SUPPORTING INFORMATION

(19 pages including this)

Title: Silaaromaticity in Polycyclic Systems: A Computational Study

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Figure S1: Selected geometric parameters ($\text{\AA}$) of the aromatic hydrocarbons and their corresponding silaaromatic compounds obtained at the B3LYP/6-31G* level. The point group, relative energies, and the number of imaginary frequencies (in parenthesis) are also given.

Figure S2: The local softness values (s_k^+ and s_k^- values are given in normal and bold faces respectively) of the aromatic hydrocarbons and their corresponding silaaromatic compounds obtained at the B3LYP/6-31G* level.

Table S1: Cartesian coordinates of the B3LYP/6-31G* optimized structures and the total energies (hartrees) of the compounds considered in this study. Only the X and Y coordinates are given for planar molecules.

Figure 1.1: Selected geometric parameters (Å) of the aromatic hydrocarbons and their corresponding silaaromatic compounds obtained at the B3LYP/6-31G* level. The point group, relative energies, and the number of imaginary frequencies (in parenthesis) are also given.

Figure S1 (contd.): Selected geometric parameters (Å) of the aromatic hydrocarbons and their corresponding silaaromatic compounds obtained at the B3LYP/6-31G* level. The point group, relative energies, and the number of imaginary frequencies (in parenthesis) are also given.

Figure S1 (contd.): Selected geometric parameters (Å) of the aromatic hydrocarbons and their corresponding silaaromatic compounds obtained at the B3LYP/6-31G* level. The point group, relative energies, and the number of imaginary frequencies (in parenthesis) are also given.

Figure S2: The local softness values (s_k^+ and s_k^- values are given in normal and bold faces respectively) of the aromatic hydrocarbons and their corresponding sila-aromatic compounds obtained at the B3LYP/6-31G* level.

Figure S2 (contd.): The local softness values (s_k^+ and s_k^- values are given in normal and bold faces respectively) of the aromatic hydrocarbons and their corresponding sila-aromatic compounds obtained at the B3LYP/6-31G* level.

Figure S2 (contd.): The local softness values (s_k^+ and s_k^- values are given in normal and bold faces respectively) of the aromatic hydrocarbons and their corresponding sila-aromatic compounds obtained at the B3LYP/6-31G* level.

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C7

C8

C9

Figure S2 (contd.): The local softness values (s_k^+ and s_k^- values are given in normal and bold faces respectively) of the aromatic hydrocarbons and their corresponding sila-aromatic compounds obtained at the B3LYP/6-31G* level.

Table S1: Cartesian coordinates of the B3LYP/6-31G* optimized structures and the total energies (hartrees) of the compounds considered in this study. Only the X and Y coordinates are given for planar molecules.

B E = -232.24863					
	X	Y			
C	1.397094	0.000000	H	1.242019	-2.491172
C	0.698547	1.209919	H	-1.242019	2.491172
C	-0.698547	1.209919	H	-1.242019	-2.491172
C	-1.397094	0.000000	H	3.379938	1.245485
C	-0.698547	-1.209919	H	3.379938	-1.245485
C	0.698547	-1.209919	H	-3.379938	-1.245485
H	-1.242070	2.151328	H	-3.379938	1.245485
H	-2.484140	0.000000			
H	-1.242070	-2.151328	N1 E = -637.23136		
H	1.242070	-2.151328		X	Y
H	2.484140	0.000000	C	2.665927	0.510656
H	1.242070	2.151328	C	1.685136	1.493275
			Si	0.000000	0.892280
			C	0.000000	-0.900989
			C	-1.685136	1.493275
			C	1.257497	-1.561324
			C	-1.257497	-1.561324
			C	2.475729	-0.901948
			C	-2.665927	0.510656
			C	-2.475729	-0.901948
			H	3.705392	0.841777
			H	1.996073	2.534134
			H	1.267745	-2.653159
			H	3.377133	-1.509698
			H	-1.996073	2.534134
			H	-3.705392	0.841777
			H	-3.377133	-1.509698
			H	-1.267745	-2.653159
			N2 E = -637.23666		
				X	Y
			C	-0.619168	0.248399
			C	0.822571	0.240310
			Si	-1.426140	-1.366229
			C	1.604188	-0.957057
			C	-1.304221	1.492893
			C	1.491693	1.499741
			C	-0.235208	-2.651198
			C	1.128265	-2.256658
			C	-0.618087	2.689315
			C	0.796447	2.687809
			H	-2.896452	-1.519044
			H	2.683088	-0.819636

B1 E = -483.59481		
	X	Y
Si	0.000000	1.389872
C	1.449357	0.369177
C	1.246096	-1.016534
C	0.000000	-1.660888
C	-1.246096	-1.016534
C	-1.449357	0.369177
H	0.000000	2.867515
H	2.471551	0.738096
H	2.126408	-1.660136
H	0.000000	-2.748022
H	-2.126408	-1.660136
H	-2.471551	0.738096

N E = -385.89223		
	X	Y
C	0.000000	0.716901
C	0.000000	-0.716901
C	1.245436	1.403344
C	1.245436	-1.403344
C	-1.245436	1.403344
C	-1.245436	-1.403344
C	2.434734	0.708853
C	2.434734	-0.708853
C	-2.434734	-0.708853
C	-2.434734	0.708853
H	1.242019	2.491172

H	-2.392506	1.498786
H	2.579473	1.504881
H	-0.460335	-3.713804
H	1.877663	-3.048478
H	-1.159653	3.631564
H	1.335789	3.631623

N3 E = -637.23754

	X	Y
C	0.757031	-0.009600
C	-0.556462	0.592559
C	0.971805	-1.421190
C	-0.652327	2.012138
C	1.885383	0.866097
C	-1.778332	-0.155913
Si	-0.410697	-2.493415
C	0.461056	2.821929
C	1.748149	2.235299
C	-1.920064	-1.527758
H	2.005962	-1.755924
H	-1.645811	2.455174
H	2.875915	0.417392
H	-2.685399	0.450153
H	-0.359752	-3.970108
H	0.354640	3.902907
H	2.631320	2.868951
H	-2.924548	-1.942103

A E = -539.52945

	X	Y
C	0.000000	1.404448
C	0.000000	-1.404448
C	-1.224550	0.722724
C	-1.224550	-0.722724
C	1.224550	0.722724
C	1.224550	-0.722724
C	2.480725	1.407942
C	2.480725	-1.407942
C	-2.480725	1.407942
C	-2.480725	-1.407942
C	3.662340	0.713559
C	3.662340	-0.713559
C	-3.662340	0.713559
C	-3.662340	-0.713559
H	0.000000	2.492972
H	0.000000	-2.492972
H	2.477429	2.495675

H	2.477429	-2.495675
H	-2.477429	2.495675
H	-2.477429	-2.495675
H	4.609611	1.246527
H	4.609611	-1.246527
H	-4.609611	1.246527
H	-4.609611	-1.246527

A1 E = -790.87281

	X	Y
Si	0.000000	1.690735
C	-1.475515	0.688476
C	-1.269141	-0.748582
C	0.000000	-1.363283
C	1.269141	-0.748582
C	1.475515	0.688476
C	2.808255	1.199104
C	2.439927	-1.580220
C	-2.808255	1.199104
C	-2.439927	-1.580220
C	3.895918	0.360393
C	3.703539	-1.049580
C	-3.895918	0.360393
C	-3.703539	-1.049580
H	0.000000	3.169257
H	0.000000	-2.451386
H	2.958673	2.276682
H	2.299881	-2.658763
H	-2.958673	2.276682
H	-2.299881	-2.658763
H	4.903412	0.767305
H	4.569129	-1.706999
H	-4.903412	0.767305
H	-4.569129	-1.706999

A2 E = -790.86757

	X	Y
C	1.180452	1.206052
C	-1.284197	-0.624107
C	-0.161955	1.661246
C	-1.335135	0.790269
Si	1.457107	-0.534817
C	-0.122014	-1.400741
C	2.794387	-1.739510
C	-0.101238	-2.830920
C	-0.401246	3.077717
C	-2.630304	1.402192

C	2.399276	-3.062757
C	1.057526	-3.575789
C	-1.663460	3.611349
C	-2.803239	2.761241
H	1.955842	1.967542
H	-2.248225	-1.138638
H	3.857179	-1.514449
H	-1.055037	-3.361783
H	0.466381	3.733345
H	-3.496624	0.744101
H	3.183576	-3.821231
H	0.961220	-4.658829
H	-1.795266	4.690542
H	-3.801671	3.189399

A3 E = -790.87526

	X	Y
C	-0.795228	1.096301
C	1.285755	-0.775802
C	0.530691	1.557944
C	1.599811	0.589180
C	-1.110471	-0.267271
C	-0.037270	-1.249496
Si	-2.800543	-0.927907
C	-0.273646	-2.667387
C	0.858966	2.948805
C	2.950003	1.061924
C	-2.778796	-2.673213
C	-1.497027	-3.301876
C	2.166683	3.362117
C	3.224862	2.405051
H	-1.596212	1.834347
H	2.099072	-1.499225
H	-3.986045	-0.045121
H	0.616152	-3.292765
H	0.048745	3.674523
H	3.755605	0.331339
H	-3.658138	-3.310556
H	-1.479138	-4.391835
H	2.406134	4.422077
H	4.255421	2.750262

A4 E = -790.87607

	X	Y
C	-1.126647	0.855882
C	1.428444	-0.258058
C	-0.017187	1.710255

C	1.305661	1.137465
C	-1.015531	-0.546858
C	0.324547	-1.121795
C	-2.205177	-1.349834
C	0.590384	-2.539595
C	-0.144002	3.135199
C	2.437929	2.008590
Si	-2.065198	-3.087067
C	-0.326576	-3.560309
C	0.967022	3.939083
C	2.275563	3.370422
H	-2.122738	1.293502
H	2.426328	-0.692504
H	-3.150014	-0.812812
H	1.649424	-2.801056
H	-1.141504	3.567975
H	3.432228	1.567934
H	-3.186391	-4.049069
H	0.039098	-4.583515
H	0.857544	5.020232
H	3.142214	4.025568

P E = -539.53744

	X	Y
C	0.680054	2.094914
C	1.423357	0.865934
C	0.729407	-0.380680
C	-0.729407	-0.380680
C	-1.423357	0.865934
C	-0.680054	2.094914
C	1.501361	-1.567764
C	2.838486	0.879716
C	-1.501361	-1.567764
C	-2.838486	0.879716
C	2.884680	-1.530206
C	3.563283	-0.296334
C	-2.884680	-1.530206
C	-3.563283	-0.296334
H	1.234079	3.030902
H	-1.234079	3.030902
H	1.007362	-2.533889
H	3.348616	1.840582
H	-1.007362	-2.533889
H	-3.348616	1.840582
H	3.449178	-2.459109
H	4.649830	-0.271962
H	-3.449178	-2.459109

H	-4.649830	-0.271962
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P1	E = -790.87833	
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	X	Y
Si	-0.769862	-0.568885
C	0.632240	-1.668273
C	1.939816	-1.076836
C	2.177029	0.273096
C	1.204055	1.349111
C	-0.222499	1.165148
C	-1.068785	2.297216
C	1.692267	2.681798
C	-0.553063	3.582689
C	0.841362	3.771804
C	-2.285716	-1.500611
C	0.372754	-3.056643
C	-2.124776	-2.887452
C	-0.905708	-3.609825
H	2.803611	-1.744101
H	3.215395	0.598009
H	-2.147546	2.155848
H	2.768871	2.837790
H	-1.220933	4.440028
H	1.252041	4.778320
H	-3.294634	-1.098840
H	1.222466	-3.742664
H	-3.032187	-3.493099
H	-0.982866	-4.694213

P2	E = -790.88301	
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	X	Y
C	-0.540584	0.809128
C	0.396834	1.885026
C	1.799355	1.587779
C	2.247344	0.304107
C	1.346289	-0.822348
C	-0.064633	-0.564858
Si	-1.102896	-2.038877
C	1.932698	-2.119715
C	-0.133184	-3.503475
C	1.267630	-3.337513
C	-1.919437	1.138850
C	-0.065578	3.222505
C	-2.350251	2.453090
C	-1.416889	3.509115
H	2.503058	2.416951
H	3.314738	0.097948

H	-2.579862	-2.028402
H	3.019651	-2.146870
H	-0.535560	-4.512362
H	1.888000	-4.233657
H	-2.659311	0.343294
H	0.667833	4.025609
H	-3.414744	2.671909
H	-1.760814	4.539704

P3	E = -790.88136	
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	X	Y
C	-0.704217	0.777445
C	0.080661	1.969306
C	1.510083	1.878142
C	2.125832	0.666273
C	1.394445	-0.569750
C	-0.044276	-0.536107
C	-0.814244	-1.728634
C	2.177493	-1.763300
C	-2.113063	0.925760
C	-0.556486	3.233790
Si	-0.027877	-3.297915
C	1.738862	-3.076255
C	-2.716197	2.171005
C	-1.932848	3.340847
H	2.090984	2.797072
H	3.211934	0.608847
H	-1.894894	-1.644725
H	3.255559	-1.595634
H	-2.752763	0.050287
H	0.065697	4.126011
H	-0.734985	-4.594510
H	2.482161	-3.868477
H	-3.800677	2.243015
H	-2.409012	4.317782

P4	E = -790.87974	
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	X	Y
Si	2.167471	2.836441
C	0.400285	3.047995
C	-0.373678	1.897108
C	0.058276	0.538108
C	1.452564	0.181003
C	2.519934	1.119308
C	-0.943007	-0.533121
C	-0.522252	-1.897682
C	0.877414	-2.203148

C	1.809979	-1.216928
C	-2.342497	-0.296738
C	-3.260588	-1.331968
C	-2.831164	-2.671958
C	-1.477123	-2.941316
H	3.164222	3.926243
H	-0.117213	4.003533
H	-1.447239	2.058671
H	3.525563	0.706028
H	2.868677	-1.464471
H	1.179354	-3.248199
H	-2.728751	0.715971
H	-1.118733	-3.968423
H	-4.323049	-1.102420
H	-3.556295	-3.481082

P5 E = -790.88030

	X	Y
C	1.878559	0.989525
C	1.381296	-0.355652
C	-0.031238	-0.603872
C	-0.933231	0.554897
C	-0.385239	1.873693
C	1.035605	2.059003
C	-0.558585	-1.925898
Si	2.476303	-1.780430
C	-2.345709	0.436657
C	-1.248620	2.996230
C	0.152597	-3.122378
C	1.555394	-3.274641
C	-3.170562	1.547427
C	-2.620604	2.843218
H	2.954627	1.151655
H	1.425791	3.074181
H	-1.636414	-2.032400
H	3.947671	-1.640537
H	-2.810194	-0.542699
H	-0.805162	3.989481
H	-0.448965	-4.031872
H	1.967053	-4.279543
H	-4.249277	1.414912
H	-3.271351	3.713575

P6 E = -790.87592

	X	Y
C	-0.558301	-0.848972
C	0.623053	-1.672158

C	1.988506	-1.180524
C	2.438602	0.113529
Si	1.149869	1.369714
C	-0.464428	0.606391
C	-1.564773	1.496877
C	1.025977	3.144685
C	-1.468741	2.886859
C	-0.273367	3.645965
C	-1.812864	-1.509871
C	0.471238	-3.082337
C	-1.923190	-2.888372
C	-0.768616	-3.690656
H	2.738533	-1.973470
H	3.510311	0.290339
H	-2.575956	1.091775
H	1.856090	3.844947
H	-2.400745	3.446577
H	-0.397525	4.729778
H	-2.721196	-0.916775
H	-2.907531	-3.349765
H	-0.849705	-4.774033
H	1.370976	-3.693864

P7 E = -790.87588

	X	Y
Si	-1.593947	1.751039
C	0.214608	1.639349
C	0.808341	0.333034
C	0.022874	-0.923803
C	-1.419806	-0.979143
C	-2.291386	0.169553
C	2.229770	0.300781
C	1.025048	2.800091
C	3.003064	1.448180
C	2.404510	2.718508
C	0.703811	-2.168875
C	-2.053269	-2.254416
C	0.057208	-3.391333
C	-1.346055	-3.437577
H	-2.295682	3.051173
H	-3.357948	-0.037404
H	2.754430	-0.645939
H	0.545394	3.777117
H	4.086442	1.358280
H	3.014418	3.617787
H	1.785952	-2.188354
H	-3.140464	-2.274227

H	0.639566	-4.308675
H	-1.869158	-4.390401

C	E = -693.18039	
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	X	Y
C	-0.657132	-0.266353
C	0.657132	0.266353
C	-1.802540	0.629196
C	1.802540	-0.629196
C	1.585545	-2.040238
C	0.246805	-2.536700
C	-0.822648	-1.689396
C	-1.585545	2.040238
C	-0.246805	2.536700
C	0.822648	1.689396
C	2.691847	-2.925976
C	3.985174	-2.446499
C	4.209646	-1.053922
C	3.146300	-0.171522
C	-3.146300	0.171522
C	-4.209646	1.053922
C	-3.985174	2.446499
C	-2.691847	2.925976
H	0.092860	-3.613451
H	-1.820651	-2.112532
H	-0.092860	3.613451
H	1.820651	2.112532
H	2.499496	-3.996690
H	4.827385	-3.133356
H	5.226779	-0.670498
H	3.358408	0.892028
H	-2.499496	3.996690
H	-4.827385	3.133356
H	-5.226779	0.670498
H	-3.358408	-0.892028

C1	E = -944.52097	
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	X	Y
Si	-0.922228	0.248818
C	0.833885	0.026524
C	-1.352199	1.989323
C	1.689148	1.197432
C	-1.809038	-1.329128
C	1.287868	-1.331719
C	-0.276178	2.846062
C	1.133864	2.529911
C	-0.963775	-2.493266

C	0.477398	-2.444590
C	2.020837	3.639140
C	3.105745	1.083624
C	3.391495	3.486492
C	3.935548	2.187298
C	-3.216049	-1.488759
C	-1.598603	-3.765367
C	-3.794647	-2.744934
C	-2.973600	-3.891662
H	2.358951	-1.527787
H	0.970890	-3.414235
H	-2.352100	2.413934
H	-0.489059	3.916670
H	1.588999	4.637801
H	3.555053	0.096191
H	4.042271	4.356548
H	5.014092	2.049878
H	-3.852864	-0.606455
H	-0.972656	-4.655188
H	-4.876508	-2.848879
H	-3.426053	-4.880211

C2	E = -944.51920	
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	X	Y
C	-0.708784	-0.132085
C	0.715477	-0.067863
Si	-1.590030	1.455151
C	1.504997	1.182441
C	-1.398160	-1.409650
C	1.409824	-1.330484
C	-0.475788	2.778418
C	0.931723	2.508523
C	-0.651254	-2.624223
C	0.769314	-2.534954
C	1.801300	3.637454
C	2.925933	1.116218
C	3.172584	3.516882
C	3.741287	2.231359
C	-2.815056	-1.516204
C	-1.319665	-3.873618
C	-3.448866	-2.743471
C	-2.697387	-3.938345
H	2.490422	-1.351946
H	1.350248	-3.454614
H	-3.057041	1.608257
H	-0.771783	3.824069
H	1.341841	4.622943

H	3.422812	0.155805
H	3.803557	4.401873
H	4.820676	2.106788
H	-3.423038	-0.616981
H	-0.723041	-4.783106
H	-4.534828	-2.788099
H	-3.204268	-4.899502

C3 E = -944.51642		
	X	Y
C	-0.043539	-0.780092
C	0.265617	0.622508
C	-1.386491	-1.285070
C	-0.734087	1.713988
C	1.055041	-1.755863
C	1.653057	0.987923
Si	-2.734428	-0.199397
C	-2.156677	1.506232
C	2.411231	-1.313550
C	2.673421	0.084022
C	-3.055875	2.601153
C	-0.322494	3.079732
C	-2.604300	3.904906
C	-1.216964	4.133329
C	0.841927	-3.160780
C	3.474108	-2.251516
C	1.890818	-4.060752
C	3.225623	-3.607218
H	1.930357	2.032501
H	3.705593	0.425951
H	-1.531715	-2.357062
H	-4.166343	-0.562367
H	-4.125825	2.401610
H	0.727843	3.336879
H	-3.302961	4.737080
H	-0.835486	5.151322
H	-0.162943	-3.565309
H	4.494766	-1.875339
H	1.680424	-5.127166
H	4.045807	-4.320254

C4 E = -944.51525		
	X	Y
C	0.701574	-0.417674
C	-0.665622	0.007235
C	1.818487	0.500365
C	-1.043823	1.411934

C	0.999885	-1.852459
C	-1.692480	-0.994002
C	1.834542	1.876266
Si	0.229115	2.663695
C	-0.070562	-2.800109
C	-1.414802	-2.326982
C	-0.462486	4.305423
C	-2.376521	1.901787
C	-1.851921	4.356247
C	-2.734745	3.245990
C	2.317436	-2.389875
C	0.195309	-4.191832
C	2.555188	-3.751488
C	1.487612	-4.671062
H	-2.729855	-0.681470
H	-2.222789	-3.055299
H	2.797777	0.033866
H	2.799867	2.373984
H	0.096931	5.236392
H	-3.206124	1.197112
H	-2.324342	5.339540
H	-3.798087	3.472443
H	3.181961	-1.737155
H	-0.649213	-4.877499
H	3.580583	-4.112381
H	1.683262	-5.739850

C5 E = -944.52298		
	X	Y
C	0.796919	0.412084
C	-0.597386	0.144177
C	1.712054	-0.685598
C	-1.085200	-1.236416
C	1.277787	1.785774
C	-1.499617	1.259303
C	1.272694	-1.978922
C	-0.116910	-2.295723
C	0.335509	2.856845
C	-1.057705	2.549894
Si	-0.719383	-3.991062
C	-2.484425	-1.514352
C	-2.471264	-4.024254
C	-3.101150	-2.759578
C	2.656096	2.125506
C	0.787858	4.199622
C	3.075406	3.442322
C	2.135313	4.493881

H	-2.568279	1.088651
H	-1.770639	3.370855
H	2.779230	-0.498432
H	1.999521	-2.788491
H	0.197791	-5.150616
H	-3.163402	-0.672119
H	-3.096364	-4.911813
H	-4.191074	-2.746909
H	3.409214	1.345758
H	0.047514	4.996237
H	4.138396	3.667975
H	2.473580	5.526371

C6	E = -944.52265	
	X	Y
C	0.562674	0.764633
C	-0.543377	-0.125567
C	1.879761	0.210720
C	-0.334986	-1.572166
C	0.357123	2.203572
C	-1.858782	0.450950
C	2.090295	-1.134272
C	1.012874	-2.080183
C	-0.972645	2.719429
C	-2.062914	1.799831
C	1.357247	-3.460841
C	-1.465686	-2.446891
Si	0.090474	-4.668903
C	-1.482662	-3.831774
C	1.422941	3.141642
C	-1.192338	4.118766
C	1.186185	4.503208
C	-0.133026	5.002465
H	-2.733645	-0.186708
H	-3.076211	2.195129
H	2.741488	0.868228
H	3.105665	-1.523147
H	2.419822	-3.691059
H	-2.442085	-1.974457
H	0.284474	-6.132797
H	-2.452406	-4.322229
H	2.451514	2.798463
H	-2.217151	4.483622
H	2.025577	5.193800
H	-0.309769	6.074660

C7	E = -944.52446	
	X	Y
C	0.452928	0.852685
C	-0.465610	-0.228791
C	1.852155	0.565284
C	0.009583	-1.614628
C	-0.032191	2.224334
C	-1.866134	0.075124
C	2.308166	-0.719587
C	1.430894	-1.845361
C	-1.437532	2.470277
C	-2.331499	1.357887
C	2.052511	-3.132763
C	-0.909628	-2.700485
C	1.446556	-4.374877
Si	-0.336199	-4.357490
C	0.831770	3.350441
C	-1.923002	3.801518
C	0.336680	4.640535
C	-1.054407	4.873379
H	-2.592198	-0.728566
H	-3.401906	1.550474
H	2.573170	1.373840
H	3.379180	-0.909422
H	3.143313	-3.105160
H	-1.970902	-2.483492
H	2.078408	-5.258566
H	-1.208029	-5.549368
H	1.906999	3.211171
H	-2.998862	3.962270
H	1.026078	5.480857
H	-1.435905	5.890976

C8	E = -944.52610	
	X	Y
C	0.868825	-0.386165
C	-0.499032	-0.013162
C	1.849440	0.653992
C	-0.883653	1.383328
C	1.242087	-1.790148
C	-1.489853	-1.049814
C	1.498991	1.971760
C	0.130596	2.399055
C	0.217663	-2.784626
C	-1.150592	-2.370916
C	-0.117369	3.803091
Si	-2.577192	2.015194

C	-1.353234	4.430084
C	-2.602289	3.770407
C	2.590010	-2.233536
C	0.567031	-4.157460
C	2.907234	-3.578736
C	1.888987	-4.554184
H	-2.540489	-0.775625
H	-1.923909	-3.135726
H	2.903332	0.399092
H	2.272720	2.736006
H	0.765632	4.437813
H	-3.793423	1.178424
H	-1.350833	5.520221
H	-3.506509	4.372692
H	3.399146	-1.511362
H	-0.230695	-4.897022
H	3.950109	-3.885108
H	2.146558	-5.609924

C9 E = -944.51916		
	X	Y
C	-0.731519	-0.315312
C	0.696106	-0.319848
C	-1.512303	0.901942
Si	1.503748	1.301321
C	-1.416898	-1.608795

C	1.420919	-1.550797
C	-1.073064	2.207218
C	0.297010	2.608829
C	-0.648645	-2.816955
C	0.777549	-2.754683
C	0.766972	3.943047
C	3.150924	1.982654
C	2.115275	4.284128
C	3.207292	3.375491
C	-2.831798	-1.743012
C	-1.305028	-4.074185
C	-3.448142	-2.979474
C	-2.680723	-4.162006
H	2.508374	-1.522893
H	1.339923	-3.685454
H	-2.588407	0.782609
H	-1.836400	2.987858
H	0.035416	4.753729
H	4.084848	1.428507
H	2.365962	5.342031
H	4.197699	3.832948
H	-3.463714	-0.863002
H	-0.695071	-4.974789
H	-4.533453	-3.037698
H	-3.171204	-5.131789

C2-m E = -944.51937			
	X	Y	Z
C	-0.717034	-0.112026	-0.001292
C	0.705870	-0.078929	0.051430
Si	-1.557355	1.497412	0.049539
C	1.523684	1.149060	-0.007271
C	-1.428279	-1.376211	-0.025893
C	1.373790	-1.347761	0.186479
C	-0.409309	2.790069	0.141246
C	0.990095	2.487989	0.071034
C	-0.706723	-2.603290	0.064935
C	0.709908	-2.539823	0.196009
C	1.893485	3.589290	0.059432
C	2.931186	1.039329	-0.173696
C	3.255315	3.427921	-0.067982
C	3.778761	2.130287	-0.204417
C	-2.841060	-1.456576	-0.148818
C	-1.398232	-3.839692	0.038879
C	-3.496752	-2.672047	-0.176836
C	-2.771864	-3.879414	-0.080744

H	2.446314	-1.373630	0.324076
H	1.265654	-3.467361	0.313971
H	-3.020642	1.682009	0.079545
H	-0.679351	3.840182	0.213814
H	1.469170	4.587082	0.140225
H	3.379014	0.064611	-0.317178
H	3.912864	4.293255	-0.080403
H	4.845675	1.978561	-0.343078
H	-3.425892	-0.545803	-0.234876
H	-0.822687	-4.759666	0.111878
H	-4.578569	-2.697664	-0.277264
H	-3.295550	-4.831132	-0.103991

C3-m	E = -944.51664		
	X	Y	Z
C	-0.780260	0.071675	-0.055827
C	0.649770	0.162438	-0.014078
C	-1.478817	-1.177039	-0.162445
C	1.568948	-0.989258	0.084908
C	-1.570262	1.307894	-0.015122
C	1.231491	1.470485	-0.102820
Si	-0.599787	-2.667327	-0.253781
C	1.166886	-2.360351	-0.063143
C	-0.922418	2.578298	-0.065602
C	0.497677	2.619423	-0.143099
C	2.120167	-3.406047	0.002969
C	2.950199	-0.780745	0.366061
C	3.456313	-3.149012	0.235991
C	3.861889	-1.817229	0.436001
C	-2.986695	1.312036	0.086637
C	-1.686452	3.772063	-0.045562
C	-3.713803	2.487073	0.116752
C	-3.061842	3.734760	0.042010
H	2.306175	1.563806	-0.187964
H	0.993251	3.582921	-0.233658
H	-2.558576	-1.154658	-0.233701
H	-1.166958	-4.022797	-0.406190
H	1.784057	-4.433224	-0.124589
H	3.316844	0.217376	0.569243
H	4.177870	-3.959884	0.285873
H	4.902094	-1.595013	0.660896
H	-3.531973	0.378892	0.165993
H	-1.160768	4.723094	-0.094593
H	-4.796381	2.444930	0.204032
H	-3.639222	4.655267	0.061529