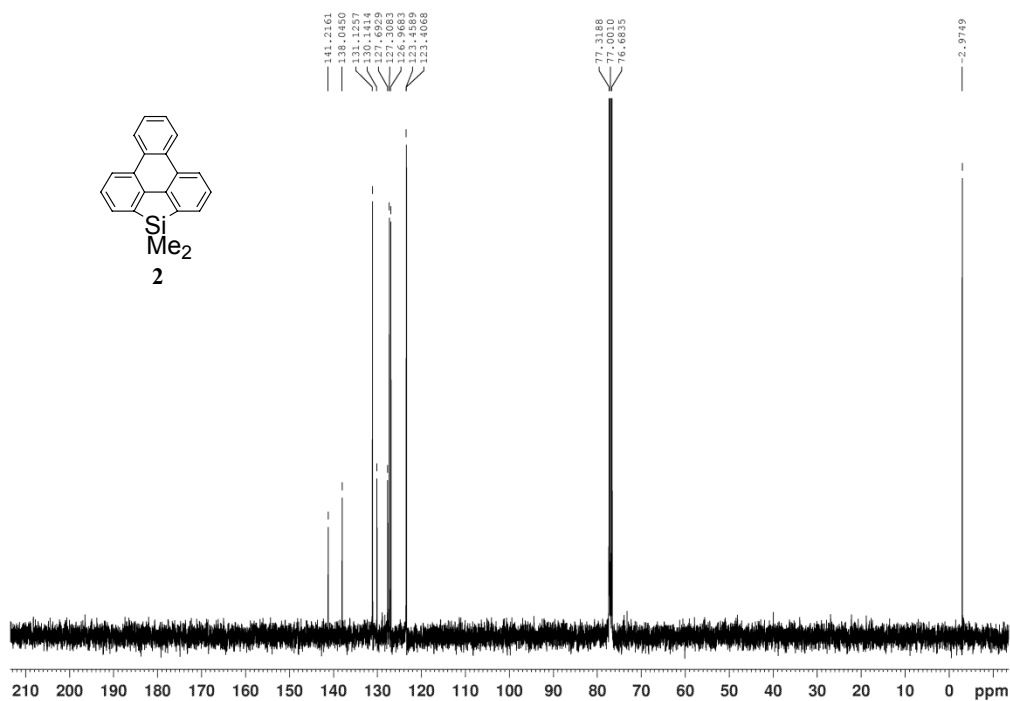
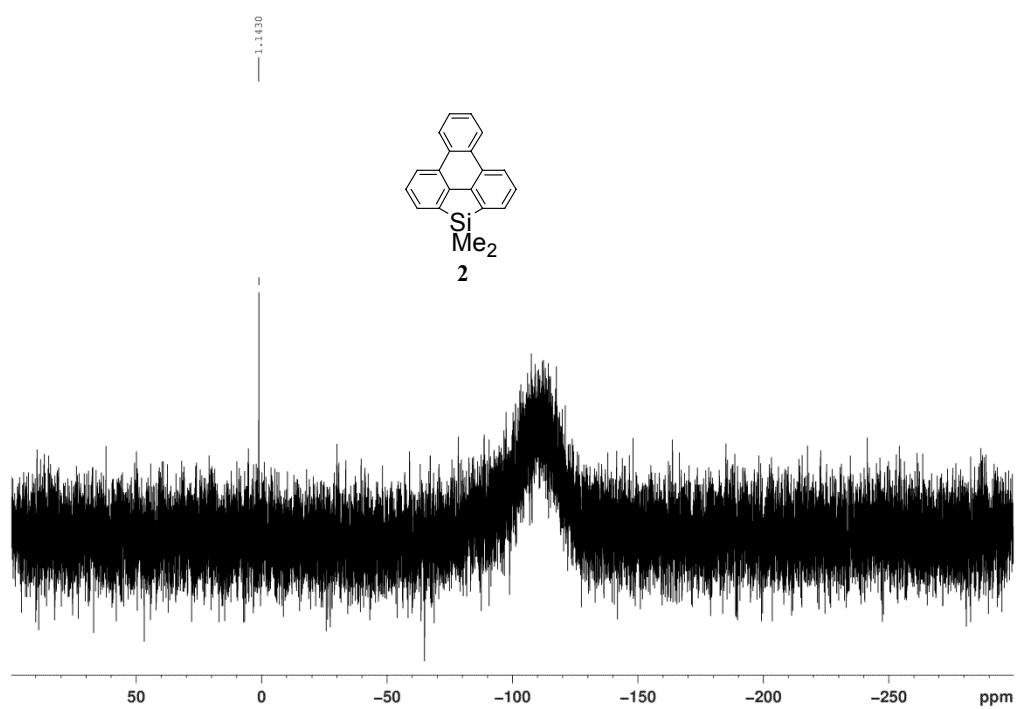


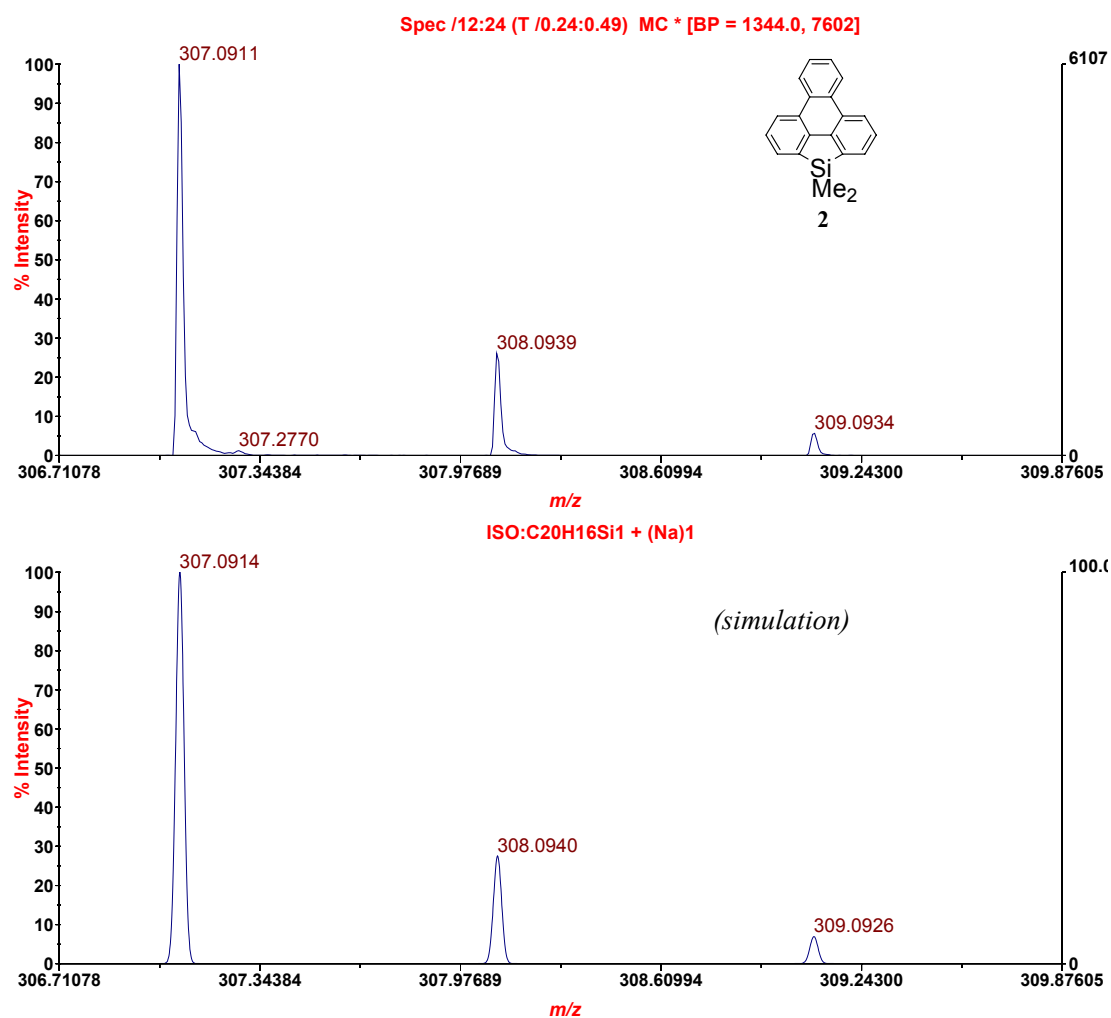
## Supplementary Material for the Communication Entitled Syntheses, Structures and Optical Properties of Trisilasumanene and its Related Compounds



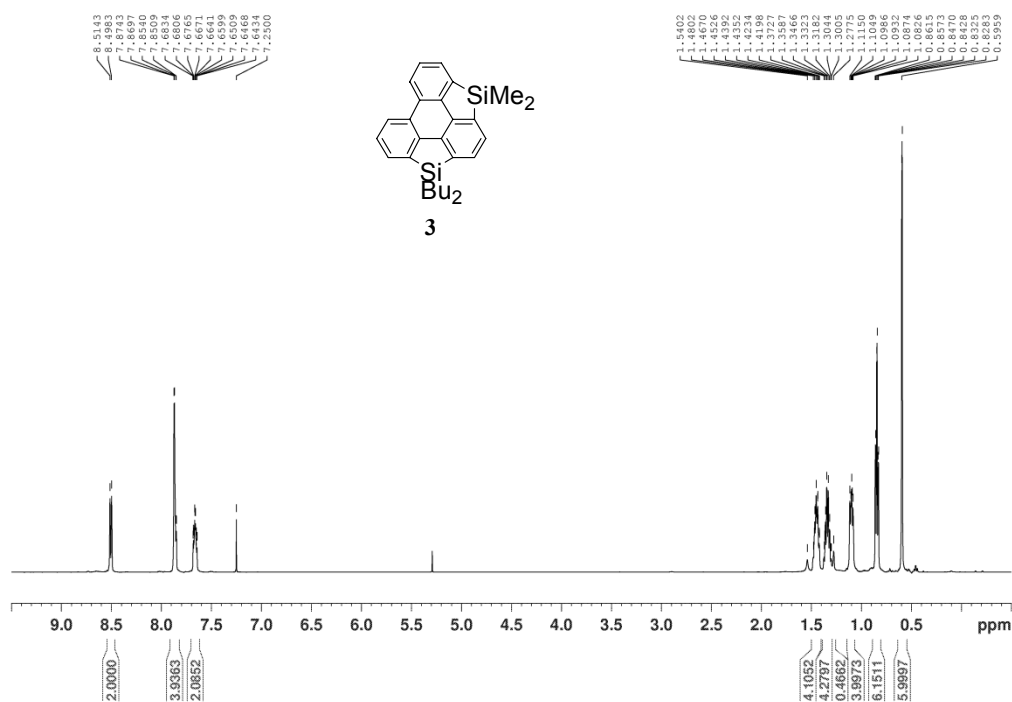
**Figure 2**  $^{13}\text{C}$  NMR Chart of Dimethyltriphenylenosilole **2**.



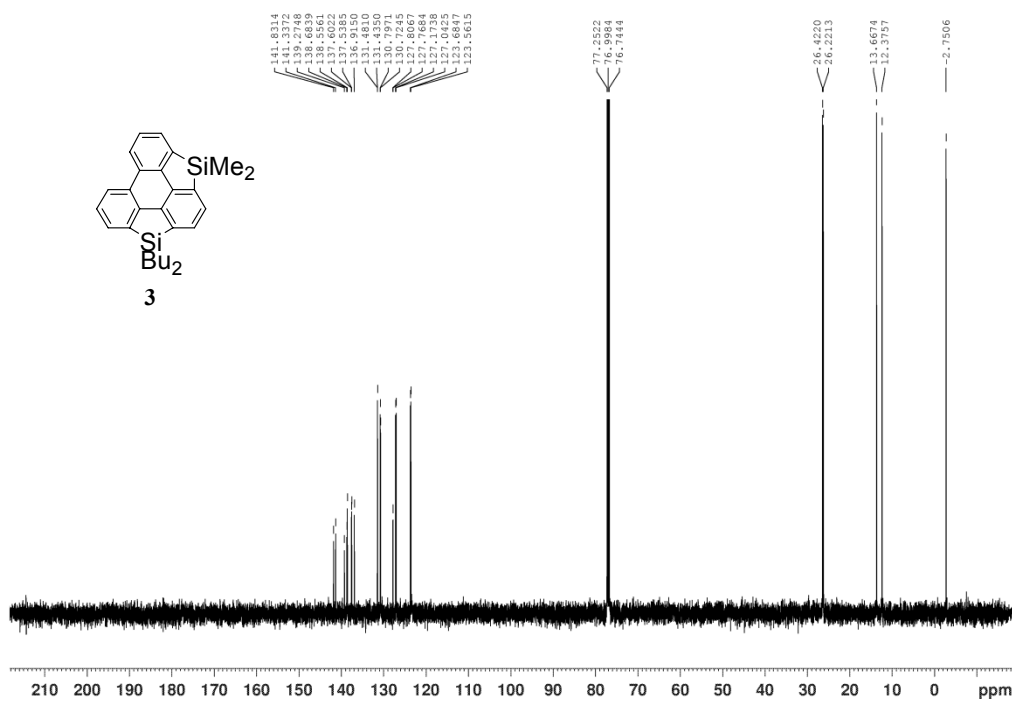
**Figure 3**  $^{29}\text{Si}$  NMR Chart of Dimethyltriphenylenosilole **2**.



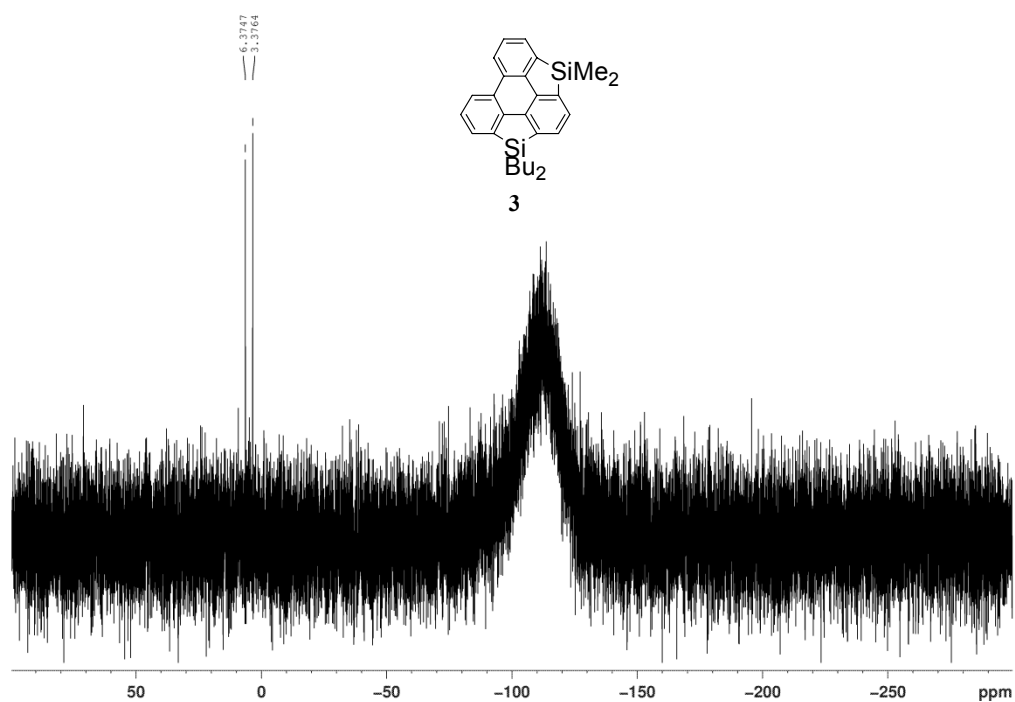
**Figure 4** High Resolution ESI-Mass Spectral Chart of Dimethyltriphenylenosilole **2**.



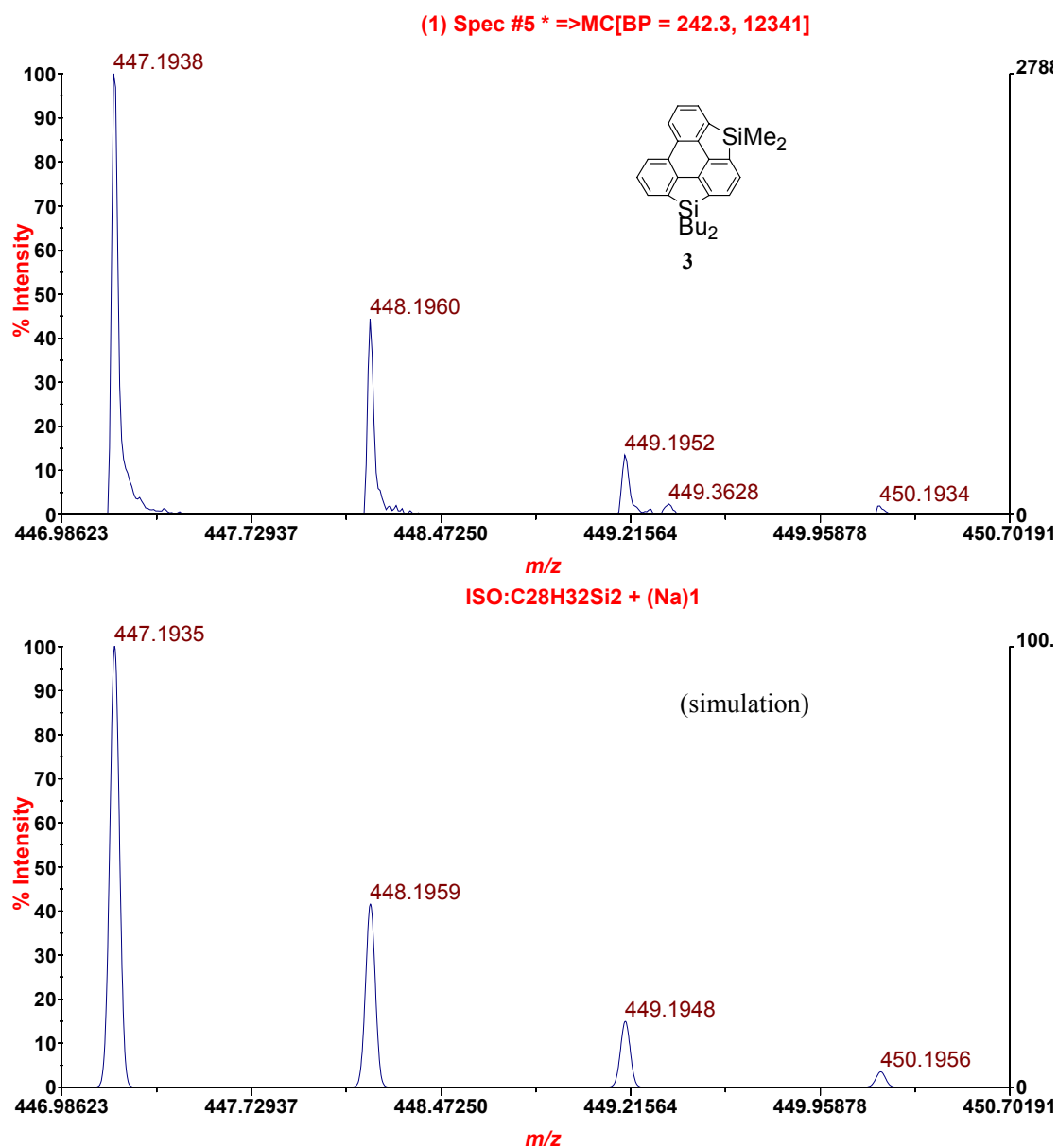
**Figure 5** <sup>1</sup>H NMR Chart of Dibutyldimethyltriphenylenodisilole **3**.



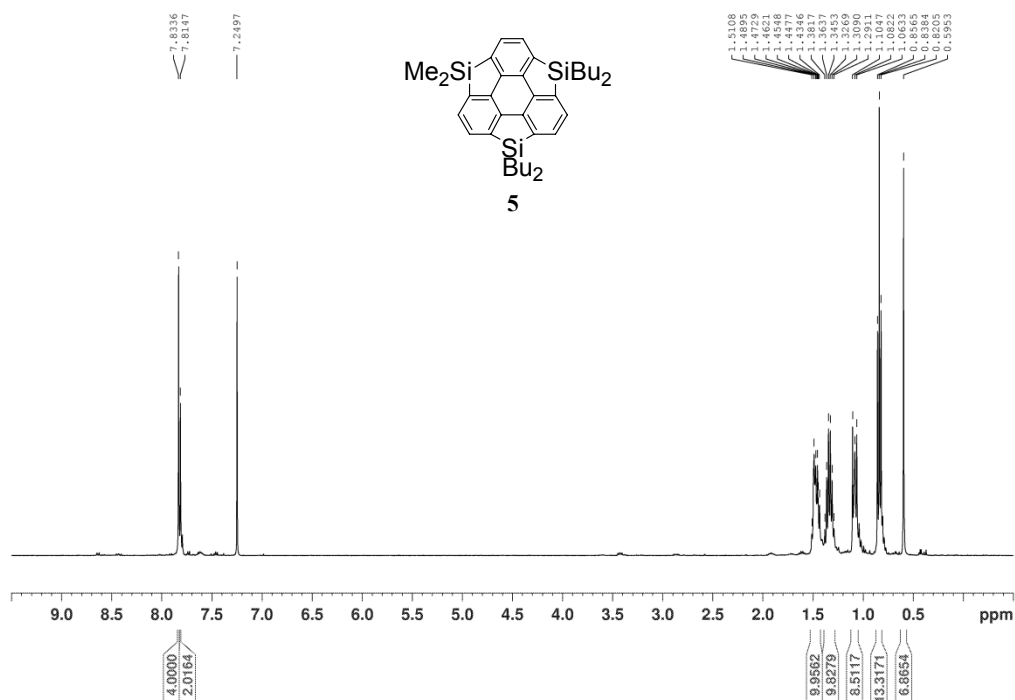
**Figure 6** <sup>13</sup>C NMR Chart of Dibutyldimethyltriphenylenodisilole **3**.



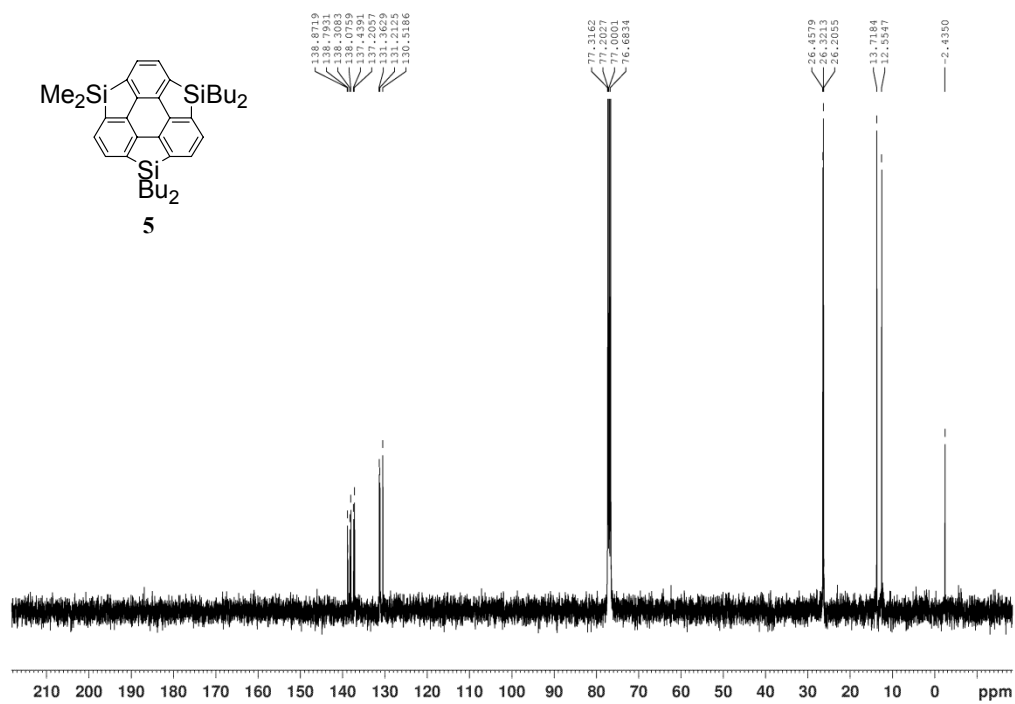
**Figure 7**  $^{29}\text{Si}$  NMR Chart of Dibutyldimethyltriphenylenodisilole **3**.



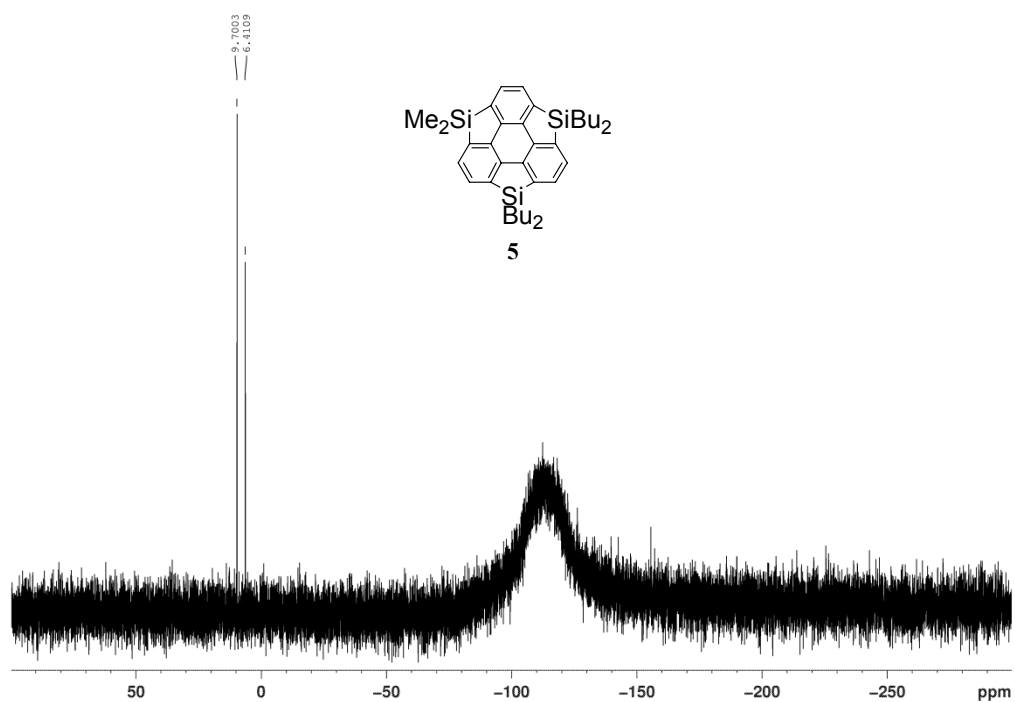
**Figure 8** High Resolution ESI-Mass Spectral Chart of Dibutyldimethyltriphenylenodisilole 3.



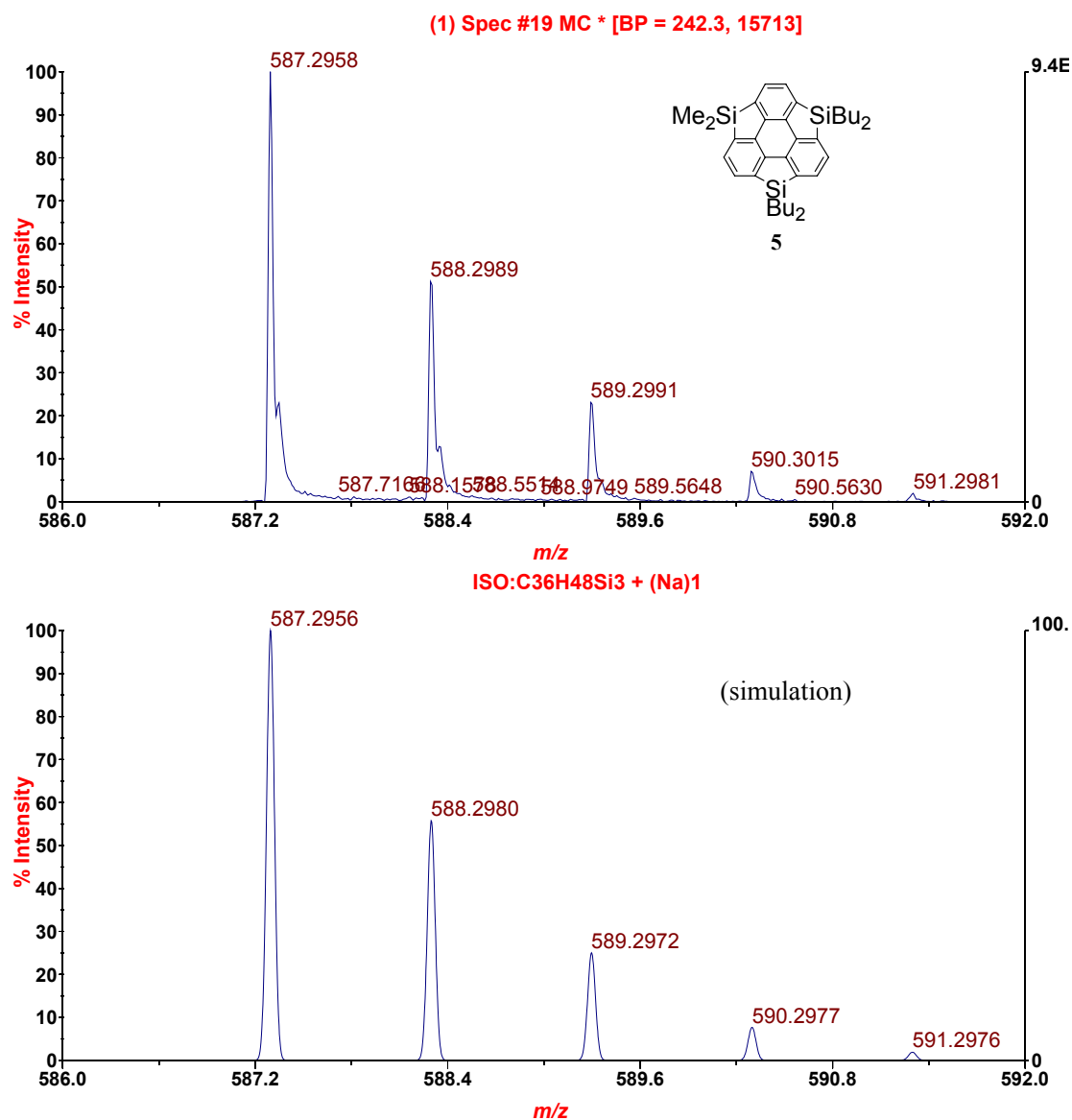
**Figure 9** <sup>1</sup>H NMR Chart of Tetrabutyltrimethylphenylene-trisilole **5**.



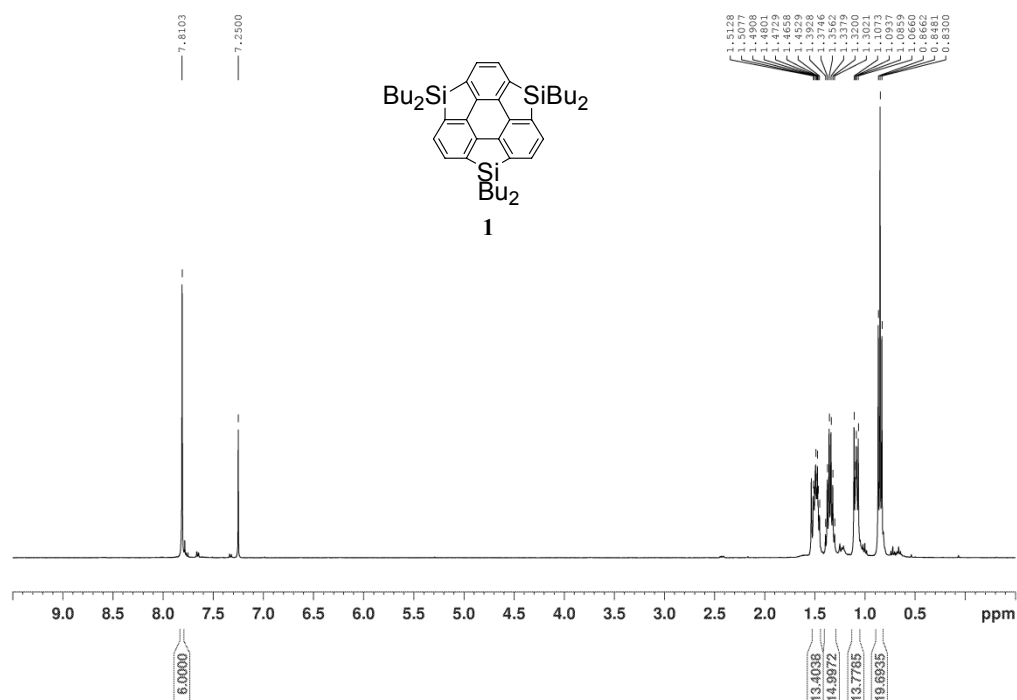
**Figure 10** <sup>13</sup>C NMR Chart of Tetrabutyltrimethylphenylene-trisilole **5**.



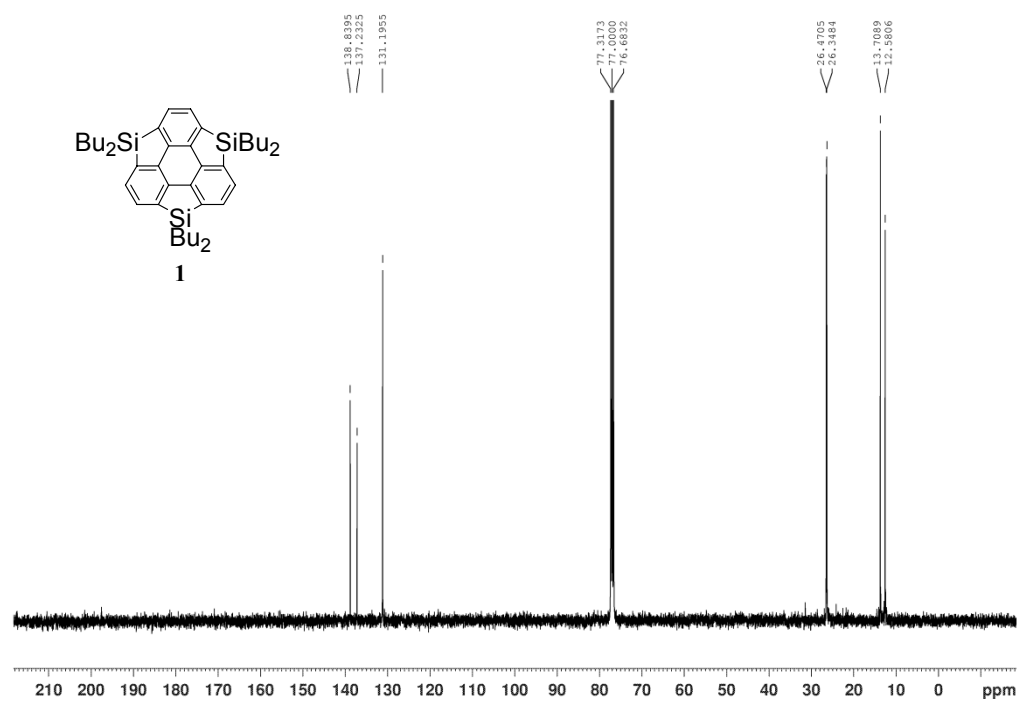
**Figure 11**  $^{29}\text{Si}$  NMR Chart of Tetrabutyltrimethyltriphenylenotrisilole **5**.



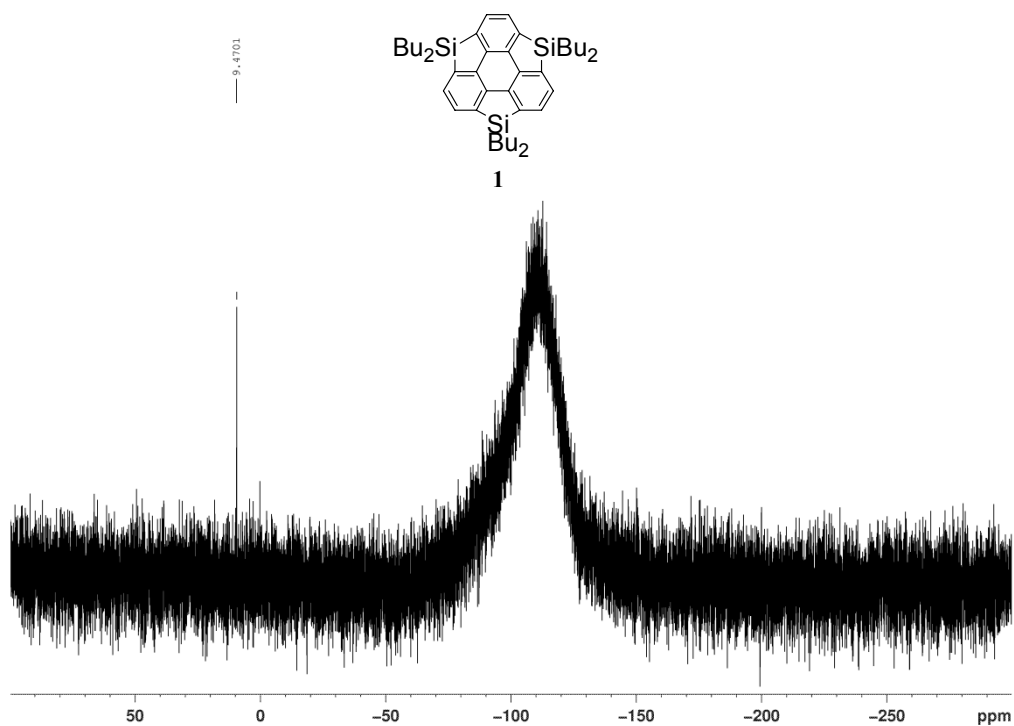
**Figure 12** High Resolution ESI-Mass Spectral Chart of Tetrabutyltrimethylphenyltrisilole 5.



**Figure 13** <sup>1</sup>H NMR Chart of Hexabutyltriphenylenotrisilole **1**.



**Figure 14** <sup>13</sup>C NMR Chart of Hexabutyltriphenylenotrisilole **1**.



**Figure 15**  $^{29}\text{Si}$  NMR Chart of Hexabutyltriphenylenotrisilole **1**.

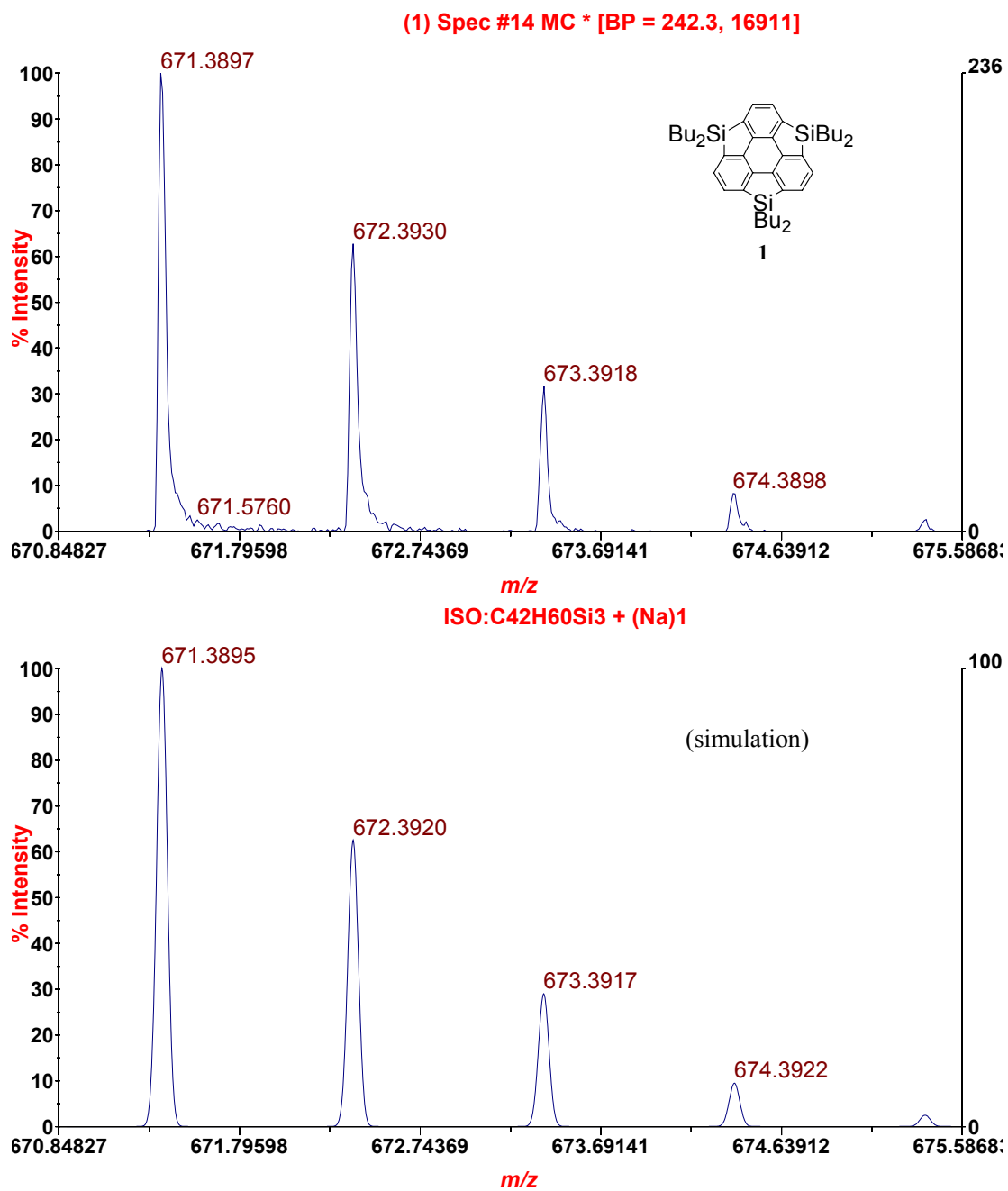


Figure 16 High Resolution ESI-Mass Spectral Chart of Hexabutyltriphenylenotrisilole 1.

The Cartesian coordinates of the optimized geometries for compounds **1**, **2**, **3** and **B**.

Compound **2**

-----

Total energy: -1061.35830910 au

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 5.003510  | -2.066602 | 0.000000  |
| C  | 3.866811  | -1.230043 | 0.000000  |
| C  | 4.063537  | 0.185436  | 0.000000  |
| C  | 5.385282  | 0.680316  | 0.000000  |
| C  | 6.482633  | -0.164719 | 0.000000  |
| C  | 6.289709  | -1.552838 | 0.000000  |
| C  | 2.909268  | 1.093254  | 0.000000  |
| C  | 1.615077  | 0.537867  | 0.000000  |
| C  | 1.415041  | -0.901431 | 0.000000  |
| C  | 2.508730  | -1.788690 | 0.000000  |
| C  | 0.066299  | -1.346216 | 0.000000  |
| Si | -1.045364 | 0.174070  | 0.000000  |
| C  | 0.438743  | 1.333592  | 0.000000  |
| C  | 2.997887  | 2.503996  | 0.000000  |
| C  | 1.856905  | 3.295097  | 0.000000  |
| C  | 0.574216  | 2.715783  | 0.000000  |
| C  | 2.209286  | -3.170131 | 0.000000  |
| C  | 0.895817  | -3.620108 | 0.000000  |
| C  | -0.180281 | -2.712965 | 0.000000  |
| H  | 3.007638  | -3.904921 | 0.000000  |
| H  | 0.698992  | -4.689172 | 0.000000  |
| H  | 5.555011  | 1.751567  | 0.000000  |
| H  | 7.486864  | 0.250219  | 0.000000  |
| H  | 7.142728  | -2.225900 | 0.000000  |
| H  | 4.874680  | -3.143538 | 0.000000  |
| H  | 3.966356  | 2.993230  | 0.000000  |
| H  | 1.959070  | 4.377317  | 0.000000  |
| C  | -2.112260 | 0.322350  | 1.539333  |
| C  | -2.112260 | 0.322350  | -1.539333 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -2.874844 | -0.465535 | 1.568279  |
| H | -1.504153 | 0.237834  | 2.446775  |
| H | -2.631089 | 1.288327  | 1.568279  |
| H | -2.631089 | 1.288327  | -1.568279 |
| H | -1.504153 | 0.237834  | -2.446775 |
| H | -2.874844 | -0.465535 | -1.568279 |
| H | -0.300089 | 3.363815  | 0.000000  |
| H | -1.198167 | -3.098017 | 0.000000  |

**Compound 3**

-----

Total energy: -1665.41617393 au

|    |           |          |           |
|----|-----------|----------|-----------|
| C  | 0.000000  | 0.000000 | 0.000000  |
| C  | 0.000000  | 0.000000 | 1.411646  |
| C  | 1.267826  | 0.000000 | 2.041412  |
| C  | 2.493557  | 0.000000 | 1.328482  |
| C  | 2.439038  | 0.000000 | -0.061409 |
| C  | 1.191902  | 0.000000 | -0.716441 |
| C  | 1.391594  | 0.000000 | 3.485372  |
| C  | 0.249755  | 0.000000 | 4.279266  |
| C  | -1.060747 | 0.000000 | 3.660131  |
| C  | -1.209546 | 0.000000 | 2.252466  |
| C  | -2.156270 | 0.000000 | 4.560277  |
| Si | -1.451450 | 0.000000 | 6.318955  |
| C  | 0.332025  | 0.000000 | 5.692576  |
| C  | 2.687853  | 0.000000 | 4.054478  |
| C  | 2.771431  | 0.000000 | 5.447513  |
| C  | 1.608184  | 0.000000 | 6.256514  |
| C  | -2.532841 | 0.000000 | 1.760935  |
| C  | -3.619604 | 0.000000 | 2.628675  |
| C  | -3.439996 | 0.000000 | 4.025736  |
| H  | -2.716703 | 0.000000 | 0.690368  |
| H  | -4.626399 | 0.000000 | 2.218614  |
| H  | 3.349115  | 0.000000 | -0.658336 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | 1.158229  | 0.000000  | -1.803040 |
| H  | -0.939641 | 0.000000  | -0.544834 |
| H  | 3.741803  | 0.000000  | 5.940997  |
| C  | -1.903732 | -1.540023 | 7.295444  |
| C  | -1.903732 | 1.540023  | 7.295444  |
| H  | -2.979920 | -1.570309 | 7.506806  |
| H  | -1.643094 | -2.446871 | 6.738429  |
| H  | -1.374063 | -1.568140 | 8.255807  |
| H  | -1.374063 | 1.568140  | 8.255807  |
| H  | -1.643094 | 2.446871  | 6.738429  |
| H  | -2.979920 | 1.570309  | 7.506806  |
| H  | 1.732896  | 0.000000  | 7.337929  |
| H  | -4.316555 | 0.000000  | 4.670791  |
| Si | 3.900913  | 0.000000  | 2.600939  |
| C  | 4.989482  | -1.540228 | 2.523005  |
| C  | 4.989482  | 1.540228  | 2.523005  |
| H  | 5.725561  | -1.471466 | 3.339157  |
| C  | 4.247224  | -2.886850 | 2.606379  |
| H  | 5.575950  | -1.495152 | 1.592155  |
| H  | 5.575950  | 1.495152  | 1.592155  |
| C  | 4.247224  | 2.886850  | 2.606379  |
| H  | 5.725561  | 1.471466  | 3.339157  |
| C  | 5.181000  | -4.105165 | 2.561582  |
| H  | 3.656120  | -2.922185 | 3.532450  |
| H  | 3.523400  | -2.958763 | 1.782229  |
| C  | 4.433522  | -5.439968 | 2.652369  |
| H  | 5.769466  | -4.075132 | 1.633195  |
| H  | 5.906489  | -4.033361 | 3.384757  |
| H  | 5.124997  | -6.289841 | 2.617822  |
| H  | 3.863645  | -5.511269 | 3.587094  |
| H  | 3.723718  | -5.553568 | 1.823627  |
| C  | 5.181000  | 4.105165  | 2.561582  |
| H  | 3.523400  | 2.958763  | 1.782229  |
| H  | 3.656120  | 2.922185  | 3.532450  |
| C  | 4.433522  | 5.439968  | 2.652369  |
| H  | 5.906489  | 4.033361  | 3.384757  |

|   |          |          |          |
|---|----------|----------|----------|
| H | 5.769466 | 4.075132 | 1.633195 |
| H | 5.124997 | 6.289841 | 2.617822 |
| H | 3.723718 | 5.553568 | 1.823627 |
| H | 3.863645 | 5.511269 | 3.587094 |

**Compound 5**

-----

Total energy: -2505.33802171 au

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 0.777646  | 2.723185  | 0.000000  |
| C  | 0.421682  | 1.356871  | 0.000000  |
| C  | 1.381782  | 0.342372  | 0.000000  |
| C  | 2.765609  | 0.622257  | 0.000000  |
| C  | 3.124044  | 1.975068  | 0.000000  |
| C  | 2.148098  | 3.006351  | 0.000000  |
| C  | 0.968924  | -1.043987 | 0.000000  |
| C  | -0.389832 | -1.367846 | 0.000000  |
| C  | -1.384043 | -0.317217 | 0.000000  |
| C  | -0.985261 | 1.021495  | 0.000000  |
| C  | -0.839405 | -2.706189 | 0.000000  |
| C  | 0.152830  | -3.692989 | 0.000000  |
| C  | 1.533914  | -3.363794 | 0.000000  |
| C  | 1.974195  | -2.035385 | 0.000000  |
| C  | -1.919423 | 2.080070  | 0.000000  |
| C  | -3.270147 | 1.714327  | 0.000000  |
| C  | -3.675650 | 0.353577  | 0.000000  |
| C  | -2.745333 | -0.691844 | 0.000000  |
| Si | 3.627210  | -1.080756 | 0.000000  |
| C  | 4.670809  | -1.388766 | 1.541880  |
| Si | -2.745265 | -2.600560 | 0.000000  |
| C  | -3.536461 | -3.347413 | 1.542080  |
| Si | -0.875228 | 3.678251  | 0.000000  |
| C  | -1.127929 | 4.734686  | 1.542623  |
| C  | -3.536461 | -3.347413 | -1.542080 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.127929 | 4.734686  | -1.542623 |
| C | 4.670809  | -1.388766 | -1.541880 |
| H | -4.047495 | 2.476685  | 0.000000  |
| H | 4.172743  | 2.267789  | 0.000000  |
| H | 2.497882  | 4.037469  | 0.000000  |
| H | 2.251772  | -4.182382 | 0.000000  |
| H | -0.118646 | -4.747345 | 0.000000  |
| H | -4.743512 | 0.141281  | 0.000000  |
| H | -0.426023 | 5.581643  | -1.490671 |
| C | -0.959594 | 4.002440  | -2.886839 |
| H | -2.133801 | 5.179304  | -1.485785 |
| H | -0.426023 | 5.581643  | 1.490671  |
| H | -2.133801 | 5.179304  | 1.485785  |
| C | -0.959594 | 4.002440  | 2.886839  |
| H | 5.063622  | -2.415951 | 1.484836  |
| H | 5.552270  | -0.730902 | 1.487980  |
| C | 3.950947  | -1.181970 | 2.887386  |
| H | 5.063622  | -2.415951 | -1.484836 |
| C | 3.950947  | -1.181970 | -2.887386 |
| H | 5.552270  | -0.730902 | -1.487980 |
| H | -3.418566 | -4.440919 | -1.486982 |
| H | -4.620766 | -3.163464 | -1.486520 |
| C | -2.992279 | -2.832613 | -2.887531 |
| H | -3.418566 | -4.440919 | 1.486982  |
| C | -2.992279 | -2.832613 | 2.887531  |
| H | -4.620766 | -3.163464 | 1.486520  |
| C | 4.848183  | -1.434204 | 4.107631  |
| H | 3.556349  | -0.157224 | 2.938092  |
| H | 3.076742  | -1.846209 | 2.941820  |
| C | 4.848183  | -1.434204 | -4.107631 |
| H | 3.076742  | -1.846209 | -2.941820 |
| H | 3.556349  | -0.157224 | -2.938092 |
| C | 4.122630  | -1.229004 | -5.441455 |
| H | 5.721283  | -0.767510 | -4.057377 |
| H | 5.244529  | -2.458773 | -4.058178 |
| H | 4.787333  | -1.416718 | -6.292720 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 3.263997  | -1.905702 | -5.533618 |
| H | 3.744926  | -0.203052 | -5.533662 |
| C | 4.122630  | -1.229004 | 5.441455  |
| H | 5.244529  | -2.458773 | 4.058178  |
| H | 5.721283  | -0.767510 | 4.057377  |
| H | 4.787333  | -1.416718 | 6.292720  |
| H | 3.744926  | -0.203052 | 5.533662  |
| H | 3.263997  | -1.905702 | 5.533618  |
| C | -3.685523 | -3.456259 | 4.107421  |
| H | -1.913090 | -3.032949 | 2.947135  |
| H | -3.100508 | -1.739568 | 2.933336  |
| C | -3.138964 | -2.937934 | 5.441629  |
| H | -4.765365 | -3.256323 | 4.049580  |
| H | -3.575978 | -4.549627 | 4.064692  |
| H | -3.652841 | -3.400408 | 6.292370  |
| H | -2.067931 | -3.153609 | 5.542270  |
| H | -3.265591 | -1.851434 | 5.526464  |
| C | -3.685523 | -3.456259 | -4.107421 |
| H | -3.100508 | -1.739568 | -2.933336 |
| H | -1.913090 | -3.032949 | -2.947135 |
| C | -3.138964 | -2.937934 | -5.441629 |
| H | -3.575978 | -4.549627 | -4.064692 |
| H | -4.765365 | -3.256323 | -4.049580 |
| H | -3.652841 | -3.400408 | -6.292370 |
| H | -3.265591 | -1.851434 | -5.526464 |
| H | -2.067931 | -3.153609 | -5.542270 |
| C | -1.167028 | 4.909532  | 4.108207  |
| H | -1.668744 | 3.164014  | 2.938031  |
| H | 0.042949  | 3.554165  | 2.938391  |
| C | -1.003391 | 4.172293  | 5.441331  |
| H | -0.455058 | 5.746262  | 4.060781  |
| H | -2.169061 | 5.359737  | 4.057133  |
| H | -1.156300 | 4.845191  | 6.293103  |
| H | -1.725607 | 3.351323  | 5.531429  |
| H | 0.000547  | 3.739714  | 5.534447  |
| C | -1.167028 | 4.909532  | -4.108207 |

|   |           |          |           |
|---|-----------|----------|-----------|
| H | 0.042949  | 3.554165 | -2.938391 |
| H | -1.668744 | 3.164014 | -2.938031 |
| C | -1.003391 | 4.172293 | -5.441331 |
| H | -2.169061 | 5.359737 | -4.057133 |
| H | -0.455058 | 5.746262 | -4.060781 |
| H | -1.156300 | 4.845191 | -6.293103 |
| H | 0.000547  | 3.739714 | -5.534447 |
| H | -1.725607 | 3.351323 | -5.531429 |

Model B

-----

Total energy: -2013.05614781 au

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 6.288949  | -0.374588 | 1.739876  |
| C  | 6.842870  | -1.585714 | 2.224783  |
| C  | 7.982880  | -2.152385 | 1.659883  |
| C  | 8.655071  | -1.554665 | 0.570655  |
| C  | 8.126398  | -0.366741 | 0.081576  |
| C  | 6.949983  | 0.212179  | 0.669211  |
| C  | 8.510377  | -3.385304 | 2.183015  |
| C  | 7.881164  | -4.010421 | 3.256662  |
| C  | 6.703672  | -3.424982 | 3.842200  |
| C  | 6.193367  | -2.233028 | 3.334121  |
| C  | 8.358712  | -5.222732 | 3.802154  |
| C  | 9.494119  | -5.770789 | 3.218633  |
| C  | 10.139296 | -5.119939 | 2.112097  |
| C  | 9.669771  | -3.928499 | 1.575272  |
| C  | 5.040211  | -1.621116 | 3.874525  |
| C  | 4.430253  | -2.264366 | 4.944245  |
| C  | 4.960856  | -3.495155 | 5.461873  |
| C  | 6.094092  | -4.096685 | 4.930945  |
| Si | 10.106066 | -2.692896 | 0.192026  |
| H  | 10.085157 | -3.308231 | -1.164787 |
| Si | 7.171414  | -5.644690 | 5.200750  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | 6.414603  | -6.914451 | 5.014528  |
| O  | 10.016081 | -6.938098 | 3.686472  |
| O  | 11.248718 | -5.803619 | 1.663174  |
| Si | 4.774274  | -0.062665 | 2.852466  |
| H  | 3.493909  | -0.023438 | 2.091470  |
| O  | 3.315366  | -1.738065 | 5.522023  |
| O  | 4.226486  | -3.992144 | 6.517151  |
| O  | 8.714635  | 0.274074  | -0.965692 |
| O  | 6.571847  | 1.387443  | 0.056051  |
| H  | 11.449019 | -2.073729 | 0.373278  |
| H  | 7.788933  | -5.694243 | 6.555845  |
| H  | 4.870437  | 1.212548  | 3.616965  |
| H  | 8.192227  | 1.074826  | -1.150223 |
| H  | 5.771344  | 1.733955  | 0.477946  |
| H  | 3.050903  | -2.330513 | 6.247834  |
| H  | 4.641971  | -4.800602 | 6.852849  |
| H  | 10.796515 | -7.150822 | 3.144816  |
| H  | 11.632404 | -5.341622 | 0.902723  |