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Trends in ionization energies for group 14 catenates and influence of substituent nature on them

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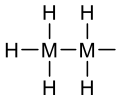
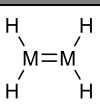
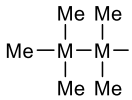
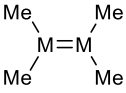
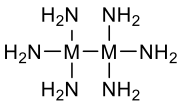
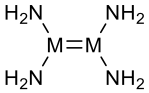
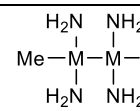
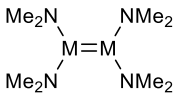
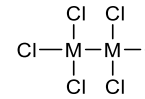
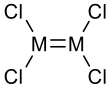
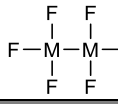
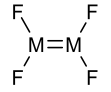
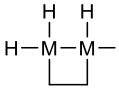
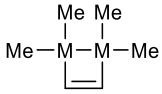
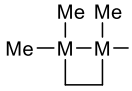
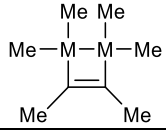
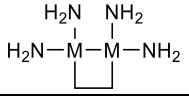
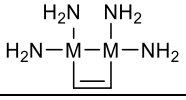
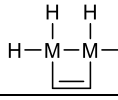
Contents

General

The adiabatic ionization potentials calculated as a difference between Gibbs free energy of an uncharged particle and the corresponding the lowest in energy cation radical. All quantum chemical calculations were performed by the ORCA [S1] ver. 5.0.4 [S2] program package using TPSS [S3] and PBE0-DH [S4] density functionals in triple-zeta basis set with two polarization functions def2-TZVPP [S5]. Atom-pairwise dispersion correction with the Becke-Johnson damping scheme (D3BJ) [S6-S7] was included in all calculations. DefGrid3 integration grids and TightSCF convergence criteria were applied throughout. RI-J and “chain of spheres” COSX approximation [S8] with the def2/J auxiliary basis set [S9] was used to speed up calculations. def2-TZVPP/C auxiliary basis set [S10] was used for MP2 part of PBE0-DH calculation. Full geometry optimization with TightOpt convergence criteria was carried out to find stationary points on the potential energy surfaces. Analytical (TPSS) and numerical (PBE0-DH) harmonic frequencies calculations were used to obtain thermodynamic quantities and verify that all stationary points found are local minima. The thermodynamic functions were calculated in the harmonic oscillator-rigid rotor approximation.

Table S1 Adiabatic ionization potentials (eV) of catenates obtained using DFT-PBE0-DH/def2-TZVPP.

		M						M			
		C	Si	Ge	Sn			C	Si	Ge	Sn
1		11.18	9.44	9.22	8.64	**8**		10.16	7.79	7.68	7.36
2		8.70	7.59	7.57	7.35	**9**		7.86	5.66	6.31	6.37
3		7.76	6.85	7.31	7.49	**10**		5.59	5.72	-*	-*
4		6.69	6.81	7.02	7.13	**11**		5.12	5.54	-*	-*
6		10.84	9.69	9.99	9.95	**13**		9.00	7.78	8.71	8.99
7		12.23	11.34	12.03	11.76	**14**		9.67	8.64	9.90	9.80
		M						M			
		C	Si	Ge	Sn			C	Si	Ge	Sn
15		9.48	8.43	7.02	7.83	**21**		8.66	7.50	7.45	7.18
16		8.24	7.25	7.25	7.00	**22**		7.67	7.35	7.29	6.99
18		5.85	6.58	6.74	6.88	**23**		4.39	6.58	7.10	6.88
20		9.08	8.70	8.52	8.05						

* structure is unstable

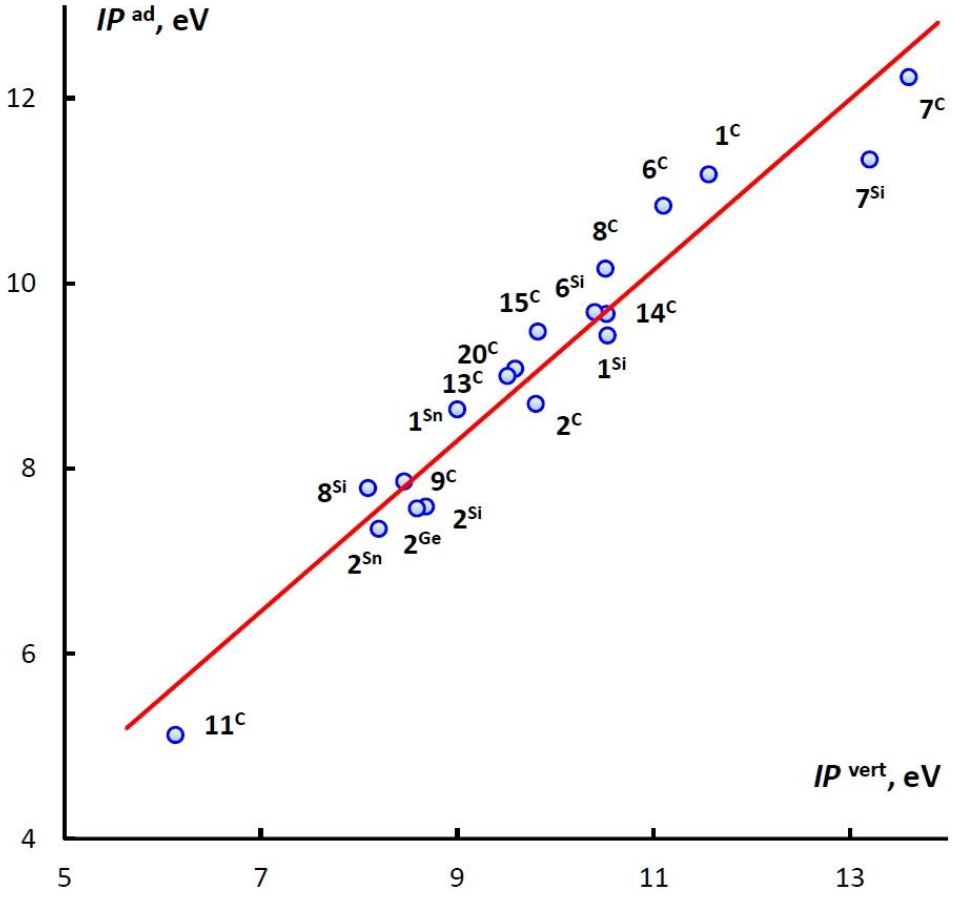


Figure S1. Correlation between the calculated using DFT-PBE0-DH/def2-TZVPP adiabatic ionization energies and the vertical values available from the literature.

Table S2. Adiabatic ionization potentials (eV) of metallylenes obtained using DFT-TPSS/D3/def2-TZVPP (above) and DFT-PBE0-DH/def2-TZVPP (below).

		M			
		C	Si	Ge	Sn
25	MH_2	9.59 9.62	8.83 8.85	8.89 8.85	8.48 8.48
26	MMe_2	7.14 7.15	7.48 7.51	7.62 7.65	7.41 7.50
27	$M(NH_2)_2$	7.44 7.45	7.94 7.95	8.24 8.43	7.96 8.32
28	$M(NMe_2)_2$	6.21 6.33	7.07 7.28	6.94 7.23	6.67 6.94
29	MPh_2	6.02 6.19	6.82 6.99	7.03 7.19	7.04 7.23
30	MCl_2	8.87 8.92	9.28 9.38	9.76 9.87	9.66 9.82
31	MF_2	11.00 11.04	10.41 10.46	11.03 11.19	10.66 10.90

Commentary on the atom M pyramidization question

The study and understanding of the principles of the spatial arrangement of atoms in molecules has attracted considerable attention since the late 19th century.[S11,S12] The unusual structures and properties of some compounds have stimulated debate on fundamental questions concerning the very definition of chemical bonding.[S13]

Traditionally, the two major bonding theories for molecular compounds valence bond (VB) and molecular orbital (MO) were in essential harmony in accounting for double or triple bonding in molecules such as ethylene or acetylene. In the heavier analogues of ethylene, these three simple bonding models are often no longer adequate. Theoretical data show that the planar forms of the heavier element ethylene analogues do not represent the most stable structures.[S14,S15,S16,S17,S18,S19,S20,S21,S22,S23] Instead, these molecules assume a trans-bent geometry with pyramidal coordination at the group 14 element. In addition, the effect of pyramidization becomes more noticeable with an increase in the atomic number.

Over the past fifty years, numerous heteroatom-containing analogues of classical organic moieties have been prepared and structurally characterized. A large number of reviews have been published on compounds containing the E-E bond.[S24,S25,S26]

Molecules involving multiple E-E bonds are often characterized by a strained geometry that is pyramidal or trans-bent compared to the idealized planar or linear structures of their carbon counterparts. These deformations are consistent with the increased nature of the non-bonding electron pairs in moving down the periodic table and the weakening of the E-E bond. The second-order Jahn-Teller effects provide an effective justification for strained geometry.

The first explanation of puckering as due to the vibronic coupling to the excited state was given for the $N_3H_3^{2+}$ radical (the authors called it pyramidalization).[S27]

The most important extension of the original JT theorem is the PJTE, which includes excited states in the vibronic coupling interactions. The first suggestion of what has been called the PJTE was given,[S28] showing that when two or more electronic states are not exactly degenerate but are very close in energy (pseudodegenerate), the JTE is not removed but modified, producing structural distortions (similar to those caused by the JTE) and further splitting of the term.

Methods of calculation of the PJTE vibronic coupling were then developed in a series of papers in applications to spectroscopic and other problems.[S29,S30,S31,S32,S33]

Trans-bent pyramidization effect, most commonly found in compounds containing the E-E bond, may also be rationalized in terms of a second-order Jahn-Teller interaction (SOJT or Pseudo Jahn-Teller Effect (PJTE)), i.e. a mixing of the inplane π- and σ^*-orbitals which have the same symmetry in the C_{2h} point group. This results in nonbonding electron density at the tetrel centers in orbitals which have lone pair character.

For example, since the effect of pyramidization is manifested everywhere from the structures discussed in the article, consider the very first – 1a (ethane C_2H_6 and the corresponding radical cation $C_2H_6^{+\cdot}$). This system has been the object of extensive experimental and theoretical research.[S34,S35,S36,S37]

Removal of an electron from the double degenerate e_g orbital of ethane, followed by PJTE distortion of the E_g state along the oscillations of the e_g mode, leads to the most energetically advantageous pyramidized structure of C_{2h} point-group symmetry with two in-plane H atoms on long C–H bonds forming a CCH angle of 81.8° and four out-of-plane H atoms on shorter C–H bonds and forming large CCH angles.[S38,S39,S40,S35,S41,S42,S43,S44,S45,S46]

The removal of an electron from the a_{1g} orbital (also shown in Figure S2) leads to the structure of the second in energy, preserving the symmetry of D_{3d} and A_{1g} electronic character, characterized by a long C-C bond.

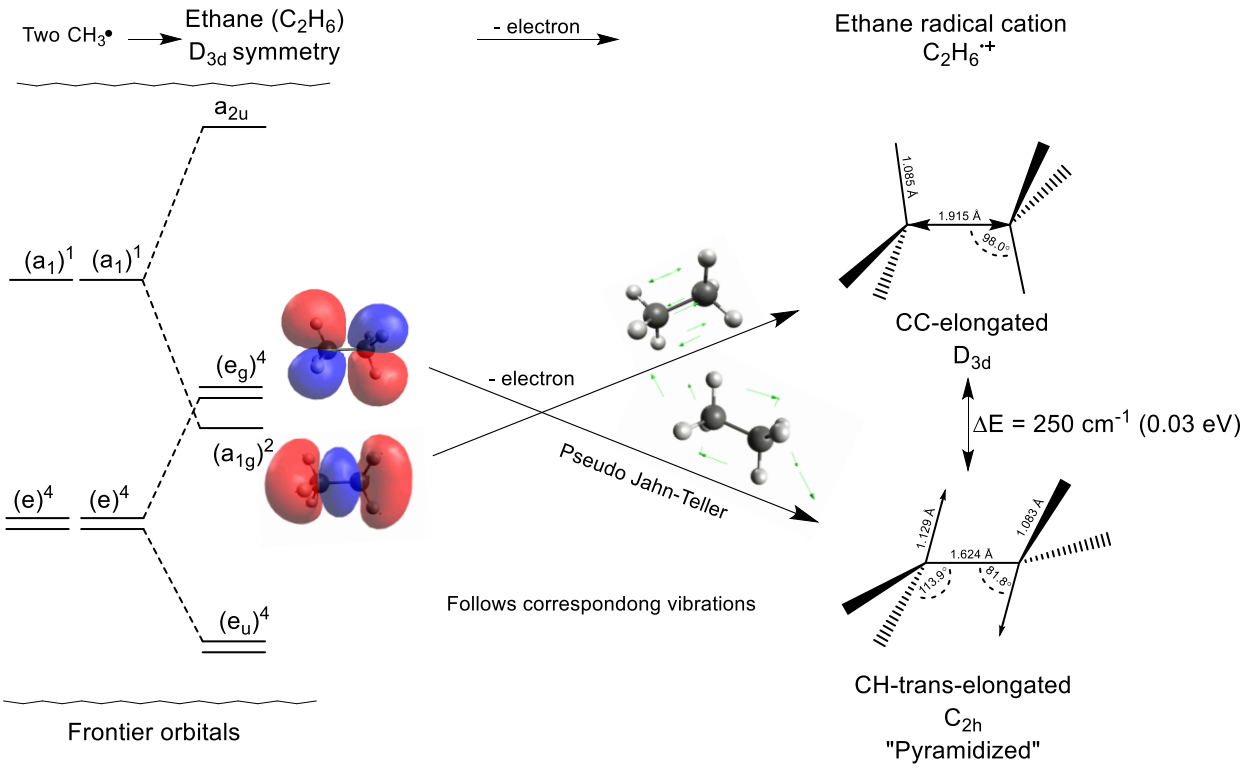


Figure S2. Schematic representation of the formation of the two lowest-lying C_{2h} and D_{3d} isomers of the ethane radical cation when an electron is removed from e_g and a_{1g} orbitals respectively. Energy and geometric parameters are taken from [S35,S37].

Cartesian coordinates and total energy values of 1-31 and its radical cations calculated by the DFT-TPSS/D3/def2-TZVPP

1C

8

Energy: -50123.9998398

C	-3.74726	-0.06708	0.82110
C	-2.40505	0.51508	0.36777
H	-1.99102	-0.05088	-0.47311
H	-1.66888	0.49221	1.17796
H	-2.51260	1.55623	0.04638
H	-3.63971	-1.10823	1.14249
H	-4.48343	-0.04421	0.01091
H	-4.16129	0.49888	1.66198

1C radical cation

8

Energy: -49861.5473237

C	-0.72346	-0.06650	0.06216
C	0.70514	0.08990	-0.06413
H	-1.29086	0.90330	-0.14560
H	-1.20979	-0.44315	-0.90079

H	-1.10895	-0.58104	0.93885
H	1.27257	-0.87970	0.14406
H	1.09057	0.60430	-0.94093
H	1.19119	0.46731	0.89867

1Si

8

Energy: -365620.0783132498

Si	-4.10462	-0.22210	0.94172
Si	-2.04769	0.67010	0.24715
H	-1.50300	-0.11049	-0.89304
H	-1.06361	0.63010	1.35888
H	-2.21447	2.08140	-0.18461
H	-3.93784	-1.63340	1.37348
H	-5.08870	-0.18210	-0.17001
H	-4.64932	0.55849	2.08192

1Si radical cation

8

Energy: -365405.6434021

Si	-4.26823	-0.29279	0.99725
Si	-1.88408	0.74079	0.19162
H	-1.60802	-0.20581	-0.90429
H	-1.14812	0.57059	1.45758
H	-2.35505	2.09251	-0.16096
H	-3.79726	-1.64451	1.34983
H	-5.00419	-0.12259	-0.26871
H	-4.54429	0.65381	2.09316

1Ge

8

Energy: -2608907.7551175

Ge	-4.13871	-0.23682	0.95300
Ge	-2.01360	0.68482	0.23587
H	-1.44727	-0.12138	-0.94485
H	-0.99238	0.64482	1.38479
H	-2.18330	2.14608	-0.21199
H	-3.96901	-1.69808	1.40086
H	-5.15993	-0.19682	-0.19592
H	-4.70504	0.56938	2.13372

1Ge radical cation

8

Energy: -2608693.6701956

Ge	-4.31191	-0.31145	1.01201

Ge	-1.84040	0.75945	0.17686
H	-1.57035	-0.22822	-0.95315
H	-1.09392	0.57630	1.49395
H	-2.34499	2.15287	-0.18268
H	-3.80732	-1.70487	1.37155
H	-5.05839	-0.12830	-0.30507
H	-4.58196	0.67622	2.14202

1Sn

8

Energy: -271096.8317096

Sn	-4.29302	-0.30473	1.00358
Sn	-1.85929	0.75273	0.18529
H	-1.22179	-0.14089	-1.13116
H	-0.71278	0.71184	1.45823
H	-2.03813	2.38125	-0.31754
H	-4.11418	-1.93325	1.50641
H	-5.43953	-0.26384	-0.26936
H	-4.93052	0.58889	2.32003

1Sn radical cation

8

Energy: -270896.2527989

Sn	-4.49019	-0.38974	1.06980
Sn	-1.66212	0.83774	0.11907
H	-1.36356	-0.26148	-1.13765
H	-0.82586	0.63639	1.58060
H	-2.21994	2.38811	-0.28273
H	-3.93237	-1.94011	1.47160
H	-5.32645	-0.18840	-0.39173
H	-4.78874	0.70948	2.32652

2C

26

Energy: -198230.1896536

C	-3.76934	-0.07678	0.82937
C	-2.38296	0.52478	0.35950
C	-1.79756	-0.27038	-0.82579
C	-1.34337	0.49204	1.49823
C	-2.53164	1.99057	-0.09560
C	-3.62066	-1.54254	1.28458
C	-4.80890	-0.04414	-0.30939
C	-4.35480	0.71844	2.01458
H	-3.20572	2.08537	-0.95192
H	-1.55348	2.37738	-0.40206
H	-2.90303	2.63389	0.70735

H	-2.45495	-0.24571	-1.69967
H	-1.61132	-1.31614	-0.56501
H	-0.83939	0.17097	-1.12121
H	-0.39931	0.91906	1.14249
H	-1.13710	-0.52867	1.83306
H	-1.66587	1.07902	2.36296
H	-3.24947	-2.18596	0.48162
H	-4.59878	-1.92926	1.59128
H	-2.94640	-1.63729	2.14076
H	-4.54081	1.76425	1.75380
H	-3.69756	0.69364	2.88856
H	-5.31309	0.27726	2.30984
H	-4.48627	-0.63097	-1.17417
H	-5.01536	0.97657	-0.64413
H	-5.75290	-0.47137	0.04627

2C radical cation

26

Energy: -198036.0870217

C	-4.16477	-0.24777	0.96070
C	-1.98754	0.69576	0.22817
C	-1.69088	-0.25141	-0.88226
C	-1.22476	0.53409	1.49645
C	-2.44177	2.06624	-0.13639
C	-3.71096	-1.61894	1.32319
C	-4.92821	-0.08407	-0.30692
C	-4.46035	0.69808	2.07255
H	-3.15861	2.07277	-0.95910
H	-1.55078	2.60895	-0.49588
H	-2.82393	2.63048	0.71591
H	-2.41875	-0.19942	-1.69358
H	-1.55964	-1.28044	-0.54359
H	-0.72345	0.06073	-1.31154
H	-0.20916	0.92080	1.30432
H	-1.10470	-0.50929	1.79273
H	-1.62949	1.12757	2.31797
H	-3.33039	-2.18255	0.46978
H	-4.60180	-2.16140	1.68345
H	-2.99295	-1.62680	2.14488
H	-4.59030	1.72778	1.73540
H	-3.73259	0.64399	2.88382
H	-5.42822	0.38653	2.50124
H	-4.52367	-0.67589	-1.12973
H	-5.04883	0.95980	-0.60123
H	-5.94355	-0.47159	-0.11503

2Si

26

Energy: -513778.4692453052

Si	-4.10725	-0.22319	0.94305
Si	-2.04506	0.67120	0.24581
C	-1.36117	-0.33142	-1.20828
C	-0.79851	0.61535	1.67072
C	-2.26909	2.47011	-0.30275
C	-3.88322	-2.02211	1.49162
C	-5.35381	-0.16734	-0.48185
C	-4.79114	0.77941	2.39715
H	-2.96959	2.54635	-1.14210
H	-1.31533	2.90557	-0.62492
H	-2.65924	3.09016	0.51225
H	-2.04725	-0.31225	-2.06260
H	-1.20507	-1.38018	-0.93144
H	-0.39801	0.07022	-1.54614
H	0.16909	1.03170	1.36502
H	-0.62629	-0.41256	2.00934
H	-1.15210	1.19349	2.53191
H	-3.49307	-2.64216	0.67661
H	-4.83697	-2.45757	1.81378
H	-3.18272	-2.09835	2.33097
H	-4.94724	1.82818	2.12031
H	-4.10506	0.76025	3.25147
H	-5.75429	0.37778	2.73501
H	-5.00021	-0.74548	-1.34305
H	-5.52602	0.86056	-0.82046
H	-6.32140	-0.58370	-0.17615

2Si radical cation

26

Energy: -513610.2697955

Si	-4.23212	-0.27737	0.98578
Si	-1.92019	0.72537	0.20309
C	-1.45827	-0.40494	-1.20457
C	-0.88497	0.56305	1.74399
C	-2.39309	2.46292	-0.27632
C	-3.75922	-2.01493	1.46517
C	-5.26734	-0.11503	-0.55512
C	-4.69403	0.85293	2.39344
H	-3.11253	2.48670	-1.09904
H	-1.48011	2.97136	-0.62004
H	-2.79015	3.03465	0.56664
H	-2.17845	-0.36329	-2.02593
H	-1.33670	-1.44289	-0.88365
H	-0.48865	-0.06444	-1.59715

H	0.11694	0.95346	1.51166
H	-0.76746	-0.47702	2.05954
H	-1.28182	1.15002	2.57645
H	-3.36216	-2.58664	0.62221
H	-4.67220	-2.52337	1.80889
H	-3.03978	-2.03871	2.28789
H	-4.81560	1.89088	2.07254
H	-3.97385	0.81127	3.21481
H	-5.66366	0.51243	2.78603
H	-4.87050	-0.70200	-1.38758
H	-5.38485	0.92504	-0.87066
H	-6.26925	-0.50545	-0.32279

2Ge

26

Energy: -2757057.1388453

Ge	-4.14474	-0.23918	0.95569
Ge	-2.00757	0.68718	0.23318
C	-1.27587	-0.34927	-1.28781
C	-0.69003	0.63699	1.71115
C	-2.22311	2.56936	-0.34463
C	-3.92920	-2.12136	1.53350
C	-5.46227	-0.18899	-0.52228
C	-4.87644	0.79727	2.47668
H	-2.92116	2.63693	-1.18401
H	-1.25838	2.97788	-0.66189
H	-2.60696	3.18300	0.47538
H	-1.96186	-0.32019	-2.13920
H	-1.12055	-1.39387	-1.00325
H	-0.31524	0.07150	-1.60151
H	0.26402	1.05805	1.37837
H	-0.51924	-0.39202	2.04022
H	-1.04716	1.21929	2.56535
H	-3.54535	-2.73500	0.71349
H	-4.89393	-2.52987	1.85076
H	-3.23115	-2.18892	2.37288
H	-5.03176	1.84187	2.19212
H	-4.19045	0.76820	3.32807
H	-5.83707	0.37651	2.79038
H	-5.10514	-0.77129	-1.37648
H	-5.63306	0.84002	-0.85135
H	-6.41632	-0.61005	-0.18951

2Ge radical cation

26

Energy: -2756883.9276790

Ge	-4.27476	-0.29642	0.99904
Ge	-1.87755	0.74443	0.18983
C	-1.40774	-0.45114	-1.28451
C	-0.80555	0.56690	1.81548
C	-2.39114	2.56410	-0.30879
C	-3.76117	-2.11610	1.49766
C	-5.34676	-0.11889	-0.62661
C	-4.74457	0.89914	2.47338
H	-3.12422	2.55875	-1.11705
H	-1.48382	3.06866	-0.66300
H	-2.78194	3.11218	0.55007
H	-2.14580	-0.39614	-2.08635
H	-1.30365	-1.48096	-0.93893
H	-0.43991	-0.11393	-1.67549
H	0.19422	0.95507	1.58507
H	-0.71249	-0.47863	2.11371
H	-1.22789	1.15497	2.63191
H	-3.37037	-2.66418	0.63880
H	-4.66849	-2.62066	1.85186
H	-3.02810	-2.11075	2.30592
H	-4.84865	1.92896	2.12780
H	-4.00651	0.84413	3.27522
H	-5.71240	0.56193	2.86436
H	-4.92442	-0.70696	-1.44304
H	-5.43982	0.92664	-0.92483
H	-6.34653	-0.50706	-0.39620

2Sn

26

Energy: -419242.4448541

Sn	-4.30004	-0.30819	1.00584
Sn	-1.85227	0.75619	0.18302
C	-1.02021	-0.36138	-1.48952
C	-0.37958	0.71478	1.78505
C	-2.05461	2.82525	-0.46128
C	-4.09770	-2.37725	1.65016
C	-5.77272	-0.26679	-0.59619
C	-5.13211	0.80938	2.67838
H	-2.75299	2.89364	-1.29913
H	-1.07915	3.20347	-0.78011
H	-2.42457	3.44396	0.36006
H	-1.70143	-0.32695	-2.34340
H	-0.86001	-1.40450	-1.20569
H	-0.06239	0.07897	-1.78080
H	0.56230	1.13690	1.42330
H	-0.20568	-0.31328	2.11238
H	-0.72929	1.30382	2.63651

H	-3.72774	-2.99596	0.82882
H	-5.07316	-2.75546	1.96899
H	-3.39932	-2.44563	2.48800
H	-5.29230	1.85251	2.39455
H	-4.45088	0.77496	3.53226
H	-6.08992	0.36904	2.96967
H	-5.42302	-0.85583	-1.44764
H	-5.94663	0.76127	-0.92352
H	-6.71461	-0.68890	-0.23443

2Sn radical cation

26

Energy: -419069.8882792579

Sn	-4.43240	-0.36666	1.05034
Sn	-1.71991	0.81466	0.13853
C	-1.23313	-0.52113	-1.48174
C	-0.56330	0.60693	1.94531
C	-2.31466	2.81405	-0.40380
C	-3.83764	-2.36603	1.59271
C	-5.58900	-0.15897	-0.75645
C	-4.91920	0.96916	2.67058
H	-3.06144	2.77981	-1.19802
H	-1.42209	3.33330	-0.76624
H	-2.70908	3.33618	0.46878
H	-1.99658	-0.45948	-2.25822
H	-1.14755	-1.54323	-1.11082
H	-0.27023	-0.20070	-1.89132
H	0.44265	0.98267	1.73432
H	-0.50477	-0.44346	2.23318
H	-1.01103	1.19763	2.74542
H	-3.44320	-2.88817	0.72015
H	-4.73021	-2.88528	1.95516
H	-3.09088	-2.33177	2.38695
H	-5.00479	1.99126	2.29963
H	-4.15576	0.90754	3.44707
H	-5.88211	0.64873	3.08016
H	-5.14125	-0.74970	-1.55655
H	-5.64752	0.89140	-1.04435
H	-6.59495	-0.53472	-0.54546

3C

20

Energy: -258647.6397619

C	-3.74478	-0.06123	0.72662
C	-2.29466	0.41506	0.22680
N	-1.57054	-0.56323	-0.58386
N	-1.45740	0.57693	1.42877

N	-2.45182	1.58760	-0.63785
N	-3.69770	-1.52944	0.84413
N	-4.76269	0.50212	-0.16486
N	-4.11440	0.39384	2.06623
H	-3.11752	2.24771	-0.24337
H	-1.55003	2.04358	-0.75801
H	-2.02422	-0.65526	-1.48947
H	-1.58900	-1.46284	-0.10539
H	-3.80405	-1.95964	-0.07204
H	-4.49127	-1.81326	1.41688
H	-4.28454	1.39644	2.04766
H	-3.34387	0.19493	2.70280
H	-4.48259	0.41818	-1.13904
H	-5.64496	0.01565	-0.02138
H	-0.48607	0.59772	1.12141
H	-1.66009	1.46505	1.88262

3C radical cation

20

Energy: -258481.1483412

C	-3.74224	-0.02554	0.72448
C	-2.31564	0.40745	0.19934
N	-1.76293	-0.33543	-0.90892
N	-1.38615	0.22818	1.29667
N	-2.42757	1.77645	-0.25985
N	-3.62681	-1.39242	1.19061
N	-4.67147	0.14569	-0.37360
N	-4.29724	0.72105	1.82893
H	-2.76610	2.45123	0.41834
H	-1.61501	2.10996	-0.77364
H	-2.27492	-0.23205	-1.77810
H	-1.55339	-1.30534	-0.69993
H	-3.28446	-2.07010	0.51730
H	-4.43812	-1.72593	1.70641
H	-4.51251	1.68834	1.61377
H	-3.78502	0.62564	2.69882
H	-4.45655	-0.36010	-1.22675
H	-5.64995	0.06499	-0.10599
H	-0.40744	0.30624	1.02892
H	-1.59865	0.73159	2.15186

3Si

20

Energy: -574291.233943401

Si	-4.08378	-0.10651	0.89462
Si	-1.96251	0.47174	0.04600
N	-1.00780	-0.67222	-0.84634

N	-0.97892	0.76927	1.44162
N	-2.28420	1.68624	-1.15830
N	-4.09542	-1.83893	0.95201
N	-5.20761	0.81473	-0.06273
N	-4.55401	0.32200	2.51044
H	-2.99330	2.38164	-0.95354
H	-1.52089	2.10028	-1.68397
H	-1.28733	-0.93555	-1.78282
H	-0.58392	-1.45017	-0.35674
H	-3.58969	-2.36392	0.24941
H	-4.90371	-2.35446	1.28206
H	-4.75298	1.28850	2.73548
H	-4.12975	-0.15854	3.29376
H	-5.02526	0.90245	-1.05639
H	-6.20525	0.74703	0.11181
H	-0.00584	1.04176	1.35915
H	-1.40000	1.16458	2.27312

3Si radical cation

20

Energy: -574143.9974740

Si	-4.16927	-0.17504	0.86344
Si	-1.88668	0.55640	0.06100
N	-1.03075	-0.87831	-0.24226
N	-1.23028	1.47012	1.33253
N	-2.17322	1.47072	-1.34074
N	-4.38095	-1.74718	0.25816
N	-5.26166	0.94636	0.20615
N	-4.09409	-0.11606	2.55880
H	-2.84111	2.22846	-1.39656
H	-1.78916	1.21639	-2.24252
H	-1.38644	-1.64325	-0.80074
H	-0.17065	-1.10989	0.23942
H	-3.70419	-2.49173	0.36344
H	-5.14230	-1.99219	-0.36288
H	-3.76212	0.68211	3.08438
H	-4.24474	-0.93322	3.13754
H	-5.28975	1.20617	-0.77114
H	-5.86152	1.52176	0.78448
H	-0.95955	2.43955	1.22177
H	-1.19375	1.15874	2.29439

3Ge

20

Energy: -2817524.7902386

Ge	-4.11299	-0.15766	0.91831
Ge	-1.90293	0.47770	0.06731

N	-0.79473	-0.73401	-0.79187
N	-0.84806	0.93809	1.53147
N	-2.25716	1.67906	-1.31684
N	-4.22293	-2.01614	0.86937
N	-5.30878	0.93127	-0.01398
N	-4.62474	0.17414	2.66861
H	-2.89683	2.42323	-1.04765
H	-1.42220	2.10108	-1.71882
H	-1.18704	-1.09314	-1.65837
H	-0.52945	-1.52108	-0.20530
H	-3.94630	-2.42608	-0.01902
H	-5.14362	-2.37395	1.11604
H	-4.65851	1.16458	2.89591
H	-4.03809	-0.29569	3.35350
H	-5.16298	0.91676	-1.02093
H	-6.28751	0.72183	0.17323
H	0.06353	1.31059	1.27303
H	-1.29083	1.58933	2.17464

3Ge radical cation

20

Energy: -2817362.2518484

Ge	-4.20883	-0.18323	0.88328
Ge	-1.84693	0.56533	0.04046
N	-0.87606	-0.90403	-0.42653
N	-0.98158	1.46513	1.36749
N	-2.03057	1.65386	-1.40894
N	-4.51293	-1.91191	0.39446
N	-5.48715	0.88675	0.14752
N	-4.28187	-0.04882	2.69895
H	-2.80831	2.30276	-1.45711
H	-1.81912	1.25718	-2.31976
H	-1.33837	-1.69927	-0.85323
H	-0.14074	-1.19765	0.20971
H	-3.74663	-2.57597	0.38703
H	-5.15143	-2.07153	-0.37919
H	-3.79590	0.70623	3.17000
H	-4.23538	-0.91201	3.23226
H	-5.37223	1.23106	-0.79931
H	-5.91089	1.58673	0.74937
H	-0.91578	2.47488	1.27899
H	-1.11145	1.18442	2.33321

3Sn

20

Energy: -479704.8076781

Sn	-4.26081	-0.22234	0.99889

Sn	-1.72995	0.50731	0.02705
N	-0.44231	-0.79231	-0.89000
N	-0.52867	1.11951	1.58654
N	-2.14949	1.75976	-1.56007
N	-4.48872	-2.26817	0.88746
N	-5.55683	1.05480	0.02289
N	-4.87418	0.07329	2.92890
H	-2.77937	2.51571	-1.29242
H	-1.30775	2.19328	-1.94002
H	-0.85144	-1.21437	-1.72240
H	-0.16128	-1.55433	-0.27457
H	-4.26823	-2.63772	-0.03645
H	-5.44822	-2.54495	1.09666
H	-4.84166	1.05630	3.19535
H	-4.29934	-0.43781	3.59733
H	-5.42357	1.03363	-0.98787
H	-6.53353	0.81921	0.20003
H	0.34519	1.51931	1.24366
H	-0.97199	1.82981	2.16768

3Sn radical cation

20

Energy: -479535.3322345524

Sn	-4.37391	-0.23341	0.93977
Sn	-1.68519	0.61670	-0.01770
N	-0.73660	-0.87492	-1.00170
N	-0.49667	1.17260	1.52260
N	-1.80667	2.19135	-1.28258
N	-4.57253	-2.24618	0.87340
N	-5.85851	0.55549	-0.18573
N	-4.69831	0.34200	2.85204
H	-2.62996	2.25665	-1.87622
H	-1.62389	3.10058	-0.86102
H	-0.78501	-0.82233	-2.01794
H	-0.92607	-1.82948	-0.70619
H	-4.07881	-2.74401	0.13659
H	-4.42417	-2.72552	1.76000
H	-5.26075	1.18438	2.96109
H	-3.89393	0.39342	3.47229
H	-5.70479	1.47545	-0.59130
H	-6.23926	-0.06589	-0.89758
H	0.16448	0.46422	1.83705
H	-0.94163	1.59880	2.33178

4C

22

Energy: -238508.3178166

C	-3.77643	-0.07282	0.79905
C	-2.38974	0.50693	0.31639
N	-1.76260	-0.29566	-0.76417
C	-1.38090	0.55423	1.46677
N	-2.63229	1.88452	-0.13102
N	-3.55655	-1.46883	1.21770
C	-4.84728	0.05200	-0.30033
N	-4.30629	0.60883	1.98769
H	-3.14000	1.87982	-1.01516
H	-1.73218	2.31923	-0.33198
H	-2.43546	-0.48593	-1.50667
H	-1.46147	-1.19828	-0.39615
H	-3.42878	-2.05905	0.39729
H	-4.40930	-1.78888	1.67695
H	-4.27676	1.61339	1.81011
H	-3.67296	0.43251	2.76739
H	-0.40241	0.84319	1.07187
H	-1.30060	-0.42729	1.93982
H	-1.68585	1.28909	2.21446
H	-4.53106	-0.43145	-1.23214
H	-5.08935	1.09836	-0.51215
H	-5.76066	-0.43758	0.04608

4C radical cation

22

Energy: -238362.0900536

C	-4.20476	-0.27042	1.00671
C	-1.99442	0.67518	0.05196
N	-1.74623	-0.17131	-0.99398
C	-1.26072	0.43972	1.33041
N	-2.43152	1.95022	-0.23387
N	-3.80106	-1.50834	1.43222
C	-4.88732	-0.15608	-0.31641
N	-4.46423	0.68902	1.94388
H	-2.47591	2.23417	-1.20571
H	-2.09335	2.68791	0.37158
H	-2.21107	-0.02312	-1.88082
H	-1.56967	-1.14184	-0.77011
H	-4.08177	-2.30674	0.87875
H	-3.74189	-1.69826	2.42479
H	-4.55791	1.63758	1.60224
H	-4.04681	0.61454	2.86327
H	-0.20758	0.73271	1.22632
H	-1.29376	-0.61715	1.60600
H	-1.69685	1.03178	2.13916
H	-4.43140	-0.82810	-1.04736
H	-4.83358	0.87024	-0.68801
H	-5.94710	-0.42538	-0.21923

4Si

22

Energy: -554115.6967146686

Si	-4.15387	-0.18028	0.89168
Si	-2.02151	0.51089	0.14500
N	-1.15875	-0.66690	-0.82017
C	-0.85322	0.83849	1.58525
N	-2.29813	1.98463	-0.72921
N	-3.96293	-1.89264	1.07368
C	-5.52180	0.38381	-0.28716
N	-4.69256	0.38198	2.45135
H	-3.16612	2.11756	-1.23219
H	-1.53867	2.46204	-1.20291
H	-1.56808	-1.06571	-1.65639
H	-0.53010	-1.32864	-0.38055
H	-3.31013	-2.38790	0.47975
H	-4.72208	-2.49142	1.37670
H	-5.12517	1.29656	2.51602
H	-4.09299	0.22767	3.25456
H	0.10095	1.24982	1.23412
H	-0.63743	-0.07991	2.14371
H	-1.29562	1.55784	2.28186
H	-5.31925	0.05346	-1.31254
H	-5.62015	1.47687	-0.30361
H	-6.49130	-0.03191	0.01282

4Si radical cation

22

Energy: -553943.1098757

Si	-4.21807	-0.22284	0.95779
Si	-1.95602	0.59439	0.08700
N	-1.58289	-0.52493	-1.13190
C	-0.87619	0.57787	1.59669
N	-2.22479	2.13485	-0.56371
N	-3.92005	-1.83214	1.40442
C	-5.34543	0.03739	-0.49371
N	-4.58030	0.72887	2.31152
H	-2.60160	2.31903	-1.48138
H	-2.15224	2.97545	-0.01009
H	-1.61670	-0.32606	-2.12071
H	-1.34755	-1.48771	-0.94454
H	-3.75023	-2.56718	0.73480
H	-3.83304	-2.15646	2.35609
H	-5.05541	1.61594	2.23560
H	-4.22926	0.56794	3.24371
H	0.13209	0.89696	1.32047
H	-0.81929	-0.42676	2.01945

H	-1.26574	1.25294	2.36077
H	-4.99349	-0.52552	-1.36004
H	-5.39331	1.09372	-0.76421
H	-6.34943	-0.30941	-0.23626

4Ge

22

Energy: -2797366.0664477

Ge	-4.19329	-0.19128	0.89819
Ge	-1.96944	0.56978	0.17834
N	-1.03233	-0.60579	-0.95621
C	-0.72902	0.89929	1.66415
N	-2.23536	2.19153	-0.70424
N	-3.95843	-2.01729	1.19814
C	-5.64182	0.29756	-0.35693
N	-4.81315	0.36514	2.56818
H	-2.98311	2.15707	-1.39318
H	-1.39760	2.52063	-1.18182
H	-1.58634	-0.94373	-1.74093
H	-0.67263	-1.42426	-0.46665
H	-3.52270	-2.50470	0.41903
H	-4.82223	-2.50237	1.43301
H	-5.05080	1.35463	2.59716
H	-4.13673	0.19129	3.30897
H	0.22340	1.26752	1.27223
H	-0.54875	-0.02364	2.22222
H	-1.14937	1.64579	2.34211
H	-5.43702	-0.10466	-1.35316
H	-5.73281	1.38574	-0.43142
H	-6.58937	-0.11194	0.00458

4Ge radical cation

22

Energy: -2797209.4123091

Ge	-4.28346	-0.19989	0.91128
Ge	-1.89603	0.60202	0.13675
N	-1.39819	-0.45235	-1.26629
C	-0.68749	0.47068	1.66229
N	-2.07633	2.30505	-0.49362
N	-4.10330	-1.90469	1.53709
C	-5.49282	-0.06640	-0.61364
N	-4.78356	0.85065	2.31658
H	-2.49049	2.47650	-1.40384
H	-2.31132	3.04593	0.15810
H	-1.82118	-0.33182	-2.18040
H	-1.17710	-1.42676	-1.09237
H	-3.86694	-2.64355	0.88362

H	-3.68957	-2.07838	2.44708
H	-5.00198	1.82584	2.14293
H	-4.35736	0.73066	3.22939
H	0.30138	0.80448	1.33967
H	-0.63613	-0.56461	2.00450
H	-1.04699	1.10675	2.47324
H	-5.13319	-0.70091	-1.42576
H	-5.54603	0.96923	-0.95445
H	-6.48085	-0.40212	-0.29037

4Sn

22

Energy: -459549.7700354

Sn	-4.37065	-0.23510	0.92199
Sn	-1.78807	0.59713	0.15344
N	-0.67854	-0.72261	-1.00378
C	-0.43805	1.11820	1.75445
N	-2.03784	2.30923	-0.97042
N	-4.18403	-2.27614	1.15145
C	-6.00244	0.40592	-0.36188
N	-5.03986	0.22729	2.81517
H	-2.81309	2.23006	-1.62713
H	-1.20676	2.50634	-1.52905
H	-1.22432	-1.11962	-1.76851
H	-0.33791	-1.51444	-0.45676
H	-3.74509	-2.72298	0.34771
H	-5.08714	-2.73011	1.28683
H	-5.20343	1.22586	2.94165
H	-4.36152	-0.04754	3.52526
H	0.50059	1.46707	1.31696
H	-0.24311	0.24797	2.38524
H	-0.87732	1.91407	2.35896
H	-5.83965	0.05085	-1.38207
H	-6.06705	1.49697	-0.36596
H	-6.93365	-0.01208	0.02823

4Sn radical cation

22

Energy: -459386.5691224141

Sn	-4.46654	-0.25196	0.89009
Sn	-1.71479	0.65887	0.15904
N	-1.11699	-0.47481	-1.41028
C	-0.34762	0.54772	1.81124
N	-1.87098	2.53661	-0.58547
N	-4.29483	-2.12167	1.65132
C	-5.82623	-0.16797	-0.76980
N	-5.08382	0.88879	2.44646

H	-2.13090	3.27819	0.05981
H	-2.35863	2.67270	-1.46736
H	-1.58491	-0.35805	-2.30546
H	-0.95178	-1.46396	-1.24305
H	-4.02737	-2.86737	1.01398
H	-3.81034	-2.24636	2.53658
H	-5.25582	1.87509	2.26933
H	-4.61943	0.78416	3.34501
H	0.61756	0.90689	1.44936
H	-0.26950	-0.48796	2.14322
H	-0.71101	1.17988	2.62192
H	-5.45413	-0.80579	-1.57204
H	-5.91019	0.86362	-1.11297
H	-6.79069	-0.53028	-0.40913

5Si

68

Energy: -1236130.0589913

Si	-4.08356	-0.23861	0.98472
Si	-2.06744	0.68761	0.20755
C	-3.75026	-2.00685	1.53240
C	-4.01258	-2.43490	2.84397
C	-3.16685	-2.92648	0.63959
C	-3.70191	-3.73251	3.25283
H	-4.45806	-1.74255	3.55316
C	-2.85856	-4.22431	1.04404
H	-2.94013	-2.62100	-0.37851
C	-3.12346	-4.62914	2.35412
H	-3.91063	-4.04348	4.27267
H	-2.40632	-4.91711	0.34005
H	-2.87880	-5.63844	2.67244
C	-4.69003	0.79568	2.43429
C	-5.96980	1.37384	2.44773
C	-3.83645	1.05250	3.52459
C	-6.38363	2.18123	3.50823
H	-6.64659	1.19381	1.61684
C	-4.24745	1.85664	4.58629
H	-2.83596	0.62822	3.53792
C	-5.52283	2.42547	4.57863
H	-7.37727	2.62043	3.49828
H	-3.57162	2.04395	5.41592
H	-5.84316	3.05636	5.40278
C	-5.33877	-0.20240	-0.41594
C	-5.62189	1.00793	-1.07798
C	-5.98039	-1.36733	-0.86734
C	-6.51019	1.04972	-2.15123
H	-5.13406	1.92485	-0.75817

C	-6.86842	-1.32921	-1.94328
H	-5.77803	-2.31459	-0.37479
C	-7.13345	-0.12104	-2.58852
H	-6.71186	1.99363	-2.64967
H	-7.35263	-2.24233	-2.27803
H	-7.82202	-0.09093	-3.42803
C	-2.40156	2.45588	-0.33968
C	-2.14016	2.88370	-1.65154
C	-2.98504	3.37545	0.55312
C	-2.45178	4.18101	-2.06065
H	-1.69465	2.19141	-2.36077
C	-3.29429	4.67298	0.14841
H	-3.21116	3.07019	1.57141
C	-3.03030	5.07758	-1.16193
H	-2.24374	4.49177	-3.08069
H	-3.74660	5.36571	0.85242
H	-3.27572	6.08664	-1.48042
C	-0.81313	0.65112	1.60896
C	-0.52988	-0.55974	2.26998
C	-0.17285	1.81601	2.06229
C	0.35720	-0.60205	3.34421
H	-1.01672	-1.47665	1.94860
C	0.71396	1.77737	3.13923
H	-0.37531	2.76364	1.57051
C	0.97907	0.56871	3.78349
H	0.55898	-1.54635	3.84188
H	1.19715	2.69047	3.47551
H	1.66667	0.53819	4.62379
C	-1.45968	-0.34564	-1.24217
C	-0.17838	-0.92034	-1.25655
C	-2.31341	-0.60481	-2.33179
C	0.23687	-1.72654	-2.31740
H	0.49850	-0.73854	-0.42611
C	-1.90102	-1.40777	-3.39384
H	-3.31508	-0.18325	-2.34428
C	-0.62405	-1.97306	-3.38718
H	1.23170	-2.16306	-2.30823
H	-2.57697	-1.59693	-4.22296
H	-0.30261	-2.60302	-4.21160

5Si radical cation

68

Energy: -1235977.6472092

Si	-4.16822	-0.27909	1.02398
Si	-1.98322	0.72852	0.16881
C	-3.64093	-1.98341	1.52267
C	-3.72158	-2.39224	2.86930
C	-3.11152	-2.88397	0.57436

C	-3.29677	-3.66194	3.25115
H	-4.13208	-1.71900	3.61518
C	-2.68611	-4.15133	0.95944
H	-3.02110	-2.58560	-0.46551
C	-2.77349	-4.54005	2.29927
H	-3.37664	-3.96939	4.28900
H	-2.28133	-4.83424	0.21933
H	-2.43555	-5.52673	2.60012
C	-4.59809	0.86311	2.41620
C	-5.76491	1.65234	2.36904
C	-3.74123	0.98945	3.53004
C	-6.06856	2.52952	3.40669
H	-6.44225	1.56689	1.52508
C	-4.04702	1.86752	4.56470
H	-2.82654	0.40691	3.57880
C	-5.20863	2.64226	4.50184
H	-6.97711	3.12187	3.36516
H	-3.38003	1.95407	5.41647
H	-5.44436	3.33172	5.30639
C	-5.25535	-0.17934	-0.47153
C	-5.57504	1.06649	-1.05159
C	-5.73387	-1.35351	-1.08737
C	-6.35249	1.13378	-2.20333
H	-5.20130	1.98375	-0.60721
C	-6.51296	-1.28262	-2.23896
H	-5.50512	-2.32245	-0.65491
C	-6.81752	-0.04089	-2.80154
H	-6.59125	2.09849	-2.63948
H	-6.88526	-2.19350	-2.69691
H	-7.41792	0.01215	-3.70429
C	-2.51063	2.43275	-0.33003
C	-2.43008	2.84151	-1.67668
C	-3.04019	3.33329	0.61823
C	-2.85508	4.11112	-2.05861
H	-2.01949	2.16829	-2.42253
C	-3.46578	4.60057	0.23307
H	-3.13057	3.03498	1.65812
C	-3.37848	4.98922	-1.10678
H	-2.77527	4.41852	-3.09649
H	-3.87066	5.28346	0.97314
H	-3.71658	5.97583	-1.40769
C	-0.89602	0.62890	1.66429
C	-0.57636	-0.61690	2.24443
C	-0.41750	1.80309	2.28009
C	0.20116	-0.68415	3.39612
H	-0.95018	-1.53417	1.80015
C	0.36166	1.73224	3.43164
H	-0.64627	2.77202	1.84762
C	0.66626	0.49054	3.99425

H	0.43992	-1.64884	3.83230
H	0.73397	2.64314	3.88954
H	1.26671	0.43754	4.89696
C	-1.55328	-0.41382	-1.22330
C	-0.38644	-1.20304	-1.17599
C	-2.40995	-0.54017	-2.33728
C	-0.08267	-2.08027	-2.21356
H	0.29080	-1.11752	-0.33196
C	-2.10403	-1.41828	-3.37187
H	-3.32463	0.04238	-2.38620
C	-0.94245	-2.19305	-3.30882
H	0.82588	-2.67261	-2.17188
H	-2.77090	-1.50484	-4.22373
H	-0.70661	-2.88252	-4.11332

5Ge

68

Energy: -3479399.8097649

Ge	-4.11803	-0.25531	1.00241
Ge	-2.03337	0.70455	0.19015
C	-3.77904	-2.10315	1.56716
C	-4.07666	-2.52973	2.86842
C	-3.17393	-3.00953	0.68140
C	-3.77744	-3.83075	3.27687
H	-4.54039	-1.84004	3.56872
C	-2.87695	-4.31063	1.08747
H	-2.92291	-2.69749	-0.32913
C	-3.17676	-4.72243	2.38754
H	-4.01236	-4.14766	4.28919
H	-2.40727	-5.00008	0.39163
H	-2.94174	-5.73386	2.70610
C	-4.75220	0.81295	2.52051
C	-6.03336	1.38071	2.52313
C	-3.89966	1.06651	3.60732
C	-6.45477	2.18249	3.58554
H	-6.70469	1.19874	1.68801
C	-4.31997	1.86602	4.67027
H	-2.89773	0.64532	3.62198
C	-5.59858	2.42701	4.65983
H	-7.45052	2.61693	3.57361
H	-3.64854	2.05450	5.50324
H	-5.92539	3.05290	5.48514
C	-5.43567	-0.21813	-0.45060
C	-5.70079	0.98302	-1.12823
C	-6.08759	-1.38565	-0.86988
C	-6.59668	1.01430	-2.19698
H	-5.19857	1.89918	-0.82829

C	-6.98290	-1.35616	-1.94074
H	-5.89067	-2.32526	-0.36032
C	-7.23790	-0.15661	-2.60623
H	-6.79014	1.95066	-2.71272
H	-7.47983	-2.26948	-2.25578
H	-7.93227	-0.13392	-3.44111
C	-2.37258	2.55229	-0.37479
C	-2.07493	2.97879	-1.67606
C	-2.97796	3.45866	0.51082
C	-2.37437	4.27970	-2.08470
H	-1.61099	2.28911	-2.37624
C	-3.27515	4.75965	0.10457
H	-3.22902	3.14668	1.52136
C	-2.97530	5.17136	-1.19552
H	-2.13942	4.59654	-3.09703
H	-3.74503	5.44909	0.80029
H	-3.21050	6.18270	-1.51422
C	-0.71603	0.66767	1.64344
C	-0.45068	-0.53347	2.32101
C	-0.06469	1.83538	2.06309
C	0.44485	-0.56455	3.39006
H	-0.95246	-1.44978	2.02079
C	0.83026	1.80609	3.13426
H	-0.26178	2.77498	1.55359
C	1.08548	0.60655	3.79969
H	0.63850	-1.50090	3.90574
H	1.32675	2.71956	3.44957
H	1.77957	0.58401	4.63480
C	-1.39868	-0.36369	-1.32774
C	-0.11733	-0.93103	-1.33010
C	-2.25095	-0.61763	-2.41468
C	0.30454	-1.73271	-2.39240
H	0.55380	-0.74878	-0.49488
C	-1.83018	-1.41705	-3.47751
H	-3.25303	-0.19679	-2.42952
C	-0.55137	-1.97759	-3.46683
H	1.30043	-2.16681	-2.38027
H	-2.50140	-1.60580	-4.31059
H	-0.22420	-2.60338	-4.29206

5Ge radical cation

68

Energy: -3479247.7789573

Ge	-4.20671	-0.29779	1.03299
Ge	-1.94446	0.74722	0.15974
C	-3.62952	-2.07106	1.54673
C	-3.68305	-2.46697	2.89441
C	-3.10478	-2.95578	0.58750

C	-3.23529	-3.73140	3.27062
H	-4.08666	-1.79469	3.64524
C	-2.65607	-4.21739	0.96947
H	-3.03348	-2.65525	-0.45333
C	-2.71780	-4.60457	2.31095
H	-3.29180	-4.03710	4.31055
H	-2.25410	-4.89643	0.22422
H	-2.36271	-5.58632	2.60787
C	-4.63333	0.90828	2.48282
C	-5.77930	1.71957	2.42114
C	-3.76665	1.01894	3.58511
C	-6.05993	2.61238	3.45314
H	-6.45712	1.64434	1.57633
C	-4.05076	1.91453	4.61260
H	-2.86401	0.41763	3.63381
C	-5.19511	2.71385	4.54560
H	-6.95354	3.22680	3.40748
H	-3.37951	1.99401	5.46177
H	-5.41304	3.41553	5.34449
C	-5.31850	-0.18303	-0.54433
C	-5.62685	1.06774	-1.10891
C	-5.77338	-1.35558	-1.17172
C	-6.38787	1.14158	-2.27266
H	-5.26082	1.98093	-0.64965
C	-6.53675	-1.27564	-2.33428
H	-5.54188	-2.32717	-0.74614
C	-6.83969	-0.02930	-2.88767
H	-6.62435	2.10937	-2.70332
H	-6.89634	-2.18357	-2.80803
H	-7.42774	0.02996	-3.79804
C	-2.52164	2.52048	-0.35400
C	-2.46806	2.91638	-1.70168
C	-3.04647	3.40519	0.60520
C	-2.91585	4.18078	-2.07792
H	-2.06438	2.24411	-2.45248
C	-3.49521	4.66678	0.22319
H	-3.11782	3.10466	1.64603
C	-3.43342	5.05395	-1.11829
H	-2.85929	4.48648	-3.11786
H	-3.89725	5.34581	0.96842
H	-3.78851	6.03569	-1.41523
C	-0.83276	0.63245	1.73713
C	-0.52356	-0.61837	2.30112
C	-0.37891	1.80503	2.36520
C	0.23735	-0.69222	3.46493
H	-0.88881	-1.53160	1.84133
C	0.38436	1.72508	3.52782
H	-0.61111	2.77666	1.94008
C	0.68818	0.47869	4.08062

H	0.47452	-1.66005	3.89514
H	0.74318	2.63304	4.00209
H	1.27611	0.41942	4.99107
C	-1.51806	-0.45885	-1.29015
C	-0.37173	-1.26968	-1.22903
C	-2.38536	-0.57001	-2.39190
C	-0.09143	-2.16261	-2.26102
H	0.30658	-1.19403	-0.38465
C	-2.10157	-1.46572	-3.41937
H	-3.28827	0.03093	-2.44014
C	-0.95690	-2.26462	-3.35292
H	0.80244	-2.77668	-2.21578
H	-2.77333	-1.54563	-4.26811
H	-0.73920	-2.96637	-4.15180

5Sn

68

Energy: -1141579.6390903

Sn	-4.25690	-0.32253	1.06142
Sn	-1.89452	0.77032	0.12958
C	-3.90465	-2.35476	1.68083
C	-4.37616	-2.83507	2.91013
C	-3.14495	-3.20897	0.86680
C	-4.10051	-4.14330	3.31460
H	-4.95699	-2.18615	3.56147
C	-2.86931	-4.51673	1.26961
H	-2.75644	-2.85526	-0.08600
C	-3.34731	-4.98481	2.49485
H	-4.47148	-4.50410	4.27005
H	-2.27930	-5.16723	0.62992
H	-3.13109	-6.00122	2.81086
C	-4.96369	0.83463	2.73472
C	-6.27938	1.31552	2.78028
C	-4.08666	1.16378	3.77971
C	-6.71210	2.10234	3.85014
H	-6.97218	1.08072	1.97557
C	-4.51829	1.94898	4.85009
H	-3.05671	0.81363	3.76170
C	-5.83230	2.41906	4.88595
H	-7.73470	2.46899	3.87375
H	-3.82870	2.19643	5.65238
H	-6.16825	3.03254	5.71687
C	-5.72887	-0.28304	-0.51025
C	-5.91537	0.88716	-1.26208
C	-6.47767	-1.42206	-0.83626
C	-6.83581	0.91974	-2.31108
H	-5.33696	1.78106	-1.03781
C	-7.39805	-1.39107	-1.88650

H	-6.34073	-2.34253	-0.27354
C	-7.57817	-0.22031	-2.62410
H	-6.96994	1.83225	-2.88539
H	-7.97225	-2.28094	-2.12959
H	-8.29236	-0.19700	-3.44207
C	-2.24830	2.80206	-0.49058
C	-1.77675	3.28255	-1.71979
C	-3.00916	3.65573	0.32295
C	-2.05353	4.59041	-2.12469
H	-1.19500	2.63405	-2.37073
C	-3.28592	4.96311	-0.08028
H	-3.39766	3.30187	1.27571
C	-2.80789	5.43137	-1.30544
H	-1.68252	4.95135	-3.08006
H	-3.87681	5.61319	0.55903
H	-3.02498	6.44749	-1.62178
C	-0.42493	0.73319	1.70356
C	-0.23968	-0.43590	2.45744
C	0.32300	1.87281	2.02945
C	0.67864	-0.46680	3.50835
H	-0.81750	-1.33022	2.23331
C	1.24127	1.84351	3.08158
H	0.18694	2.79248	1.46521
C	1.42013	0.67385	3.82124
H	0.81178	-1.37845	4.08425
H	1.81478	2.73385	3.32457
H	2.13265	0.65187	4.64069
C	-1.18368	-0.38613	-1.54248
C	0.13239	-0.86627	-1.58505
C	-2.05798	-0.71534	-2.58973
C	0.56814	-1.65247	-2.65413
H	0.82313	-0.63133	-0.77861
C	-1.62331	-1.49993	-3.65934
H	-3.08810	-0.36563	-2.57420
C	-0.30898	-1.96932	-3.69217
H	1.59100	-2.01853	-2.67539
H	-2.31080	-1.74742	-4.46342
H	0.02931	-2.58230	-4.52250

5Sn radical cation

68

Energy: -1141415.484006814

Sn	-4.35194	-0.36088	1.08870
Sn	-1.79962	0.81010	0.10404
C	-3.60919	-2.28261	1.61327
C	-3.51863	-2.66706	2.96041
C	-3.09968	-3.12604	0.61191
C	-2.94405	-3.89190	3.29763

H	-3.89927	-2.02072	3.74618
C	-2.52406	-4.34799	0.95655
H	-3.13716	-2.83111	-0.43292
C	-2.44487	-4.72982	2.29785
H	-2.88589	-4.19233	4.33918
H	-2.13454	-4.99894	0.18005
H	-1.99320	-5.68009	2.56436
C	-4.73358	1.02799	2.65220
C	-5.81782	1.91555	2.56768
C	-3.82851	1.13315	3.72146
C	-6.00375	2.88333	3.55413
H	-6.52203	1.85180	1.74291
C	-4.01856	2.10541	4.70223
H	-2.97051	0.47034	3.78855
C	-5.10376	2.98068	4.61776
H	-6.85016	3.56037	3.49328
H	-3.31958	2.18162	5.52932
H	-5.24858	3.73872	5.38095
C	-5.48919	-0.17349	-0.69769
C	-5.75583	1.10630	-1.21247
C	-5.87454	-1.31075	-1.42477
C	-6.41589	1.24304	-2.43268
H	-5.44110	1.99592	-0.67405
C	-6.53680	-1.16666	-2.64325
H	-5.66773	-2.30672	-1.04349
C	-6.80396	0.10800	-3.14837
H	-6.62308	2.23343	-2.82586
H	-6.84370	-2.04764	-3.19835
H	-7.31421	0.21643	-4.10019
C	-2.54393	2.72919	-0.42798
C	-2.61687	3.11562	-1.77564
C	-3.07200	3.56839	0.56732
C	-3.19238	4.33829	-2.11905
H	-2.22165	2.47259	-2.55691
C	-3.64846	4.78817	0.21646
H	-3.04854	3.27166	1.61205
C	-3.71003	5.17202	-1.12518
H	-3.23685	4.64031	-3.16082
H	-4.05243	5.43581	0.98833
H	-4.16239	6.12058	-1.39658
C	-0.66511	0.62992	1.89291
C	-0.41422	-0.64686	2.42289
C	-0.26610	1.77089	2.60672
C	0.24386	-0.77723	3.64487
H	-0.73990	-1.53887	1.89504
C	0.39411	1.63313	3.82704
H	-0.46044	2.76474	2.21356
C	0.64562	0.36136	4.34725
H	0.43880	-1.76535	4.04982

H	0.71167	2.51679	4.37179
H	1.15429	0.25795	5.30046
C	-1.41400	-0.58357	-1.45425
C	-0.32045	-1.45983	-1.37170
C	-2.32476	-0.70384	-2.51708
C	-0.13107	-2.43125	-2.35389
H	0.38842	-1.38430	-0.55194
C	-2.13121	-1.67970	-3.49357
H	-3.18989	-0.05017	-2.58229
C	-1.03677	-2.54360	-3.41117
H	0.72246	-3.09943	-2.29469
H	-2.83466	-1.76761	-4.31569
H	-0.88922	-3.30447	-4.17101

6C

8

Energy: -1780621.359735635

C	-3.77054	-0.07734	0.82888
C	-2.38178	0.52534	0.35999
Cl	-1.75124	-0.42824	-1.00669
Cl	-1.22117	0.46529	1.71035
Cl	-2.60971	2.21645	-0.15198
Cl	-3.54261	-1.76846	1.34082
Cl	-4.93115	-0.01727	-0.52147
Cl	-4.40106	0.87623	2.19557

6C radical cation

8

Energy: -1780414.2290710

C	-3.76635	-0.07560	0.82746
C	-2.38595	0.52360	0.36141
Cl	-1.75535	-0.42100	-0.99655
Cl	-1.22931	0.46604	1.70013
Cl	-2.60753	2.20406	-0.14848
Cl	-3.54482	-1.75617	1.33709
Cl	-4.92310	-0.01778	-0.51120
Cl	-4.39683	0.86885	2.18562

6Si

8

Energy: -2096353.492498974

Si	-4.09837	-0.21960	0.93963
Si	-2.05394	0.66760	0.24924
Cl	-1.33431	-0.43019	-1.31987
Cl	-0.72534	0.59632	1.80295

Cl	-2.32070	2.60894	-0.33772
Cl	-3.83161	-2.16094	1.52659
Cl	-5.42697	-0.14832	-0.61408
Cl	-4.81801	0.87819	2.50874

6Si radical cation

8

Energy: -2096162.9770594

Si	-4.22161	-0.27220	0.98150
Si	-1.93070	0.72020	0.20736
Cl	-1.43894	-0.49609	-1.30388
Cl	-0.82162	0.54563	1.86427
Cl	-2.44001	2.58619	-0.30663
Cl	-3.71230	-2.13819	1.49550
Cl	-5.33069	-0.09763	-0.67540
Cl	-4.71336	0.94409	2.49275

6Ge

8

Energy: -4339582.15689186

Ge	-4.15233	-0.24279	0.95776
Ge	-1.99998	0.69079	0.23111
Cl	-1.23237	-0.45080	-1.41477
Cl	-0.59513	0.62314	1.85059
Cl	-2.26413	2.72764	-0.38750
Cl	-3.88818	-2.27964	1.57637
Cl	-5.55718	-0.17514	-0.66172
Cl	-4.91994	0.89880	2.60364

6Ge radical cation

8

Energy: -4339415.2928668

Ge	-4.26369	-0.29095	0.99642
Ge	-1.88862	0.73895	0.19245
Cl	-1.35552	-0.53161	-1.39936
Cl	-0.70769	0.56260	1.92697
Cl	-2.40611	2.70574	-0.35224
Cl	-3.74620	-2.25774	1.54111
Cl	-5.44462	-0.11460	-0.73810
Cl	-4.79679	0.97961	2.58823

6Sn

8

Energy: -2001829.893848922

Sn	-4.31312	-0.31351	1.01049

Sn	-1.83919	0.76151	0.17838
Cl	-0.98363	-0.45733	-1.60543
Cl	-0.29264	0.70207	1.91105
Cl	-2.09270	2.96935	-0.49949
Cl	-4.05960	-2.52135	1.68838
Cl	-5.85966	-0.25409	-0.72219
Cl	-5.16869	0.90534	2.79429

6Sn radical cation

8

Energy: -2001633.4794435

Sn	-4.42979	-0.36417	1.04957
Sn	-1.72252	0.81217	0.13930
Cl	-1.16174	-0.58029	-1.58849
Cl	-0.44786	0.61533	2.02964
Cl	-2.29982	2.94680	-0.44995
Cl	-3.85250	-2.49880	1.63881
Cl	-5.70445	-0.16733	-0.84076
Cl	-4.99057	1.02828	2.77736

7C

8

Energy: -423964.1990591

C	-3.75926	-0.07238	0.82517
C	-2.39305	0.52038	0.36370
F	-1.90850	-0.19213	-0.66767
F	-1.51001	0.47974	1.37587
F	-2.55401	1.79670	-0.02485
F	-3.59830	-1.34870	1.21372
F	-4.64230	-0.03174	-0.18700
F	-4.24381	0.64012	1.85654

7C radical cation

8

Energy: -423693.1005682

C	-4.03546	-0.19180	0.91847
C	-2.11686	0.63981	0.27040
F	-1.81884	-0.15415	-0.69873
F	-1.42006	0.51840	1.34657
F	-2.46496	1.83619	-0.05524
F	-3.68730	-1.38820	1.24404
F	-4.73225	-0.07034	-0.15769
F	-4.33350	0.60209	1.88766

7Si

8

Energy: -739725.2627649

Si	-4.09979	-0.22000	0.93979
Si	-2.05252	0.66800	0.24908
F	-1.46479	-0.16328	-0.97068
F	-0.99474	0.62833	1.43380
F	-2.22467	2.17801	-0.21396
F	-3.92765	-1.73001	1.40283
F	-5.15757	-0.18033	-0.24493
F	-4.68752	0.61128	2.15955

7Si radical cation

8

Energy: -739468.1824017

Si	-4.27153	-0.29505	0.99874
Si	-1.88078	0.74305	0.19012
F	-1.52196	-0.21743	-0.98001
F	-1.03965	0.59652	1.49089
F	-2.29976	2.18898	-0.20245
F	-3.85255	-1.74098	1.39131
F	-5.11266	-0.14852	-0.30202
F	-4.63035	0.66543	2.16888

7Ge

8

Energy: -2982906.9992755

Ge	-4.14900	-0.24106	0.95624
Ge	-2.00331	0.68906	0.23263
F	-1.34691	-0.19849	-1.09093
F	-0.83915	0.65652	1.50302
F	-2.16715	2.32834	-0.27405
F	-3.98516	-1.88034	1.46292
F	-5.31316	-0.20852	-0.31415
F	-4.80540	0.64649	2.27980

7Ge radical cation

8

Energy: -2982638.9951223

Ge	-4.30772	-0.31165	1.01174
Ge	-1.84458	0.75965	0.17713
F	-1.43631	-0.27778	-1.10000
F	-0.91299	0.60668	1.58529
F	-2.28214	2.33923	-0.25531
F	-3.87017	-1.89123	1.44418
F	-5.23932	-0.15868	-0.39642
F	-4.71600	0.72578	2.28887

7Sn

8

Energy: -645091.9928296

Sn	-4.30728	-0.31115	1.01231
Sn	-1.84504	0.75917	0.17657
F	-1.09670	-0.20640	-1.29136
F	-0.54345	0.72627	1.57361
F	-2.00219	2.57561	-0.39188
F	-4.14972	-2.12694	1.58270
F	-5.60823	-0.28023	-0.38537
F	-5.05664	0.65566	2.47891

7Sn radical cation

8

Energy: -644831.0165586

Sn	-4.53620	-0.37595	1.09786
Sn	-1.61611	0.82394	0.09103
F	-1.14145	-0.30471	-1.34147
F	-0.61559	0.65306	1.68051
F	-2.17692	2.56673	-0.36766
F	-3.97551	-2.11886	1.55624
F	-5.53672	-0.20471	-0.49158
F	-5.01074	0.75251	2.53055

8C

6

Energy: -49345.2323612

C	-3.72769	0.20451	0.72797
C	-2.42462	0.24362	0.46093
H	-2.03320	-0.02373	-0.51676
H	-1.69655	0.54430	1.20916
H	-4.45584	-0.09636	-0.02030
H	-4.11904	0.47167	1.70559

8C radical cation

6

Energy: -49108.4842965

C	-3.77289	0.20307	0.73723
C	-2.37942	0.24494	0.45164
H	-2.00610	-0.02675	-0.53465
H	-1.66479	0.54913	1.21499
H	-4.48753	-0.10109	-0.02614
H	-4.14621	0.47472	1.72353

8Si

6

Energy: -364826.1844040958

Si	-4.09902	0.00001	0.86776
Si	-2.05329	0.44799	0.32112
H	-1.48777	-0.14858	-0.91099
H	-1.03927	0.60769	1.38891
H	-5.11303	-0.15981	-0.20001
H	-4.66456	0.59671	2.09981

8Si radical cation

6

Energy: -364649.6454303

Si	-4.17558	0.18607	0.82136
Si	-1.97673	0.26193	0.36750
H	-1.48544	-0.10448	-0.97092
H	-1.02143	0.67781	1.40742
H	-5.13090	-0.22974	-0.21857
H	-4.66686	0.55241	2.15981

8Ge

6

Energy: -2608127.3620048

Ge	-4.12384	-0.10753	0.90782
Ge	-2.02847	0.55553	0.28103
H	-1.42357	-0.18223	-0.93251
H	-0.96798	0.58587	1.40234
H	-5.18435	-0.13781	-0.21348
H	-4.72873	0.63018	2.12140

8Ge radical cation

6

Energy: -2607946.5464500

Ge	-4.21872	0.18230	0.83043
Ge	-1.93359	0.26570	0.35844
H	-1.43351	-0.11436	-1.02893
H	-0.95099	0.69761	1.43870
H	-5.20134	-0.24940	-0.24990
H	-4.71878	0.56217	2.21786

8Sn

6

Energy: -270333.6523028

Sn	-4.28506	-0.23730	0.97893

Sn	-1.86724	0.68535	0.21009
H	-1.15914	-0.23755	-1.07739
H	-0.65990	0.59542	1.45240
H	-5.49226	-0.14779	-0.26354
H	-4.99334	0.68587	2.26612

8Sn radical cation

6

Energy: -270159.3960490

Sn	-4.38006	0.03930	0.91098
Sn	-1.77224	0.40871	0.27795
H	-1.18840	-0.18200	-1.20292
H	-0.65910	0.71435	1.52336
H	-5.49311	-0.26683	-0.33439
H	-4.96403	0.63048	2.39161

9C

18

Energy: -148092.6795305

C	-3.73790	0.30186	0.69799
C	-2.41438	0.14654	0.49065
C	-1.81028	-0.33398	-0.80745
C	-1.35481	0.43008	1.52903
C	-4.79756	0.01784	-0.34015
C	-4.34198	0.78212	1.99628
H	-5.02875	0.02522	2.39858
H	-4.94356	1.68462	1.82358
H	-3.60759	1.01205	2.76803
H	-4.40093	-0.33775	-1.29088
H	-5.38717	0.92312	-0.53771
H	-5.50380	-0.73563	0.03381
H	-2.54463	-0.56396	-1.57922
H	-1.20880	-1.23651	-0.63457
H	-1.12342	0.42279	-1.20981
H	-0.64843	1.18359	1.15543
H	-0.76533	-0.47534	1.72637
H	-1.75153	0.78539	2.47983

9C radical cation

18

Energy: -147912.2662074

C	-3.76910	0.37385	0.68902
C	-2.38415	0.07450	0.50021
C	-1.89084	-0.48814	-0.77925
C	-1.39586	0.31676	1.57811
C	-4.71544	0.36269	-0.45178

C	-4.30325	0.70510	2.03118
H	-3.72127	0.28699	2.85354
H	-5.35335	0.41316	2.11687
H	-4.28526	1.80492	2.14104
H	-4.24678	0.56790	-1.41536
H	-5.54794	1.04901	-0.27641
H	-5.16152	-0.64685	-0.51282
H	-2.64640	-1.04012	-1.33980
H	-1.00481	-1.10773	-0.61693
H	-1.55877	0.35325	-1.41459
H	-0.40744	0.52765	1.16149
H	-1.28790	-0.61942	2.15587
H	-1.69076	1.09853	2.27937

9Si

18

Energy: -463596.9262935319

Si	-4.12561	0.10902	0.83780
Si	-2.02640	0.33951	0.35265
C	-1.31091	-0.44937	-1.20975
C	-0.73752	0.50947	1.72581
C	-5.41379	-0.06723	-0.53521
C	-4.84240	0.90316	2.39694
H	-5.57588	0.23689	2.86557
H	-5.34799	1.84793	2.16752
H	-4.05565	1.10416	3.12996
H	-4.95087	-0.41699	-1.46260
H	-5.91346	0.88659	-0.73853
H	-6.18351	-0.79343	-0.24932
H	-2.09810	-0.64682	-1.94326
H	-0.80618	-1.39550	-0.98408
H	-0.57692	0.21795	-1.67610
H	0.03262	1.23618	1.44239
H	-0.23849	-0.44550	1.92526
H	-1.19979	0.85603	2.65473

9Si radical cation

18

Energy: -463457.0765511

Si	-4.17911	0.34651	0.76951
Si	-1.97320	0.10151	0.41935
C	-1.32553	-0.49109	-1.21681
C	-0.74545	0.48461	1.75862
C	-5.40690	-0.03741	-0.56948
C	-4.82675	0.93991	2.40540
H	-5.49782	0.18453	2.83259
H	-5.41497	1.85434	2.26009

H	-4.02871	1.14571	3.12208
H	-4.92917	-0.38192	-1.48923
H	-6.00042	0.85735	-0.79421
H	-6.10219	-0.81158	-0.22218
H	-2.12354	-0.69634	-1.93367
H	-0.73752	-1.40573	-1.07195
H	-0.65425	0.26437	-1.64351
H	-0.05009	1.25891	1.41175
H	-0.15202	-0.41031	1.98291
H	-1.22321	0.82869	2.67852

9Ge

18

Energy: -2706893.4486045

Ge	-4.15079	-0.07332	0.90303
Ge	-2.00150	0.52138	0.28598
C	-1.21594	-0.44887	-1.26074
C	-0.63354	0.53428	1.72803
C	-5.51858	-0.08631	-0.53919
C	-4.93659	0.89692	2.44964
H	-5.71998	0.27839	2.89851
H	-5.38385	1.83967	2.12157
H	-4.17566	1.10194	3.20575
H	-5.08710	-0.43862	-1.47858
H	-5.93023	0.91672	-0.68393
H	-6.33367	-0.75835	-0.25328
H	-1.97698	-0.65391	-2.01672
H	-0.76861	-1.39162	-0.93274
H	-0.43262	0.16965	-1.70975
H	0.18157	1.20625	1.44200
H	-0.22194	-0.46878	1.87273
H	-1.06486	0.88664	2.66747

9Ge radical cation

18

Energy: -2706744.5446500

Ge	-4.22806	0.34828	0.77893
Ge	-1.92426	0.09973	0.40993
C	-1.24775	-0.52418	-1.30724
C	-0.63894	0.50135	1.81787
C	-5.51338	-0.05315	-0.62907
C	-4.90457	0.97199	2.49617
H	-5.56897	0.20666	2.90858
H	-5.48326	1.88596	2.33172
H	-4.08968	1.16935	3.19275
H	-5.01195	-0.39877	-1.53317
H	-6.08776	0.85268	-0.84563

H	-6.19972	-0.82434	-0.26663
H	-2.06264	-0.72166	-2.00379
H	-0.66902	-1.43810	-1.14268
H	-0.58338	0.24113	-1.71976
H	0.04738	1.27251	1.45533
H	-0.06454	-0.40445	2.03453
H	-1.14037	0.84706	2.72193

9Sn

18

Energy: -369098.3220321

Sn	-4.31060	-0.22516	0.97840
Sn	-1.84171	0.67306	0.21063
C	-0.92373	-0.48984	-1.40862
C	-0.30126	0.55122	1.76859
C	-5.85103	-0.10350	-0.57960
C	-5.22862	0.93813	2.59735
H	-6.06393	0.36562	3.01134
H	-5.61122	1.88079	2.19653
H	-4.50585	1.14177	3.38981
H	-5.47775	-0.48873	-1.53037
H	-6.16497	0.93685	-0.70077
H	-6.71376	-0.69805	-0.26459
H	-1.64649	-0.69327	-2.20113
H	-0.54114	-1.43260	-1.00803
H	-0.08841	0.08276	-1.82246
H	0.56144	1.14585	1.45368
H	0.01273	-0.48914	1.88958
H	-0.67454	0.93627	2.71943

9Sn radical cation

18

Energy: -368949.2158552

Sn	-4.40920	0.11890	0.88817
Sn	-1.74314	0.32908	0.30064
C	-0.97333	-0.53862	-1.51581
C	-0.30909	0.57835	1.89006
C	-5.84327	-0.13004	-0.70129
C	-5.17895	0.98632	2.70477
H	-5.99818	0.35808	3.06076
H	-5.55890	1.98278	2.46384
H	-4.39297	1.04994	3.45651
H	-5.37696	-0.61219	-1.55981
H	-6.21370	0.86156	-0.97496
H	-6.66778	-0.73774	-0.32266
H	-1.75930	-0.60242	-2.26755
H	-0.59333	-1.53502	-1.27470

H	-0.15413	0.08959	-1.87190
H	0.51539	1.18604	1.51133
H	0.06140	-0.41319	2.16389
H	-0.77543	1.06062	2.74850

10C

14

Energy: -188369.7086774292

C	0.34032	1.08862	0.35047
C	-0.87290	0.68125	-0.07778
N	-1.07441	-0.68565	-0.44066
N	-2.01433	1.52618	-0.09002
N	1.48175	0.24369	0.36271
N	0.54183	2.45552	0.71335
H	-1.72529	2.48138	0.12312
H	-2.47421	1.51856	-1.00153
H	-2.00566	-0.99235	-0.16317
H	-0.98800	-0.83243	-1.44608
H	1.19272	-0.71152	0.14958
H	1.94163	0.25131	1.27422
H	0.45545	2.60230	1.71876
H	1.47307	2.76222	0.43583

10C radical cation

14

Energy: -188239.7202339

C	0.38450	1.05821	0.36057
C	-0.91708	0.71166	-0.08789
N	-1.20016	-0.58201	-0.44218
N	-1.92847	1.62149	-0.03540
N	1.39592	0.14840	0.30805
N	0.66755	2.35187	0.71490
H	-1.69439	2.60452	0.00881
H	-2.78313	1.42548	-0.54093
H	-2.15749	-0.80405	-0.68591
H	-0.52524	-1.07781	-1.01220
H	1.16189	-0.83463	0.26376
H	2.25056	0.34441	0.81364
H	-0.00736	2.84760	1.28501
H	1.62488	2.57395	0.95857

10Si

14

Energy: -503943.8700286

Si	-4.20865	-0.47200	0.77163
Si	-1.88994	0.47496	0.14144

N	-1.18175	-0.55088	-1.06026
N	-2.00559	1.97607	-0.71158
N	-4.00125	-2.06507	1.41737
N	-4.91270	0.35565	2.11834
H	-2.39544	2.79653	-0.26753
H	-1.92324	2.10322	-1.71399
H	-1.11666	-0.36102	-2.05385
H	-0.95005	-1.51242	-0.85102
H	-3.63230	-2.81275	0.84560
H	-4.04123	-2.33051	2.39485
H	-5.15283	1.33594	2.05804
H	-4.92948	0.03011	3.07830

10Si radical cation

14

Energy: -503811.6908906

Si	-3.99363	-0.40992	1.01717
Si	-2.13064	0.47805	-0.09052
N	-1.11023	-0.59020	-0.90072
N	-2.38962	1.89495	-0.96913
N	-4.05429	-2.07803	1.24645
N	-4.52797	0.43506	2.37630
H	-3.15860	2.53037	-0.79486
H	-1.69398	2.30197	-1.58466
H	-0.80498	-0.47572	-1.86129
H	-0.63166	-1.34955	-0.43154
H	-4.03524	-2.73569	0.47647
H	-4.24170	-2.52911	2.13549
H	-4.32597	1.41302	2.54449
H	-5.24260	0.08262	3.00366

11C

38

Energy: -385806.1207748797

C	-0.37514	0.24559	1.72173
C	-0.96164	0.41449	0.49673
N	-0.44804	-0.13167	-0.69845
N	-2.14666	1.15195	0.29519
N	-1.10346	0.13764	2.92448
N	1.01919	0.16049	1.91698
C	-2.42080	2.31185	1.11694
C	-3.29257	0.51965	-0.34106
C	-0.13437	0.74737	-1.81563
C	0.23843	-1.40617	-0.66658
C	-2.40486	-0.49623	2.92194
C	-0.82308	1.04893	4.02388

C	1.91216	0.90820	1.05686
C	1.58510	-1.00592	2.57925
H	-2.41843	-1.26188	2.14192
H	-3.24315	0.19471	2.73754
H	-2.57738	-0.97129	3.89681
H	-0.98638	0.53957	4.98134
H	-1.45313	1.95406	4.00704
H	0.22466	1.35015	3.95963
H	1.40551	1.82191	0.73593
H	2.23223	0.35912	0.15661
H	2.81668	1.17578	1.61915
H	-3.00755	3.03581	0.53589
H	-1.47046	2.76874	1.40492
H	-2.98654	2.09042	2.03641
H	-3.85029	1.26081	-0.92633
H	-3.98901	0.06143	0.38105
H	-2.92533	-0.25706	-1.01531
H	0.90963	1.10273	-1.80483
H	-0.79951	1.61228	-1.76869
H	-0.30419	0.22176	-2.76308
H	1.32153	-1.33063	-0.47827
H	0.10601	-1.91200	-1.63210
H	-0.20130	-2.02051	0.12348
H	0.83740	-1.40680	3.26685
H	2.47354	-0.71529	3.15290
H	1.87896	-1.80023	1.87300

11C radical cation

38

Energy: -385694.0772516453

C	-0.36406	0.24339	1.74956
C	-0.97250	0.41987	0.47437
N	-0.43812	-0.16201	-0.64646
N	-2.10821	1.17466	0.33276
N	-1.12715	0.11532	2.88172
N	0.99995	0.20001	1.87867
C	-2.36170	2.35346	1.15710
C	-3.16138	0.81956	-0.61824
C	-0.45157	0.50510	-1.94829
C	0.22624	-1.46162	-0.59939
C	-2.42408	-0.55609	2.86660
C	-0.70925	0.67499	4.16697
C	1.88152	0.97523	1.00978
C	1.66069	-0.68297	2.84013
H	-2.57928	-1.03165	1.89910
H	-3.23835	0.15068	3.06274
H	-2.44366	-1.32503	3.64682
H	-0.45775	-0.11027	4.88868

H	-1.53080	1.27089	4.57930
H	0.15781	1.31791	4.01821
H	1.29604	1.70036	0.44582
H	2.42727	0.32586	0.31554
H	2.61282	1.51137	1.62398
H	-2.60024	3.20408	0.50914
H	-1.47267	2.59272	1.73919
H	-3.20927	2.18991	1.83235
H	-3.22312	1.53915	-1.44230
H	-4.12441	0.81122	-0.09609
H	-2.96683	-0.17375	-1.02167
H	0.56252	0.49799	-2.36269
H	-0.77763	1.53754	-1.82491
H	-1.11637	-0.00224	-2.65624
H	1.30309	-1.36451	-0.77948
H	-0.19312	-2.11094	-1.37561
H	0.06080	-1.92353	0.37324
H	0.92805	-1.36433	3.27201
H	2.14498	-0.11597	3.64276
H	2.42747	-1.26656	2.31898

11Si

38

Energy: -701382.1114091

Si	-4.22399	-0.49085	0.58544
Si	-1.80815	0.24140	0.20031
N	-1.04157	-0.73477	-1.02614
N	-1.89528	1.83557	-0.49505
N	-4.14546	-2.10539	1.23308
N	-4.96089	0.45756	1.85166
C	-2.84686	2.78287	0.06634
C	-1.17036	2.34465	-1.64736
C	-1.38935	-0.73945	-2.44261
C	-0.11489	-1.79834	-0.65911
C	-3.23663	-3.05785	0.61213
C	-4.84346	-2.63381	2.39343
C	-5.88823	1.53540	1.53164
C	-4.57534	0.43106	3.25824
H	-2.85657	-2.64057	-0.32576
H	-3.75129	-4.00373	0.39264
H	-2.37481	-3.27671	1.26174
H	-4.16393	-2.80450	3.24427
H	-5.31266	-3.59608	2.14374
H	-5.62435	-1.93817	2.70500
H	-6.06010	1.56642	0.45135
H	-5.49586	2.51366	1.85131
H	-6.85826	1.38561	2.02885
H	-2.36641	3.75170	0.26128

H	-3.23779	2.39091	1.01059
H	-3.69891	2.94932	-0.61161
H	-0.72279	3.32016	-1.40964
H	-1.82615	2.48252	-2.52248
H	-0.37058	1.65286	-1.91678
H	-0.51900	-0.52859	-3.08282
H	-2.15913	0.00835	-2.63956
H	-1.78744	-1.72463	-2.73322
H	0.86864	-1.64823	-1.12896
H	-0.48939	-2.78501	-0.97344
H	0.02380	-1.80888	0.42637
H	-3.80483	-0.32451	3.41954
H	-5.42988	0.21116	3.91650
H	-4.16360	1.40758	3.55859

11Si radical cation

38

Energy: -701257.6027044

Si	-4.17227	-0.40303	0.90280
Si	-2.23908	0.27822	-0.24770
N	-1.10516	-0.74699	-0.98360
N	-2.38142	1.78120	-1.02029
N	-4.18047	-2.08284	1.20783
N	-4.59771	0.52326	2.26375
C	-3.60670	2.59116	-1.02399
C	-1.22965	2.48145	-1.61441
C	-0.67714	-0.68322	-2.38976
C	-0.40602	-1.77905	-0.20069
C	-3.63511	-3.05443	0.25328
C	-4.91977	-2.70127	2.31614
C	-5.49544	1.68382	2.18661
C	-4.03412	0.30717	3.60540
H	-3.16313	-2.53589	-0.58549
H	-4.43638	-3.69256	-0.13502
H	-2.88912	-3.68949	0.74415
H	-4.23155	-3.25473	2.96597
H	-5.66578	-3.39988	1.92163
H	-5.42765	-1.93505	2.90216
H	-5.89698	1.78500	1.17520
H	-4.96468	2.60575	2.45360
H	-6.33849	1.55504	2.87544
H	-3.48243	3.48711	-0.40641
H	-4.44590	2.00387	-0.64434
H	-3.83831	2.89841	-2.05009
H	-1.08628	3.44569	-1.11487
H	-1.40548	2.66181	-2.68079
H	-0.32188	1.88841	-1.49598
H	0.37396	-0.38262	-2.46611

H	-1.29589	0.02687	-2.93940
H	-0.78868	-1.67357	-2.84554
H	0.66412	-1.55238	-0.14016
H	-0.53207	-2.75953	-0.67205
H	-0.81063	-1.81491	0.81478
H	-3.34268	-0.53807	3.59507
H	-4.82908	0.10316	4.33269
H	-3.48670	1.20081	3.92970

12C

46

Energy: -629663.2768535

C	-3.75053	0.28964	0.70740
C	-2.40529	0.16720	0.48948
C	-4.75536	-0.15764	-0.28988
C	-4.63603	-1.40394	-0.92609
C	-5.87343	0.63879	-0.58677
C	-5.58863	-1.82867	-1.84726
H	-3.78738	-2.03716	-0.68943
C	-6.82065	0.21976	-1.51827
H	-5.98856	1.59583	-0.08668
C	-6.68138	-1.01517	-2.15412
H	-5.48088	-2.79821	-2.32454
H	-7.67030	0.85683	-1.74595
H	-7.42300	-1.34477	-2.87552
C	-4.30566	0.87136	1.95481
C	-5.41006	0.27703	2.58710
C	-3.77291	2.04693	2.50876
C	-5.94042	0.81847	3.75581
H	-5.84527	-0.62087	2.15863
C	-4.31006	2.59486	3.66974
H	-2.93315	2.52811	2.01830
C	-5.39134	1.97886	4.30353
H	-6.78534	0.33564	4.23812
H	-3.88680	3.50732	4.07928
H	-5.80799	2.40528	5.21107
C	-1.84567	-0.14098	-0.85082
C	-2.30073	0.52894	-1.99809
C	-0.81309	-1.08228	-0.99338
C	-1.75916	0.24901	-3.24916
H	-3.08288	1.27438	-1.89815
C	-0.27981	-1.37232	-2.24703
H	-0.43753	-1.59241	-0.11139
C	-0.75183	-0.70913	-3.38098
H	-2.12104	0.78230	-4.12329
H	0.50756	-2.11476	-2.33893
H	-0.33186	-0.92983	-4.35768

C	-1.40337	0.33222	1.57221
C	-0.22261	1.05773	1.34424
C	-1.58547	-0.26783	2.82902
C	0.72762	1.21001	2.35133
H	-0.05955	1.50950	0.37034
C	-0.63058	-0.12631	3.83154
H	-2.48397	-0.84834	3.01071
C	0.52705	0.61982	3.60023
H	1.62769	1.78700	2.16008
H	-0.78763	-0.60317	4.79455
H	1.27050	0.73184	4.38365

12C radical cation

46

Energy: -629514.4210814

C	-3.76691	0.29725	0.70617
C	-2.37318	0.17258	0.48071
C	-4.73548	-0.24690	-0.24057
C	-4.49964	-1.47447	-0.90327
C	-5.95038	0.43404	-0.48688
C	-5.44271	-1.99607	-1.77491
H	-3.58822	-2.02452	-0.69726
C	-6.87657	-0.07880	-1.38404
H	-6.13249	1.38540	0.00156
C	-6.62864	-1.29630	-2.02666
H	-5.26285	-2.95077	-2.25762
H	-7.79136	0.46743	-1.58822
H	-7.35910	-1.70095	-2.71969
C	-4.28558	0.96641	1.89423
C	-5.46525	0.49283	2.51512
C	-3.64746	2.10900	2.43299
C	-5.96761	1.11978	3.64627
H	-5.95010	-0.39452	2.12259
C	-4.17142	2.74771	3.54594
H	-2.76206	2.50230	1.94619
C	-5.32604	2.25064	4.16222
H	-6.85561	0.72971	4.13221
H	-3.68794	3.63728	3.93551
H	-5.72534	2.74604	5.04129
C	-1.84396	-0.02712	-0.86453
C	-2.42539	0.61686	-1.98244
C	-0.71743	-0.85741	-1.07050
C	-1.90053	0.43334	-3.25197
H	-3.26754	1.28315	-1.83358
C	-0.21534	-1.05984	-2.34822
H	-0.27677	-1.37109	-0.22278
C	-0.80191	-0.41331	-3.44128
H	-2.33989	0.95031	-4.09846

H	0.62911	-1.72403	-2.49868
H	-0.40260	-0.56646	-4.43862
C	-1.42107	0.23128	1.58483
C	-0.15493	0.83539	1.40307
C	-1.72576	-0.33965	2.84320
C	0.75566	0.89197	2.44857
H	0.08085	1.29294	0.44817
C	-0.80025	-0.30495	3.87422
H	-2.67852	-0.83717	2.98503
C	0.43849	0.31896	3.68465
H	1.71185	1.38442	2.30688
H	-1.03478	-0.76754	4.82701
H	1.15588	0.35570	4.49804

12Si

46

Energy: -945166.4633856

Si	-4.12496	0.18446	0.85344
Si	-2.00448	0.29561	0.41442
C	-5.36190	-0.23815	-0.47466
C	-5.08343	-1.24593	-1.41979
C	-6.59560	0.43634	-0.56936
C	-5.99209	-1.55331	-2.42872
H	-4.14354	-1.78789	-1.36014
C	-7.51000	0.11904	-1.57207
H	-6.83625	1.21946	0.14435
C	-7.20998	-0.87348	-2.50666
H	-5.75512	-2.33042	-3.14969
H	-8.45521	0.65145	-1.62830
H	-7.92224	-1.11870	-3.28889
C	-4.84763	0.95428	2.38829
C	-6.08807	0.51239	2.89211
C	-4.16167	1.95455	3.10639
C	-6.61980	1.04944	4.06306
H	-6.63936	-0.26136	2.36407
C	-4.68837	2.48209	4.28224
H	-3.21044	2.32342	2.73280
C	-5.92051	2.03328	4.76370
H	-7.57852	0.69602	4.43177
H	-4.14239	3.25272	4.81881
H	-6.33445	2.45103	5.67658
C	-1.33986	-0.24405	-1.24081
C	-2.02065	0.09016	-2.42866
C	-0.15520	-1.00000	-1.34560
C	-1.54735	-0.33083	-3.66841
H	-2.92986	0.68263	-2.37345
C	0.32462	-1.41016	-2.58811
H	0.38890	-1.27356	-0.44578

C	-0.37158	-1.08051	-3.75226
H	-2.09025	-0.06664	-4.57134
H	1.23925	-1.99318	-2.64772
H	0.00189	-1.40222	-4.71993
C	-0.73333	0.44885	1.76728
C	0.56098	0.92956	1.48173
C	-1.04058	0.13622	3.10705
C	1.50767	1.08777	2.49231
H	0.82731	1.18484	0.45933
C	-0.09806	0.30628	4.11737
H	-2.02583	-0.24972	3.35342
C	1.18054	0.78013	3.81369
H	2.49994	1.45660	2.24870
H	-0.35702	0.05805	5.14267
H	1.91771	0.90432	4.60132

12Si radical cation

46

Energy: -945033.4292394

Si	-4.17185	0.34145	0.78880
Si	-1.96374	0.14599	0.42645
C	-5.35839	-0.28204	-0.46575
C	-5.00891	-1.35983	-1.30972
C	-6.63061	0.31496	-0.61473
C	-5.90485	-1.82732	-2.26396
H	-4.03726	-1.83531	-1.21000
C	-7.51926	-0.15421	-1.57654
H	-6.91560	1.15300	0.01448
C	-7.15875	-1.22487	-2.39860
H	-5.63093	-2.66199	-2.90088
H	-8.49164	0.31424	-1.68788
H	-7.85626	-1.59051	-3.14537
C	-4.81302	1.10970	2.32659
C	-6.08635	0.74838	2.82239
C	-4.04465	2.05339	3.04479
C	-6.56962	1.31381	3.99761
H	-6.68857	0.01597	2.29304
C	-4.53682	2.61755	4.21575
H	-3.06563	2.34882	2.67825
C	-5.79759	2.24783	4.69293
H	-7.54566	1.02626	4.37448
H	-3.94287	3.34748	4.75592
H	-6.17888	2.68909	5.60822
C	-1.34550	-0.19282	-1.26819
C	-2.08358	0.22347	-2.39894
C	-0.13360	-0.89259	-1.46567
C	-1.62139	-0.04717	-3.68133
H	-3.01566	0.76616	-2.26954

C	0.31961	-1.16436	-2.75226
H	0.44350	-1.23347	-0.61119
C	-0.42142	-0.74147	-3.85873
H	-2.19124	0.28416	-4.54322
H	1.24815	-1.70747	-2.89456
H	-0.06311	-0.95305	-4.86107
C	-0.76786	0.30544	1.80864
C	0.55543	0.73854	1.56559
C	-1.15458	0.00768	3.13463
C	1.45748	0.86638	2.61642
H	0.87023	0.98543	0.55599
C	-0.24588	0.13336	4.17866
H	-2.16565	-0.33091	3.34268
C	1.05909	0.56267	3.92072
H	2.46987	1.20459	2.42144
H	-0.54958	-0.10625	5.19243
H	1.76662	0.66069	4.73780

12Ge

46

Energy: -3188453.9612650

Ge	-4.10290	-0.14210	1.03010
Ge	-2.00061	0.61526	0.39145
C	-5.39295	-0.32998	-0.43906
C	-5.15873	-1.27014	-1.45601
C	-6.55709	0.45274	-0.49897
C	-6.05697	-1.41398	-2.51249
H	-4.26444	-1.88700	-1.42473
C	-7.45777	0.30600	-1.55379
H	-6.75511	1.18646	0.27731
C	-7.20876	-0.62634	-2.56259
H	-5.86009	-2.14162	-3.29471
H	-8.35198	0.92190	-1.59122
H	-7.91023	-0.73995	-3.38393
C	-4.97877	0.78020	2.52342
C	-6.25687	0.36813	2.93899
C	-4.33294	1.79179	3.25472
C	-6.87411	0.95548	4.04364
H	-6.77705	-0.41673	2.39545
C	-4.94958	2.37870	4.35817
H	-3.34820	2.13575	2.95079
C	-6.22188	1.96229	4.75607
H	-7.86374	0.62620	4.34756
H	-4.43960	3.16683	4.90494
H	-6.70244	2.42182	5.61464
C	-1.30723	-0.17910	-1.26496
C	-1.98201	0.05393	-2.47468
C	-0.14730	-0.97053	-1.28184

C	-1.51769	-0.49898	-3.66718
H	-2.88041	0.66560	-2.48155
C	0.32016	-1.51971	-2.47576
H	0.38713	-1.16580	-0.35642
C	-0.36427	-1.28590	-3.66984
H	-2.05315	-0.31386	-4.59404
H	1.21625	-2.13399	-2.47376
H	0.00057	-1.71411	-4.59884
C	-0.58147	0.62560	1.74377
C	0.71374	1.03948	1.38715
C	-0.83798	0.32249	3.09219
C	1.72290	1.13672	2.34544
H	0.93792	1.28873	0.35302
C	0.17020	0.41950	4.04934
H	-1.82849	-0.00563	3.39499
C	1.45376	0.82697	3.67892
H	2.71867	1.45554	2.05051
H	-0.04431	0.17150	5.08502
H	2.23909	0.90070	4.42528

12Ge radical cation

46

Energy: -3188317.1034927

Ge	-4.21902	0.33849	0.80046
Ge	-1.92030	0.15212	0.41566
C	-5.45819	-0.29064	-0.52337
C	-5.09197	-1.33164	-1.39731
C	-6.73558	0.29217	-0.63063
C	-5.99254	-1.78492	-2.35591
H	-4.11055	-1.79096	-1.32305
C	-7.62746	-0.16386	-1.59779
H	-7.02628	1.10511	0.02791
C	-7.25826	-1.20145	-2.45695
H	-5.71085	-2.59359	-3.02243
H	-8.60905	0.29081	-1.68283
H	-7.95808	-1.55577	-3.20687
C	-4.89169	1.11052	2.42216
C	-6.17190	0.75057	2.88544
C	-4.11369	2.02219	3.16082
C	-6.66008	1.29654	4.06943
H	-6.77705	0.03866	2.33232
C	-4.61275	2.56622	4.33998
H	-3.12699	2.31146	2.81102
C	-5.88347	2.20327	4.79452
H	-7.64428	1.01358	4.42827
H	-4.01426	3.27455	4.90353
H	-6.26902	2.62833	5.71557
C	-1.27613	-0.22836	-1.35111

C	-2.03570	0.13568	-2.47910
C	-0.04332	-0.88678	-1.52368
C	-1.56505	-0.15025	-3.75652
H	-2.98651	0.64654	-2.35872
C	0.41652	-1.17348	-2.80614
H	0.54601	-1.18530	-0.66197
C	-0.34114	-0.80462	-3.92022
H	-2.14890	0.13844	-4.62445
H	1.36379	-1.68630	-2.93712
H	0.02260	-1.02767	-4.91802
C	-0.66523	0.35074	1.85264
C	0.65138	0.77124	1.58279
C	-1.05314	0.08305	3.17919
C	1.56075	0.91794	2.62669
H	0.95995	0.99496	0.56607
C	-0.13551	0.22746	4.21479
H	-2.06458	-0.24574	3.39954
C	1.16951	0.64470	3.93949
H	2.57326	1.24724	2.41730
H	-0.43463	0.01218	5.23543
H	1.88259	0.75743	4.74971

12Sn

46

Energy: -850655.8637910

Sn	-4.19035	-0.36527	1.26346
Sn	-1.88532	0.90039	0.41597
C	-5.55298	-0.40654	-0.43936
C	-5.29508	-1.29050	-1.49994
C	-6.65681	0.45522	-0.53909
C	-6.11459	-1.31291	-2.62926
H	-4.44053	-1.96180	-1.45356
C	-7.47757	0.43485	-1.66819
H	-6.87499	1.15578	0.26266
C	-7.20831	-0.44989	-2.71382
H	-5.89866	-2.00073	-3.44226
H	-8.32517	1.11176	-1.73358
H	-7.84757	-0.46536	-3.59181
C	-5.32884	0.67360	2.79982
C	-6.69744	0.41398	2.97953
C	-4.69692	1.55922	3.68860
C	-7.41565	1.03234	4.00502
H	-7.21474	-0.27354	2.31436
C	-5.41364	2.18417	4.70919
H	-3.63693	1.77833	3.57916
C	-6.77545	1.92069	4.86952
H	-8.47444	0.82107	4.12768
H	-4.91084	2.87659	5.37877

H	-7.33396	2.40456	5.66537
C	-1.17505	-0.13914	-1.36212
C	-1.92675	-0.04862	-2.54549
C	-0.01895	-0.93565	-1.36207
C	-1.53743	-0.73651	-3.69528
H	-2.83220	0.55344	-2.57067
C	0.37304	-1.62336	-2.51195
H	0.57597	-1.03210	-0.45766
C	-0.38507	-1.52420	-3.67986
H	-2.13303	-0.65926	-4.60079
H	1.26779	-2.23981	-2.49520
H	-0.07945	-2.05980	-4.57400
C	-0.18306	0.83256	1.76959
C	1.11655	1.08836	1.30179
C	-0.36388	0.61364	3.14560
C	2.20323	1.10903	2.17825
H	1.29047	1.27233	0.24407
C	0.72110	0.62626	4.02232
H	-1.35803	0.41668	3.54085
C	2.00742	0.87482	3.53960
H	3.20163	1.30696	1.79795
H	0.56353	0.44182	5.08146
H	2.85223	0.88743	4.22192

12Sn radical cation

46

Energy: -850514.4863000

Sn	-4.36025	-0.04103	1.01333
Sn	-1.75266	0.48947	0.33078
C	-5.73639	-0.39901	-0.57372
C	-5.39398	-1.25992	-1.63004
C	-6.98518	0.24556	-0.57207
C	-6.29061	-1.46540	-2.67664
H	-4.43586	-1.77249	-1.63964
C	-7.87378	0.03698	-1.62604
H	-7.26209	0.91933	0.23351
C	-7.52816	-0.81775	-2.67443
H	-6.02583	-2.13227	-3.49110
H	-8.83431	0.54239	-1.62856
H	-8.22488	-0.98108	-3.49028
C	-5.18761	0.91787	2.72440
C	-6.50592	0.62683	3.11638
C	-4.41784	1.81771	3.48115
C	-7.04900	1.24582	4.24105
H	-7.11014	-0.08005	2.55458
C	-4.97105	2.43731	4.59981
H	-3.39459	2.04951	3.19718
C	-6.28398	2.15037	4.98000

H	-8.06762	1.02094	4.54068
H	-4.37849	3.14189	5.17469
H	-6.71007	2.62986	5.85531
C	-1.03931	-0.24233	-1.53723
C	-1.83851	-0.13566	-2.68804
C	0.22761	-0.84540	-1.61735
C	-1.37573	-0.63543	-3.90346
H	-2.81662	0.33554	-2.64255
C	0.68016	-1.34587	-2.83744
H	0.85431	-0.94164	-0.73553
C	-0.11847	-1.23944	-3.97770
H	-1.99327	-0.55131	-4.79213
H	1.65494	-1.81950	-2.89671
H	0.24010	-1.62644	-4.92606
C	-0.30324	0.61120	1.88483
C	1.02487	0.96171	1.58544
C	-0.67635	0.36975	3.21818
C	1.96764	1.04932	2.60849
H	1.32860	1.17088	0.56354
C	0.27404	0.45227	4.23366
H	-1.70013	0.10403	3.46914
C	1.59376	0.79307	3.92916
H	2.99269	1.31862	2.37465
H	-0.01438	0.25205	5.26068
H	2.33080	0.86259	4.72260

13C

6

Energy: -1203022.396986132

C	-3.73733	0.21256	0.72715
C	-2.41499	0.23544	0.46172
Cl	-1.78386	-0.19611	-1.07781
Cl	-1.25347	0.69814	1.64123
Cl	-4.89884	-0.25016	-0.45236
Cl	-4.36845	0.64414	2.26667

13C radical cation

6

Energy: -1202836.4896932

C	-3.77717	0.21184	0.73519
C	-2.37514	0.23617	0.45368
Cl	-1.80552	-0.19201	-1.05911
Cl	-1.28051	0.69319	1.63233
Cl	-4.87181	-0.24519	-0.44346
Cl	-4.34679	0.64002	2.24798

13Si

6

Energy: -1518648.496866448

Si	-4.08459	-0.28458	0.95766
Si	-2.06800	0.73213	0.22979
Cl	-1.26826	-0.34240	-1.35091
Cl	-0.66459	0.68192	1.75303
Cl	-5.48939	-0.23047	-0.56417
Cl	-4.88211	0.78742	2.54120

13Si radical cation

6

Energy: -1518486.4878238

Si	-4.15582	-0.06075	0.89871
Si	-1.99649	0.50875	0.29017
Cl	-1.31167	-0.28969	-1.40565
Cl	-0.69058	0.75733	1.77844
Cl	-5.46174	-0.30952	-0.58952
Cl	-4.84064	0.73789	2.59444

13Ge

6

Energy: -3761918.858508289

Ge	-4.17874	-0.39340	1.01209
Ge	-1.97354	0.84148	0.17675
Cl	-1.10971	-0.36698	-1.42682
Cl	-0.48519	0.68474	1.76994
Cl	-5.66715	-0.23677	-0.58105
Cl	-5.04262	0.81494	2.61571

13Ge radical cation

6

Energy: -3761765.4162627

Ge	-4.23640	-0.17608	0.95210
Ge	-1.91590	0.62412	0.23675
Cl	-1.15873	-0.32052	-1.49060
Cl	-0.51491	0.76444	1.80733
Cl	-5.63742	-0.31645	-0.61846
Cl	-4.99359	0.76850	2.67947

13Sn

6

Energy: -1424185.863012453

Sn	-4.41060	-0.52494	1.09922
Sn	-1.74172	0.97293	0.08965
Cl	-0.79618	-0.41317	-1.58803

Cl	-0.12995	0.70534	1.80981
Cl	-6.02237	-0.25733	-0.62094
Cl	-5.35612	0.86117	2.77689

13Sn radical cation

6

Energy: -1423998.1011715

Sn	-4.47894	-0.26210	1.02376
Sn	-1.67337	0.71008	0.16513
Cl	-0.80251	-0.35741	-1.68437
Cl	-0.10447	0.80796	1.85249
Cl	-6.04782	-0.36000	-0.66362
Cl	-5.34982	0.80547	2.87321

14C

6

Energy: -298551.6757913

C	-3.72752	0.21284	0.72513
C	-2.42479	0.23516	0.46374
F	-1.90971	-0.09270	-0.71550
F	-1.50561	0.58828	1.35496
F	-4.64670	-0.14028	-0.16609
F	-4.24261	0.54071	1.90437

14C radical cation

6

Energy: -298332.0760555

C	-3.77343	0.21188	0.73443
C	-2.37888	0.23612	0.45444
F	-1.93611	-0.08854	-0.69530
F	-1.53775	0.58299	1.34645
F	-4.61456	-0.13499	-0.15758
F	-4.21621	0.53654	1.88417

14Si

6

Energy: -614221.9424342

Si	-4.16602	-0.29433	0.97746
Si	-1.98632	0.74239	0.21151
F	-1.39063	-0.20571	-0.94766
F	-0.92928	0.57152	1.41586
F	-5.22295	-0.12374	-0.22691
F	-4.76174	0.65387	2.13634

14Si radical cation

6

Energy: -614021.5160492

Si	-4.18782	-0.10657	0.91911
Si	-1.96449	0.55457	0.26975
F	-1.42394	-0.18080	-0.99957
F	-0.94398	0.62581	1.45192
F	-5.20834	-0.17781	-0.26305
F	-4.72837	0.62881	2.18844

14Ge

6

Energy: -2857482.4674530

Ge	-4.32270	-0.40140	1.04411
Ge	-1.82962	0.84939	0.14476
F	-1.14480	-0.22944	-1.06144
F	-0.66076	0.58966	1.43094
F	-5.49155	-0.14165	-0.24208
F	-5.00751	0.67744	2.25031

14Ge radical cation

6

Energy: -2857253.9993116

Ge	-4.29627	-0.18683	0.96574
Ge	-1.85603	0.63485	0.22312
F	-1.21516	-0.20375	-1.11887
F	-0.70393	0.65292	1.48289
F	-5.44839	-0.20492	-0.29402
F	-4.93715	0.65175	2.30774

14Sn

6

Energy: -519702.5455161

Sn	-4.60332	-0.50328	1.08019
Sn	-1.54900	0.95127	0.10869
F	-0.82593	-0.26839	-1.22555
F	-0.19296	0.64933	1.47178
F	-5.95935	-0.20133	-0.28292
F	-5.32638	0.71640	2.41442

14Sn radical cation

6

Energy: -519474.7865214

Sn	-4.42718	0.15572	0.85122
Sn	-1.44065	0.97250	-0.05460

F	-0.99028	-0.51662	-1.16186
F	-0.55716	0.72667	1.62096
F	-5.87904	-0.30104	-0.28412
F	-5.16263	0.30677	2.59501

15C

12

Energy: -98712.9597817

C	-3.86675	-0.22389	0.10457
C	-2.35216	0.11865	0.13083
C	-2.06502	-1.33667	-0.32924
C	-3.47842	-1.72564	0.18409
H	-2.00756	-1.40328	-1.42010
H	-1.20145	-1.85167	0.10038
H	-3.44174	-2.07061	1.22201
H	-4.06120	-2.43991	-0.40386
H	-4.50125	0.18647	0.89484
H	-4.31107	0.01934	-0.86551
H	-1.99840	0.93786	-0.50105
H	-2.00194	0.28692	1.15393

15C radical cation

12

Energy: -98495.7557081

C	-3.75742	-0.28474	0.22397
C	-2.29844	0.25624	-0.00869
C	-2.12337	-1.29944	-0.17601
C	-3.58320	-1.83975	0.05134
H	-1.83571	-1.50426	-1.21044
H	-1.48875	-1.66429	0.63546
H	-3.72882	-2.42851	0.95113
H	-4.06384	-2.26878	-0.82182
H	-4.04042	-0.08220	1.25997
H	-4.39518	0.08264	-0.58408
H	-2.15581	0.84131	-0.91138
H	-1.81601	0.68937	0.86142

15Si

12

Energy: -414229.1009134

Si	-4.27122	0.04455	0.12410
Si	-2.00419	0.53553	-0.17058
C	-1.97853	-1.38696	-0.17211
C	-3.51217	-1.71885	0.01994
H	-1.37229	-1.80342	0.63838
H	-1.58937	-1.80647	-1.10507

H	-1.55313	1.16392	-1.44193
H	-1.24253	1.16691	0.94112
H	-5.23688	0.37104	-0.96012
H	-4.92396	0.36423	1.42270
H	-3.68612	-2.31065	0.92404
H	-3.90592	-2.30098	-0.81907

15Si radical cation

12

Energy: -414035.2891681

Si	-4.40081	-0.11052	0.25874
Si	-1.82440	0.45442	-0.31168
C	-1.99451	-1.37268	0.08183
C	-3.50651	-1.68542	-0.23285
H	-1.77797	-1.53746	1.14161
H	-1.32296	-2.00855	-0.50572
H	-1.90463	0.85487	-1.73080
H	-1.17630	1.40644	0.60997
H	-5.39241	0.54341	-0.61583
H	-4.47162	0.21051	1.69841
H	-3.85430	-2.57114	0.31036
H	-3.64988	-1.86502	-1.30264

15Ge

12

Energy: -2657511.1281621

Ge	-4.32273	0.06588	0.12976
Ge	-1.96594	0.57630	-0.17485
C	-1.97677	-1.43430	-0.17335
C	-3.49449	-1.76287	0.01903
H	-1.36304	-1.83515	0.63761
H	-1.58425	-1.83614	-1.11114
H	-1.48910	1.21996	-1.49367
H	-1.16851	1.22071	0.97831
H	-5.32664	0.39154	-0.99586
H	-5.00490	0.38693	1.47605
H	-3.67864	-2.33990	0.92906
H	-3.90131	-2.33408	-0.81954

15Ge radical cation

12

Energy: -2657320.6174822

Ge	-4.46371	-0.10236	0.26959
Ge	-1.77179	0.48957	-0.32089
C	-1.99249	-1.42929	0.07518
C	-3.48476	-1.73903	-0.23008

H	-1.75906	-1.57606	1.13201
H	-1.31227	-2.04039	-0.52550
H	-1.83545	0.93914	-1.78273
H	-1.13473	1.46137	0.67207
H	-5.45587	0.57764	-0.67348
H	-4.56648	0.25427	1.75465
H	-3.84925	-2.60730	0.32685
H	-3.65043	-1.90870	-1.29627

15Sn

12

Energy: -319701.5187313

Sn	-4.50974	0.10756	0.15078
Sn	-1.81284	0.69207	-0.19254
C	-1.96594	-1.51668	-0.17817
C	-3.47058	-1.84284	0.02074
H	-1.34925	-1.91970	0.62917
H	-1.58234	-1.91387	-1.12136
H	-1.21725	1.36957	-1.66049
H	-0.86515	1.36410	1.07966
H	-5.66196	0.40344	-1.09543
H	-5.31383	0.40489	1.64531
H	-3.64855	-2.41093	0.93734
H	-3.87888	-2.41876	-0.81360

15Sn radical cation

12

Energy: -319521.0890507

Sn	-4.68446	-0.08186	0.06389
Sn	-1.57183	0.58181	-0.11316
C	-2.06426	-1.51347	-0.45109
C	-3.37966	-1.81235	0.29194
H	-1.24192	-2.14725	-0.10678
H	-2.16690	-1.62686	-1.53234
H	-1.10947	1.62478	-1.37606
H	-1.13477	1.05995	1.46372
H	-5.29865	0.26314	-1.48856
H	-5.51738	0.60824	1.37782
H	-3.22751	-1.93203	1.36669
H	-3.87950	-2.70525	-0.09466

16C

24

Energy: -197457.5686531

C	-3.84719	-0.12745	0.12089
C	-2.30741	0.23162	-0.03937

C	-2.00486	-1.28907	0.11086
C	-1.68081	1.17199	0.98592
C	-1.96166	0.70820	-1.45384
C	-3.47737	-1.59256	-0.25808
C	-4.84783	0.59293	-0.77802
C	-4.31801	-0.05387	1.57712
H	-1.77910	-1.55773	1.14715
H	-1.22402	-1.70154	-0.53540
H	-3.98599	-2.38700	0.29651
H	-3.60110	-1.77847	-1.32920
H	-4.38199	0.98316	1.92490
H	-3.64792	-0.59631	2.25183
H	-5.31457	-0.50127	1.66691
H	-0.59580	1.22573	0.83624
H	-1.85976	0.83693	2.01139
H	-2.07898	2.18906	0.88560
H	-4.57522	0.51931	-1.83446
H	-4.91996	1.65615	-0.51829
H	-5.84624	0.15535	-0.65897
H	-2.35779	0.03459	-2.22051
H	-0.87304	0.74737	-1.57518
H	-2.35840	1.71117	-1.64606

16C radical cation

24

Energy: -197273.4586594

C	-4.14649	-0.25659	0.17203
C	-1.98352	0.25135	-0.09891
C	-2.00633	-1.24709	0.09757
C	-1.56463	1.15483	1.00324
C	-1.88646	0.76887	-1.49149
C	-3.49383	-1.55637	-0.23848
C	-4.94655	0.53018	-0.80122
C	-4.40994	-0.03660	1.62075
H	-1.77290	-1.51474	1.12921
H	-1.31814	-1.76970	-0.57543
H	-3.87117	-2.41385	0.32898
H	-3.62514	-1.74535	-1.30504
H	-4.44423	1.02315	1.88576
H	-3.71603	-0.57068	2.27242
H	-5.41512	-0.44346	1.82282
H	-0.46160	1.20115	0.97012
H	-1.83093	0.78069	1.99239
H	-1.92517	2.17748	0.86647
H	-4.57579	0.45614	-1.82419
H	-5.05722	1.57621	-0.50467
H	-5.96046	0.09198	-0.80133
H	-2.30938	0.09092	-2.23506

H	-0.81087	0.86056	-1.71852
H	-2.31314	1.76922	-1.59950

16Si

24

Energy: -513005.9517202

Si	-4.24394	-0.07561	0.12923
Si	-1.96641	0.43422	-0.02803
C	-1.99038	-1.47229	0.18845
C	-0.98004	1.41904	1.24615
C	-1.39812	0.90134	-1.77106
C	-3.43718	-1.74686	-0.35896
C	-5.58908	0.58224	-1.02148
C	-4.90118	-0.14284	1.90200
H	-1.94822	-1.71778	1.25731
H	-1.20963	-2.05987	-0.30841
H	-3.88771	-2.67067	0.02228
H	-3.40708	-1.83025	-1.45290
H	-5.16384	0.85619	2.26753
H	-4.15617	-0.56229	2.58652
H	-5.80050	-0.76807	1.96162
H	0.09480	1.22413	1.14613
H	-1.27644	1.15762	2.26736
H	-1.13503	2.49644	1.11779
H	-1.92486	0.31455	-2.53122
H	-0.32323	0.71959	-1.89255
H	-1.58395	1.96072	-1.98036
H	-5.23985	0.62489	-2.05843
H	-5.89828	1.59258	-0.73014
H	-6.47872	-0.05874	-0.99089

16Si radical cation

24

Energy: -512837.7887745

Si	-4.37255	-0.24675	0.13469
Si	-1.77899	0.33615	-0.05446
C	-1.96953	-1.52633	0.16375
C	-1.07887	1.37442	1.31731
C	-1.51805	0.94363	-1.79360
C	-3.43152	-1.80846	-0.34298
C	-5.48301	0.59309	-1.09488
C	-4.80964	-0.05982	1.93350
H	-1.87875	-1.78087	1.22446
H	-1.22781	-2.11747	-0.38424
H	-3.84244	-2.72655	0.09074
H	-3.44125	-1.92249	-1.43152
H	-4.97079	0.98734	2.20543

H	-4.05047	-0.48787	2.59373
H	-5.75112	-0.59799	2.11583
H	0.01543	1.26616	1.30891
H	-1.43666	1.05468	2.29962
H	-1.30819	2.43491	1.17829
H	-2.05674	0.34169	-2.53050
H	-0.44546	0.87128	-2.02504
H	-1.80981	1.99181	-1.90591
H	-5.05446	0.59943	-2.10059
H	-5.71279	1.61971	-0.79515
H	-6.43157	0.03858	-1.13945

16Ge

24

Energy: -2756243.10488597

Ge	-4.28427	-0.09918	0.20247
Ge	-1.91994	0.43674	-0.09763
C	-1.92418	-1.57837	-0.14901
C	-0.85993	1.19969	1.38979
C	-1.31944	1.27030	-1.78981
C	-3.44796	-1.91728	-0.04129
C	-5.60100	0.36943	-1.19948
C	-5.13446	0.15130	1.97245
H	-1.35526	-1.99310	0.68915
H	-1.47663	-1.96893	-1.06842
H	-3.66464	-2.58685	0.79708
H	-3.82241	-2.40257	-0.94816
H	-5.45128	1.19032	2.10026
H	-4.43567	-0.10231	2.77391
H	-6.01450	-0.49441	2.05683
H	0.20552	1.00933	1.22487
H	-1.15351	0.74834	2.34113
H	-1.01450	2.28065	1.45308
H	-5.17694	0.20411	-2.19337
H	-5.89173	1.42039	-1.11386
H	-6.49761	-0.24966	-1.09264
H	-1.85856	0.84359	-2.63972
H	-0.24767	1.09764	-1.93134
H	-1.49844	2.34909	-1.76838

16Ge radical cation

24

Energy: -2756113.3358136

Ge	-4.42889	-0.26865	0.14851
Ge	-1.71724	0.33778	-0.06898
C	-1.96057	-1.61717	0.15108
C	-0.99092	1.41600	1.38525

C	-1.46023	0.99833	-1.88892
C	-3.40634	-1.89467	-0.34196
C	-5.57687	0.61248	-1.15954
C	-4.88614	-0.04558	2.03419
H	-1.85257	-1.84922	1.21370
H	-1.21163	-2.19007	-0.40402
H	-3.83387	-2.79870	0.10211
H	-3.44168	-1.99637	-1.42963
H	-5.02164	1.01093	2.27367
H	-4.11956	-0.47947	2.67848
H	-5.83347	-0.56884	2.21040
H	0.10037	1.31132	1.36417
H	-1.36044	1.06681	2.35068
H	-1.24577	2.46796	1.24300
H	-5.12124	0.59694	-2.15086
H	-5.78043	1.64095	-0.85524
H	-6.52394	0.06106	-1.19584
H	-2.00785	0.38817	-2.60925
H	-0.38936	0.93738	-2.11640
H	-1.77473	2.04091	-1.96668

16Sn

24

Energy: -418466.5777364

Sn	-4.47929	-0.05709	0.17203
Sn	-1.75645	0.53774	-0.06225
C	-1.95139	-1.66532	0.10352
C	-0.50303	1.48338	1.44745
C	-1.00046	1.15884	-2.00795
C	-3.41682	-1.94540	-0.30148
C	-6.05211	0.50853	-1.22472
C	-5.36175	-0.07592	2.16293
H	-1.78206	-1.91338	1.15702
H	-1.22313	-2.22640	-0.49198
H	-3.83826	-2.83193	0.18456
H	-3.50390	-2.08578	-1.38443
H	-5.68121	0.93143	2.44127
H	-4.63245	-0.43408	2.89311
H	-6.23114	-0.73954	2.16770
H	0.54261	1.21782	1.26726
H	-0.79429	1.14480	2.44420
H	-0.60869	2.56978	1.39270
H	-1.54585	0.64599	-2.80347
H	0.06154	0.90746	-2.08032
H	-1.12019	2.23813	-2.13056
H	-5.67848	0.46407	-2.25009
H	-6.39271	1.52476	-1.01093
H	-6.89550	-0.17961	-1.11763

16Sn radical cation

24

Energy: -418306.4879236

Sn	-4.61464	-0.27861	0.14945
Sn	-1.53983	0.38655	-0.06838
C	-1.96408	-1.74880	0.17741
C	-0.67242	1.52799	1.53779
C	-1.18210	1.08831	-2.07392
C	-3.37441	-2.00411	-0.38503
C	-5.91865	0.63003	-1.30273
C	-5.16374	-0.07527	2.22304
H	-1.91214	-1.94889	1.25055
H	-1.19889	-2.34987	-0.32342
H	-3.81833	-2.92675	0.00149
H	-3.37351	-2.05293	-1.47680
H	-5.33362	0.97690	2.45611
H	-4.37920	-0.48383	2.86093
H	-6.09080	-0.63587	2.37597
H	0.41193	1.38913	1.49438
H	-1.05165	1.17079	2.49559
H	-0.91042	2.58404	1.40219
H	-1.75770	0.49693	-2.78688
H	-0.11360	0.97289	-2.27897
H	-1.45379	2.14235	-2.14763
H	-5.45397	0.60351	-2.28873
H	-6.13012	1.65876	-1.00735
H	-6.84933	0.05504	-1.31713

17C

36

Energy: -296195.3251044

C	-3.82784	-0.12919	0.23935
C	-2.33339	0.21795	-0.15523
C	-1.97823	-1.32303	-0.07015
C	-1.57049	1.15469	0.78673
C	-2.19315	0.80198	-1.56779
C	-3.52656	-1.65584	-0.05792
C	-4.93206	0.52949	-0.59314
C	-4.15397	0.15483	1.71206
C	-1.25910	-1.71361	1.22862
C	-1.15598	-1.90531	-1.22381
C	-4.00638	-2.67019	0.98455
C	-4.06088	-2.13257	-1.41609
H	-4.19561	1.23536	1.88733
H	-3.42456	-0.26523	2.40750
H	-5.13472	-0.26127	1.96661

H	-0.51633	1.21347	0.49162
H	-1.60756	0.83871	1.83069
H	-1.98306	2.16881	0.72971
H	-4.80144	0.38903	-1.66771
H	-4.96351	1.60760	-0.39718
H	-5.91063	0.11846	-0.31845
H	-2.70166	0.21335	-2.33352
H	-1.13565	0.86633	-1.84648
H	-2.60680	1.81577	-1.59854
H	-1.58063	-1.68876	-2.20567
H	-1.08000	-2.99443	-1.12456
H	-0.13642	-1.50294	-1.20344
H	-0.23929	-1.31376	1.22941
H	-1.18760	-2.80392	1.30766
H	-1.75806	-1.34901	2.12883
H	-3.62671	-3.66999	0.74351
H	-5.10114	-2.72732	0.98284
H	-3.68683	-2.42771	1.99939
H	-3.78206	-1.48163	-2.24686
H	-5.15455	-2.18989	-1.39210
H	-3.68058	-3.13556	-1.63801

17C radical cation

36

Energy: -296015.4534849

C	-3.83888	0.13394	0.28689
C	-2.38186	0.23438	-0.15505
C	-2.01251	-1.35828	-0.05824
C	-1.51979	1.09673	0.78739
C	-2.22384	0.79589	-1.57411
C	-3.43630	-1.90449	-0.11689
C	-4.95939	0.55626	-0.60925
C	-4.16572	0.21593	1.74527
C	-1.28637	-1.71934	1.24394
C	-1.13301	-1.82848	-1.23290
C	-4.01249	-2.71010	1.00339
C	-4.05407	-2.19400	-1.44916
H	-4.20183	1.28587	2.00393
H	-3.41859	-0.23662	2.39551
H	-5.15200	-0.19907	1.96370
H	-0.47273	1.04198	0.47988
H	-1.58731	0.80272	1.83382
H	-1.83911	2.14045	0.70313
H	-4.78729	0.36492	-1.66644
H	-5.06438	1.64760	-0.49352
H	-5.90979	0.11577	-0.29776
H	-2.75697	0.23050	-2.33956
H	-1.16761	0.81593	-1.84926

H	-2.59545	1.82468	-1.60044
H	-1.57743	-1.64738	-2.21060
H	-0.95084	-2.90309	-1.13143
H	-0.16657	-1.32005	-1.19312
H	-0.28705	-1.27995	1.24395
H	-1.17352	-2.80583	1.30823
H	-1.79801	-1.38460	2.14761
H	-3.67896	-3.74982	0.85074
H	-5.10466	-2.72404	0.96675
H	-3.67484	-2.41168	1.99351
H	-3.75373	-1.50794	-2.23955
H	-5.14355	-2.23968	-1.38844
H	-3.70697	-3.19443	-1.75217

17Si

36

Energy: -611743.2578625

Si	-4.21823	-0.02177	0.36085
Si	-2.02711	0.49307	-0.24924
C	-1.94717	-1.42915	-0.00318
C	-0.86050	1.47004	0.87454
C	-1.71080	1.06623	-2.02658
C	-3.51078	-1.75614	-0.14208
C	-5.71503	0.53163	-0.65473
C	-4.68909	0.13007	2.18920
C	-1.46754	-1.69030	1.43882
C	-1.05237	-2.23187	-0.95747
C	-3.97038	-2.97369	0.67175
C	-3.88393	-1.99677	-1.61846
H	-5.00048	1.15602	2.41721
H	-3.86630	-0.12385	2.86348
H	-5.53149	-0.53209	2.42417
H	0.18842	1.26777	0.62474
H	-1.00793	1.22641	1.93085
H	-1.02666	2.54657	0.75291
H	-2.36235	0.57409	-2.75407
H	-0.67235	0.86247	-2.31561
H	-1.87264	2.14687	-2.11280
H	-5.51459	0.50318	-1.72985
H	-5.99425	1.55883	-0.39346
H	-6.58458	-0.10718	-0.45634
H	-3.58044	-1.16899	-2.26908
H	-4.96716	-2.11758	-1.72560
H	-3.40833	-2.90801	-2.00180
H	-1.26408	-2.02024	-2.00914
H	-1.17155	-3.31354	-0.80073
H	0.00243	-1.99268	-0.77802
H	-0.43126	-1.35962	1.56585

H	-1.50715	-2.75987	1.67981
H	-2.07434	-1.16360	2.18366
H	-3.42896	-3.88210	0.37118
H	-5.03722	-3.16114	0.50163
H	-3.82723	-2.83838	1.74739

17Si radical cation

36

Energy: -611578.0139019

Si	-4.31914	-0.16321	0.38715
Si	-1.88107	0.41334	-0.28971
C	-1.94000	-1.47622	-0.00504
C	-1.01229	1.48750	0.96130
C	-1.80688	1.08798	-2.02612
C	-3.50500	-1.80758	-0.14285
C	-5.58118	0.62436	-0.73619
C	-4.61069	0.19054	2.19445
C	-1.43042	-1.74065	1.42732
C	-1.06221	-2.25689	-1.00276
C	-3.94957	-3.00955	0.71236
C	-3.89983	-2.06412	-1.61232
H	-4.77386	1.25959	2.36184
H	-3.80352	-0.15170	2.84508
H	-5.52782	-0.33378	2.49884
H	0.07209	1.40731	0.79894
H	-1.21649	1.19189	1.99275
H	-1.28651	2.53859	0.82964
H	-2.40674	0.52368	-2.74284
H	-0.76104	1.04771	-2.36270
H	-2.11713	2.13722	-2.05096
H	-5.30740	0.56814	-1.79201
H	-5.74475	1.67160	-0.46450
H	-6.53812	0.09796	-0.61017
H	-3.59834	-1.25448	-2.28374
H	-4.98258	-2.18817	-1.70577
H	-3.43043	-2.98499	-1.97138
H	-1.29113	-2.02774	-2.04587
H	-1.19725	-3.33503	-0.85564
H	-0.00471	-2.03357	-0.83032
H	-0.39404	-1.40905	1.53862
H	-1.45797	-2.81313	1.64281
H	-2.02673	-1.23393	2.19182
H	-3.38871	-3.90532	0.42038
H	-5.01038	-3.22052	0.54411
H	-3.80159	-2.85306	1.78322

17Ge

36

Energy: -2855018.4564436

Ge	-4.26940	0.00433	0.37905
Ge	-1.98592	0.53631	-0.26360
C	-1.94909	-1.48057	0.00984
C	-0.73835	1.51785	0.91934
C	-1.62670	1.12929	-2.11962
C	-3.49262	-1.79778	-0.16109
C	-5.84252	0.54283	-0.69558
C	-4.78586	0.14799	2.28665
C	-1.49733	-1.71004	1.46134
C	-1.03472	-2.28132	-0.92335
C	-3.97619	-3.01642	0.63224
C	-3.85447	-1.99394	-1.64201
H	-5.14054	1.16077	2.49866
H	-3.94676	-0.07286	2.94992
H	-5.59621	-0.55635	2.50040
H	0.29676	1.27335	0.65943
H	-0.90790	1.25953	1.96699
H	-0.88087	2.59530	0.79644
H	-5.61693	0.51041	-1.76379
H	-6.14087	1.56138	-0.43116
H	-6.68371	-0.12805	-0.49272
H	-2.31143	0.66210	-2.83065
H	-0.60072	0.86659	-2.39692
H	-1.73831	2.21515	-2.18951
H	-1.22900	-2.07636	-1.97972
H	-1.15266	-3.36347	-0.76414
H	0.01573	-2.03837	-0.72568
H	-0.46589	-1.37158	1.60558
H	-1.53563	-2.77521	1.72406
H	-2.12559	-1.17260	2.18123
H	-3.43722	-3.92701	0.33139
H	-5.04127	-3.19418	0.44341
H	-3.84717	-2.89335	1.71117
H	-3.52435	-1.15361	-2.26396
H	-4.93798	-2.09199	-1.76701
H	-3.39173	-2.90344	-2.04686

17Ge radical cation

36

Energy: -2854855.9216762

Ge	-4.36663	-0.16034	0.41752
Ge	-1.83301	0.43230	-0.31990
C	-1.93689	-1.55860	0.01085
C	-0.92109	1.54969	1.00333
C	-1.75385	1.16133	-2.13511
C	-3.47440	-1.87443	-0.17094

C	-5.68715	0.65958	-0.77222
C	-4.68334	0.22598	2.31044
C	-1.47142	-1.76863	1.45981
C	-1.02692	-2.34059	-0.94648
C	-3.95952	-3.07881	0.64773
C	-3.85590	-2.05960	-1.64743
H	-4.87135	1.29391	2.44168
H	-3.84926	-0.08333	2.94066
H	-5.57982	-0.32578	2.61624
H	0.15667	1.49202	0.81113
H	-1.11740	1.20793	2.02012
H	-1.23751	2.58908	0.89212
H	-5.39177	0.57453	-1.81852
H	-5.82213	1.71051	-0.50744
H	-6.64160	0.13949	-0.62946
H	-2.39003	0.61200	-2.82935
H	-0.71465	1.09003	-2.47659
H	-2.04247	2.21474	-2.12151
H	-1.23164	-2.13108	-1.99890
H	-1.15493	-3.41910	-0.78855
H	0.02418	-2.10815	-0.74956
H	-0.44094	-1.42840	1.59603
H	-1.49958	-2.83399	1.71173
H	-2.09886	-1.24087	2.18508
H	-3.41116	-3.98123	0.34889
H	-5.02037	-3.26825	0.45664
H	-3.82476	-2.94745	1.72389
H	-3.51971	-1.22969	-2.27720
H	-4.93931	-2.15313	-1.76450
H	-3.40491	-2.97697	-2.04045

17Sn

36

Energy: -517198.9643424869

Sn	-4.45485	0.05916	0.43261
Sn	-1.84110	0.66684	-0.30188
C	-1.95410	-1.54516	0.06233
C	-0.38333	1.63866	0.99304
C	-1.34020	1.25230	-2.34095
C	-3.46555	-1.84643	-0.22150
C	-6.21861	0.51424	-0.76247
C	-5.08652	0.12171	2.51777
C	-1.62973	-1.70963	1.55399
C	-0.98364	-2.39706	-0.76471
C	-3.98352	-3.12101	0.45580
C	-3.73985	-1.92487	-1.72999
H	-5.57818	1.07566	2.72425
H	-4.23005	0.00701	3.18500

H	-5.79480	-0.69184	2.69923
H	0.62296	1.30624	0.72173
H	-0.57639	1.38644	2.03771
H	-0.44434	2.72273	0.86870
H	-2.08309	0.87489	-3.04636
H	-0.35979	0.84022	-2.59682
H	-1.29856	2.34210	-2.41150
H	-5.97188	0.48926	-1.82583
H	-6.59381	1.50771	-0.50452
H	-6.99839	-0.22469	-0.55587
H	-3.36997	-1.03644	-2.25931
H	-4.81197	-2.01203	-1.93611
H	-3.24798	-2.79823	-2.18057
H	-3.41674	-4.00643	0.12819
H	-5.03242	-3.29536	0.19012
H	-3.92152	-3.07205	1.54653
H	-0.60927	-1.38104	1.77780
H	-1.71206	-2.75994	1.86626
H	-2.31354	-1.12900	2.18773
H	-1.08979	-2.23102	-1.84041
H	-1.13405	-3.47156	-0.57614
H	0.05321	-2.16668	-0.49409

17Sn radical cation

36

Energy: -517056.7791286

Sn	-4.48129	0.21825	0.39115
Sn	-1.88116	0.82574	-0.23655
C	-1.98596	-1.59648	0.03415
C	-0.39277	1.50195	1.17575
C	-1.33421	1.19578	-2.29334
C	-3.42117	-1.88535	-0.19674
C	-6.15013	0.42860	-0.96492
C	-5.07145	0.06458	2.46364
C	-1.47409	-1.81035	1.45025
C	-0.99638	-2.05989	-1.03662
C	-4.10250	-2.85619	0.77093
C	-3.84133	-2.09737	-1.64342
H	-5.53757	1.00945	2.75313
H	-4.20393	-0.12336	3.09684
H	-5.79494	-0.74701	2.56368
H	0.56332	1.03628	0.92741
H	-0.68890	1.24411	2.19223
H	-0.30856	2.58680	1.07593
H	-2.04636	0.72244	-2.96986
H	-0.33015	0.80356	-2.46664
H	-1.33908	2.27642	-2.45505
H	-5.79993	0.43197	-1.99680

H	-6.64847	1.37383	-0.73701
H	-6.84238	-0.39975	-0.80003
H	-3.48583	-1.30269	-2.30781
H	-4.92800	-2.16008	-1.73780
H	-3.42793	-3.04366	-2.02055
H	-3.68809	-3.86269	0.60484
H	-5.17806	-2.91292	0.58259
H	-3.94538	-2.60936	1.82192
H	-0.45458	-1.43583	1.56839
H	-1.45387	-2.88489	1.68160
H	-2.10550	-1.33058	2.20531
H	-1.27027	-1.75559	-2.04776
H	-0.96086	-3.16049	-1.02430
H	0.01430	-1.70054	-0.82479

18C

20

Energy: -237732.0146534

C	-3.85603	-0.11950	0.16788
C	-2.28568	0.12412	-0.02759
C	-2.15942	-1.37868	-0.41063
N	-1.66106	0.35777	1.26649
N	-1.94547	1.18494	-0.97923
C	-3.54601	-1.63485	0.23497
N	-4.65550	0.22284	-1.00402
N	-4.50646	0.43496	1.34051
H	-1.30359	-1.92084	0.00170
H	-2.17251	-1.50887	-1.49681
H	-3.45779	-1.95673	1.27356
H	-4.24718	-2.29038	-0.28891
H	-2.23796	0.92958	-1.92198
H	-0.93388	1.31128	-1.01335
H	-1.72834	1.34935	1.49640
H	-0.67078	0.11778	1.23796
H	-4.85712	1.37078	1.14514
H	-3.83304	0.48955	2.10405
H	-4.50944	-0.44405	-1.75732
H	-4.39121	1.14594	-1.34878

18C radical cation

20

Energy: -237603.5928492

C	-4.44894	-0.21946	0.01280
C	-1.34087	0.04705	-0.02464
C	-2.08870	-1.14856	-0.51967
N	-1.43556	0.31346	1.38216
N	-1.41608	1.21263	-0.81728

C	-3.52427	-1.38663	0.10571
N	-5.51061	-0.27311	-0.79059
N	-4.17751	0.84304	0.74594
H	-1.53781	-2.06867	-0.29704
H	-2.17744	-1.08937	-1.60792
H	-3.39806	-1.62224	1.16655
H	-3.97471	-2.25784	-0.37511
H	-1.27448	1.01846	-1.80392
H	-0.77096	1.94720	-0.53419
H	-0.80907	1.06238	1.67506
H	-1.19333	-0.50828	1.93243
H	-4.72234	1.69448	0.69542
H	-3.27497	0.84490	1.25838
H	-5.72939	-1.12570	-1.28576
H	-6.15337	0.50125	-0.89829

18Si

20

Energy: -553345.6261168

Si	-4.14846	0.05302	0.08183
Si	-1.81414	0.31773	-0.05440
C	-2.03727	-1.57277	0.16400
N	-0.61333	0.91057	1.04742
N	-1.34164	0.94320	-1.59567
C	-3.52264	-1.71286	-0.31858
N	-5.46951	0.47182	-0.96059
N	-4.71677	0.40869	1.67569
H	-1.96881	-1.82962	1.23007
H	-1.33848	-2.22471	-0.37143
H	-4.05679	-2.55138	0.14136
H	-3.54489	-1.87064	-1.40568
H	-5.55273	-0.01981	2.05611
H	-4.06851	0.67306	2.40511
H	-0.37841	1.89598	1.06091
H	-0.51608	0.50091	1.96820
H	-2.03322	1.12478	-2.31047
H	-0.43244	0.74605	-1.99779
H	-5.49082	0.14224	-1.91774
H	-5.91356	1.37875	-0.87829

18Si radical cation

20

Energy: -553195.1394624

Si	-4.27585	-0.09276	0.13831
Si	-1.65715	0.20846	-0.11876
C	-2.01949	-1.62626	0.11999
N	-0.71515	0.95427	1.07000

N	-1.29873	0.80474	-1.66468
C	-3.52627	-1.77198	-0.27777
N	-5.37177	0.54238	-0.98083
N	-4.73705	0.25757	1.73155
H	-1.88782	-1.85014	1.18611
H	-1.36050	-2.29559	-0.44018
H	-4.01814	-2.62138	0.20452
H	-3.61799	-1.90988	-1.36250
H	-5.54512	0.82716	1.95533
H	-4.12364	0.14885	2.52923
H	-0.43531	1.92755	1.05457
H	-0.49034	0.50945	1.95098
H	-1.88079	0.64237	-2.47661
H	-0.63777	1.55692	-1.82220
H	-5.50316	0.14807	-1.90374
H	-5.85643	1.42520	-0.87330

18Ge

20

Energy: -2796587.5659368

Ge	-4.22498	0.00961	0.12003
Ge	-1.78544	0.35811	-0.02627
C	-2.01220	-1.65204	0.10576
N	-0.70145	1.12924	1.26459
N	-1.17806	1.12315	-1.61922
C	-3.49975	-1.81837	-0.29009
N	-5.69958	0.43376	-0.94838
N	-4.81541	0.14902	1.87802
H	-1.85004	-1.93790	1.15053
H	-1.31873	-2.22358	-0.51815
H	-4.01131	-2.61793	0.25200
H	-3.60563	-2.00978	-1.36363
H	-1.85443	1.07092	-2.37728
H	-0.30270	0.72468	-1.95503
H	-0.02201	1.78495	0.88993
H	-0.24912	0.48716	1.90719
H	-5.82961	0.16770	1.96049
H	-4.43233	0.94795	2.37491
H	-5.55399	0.26109	-1.94114
H	-6.01169	1.39727	-0.84421

18Ge radical cation

20

Energy: -2796436.7047370

Ge	-4.33348	-0.08059	0.15710
Ge	-1.60135	0.22699	-0.13439
C	-2.02051	-1.69937	0.10059

N	-0.55463	1.05181	1.09710
N	-1.03119	0.70441	-1.78953
C	-3.51710	-1.84313	-0.25368
N	-5.53885	0.61468	-1.00745
N	-4.98270	0.10794	1.84106
H	-1.82735	-1.93247	1.15155
H	-1.36564	-2.32375	-0.51197
H	-4.01846	-2.64743	0.29005
H	-3.66740	-2.01070	-1.32399
H	-1.40677	0.22016	-2.59754
H	-0.84193	1.67797	-2.00444
H	-0.17131	1.96785	0.88267
H	-0.82685	0.99797	2.07319
H	-5.37423	0.99477	2.14128
H	-4.50514	-0.35575	2.60621
H	-5.26875	0.70712	-1.98123
H	-6.10484	1.40652	-0.71652

18Sn

20

Energy: -458774.4137474

Sn	-4.42009	0.03775	0.23687
Sn	-1.63621	0.53385	-0.19183
C	-1.95158	-1.70834	-0.25787
N	-0.38647	1.16647	1.31457
N	-0.89300	1.64930	-1.77065
C	-3.40837	-1.95295	0.11230
N	-6.00563	0.14130	-1.08692
N	-5.40986	0.37744	2.00907
H	-1.24119	-2.16822	0.43377
H	-1.70949	-2.02502	-1.27551
H	-3.52317	-2.40678	1.09976
H	-3.94578	-2.56319	-0.61824
H	0.32552	1.81354	0.98062
H	0.07640	0.41651	1.82304
H	-6.35262	0.73141	1.84936
H	-4.93405	1.03697	2.62182
H	-5.74635	-0.14121	-2.03181
H	-6.38631	1.08456	-1.16324
H	-1.45721	1.56718	-2.61558
H	0.05714	1.37411	-2.02158

18Sn radical cation

20

Energy: -458621.8940200

Sn	-4.51118	-0.05035	0.28350
Sn	-1.45458	0.42682	-0.32666

C	-2.02293	-1.70062	-0.44631
N	-0.20153	0.91472	1.17917
N	-0.65363	1.27253	-1.97503
C	-3.34083	-1.91976	0.28925
N	-5.86943	0.13048	-1.19890
N	-5.51000	0.42950	1.97055
H	-1.19701	-2.28423	-0.03272
H	-2.10025	-1.90489	-1.51682
H	-3.19779	-2.15066	1.34752
H	-3.96197	-2.69672	-0.16272
H	0.11604	1.87949	1.24162
H	-0.43572	0.58111	2.11074
H	-6.15749	1.21373	1.92521
H	-4.96733	0.49748	2.82808
H	-5.55943	-0.06725	-2.14690
H	-6.45820	0.96038	-1.20778
H	-1.19776	1.22327	-2.83291
H	-0.26730	2.20964	-1.88092

19C

44

Energy: -435158.8141575

C	-3.80642	-0.09610	-0.10757
C	-2.17830	0.12109	-0.09343
C	-2.05661	-1.43029	0.00099
N	-1.70734	0.85855	1.06449
N	-1.59343	0.67926	-1.34735
C	-3.51895	-1.58450	-0.46153
N	-4.59028	0.59043	-1.12288
N	-4.47059	-0.02978	1.20832
H	-1.91146	-1.78767	1.02079
H	-1.28543	-1.87144	-0.63606
H	-4.12843	-2.33900	0.03931
H	-3.59996	-1.72455	-1.53935
C	-2.00581	0.05434	-2.60983
C	-0.12993	0.68705	-1.29461
C	-1.74994	2.31032	0.97819
C	-0.57444	0.38693	1.84644
C	-4.77949	1.29223	1.74131
C	-4.04968	-0.90782	2.29507
C	-5.98383	0.17371	-1.18434
C	-4.38649	1.99396	-1.45133
H	-1.59224	0.65013	-3.42986
H	-3.09253	0.04802	-2.68462
H	-1.62538	-0.97781	-2.72437
H	0.24294	1.12509	-2.22506
H	0.30682	-0.32478	-1.19911
H	0.22656	1.29734	-0.46537

H	-6.61487	0.63698	-0.40731
H	-6.04922	-0.91056	-1.06423
H	-6.38925	0.44521	-2.16614
H	-5.10322	1.95706	0.94300
H	-3.93486	1.75712	2.27212
H	-5.60836	1.18956	2.45255
H	-3.94300	-1.93812	1.95612
H	-4.83621	-0.89259	3.05872
H	-3.10814	-0.58750	2.77126
H	-4.93579	2.70227	-0.80477
H	-4.73814	2.16058	-2.47793
H	-3.32102	2.22184	-1.41586
H	-0.55090	-0.70271	1.87532
H	-0.68085	0.75112	2.87599
H	0.40415	0.73650	1.47234
H	-2.66427	2.63037	0.48122
H	-0.89480	2.74481	0.43241
H	-1.74569	2.72371	1.99398

19C radical cation

44

Energy: -435040.4565226

C	-4.23463	-0.04957	0.19841
C	-1.66068	-0.16443	-0.20719
C	-2.23899	-1.55608	0.00752
N	-1.00757	0.47820	0.82601
N	-1.35619	0.23633	-1.48523
C	-3.78342	-1.48643	-0.02220
N	-4.82668	0.65261	-0.83270
N	-4.50447	0.36895	1.47890
H	-1.90501	-1.91698	0.98300
H	-1.85614	-2.26856	-0.73194
H	-4.22956	-2.16489	0.71378
H	-4.14762	-1.81204	-0.99920
C	-2.06803	-0.26438	-2.65319
C	-0.42168	1.32041	-1.76917
C	-1.20248	1.90619	1.07064
C	-0.35989	-0.24574	1.91859
C	-5.33706	1.53142	1.76961
C	-3.83556	-0.19542	2.64318
C	-5.53358	-0.00542	-1.93029
C	-4.51478	2.06115	-1.06687
H	-2.69360	0.52110	-3.09739
H	-2.70111	-1.10680	-2.38626
H	-1.34294	-0.58859	-3.40549
H	-0.92818	2.28883	-1.88063
H	0.08610	1.09182	-2.70961
H	0.31374	1.38588	-0.96852

H	-6.35117	0.64908	-2.24683
H	-5.97029	-0.94572	-1.59492
H	-4.89195	-0.18857	-2.80285
H	-6.06445	1.66871	0.97068
H	-4.74518	2.44951	1.88651
H	-5.86308	1.34396	2.70910
H	-3.30132	-1.10443	2.37820
H	-4.58300	-0.43373	3.40544
H	-3.12367	0.52082	3.07444
H	-5.42882	2.65487	-1.17274
H	-3.92638	2.16906	-1.98951
H	-3.93023	2.45356	-0.23711
H	0.00647	-1.21212	1.57272
H	-1.01802	-0.39159	2.78600
H	0.50259	0.34158	2.24701
H	-1.74791	2.35162	0.24106
H	-0.24274	2.42060	1.18530
H	-1.78589	2.05558	1.99078

19Si

44

Energy: -750781.6826377

Si	-4.10429	0.09888	0.18192
Si	-1.77731	0.01337	-0.19944
C	-2.34011	-1.80610	-0.43360
N	-0.60230	0.08419	1.08370
N	-1.09454	0.92008	-1.50411
C	-3.68184	-1.76313	0.37586
N	-5.27190	0.29142	-1.09527
N	-4.71262	1.02634	1.50905
H	-1.66982	-2.62520	-0.14986
H	-2.56277	-1.93228	-1.50255
H	-3.46962	-1.92641	1.44199
H	-4.41194	-2.52369	0.07705
C	-1.90763	1.67897	-2.44150
C	0.28836	0.74955	-1.93157
C	0.00505	1.35210	1.46845
C	-0.45685	-0.94386	2.10296
C	-6.10455	0.95639	1.93584
C	-3.83813	1.67892	2.47101
C	-5.49858	-0.69919	-2.13645
C	-5.76878	1.61424	-1.45410
H	-1.48697	2.68377	-2.59806
H	-2.92086	1.78623	-2.04610
H	-1.97246	1.18721	-3.42560
H	0.78099	1.72508	-2.06042
H	0.35610	0.21100	-2.89022
H	0.83826	0.18358	-1.17519

H	-6.57449	-0.80502	-2.33966
H	-5.11430	-1.67186	-1.82435
H	-5.00734	-0.42161	-3.08371
H	-6.70110	0.46857	1.16065
H	-6.51227	1.96444	2.10431
H	-6.21670	0.38882	2.87342
H	-2.81969	1.71562	2.07614
H	-3.81392	1.14742	3.43623
H	-4.17293	2.70885	2.66616
H	-6.85835	1.59034	-1.60299
H	-5.31468	1.98760	-2.38686
H	-5.54543	2.32133	-0.65133
H	-0.92073	-1.87473	1.77213
H	-0.92190	-0.64673	3.05741
H	0.60693	-1.14289	2.30035
H	-0.15987	2.09315	0.68241
H	1.08930	1.23331	1.61150
H	-0.41253	1.74229	2.41143

19Si radical cation

44

Energy: -750644.6989191

Si	-4.15800	-0.00030	0.29332
Si	-1.72704	-0.08944	-0.31014
C	-2.40286	-1.84346	-0.51905
N	-0.74818	0.12727	1.07777
N	-1.12353	0.74230	-1.67541
C	-3.62562	-1.80784	0.45500
N	-5.11564	0.32736	-1.08765
N	-4.69398	0.84245	1.67977
H	-1.70691	-2.66698	-0.33207
H	-2.74438	-1.94265	-1.55632
H	-3.29541	-1.96303	1.48897
H	-4.38523	-2.56717	0.24574
C	-1.96360	0.91661	-2.86245
C	0.15138	1.45857	-1.73531
C	-0.39552	1.46541	1.56108
C	-0.29497	-0.95550	1.95151
C	-5.90948	1.65396	1.75948
C	-3.84356	0.91921	2.86970
C	-5.65188	-0.69474	-1.98737
C	-5.36615	1.70027	-1.53566
H	-2.21167	1.97343	-3.02081
H	-2.89449	0.35565	-2.74602
H	-1.43714	0.54660	-3.74970
H	0.00440	2.54625	-1.73030
H	0.67209	1.18829	-2.66141
H	0.77874	1.17774	-0.88909

H	-6.74500	-0.61814	-2.03831
H	-5.39451	-1.69262	-1.62948
H	-5.25392	-0.56689	-3.00227
H	-6.55560	1.44353	0.90701
H	-5.67842	2.72665	1.78157
H	-6.45066	1.40176	2.67894
H	-2.96165	0.28694	2.73835
H	-4.39905	0.57151	3.74821
H	-3.51060	1.94816	3.05354
H	-6.44069	1.91969	-1.53045
H	-4.99343	1.84430	-2.55693
H	-4.86115	2.41100	-0.87703
H	-0.62740	-1.92104	1.56777
H	-0.68482	-0.82337	2.96906
H	0.80063	-0.96419	2.00572
H	-0.83943	2.22873	0.91740
H	0.69274	1.60098	1.56677
H	-0.76349	1.61313	2.58354

19Ge

44

Energy: -2994024.8089833

Ge	-4.16099	0.13304	0.19318
Ge	-1.71615	0.04103	-0.19829
C	-2.32068	-1.88431	-0.36600
N	-0.38527	0.19028	1.09263
N	-0.97299	0.95841	-1.62683
C	-3.71263	-1.83828	0.30771
N	-5.46623	0.42080	-1.10141
N	-4.84132	1.06889	1.64034
H	-1.63955	-2.62523	0.06224
H	-2.41003	-2.09217	-1.43828
H	-3.64162	-2.08369	1.37337
H	-4.45027	-2.50948	-0.14135
C	-1.84506	1.42929	-2.69179
C	0.36249	0.59342	-2.08612
C	0.14574	1.51676	1.38803
C	-0.43739	-0.67131	2.26580
C	-6.20292	0.79388	2.08569
C	-3.94382	1.45359	2.71884
C	-5.46862	-0.40956	-2.29836
C	-5.88239	1.79426	-1.36611
H	-1.42453	2.33460	-3.15316
H	-2.82809	1.68265	-2.28243
H	-1.98945	0.68475	-3.49491
H	0.86868	1.47212	-2.51171
H	0.34424	-0.19037	-2.86360
H	0.95341	0.23013	-1.24109

H	-6.48947	-0.48472	-2.69923
H	-5.12621	-1.41964	-2.05847
H	-4.82571	-0.00806	-3.10109
H	-6.81469	0.49603	1.23002
H	-6.64428	1.69768	2.53046
H	-6.24725	-0.00707	2.84436
H	-2.94176	1.64019	2.32000
H	-3.86155	0.68579	3.50869
H	-4.29945	2.37907	3.19445
H	-6.92458	1.80723	-1.71553
H	-5.26593	2.28411	-2.14047
H	-5.81547	2.38065	-0.44638
H	-0.86195	-1.64355	2.00213
H	-1.03787	-0.24304	3.08736
H	0.57812	-0.83930	2.65188
H	0.11496	2.13326	0.48623
H	1.19043	1.43494	1.72058
H	-0.41698	2.03330	2.18565

19Ge radical cation

44

Energy: -2993884.8214591

Ge	-4.27770	0.18034	0.13793
Ge	-1.75692	-0.29256	-0.37033
C	-2.69975	-2.03752	-0.54097
N	-0.77446	-0.10502	1.16506
N	-0.74111	0.27043	-1.79488
C	-4.02410	-1.79981	0.22570
N	-5.44839	0.69457	-1.18731
N	-4.70631	1.09945	1.66469
H	-2.12227	-2.88746	-0.16969
H	-2.87767	-2.19659	-1.60841
H	-3.92508	-2.07175	1.28027
H	-4.87322	-2.34679	-0.18946
C	-1.37354	0.46186	-3.09750
C	0.51635	0.99184	-1.61819
C	-0.45582	1.22668	1.67879
C	-0.71599	-1.15857	2.17540
C	-4.73870	0.43010	2.96417
C	-4.44080	2.53685	1.75281
C	-5.26576	0.19068	-2.54490
C	-6.26517	1.90005	-1.09129
H	-1.65249	1.50992	-3.27426
H	-2.27167	-0.15628	-3.17583
H	-0.67361	0.15730	-3.88417
H	0.37976	2.08265	-1.62536
H	1.18565	0.73142	-2.44680
H	0.98421	0.69239	-0.67936

H	-6.24796	-0.01549	-2.98636
H	-4.69670	-0.74311	-2.52900
H	-4.74645	0.91112	-3.19172
H	-4.93199	-0.63744	2.84193
H	-5.55084	0.85333	3.56794
H	-3.79945	0.56282	3.51995
H	-4.35168	2.97375	0.75545
H	-3.51322	2.74353	2.30473
H	-5.26577	3.03510	2.27660
H	-7.20187	1.72942	-1.63499
H	-5.77411	2.77873	-1.53373
H	-6.49810	2.10432	-0.04533
H	-0.98582	-2.12266	1.74048
H	-1.38319	-0.95110	3.02411
H	0.30757	-1.23740	2.56281
H	-0.57374	1.97878	0.89498
H	0.58203	1.25444	2.03303
H	-1.10921	1.49806	2.52005

19Sn

44

Energy: -656207.3841451

Sn	-4.33381	0.20246	-0.00650
Sn	-1.48788	0.38983	-0.14677
C	-2.02278	-1.79571	0.01593
N	0.11509	0.90579	1.03757
N	-0.78014	1.09579	-1.93934
C	-3.52024	-1.88962	-0.23000
N	-6.00085	0.52752	-1.16911
N	-5.11692	0.75743	1.80817
H	-1.74061	-2.11942	1.02071
H	-1.42229	-2.34289	-0.71493
H	-4.04321	-2.53063	0.48401
H	-3.76021	-2.21853	-1.24399
C	0.65039	2.25993	0.94359
C	0.18703	0.37074	2.39093
C	-6.39730	0.20700	2.23591
C	-4.22004	1.03656	2.91908
C	-6.00694	0.03166	-2.53907
C	-6.72428	1.78641	-1.02639
C	-1.69822	1.25181	-3.05673
C	0.57628	0.76561	-2.35872
H	-0.24424	-0.63479	2.42696
H	-0.33738	0.99691	3.13441
H	1.23801	0.29533	2.70914
H	0.99665	1.58171	-2.96721
H	0.62330	-0.15616	-2.96647
H	1.21547	0.62975	-1.48158

H	0.51047	2.64550	-0.07007
H	1.72869	2.25330	1.16521
H	0.17151	2.95853	1.65192
H	-1.36364	2.06809	-3.71577
H	-2.69947	1.50724	-2.69023
H	-1.78632	0.34276	-3.67928
H	-7.03816	-0.18897	-2.85440
H	-5.43153	-0.89695	-2.61099
H	-5.58877	0.75274	-3.26358
H	-7.79319	1.63187	-1.23981
H	-6.35960	2.56863	-1.71510
H	-6.62836	2.15588	-0.00162
H	-7.01946	-0.01263	1.36353
H	-6.93384	0.93392	2.86575
H	-6.28692	-0.72102	2.82554
H	-3.27712	1.45487	2.54792
H	-3.98092	0.14170	3.52224
H	-4.67208	1.77658	3.59769

19Sn radical cation

44

Energy: -656065.7691651

Sn	-4.33014	0.09922	0.12177
Sn	-1.47746	0.30599	-0.27791
C	-1.99438	-1.87501	-0.11817
N	-0.04285	0.85385	1.10117
N	-0.68953	1.20913	-1.94471
C	-3.50915	-1.98237	-0.10163
N	-5.84258	0.48126	-1.22733
N	-5.20613	0.85418	1.81604
H	-1.52751	-2.24329	0.79695
H	-1.53544	-2.36821	-0.97715
H	-3.89340	-2.55902	0.74184
H	-3.92153	-2.38547	-1.02818
C	0.73277	2.07733	0.94976
C	-0.03041	0.29460	2.44481
C	-6.32439	0.10471	2.39535
C	-4.35442	1.48046	2.82746
C	-5.80657	-0.05268	-2.58064
C	-6.77445	1.58448	-1.03804
C	-1.60443	1.77007	-2.93939
C	0.49928	0.59714	-2.54501
H	-0.63696	-0.61345	2.49072
H	-0.41067	1.01337	3.18486
H	0.99967	0.03954	2.72881
H	1.03243	1.35545	-3.13360
H	0.26138	-0.24073	-3.21890
H	1.17514	0.23655	-1.76377

H	0.67895	2.42493	-0.08369
H	1.77961	1.87941	1.21776
H	0.36405	2.87126	1.61576
H	-1.08473	2.55845	-3.49925
H	-2.47172	2.21931	-2.44532
H	-1.96194	1.02521	-3.66794
H	-6.79910	-0.43708	-2.85251
H	-5.08650	-0.87165	-2.65332
H	-5.53846	0.72191	-3.31356
H	-7.79113	1.24849	-1.28396
H	-6.53512	2.42950	-1.70016
H	-6.74231	1.92348	-0.00094
H	-6.95508	-0.30729	1.60191
H	-6.93774	0.78760	2.99801
H	-6.00007	-0.71861	3.05073
H	-3.53827	2.02909	2.34640
H	-3.92083	0.75831	3.53735
H	-4.95169	2.19708	3.40616

20C

10

Energy: -97935.4834286

C	-3.87322	-0.00307	0.06781
C	-2.34859	0.32714	-0.12815
C	-2.14504	-1.17659	-0.15473
C	-3.44639	-1.45849	0.01257
H	-4.00835	-2.38552	0.08467
H	-1.25505	-1.78914	-0.26927
H	-4.52385	0.33585	-0.74595
H	-4.29681	0.33537	1.01987
H	-2.11031	0.85866	-1.05610
H	-1.88333	0.85805	0.70976

20C radical cation

10

Energy: -97725.6635350

C	-3.87310	-0.00699	0.06791
C	-2.34712	0.32353	-0.12839
C	-2.10891	-1.14071	-0.15916
C	-3.49395	-1.44070	0.01859
H	-4.04742	-2.37504	0.08905
H	-1.22368	-1.76340	-0.27281
H	-4.56298	0.30565	-0.73035
H	-4.33826	0.30506	1.01507
H	-2.06004	0.84751	-1.05245
H	-1.83547	0.84735	0.69303

20Si

10

Energy: -413459.4985162

Si	-4.27527	0.05960	0.11969
Si	-2.00739	0.55058	-0.17216
C	-2.10274	-1.33440	-0.16004
C	-3.42072	-1.61975	0.00932
H	-3.80836	-2.63923	0.05895
H	-1.33414	-2.10350	-0.25895
H	-5.25373	0.34357	-0.96425
H	-4.94715	0.34313	1.41627
H	-1.52391	1.15099	-1.44445
H	-1.21752	1.15127	0.93610

20Si radical cation

10

Energy: -413256.9774457

Si	-4.43997	-0.07220	0.14091
Si	-1.80352	0.49860	-0.19833
C	-2.10553	-1.33471	-0.15967
C	-3.41787	-1.61878	0.00917
H	-3.79640	-2.64063	0.05767
H	-1.34441	-2.10985	-0.25781
H	-5.20734	0.40512	-1.02561
H	-4.88785	0.40444	1.46363
H	-1.60483	1.18521	-1.48927
H	-1.28323	1.18506	0.99979

20Ge

10

Energy: -2656738.0294077

Ge	-4.32906	0.07541	0.12643
Ge	-1.96485	0.58732	-0.17757
C	-2.09726	-1.38252	-0.16049
C	-3.40611	-1.66590	0.00729
H	-3.80472	-2.68016	0.05828
H	-1.32076	-2.14234	-0.26014
H	-5.34153	0.35792	-1.00186
H	-5.02218	0.35708	1.47484
H	-1.46176	1.19728	-1.50152
H	-1.14271	1.19816	0.97522

20Ge radical cation

10

Energy: -2656540.1883553

Ge	-4.50656	-0.07192	0.14941
Ge	-1.74285	0.52642	-0.20622
C	-2.10088	-1.38439	-0.16012
C	-3.40194	-1.66603	0.00708
H	-3.79742	-2.68015	0.05760
H	-1.32741	-2.14543	-0.25984
H	-5.28871	0.42634	-1.06630
H	-4.95523	0.42625	1.52361
H	-1.55171	1.23545	-1.54736
H	-1.21823	1.23573	1.04262

20Sn

10

Energy: -318927.8779727

Sn	-4.51176	0.10490	0.14941
Sn	-1.81071	0.69030	-0.19717
C	-2.08127	-1.46593	-0.16194
C	-3.38649	-1.74872	0.00534
H	-3.76184	-2.77325	0.05347
H	-1.32177	-2.24474	-0.25930
H	-5.67087	0.35021	-1.09762
H	-5.31710	0.34978	1.64962
H	-1.19215	1.31875	-1.67420
H	-0.83698	1.32096	1.07287

20Sn radical cation

10

Energy: -318741.2350204

Sn	-4.69287	-0.06318	0.17278
Sn	-1.57682	0.61168	-0.22770
C	-2.08468	-1.46982	-0.16170
C	-3.38191	-1.75085	0.00471
H	-3.75748	-2.77343	0.05307
H	-1.32555	-2.24657	-0.25889
H	-5.60624	0.43305	-1.17424
H	-5.23469	0.43158	1.70800
H	-1.30036	1.36331	-1.72897
H	-0.93034	1.36647	1.15340

21C

22

Energy: -196679.0113400

C	-3.85481	-0.13219	0.14246
C	-2.29508	0.23931	-0.06909
C	-2.09449	-1.26682	-0.16952
C	-1.60089	0.90254	1.12547

C	-1.96431	1.01874	-1.34660
C	-3.38546	-1.57434	0.00558
C	-4.80787	0.34155	-0.96023
C	-4.44362	0.22563	1.51147
H	-3.93451	-2.51275	0.04205
H	-1.19714	-1.86072	-0.32914
H	-4.53316	1.31194	1.62921
H	-3.83599	-0.16177	2.33260
H	-5.44790	-0.20307	1.60806
H	-0.52195	0.96241	0.94127
H	-1.75022	0.34048	2.05031
H	-1.96948	1.92379	1.27731
H	-2.37831	0.54031	-2.23729
H	-0.87718	1.07849	-1.47409
H	-2.34970	2.04363	-1.29274
H	-4.46376	0.04742	-1.95450
H	-4.92112	1.43183	-0.94068
H	-5.80021	-0.09807	-0.80657

21C radical cation

22

Energy: -196481.9943673

C	-3.86456	-0.09743	0.09610
C	-2.29916	0.26752	-0.01737
C	-2.07605	-1.21077	-0.14484
C	-1.63555	1.04509	1.11592
C	-1.87849	0.86046	-1.40378
C	-3.42685	-1.52863	-0.01010
C	-4.83711	0.48163	-0.92768
C	-4.45152	0.03930	1.54139
H	-3.96422	-2.46367	0.13631
H	-1.19492	-1.78984	-0.41465
H	-4.48499	1.11218	1.76466
H	-3.84657	-0.45464	2.30477
H	-5.46126	-0.37384	1.56080
H	-0.55080	1.05500	0.98346
H	-1.85840	0.61061	2.09217
H	-1.99019	2.07929	1.10380
H	-2.24331	0.27907	-2.25326
H	-0.79034	0.92531	-1.45436
H	-2.31227	1.86596	-1.45868
H	-4.48224	0.34180	-1.95038
H	-4.96377	1.55209	-0.74451
H	-5.81460	0.00186	-0.83446

21Si

22

Energy: -512235.3772737

Si	-4.23445	-0.09610	0.19494
Si	-1.96594	0.42379	-0.10416
C	-2.05340	-1.46475	-0.18128
C	-0.94398	1.09823	1.33578
C	-1.37579	1.24211	-1.70254
C	-3.36824	-1.76604	-0.00779
C	-5.49232	0.29782	-1.15986
C	-5.05745	0.15464	1.87796
H	-3.74255	-2.79385	-0.00302
H	-1.28655	-2.23102	-0.32709
H	-5.39343	1.19103	1.99892
H	-4.36798	-0.07464	2.69662
H	-5.93627	-0.49301	1.98428
H	0.12431	0.90039	1.18512
H	-1.24161	0.64026	2.28438
H	-1.06953	2.18313	1.43020
H	-1.93030	0.86896	-2.56938
H	-0.31004	1.04626	-1.87258
H	-1.50947	2.32920	-1.65799
H	-5.06394	0.15068	-2.15632
H	-5.83230	1.33748	-1.08804
H	-6.37593	-0.34620	-1.07283

21Si radical cation

22

Energy: -512062.0845839

Si	-4.36994	-0.25160	0.20821
Si	-1.77876	0.34394	-0.13476
C	-2.04727	-1.50174	-0.18373
C	-1.02994	1.08777	1.39412
C	-1.47773	1.23793	-1.73530
C	-3.35579	-1.80250	-0.00949
C	-5.40946	0.33202	-1.21672
C	-4.96491	0.18644	1.91278
H	-3.72267	-2.83024	-0.00488
H	-1.28633	-2.27022	-0.32947
H	-5.22555	1.24631	1.98762
H	-4.23220	-0.06438	2.68359
H	-5.87659	-0.39504	2.11476
H	0.06101	0.95972	1.33508
H	-1.37451	0.59274	2.30525
H	-1.23405	2.16042	1.46162
H	-2.07101	0.82727	-2.55588
H	-0.41596	1.11877	-1.99693
H	-1.67718	2.30944	-1.64106
H	-4.92130	0.16485	-2.17989
H	-5.67009	1.38990	-1.11799

H	-6.34694	-0.24343	-1.21159

21Ge

22

Energy: -2755506.4747144

Ge	-4.28936	-0.09091	0.20192
Ge	-1.91852	0.45074	-0.10929
C	-2.04582	-1.52621	-0.18456
C	-0.83305	1.13757	1.39492
C	-1.28200	1.28785	-1.78461
C	-3.35226	-1.82471	-0.01298
C	-5.61259	0.29717	-1.21623
C	-5.15798	0.14919	1.96273
H	-3.73722	-2.84763	-0.00637
H	-1.27210	-2.28431	-0.33017
H	-5.49206	1.18396	2.08146
H	-4.45905	-0.09097	2.76751
H	-6.02895	-0.50891	2.04305
H	0.22558	0.91867	1.22309
H	-1.14232	0.66912	2.33234
H	-0.95388	2.22104	1.48442
H	-1.84865	0.90933	-2.63869
H	-0.22173	1.06181	-1.93583
H	-1.40200	2.37388	-1.73374
H	-5.16855	0.14597	-2.20303
H	-5.95786	1.33216	-1.13846
H	-6.47682	-0.36646	-1.11217

21Ge radical cation

22

Energy: -2755335.5650913

Ge	-4.43253	-0.27537	0.21434
Ge	-1.71173	0.34768	-0.14342
C	-2.03660	-1.58055	-0.18855
C	-0.94453	1.12419	1.47321
C	-1.41206	1.28156	-1.82957
C	-3.33534	-1.87790	-0.01744
C	-5.50782	0.34277	-1.29122
C	-5.03655	0.18920	2.01005
H	-3.71829	-2.89881	-0.01136
H	-1.26518	-2.33717	-0.33463
H	-5.27858	1.25222	2.06614
H	-4.27940	-0.06886	2.75154
H	-5.94505	-0.39104	2.21190
H	0.14251	0.98968	1.41856
H	-1.31999	0.61502	2.36174

H	-1.16505	2.19212	1.52377
H	-2.02498	0.85215	-2.62308
H	-0.35409	1.15795	-2.09058
H	-1.62492	2.34634	-1.71717
H	-4.98902	0.16741	-2.23451
H	-5.74631	1.40204	-1.17825
H	-6.44164	-0.23229	-1.28615

21Sn

22

Energy: -417693.3509591

Sn	-4.47304	-0.06688	0.22557
Sn	-1.76209	0.54797	-0.12454
C	-2.03095	-1.61784	-0.18945
C	-0.48644	1.23183	1.50036
C	-0.97236	1.39520	-1.96681
C	-3.33507	-1.91359	-0.02145
C	-5.97243	0.26264	-1.31661
C	-5.47685	0.10299	2.14888
H	-3.69860	-2.94545	-0.01972
H	-1.27531	-2.39609	-0.33161
H	-5.85461	1.11965	2.28310
H	-4.77902	-0.13237	2.95507
H	-6.31709	-0.59632	2.18205
H	0.54919	0.95108	1.28880
H	-0.80068	0.77211	2.43959
H	-0.54903	2.31909	1.59122
H	-1.54208	1.02464	-2.82142
H	0.07621	1.10485	-2.07773
H	-1.03820	2.48556	-1.93367
H	-5.52918	0.12082	-2.30436
H	-6.36845	1.27835	-1.24030
H	-6.79108	-0.44990	-1.18166

21Sn radical cation

22

Energy: -417528.9688406

Sn	-4.61212	-0.29616	0.23582
Sn	-1.53948	0.39904	-0.16353
C	-2.01620	-1.70444	-0.19652
C	-0.64284	1.21357	1.61542
C	-1.15416	1.38785	-2.03594
C	-3.31268	-1.99766	-0.02817
C	-5.82694	0.32725	-1.42770
C	-5.30455	0.15937	2.22219
H	-3.67939	-3.02565	-0.02603

H	-1.26029	-2.47849	-0.34017
H	-5.55917	1.21814	2.28545
H	-4.53197	-0.09632	2.94745
H	-6.19870	-0.44448	2.40388
H	0.43594	1.04503	1.54485
H	-1.03999	0.70314	2.49291
H	-0.84336	2.28451	1.66710
H	-1.77746	0.95121	-2.81638
H	-0.09766	1.23500	-2.27586
H	-1.35517	2.45495	-1.93231
H	-5.29092	0.14959	-2.36011
H	-6.07704	1.38357	-1.32060
H	-6.74302	-0.27065	-1.40643

22C

28

Energy: -246056.2008552761

C	-3.83448	-0.15365	0.13699
C	-2.28423	0.19837	-0.10709
C	-2.08649	-1.31545	-0.16762
C	-1.56567	0.89339	1.05570
C	-1.96625	0.93905	-1.41159
C	-3.38334	-1.60997	0.03490
C	-4.80366	0.29733	-0.96225
C	-4.40120	0.24713	1.50423
C	-4.17122	-2.87249	0.13657
C	-0.84707	-2.11768	-0.38099
H	-4.47901	1.33673	1.59690
H	-3.78514	-0.12487	2.32676
H	-5.40875	-0.16692	1.62868
H	-0.48923	0.94271	0.85375
H	-1.70310	0.35970	1.99949
H	-1.92420	1.92125	1.18534
H	-2.39318	0.43488	-2.28228
H	-0.88080	0.99329	-1.55588
H	-2.34722	1.96662	-1.38600
H	-4.48029	-0.03005	-1.95357
H	-4.90750	1.38862	-0.97545
H	-5.79849	-0.12547	-0.77920
H	-3.53383	-3.75365	0.01458
H	-4.95599	-2.91265	-0.62983
H	-4.67381	-2.94914	1.10941
H	-0.09850	-1.90346	0.39268
H	-0.38183	-1.88019	-1.34641
H	-1.05606	-3.19170	-0.36141

22C radical cation

28

Energy: -245878.5512004143

C	-3.83735	-0.15922	0.13413
C	-2.28161	0.19660	-0.10020
C	-2.06011	-1.28510	-0.22134
C	-1.55228	0.76813	1.14107
C	-1.91429	1.03299	-1.33845
C	-3.41418	-1.60115	0.09478
C	-4.76593	0.17822	-1.05869
C	-4.49318	0.31436	1.44283
C	-4.13591	-2.85786	0.30842
C	-0.88395	-2.09270	-0.55365
H	-4.59279	1.40306	1.42074
H	-3.91191	0.03473	2.32323
H	-5.49435	-0.11470	1.53680
H	-0.48024	0.83546	0.94053
H	-1.70083	0.15630	2.03341
H	-1.93162	1.77419	1.33941
H	-2.34826	0.62983	-2.25525
H	-0.82793	1.07039	-1.45545
H	-2.27512	2.05609	-1.20135
H	-4.39045	-0.21511	-2.00571
H	-4.85287	1.26508	-1.14109
H	-5.76134	-0.23566	-0.87985
H	-3.52563	-3.74240	0.12193
H	-5.03763	-2.88489	-0.32005
H	-4.51201	-2.88937	1.34324
H	-0.03239	-1.79531	0.07445
H	-0.56843	-1.86456	-1.58430
H	-1.05801	-3.16565	-0.46321

22Si

28

Energy: -561611.8093359

Si	-4.25341	0.01158	0.20153
Si	-1.99901	0.52249	-0.09508
C	-2.07642	-1.36654	-0.17149
C	-0.96412	1.19457	1.33950
C	-1.39280	1.33591	-1.69243
C	-3.39969	-1.66678	0.00138
C	-5.52127	0.39914	-1.14888
C	-5.08546	0.25521	1.88366
C	-3.98648	-3.05356	0.02100
C	-0.97659	-2.38661	-0.37206
H	-5.43384	1.28730	2.00556
H	-4.39634	0.03289	2.70470
H	-5.95800	-0.40157	1.98776
H	0.10012	0.97160	1.19348

H	-1.27226	0.75489	2.29345
H	-1.06403	2.28314	1.42120
H	-1.95704	0.97957	-2.56014
H	-0.33213	1.11573	-1.86596
H	-1.49910	2.42586	-1.64441
H	-5.09521	0.25999	-2.14763
H	-5.87301	1.43456	-1.07354
H	-6.39856	-0.25376	-1.06171
H	-3.23394	-3.83718	-0.11716
H	-4.74185	-3.16451	-0.76751
H	-4.50332	-3.24114	0.97087
H	0.00509	-1.91306	-0.46320
H	-1.14326	-2.97943	-1.28025
H	-0.92809	-3.09193	0.46687

22Si radical cation

28

Energy: -561443.0455835

Si	-4.35983	-0.14683	0.22506
Si	-1.83902	0.42016	-0.14933
C	-2.06811	-1.43638	-0.17289
C	-1.05532	1.20230	1.34637
C	-1.55539	1.30836	-1.76016
C	-3.38557	-1.73184	0.02468
C	-5.42292	0.43187	-1.18873
C	-4.95767	0.32581	1.92269
C	-4.00968	-3.10235	0.08468
C	-0.94026	-2.41426	-0.37658
H	-5.20131	1.39079	1.98260
H	-4.23206	0.07569	2.70052
H	-5.88059	-0.23493	2.13107
H	0.03522	1.08669	1.26292
H	-1.37158	0.72239	2.27578
H	-1.26835	2.27407	1.40048
H	-2.14424	0.88265	-2.57627
H	-0.49252	1.20795	-2.02448
H	-1.77252	2.37732	-1.67504
H	-4.95913	0.23959	-2.15923
H	-5.66213	1.49621	-1.10506
H	-6.37202	-0.12278	-1.15364
H	-3.27566	-3.89920	-0.05235
H	-4.77845	-3.20935	-0.68942
H	-4.50578	-3.25715	1.04987
H	-0.17326	-2.28451	0.39581
H	-0.45148	-2.24239	-1.34267
H	-1.28037	-3.45154	-0.34715

22Ge

28

Energy: -2804882.6154506

Ge	-4.30955	0.03025	0.21039
Ge	-1.95388	0.56144	-0.10142
C	-2.06929	-1.41846	-0.16784
C	-0.85146	1.25030	1.39193
C	-1.30781	1.38890	-1.78033
C	-3.38440	-1.71429	0.00299
C	-5.64615	0.40486	-1.20150
C	-5.18303	0.26201	1.97218
C	-3.98545	-3.09345	0.02308
C	-0.96280	-2.42971	-0.36893
H	-5.53783	1.28993	2.08984
H	-4.47975	0.03733	2.77781
H	-6.04165	-0.41214	2.05531
H	0.20120	0.99853	1.22683
H	-1.17388	0.81033	2.33873
H	-0.94010	2.33846	1.45928
H	-1.88641	1.02427	-2.63253
H	-0.25328	1.14037	-1.93797
H	-1.40266	2.47738	-1.72842
H	-5.20621	0.26161	-2.19146
H	-6.00629	1.43452	-1.12113
H	-6.50138	-0.27018	-1.09429
H	-3.23685	-3.88320	-0.10581
H	-4.73110	-3.20208	-0.77499
H	-4.51357	-3.27546	0.96776
H	0.02601	-1.96548	-0.31402
H	-1.04283	-2.91251	-1.35149
H	-0.99957	-3.22517	0.38554

22Ge radical cation

28

Energy: -2804716.5411210

Ge	-4.42155	-0.15695	0.22917
Ge	-1.77753	0.43651	-0.15485
C	-2.05796	-1.50840	-0.17180
C	-0.97450	1.25853	1.42516
C	-1.50025	1.36620	-1.85118
C	-3.36549	-1.80106	0.01800
C	-5.51742	0.46109	-1.26589
C	-5.03400	0.34592	2.01502
C	-4.00474	-3.16146	0.07780
C	-0.92022	-2.47162	-0.37017
H	-5.25208	1.41501	2.05596
H	-4.28953	0.08289	2.76770
H	-5.95841	-0.20738	2.21925

H	0.11287	1.14145	1.34585
H	-1.31853	0.76425	2.33472
H	-1.20892	2.32425	1.46162
H	-2.10215	0.91614	-2.64175
H	-0.43963	1.27215	-2.11309
H	-1.74141	2.42612	-1.74858
H	-5.02254	0.26135	-2.21722
H	-5.73106	1.52722	-1.16671
H	-6.46476	-0.09022	-1.23412
H	-3.27333	-3.96385	-0.04653
H	-4.76267	-3.26884	-0.70676
H	-4.51176	-3.31054	1.03808
H	-0.15761	-2.33816	0.40580
H	-0.43037	-2.30063	-1.33578
H	-1.25442	-3.51163	-0.34018

22Sn

28

Energy: -467068.2386395

Sn	-4.49776	0.08353	0.23626
Sn	-1.80774	0.69204	-0.11133
C	-2.05766	-1.47992	-0.17640
C	-0.51682	1.36646	1.50767
C	-0.99816	1.52564	-1.95315
C	-3.36917	-1.77551	-0.00658
C	-6.00497	0.39233	-1.30474
C	-5.51089	0.23790	2.15783
C	-3.94615	-3.16875	0.00807
C	-0.97060	-2.51847	-0.37815
H	-5.90951	1.24658	2.29180
H	-4.81081	0.01666	2.96625
H	-6.33761	-0.47770	2.18994
H	0.51026	1.04881	1.30556
H	-0.84812	0.93420	2.45413
H	-0.54352	2.45668	1.57911
H	-1.60389	1.20870	-2.80462
H	0.02773	1.17077	-2.08836
H	-0.99198	2.61718	-1.89962
H	-5.55494	0.28571	-2.29399
H	-6.43812	1.39124	-1.21082
H	-6.79831	-0.35149	-1.18673
H	-3.18442	-3.94554	-0.12757
H	-4.69450	-3.28792	-0.78594
H	-4.46426	-3.36565	0.95534
H	0.01747	-2.06317	-0.48864
H	-1.15634	-3.12032	-1.27712
H	-0.91920	-3.21165	0.47130

22Sn radical cation

28

Energy: -466902.3973982629

Sn	-4.60351	-0.14200	0.21104
Sn	-1.61183	0.51690	-0.13880
C	-2.04466	-1.60847	-0.22347
C	-0.90631	1.36087	1.71762
C	-0.98382	1.51627	-1.93984
C	-3.35435	-1.89562	-0.07022
C	-5.97732	0.40231	-1.35506
C	-5.17231	0.42328	2.21443
C	-3.99621	-3.25779	-0.11131
C	-0.92501	-2.58534	-0.46826
H	-5.37465	1.49490	2.24678
H	-4.37698	0.16160	2.91248
H	-6.08380	-0.12755	2.46510
H	0.18083	1.23985	1.74144
H	-1.35646	0.83211	2.55794
H	-1.15532	2.42245	1.75357
H	-1.49836	1.08614	-2.79943
H	0.09558	1.37093	-2.04325
H	-1.19957	2.58270	-1.85840
H	-5.53547	0.18236	-2.32717
H	-6.21916	1.46327	-1.27550
H	-6.88805	-0.18865	-1.21974
H	-3.27138	-4.05262	-0.30763
H	-4.76275	-3.30300	-0.89398
H	-4.49252	-3.48210	0.84004
H	-0.40327	-2.35357	-1.40438
H	-1.28108	-3.61726	-0.53076
H	-0.18222	-2.53361	0.33628

23C

18

Energy: -236953.6576697

C	-3.88095	-0.10682	0.16820
C	-2.27264	0.13914	-0.00975
C	-2.20711	-1.37241	-0.17150
N	-1.63565	0.63303	1.20264
N	-1.94997	1.01046	-1.14420
C	-3.52270	-1.57551	-0.01636
N	-4.75185	0.43597	-0.86865
N	-4.42264	0.23585	1.46964
H	-4.14880	-2.46318	0.00966
H	-1.36590	-2.03767	-0.35608
H	-1.51661	1.64339	1.13653
H	-0.71881	0.21419	1.34079

H	-5.04076	1.03863	1.38591
H	-3.65150	0.45708	2.10137
H	-4.68052	-0.11304	-1.72212
H	-4.45983	1.38840	-1.09304
H	-2.37315	0.65041	-1.99870
H	-0.94125	1.02716	-1.29694

23C radical cation

18

Energy: -236858.5100789

C	-4.57530	-0.16029	0.23456
C	-1.35108	0.23118	-0.32602
C	-2.29501	-0.73523	-0.76438
N	-1.67855	1.39894	0.26106
N	-0.03764	-0.00852	-0.55526
C	-3.68872	-0.79533	-0.65098
N	-5.89499	-0.07640	-0.05257
N	-4.15031	0.44098	1.40666
H	-4.17380	-1.48236	-1.33883
H	-1.85868	-1.50385	-1.39536
H	-0.96347	2.01952	0.61351
H	-2.62722	1.54137	0.59354
H	-4.86730	0.83756	2.00415
H	-3.45105	-0.07961	1.92598
H	-6.23302	-0.38519	-0.95278
H	-6.58756	0.06748	0.66970
H	0.23444	-0.82030	-1.08944
H	0.65865	0.71515	-0.44610

23Si

18

Energy: -552576.8649745

Si	-4.14706	0.05001	0.14641
Si	-1.82323	0.29430	-0.12005
C	-2.13325	-1.57349	-0.16288
N	-0.62027	0.63709	1.08346
N	-1.27130	1.19940	-1.48488
C	-3.47585	-1.71557	0.01026
N	-5.40389	0.26724	-1.03116
N	-4.85419	0.69111	1.58715
H	-3.96371	-2.69349	0.04315
H	-1.46309	-2.42858	-0.28590
H	-1.89085	1.36583	-2.26751
H	-0.30440	1.14661	-1.78509
H	-0.37707	1.60008	1.28514
H	-0.58308	0.07360	1.92426

H	-5.78945	0.42060	1.86986
H	-4.27268	0.89705	2.38935
H	-5.33493	-0.20596	-1.92404
H	-5.83232	1.17925	-1.14012

23Si radical cation

18

Energy: -552422.9264163

Si	-4.25496	-0.07215	0.20637
Si	-1.69375	0.20204	-0.19032
C	-2.13904	-1.60790	-0.20586
N	-0.76902	0.70599	1.13359
N	-1.23998	0.99884	-1.61095
C	-3.46314	-1.75217	0.04949
N	-5.27022	0.36898	-1.07291
N	-4.84515	0.47648	1.69287
H	-3.95167	-2.72385	0.12548
H	-1.46997	-2.45253	-0.37182
H	-1.77273	0.93293	-2.46919
H	-0.55992	1.74951	-1.64242
H	-0.40866	1.64370	1.26364
H	-0.65281	0.13465	1.96131
H	-5.65800	1.07390	1.78957
H	-4.30358	0.43135	2.54693
H	-5.27881	-0.13028	-1.95365
H	-5.80919	1.22560	-1.11470

23Ge

18

Energy: -2795814.8554911

Ge	-4.24190	-0.00924	0.21046
Ge	-1.81099	0.34628	-0.08360
C	-2.11266	-1.62599	-0.18042
N	-0.71140	0.86189	1.31681
N	-1.15471	1.33864	-1.52067
C	-3.43676	-1.80957	-0.00786
N	-5.62045	0.24851	-1.02041
N	-5.06172	0.33022	1.83764
H	-3.91683	-2.78913	0.00474
H	-1.40359	-2.44247	-0.32926
H	0.00129	1.53897	1.06190
H	-0.29902	0.10641	1.85402
H	-6.00155	0.70603	1.74090
H	-4.52524	0.92327	2.46363
H	-5.39330	-0.10128	-1.94893

H	-5.89689	1.22350	-1.11841
H	-1.74477	1.28587	-2.34792
H	-0.21013	1.07317	-1.79521

23Ge radical cation

18

Energy: -2795660.1675013

Ge	-4.33158	-0.06860	0.20313
Ge	-1.61953	0.22303	-0.18687
C	-2.13247	-1.66555	-0.17459
N	-0.55404	0.78944	1.16665
N	-0.98208	0.88187	-1.75104
C	-3.45414	-1.80762	0.01377
N	-5.50134	0.40303	-1.09961
N	-5.07180	0.29651	1.81753
H	-3.96524	-2.76803	0.05583
H	-1.44119	-2.49672	-0.30378
H	-0.20283	1.74228	1.16498
H	-0.77629	0.48650	2.10916
H	-5.59522	1.15666	1.94916
H	-4.54171	0.06308	2.65058
H	-5.23367	0.24076	-2.06474
H	-6.03423	1.26281	-1.01012
H	-1.46185	0.62816	-2.60828
H	-0.64140	1.83747	-1.79432

23Sn

18

Energy: -458000.4265644

Sn	-4.41377	0.02922	0.23509
Sn	-1.65324	0.55756	-0.19044
C	-2.02209	-1.62155	-0.19271
N	-0.38345	1.20937	1.28355
N	-0.89626	1.58020	-1.81864
C	-3.32299	-1.85557	0.01842
N	-6.01747	0.11074	-1.05948
N	-5.37959	0.26745	2.03140
H	-3.75140	-2.85797	0.07309
H	-1.28494	-2.41526	-0.33044
H	-1.46302	1.44753	-2.65564
H	0.04707	1.26837	-2.05237
H	0.38047	1.77472	0.91801
H	0.01207	0.46296	1.85067
H	-6.31694	0.64736	1.90307
H	-4.88560	0.88094	2.67677
H	-5.75547	-0.14592	-2.01097

H	-6.42384	1.04459	-1.11405

23Sn radical cation

18

Energy: -457844.2877349

Sn	-4.50630	-0.04891	0.22693
Sn	-1.45964	0.43270	-0.27162
C	-2.03381	-1.65068	-0.18569
N	-0.16915	1.06709	1.14225
N	-0.71223	1.07783	-2.03029
C	-3.33522	-1.85625	0.02503
N	-5.93936	0.24798	-1.16069
N	-5.39679	0.23442	2.01432
H	-3.78559	-2.84620	0.09305
H	-1.30838	-2.45469	-0.30715
H	-1.24775	0.85417	-2.86576
H	-0.39556	2.04365	-2.08460
H	0.14626	2.03370	1.09472
H	-0.39713	0.83730	2.10666
H	-5.98907	1.05492	2.12404
H	-4.81012	0.13314	2.83919
H	-5.65992	0.15417	-2.13435
H	-6.53070	1.07043	-1.06070

24C

42

Energy: -434378.8221066

C	-3.82189	-0.04946	0.14050
C	-2.10628	-0.13214	-0.14316
C	-2.37960	-1.62554	-0.10970
N	-1.10742	0.23143	0.85860
N	-1.80154	0.34592	-1.46845
C	-3.69451	-1.56242	0.09826
N	-4.77839	0.41684	-0.85967
N	-4.08181	0.44637	1.46893
H	-4.46969	-2.32148	0.16023
H	-1.68174	-2.45590	-0.17548
C	-2.03495	1.74378	-1.79471
C	-0.63569	-0.22227	-2.12460
C	-0.37638	1.48069	0.78803
C	-1.20908	-0.30836	2.20804
C	-5.30724	-0.00080	2.11086
C	-3.70897	1.81049	1.80933
C	-4.73202	-0.12535	-2.21117
C	-5.37925	1.73354	-0.78343

H	-5.75714	-0.22726	-2.59291
H	-4.26220	-1.10875	-2.19715
H	-4.16871	0.50554	-2.91582
H	-6.27026	1.73667	-1.42164
H	-4.73078	2.56098	-1.12605
H	-5.70189	1.95185	0.23404
H	-5.46458	-1.06196	1.90692
H	-6.20606	0.55018	1.77941
H	-5.21271	0.13063	3.19515
H	-2.94797	2.16828	1.11631
H	-3.29176	1.84453	2.82526
H	-4.55476	2.51677	1.77876
H	-1.77734	-1.23850	2.19178
H	-1.70398	0.37493	2.91505
H	-0.19969	-0.51634	2.58873
H	-0.03122	1.66854	-0.22818
H	0.50890	1.39018	1.42771
H	-0.93819	2.36829	1.13362
H	0.31943	0.22731	-1.79748
H	-0.72449	-0.07222	-3.20701
H	-0.59028	-1.29589	-1.93057
H	-1.12045	2.35862	-1.76969
H	-2.74627	2.17267	-1.08931
H	-2.45842	1.83004	-2.80494

24C radical cation

42

Energy: -434307.9023159

C	-4.51374	0.04588	-0.42699
C	-1.40531	-0.08250	0.43052
C	-2.35966	-1.11807	0.27665
N	-0.43693	-0.19309	1.38749
N	-1.37810	1.03016	-0.36531
C	-3.65304	-1.06686	-0.25937
N	-5.48884	0.01062	-1.38246
N	-4.44262	1.16451	0.35812
H	-4.08665	-2.02238	-0.54044
H	-2.00904	-2.10334	0.57056
C	-0.87684	2.32149	0.10271
C	-1.79925	0.99379	-1.76363
C	0.94381	0.24501	1.15706
C	-0.62738	-1.05428	2.55398
C	-4.02986	1.10073	1.75800
C	-4.81534	2.49276	-0.12557
C	-5.37985	-0.88032	-2.53705
C	-6.82249	0.57925	-1.16005
H	-5.91165	-1.82450	-2.36515
H	-4.33010	-1.08817	-2.74226

H	-5.82464	-0.38654	-3.40596
H	-7.56806	-0.20269	-1.33780
H	-7.02513	1.41371	-1.83915
H	-6.91080	0.91712	-0.12871
H	-3.99406	0.06129	2.07861
H	-4.76161	1.64106	2.36753
H	-3.04681	1.56052	1.90843
H	-4.90923	2.47494	-1.21107
H	-4.02893	3.20144	0.15469
H	-5.75737	2.84221	0.31194
H	-1.69178	-1.15957	2.76214
H	-0.13691	-0.59264	3.41594
H	-0.18716	-2.04671	2.39526
H	1.06249	0.55814	0.12096
H	1.61316	-0.60065	1.34615
H	1.22466	1.06652	1.82403
H	-1.01274	1.43779	-2.38287
H	-2.72262	1.56323	-1.91613
H	-1.95698	-0.03845	-2.06996
H	0.09471	2.57174	-0.33822
H	-0.78465	2.30673	1.18834
H	-1.58992	3.10056	-0.18657

24Si

42

Energy: -750013.5196419

Si	-4.12846	0.13855	0.10964
Si	-1.78358	0.02258	-0.10879
C	-2.36911	-1.77888	-0.05106
N	-0.56666	0.27523	1.10499
N	-1.11900	0.69391	-1.55858
C	-3.72511	-1.71170	0.04032
N	-5.31023	0.51969	-1.10523
N	-4.72772	0.86385	1.56174
H	-4.35337	-2.60581	0.07746
H	-1.83264	-2.73062	-0.09515
C	-1.94824	1.27195	-2.60561
C	0.25124	0.43167	-1.98187
C	0.11499	1.55383	1.25475
C	-0.43751	-0.58613	2.27163
C	-6.11876	0.73646	1.97894
C	-3.84974	1.35761	2.61215
C	-5.52736	-0.31709	-2.27668
C	-5.85537	1.86284	-1.25010
H	-6.60340	-0.44965	-2.46306
H	-5.07899	-1.30134	-2.12194
H	-5.08216	0.12194	-3.18444
H	-6.94471	1.82654	-1.39861

H	-5.41938	2.39182	-2.11380
H	-5.64805	2.44291	-0.34764
H	-6.71939	0.36473	1.14496
H	-6.52356	1.71096	2.29088
H	-6.22760	0.04178	2.82683
H	-2.83167	1.45664	2.22660
H	-3.82325	0.68116	3.48145
H	-4.18596	2.34373	2.96587
H	-0.98970	-1.51535	2.11258
H	-0.83063	-0.10676	3.18301
H	0.61845	-0.83481	2.45423
H	-0.03134	2.15526	0.35436
H	1.19473	1.40408	1.40255
H	-0.26359	2.12206	2.12050
H	0.74615	1.36179	-2.29916
H	0.28830	-0.27285	-2.82787
H	0.81761	0.00609	-1.14969
H	-1.52289	2.22466	-2.95489
H	-2.95275	1.46216	-2.21873
H	-2.03684	0.60495	-3.47814

24Si radical cation

42

Energy: -749872.1400688

Si	-4.19193	0.01018	0.19374
Si	-1.73843	-0.10823	-0.19558
C	-2.38375	-1.86382	-0.12176
N	-0.72704	0.34701	1.10674
N	-1.14489	0.46828	-1.69475
C	-3.72035	-1.79943	0.11432
N	-5.15067	0.56787	-1.10860
N	-4.72825	0.63074	1.69710
H	-4.34434	-2.68647	0.22996
H	-1.84837	-2.80659	-0.24074
C	-1.99732	0.44054	-2.88513
C	0.12696	1.16658	-1.88631
C	-0.37998	1.74695	1.36069
C	-0.27167	-0.58286	2.14081
C	-5.90845	1.47382	1.89087
C	-3.88907	0.49298	2.88925
C	-5.69525	-0.31195	-2.14339
C	-5.35067	1.99578	-1.36591
H	-6.79069	-0.25047	-2.15587
H	-5.40944	-1.34755	-1.94785
H	-5.32489	-0.02150	-3.13442
H	-6.41865	2.24590	-1.36226
H	-4.93836	2.26770	-2.34523
H	-4.85125	2.59268	-0.59876

H	-6.55592	1.41960	1.01540
H	-5.63353	2.52104	2.07242
H	-6.46618	1.11223	2.76270
H	-3.06227	-0.19182	2.68676
H	-4.48516	0.08621	3.71400
H	-3.47721	1.46074	3.20240
H	-0.65548	-1.58585	1.94313
H	-0.61356	-0.25960	3.13189
H	0.82458	-0.62725	2.15473
H	-0.82079	2.39119	0.59598
H	0.70804	1.88568	1.34954
H	-0.75533	2.06064	2.34245
H	-0.02101	2.24152	-2.05290
H	0.63247	0.75172	-2.76620
H	0.76727	1.02305	-1.01569
H	-2.29814	1.45241	-3.18478
H	-2.89540	-0.14887	-2.68726
H	-1.45282	-0.02035	-3.71705

24Ge

42

Energy: -2993252.7401319

Ge	-4.18632	0.18514	0.11226
Ge	-1.71985	0.06854	-0.11444
C	-2.37209	-1.81432	-0.05549
N	-0.35717	0.31534	1.11842
N	-0.98211	0.79383	-1.65007
C	-3.71554	-1.75075	0.03772
N	-5.51474	0.57039	-1.12192
N	-4.85500	0.96497	1.65318
H	-4.35919	-2.63124	0.07519
H	-1.81498	-2.75160	-0.10123
C	0.23024	1.64116	1.26809
C	-0.37130	-0.45353	2.35520
C	-6.21533	0.65144	2.07742
C	-3.94833	1.22467	2.76168
C	-5.56484	-0.18096	-2.36838
C	-5.98343	1.94432	-1.25478
C	-1.85952	1.16792	-2.74901
C	0.33811	0.35010	-2.08406
H	-2.95155	1.46595	2.37896
H	-3.85295	0.36767	3.45075
H	-4.30581	2.08427	3.34651
H	-0.86412	-1.41607	2.19209
H	-0.89565	0.06510	3.17592
H	0.65858	-0.64627	2.68852
H	0.17127	2.17617	0.31683
H	1.28806	1.55382	1.55477

H	-0.27607	2.24349	2.04265
H	0.85789	1.16671	-2.60594
H	0.28889	-0.50979	-2.77436
H	0.93220	0.06347	-1.21243
H	-1.41687	1.99819	-3.31776
H	-2.82525	1.50199	-2.35661
H	-2.04499	0.34010	-3.45542
H	-6.60684	-0.28058	-2.70489
H	-5.15629	-1.18418	-2.21774
H	-4.99662	0.30151	-3.18194
H	-6.83340	0.44249	1.20044
H	-6.64955	1.50815	2.61299
H	-6.25790	-0.22109	2.75224
H	-7.04469	1.95389	-1.54196
H	-5.42601	2.50985	-2.02196
H	-5.87814	2.46018	-0.29703

24Ge radical cation

42

Energy: -2993109.2086693

Ge	-4.21043	-0.02577	0.17847
Ge	-1.66403	0.09437	-0.11657
C	-2.18128	-1.81358	-0.05911
N	-0.42218	0.46226	1.19835
N	-1.00986	0.96244	-1.60583
C	-3.51934	-1.86624	0.07945
N	-5.34917	0.44442	-1.17683
N	-4.97325	0.45615	1.78500
H	-4.09676	-2.78787	0.13634
H	-1.54875	-2.69689	-0.13845
C	0.30353	1.72697	1.23641
C	-0.34792	-0.33057	2.41823
C	-6.24700	1.15921	1.88784
C	-4.11737	0.55724	2.96235
C	-5.58992	-0.44441	-2.31052
C	-5.76684	1.82723	-1.38727
C	-1.95744	1.57572	-2.53886
C	0.13913	0.33531	-2.27537
H	-3.22823	-0.06531	2.83302
H	-4.66591	0.19640	3.84033
H	-3.79966	1.59140	3.15804
H	-0.94697	-1.23838	2.31739
H	-0.69724	0.24059	3.28867
H	0.69499	-0.61844	2.60300
H	0.21118	2.22962	0.27270
H	1.36195	1.52924	1.44736
H	-0.08173	2.38112	2.03039
H	0.66440	1.09854	-2.86165

H	-0.15384	-0.47644	-2.95729
H	0.83422	-0.06221	-1.53078
H	-1.42965	2.33501	-3.12725
H	-2.75904	2.06996	-1.98414
H	-2.40386	0.85423	-3.23995
H	-6.66956	-0.55425	-2.47545
H	-5.16843	-1.43262	-2.11510
H	-5.14335	-0.04401	-3.23033
H	-6.87289	0.92214	1.02629
H	-6.12245	2.24989	1.95407
H	-6.75798	0.82458	2.79872
H	-6.85669	1.88199	-1.50566
H	-5.30771	2.24224	-2.29498
H	-5.47983	2.44914	-0.53661

24Sn

42

Energy: -655433.4506867

Sn	-4.30987	0.18933	0.07894
Sn	-1.50419	0.46106	-0.26675
C	-2.05024	-1.67288	-0.20308
N	0.06625	0.83337	0.99946
N	-0.77711	1.32609	-1.97599
C	-3.37726	-1.80058	-0.07967
N	-5.96331	0.30516	-1.12925
N	-5.13975	0.83271	1.83898
H	-3.88504	-2.76650	-0.04570
H	-1.37061	-2.52437	-0.27401
C	-1.69107	1.53793	-3.08977
C	0.58225	1.01719	-2.40703
C	0.61079	2.18504	1.07215
C	0.07223	0.15492	2.29023
C	-6.39079	0.23702	2.29602
C	-4.25487	1.20271	2.93451
C	-5.89059	-0.31326	-2.44756
C	-6.76092	1.52669	-1.12316
H	-7.80927	1.28906	-1.35948
H	-6.41486	2.26784	-1.86487
H	-6.72824	1.98807	-0.13221
H	-1.36153	2.39841	-3.69188
H	-2.69806	1.75680	-2.71664
H	-1.76066	0.66755	-3.76633
H	1.00594	1.87015	-2.95937
H	0.63036	0.13589	-3.07127
H	1.21606	0.82520	-1.53667
H	-0.37999	-0.83790	2.19846
H	-0.47358	0.71008	3.07342
H	1.10755	0.02476	2.63956

H	-3.32756	1.63590	2.54257
H	-3.98437	0.34995	3.58265
H	-4.73713	1.96041	3.57079
H	-7.00074	-0.05736	1.43728
H	-6.96256	0.96739	2.88917
H	-6.23264	-0.65319	2.93059
H	-6.89504	-0.62779	-2.76877
H	-5.25357	-1.20298	-2.41362
H	-5.49334	0.36502	-3.22325
H	0.52062	2.67648	0.09933
H	1.67723	2.14412	1.34099
H	0.10354	2.81109	1.82712

24Sn radical cation

42

Energy: -655292.8710817

Sn	-4.27026	-0.08558	0.24104
Sn	-1.41040	0.57059	-0.27295
C	-1.75274	-1.57314	-0.15716
N	-0.04521	1.19560	1.12044
N	-0.69629	1.21937	-2.07525
C	-3.03649	-1.86778	0.07474
N	-5.73729	0.06118	-1.17511
N	-5.22865	0.00352	2.04995
H	-3.40756	-2.88728	0.18129
H	-0.97309	-2.32832	-0.25856
C	-0.70758	2.63773	-2.42848
C	-0.82178	0.33914	-3.23613
C	0.85547	2.31451	0.86458
C	-0.35373	0.99274	2.53335
C	-6.53718	0.63221	2.19712
C	-4.41546	0.03813	3.26280
C	-5.63658	-0.76403	-2.37781
C	-6.44755	1.31856	-1.40107
H	-7.48237	1.10307	-1.69832
H	-5.98612	1.91436	-2.20257
H	-6.47084	1.92080	-0.48976
H	0.15477	2.85823	-3.07142
H	-0.63718	3.26208	-1.53457
H	-1.61679	2.91884	-2.98051
H	0.05720	0.46723	-3.88187
H	-1.71506	0.56703	-3.83670
H	-0.86485	-0.70730	-2.92337
H	-0.99485	0.11498	2.65815
H	-0.84959	1.86227	2.98906
H	0.58158	0.81474	3.07936
H	-3.47032	-0.48824	3.09988
H	-4.95844	-0.47356	4.06773

H	-4.19901	1.06201	3.60124
H	-7.13678	0.46160	1.30071
H	-6.47373	1.71329	2.39212
H	-7.04976	0.17163	3.05169
H	-6.64383	-1.07180	-2.68896
H	-5.05120	-1.66534	-2.17895
H	-5.17786	-0.22045	-3.21722
H	1.13221	2.33688	-0.19137
H	1.76608	2.17121	1.46081
H	0.42312	3.28588	1.14795

25C

3

Energy: -24569.1077276

C	-3.63793	0.20738	0.70947
H	-4.48969	-0.07854	0.04485
H	-4.17487	0.45231	1.65851

25C radical cation

3

Energy: -24346.0568787

C	-3.89838	0.19932	0.76294
H	-4.44355	-0.13087	-0.13521
H	-4.06470	0.50825	1.80689

25Si

3

Energy: -182379.6797751

Si	-2.20601	0.49027	0.33691
H	-1.38605	-0.12742	-0.78925
H	-0.98828	0.54427	1.25136

25Si radical cation

3

Energy: -182174.5086999

Si	-4.16726	0.18636	0.81965
H	-5.13763	-0.23421	-0.23088
H	-4.66845	0.55660	2.17383

25Ge

3

Energy: -1304036.7116809

Ge	-3.98936	-0.16460	0.90039
H	-5.23054	-0.07432	-0.10242

H -4.81690 0.62335 2.01781

25Ge radical cation

3
Energy: -1303830.0553859
Ge -4.20740 0.18226 0.82826
H -5.21241 -0.25889 -0.27641
H -4.71905 0.57152 2.24660

25Sn

3
Energy: -135150.2147886
Sn -4.20186 -0.30415 0.98539
H -5.53530 -0.08892 -0.17580
H -5.07126 0.68790 2.18243

25Sn radical cation

3
Energy: -134952.8641976
Sn -4.37633 0.03865 0.91039
H -5.50284 -0.27988 -0.37472
H -4.95803 0.64418 2.43253

26C

9
Energy: -73964.6295278
C -1.99726 0.73704 0.24349
C -1.65263 -0.19896 -0.83896
C -1.41264 0.33056 1.53178
H -2.58280 -0.80823 -0.83057
H -0.81318 -0.90078 -0.67882
H -1.62231 0.25335 -1.83447
H -0.51267 0.98353 1.51584
H -1.04791 -0.70795 1.63848
H -1.98042 0.65606 2.40821

26C radical cation

9
Energy: -73797.3835374
C -2.00717 0.00110 0.47308
C -1.80523 -0.47878 -0.83984
C -1.35769 0.29951 1.69123
H -2.46457 0.00703 -1.57375
H -2.19477 -1.52445 -0.77718

H	-0.75423	-0.51905	-1.16214
H	-1.29775	1.41525	1.66597
H	-0.33703	-0.10050	1.78268
H	-1.98597	0.08694	2.56845

26Si

9

Energy: -231769.6681991

Si	-3.89629	0.14963	0.78154
C	-5.37076	0.00546	-0.42326
C	-4.86412	0.82435	2.28315
H	-5.35411	-0.05532	2.73757
H	-5.66928	1.52261	2.02071
H	-4.22975	1.27032	3.05476
H	-5.16926	-0.62221	-1.29630
H	-5.54808	1.02980	-0.79695
H	-6.30750	-0.31455	0.05091

26Si radical cation

9

Energy: -231595.7992149

Si	-4.20841	0.35011	0.77405
C	-5.40541	-0.03766	-0.57784
C	-4.82289	0.93942	2.41285
H	-5.47715	0.15522	2.82485
H	-5.43683	1.83672	2.23996
H	-4.02301	1.16422	3.12065
H	-4.92749	-0.40170	-1.48909
H	-5.97246	0.88121	-0.79441
H	-6.11261	-0.79021	-0.19636

26Ge

9

Energy: -1353423.1666171

Ge	-3.92462	0.00828	0.83142
C	-5.48009	-0.01910	-0.44464
C	-4.95945	0.81886	2.35493
H	-5.56806	0.00693	2.78298
H	-5.65589	1.59609	2.01939
H	-4.31792	1.21162	3.14788
H	-5.30574	-0.65071	-1.31941
H	-5.61346	1.01634	-0.79496
H	-6.41545	-0.31228	0.04619

26Ge radical cation

9

Energy: -1353246.2759687

Ge	-4.23371	0.35260	0.77858
C	-5.51525	-0.05567	-0.64088
C	-4.90239	0.97425	2.50785
H	-5.55692	0.17887	2.88860
H	-5.49682	1.87475	2.30409
H	-4.09349	1.18525	3.20614
H	-5.02341	-0.41653	-1.54328
H	-6.06485	0.87510	-0.83526
H	-6.20070	-0.80981	-0.23217

26Sn

9

Energy: -184533.9009221

Sn	-4.11015	-0.15282	0.91568
C	-5.82636	-0.07935	-0.48155
C	-5.24151	0.89696	2.50369
H	-6.12950	0.30610	2.76278
H	-5.59539	1.86163	2.11860
H	-4.65140	1.06709	3.40755
H	-5.61239	-0.54865	-1.44493
H	-6.11048	0.96748	-0.64843
H	-6.68819	-0.58003	-0.02231

26Sn radical cation

9

Energy: -184361.0732253

Sn	-4.41906	0.12511	0.88799
C	-5.85173	-0.13870	-0.72884
C	-5.17609	0.99715	2.73272
H	-5.99913	0.34857	3.05136
H	-5.54787	1.99061	2.45930
H	-4.39162	1.05451	3.48515
H	-5.38439	-0.61952	-1.58631
H	-6.20900	0.86725	-0.97447
H	-6.66101	-0.74736	-0.31157

27C

7

Energy: -94162.2236363

C	-0.82705	0.73591	-0.36772
N	-1.23356	-0.50026	-0.69408
N	-1.84876	1.58499	-0.18034
H	-1.64962	2.54019	0.06860

H	-2.84224	1.34420	-0.26964
H	-2.21145	-0.79388	-0.79621
H	-0.54199	-1.21408	-0.85606

27C radical cation

7

Energy: -93988.7423918

C	-2.45231	0.27156	-0.24095
N	-2.00735	-0.67050	-1.00498
N	-2.33300	1.55472	-0.14889
H	-2.82152	2.05505	0.58987
H	-1.76395	2.11543	-0.78724
H	-1.37738	-0.50667	-1.79364
H	-2.28436	-1.63379	-0.83159

27Si

7

Energy: -251968.0219065

Si	-4.28299	-0.48889	0.73086
N	-3.96432	-2.03730	1.43045
N	-4.85027	0.35708	2.12773
H	-3.60623	-2.79420	0.86221
H	-4.08821	-2.32626	2.39576
H	-5.13328	1.32643	2.06250
H	-4.95295	0.00472	3.07430

27Si radical cation

7

Energy: -251783.0863441

Si	-3.99136	-0.45826	1.12885
N	-4.09956	-2.11504	1.23962
N	-4.57301	0.47176	2.38007
H	-3.61223	-2.73783	0.60077
H	-4.79015	-2.60074	1.80961
H	-4.69600	1.47783	2.30145
H	-4.65888	0.14033	3.33950

27Ge

7

Energy: -1373607.9201178

Ge	-1.69345	0.12159	0.61605
N	-1.04167	-0.76882	-0.86107
N	-2.78137	1.29662	-0.29763

H	-3.33537	1.98526	0.19474
H	-2.91150	1.35475	-1.30170
H	-1.27140	-0.59045	-1.83261
H	-0.37959	-1.52756	-0.76354

27Ge radical cation

7

Energy: -1373416.4809671

Ge	-4.04546	-0.33417	1.02896
N	-4.17342	-2.14362	1.24387
N	-4.72554	0.34887	2.58087
H	-3.95679	-2.75167	0.45375
H	-3.85016	-2.55605	2.12175
H	-4.65607	1.35252	2.75078
H	-5.61274	-0.02000	2.93038

27Sn

7

Energy: -204712.2503613

Sn	-4.24270	-0.40342	0.48975
N	-3.91406	-2.19899	1.39929
N	-4.90685	0.50702	2.18965
H	-3.54610	-3.00474	0.90787
H	-4.06571	-2.41270	2.37923
H	-5.21096	1.47304	2.21199
H	-4.99207	0.08116	3.10636

27Sn radical cation

7

Energy: -204527.2656531

Sn	-4.05728	-0.35485	0.58794
N	-4.04353	-2.26086	1.40808
N	-4.80729	0.51832	2.31431
H	-3.78492	-3.06409	0.83131
H	-3.69083	-2.40420	2.35779
H	-4.91403	1.53337	2.36910
H	-5.58057	0.07367	2.81560

28C

19

Energy: -192617.1881910

C	-0.78213	0.08605	0.08820
N	-1.66498	-0.88343	-0.17415
N	-1.23177	1.26234	0.53805
C	-3.02713	-1.03999	0.30031

H	-3.77567	-0.84252	-0.46858
H	-3.15927	-2.07046	0.62797
H	-3.21413	-0.39812	1.15193
C	-0.23173	2.21859	0.94696
H	-0.22509	3.08602	0.28250
H	-0.42533	2.57224	1.96094
H	0.73453	1.73113	0.91656
C	-2.56024	1.83729	0.43922
H	-3.09928	1.84023	1.38783
H	-2.46191	2.87292	0.11594
H	-3.15077	1.31624	-0.30377
C	-1.14437	-2.07458	-0.79993
H	-1.22105	-2.93415	-0.12973
H	-1.69795	-2.30710	-1.71111
H	-0.10511	-1.89936	-1.04781

28C radical cation

19

Energy: -192470.0980158

C	0.99110	0.01064	0.08725
N	1.49145	-1.16878	0.19320
N	1.46703	1.20464	0.06398
C	2.85908	-1.50957	-0.18924
H	3.44077	-1.75588	0.69584
H	2.82351	-2.37567	-0.84341
H	3.31771	-0.68370	-0.71856
C	0.67382	2.28695	-0.50746
H	0.45256	3.01633	0.26700
H	1.24198	2.76391	-1.30120
H	-0.24895	1.88660	-0.90928
C	2.74095	1.58365	0.66931
H	3.45534	1.84896	-0.10634
H	2.57130	2.44645	1.30657
H	3.12807	0.76977	1.26961
C	0.64577	-2.27512	0.62710
H	0.57899	-3.00934	-0.17118
H	1.08665	-2.73653	1.50635
H	-0.34269	-1.90296	0.86730

28Si

19

Energy: -350361.3892956

Si	-1.08301	0.39271	-0.33341
N	-2.13380	-0.97136	-0.26015
N	-1.97826	1.67724	0.38689
C	-3.20571	-1.26771	0.65388
H	-4.17509	-1.33672	0.15138

H	-3.02509	-2.22973	1.14025
H	-3.27301	-0.51214	1.42917
C	-1.23089	2.83058	0.82695
H	-1.55147	3.73368	0.30099
H	-1.35712	3.00594	1.89830
H	-0.16858	2.68330	0.63728
C	-3.40090	1.87319	0.48594
H	-3.74879	1.88676	1.52310
H	-3.67654	2.83242	0.04035
H	-3.93650	1.09468	-0.04660
C	-1.82681	-2.08260	-1.12810
H	-1.62550	-2.98995	-0.55262
H	-2.65182	-2.29741	-1.81204
H	-0.94720	-1.85665	-1.72924

28Si radical cation

19

Energy: -350191.8892025

Si	-1.28930	0.26559	-0.02366
N	-2.25508	-1.05864	-0.25602
N	-1.89089	1.68775	0.57298
C	-3.44816	-1.35703	0.52437
H	-4.30803	-1.43229	-0.13934
H	-3.31911	-2.30543	1.04144
H	-3.63651	-0.58306	1.26143
C	-1.00691	2.66844	1.19255
H	-0.99404	3.58472	0.60680
H	-1.36222	2.89314	2.19603
H	0.00811	2.28545	1.26407
C	-3.26098	2.14664	0.38784
H	-3.72449	2.31053	1.35931
H	-3.26108	3.08407	-0.16422
H	-3.84570	1.41859	-0.16509
C	-1.85912	-2.11588	-1.17920
H	-1.69750	-3.04542	-0.63829
H	-2.64504	-2.26556	-1.91658
H	-0.94276	-1.85178	-1.70139

28Ge

19

Energy: -1471892.9730189

Ge	-1.51976	0.28855	0.26410
N	-0.88863	-0.75015	-1.11028
N	-1.87924	1.87580	-0.58288
C	-2.74688	2.80195	0.09527
C	-1.28865	2.43274	-1.76801
C	-1.15938	-0.66422	-2.51836

C	-0.13979	-1.92662	-0.75645
H	-2.23667	3.74684	0.30643
H	-3.08560	2.38220	1.04213
H	-3.63616	3.03492	-0.49817
H	-0.85828	3.41455	-1.54784
H	-2.01713	2.57518	-2.57342
H	-0.49005	1.79833	-2.13827
H	-0.26026	-0.45331	-3.10730
H	-1.89220	0.10877	-2.72562
H	-1.56524	-1.61328	-2.88183
H	0.87256	-1.90399	-1.17118
H	-0.62508	-2.83572	-1.12475
H	-0.04816	-2.00757	0.32638

28Ge radical cation

19

Energy: -1471722.7174831

Ge	-2.31017	0.15402	-0.02260
N	-1.05581	-0.75834	-1.31026
N	-1.99072	1.82199	-0.56526
C	-2.76489	2.86074	0.09755
C	-1.05126	2.35468	-1.52711
C	-1.45469	-1.03649	-2.65724
C	0.05983	-1.50722	-0.81665
H	-2.10506	3.55058	0.62135
H	-3.45543	2.43008	0.82095
H	-3.34364	3.42157	-0.63504
H	-0.35770	3.03635	-1.03517
H	-1.58171	2.91513	-2.29691
H	-0.47741	1.56549	-1.99975
H	-0.58872	-0.98077	-3.31811
H	-2.22087	-0.34237	-2.98748
H	-1.84265	-2.05700	-2.72202
H	0.94262	-1.26365	-1.41179
H	-0.12041	-2.57861	-0.93146
H	0.25411	-1.28121	0.22694

28Sn

19

Energy: -303214.0886404

Sn	-5.26068	-0.50008	-0.13962
N	-4.02324	-1.64279	0.99152
N	-5.87283	0.81736	1.27624
C	-3.66569	-2.95006	0.51377
C	-3.30043	-1.27944	2.17687
C	-6.45171	2.06382	0.85630
C	-5.94549	0.63536	2.69803

H	-4.16039	-3.16707	-0.43385
H	-3.95465	-3.73812	1.21809
H	-2.58538	-3.04090	0.35375
H	-2.22350	-1.42020	2.03014
H	-3.58486	-1.88686	3.04450
H	-3.46314	-0.23554	2.42883
H	-6.46408	2.14086	-0.23163
H	-5.89166	2.92567	1.23608
H	-7.48379	2.16949	1.20932
H	-5.65121	-0.37194	2.97805
H	-6.96985	0.79193	3.05481
H	-5.30764	1.34045	3.24458

28Sn radical cation

19

Energy: -303050.7482009

Sn	-6.07578	-0.83415	0.17487
N	-4.29781	-1.82759	1.17648
N	-5.87764	0.81362	1.25960
C	-3.12366	-2.16565	0.43443
C	-4.36402	-2.37249	2.49687
C	-6.87277	1.84861	1.04818
C	-4.87595	1.20937	2.21992
H	-3.19510	-1.83291	-0.59636
H	-2.94864	-3.24335	0.46189
H	-2.25680	-1.69007	0.90168
H	-3.41648	-2.23104	3.01877
H	-4.53308	-3.45189	2.43007
H	-5.17286	-1.92547	3.06606
H	-7.61763	1.53909	0.31447
H	-6.40729	2.76631	0.68749
H	-7.39504	2.07481	1.97851
H	-4.12730	0.43547	2.35661
H	-5.33557	1.42292	3.18664
H	-4.36683	2.11633	1.88960

29C

23

Energy: -314321.6627786

C	-3.93517	0.29494	0.74355
C	-4.87897	-0.16080	-0.22555
C	-4.53062	-1.26780	-1.01826
C	-6.10829	0.47557	-0.47963
C	-5.40233	-1.76428	-1.96218
H	-3.56608	-1.72307	-0.85073
C	-6.94191	0.02267	-1.48159
H	-6.37398	1.35076	0.09436

C	-6.60207	-1.10916	-2.20670
H	-5.13756	-2.63780	-2.53900
H	-7.86668	0.53968	-1.69129
H	-7.26593	-1.47287	-2.97727
C	-4.44489	0.88375	1.93989
C	-5.63503	0.47213	2.56855
C	-3.67904	1.88397	2.56319
C	-6.03139	1.03587	3.76405
H	-6.21557	-0.32207	2.12331
C	-4.12017	2.49886	3.71416
H	-2.74358	2.16213	2.10145
C	-5.28913	2.06397	4.32490
H	-6.92804	0.68824	4.25559
H	-3.53946	3.29075	4.16305
H	-5.61237	2.51666	5.25084

29C radical cation

23

Energy: -314178.1796686

C	-4.48349	0.35279	0.82563
C	-5.12628	-0.25704	-0.22992
C	-4.41121	-1.18113	-1.02493
C	-6.47403	0.04590	-0.54283
C	-5.04103	-1.81402	-2.06676
H	-3.37912	-1.38848	-0.78767
C	-7.07801	-0.57786	-1.60311
H	-7.00240	0.78878	0.03442
C	-6.36692	-1.51045	-2.35464
H	-4.50804	-2.53381	-2.66753
H	-8.09936	-0.34445	-1.85998
H	-6.85336	-1.99928	-3.18590
C	-4.65581	1.03357	2.01143
C	-5.87429	0.95944	2.72991
C	-3.58216	1.79519	2.52588
C	-6.00592	1.64504	3.90922
H	-6.67515	0.33779	2.36064
C	-3.74186	2.49441	3.69562
H	-2.65277	1.82775	1.97845
C	-4.94759	2.41651	4.38362
H	-6.92389	1.58448	4.47253
H	-2.93343	3.09161	4.08664
H	-5.06289	2.95605	5.31214

29Si

23

Energy: -472058.2568030

Si	-3.93495	0.27602	0.77785

C	-5.33917	-0.16485	-0.39415
C	-5.06726	-1.16019	-1.33878
C	-6.57856	0.47989	-0.47118
C	-6.00359	-1.53361	-2.28614
H	-4.10066	-1.64836	-1.32820
C	-7.50516	0.13576	-1.43771
H	-6.81503	1.26889	0.22850
C	-7.22302	-0.88010	-2.33789
H	-5.77848	-2.31802	-2.99360
H	-8.45131	0.65455	-1.48933
H	-7.95147	-1.15469	-3.08681
C	-4.85104	0.94727	2.27786
C	-6.11201	0.53500	2.72204
C	-4.15730	1.87206	3.06511
C	-6.65728	1.03420	3.89018
H	-6.66838	-0.19381	2.14984
C	-4.71276	2.40303	4.21545
H	-3.16273	2.17943	2.76657
C	-5.96326	1.97848	4.63076
H	-7.62653	0.69327	4.22384
H	-4.16692	3.13148	4.79672
H	-6.39478	2.37576	5.53786

29Si radical cation

23

Energy: -471895.8914166

Si	-4.38756	0.30983	0.84827
C	-5.47289	-0.31702	-0.44823
C	-4.95568	-1.23809	-1.37160
C	-6.79868	0.13072	-0.57174
C	-5.76175	-1.72815	-2.37647
H	-3.92977	-1.57026	-1.29794
C	-7.58878	-0.35797	-1.58854
H	-7.19878	0.86622	0.11022
C	-7.07252	-1.28762	-2.48196
H	-5.37145	-2.44441	-3.08244
H	-8.60639	-0.01463	-1.69277
H	-7.69908	-1.66603	-3.27575
C	-4.93093	1.10563	2.37269
C	-6.22913	0.91736	2.87515
C	-4.01579	1.90261	3.07664
C	-6.60018	1.53791	4.04741
H	-6.93249	0.27838	2.36217
C	-4.40531	2.52851	4.24127
H	-3.00790	2.03421	2.70905
C	-5.69295	2.34451	4.72225
H	-7.59396	1.39381	4.44222
H	-3.70858	3.15167	4.77976

H	-5.99284	2.82849	5.63966

29Ge

23

Energy: -1593603.3367107

Ge	-3.94486	0.12874	0.89856
C	-5.38626	-0.20254	-0.40384
C	-5.15264	-1.18984	-1.36352
C	-6.56842	0.53498	-0.50183
C	-6.07803	-1.46428	-2.35516
H	-4.22856	-1.75374	-1.33382
C	-7.48349	0.28656	-1.50927
H	-6.77334	1.31859	0.21395
C	-7.24392	-0.72114	-2.42988
H	-5.88558	-2.24407	-3.07742
H	-8.38721	0.87484	-1.57605
H	-7.96288	-0.92098	-3.21090
C	-4.97793	0.85068	2.41397
C	-6.28706	0.49131	2.74233
C	-4.30439	1.71815	3.27649
C	-6.89988	0.98822	3.87888
H	-6.83258	-0.19098	2.10562
C	-4.92267	2.24428	4.39719
H	-3.27649	1.98690	3.06664
C	-6.22197	1.87449	4.70070
H	-7.90905	0.68981	4.12340
H	-4.38960	2.92828	5.04120
H	-6.70446	2.26999	5.58251

29Ge radical cation

23

Energy: -1593436.3452296

Ge	-4.38403	0.29585	0.85356
C	-5.53845	-0.33585	-0.50354
C	-5.05442	-1.25055	-1.44310
C	-6.84976	0.14819	-0.58756
C	-5.89216	-1.70577	-2.43980
H	-4.03538	-1.60602	-1.39356
C	-7.67108	-0.30770	-1.59752
H	-7.22047	0.87969	0.11530
C	-7.19411	-1.23380	-2.51450
H	-5.53151	-2.41986	-3.16366
H	-8.68260	0.06019	-1.67474
H	-7.84384	-1.58520	-3.30189
C	-4.97381	1.10289	2.45863
C	-6.27029	0.86034	2.92874
C	-4.09434	1.91597	3.17885

C	-6.68100	1.45430	4.10390
H	-6.94481	0.20783	2.39411
C	-4.52494	2.51337	4.34523
H	-3.08613	2.08466	2.82906
C	-5.81307	2.28092	4.80356
H	-7.67665	1.27264	4.47823
H	-3.85781	3.15255	4.90230
H	-6.14342	2.74292	5.72171

29Sn

23

Energy: -424930.8558714

Sn	-3.97217	-0.11383	1.42952
C	-5.25876	-0.32245	-0.30097
C	-4.93633	-1.30951	-1.23388
C	-6.33361	0.51898	-0.59333
C	-5.67257	-1.47535	-2.39502
H	-4.09197	-1.96471	-1.05614
C	-7.06027	0.37430	-1.76316
H	-6.60911	1.30316	0.09876
C	-6.73553	-0.62928	-2.66118
H	-5.41200	-2.25469	-3.09649
H	-7.88338	1.04182	-1.97433
H	-7.30653	-0.74712	-3.57051
C	-5.42030	0.74722	2.79113
C	-6.79322	0.49929	2.74382
C	-4.93905	1.52963	3.84217
C	-7.64933	1.01874	3.70009
H	-7.20435	-0.11130	1.95141
C	-5.79156	2.07129	4.78948
H	-3.87641	1.72217	3.92886
C	-7.14976	1.81262	4.71946
H	-8.70792	0.80775	3.64968
H	-5.39758	2.68441	5.58707
H	-7.81795	2.22379	5.46193

29Sn radical cation

23

Energy: -424762.7837131

Sn	-4.46323	0.24320	0.91039
C	-5.77254	-0.28892	-0.63472
C	-5.38233	-1.19852	-1.61545
C	-7.03595	0.30427	-0.66828
C	-6.27324	-1.53607	-2.61592
H	-4.39857	-1.64488	-1.60479
C	-7.91203	-0.03585	-1.68188
H	-7.34000	1.02793	0.07492

C	-7.53156	-0.95500	-2.64721
H	-5.98483	-2.24661	-3.37517
H	-8.89086	0.41736	-1.71872
H	-8.22108	-1.21637	-3.43557
C	-5.20963	1.04443	2.69538
C	-6.54004	0.79207	3.03496
C	-4.38540	1.79001	3.53589
C	-7.04309	1.30959	4.21380
H	-7.18121	0.19543	2.40145
C	-4.90596	2.30919	4.70547
H	-3.34958	1.97030	3.28741
C	-6.22915	2.06768	5.04101
H	-8.06973	1.11974	4.48740
H	-4.27881	2.89559	5.35915
H	-6.62882	2.46880	5.96005

30C

3

Energy: -601213.6290040

C	-3.69481	0.21330	0.71861
Cl	-4.90779	-0.22976	-0.38494
Cl	-4.40204	0.62299	2.20780

30C radical cation

3

Energy: -601006.9085730

C	-3.94371	0.20894	0.76862
Cl	-4.79223	-0.24996	-0.47908
Cl	-4.25984	0.64768	2.25017

30Si

3

Energy: -759021.4073891

Si	-4.03877	-0.30694	0.95890
Cl	-5.49761	-0.20382	-0.50210
Cl	-4.91969	0.78312	2.47789

30Si radical cation

3

Energy: -758803.5299501

Si	-4.26000	-0.19427	0.96404
Cl	-5.40791	-0.29610	-0.61304
Cl	-4.78818	0.76273	2.58368

30Ge

3

Energy: -1880567.8712972

Ge	-4.15604	-0.40667	1.01175
Cl	-5.66830	-0.21319	-0.52922
Cl	-5.06414	0.80463	2.56420

30Ge radical cation

3

Energy: -1880338.4498833

Ge	-4.32262	-0.14388	0.95852
Cl	-5.59941	-0.34103	-0.64753
Cl	-4.94539	0.76090	2.70213

30Sn

3

Energy: -711907.7375703

Sn	-4.39763	-0.53353	1.09900
Cl	-6.01892	-0.23674	-0.57098
Cl	-5.37254	0.84916	2.72715

30Sn radical cation

3

Energy: -711679.2681879

Sn	-4.61927	-0.39007	1.09559
Cl	-5.93937	-0.36071	-0.72822
Cl	-5.23045	0.82969	2.88780

31C

3

Energy: -149077.3958913

C	-3.69167	0.21348	0.71794
F	-4.64862	-0.11370	-0.08072
F	-4.27652	0.51352	1.82627

31C radical cation

3

Energy: -148821.5731262

C	-3.83496	0.21081	0.74677
F	-4.57965	-0.12750	-0.14260
F	-4.18958	0.53013	1.85687

31Si

3

Energy: -306888.8998945

Si	-4.15256	-0.30347	0.97774
F	-5.22166	-0.10526	-0.18547
F	-4.77650	0.64455	2.09466

31Si radical cation

3

Energy: -306645.4062259

Si	-4.29248	-0.20875	0.97388
F	-5.16923	-0.18217	-0.27337
F	-4.68901	0.62674	2.18642

31Ge

3

Energy: -1428411.9468775

Ge	-4.31868	-0.40436	1.04417
F	-5.48647	-0.12821	-0.20564
F	-5.01665	0.66697	2.21380

31Ge radical cation

3

Energy: -1428152.1511555

Ge	-4.46972	-0.29525	1.03771
F	-5.43324	-0.22045	-0.31711
F	-4.91884	0.65010	2.33173

31Sn

3

Energy: -259740.3859545

Sn	-4.60204	-0.50400	1.08063
F	-5.95206	-0.18911	-0.24864
F	-5.33496	0.70491	2.37971

31Sn radical cation

3

Energy: -259486.7049680

Sn	-4.77981	-0.37407	1.07782
F	-5.89982	-0.30736	-0.40369
F	-5.20942	0.69322	2.53756

Cartesian coordinates and total energy values of 1-31 and its radical cations calculated by the DFT-PBE0-DH/def2-TZVPP

1C

8

Energy: -50053.1317646

C	-3.74005	-0.06398	0.81865
C	-2.41226	0.51197	0.37022
H	-1.99893	-0.04900	-0.46548
H	-1.67910	0.49020	1.17390
H	-2.51679	1.54669	0.05030
H	-3.63552	-1.09869	1.13857
H	-4.47321	-0.04220	0.01498
H	-4.15338	0.49700	1.65435

1C cation radical

8

Energy: -49784.9967839

C	0.78227	-0.00678	-0.00000
C	-0.78227	0.00678	-0.00000
H	0.65506	1.12386	0.00000
H	1.24722	-0.34354	0.91656
H	1.24722	-0.34354	-0.91656
H	-0.65506	-1.12386	0.00000
H	-1.24722	0.34354	0.91656
H	-1.24722	0.34354	-0.91656

1Si

8

Energy: -365425.0725386

Si	-4.09990	-0.21997	0.94055
Si	-2.05240	0.66797	0.24832
H	-1.51137	-0.11292	-0.88900
H	-1.07327	0.62666	1.36003
H	-2.22217	2.07610	-0.18127
H	-3.93015	-1.62810	1.37012
H	-5.07904	-0.17864	-0.17115
H	-4.64093	0.56091	2.07789

1Si cation radical

8

Energy: -365203.2065041

Si	-4.25093	-0.28539	0.99149
Si	-1.90139	0.73339	0.19739
H	-1.62721	-0.21077	-0.89466

H	-1.16877	0.56332	1.45978
H	-2.37160	2.08055	-0.15376
H	-3.78073	-1.63257	1.34257
H	-4.98356	-0.11526	-0.27090
H	-4.52508	0.65873	2.08357

1Ge

8

Energy: -2608500.2339271

Ge	-4.13344	-0.23374	0.95206
Ge	-2.01887	0.68174	0.23681
H	-1.45898	-0.12323	-0.93779
H	-1.00728	0.64034	1.38434
H	-2.19368	2.13603	-0.20644
H	-3.95863	-1.68803	1.39528
H	-5.14503	-0.19232	-0.19547
H	-4.69333	0.57122	2.12668

1Ge cation radical

8

Energy: -2608283.6001066

Ge	-4.29433	-0.30336	1.00654
Ge	-1.85798	0.75136	0.18234
H	-1.58611	-0.22916	-0.94234
H	-1.11385	0.57055	1.49164
H	-2.35761	2.13813	-0.17557
H	-3.79472	-1.69016	1.36436
H	-5.03848	-0.12247	-0.30274
H	-4.56616	0.67711	2.13126

1Sn

8

Energy: -271128.3148049

Sn	-4.28340	-0.29926	1.00169
Sn	-1.86891	0.74727	0.18718
H	-1.24205	-0.14181	-1.11680
H	-0.73951	0.70454	1.45458
H	-2.05465	2.36119	-0.30738
H	-4.09764	-1.91317	1.49629
H	-5.41279	-0.25658	-0.26572
H	-4.91028	0.58983	2.30565

1Sn cation radical

8

Energy: -270925.2614404

Sn	-4.46855	-0.37771	1.06620
Sn	-1.68376	0.82571	0.12268
H	-1.38077	-0.25908	-1.12346
H	-0.86038	0.62595	1.57346
H	-2.23834	2.36164	-0.27261
H	-3.91398	-1.91365	1.46145
H	-5.29193	-0.17792	-0.38458
H	-4.77152	0.70705	2.31235

2C

26

Energy: -197959.1674778

C	-3.76214	-0.07377	0.82598
C	-2.39017	0.52177	0.36290
C	-1.80670	-0.26454	-0.80878
C	-1.35974	0.49460	1.48952
C	-2.53394	1.97367	-0.08778
C	-3.61901	-1.52674	1.27342
C	-4.79357	-0.04345	-0.29964
C	-4.34397	0.71046	1.99987
H	-3.20846	2.07661	-0.93462
H	-1.56221	2.35360	-0.40098
H	-2.88959	2.61874	0.71231
H	-2.45584	-0.24435	-1.68110
H	-1.61389	-1.30331	-0.55095
H	-0.85550	0.17689	-1.10378
H	-0.41987	0.91265	1.13100
H	-1.15289	-0.51629	1.83303
H	-1.67112	1.08891	2.34542
H	-3.26641	-2.17065	0.47107
H	-4.59035	-1.90604	1.58854
H	-2.94227	-1.63225	2.11819
H	-4.53451	1.75040	1.74502
H	-3.69492	0.68634	2.87213
H	-5.29615	0.27025	2.29356
H	-4.48257	-0.63460	-1.15787
H	-5.00141	0.96847	-0.63945
H	-5.73285	-0.46336	0.05828

2C cation radical

26

Energy: -197752.6635693

C	-4.06407	-0.20407	0.92908
C	-2.08854	0.65194	0.26008
C	-1.65337	-0.37741	-0.71231
C	-1.35409	0.69978	1.54576
C	-2.52338	1.95168	-0.30230

C	-3.70537	-1.63013	1.10919
C	-4.91775	0.12090	-0.23715
C	-4.30324	0.57914	2.16359
H	-3.07414	1.85413	-1.23105
H	-1.60431	2.50354	-0.52886
H	-3.07380	2.56264	0.40686
H	-2.37335	-0.54749	-1.50720
H	-1.36967	-1.31438	-0.24638
H	-0.75705	0.02637	-1.19625
H	-0.32415	0.97538	1.29309
H	-1.29423	-0.26466	2.04118
H	-1.72920	1.45624	2.22586
H	-3.52050	-2.14697	0.17420
H	-4.57847	-2.10325	1.57224
H	-2.88066	-1.78067	1.79941
H	-4.29563	1.65235	1.99825
H	-3.63640	0.31285	2.97595
H	-5.32027	0.32929	2.48575
H	-4.53457	-0.27656	-1.17225
H	-5.13100	1.17977	-0.33060
H	-5.87282	-0.38636	-0.06086

2Si

26

Energy: -513389.6769709

Si	-4.10694	-0.22325	0.94321
Si	-2.04537	0.67124	0.24566
C	-1.36277	-0.32121	-1.19731
C	-0.80637	0.61732	1.65788
C	-2.26341	2.45721	-0.29809
C	-3.88895	-2.00928	1.48676
C	-5.34600	-0.16911	-0.46895
C	-4.78943	0.76908	2.38632
H	-2.95984	2.53572	-1.13163
H	-1.31171	2.88066	-0.61921
H	-2.64448	3.07487	0.51387
H	-2.04509	-0.30774	-2.04598
H	-1.19669	-1.36112	-0.91981
H	-0.40983	0.08990	-1.53060
H	0.15429	1.02525	1.34338
H	-0.63805	-0.40317	1.99882
H	-1.15184	1.20071	2.51010
H	-3.50794	-2.62687	0.67471
H	-4.84065	-2.43272	1.80788
H	-3.19248	-2.08791	2.32025
H	-4.95548	1.80903	2.10893
H	-4.10707	0.75550	3.23495
H	-5.74237	0.35798	2.71960

H	-5.00059	-0.75243	-1.32124
H	-5.51429	0.85142	-0.80977
H	-6.30666	-0.57705	-0.15445

2Si cation radical

26

Energy: -513211.5747417

Si	-4.24348	-0.28094	0.98893
Si	-1.90883	0.72894	0.19994
C	-1.45993	-0.39526	-1.19486
C	-0.88967	0.56459	1.73168
C	-2.38435	2.44933	-0.27436
C	-3.76796	-2.00133	1.46324
C	-5.26262	-0.11659	-0.54282
C	-4.69238	0.84325	2.38373
H	-3.09622	2.46992	-1.09554
H	-1.47807	2.95824	-0.61315
H	-2.78269	3.01588	0.56337
H	-2.18225	-0.35661	-2.00620
H	-1.33375	-1.42565	-0.87250
H	-0.50003	-0.05668	-1.59356
H	0.10406	0.96189	1.50880
H	-0.76554	-0.47100	2.03771
H	-1.29266	1.14055	2.56079
H	-3.36966	-2.56790	0.62549
H	-4.67424	-2.51023	1.80205
H	-3.05607	-2.02192	2.28439
H	-4.81855	1.87366	2.06138
H	-3.97008	0.80459	3.19509
H	-5.65230	0.50469	2.78241
H	-4.85963	-0.69255	-1.37192
H	-5.38674	0.91900	-0.84885
H	-6.25636	-0.51388	-0.31994

2Ge

26

Energy: -2756449.2044892

Ge	-4.14169	-0.23707	0.95533
Ge	-2.01062	0.68507	0.23354
C	-1.28841	-0.34002	-1.27084
C	-0.71033	0.63534	1.69708
C	-2.22318	2.54718	-0.33518
C	-3.92915	-2.09923	1.52386
C	-5.44205	-0.18716	-0.50815
C	-4.86380	0.78790	2.45983
H	-2.91557	2.62035	-1.17053
H	-1.26398	2.95399	-0.64956

H	-2.60340	3.15923	0.47938
H	-1.97504	-0.32637	-2.11401
H	-1.11563	-1.37534	-0.98649
H	-0.34147	0.08808	-1.59409
H	0.24127	1.04709	1.36635
H	-0.54278	-0.38555	2.03213
H	-1.05986	1.22089	2.54418
H	-3.54899	-2.71122	0.70923
H	-4.88835	-2.50606	1.83825
H	-3.23672	-2.17251	2.35918
H	-5.03658	1.82325	2.17558
H	-4.17713	0.77416	3.30297
H	-5.81074	0.35979	2.78309
H	-5.09260	-0.77268	-1.35530
H	-5.60954	0.83376	-0.84313
H	-6.39366	-0.59887	-0.17740

2Ge cation radical

26

Energy: -2756271.7238182

Ge	-4.28265	-0.29814	1.00309
Ge	-1.86967	0.74613	0.18578
C	-1.41764	-0.43805	-1.27021
C	-0.82093	0.56705	1.79710
C	-2.38445	2.54046	-0.30648
C	-3.76789	-2.09251	1.49524
C	-5.33141	-0.11894	-0.60820
C	-4.73461	0.88598	2.45915
H	-3.10279	2.53690	-1.12028
H	-1.48545	3.05568	-0.64704
H	-2.78774	3.08534	0.54127
H	-2.15332	-0.38464	-2.06655
H	-1.31364	-1.46374	-0.93042
H	-0.45674	-0.11218	-1.67019
H	0.17224	0.96536	1.58620
H	-0.71495	-0.47323	2.08829
H	-1.24969	1.13878	2.61417
H	-3.36468	-2.63736	0.64744
H	-4.66689	-2.60771	1.83584
H	-3.04950	-2.08900	2.30899
H	-4.83856	1.91170	2.11942
H	-3.99893	0.83249	3.25548
H	-5.69552	0.56013	2.85911
H	-4.90267	-0.69061	-1.42532
H	-5.43739	0.92137	-0.89931
H	-6.32458	-0.51726	-0.39731

2Sn

26

Energy: -419068.6784506

Sn	-4.29324	-0.30398	1.00509
Sn	-1.85907	0.75197	0.18377
C	-1.04785	-0.35238	-1.46513
C	-0.41585	0.71040	1.76876
C	-2.06054	2.79180	-0.44567
C	-4.09171	-2.34369	1.63487
C	-5.73636	-0.26271	-0.57999
C	-5.10462	0.80059	2.65377
H	-2.75026	2.86734	-1.28195
H	-1.09176	3.17472	-0.75788
H	-2.43214	3.40795	0.36861
H	-1.73468	-0.33993	-2.30708
H	-0.86542	-1.38504	-1.18021
H	-0.10645	0.09382	-1.77702
H	0.52584	1.12557	1.41740
H	-0.24331	-0.30916	2.10265
H	-0.76168	1.29940	2.61394
H	-3.72001	-2.95995	0.82070
H	-5.06048	-2.72662	1.94706
H	-3.40205	-2.41906	2.47120
H	-5.28709	1.83320	2.36869
H	-4.41784	0.78831	3.49577
H	-6.04601	0.35439	2.96568
H	-5.39047	-0.85185	-1.42505
H	-5.90892	0.75679	-0.91408
H	-6.67806	-0.67785	-0.22861

2Sn cation radical

26

Energy: -418897.1537943

Sn	-4.44383	-0.36796	1.06159
Sn	-1.70849	0.81596	0.12728
C	-1.23150	-0.49286	-1.46961
C	-0.57814	0.61070	1.90901
C	-2.29401	2.78089	-0.40934
C	-3.85827	-2.33284	1.59834
C	-5.57415	-0.16285	-0.72017
C	-4.92087	0.94096	2.65839
H	-3.02131	2.75500	-1.21403
H	-1.40672	3.30881	-0.75433
H	-2.70381	3.30632	0.44684
H	-1.97383	-0.41840	-2.25732
H	-1.16254	-1.51697	-1.11807
H	-0.26398	-0.19215	-1.86760
H	0.41684	1.00920	1.71906

H	-0.49040	-0.43404	2.18797
H	-1.03378	1.17525	2.71575
H	-3.44843	-2.85831	0.74221
H	-4.74556	-2.86076	1.94333
H	-3.13100	-2.30688	2.40306
H	-4.98987	1.96504	2.30677
H	-4.17853	0.86659	3.44610
H	-5.88838	0.64023	3.05640
H	-5.11848	-0.72744	-1.52686
H	-5.66190	0.88187	-0.99921
H	-6.56912	-0.56135	-0.53022

3C

20

Energy: -258334.1776983

C	-3.73567	-0.05752	0.72256
C	-2.30353	0.41220	0.22876
N	-1.61425	-0.54617	-0.60084
N	-1.46518	0.54634	1.40580
N	-2.45265	1.59403	-0.58998
N	-3.68825	-1.50053	0.86979
N	-4.73790	0.46203	-0.18001
N	-4.10579	0.42899	2.02955
H	-3.11880	2.24058	-0.20228
H	-1.56005	2.04480	-0.70670
H	-2.05722	-0.61553	-1.50121
H	-1.60492	-1.44488	-0.14549
H	-3.77316	-1.95471	-0.02442
H	-4.46862	-1.78030	1.44311
H	-4.28467	1.41832	1.99943
H	-3.37077	0.22641	2.68822
H	-4.45683	0.38295	-1.14274
H	-5.61138	-0.01679	-0.03383
H	-0.50400	0.56026	1.10267
H	-1.65854	1.40944	1.88622

3C cation radical

20

Energy: -258151.2256210

C	-3.77708	0.02329	0.64594
C	-2.36375	0.48135	0.15393
N	-1.86625	-0.14433	-1.02706
N	-1.51483	-0.02366	1.24636
N	-2.31618	1.86890	-0.05704
N	-3.43473	-1.23245	1.33500
N	-4.67967	-0.09928	-0.42288
N	-4.40181	0.83620	1.63721

H	-2.62586	2.44133	0.70609
H	-1.45003	2.19041	-0.45469
H	-2.29608	0.22526	-1.85773
H	-1.86749	-1.14946	-1.02674
H	-3.20529	-2.02689	0.76029
H	-4.00546	-1.46881	2.13529
H	-4.78958	1.67672	1.24407
H	-3.85346	1.03103	2.45675
H	-4.37513	-0.66358	-1.19409
H	-5.62127	-0.30924	-0.13829
H	-0.58447	-0.32019	0.98454
H	-1.54376	0.47331	2.12169

3Si

20

Energy: -573861.7297339

Si	-4.08144	-0.10973	0.89427
Si	-1.96212	0.47106	0.04792
N	-1.02693	-0.66907	-0.83752
N	-0.98588	0.78143	1.42611
N	-2.28041	1.68411	-1.13525
N	-4.11282	-1.82600	0.94058
N	-5.19432	0.79473	-0.06268
N	-4.53203	0.32616	2.49597
H	-2.98896	2.36818	-0.94105
H	-1.52676	2.08588	-1.66439
H	-1.28384	-0.91577	-1.77388
H	-0.57917	-1.42720	-0.35933
H	-3.60929	-2.35796	0.25671
H	-4.90584	-2.33023	1.29278
H	-4.75428	1.27710	2.71916
H	-4.13942	-0.16175	3.27798
H	-5.01286	0.88896	-1.04550
H	-6.18112	0.73567	0.11706
H	-0.01787	1.03262	1.34244
H	-1.39680	1.16173	2.25727

3Si cation radical

20

Energy: -573700.8494700

Si	-4.20906	-0.18516	0.87593
Si	-1.85064	0.56962	0.05083
N	-1.04867	-0.88636	-0.16376
N	-1.28262	1.51517	1.31213
N	-2.18371	1.41013	-1.35983
N	-4.37460	-1.70507	0.19110
N	-5.24218	0.97731	0.25268

N	-4.04653	-0.16898	2.54385
H	-2.77499	2.21758	-1.40901
H	-1.81109	1.13686	-2.25011
H	-1.35302	-1.61157	-0.78458
H	-0.19824	-1.10869	0.31945
H	-3.74451	-2.46746	0.35125
H	-5.13642	-1.94060	-0.41736
H	-3.79974	0.64186	3.07837
H	-4.18713	-0.98737	3.10648
H	-5.33264	1.18546	-0.72330
H	-5.81965	1.55351	0.83620
H	-1.01030	2.47216	1.18512
H	-1.16640	1.19152	2.25321

3Ge

20

Energy: -2816872.7305187

Ge	-4.10443	-0.15685	0.92028
Ge	-1.90875	0.47786	0.07599
N	-0.83117	-0.74702	-0.74516
N	-0.87486	0.99414	1.49704
N	-2.26080	1.64491	-1.29848
N	-4.24069	-1.98027	0.81490
N	-5.27719	0.92507	0.01001
N	-4.58528	0.15134	2.65495
H	-2.90769	2.38152	-1.07103
H	-1.44980	2.04038	-1.74534
H	-1.18378	-1.10598	-1.61542
H	-0.53219	-1.50911	-0.16156
H	-3.93994	-2.39798	-0.04838
H	-5.13515	-2.35931	1.07796
H	-4.64959	1.12118	2.91148
H	-4.04023	-0.34359	3.33967
H	-5.13710	0.95483	-0.98613
H	-6.25188	0.76490	0.20503
H	0.04273	1.33207	1.25888
H	-1.30436	1.62184	2.15395

3Ge cation radical

20

Energy: -2816700.0541604

Ge	-4.24568	-0.18943	0.89574
Ge	-1.81278	0.57887	0.03165
N	-0.88709	-0.93142	-0.17358
N	-1.12954	1.63345	1.29743
N	-2.08182	1.44108	-1.50666
N	-4.52229	-1.79460	0.17038

N	-5.41023	1.02868	0.31033
N	-4.14678	-0.24266	2.67654
H	-2.76399	2.17106	-1.58977
H	-1.89458	0.97738	-2.37717
H	-1.25415	-1.71640	-0.67701
H	-0.18920	-1.18561	0.50173
H	-3.83531	-2.52307	0.21502
H	-5.14701	-1.88811	-0.60985
H	-3.76856	0.52000	3.20622
H	-4.05088	-1.12755	3.14133
H	-5.40557	1.34600	-0.64073
H	-5.77105	1.71446	0.94898
H	-1.11935	2.62846	1.16347
H	-1.13631	1.36933	2.26458

3Sn

20

Energy: -479482.2880492

Sn	-4.25596	-0.20231	0.98487
Sn	-1.75184	0.51606	0.02026
N	-0.48904	-0.81602	-0.79813
N	-0.61680	1.19743	1.54390
N	-2.09794	1.70827	-1.57618
N	-4.49249	-2.19533	0.77810
N	-5.57176	1.04988	0.09517
N	-4.78614	0.02362	2.91052
H	-2.72593	2.47604	-1.39997
H	-1.26233	2.07835	-2.00155
H	-0.83453	-1.25420	-1.63623
H	-0.18283	-1.53882	-0.16742
H	-4.25953	-2.56901	-0.12710
H	-5.41058	-2.52654	1.02916
H	-4.79908	0.97935	3.22720
H	-4.23384	-0.51527	3.55752
H	-5.49346	1.09609	-0.90820
H	-6.53531	0.86302	0.32522
H	0.28042	1.55459	1.25547
H	-1.05316	1.88473	2.13603

3Sn cation radical

20

Energy: -479306.9837077

Sn	-4.40667	-0.26007	0.93863
Sn	-1.64944	0.61527	-0.02622
N	-0.93864	-0.72699	-1.29123
N	-0.48975	0.77673	1.56643

N	-1.87469	2.36604	-0.91373
N	-4.40450	-2.21630	1.21851
N	-5.73748	0.25880	-0.42658
N	-4.72668	0.70109	2.63529
H	-2.61266	2.49013	-1.58498
H	-1.76955	3.19273	-0.34902
H	-1.13101	-0.58399	-2.26921
H	-1.01082	-1.70330	-1.06129
H	-4.02481	-2.81430	0.50494
H	-4.14733	-2.55351	2.13160
H	-5.18984	1.59357	2.58721
H	-4.00898	0.71502	3.33910
H	-5.68900	1.17545	-0.83686
H	-5.98102	-0.42513	-1.12387
H	0.06464	-0.02430	1.82063
H	-0.84393	1.23300	2.38928

4C

22

Energy: -238208.9547795

C	-3.76757	-0.07352	0.79680
C	-2.39706	0.50322	0.31541
N	-1.77987	-0.29627	-0.73893
C	-1.39938	0.55716	1.45683
N	-2.63233	1.85976	-0.13496
N	-3.55948	-1.45500	1.19678
C	-4.83024	0.05603	-0.29007
N	-4.28446	0.59817	1.97062
H	-3.13274	1.86011	-1.01049
H	-1.74298	2.29844	-0.31998
H	-2.42041	-0.47222	-1.49724
H	-1.47227	-1.18652	-0.37915
H	-3.45173	-2.04534	0.38773
H	-4.38834	-1.76537	1.68152
H	-4.27637	1.59345	1.80364
H	-3.66932	0.42059	2.74987
H	-0.42634	0.83978	1.06073
H	-1.31456	-0.41450	1.93542
H	-1.69537	1.29436	2.19640
H	-4.52335	-0.41518	-1.22337
H	-5.07923	1.09607	-0.48978
H	-5.73554	-0.43687	0.05399

4C cation radical

22

Energy: -238049.4865724

C	-4.12255	-0.22386	0.98172
C	-2.05733	0.62533	0.06570
N	-1.81194	-0.26626	-0.92106
C	-1.29374	0.46514	1.32785
N	-2.44084	1.88050	-0.29101
N	-3.73901	-1.47910	1.33814
C	-4.88623	-0.06340	-0.28035
N	-4.36787	0.66752	1.96868
H	-2.49657	2.11310	-1.26503
H	-2.13073	2.63630	0.28898
H	-2.23068	-0.14882	-1.82380
H	-1.61552	-1.21175	-0.65503
H	-4.04921	-2.23479	0.75804
H	-3.68320	-1.71189	2.31211
H	-4.56445	1.61304	1.70289
H	-3.94910	0.54990	2.87138
H	-0.25028	0.73198	1.15555
H	-1.32523	-0.56424	1.67249
H	-1.68356	1.11659	2.10426
H	-4.49638	-0.71460	-1.05696
H	-4.85487	0.96607	-0.62472
H	-5.92966	-0.33041	-0.10806

4Si

22

Energy: -553700.3690613

Si	-4.19134	-0.18604	0.89788
Si	-2.04902	0.48239	0.18777
N	-1.39707	-0.85324	-0.71201
C	-0.81157	0.76893	1.55813
N	-2.23122	2.01325	-0.59425
N	-4.00681	-1.87071	1.12522
C	-5.49954	0.31621	-0.34664
N	-4.75996	0.47837	2.38494
H	-2.95383	2.14864	-1.27674
H	-1.43072	2.57720	-0.81744
H	-1.90113	-1.20642	-1.50554
H	-0.40925	-0.89228	-0.89453
H	-3.21561	-2.35223	0.74387
H	-4.72612	-2.48330	1.45755
H	-5.19868	1.38059	2.38719
H	-4.22032	0.34584	3.22058
H	0.15043	1.08602	1.15222
H	-0.64534	-0.13995	2.13222
H	-1.15658	1.54791	2.23430
H	-5.27564	-0.08381	-1.33451
H	-5.57306	1.40055	-0.43251
H	-6.47657	-0.06160	-0.04593

4Si cation radical

22

Energy: -553541.3243299

Si	-4.25731	-0.20932	0.94319
Si	-1.92262	0.61048	0.10423
N	-1.52415	-0.43133	-1.15311
C	-0.89506	0.43485	1.62361
N	-2.23290	2.16791	-0.44711
N	-3.94509	-1.76848	1.48868
C	-5.28512	-0.02683	-0.57532
N	-4.65740	0.82608	2.20519
H	-2.46409	2.93072	0.16109
H	-2.24264	2.43160	-1.41483
H	-1.81689	-0.32367	-2.10602
H	-0.97428	-1.25859	-1.01431
H	-3.70923	-2.52820	0.87844
H	-3.94178	-2.03661	2.45523
H	-5.20786	1.65361	2.07039
H	-4.36175	0.71581	3.15690
H	0.12963	0.72327	1.39161
H	-0.90218	-0.59019	1.98567
H	-1.26279	1.08518	2.41385
H	-4.91727	-0.67309	-1.36883
H	-5.27853	1.00002	-0.93224
H	-6.30964	-0.31687	-0.34456

4Ge

22

Energy: -2796728.1923082

Ge	-4.19051	-0.18175	0.90025
Ge	-1.97699	0.56393	0.18632
N	-1.11737	-0.58123	-0.98738
C	-0.71732	0.80135	1.64359
N	-2.22689	2.19660	-0.61949
N	-3.98483	-1.96841	1.27544
C	-5.58613	0.24108	-0.39866
N	-4.82275	0.47735	2.49499
H	-2.98223	2.23098	-1.28282
H	-1.40242	2.56990	-1.06200
H	-1.66114	-0.90338	-1.77001
H	-0.67764	-1.37700	-0.55480
H	-3.52322	-2.50792	0.56351
H	-4.82818	-2.44232	1.55390
H	-5.08404	1.44906	2.47398
H	-4.20059	0.33214	3.27296

H	0.23488	1.15147	1.25158
H	-0.55452	-0.13701	2.16812
H	-1.09647	1.53401	2.35051
H	-5.36136	-0.19925	-1.36724
H	-5.68145	1.31800	-0.52352
H	-6.53777	-0.15126	-0.04750

4Ge cation radical

22

Energy: -2796563.3971732

Ge	-4.30507	-0.20607	0.94815
Ge	-1.87483	0.60752	0.09931
N	-1.46017	-0.47005	-1.26496
C	-0.75215	0.45095	1.65481
N	-2.12763	2.26700	-0.51116
N	-4.05223	-1.86565	1.55832
C	-5.42778	-0.04918	-0.60731
N	-4.71978	0.87126	2.31259
H	-2.45408	2.45738	-1.44018
H	-2.26629	3.03839	0.11410
H	-1.80204	-0.31595	-2.19533
H	-1.19459	-1.42415	-1.10641
H	-3.91343	-2.63692	0.93294
H	-3.72592	-2.05619	2.48736
H	-4.98546	1.82535	2.15415
H	-4.37772	0.71714	3.24289
H	0.25790	0.74041	1.37535
H	-0.75004	-0.57426	2.01171
H	-1.11267	1.10713	2.44094
H	-5.06726	-0.70518	-1.39360
H	-5.42990	0.97611	-0.96397
H	-6.43782	-0.33872	-0.32791

4Sn

22

Energy: -459343.0937634

Sn	-4.35759	-0.22500	0.92228
Sn	-1.80706	0.60596	0.16666
N	-0.84338	-0.62735	-1.13400
C	-0.39841	0.90438	1.72837
N	-2.03855	2.39287	-0.75580
N	-4.16553	-2.19384	1.35045
C	-5.91468	0.23492	-0.46544
N	-5.07744	0.44845	2.68802
H	-2.80918	2.43369	-1.40266
H	-1.21432	2.69630	-1.25133
H	-1.40220	-0.96358	-1.90161

H	-0.41077	-1.42859	-0.70131
H	-3.71355	-2.74513	0.63956
H	-5.03266	-2.64695	1.59221
H	-5.31356	1.42801	2.69657
H	-4.45959	0.27930	3.46599
H	0.55189	1.20027	1.29185
H	-0.25769	-0.00776	2.30105
H	-0.74592	1.69028	2.39210
H	-5.70698	-0.20676	-1.43599
H	-6.01145	1.31128	-0.58216
H	-6.85031	-0.16441	-0.08303

4Sn cation radical

22

Energy: -459176.3313317

Sn	-4.47605	-0.22276	0.98634
Sn	-1.71608	0.68641	0.06806
N	-1.38997	-0.38386	-1.56297
C	-0.38170	0.32617	1.66365
N	-1.87941	2.57664	-0.49081
N	-4.15075	-1.96639	1.85963
C	-5.73314	-0.29139	-0.70781
N	-5.01932	1.04543	2.40365
H	-2.34272	2.81455	-1.35054
H	-2.03489	3.28648	0.20351
H	-1.84716	-0.15894	-2.42904
H	-1.21873	-1.37143	-1.49347
H	-3.94329	-2.77847	1.30564
H	-3.70296	-2.02097	2.75743
H	-5.22269	2.00075	2.16718
H	-4.61420	0.98528	3.32168
H	0.61312	0.60259	1.32592
H	-0.40595	-0.72568	1.92696
H	-0.66303	0.93046	2.51931
H	-5.30231	-0.94954	-1.45438
H	-5.85185	0.70668	-1.11543
H	-6.69586	-0.67567	-0.38274

6C

8

Energy: -1779950.7272788

C	-3.76461	-0.07444	0.82681
C	-2.38770	0.52245	0.36206
Cl	-1.76371	-0.41419	-0.98367
Cl	-1.24198	0.46518	1.68939
Cl	-2.60880	2.18800	-0.14256
Cl	-3.54351	-1.74000	1.33142

Cl	-4.91033	-0.01717	-0.50052
Cl	-4.38859	0.86218	2.17255

6C cation radical

8

Energy: -1779697.5472025

C	-3.75884	-0.07200	0.82487
C	-2.39348	0.52000	0.36401
Cl	-1.77335	-0.40881	-0.97169
Cl	-1.25557	0.46334	1.68053
Cl	-2.61177	2.17305	-0.13689
Cl	-3.54048	-1.72494	1.32612
Cl	-4.89663	-0.01569	-0.49177
Cl	-4.37915	0.85704	2.16031

6Si

8

Energy: -2095573.3264579

Si	-4.09733	-0.21810	0.93698
Si	-2.05498	0.66611	0.25190
Cl	-1.33956	-0.41936	-1.30100
Cl	-0.73280	0.60124	1.78551
Cl	-2.31616	2.58783	-0.33076
Cl	-3.83656	-2.14059	1.51726
Cl	-5.42023	-0.15096	-0.59590
Cl	-4.81161	0.86582	2.49149

6Si cation radical

8

Energy: -2095347.6292384

Si	-4.24155	-0.28011	0.98137
Si	-1.91076	0.72811	0.20750
Cl	-1.44527	-0.49027	-1.27970
Cl	-0.81757	0.55183	1.84623
Cl	-2.43795	2.56792	-0.29253
Cl	-3.71436	-2.11995	1.48131
Cl	-5.33478	-0.10374	-0.65733
Cl	-4.70701	0.93820	2.46863

6Ge

8

Energy: -4338614.7859390

Ge	-4.14354	-0.23760	0.95092
Ge	-2.00877	0.68560	0.23795
Cl	-1.24737	-0.43746	-1.38640

Cl	-0.61034	0.62766	1.82692
Cl	-2.26237	2.69613	-0.37304
Cl	-3.89000	-2.24823	1.56162
Cl	-5.54207	-0.17937	-0.63796
Cl	-4.90480	0.88528	2.57546

6Ge cation radical

8

Energy: -4338381.8814892

Ge	-4.28656	-0.29657	0.99340
Ge	-1.86575	0.74453	0.19547
Cl	-1.36922	-0.52679	-1.36593
Cl	-0.70883	0.56459	1.90638
Cl	-2.41687	2.67351	-0.33066
Cl	-3.73560	-2.22555	1.51973
Cl	-5.44351	-0.11680	-0.71750
Cl	-4.78291	0.97507	2.55460

6Sn

8

Energy: -2001265.2006327

Sn	-4.30731	-0.30593	0.97616
Sn	-1.86217	0.74162	0.16222
Cl	-1.07884	-0.15772	-1.78883
Cl	-0.28974	0.32558	1.77291
Cl	-2.03789	3.00623	-0.12449
Cl	-3.97739	-2.32596	1.99866
Cl	-5.80280	-0.62625	-0.72526
Cl	-5.25308	1.13443	2.48412

6Sn cation radical

8

Energy: -2001033.0623319

Sn	-4.46757	-0.34501	1.04850
Sn	-1.68545	0.82542	0.15029
Cl	-1.22827	-0.64663	-1.49087
Cl	-0.40235	0.66501	1.98883
Cl	-2.26733	2.90907	-0.46856
Cl	-3.76964	-2.42517	1.55255
Cl	-5.70432	-0.12306	-0.81715
Cl	-5.08432	0.93234	2.79188

7C

8

Energy: -423531.9139339

C	-3.75113	-0.06910	0.82259
C	-2.40118	0.51710	0.36628
F	-1.93058	-0.18440	-0.64521
F	-1.53929	0.47560	1.36214
F	-2.56269	1.76863	-0.01387
F	-3.58962	-1.32062	1.20275
F	-4.61302	-0.02761	-0.17327
F	-4.22173	0.63240	1.83408

7C cation radical

8

Energy: -423245.9094128

C	-3.99134	-0.17267	0.90428
C	-2.16097	0.62067	0.28460
F	-1.87023	-0.15909	-0.66702
F	-1.48084	0.49969	1.34356
F	-2.50489	1.79437	-0.03497
F	-3.64742	-1.34638	1.22380
F	-4.67147	-0.05164	-0.15468
F	-4.28207	0.60706	1.85593

7Si

8

Energy: -739176.7763306

Si	-4.09142	-0.22109	0.93966
Si	-2.06093	0.66909	0.24905
F	-1.49032	-0.15332	-0.95655
F	-1.02760	0.62826	1.42618
F	-2.22031	2.15938	-0.20881
F	-3.93155	-1.71098	1.39864
F	-5.12496	-0.18149	-0.23733
F	-4.66215	0.60215	2.14464

7Si cation radical

8

Energy: -738912.0571601

Si	-4.26807	-0.29392	1.01385
Si	-1.88425	0.74193	0.17501
F	-1.52445	-0.19333	-0.98380
F	-1.09649	0.58054	1.48081
F	-2.29731	2.16467	-0.21490
F	-3.85495	-1.71663	1.40383
F	-5.05582	-0.13262	-0.29195
F	-4.62791	0.64136	2.17263

7Ge

8

Energy: -2982135.7245734

Ge	-4.13652	-0.23757	0.96853
Ge	-2.00645	0.67742	0.25125
F	-1.25827	-0.30858	-0.90536
F	-0.88544	0.88552	1.50357
F	-2.24640	2.19304	-0.46789
F	-4.04897	-1.90818	1.24079
F	-5.30587	0.02558	-0.23103
F	-4.72133	0.46476	2.39563

7Ge cation radical

8

Energy: -2981855.4106422

Ge	-4.30143	-0.30286	1.05626
Ge	-1.85089	0.75086	0.13260
F	-1.41375	-0.23578	-1.13149
F	-1.03473	0.56019	1.57362
F	-2.28862	2.29917	-0.28806
F	-3.86372	-1.85121	1.47681
F	-5.11763	-0.11207	-0.38471
F	-4.73848	0.68370	2.32044

7Sn

8

Energy: -644747.5534887

Sn	-4.29142	-0.29518	0.98808
Sn	-1.87211	0.74582	0.14954
F	-0.95071	-0.22614	-1.16771
F	-0.71681	0.84651	1.62772
F	-2.04505	2.48340	-0.53687
F	-4.10765	-2.11718	1.38929
F	-5.68494	-0.15406	-0.25057
F	-4.94056	0.50881	2.55601

7Sn cation radical

8

Energy: -644472.8321096

Sn	-4.52094	-0.37526	1.11935
Sn	-1.64733	0.85179	0.08307
F	-1.38049	-0.07969	-1.49014
F	-0.63662	0.33474	1.54543
F	-2.02555	2.65363	-0.09722

F	-3.82312	-1.94109	1.81777
F	-5.32738	-0.47748	-0.54402
F	-5.24780	0.82538	2.32125

8C

6

Energy: -49273.4087780

C	-3.72279	0.20489	0.72687
C	-2.42952	0.24312	0.46199
H	-2.04316	-0.02323	-0.51086
H	-1.70786	0.54220	1.20793
H	-4.44445	-0.09419	-0.01907
H	-4.10916	0.47124	1.69972

8C cation radical

6

Energy: -49035.2500303

C	-3.76461	0.20336	0.73552
C	-2.38770	0.24464	0.45335
H	-2.01689	-0.02550	-0.52721
H	-1.67755	0.54720	1.21237
H	-4.47478	-0.09904	-0.02355
H	-4.13541	0.47335	1.71612

8Si

6

Energy: -364634.2684462

Si	-4.10502	0.09411	0.83771
Si	-2.04732	0.35385	0.35099
H	-1.49464	-0.12546	-0.92819
H	-1.04242	0.63859	1.39049
H	-5.11019	-0.18930	-0.20190
H	-4.65735	0.57222	2.11749

8Si cation radical

6

Energy: -364453.3524343

Si	-4.16602	0.18676	0.81944
Si	-1.98629	0.26124	0.36943
H	-1.49869	-0.10397	-0.96564
H	-1.03594	0.67648	1.40771
H	-5.11636	-0.22856	-0.21881
H	-4.65363	0.55205	2.15448

8Ge

6

Energy: -2607719.4841431

Ge	-4.12419	-0.05556	0.89098
Ge	-2.02813	0.50356	0.29788
H	-1.43878	-0.16960	-0.94205
H	-0.98072	0.60310	1.40739
H	-5.17161	-0.15508	-0.21853
H	-4.71351	0.61760	2.13091

8Ge cation radical

6

Energy: -2607540.8156226

Ge	-4.20728	0.18754	0.82788
Ge	-1.94504	0.26046	0.36099
H	-1.44830	-0.11267	-1.01943
H	-0.97084	0.69456	1.43541
H	-5.18146	-0.24664	-0.24652
H	-4.70402	0.56077	2.20827

8Sn

6

Energy: -270363.3861980

Sn	-4.27434	-0.20064	0.96694
Sn	-1.87794	0.64870	0.22211
H	-1.18522	-0.22868	-1.07464
H	-0.68993	0.60308	1.45386
H	-5.46218	-0.15551	-0.26500
H	-4.96734	0.67706	2.26333

8Sn cation radical

6

Energy: -270191.9788277

Sn	-4.37040	0.16701	0.86506
Sn	-1.78206	0.28256	0.32332
H	-1.23087	-0.14294	-1.20215
H	-0.69966	0.74957	1.51570
H	-5.45240	-0.30414	-0.32605
H	-4.92155	0.59196	2.39071

9C

18

Energy: -147887.6562778

C	-3.73240	0.30151	0.69693
C	-2.41992	0.14649	0.49194
C	-1.81805	-0.33014	-0.79372
C	-1.36714	0.42794	1.51897
C	-4.78517	0.02009	-0.33011
C	-4.33427	0.77813	1.98259
H	-5.02417	0.02898	2.37471
H	-4.92607	1.67849	1.80943
H	-3.61165	1.00063	2.75787
H	-4.40015	-0.33584	-1.27764
H	-5.37041	0.92042	-0.52468
H	-5.48707	-0.72590	0.04630
H	-2.54069	-0.55281	-1.56894
H	-1.22612	-1.23041	-0.62051
H	-1.12827	0.41907	-1.18594
H	-0.66517	1.17382	1.14248
H	-0.78199	-0.47242	1.71366
H	-1.75215	0.78403	2.46645

9C cation radical

18

Energy: -147703.5008752

C	-3.76594	0.36805	0.67228
C	-2.38694	0.07944	0.51657
C	-1.86046	-0.45374	-0.74806
C	-1.43512	0.30390	1.61391
C	-4.75016	-0.06131	-0.33146
C	-4.25926	1.10715	1.84326
H	-4.54945	0.37110	2.60437
H	-5.16281	1.65911	1.59850
H	-3.52305	1.76597	2.29043
H	-4.88800	0.76690	-1.03881
H	-5.72090	-0.22842	0.12784
H	-4.44699	-0.93194	-0.90233
H	-2.45207	-0.19006	-1.61778
H	-1.85469	-1.54889	-0.67184
H	-0.82475	-0.15671	-0.89004
H	-1.00725	1.30655	1.48410
H	-0.60072	-0.38938	1.54791
H	-1.88231	0.26433	2.60096

9Si

18

Energy: -2706351.0362204

Ge	-4.15395	-0.00048	0.87673

Ge	-1.99832	0.44859	0.31246
C	-1.23594	-0.45664	-1.24666
C	-0.65369	0.52020	1.73302
C	-5.49842	-0.07299	-0.54394
C	-4.91659	0.90544	2.43531
H	-5.66182	0.26052	2.89590
H	-5.39987	1.83462	2.14364
H	-4.14683	1.12114	3.17016
H	-5.05777	-0.41568	-1.47522
H	-5.94659	0.90502	-0.70078
H	-6.28395	-0.76891	-0.25732
H	-2.00581	-0.67199	-1.98148
H	-0.75264	-1.38595	-0.95546
H	-0.49076	0.18847	-1.70707
H	0.13196	1.21606	1.44660
H	-0.20571	-0.45797	1.88941
H	-1.09416	0.86261	2.66449

9Si cation radical

18

Energy: -2706203.9821486

Ge	-4.21572	0.35940	0.77250
Ge	-1.93658	0.08881	0.41631
C	-1.26385	-0.52277	-1.27796
C	-0.66342	0.49157	1.80035
C	-5.48885	-0.04291	-0.61171
C	-4.88853	0.97013	2.46705
H	-5.54258	0.20568	2.88203
H	-5.47538	1.87281	2.30986
H	-4.08553	1.17687	3.16570
H	-5.00009	-0.36157	-1.52552
H	-6.08716	0.84422	-0.80927
H	-6.15256	-0.83085	-0.26096
H	-2.06687	-0.72980	-1.97649
H	-0.67705	-1.42540	-1.12036
H	-0.60975	0.24144	-1.69332
H	0.00036	1.27932	1.44929
H	-0.06518	-0.39553	1.99826
H	-1.15215	0.81063	2.71404

9Ge

18

Energy: -463262.1121531

Si	-4.12069	0.34558	0.75765
Si	-2.03163	0.10239	0.43122
C	-1.31991	-0.48570	-1.19527
C	-0.74739	0.47657	1.73848

C	-5.40507	-0.03104	-0.54878
C	-4.83226	0.93617	2.38330
H	-5.49599	0.18645	2.81349
H	-5.40458	1.85362	2.24760
H	-4.03693	1.13545	3.09883
H	-4.92934	-0.36968	-1.46703
H	-5.99655	0.85474	-0.77950
H	-6.08655	-0.81168	-0.21131
H	-2.11516	-0.68356	-1.91128
H	-0.74790	-1.40354	-1.06097
H	-0.65588	0.26453	-1.62409
H	-0.06573	1.25766	1.40242
H	-0.15609	-0.40970	1.96781
H	-1.22320	0.81377	2.65722

9Ge cation radical

18

Energy: -463130.0836067

Si	-4.17139	0.34825	0.76639
Si	-1.98092	0.09991	0.42242
C	-1.33610	-0.48798	-1.19770
C	-0.76110	0.48087	1.74662
C	-5.39121	-0.03267	-0.55783
C	-4.81623	0.93581	2.38663
H	-5.48321	0.18350	2.80861
H	-5.40116	1.84414	2.24026
H	-4.02527	1.14106	3.10177
H	-4.92039	-0.36397	-1.47845
H	-5.98964	0.85395	-0.76888
H	-6.07282	-0.81068	-0.21282
H	-2.12707	-0.69336	-1.91280
H	-0.75119	-1.39630	-1.05115
H	-0.66910	0.26422	-1.61983
H	-0.07938	1.25875	1.40152
H	-0.16279	-0.40578	1.95783
H	-1.23191	0.81237	2.66718

9Sn

18

Energy: -368990.6222488

Sn	-4.30560	-0.17863	0.96540
Sn	-1.84670	0.62670	0.22357
C	-0.95383	-0.49128	-1.38829
C	-0.33843	0.54300	1.76107
C	-5.81383	-0.09522	-0.57215
C	-5.19855	0.93951	2.57709
H	-6.01433	0.35516	2.99692

H	-5.60097	1.87726	2.20262
H	-4.47439	1.14372	3.35941
H	-5.42982	-0.46566	-1.51738
H	-6.16160	0.92688	-0.69835
H	-6.65582	-0.71318	-0.26820
H	-1.67800	-0.69530	-2.17065
H	-0.55149	-1.42913	-1.01395
H	-0.13799	0.09306	-1.80801
H	0.50360	1.16094	1.45717
H	0.00927	-0.47913	1.88714
H	-0.72239	0.91335	2.70635

9Sn cation radical

18

Energy: -368843.3227220

Sn	-4.38817	0.24647	0.84136
Sn	-1.76431	0.19996	0.34787
C	-1.01401	-0.56465	-1.47553
C	-0.35598	0.54816	1.88661
C	-5.79639	-0.09869	-0.69815
C	-5.13826	1.01118	2.66480
H	-5.89329	0.32607	3.04032
H	-5.59820	1.97696	2.47240
H	-4.34238	1.11845	3.39251
H	-5.31001	-0.48731	-1.58512
H	-6.29309	0.84044	-0.92786
H	-6.53285	-0.81116	-0.33695
H	-1.80997	-0.67276	-2.20303
H	-0.55325	-1.53000	-1.28295
H	-0.25962	0.12097	-1.85141
H	0.37987	1.26073	1.52434
H	0.14148	-0.39031	2.11738
H	-0.84243	0.93753	2.77321

10C

14

Energy: -188138.2150844

C	0.33483	1.08622	0.34683
C	-0.86741	0.68365	-0.07415
N	-1.07107	-0.66418	-0.44380
N	-1.99369	1.52229	-0.09571
N	1.46111	0.24758	0.36840
N	0.53849	2.43405	0.71648
H	-1.71899	2.46955	0.11592
H	-2.45441	1.50179	-0.99310
H	-1.98234	-0.97900	-0.15011
H	-0.99564	-0.80424	-1.43954

H	1.18642	-0.69968	0.15678
H	1.92184	0.26808	1.26579
H	0.46309	2.57410	1.71223
H	1.44975	2.74888	0.42277

10C cation radical

14

Energy: -188007.8996548

C	0.37438	1.04139	0.37590
C	-0.90743	0.72880	-0.10263
N	-1.20947	-0.54500	-0.42145
N	-1.82666	1.70433	-0.24018
N	1.37462	0.14873	0.23953
N	0.59558	2.23119	0.96843
H	-1.52063	2.62921	-0.47836
H	-2.76520	1.47050	-0.50038
H	-2.09316	-0.75667	-0.84276
H	-0.77586	-1.28955	0.09176
H	1.37858	-0.45700	-0.55978
H	2.26675	0.33417	0.65547
H	-0.14597	2.65852	1.49116
H	1.52644	2.49050	1.23207

10Si

14

Energy: -503584.1141548

Si	0.55223	0.95833	1.11566
Si	-1.08451	0.81062	-0.84315
N	-1.71758	-0.76983	-1.02614
N	-2.50541	1.72573	-0.56689
N	1.97386	0.04458	0.83864
N	1.18402	2.53916	1.29975
H	-2.46600	2.71950	-0.45264
H	-3.40157	1.35523	-0.30967
H	-2.63474	-1.07029	-0.75214
H	-1.11616	-1.54529	-1.22477
H	1.93526	-0.94915	0.72375
H	2.86970	0.41598	0.58164
H	0.58197	3.31400	1.49888
H	2.10092	2.84055	1.02589

10Si cation radical

14

Energy: -503453.2997019

Si	0.67613	0.99139	0.79156
Si	-1.16929	0.64750	-0.53751

N	-1.79343	-0.89787	-0.59537
N	-2.33476	1.82874	-0.68159
N	2.05241	0.12832	0.41521
N	1.00183	2.50284	1.41216
H	-2.12462	2.77156	-0.95267
H	-3.32029	1.66450	-0.57522
H	-2.63829	-1.12815	-1.08754
H	-1.31359	-1.71110	-0.25722
H	2.07344	-0.65090	-0.21584
H	2.92789	0.26092	0.88964
H	0.33790	3.02558	1.95294
H	1.89666	2.95576	1.35024

11C

38

Energy: -385289.7661542

C	-0.73110	0.07773	0.08026
C	0.59605	-0.13108	-0.10306
N	1.48350	0.86980	-0.50301
N	1.21345	-1.36863	0.08832
N	-1.70198	-0.90006	-0.14576
N	-1.26469	1.29282	0.51366
C	-2.59677	-1.27354	0.91202
H	-3.57002	-1.54819	0.50287
H	-2.23440	-2.12056	1.50662
H	-2.73331	-0.42356	1.57472
C	-0.55595	2.09522	1.46006
H	0.12749	2.82578	1.01433
H	-1.26928	2.65203	2.07143
H	0.02849	1.44907	2.11093
C	2.63183	1.16950	0.30336
H	3.46779	1.47267	-0.32864
H	2.45376	1.97324	1.02770
H	2.92308	0.27572	0.84785
C	0.76790	-2.24457	1.12569
H	-0.01672	-2.94561	0.82173
H	1.60996	-2.83942	1.48581
H	0.38201	-1.65338	1.95287
C	1.95685	-1.96806	-0.98249
H	2.79892	-2.53652	-0.58513
H	1.35626	-2.64876	-1.59752
H	2.34801	-1.18258	-1.62294
C	1.06159	1.88385	-1.41723
H	0.63468	2.77377	-0.94267
H	1.91517	2.21388	-2.01299
H	0.30961	1.47250	-2.08655
C	-2.25981	1.95851	-0.27688
H	-2.96222	2.48805	0.36842

H	-1.83813	2.68784	-0.97873
H	-2.81275	1.21601	-0.84530
C	-1.54226	-1.83982	-1.21047
H	-1.00736	-2.75427	-0.93290
H	-2.52484	-2.14024	-1.58014
H	-0.99450	-1.36951	-2.02383

11C cation radical

38

Energy: -385172.8177088

C	-0.74555	-0.01689	-0.05968
C	0.66696	0.00576	0.06156
N	1.37061	-1.14670	0.16482
N	1.34217	1.17956	0.07623
N	-1.50815	0.92146	0.55004
N	-1.36083	-0.97767	-0.78947
C	-2.71750	1.43359	-0.04886
H	-3.60766	1.11875	0.49541
H	-2.68710	2.52277	-0.04221
H	-2.79576	1.09681	-1.07631
C	-0.76370	-1.54203	-1.97369
H	-0.46078	-2.57768	-1.81829
H	-1.48787	-1.52541	-2.78758
H	0.09959	-0.95951	-2.27451
C	2.67238	-1.30589	-0.43805
H	3.46227	-1.38038	0.30910
H	2.68322	-2.21992	-1.03117
H	2.88468	-0.46782	-1.09214
C	0.90396	2.32740	-0.67745
H	0.54338	3.12338	-0.02571
H	1.73939	2.72233	-1.25467
H	0.11611	2.04713	-1.36719
C	2.52122	1.37577	0.88545
H	3.42173	1.47143	0.27903
H	2.40845	2.29055	1.46660
H	2.64518	0.54488	1.57065
C	0.84458	-2.31104	0.83182
H	0.61529	-3.11048	0.12694
H	1.58476	-2.68986	1.53582
H	-0.05191	-2.05575	1.38519
C	-2.63275	-1.53916	-0.40176
H	-3.43061	-1.25573	-1.08795
H	-2.55952	-2.62636	-0.40191
H	-2.89541	-1.21158	0.59771
C	-1.14094	1.50883	1.81405
H	-0.85605	2.55531	1.70399
H	-1.99090	1.46495	2.49430
H	-0.31912	0.96055	2.26016

11Si

38

Energy: -700733.0481850

Si	-1.12340	0.41914	-0.43080
Si	1.07126	0.05226	0.41956
N	2.26912	0.99358	-0.39571
N	1.58693	-1.57577	0.22969
N	-2.12395	-0.96986	-0.28572
N	-1.97103	1.67164	0.40245
C	-2.97618	-1.27843	0.83115
H	-4.00793	-1.45866	0.51424
H	-2.62973	-2.17950	1.34725
H	-2.97447	-0.45920	1.54350
C	-1.28787	2.77794	1.01262
H	-1.26909	3.66723	0.37414
H	-1.78041	3.05688	1.94867
H	-0.26141	2.50494	1.25164
C	3.67748	0.77903	-0.19924
H	4.21150	0.77412	-1.15451
H	4.12443	1.56311	0.42092
H	3.85536	-0.17435	0.29110
C	1.14312	-2.59055	1.14725
H	0.51447	-3.33514	0.64962
H	1.98914	-3.12064	1.59443
H	0.56436	-2.14110	1.95209
C	2.30776	-2.10110	-0.89872
H	3.23294	-2.59802	-0.59113
H	1.70356	-2.83797	-1.43748
H	2.56094	-1.30149	-1.58806
C	1.96881	2.26870	-0.98484
H	2.19809	3.10806	-0.31991
H	2.55169	2.40821	-1.89986
H	0.91543	2.32247	-1.25507
C	-3.38017	1.90027	0.23120
H	-3.87915	2.02771	1.19699
H	-3.57440	2.80225	-0.35829
H	-3.84521	1.06209	-0.28068
C	-2.00282	-2.05013	-1.22788
H	-1.63036	-2.96095	-0.74938
H	-2.96715	-2.28907	-1.68553
H	-1.31137	-1.77807	-2.02325

11Si cation radical

38

Si	-1.15869	0.27708	-0.11716

Si	1.07861	-0.07598	0.12306
N	2.13997	1.04570	-0.53073
N	1.63854	-1.65369	0.17774
N	-2.17700	-1.05110	-0.18277
N	-1.82697	1.66919	0.53632
C	-3.31846	-1.26695	0.68344
H	-4.24747	-1.28316	0.11113
H	-3.21994	-2.22557	1.19543
H	-3.38624	-0.48608	1.43540
C	-1.06048	2.66723	1.25137
H	-1.03377	3.60847	0.70037
H	-1.50946	2.85581	2.22799
H	-0.03855	2.33047	1.41457
C	3.57365	0.98322	-0.32095
H	4.09947	0.93452	-1.27589
H	3.91646	1.87125	0.21187
H	3.84308	0.11036	0.26743
C	1.11704	-2.60069	1.14279
H	0.69513	-3.46961	0.63577
H	1.90665	-2.94557	1.81206
H	0.33829	-2.14177	1.74971
C	2.64554	-2.21027	-0.70315
H	3.52859	-2.52073	-0.14225
H	2.24610	-3.08618	-1.21708
H	2.94676	-1.48480	-1.45336
C	1.71034	2.24300	-1.22115
H	1.98158	3.13753	-0.65850
H	2.18366	2.30012	-2.20277
H	0.63241	2.24042	-1.37130
C	-3.20668	2.05503	0.30921
H	-3.73704	2.16072	1.25702
H	-3.24981	3.01136	-0.21385
H	-3.72336	1.31479	-0.29567
C	-1.96631	-2.11059	-1.14873
H	-1.84090	-3.06897	-0.64288
H	-2.81740	-2.19095	-1.82666
H	-1.07745	-1.91498	-1.74626

13C

6

Energy: -1202551.7278297

C	-3.73054	0.21256	0.72576
C	-2.42177	0.23544	0.46310
Cl	-1.79662	-0.19068	-1.05707
Cl	-1.27277	0.69217	1.62713
Cl	-4.87954	-0.24417	-0.43827
Cl	-4.35570	0.63868	2.24593

13C cation radical

6

Energy: -1202342.6804684

C	-3.77253	0.21218	0.73405
C	-2.37984	0.23649	0.45460
Cl	-1.81838	-0.18686	-1.03871
Cl	-1.29976	0.68718	1.61867
Cl	-4.85254	-0.23949	-0.42970
Cl	-4.33390	0.63451	2.22768

13Si

6

Energy: -1518060.6363051

Si	-4.08306	-0.25685	0.94757
Si	-2.06920	0.70492	0.24150
Cl	-1.26498	-0.32703	-1.33050
Cl	-0.66417	0.67981	1.72885
Cl	-5.48774	-0.23190	-0.54014
Cl	-4.88779	0.77507	2.51933

13Si cation radical

6

Energy: -1517880.0364003

Si	-4.14813	-0.01862	0.88241
Si	-2.00422	0.46663	0.30644
Cl	-1.32302	-0.27392	-1.38940
Cl	-0.70637	0.76284	1.76172
Cl	-5.44597	-0.31477	-0.57289
Cl	-4.82923	0.72185	2.57833

13Ge

6

Energy: -3761141.9430554

Ge	-4.17655	-0.37573	1.00655
Ge	-1.97569	0.82387	0.18265
Cl	-1.10557	-0.35234	-1.39707
Cl	-0.49428	0.67791	1.73752
Cl	-5.65767	-0.23070	-0.54868
Cl	-5.04717	0.80100	2.58561

13Ge cation radical

6

Energy: -3760940.7891460

Ge	-4.21509	-0.14185	0.93968

Ge	-1.93734	0.58974	0.24900
Cl	-1.18346	-0.30662	-1.46513
Cl	-0.55391	0.76361	1.78753
Cl	-5.59859	-0.31447	-0.59894
Cl	-4.96856	0.75360	2.65446

13Sn

6

Energy: -1423816.5997283

Sn	-4.38680	-0.40491	1.12993
Sn	-1.66376	1.03252	0.04574
Cl	-0.80751	-0.44590	-1.55162
Cl	-0.08324	0.66407	1.73080
Cl	-5.97431	-0.26872	-0.57375
Cl	-5.54133	0.76693	2.78550

13Sn cation radical

6

Energy: -1423607.9321067

Sn	-4.57741	-0.56758	1.14181
Sn	-1.84607	0.27042	0.28654
Cl	-0.82794	-0.15903	-1.68251
Cl	-0.31312	1.01425	1.76834
Cl	-5.82686	-0.16326	-0.71747
Cl	-5.06553	0.94920	2.76990

14C

6

Energy: -298235.0920632

C	-3.72082	0.21289	0.72389
C	-2.43150	0.23512	0.46498
F	-1.92641	-0.08719	-0.69357
F	-1.52962	0.58197	1.34101
F	-4.62269	-0.13396	-0.15215
F	-4.22590	0.53520	1.88244

14C cation radical

6

Energy: -298010.9885208

C	-3.76692	0.21141	0.73330
C	-2.38530	0.23534	0.45596
F	-1.95329	-0.08300	-0.67437
F	-1.56156	0.57739	1.33352
F	-4.59081	-0.12877	-0.14485
F	-4.19906	0.53163	1.86304

14Si

6

Energy: -613785.2152728

Si	-4.20559	-0.25041	0.93360
Si	-1.95361	0.68630	0.20362
F	-1.33997	-0.29815	-0.88043
F	-0.94701	0.53815	1.42094
F	-5.26467	0.00089	-0.22075
F	-4.74610	0.66724	2.10964

14Si cation radical

6

Energy: -613585.4451643

Si	-4.17625	-0.08886	0.91462
Si	-1.97608	0.53680	0.27426
F	-1.43190	-0.17057	-0.98112
F	-0.96646	0.62268	1.43396
F	-5.18587	-0.17466	-0.24509
F	-4.72038	0.61860	2.16997

14Ge

6

Energy: -2856824.6270934

Ge	-4.50357	0.03859	0.80077
Ge	-1.05752	1.17928	-0.03934
F	-0.97577	-0.20559	-1.07624
F	-0.78421	0.34513	1.45842
F	-5.95245	-0.63138	0.14346
F	-5.18343	0.61799	2.27953

14Ge cation radical

6

Energy: -2856594.5006938

Ge	-4.24327	-0.16914	0.96121
Ge	-1.90901	0.61719	0.22748
F	-1.27971	-0.19885	-1.09290
F	-0.79715	0.64381	1.48028
F	-5.35540	-0.19552	-0.29135
F	-4.87241	0.64653	2.28188

14Sn

6

Energy: -519508.2366417

Sn	-3.94045	-0.82923	0.82702
Sn	-1.48538	1.33892	0.33850
F	-2.16124	-0.11562	-0.85894
F	-1.52751	-0.03040	1.77207
F	-5.78857	-0.26737	0.70186
F	-3.55377	1.24770	0.78610

14Sn cation radical

6

Energy: -519246.1584439

Sn	-4.31237	0.16380	0.81325
Sn	-1.52909	0.85386	-0.21302
F	-1.04728	-0.87555	-0.74284
F	-0.75416	1.18793	1.45728
F	-5.84228	0.29612	-0.23862
F	-4.97175	-0.28216	2.49056

15C

12

Energy: -98578.5386093

C	-3.85704	-0.22987	0.10224
C	-2.35822	0.10876	0.13117
C	-2.07475	-1.33069	-0.32683
C	-3.47230	-1.71559	0.18373
H	-2.02294	-1.39365	-1.41196
H	-1.21419	-1.84420	0.09367
H	-3.43244	-2.05392	1.21721
H	-4.05252	-2.42963	-0.39469
H	-4.49220	0.18051	0.88277
H	-4.29423	0.00921	-0.86516
H	-2.00346	0.92580	-0.49145
H	-2.01271	0.27088	1.15020

15C cation radical

12

Energy: -98353.5619249

C	-3.74300	-0.29371	0.22031
C	-2.30338	0.24796	-0.00831
C	-2.13772	-1.29025	-0.17279
C	-3.57818	-1.83151	0.05137
H	-1.85242	-1.49415	-1.20189
H	-1.50660	-1.65346	0.63437
H	-3.72320	-2.41767	0.94621
H	-4.05660	-2.25929	-0.81669
H	-4.02468	-0.09195	1.25070
H	-4.37692	0.07133	-0.58399

H	-2.16084	0.83108	-0.90556
H	-1.82343	0.67921	0.85716

15Si

12

Energy: -413969.5877500

Si	-4.23533	0.01244	0.23547
Si	-2.02537	0.49815	-0.28384
C	-2.01040	-1.36672	0.08857
C	-3.49429	-1.67366	-0.23885
H	-1.83044	-1.50090	1.15586
H	-1.29517	-1.98964	-0.44416
H	-1.80986	0.76160	-1.72909
H	-1.12168	1.37606	0.49853
H	-5.42671	0.48890	-0.50828
H	-4.52277	0.08537	1.69030
H	-3.88769	-2.56180	0.25078
H	-3.61658	-1.81091	-1.31390

15Si cation radical

12

Energy: -413772.1192001

Si	-4.38545	-0.11750	0.26074
Si	-1.83526	0.44111	-0.31419
C	-2.00909	-1.36820	0.08868
C	-3.49444	-1.67397	-0.23932
H	-1.80410	-1.51638	1.14768
H	-1.32537	-2.00213	-0.47461
H	-1.92268	0.82742	-1.73218
H	-1.18144	1.39604	0.59241
H	-5.38326	0.53524	-0.59921
H	-4.44617	0.19228	1.69877
H	-3.85503	-2.56119	0.27987
H	-3.63400	-1.83386	-1.30724

15Ge

12

Energy: -2657040.6953903

Ge	-4.29077	0.03840	0.22949
Ge	-1.98409	0.54243	-0.27675
C	-1.99849	-1.41458	0.05290
C	-3.48611	-1.72343	-0.20529
H	-1.75207	-1.56916	1.10234
H	-1.31037	-2.01260	-0.53959
H	-1.71224	0.88959	-1.74602
H	-1.07239	1.39736	0.60986

H	-5.48227	0.49489	-0.61906
H	-4.66249	0.16437	1.71243
H	-3.86475	-2.58091	0.34558
H	-3.66026	-1.90749	-1.26445

15Ge cation radical

12

Energy: -2656847.2354990

Ge	-4.44595	-0.10682	0.27114
Ge	-1.78483	0.47662	-0.32278
C	-2.00405	-1.41585	0.08089
C	-3.47822	-1.71939	-0.23506
H	-1.78475	-1.55650	1.13634
H	-1.31974	-2.03463	-0.49582
H	-1.85279	0.90673	-1.78065
H	-1.14206	1.44500	0.65495
H	-5.44276	0.56437	-0.65768
H	-4.54195	0.23145	1.75148
H	-3.84524	-2.59424	0.29780
H	-3.63396	-1.87788	-1.29923

15Sn

12

Energy: -319667.7051029

Sn	-4.49639	0.07778	0.06241
Sn	-1.81135	0.65412	-0.10637
C	-2.04291	-1.49021	-0.39141
C	-3.40918	-1.79868	0.23595
H	-1.23629	-2.09722	0.01381
H	-2.06504	-1.65095	-1.46817
H	-1.07116	1.51182	-1.37694
H	-1.01239	1.06660	1.34012
H	-5.41014	0.20643	-1.36911
H	-5.50733	0.49142	1.36799
H	-3.31102	-1.99298	1.30289
H	-3.90312	-2.65926	-0.20976

15Sn cation radical

12

Energy: -319484.8138759

Sn	-4.66483	-0.09185	0.05823
Sn	-1.58703	0.56688	-0.10693
C	-2.07716	-1.48985	-0.45000
C	-3.37880	-1.78839	0.29330
H	-1.26284	-2.13544	-0.12753
H	-2.19015	-1.60200	-1.52535

H	-1.12765	1.59483	-1.35878
H	-1.15748	1.02690	1.45814
H	-5.26055	0.23991	-1.48485
H	-5.48770	0.59249	1.35800
H	-3.21766	-1.90481	1.36199
H	-3.86444	-2.68980	-0.07481

16C

24

Energy: -197189.8657025

C	-3.83857	-0.12616	0.11961
C	-2.31625	0.22906	-0.03855
C	-2.01340	-1.27609	0.10487
C	-1.69292	1.15839	0.97766
C	-1.97103	0.70543	-1.43703
C	-3.47486	-1.57842	-0.24956
C	-4.83146	0.58435	-0.77151
C	-4.30834	-0.05016	1.56026
H	-1.77750	-1.54752	1.13184
H	-1.24181	-1.68275	-0.54578
H	-3.97765	-2.36476	0.30986
H	-3.60574	-1.77299	-1.31214
H	-4.36692	0.98071	1.90769
H	-3.65168	-0.59479	2.23615
H	-5.30284	-0.48740	1.64629
H	-0.61377	1.20607	0.83047
H	-1.87180	0.83124	1.99887
H	-2.08077	2.17260	0.87595
H	-4.56349	0.51575	-1.82287
H	-4.90991	1.64071	-0.51197
H	-5.82251	0.14559	-0.65409
H	-2.35495	0.03705	-2.20546
H	-0.88841	0.75100	-1.55309
H	-2.36846	1.70134	-1.62952

16C cation radical

24

Energy: -196995.5438899

C	-4.09010	-0.24106	0.16467
C	-2.04097	0.23982	-0.09177
C	-2.01323	-1.24702	0.08788
C	-1.61909	1.14313	0.99660
C	-1.91834	0.75578	-1.47251
C	-3.48712	-1.55476	-0.22852
C	-4.89259	0.54266	-0.79461
C	-4.37606	-0.03192	1.60070
H	-1.75920	-1.52039	1.10700

H	-1.32677	-1.73925	-0.59891
H	-3.87555	-2.38601	0.35742
H	-3.63335	-1.76023	-1.28412
H	-4.41144	1.01896	1.87424
H	-3.70300	-0.57288	2.25816
H	-5.37999	-0.43613	1.77181
H	-0.52558	1.20351	0.93382
H	-1.85593	0.77044	1.98649
H	-1.99543	2.15459	0.86766
H	-4.55139	0.45497	-1.81967
H	-4.98070	1.58733	-0.50793
H	-5.90432	0.12014	-0.76000
H	-2.31809	0.08075	-2.22248
H	-0.84402	0.84689	-1.66776
H	-2.34275	1.74896	-1.59025

16Si

24

Energy: -512614.4790984

Si	-4.24124	-0.07767	0.13317
Si	-1.96843	0.43217	-0.03016
C	-2.00067	-1.46061	0.18395
C	-0.98390	1.40367	1.23299
C	-1.40611	0.90327	-1.75760
C	-3.43157	-1.73317	-0.35033
C	-5.57416	0.57058	-1.01231
C	-4.90004	-0.13986	1.88942
H	-1.95245	-1.69470	1.24900
H	-1.22318	-2.04518	-0.30693
H	-3.88029	-2.65169	0.02675
H	-3.41184	-1.81018	-1.43894
H	-5.16524	0.85434	2.24566
H	-4.16193	-0.55368	2.57416
H	-5.79267	-0.76316	1.94248
H	0.08195	1.19962	1.13149
H	-1.28118	1.14865	2.24822
H	-1.13087	2.47450	1.09949
H	-1.92778	0.32192	-2.51576
H	-0.33727	0.72499	-1.87522
H	-1.59308	1.95707	-1.95816
H	-5.22477	0.61413	-2.04190
H	-5.88285	1.57333	-0.72020
H	-6.45545	-0.07004	-0.98131

16Si cation radical

24

Energy: -512444.3529628

Si	-4.37988	-0.24228	0.13519
Si	-1.77412	0.34161	-0.05450
C	-1.99129	-1.50083	0.17398
C	-1.06107	1.37023	1.29571
C	-1.50055	0.93083	-1.78068
C	-3.42375	-1.77347	-0.35044
C	-5.50010	0.57788	-1.07405
C	-4.81700	-0.07417	1.91928
H	-1.91799	-1.73961	1.23401
H	-1.24149	-2.09668	-0.34526
H	-3.84232	-2.69493	0.05290
H	-3.42515	-1.86474	-1.43569
H	-4.98827	0.96366	2.19555
H	-4.06153	-0.49823	2.57582
H	-5.74894	-0.61805	2.09232
H	0.02420	1.24198	1.28540
H	-1.42016	1.06989	2.27655
H	-1.26873	2.42711	1.14539
H	-2.03147	0.33089	-2.51541
H	-0.43263	0.85332	-1.99946
H	-1.78342	1.97417	-1.89968
H	-5.07957	0.60053	-2.07597
H	-5.74805	1.59092	-0.76586
H	-6.43177	0.00824	-1.11715

16Ge
24
Energy: -2755674.6792206

Ge	-4.28888	-0.08186	0.14537
Ge	-1.92485	0.44813	-0.04145
C	-1.97921	-1.53296	0.14020
C	-0.88702	1.41261	1.30315
C	-1.32490	0.99234	-1.82176
C	-3.42424	-1.81297	-0.31941
C	-5.66946	0.55006	-1.08357
C	-5.00602	-0.09868	1.96528
H	-1.86204	-1.77514	1.19672
H	-1.22312	-2.09411	-0.40669
H	-3.86251	-2.70992	0.11534
H	-3.46411	-1.92512	-1.40317
H	-5.27508	0.90641	2.28090
H	-4.27200	-0.49308	2.66336
H	-5.89592	-0.72344	2.01092
H	0.17301	1.19775	1.18229
H	-1.18789	1.12169	2.30594
H	-1.03294	2.48490	1.19625
H	-5.30137	0.55925	-2.10592
H	-5.97927	1.55837	-0.81930

H	-6.54115	-0.09968	-1.03422
H	-1.84469	0.42810	-2.59196
H	-0.25628	0.81504	-1.92638
H	-1.51510	2.05054	-1.98396

16Ge cation radical

24

Energy: -2755505.7801028

Ge	-4.43470	-0.26216	0.14555
Ge	-1.71702	0.34436	-0.06793
C	-1.98300	-1.58024	0.16146
C	-0.98376	1.40808	1.35975
C	-1.43680	0.97924	-1.86705
C	-3.40525	-1.84904	-0.35410
C	-5.59600	0.59110	-1.13146
C	-4.88193	-0.05996	2.01085
H	-1.89947	-1.80572	1.22233
H	-1.23072	-2.16627	-0.36325
H	-3.83216	-2.76305	0.05474
H	-3.42251	-1.93069	-1.43868
H	-5.03009	0.98637	2.26073
H	-4.11721	-0.48563	2.65288
H	-5.81774	-0.58991	2.19014
H	0.10002	1.28926	1.34370
H	-1.35252	1.08055	2.32637
H	-1.21526	2.45873	1.21291
H	-5.15977	0.58860	-2.12512
H	-5.81715	1.60996	-0.82812
H	-6.53087	0.03070	-1.16166
H	-1.97717	0.37761	-2.59113
H	-0.37091	0.90654	-2.08481
H	-1.73302	2.01977	-1.96019

16Sn

24

Energy: -418295.3497081

Sn	-4.46511	-0.06125	0.16825
Sn	-1.76957	0.52691	-0.06926
C	-1.96734	-1.63917	0.10810
C	-0.56101	1.46899	1.42708
C	-1.01966	1.12937	-1.98386
C	-3.41724	-1.91316	-0.31585
C	-6.01490	0.50673	-1.19662
C	-5.30931	-0.07740	2.13835
H	-1.82278	-1.87667	1.16220
H	-1.23714	-2.21805	-0.45581
H	-3.83451	-2.81394	0.13212

H	-3.48660	-2.02936	-1.39768
H	-5.62306	0.92364	2.42149
H	-4.58007	-0.43299	2.86053
H	-6.17554	-0.73442	2.16005
H	0.48236	1.20066	1.27848
H	-0.86885	1.15232	2.41922
H	-0.65560	2.54936	1.35836
H	-1.54586	0.60786	-2.77822
H	0.04004	0.89453	-2.05087
H	-1.14949	2.19930	-2.12173
H	-5.64939	0.48037	-2.21895
H	-6.35989	1.51274	-0.97351
H	-6.85451	-0.17813	-1.10392

16Sn cation radical

24

Energy: -418132.6625502

Sn	-4.61461	-0.27634	0.15223
Sn	-1.54320	0.38799	-0.07651
C	-1.98422	-1.70276	0.17759
C	-0.69649	1.51067	1.50464
C	-1.15837	1.06316	-2.04729
C	-3.38055	-1.95333	-0.39083
C	-5.91449	0.60882	-1.26342
C	-5.14809	-0.08601	2.19380
H	-1.94641	-1.89979	1.24676
H	-1.22647	-2.32179	-0.29963
H	-3.81102	-2.88701	-0.03291
H	-3.36925	-1.99017	-1.47799
H	-5.33162	0.95609	2.43485
H	-4.36723	-0.48197	2.83420
H	-6.06342	-0.65164	2.35651
H	0.38403	1.38717	1.46702
H	-1.06377	1.15759	2.46201
H	-0.93508	2.56204	1.37969
H	-1.72563	0.48587	-2.76949
H	-0.09578	0.93535	-2.24448
H	-1.40771	2.11562	-2.13639
H	-5.46973	0.59083	-2.25240
H	-6.13572	1.63099	-0.97367
H	-6.84018	0.03687	-1.27635

18C

20

Energy: -237435.7315325

C	-3.84238	-0.11601	0.16719
C	-2.29360	0.12350	-0.02802

C	-2.17098	-1.36256	-0.41557
N	-1.66850	0.34235	1.24714
N	-1.95104	1.16757	-0.96475
C	-3.53624	-1.61700	0.23894
N	-4.62511	0.20997	-0.99599
N	-4.48302	0.44470	1.31820
H	-1.31449	-1.90299	-0.01899
H	-2.19581	-1.49021	-1.49587
H	-3.43633	-1.93088	1.27265
H	-4.23990	-2.27194	-0.26903
H	-2.23270	0.92631	-1.90178
H	-0.95315	1.31325	-0.98172
H	-1.74155	1.31665	1.49977
H	-0.68999	0.10109	1.21950
H	-4.85808	1.35770	1.12000
H	-3.83569	0.50245	2.08802
H	-4.50024	-0.45673	-1.73789
H	-4.38965	1.12780	-1.34179

18C cation radical

20

Energy: -237299.7202665

C	-4.42356	-0.20776	0.01580
C	-1.35866	0.04273	-0.02694
C	-2.10790	-1.15279	-0.50675
N	-1.44459	0.30841	1.36432
N	-1.46092	1.19599	-0.81236
C	-3.51048	-1.37826	0.11105
N	-5.45867	-0.25736	-0.79404
N	-4.17067	0.83129	0.75744
H	-1.54776	-2.06199	-0.28895
H	-2.19231	-1.10204	-1.59035
H	-3.40357	-1.61185	1.16845
H	-3.97413	-2.24052	-0.36099
H	-1.31720	1.00758	-1.78986
H	-0.83164	1.93194	-0.53322
H	-0.82307	1.05217	1.64616
H	-1.19751	-0.50268	1.91046
H	-4.71270	1.67384	0.70108
H	-3.27637	0.83711	1.26228
H	-5.65130	-1.09149	-1.31299
H	-6.09546	0.51071	-0.90056

18Si

20

Energy: -552926.0163904

Si	-4.14541	0.04481	0.08817

Si	-1.81943	0.31107	-0.06944
C	-2.04876	-1.56355	0.15509
N	-0.65853	0.91484	1.04165
N	-1.33344	0.91806	-1.59625
C	-3.51765	-1.70362	-0.31578
N	-5.44685	0.47624	-0.94538
N	-4.69931	0.38312	1.67374
H	-1.97543	-1.80214	1.21874
H	-1.35134	-2.21569	-0.36845
H	-4.04953	-2.54111	0.13291
H	-3.54816	-1.84636	-1.39868
H	-5.54769	-0.00772	2.03913
H	-4.06643	0.66068	2.39746
H	-0.39638	1.88240	1.03085
H	-0.54730	0.50859	1.95059
H	-2.00088	1.09979	-2.31959
H	-0.41380	0.75531	-1.96275
H	-5.48530	0.14934	-1.89185
H	-5.90686	1.36092	-0.84011

18Si cation radical

20

Si	-4.29001	-0.09588	0.16838
Si	-1.65106	0.21700	-0.13336
C	-2.05271	-1.58209	0.15838
N	-0.84035	1.16911	0.97506
N	-1.26617	0.58801	-1.72026
C	-3.51099	-1.71423	-0.33217
N	-5.30320	0.75696	-0.84966
N	-4.70026	0.04170	1.78630
H	-1.98640	-1.76272	1.23147
H	-1.36615	-2.27626	-0.32369
H	-4.02364	-2.59356	0.05404
H	-3.55036	-1.77286	-1.42021
H	-5.21930	0.80516	2.17862
H	-4.53284	-0.68753	2.45408
H	-0.13529	1.83300	0.71113
H	-1.10518	1.25153	1.93858
H	-1.20619	-0.10192	-2.44561
H	-1.03652	1.50815	-2.04701
H	-5.13559	0.85061	-1.83404
H	-6.04628	1.35081	-0.53004

18Ge

20

Energy: -2795952.4182737

Ge	-4.21771	0.00087	0.11915
Ge	-1.80268	0.34887	-0.04502
C	-2.02542	-1.62901	0.10983
N	-0.73482	1.10408	1.22657
N	-1.19299	1.06559	-1.62265
C	-3.49786	-1.79932	-0.29888
N	-5.65188	0.45152	-0.93729
N	-4.77971	0.16462	1.85236
H	-1.88535	-1.89482	1.15765
H	-1.32972	-2.22194	-0.48020
H	-4.00425	-2.61561	0.21014
H	-3.58787	-1.96898	-1.37218
H	-1.84054	1.03536	-2.39094
H	-0.29962	0.72188	-1.93485
H	-0.08449	1.79557	0.89933
H	-0.31165	0.50006	1.90647
H	-5.77466	0.11526	1.99139
H	-4.40026	0.94325	2.36035
H	-5.54026	0.27952	-1.92230
H	-5.99670	1.38820	-0.80890

18Ge cation radical

20

Energy: -2795795.8317742

Ge	-4.35445	-0.10515	0.16034
Ge	-1.58078	0.20809	-0.14859
C	-2.03729	-1.67561	0.11184
N	-0.63221	1.08175	1.07697
N	-1.06839	0.69001	-1.78274
C	-3.51316	-1.81661	-0.26926
N	-5.49823	0.64586	-0.97759
N	-4.91445	0.11295	1.83542
H	-1.87198	-1.89105	1.16596
H	-1.38050	-2.32432	-0.46288
H	-4.01128	-2.64123	0.23500
H	-3.63885	-1.96236	-1.34067
H	-1.35655	0.17140	-2.59120
H	-0.82115	1.63693	-2.00455
H	-0.19357	1.95737	0.85378
H	-0.87472	1.01937	2.04851
H	-5.34224	0.96614	2.14547
H	-4.50309	-0.40344	2.59030
H	-5.26717	0.72245	-1.95110
H	-6.09841	1.39247	-0.67496

18Sn

20

Energy: -458568.9638831

Sn	-4.39449	0.01843	0.25085
Sn	-1.67669	0.51842	-0.19433
C	-1.98390	-1.65651	-0.35694
N	-0.45557	1.03588	1.32486
N	-0.93476	1.63788	-1.70909
C	-3.37679	-1.91651	0.20437
N	-5.90024	0.11080	-1.09993
N	-5.37914	0.46687	1.94866
H	-1.20154	-2.21169	0.15587
H	-1.92200	-1.89954	-1.41656
H	-3.33992	-2.25747	1.23744
H	-3.94304	-2.64941	-0.36592
H	0.19040	1.77620	1.10680
H	0.04102	0.28540	1.77369
H	-6.33521	0.74742	1.80197
H	-4.93304	1.13177	2.55733
H	-5.68433	-0.29099	-1.99819
H	-6.25393	1.04052	-1.26200
H	-1.48427	1.64871	-2.55242
H	0.01909	1.42847	-1.95851

18Sn cation radical

20

Energy: -458410.1938385

Sn	-4.51420	-0.10460	0.26478
Sn	-1.43519	0.37432	-0.32584
C	-2.03655	-1.68931	-0.47358
N	-0.32005	0.91831	1.20554
N	-0.73082	1.28847	-1.92116
C	-3.32947	-1.90487	0.29476
N	-5.80779	0.14185	-1.20059
N	-5.38767	0.49337	1.92574
H	-1.22559	-2.32032	-0.11783
H	-2.15922	-1.86876	-1.53952
H	-3.15060	-2.10273	1.34941
H	-3.92401	-2.72336	-0.10411
H	-0.00066	1.86949	1.27471
H	-0.51335	0.54688	2.11907
H	-6.05763	1.24282	1.88610
H	-4.85496	0.54416	2.77627
H	-5.55325	-0.11829	-2.13740
H	-6.39634	0.95737	-1.21200
H	-1.22613	1.21610	-2.79262
H	-0.32487	2.20379	-1.82380

20C

10

Energy: -97799.8818548

C	-3.86348	-0.00529	0.06654
C	-2.35658	0.32109	-0.12712
C	-2.15196	-1.16943	-0.15385
C	-3.44300	-1.44905	0.01211
H	-4.00006	-2.37143	0.08363
H	-1.26834	-1.77976	-0.26755
H	-4.51064	0.33023	-0.74222
H	-4.28491	0.32976	1.01290
H	-2.11875	0.84836	-1.04955
H	-1.89321	0.84775	0.70559

20C cation radical

10

Energy: -97586.5659808

C	-3.86305	-0.00599	0.06655
C	-2.35668	0.32028	-0.12711
C	-2.11689	-1.13416	-0.15815
C	-3.48934	-1.43139	0.01790
H	-4.03867	-2.36104	0.08805
H	-1.23737	-1.75434	-0.27104
H	-4.54589	0.29976	-0.72988
H	-4.32178	0.29900	1.01027
H	-2.07259	0.83512	-1.04813
H	-1.84870	0.83503	0.69205

20Si

10

Energy: -413197.0756259

Si	-4.26842	0.05537	0.11876
Si	-2.01220	0.54416	-0.17164
C	-2.10964	-1.32960	-0.15923
C	-3.41647	-1.61273	0.00889
H	-3.79963	-2.62656	0.05800
H	-1.34730	-2.09529	-0.25735
H	-5.24263	0.34014	-0.96390
H	-4.93642	0.33985	1.41304
H	-1.53199	1.14351	-1.44148
H	-1.22626	1.14341	0.93540

20Si cation radical

10

Energy: -412992.4043049

Si	-4.42119	-0.07183	0.13838
Si	-1.82098	0.49125	-0.19610

C	-2.11217	-1.33234	-0.15876
C	-3.41285	-1.61391	0.00830
H	-3.79012	-2.62935	0.05655
H	-1.35477	-2.10214	-0.25628
H	-5.18382	0.40496	-1.02525
H	-4.86381	0.40479	1.45744
H	-1.62552	1.17537	-1.48326
H	-1.30571	1.17547	0.99946

20Ge

10

Energy: -2656265.8804433

Ge	-4.31959	0.07044	0.12571
Ge	-1.97150	0.57874	-0.17762
C	-2.10385	-1.37379	-0.16015
C	-3.40381	-1.65532	0.00760
H	-3.79330	-2.66594	0.05780
H	-1.33693	-2.13384	-0.25887
H	-5.32065	0.35434	-1.00018
H	-5.00373	0.35426	1.46796
H	-1.47694	1.18719	-1.49492
H	-1.16067	1.18617	0.97314

20Ge cation radical

10

Energy: -2656065.8435526

Ge	-4.48477	-0.06974	0.14703
Ge	-1.76372	0.51945	-0.20407
C	-2.10740	-1.37570	-0.15965
C	-3.39949	-1.65546	0.00688
H	-3.78668	-2.66614	0.05670
H	-1.34293	-2.13707	-0.25827
H	-5.26016	0.42272	-1.06357
H	-4.92902	0.42247	1.51434
H	-1.57313	1.22079	-1.53854
H	-1.24365	1.22093	1.03963

20Sn

10

Energy: -318892.8758434

Sn	-4.49456	0.09758	0.14718
Sn	-1.82330	0.67646	-0.19594
C	-2.08810	-1.45307	-0.16126
C	-3.38603	-1.73419	0.00497
H	-3.74975	-2.75576	0.05201
H	-1.34010	-2.23378	-0.25679

H	-5.63275	0.34864	-1.09297
H	-5.28061	0.34890	1.63576
H	-1.22360	1.30283	-1.66045
H	-0.87214	1.30467	1.06796

20Sn cation radical

10

Energy: -318704.2776297

Sn	-4.66926	-0.06448	0.17000
Sn	-1.59771	0.60117	-0.22505
C	-2.09198	-1.45379	-0.16063
C	-3.38170	-1.73375	0.00446
H	-3.74474	-2.75430	0.05124
H	-1.34506	-2.23386	-0.25616
H	-5.56653	0.42670	-1.16741
H	-5.19851	0.42702	1.69100
H	-1.33205	1.34300	-1.71295
H	-0.96340	1.34455	1.14597

21C

22

Energy: -196409.9858638

C	-3.84553	-0.12448	0.14147
C	-2.30694	0.24177	-0.06725
C	-2.10348	-1.25112	-0.16712
C	-1.61394	0.89573	1.11335
C	-1.97355	1.01066	-1.33194
C	-3.38466	-1.55609	0.00632
C	-4.79243	0.34020	-0.94913
C	-4.43266	0.22390	1.49646
H	-3.92983	-2.48959	0.04236
H	-1.21185	-1.84264	-0.32528
H	-4.53518	1.30247	1.61617
H	-3.82953	-0.15538	2.31632
H	-5.42718	-0.21166	1.59094
H	-0.54161	0.95196	0.92714
H	-1.75776	0.33956	2.03519
H	-1.97309	1.91336	1.26695
H	-2.38338	0.53943	-2.22063
H	-0.89227	1.06441	-1.45719
H	-2.34828	2.03305	-1.28194
H	-4.45624	0.04646	-1.93933
H	-4.90948	1.42384	-0.93412
H	-5.77829	-0.09749	-0.79344

21C cation radical

22

Energy: -196206.3671803

C	-3.85604	-0.09329	0.09310
C	-2.30945	0.26688	-0.01384
C	-2.07373	-1.19356	-0.09360
C	-1.65245	1.06478	1.09206
C	-1.89600	0.82514	-1.39078
C	-3.43855	-1.50660	-0.05926
C	-4.82927	0.50361	-0.90077
C	-4.42116	0.01573	1.52374
H	-3.97967	-2.44433	-0.03566
H	-1.18343	-1.79213	-0.24119
H	-4.46741	1.07325	1.78009
H	-3.81385	-0.48818	2.27156
H	-5.42440	-0.39926	1.55436
H	-0.57313	1.07076	0.96183
H	-1.87349	0.66872	2.07789
H	-1.99830	2.09501	1.04852
H	-2.25216	0.22926	-2.22744
H	-0.81356	0.89282	-1.44876
H	-2.31876	1.82478	-1.48139
H	-4.49565	0.39174	-1.92732
H	-4.95371	1.56370	-0.69195
H	-5.80298	0.02952	-0.80585

21Si

22

Energy: -511842.8889806

Si	-4.23233	-0.09323	0.19446
Si	-1.96988	0.42639	-0.10311
C	-2.06134	-1.45179	-0.17820
C	-0.95320	1.09432	1.32339
C	-1.38200	1.23616	-1.68847
C	-3.36544	-1.75133	-0.00774
C	-5.48166	0.29583	-1.14801
C	-5.05070	0.15355	1.86285
H	-3.73316	-2.77416	-0.00413
H	-1.30139	-2.21553	-0.32172
H	-5.38264	1.18423	1.98137
H	-4.36715	-0.07714	2.67708
H	-5.92516	-0.48921	1.96296
H	0.10709	0.89544	1.16812
H	-1.24768	0.63918	2.26653
H	-1.07736	2.17265	1.41468
H	-1.93446	0.86748	-2.54998
H	-0.32348	1.03650	-1.85444
H	-1.51108	2.31674	-1.64075
H	-5.05684	0.15006	-2.13876

H	-5.81975	1.32862	-1.07319
H	-6.35757	-0.34641	-1.05760

21Si cation radical

22

Energy: -511667.2591846

Si	-4.37435	-0.24643	0.20707
Si	-1.77914	0.34954	-0.13430
C	-2.05937	-1.48329	-0.18096
C	-1.03029	1.08526	1.37837
C	-1.46763	1.23100	-1.72052
C	-3.35675	-1.78147	-0.01130
C	-5.41324	0.32592	-1.20125
C	-4.96514	0.18145	1.89780
H	-3.71860	-2.80431	-0.00934
H	-1.30501	-2.24975	-0.32473
H	-5.23275	1.23310	1.97203
H	-4.23472	-0.06305	2.66392
H	-5.86706	-0.40289	2.09760
H	0.05304	0.95346	1.31614
H	-1.37209	0.59774	2.28705
H	-1.22741	2.15308	1.44175
H	-2.05175	0.82370	-2.54095
H	-0.41052	1.11027	-1.97108
H	-1.66279	2.29711	-1.62854
H	-4.92938	0.16796	-2.16106
H	-5.68281	1.37456	-1.09750
H	-6.33938	-0.25462	-1.19491

21Ge

22

Energy: -2754900.9239758

Ge	-4.28189	-0.09080	0.20081
Ge	-1.92402	0.44606	-0.10980
C	-2.05375	-1.51324	-0.18260
C	-0.85554	1.12908	1.37727
C	-1.29655	1.27640	-1.76391
C	-3.35200	-1.80907	-0.01287
C	-5.58923	0.29824	-1.19865
C	-5.13920	0.14933	1.94033
H	-3.72719	-2.82832	-0.00741
H	-1.29070	-2.27278	-0.32589
H	-5.47316	1.17752	2.05866
H	-4.44856	-0.08704	2.74492
H	-6.00605	-0.50325	2.02345
H	0.19904	0.92051	1.20839
H	-1.15650	0.66356	2.31159

H	-0.98033	2.20558	1.46872
H	-1.84978	0.89704	-2.61839
H	-0.23949	1.06439	-1.91161
H	-1.42501	2.35534	-1.71686
H	-5.15443	0.14838	-2.18285
H	-5.93052	1.32795	-1.12156
H	-6.45233	-0.35657	-1.09640

21Ge cation radical

22

Energy: -2754726.9407602

Ge	-4.43262	-0.26981	0.21312
Ge	-1.71670	0.35169	-0.14362
C	-2.04903	-1.55575	-0.18728
C	-0.95069	1.11691	1.44899
C	-1.40216	1.27143	-1.80585
C	-3.33884	-1.85121	-0.01813
C	-5.50720	0.33218	-1.26724
C	-5.03231	0.18457	1.98585
H	-3.71083	-2.86956	-0.01487
H	-1.28873	-2.31496	-0.33215
H	-5.27298	1.24159	2.04887
H	-4.28708	-0.07427	2.73052
H	-5.93909	-0.38690	2.18688
H	0.13095	0.99059	1.39159
H	-1.31137	0.61282	2.33934
H	-1.16875	2.17915	1.50629
H	-1.99426	0.84535	-2.60883
H	-0.34627	1.15826	-2.05381
H	-1.61786	2.33076	-1.70332
H	-5.00235	0.16328	-2.21255
H	-5.75449	1.38387	-1.15790
H	-6.43449	-0.24162	-1.26061

21Sn

22

Energy: -417521.7262597

Sn	-4.45688	-0.07689	0.22264
Sn	-1.77358	0.52951	-0.12387
C	-2.03904	-1.60903	-0.18579
C	-0.53191	1.22360	1.47598
C	-1.00663	1.37488	-1.93521
C	-3.33681	-1.90218	-0.02314
C	-5.92601	0.27480	-1.29442
C	-5.43715	0.10067	2.11774
H	-3.68838	-2.93077	-0.02431
H	-1.29606	-2.39042	-0.32400

H	-5.81193	1.11196	2.25108
H	-4.74643	-0.12922	2.92327
H	-6.27574	-0.59007	2.16252
H	0.50417	0.96066	1.27667
H	-0.83709	0.77225	2.41512
H	-0.60601	2.30433	1.56288
H	-1.55380	0.99364	-2.79198
H	0.04435	1.11763	-2.04297
H	-1.09897	2.45738	-1.90993
H	-5.49446	0.12577	-2.27951
H	-6.30031	1.29243	-1.22253
H	-6.75850	-0.41260	-1.16493

21Sn cation radical

22

Energy: -417354.4017512

Sn	-4.60836	-0.29401	0.23392
Sn	-1.54789	0.40144	-0.16618
C	-2.02882	-1.66879	-0.19859
C	-0.66992	1.20503	1.58213
C	-1.14550	1.37058	-2.00212
C	-3.31735	-1.96208	-0.03086
C	-5.81639	0.31607	-1.39181
C	-5.28660	0.15137	2.18761
H	-3.66822	-2.98891	-0.03247
H	-1.28662	-2.44725	-0.34222
H	-5.53004	1.20609	2.26371
H	-4.53022	-0.11387	2.91777
H	-6.18569	-0.43365	2.37139
H	0.40554	1.05150	1.51785
H	-1.05196	0.69921	2.46185
H	-0.87212	2.26943	1.64247
H	-1.74442	0.93767	-2.79559
H	-0.09071	1.23014	-2.23028
H	-1.34936	2.43265	-1.91332
H	-5.30786	0.12618	-2.33045
H	-6.05608	1.37045	-1.30038
H	-6.73855	-0.26086	-1.35912

22C

28

Energy: -245721.2763178

C	-3.85548	-0.11394	0.14277
C	-2.31756	0.23753	-0.06417
C	-2.11628	-1.26282	-0.16203
C	-1.61713	0.89082	1.11857
C	-1.97263	1.00247	-1.33381

C	-3.41305	-1.55881	0.01209
C	-4.79966	0.35770	-0.95366
C	-4.44358	0.24387	1.50004
C	-4.20338	-2.81253	0.06978
C	-0.87623	-2.05976	-0.37813
H	-4.53549	1.33147	1.62378
H	-3.84106	-0.14402	2.32816
H	-5.45131	-0.18235	1.59864
H	-0.53386	0.93034	0.93961
H	-1.77512	0.33935	2.05115
H	-1.96068	1.92343	1.26816
H	-2.39579	0.53435	-2.22871
H	-0.88259	1.03937	-1.46656
H	-2.33071	2.04002	-1.28746
H	-4.46373	0.05146	-1.95002
H	-4.90583	1.45104	-0.94940
H	-5.80050	-0.06817	-0.79890
H	-3.56721	-3.69559	-0.06167
H	-4.97617	-2.83269	-0.71172
H	-4.72410	-2.91087	1.03294
H	0.00254	-1.40949	-0.46227
H	-0.93198	-2.65721	-1.29784
H	-0.69140	-2.75660	0.45019

22C cation radical

28

Energy: -245540.3697210

C	-3.85388	-0.11832	0.14226
C	-2.32065	0.23604	-0.08650
C	-2.09309	-1.23486	-0.21413
C	-1.59794	0.78157	1.14615
C	-1.95328	1.06638	-1.30553
C	-3.43466	-1.55161	0.10568
C	-4.76948	0.19941	-1.04093
C	-4.50791	0.34233	1.43490
C	-4.15265	-2.79599	0.32179
C	-0.92114	-2.02828	-0.54286
H	-4.62121	1.42404	1.41935
H	-3.93612	0.07266	2.31755
H	-5.50110	-0.09124	1.52680
H	-0.53146	0.85485	0.94795
H	-1.73751	0.16427	2.02962
H	-1.96883	1.78000	1.36628
H	-2.37761	0.67697	-2.22589
H	-0.87233	1.10627	-1.41888
H	-2.30784	2.08589	-1.17106
H	-4.40362	-0.20133	-1.98252
H	-4.86162	1.27830	-1.14295

H	-5.76146	-0.20774	-0.86136
H	-3.54445	-3.67862	0.15680
H	-5.03529	-2.82675	-0.32191
H	-4.54370	-2.80996	1.34360
H	-0.10148	-1.76525	0.13090
H	-0.56946	-1.75346	-1.54154
H	-1.10019	-3.09720	-0.50404

22Si

28

Energy: -561152.1387113

Si	-4.24833	-0.00142	0.20885
Si	-2.00392	0.50518	-0.11975
C	-2.08621	-1.37734	-0.16167
C	-0.96003	1.19762	1.27801
C	-1.42325	1.28342	-1.72622
C	-3.39701	-1.67307	0.02420
C	-5.52226	0.36506	-1.12002
C	-5.05400	0.26927	1.88233
C	-4.00628	-3.03601	0.06953
C	-0.97067	-2.35102	-0.35713
H	-5.38883	1.30046	1.98781
H	-4.36195	0.05500	2.69410
H	-5.92609	-0.37361	2.00239
H	0.09682	0.98658	1.11406
H	-1.24581	0.76778	2.23579
H	-1.07235	2.27895	1.34644
H	-1.98855	0.90649	-2.57595
H	-0.36820	1.07204	-1.90081
H	-1.54086	2.36596	-1.69607
H	-5.11196	0.21034	-2.11571
H	-5.86530	1.39677	-1.05282
H	-6.39444	-0.27939	-1.00928
H	-3.28549	-3.83812	-0.07571
H	-4.77601	-3.13561	-0.69660
H	-4.50249	-3.20134	1.02659
H	-0.20859	-2.21759	0.41151
H	-0.47563	-2.17789	-1.31342
H	-1.29231	-3.39017	-0.33091

22Si cation radical

28

Energy: -560979.9035885

Si	-4.36928	-0.15157	0.22407
Si	-1.83248	0.42023	-0.14918
C	-2.08053	-1.42371	-0.16344
C	-1.05152	1.20176	1.32781

C	-1.53619	1.28632	-1.75071
C	-3.38710	-1.71813	0.01871
C	-5.43695	0.41945	-1.16756
C	-4.95203	0.31116	1.91203
C	-4.00480	-3.07789	0.06289
C	-0.95911	-2.39209	-0.35651
H	-5.20316	1.36793	1.97144
H	-4.22312	0.06878	2.68035
H	-5.86332	-0.25338	2.12480
H	0.03198	1.08814	1.24096
H	-1.36226	0.73148	2.25658
H	-1.26348	2.26779	1.37334
H	-2.12033	0.86340	-2.56321
H	-0.47909	1.17817	-2.00614
H	-1.74363	2.35129	-1.67152
H	-4.98197	0.23916	-2.13750
H	-5.68284	1.47496	-1.07354
H	-6.37555	-0.13904	-1.12883
H	-3.27874	-3.87091	-0.08565
H	-4.77099	-3.17687	-0.70571
H	-4.49536	-3.24702	1.02126
H	-0.20151	-2.26144	0.41589
H	-0.46608	-2.22441	-1.31385
H	-1.29053	-3.42526	-0.32728

22Ge

28

Energy: -2804210.1053923

Ge	-4.29973	0.01299	0.21623
Ge	-1.96130	0.53836	-0.12498
C	-2.07971	-1.42683	-0.16583
C	-0.86592	1.24253	1.33489
C	-1.34197	1.33865	-1.79926
C	-3.38382	-1.72026	0.02075
C	-5.62915	0.37814	-1.17177
C	-5.14661	0.27748	1.95965
C	-3.99897	-3.07913	0.06861
C	-0.96102	-2.39458	-0.36337
H	-5.48856	1.30475	2.06234
H	-4.44765	0.06241	2.76324
H	-6.00801	-0.37973	2.06294
H	0.18417	1.01499	1.16129
H	-1.16394	0.80474	2.28364
H	-0.97309	2.32271	1.40202
H	-1.91166	0.95659	-2.64184
H	-0.28973	1.11060	-1.95851
H	-1.45409	2.41991	-1.76573
H	-5.20521	0.22359	-2.16016

H	-5.97859	1.40554	-1.10028
H	-6.48648	-0.28192	-1.05388
H	-3.27840	-3.88245	-0.07454
H	-4.76721	-3.18006	-0.69881
H	-4.49540	-3.24309	1.02576
H	-0.19906	-2.26260	0.40565
H	-0.46698	-2.22054	-1.31999
H	-1.28190	-3.43446	-0.33852

22Ge cation radical

28

Energy: -2804039.7017466

Ge	-4.42730	-0.16101	0.22870
Ge	-1.77505	0.43506	-0.15511
C	-2.07076	-1.48782	-0.16387
C	-0.97654	1.25306	1.39845
C	-1.47883	1.33980	-1.83282
C	-3.36986	-1.77962	0.01361
C	-5.52609	0.44330	-1.23715
C	-5.02577	0.32920	1.99565
C	-3.99771	-3.13252	0.05858
C	-0.94344	-2.44700	-0.35283
H	-5.25178	1.39047	2.04250
H	-4.28504	0.07357	2.74609
H	-5.94149	-0.22394	2.20644
H	0.10548	1.14578	1.31715
H	-1.30568	0.76823	2.31157
H	-1.21069	2.31299	1.43542
H	-2.06825	0.89656	-2.62855
H	-0.42250	1.24330	-2.08529
H	-1.71081	2.39702	-1.74270
H	-5.04672	0.25470	-2.19200
H	-5.75007	1.50123	-1.13614
H	-6.46570	-0.10890	-1.20365
H	-3.27326	-3.92932	-0.08138
H	-4.75671	-3.23201	-0.71703
H	-4.49530	-3.29739	1.01401
H	-0.19105	-2.31676	0.42468
H	-0.44678	-2.27800	-1.30800
H	-1.27228	-3.48164	-0.32678

22Sn

28

Energy: -466828.5826129

Sn	-4.48094	0.06420	0.23328
Sn	-1.81805	0.66720	-0.11250
C	-2.06335	-1.47855	-0.17298

C	-0.56003	1.35554	1.47916
C	-1.03913	1.50425	-1.92471
C	-3.36786	-1.77315	-0.01048
C	-5.95813	0.40882	-1.28021
C	-5.46903	0.23040	2.12738
C	-3.92908	-3.15937	0.00134
C	-0.99031	-2.51410	-0.36545
H	-5.85881	1.23618	2.25853
H	-4.77682	0.01204	2.93484
H	-6.29793	-0.47205	2.17152
H	0.46677	1.04967	1.29293
H	-0.88657	0.93870	2.42698
H	-0.59389	2.44001	1.53922
H	-1.60708	1.15047	-2.77968
H	0.00128	1.21177	-2.04529
H	-1.09303	2.58896	-1.88840
H	-5.52685	0.27098	-2.26705
H	-6.34273	1.42202	-1.20138
H	-6.78377	-0.28739	-1.15381
H	-3.16782	-3.92679	-0.13377
H	-4.67124	-3.28356	-0.78829
H	-4.44439	-3.36186	0.94110
H	0.00017	-2.07178	-0.43613
H	-1.15273	-3.08921	-1.27808
H	-0.96860	-3.22504	0.46145

22Sn cation radical

28

Energy: -466665.3760029

Sn	-4.60518	-0.15497	0.22622
Sn	-1.61009	0.50769	-0.11892
C	-2.05588	-1.58312	-0.18751
C	-0.74545	1.32402	1.63430
C	-1.16261	1.51547	-1.92713
C	-3.35779	-1.87074	-0.04658
C	-5.82454	0.49338	-1.38024
C	-5.30329	0.29981	2.17451
C	-3.97925	-3.23002	-0.06588
C	-0.94314	-2.56054	-0.38892
H	-5.52507	1.35965	2.24901
H	-4.56353	0.01971	2.91622
H	-6.21803	-0.26381	2.34711
H	0.33304	1.19250	1.57294
H	-1.11926	0.81423	2.51533
H	-0.96652	2.38497	1.69426
H	-1.73338	1.09444	-2.74746
H	-0.10014	1.39420	-2.12883
H	-1.38122	2.57360	-1.82421

H	-5.32953	0.31300	-2.32808
H	-6.04910	1.54964	-1.27127
H	-6.75547	-0.06920	-1.34799
H	-3.25169	-4.02206	-0.21957
H	-4.72077	-3.30500	-0.86125
H	-4.49653	-3.43380	0.87165
H	-0.42524	-2.37074	-1.32906
H	-1.28783	-3.59070	-0.40503
H	-0.20250	-2.47329	0.40592

23C

18

Energy: -236655.6837146

C	-3.86542	-0.10006	0.16553
C	-2.28434	0.14232	-0.01343
C	-2.21376	-1.35880	-0.17413
N	-1.64143	0.61886	1.18058
N	-1.96073	0.99676	-1.13260
C	-3.51701	-1.56003	-0.00829
N	-4.72301	0.42152	-0.86456
N	-4.40141	0.24972	1.44636
H	-4.14054	-2.44172	0.02585
H	-1.37769	-2.02158	-0.35448
H	-1.52700	1.61987	1.13735
H	-0.73806	0.19666	1.31646
H	-5.03377	1.02718	1.36742
H	-3.65226	0.46343	2.08708
H	-4.64672	-0.11145	-1.71417
H	-4.47955	1.37946	-1.07064
H	-2.37574	0.65262	-1.98374
H	-0.96219	1.03032	-1.27320

23C cation radical

18

Energy: -236552.6786702

C	-4.61305	-0.07975	0.11928
C	-1.35861	0.14796	-0.19497
C	-2.31867	-0.60870	-0.87086
N	-1.55406	0.63367	1.05669
N	-0.19559	0.43794	-0.78714
C	-3.66609	-0.82835	-0.60705
N	-5.84110	-0.58542	0.27336
N	-4.37493	1.12354	0.64034
H	-4.10260	-1.65732	-1.14427
H	-1.92101	-1.16782	-1.70550
H	-0.78737	1.09095	1.51430
H	-2.13111	0.08296	1.66519

H	-5.08635	1.63069	1.12768
H	-3.47827	1.55479	0.53349
H	-6.06454	-1.48027	-0.11203
H	-6.59532	-0.04123	0.64192
H	-0.05022	0.19770	-1.74715
H	0.59825	0.75374	-0.26588

23Si

20

Energy: -552926.0166530

Si	-4.14534	0.04482	0.08780
Si	-1.81944	0.31109	-0.06884
C	-2.04904	-1.56326	0.15630
N	-0.65848	0.91508	1.04185
N	-1.33413	0.91654	-1.59638
C	-3.51729	-1.70316	-0.31698
N	-5.44671	0.47650	-0.94556
N	-4.69856	0.38137	1.67385
H	-1.97805	-1.80115	1.22028
H	-1.35105	-2.21618	-0.36551
H	-4.04955	-2.54136	0.12993
H	-3.54569	-1.84468	-1.40011
H	-5.54691	-0.00859	2.04019
H	-4.06651	0.66222	2.39702
H	-0.39441	1.88210	1.03055
H	-0.54626	0.50880	1.95066
H	-2.00193	1.10111	-2.31866
H	-0.41503	0.75406	-1.96434
H	-5.48585	0.14936	-1.89193
H	-5.90825	1.36034	-0.84007

23Si cation radical

20

Energy: -552773.3718136

Si	-4.28343	-0.09491	0.15670
Si	-1.65094	0.21206	-0.13838
C	-2.04105	-1.58965	0.14640
N	-0.85257	1.15379	0.98738
N	-1.26091	0.61045	-1.71764
C	-3.51273	-1.73047	-0.30223
N	-5.28433	0.75511	-0.87640
N	-4.72525	0.05359	1.76559
H	-1.93942	-1.78647	1.21355
H	-1.36528	-2.27071	-0.36832
H	-4.01724	-2.59114	0.13372
H	-3.58033	-1.83664	-1.38490
H	-5.11991	0.88132	2.17221

H	-4.58445	-0.67453	2.44067
H	-0.19999	1.87450	0.73806
H	-1.07163	1.15535	1.96584
H	-1.24749	-0.06047	-2.46297
H	-1.05938	1.53996	-2.03652
H	-5.08683	0.89607	-1.84935
H	-6.07530	1.28778	-0.56340

23Ge

20

Energy: -2795952.4182830

Ge	-4.21771	0.00088	0.11919
Ge	-1.80267	0.34888	-0.04500
C	-2.02541	-1.62900	0.10983
N	-0.73477	1.10405	1.22658
N	-1.19301	1.06560	-1.62264
C	-3.49786	-1.79931	-0.29886
N	-5.65186	0.45154	-0.93728
N	-4.77977	0.16462	1.85237
H	-1.88533	-1.89482	1.15764
H	-1.32972	-2.22193	-0.48022
H	-4.00424	-2.61560	0.21017
H	-3.58788	-1.96895	-1.37216
H	-1.84059	1.03537	-2.39092
H	-0.29967	0.72186	-1.93487
H	-0.08451	1.79560	0.89935
H	-0.31149	0.50001	1.90639
H	-5.77472	0.11520	1.99137
H	-4.40042	0.94330	2.36036
H	-5.54026	0.27945	-1.92227
H	-5.99658	1.38826	-0.80898

23Ge cation radical

20

Energy: -2795787.1573658

Ge	-4.35404	-0.10423	0.16154
Ge	-1.58096	0.20910	-0.14859
C	-2.03725	-1.67504	0.11311
N	-0.63449	1.08855	1.07388
N	-1.07396	0.68967	-1.78429
C	-3.51247	-1.81591	-0.26940
N	-5.49374	0.65375	-0.97530
N	-4.91318	0.11183	1.83659
H	-1.87223	-1.88952	1.16854
H	-1.37894	-2.32501	-0.46058
H	-4.01183	-2.64191	0.23379
H	-3.63818	-1.96059	-1.34200

H	-1.33848	0.15639	-2.59226
H	-0.82070	1.63463	-2.01117
H	-0.17629	1.95308	0.84290
H	-0.87825	1.03634	2.04663
H	-5.34829	0.96069	2.15093
H	-4.52325	-0.42357	2.59063
H	-5.26068	0.74198	-1.94826
H	-6.11127	1.38478	-0.66661

23Sn

20

Energy: -458568.9639055

Sn	-4.39449	0.01844	0.25094
Sn	-1.67669	0.51842	-0.19427
C	-1.98394	-1.65650	-0.35698
N	-0.45545	1.03577	1.32486
N	-0.93481	1.63797	-1.70900
C	-3.37678	-1.91650	0.20447
N	-5.90013	0.11078	-1.09996
N	-5.37925	0.46693	1.94867
H	-1.20154	-2.21174	0.15570
H	-1.92217	-1.89944	-1.41663
H	-3.33981	-2.25741	1.23754
H	-3.94308	-2.64943	-0.36574
H	0.19047	1.77614	1.10683
H	0.04122	0.28527	1.77356
H	-6.33531	0.74747	1.80189
H	-4.93321	1.13185	2.55735
H	-5.68427	-0.29131	-1.99810
H	-6.25359	1.04053	-1.26231
H	-1.48446	1.64903	-2.55224
H	0.01896	1.42842	-1.95862

23Sn cation radical

20

Energy: -458410.1938734

Sn	-4.51417	-0.10461	0.26487
Sn	-1.43520	0.37430	-0.32580
C	-2.03655	-1.68933	-0.47353
N	-0.31998	0.91834	1.20550
N	-0.73098	1.28844	-1.92120
C	-3.32947	-1.90490	0.29480
N	-5.80758	0.14197	-1.20064
N	-5.38778	0.49331	1.92576
H	-1.22558	-2.32034	-0.11780
H	-2.15923	-1.86876	-1.53948
H	-3.15060	-2.10278	1.34945

H	-3.92403	-2.72337	-0.10408
H	-0.00061	1.86953	1.27465
H	-0.51320	0.54691	2.11904
H	-6.05770	1.24279	1.88611
H	-4.85516	0.54401	2.77635
H	-5.55296	-0.11813	-2.13744
H	-6.39613	0.95748	-1.21207
H	-1.22637	1.21604	-2.79261
H	-0.32505	2.20378	-1.82391

25C

3

Energy: -24531.0540338

C	-3.64640	0.20713	0.71121
H	-4.48459	-0.07696	0.04839
H	-4.17149	0.45098	1.65323

25C cation radical

3

Energy: -24307.2117611

C	-3.89666	0.19937	0.76259
H	-4.44253	-0.12772	-0.12539
H	-4.06744	0.50505	1.79742

25Si

3

Energy: -182281.9830553

Si	-2.20287	0.48940	0.33658
H	-1.38688	-0.12574	-0.78531
H	-0.99058	0.54346	1.24776

25Si cation radical

3

Energy: -182076.3537488

Si	-4.17274	0.18617	0.82078
H	-5.13402	-0.23265	-0.22699
H	-4.66658	0.55522	2.16881

25Ge

3

Energy: -1303832.4018507

Ge	-3.99956	-0.16027	0.90097
H	-5.22479	-0.07538	-0.09936

H -4.81245 0.62008 2.01418

25Ge cation radical

3

Energy: -1303626.6300108

Ge -4.21896 0.18187 0.83064
H -5.20486 -0.25572 -0.26854
H -4.71504 0.56874 2.23636

25Sn

3

Energy: -135165.1377266

Sn -4.21473 -0.29710 0.98562
H -5.52730 -0.08980 -0.16790
H -5.06639 0.68173 2.17431

25Sn cation radical

3

Energy: -134967.9682991

Sn -4.39239 0.04134 0.91261
H -5.49146 -0.27555 -0.35857
H -4.95336 0.63716 2.41417

26C

9

C -2.39518 0.21517 0.46368
C -1.80977 -0.32966 -0.76960
C -1.37170 0.40250 1.50395
H -2.53960 -0.62914 -1.51482
H -1.10272 -1.14675 -0.58251
H -1.20398 0.48154 -1.19622
H -0.60268 1.08119 1.11327
H -0.84311 -0.53801 1.70173
H -1.75306 0.80778 2.43549

26C cation radical

9

Energy: -73689.0002977

C -2.02012 0.00310 0.47484
C -1.80654 -0.45804 -0.83271
C -1.36882 0.28122 1.68573
H -2.49144 -0.02094 -1.56060
H -2.12960 -1.51724 -0.73687

H	-0.76204	-0.45078	-1.15256
H	-1.25133	1.38407	1.61155
H	-0.37343	-0.15919	1.77834
H	-2.00108	0.12483	2.56077

26Si

9

Energy: -231606.5687257

Si	-3.91213	0.15275	0.78206
C	-5.37129	0.00598	-0.41126
C	-4.86475	0.82363	2.27118
H	-5.36804	-0.04479	2.71355
H	-5.64903	1.53296	2.00514
H	-4.22731	1.25263	3.03978
H	-5.16142	-0.60552	-1.28481
H	-5.56269	1.02591	-0.76684
H	-6.29249	-0.33343	0.06334

26Si cation radical

9

Energy: -231431.5425991

Si	-4.22776	0.35402	0.77639
C	-5.40377	-0.03704	-0.56665
C	-4.82538	0.93884	2.40138
H	-5.49691	0.17599	2.80684
H	-5.41106	1.84840	2.23766
H	-4.02375	1.13705	3.10600
H	-4.91826	-0.37776	-1.47567
H	-5.98959	0.86401	-0.77219
H	-6.08977	-0.80616	-0.19911

26Ge

9

Energy: -1353152.0643358

Ge	-3.94504	0.03164	0.82851
C	-5.47771	-0.01903	-0.42944
C	-4.95899	0.81650	2.34166
H	-5.58612	0.01770	2.74834
H	-5.63044	1.60986	2.01437
H	-4.31945	1.18135	3.13995
H	-5.29308	-0.64267	-1.29928
H	-5.62748	1.00741	-0.77785
H	-6.40236	-0.32671	0.05752

26Ge cation radical

9

Energy: -1352974.2282719

Ge	-4.26637	0.36571	0.78064
C	-5.50925	-0.05428	-0.62544
C	-4.90236	0.97170	2.49109
H	-5.57508	0.20207	2.87436
H	-5.47131	1.88672	2.31495
H	-4.09050	1.15311	3.18565
H	-5.00820	-0.39678	-1.52311
H	-6.08265	0.85315	-0.82518
H	-6.18183	-0.82260	-0.23930

26Sn

9

Energy: -184480.8648514

Sn	-4.13715	-0.12349	0.91159
C	-5.82278	-0.07832	-0.46449
C	-5.24182	0.89342	2.48718
H	-6.13880	0.32141	2.72719
H	-5.57056	1.86802	2.12409
H	-4.65764	1.03282	3.39191
H	-5.60125	-0.54488	-1.41985
H	-6.12160	0.95643	-0.63650
H	-6.67377	-0.58699	-0.01005

26Sn cation radical

9

Energy: -184306.1721653

Sn	-4.47369	0.10886	0.90409
C	-5.84189	-0.13337	-0.70750
C	-5.17414	0.99006	2.71005
H	-5.99316	0.36624	3.06565
H	-5.54593	1.98043	2.45004
H	-4.38195	1.05173	3.44591
H	-5.35880	-0.59063	-1.56226
H	-6.21489	0.86014	-0.95335
H	-6.65545	-0.75586	-0.33729

27C

7

Energy: -94042.3367219

C	-0.83770	0.73306	-0.36884
N	-1.23796	-0.49135	-0.69193
N	-1.84756	1.57529	-0.18295
H	-1.64909	2.52106	0.06384
H	-2.82530	1.32949	-0.27279

H	-2.20509	-0.77301	-0.79079
H	-0.55199	-1.19748	-0.85200

27C cation radical

7

Energy: -93868.1314289

C	-2.45168	0.27190	-0.24160
N	-2.00903	-0.65862	-1.00061
N	-2.33107	1.54295	-0.15336
H	-2.81512	2.04060	0.57730
H	-1.76477	2.08949	-0.78958
H	-1.38640	-0.48679	-1.77969
H	-2.28180	-1.61375	-0.82987

27Si

7

Energy: -251789.6230360

Si	-4.28484	-0.49393	0.74613
N	-3.96802	-2.02685	1.43468
N	-4.84603	0.34582	2.12612
H	-3.61386	-2.77385	0.86859
H	-4.09344	-2.30795	2.39070
H	-5.12624	1.30528	2.05646
H	-4.94581	-0.00694	3.06115

27Si cation radical

7

Energy: -251604.0948865

Si	-4.00660	-0.47444	1.15924
N	-4.11422	-2.11140	1.22022
N	-4.54975	0.47782	2.38115
H	-3.78403	-2.69923	0.47236
H	-4.50576	-2.63550	1.98778
H	-4.48358	1.48202	2.34976
H	-4.97725	0.13880	3.22937

27Ge

7

Energy: -1373320.6938698

Ge	-1.69761	0.12382	0.59361
N	-1.05258	-0.75768	-0.85870
N	-2.77352	1.28383	-0.29994
H	-3.31877	1.96635	0.18990
H	-2.89551	1.34131	-1.29444
H	-1.28200	-0.58049	-1.81942

H -0.39436 -1.50574 -0.75675

27Ge cation radical

7

Energy: -1373124.8669583

Ge	-4.09427	-0.39913	1.12988
N	-4.13396	-2.15920	1.21681
N	-4.74323	0.39097	2.56690
H	-3.88025	-2.71569	0.41611
H	-3.92992	-2.61776	2.09360
H	-4.67708	1.39124	2.66989
H	-5.56146	0.00546	3.01716

27Sn

7

Energy: -204642.4413585

Sn	-4.24548	-0.41081	0.51210
N	-3.90440	-2.17399	1.40809
N	-4.90909	0.48404	2.18172
H	-3.56502	-2.97816	0.91466
H	-4.07772	-2.38762	2.37360
H	-5.19570	1.44468	2.20371
H	-4.98103	0.06323	3.09025

27Sn cation radical

7

Energy: -204448.0874199

Sn	-3.62854	-0.07121	0.79407
N	-3.89781	-2.21557	1.54020
N	-4.95479	0.51387	2.11816
H	-4.50798	-2.90395	1.10346
H	-3.22978	-2.70819	2.12996
H	-5.21946	1.48145	2.20825
H	-5.44007	-0.05502	2.79004

28C

19

Energy: -192617.1881910

C	-0.78213	0.08605	0.08820
N	-1.66498	-0.88343	-0.17415
N	-1.23177	1.26234	0.53805
C	-3.02713	-1.03999	0.30031
H	-3.77567	-0.84252	-0.46858
H	-3.15927	-2.07046	0.62797
H	-3.21413	-0.39812	1.15193

C	-0.23173	2.21859	0.94696
H	-0.22509	3.08602	0.28250
H	-0.42533	2.57224	1.96094
H	0.73453	1.73113	0.91656
C	-2.56024	1.83729	0.43922
H	-3.09928	1.84023	1.38783
H	-2.46191	2.87292	0.11594
H	-3.15077	1.31624	-0.30377
C	-1.14437	-2.07458	-0.79993
H	-1.22105	-2.93415	-0.12973
H	-1.69795	-2.30710	-1.71111
H	-0.10511	-1.89936	-1.04781

28C cation radical

19

Energy: -192470.0980158

C	0.99110	0.01064	0.08725
N	1.49145	-1.16878	0.19320
N	1.46703	1.20464	0.06398
C	2.85908	-1.50957	-0.18924
H	3.44077	-1.75588	0.69584
H	2.82351	-2.37567	-0.84341
H	3.31771	-0.68370	-0.71856
C	0.67382	2.28695	-0.50746
H	0.45256	3.01633	0.26700
H	1.24198	2.76391	-1.30120
H	-0.24895	1.88660	-0.90928
C	2.74095	1.58365	0.66931
H	3.45534	1.84896	-0.10634
H	2.57130	2.44645	1.30657
H	3.12807	0.76977	1.26961
C	0.64577	-2.27512	0.62710
H	0.57899	-3.00934	-0.17118
H	1.08665	-2.73653	1.50635
H	-0.34269	-1.90296	0.86730

28Si

19

Energy: -350361.3892956

Si	-1.08301	0.39271	-0.33341
N	-2.13380	-0.97136	-0.26015
N	-1.97826	1.67724	0.38689
C	-3.20571	-1.26771	0.65388
H	-4.17509	-1.33672	0.15138
H	-3.02509	-2.22973	1.14025
H	-3.27301	-0.51214	1.42917
C	-1.23089	2.83058	0.82695

H	-1.55147	3.73368	0.30099
H	-1.35712	3.00594	1.89830
H	-0.16858	2.68330	0.63728
C	-3.40090	1.87319	0.48594
H	-3.74879	1.88676	1.52310
H	-3.67654	2.83242	0.04035
H	-3.93650	1.09468	-0.04660
C	-1.82681	-2.08260	-1.12810
H	-1.62550	-2.98995	-0.55262
H	-2.65182	-2.29741	-1.81204
H	-0.94720	-1.85665	-1.72924

28Si cation radical

19

Energy: -350191.8892025

Si	-1.28930	0.26559	-0.02366
N	-2.25508	-1.05864	-0.25602
N	-1.89089	1.68775	0.57298
C	-3.44816	-1.35703	0.52437
H	-4.30803	-1.43229	-0.13934
H	-3.31911	-2.30543	1.04144
H	-3.63651	-0.58306	1.26143
C	-1.00691	2.66844	1.19255
H	-0.99404	3.58472	0.60680
H	-1.36222	2.89314	2.19603
H	0.00811	2.28545	1.26407
C	-3.26098	2.14664	0.38784
H	-3.72449	2.31053	1.35931
H	-3.26108	3.08407	-0.16422
H	-3.84570	1.41859	-0.16509
C	-1.85912	-2.11588	-1.17920
H	-1.69750	-3.04542	-0.63829
H	-2.64504	-2.26556	-1.91658
H	-0.94276	-1.85178	-1.70139

28Ge

19

Energy: -1471892.9730189

Ge	-1.51976	0.28855	0.26410
N	-0.88863	-0.75015	-1.11028
N	-1.87924	1.87580	-0.58288
C	-2.74688	2.80195	0.09527
C	-1.28865	2.43274	-1.76801
C	-1.15938	-0.66422	-2.51836
C	-0.13979	-1.92662	-0.75645
H	-2.23667	3.74684	0.30643
H	-3.08560	2.38220	1.04213

H	-3.63616	3.03492	-0.49817
H	-0.85828	3.41455	-1.54784
H	-2.01713	2.57518	-2.57342
H	-0.49005	1.79833	-2.13827
H	-0.26026	-0.45331	-3.10730
H	-1.89220	0.10877	-2.72562
H	-1.56524	-1.61328	-2.88183
H	0.87256	-1.90399	-1.17118
H	-0.62508	-2.83572	-1.12475
H	-0.04816	-2.00757	0.32638

28Ge cation radical

19

Energy: -1471722.7174831

Ge	-2.31017	0.15402	-0.02260
N	-1.05581	-0.75834	-1.31026
N	-1.99072	1.82199	-0.56526
C	-2.76489	2.86074	0.09755
C	-1.05126	2.35468	-1.52711
C	-1.45469	-1.03649	-2.65724
C	0.05983	-1.50722	-0.81665
H	-2.10506	3.55058	0.62135
H	-3.45543	2.43008	0.82095
H	-3.34364	3.42157	-0.63504
H	-0.35770	3.03635	-1.03517
H	-1.58171	2.91513	-2.29691
H	-0.47741	1.56549	-1.99975
H	-0.58872	-0.98077	-3.31811
H	-2.22087	-0.34237	-2.98748
H	-1.84265	-2.05700	-2.72202
H	0.94262	-1.26365	-1.41179
H	-0.12041	-2.57861	-0.93146
H	0.25411	-1.28121	0.22694

28Sn

19

Energy: -303214.0886404

Sn	-5.26068	-0.50008	-0.13962
N	-4.02324	-1.64279	0.99152
N	-5.87283	0.81736	1.27624
C	-3.66569	-2.95006	0.51377
C	-3.30043	-1.27944	2.17687
C	-6.45171	2.06382	0.85630
C	-5.94549	0.63536	2.69803
H	-4.16039	-3.16707	-0.43385
H	-3.95465	-3.73812	1.21809
H	-2.58538	-3.04090	0.35375

H	-2.22350	-1.42020	2.03014
H	-3.58486	-1.88686	3.04450
H	-3.46314	-0.23554	2.42883
H	-6.46408	2.14086	-0.23163
H	-5.89166	2.92567	1.23608
H	-7.48379	2.16949	1.20932
H	-5.65121	-0.37194	2.97805
H	-6.96985	0.79193	3.05481
H	-5.30764	1.34045	3.24458

28Sn cation radical

19

Energy: -303050.7482009

Sn	-6.07578	-0.83415	0.17487
N	-4.29781	-1.82759	1.17648
N	-5.87764	0.81362	1.25960
C	-3.12366	-2.16565	0.43443
C	-4.36402	-2.37249	2.49687
C	-6.87277	1.84861	1.04818
C	-4.87595	1.20937	2.21992
H	-3.19510	-1.83291	-0.59636
H	-2.94864	-3.24335	0.46189
H	-2.25680	-1.69007	0.90168
H	-3.41648	-2.23104	3.01877
H	-4.53308	-3.45189	2.43007
H	-5.17286	-1.92547	3.06606
H	-7.61763	1.53909	0.31447
H	-6.40729	2.76631	0.68749
H	-7.39504	2.07481	1.97851
H	-4.12730	0.43547	2.35661
H	-5.33557	1.42292	3.18664
H	-4.36683	2.11633	1.88960

29C

23

Energy: -314321.6627786

C	-3.93517	0.29494	0.74355
C	-4.87897	-0.16080	-0.22555
C	-4.53062	-1.26780	-1.01826
C	-6.10829	0.47557	-0.47963
C	-5.40233	-1.76428	-1.96218
H	-3.56608	-1.72307	-0.85073
C	-6.94191	0.02267	-1.48159
H	-6.37398	1.35076	0.09436
C	-6.60207	-1.10916	-2.20670
H	-5.13756	-2.63780	-2.53900
H	-7.86668	0.53968	-1.69129

H	-7.26593	-1.47287	-2.97727
C	-4.44489	0.88375	1.93989
C	-5.63503	0.47213	2.56855
C	-3.67904	1.88397	2.56319
C	-6.03139	1.03587	3.76405
H	-6.21557	-0.32207	2.12331
C	-4.12017	2.49886	3.71416
H	-2.74358	2.16213	2.10145
C	-5.28913	2.06397	4.32490
H	-6.92804	0.68824	4.25559
H	-3.53946	3.29075	4.16305
H	-5.61237	2.51666	5.25084

29C cation radical

23

Energy: -314178.1796686

C	-4.48349	0.35279	0.82563
C	-5.12628	-0.25704	-0.22992
C	-4.41121	-1.18113	-1.02493
C	-6.47403	0.04590	-0.54283
C	-5.04103	-1.81402	-2.06676
H	-3.37912	-1.38848	-0.78767
C	-7.07801	-0.57786	-1.60311
H	-7.00240	0.78878	0.03442
C	-6.36692	-1.51045	-2.35464
H	-4.50804	-2.53381	-2.66753
H	-8.09936	-0.34445	-1.85998
H	-6.85336	-1.99928	-3.18590
C	-4.65581	1.03357	2.01143
C	-5.87429	0.95944	2.72991
C	-3.58216	1.79519	2.52588
C	-6.00592	1.64504	3.90922
H	-6.67515	0.33779	2.36064
C	-3.74186	2.49441	3.69562
H	-2.65277	1.82775	1.97845
C	-4.94759	2.41651	4.38362
H	-6.92389	1.58448	4.47253
H	-2.93343	3.09161	4.08664
H	-5.06289	2.95605	5.31214

29Si

23

Energy: -472058.2568030

Si	-3.93495	0.27602	0.77785
C	-5.33917	-0.16485	-0.39415
C	-5.06726	-1.16019	-1.33878
C	-6.57856	0.47989	-0.47118

C	-6.00359	-1.53361	-2.28614
H	-4.10066	-1.64836	-1.32820
C	-7.50516	0.13576	-1.43771
H	-6.81503	1.26889	0.22850
C	-7.22302	-0.88010	-2.33789
H	-5.77848	-2.31802	-2.99360
H	-8.45131	0.65455	-1.48933
H	-7.95147	-1.15469	-3.08681
C	-4.85104	0.94727	2.27786
C	-6.11201	0.53500	2.72204
C	-4.15730	1.87206	3.06511
C	-6.65728	1.03420	3.89018
H	-6.66838	-0.19381	2.14984
C	-4.71276	2.40303	4.21545
H	-3.16273	2.17943	2.76657
C	-5.96326	1.97848	4.63076
H	-7.62653	0.69327	4.22384
H	-4.16692	3.13148	4.79672
H	-6.39478	2.37576	5.53786

29Si cation radical

23

Energy: -471895.8914166

Si	-4.38756	0.30983	0.84827
C	-5.47289	-0.31702	-0.44823
C	-4.95568	-1.23809	-1.37160
C	-6.79868	0.13072	-0.57174
C	-5.76175	-1.72815	-2.37647
H	-3.92977	-1.57026	-1.29794
C	-7.58878	-0.35797	-1.58854
H	-7.19878	0.86622	0.11022
C	-7.07252	-1.28762	-2.48196
H	-5.37145	-2.44441	-3.08244
H	-8.60639	-0.01463	-1.69277
H	-7.69908	-1.66603	-3.27575
C	-4.93093	1.10563	2.37269
C	-6.22913	0.91736	2.87515
C	-4.01579	1.90261	3.07664
C	-6.60018	1.53791	4.04741
H	-6.93249	0.27838	2.36217
C	-4.40531	2.52851	4.24127
H	-3.00790	2.03421	2.70905
C	-5.69295	2.34451	4.72225
H	-7.59396	1.39381	4.44222
H	-3.70858	3.15167	4.77976
H	-5.99284	2.82849	5.63966

29Ge

23

Energy: -1593603.3367107

Ge	-3.94486	0.12874	0.89856
C	-5.38626	-0.20254	-0.40384
C	-5.15264	-1.18984	-1.36352
C	-6.56842	0.53498	-0.50183
C	-6.07803	-1.46428	-2.35516
H	-4.22856	-1.75374	-1.33382
C	-7.48349	0.28656	-1.50927
H	-6.77334	1.31859	0.21395
C	-7.24392	-0.72114	-2.42988
H	-5.88558	-2.24407	-3.07742
H	-8.38721	0.87484	-1.57605
H	-7.96288	-0.92098	-3.21090
C	-4.97793	0.85068	2.41397
C	-6.28706	0.49131	2.74233
C	-4.30439	1.71815	3.27649
C	-6.89988	0.98822	3.87888
H	-6.83258	-0.19098	2.10562
C	-4.92267	2.24428	4.39719
H	-3.27649	1.98690	3.06664
C	-6.22197	1.87449	4.70070
H	-7.90905	0.68981	4.12340
H	-4.38960	2.92828	5.04120
H	-6.70446	2.26999	5.58251

29Ge cation radical

23

Energy: -1593436.3452296

Ge	-4.38403	0.29585	0.85356
C	-5.53845	-0.33585	-0.50354
C	-5.05442	-1.25055	-1.44310
C	-6.84976	0.14819	-0.58756
C	-5.89216	-1.70577	-2.43980
H	-4.03538	-1.60602	-1.39356
C	-7.67108	-0.30770	-1.59752
H	-7.22047	0.87969	0.11530
C	-7.19411	-1.23380	-2.51450
H	-5.53151	-2.41986	-3.16366
H	-8.68260	0.06019	-1.67474
H	-7.84384	-1.58520	-3.30189
C	-4.97381	1.10289	2.45863
C	-6.27029	0.86034	2.92874
C	-4.09434	1.91597	3.17885
C	-6.68100	1.45430	4.10390
H	-6.94481	0.20783	2.39411
C	-4.52494	2.51337	4.34523

H	-3.08613	2.08466	2.82906
C	-5.81307	2.28092	4.80356
H	-7.67665	1.27264	4.47823
H	-3.85781	3.15255	4.90230
H	-6.14342	2.74292	5.72171

29Sn

23

Energy: -424930.8558714

Sn	-3.97217	-0.11383	1.42952
C	-5.25876	-0.32245	-0.30097
C	-4.93633	-1.30951	-1.23388
C	-6.33361	0.51898	-0.59333
C	-5.67257	-1.47535	-2.39502
H	-4.09197	-1.96471	-1.05614
C	-7.06027	0.37430	-1.76316
H	-6.60911	1.30316	0.09876
C	-6.73553	-0.62928	-2.66118
H	-5.41200	-2.25469	-3.09649
H	-7.88338	1.04182	-1.97433
H	-7.30653	-0.74712	-3.57051
C	-5.42030	0.74722	2.79113
C	-6.79322	0.49929	2.74382
C	-4.93905	1.52963	3.84217
C	-7.64933	1.01874	3.70009
H	-7.20435	-0.11130	1.95141
C	-5.79156	2.07129	4.78948
H	-3.87641	1.72217	3.92886
C	-7.14976	1.81262	4.71946
H	-8.70792	0.80775	3.64968
H	-5.39758	2.68441	5.58707
H	-7.81795	2.22379	5.46193

29Sn cation radical

23

Energy: -424762.7837131

Sn	-4.46323	0.24320	0.91039
C	-5.77254	-0.28892	-0.63472
C	-5.38233	-1.19852	-1.61545
C	-7.03595	0.30427	-0.66828
C	-6.27324	-1.53607	-2.61592
H	-4.39857	-1.64488	-1.60479
C	-7.91203	-0.03585	-1.68188
H	-7.34000	1.02793	0.07492
C	-7.53156	-0.95500	-2.64721
H	-5.98483	-2.24661	-3.37517
H	-8.89086	0.41736	-1.71872

H	-8.22108	-1.21637	-3.43557
C	-5.20963	1.04443	2.69538
C	-6.54004	0.79207	3.03496
C	-4.38540	1.79001	3.53589
C	-7.04309	1.30959	4.21380
H	-7.18121	0.19543	2.40145
C	-4.90596	2.30919	4.70547
H	-3.34958	1.97030	3.28741
C	-6.22915	2.06768	5.04101
H	-8.06973	1.11974	4.48740
H	-4.27881	2.89559	5.35915
H	-6.62882	2.46880	5.96005

30C

3

Energy: -601213.6290040

C	-3.69481	0.21330	0.71861
Cl	-4.90779	-0.22976	-0.38494
Cl	-4.40204	0.62299	2.20780

30C cation radical

3

Energy: -601006.9085730

C	-3.94371	0.20894	0.76862
Cl	-4.79223	-0.24996	-0.47908
Cl	-4.25984	0.64768	2.25017

30Si

3

Energy: -759021.4073891

Si	-4.03877	-0.30694	0.95890
Cl	-5.49761	-0.20382	-0.50210
Cl	-4.91969	0.78312	2.47789

30Si cation radical

3

Energy: -758803.5299501

Si	-4.26000	-0.19427	0.96404
Cl	-5.40791	-0.29610	-0.61304
Cl	-4.78818	0.76273	2.58368

30Ge

3

Energy: -1880567.8712972

Ge -4.15604 -0.40667 1.01175
Cl -5.66830 -0.21319 -0.52922
Cl -5.06414 0.80463 2.56420

30Ge cation radical

3
Energy: -1880338.4498833
Ge -4.32262 -0.14388 0.95852
Cl -5.59941 -0.34103 -0.64753
Cl -4.94539 0.76090 2.70213

30Sn

3
Energy: -711907.7375703
Sn -4.39763 -0.53353 1.09900
Cl -6.01892 -0.23674 -0.57098
Cl -5.37254 0.84916 2.72715

30Sn cation radical

3
Energy: -711679.2681879
Sn -4.61927 -0.39007 1.09559
Cl -5.93937 -0.36071 -0.72822
Cl -5.23045 0.82969 2.88780

31C

3
Energy: -149077.3958913
C -3.69167 0.21348 0.71794
F -4.64862 -0.11370 -0.08072
F -4.27652 0.51352 1.82627

31C cation radical

3
Energy: -148821.5731262
C -3.83496 0.21081 0.74677
F -4.57965 -0.12750 -0.14260
F -4.18958 0.53013 1.85687

31Si

3
Energy: -306888.8998945
Si -4.15256 -0.30347 0.97774

F -5.22166 -0.10526 -0.18547
F -4.77650 0.64455 2.09466

31Si cation radical

3
Energy: -306645.4062259
Si -4.29248 -0.20875 0.97388
F -5.16923 -0.18217 -0.27337
F -4.68901 0.62674 2.18642

31Ge

3
Energy: -1428411.9468775
Ge -4.31868 -0.40436 1.04417
F -5.48647 -0.12821 -0.20564
F -5.01665 0.66697 2.21380

31Ge cation radical

3
Energy: -1428152.1511555
Ge -4.46972 -0.29525 1.03771
F -5.43324 -0.22045 -0.31711
F -4.91884 0.65010 2.33173

31Sn

3
Energy: -259740.3859545
Sn -4.60204 -0.50400 1.08063
F -5.95206 -0.18911 -0.24864
F -5.33496 0.70491 2.37971

31Sn cation radical

3
Energy: -259486.7049680
Sn -4.77981 -0.37407 1.07782
F -5.89982 -0.30736 -0.40369
F -5.20942 0.69322 2.53756

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