On the Power of the Geometry over the Tetrel Bond

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$E^2_{n\rightarrow\sigma^*}$ for $\mathbf{1}_{Si}$

$E^2_{n\rightarrow\sigma^*}$ was taken directly from the NBO analyses for all dimers in which the T···N interaction is noncovalent. According to NBO analyses the complex formed between 1_{Si} at α=90° and HCN is covalent, so the $E^2_{n\rightarrow\sigma^*}$ value for it was computed by extrapolation. This was done by increasing the Si-N distance by steps of 0.1 Å (while keeping α constant) until the resulting complex was considered noncovalent in the NBO analyses. From four such complexes, and assuming a linear relationship between the $E^2_{n\rightarrow\sigma^*}$ and the Si-N distance, we extrapolated the value for the optimized Si-N distance.

Frontier orbitals and ESP for $\mathbf{1}_T$:

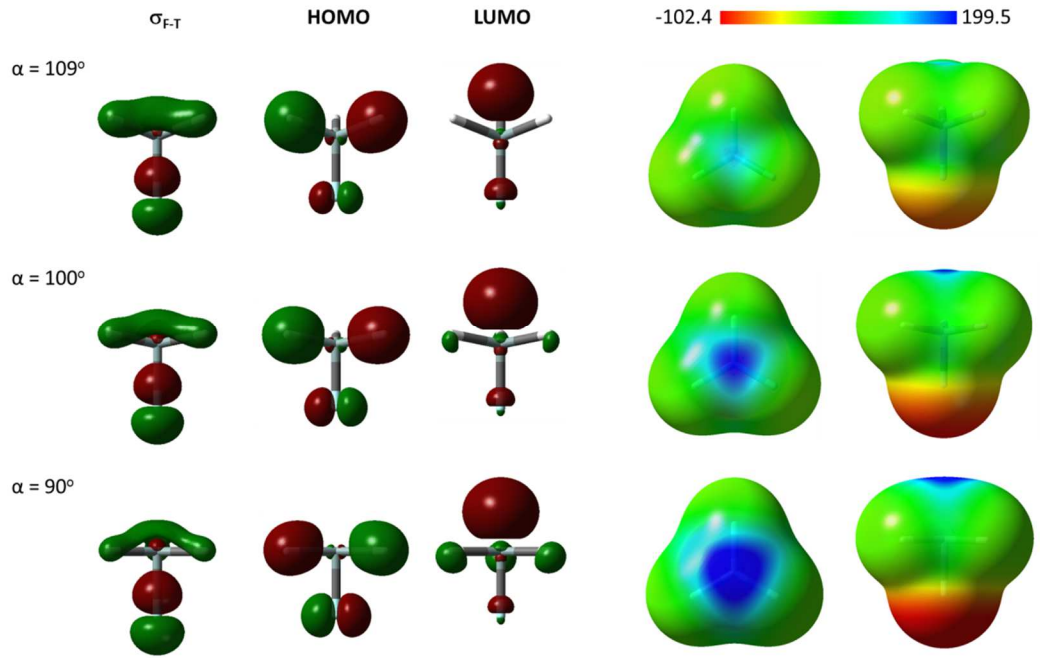

Figure S1. Chosen MOs and ESP maps for $\mathbf{1}_{Si}$ with three different F-Si-H angles (α). The ESP maps are on the 0.001 density isosurface. The color scale is in kJ mol^{-1}. $\sigma_{F\text{-}T}$ corresponds to the bonding F-T σ orbital, irrespective of its position. The HOMO is doubly degenerate.

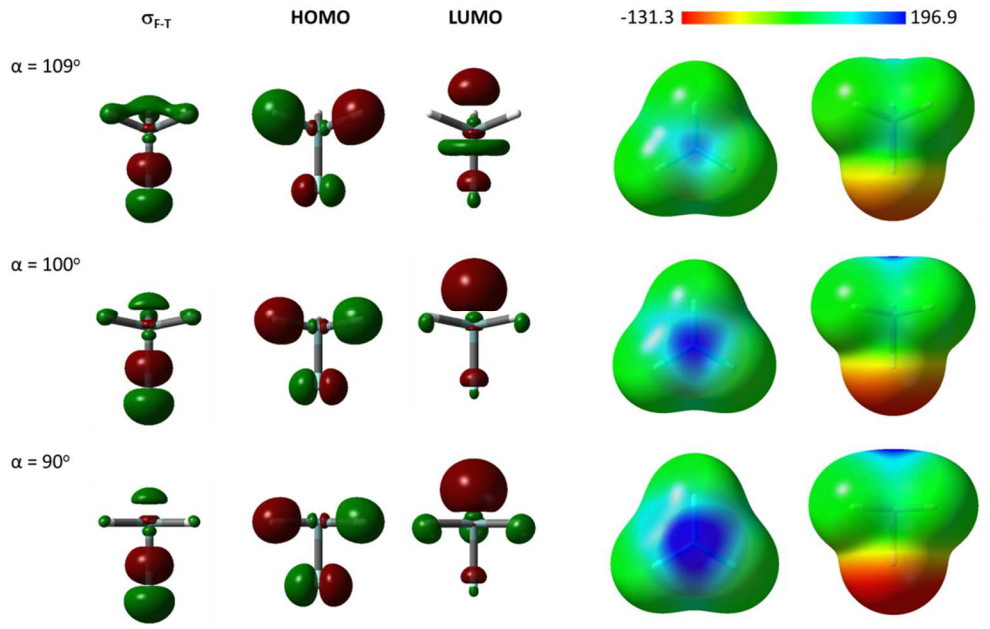

Figure S2. Chosen MOs and ESP maps for **1**$_{Ge}$ with three different F-Ge-H angles (α). The ESP maps are on the 0.001 density isosurface. The color scale is in kJ mol^{-1}. $\sigma_{F\text{-}T}$ corresponds to the bonding F-T σ orbital, irrespective of its position. The HOMO is doubly degenerate.

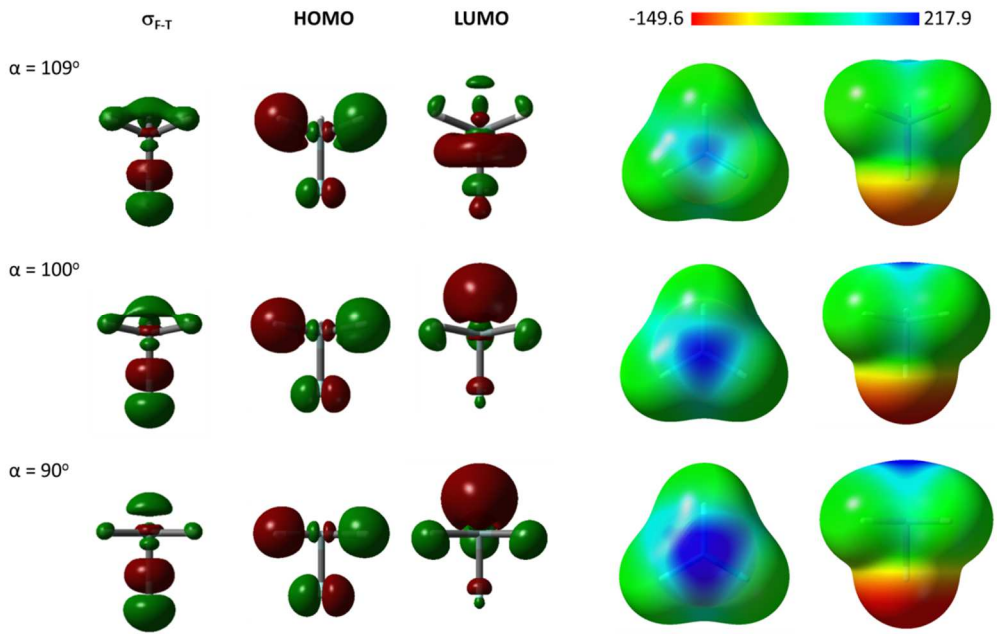

Figure S3. Chosen MOs and ESP maps for **1**$_{Sn}$ with three different F-Sn-H angles (α). The ESP maps are on the 0.001 density isosurface. The color scale is in kJ mol^{-1}. $\sigma_{F\text{-}T}$ corresponds to the bonding F-T σ orbital, irrespective of its position. The HOMO is doubly degenerate.

Trends in 1T and 2T*n*:

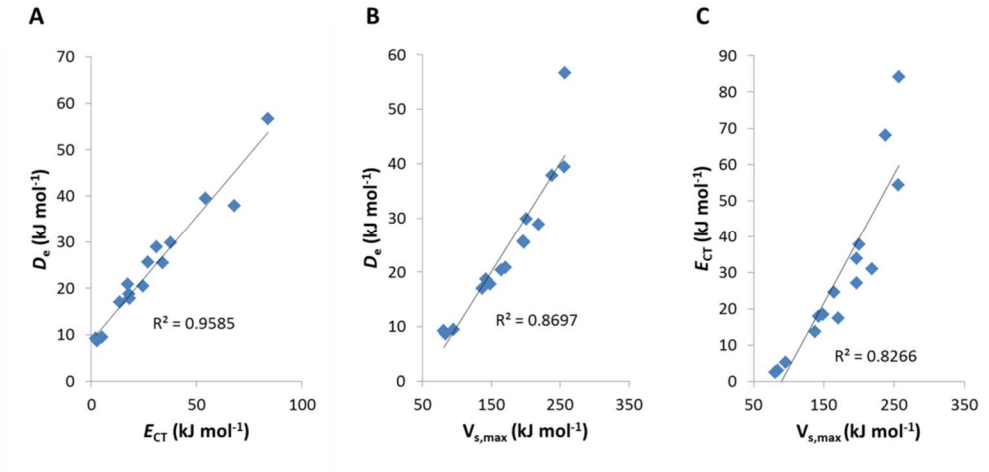

Figure S4. Complexation of **1T** with HCN: A) Dissociation energy as a function of the NBO $n \rightarrow \sigma^*$ charge transfer energy; B) Dissociation energy as a function of $V_{s,max}$; C) $n \rightarrow \sigma^*$ charge transfer energy as a function of of $V_{s,max}$.

Table S1. Distortion energies (in kJ mol^{-1}) relative to the unconstrained (optimized) reference structure, of the monomer and complex of **1T** with HCN at different α angles.

T	α	E_{dist} monomer	E_{dist} complex	ΔE_{dist}
C	109º	0.0	0.0	-0.0
	100º	26.7	27.3	-0.6
	90º	108.5	108.3	0.2
Si	109º	0.2	1.9	-1.7
	100º	21.0	9.9	11.1
	90º	99.6	61.6	38.0
Ge	109º	2.2	4.8	-2.6
	100º	10.2	5.2	5.0
	90º	67.9	50.5	17.4
Sn	109º	4.8	9.7	-4.8
	100º	4.3	1.1	3.2
	90º	46.0	32.2	13.8

Table S2. Tetrel bond dissociation energies (in kJ mol^{-1}) for the complexes of **1T** (T = Si, Ge) with HCN at different α angles, computed at CCSD(T)/CBS//MN15/Def2-TZVPD, at MN15/Def2-TZVPD, and the difference between them.

T	α	D_e[a]	D_e[b]	D_{Diff}[c]
Si	109º	13.6	17.0	3.3
	100º	24.6	29.8	5.2
	90º	48.5	56.7	8.2
Ge	109º	17.5	17.8	0.3
	100º	26.6	25.4	1.2
	90º	41.2	37.8	3.4

[a] At CCSD(T)/CBS//MN15/Def2-TZVPD

[b] At MN15/Def2-TZVPD

[c] The absolute value of the difference in dissociation energies for the two methods

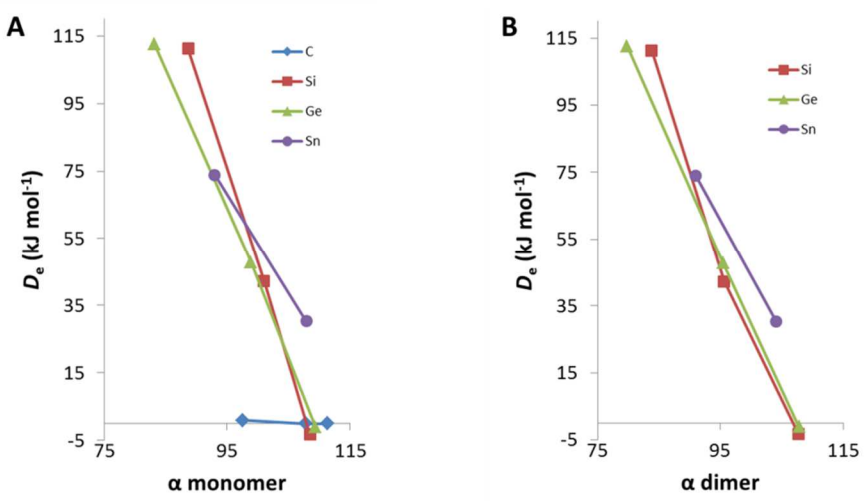

Figure S5. Complexation of **2**$_{Tn}$ with HCN: dissociation energy as a function of the α angle in the A) monomer and B) dimer.

Geometries:

1_C α=90°:

C	0.000000	0.000000	-0.755472
H	0.000000	1.083039	-0.755473
H	0.937939	-0.541519	-0.755473
H	-0.937939	-0.541519	-0.755473
F	0.000000	0.000000	0.755472

1_C α=100°:

C	0.000000	0.000000	-0.681405
H	-0.000000	1.069603	-0.870006
H	0.926304	-0.534802	-0.870006
H	-0.926304	-0.534802	-0.870006
F	0.000000	0.000000	0.744272

1_C α=109°:

C	0.000000	0.000000	-0.629039
H	0.000000	1.030579	-0.983895
H	0.892508	-0.515290	-0.983895
H	-0.892508	-0.515290	-0.983895
F	0.000000	0.000000	0.747324

1_C fully optimized:

C	0.000000	0.000000	-0.628620
H	0.000000	1.030265	-0.984627
H	0.892235	-0.515132	-0.984627
H	-0.892235	-0.515132	-0.984627
F	0.000000	0.000000	0.747289

1_C ⋯ NCH α=90°:

C	0.000000	-0.000000	1.174332
H	0.000000	1.081632	1.174323
H	0.936720	-0.540816	1.174323
H	-0.936720	-0.540816	1.174323
F	0.000000	-0.000000	2.695395
N	-0.000000	0.000000	-1.838215
C	-0.000000	0.000000	-2.984634
H	-0.000000	0.000000	-4.052203

1_C ⋯ NCH α=100°:

C	-0.000000	-0.000000	1.262446
H	0.000000	1.068300	1.074068
H	0.925175	-0.534150	1.074068
H	-0.925175	-0.534150	1.074068
F	-0.000000	-0.000000	2.694380
N	0.000000	0.000000	-1.853786
C	0.000000	0.000000	-3.000324
H	0.000000	0.000000	-4.067853

1_C ⋯ NCH α=109°:

C	0.000000	-0.000000	1.309149
H	-0.000000	1.029740	0.954578
H	0.891781	-0.514870	0.954578
H	-0.891781	-0.514870	0.954578
F	0.000000	-0.000000	2.690398
N	-0.000000	0.000000	-1.845633
C	-0.000000	0.000000	-2.992178
H	-0.000000	0.000000	-4.059711

1_C ⋯ NCH fully optimized:

C	-0.000000	0.000000	1.309744
H	0.000000	1.028195	0.950218
H	0.890443	-0.514098	0.950218
H	-0.890443	-0.514098	0.950218
F	-0.000000	0.000000	2.689760
N	0.000000	-0.000000	-1.844545
C	0.000000	-0.000000	-2.991088
H	0.000000	-0.000000	-4.058621

1_{Si} α=90°:

H	-0.000000	1.466232	0.572924
H	-1.269794	-0.733116	0.572924
H	1.269794	-0.733116	0.572924
F	0.000000	0.000000	-1.082190
Si	0.000000	0.000000	0.572924

1_{Si} α=100°:

H	0.000000	1.440434	0.784320
H	-1.247452	-0.720217	0.784320
H	1.247452	-0.720217	0.784320
F	0.000000	0.000000	-1.086402
Si	0.000000	0.000000	0.530333

1_{Si} α=109°:

H	0.000000	1.383161	0.973890
H	-1.197852	-0.691580	0.973890
H	1.197852	-0.691580	0.973890
F	0.000000	0.000000	-1.098721
Si	0.000000	0.000000	0.497630

1_{Si} fully optimized:

Si	0.000000	0.000000	0.500026
H	-0.000000	1.388888	0.959059
H	-1.202813	-0.694444	0.959059
H	1.202813	-0.694444	0.959059
F	0.000000	0.000000	-1.097505

1_{Si} ⋯ NCH α=90°:

Si	-0.000000	0.000000	0.607414
H	-0.000000	1.465849	0.607404
H	1.269463	-0.732925	0.607404
H	-1.269463	-0.732925	0.607404
F	-0.000000	0.000000	2.277133
N	0.000000	-0.000000	-1.554218
C	0.000000	-0.000000	-2.696003
H	0.000000	-0.000000	-3.764671

1_{Si} ⋯ NCH α=100°:

Si	0.000000	-0.000000	0.781847
H	0.000000	1.439174	0.528073
H	1.246361	-0.719587	0.528073
H	-1.246361	-0.719587	0.528073
F	0.000000	-0.000000	2.407192
N	-0.000000	0.000000	-1.794049
C	-0.000000	0.000000	-2.938358
H	-0.000000	0.000000	-4.006316

1_{Si} ⋯ NCH α=109°:

Si	-0.000000	-0.000000	0.932964
H	-0.000000	1.382198	0.457046
H	1.197018	-0.691099	0.457046
H	-1.197018	-0.691099	0.457046
F	-0.000000	-0.000000	2.535132
N	0.000000	0.000000	-2.011491
C	0.000000	0.000000	-3.157257
H	0.000000	0.000000	-4.224836

1_{Si} ⋯ NCH fully optimized:

Si	-0.000000	0.000000	0.892493
H	-0.000000	1.402275	0.481864
H	1.214406	-0.701138	0.481864
H	-1.214406	-0.701138	0.481864
F	-0.000000	0.000000	2.500362
N	0.000000	-0.000000	-1.954139
C	0.000000	-0.000000	-3.099589
H	0.000000	-0.000000	-4.167250

1_{Ge} α=90°:

H	0.000000	1.519678	0.365633
H	-1.316080	-0.759839	0.365633
H	1.316080	-0.759839	0.365633
F	0.000000	0.000000	-1.421905
Ge	0.000000	0.000000	0.365633

1_{Ge} α=100°:

H	-0.000000	1.496210	0.604012
H	-1.295756	-0.748105	0.604012
H	1.295756	-0.748105	0.604012
F	0.000000	0.000000	-1.410901
Ge	0.000000	0.000000	0.340190

1_{Ge} α=109°:

H	0.000000	1.438734	0.815650
H	-1.245980	-0.719367	0.815650
H	1.245980	-0.719367	0.815650
F	0.000000	0.000000	-1.410564
Ge	0.000000	0.000000	0.320254

1_{Ge} fully optimized:

H	0.000000	1.460188	0.749689
H	-1.264560	-0.730094	0.749689
H	1.264560	-0.730094	0.749689
F	0.000000	0.000000	-1.410193
Ge	0.000000	0.000000	0.326333

1_{Ge} ⋯ NCH α=90°:

Ge	0.000000	-0.000000	0.487146
H	0.000000	1.517418	0.487137
H	1.314123	-0.758709	0.487137

H	−1.314123	−0.758709	0.487137
F	0.000000	−0.000000	2.295085
N	−0.000000	0.000000	−2.045136
C	−0.000000	0.000000	−3.188781
H	−0.000000	0.000000	−4.257209

1_{Ge} ⋯ NCH α=100°:

Ge	−0.000000	−0.000000	0.573495
H	0.000000	1.494285	0.310004
H	1.294088	−0.747142	0.310004
H	−1.294088	−0.747142	0.310004
F	−0.000000	−0.000000	2.336852
N	0.000000	0.000000	−2.230746
C	0.000000	0.000000	−3.375766
H	0.000000	0.000000	−4.443694

1_{Ge} ⋯ NCH α=109°:

Ge	−0.000000	0.000000	0.646989
H	0.000000	1.437976	0.151840
H	1.245324	−0.718988	0.151840
H	−1.245324	−0.718988	0.151840
F	−0.000000	0.000000	2.385213
N	0.000000	−0.000000	−2.395541
C	0.000000	−0.000000	−3.541378
H	0.000000	−0.000000	−4.609024

1_{Ge} ⋯ NCH fully optimized:

Ge	0.000000	−0.000000	0.612460
H	0.000000	1.469487	0.229190
H	1.272613	−0.734744	0.229190
H	−1.272613	−0.734744	0.229190
F	0.000000	−0.000000	2.361845
N	−0.000000	0.000000	−2.318334
C	−0.000000	0.000000	−3.463826
H	−0.000000	0.000000	−4.531601

1_{Sn} α=90°:

H	−0.000000	1.686842	0.284764
H	−1.460848	−0.843421	0.284764
H	1.460848	−0.843421	0.284764
F	0.000000	0.000000	−1.676946
Sn	0.000000	0.000000	0.284764

1_{Sn} α=100°:

H	0.000000	1.662037	0.559796
H	−1.439366	−0.831018	0.559796
H	1.439366	−0.831018	0.559796
F	0.000000	0.000000	−1.668453
Sn	0.000000	0.000000	0.266734

1_{Sn} α=109°:

H	−0.000000	1.600642	0.803116
H	−1.386196	−0.800321	0.803116
H	1.386196	−0.800321	0.803116
F	0.000000	0.000000	−1.667539
Sn	0.000000	0.000000	0.251970

1_{Sn} fully optimized:

H	−0.000000	1.636704	0.679241
H	−1.417427	−0.818352	0.679241
H	1.417427	−0.818352	0.679241
F	0.000000	0.000000	−1.667476
Sn	0.000000	0.000000	0.259391

1_{Sn} ⋯ NCH α=90°:

Sn	−0.000000	0.000000	0.382533
H	0.000000	1.686241	0.382524
H	1.460328	−0.843121	0.382524
H	−1.460328	−0.843121	0.382524
F	−0.000000	0.000000	2.364746
N	0.000000	0.000000	−2.320115
C	0.000000	0.000000	−3.463937
H	0.000000	0.000000	−4.532509

1_{Sn} ⋯ NCH α=100°:

Sn	0.000000	0.000000	0.431890
H	−0.000000	1.661370	0.138941
H	1.438789	−0.830685	0.138941
H	−1.438789	−0.830685	0.138941
F	0.000000	0.000000	2.382010
N	−0.000000	−0.000000	−2.454840
C	−0.000000	−0.000000	−3.599632
H	−0.000000	−0.000000	−4.667715

1_{Sn} ⋯ NCH α=109°:

Sn	−0.000000	−0.000000	0.481190
H	0.000000	1.599771	−0.069659
H	1.385442	−0.799886	−0.069659
H	−1.385442	−0.799886	−0.069659
F	−0.000000	−0.000000	2.411590
N	0.000000	0.000000	−2.604857
C	0.000000	0.000000	−3.750442
H	0.000000	0.000000	−4.818200

1_{Sn} ⋯ NCH fully optimized:

Sn	−0.000000	−0.000000	0.443836
H	0.000000	1.649484	0.086319
H	1.428495	−0.824742	0.086319
H	−1.428495	−0.824742	0.086319
F	−0.000000	−0.000000	2.388409
N	0.000000	0.000000	−2.490243
C	0.000000	0.000000	−3.635250
H	0.000000	0.000000	−4.703241

2_{C1} :

C	0.000000	0.000000	0.619422
C	0.000000	0.000000	−0.861707
C	−1.318537	0.761025	−0.656471
H	−1.318698	1.795903	−0.999146
H	−2.214727	0.243369	−0.998929
C	0.000201	−1.522399	−0.656471
C	1.318335	0.761374	−0.656471
H	0.896600	−2.039694	−0.998929
H	−0.895948	−2.039977	−0.999146
H	1.318127	1.796325	−0.998929
H	2.214646	0.244075	−0.999146
O	−1.196400	0.690742	0.802684
O	−0.000000	−1.381483	0.802684
O	1.196400	0.690742	0.802684

2_{C2} :

C	0.000000	0.000000	0.730197
C	0.000000	0.000000	−0.830641
C	1.477389	1.582397	0.129294
C	−2.109090	0.488258	0.129294
C	0.631701	−2.070654	0.129294
C	−1.314549	0.707676	−1.154892
H	−2.913834	1.202018	0.292148
H	−2.519097	−0.528600	0.168937
H	−1.143376	1.778688	−1.296150
H	−1.806131	0.311760	−2.044461
C	0.044409	−1.492271	−1.154892
C	1.270140	0.784595	−1.154892
H	1.717329	−1.917303	0.168937
H	0.415939	−3.124463	0.292148
H	0.633073	−1.720036	−2.044461
H	−0.968701	−1.879536	−1.296150
H	2.497895	1.922445	0.292148
H	0.801768	2.445902	0.168937
H	1.173058	1.408275	−2.044461
H	2.112077	0.100849	−1.296150
O	1.142373	0.659549	1.154251
O	−1.142373	0.659549	1.154251
O	0.000000	−1.319098	1.154251

2_{C3} :

C	0.000000	0.000000	0.720326
C	0.000000	0.000000	−0.822103
C	2.361066	−0.070681	0.849087
C	−1.119321	2.080084	0.849087
C	−1.241745	−2.009403	0.849087
C	−1.140513	0.896301	−1.322019
H	−1.011043	3.027776	1.375103
H	−2.037397	1.593395	1.193683
C	−0.205963	−1.435864	−1.322019
C	1.346476	0.539563	−1.322019
H	−0.361222	−2.561135	1.193683
H	−2.116610	−2.389477	1.375103
H	3.127652	−0.638299	1.375103
H	2.398619	0.967740	1.193683

C	2.537321	-0.137662	-0.655001
C	-1.387879	-2.128554	-0.655001
C	-1.149442	2.266215	-0.655001
H	-2.335307	-1.681053	-0.964525
H	-1.421845	-3.182765	-0.939718
H	2.623488	-1.181909	-0.964525
H	3.467278	0.360028	-0.939718
H	-2.045432	2.822736	-0.939718
H	-0.288181	2.862962	-0.964525
H	0.693839	-2.020445	-1.111294
H	-0.325428	-1.406615	-2.410831
H	1.380879	0.421479	-2.410831
H	1.402837	1.611105	-1.111294
H	-2.096676	0.409340	-1.111294
H	-1.055451	0.985137	-2.410831
O	0.000000	1.294336	1.228592
O	-1.120928	-0.647168	1.228592
O	1.120928	-0.647168	1.228592

2_{C1} ⋯ NCH :

C	0.000000	0.000000	-0.172349
C	0.000000	0.000000	-1.658067
C	-1.415952	-0.555519	-1.456447
H	-2.224031	0.090197	-1.802663
H	-1.570138	-1.577926	-1.803839
C	1.189069	-0.948491	-1.456447
C	0.226882	1.504010	-1.456447
H	2.151593	-0.570816	-1.803839
H	1.033903	-1.971166	-1.802663
H	-0.581455	2.148743	-1.803839
H	1.190129	1.880969	-1.802663
N	0.000000	0.000000	2.781072
C	0.000000	0.000000	3.927526
H	0.000000	0.000000	4.994341
O	-1.288921	-0.506723	-0.000373
O	1.083295	-0.862877	-0.000373
O	0.205626	1.369600	-0.000373

2_{Si1} :

Si	0.000000	0.000000	0.767793
C	0.000000	0.000000	-1.116337
C	0.000061	1.476967	-0.815534
H	0.898427	1.989664	-1.150611
H	-0.898214	1.989755	-1.150725
C	-1.279122	-0.738431	-0.815534
C	1.279061	-0.738536	-0.815534
H	-1.274071	-1.772753	-1.150725
H	-2.172313	-0.216771	-1.150611
H	2.172285	-0.217001	-1.150725
H	1.273886	-1.772893	-1.150611
O	0.000000	1.609000	0.730523
O	-1.393435	-0.804500	0.730523
O	1.393435	-0.804500	0.730523

2_{Si2} :

Si	0.000000	0.000000	0.856306
C	0.000000	0.000000	-0.974109
C	0.000000	2.303015	-0.046204
C	-1.994469	-1.151507	-0.046204
C	1.994469	-1.151507	-0.046204
C	-1.470025	-0.344776	-1.251546
H	-3.082753	-1.169763	-0.000237
H	-1.636467	-2.186223	-0.097962
H	-2.045988	0.584679	-1.319537
H	-1.628861	-0.898551	-2.182162
C	1.033597	-1.100691	-1.251546
C	0.436428	1.445467	-1.251546
H	2.711558	-0.324110	-0.097962
H	2.554421	-2.084861	-0.000237
H	1.592599	-0.961360	-2.182162
H	0.516647	-2.064217	-1.319537
H	0.528332	3.254624	-0.000237
H	-1.075091	2.510333	-0.097962
H	0.036262	1.859911	-2.182162
H	1.529341	1.479538	-1.319537
O	0.275997	1.580770	1.167315
O	-1.506985	-0.551364	1.167315
O	1.230988	-1.029406	1.167315

2_{Si3} :

Si	0.000000	0.000000	0.878365
C	0.000000	0.000000	-0.975652
C	0.000000	2.615475	0.709908
C	-2.265067	-1.307737	0.709908
C	2.265067	-1.307737	0.709908
C	-1.028949	-1.026834	-1.485337
H	-3.250529	-1.347590	1.175691
H	-1.790173	-2.288474	0.845396
C	1.403738	-0.377679	-1.485337
C	-0.374790	1.404512	-1.485337
H	2.876963	-0.406098	0.845396
H	2.792312	-2.141245	1.175691
H	0.458217	3.488836	1.175691
H	-1.086790	2.694572	0.845396
C	0.334281	2.556753	-0.772495
C	2.047073	-1.567872	-0.772495
C	-2.381354	-0.988881	-0.772495
H	1.429947	-2.465533	-0.877210
H	3.012990	-1.792775	-1.232759
H	1.420241	2.471137	-0.877210
H	0.046094	3.505713	-1.232759
H	-3.059083	-1.712938	-1.232759
H	-2.850188	-0.005604	-0.877210
H	2.074087	0.482240	-1.370132
H	1.335830	-0.574067	-2.564756
H	-0.170759	1.443896	-2.564756
H	-1.454676	1.555092	-1.370132
H	-0.619411	-2.037333	-1.370132
H	-1.165071	-0.869829	-2.564756
O	-1.510726	-0.315984	1.395447
O	1.029013	-1.150335	1.395447
O	0.481713	1.466319	1.395447

2_{Si1} ⋯ NCH :

Si	0.000000	0.000000	0.272760
C	0.000000	0.000000	-1.681111
C	-1.375466	-0.539666	-1.405430
H	-2.173122	0.107698	-1.771496
H	-1.519939	-1.556877	-1.771135
C	1.155098	-0.921356	-1.405430
C	0.220368	1.461022	-1.405430
H	2.108265	-0.537868	-1.771135
H	0.993292	-1.935828	-1.771496
H	-0.588325	2.094745	-1.771135
H	1.179831	1.828130	-1.771496
N	0.000000	0.000000	2.204119
C	0.000000	0.000000	3.341147
H	0.000000	0.000000	4.410676
O	-1.513413	-0.593449	0.096136
O	1.270649	-1.013930	0.096136
O	0.242764	1.607379	0.096136

2_{Si2} ⋯ NCH :

Si	0.000000	0.000000	0.484693
C	0.000000	0.000000	-1.394714
C	0.457164	2.278782	-0.596403
C	-2.202065	-0.743476	-0.596403
C	1.744901	-1.535306	-0.596403
C	-1.490559	0.015518	-1.724558
H	-3.266697	-0.508139	-0.548318
H	-2.106226	-1.825482	-0.749405
H	-1.847951	1.051934	-1.725092
H	-1.738397	-0.415363	-2.701453
C	0.731840	-1.298621	-1.724558
C	0.758718	1.283102	-1.724558
H	2.634027	-0.911304	-0.749405
H	2.073410	-2.574974	-0.548318
H	1.228913	-1.297814	-2.701453
H	0.012974	-2.126339	-1.725092
H	1.193288	3.083112	-0.548318
H	-0.527801	2.736786	-0.749405
H	0.509484	1.713177	-2.701453
H	1.834977	1.074405	-1.725092
N	0.000000	0.000000	2.568779
C	0.000000	0.000000	3.707518
H	0.000000	0.000000	4.775091

O	−1.603528	−0.397832	0.647127
O	0.457231	1.587612	0.647127
O	1.146297	−1.189780	0.647127

2_{Si3} ⋯ NCH :

Si	0.000000	0.000000	0.344652
C	0.000000	0.000000	−1.514954
C	2.612037	0.112482	0.159181
C	−1.403431	2.205850	0.159181
C	−1.208607	−2.318331	0.159181
C	−1.077748	0.972740	−2.028511
H	−1.488436	3.191009	0.620385
H	−2.359291	1.684868	0.304734
C	−0.303543	−1.419727	−2.028511
C	1.381292	0.446987	−2.028511
H	−0.279493	−2.885640	0.304734
H	−2.019277	−2.884528	0.620385
H	3.507713	−0.306481	0.620385
H	2.638784	1.200772	0.304734
C	2.570578	−0.208901	−1.326579
C	−1.466203	−2.121736	−1.326579
C	−1.104375	2.330637	−1.326579
H	−2.393778	−1.552891	−1.443001
H	−1.635243	−3.100187	−1.784780
H	2.541732	−1.296627	−1.443001
H	3.502462	0.133932	−1.784780
H	−1.867219	2.966255	−1.784780
H	−0.147954	2.849518	−1.443001
H	0.587005	−2.047289	−1.904838
H	−0.492920	−1.361409	−3.110170
H	1.425475	0.253823	−3.110170
H	1.479502	1.532006	−1.904838
H	−2.066507	0.515283	−1.904838
H	−0.932555	1.107586	−3.110170
N	0.000000	0.000000	3.893924
C	0.000000	0.000000	5.040992
H	0.000000	0.000000	6.107870
O	−1.118107	−1.074880	0.838861
O	1.489927	−0.430870	0.838861
O	−0.371819	1.505749	0.838861

2_{Ge1} :

Ge	0.000000	0.000000	0.704037
C	0.000000	0.000000	−1.269894
C	0.000000	1.489802	−1.025291
H	0.896349	1.984103	−1.396516
H	−0.896554	1.983901	−1.396287
C	−1.290207	−0.744901	−1.025291
C	1.290207	−0.744901	−1.025291
H	−1.269831	−1.768389	−1.396287
H	−2.166458	−0.215791	−1.396516
H	2.166385	−0.215512	−1.396287
H	1.270109	−1.768312	−1.396516
O	0.000134	1.738274	0.496826
O	−1.505457	−0.869021	0.496826
O	1.505323	−0.869253	0.496826

2_{Ge2} :

Ge	0.000000	0.000000	0.760937
C	0.000000	0.000000	−1.138248
C	0.000000	2.337331	−0.226642
C	−2.024188	−1.168665	−0.226642
C	2.024188	−1.168665	−0.226642
C	−1.474139	−0.333745	−1.404295
H	−3.113164	−1.214005	−0.244661
H	−1.640224	−2.194596	−0.289195
H	−2.043709	0.600744	−1.455980
H	−1.636134	−0.868651	−2.345613
C	1.026101	−1.109769	−1.404295
C	0.448038	1.443514	−1.404295
H	2.720688	−0.323178	−0.289195
H	2.607942	−2.089077	−0.244661
H	1.570341	−0.982608	−2.345613
H	0.501595	−2.070276	−1.455980
H	0.505223	3.303082	−0.244661
H	−1.080464	2.517774	−0.289195
H	0.065793	1.851259	−2.345613
H	1.542115	1.469532	−1.455980
O	0.300006	1.716326	1.035113
O	−1.636385	−0.598350	1.035113
O	1.336379	−1.117976	1.035113

2_{Ge3} :

Ge	0.000000	0.000000	0.778694
C	0.000000	0.000000	−1.154823
C	0.000000	2.672026	0.560909
C	−2.314042	−1.336013	0.560909
C	2.314042	−1.336013	0.560909
C	−1.079389	−0.978149	−1.645316
H	−3.312350	−1.431633	0.991746
H	−1.832687	−2.322834	0.621843
C	1.386797	−0.445704	−1.645316
C	−0.307408	1.423853	−1.645316
H	2.927977	−0.425736	0.621843
H	2.896006	−2.152763	0.991746
H	0.416344	3.584396	0.991746
H	−1.095290	2.748570	0.621843
C	0.421146	2.543121	−0.898406
C	1.991834	−1.636284	−0.898406
C	−2.412980	−0.906837	−0.898406
H	1.318736	−2.499639	−0.928506
H	2.915466	−1.939918	−1.398548
H	1.505383	2.391878	−0.928506
H	0.222285	3.494826	−1.398548
H	−3.137751	−1.554908	−1.398548
H	−2.824119	0.107761	−0.928506
H	2.087228	0.393692	−1.562981
H	1.303709	−0.673085	−2.717436
H	−0.068946	1.465587	−2.717436
H	−1.384561	1.610747	−1.562981
H	−0.702667	−2.004439	−1.562981
H	−1.234763	−0.792503	−2.717436
O	−1.607055	−0.398860	1.361793
O	1.148951	−1.192320	1.361793
O	0.458104	1.591181	1.361793

2_{Ge1} ⋯ NCH :

Ge	0.000000	0.000000	0.277302
C	0.000000	0.000000	−1.766070
C	−0.542027	1.381508	−1.530223
H	0.109794	2.165557	−1.918845
H	−1.552925	1.513357	−1.919239
C	−0.925408	−1.160164	−1.530223
C	1.467435	−0.221345	−1.530223
H	−0.534143	−2.101551	−1.919239
H	−1.930324	−0.987694	−1.918845
H	2.087068	0.588194	−1.919239
H	1.820530	−1.177862	−1.918845
N	0.000000	0.000000	2.324030
C	0.000000	0.000000	3.461996
H	0.000000	0.000000	4.532222
O	−0.632945	1.612327	−0.032973
O	−1.079843	−1.354310	−0.032973
O	1.712788	−0.258017	−0.032973

2_{Ge2} ⋯ NCH :

Ge	0.000000	0.000000	0.412201
C	0.000000	0.000000	−1.522362
C	0.475137	2.305683	−0.696467
C	−2.234348	−0.741361	−0.696467
C	1.759211	−1.564322	−0.696467
C	−1.497741	0.006808	−1.824018
H	−3.306177	−0.536316	−0.724375
H	−2.098740	−1.823680	−0.824139
H	−1.852678	1.043890	−1.835880
H	−1.749891	−0.435376	−2.794653
C	0.742975	−1.300486	−1.824018
C	0.754767	1.293678	−1.824018
H	2.628724	−0.905722	−0.824139
H	2.117552	−2.595076	−0.724375
H	1.251992	−1.297762	−2.794653
H	0.022304	−2.126411	−1.835880
H	1.188625	3.131392	−0.724375
H	−0.529983	2.729403	−0.824139
H	0.497898	1.733138	−2.794653
H	1.830374	1.082521	−1.835880
N	0.000000	0.000000	2.632344

C	0.000000	0.000000	3.772148
H	0.000000	0.000000	4.840009
O	-1.740243	-0.353226	0.581263
O	0.564219	1.683708	0.581263
O	1.176024	-1.330482	0.581263

2_{Ge3} ⋯ NCH :

Ge	0.000000	0.000000	0.366261
C	0.000000	0.000000	-1.577266
C	2.670599	0.160338	0.108966
C	-1.474156	2.232637	0.108966
C	-1.196443	-2.392975	0.108966
C	-1.055343	0.997900	-2.078303
H	-1.633802	3.226916	0.531447
H	-2.425342	1.685707	0.187599
C	-0.336535	-1.412903	-2.078303
C	1.391878	0.415004	-2.078303
H	-0.247194	-2.943262	0.187599
H	-1.977690	-3.028372	0.531447
H	3.611492	-0.198544	0.531447
H	2.672536	1.257554	0.187599
C	2.569143	-0.241720	-1.356841
C	-1.493907	-2.104083	-1.356841
C	-1.075236	2.345803	-1.356841
H	-2.405734	-1.500170	-1.408663
H	-1.713932	-3.051247	-1.857447
H	2.502052	-1.333342	-1.408663
H	3.499423	0.041315	-1.857447
H	-1.785492	3.009932	-1.857447
H	-0.096318	2.833511	-1.408663
H	0.548152	-2.053036	-1.980078
H	-0.547652	-1.342914	-3.155305
H	1.436824	0.197177	-3.155305
H	1.503906	1.501231	-1.980078
H	-2.052057	0.551805	-1.980078
H	-0.889172	1.145737	-3.155305
N	0.000000	0.000000	3.564573
C	0.000000	0.000000	4.711109
H	0.000000	0.000000	5.777885
O	-1.147113	-1.218437	0.902718
O	1.628754	-0.384211	0.902718
O	-0.481640	1.602648	0.902718

2_{Sn2} :

Sn	0.000000	0.000000	0.771849
C	0.000000	0.000000	-1.304658
C	0.000000	2.398235	-0.441957
C	-2.076933	-1.199118	-0.441957
C	2.076933	-1.199118	-0.441957
C	-1.475268	-0.320110	-1.567437
H	-3.158382	-1.277894	-0.567570
H	-1.656206	-2.211378	-0.512897
H	-2.038486	0.619859	-1.595392
H	-1.639937	-0.823792	-2.527337
C	1.014857	-1.117565	-1.567437
C	0.460411	1.437675	-1.567437
H	2.743212	-0.328628	-0.512897
H	2.685879	-2.096292	-0.567570
H	1.533393	-1.008331	-2.527337
H	0.482429	-2.075311	-1.595392
H	0.472503	3.374186	-0.567570
H	-1.087006	2.540005	-0.512897
H	0.106543	1.832123	-2.527337
H	1.556057	1.455451	-1.595392
O	0.334309	1.940524	0.875592
O	-1.847698	-0.680742	0.875592
O	1.513388	-1.259782	0.875592

2_{Sn3} :

Sn	0.000000	0.000000	0.762114
C	0.000000	0.000000	-1.355621
C	2.596330	1.095304	0.366899
C	-2.246726	1.700835	0.366899
C	-0.349604	-2.796140	0.366899
C	-1.266639	0.731294	-1.818385
H	-2.731850	2.610371	0.730805
H	-3.032263	0.937658	0.257859
C	0.000000	-1.462589	-1.818385
C	1.266639	0.731294	-1.818385
H	0.704096	-3.094846	0.257859
H	-0.894722	-3.671037	0.730805
H	3.626572	1.060666	0.730805
H	2.328167	2.157188	0.257859
C	2.533518	0.427530	-1.009895
C	-0.896507	-2.407856	-1.009895
C	-1.637011	1.980325	-1.009895
H	-1.893454	-1.969996	-0.871558
H	-1.041409	-3.330101	-1.578964
H	2.652794	-0.654781	-0.871558
H	3.404657	0.763164	-1.578964
H	-2.363248	2.566937	-1.578964
H	-0.759340	2.624777	-0.871558
H	1.023595	-1.854958	-1.786766
H	-0.297283	-1.473708	-2.877155
H	1.424910	0.479399	-2.877155
H	1.094643	1.813938	-1.786766
H	-2.118238	0.041020	-1.786766
H	-1.127627	0.994309	-2.877155
O	-1.316466	1.309550	1.362925
O	-0.475871	-1.794868	1.362925
O	1.792336	0.485318	1.362925

2_{Sn2} ⋯ NCH :

Sn	0.000000	0.000000	0.437276
C	0.000000	0.000000	-1.666336
C	0.493288	2.363951	-0.850721
C	-2.293885	-0.754776	-0.850721
C	1.800597	-1.609175	-0.850721
C	-1.501797	0.005970	-1.944738
H	-3.363415	-0.579547	-0.991131
H	-2.118379	-1.833559	-0.972966
H	-1.852032	1.045185	-1.949241
H	-1.756200	-0.424313	-2.921809
C	0.745728	-1.303579	-1.944738
C	0.756068	1.297609	-1.944738
H	2.647098	-0.917790	-0.972966
H	2.183610	-2.623030	-0.991131
H	1.245566	-1.308757	-2.921809
H	0.020859	-2.126500	-1.949241
H	1.179806	3.202577	-0.991131
H	-0.528719	2.751349	-0.972966
H	0.510634	1.733070	-2.921809
H	1.831173	1.081314	-1.949241
N	0.000000	0.000000	2.755279
C	0.000000	0.000000	3.894930
H	0.000000	0.000000	4.963941
O	-1.953351	-0.363762	0.472394
O	0.661648	1.873532	0.472394
O	1.291702	-1.509770	0.472394

2_{Sn3} ⋯ NCH :

Sn	0.000000	0.000000	0.494414
C	0.000000	0.000000	-1.652695
C	2.867790	0.361658	-0.037083
C	-1.747100	2.302750	-0.037083
C	-1.120690	-2.664408	-0.037083
C	-1.002016	1.050476	-2.141822
H	-1.865458	3.320294	0.350742
H	-2.758448	1.915919	-0.235399
C	-0.408731	-1.393009	-2.141822
C	1.410747	0.342533	-2.141822
H	-0.280010	-3.346845	-0.235399
H	-1.942730	-3.275681	0.350742
H	3.808188	-0.044613	0.350742
H	3.038458	1.430927	-0.235399
C	2.544719	-0.324788	-1.361685
C	-1.553634	-2.041397	-1.361685
C	-0.991085	2.366185	-1.361685
H	-2.345844	-1.307707	-1.161795
H	-2.007806	-2.831364	-1.966424
H	2.305430	-1.377707	-1.161795
H	3.455936	-0.323129	-1.966424
H	-1.448130	3.154493	-1.966424
H	0.040414	2.685414	-1.161795
H	0.455136	-2.067871	-2.102547
H	-0.672599	-1.300339	-3.206422
H	1.462426	0.067682	-3.206422

H	1.563260	1.428095	-2.102547
H	-2.018396	0.639776	-2.102547
H	-0.789827	1.232657	-3.206422
N	0.000000	0.000000	2.964748
C	0.000000	0.000000	4.105992
H	0.000000	0.000000	5.173103
O	-0.766723	-1.747247	0.972056
O	1.896522	0.209622	0.972056
O	-1.129799	1.537625	0.972056