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

SUPPLEMENTARY INFORMATION

Influence of Monomer Deformation on the Competition Between Two Types of σ-Holes in Tetrel Bonds

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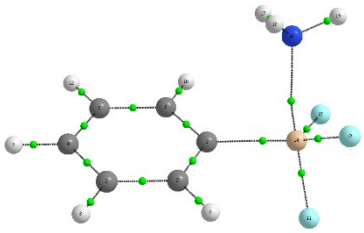
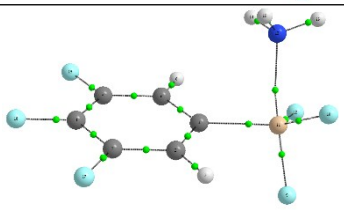
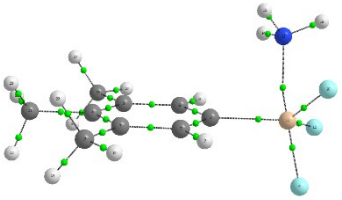
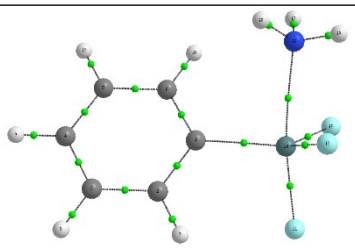
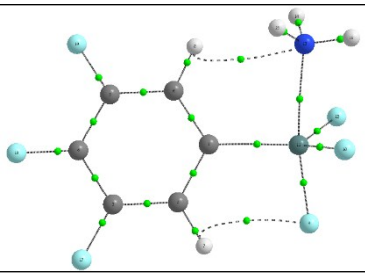
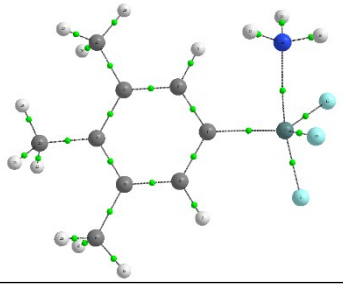
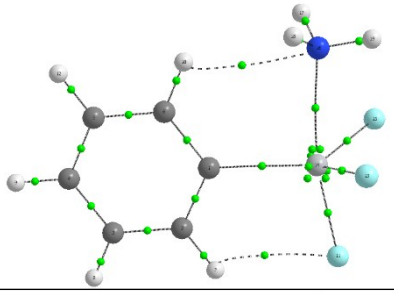
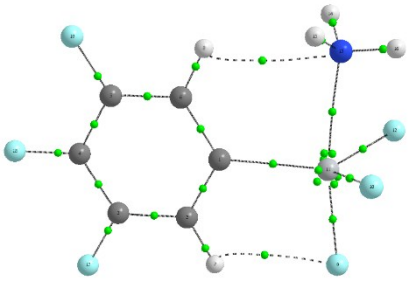
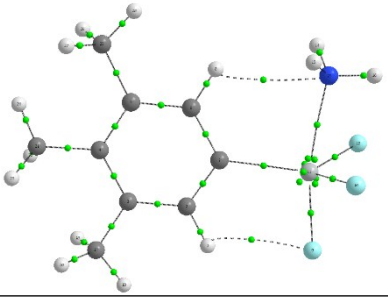
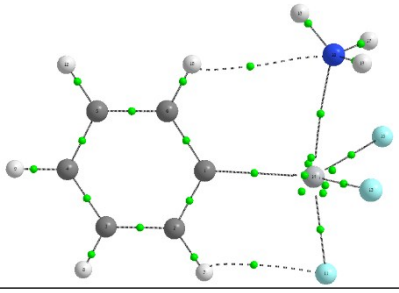
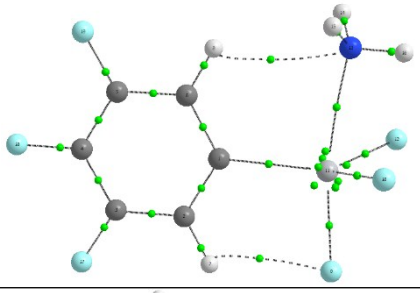
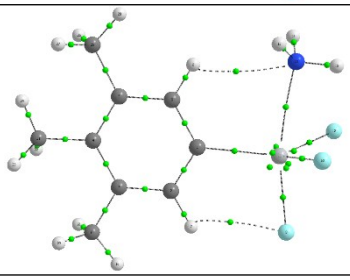
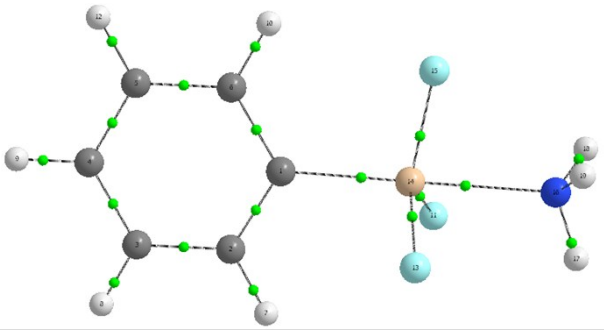
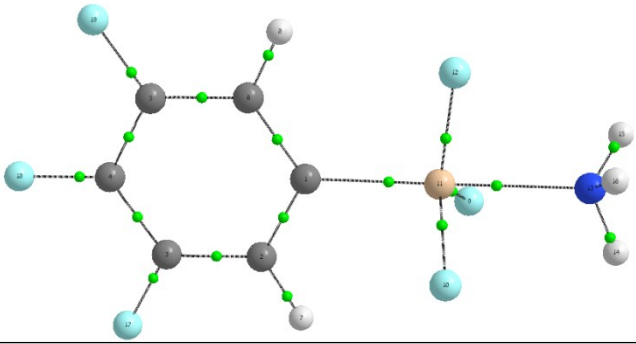
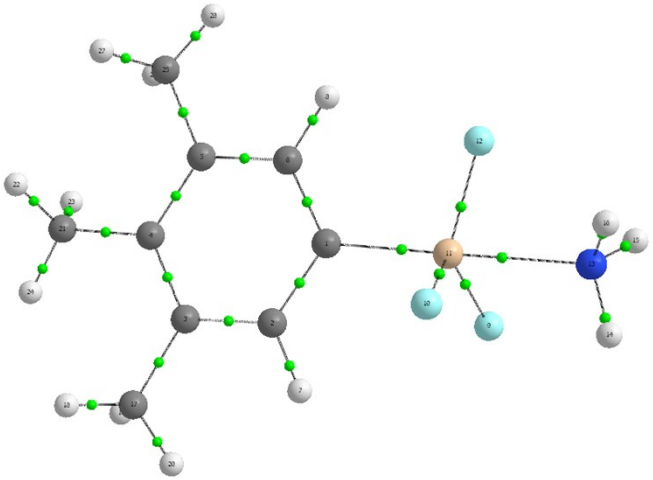
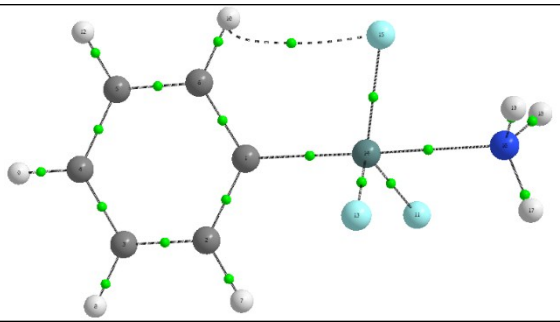
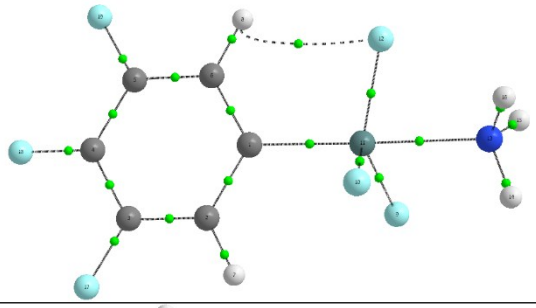
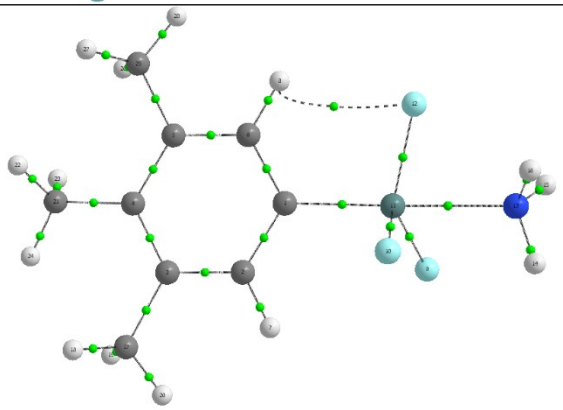
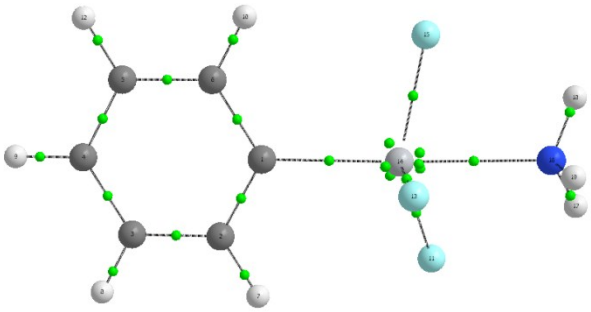
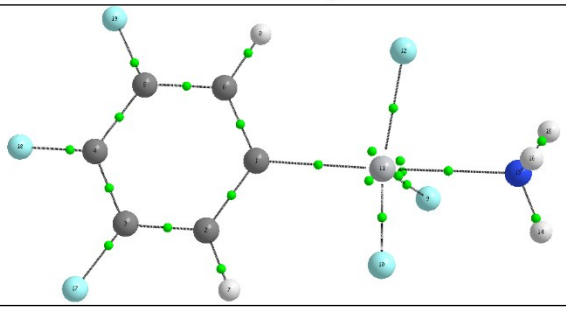
T-F σ-hole bonded complexes	
$SiF_3C_6H_5$	
$SiF_3C_6H_2F_3$	
$SiF_3C_6H_2(CH_3)_3$	
$GeF_3C_6H_5$	

$GeF_3C_6H_2F_3$	
$GeF_3C_6H_2(CH_3)_3$	
$SnF_3C_6H_5$	
$SnF_3C_6H_2F_3$	
$SnF_3C_6H_2(CH_3)_3$	
$PbF_3C_6H_5$	

$PbF_3C_6H_2F_3$	
$PbF_3C_6H_2(CH_3)_3$	
T-C σ-hole bonded complexes	
$SiF_3C_6H_5$	
$SiF_3C_6H_2F_3$	
$SiF_3C_6H_2(CH_3)_3$	

$GeF_3C_6H_5$	
$GeF_3C_6H_2F_3$	
$GeF_3C_6H_2(CH_3)_3$	
$SnF_3C_6H_5$	
$SnF_3C_6H_2F_3$	

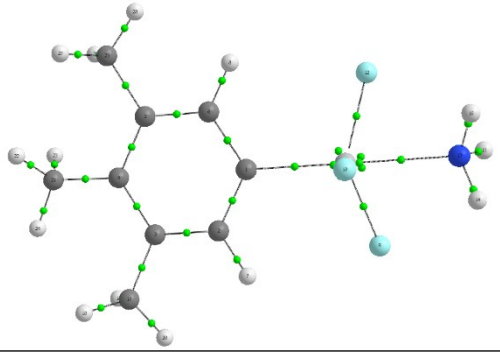
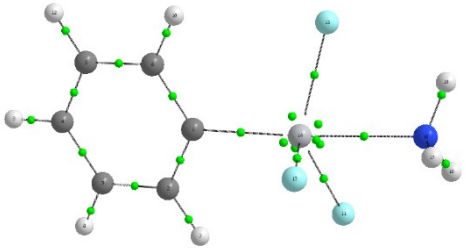
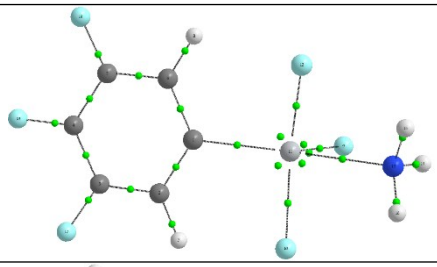
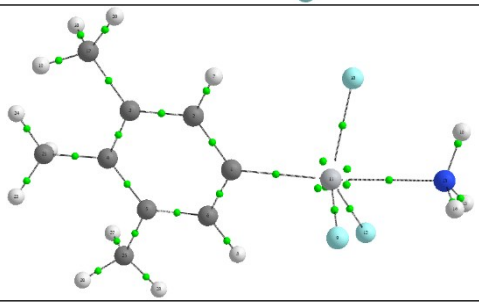
$SnF_3C_6H_2(CH_3)_3$	
$PbF_3C_6H_5$	
$PbF_3C_6H_2F_3$	
$PbF_3C_6H_2(CH_3)_3$	

Fig. S1. AIM molecular graphs of σ-hole tetrel bonded complexes with ammonia obtained at the MP2/aug-cc-pVDZ level. Small green dots represent bond critical points.

Table S1. AIM bond critical point (BCP) properties of the T···N interactions in systems studied: electron density ρ, Laplacian of electron density $\nabla^2\rho$, total electron energy (H) were obtained at the MP2/aug-cc-pVDZ level. Data given in atomic units.

		ρ	$\nabla^2\rho$	H
T-F σ-hole				
$GeF_3C_6H_2F_3$	N···H	0.010	0.041	0.002
	F···H	0.012	0.056	0.002
$SnF_3C_6H_5$	N···H	0.009	0.033	0.001
	F···H	0.010	0.042	0.001

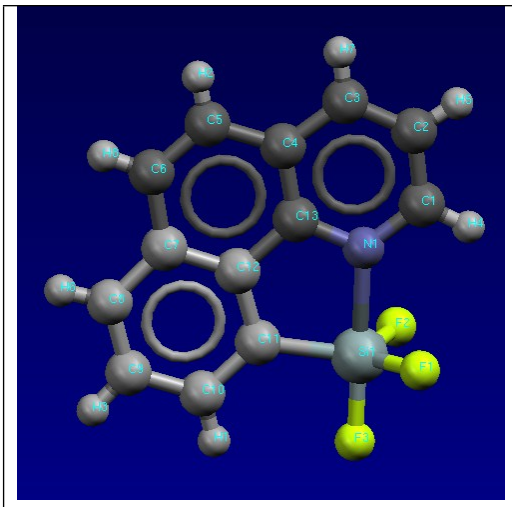
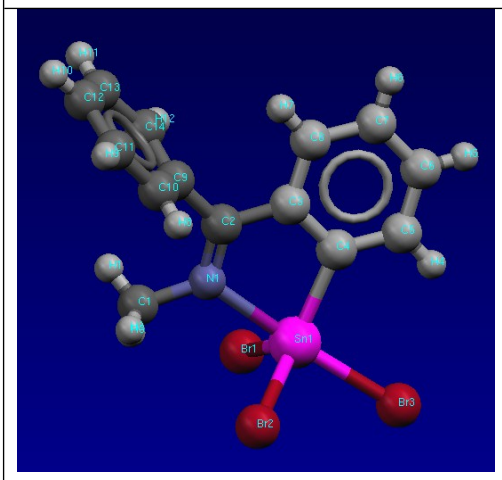
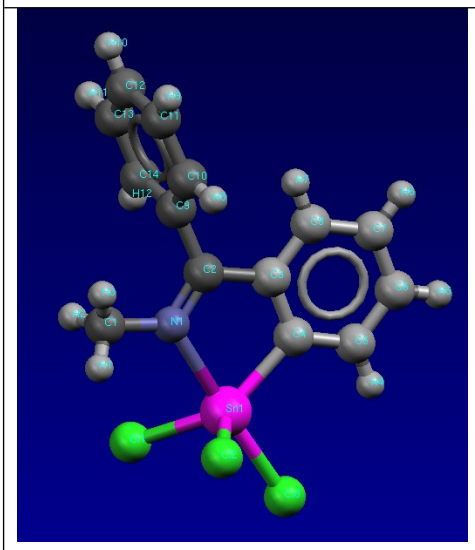
$SnF_3C_6H_2F_3$	N···H	0.009	0.032	0.001
	F···H	0.011	0.044	0.001
$SnF_3C_6H_2(CH_3)_3$	N···H	0.009	0.033	0.001
	F···H	0.010	0.041	0.001
$PbF_3C_6H_5$	N···H	0.007	0.025	0.001
	F···H	0.010	0.040	0.001
$PbF_3C_6H_2F_3$	N···H	0.008	0.026	0.001
	F···H	0.011	0.041	0.001
$PbF_3C_6H_2(CH_3)_3$	N···H	0.008	0.027	0.001
	F···H	0.010	0.038	0.001
T-C σ-hole				
$GeF_3C_6H_5$	F···H	0.011	0.048	0.002
$GeF_3C_6H_2F_3$	F···H	0.011	0.050	0.002
$GeF_3C_6H_2(CH_3)_3$	F···H	0.010	0.048	0.002

Table S2. EDA/BLYP-D3/ZORA/TZ2P decomposition of the interaction energy of σ-hole (T-F and T-C) complexes studied into Pauli repulsion (E_{Pauli}), electrostatic (E_{elec}), orbital interaction (E_{oi}) and dispersion (E_{disp}) terms. All energies in kcal/mol. The relative values in percent express the contribution of each to the sum of all attractive energy terms.

Complex	E_{int}	E_{Pauli}	E_{elec}	%	E_{oi}	%	E_{disp}	%
	(T-F) σ-hole							
$SiF_3C_6H_5$	-16.64	91.38	-65.38	61	-38.20	35	-4.44	4
$SiF_3C_6H_2F_3$	-18.99	93.56	-67.76	60	-40.36	36	-4.42	4
$SiF_3C_6H_2(CH_3)_3$	-15.86	91.39	-64.97	61	-37.76	35	-4.52	4
$GeF_3C_6H_5$	-16.08	89.08	-65.29	62	-35.53	34	-4.33	4
$GeF_3C_6H_2F_3$	-18.49	91.45	-67.87	62	-37.77	34	-4.30	4
$GeF_3C_6H_2(CH_3)_3$	-15.34	89.24	-65.03	62	-35.15	34	-4.40	4
$SnF_3C_6H_5$	-19.37	80.27	-64.82	65	-30.96	31	-3.86	4
$SnF_3C_6H_2F_3$	-21.48	81.14	-66.41	65	-32.34	32	-3.87	4
$SnF_3C_6H_2(CH_3)_3$	-18.54	79.89	-64.09	65	-30.40	31	-3.94	4

$PbF_3C_6H_5$	-15.59	63.37	-51.24	65	-24.25	31	-3.47	4
$PbF_3C_6H_2F_3$	-16.77	65.23	-53.28	65	-25.03	31	-3.68	4
$PbF_3C_6H_2(CH_3)_3$	-14.04	62.42	-50.01	65	-22.70	30	-3.75	5
(T-C) σ-hole								
$SiF_3C_6H_5$	-23.04	102.19	-77.32	62	-44.80	36	-3.11	2
$SiF_3C_6H_2F_3$	-26.49	105.25	-80.61	61	-48.02	36	-3.10	2
$SiF_3C_6H_2(CH_3)_3$	-21.76	101.00	-76.05	62	-43.59	36	-3.12	3
$GeF_3C_6H_5$	-22.68	111.32	-83.78	63	-47.13	35	-3.09	2
$GeF_3C_6H_2F_3$	-25.53	113.15	-86.13	62	-49.47	36	-3.08	2
$GeF_3C_6H_2(CH_3)_3$	-21.56	110.98	-83.07	63	-46.37	35	-3.11	2
$SnF_3C_6H_5$	-27.00	102.99	-85.33	66	-41.87	32	-2.80	2
$SnF_3C_6H_2F_3$	-32.66	80.33	-64.25	57	-45.87	41	-2.88	3
$SnF_3C_6H_2(CH_3)_3$	-24.68	101.07	-82.94	66	-39.97	32	-2.84	2
$PbF_3C_6H_5$	-24.03	116.26	-91.22	65	-46.26	33	-2.81	2
$PbF_3C_6H_2F_3$	-26.10	115.76	-91.78	65	-47.29	33	-2.79	2
$PbF_3C_6H_2(CH_3)_3$	-23.13	116.81	-91.16	65	-45.96	33	-2.82	2

Table S3. The crystal structures of TX_3R complexes with Lewis bases attached via T-X or T-C σ-hole found in CSD.

	VEGGIZ[100] R(N···Si)= 2.055 Å
	AVERUQ[101] R(N···Sn) = 2.283 Å
	FIKSUN[102] R(N···Sn) = 2.284 Å

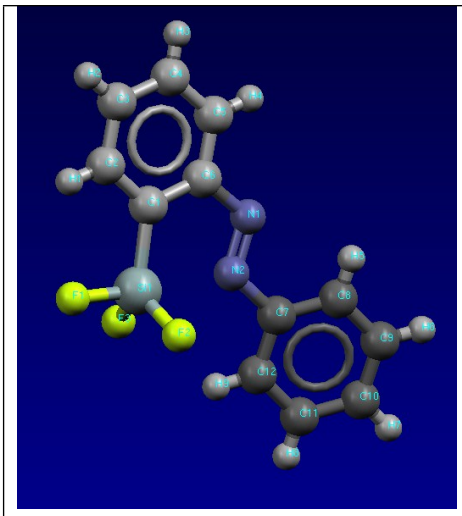
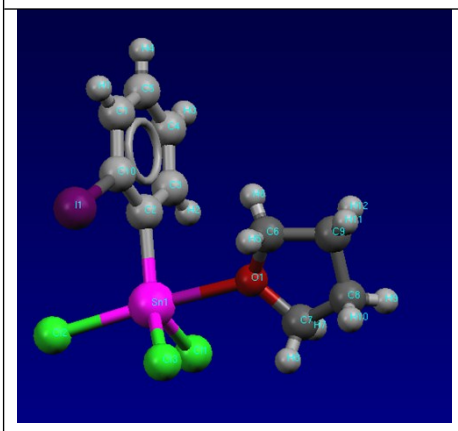
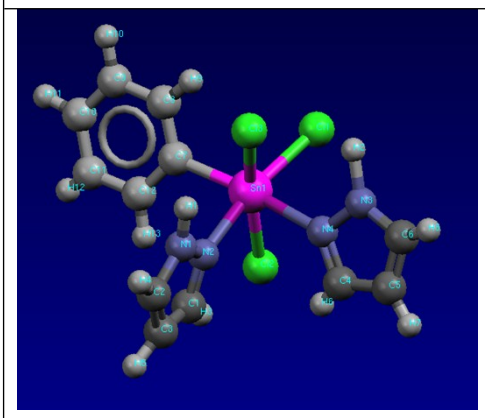
	QELCIU[103] R(N···Si) = 2.303 Å
	RIGHAQ[104] R(O···Sn) = 2.357 Å
	TOQGAH[105] R(N···Sn) = 2.284 Å

Table S4. The cartesian atomic coordinates for optimized equilibrium geometries of all model species (MP2/aug-cc-pVDZ)

	(T-F) σ-hole				(T-C) σ-hole			
$SiF_3C_6H_5$	C	-0.607986	-1.712666	0.324541	C	-0.777451	-1.748262	0.338633
	C	0.276998	-2.790495	0.567211	C	0.156399	-2.779164	0.612410
	C	1.668650	-2.583160	0.609602	C	1.541676	-2.547188	0.537978
	C	2.195917	-1.290967	0.426066	C	2.023032	-1.271700	0.186140
	C	1.328211	-0.205385	0.202169	C	1.112454	-0.235427	-0.089311
	C	-0.061786	-0.419026	0.143014	C	-0.273654	-0.473689	-0.013237
	H	-0.121731	-3.796618	0.733801	H	-0.199445	-3.777913	0.887846
	H	2.340563	-3.427205	0.792710	H	2.244795	-3.357884	0.753578
	H	3.277163	-1.128839	0.466455	H	3.100200	-1.087493	0.127286
	H	-0.724504	0.440117	-0.015531	H	-0.969341	0.341811	-0.230067
	F	-2.716911	-2.604304	1.778841	F	-2.685000	-2.624768	2.044613
	H	1.733166	0.803534	0.077024	H	1.480968	0.758197	-0.363317
	F	-2.999249	-3.383442	-0.530821	F	-2.707778	-3.355703	-0.665817
	Si	-2.452341	-2.024680	0.241969	Si	-2.620447	-2.125053	0.455425
	F	-3.473894	-0.729350	0.339147	F	-3.212362	-0.618119	0.052986
	N	-2.335800	-1.356124	-1.816993	N	-4.666547	-2.527909	0.581564
	H	-2.020570	-0.390985	-1.920229	H	-4.820034	-3.501166	0.846268
	H	-1.697563	-1.948371	-2.350564	H	-5.118291	-1.937069	1.279907
	H	-3.257356	-1.429223	-2.252037	H	-5.131489	-2.368111	-0.312397
$SiF_3C_6H_2F_3$	C	-0.599243	-1.713684	0.310278	C	-0.780011	-1.754103	0.340340
	C	0.272472	-2.795553	0.572695	C	0.147240	-2.788681	0.615053
	C	1.651691	-2.574630	0.628002	C	1.518422	-2.538682	0.535761
	C	2.192942	-1.294369	0.443854	C	2.007655	-1.272458	0.186374
	C	1.321557	-0.224270	0.200339	C	1.088140	-0.251972	-0.084589
	C	-0.060374	-0.419622	0.123497	C	-0.289914	-0.476112	-0.012307
	H	-0.102632	-3.807447	0.747942	H	-0.178449	-3.794882	0.892258
	H	-0.694750	0.455933	-0.045152	H	-0.965006	0.353233	-0.233018
	F	-2.683550	-2.623365	1.757827	F	-2.675119	-2.627037	2.044965
	F	-2.979412	-3.388383	-0.551480	F	-2.697534	-3.358742	-0.663912
	Si	-2.447463	-2.027800	0.224602	Si	-2.628788	-2.130169	0.457003
	F	-3.458874	-0.730001	0.354546	F	-3.193630	-0.615841	0.052082
	N	-2.359094	-1.345283	-1.814457	N	-4.656434	-2.520808	0.579384
	H	-2.069407	-0.372717	-1.924470	H	-4.815286	-3.493713	0.843522
	H	-1.723307	-1.922804	-2.367211	H	-5.107756	-1.928861	1.277547
	H	-3.288139	-1.435524	-2.230780	H	-5.120877	-2.359030	-0.314845
	F	2.505889	-3.599075	0.867002	F	2.419069	-3.522265	0.796838
	F	3.524136	-1.095271	0.504871	F	3.335874	-1.043372	0.113177
	F	1.853096	1.013051	0.037476	F	1.571738	0.972554	-0.422509
	C	-0.603299	-1.739901	0.285486	C	-0.775764	-1.750167	0.342120
	C	0.290335	-2.803461	0.539949	C	0.160566	-2.779058	0.595372
	C	1.681958	-2.595318	0.609251	C	1.551889	-2.565743	0.523560
	C	2.209311	-1.287875	0.438782	C	2.039222	-1.276599	0.185838
	C	1.326867	-0.201065	0.207404	C	1.118188	-0.228773	-0.072568
	C	-0.059213	-0.446726	0.121088	C	-0.266970	-0.476468	0.007947
	H	-0.099372	-3.815055	0.701042	H	-0.194077	-3.782879	0.858193
	H	-0.724881	0.411352	-0.038795	H	-0.959368	0.346962	-0.195300

	F	-2.696367	-2.771268	1.667053	F	-2.682850	-2.660854	2.037188
	F	-2.969105	-3.384497	-0.691556	F	-2.716819	-3.338698	-0.683021
	S	-2.438625	-2.075870	0.176428	Si	-2.614173	-2.126996	0.458506
	F	-3.491867	-0.814876	0.361451	F	-3.209730	-0.612610	0.087276
	N	-2.339598	-1.262970	-1.833217	N	-4.669380	-2.525710	0.583694
	H	-2.065516	-0.280842	-1.869812	H	-4.825280	-3.503506	0.828968
	H	-1.672435	-1.791547	-2.397153	H	-5.115990	-1.947346	1.295439
	H	-3.254743	-1.347480	-2.279302	H	-5.135972	-2.345684	-0.305366
	C	2.607659	-3.761659	0.877087	C	2.495602	-3.717571	0.808480
	H	3.230318	-3.581266	1.769346	H	3.136742	-3.940506	-0.060635
	H	2.031433	-4.684003	1.041492	H	3.157638	-3.497161	1.662444
	H	3.293214	-3.932627	0.029604	H	1.924415	-4.626713	1.049339
	C	3.706155	-1.082946	0.535806	C	3.522726	-0.987117	0.093349
	H	4.059800	-1.264953	1.565708	H	3.791809	-0.633781	-0.916898
	H	4.242929	-1.788892	-0.118980	H	3.812414	-0.190799	0.800316
	H	4.005835	-0.065573	0.252941	H	4.134234	-1.871478	0.314140
	C	1.841244	1.217195	0.060856	C	1.619241	1.152739	-0.434093
	H	2.401899	1.536417	0.954683	H	2.250596	1.574231	0.366744
	H	2.514648	1.317152	-0.806706	H	2.230428	1.131645	-1.352568
	H	1.002706	1.916125	-0.078472	H	0.775661	1.838972	-0.600836
	C	-0.505373	-1.756269	0.278231	C	-0.732945	-1.755951	0.340305
	C	0.323145	-2.722286	0.895421	C	0.196914	-2.785735	0.613820
	C	1.713066	-2.519072	0.976273	C	1.579495	-2.539411	0.535573
	C	2.288100	-1.342143	0.461526	C	2.047989	-1.259514	0.182639
	C	1.469431	-0.365142	-0.134608	C	1.130331	-0.228777	-0.091240
	C	0.081756	-0.577159	-0.233487	C	-0.253960	-0.474881	-0.013059
	H	-0.122832	-3.624583	1.322766	H	-0.155342	-3.784901	0.889294
	H	2.345899	-3.276468	1.448394	H	2.290085	-3.343750	0.749365
	H	3.367986	-1.182245	0.532663	H	3.123419	-1.067031	0.121556
$GeF_3C_6H_5$	H	-0.537164	0.204490	-0.685127	H	-0.962246	0.329796	-0.226866
	F	-2.611139	-3.004184	1.701420	F	-2.733616	-2.687865	2.150277
	H	1.909323	0.559837	-0.519388	H	1.491322	0.767223	-0.365829
	F	-3.024191	-3.419938	-0.819772	F	-2.757690	-3.463885	-0.723759
	Ge	-2.405533	-2.108236	0.186298	Ge	-2.631047	-2.137265	0.458840
	F	-3.581740	-0.852132	0.559258	F	-3.269535	-0.525770	0.028333
	N	-2.541780	-1.102349	-1.789697	N	-4.709898	-2.518457	0.579282
	H	-2.639594	-0.088240	-1.737730	H	-4.864745	-3.491596	0.843285
	H	-1.777652	-1.326179	-2.428627	H	-5.148749	-1.918791	1.278127
	H	-3.400730	-1.474889	-2.197442	H	-5.162097	-2.350053	-0.319457
	C	-0.487278	-1.805446	0.228169	C	-0.734705	-1.762867	0.342173
	C	0.329277	-2.742637	0.901854	C	0.189702	-2.795642	0.616468
	C	1.692208	-2.478135	1.058574	C	1.558458	-2.531799	0.533574
	C	2.267751	-1.294138	0.575138	C	2.034143	-1.260421	0.183006
	C	1.445736	-0.366020	-0.077001	C	1.107326	-0.245260	-0.086481
	C	0.082434	-0.610128	-0.262216	C	-0.268980	-0.478428	-0.011895
	H	-0.087766	-3.663366	1.315091	H	-0.132213	-3.802527	0.893738
	H	-0.502339	0.166146	-0.759124	H	-0.957965	0.339926	-0.229524
	F	-2.505424	-3.369936	1.396196	F	-2.722135	-2.691723	2.149209
$GeF_3C_6H_2F_3$	F	-2.884525	-3.423972	-1.165265	F	-2.746055	-3.467195	-0.720579
	Ge	-2.367030	-2.243385	0.036566	Ge	-2.636848	-2.142977	0.460426

	F	-3.616122	-1.139148	0.596243	F	-3.245503	-0.524170	0.027392
	N	-2.581587	-0.962755	-1.745537	N	-4.705710	-2.510543	0.577094
	H	-2.684633	0.033719	-1.550610	H	-4.867613	-3.482912	0.841159
	H	-1.863291	-1.088382	-2.460387	H	-5.143888	-1.908746	1.275074
	H	-3.463625	-1.283858	-2.149034	H	-5.157182	-2.340247	-0.322076
	F	2.496906	-3.362600	1.691402	F	2.467508	-3.505326	0.791873
	F	3.581059	-1.050151	0.739039	F	3.359230	-1.020541	0.107032
	F	2.003790	0.783376	-0.529715	F	1.581764	0.980456	-0.424538
$GeF_3C_6H_2(CH_3)_3$	C	-0.509131	-1.840877	0.169223	C	-0.740136	-1.762457	0.344025
	C	0.370562	-2.857068	0.599288	C	0.189194	-2.792614	0.597860
	C	1.751275	-2.614654	0.734667	C	1.578649	-2.568330	0.523649
	C	2.275551	-1.325521	0.451830	C	2.056682	-1.275613	0.185433
	C	1.398947	-0.287499	0.043638	C	1.130844	-0.231003	-0.072206
	C	0.024236	-0.564626	-0.104691	C	-0.253251	-0.483120	0.009056
	H	-0.026795	-3.845857	0.847722	H	-0.164530	-3.795934	0.860293
	H	-0.630521	0.261333	-0.403074	H	-0.955976	0.331247	-0.191824
	F	-2.510719	-3.550635	1.216954	F	-2.743523	-2.726332	2.141541
	F	-2.951679	-3.307719	-1.321588	F	-2.780270	-3.446631	-0.742119
	Ge	-2.382663	-2.273330	-0.007228	Ge	-2.634446	-2.138955	0.461347
	F	-3.636612	-1.246375	0.685287	F	-3.271644	-0.516925	0.062356
	N	-2.633347	-0.791462	-1.644062	N	-4.719359	-2.507883	0.580336
	H	-2.781307	0.165450	-1.323205	H	-4.879511	-3.484746	0.826271
	H	-1.882661	-0.795519	-2.335682	H	-5.151572	-1.918216	1.291523
	H	-3.486869	-1.095239	-2.115055	H	-5.171943	-2.319015	-0.313979
	C	2.668833	-3.728099	1.188892	C	2.529275	-3.714377	0.807124
	H	3.229942	-3.438980	2.093171	H	3.170084	-3.932198	-0.063303
	H	2.092352	-4.636304	1.416717	H	3.190501	-3.488955	1.660173
	H	3.409095	-3.977754	0.409932	H	1.964232	-4.626984	1.048527
	C	3.760489	-1.085771	0.619227	C	3.538235	-0.977980	0.091264
	H	4.050270	-1.159374	1.681865	H	3.803332	-0.622681	-0.919218
	H	4.343838	-1.844804	0.072696	H	3.823613	-0.180228	0.798181
	H	4.066749	-0.096872	0.254792	H	4.154921	-1.858820	0.310907
	C	1.907547	1.113073	-0.233063	C	1.624587	1.152740	-0.433907
	H	2.406414	1.542068	0.651243	H	2.254694	1.575988	0.366744
	H	2.633982	1.122657	-1.062435	H	2.234703	1.133612	-1.352931
	H	1.073511	1.777329	-0.505598	H	0.777614	1.834745	-0.599497
$SnF_3C_6H_5$	C	-0.356425	-1.862723	0.199323	C	-0.618787	-1.761093	0.336897
	C	0.393237	-2.605750	1.142352	C	0.313770	-2.791090	0.596122
	C	1.755881	-2.316430	1.345158	C	1.693873	-2.522779	0.522133
	C	2.379614	-1.288885	0.613024	C	2.146252	-1.231424	0.191677
	C	1.639814	-0.546601	-0.326025	C	1.218871	-0.202988	-0.060773
	C	0.276802	-0.832734	-0.531856	C	-0.162837	-0.463478	0.011248
	H	-0.090294	-3.404547	1.711874	H	-0.031708	-3.793031	0.868127
	H	2.330000	-2.894358	2.075589	H	2.414868	-3.320654	0.725096
	H	3.438757	-1.066629	0.773100	H	3.219458	-1.025765	0.135574
	H	-0.275834	-0.241318	-1.267493	H	-0.878744	0.343598	-0.171326
	F	-2.491040	-3.817867	1.264507	F	-2.654958	-3.687046	1.661391
	H	2.122066	0.252748	-0.896650	H	1.570587	0.802654	-0.310998
	F	-3.050557	-3.412407	-1.532445	F	-3.186539	-2.724145	-1.399426
	Sn	-2.390403	-2.370149	-0.033329	Sn	-2.685795	-2.166497	0.408132

	F	-3.830325	-1.321235	0.738650	F	-3.337528	-0.353350	0.822162
	N	-2.778600	-0.736108	-1.671401	N	-4.879497	-2.539227	0.712605
	H	-2.679957	0.232396	-1.364114	H	-5.024415	-3.268183	1.412472
	H	-2.272575	-0.859221	-2.549439	H	-5.350817	-1.681647	1.003475
	H	-3.769181	-0.885370	-1.874450	H	-5.272164	-2.849660	-0.177967
$SnF_3C_6H_2F_3$	C	-0.356718	-1.866559	0.188882	C	-0.619115	-1.760586	0.356817
	C	0.390204	-2.629777	1.115895	C	0.293607	-2.836400	0.289955
	C	1.744318	-2.336611	1.303165	C	1.660031	-2.557819	0.191756
	C	2.374082	-1.304096	0.592189	C	2.134215	-1.238873	0.156422
	C	1.620369	-0.556849	-0.322805	C	1.212223	-0.184437	0.218323
	C	0.264429	-0.824577	-0.533350	C	-0.161363	-0.425016	0.316955
	H	-0.068536	-3.441212	1.686636	H	-0.035063	-3.878638	0.297215
	H	-0.264862	-0.205280	-1.260069	H	-0.847152	0.425408	0.345407
	F	-2.439456	-3.829254	1.248037	F	-3.043588	-2.241534	2.457628
	F	-3.048577	-3.399549	-1.543044	F	-2.708884	-3.931424	-0.286958
	Sn	-2.394251	-2.370582	-0.037215	Sn	-2.682948	-2.152307	0.544524
	F	-3.817465	-1.335126	0.773051	F	-3.358856	-0.487722	-0.248977
	N	-2.787968	-0.717235	-1.641650	N	-4.878423	-2.566302	0.479315
	H	-2.692429	0.248229	-1.322684	H	-5.078351	-3.447848	0.954043
	H	-2.291106	-0.825103	-2.527358	H	-5.386642	-1.817284	0.951672
	H	-3.780071	-0.864542	-1.840963	H	-5.226836	-2.633753	-0.477833
	F	2.488149	-3.046490	2.181567	F	2.566311	-3.563433	0.122031
	F	3.678255	-1.034763	0.784116	F	3.454649	-0.988624	0.058082
	F	2.237171	0.438562	-1.005018	F	1.689554	1.083499	0.174082
$SnF_3C_6H_2(CH_3)_3$	C	-0.384110	-1.934550	0.013587	C	-0.657055	-1.779044	0.319991
	C	0.456660	-2.877588	0.643643	C	0.270946	-2.780301	0.671984
	C	1.815248	-2.587808	0.879532	C	1.659318	-2.537571	0.607791
	C	2.352889	-1.334679	0.481872	C	2.126496	-1.266679	0.182172
	C	1.516118	-0.380205	-0.152046	C	1.194537	-0.252586	-0.164640
	C	0.159074	-0.693703	-0.377293	C	-0.188050	-0.515100	-0.092835
	H	0.049970	-3.845634	0.953128	H	-0.080900	-3.759055	1.014961
	H	-0.463049	0.061867	-0.868419	H	-0.895967	0.280468	-0.348706
	F	-2.363719	-4.259756	0.490466	F	-2.735491	-3.607176	1.737215
	F	-3.095590	-3.034565	-2.011334	F	-3.216300	-2.867209	-1.380671
	Sn	-2.395064	-2.473989	-0.287966	Sn	-2.720326	-2.177526	0.381033
	F	-3.848096	-1.813675	0.820043	F	-3.396990	-0.345898	0.645845
	N	-2.951532	-0.435333	-1.314828	N	-4.918214	-2.522677	0.681731
	H	-2.880613	0.392095	-0.721301	H	-5.131923	-3.511998	0.551626
	H	-2.486977	-0.247299	-2.204082	H	-5.222244	-2.248643	1.616342
	H	-3.943308	-0.575274	-1.517755	H	-5.447418	-1.978331	-0.000188
	C	2.694873	-3.615231	1.556300	C	2.619600	-3.642298	1.001452
	H	3.119813	-3.220351	2.494418	H	3.273956	-3.925688	0.160505
	H	2.119149	-4.521217	1.794189	H	3.266775	-3.334288	1.839161
	H	3.540631	-3.903854	0.909799	H	2.062635	-4.537900	1.314166
	C	3.815472	-1.051517	0.748225	C	3.605756	-0.955828	0.098488
	H	4.034384	-1.114720	1.827579	H	3.874944	-0.601800	-0.910765
	H	4.454570	-1.797184	0.245777	H	3.877603	-0.152833	0.805264
	H	4.119287	-0.056447	0.399609	H	4.228515	-1.830123	0.326601
	C	2.046818	0.969161	-0.593050	C	1.679527	1.110247	-0.607909
	H	2.440283	1.545928	0.259953	H	2.312913	1.580343	0.163141

	H	2.861824	0.861361	-1.327377	H	2.283444	1.039516	-1.528431
	H	1.246288	1.561737	-1.061205	H	0.828912	1.778311	-0.807696
$PbF_3C_6H_5$	C	-0.253115	-1.853413	0.230977	C	-0.568842	-1.767639	0.301439
	C	0.444071	-2.584044	1.212238	C	0.328254	-2.666913	0.904897
	C	1.810547	-2.306466	1.410488	C	1.704632	-2.372674	0.850649
	C	2.456022	-1.319959	0.641082	C	2.156479	-1.205140	0.206677
	C	1.741433	-0.600598	-0.334845	C	1.237366	-0.316550	-0.382942
	C	0.374268	-0.865067	-0.546600	C	-0.143521	-0.590961	-0.340575
	H	-0.072367	-3.346884	1.801221	H	-0.035116	-3.561276	1.418273
	H	2.368618	-2.864021	2.168398	H	2.421444	-3.056527	1.314898
	H	3.517523	-1.111079	0.801905	H	3.227143	-0.984190	0.169397
	H	-0.180755	-0.307026	-1.303870	H	-0.867423	0.101282	-0.779029
	F	-2.463277	-3.800190	1.423176	F	-2.720448	-3.409495	2.068800
	H	2.244234	0.165766	-0.932040	H	1.591866	0.593929	-0.875239
	F	-3.169499	-3.443073	-1.501826	F	-3.201027	-3.323354	-1.296008
	Pb	-2.337724	-2.336412	-0.011278	Pb	-2.671244	-2.210411	0.359319
	F	-3.926569	-1.258405	0.660831	F	-3.432807	-0.273143	0.188091
	N	-2.848923	-0.705809	-1.837382	N	-4.903000	-2.510900	0.704054
	H	-3.631201	-0.211782	-1.401209	H	-5.242256	-3.062299	-0.086614
	H	-2.269898	-0.023908	-2.325795	H	-5.040226	-3.020516	1.578207
	H	-3.238666	-1.351952	-2.527958	H	-5.363590	-1.599835	0.726193
$PbF_3C_6H_2F_3$	C	-0.286592	-1.872847	0.226529	C	-0.574011	-1.753130	0.381133
	C	0.432710	-2.632984	1.167871	C	0.313062	-2.841627	0.306939
	C	1.785870	-2.328893	1.351250	C	1.677228	-2.555324	0.188794
	C	2.411731	-1.302943	0.625610	C	2.145634	-1.233624	0.143911
	C	1.661539	-0.567897	-0.303296	C	1.225133	-0.177170	0.213888
	C	0.305926	-0.838723	-0.517975	C	-0.148469	-0.413815	0.332584
	H	-0.039305	-3.435163	1.741161	H	-0.028984	-3.879165	0.318606
	H	-0.242407	-0.243486	-1.250029	H	-0.847296	0.425391	0.364082
	F	-2.412920	-3.899080	1.355803	F	-3.182266	-2.272219	2.568558
	F	-3.169679	-3.420931	-1.560029	F	-2.701109	-4.053385	-0.273063
	Pb	-2.364068	-2.379149	-0.018936	Pb	-2.674448	-2.154626	0.580196
	F	-3.944920	-1.341529	0.711561	F	-3.399295	-0.381217	-0.234450
	N	-2.823091	-0.661906	-1.747478	N	-4.903988	-2.576987	0.424345
	H	-2.788138	0.321510	-1.474969	H	-5.249941	-2.653003	1.383320
	H	-2.383235	-0.766366	-2.663013	H	-5.363145	-1.800818	-0.055398
	H	-3.810756	-0.898484	-1.867442	H	-5.047863	-3.457549	-0.072980
	F	2.530123	-3.021499	2.239280	F	2.583658	-3.555671	0.109154
	F	3.713402	-1.027713	0.817840	F	3.462371	-0.982077	0.027226
	F	2.279349	0.417269	-0.994356	F	1.701004	1.087384	0.158204
	C	-0.322468	-1.940500	0.055735	C	-0.604189	-1.796913	0.522564
	C	0.492105	-2.890907	0.691953	C	0.240078	-2.690064	-0.152921
	C	1.853173	-2.591910	0.905835	C	1.627642	-2.432981	-0.187728
	C	2.385817	-1.344345	0.482034	C	2.145521	-1.279653	0.458844
	C	1.545882	-0.395714	-0.157956	C	1.266718	-0.386131	1.128555
	C	0.184499	-0.704138	-0.368705	C	-0.118554	-0.646212	1.160550
	H	0.073179	-3.848168	1.016560	H	-0.168875	-3.566850	-0.663759
	H	-0.459809	0.029840	-0.861278	H	-0.799724	0.049455	1.659676
	F	-2.361614	-4.329366	0.650787	F	-3.159272	-3.350389	2.251420
	F	-3.269719	-3.073614	-1.958478	F	-2.889754	-3.382730	-1.134637

	Pb	-2.383353	-2.472532	-0.229733	Pb	-2.706879	-2.209889	0.588278
	F	-3.972819	-1.751465	0.813763	F	-3.439522	-0.268208	0.853225
	N	-3.019358	-0.355500	-1.399516	N	-4.960467	-2.473626	0.377718
	H	-3.083011	0.487744	-0.828031	H	-5.253418	-3.036965	1.178277
	H	-2.583248	-0.118297	-2.291156	H	-5.407449	-1.556110	0.403983
	H	-3.976453	-0.648858	-1.606358	H	-5.158691	-2.963798	-0.495635
	C	2.739394	-3.608591	1.589488	C	2.530724	-3.401203	-0.924955
	H	3.176210	-3.196174	2.514269	H	3.077116	-2.898287	-1.739447
	H	2.166012	-4.509306	1.850904	H	3.275834	-3.848847	-0.247101
	H	3.575865	-3.908714	0.936483	H	1.938170	-4.216425	-1.365104
	C	3.851097	-1.059299	0.729457	C	3.626144	-0.966798	0.445540
	H	4.078597	-1.098880	1.808070	H	3.818146	-0.007769	-0.065234
	H	4.483581	-1.817666	0.238160	H	4.013576	-0.868751	1.473458
	H	4.153899	-0.073160	0.356099	H	4.211023	-1.743088	-0.063264
	C	2.074347	0.946227	-0.622669	C	1.808406	0.851585	1.808627
	H	2.478859	1.531370	0.219136	H	2.521111	0.586300	2.607434
	H	2.880488	0.824909	-1.364378	H	2.343398	1.497263	1.092356
	H	1.270136	1.534584	-1.089012	H	0.992689	1.437005	2.256901