The Ditetrel Bond between Propellane Derivatives and TH_3F

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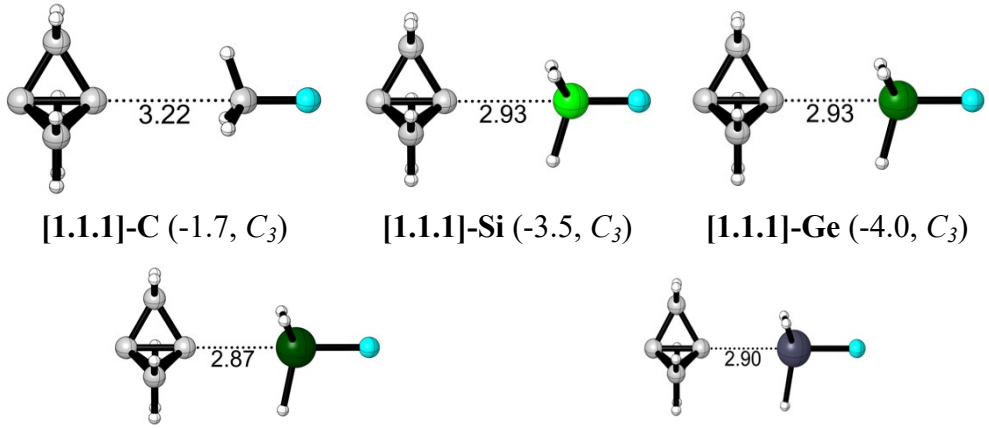
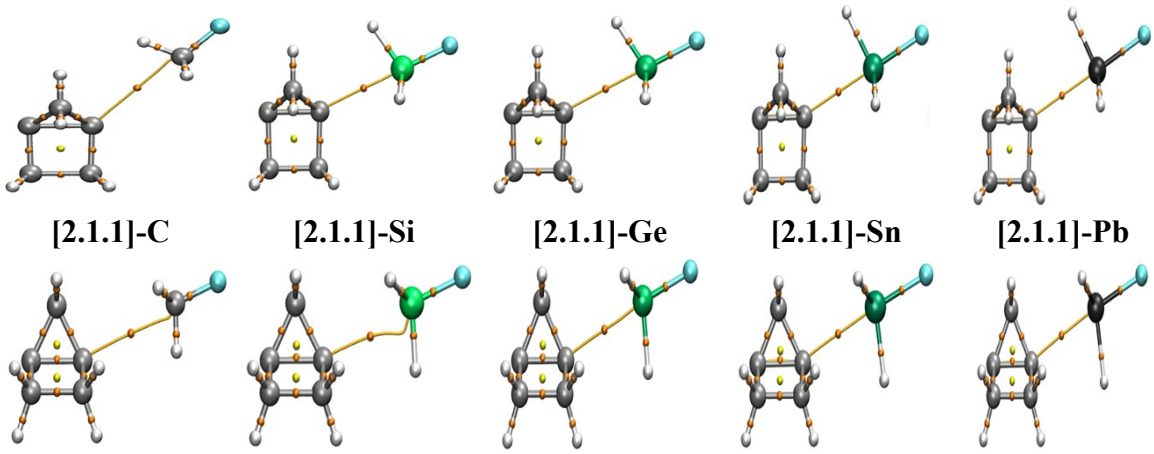


[1.1.1]-C (-1.7, C_3) **[1.1.1]-Si** (-3.5, C_3) **[1.1.1]-Ge** (-4.0, C_3)

[1.1.1]-Sn (-5.8, C_3) **[1.1.1]-Pb** (-6.0, C_{3v})

Figure S1. The optimized structures, binding energy (kcal mol^{-1}) and symmetry of **[1.1.1]-T** binary systems (T=C, Si, Ge, Sn, Pb) at MP2/def2tzvp level.



[2.1.1]-C **[2.1.1]-Si** **[2.1.1]-Ge** **[2.1.1]-Sn** **[2.1.1]-Pb**

[2.2.1]-C **[2.2.1]-Si** **[2.2.1]-Ge** **[2.2.1]-Sn** **[2.2.1]-Pb**

Figure S2. Atoms in molecules (AIM) diagrams of **[2.1.1]-T** and **[2.2.1]-T** complexes.

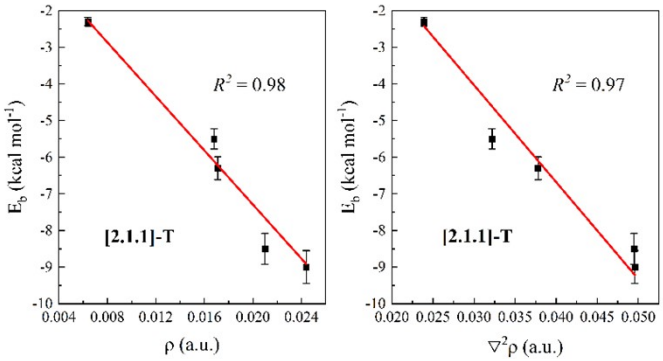


Figure S3. Linear plot of E_b with ρ and $\nabla^2\rho$ in **[2.1.1]-T** binary system.

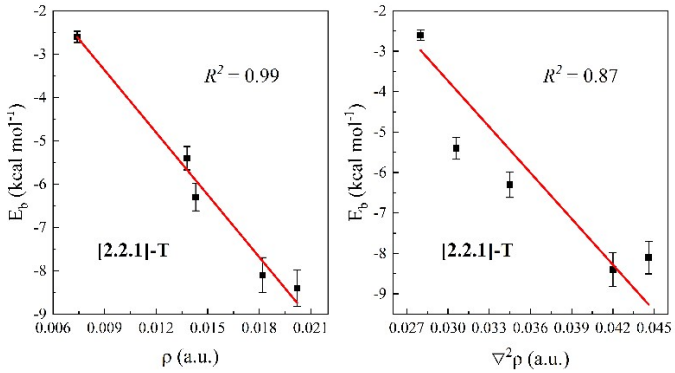
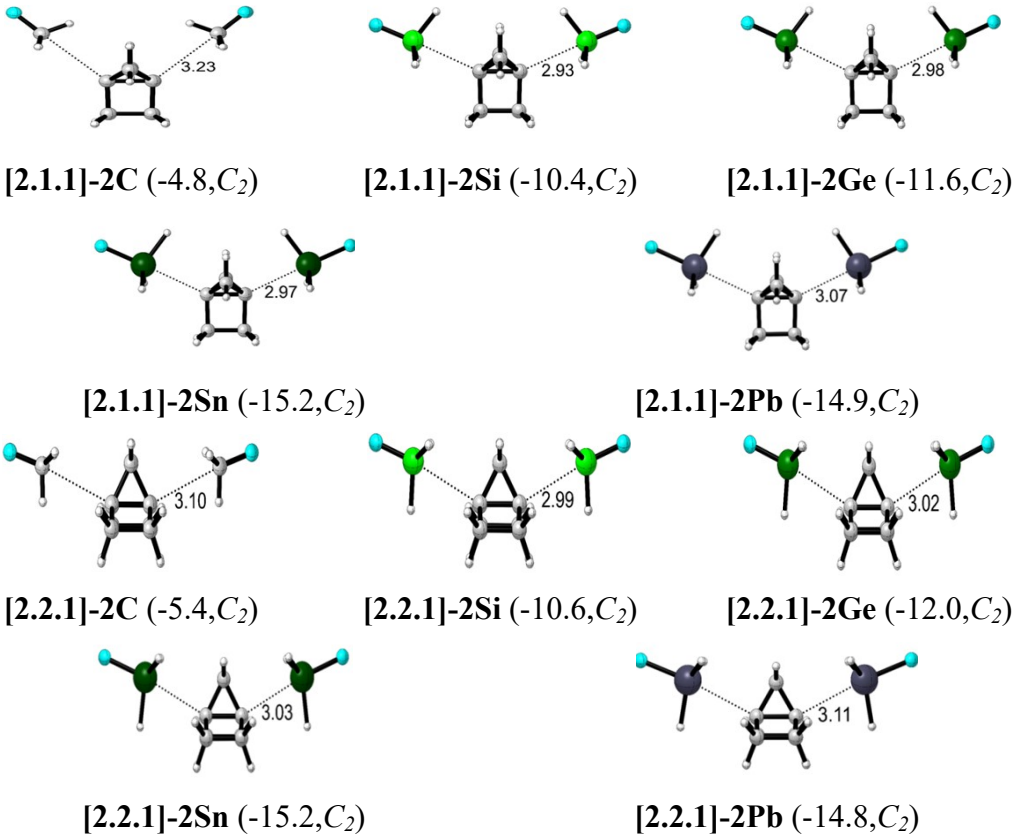


Figure S4. Linear plot of E_b with ρ and$\nabla^2\rho$ in **[2.2.1]-T** binary system.



[2.1.1]-2C (-4.8,C_2) **[2.1.1]-2Si** (-10.4,C_2) **[2.1.1]-2Ge** (-11.6,C_2)

[2.1.1]-2Sn (-15.2,C_2) **[2.1.1]-2Pb** (-14.9,C_2)

[2.2.1]-2C (-5.4,C_2) **[2.2.1]-2Si** (-10.6,C_2) **[2.2.1]-2Ge** (-12.0,C_2)

[2.2.1]-2Sn (-15.2,C_2) **[2.2.1]-2Pb** (-14.8,C_2)

Figure S5. The optimized structures, the interaction energy (kcal mol^{-1}) and symmetry of **[2.1.1]-2T** and **[2.2.1]-2T** ternary system.

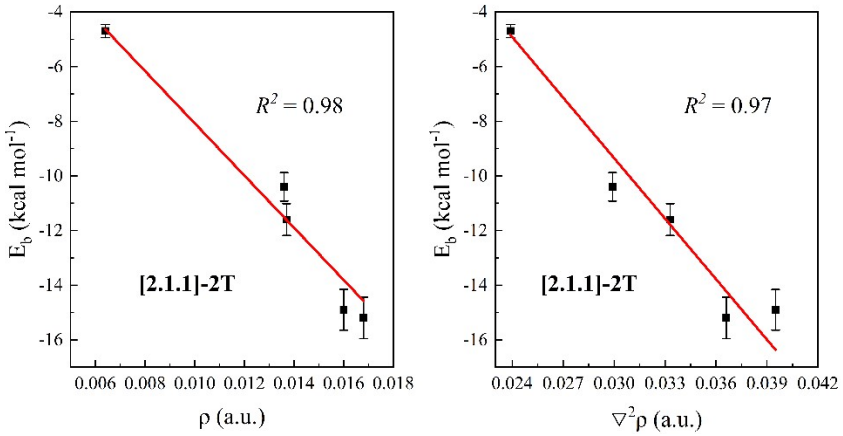


Figure S6. Linear plot of E_b with ρ and$\nabla^2\rho$ in **[2.1.1]-2T** binary system.

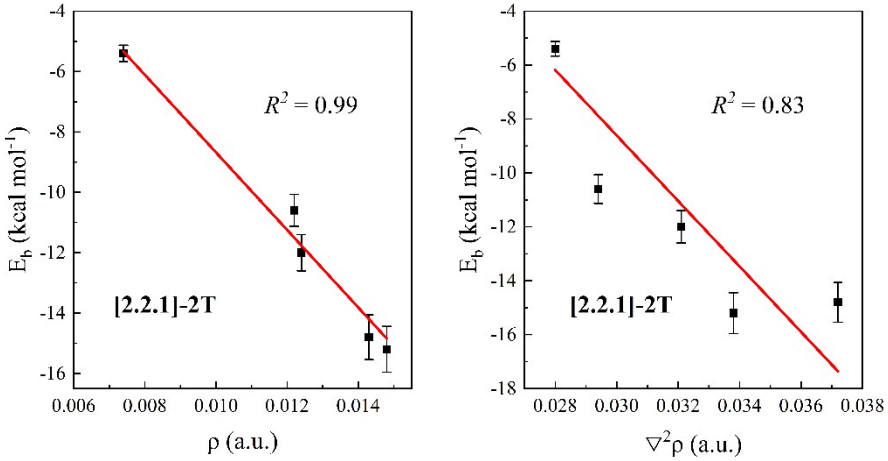


Figure S7. Linear plot of E_b with ρ and$\nabla^2\rho$ in **[2.2.1]-2T** binary system.

Table S1. Comparison of binding energy (E_b, kcal mol^{-1}) for **[1.1.1]-T** complexes at wB97XD/def2-TZVP and MP2/def2-TZVP levels.

	wB97XD	MP2
[1.1.1]-C	-1.9	-1.7
[1.1.1]-Si	-4.0	-3.5
[1.1.1]-Ge	-4.8	-4.0
[1.1.1]-Sn	-6.7	-5.9
[1.1.1]-Pb	-6.8	-6.0

Table S2. Binding energy of ternary system (E_b), sum of binding energy of the corresponding binary system (ΣE_b), cooperative energy (E_{coop}) of **[1.1.1]-CT** ternary complexes. All in kcal mol^{-1}.

	E_b	ΣE_b'	E_{coop}
[1.1.1]-CSi	-5.8	-5.9	-0.1
[1.1.1]-CGe	-6.4	-6.7	-0.3
[1.1.1]-CSn	-8.1	-8.6	-0.5
[1.1.1]-CPb	-8.1	-8.7	-0.6

Table S3. Binding energy (E_b, kcal mol^{-1}), electron density (ρ, a.u.), Laplace electron density ($\nabla^2\rho$, a.u.) at the BCPs of **[1.1.1]-CT** ternary complexes and their change ($\Delta\rho$ and $\Delta(\nabla^2\rho)$, a.u.) related to the binary analogues.

	E_b	ρ	$\Delta\rho$	$\nabla^2\rho$	$\Delta(\nabla^2\rho)$
[1.1.1]-CSi/C2···C	-5.8	0.0056	-0.0001	0.0219	0.0002
[1.1.1]-CSi/C1···Si		0.0108	-0.0009	0.0274	-0.0013
[1.1.1]-CGe/C2···C	-6.4	0.0054	-0.0003	0.0211	-0.0006
[1.1.1]-CGe/C1···Ge		0.0119	-0.0005	0.0316	-0.0009
[1.1.1]-CSn/C2···C	-8.1	0.0053	-0.0004	0.0210	-0.0007
[1.1.1]-CSnC1···Sn		0.0158	-0.0009	0.0369	-0.0017
[1.1.1]-CPbC2···C	-8.1	0.0053	-0.0004	0.0209	-0.0008
[1.1.1]-CPb/C1···Pb		0.0152	-0.0007	0.0398	-0.0016

Cartesian coordinates of the optimized **[1.1.1]-T** species at MP2/def2-TZVP

[1.1.1]

C	0.000000	0.000000	0.796478
C	0.000000	0.000000	-0.796478
C	0.000000	1.290434	0.000000
H	0.919008	1.866953	0.000000
H	-0.919008	1.866953	0.000000
C	1.117548	-0.645217	0.000000
C	-1.117548	-0.645217	0.000000
H	1.157324	-1.729361	0.000000
H	2.076333	-0.137592	0.000000
H	-1.157324	-1.729361	0.000000
H	-2.076333	-0.137592	0.000000

CH_3F

C	0.000000	0.000000	-0.633542
F	0.000000	0.000000	0.750969
H	0.000000	1.030256	-0.985822
H	-0.892228	-0.515128	-0.985822
H	0.892228	-0.515128	-0.985822

SiH_3F

H	0.000000	-1.397846	0.965213
H	-1.210570	0.698923	0.965213
H	1.210570	0.698923	0.965213
F	0.000000	0.000000	-1.101806
Si	0.000000	0.000000	0.501472

GeH_3F

H	0.000000	1.460843	0.757085
H	1.265127	-0.730421	0.757085
H	-1.265127	-0.730421	0.757085
F	0.000000	0.000000	-1.414854
Ge	0.000000	0.000000	0.326951

SnH_3F

H	0.000000	-1.626732	0.686142
H	-1.408791	0.813366	0.686142
H	1.408791	0.813366	0.686142
F	0.000000	0.000000	-1.664277
Sn	0.000000	0.000000	0.258401

PbH_3F

H	0.000000	1.686782	0.519015
H	1.460796	-0.843391	0.519015
H	-1.460796	-0.843391	0.519015
F	0.000000	0.000000	-1.845400
Pb	0.000000	0.000000	0.183556

[1.1.1]-C

C	0.000000	0.000000	-2.344783
C	0.000000	0.000000	-0.752285
C	1.291474	0.000003	-1.551616
H	1.867447	0.919182	-1.552601
H	1.867444	-0.919179	-1.552629
C	-0.645739	1.118448	-1.551616
C	-0.645735	-1.118450	-1.551616
H	-1.729758	1.157665	-1.552601
H	-0.137690	2.076843	-1.552629
H	-1.729754	-1.157664	-1.552629
H	-0.137688	-2.076847	-1.552601
C	0.000000	0.000000	2.466240
H	1.029236	0.000103	2.112064
H	-0.514707	0.891293	2.112064
H	-0.514529	-0.891396	2.112064

F	0.000000	0.000000	3.854839

[1.1.1]-Si

C	0.000000	0.000000	-2.567804
C	0.000000	0.000000	-0.977978
C	1.274008	-0.216677	-1.779990
H	1.995017	0.593729	-1.777803
H	1.686570	-1.219874	-1.777796
C	-0.449356	1.211661	-1.779990
C	-0.824652	-0.994984	-1.779990
H	-1.511693	1.430871	-1.777803
H	0.213156	2.070549	-1.777796
H	-1.899727	-0.850676	-1.777796
H	-0.483324	-2.024600	-1.777803
H	0.898927	1.087385	1.530328
H	-1.391167	0.234802	1.530328
H	0.492239	-1.322186	1.530328
F	0.000000	0.000000	3.563973
Si	0.000000	0.000000	1.951040

[1.1.1]-Ge

C	0.000000	0.000000	-3.023364
C	0.000000	0.000000	-1.434970
C	-0.000338	1.292742	-2.236952
H	-0.920426	1.867257	-2.235221
H	0.919449	1.867737	-2.235222
C	-1.119378	-0.646664	-2.236952
C	1.119716	-0.646078	-2.236952
H	-1.156879	-1.730740	-2.235221
H	-2.077232	-0.137602	-2.235222
H	1.157783	-1.730135	-2.235222
H	2.077305	-0.136516	-2.235221
H	-1.275920	0.736413	1.112933
H	0.000208	-1.473186	1.112933
H	1.275713	0.736773	1.112933
F	0.000000	0.000000	3.250364
Ge	0.000000	0.000000	1.494825

[1.1.1]-Sn

C	0.000000	0.000000	-3.273875
C	0.000000	0.000000	-1.689123
C	0.369046	1.240287	-2.493268
H	-0.349541	2.052805	-2.490239
H	1.414943	1.527782	-2.490259
C	-1.258643	-0.300540	-2.493268
C	0.889597	-0.939747	-2.493268
H	-1.603011	-1.329114	-2.490239
H	-2.030570	0.461485	-2.490259
H	0.615627	-1.989268	-2.490259
H	1.952552	-0.723691	-2.490239
H	-1.130132	1.198920	0.841549
H	-0.473229	-1.578184	0.841549
H	1.603362	0.379263	0.841549
F	0.000000	0.000000	3.122564
Sn	0.000000	0.000000	1.179412

[1.1.1]-Pb

C	0.000000	0.000000	-3.593505
C	0.000000	0.000000	-2.008676
C	1.293984	0.000289	-2.811579
H	1.867855	0.920801	-2.809698
H	1.868266	-0.919966	-2.809698
C	-0.647242	1.120478	-2.811579
C	-0.646742	-1.120768	-2.811579
H	-1.731365	1.157209	-2.809698
H	-0.137419	2.077949	-2.809698
H	-1.730847	-1.157983	-2.809698
H	-0.136490	-2.078011	-2.809698
H	0.848939	1.471146	0.622907
H	-1.698519	-0.000370	0.622907
H	0.849580	-1.470776	0.622907
F	0.000000	0.000000	2.942669
Pb	0.000000	0.000000	0.886914

Cartesian coordinates of the optimized species at wB97XD/def2-TZVP

[1.1.1]

C	0.000000	0.000000	0.778348
C	0.000000	0.000000	-0.778348
C	0.000000	1.295119	0.000000
H	0.914729	1.875242	0.000000
H	-0.914729	1.875242	0.000000
C	1.121606	-0.647560	0.000000
C	-1.121606	-0.647560	0.000000
H	1.166643	-1.729800	0.000000
H	2.081372	-0.145442	0.000000
H	-1.166643	-1.729800	0.000000
H	-2.081372	-0.145442	0.000000

[2.1.1]

C	-0.808999	0.000000	-0.367028
C	0.808999	0.000000	-0.367028
C	0.000000	1.123198	-0.943117
H	0.000000	2.073084	-0.420179
H	0.000000	1.208880	-2.024064
C	0.000000	-1.123198	-0.943117
H	0.000000	-2.073084	-0.420179
H	0.000000	-1.208880	-2.024064
C	0.767792	0.000000	1.180535
C	-0.767792	0.000000	1.180535
H	1.237215	-0.882663	1.610955
H	-1.237215	0.882663	1.610955
H	1.237215	0.882663	1.610955
H	-1.237215	-0.882663	1.610955

[2.2.1]

C	0.000000	0.782628	0.253037
C	0.000000	-0.782628	0.253037
C	0.000000	0.000000	1.515012
H	0.909375	0.000000	2.103609
H	-0.909375	0.000000	2.103609
H	2.173198	-1.274774	0.087989
H	1.317094	1.199829	-1.455830
C	-1.364929	0.778118	-0.452599
C	-1.364929	-0.778118	-0.452599
C	1.364929	0.778118	-0.452599
C	1.364929	-0.778118	-0.452599
H	-1.317094	1.199829	-1.455830
H	-1.317094	-1.199829	-1.455830
H	-2.173198	1.274774	0.087989
H	-2.173198	-1.274774	0.087989
H	1.317094	-1.199829	-1.455830
H	2.173198	1.274774	0.087989

CH_3F

C	0.000000	0.000000	-0.630163
F	0.000000	0.000000	0.748517
H	0.000000	1.031946	-0.985224
H	-0.893691	-0.515973	-0.985224
H	0.893691	-0.515973	-0.985224

SiH_3F

F	0.000000	0.000000	-1.100202
H	0.000000	1.402191	0.965945
H	1.214333	-0.701096	0.965945
H	-1.214333	-0.701096	0.965945
Si	0.000000	0.000000	0.500284

GeH_3F

F	0.000000	0.000000	-1.416702
H	0.000000	1.469617	0.756316
H	1.272725	-0.734808	0.756316
H	-1.272725	-0.734808	0.756316
Ge	0.000000	0.000000	0.327543

SnH_3F

H	0.000000	1.643489	0.691735
H	1.423303	-0.821745	0.691735
H	-1.423303	-0.821745	0.691735
F	0.000000	0.000000	-1.669694
Sn	0.000000	0.000000	0.259041

PbH_3F

F	0.000000	0.000000	-1.852795
H	0.000000	1.706474	0.541377
H	1.477850	-0.853237	0.541377
H	-1.477850	-0.853237	0.541377
Pb	0.000000	0.000000	0.183549

[1.1.1]-C

C	0.000000	0.000000	-2.326141
C	0.000000	0.000000	-0.771504
C	-1.098349	-0.687513	-1.553289
H	-1.104382	-1.770621	-1.553596
H	-2.075182	-0.219609	-1.553590
C	1.144578	-0.607442	-1.553289
C	-0.046229	1.294955	-1.553289
H	2.085594	-0.071112	-1.553596
H	1.227778	-1.687356	-1.553590
H	0.847404	1.906965	-1.553590
H	-0.981212	1.841733	-1.553596
C	0.000000	0.000000	2.472100
H	-0.865990	-0.558007	2.114457
H	0.916243	-0.470966	2.114457
H	-0.050253	1.028973	2.114457
F	0.000000	0.000000	3.854518

[1.1.1]-Si

C	0.000000	0.000000	-2.566112
C	0.000000	0.000000	-1.013749
C	0.217476	1.278191	-1.802422

H	-0.587868	2.002244	-1.799379
H	1.216959	1.695141	-1.799381
C	-1.215684	-0.450755	-1.802422
C	0.998208	-0.827435	-1.802422
H	-1.440060	-1.510231	-1.799379
H	-2.076515	0.206347	-1.799381
H	0.859556	-1.901488	-1.799381
H	2.027928	-0.492014	-1.799379
H	-1.089528	0.900033	1.556164
H	-0.234687	-1.393575	1.556164
H	1.324215	0.493542	1.556164
F	0.000000	0.000000	3.590677
Si	0.000000	0.000000	1.981033

[1.1.1]-Ge

C	0.000000	0.000000	-3.040175
C	0.000000	0.000000	-1.488686
C	-1.296944	-0.000347	-2.279091
H	-1.875257	-0.915953	-2.276330
H	-1.875798	0.914908	-2.276322
C	0.648773	-1.123013	-2.279091
C	0.648171	1.123360	-2.279091
H	1.730867	-1.166044	-2.276330
H	0.145565	-2.081942	-2.276322
H	1.730232	1.167034	-2.276322
H	0.144390	2.081997	-2.276330
H	-0.739621	-1.281225	1.140930
H	1.479384	0.000082	1.140930
H	-0.739763	1.281143	1.140930
F	0.000000	0.000000	3.284537
Ge	0.000000	0.000000	1.527223

[1.1.1]-Sn

C	0.000000	0.000000	-3.303560
C	0.000000	0.000000	-1.754050
C	1.244152	-0.369947	-2.551956
H	2.058962	0.343216	-2.547651
H	1.536839	-1.412481	-2.547661
C	-0.301692	1.262441	-2.551956
C	-0.942460	-0.892493	-2.551956
H	-1.326715	1.611506	-2.547651
H	0.454825	2.037182	-2.547661
H	-1.991664	-0.624701	-2.547661
H	-0.732247	-1.954722	-2.547651
H	1.210017	1.139125	0.863231
H	-1.591519	0.478343	0.863231
H	0.381503	-1.617468	0.863231
F	0.000000	0.000000	3.158971
Sn	0.000000	0.000000	1.210928

[1.1.1]-Pb

C	0.000000	0.000000	-3.676817
C	0.000000	0.000000	-2.126895
C	0.000499	1.297963	-2.923919
H	-0.914984	1.876314	-2.920859
H	0.916404	1.875631	-2.920841
C	-1.124319	-0.648549	-2.923919
C	1.123820	-0.649414	-2.923919
H	-1.167444	-1.730556	-2.920859
H	-2.082546	-0.144186	-2.920841
H	1.166142	-1.731445	-2.920841
H	2.082428	-0.145758	-2.920859
H	-1.488223	0.854511	0.633647
H	0.004084	-1.716094	0.633647
H	1.484139	0.861584	0.633647
F	0.000000	0.000000	2.989634
Pb	0.000000	0.000000	0.928906

[2.1.1]-C

C	-0.037658	0.565170	0.000000
C	-1.558005	1.114141	0.000000
C	-0.999701	0.298966	1.123264
H	-0.824098	0.790029	2.073775
H	-1.366319	-0.718334	1.208171
C	-0.999701	0.298966	-1.123264
H	-0.824098	0.790029	-2.073775
H	-1.366319	-0.718334	-1.208171
C	-0.999701	2.557092	0.000000
C	0.445195	2.036724	0.000000
H	-1.296198	3.120170	-0.882794
H	1.032417	2.283168	0.882609
H	-1.296198	3.120170	0.882794
H	1.032417	2.283168	-0.882609
H	1.704359	-1.783699	-0.892136
H	1.704359	-1.783699	0.892136
H	0.305179	-2.438392	0.000000
F	1.972356	-3.579464	0.000000
C	1.390119	-2.325909	0.000000

[2.1.1]-Si

C	-0.156616	0.655588	0.000000
C	-1.117410	1.959152	0.000000

C	-1.117410	0.986303	1.123449
H	-0.700629	1.298068	2.074203
H	-1.976966	0.329856	1.201485
C	-1.117410	0.986303	-1.123449
H	-0.700629	1.298068	-2.074203
H	-1.976966	0.329856	-1.201485
C	0.135886	2.860318	0.000000
C	1.051787	1.626419	0.000000
H	0.198495	3.492003	-0.883548
H	1.676406	1.506913	0.883325
H	0.198495	3.492003	0.883548
H	1.676406	1.506913	-0.883325
Si	0.472395	-2.106921	0.000000
H	1.066753	-1.544063	-1.228409
H	1.066753	-1.544063	1.228409
H	-1.003224	-2.067790	0.000000
F	0.865402	-3.671707	0.000000

[2.1.1]-Ge

C	-0.244602	1.129819	0.000000
C	-1.206848	2.430509	0.000000
C	-1.206848	1.458748	1.123771
H	-0.791154	1.771541	2.074627
H	-2.066084	0.801746	1.201707
C	-1.206848	1.458748	-1.123771
H	-0.791154	1.771541	-2.074627
H	-2.066084	0.801746	-1.201707
C	0.043897	3.335087	0.000000
C	0.962431	2.103305	0.000000
H	0.104900	3.966816	-0.883542
H	1.587471	1.985525	0.883247
H	0.104900	3.966816	0.883542
H	1.587471	1.985525	-0.883247
H	1.009366	-1.161021	-1.284737
H	1.009366	-1.161021	1.284737
H	-1.163150	-1.672428	0.000000
F	0.767075	-3.401591	0.000000
Ge	0.366356	-1.685618	0.000000

[2.1.1]-Sn

C	-0.238931	-1.395392	0.000000
C	0.172339	-2.963121	0.000000
C	0.538047	-2.076771	1.124420
H	0.037754	-2.215226	2.075607
H	1.577306	-1.775872	1.197714
C	0.538047	-2.076771	-1.124420
H	0.037754	-2.215226	-2.075607
H	1.577306	-1.775872	-1.197714
C	-1.317714	-3.352880	0.000000
C	-1.718385	-1.868836	0.000000
H	-1.605092	-3.917138	-0.884173
H	-2.256101	-1.530817	0.883776
H	-1.605092	-3.917138	0.884173
H	-2.256101	-1.530817	-0.883776
H	-0.656240	1.197945	-1.443488
H	-0.656240	1.197945	1.443488
H	1.831241	0.806247	0.000000
F	0.538047	3.298571	0.000000
Sn	0.225813	1.367829	0.000000

[2.1.1]-Pb

C	-0.294162	-1.819638	0.000000
C	0.148185	-3.376770	0.000000
C	0.494401	-2.477060	1.124522
H	-0.003688	-2.625184	2.075528
H	1.529574	-2.162844	1.200665
C	0.494401	-2.477060	-1.124522
H	-0.003688	-2.625184	-2.075528
H	1.529574	-2.162844	-1.200665
C	-1.336658	-3.791469	0.000000
C	-1.765988	-2.316236	0.000000
H	-1.613712	-4.361549	-0.883839
H	-2.310674	-1.988532	0.883397
H	-1.613712	-4.361549	0.883839
H	-2.310674	-1.988532	-0.883397
H	-0.731816	0.956346	-1.487288
H	-0.731816	0.956346	1.487288
H	1.824336	0.554070	0.000000
F	0.494401	3.128936	0.000000
Pb	0.165190	1.087786	0.000000

[2.2.1]-C

C	-1.790499	0.001339	0.540311
C	-0.351967	-0.001128	-0.072669
C	-0.579157	-0.000786	1.396705
H	-0.346423	0.908307	1.938014
H	-0.349536	-0.910712	1.937943
H	0.041332	2.171282	-0.415412
H	-2.842730	1.322115	-0.866020
C	-2.066296	-1.363838	-0.108612
C	-0.634464	-1.366046	-0.719082
C	-2.061579	1.367512	-0.108482

C	-0.629758	1.364790	-0.719001
H	-2.847256	-1.315650	-0.866174
H	-0.639002	-1.319422	-1.807339
H	-2.311621	-2.170606	0.584544
H	0.033800	-2.174881	-0.415503
H	-0.634506	1.318232	-1.807262
H	-2.304063	2.175068	0.584757
H	2.351593	0.004310	-0.994834
H	2.416046	0.888266	0.554722
H	2.416161	-0.895874	0.545361
F	4.132103	-0.000607	-0.038696
C	2.751600	-0.001003	0.020074

[2.2.1]-Si

C	-0.313647	-2.088271	0.000000
C	-0.303967	-0.502785	0.000000
C	0.946354	-1.326056	0.000000
H	1.533910	-1.319498	0.910065
H	1.533910	-1.319498	-0.910065
H	-0.489571	-0.040870	2.173343
H	-2.026264	-2.512718	1.307008
C	-1.025791	-2.086232	-1.359086
C	-1.025791	-0.533617	-1.359504
C	-1.025791	-2.086232	1.359086
C	-1.025791	-0.533617	1.359504
H	-2.026264	-2.512718	-1.307008
H	-2.025980	-0.106789	-1.302585
H	-0.483215	-2.580429	-2.166614
H	-0.489571	-0.040870	-2.173343
H	-2.025980	-0.106789	1.302585
H	-0.483215	-2.580429	2.166614
H	-0.513518	2.252132	0.000000
H	1.470394	1.500995	1.227433
H	1.470394	1.500995	-1.227433
F	1.530238	3.646726	0.000000
Si	0.959240	2.141915	0.000000

[2.2.1]-Ge

C	-0.506365	-2.512246	0.000000
C	-0.496016	-0.928616	0.000000
C	0.754936	-1.752555	0.000000
H	1.342482	-1.747040	0.910165
H	1.342482	-1.747040	-0.910165
H	-0.681001	-0.466834	2.174892
H	-2.217818	-2.937760	1.308332
C	-1.217288	-2.511533	-1.359710
C	-1.217288	-0.958852	-1.360459
C	-1.217288	-2.511533	1.359710
C	-1.217288	-0.958852	1.360459
H	-2.217818	-2.937760	-1.308332
H	-2.217468	-0.531983	-1.304239
H	-0.673925	-3.005926	-2.166433
H	-0.681001	-0.466834	-2.174892
H	-2.217468	-0.531983	1.304239
H	-0.673925	-3.005926	2.166433
H	-0.740136	1.915586	0.000000
H	1.331907	1.118421	1.284925
H	1.331907	1.118421	-1.284925
F	1.412128	3.377767	0.000000
Ge	0.780069	1.738496	0.000000

[2.2.1]-Sn

C	0.631651	2.772898	0.000000
C	0.611861	1.171734	0.000000
C	-0.628919	2.028440	0.000000
H	-1.215661	2.020746	0.910769
H	-1.215661	2.020746	-0.910769
H	0.816656	0.738150	2.178297
H	2.345792	3.204059	1.300041
C	1.347330	2.774233	-1.354753
C	1.347330	1.224480	-1.356861
C	1.347330	2.774233	1.354753
C	1.347330	1.224480	1.356861
H	2.345792	3.204059	-1.300041
H	2.345649	0.795023	-1.293497
H	0.802571	3.267000	-2.160977
H	0.816656	0.738150	-2.178297
H	2.345649	0.795023	1.293497
H	0.802571	3.267000	2.160977
H	1.026219	-1.730700	0.000000
H	-1.293030	-0.812290	1.446839
H	-1.293030	-0.812290	-1.446839
F	-1.367332	-3.238200	0.000000
Sn	-0.646953	-1.427477	0.000000

[2.2.1]-Pb

C	0.788617	3.158427	0.000000
C	0.771720	1.567819	0.000000
C	-0.474478	2.410024	0.000000
H	-1.061669	2.406589	0.910560
H	-1.061669	2.406589	-0.910560
H	0.969199	1.121649	2.180170

H	2.500370	3.587975	1.305210
C	1.500808	3.160258	-1.357651
C	1.500808	1.609211	-1.359843
C	1.500808	3.160258	1.357651
C	1.500808	1.609211	1.359843
H	2.500370	3.587975	-1.305210
H	2.500109	1.181298	-1.299513
H	0.956058	3.654151	-2.163307
H	0.969199	1.121649	-2.180170
H	2.500109	1.181298	1.299513
H	0.956058	3.654151	2.163307
H	1.199884	-1.484308	0.000000
H	-1.203271	-0.567558	1.492129
H	-1.203271	-0.567558	-1.492129
F	-1.248414	-3.065945	0.000000
Pb	-0.510003	-1.143191	0.000000

[1.1.1]-2C

C	0.376191	-0.679548	-0.093760
C	-0.376191	0.679548	-0.093760
C	0.000000	0.000000	1.202376
H	-0.800878	-0.442233	1.782192
H	0.800878	0.442233	1.782192
C	-0.983387	-0.541014	-0.741971
C	0.983387	0.541014	-0.741971
H	-1.022856	-0.562858	-1.824122
H	-1.823321	-1.005044	-0.239448
H	1.022856	0.562858	-1.824122
H	1.823321	1.005044	-0.239448
H	0.523263	3.438787	0.768768
H	-1.162739	3.638396	0.222937
H	0.164300	3.625320	-0.970300
F	0.000000	5.292440	0.159821
H	-0.523263	-3.438787	0.768768
H	-0.164300	-3.625320	-0.970300
H	1.162739	-3.638396	0.222937
F	0.000000	-5.292440	0.159821
C	-0.126248	3.922740	0.038140
C	0.126248	-3.922740	0.038140

[1.1.1]-2Si

C	-0.006025	-0.774266	0.092080
C	0.006025	0.774266	0.092080
C	0.000000	0.000000	1.389754
H	0.915820	-0.007148	1.967437
H	-0.915820	0.007148	1.967437
C	1.123782	-0.008502	-0.556897
C	-1.123782	0.008502	-0.556897
H	1.165853	-0.008905	-1.638920
H	2.082016	-0.016084	-0.052675
H	-1.165853	0.008905	-1.638920
H	-2.082016	0.016084	-0.052675
H	-1.218683	3.414966	0.684794
H	1.224674	3.418195	0.684038
H	0.002364	3.318639	-1.429223
F	0.000000	5.423437	-0.114981
Si	0.002271	3.817990	-0.040070
Si	-0.002271	-3.817990	-0.040070
H	1.218683	-3.414966	0.684794
H	-0.002364	-3.318639	-1.429223
H	-1.224674	-3.418195	0.684038
F	0.000000	-5.423437	-0.114981

[1.1.1]-2Ge

C	-0.000592	-0.004819	0.773508
C	-0.000592	-0.004819	-0.773508
C	1.254870	-0.335931	0.000000
H	2.046808	0.402487	0.000000
H	1.579601	-1.368876	0.000000
C	-0.341574	1.248015	0.000000
C	-0.915072	-0.926519	0.000000
H	-1.377010	1.564712	0.000000
H	0.390657	2.045679	0.000000
H	-1.972000	-0.691251	0.000000
H	-0.671597	-1.981574	0.000000
H	0.386869	-1.425282	-3.438202
H	1.041450	1.047804	-3.432256
H	-1.427573	0.378101	-3.433816
Ge	0.000242	0.001167	-3.832035
Ge	0.000242	0.001167	3.832035
H	1.041450	1.047804	3.432256
H	0.386869	-1.425282	3.438202
H	-1.427573	0.378101	3.433816
F	0.000242	0.005405	5.585586
F	0.000242	0.005405	-5.585586

[1.1.1]-2Sn

C	0.000164	0.771992	0.131780
C	-0.000164	-0.771992	0.131780
C	-1.125602	0.000229	-0.518413

H	-1.166118	0.000250	-1.600374
H	-2.083161	0.000429	-0.013176
C	1.125602	-0.000229	-0.518413
C	0.000000	0.000000	1.431469
H	2.083161	-0.000429	-0.013176
H	1.166118	-0.000250	-1.600374
H	0.916431	-0.000205	2.007914
H	-0.916431	0.000205	2.007914
H	-1.434036	-3.505700	0.822622
H	0.000578	-3.367886	-1.655363
H	1.433378	-3.505532	0.823683
H	-0.000578	3.367886	-1.655363
H	-1.433378	3.505532	0.823683
H	1.434036	3.505700	0.822622
F	-0.000161	5.776048	-0.131899
F	0.000161	-5.776048	-0.131899
Sn	0.000000	-3.838715	-0.023456
Sn	0.000000	3.838715	-0.023456

[1.1.1]-2Pb

C	0.000070	0.772172	-0.012095
C	-0.000070	-0.772172	-0.012095
C	-1.125836	0.000098	-0.662034
H	-1.167199	0.000113	-1.743938
H	-2.083410	0.000185	-0.156753
C	1.125836	-0.000098	-0.662034
C	0.000000	0.000000	1.287881
H	2.083410	-0.000185	-0.156753
H	1.167199	-0.000113	-1.743938
H	0.916318	-0.000084	1.864613
H	-0.916318	0.000084	1.864613
H	-1.483102	-3.587924	0.856459
H	-0.000060	-3.600254	-1.712408
H	1.483138	-3.587844	0.856369
H	0.000060	3.600254	-1.712408
H	-1.483138	3.587844	0.856369
H	1.483102	3.587924	0.856459
F	-0.000058	5.962036	0.011252
F	0.000058	-5.962036	0.011252
Pb	0.000000	3.910595	0.001409
Pb	0.000000	-3.910595	0.001409

[2.1.1]-2C

C	0.666704	0.455724	1.015871
C	-0.666704	-0.455724	1.015871
C	-0.633855	0.927331	0.437854
H	-1.170519	1.712584	0.957989
H	-0.681536	0.996651	-0.643881
C	0.633855	-0.927331	0.437854
H	1.170519	-1.712584	0.957989
H	0.681536	-0.996651	-0.643881
C	-0.633855	-0.433436	2.563214
C	0.633855	0.433436	2.563214
H	-0.522857	-1.427070	2.992788
H	0.522857	1.427070	2.992788
H	-1.519507	0.030164	2.993149
H	1.519507	-0.030164	2.993149
H	3.170775	1.034273	-0.635955
H	2.215824	2.541500	-0.606617
H	1.751726	1.212497	-1.702601
F	3.394833	2.263608	-2.226065
H	-1.751726	-1.212497	-1.702601
H	-3.170775	-1.034273	-0.635955
H	-2.215824	-2.541500	-0.606617
F	-3.394833	-2.263608	-2.226065
C	2.589275	1.733964	-1.236987
C	-2.589275	-1.733964	-1.236987

[2.1.1]-2Si

C	0.000358	0.808228	0.581270
C	-0.000358	-0.808228	0.581270
C	-1.123813	0.000472	0.002630
H	-2.074856	0.000914	0.522135
H	-1.198418	0.000519	-1.079229
C	1.123813	-0.000472	0.002630
H	2.074856	-0.000914	0.522135
H	1.198418	-0.000519	-1.079229
C	-0.000343	-0.768572	2.127127
C	0.000343	0.768572	2.127127
H	0.883184	-1.238493	2.554173
H	-0.883184	1.238493	2.554173
H	-0.884293	-1.237704	2.554163
H	0.884293	1.237704	2.554163
H	1.222620	3.367050	0.210393
H	-1.224094	3.366161	0.208107
H	0.001358	2.562539	-1.757555
F	0.000017	4.977230	-1.218253
H	-0.001358	-2.562539	-1.757555
H	-1.222620	-3.367050	0.210393
H	1.224094	-3.366161	0.208107
F	-0.000017	-4.977230	-1.218253

Si	-0.000017	3.488740	-0.608148
Si	0.000017	-3.488740	-0.608148

[2.1.1]-2Ge

C	0.666485	0.455385	0.815607
C	-0.666485	-0.455385	0.815607
C	-0.634335	0.928340	0.235807
H	-1.170989	1.713759	0.754786
H	-0.676318	0.989696	-0.846222
C	0.634335	-0.928340	0.235807
H	1.170989	-1.713759	0.754786
H	0.676318	-0.989696	-0.846222
C	-0.634335	-0.433567	2.361933
C	0.634335	0.433567	2.361933
H	-0.523089	-1.428014	2.788983
H	0.523089	1.428014	2.788983
H	-1.520457	0.030985	2.789295
H	1.520457	-0.030985	2.789295
H	3.573211	0.888229	0.380413
H	2.130509	3.003950	0.381413
H	2.105314	1.438057	-1.649589
F	4.219128	2.879038	-1.169902
H	-2.105314	-1.438057	-1.649589
H	-3.573211	-0.888229	0.380413
H	-2.130509	-3.003950	0.381413
F	-4.219128	-2.879038	-1.169902
Ge	2.894912	1.975845	-0.454689
Ge	-2.894912	-1.975845	-0.454689

[2.1.1]-2Sn

C	0.666715	0.455188	0.925804
C	-0.666715	-0.455188	0.925804
C	-0.634513	0.929304	0.344749
H	-1.170970	1.715079	0.862906
H	-0.674221	0.987301	-0.737646
C	0.634513	-0.929304	0.344749
H	1.170970	-1.715079	0.862906
H	0.674221	-0.987301	-0.737646
C	-0.634513	-0.433364	2.472244
C	0.634513	0.433364	2.472244
H	-0.523102	-1.428100	2.898049
H	0.523102	1.428100	2.898049
H	-1.520553	0.032023	2.898336
H	1.520553	-0.032023	2.898336
H	3.704080	0.796348	0.570061
H	2.086712	3.165097	0.555187
H	2.052633	1.390921	-1.710964
F	4.350102	2.963126	-1.152554
H	-2.052633	-1.390921	-1.710964
H	-3.704080	-0.796348	0.570061
H	-2.086712	-3.165097	0.555187
F	-4.350102	-2.963126	-1.152554
Sn	-2.887286	-1.969488	-0.348394

[2.1.1]-2Pb

C	-0.001685	-0.806414	1.045038
C	0.001685	0.806414	1.045038
C	1.125748	-0.002267	0.463541
H	2.076982	-0.004338	0.982230
H	1.198552	-0.002338	-0.618733
C	-1.125748	0.002267	0.463541
H	-2.076982	0.004338	0.982230
H	-1.198552	0.002338	-0.618733
C	0.001610	0.768207	2.592301
C	-0.001610	-0.768207	2.592301
H	-0.881319	1.238984	3.018948
H	0.881319	-1.238984	3.018948
H	0.886507	1.235330	3.018873
H	-0.886507	-1.235330	3.018873
H	-1.472416	-3.662926	0.677918
H	1.494660	-3.648858	0.638558
H	-0.025210	-2.595341	-1.688945
F	-0.004291	-5.453550	-1.100904
H	0.025210	2.595341	-1.688945
H	1.472416	3.662926	0.677918
H	-1.494660	3.648858	0.638558
F	0.004291	5.453550	-1.100904
Pb	0.001610	3.583241	-0.252756
Pb	-0.001610	-3.583241	-0.252756

[2.2.1]-2C

C	-0.678904	-0.386631	-0.411212
C	0.678904	0.386631	-0.411212
C	0.000000	0.000000	0.852086
H	-0.450595	0.790241	1.440503
H	0.450595	-0.790241	1.440503
H	0.032311	2.518868	-0.572644
H	-1.697127	0.552537	-2.117358
C	0.000000	-1.571793	-1.115178
C	1.352548	-0.801628	-1.114713

C	-1.352548	0.801628	-1.114713
C	0.000000	1.571793	-1.115178
H	-0.389671	-1.740472	-2.118096
H	1.697127	-0.552537	-2.117358
H	-0.032311	-2.518868	-0.572644
H	2.183005	-1.257162	-0.571576
H	0.389671	1.740472	-2.118096
H	-2.183005	1.257162	-0.571576
H	3.065030	1.927395	-0.324152
H	2.217383	2.365809	1.184480
H	3.190060	0.871644	1.110197
F	4.224139	2.606637	1.185016
H	-2.217383	-2.365809	1.184480
H	-3.065030	-1.927395	-0.324152
H	-3.190060	-0.871644	1.110197
F	-4.224139	-2.606637	1.185016
C	-3.112045	-1.903489	0.765644
C	3.112045	1.903489	0.765644

[2.2.1]-2Si

C	0.000006	0.796683	-0.608275
C	-0.000006	-0.796683	-0.608275
C	0.000000	0.000000	0.644965
H	0.910518	0.000013	1.231866
H	-0.910518	-0.000013	1.231866
H	2.168369	-1.267564	-0.789335
H	1.300219	1.205140	-2.328042
C	-1.357455	0.775486	-1.329443
C	-1.357457	-0.775463	-1.329444
C	1.357457	0.775463	-1.329444
C	1.357455	-0.775486	-1.329443
H	-1.300249	1.205173	-2.328036
H	-1.300219	-1.205140	-2.328042
H	-2.168369	1.267564	-0.789335
H	-2.168404	-1.267535	-0.789372
H	1.300249	-1.205173	-2.328036
H	2.168404	1.267535	-0.789372
H	0.000460	-3.577293	-0.779491
H	1.224126	-2.836326	1.203158
H	-1.224365	-2.836526	1.202493
F	0.000000	-4.991227	1.257483
H	-1.224126	2.836326	1.203158
H	-0.000460	3.577293	-0.779491
H	1.224365	2.836526	1.202493
F	0.000000	4.991227	1.257483
Si	-0.000070	3.486366	0.694821
Si	0.000070	-3.486366	0.694821

[2.2.1]-2Ge

C	0.000007	0.794562	-0.798750
C	-0.000007	-0.794562	-0.798750
C	0.000000	0.000000	0.456537
H	0.910674	0.000004	1.043468
H	-0.910674	-0.000004	1.043468
H	2.169850	-1.267247	-0.977560
H	1.302918	1.204943	-2.516908
C	-1.358997	0.775584	-1.518210
C	-1.358997	-0.775567	-1.518211
C	1.358997	0.775567	-1.518211
C	1.358997	-0.775584	-1.518210
H	-1.302922	1.204957	-2.516902
H	-1.302918	-1.204943	-2.516908
H	-2.169850	1.267247	-0.977560
H	-2.169888	-1.267236	-0.977607
H	1.302922	-1.204957	-2.516902
H	2.169888	1.267236	-0.977607
H	0.000298	-3.660929	-1.012655
H	1.281416	-2.885369	1.062718
H	-1.281652	-2.885549	1.062243
F	0.000000	-5.155157	1.124568
H	-1.281416	2.885369	1.062718
H	-0.000298	3.660929	-1.012655
H	1.281652	2.885549	1.062243
F	0.000000	5.155157	1.124568
Ge	-0.000028	3.513637	0.511047
Ge	0.000028	-3.513637	0.511047

[2.2.1]-2Sn

C	0.000169	0.799770	-0.922032
C	-0.000169	-0.799770	-0.922032
C	0.000000	0.000000	0.331222
H	0.911355	-0.000117	0.917283
H	-0.911355	0.000117	0.917283
H	2.170007	-1.263604	-1.108880
H	1.297157	1.206358	-2.644722
C	-1.356805	0.774605	-1.648038
C	-1.357213	-0.774146	-1.647838
C	1.357213	0.774146	-1.647838
C	1.356805	-0.774605	-1.648038
H	-1.296330	1.206407	-2.645082

H	-1.297157	-1.206358	-2.644722
H	-2.170007	1.263604	-1.108880
H	-2.170650	-1.262513	-1.108442
H	1.296330	-1.206407	-2.645082
H	2.170650	1.262513	-1.108442
H	-0.018012	-3.751561	-1.278486
H	1.445566	-2.884316	1.030139
H	-1.428862	-2.875917	1.059302
F	0.001699	-5.338806	1.087601
H	-1.445566	2.884316	1.030139
H	0.018012	3.751561	-1.278486
H	1.428862	2.875917	1.059302
F	-0.001699	5.338806	1.087601
Sn	0.000000	3.523262	0.406085
Sn	0.000000	-3.523262	0.406085

[2.2.1]-2Pb

C	-0.000014	-0.795845	-1.052291
C	0.000014	0.795845	-1.052291
C	0.000000	0.000000	0.204033
H	-0.911225	-0.000007	0.790563
H	0.911225	0.000007	0.790563
H	-2.172852	1.263854	-1.235612
H	-1.301541	-1.205073	-2.772503
C	1.359413	-0.774833	-1.774661
C	1.359469	0.774807	-1.774599
C	-1.359469	-0.774807	-1.774599
C	-1.359413	0.774833	-1.774661
H	1.301379	-1.204985	-2.772607
H	1.301541	1.205073	-2.772503
H	2.172852	-1.263854	-1.235612
H	2.172900	1.263714	-1.235435
H	-1.301379	1.204985	-2.772607
H	-2.172900	-1.263714	-1.235435
H	-0.000173	3.896340	-1.418318
H	-1.486728	2.991384	0.982905
H	1.486772	2.991140	0.982593
F	0.000242	5.509003	1.021971
H	1.486728	-2.991384	0.982905
H	0.000173	-3.896340	-1.418318
H	-1.486772	-2.991140	0.982593
F	-0.000242	-5.509003	1.021971
Pb	0.000000	3.591728	0.298511
Pb	0.000000	-3.591728	0.298511

[1.1.1]-CSi

C	0.145888	0.460621	0.000000
C	1.136630	-0.732695	0.000000
C	0.145888	-0.555015	1.123072
H	0.530976	-0.231787	2.082194
H	-0.689280	-1.243331	1.166402
C	1.645653	0.684346	0.000000
C	0.145888	-0.555015	-1.123072
H	2.088525	1.056364	-0.915493
H	2.088525	1.056364	0.915493
H	0.530976	-0.231787	-2.082194
H	-0.689280	-1.243331	-1.166402
H	0.321509	-3.663670	0.000000
H	1.865477	-3.586867	0.892149
H	1.865477	-3.586867	-0.892149
F	1.433253	-5.348892	0.000000
Si	-1.573930	2.958904	0.000000
H	-0.747377	3.001753	1.222187
H	-0.747377	3.001753	-1.222187
H	-2.496585	1.807313	0.000000
F	-2.479881	4.287384	0.000000
C	1.368904	-3.970073	0.000000

[1.1.1]-CGe

C	-0.123226	0.576478	0.000000
C	0.879280	1.758781	0.000000
C	0.879280	0.754993	1.123312
H	0.494282	1.078098	2.082481
H	1.702080	0.051907	1.166141
C	-0.604198	2.014913	0.000000
C	0.879280	0.754993	-1.123312
H	-1.046746	2.387167	-0.915502
H	-1.046746	2.387167	0.915502
H	0.494282	1.078098	-2.082481
H	1.702080	0.051907	-1.166141
H	3.941185	1.454905	0.000000
H	3.579790	2.958541	0.892201
H	3.579790	2.958541	-0.892201
F	5.390781	2.859023	0.000000
H	-2.350328	-1.031884	1.280428
H	-2.350328	-1.031884	-1.280428
H	-0.611565	-2.407968	0.000000
F	-3.102339	-3.174227	0.000000
C	4.047922	2.541076	0.000000
Ge	-2.013556	-1.797036	0.000000

[1.1.1]-CSn

C	0.215395	0.826314	0.000000
C	1.223897	2.001037	0.000000
C	1.223897	1.003760	1.124153
H	0.839354	1.328634	2.082809
H	2.041397	0.294630	1.166164
C	-0.252706	2.273899	0.000000
C	1.223897	1.003760	-1.124153
H	-0.693365	2.647178	-0.915895
H	-0.693365	2.647178	0.915895
H	0.839354	1.328634	-2.082809
H	2.041397	0.294630	-1.166164
H	4.292616	1.667711	0.000000
H	3.934540	3.172392	0.892319
H	3.934540	3.172392	-0.892319
F	5.744625	3.068571	0.000000
H	-2.114849	-0.657056	1.437786
H	-2.114849	-0.657056	-1.437786
H	-0.205770	-2.254753	0.000000
F	-2.956220	-2.956072	0.000000
C	4.401760	2.753795	0.000000
Sn	-1.708270	-1.463448	0.000000

[1.1.1]-CPb

C	1.221176	0.559573	-0.008217
C	2.731419	0.901478	0.016636
C	2.096600	0.190241	1.178736
H	1.951299	0.753333	2.092127
H	2.327055	-0.859683	1.311083
C	1.710682	1.996731	-0.103792
C	2.171972	0.014978	-1.061437
H	1.612780	2.486571	-1.064461
H	1.550246	2.629040	0.760427
H	2.091493	0.428967	-2.058775
H	2.406344	-1.041313	-1.013462
H	4.971570	-1.151253	0.291869
H	5.717450	0.421389	0.686259
H	5.509158	-0.063587	-1.018763
F	6.964940	-1.016645	0.007554
H	-1.703057	0.962009	1.369773
H	-1.641858	0.614527	-1.580600
H	-1.115968	-1.703792	0.199911
F	-3.791118	-0.554274	0.008371
C	5.722357	-0.418574	-0.009524
Pb	-1.782514	-0.107372	-0.002355