	C	0.08145800	-1.03371300	0.19401200
	C	-0.99362300	-0.05382100	0.20549500
	C	1.06271200	0.04228000	0.21586200
	C	-0.01500800	1.02269700	0.22517300
	H	0.12967900	-2.10205100	0.31823500
	H	-2.05902600	-0.10626800	0.35027500
	H	2.13196700	0.09021300	0.33602700
	H	-0.06705800	2.08804200	0.37265400
	Cl	0.10413100	-0.03692800	3.71670600
	H	0.30768700	0.04723500	2.45031200
	Pb	0.03772500	0.02623400	-1.99300100
HBr	C	0.08095500	-0.99469100	0.21627400
	C	-0.99091000	-0.01233500	0.19904600
	C	1.06561100	0.07656300	0.19395500
	C	-0.00880000	1.06139500	0.17682600
	H	0.12675800	-2.05690800	0.38489600
	H	-2.05588200	-0.05667500	0.34978400
	H	2.13507100	0.12392700	0.31180300
	H	-0.05650100	2.13272200	0.27620100
	Br	0.10461300	0.17347700	3.84255400
	H	0.29875400	0.36849700	2.43899600
	Pb	0.02907600	-0.01395100	-2.00668200
FCl	C	0.87948900	0.02415800	0.43627700
	C	-0.10272900	-1.02566500	0.19489200
	C	-0.14196000	1.03363800	0.18401800
	C	-1.12387800	-0.01623400	-0.02230400
	H	1.92789000	0.04514000	0.68762500
	H	-0.11805100	-2.09116400	0.34675600
	H	-0.19904000	2.09892700	0.32728400
	H	-2.19854400	-0.03695100	-0.08047500
	F	0.23243200	0.04624100	4.74981300
	Cl	0.47587500	0.03782300	3.12796000
	Pb	0.34269800	0.00235400	-1.95937700
FBr	C	0.83601500	0.02800800	0.51783700
	C	-0.12064500	-1.02760600	0.17603700
	C	-0.17028500	1.03470300	0.17233700
	C	-1.12921700	-0.02020800	-0.08112900
	H	1.90227000	0.05382900	0.69299400
	H	-0.15053600	-2.09124700	0.33816800
	H	-0.24944700	2.09726700	0.32494300
	H	-2.20075900	-0.04591400	-0.18557200
	F	0.28381600	0.03642000	4.87755600
	Br	0.51429800	0.04033500	3.09113800
	Pb	0.45867300	0.01268000	-1.93184000
FI	C	0.82446800	0.01746300	0.49923200

	C	-0.13553000	-1.03142100	0.13948700
	C	-0.17168600	1.03183800	0.13472000
	C	-1.13222700	-0.01820400	-0.13217200
	H	1.89520700	0.03595700	0.65388700
	H	-0.17186400	-2.09660500	0.29038700
	H	-0.25034700	2.09374300	0.29234400
	H	-2.20258200	-0.03712700	-0.25008000
	F	0.31074300	0.06286500	5.13109600
	I	0.52278100	0.04537900	3.19260600
	Pb	0.48522100	0.01437900	-1.95903600
$Fe(CO)_4$	Fe	9.56437800	-0.07375300	8.07501800
	Pb	12.39072400	0.82983500	4.20401100
	O	7.78171900	2.09133700	6.99867800
	O	7.37896400	-2.02516000	8.12949700
	O	11.61248000	-2.16465500	8.80017900
	O	9.82328300	1.25379800	10.67459700
	C	12.56592000	0.04616600	6.43829200
	C	11.81888900	-0.95654000	5.65858800
	C	10.62635100	-0.11207300	5.74111700
	C	11.35968400	0.87199600	6.50647400
	C	8.43338500	1.27283400	7.42654000
	C	8.24370100	-1.29207600	8.01517200
	C	10.83794600	-1.38645500	8.54200600
	C	9.79765100	0.79230200	9.63317000
	H	11.96020200	-2.01173600	5.49683600
	H	13.45083800	-0.01160400	7.04913400
	H	11.17341100	1.88391200	6.83193400
	H	9.66239000	-0.14341900	5.25703900
$Ru(CO)_4$	Ru	9.45284900	-0.05937400	8.15896500
	Pb	12.53522100	0.79071800	4.11255800
	O	7.45741900	2.08782700	7.24808500
	O	7.27886000	-2.14726900	8.10499600
	O	11.59602200	-2.16979100	8.87899500
	O	9.84386200	1.37204700	10.78315600
	C	12.64851100	0.01802000	6.38072400
	C	11.89647100	-0.97359400	5.60710300
	C	10.74421600	-0.08043100	5.59504900
	C	11.49007700	0.90265000	6.36080100
	C	8.18189600	1.29297900	7.59931100
	C	8.12718600	-1.39462400	7.97967700
	C	10.79977200	-1.40694400	8.63931400
	C	9.81115400	0.91548500	9.73799700
	H	12.02476200	-2.02645700	5.42328700
	H	13.53954000	-0.02877300	6.98296900
	H	11.29242300	1.89528500	6.73318400
	H	9.76167600	-0.12304600	5.15211000
$Os(CO)_4$	Os	9.39204900	-0.10454700	8.07663600
	Pb	12.42011400	0.80742600	4.12944200
	O	7.00347900	1.45817400	6.90018500
	O	7.71173200	-2.62379400	8.19313000
	O	11.87729400	-1.63172400	9.10686300
	O	9.41587500	1.71204400	10.50225400
	C	12.66610400	-0.42334600	6.20781500
	C	11.41253000	-0.82974000	5.60514900
	C	10.80331800	0.44450500	6.01762800
	C	12.11354500	0.87753300	6.52964900
	C	7.87519500	0.88206400	7.34082400
	C	8.38059700	-1.70834300	8.03096900
	C	10.95683000	-1.07804000	8.74836000
	C	9.48779200	1.10922100	9.53112000
	H	11.01583500	-1.77152700	5.26596200
	H	13.54463600	-0.95837100	6.52966800
	H	12.43877500	1.69563900	7.14956500
	H	9.96621600	1.00753900	5.61306400