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## ***SUPPORTING INFORMATION***

***Title:*** Ab initio Study of Some Intramolecularly Donor-Stabilized Silenes
***Author(s):*** Dirk Wandschneider, Manfred Michalik, Hartmut Oehme, Andreas Heintz*
***Ref. No.:*** I200500126

The following material contains the geometric structures, energies and some thermodynamic properties of the following compounds:

1-(2-dimethylaminomethylphenyl)-1,2,2-tris(trimethylsilyl)silene (**1**),

1-(2-dimethylaminomethylphenyl)-1-methyl,2,2-bis(trimethylsilyl)silene (**2**),

1-[2,6-bis(dimethylaminomethyl)phenyl]-1,2,2-tris(trimethylsilyl)silene (**3**) and

1-(2-isobutylphenyl)-1,2,2-tris(trimethylsilyl)silene (**5**),

1 hartree = $4.3597482 \cdot 10^{-18}$ J
1 cal = 4.184 J

Compound **1**, HF/6-31++G(d,p) optimized geometric structure with short Si-N distance
E(HF/6-31++G(d,p))=-1952.460209 hartrees
E(MP2/6-31++G(d,p))=-1955.769434 hartrees
Cartesian coordinates:

| | | | |
|---|---|---|---|
| Si | 0.299953 | 0.280464 | 0.060868 |
| Si | 1.028857 | 2.342695 | -0.999390 |
| C | 0.091031 | 2.443896 | -2.645488 |
| H | 0.253361 | 1.546211 | -3.236822 |
| H | 0.456814 | 3.289411 | -3.225489 |
| H | -0.979566 | 2.560322 | -2.522947 |
| C | 2.870016 | 2.191679 | -1.453638 |
| H | 3.522075 | 2.154147 | -0.584977 |
| H | 3.157765 | 3.067221 | -2.033851 |
| H | 3.078166 | 1.313490 | -2.055834 |
| C | 0.902641 | 4.006743 | -0.083332 |
| H | 1.660386 | 4.090183 | 0.692637 |
| H | -0.063285 | 4.206674 | 0.362346 |
| H | 1.103045 | 4.801521 | -0.799838 |
| N | 1.034323 | 0.359675 | 2.022669 |
| C | 2.501918 | 0.240783 | 1.875389 |
| C | 2.805570 | -0.702241 | 0.733840 |
| C | 1.826879 | -0.818141 | -0.252172 |
| C | 2.111733 | -1.606207 | -1.365567 |
| C | 3.322065 | -2.273660 | -1.477608 |
| C | 4.272529 | -2.165312 | -0.471371 |
| C | 4.014430 | -1.376780 | 0.639022 |
| H | 4.751907 | -1.288407 | 1.419456 |
| H | 5.206990 | -2.691832 | -0.551663 |
| H | 3.520976 | -2.883225 | -2.341348 |
| H | 1.386699 | -1.709713 | -2.152328 |
| H | 2.947665 | -0.084380 | 2.811345 |
| H | 2.894599 | 1.227771 | 1.654936 |

| | | | |
|---|---|---|---|
| C | 0.512437 | -0.805239 | 2.771717 |
| H | 0.837313 | -1.719137 | 2.301363 |
| H | -0.565849 | -0.775787 | 2.767459 |
| H | 0.885037 | -0.772536 | 3.791462 |
| C | 0.666448 | 1.581359 | 2.756705 |
| H | 1.009722 | 2.455061 | 2.225696 |
| H | 1.108096 | 1.571499 | 3.748989 |
| H | -0.409127 | 1.626701 | 2.853287 |
| C | -1.341947 | -0.335607 | -0.012651 |
| Si | -1.703667 | -2.126369 | -0.387427 |
| C | -0.544806 | -3.418856 | 0.407088 |
| H | -0.821912 | -4.403334 | 0.032817 |
| H | -0.677597 | -3.445145 | 1.486938 |
| H | 0.509807 | -3.281513 | 0.200498 |
| C | -3.407916 | -2.734817 | 0.215946 |
| H | -3.532431 | -3.764617 | -0.115676 |
| H | -4.252646 | -2.172447 | -0.167372 |
| H | -3.474849 | -2.736694 | 1.300939 |
| C | -1.712275 | -2.483140 | -2.260809 |
| H | -1.958802 | -3.524126 | -2.464740 |
| H | -0.754010 | -2.275286 | -2.729548 |
| H | -2.451707 | -1.863579 | -2.762793 |
| Si | -2.822064 | 0.770620 | 0.140533 |
| C | -2.454490 | 2.632176 | 0.340277 |
| H | -3.406694 | 3.137480 | 0.491815 |
| H | -1.993661 | 3.087333 | -0.528587 |
| H | -1.839949 | 2.859285 | 1.207623 |
| C | -3.994044 | 0.696062 | -1.359306 |
| H | -4.854683 | 1.345424 | -1.206225 |
| H | -4.372795 | -0.301500 | -1.559347 |
| H | -3.482643 | 1.032333 | -2.258939 |
| C | -3.875695 | 0.421168 | 1.694356 |
| H | -4.709113 | 1.120458 | 1.747439 |
| H | -3.283139 | 0.556218 | 2.598803 |
| H | -4.288490 | -0.580124 | 1.725224 |

Compound **1**, B3LYP/6-31++G(d,p) optimized geometric structure with short Si-N distance
E(B3LYP/6-31++G(d,p))=-1960.4143739 hartrees
Cartesian coordinates:

| | | | |
|---|---|---|---|
| Si | 0.287466 | 0.301080 | 0.022327 |
| Si | 1.001917 | 2.378080 | -0.997736 |
| C | 0.064101 | 2.529537 | -2.643631 |
| H | 0.244607 | 1.653017 | -3.275508 |
| H | 0.416982 | 3.413921 | -3.189170 |
| H | -1.017224 | 2.619562 | -2.511912 |
| C | 2.845938 | 2.213998 | -1.449146 |
| H | 3.497100 | 2.166756 | -0.569164 |
| H | 3.149350 | 3.091797 | -2.034019 |
| H | 3.044575 | 1.322660 | -2.051781 |
| C | 0.872055 | 4.023519 | -0.042207 |
| H | 1.619636 | 4.082389 | 0.757499 |

| | | | |
|---|---|---|---|
| H | -0.112243 | 4.211769 | 0.392163 |
| H | 1.089743 | 4.842479 | -0.739850 |
| N | 1.065433 | 0.378583 | 2.052434 |
| C | 2.537403 | 0.239402 | 1.871400 |
| C | 2.811766 | -0.704840 | 0.720014 |
| C | 1.821599 | -0.795722 | -0.277471 |
| C | 2.095560 | -1.587261 | -1.403861 |
| C | 3.301404 | -2.284340 | -1.521602 |
| C | 4.259639 | -2.203101 | -0.506649 |
| C | 4.013710 | -1.410976 | 0.617587 |
| H | 4.758068 | -1.343148 | 1.408349 |
| H | 5.191468 | -2.754984 | -0.588792 |
| H | 3.488976 | -2.897899 | -2.398312 |
| H | 1.358771 | -1.671388 | -2.197405 |
| H | 3.010099 | -0.090702 | 2.806700 |
| H | 2.932532 | 1.236173 | 1.640708 |
| C | 0.521850 | -0.794504 | 2.784902 |
| H | 0.857196 | -1.713168 | 2.305337 |
| H | -0.567965 | -0.761418 | 2.746184 |
| H | 0.869914 | -0.774804 | 3.825391 |
| C | 0.712148 | 1.611112 | 2.791422 |
| H | 1.082109 | 2.486771 | 2.258515 |
| H | 1.141771 | 1.592204 | 3.801309 |
| H | -0.375018 | 1.678532 | 2.869534 |
| C | -1.349389 | -0.346305 | -0.021265 |
| Si | -1.684309 | -2.152072 | -0.366805 |
| C | -0.486652 | -3.408308 | 0.430723 |
| H | -0.745456 | -4.412494 | 0.070717 |
| H | -0.597927 | -3.421818 | 1.521745 |
| H | 0.567053 | -3.237918 | 0.196261 |
| C | -3.383118 | -2.763444 | 0.253199 |
| H | -3.507139 | -3.807186 | -0.062876 |
| H | -4.232887 | -2.200711 | -0.144325 |
| H | -3.449648 | -2.743419 | 1.346734 |
| C | -1.692433 | -2.514633 | -2.240888 |
| H | -1.954789 | -3.560805 | -2.444997 |
| H | -0.718205 | -2.318761 | -2.702611 |
| H | -2.423978 | -1.877288 | -2.750734 |
| Si | -2.839787 | 0.752661 | 0.133040 |
| C | -2.466030 | 2.615286 | 0.320107 |
| H | -3.418210 | 3.136004 | 0.481680 |
| H | -2.002312 | 3.061645 | -0.563127 |
| H | -1.831082 | 2.835388 | 1.185805 |
| C | -4.018436 | 0.642752 | -1.362222 |
| H | -4.895172 | 1.286511 | -1.215605 |
| H | -4.384250 | -0.373674 | -1.541383 |
| H | -3.510929 | 0.971096 | -2.277120 |
| C | -3.874539 | 0.390500 | 1.698550 |
| H | -4.725163 | 1.082034 | 1.758410 |
| H | -3.269788 | 0.535261 | 2.603237 |
| H | -4.272057 | -0.626980 | 1.730047 |

Compound **1**, X-Ray structure
(position of the hydrogen atoms optimized with HF/6-31++G(d,p))
E(HF/6-31++G(d,p))=-1952.452114 hartrees
E(MP2/6-31++G(d,p))=-1955.764 hartrees
Cartesian coordinates:

| | | | |
|---|---|---|---|
| Si | -0.000000 | -0.000000 | -0.000000 |
| Si | 2.3808500 | 0.000000 | -0.000000 |
| C | 2.8346799 | 1.812309 | 0.000000 |
| H | 2.2956452 | 2.347396 | -0.777607 |
| H | 3.8986966 | 1.936495 | -0.198774 |
| H | 2.6166727 | 2.308931 | 0.936821 |
| C | 2.9399999 | -0.737050 | -1.625239 |
| H | 2.6672118 | -1.784230 | -1.728835 |
| H | 4.0261095 | -0.683712 | -1.695955 |
| H | 2.5333710 | -0.213931 | -2.483996 |
| C | 3.3892349 | -0.931800 | 1.322416 |
| H | 3.3560183 | -2.007165 | 1.158637 |
| H | 3.0897165 | -0.735436 | 2.344573 |
| H | 4.4325401 | -0.635642 | 1.226188 |
| N | -0.6131799 | -1.831190 | 0.535660 |
| C | -0.2782399 | -2.713139 | -0.616060 |
| C | -0.4618701 | -1.929180 | -1.899699 |
| C | -0.3489899 | -0.547149 | -1.775149 |
| C | -0.3842178 | 0.206641 | -2.944340 |
| C | -0.5554100 | -0.404799 | -4.175150 |
| C | -0.6941700 | -1.767500 | -4.263849 |
| C | -0.6434099 | -2.535309 | -3.128220 |
| H | -0.7407992 | -3.606534 | -3.197018 |
| H | -0.8379146 | -2.234725 | -5.222251 |
| H | -0.5875429 | 0.197347 | -5.066468 |
| H | -0.2843734 | 1.274143 | -2.907234 |
| H | -0.8848020 | -3.612728 | -0.578628 |
| H | 0.7590938 | -3.012821 | -0.510553 |
| C | -2.0849700 | -1.789409 | 0.710549 |
| H | -2.5542218 | -1.497725 | -0.215056 |
| H | -2.3326626 | -1.064232 | 1.468231 |
| H | -2.4361281 | -2.775521 | 0.999103 |
| C | -0.0043600 | -2.340760 | 1.783200 |
| H | 1.0706710 | -2.317001 | 1.710908 |
| H | -0.3302239 | -3.360804 | 1.960882 |
| H | -0.3230525 | -1.723972 | 2.609270 |
| C | -0.9187500 | 1.284159 | 0.750760 |
| Si | -2.1872899 | 2.195730 | -0.206720 |
| C | -3.3531299 | 1.141459 | -1.237189 |
| H | -4.0342168 | 1.793113 | -1.783995 |
| H | -3.9724406 | 0.520318 | -0.591241 |
| H | -2.8809354 | 0.494335 | -1.964833 |
| C | -3.3714400 | 3.186529 | 0.860550 |
| H | -4.0282579 | 3.761318 | 0.207986 |

| | | | |
|---|---|---|---|
| H | -2.8938741 | 3.896223 | 1.526753 |
| H | -4.0104980 | 2.547285 | 1.465106 |
| C | -1.4293800 | 3.497020 | -1.335900 |
| H | -2.1819018 | 3.992289 | -1.949192 |
| H | -0.6657494 | 3.112916 | -2.004676 |
| H | -0.9497932 | 4.265358 | -0.732214 |
| Si | -0.4780699 | 1.924360 | 2.401079 |
| C | 0.9754599 | 1.060819 | 3.225270 |
| H | 1.0616404 | 1.454458 | 4.237488 |
| H | 1.9283588 | 1.247516 | 2.746621 |
| H | 0.8598462 | -0.013694 | 3.327975 |
| C | 0.0022699 | 3.750299 | 2.406450 |
| H | 0.2624448 | 4.083968 | 3.410689 |
| H | -0.7911629 | 4.400477 | 2.051759 |
| H | 0.8660163 | 3.928739 | 1.769976 |
| C | -1.8507800 | 1.726899 | 3.658970 |
| H | -1.5389190 | 2.097163 | 4.635383 |
| H | -2.1173093 | 0.677554 | 3.786954 |
| H | -2.7589362 | 2.254432 | 3.391788 |

Compound **1b**, HF/6-31++G(d,p) optimized geometric structure with long Si-N distance

E(HF/6-31++G(d,p))=-1952.446059 hartrees

E(MP2/6-31++G(d,p))=-1955.740197 hartrees

Cartesian coordinates:

| | | | |
|---|---|---|---|
| Si | -0.173956 | 0.434022 | -0.367261 |
| Si | 0.392186 | 2.738537 | -0.782707 |
| C | -0.792999 | 3.558282 | -2.010908 |
| H | -0.776430 | 3.034226 | -2.963543 |
| H | -0.476274 | 4.582912 | -2.198040 |
| H | -1.819698 | 3.582545 | -1.665781 |
| C | 2.096712 | 2.672483 | -1.610620 |
| H | 2.854529 | 2.231622 | -0.968628 |
| H | 2.412528 | 3.687361 | -1.847124 |
| H | 2.086070 | 2.105140 | -2.535727 |
| C | 0.580040 | 3.784761 | 0.784019 |
| H | 1.236395 | 3.304810 | 1.505158 |
| H | -0.362232 | 3.995729 | 1.275364 |
| H | 1.035988 | 4.735790 | 0.514597 |
| N | 3.579840 | -0.491282 | 2.098369 |
| C | 2.301586 | -0.640509 | 1.434907 |
| C | 2.397109 | -0.915659 | -0.059648 |
| C | 1.351945 | -0.555186 | -0.923256 |
| C | 1.468017 | -0.882757 | -2.277986 |
| C | 2.570178 | -1.559286 | -2.774115 |
| C | 3.588062 | -1.922828 | -1.906741 |
| C | 3.498758 | -1.602062 | -0.561476 |
| H | 4.286550 | -1.882118 | 0.112645 |
| H | 4.448857 | -2.453978 | -2.273750 |
| H | 2.631507 | -1.798855 | -3.821100 |
| H | 0.685712 | -0.605693 | -2.965247 |

| | | | |
|---|---|---|---|
| H | 1.780276 | -1.475036 | 1.891295 |
| H | 1.670397 | 0.238942 | 1.611937 |
| C | 4.230822 | 0.763653 | 1.781155 |
| H | 4.353705 | 0.866698 | 0.710677 |
| H | 5.214624 | 0.790328 | 2.235868 |
| H | 3.665633 | 1.628588 | 2.145134 |
| C | 3.477726 | -0.688387 | 3.529717 |
| H | 3.073488 | -1.671450 | 3.741824 |
| H | 2.840181 | 0.057105 | 4.016835 |
| H | 4.463943 | -0.628646 | 3.975833 |
| C | -1.648164 | -0.339279 | 0.073902 |
| Si | -1.850999 | -2.207828 | -0.203588 |
| C | -0.449709 | -3.265104 | 0.512755 |
| H | -0.716977 | -4.316146 | 0.416149 |
| H | -0.311446 | -3.063335 | 1.572848 |
| H | 0.501031 | -3.123611 | 0.012728 |
| C | -3.413844 | -2.943278 | 0.587686 |
| H | -3.483681 | -3.979370 | 0.260482 |
| H | -4.337415 | -2.453929 | 0.295468 |
| H | -3.365084 | -2.952048 | 1.672037 |
| C | -2.014516 | -2.593411 | -2.055095 |
| H | -2.239382 | -3.648063 | -2.204766 |
| H | -1.106097 | -2.372780 | -2.606107 |
| H | -2.821754 | -2.017171 | -2.501856 |
| Si | -3.130846 | 0.618688 | 0.724309 |
| C | -2.780306 | 2.429333 | 1.175898 |
| H | -3.707710 | 2.855835 | 1.553790 |
| H | -2.457504 | 3.073292 | 0.363058 |
| H | -2.046458 | 2.501230 | 1.976478 |
| C | -4.544539 | 0.639876 | -0.542795 |
| H | -5.425151 | 1.130459 | -0.131699 |
| H | -4.841661 | -0.357303 | -0.854831 |
| H | -4.252914 | 1.183663 | -1.438143 |
| C | -3.794066 | -0.087092 | 2.360518 |
| H | -4.409964 | 0.667776 | 2.846163 |
| H | -2.982991 | -0.332183 | 3.042866 |
| H | -4.405732 | -0.972536 | 2.240495 |

Compound **5**, HF/6-31++G(d,p) optimized geometric structure with short Si-C(iPr) distance
E(HF/6-31++G(d,p))=-1936.418494 hartrees
E(MP2/6-31++G(d,p))=-1939.706605 hartrees
Cartesian coordinates:

| | | | |
|---|---|---|---|
| Si | 0.000000 | 0.000000 | 0.000000 |
| Si | 0.000000 | 0.000000 | 2.428878 |
| C | 1.790699 | 0.000000 | 3.049195 |
| H | 2.353128 | -0.813886 | 2.599093 |
| H | 1.797262 | -0.153385 | 4.127009 |
| H | 2.325801 | 0.918974 | 2.842414 |
| C | -0.757922 | -1.643602 | 3.001013 |
| H | -1.797884 | -1.753902 | 2.708494 |
| H | -0.713641 | -1.694588 | 4.087819 |

| | | | |
|---|---|---|---|
| H | -0.217945 | -2.500447 | 2.609352 |
| C | -0.999943 | 1.370644 | 3.284893 |
| H | -2.066118 | 1.251384 | 3.108620 |
| H | -0.718850 | 2.373897 | 2.986778 |
| H | -0.847074 | 1.293369 | 4.359926 |
| C | -2.948536 | -0.172765 | -0.071730 |
| C | -2.333842 | -1.514188 | -0.377080 |
| C | -0.945048 | -1.583254 | -0.413746 |
| C | -0.342996 | -2.826167 | -0.609455 |
| C | -1.109006 | -3.966166 | -0.793467 |
| C | -2.494051 | -3.877000 | -0.783769 |
| C | -3.106247 | -2.651480 | -0.575311 |
| H | -4.180993 | -2.583189 | -0.562909 |
| H | -3.092694 | -4.757558 | -0.936811 |
| H | -0.629369 | -4.915776 | -0.951611 |
| H | 0.727567 | -2.913972 | -0.627074 |
| C | -2.103459 | 1.025213 | -0.533291 |
| H | -3.132490 | -0.092480 | 0.997967 |
| C | 1.275420 | 0.650639 | -0.989923 |
| Si | 1.991049 | -0.277095 | -2.448320 |
| C | 0.744102 | -1.122513 | -3.613838 |
| H | 1.298687 | -1.693433 | -4.357206 |
| H | 0.161487 | -0.379721 | -4.154570 |
| H | 0.052191 | -1.803760 | -3.133548 |
| C | 2.997712 | 0.796823 | -3.656434 |
| H | 3.431462 | 0.133648 | -4.403312 |
| H | 3.818111 | 1.339493 | -3.197855 |
| H | 2.375389 | 1.513068 | -4.185190 |
| C | 3.234169 | -1.604517 | -1.876307 |
| H | 3.666160 | -2.132741 | -2.724939 |
| H | 2.794777 | -2.347879 | -1.216807 |
| H | 4.050343 | -1.139151 | -1.327706 |
| Si | 2.067407 | 2.277835 | -0.551521 |
| C | 1.249232 | 3.181694 | 0.917534 |
| H | 1.719550 | 4.159200 | 1.005991 |
| H | 1.372326 | 2.689947 | 1.874210 |
| H | 0.187002 | 3.363294 | 0.763834 |
| C | 3.908484 | 2.134519 | -0.098432 |
| H | 4.329282 | 3.111471 | 0.134225 |
| H | 4.501285 | 1.709710 | -0.903728 |
| H | 4.045944 | 1.497750 | 0.772435 |
| C | 1.926132 | 3.588032 | -1.928747 |
| H | 2.273093 | 4.549048 | -1.551615 |
| H | 0.891361 | 3.717056 | -2.241508 |
| H | 2.507715 | 3.359939 | -2.813223 |
| C | -2.843752 | 2.321752 | -0.114018 |
| C | -1.898884 | 1.069974 | -2.049975 |
| H | -3.918010 | -0.080238 | -0.551750 |
| H | -2.872517 | 1.222390 | -2.507058 |
| H | -1.254601 | 1.892709 | -2.329660 |
| H | -3.821065 | 2.358186 | -0.584613 |

| | | | |
|---|---|---|---|
| H | -2.983146 | 2.371819 | 0.960007 |
| H | -2.289480 | 3.199860 | -0.425988 |
| H | -1.480275 | 0.164050 | -2.457433 |
| H | -1.209601 | 1.215962 | 0.059506 |

Compound **5b**, HF/6-31++G(d,p) optimized geometric structure with long Si-C(iPr) distance
E(HF/6-31++G(d,p))=-1936.465143 hartrees
E(MP2/6-31++G(d,p))=-1939.734984 hartrees
Cartesian coordinates:

| | | | |
|---|---|---|---|
| Si | 0.277494 | 0.541879 | 0.283676 |
| Si | -0.138073 | 2.917217 | 0.393025 |
| C | 0.856602 | 3.678544 | 1.816459 |
| H | 0.609828 | 3.197783 | 2.759864 |
| H | 0.600490 | 4.732212 | 1.911906 |
| H | 1.930018 | 3.611479 | 1.681891 |
| C | -1.968126 | 3.108315 | 0.847768 |
| H | -2.633618 | 2.744525 | 0.070954 |
| H | -2.180244 | 4.166955 | 0.989582 |
| H | -2.224076 | 2.592168 | 1.767131 |
| C | 0.128565 | 3.885125 | -1.213734 |
| H | -0.271657 | 3.360433 | -2.077355 |
| H | 1.170108 | 4.106404 | -1.409051 |
| H | -0.400473 | 4.833063 | -1.135374 |
| C | -2.361527 | -0.247193 | -1.321428 |
| C | -2.453998 | -0.509067 | 0.180349 |
| C | -1.312267 | -0.245645 | 0.967215 |
| C | -1.366114 | -0.484534 | 2.338906 |
| C | -2.507119 | -0.986581 | 2.950896 |
| C | -3.618150 | -1.249771 | 2.175453 |
| C | -3.587243 | -1.010838 | 0.805952 |
| H | -4.468163 | -1.227617 | 0.238024 |
| H | -4.514319 | -1.640518 | 2.624764 |
| H | -2.520385 | -1.167311 | 4.011110 |
| H | -0.503691 | -0.281558 | 2.952254 |
| C | -3.556674 | -0.440123 | -2.278963 |
| H | -2.031408 | 0.783501 | -1.450518 |
| C | 1.658799 | -0.420861 | -0.077385 |
| Si | 1.629042 | -2.289216 | 0.267536 |
| C | 0.025605 | -3.180467 | -0.213939 |
| H | 0.184359 | -4.251048 | -0.093834 |
| H | -0.225191 | -3.009409 | -1.258296 |
| H | -0.830784 | -2.908092 | 0.389882 |
| C | 2.954085 | -3.259881 | -0.689733 |
| H | 2.899081 | -4.296889 | -0.362706 |
| H | 3.972517 | -2.926440 | -0.523815 |
| H | 2.767654 | -3.251132 | -1.759968 |
| C | 1.958543 | -2.621890 | 2.107133 |
| H | 2.024940 | -3.691606 | 2.298069 |
| H | 1.167116 | -2.225559 | 2.736600 |
| H | 2.892892 | -2.169322 | 2.429523 |
| Si | 3.288709 | 0.293844 | -0.686873 |

| | | | |
|---|---|---|---|
| C | 3.314130 | 2.174969 | -0.912939 |
| H | 4.328409 | 2.460860 | -1.185666 |
| H | 3.056142 | 2.735570 | -0.021988 |
| H | 2.667031 | 2.492395 | -1.723814 |
| C | 4.692932 | -0.083330 | 0.534917 |
| H | 5.639782 | 0.289577 | 0.148290 |
| H | 4.819269 | -1.141894 | 0.737587 |
| H | 4.510094 | 0.410428 | 1.487085 |
| C | 3.764000 | -0.352330 | -2.408535 |
| H | 4.616087 | 0.212367 | -2.783617 |
| H | 2.944449 | -0.210011 | -3.109883 |
| H | 4.035754 | -1.400365 | -2.427163 |
| C | -3.998043 | -1.899375 | -2.452435 |
| C | -4.736973 | 0.503148 | -2.014957 |
| H | -1.549617 | -0.860063 | -1.704052 |
| H | -4.402968 | 1.535483 | -1.957248 |
| H | -5.455791 | 0.436820 | -2.826867 |
| H | -3.146828 | -2.537682 | -2.670341 |
| H | -4.493085 | -2.303763 | -1.577821 |
| H | -4.692021 | -1.980130 | -3.284467 |
| H | -5.263683 | 0.278740 | -1.095078 |
| H | -3.150578 | -0.141765 | -3.244693 |

Compound **3**, HF/6-31++G(d,p) optimized geometric structure
E(HF/6-31++G(d,p))=-2124.5784029 hartrees
E(MP2/6-31++G(d,p))=-2128.5176029 hartrees
Cartesian coordinates:

| | | | |
|---|---|---|---|
| Si | -0.012004 | 0.389285 | -0.493922 |
| Si | -0.825185 | 2.579764 | 0.221972 |
| C | -0.293163 | 2.953052 | 2.000685 |
| H | 0.763069 | 3.173248 | 2.099921 |
| H | -0.533115 | 2.126483 | 2.658579 |
| H | -0.844956 | 3.825819 | 2.347150 |
| C | -0.391695 | 4.111033 | -0.833480 |
| H | -1.022893 | 4.185196 | -1.715856 |
| H | 0.643115 | 4.171153 | -1.149455 |
| H | -0.597753 | 4.993664 | -0.230433 |
| C | -2.724159 | 2.531407 | 0.232927 |
| H | -3.157604 | 2.362620 | -0.748875 |
| H | -3.094812 | 3.491457 | 0.589628 |
| H | -3.098712 | 1.761558 | 0.896750 |
| N | -0.219638 | 0.457972 | -2.602098 |
| C | -1.676741 | 0.394554 | -2.824210 |
| C | -2.294332 | -0.521178 | -1.792622 |
| C | -1.638452 | -0.626001 | -0.565374 |
| C | -2.245455 | -1.383476 | 0.449639 |
| C | -1.637364 | -1.509964 | 1.835780 |
| N | -1.921492 | -0.381792 | 2.713666 |
| C | -3.316136 | -0.291063 | 3.097201 |
| H | -3.947924 | -0.196839 | 2.224196 |
| H | -3.464934 | 0.588733 | 3.713282 |

| | | | |
|---|---|---|---|
| H | -3.649713 | -1.165158 | 3.667663 |
| C | -1.069765 | -0.428987 | 3.888003 |
| H | -0.028010 | -0.417441 | 3.592326 |
| H | -1.245143 | -1.322403 | 4.496514 |
| H | -1.254768 | 0.439674 | 4.509983 |
| H | -1.978768 | -2.447617 | 2.286318 |
| H | -0.564101 | -1.573399 | 1.743605 |
| C | -3.433477 | -2.052638 | 0.178285 |
| C | -4.052098 | -1.962754 | -1.059957 |
| C | -3.485099 | -1.184522 | -2.051937 |
| H | -3.959793 | -1.100278 | -3.015229 |
| H | -4.967349 | -2.496645 | -1.245218 |
| H | -3.882899 | -2.659394 | 0.945462 |
| H | -1.891318 | 0.072400 | -3.839603 |
| H | -2.074975 | 1.397282 | -2.712766 |
| C | 0.426943 | -0.731956 | -3.191005 |
| H | -0.006489 | -1.630926 | -2.784049 |
| H | 1.479366 | -0.710095 | -2.961754 |
| H | 0.282902 | -0.724935 | -4.267772 |
| C | 0.374845 | 1.644834 | -3.236811 |
| H | -0.094777 | 2.541534 | -2.871561 |
| H | 0.251672 | 1.594951 | -4.315090 |
| H | 1.430153 | 1.678278 | -3.004883 |
| C | 1.536364 | -0.319760 | -0.050152 |
| Si | 1.925556 | -2.145419 | -0.100900 |
| C | 2.716095 | -2.759008 | 1.523059 |
| H | 2.881292 | -3.833892 | 1.467805 |
| H | 2.060489 | -2.572295 | 2.371019 |
| H | 3.673039 | -2.297974 | 1.745828 |
| C | 0.485234 | -3.376229 | -0.350985 |
| H | 0.938971 | -4.349589 | -0.533763 |
| H | -0.167239 | -3.166737 | -1.191497 |
| H | -0.143005 | -3.483725 | 0.526193 |
| C | 3.130062 | -2.661837 | -1.495996 |
| H | 3.532804 | -3.651192 | -1.283034 |
| H | 3.969184 | -1.987816 | -1.621235 |
| H | 2.619987 | -2.733022 | -2.454748 |
| Si | 2.940693 | 0.737986 | 0.562185 |
| C | 3.033409 | 0.874748 | 2.460690 |
| H | 3.851537 | 1.525873 | 2.766111 |
| H | 3.201434 | -0.096732 | 2.917771 |
| H | 2.116663 | 1.275892 | 2.882829 |
| C | 2.958469 | 2.533027 | -0.086464 |
| H | 3.880187 | 3.005855 | 0.248380 |
| H | 2.145167 | 3.151950 | 0.269757 |
| H | 2.958878 | 2.571286 | -1.173855 |
| C | 4.670826 | 0.131873 | 0.031203 |
| H | 5.414670 | 0.790951 | 0.476370 |
| H | 4.798587 | 0.183915 | -1.047769 |
| H | 4.913079 | -0.878488 | 0.342464 |

Compound **3**, B3LYP/6-31++G(d,p) optimized geometric structure

E(B3LYP/6-31++G(d,p))=-2133.6991301 hartrees

Cartesian coordinates:

| | | | |
|---|---|---|---|
| Si | -0.004452 | 0.400605 | -0.482180 |
| Si | -0.772032 | 2.597533 | 0.212026 |
| C | -0.235601 | 2.960243 | 1.994352 |
| H | 0.845360 | 3.072402 | 2.106419 |
| H | -0.571577 | 2.160711 | 2.659887 |
| H | -0.707406 | 3.896541 | 2.319577 |
| C | -0.298732 | 4.113740 | -0.853702 |
| H | -0.916443 | 4.187843 | -1.756175 |
| H | 0.752031 | 4.146483 | -1.152673 |
| H | -0.500031 | 5.014945 | -0.260288 |
| C | -2.674419 | 2.567939 | 0.215800 |
| H | -3.105265 | 2.378950 | -0.773618 |
| H | -3.046267 | 3.542714 | 0.556893 |
| H | -3.052003 | 1.801674 | 0.897819 |
| N | -0.238244 | 0.458551 | -2.667669 |
| C | -1.709309 | 0.380479 | -2.859036 |
| C | -2.307816 | -0.522672 | -1.800571 |
| C | -1.636907 | -0.605522 | -0.564198 |
| C | -2.238242 | -1.352338 | 0.474621 |
| C | -1.614521 | -1.450025 | 1.856047 |
| N | -1.928032 | -0.313251 | 2.737078 |
| C | -3.340169 | -0.246980 | 3.099633 |
| H | -3.961506 | -0.154387 | 2.205723 |
| H | -3.512999 | 0.632837 | 3.727294 |
| H | -3.676592 | -1.141143 | 3.661920 |
| C | -1.092271 | -0.362342 | 3.935259 |
| H | -0.035770 | -0.346465 | 3.653499 |
| H | -1.276773 | -1.268663 | 4.544571 |
| H | -1.295231 | 0.511957 | 4.561875 |
| H | -1.927546 | -2.403939 | 2.326227 |
| H | -0.526967 | -1.475003 | 1.756526 |
| C | -3.438385 | -2.033388 | 0.225311 |
| C | -4.071485 | -1.967269 | -1.017250 |
| C | -3.507468 | -1.199943 | -2.035661 |
| H | -3.993381 | -1.134191 | -3.006817 |
| H | -4.994609 | -2.513048 | -1.189370 |
| H | -3.877708 | -2.635638 | 1.016834 |
| H | -1.949734 | 0.042459 | -3.876747 |
| H | -2.107231 | 1.396785 | -2.751695 |
| C | 0.421082 | -0.746683 | -3.226443 |
| H | -0.035838 | -1.644283 | -2.811672 |
| H | 1.475729 | -0.728957 | -2.952324 |
| H | 0.313128 | -0.756916 | -4.318858 |
| C | 0.349492 | 1.652106 | -3.312759 |
| H | -0.141647 | 2.553254 | -2.951755 |
| H | 0.241957 | 1.593863 | -4.403798 |
| H | 1.411152 | 1.701254 | -3.060652 |
| C | 1.539645 | -0.338101 | -0.049710 |

| | | | |
|---|---|---|---|
| Si | 1.890844 | -2.174349 | -0.097671 |
| C | 2.658054 | -2.793655 | 1.537794 |
| H | 2.822303 | -3.877466 | 1.485162 |
| H | 1.988307 | -2.600174 | 2.383982 |
| H | 3.621149 | -2.327998 | 1.769873 |
| C | 0.412547 | -3.356703 | -0.363099 |
| H | 0.831667 | -4.356340 | -0.536668 |
| H | -0.221754 | -3.117375 | -1.221719 |
| H | -0.240793 | -3.430686 | 0.510655 |
| C | 3.105027 | -2.706459 | -1.479658 |
| H | 3.419794 | -3.744440 | -1.309461 |
| H | 4.006365 | -2.090109 | -1.525005 |
| H | 2.631325 | -2.675495 | -2.468260 |
| Si | 2.957511 | 0.706604 | 0.565148 |
| C | 3.020116 | 0.833995 | 2.467924 |
| H | 3.840808 | 1.484625 | 2.796793 |
| H | 3.175379 | -0.151582 | 2.920695 |
| H | 2.086406 | 1.236573 | 2.874205 |
| C | 2.998091 | 2.498577 | -0.096594 |
| H | 3.931614 | 2.969833 | 0.236381 |
| H | 2.180552 | 3.130579 | 0.256422 |
| H | 2.995977 | 2.523423 | -1.193109 |
| C | 4.679974 | 0.059612 | 0.051832 |
| H | 5.440910 | 0.724306 | 0.480388 |
| H | 4.807392 | 0.073607 | -1.036831 |
| H | 4.901301 | -0.953596 | 0.400122 |

Compound **3**, X-Ray structure
(position of the hydrogen atoms optimized with HF/6-31++G(d,p)
E(HF/6-31++G(d,p))=-2124.566999 hartrees
Cartesian coordinates:

| | | | |
|---|---|---|---|
| Si | 0.000000 | -0.000000 | -0.000000 |
| Si | 2.402367 | 0.000000 | -0.000002 |
| C | 3.025269 | 1.761353 | 0.000001 |
| H | 2.432744 | 2.440998 | 0.593995 |
| H | 3.050395 | 2.146493 | -1.009401 |
| H | 4.042491 | 1.792229 | 0.388477 |
| C | 3.350014 | -0.917450 | 1.357440 |
| H | 3.356250 | -1.994592 | 1.205324 |
| H | 3.008605 | -0.722757 | 2.367117 |
| H | 4.389355 | -0.598020 | 1.302990 |
| C | 2.980893 | -0.805921 | -1.604769 |
| H | 2.834210 | -1.883105 | -1.614073 |
| H | 4.051073 | -0.635180 | -1.720769 |
| H | 2.485823 | -0.401831 | -2.475863 |
| N | -0.477444 | -1.913092 | 0.504091 |
| C | -0.087994 | -2.740126 | -0.678442 |
| C | -0.377782 | -1.938931 | -1.926168 |
| C | -0.374230 | -0.553480 | -1.770490 |
| C | -0.549649 | 0.244990 | -2.920210 |
| C | -0.485879 | 1.741347 | -2.794610 |

| | | | |
|---|---|---|---|
| N | 0.866788 | 2.204106 | -2.496119 |
| C | 1.752481 | 2.054227 | -3.639229 |
| H | 1.762460 | 1.031251 | -3.987441 |
| H | 2.764519 | 2.325571 | -3.360518 |
| H | 1.452041 | 2.692078 | -4.477128 |
| C | 0.840772 | 3.593106 | -2.064418 |
| H | 0.241933 | 3.687737 | -1.169696 |
| H | 0.429250 | 4.255292 | -2.832956 |
| H | 1.845008 | 3.930184 | -1.839183 |
| H | -0.868305 | 2.208382 | -3.707904 |
| H | -1.114004 | 2.063997 | -1.982627 |
| C | -0.757560 | -0.369239 | -4.143350 |
| C | -0.781069 | -1.744049 | -4.265170 |
| C | -0.587400 | -2.534570 | -3.157299 |
| H | -0.598824 | -3.608172 | -3.249998 |
| H | -0.949948 | -2.194975 | -5.227178 |
| H | -0.905025 | 0.239302 | -5.019756 |
| H | -0.614776 | -3.689276 | -0.656116 |
| H | 0.972103 | -2.950456 | -0.601089 |
| C | -1.940210 | -2.008919 | 0.714829 |
| H | -2.461820 | -1.728310 | -0.182835 |
| H | -2.221787 | -1.349004 | 1.517518 |
| H | -2.198426 | -3.032675 | 0.969075 |
| C | 0.197562 | -2.415928 | 1.739849 |
| H | 1.264809 | -2.392933 | 1.613879 |
| H | -0.121423 | -3.433316 | 1.940933 |
| H | -0.081944 | -1.783564 | 2.570213 |
| C | -1.009618 | 1.165119 | 0.846319 |
| Si | -2.749069 | 1.538059 | 0.378569 |
| C | -3.050060 | 3.376250 | 0.164620 |
| H | -4.065038 | 3.554261 | -0.189070 |
| H | -2.372608 | 3.824687 | -0.558252 |
| H | -2.940217 | 3.930518 | 1.092685 |
| C | -3.436510 | 0.777009 | -1.206069 |
| H | -4.520373 | 0.876552 | -1.148453 |
| H | -3.229861 | -0.272711 | -1.368074 |
| H | -3.134429 | 1.298498 | -2.107243 |
| C | -4.031209 | 0.975780 | 1.660660 |
| H | -5.001740 | 1.409722 | 1.419292 |
| H | -3.800617 | 1.252511 | 2.679605 |
| H | -4.168395 | -0.104535 | 1.643041 |
| Si | -0.371328 | 2.120694 | 2.279205 |
| C | 0.182696 | 3.868324 | 1.886847 |
| H | 0.541680 | 4.366962 | 2.787208 |
| H | -0.628231 | 4.473819 | 1.491484 |
| H | 0.986835 | 3.904226 | 1.159655 |
| C | 1.102253 | 1.337740 | 3.152166 |
| H | 1.290606 | 1.893529 | 4.069855 |
| H | 2.024505 | 1.367328 | 2.586877 |
| H | 0.920329 | 0.306407 | 3.446117 |
| C | -1.627809 | 2.322839 | 3.667939 |

| | | | |
|---|---|---|---|
| H | -1.153060 | 2.845767 | 4.497735 |
| H | -1.975965 | 1.366005 | 4.049311 |
| H | -2.500541 | 2.905945 | 3.392077 |

**Calculation of the rotational barrier about the Si=C double bond**

All following geometric structures were optimized with HF/6-31G(d)-method.

Compound **1**, structure representing minimum of the rotational barrier
Cartesian coordinates:

| | | | |
|---|---|---|---|
| Si | 0.297319 | 0.278388 | 0.058721 |
| Si | 1.029976 | 2.329350 | -1.002567 |
| C | 0.921381 | 3.997684 | -0.088338 |
| H | -0.040523 | 4.207180 | 0.361400 |
| H | 1.125746 | 4.791733 | -0.803875 |
| H | 1.681279 | 4.077041 | 0.685718 |
| C | 0.084119 | 2.434180 | -2.646355 |
| H | 0.244481 | 1.538206 | -3.240344 |
| H | 0.444627 | 3.279499 | -3.229116 |
| H | -0.986374 | 2.548651 | -2.522215 |
| C | 2.868196 | 2.166842 | -1.473447 |
| H | 3.064590 | 1.290534 | -2.081727 |
| H | 3.528847 | 2.117496 | -0.612264 |
| H | 3.161292 | 3.041246 | -2.051748 |
| N | 1.036114 | 0.363034 | 2.024705 |
| C | 2.503152 | 0.256199 | 1.869104 |
| C | 2.806815 | -0.693857 | 0.733225 |
| C | 1.825093 | -0.819062 | -0.248498 |
| C | 2.108436 | -1.612339 | -1.357572 |
| C | 3.319182 | -2.277319 | -1.467567 |
| C | 4.271726 | -2.158599 | -0.466867 |
| C | 4.016147 | -1.364074 | 0.637816 |
| H | 4.756246 | -1.267421 | 1.414263 |
| H | 5.207410 | -2.682360 | -0.547159 |
| H | 3.517453 | -2.891915 | -2.327494 |
| H | 1.380892 | -1.721629 | -2.140794 |
| H | 2.957101 | -0.054870 | 2.805270 |
| H | 2.883810 | 1.245122 | 1.638953 |
| C | 0.527285 | -0.807714 | 2.771206 |
| H | 0.861712 | -1.716212 | 2.298635 |
| H | -0.550567 | -0.789872 | 2.768170 |
| H | 0.899633 | -0.774281 | 3.790519 |
| C | 0.658415 | 1.579463 | 2.760207 |
| H | 0.994045 | 2.456569 | 2.230698 |
| H | 1.100136 | 1.572717 | 3.751847 |
| H | -0.416990 | 1.615863 | 2.856204 |
| C | -1.342942 | -0.334561 | -0.014988 |
| Si | -1.708747 | -2.124376 | -0.384838 |
| C | -3.414749 | -2.726555 | 0.224054 |
| H | -3.479882 | -2.725643 | 1.308914 |
| H | -3.547672 | -3.756493 | -0.102762 |

| | | | |
|---|---|---|---|
| H | -4.259346 | -2.162206 | -0.156399 |
| C | -1.720963 | -2.488457 | -2.258338 |
| H | -0.763811 | -2.285962 | -2.731809 |
| H | -2.459166 | -1.871708 | -2.765111 |
| H | -1.969313 | -3.529133 | -2.459724 |
| C | -0.552569 | -3.421035 | 0.409580 |
| H | -0.841239 | -4.406911 | 0.049161 |
| H | -0.670695 | -3.437702 | 1.491059 |
| H | 0.501034 | -3.296684 | 0.190424 |
| Si | -2.818455 | 0.776090 | 0.140119 |
| C | -3.873516 | 0.434299 | 1.696268 |
| H | -4.700563 | 1.140274 | 1.753384 |
| H | -3.280842 | 0.563028 | 2.601366 |
| H | -4.297301 | -0.562270 | 1.729968 |
| C | -2.443591 | 2.637544 | 0.341208 |
| H | -3.391911 | 3.151367 | 0.485484 |
| H | -1.972372 | 3.091310 | -0.522756 |
| H | -1.833721 | 2.863154 | 1.212334 |
| C | -3.993245 | 0.706986 | -1.359289 |
| H | -4.853368 | 1.356719 | -1.207559 |
| H | -4.374702 | -0.288995 | -1.562310 |
| H | -3.484297 | 1.043252 | -2.260062 |

E(HF/6-31G(d)) = -1952.377657 hartrees
ZPE(HF/6-31G(d)) = 0.575626 hartrees
$E_{vib}$(HF/6-31G(d)) = 19.052 kcal/mol
$E_{rot}$(HF/6-31G(d)) =0.889 kcal/mol
S(HF/6-31G(d)) = 199.679 cal/(mol K)
E(HF/6-31++G(d,p)) = -1952.4602707 hartrees
E(MP2/6-31++G(d,p)) = -1955.7701315 hartrees

Compound **1**, structure representing maximum of the rotational barrier
Cartesian coordinates:

| | | | |
|---|---|---|---|
| Si | -0.409478 | 0.103151 | -0.165981 |
| Si | -1.118740 | 2.265462 | -1.012863 |
| C | -0.989830 | 3.665264 | 0.264790 |
| H | -1.651733 | 3.523344 | 1.113642 |
| H | -1.285372 | 4.591074 | -0.225105 |
| H | 0.014494 | 3.806165 | 0.645691 |
| C | -2.916698 | 2.390078 | -1.651119 |
| H | -3.104357 | 1.844708 | -2.572053 |
| H | -3.132658 | 3.435246 | -1.861527 |
| H | -3.640639 | 2.059026 | -0.910947 |
| C | 0.043807 | 2.731898 | -2.443769 |
| H | -0.091643 | 2.117325 | -3.329186 |
| H | 1.082057 | 2.639058 | -2.141706 |
| H | -0.126777 | 3.764640 | -2.740668 |
| N | -1.262307 | -1.164561 | -1.545182 |
| C | -2.714221 | -1.121044 | -1.219825 |
| C | -2.846492 | -1.153355 | 0.280982 |
| C | -1.760185 | -0.631904 | 0.982702 |
| C | -1.802194 | -0.686210 | 2.372878 |

| | | | |
|---|---|---|---|
| C | -2.899721 | -1.220009 | 3.032336 |
| C | -3.974342 | -1.715618 | 2.312243 |
| C | -3.944683 | -1.693634 | 0.926894 |
| H | -4.765194 | -2.103293 | 0.362268 |
| H | -4.822369 | -2.133188 | 2.824965 |
| H | -2.912357 | -1.255487 | 4.107152 |
| H | -0.976362 | -0.321869 | 2.951790 |
| H | -3.215906 | -1.954987 | -1.699622 |
| H | -3.124347 | -0.211378 | -1.631091 |
| C | -0.793605 | -2.556839 | -1.330401 |
| H | -0.943792 | -2.840582 | -0.302402 |
| H | 0.247321 | -2.632157 | -1.569682 |
| H | -1.357055 | -3.223812 | -1.974182 |
| C | -1.039176 | -0.800314 | -2.958020 |
| H | -1.477009 | 0.163068 | -3.161602 |
| H | -1.500118 | -1.537551 | -3.606885 |
| H | 0.018413 | -0.758381 | -3.159142 |
| C | 1.341913 | -0.077854 | 0.013758 |
| Si | 2.563644 | -1.314869 | -0.609121 |
| C | 2.506969 | -1.702014 | -2.495450 |
| H | 3.441203 | -2.194407 | -2.757352 |
| H | 2.470684 | -0.776823 | -3.067397 |
| H | 1.717292 | -2.348454 | -2.864523 |
| C | 4.371614 | -0.699772 | -0.532175 |
| H | 5.024078 | -1.514999 | -0.840466 |
| H | 4.726250 | -0.357512 | 0.430740 |
| H | 4.520639 | 0.111790 | -1.240484 |
| C | 2.563851 | -3.005957 | 0.280713 |
| H | 3.284184 | -3.687300 | -0.169283 |
| H | 1.595548 | -3.500055 | 0.266930 |
| H | 2.838620 | -2.886842 | 1.325443 |
| Si | 2.030503 | 0.938660 | 1.418824 |
| C | 0.721985 | 1.770733 | 2.563264 |
| H | 1.070425 | 2.761228 | 2.846918 |
| H | 0.630523 | 1.200258 | 3.483793 |
| H | -0.279348 | 1.897668 | 2.170800 |
| C | 3.010421 | -0.059575 | 2.722638 |
| H | 3.335113 | 0.612376 | 3.516162 |
| H | 3.891245 | -0.575879 | 2.361446 |
| H | 2.363406 | -0.806042 | 3.179221 |
| C | 3.148502 | 2.378542 | 0.858378 |
| H | 3.560429 | 2.910546 | 1.714605 |
| H | 2.586281 | 3.100174 | 0.268586 |
| H | 3.981124 | 2.048449 | 0.246472 |

E(HF/6-31G(d)) = - 1952.3523164 hartrees
ZPE(HF/6-31G(d)) = 0.577163 hartrees
$E_{vib}$(HF/6-31G(d)) = 18.745 kcal/mol
$E_{rot}$(HF/6-31G(d)) = 0.889 kcal/mol
S(HF/6-31G(d)) = 196.824 cal/(mol K)
E(HF/6-31++G(d,p)) = -1952.4354464 hartrees
E(MP2/6-31++G(d,p)) = -1955.7456573 hartrees

Compound **2**, structure representing minimum of the rotational barrier

Cartesian coordinates:

| | | | |
|---|---|---|---|
| Si | -0.365637 | -0.636484 | -0.545716 |
| N | -1.211352 | -1.765372 | 0.999087 |
| C | -2.664088 | -1.778399 | 0.706592 |
| C | -3.055648 | -0.461437 | 0.073206 |
| C | -2.047105 | 0.237135 | -0.587404 |
| C | -2.389045 | 1.409425 | -1.256568 |
| C | -3.692475 | 1.878770 | -1.246783 |
| C | -4.677141 | 1.180049 | -0.564365 |
| C | -4.360503 | 0.006070 | 0.097816 |
| H | -5.125916 | -0.537605 | 0.625592 |
| H | -5.686951 | 1.549459 | -0.547841 |
| H | -3.939960 | 2.788845 | -1.763382 |
| H | -1.635364 | 1.965627 | -1.784023 |
| H | -3.223604 | -1.983655 | 1.614057 |
| H | -2.857673 | -2.591857 | 0.017717 |
| C | -0.969302 | -1.077465 | 2.284822 |
| H | -1.429581 | -0.103251 | 2.267400 |
| H | 0.092580 | -0.959719 | 2.430725 |
| H | -1.395463 | -1.661173 | 3.094653 |
| C | -0.666293 | -3.129826 | 1.089018 |
| H | -0.845281 | -3.664139 | 0.169211 |
| H | -1.131973 | -3.668761 | 1.908104 |
| H | 0.398906 | -3.075197 | 1.265772 |
| C | 1.139989 | 0.137407 | -0.133951 |
| Si | 1.212453 | 1.877962 | 0.521957 |
| C | -0.241841 | 2.438674 | 1.627766 |
| H | -0.117687 | 3.498693 | 1.842212 |
| H | -0.232797 | 1.924933 | 2.586495 |
| H | -1.225958 | 2.316060 | 1.190333 |
| C | 2.706675 | 2.217503 | 1.659868 |
| H | 2.677543 | 3.259467 | 1.973935 |
| H | 3.674291 | 2.051789 | 1.198557 |
| H | 2.666098 | 1.610374 | 2.561085 |
| C | 1.325322 | 3.181800 | -0.866170 |
| H | 1.434769 | 4.185617 | -0.459113 |
| H | 0.437700 | 3.182989 | -1.494601 |
| H | 2.174731 | 2.997370 | -1.517964 |
| Si | 2.781072 | -0.665088 | -0.463012 |
| C | 2.758940 | -2.281749 | -1.480242 |
| H | 3.790867 | -2.604979 | -1.602723 |
| H | 2.342441 | -2.161965 | -2.475445 |
| H | 2.234141 | -3.099418 | -0.991783 |
| C | 3.978273 | 0.444695 | -1.447737 |
| H | 4.931639 | -0.060849 | -1.590875 |
| H | 4.188690 | 1.397156 | -0.972213 |
| H | 3.572768 | 0.660053 | -2.433964 |
| C | 3.693137 | -1.197637 | 1.129271 |
| H | 4.649670 | -1.659534 | 0.890077 |

| | | | |
|---|---|---|---|
| H | 3.110946 | -1.935221 | 1.680833 |
| H | 3.890698 | -0.374563 | 1.807235 |
| C | -0.515874 | -1.940148 | -1.915431 |
| H | 0.144706 | -2.790719 | -1.827254 |
| H | -1.535317 | -2.305626 | -2.002921 |
| H | -0.278747 | -1.451248 | -2.856948 |

E(HF/6-31G(d)) = -1584.2209157 hartrees
ZPE(HF/6-31G(d)) = 0.495523 hartrees
$E_{vib}$(HF/6-31G(d)) = 15.209 kcal/mol
$E_{rot}$(HF/6-31G(d)) = 0.889 kcal/mol
S(HF/6-31G(d)) = 172.687 cal/(mol K)
E(HF/6-31++G(d,p)) = -1584.291707 hartrees
E(MP2/6-31++G(d,p)) = -1587.195066 hartrees

Compound **2**, structure representing maximum of the rotational barrier
Cartesian coordinates:

| | | | |
|---|---|---|---|
| Si | -0.473437 | 0.009811 | 0.761785 |
| N | -1.522225 | 1.753881 | 0.693050 |
| C | -2.944705 | 1.316504 | 0.808690 |
| C | -3.117889 | 0.066727 | -0.022288 |
| C | -1.967308 | -0.702761 | -0.181550 |
| C | -2.048164 | -1.850486 | -0.962822 |
| C | -3.249789 | -2.226630 | -1.544531 |
| C | -4.385003 | -1.452038 | -1.362838 |
| C | -4.320593 | -0.292370 | -0.606184 |
| H | -5.196965 | 0.321617 | -0.483808 |
| H | -5.313566 | -1.741430 | -1.821630 |
| H | -3.299578 | -3.116570 | -2.146253 |
| H | -1.172664 | -2.451629 | -1.129088 |
| H | -3.593596 | 2.124119 | 0.487280 |
| H | -3.154261 | 1.126658 | 1.852349 |
| C | -1.364538 | 2.436454 | -0.614018 |
| H | -1.627597 | 1.760550 | -1.411020 |
| H | -0.348531 | 2.755381 | -0.739328 |
| H | -2.016893 | 3.302188 | -0.646312 |
| C | -1.172567 | 2.697594 | 1.774873 |
| H | -1.348564 | 2.236889 | 2.733695 |
| H | -1.778667 | 3.593551 | 1.693733 |
| H | -0.129705 | 2.962625 | 1.696566 |
| C | 1.190513 | 0.013740 | 0.195910 |
| Si | 2.032444 | -1.632356 | 0.409841 |
| C | 1.002517 | -2.984224 | 1.301939 |
| H | 1.484952 | -3.938483 | 1.099203 |
| H | -0.030714 | -3.086155 | 0.979809 |
| H | 1.003222 | -2.860785 | 2.380879 |
| C | 2.447095 | -2.476906 | -1.253939 |
| H | 3.040947 | -3.375873 | -1.095866 |
| H | 2.993171 | -1.845624 | -1.946873 |
| H | 1.531242 | -2.779451 | -1.758883 |
| C | 3.627242 | -1.610536 | 1.454114 |
| H | 3.961056 | -2.629304 | 1.645560 |

| | | | |
|---|---|---|---|
| H | 3.444103 | -1.141222 | 2.418375 |
| H | 4.451413 | -1.084072 | 0.987322 |
| Si | 2.134775 | 1.247106 | -0.796947 |
| C | 2.233888 | 3.011480 | -0.038576 |
| H | 2.982995 | 3.584998 | -0.581184 |
| H | 2.569784 | 2.945680 | 0.994367 |
| H | 1.330077 | 3.613427 | -0.045842 |
| C | 4.000006 | 0.879154 | -0.959271 |
| H | 4.423450 | 1.607320 | -1.648992 |
| H | 4.250371 | -0.102686 | -1.343099 |
| H | 4.514144 | 1.004024 | -0.010785 |
| C | 1.560636 | 1.449656 | -2.610601 |
| H | 2.120995 | 2.233246 | -3.118184 |
| H | 0.504958 | 1.679437 | -2.723764 |
| H | 1.735913 | 0.523258 | -3.153246 |
| C | -0.798345 | -0.397237 | 2.590750 |
| H | -0.110540 | 0.142837 | 3.234706 |
| H | -1.812497 | -0.202148 | 2.926176 |
| H | -0.623808 | -1.452119 | 2.759330 |

E(HF/6-31G(d)) = -1584.200896 hartrees
ZPE(HF/6-31G(d)) = 0.495853hartrees
$E_{vib}$(HF/6-31G(d)) = 15.246 kcal/mol
$E_{rot}$(HF/6-31G(d)) = 0.889 kcal/mol
S(HF/6-31G(d)) = 173.375 cal/(mol K)
E(HF/6-31++G(d,p)) = -1584.269842 hartrees
E(MP2/6-31++G(d,p)) = -1587.173683 hartrees

Compound **3**, structure representing minimum of the rotational barrier
Cartesian coordinates:

| | | | |
|---|---|---|---|
| Si | -0.006501 | 0.389604 | -0.486303 |
| Si | -0.793022 | 2.580618 | 0.224024 |
| C | -0.262157 | 2.943720 | 2.006995 |
| H | 0.797942 | 3.139250 | 2.114736 |
| H | -0.523630 | 2.122259 | 2.662683 |
| H | -0.794382 | 3.827317 | 2.355143 |
| C | -0.339428 | 4.111356 | -0.826518 |
| H | -0.965279 | 4.195784 | -1.711480 |
| H | 0.696409 | 4.163125 | -1.139759 |
| H | -0.538020 | 4.995893 | -0.224476 |
| C | -2.694308 | 2.555864 | 0.232294 |
| H | -3.131198 | 2.393772 | -0.748895 |
| H | -3.057441 | 3.517392 | 0.591055 |
| H | -3.078363 | 1.789166 | 0.893707 |
| N | -0.207022 | 0.467166 | -2.605022 |
| C | -1.663969 | 0.424213 | -2.827590 |
| C | -2.294034 | -0.489318 | -1.801531 |
| C | -1.644403 | -0.604404 | -0.572514 |
| C | -2.263997 | -1.357447 | 0.437396 |
| C | -1.665761 | -1.491730 | 1.827023 |
| N | -1.941978 | -0.359028 | 2.701197 |
| C | -3.337758 | -0.253774 | 3.074766 |

| | | | |
|---|---|---|---|
| H | -3.961258 | -0.158048 | 2.196771 |
| H | -3.482662 | 0.630379 | 3.684603 |
| H | -3.684733 | -1.120355 | 3.646654 |
| C | -1.100873 | -0.414514 | 3.882039 |
| H | -0.057287 | -0.414105 | 3.594292 |
| H | -1.289190 | -1.303871 | 4.490664 |
| H | -1.280980 | 0.456957 | 4.500679 |
| H | -2.019793 | -2.424276 | 2.276227 |
| H | -0.593282 | -1.568006 | 1.742993 |
| C | -3.457311 | -2.012043 | 0.159106 |
| C | -4.069318 | -1.911333 | -1.080096 |
| C | -3.490491 | -1.137902 | -2.066209 |
| H | -3.960420 | -1.044609 | -3.030596 |
| H | -4.990063 | -2.433411 | -1.270164 |
| H | -3.916381 | -2.614797 | 0.923227 |
| H | -1.881904 | 0.113456 | -3.845267 |
| H | -2.047490 | 1.431465 | -2.710503 |
| C | 0.422850 | -0.731802 | -3.190154 |
| H | -0.025175 | -1.622491 | -2.782717 |
| H | 1.474164 | -0.725898 | -2.958076 |
| H | 0.282462 | -0.725208 | -4.266970 |
| C | 0.407646 | 1.644667 | -3.234821 |
| H | -0.052667 | 2.547461 | -2.873795 |
| H | 0.293096 | 1.597309 | -4.313609 |
| H | 1.460637 | 1.664520 | -2.993421 |
| C | 1.529244 | -0.340332 | -0.042812 |
| Si | 1.894861 | -2.169446 | -0.099188 |
| C | 2.676906 | -2.799747 | 1.524205 |
| H | 2.833343 | -3.875526 | 1.467787 |
| H | 2.023203 | -2.611338 | 2.373074 |
| H | 3.637421 | -2.349275 | 1.752906 |
| C | 0.439510 | -3.384151 | -0.354093 |
| H | 0.879180 | -4.365443 | -0.525914 |
| H | -0.203344 | -3.174426 | -1.201872 |
| H | -0.199614 | -3.478561 | 0.516600 |
| C | 3.093372 | -2.701979 | -1.495425 |
| H | 3.478939 | -3.698694 | -1.286894 |
| H | 3.945826 | -2.044603 | -1.619079 |
| H | 2.586360 | -2.761772 | -2.456378 |
| Si | 2.945315 | 0.696974 | 0.574144 |
| C | 3.041148 | 0.827990 | 2.474350 |
| H | 3.864178 | 1.470678 | 2.783115 |
| H | 3.201511 | -0.144632 | 2.931498 |
| H | 2.129639 | 1.235678 | 2.901607 |
| C | 2.987673 | 2.494559 | -0.070194 |
| H | 3.908439 | 2.961438 | 0.274163 |
| H | 2.175665 | 3.121705 | 0.274723 |
| H | 3.001246 | 2.535849 | -1.157387 |
| C | 4.669190 | 0.072445 | 0.040136 |
| H | 5.423738 | 0.720495 | 0.482766 |
| H | 4.796772 | 0.123795 | -1.038590 |

| | | | |
|---|---|---|---|
| H | 4.902006 | -0.941104 | 0.348011 |

E(HF/6-31G(d)) = -2124.484345 hartrees
ZPE(HF/6-31G(d)) = 0.686400 hartrees
$E_{vib}$(HF/6-31G(d)) = 21.973 kcal/mol
$E_{rot}$(HF/6-31G(d)) = 0.889 kcal/mol
S(HF/6-31G(d)) = 218.883 cal/(mol K)
E(HF/6-31++G(d,p)) = -2124.578921 hartrees
E(MP2/6-31++G(d,p)) = -2128.522059 hartrees

Compound **3**, structure representing maximum of the rotational barrier
Cartesian coordinates:

| | | | |
|---|---|---|---|
| Si | 0.002304 | -0.567128 | 0.240120 |
| Si | 1.013864 | 0.150582 | 2.407539 |
| C | 0.762455 | 1.983048 | 2.833091 |
| H | -0.257821 | 2.279773 | 3.028970 |
| H | 1.156402 | 2.621095 | 2.050171 |
| H | 1.340978 | 2.179103 | 3.734410 |
| C | 0.558529 | -0.849544 | 3.977663 |
| H | 1.101169 | -1.790664 | 4.034126 |
| H | -0.497325 | -1.065584 | 4.097093 |
| H | 0.864565 | -0.267907 | 4.844545 |
| C | 2.920741 | 0.048489 | 2.338586 |
| H | 3.339750 | -0.947723 | 2.252595 |
| H | 3.296821 | 0.469486 | 3.269476 |
| H | 3.327727 | 0.643177 | 1.528298 |
| N | 0.274491 | -2.594664 | 0.368076 |
| C | 1.749552 | -2.695419 | 0.515403 |
| C | 2.401143 | -1.705430 | -0.425418 |
| C | 1.678404 | -0.537407 | -0.703074 |
| C | 2.247216 | 0.392900 | -1.581954 |
| C | 1.540799 | 1.663429 | -2.018275 |
| N | 1.716977 | 2.799134 | -1.119969 |
| C | 3.098171 | 3.185918 | -0.918824 |
| H | 3.663385 | 2.379688 | -0.473175 |
| H | 3.135116 | 4.031383 | -0.241656 |
| H | 3.596275 | 3.479388 | -1.849024 |
| C | 0.950889 | 3.928376 | -1.611345 |
| H | -0.081721 | 3.642483 | -1.751792 |
| H | 1.334719 | 4.306254 | -2.564348 |
| H | 0.981396 | 4.737394 | -0.891070 |
| H | 1.892752 | 1.914681 | -3.023901 |
| H | 0.480180 | 1.470270 | -2.084515 |
| C | 3.504222 | 0.126664 | -2.122904 |
| C | 4.207745 | -1.023775 | -1.817773 |
| C | 3.649252 | -1.957049 | -0.963758 |
| H | 4.173402 | -2.869593 | -0.735022 |
| H | 5.172601 | -1.199140 | -2.258944 |
| H | 3.933942 | 0.833112 | -2.811145 |
| H | 2.063921 | -3.714924 | 0.319083 |
| H | 1.993103 | -2.475600 | 1.545219 |
| C | -0.111474 | -3.350225 | -0.846025 |

| | | | |
|---|---|---|---|
| H | 0.422398 | -2.971836 | -1.699804 |
| H | -1.168744 | -3.264059 | -1.011948 |
| H | 0.141758 | -4.394924 | -0.701979 |
| C | -0.430780 | -3.199908 | 1.516287 |
| H | -0.132519 | -2.722287 | 2.431438 |
| H | -0.199414 | -4.258006 | 1.573778 |
| H | -1.494641 | -3.074105 | 1.385974 |
| C | -1.489122 | 0.161870 | -0.417593 |
| Si | -2.691098 | -0.789016 | -1.474779 |
| C | -4.000027 | 0.229451 | -2.424282 |
| H | -4.316018 | -0.369587 | -3.276583 |
| H | -3.586582 | 1.153969 | -2.820041 |
| H | -4.892119 | 0.475148 | -1.865359 |
| C | -1.796125 | -1.617028 | -2.972082 |
| H | -2.084845 | -2.652725 | -3.144806 |
| H | -0.714388 | -1.574573 | -2.913843 |
| H | -2.068759 | -1.067354 | -3.868976 |
| C | -3.751278 | -2.117610 | -0.590521 |
| H | -4.466118 | -2.546923 | -1.290450 |
| H | -4.325157 | -1.672835 | 0.219205 |
| H | -3.192917 | -2.945453 | -0.161081 |
| Si | -2.387103 | 1.358287 | 0.727895 |
| C | -1.635015 | 3.106774 | 0.725466 |
| H | -1.952945 | 3.680478 | 1.594149 |
| H | -2.002063 | 3.632891 | -0.153427 |
| H | -0.555885 | 3.125814 | 0.681663 |
| C | -2.617194 | 0.747174 | 2.529273 |
| H | -3.105214 | 1.517522 | 3.123829 |
| H | -1.722728 | 0.458544 | 3.061822 |
| H | -3.279236 | -0.117539 | 2.524759 |
| C | -4.208673 | 1.765412 | 0.327356 |
| H | -4.529273 | 2.456865 | 1.105520 |
| H | -4.885437 | 0.917662 | 0.363788 |
| H | -4.348885 | 2.271048 | -0.620409 |

E(HF/6-31G(d)) = -2124.443208 hartrees
ZPE(HF/6-31G(d)) = 0.688628 hartrees
$E_{vib}$(HF/6-31G(d)) = 21.424 kcal/mol
$E_{rot}$(HF/6-31G(d)) = 0.889 kcal/mol
S(HF/6-31G(d)) = 216.214 cal/(mol K)
E(HF/6-31++G(d,p)) = -2124.537953 hartrees
E(MP2/6-31++G(d,p)) = -2128.486342 hartrees