Geometric and Electronic Structures as well as Thermodynamic Stability of Hexyl-Modified Silicon Nanosheet

Feng Li,[†] Ruifeng Lu,[,†,‡] Qiushi Yao,[†] Erjun Kan,[†,‡] Yuzhen Liu,[†] Haiping Wu,[†] Yongbo Yuan,[†] Chuanyun Xiao,[†,‡] and Kaiming Deng[*,†,‡]*

[†]Department of Applied Physics, Nanjing University of Science and Technology, Nanjing 210094, China.

[‡]Key Laboratory of Soft Chemistry and Functional Materials, Ministry of Education, Nanjing University of Science and Technology, Nanjing 210094, China.

E-mail address: rflu@njust.edu.cn; kmdeng@njust.edu.cn

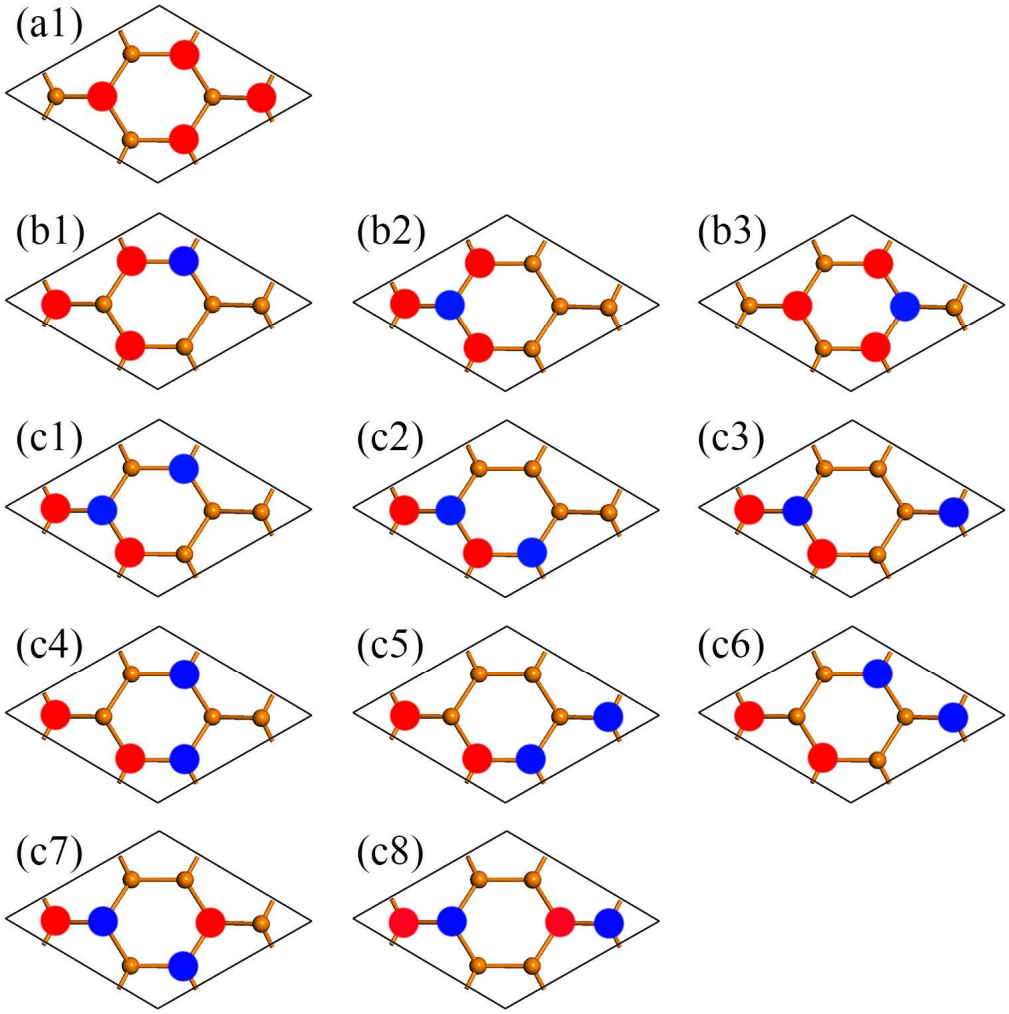

Figure S1. All twelve possible configurations of geometric structures of $Si_8H_4(C_6H_{13})_4$. The circles represent the connecting positions of the alkyl groups on the Si-NS: red circle is on top, blue circle is below. (a1) all the four hexyl groups are on top. (b1-b3) three hexyl groups are on top, and the other one hexyl group is below. (c1-c8) half of hexyl groups are on top, half are below. Looking carefully at the geometric structures, there are several structures are equivalent: b1 and b3; c1, c3, c4 and c5; c8 and c6. Thus, there are totally six different geometric structures.

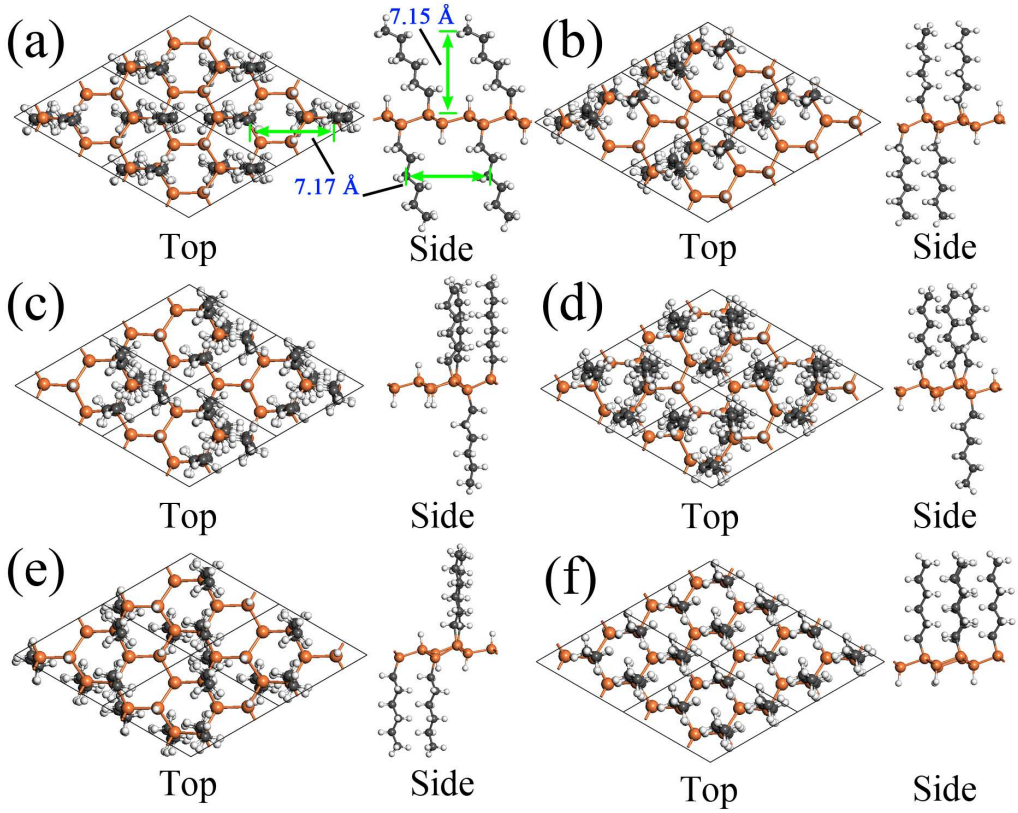

Figure S2. Six types of geometric structures of $Si_8H_4(C_6H_{13})_4$. Left is top view, right is side view. (a) The ground state of $Si_8H_4(C_6H_{13})_4$, in which the hexyls groups most uniformly distribute on both sides of the sheets. (b) The attaching hexyl groups stand in zigzag line on the sheet. (c)-(d) The numbers of the attaching hexyl groups on the two sides of the sheet are not equal. (e) Four hexyl groups gather on the same side of the silicon six-membered ring. (f) The highest-energy structure, in which all hexyl-groups are concentrated on one side of Si-NSs.

Table S1. Bond lengths (Å) and angles (°) for the most stable structure of $Si_8H_4(C_6H_{13})_4$.

	Si-Si	Si-H	Si-C	C-H	C-C
length	2.39	1.51	1.91	1.11	1.54
	Si-Si-Si	Si-Si-C	Si-Si-H	C-C-C	C-C-H
angle	108.5	107.4	105.3	114.6	109.3

Table S2. Relative energy (E_r) of the $Si_8H_4(C_6H_{13})_4$ and $Si_8H_4(CH_3)_4$ isomers.

Isomers of $Si_8H_4(C_6H_{13})_4$	E_r /eV	Isomers of $Si_8H_4(CH_3)_4$	E_r /eV
$Si_8H_4(C_6H_{13})_4$-a	0	$Si_8H_4(CH_3)_4$-a	0
$Si_8H_4(C_6H_{13})_4$-b	0.76	$Si_8H_4(CH_3)_4$-b	0.07
$Si_8H_4(C_6H_{13})_4$-c	0.87	$Si_8H_4(CH_3)_4$-c	0.13
$Si_8H_4(C_6H_{13})_4$-d	0.94	$Si_8H_4(CH_3)_4$-d	0.09
$Si_8H_4(C_6H_{13})_4$-e	2.23	$Si_8H_4(CH_3)_4$-e	0.12
$Si_8H_4(C_6H_{13})_4$-f	2.66	$Si_8H_4(CH_3)_4$-f	0.32

Optimized cartesian coordinates (in Å) of $Si_8H_4(C_6H_{13})_4$-a

a = 7.8745 Å b = 7.8745 Å c = 35 Å

α = 90° β = 90° γ = 120°

C	0.065863033	4.438569135	2.903733771
C	-1.150804359	4.758258455	3.783192574
C	-0.820631982	4.648386349	5.279861373
C	-1.978299651	5.060760346	6.196073496
C	-1.66172952	4.873195209	7.685478563
C	-2.775790823	5.35787572	8.629034241
C	6.048687	1.053651698	2.875818982
C	4.976878775	1.174796979	3.975207892
C	5.601934394	0.831565751	5.342566731
C	4.732218349	1.185239356	6.560550981
C	5.373808013	0.796096872	7.904242338
C	4.534050272	1.231384346	9.122037632
C	-0.267770237	5.157455639	-7.745658931
C	-1.261901069	5.607016922	-6.666024601
C	-0.715865163	5.341876729	-5.253459775
C	-1.739067007	5.616073372	-4.126583872
C	-1.228892805	5.370083964	-2.6878512
C	-2.392598125	5.573180051	-1.680615573
C	6.27376757	1.467600641	-7.455463892
C	5.198646115	1.89267022	-6.445409803
C	5.616590699	1.728046037	-4.983425134
C	4.455545462	2.093918214	-4.043167947
C	4.745188007	1.958696911	-2.540887256
C	3.50168251	2.236741283	-1.670062177
H	-0.177042263	2.243122572	-1.244991114
H	1.707768623	1.112168717	2.48897929
H	1.789966483	5.605625461	-1.240744685

H	3.67998941	4.500862481	2.503888717
H	0.465294151	3.443675911	3.158324563
H	0.877540932	5.145527363	3.143092446
H	-1.993155775	4.087997991	3.543406136
H	-1.512954829	5.773352685	3.551117562
H	0.062781606	5.267330353	5.505782354
H	-0.523509035	3.610661544	5.508099918
H	-2.87963476	4.485236399	5.925485649
H	-2.221107746	6.118781632	6.006261304
H	-0.725207064	5.407504635	7.912365708
H	-1.449842572	3.80910928	7.874822968
H	-2.96529243	6.429693086	8.478499506
H	-2.500883625	5.193409803	9.679443925
H	-3.717416369	4.824400305	8.433206725
H	6.595640674	0.103538319	3.01195616
H	6.803189874	1.83657593	3.048992981
H	4.122647629	0.509194951	3.777187792
H	4.578836558	2.202745795	3.994208277
H	6.573809107	1.348696008	5.410897626
H	5.83141061	-0.248042599	5.352216701
H	3.749876581	0.694848312	6.451881195
H	4.531609085	2.268045705	6.564117678
H	6.382342607	1.239975597	7.942864025
H	5.513271211	-0.296903329	7.927984881
H	4.45105931	2.324313456	9.17376116
H	4.973782954	0.883265004	10.05881166
H	3.516406101	0.82517079	9.037657913
H	-0.031996704	4.091061697	-7.650461001
H	0.675572101	5.714591652	-7.683297966
H	-0.696165515	5.31982621	-8.7399851
H	-2.209517212	5.060671091	-6.80508616
H	-1.498560431	6.673478666	-6.808727055
H	0.196984038	5.941125755	-5.096556283
H	-0.399191424	4.286604249	-5.208956696
H	-2.628470622	4.988770989	-4.300837904
H	-2.079923769	6.662803979	-4.218270762
H	-0.384328496	6.043596407	-2.477485439
H	-0.835461287	4.343281102	-2.614647398
H	-2.89851117	6.518172383	-1.946216187
H	-3.147992905	4.794425435	-1.88288011
H	6.523680367	0.404071572	-7.348560284
H	7.201661862	2.042533087	-7.347603825
H	5.906169646	1.61307788	-8.478226957
H	4.286383203	1.303006937	-6.622427128

H	4.916722316	2.939932517	-6.631507902
H	6.501400122	2.352094467	-4.772732461
H	5.917729726	0.68263217	-4.808215615
H	3.590689988	1.457270087	-4.299491315
H	4.143107194	3.129466988	-4.259019627
H	5.565020636	2.639356855	-2.270654738
H	5.109526928	0.941255773	-2.332214136
H	3.059296799	3.203860114	-1.965041174
H	2.728193748	1.48742181	-1.913681728
Si	-0.249958005	2.251667666	0.256135973
Si	1.720377553	1.124342893	0.988047199
Si	3.678432233	2.258659947	0.244566606
Si	5.661331903	1.119294031	1.004364086
Si	-2.196801694	5.633880157	0.239631288
Si	-0.218457355	4.503831668	1.016978023
Si	1.731638272	5.637669433	0.260433629
Si	3.702058636	4.516459596	1.002676012

Optimized cartesian coordinates (in Å) of $Si_8H_4(C_6H_{13})_4$-b

a = 7.8745 Å b = 7.8745 Å c = 35 Å

α = 90° β = 90° γ = 120°

C	-2.401716185	5.565486378	-1.954549248
C	1.586726136	5.542023196	-2.154681665
C	-0.017269396	5.156656193	2.613672018
C	-1.485152364	5.795586603	-3.190100924
C	-2.270267059	5.938070723	-4.518095709
C	-1.429009972	5.816938229	-5.807773602
C	-2.244623519	5.958035556	-7.106985706
C	-1.431392222	5.810715626	-8.404651886
C	2.480500447	5.546661568	-3.426496612
C	1.673282249	5.682483035	-4.74549316
C	2.509357889	5.559667963	-6.041263124
C	1.707335832	5.709814313	-7.350593303
C	2.542514932	5.561380644	-8.640227015
C	3.50941733	4.542089672	2.690435489
C	4.470390108	4.355456978	3.90957479
C	3.709579254	4.220890176	5.258320985
C	4.571105928	4.336518004	6.543466208
C	3.771698021	4.216001245	7.858834683
C	4.631077798	4.369645449	9.133182875
C	0.228288167	4.370906047	3.927658726
C	0.174648643	5.3395453	5.135364052

C	0.30605448	4.686277931	6.532655264
C	0.262792219	5.704818323	7.695089219
C	0.399869919	5.085930205	9.11203488
H	0.037556284	2.399355696	-1.43685146
H	2.009281002	1.091906745	2.194089282
H	3.934964419	2.304051368	-1.46969169
H	5.96910314	0.965911633	2.095346846
H	-3.230233269	6.291260669	-2.000831933
H	-2.889827999	4.580548779	-2.079365891
H	0.876590698	6.375490716	-2.226988239
H	-1.02848702	5.592767538	2.699667763
H	0.653852498	6.035577649	2.606938779
H	0.957774203	4.641513928	-2.209521198
H	-0.794348185	4.947611166	-3.278705591
H	-0.868172648	6.697199134	-3.064748311
H	-2.782918098	6.917782675	-4.517668264
H	-3.056749659	5.173507062	-4.550701208
H	-0.935631338	4.828510287	-5.819260397
H	-0.627839256	6.568939749	-5.809591346
H	-2.742272504	6.945562611	-7.106821956
H	-3.038934939	5.202125503	-7.11091369
H	-2.058319621	5.903231466	-9.310648859
H	-0.952055578	4.819592221	-8.449188331
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H	3.211437432	6.363234294	-3.393993237
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H	0.880880056	4.923921911	-4.762033322
H	3.014494554	4.576303099	-6.045190083
H	3.299616258	6.322365385	-6.032118808
H	1.228824434	6.70344435	-7.355934878
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H	1.928147445	5.685615134	-9.546372926
H	2.999146716	4.561633119	-8.691305201
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H	2.927573139	5.461749648	2.86711331
H	5.148331387	5.221242389	3.96356002
H	5.098921312	3.466670477	3.752482873
H	3.187446338	3.246634374	5.268995012
H	2.918788995	4.984779021	5.294691866
H	5.102336758	5.304237568	6.536844912
H	5.360722393	3.568303365	6.530609243
H	3.256678156	3.239189766	7.881573042

H	2.980346794	4.977300715	7.866957583
H	5.127636819	5.350409081	9.166012405
H	5.413876142	3.60001805	9.182331912
H	4.027167101	4.284375745	10.04530546
H	1.192459473	3.84534513	3.920295904
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H	0.967321175	6.097208824	5.005939016
H	1.245460747	4.111831594	6.579295461
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H	-0.668779319	6.293985615	7.632775451
H	1.07018974	6.44121871	7.555440654
H	0.404093927	5.858752134	9.897932725
H	1.337668103	4.518617733	9.197275095
H	-0.420762736	4.395269966	9.343768875
Si	0.013625382	2.291472787	0.068941631
Si	1.987600465	1.112205186	0.686376614
Si	3.951124544	2.274310959	0.033301072
Si	5.933997481	1.075799609	0.581585338
Si	-1.953337233	5.628350124	-0.073417124
Si	0.038295712	4.576699296	0.763927385
Si	2.005649095	5.60723223	-0.25868383
Si	3.946035058	4.539943107	0.792764709

Optimized cartesian coordinates (in Å) of $Si_8H_4(C_6H_{13})_4$-c

a = 7.8745 Å b = 7.8745 Å c = 35 Å

α = 90° β = 90° γ = 120°

C	4.599653181	2.297373983	-1.818516217
C	3.784731965	2.185104705	-3.13772085
C	4.696766018	2.404412441	-4.37630937
C	4.005549207	2.155801701	-5.744792495
C	4.853039964	2.568759172	-6.964598647
C	4.22795809	2.160287388	-8.32561875
C	5.713147494	0.380998372	2.931720608
C	5.82159847	1.232966173	4.224107233
C	5.717638757	0.390854541	5.530529302
C	5.822897509	1.214880106	6.834217978
C	5.723106952	0.385664946	8.136362417
C	5.843947793	1.235105212	9.418671007
C	1.477042767	1.406212642	2.701303202
C	2.254315098	1.029473228	3.981540389
C	1.482837981	1.402663088	5.278980299

C	2.23563453	1.079569714	6.585285905
C	1.44272017	1.420713596	7.865673601
C	2.188630309	1.159264255	9.183915065
C	3.769243925	4.071682994	2.76604767
C	4.563623071	4.64507491	3.966160327
C	3.930475743	4.183645978	5.298336511
C	4.634410231	4.662785558	6.581920936
C	3.948515993	4.184051626	7.879356191
C	4.661840218	4.657699562	9.158861045
H	-0.281180972	2.005191704	-1.357177299
H	-2.005775137	5.633879521	-1.312903382
H	2.091211217	5.639246938	-1.431220485
H	5.394997839	1.537395587	-1.86310027
H	5.143016923	3.261422149	-1.822779944
H	2.966256275	2.922325956	-3.160606321
H	3.314296689	1.187863436	-3.199665274
H	5.584595672	1.752537827	-4.301693947
H	5.088368197	3.436098746	-4.347106759
H	3.054678067	2.711072716	-5.782265269
H	3.735182012	1.090924267	-5.821725186
H	5.86178514	2.13411784	-6.884779722
H	5.006020161	3.65651019	-6.940667552
H	4.147891045	1.069829642	-8.406374638
H	4.813995835	2.525241387	-9.182526858
H	3.207420722	2.554886787	-8.420059862
H	6.497285648	-0.389495607	2.963066247
H	4.771010027	-0.195453306	2.956202754
H	5.030642671	1.986589771	4.233430717
H	6.765370627	1.797740958	4.229701358
H	6.50531829	-0.37189577	5.532506512
H	4.769257437	-0.170946084	5.528904667
H	5.030762649	1.96964362	6.837656043
H	6.766064429	1.782678527	6.837132233
H	6.507233041	-0.379233999	8.142762004
H	4.77266925	-0.170202124	8.142905772
H	5.778949016	0.636540457	10.34277035
H	5.049254834	1.985792287	9.460697979
H	6.80001955	1.777988688	9.441045877
H	0.505444546	0.883284232	2.717451735
H	1.220230466	2.475666875	2.746575464
H	3.224486567	1.535517724	3.991162866
H	2.47033598	-0.047568061	3.989053339
H	0.51723683	0.877234837	5.281018941
H	1.244707147	2.479411716	5.261398088

H	3.189310174	1.620008722	6.591642577
H	2.492989693	0.009485914	6.600302131
H	0.509071755	0.842806656	7.862860274
H	1.145385069	2.481231884	7.842255466
H	2.877745321	1.978539406	9.424594534
H	2.765572222	0.224803347	9.15606119
H	1.480830358	1.074671412	10.01934323
H	0.0973308	4.411443196	2.210939453
H	3.870559956	2.976588816	2.790482116
H	2.69942505	4.24412318	2.972786786
H	4.581343729	5.741514228	3.941643268
H	5.615429214	4.320173891	3.923515833
H	3.892367163	3.088493338	5.305064776
H	2.880292546	4.510739142	5.30527456
H	4.677286497	5.759903241	6.58638311
H	5.680462578	4.318694364	6.576823031
H	3.905156036	3.090072271	7.881469145
H	2.901931869	4.517420234	7.874548556
H	4.685295753	5.750825131	9.208448893
H	5.703311121	4.313588564	9.170524312
H	4.186839594	4.284988423	10.07930485
Si	-0.137172643	2.072578313	0.144893069
Si	1.949630601	1.14889446	0.816686461
Si	3.972587795	2.242070443	0.021402457
Si	5.776747369	0.962459551	1.052130769
Si	-1.934463417	5.632809714	0.204742109
Si	0.045901948	4.393091238	0.70255737
Si	2.015301609	5.584990861	0.069721524
Si	3.981290693	4.461918781	0.892570015

Optimized cartesian coordinates (in Å) of $Si_8H_4(C_6H_{13})_4$-d

a = 7.8745 Å b = 7.8745 Å c = 35 Å

α = 90° β = 90° γ = 120°

C	-0.351045529	5.804464698	2.891603865
C	0.942321314	1.87871309	2.712348939
C	4.214542135	4.649434473	2.639744945
C	3.823884486	2.225259335	-1.9386449
C	3.039569621	2.829273317	-3.142891216
C	3.727246754	2.497475847	-4.496212649
C	2.98829556	3.000003533	-5.762537512
C	3.733918185	2.671207177	-7.08431077
C	2.988571017	3.201479227	-8.327831813

C	0.727767803	5.609246947	3.980880147
C	0.25594887	6.229544601	5.316175291
C	0.97061723	5.76126596	6.597114932
C	0.224571607	6.247391381	7.856361521
C	0.734957703	5.687946149	9.188159334
C	1.363267807	1.268905505	4.071571288
C	0.458573712	1.730038379	5.255405444
C	0.925212495	1.218252762	6.632185751
C	0.06165555	1.673074754	7.832110374
C	0.554880179	1.113251849	9.179185527
C	3.757227892	3.742950834	3.793224702
C	4.689821341	3.920943208	5.021227925
C	4.054170961	3.552406973	6.37940101
C	4.894834406	3.991219266	7.590124709
C	4.345968964	3.596495374	8.969696966
H	-0.505264322	3.177031057	-1.247867103
H	5.475061205	1.598428015	2.325284034
H	-2.221101148	6.115533925	-1.381285082
H	1.753233675	6.012323151	-1.291161824
H	-1.299797257	5.454624119	3.309468764
H	-0.489128847	6.890915233	2.735159141
H	-0.137213678	1.677909861	2.601527498
H	1.016635589	2.975658915	2.795265096
H	5.268582401	4.391094904	2.449843796
H	4.221700239	5.691324991	2.999916584
H	3.836759185	1.124896078	-2.028574549
H	4.879369513	2.534298611	-2.04814835
H	2.971464037	3.923474907	-3.02986295
H	2.005446242	2.456008928	-3.160098052
H	3.871819705	1.406708692	-4.565388406
H	4.737714401	2.939648717	-4.491440334
H	2.854487847	4.091543206	-5.674651221
H	1.980388069	2.552374516	-5.804727293
H	3.856920557	1.578117562	-7.156446679
H	4.743732143	3.113351658	-7.067701858
H	3.550697591	3.047878914	-9.252591215
H	2.808344982	4.279733629	-8.217660865
H	2.012076801	2.71073231	-8.430010177
H	1.689012339	6.054837719	3.6867246
H	0.892355577	4.534090124	4.113747694
H	-0.805949969	5.980744563	5.459355389
H	0.303417559	7.329327072	5.247290727
H	2.020952981	6.098212545	6.616242888
H	0.982652844	4.658702069	6.612920548

H	-0.83064644	5.970433195	7.724132996
H	0.25118944	7.347340246	7.885277021
H	1.706498781	6.119402242	9.464217421
H	0.846329319	4.593446142	9.158598077
H	0.02151789	5.906128727	9.99633278
H	2.396815718	1.53663513	4.320001669
H	1.331121341	0.174911892	4.02995489
H	-0.578555653	1.394671329	5.07251616
H	0.423091732	2.832664742	5.273834988
H	1.956831274	1.549248886	6.817731328
H	0.954182357	0.116428276	6.612608894
H	-0.983309774	1.36641865	7.66907677
H	0.057579966	2.774202961	7.875331338
H	1.556368192	1.487821398	9.433830161
H	0.605909882	0.015509289	9.168005793
H	-0.122442874	1.395171129	9.994232209
H	3.760247051	2.694691511	3.46767114
H	2.736828998	3.98766865	4.105124795
H	4.988600696	4.983160939	5.059964323
H	5.622713758	3.351139577	4.867197356
H	3.883245858	2.467002484	6.444474738
H	3.054787513	4.013290744	6.435702949
H	4.996935455	5.086997927	7.57452231
H	5.913240569	3.598604957	7.469195382
H	4.22212707	2.513761488	9.10075218
H	3.368113175	4.056695708	9.161979608
H	5.035147718	3.939706833	9.758574647
Si	-0.402858359	2.940146565	0.233912489
Si	1.467146779	1.58353516	0.835812241
Si	3.528422248	2.521720917	-0.044868209
Si	5.579241985	1.60697913	0.81610665
Si	-2.390410839	6.089315663	0.120836014
Si	-0.336228809	5.201781684	1.051175539
Si	1.720588099	6.088778345	0.22412396
Si	3.615901604	4.750215	0.808663354

Optimized cartesian coordinates (in Å) of $Si_8H_4(C_6H_{13})_4$-e

a = 7.8745 Å b = 7.8745 Å c = 35 Å

α = 90° β = 90° γ = 120°

C	-2.579961777	6.123545288	-1.912065594
C	-0.379074768	2.779363038	-2.137810628
C	4.107738821	4.899888818	2.823086967

C	3.510588346	4.20999869	4.063261892
C	4.163428349	4.736547305	5.362055612
C	3.730340356	4.017726993	6.648697186
C	4.500848402	4.507412412	7.886376813
C	4.062288691	3.869758276	9.21183238
C	1.181943357	1.568868446	2.696305057
C	1.896827986	1.029459152	3.964356908
C	1.259887441	1.588936254	5.269360837
C	1.855768336	1.025398568	6.578050733
C	1.261541218	1.650149326	7.86351007
C	1.738735681	0.981925088	9.17392332
C	-2.491339212	5.19182582	-3.157164069
C	-2.847544902	5.912740892	-4.483523613
C	-2.668890397	5.080157701	-5.768823983
C	-3.004190159	5.845545723	-7.065508399
C	-2.961429586	5.027850777	-8.367512468
C	-0.187494928	1.952299405	-3.429910412
C	-0.364814639	2.784587967	-4.732860014
C	-0.165780928	2.000112294	-6.049295691
C	-0.373611655	2.806771471	-7.352689325
C	-0.231681552	1.972196386	-8.642467321
H	3.606557939	2.391698085	-1.22079754
H	-0.401294414	4.48693218	2.110572396
H	1.894471334	5.569429445	-1.375018384
H	-1.897236192	6.978403622	-2.082522237
H	-3.588844626	6.567031765	-1.873117218
H	0.30442526	3.64659139	-2.171209942
H	-1.389854343	3.209942253	-2.142935294
H	3.960494388	5.987794041	2.916235893
H	5.19975369	4.751300897	2.854931749
H	3.667441943	3.127313427	3.997766419
H	2.423029731	4.367249243	4.115806727
H	3.959893154	5.81323594	5.47738758
H	5.259161822	4.652779345	5.271726942
H	3.880661081	2.934737132	6.545507574
H	2.654161216	4.16828166	6.822562845
H	4.399050517	5.596162776	7.964235852
H	5.57038951	4.303988941	7.721185238
H	4.132976671	2.774654307	9.184934849
H	3.030435905	4.131895367	9.474425438
H	4.711443834	4.223500618	10.02300161
H	5.875285257	1.178031572	2.203170217
H	0.10658358	1.351940175	2.799612117
H	1.243047313	2.672858855	2.696969753

H	2.961536734	1.308054723	3.948549557
H	1.880868555	-0.067450428	3.98430597
H	0.170396611	1.384940431	5.260948865
H	1.347007629	2.689797823	5.265505908
H	2.945204166	1.195468695	6.597846716
H	1.725220754	-0.06820069	6.595061638
H	0.159158592	1.598778039	7.821323294
H	1.510859373	2.722036016	7.883485597
H	2.751799595	0.561060935	9.08277426
H	1.066408375	0.163923298	9.467793684
H	1.763575443	1.697237605	10.0050354
H	-3.14033529	4.309963167	-3.01553444
H	-1.467931248	4.815211918	-3.234921435
H	-2.203011772	6.802106615	-4.560103352
H	-3.880185888	6.27785242	-4.420203448
H	-3.292897876	4.173130237	-5.689069523
H	-1.630477979	4.743051527	-5.825596143
H	-2.312614286	6.700103116	-7.146011895
H	-4.006844542	6.279824479	-6.966940802
H	-1.941582806	4.782599844	-8.681260191
H	-3.439048076	5.578397721	-9.18752995
H	-3.504644365	4.080207828	-8.233136996
H	-0.900086165	1.115565665	-3.442871721
H	0.807775218	1.503918175	-3.419161332
H	0.323065098	3.648826528	-4.711408673
H	-1.37589383	3.195450679	-4.728598156
H	-0.873891563	1.155766316	-6.053322055
H	0.840942091	1.564662637	-6.054926472
H	0.322275756	3.661761727	-7.376404206
H	-1.377666324	3.240024117	-7.348640926
H	0.763396109	1.518473574	-8.720040545
H	-0.402962183	2.569478991	-9.552783015
H	-0.964317046	1.154739782	-8.661037841
Si	-0.253625617	2.271906661	-0.251317789
Si	1.612569099	1.149726567	0.842714836
Si	3.652288358	2.267363809	0.278585334
Si	5.698293352	1.136624453	0.702702563
Si	-2.298242347	5.675378858	-0.048700089
Si	-0.304259915	4.516956931	0.594723582
Si	1.751707057	5.621112978	0.133079644
Si	3.712143811	4.530987936	0.996517585

Optimized cartesian coordinates (in Å) of $Si_8H_4(C_6H_{13})_4$-f

a = 7.8745 Å b = 7.8745 Å c = 35 Å

α = 90° β = 90° γ = 120°

C	-0.070621261	5.420475835	3.021263679
C	3.754005433	5.353773846	3.022172735
C	1.896231285	2.03745807	3.019671862
C	5.694569535	1.95515087	3.021318257
C	6.295428756	1.355545404	4.302014543
C	5.77845778	2.033302837	5.594105334
C	6.31435415	1.422881273	6.9010937
C	5.749271675	2.066703526	8.185554918
C	6.207485664	1.439867198	9.512355651
C	2.228488883	1.271395607	4.306404891
C	1.979464813	2.085231374	5.592651723
C	2.254878241	1.320612799	6.896685634
C	2.018441948	2.147201417	8.171025455
C	2.378687425	1.468829785	9.497146363
C	4.354338653	4.753987608	4.303878404
C	3.827109238	5.426349955	5.593882644
C	4.371946312	4.824147191	6.89929481
C	3.816766783	5.47122671	8.184554765
C	4.327327974	4.869435666	9.504642352
C	0.271715413	4.659699688	4.308283285
C	0.027828892	5.476986602	5.596564131
C	0.280101158	4.700960731	6.898520641
C	0.018838248	5.494400195	8.193206945
C	0.26886996	4.693266799	9.482739327
H	-1.124633659	5.729709184	3.067662356
H	0.499009889	6.36288451	2.993742329
H	2.657046248	5.349816333	3.100851902
H	4.018264455	6.424748819	2.966472013
H	0.851121219	2.374749015	3.060538482
H	4.598359877	1.939027309	3.096984088
H	5.949853413	3.027869766	2.970096152
H	2.483316661	2.969155281	2.987935672
H	7.389623827	1.406051292	4.276004748
H	6.060370706	0.28654243	4.343426507
H	4.681354165	1.985583156	5.600839921
H	6.027428212	3.101095146	5.57538755
H	7.409801136	1.506061617	6.908131826
H	6.093128866	0.348912454	6.907531912
H	4.655635461	2.034312581	8.152240249
H	6.011541901	3.130670547	8.193083323
H	5.906157414	2.041998778	10.39288028

H	7.298130167	1.338427382	9.543151001
H	3.270571794	0.936531244	4.295873033
H	1.626122966	0.354023055	4.342106762
H	0.948735302	2.453865646	5.594782839
H	2.609651567	2.985229332	5.575901321
H	3.289594431	0.959352445	6.891158175
H	1.626222348	0.420054772	6.929414811
H	0.974205487	2.47386323	8.201853933
H	2.608943131	3.072129601	8.106877675
H	2.352035129	2.205512937	10.31392211
H	3.390522209	1.050365235	9.482952792
H	5.448524117	4.812083903	4.285626389
H	4.1225023	3.68369622	4.341950363
H	2.730766873	5.365385161	5.599019156
H	4.063172145	6.49651804	5.576504013
H	5.465423318	4.915848716	6.902963013
H	4.157293416	3.749454068	6.913584219
H	2.71980461	5.422899878	8.173380046
H	4.066171474	6.53794498	8.178210598
H	4.048852483	5.487543631	10.38009617
H	5.417371947	4.77350373	9.502642864
H	1.311443785	4.319146283	4.288373976
H	-0.332510737	3.744518974	4.344526802
H	-0.999144212	5.856704327	5.594019585
H	0.669558435	6.368059569	5.585834542
H	1.313017169	4.334861218	6.902208431
H	-0.351807699	3.803449069	6.899505836
H	-1.011437169	5.86439961	8.192079977
H	0.651811662	6.391372109	8.198317632
H	0.032043322	5.258154492	10.40466396
H	1.317936242	4.380662818	9.542654358
H	5.774259874	0.443764656	9.679722251
H	1.691388534	0.65524751	9.758401996
H	3.909483313	3.870429786	9.695548583
H	-0.340283108	3.781755326	9.494168086
Si	0.101079453	2.515723688	0.453773637
Si	2.075311385	1.409855532	1.179697531
Si	4.047995509	2.516798678	0.431713775
Si	6.008940967	1.399989016	1.188178149
Si	-1.853437415	5.906276561	0.455344475
Si	0.120493581	4.798384318	1.180313665
Si	2.091935408	5.907175878	0.433231501
Si	4.054345232	4.790000362	1.189321732

Optimized cartesian coordinates (in Å) of $Si_8H_4(CH_3)_4$-a

a = 7.40 Å b = 7.40 Å c = 35 Å

α = 90° β = 90° γ = 120°

C	0.37693364	0.76184144	0.08374162
C	0.87464078	0.76019757	0.08395448
C	0.37403631	0.2585455	0.08355983
C	0.87592645	0.26179934	0.08385537
H	0.50977661	0.90462087	0.09494419
H	0.39045548	0.63546038	0.09510856
H	0.21320534	0.42996469	0.96290096
H	0.71520217	0.43047637	0.96301882
H	0.21077338	0.92655784	0.96293829
H	0.71542435	0.92979714	0.96308571
H	0.89736219	0.63947329	0.09540394
H	0.72442595	0.73479371	0.09510069
H	0.50631959	0.40070365	0.09507323
H	0.00958833	0.40371421	0.09512254
H	0.88693014	0.13415332	0.09531738
H	0.38679575	0.1312295	0.09466937
H	0.23106273	0.74609395	0.09506086
H	0.000918	0.906445	0.09531208
H	0.22751395	0.24200769	0.09473367
H	0.73058582	0.24794985	0.09502662
Si	0.21489467	0.43046415	0.00574333
Si	0.37589937	0.26039094	0.0288504
Si	0.71506612	0.42992658	0.00583893
Si	0.87672011	0.26087972	0.02916884
Si	0.21422879	0.9293567	0.00575408
Si	0.37689463	0.76123119	0.02906131
Si	0.71554141	0.93002972	0.00590838
Si	0.87620895	0.76032769	0.0293315