# Supporting Information

# Studies on the Detailed Structure of Poly(dimethylsilylene)

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## Contents

## 1. Spectral Data

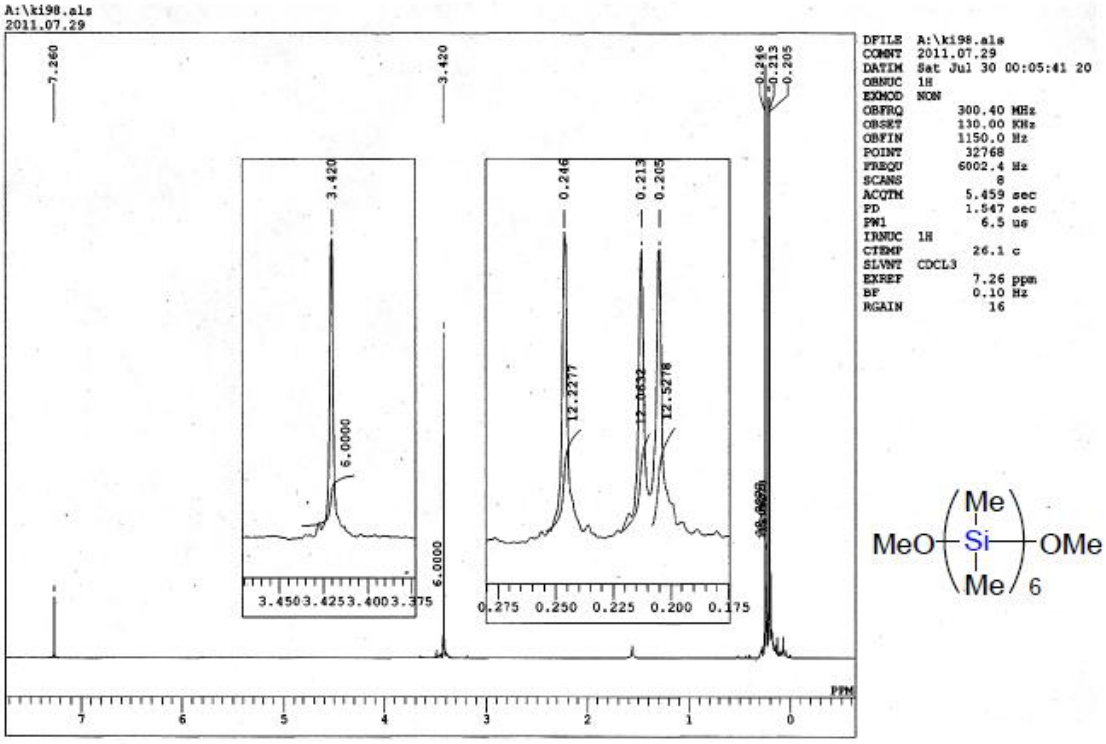



**Figure S1.** $^{1}$H NMR spectrum of **6** in $CDCl_3$ at room temperature.

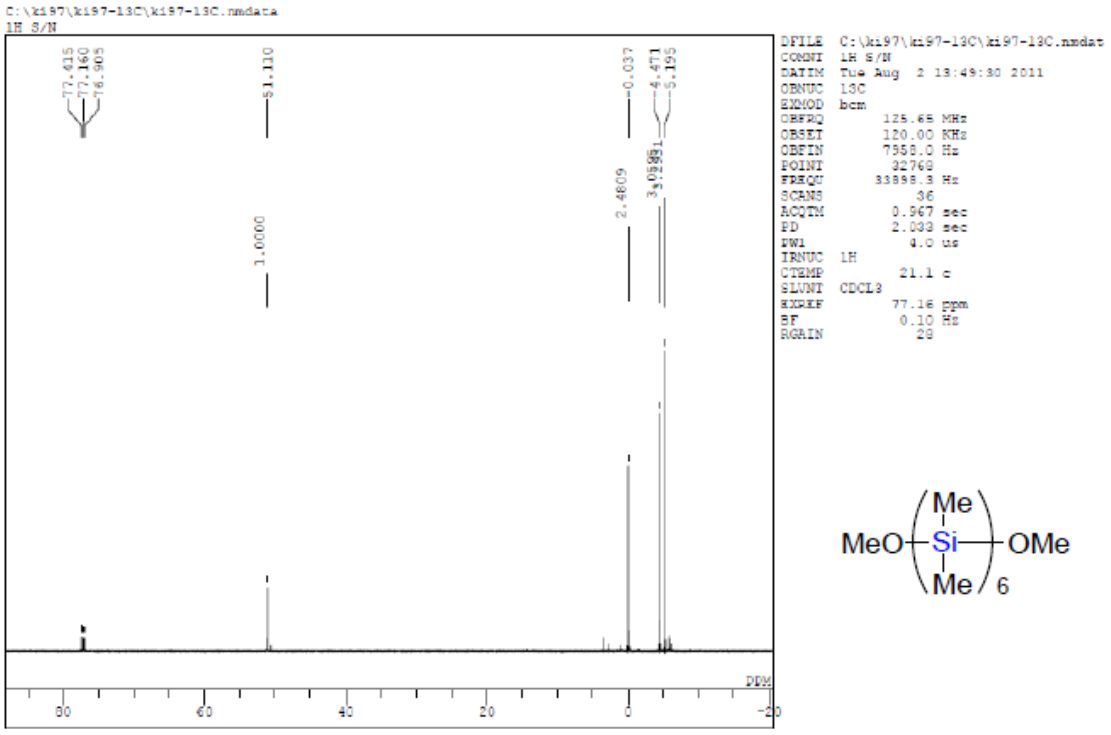



**Figure S2.** $^{13}$C NMR spectrum of **6** in $CDCl_3$ at room temperature.

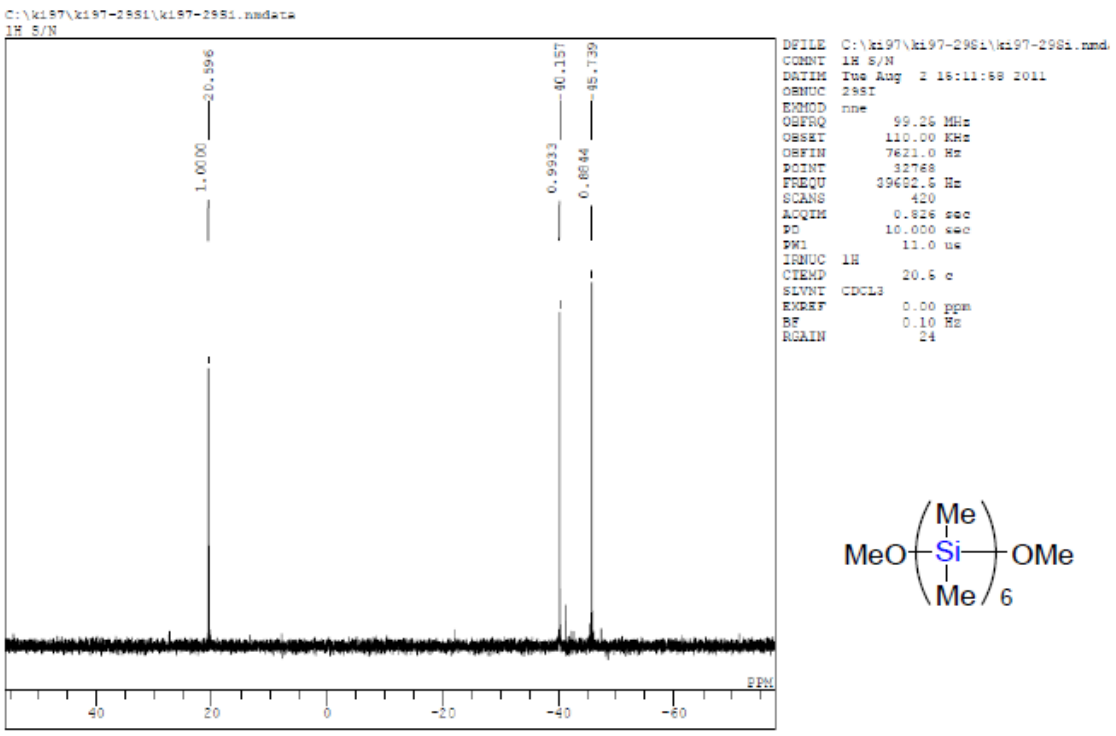



**Figure S3.** $^{29}$Si NMR spectrum of **6** in $CDCl_3$ at room temperature.

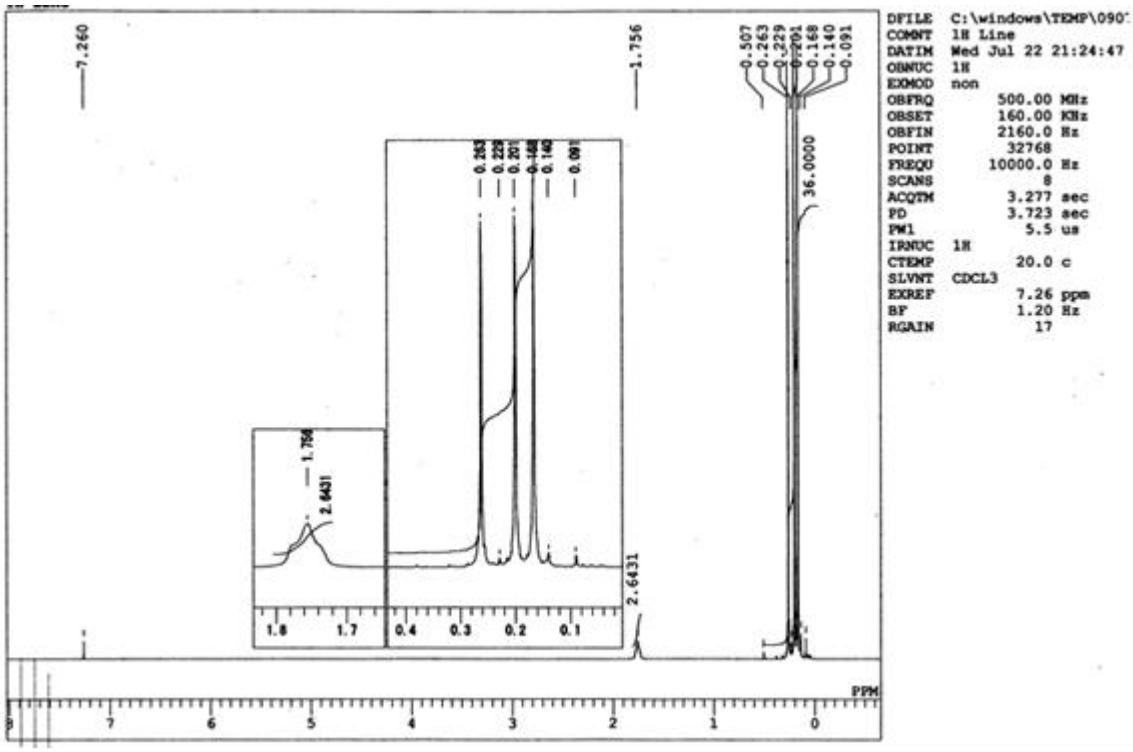



**Figure S4.** $^{1}$H NMR spectrum of **7** in $CDCl_3$ at room temperature.

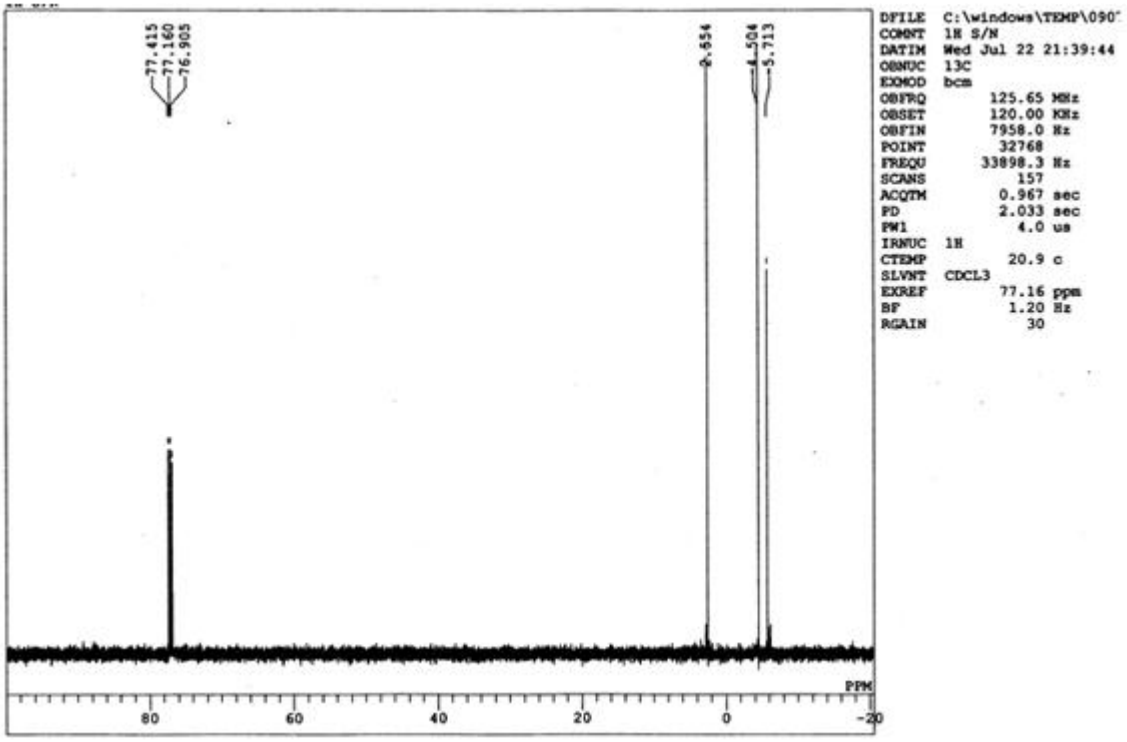



**Figure S5.** $^{13}C$ NMR spectrum of **7** in $CDCl_3$ at room temperature.

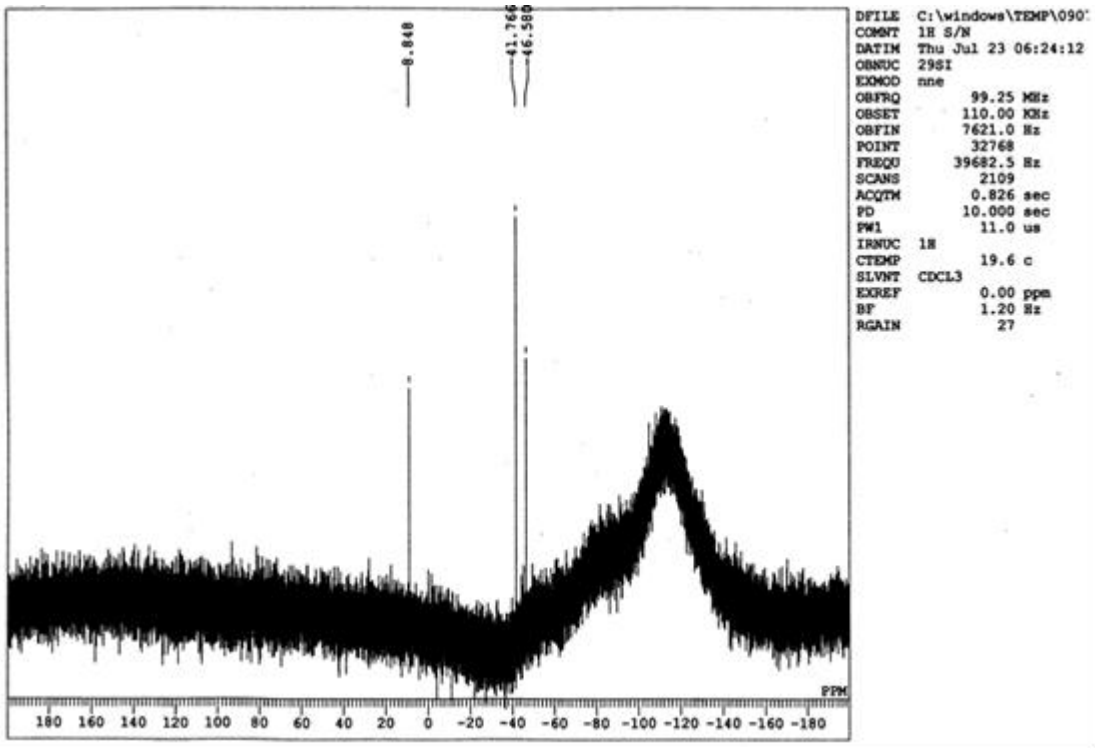



**Figure S6.** $^{29}Si$ NMR spectrum of **7** in $CDCl_3$ at room temperature.

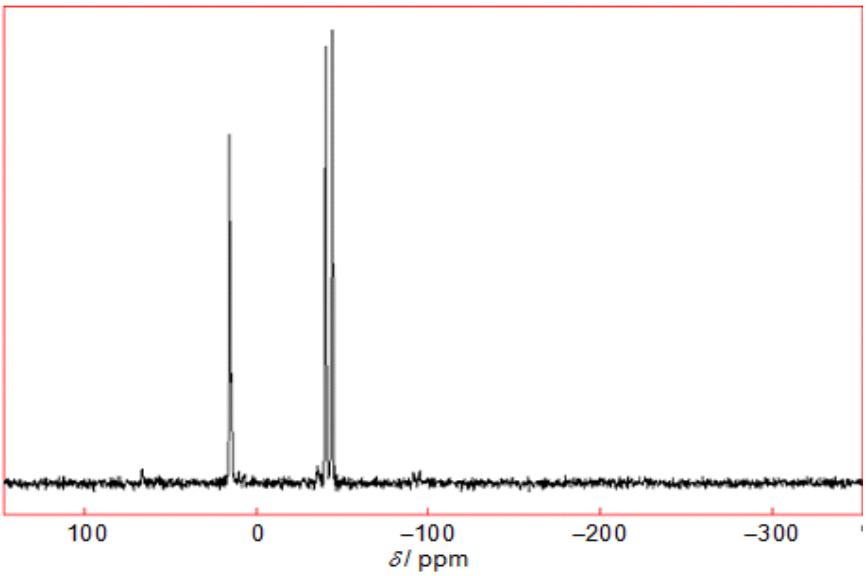
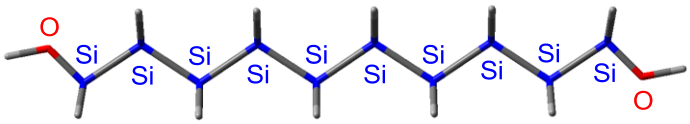



**Figure S7.** $^{29}$Si CP/MAS NMR spectrum of **7** at room temperature.

## 2. Theoretical Calculations

All theoretical calculations were performed using Gaussian 03[S1] and 09.[S2] The optimized structures were calculated at the B3LYP/6-31G(d) level. The structures of **1**–**5** were optimized by assuming the all-anti conformation. The magnetic shielding tensors of the $^{13}C$ and $^{29}Si$ nuclei were calculated by the GIAO method at the B3LYP/6-311+G(2d,p) level using the optimized structures. All calculations were carried out on an HPC Systems HPC-5000-XW208T computer and a PRIMERGY system of the Research Center for Computational Science, Japan.

**Table S1. Atomic Coordinates of the Optimized Structure of 1**




| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | C | 1.560760 | -9.179095 | 1.535716 |
| 2 | H | 2.025235 | -10.173238 | 1.559938 |
| 3 | H | 2.372799 | -8.441561 | 1.548659 |
| 4 | H | 0.985540 | -9.057709 | 2.460597 |
| 5 | C | 1.560760 | -9.179095 | -1.535716 |
| 6 | H | 2.025235 | -10.173238 | -1.559938 |
| 7 | H | 0.985540 | -9.057709 | -2.460597 |
| 8 | H | 2.372799 | -8.441561 | -1.548659 |
| 9 | C | -1.912608 | -7.014130 | -1.547807 |
| 10 | H | -2.667971 | -6.219815 | -1.530283 |
| 11 | H | -1.337113 | -6.905192 | -2.474273 |
| 12 | H | -2.437252 | -7.975612 | -1.590879 |
| 13 | C | -1.912608 | -7.014130 | 1.547807 |
| 14 | H | -1.337113 | -6.905192 | 2.474273 |
| 15 | H | -2.667971 | -6.219815 | 1.530283 |
| 16 | H | -2.437252 | -7.975612 | 1.590879 |
| 17 | C | 1.703177 | -5.051648 | 1.545572 |
| 18 | H | 1.122712 | -4.988392 | 2.473151 |
| 19 | H | 2.280957 | -5.983021 | 1.580494 |
| 20 | H | 2.418362 | -4.221009 | 1.545635 |
| 21 | C | 1.703177 | -5.051648 | -1.545572 |
| 22 | H | 2.280957 | -5.983021 | -1.580494 |
| 23 | H | 1.122712 | -4.988392 | -2.473151 |
| 24 | H | 2.418362 | -4.221009 | -1.545635 |
| 25 | C | -1.837830 | -2.982902 | -1.547164 |
| 26 | H | -1.252597 | -2.954212 | -2.473507 |
| 27 | H | -2.462210 | -3.883151 | -1.578636 |
| 28 | H | -2.508002 | -2.115661 | -1.552405 |
| 29 | C | -1.837830 | -2.982902 | 1.547164 |
| 30 | H | -2.462210 | -3.883151 | 1.578636 |
| 31 | H | -1.252597 | -2.954212 | 2.473507 |
| 32 | H | -2.508002 | -2.115661 | 1.552405 |
| 33 | C | 1.773364 | -1.030145 | 1.546688 |
| 34 | H | 1.188462 | -1.016186 | 2.473566 |
| 35 | H | 2.402374 | -1.927482 | 1.566182 |
| 36 | H | 2.439724 | -0.160182 | 1.563347 |
| 37 | C | 1.773364 | -1.030145 | -1.546688 |
| 38 | H | 2.402374 | -1.927482 | -1.566182 |
| 39 | H | 1.188462 | -1.016186 | -2.473566 |
| 40 | H | 2.439724 | -0.160182 | -1.563347 |
| 41 | C | -1.773127 | 1.029922 | 1.546674 |
| 42 | H | -2.439314 | 0.159821 | 1.563361 |
| 43 | H | -1.188232 | 1.016112 | 2.473558 |
| 44 | H | -2.402316 | 1.927130 | 1.566128 |
| 45 | C | -1.773127 | 1.029922 | -1.546674 |
| 46 | H | -1.188232 | 1.016112 | -2.473558 |
| 47 | H | -2.439314 | 0.159821 | -1.563361 |
| 48 | H | -2.402316 | 1.927130 | -1.566128 |
| 49 | C | 1.837921 | 2.983168 | -1.547156 |
| 50 | H | 2.508240 | 2.116045 | -1.552401 |
| 51 | H | 1.252691 | 2.954387 | -2.473498 |

| | | | | |
|---|---|---|---|---|
| 52 | H | 2.462153 | 3.883523 | -1.578625 |
| 53 | C | 1.837921 | 2.983168 | 1.547156 |
| 54 | H | 1.252691 | 2.954387 | 2.473498 |
| 55 | H | 2.508240 | 2.116045 | 1.552401 |
| 56 | H | 2.462153 | 3.883523 | 1.578625 |
| 57 | C | -1.703228 | 5.051619 | 1.545578 |
| 58 | H | -2.418523 | 4.221078 | 1.545540 |
| 59 | H | -1.122777 | 4.988182 | 2.473154 |
| 60 | H | -2.280886 | 5.983064 | 1.580604 |
| 61 | C | -1.703228 | 5.051619 | -1.545578 |
| 62 | H | -1.122777 | 4.988182 | -2.473154 |
| 63 | H | -2.418523 | 4.221078 | -1.545540 |
| 64 | H | -2.280886 | 5.983064 | -1.580604 |
| 65 | C | 1.912514 | 7.014099 | -1.547808 |
| 66 | H | 2.667828 | 6.219736 | -1.530300 |
| 67 | H | 1.337007 | 6.905208 | -2.474272 |
| 68 | H | 2.437216 | 7.975549 | -1.590871 |
| 69 | C | 1.912514 | 7.014099 | 1.547808 |
| 70 | H | 1.337007 | 6.905208 | 2.474272 |
| 71 | H | 2.667828 | 6.219736 | 1.530300 |
| 72 | H | 2.437216 | 7.975549 | 1.590871 |
| 73 | C | -1.560876 | 9.179084 | 1.535718 |
| 74 | H | -2.372918 | 8.441554 | 1.548650 |
| 75 | H | -0.985662 | 9.057686 | 2.460600 |
| 76 | H | -2.025349 | 10.173228 | 1.559949 |
| 77 | C | -1.560876 | 9.179084 | -1.535718 |
| 78 | H | -0.985662 | 9.057686 | -2.460600 |
| 79 | H | -2.372918 | 8.441554 | -1.548650 |
| 80 | H | -2.025349 | 10.173228 | -1.559949 |
| 81 | O | 0.754691 | 10.124360 | 0.000000 |
| 82 | O | -0.754813 | -10.124343 | 0.000000 |
| 83 | Si | 0.466595 | -8.957541 | 0.000000 |
| 84 | Si | -0.792625 | -6.950411 | 0.000000 |
| 85 | Si | 0.575198 | -4.996375 | 0.000000 |
| 86 | Si | -0.712151 | -2.980455 | 0.000000 |
| 87 | Si | 0.646836 | -1.008481 | 0.000000 |
| 88 | Si | -0.646576 | 1.008404 | 0.000000 |
| 89 | Si | 0.712231 | 2.980544 | 0.000000 |
| 90 | Si | -0.575260 | 4.996374 | 0.000000 |
| 91 | Si | 0.792527 | 6.950420 | 0.000000 |
| 92 | Si | -0.466706 | 8.957545 | 0.000000 |
| 93 | C | -0.520716 | -11.522151 | 0.000000 |
| 94 | H | -1.490121 | -12.031710 | 0.000000 |
| 95 | H | 0.036336 | -11.844025 | -0.891572 |
| 96 | H | 0.036336 | -11.844025 | 0.891572 |
| 97 | C | 0.520589 | 11.522165 | 0.000000 |
| 98 | H | 1.489993 | 12.031726 | 0.000000 |
| 99 | H | -0.036465 | 11.844035 | -0.891572 |
| 100 | H | -0.036465 | 11.844035 | 0.891572 |

**Table S2. Magnetic Shielding Tensors of $^{29}$Si and $^{13}$C Nuclei of 1 Calculated by the GIAO Method**

```
SCF GIAO Magnetic shielding tensor (ppm):
  1  C    Isotropic =   182.3730   Anisotropy =    10.5485
   XX=   181.2775   YX=     6.9049   ZX=     3.0943
   XY=     2.5944   YY=   178.9611   ZY=    -4.2830
   XZ=    -1.2803   YZ=    -5.3993   ZZ=   186.8805
   Eigenvalues:   173.7277   183.9860   189.4053
   Eigenvectors:
      (1)  -0.531292   0.782513   0.324657
      (2)   0.826564   0.394741   0.401213
```

```
     (3)  -0.185799  -0.481510   0.856520
 5  C    Isotropic =   182.3730   Anisotropy =    10.5484
  XX=   181.2775   YX=     6.9049   ZX=    -3.0943
  XY=     2.5944   YY=   178.9611   ZY=     4.2830
  XZ=     1.2803   YZ=     5.3993   ZZ=   186.8805
  Eigenvalues:   173.7277   183.9860   189.4053
  Eigenvectors:
     (1)  -0.531292   0.782513  -0.324656
     (2)   0.826564   0.394741  -0.401213
     (3)   0.185799   0.481511   0.856520
 9  C    Isotropic =   185.8358   Anisotropy =     3.7988
  XX=   186.0103   YX=    -2.2014   ZX=     1.8505
  XY=    -1.0285   YY=   184.9616   ZY=     0.9195
  XZ=    -3.9733   YZ=     1.1581   ZZ=   186.5355
  Eigenvalues:   183.7661   185.3729   188.3683
  Eigenvectors:
     (1)   0.549357   0.829510  -0.100600
     (2)   0.568809  -0.283049   0.772231
     (3)  -0.612098   0.481452   0.627327
13  C    Isotropic =   185.8358   Anisotropy =     3.7988
  XX=   186.0103   YX=    -2.2014   ZX=    -1.8505
  XY=    -1.0285   YY=   184.9616   ZY=    -0.9195
  XZ=     3.9733   YZ=    -1.1581   ZZ=   186.5355
  Eigenvalues:   183.7661   185.3729   188.3683
  Eigenvectors:
     (1)   0.549357   0.829510   0.100600
     (2)  -0.568808   0.283050   0.772231
     (3)   0.612098  -0.481452   0.627327
17  C    Isotropic =   183.5466   Anisotropy =     3.3279
  XX=   183.2270   YX=     0.4701   ZX=     3.5040
  XY=    -0.3124   YY=   185.7617   ZY=    -0.2966
  XZ=    -1.5164   YZ=     0.3607   ZZ=   181.6512
  Eigenvalues:   181.1708   183.7038   185.7652
  Eigenvectors:
     (1)  -0.435205   0.001191   0.900330
     (2)   0.899544  -0.041238   0.434880
     (3)   0.037646   0.999149   0.016876
21  C    Isotropic =   183.5466   Anisotropy =     3.3279
  XX=   183.2270   YX=     0.4701   ZX=    -3.5040
  XY=    -0.3124   YY=   185.7617   ZY=     0.2966
  XZ=     1.5164   YZ=    -0.3607   ZZ=   181.6512
  Eigenvalues:   181.1708   183.7038   185.7652
  Eigenvectors:
     (1)   0.435205  -0.001191   0.900330
     (2)   0.899544  -0.041240  -0.434880
     (3)   0.037647   0.999149  -0.016876
25  C    Isotropic =   182.9744   Anisotropy =     4.5876
  XX=   182.7048   YX=    -0.5554   ZX=     4.0450
  XY=     0.0213   YY=   186.0051   ZY=     0.0748
  XZ=    -1.2136   YZ=    -0.2089   ZZ=   180.2133
  Eigenvalues:   179.5729   183.3175   186.0328
  Eigenvectors:
     (1)  -0.412423  -0.007627   0.910961
     (2)   0.906079   0.100290   0.411052
     (3)  -0.094495   0.994929  -0.034451
29  C    Isotropic =   182.9744   Anisotropy =     4.5876
  XX=   182.7048   YX=    -0.5554   ZX=    -4.0450
  XY=     0.0213   YY=   186.0051   ZY=    -0.0748
  XZ=     1.2136   YZ=     0.2089   ZZ=   180.2133
  Eigenvalues:   179.5729   183.3175   186.0328
  Eigenvectors:
     (1)   0.412423   0.007627   0.910961
     (2)   0.906078   0.100290  -0.411052
     (3)  -0.094495   0.994929   0.034451
33  C    Isotropic =   182.9068   Anisotropy =     4.8470
  XX=   182.5069   YX=     0.0847   ZX=     4.0413
```

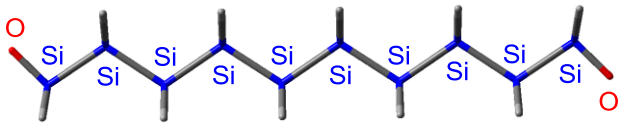
```
  XY=    -0.0183   YY=   186.1375   ZY=    -0.1165
  XZ=    -1.2851   YZ=     0.0018   ZZ=   180.0759
  Eigenvalues:   179.4533   183.1290   186.1381
  Eigenvectors:
     (1)  -0.411405   0.009859   0.911399
     (2)   0.911432  -0.002217   0.411444
     (3)   0.006077   0.999949  -0.008074
37  C    Isotropic =   182.9068   Anisotropy =     4.8470
  XX=   182.5069   YX=     0.0847   ZX=    -4.0413
  XY=    -0.0183   YY=   186.1375   ZY=     0.1165
  XZ=     1.2851   YZ=    -0.0018   ZZ=   180.0759
  Eigenvalues:   179.4533   183.1290   186.1381
  Eigenvectors:
     (1)   0.411405  -0.009859   0.911399
     (2)   0.911432  -0.002217  -0.411444
     (3)   0.006077   0.999949   0.008074
41  C    Isotropic =   182.9056   Anisotropy =     4.8482
  XX=   182.5048   YX=     0.0864   ZX=    -4.0412
  XY=    -0.0178   YY=   186.1370   ZY=     0.1162
  XZ=     1.2852   YZ=    -0.0012   ZZ=   180.0749
  Eigenvalues:   179.4521   183.1269   186.1377
  Eigenvectors:
     (1)   0.411497  -0.009945   0.911357
     (2)   0.911389  -0.002515  -0.411539
     (3)   0.006385   0.999947   0.008029
45  C    Isotropic =   182.9056   Anisotropy =     4.8482
  XX=   182.5048   YX=     0.0864   ZX=     4.0412
  XY=    -0.0178   YY=   186.1370   ZY=    -0.1162
  XZ=    -1.2852   YZ=     0.0012   ZZ=   180.0749
  Eigenvalues:   179.4521   183.1269   186.1377
  Eigenvectors:
     (1)  -0.411498   0.009945   0.911357
     (2)   0.911388  -0.002515   0.411540
     (3)   0.006385   0.999947  -0.008029
49  C    Isotropic =   182.9754   Anisotropy =     4.5856
  XX=   182.7058   YX=    -0.5528   ZX=    -4.0456
  XY=     0.0221   YY=   186.0050   ZY=    -0.0749
  XZ=     1.2131   YZ=     0.2100   ZZ=   180.2154
  Eigenvalues:   179.5744   183.3193   186.0324
  Eigenvectors:
     (1)   0.412599   0.007460   0.910882
     (2)   0.906046   0.099864  -0.411226
     (3)  -0.094032   0.994973   0.034445
53  C    Isotropic =   182.9754   Anisotropy =     4.5856
  XX=   182.7058   YX=    -0.5528   ZX=     4.0456
  XY=     0.0221   YY=   186.0050   ZY=     0.0749
  XZ=    -1.2131   YZ=    -0.2100   ZZ=   180.2154
  Eigenvalues:   179.5744   183.3193   186.0324
  Eigenvectors:
     (1)  -0.412599  -0.007460   0.910882
     (2)   0.906046   0.099865   0.411226
     (3)  -0.094033   0.994973  -0.034445
57  C    Isotropic =   183.5478   Anisotropy =     3.3259
  XX=   183.2291   YX=     0.4718   ZX=    -3.5040
  XY=    -0.3114   YY=   185.7615   ZY=     0.2972
  XZ=     1.5160   YZ=    -0.3604   ZZ=   181.6528
  Eigenvalues:   181.1724   183.7059   185.7651
  Eigenvectors:
     (1)   0.435174  -0.001411   0.900345
     (2)   0.899534  -0.041798  -0.434847
     (3)   0.038246   0.999125  -0.016920
61  C    Isotropic =   183.5478   Anisotropy =     3.3259
  XX=   183.2291   YX=     0.4718   ZX=     3.5040
  XY=    -0.3114   YY=   185.7615   ZY=    -0.2972
  XZ=    -1.5160   YZ=     0.3604   ZZ=   181.6528
  Eigenvalues:   181.1724   183.7059   185.7651
```

```
  Eigenvectors:
     (1)  -0.435174   0.001411   0.900345
     (2)   0.899534  -0.041799   0.434847
     (3)   0.038247   0.999125   0.016921
65  C    Isotropic =   185.8343   Anisotropy =     3.7991
  XX=   186.0077   YX=    -2.2021   ZX=    -1.8507
  XY=    -1.0286   YY=   184.9619   ZY=    -0.9197
  XZ=     3.9732   YZ=    -1.1589   ZZ=   186.5333
  Eigenvalues:   183.7650   185.3708   188.3670
  Eigenvectors:
     (1)   0.549702   0.829279   0.100619
     (2)  -0.568618   0.283212   0.772311
     (3)   0.611965  -0.481755   0.627225
69  C    Isotropic =   185.8343   Anisotropy =     3.7991
  XX=   186.0077   YX=    -2.2021   ZX=     1.8507
  XY=    -1.0286   YY=   184.9619   ZY=     0.9197
  XZ=    -3.9732   YZ=     1.1589   ZZ=   186.5333
  Eigenvalues:   183.7650   185.3708   188.3670
  Eigenvectors:
     (1)   0.549703   0.829278  -0.100619
     (2)   0.568618  -0.283212   0.772311
     (3)  -0.611965   0.481755   0.627225
73  C    Isotropic =   182.3730   Anisotropy =    10.5486
  XX=   181.2773   YX=     6.9052   ZX=    -3.0943
  XY=     2.5945   YY=   178.9611   ZY=     4.2830
  XZ=     1.2801   YZ=     5.3992   ZZ=   186.8806
  Eigenvalues:   173.7275   183.9861   189.4053
  Eigenvectors:
     (1)  -0.531308   0.782505  -0.324649
     (2)   0.826554   0.394757  -0.401218
     (3)   0.185797   0.481510   0.856520
77  C    Isotropic =   182.3730   Anisotropy =    10.5486
  XX=   181.2773   YX=     6.9052   ZX=     3.0943
  XY=     2.5945   YY=   178.9611   ZY=    -4.2830
  XZ=    -1.2801   YZ=    -5.3992   ZZ=   186.8806
  Eigenvalues:   173.7275   183.9861   189.4053
  Eigenvectors:
     (1)  -0.531308   0.782505   0.324649
     (2)   0.826554   0.394757   0.401218
     (3)  -0.185798  -0.481511   0.856520
83  Si   Isotropic =   309.4931   Anisotropy =    63.3594
  XX=   317.5079   YX=    24.3089   ZX=     0.0000
  XY=    32.1982   YY=   328.4086   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   282.5627
  Eigenvalues:   282.5627   294.1838   351.7327
  Eigenvectors:
     (1)   0.000000   0.000000   1.000000
     (2)   0.771173  -0.636626   0.000000
     (3)   0.636626   0.771173   0.000000
84  Si   Isotropic =   358.8347   Anisotropy =    25.8145
  XX=   372.5573   YX=    10.3345   ZX=     0.0000
  XY=    10.7349   YY=   344.2180   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   359.7288
  Eigenvalues:   340.7310   359.7288   376.0444
  Eigenvectors:
     (1)  -0.314239   0.949344   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.949344   0.314239   0.000000
85  Si   Isotropic =   357.3796   Anisotropy =    20.7890
  XX=   370.4534   YX=    -6.0377   ZX=     0.0000
  XY=    -3.3180   YY=   343.3823   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   358.3031
  Eigenvalues:   342.5968   358.3031   371.2389
  Eigenvectors:
     (1)   0.165607   0.986192   0.000000
     (2)   0.000000   0.000000   1.000000
```

```
     (3)    0.986192   -0.165607    0.000000
86  Si    Isotropic =    352.1410    Anisotropy =     18.7685
  XX=    364.6201    YX=      0.7914    ZX=      0.0000
  XY=      0.9581    YY=    341.6193    ZY=      0.0000
  XZ=      0.0000    YZ=      0.0000    ZZ=    350.1836
  Eigenvalues:    341.5860    350.1836    364.6533
  Eigenvectors:
     (1)   -0.037948    0.999280    0.000000
     (2)    0.000000    0.000000    1.000000
     (3)    0.999280    0.037948    0.000000
87  Si    Isotropic =    352.0293    Anisotropy =     19.0330
  XX=    364.6941    YX=     -0.6068    ZX=      0.0000
  XY=     -0.8724    YY=    341.8113    ZY=      0.0000
  XZ=      0.0000    YZ=      0.0000    ZZ=    349.5826
  Eigenvalues:    341.7874    349.5826    364.7180
  Eigenvectors:
     (1)    0.032271    0.999479    0.000000
     (2)    0.000000    0.000000    1.000000
     (3)    0.999479   -0.032271    0.000000
88  Si    Isotropic =    352.0255    Anisotropy =     19.0348
  XX=    364.6921    YX=     -0.5977    ZX=      0.0000
  XY=     -0.8640    YY=    341.8134    ZY=      0.0000
  XZ=      0.0000    YZ=      0.0000    ZZ=    349.5710
  Eigenvalues:    341.7901    349.5710    364.7154
  Eigenvectors:
     (1)    0.031896    0.999491    0.000000
     (2)    0.000000    0.000000    1.000000
     (3)    0.999491   -0.031896    0.000000
89  Si    Isotropic =    352.1407    Anisotropy =     18.7684
  XX=    364.6191    YX=      0.7988    ZX=      0.0000
  XY=      0.9675    YY=    341.6200    ZY=      0.0000
  XZ=      0.0000    YZ=      0.0000    ZZ=    350.1830
  Eigenvalues:    341.5861    350.1830    364.6529
  Eigenvectors:
     (1)   -0.038315    0.999266    0.000000
     (2)    0.000000    0.000000    1.000000
     (3)    0.999266    0.038315    0.000000
90  Si    Isotropic =    357.3798    Anisotropy =     20.7928
  XX=    370.4557    YX=     -6.0429    ZX=      0.0000
  XY=     -3.3167    YY=    343.3802    ZY=      0.0000
  XZ=      0.0000    YZ=      0.0000    ZZ=    358.3036
  Eigenvalues:    342.5941    358.3036    371.2417
  Eigenvectors:
     (1)    0.165646    0.986185    0.000000
     (2)    0.000000    0.000000    1.000000
     (3)    0.986185   -0.165646    0.000000
91  Si    Isotropic =    358.8341    Anisotropy =     25.8091
  XX=    372.5559    YX=     10.3285    ZX=      0.0000
  XY=     10.7309    YY=    344.2189    ZY=      0.0000
  XZ=      0.0000    YZ=      0.0000    ZZ=    359.7276
  Eigenvalues:    340.7346    359.7276    376.0402
  Eigenvectors:
     (1)   -0.314148    0.949374    0.000000
     (2)    0.000000    0.000000    1.000000
     (3)    0.949374    0.314148    0.000000
92  Si    Isotropic =    309.4929    Anisotropy =     63.3603
  XX=    317.5069    YX=     24.3087    ZX=      0.0000
  XY=     32.1990    YY=    328.4095    ZY=      0.0000
  XZ=      0.0000    YZ=      0.0000    ZZ=    282.5623
  Eigenvalues:    282.5623    294.1833    351.7331
  Eigenvectors:
     (1)    0.000000    0.000000    1.000000
     (2)    0.771183   -0.636614    0.000000
     (3)    0.636614    0.771183    0.000000
93  C     Isotropic =    130.7327    Anisotropy =     79.9144
  XX=    103.8606    YX=     -9.1468    ZX=      0.0000
```

```
  XY=   -10.2337   YY=   182.8374   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   105.5000
  Eigenvalues:   102.6890   105.5000   184.0089
  Eigenvectors:
     (1)   0.992770   0.120030   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)  -0.120030   0.992770   0.000000
97  C    Isotropic =   130.7327   Anisotropy =    79.9142
  XX=   103.8608   YX=    -9.1471   ZX=     0.0000
  XY=   -10.2339   YY=   182.8372   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   105.5001
  Eigenvalues:   102.6892   105.5001   184.0088
  Eigenvectors:
     (1)   0.992770   0.120033   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)  -0.120033   0.992770   0.000000
```

**Table S3. Atomic Coordinates of the Optimized Structure of 2**




| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | C | -1.488748 | 9.188759 | 1.531034 |
| 2 | H | -1.943620 | 10.188457 | 1.546666 |
| 3 | H | -2.308363 | 8.459538 | 1.547064 |
| 4 | H | -0.916671 | 9.069670 | 2.458006 |
| 5 | C | -1.488748 | 9.188759 | -1.531034 |
| 6 | H | -1.943620 | 10.188457 | -1.546666 |
| 7 | H | -0.916671 | 9.069670 | -2.458006 |
| 8 | H | -2.308363 | 8.459538 | -1.547064 |
| 9 | C | 1.969075 | 6.995069 | -1.548919 |
| 10 | H | 2.710398 | 6.187600 | -1.536134 |
| 11 | H | 1.389686 | 6.899736 | -2.474455 |
| 12 | H | 2.510446 | 7.947341 | -1.589380 |
| 13 | C | 1.969075 | 6.995069 | 1.548919 |
| 14 | H | 1.389686 | 6.899736 | 2.474455 |
| 15 | H | 2.710398 | 6.187600 | 1.536134 |
| 16 | H | 2.510446 | 7.947341 | 1.589380 |
| 17 | C | -1.661636 | 5.064273 | 1.545789 |
| 18 | H | -1.081299 | 4.996417 | 2.473135 |
| 19 | H | -2.233160 | 5.999470 | 1.581487 |
| 20 | H | -2.382495 | 4.238537 | 1.545526 |
| 21 | C | -1.661636 | 5.064273 | -1.545789 |
| 22 | H | -2.233160 | 5.999470 | -1.581487 |
| 23 | H | -1.081299 | 4.996417 | -2.473135 |
| 24 | H | -2.382495 | 4.238537 | -1.545526 |
| 25 | C | 1.861578 | 2.967781 | -1.547225 |
| 26 | H | 1.276086 | 2.943490 | -2.473536 |
| 27 | H | 2.493107 | 3.862999 | -1.578989 |
| 28 | H | 2.524900 | 2.095306 | -1.552206 |
| 29 | C | 1.861578 | 2.967781 | 1.547225 |
| 30 | H | 2.493107 | 3.862999 | 1.578989 |
| 31 | H | 1.276086 | 2.943490 | 2.473536 |
| 32 | H | 2.524900 | 2.095306 | 1.552206 |

| | | | | |
|---|---|---|---|---|
| 33 | C | −1.764832 | 1.043799 | 1.546703 |
| 34 | H | −1.180032 | 1.025783 | 2.473584 |
| 35 | H | −2.387561 | 1.945521 | 1.566101 |
| 36 | H | −2.437289 | 0.178547 | 1.563411 |
| 37 | C | −1.764832 | 1.043799 | −1.546703 |
| 38 | H | −2.387561 | 1.945521 | −1.566101 |
| 39 | H | −1.180032 | 1.025783 | −2.473584 |
| 40 | H | −2.437289 | 0.178547 | −1.563411 |
| 41 | C | 1.764595 | −1.044015 | 1.546709 |
| 42 | H | 2.437264 | −0.178930 | 1.563331 |
| 43 | H | 1.179801 | −1.025770 | 2.473589 |
| 44 | H | 2.387102 | −1.945897 | 1.566190 |
| 45 | C | 1.764595 | −1.044015 | −1.546709 |
| 46 | H | 1.179801 | −1.025770 | −2.473589 |
| 47 | H | 2.437264 | −0.178930 | −1.563331 |
| 48 | H | 2.387102 | −1.945897 | −1.566190 |
| 49 | C | −1.861835 | −2.967654 | −1.547250 |
| 50 | H | −2.524978 | −2.095039 | −1.552304 |
| 51 | H | −1.276322 | −2.943542 | −2.473553 |
| 52 | H | −2.493543 | −3.862739 | −1.578967 |
| 53 | C | −1.861835 | −2.967654 | 1.547250 |
| 54 | H | −1.276322 | −2.943542 | 2.473553 |
| 55 | H | −2.524978 | −2.095039 | 1.552304 |
| 56 | H | −2.493543 | −3.862739 | 1.578967 |
| 57 | C | 1.661470 | −5.064009 | 1.545767 |
| 58 | H | 2.382148 | −4.238106 | 1.545508 |
| 59 | H | 1.081135 | −4.996296 | 2.473123 |
| 60 | H | 2.233204 | −5.999079 | 1.581441 |
| 61 | C | 1.661470 | −5.064009 | −1.545767 |
| 62 | H | 1.081135 | −4.996296 | −2.473123 |
| 63 | H | 2.382148 | −4.238106 | −1.545508 |
| 64 | H | 2.233204 | −5.999079 | −1.581441 |
| 65 | C | −1.969011 | −6.995421 | −1.548926 |
| 66 | H | −2.710505 | −6.188117 | −1.536116 |
| 67 | H | −1.389638 | −6.899933 | −2.474456 |
| 68 | H | −2.510176 | −7.947809 | −1.589425 |
| 69 | C | −1.969011 | −6.995421 | 1.548926 |
| 70 | H | −1.389638 | −6.899933 | 2.474456 |
| 71 | H | −2.710505 | −6.188117 | 1.536116 |
| 72 | H | −2.510176 | −7.947809 | 1.589425 |
| 73 | C | 1.489203 | −9.188447 | 1.531031 |
| 74 | H | 2.308645 | −8.459031 | 1.547074 |
| 75 | H | 0.917099 | −9.069518 | 2.458006 |
| 76 | H | 1.944314 | −10.188038 | 1.546638 |
| 77 | C | 1.489203 | −9.188447 | −1.531031 |
| 78 | H | 0.917099 | −9.069518 | −2.458006 |
| 79 | H | 2.308645 | −8.459031 | −1.547074 |
| 80 | H | 1.944314 | −10.188038 | −1.546638 |
| 81 | O | −0.836007 | −10.125377 | 0.000000 |
| 82 | H | −0.538037 | −11.047231 | 0.000000 |
| 83 | O | 0.836668 | 10.125188 | 0.000000 |
| 84 | H | 0.538906 | 11.047108 | 0.000000 |
| 85 | Si | −0.391995 | 8.958935 | 0.000000 |
| 86 | Si | 0.850478 | 6.943165 | 0.000000 |
| 87 | Si | −0.534224 | 5.001635 | 0.000000 |
| 88 | Si | 0.735880 | 2.974840 | 0.000000 |
| 89 | Si | −0.638330 | 1.013790 | 0.000000 |
| 90 | Si | 0.638109 | −1.013878 | 0.000000 |
| 91 | Si | −0.736169 | −2.974826 | 0.000000 |
| 92 | Si | 0.534011 | −5.001566 | 0.000000 |
| 93 | Si | −0.850433 | −6.943315 | 0.000000 |
| 94 | Si | 0.392400 | −8.958858 | 0.000000 |

**Table S4. Magnetic Shielding Tensors of $^{29}$Si and $^{13}$C Nuclei of 2 Calculated by the GIAO Method**

```
SCF GIAO Magnetic shielding tensor (ppm):
  1  C    Isotropic =   177.1692   Anisotropy =    12.8865
   XX=   175.1102   YX=     7.5732   ZX=    -9.8566
   XY=     3.0889   YY=   178.3409   ZY=     5.8715
   XZ=    -8.2585   YZ=     3.2837   ZZ=   178.0565
   Eigenvalues:   163.9709   181.7765   185.7602
   Eigenvectors:
      (1)   0.683888  -0.439277   0.582523
      (2)   0.339460   0.898324   0.278891
      (3)  -0.645805   0.007013   0.763471
  5  C    Isotropic =   177.1692   Anisotropy =    12.8865
   XX=   175.1102   YX=     7.5732   ZX=     9.8566
   XY=     3.0889   YY=   178.3409   ZY=    -5.8715
   XZ=     8.2585   YZ=    -3.2837   ZZ=   178.0565
   Eigenvalues:   163.9709   181.7765   185.7602
   Eigenvectors:
      (1)   0.683888  -0.439277  -0.582523
      (2)   0.339460   0.898324  -0.278891
      (3)   0.645805  -0.007013   0.763470
  9  C    Isotropic =   185.7307   Anisotropy =     3.6724
   XX=   185.9261   YX=    -2.0403   ZX=    -1.9860
   XY=    -0.8259   YY=   184.7939   ZY=    -0.9366
   XZ=     3.9667   YZ=    -1.3503   ZZ=   186.4721
   Eigenvalues:   183.7455   185.2676   188.1790
   Eigenvectors:
      (1)   0.479419   0.857739   0.185585
      (2)  -0.651004   0.205781   0.730649
      (3)   0.588516  -0.471104   0.657046
 13  C    Isotropic =   185.7307   Anisotropy =     3.6724
   XX=   185.9261   YX=    -2.0403   ZX=     1.9860
   XY=    -0.8259   YY=   184.7939   ZY=     0.9366
   XZ=    -3.9667   YZ=     1.3503   ZZ=   186.4721
   Eigenvalues:   183.7455   185.2676   188.1790
   Eigenvectors:
      (1)   0.479420   0.857738  -0.185584
      (2)   0.651003  -0.205782   0.730650
      (3)  -0.588516   0.471104   0.657046
 17  C    Isotropic =   183.6403   Anisotropy =     3.0835
   XX=   183.2971   YX=     0.4806   ZX=    -3.4916
   XY=    -0.3433   YY=   185.6939   ZY=     0.3560
   XZ=     1.5581   YZ=    -0.3335   ZZ=   181.9298
   Eigenvalues:   181.4290   183.7958   185.6959
   Eigenvectors:
      (1)   0.459873  -0.009748   0.887931
      (2)   0.887459  -0.029365  -0.459951
      (3)   0.030558   0.999521  -0.004853
 21  C    Isotropic =   183.6403   Anisotropy =     3.0835
   XX=   183.2971   YX=     0.4806   ZX=     3.4916
   XY=    -0.3433   YY=   185.6939   ZY=    -0.3560
   XZ=    -1.5581   YZ=     0.3335   ZZ=   181.9298
   Eigenvalues:   181.4290   183.7958   185.6959
   Eigenvectors:
      (1)  -0.459873   0.009748   0.887931
      (2)   0.887458  -0.029366   0.459951
      (3)   0.030559   0.999521   0.004854
 25  C    Isotropic =   182.9011   Anisotropy =     4.5772
   XX=   182.6445   YX=    -0.5079   ZX=    -4.0807
   XY=     0.0498   YY=   185.9317   ZY=    -0.0456
   XZ=     1.1801   YZ=     0.1681   ZZ=   180.1271
   Eigenvalues:   179.4653   183.2855   185.9526
   Eigenvectors:
      (1)   0.415386   0.006096   0.909625
```

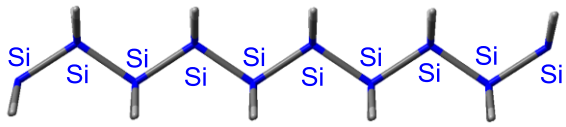
```
     (2)    0.905891    0.087992   -0.414270
     (3)   -0.082565    0.996103    0.031029
29  C    Isotropic =    182.9011    Anisotropy =      4.5772
  XX=    182.6445    YX=     -0.5079    ZX=      4.0807
  XY=      0.0498    YY=    185.9317    ZY=      0.0456
  XZ=     -1.1801    YZ=     -0.1681    ZZ=    180.1271
  Eigenvalues:    179.4653    183.2855    185.9526
  Eigenvectors:
     (1)   -0.415386   -0.006096    0.909625
     (2)    0.905891    0.087992    0.414270
     (3)   -0.082565    0.996103   -0.031029
33  C    Isotropic =    182.8684    Anisotropy =      4.8235
  XX=    182.4773    YX=      0.1001    ZX=     -4.0707
  XY=     -0.0055    YY=    186.0826    ZY=      0.1626
  XZ=      1.2816    YZ=      0.0066    ZZ=    180.0452
  Eigenvalues:    179.4095    183.1115    186.0841
  Eigenvectors:
     (1)    0.413981   -0.014473    0.910170
     (2)    0.910246   -0.002698   -0.414059
     (3)    0.008449    0.999892    0.012057
37  C    Isotropic =    182.8684    Anisotropy =      4.8235
  XX=    182.4773    YX=      0.1001    ZX=      4.0707
  XY=     -0.0055    YY=    186.0826    ZY=     -0.1626
  XZ=     -1.2816    YZ=     -0.0066    ZZ=    180.0452
  Eigenvalues:    179.4095    183.1115    186.0841
  Eigenvectors:
     (1)   -0.413981    0.014473    0.910170
     (2)    0.910246   -0.002699    0.414058
     (3)    0.008449    0.999892   -0.012057
41  C    Isotropic =    182.8680    Anisotropy =      4.8244
  XX=    182.4772    YX=      0.0991    ZX=      4.0710
  XY=     -0.0057    YY=    186.0828    ZY=     -0.1630
  XZ=     -1.2816    YZ=     -0.0058    ZZ=    180.0439
  Eigenvalues:    179.4084    183.1113    186.0842
  Eigenvectors:
     (1)   -0.413890    0.014406    0.910213
     (2)    0.910289   -0.002550    0.413965
     (3)    0.008285    0.999893   -0.012059
45  C    Isotropic =    182.8680    Anisotropy =      4.8244
  XX=    182.4772    YX=      0.0991    ZX=     -4.0710
  XY=     -0.0057    YY=    186.0828    ZY=      0.1630
  XZ=      1.2816    YZ=      0.0058    ZZ=    180.0439
  Eigenvalues:    179.4084    183.1113    186.0842
  Eigenvectors:
     (1)    0.413890   -0.014407    0.910213
     (2)    0.910289   -0.002550   -0.413965
     (3)    0.008285    0.999893    0.012059
49  C    Isotropic =    182.9017    Anisotropy =      4.5775
  XX=    182.6464    YX=     -0.5087    ZX=      4.0799
  XY=      0.0496    YY=    185.9324    ZY=      0.0456
  XZ=     -1.1799    YZ=     -0.1669    ZZ=    180.1263
  Eigenvalues:    179.4651    183.2866    185.9534
  Eigenvectors:
     (1)   -0.415108   -0.006200    0.909751
     (2)    0.906003    0.088107    0.413999
     (3)   -0.082723    0.996092   -0.030957
53  C    Isotropic =    182.9017    Anisotropy =      4.5775
  XX=    182.6464    YX=     -0.5087    ZX=     -4.0799
  XY=      0.0496    YY=    185.9324    ZY=     -0.0456
  XZ=      1.1799    YZ=      0.1669    ZZ=    180.1263
  Eigenvalues:    179.4651    183.2866    185.9534
  Eigenvectors:
     (1)    0.415108    0.006200    0.909751
     (2)    0.906003    0.088108   -0.413999
     (3)   -0.082723    0.996092    0.030957
57  C    Isotropic =    183.6376    Anisotropy =      3.0871
```

```
  XX=   183.2923   YX=     0.4829   ZX=     3.4914
  XY=    -0.3422   YY=   185.6935   ZY=    -0.3560
  XZ=    -1.5597   YZ=     0.3333   ZZ=   181.9271
  Eigenvalues:   181.4265   183.7907   185.6957
  Eigenvectors:
     (1)  -0.460007   0.009939   0.887859
     (2)   0.887365  -0.030052   0.460088
     (3)   0.031255   0.999499   0.005005
61  C    Isotropic =   183.6376   Anisotropy =     3.0871
  XX=   183.2923   YX=     0.4829   ZX=    -3.4914
  XY=    -0.3422   YY=   185.6935   ZY=     0.3560
  XZ=     1.5597   YZ=    -0.3333   ZZ=   181.9271
  Eigenvalues:   181.4265   183.7907   185.6957
  Eigenvectors:
     (1)   0.460008  -0.009939   0.887859
     (2)   0.887365  -0.030053  -0.460088
     (3)   0.031256   0.999499  -0.005005
65  C    Isotropic =   185.7334   Anisotropy =     3.6714
  XX=   185.9311   YX=    -2.0384   ZX=     1.9860
  XY=    -0.8247   YY=   184.7930   ZY=     0.9365
  XZ=    -3.9670   YZ=     1.3486   ZZ=   186.4763
  Eigenvalues:   183.7477   185.2716   188.1810
  Eigenvectors:
     (1)   0.478463   0.858249  -0.185693
     (2)   0.651528  -0.205199   0.730345
     (3)  -0.588714   0.470427   0.657354
69  C    Isotropic =   185.7334   Anisotropy =     3.6714
  XX=   185.9311   YX=    -2.0384   ZX=    -1.9859
  XY=    -0.8247   YY=   184.7930   ZY=    -0.9365
  XZ=     3.9670   YZ=    -1.3486   ZZ=   186.4763
  Eigenvalues:   183.7477   185.2716   188.1810
  Eigenvectors:
     (1)   0.478464   0.858249   0.185692
     (2)  -0.651527   0.205200   0.730346
     (3)   0.588714  -0.470427   0.657353
73  C    Isotropic =   177.1687   Anisotropy =    12.8866
  XX=   175.1072   YX=     7.5725   ZX=     9.8582
  XY=     3.0884   YY=   178.3431   ZY=    -5.8694
  XZ=     8.2595   YZ=    -3.2834   ZZ=   178.0557
  Eigenvalues:   163.9696   181.7768   185.7597
  Eigenvectors:
     (1)   0.683974  -0.439128  -0.582534
     (2)   0.339331   0.898398  -0.278813
     (3)   0.645782  -0.006971   0.763490
77  C    Isotropic =   177.1687   Anisotropy =    12.8866
  XX=   175.1072   YX=     7.5726   ZX=    -9.8582
  XY=     3.0884   YY=   178.3431   ZY=     5.8694
  XZ=    -8.2595   YZ=     3.2834   ZZ=   178.0557
  Eigenvalues:   163.9696   181.7768   185.7597
  Eigenvectors:
     (1)   0.683974  -0.439128   0.582534
     (2)   0.339330   0.898398   0.278813
     (3)  -0.645782   0.006971   0.763490
85  Si   Isotropic =   310.1437   Anisotropy =    56.1615
  XX=   317.0014   YX=    20.9488   ZX=     0.0000
  XY=    31.6258   YY=   324.9899   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   288.4398
  Eigenvalues:   288.4398   294.4066   347.5847
  Eigenvectors:
     (1)   0.000000   0.000000   1.000000
     (2)   0.758361  -0.651835   0.000000
     (3)   0.651835   0.758361   0.000000
86  Si   Isotropic =   358.5568   Anisotropy =    25.6808
  XX=   372.4052   YX=    10.0950   ZX=     0.0000
  XY=    10.4487   YY=   343.4317   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   359.8334
```

```
  Eigenvalues:   340.1596   359.8334   375.6773
  Eigenvectors:
     (1)  -0.303523   0.952824   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.952824   0.303523   0.000000
87  Si   Isotropic =   358.1022   Anisotropy =    20.7906
  XX=   371.0988   YX=    -6.4516   ZX=     0.0000
  XY=    -3.5009   YY=   343.2987   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   359.9092
  Eigenvalues:   342.4348   359.9092   371.9627
  Eigenvectors:
     (1)   0.171049   0.985262   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.985262  -0.171049   0.000000
88  Si   Isotropic =   351.9099   Anisotropy =    19.0887
  XX=   364.6245   YX=     0.4996   ZX=     0.0000
  XY=     0.5178   YY=   341.4657   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   349.6394
  Eigenvalues:   341.4546   349.6394   364.6357
  Eigenvectors:
     (1)  -0.021951   0.999759   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.999759   0.021951   0.000000
89  Si   Isotropic =   352.0379   Anisotropy =    19.3124
  XX=   364.8717   YX=    -0.8388   ZX=     0.0000
  XY=    -1.1138   YY=   341.7502   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   349.4919
  Eigenvalues:   341.7090   349.4919   364.9129
  Eigenvectors:
     (1)   0.042113   0.999113   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.999113  -0.042113   0.000000
90  Si   Isotropic =   352.0438   Anisotropy =    19.3139
  XX=   364.8778   YX=    -0.8494   ZX=     0.0000
  XY=    -1.1216   YY=   341.7503   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   349.5032
  Eigenvalues:   341.7084   349.5032   364.9197
  Eigenvectors:
     (1)   0.042498   0.999097   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.999097  -0.042498   0.000000
91  Si   Isotropic =   351.9108   Anisotropy =    19.0937
  XX=   364.6291   YX=     0.4917   ZX=     0.0000
  XY=     0.5099   YY=   341.4615   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   349.6418
  Eigenvalues:   341.4506   349.6418   364.6399
  Eigenvectors:
     (1)  -0.021602   0.999767   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.999767   0.021602   0.000000
92  Si   Isotropic =   358.0926   Anisotropy =    20.7831
  XX=   371.0882   YX=    -6.4345   ZX=     0.0000
  XY=    -3.4908   YY=   343.3026   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   359.8869
  Eigenvalues:   342.4428   359.8869   371.9480
  Eigenvectors:
     (1)   0.170702   0.985323   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.985323  -0.170702   0.000000
93  Si   Isotropic =   358.5651   Anisotropy =    25.6899
  XX=   372.4146   YX=    10.1081   ZX=     0.0000
  XY=    10.4558   YY=   343.4316   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   359.8491
  Eigenvalues:   340.1545   359.8491   375.6917
  Eigenvectors:
     (1)  -0.303670   0.952777   0.000000
```

```
     (2)    0.000000    0.000000    1.000000
     (3)    0.952777    0.303670    0.000000
94  Si    Isotropic =   310.1398   Anisotropy =    56.1675
  XX=   316.9871   YX=    20.9476   ZX=     0.0000
  XY=    31.6250   YY=   325.0024   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   288.4300
  Eigenvalues:   288.4300   294.4047   347.5848
  Eigenvectors:
     (1)    0.000000    0.000000    1.000000
     (2)    0.758525   -0.651644    0.000000
     (3)    0.651644    0.758525    0.000000
```

**Table S5. Atomic Coordinates of the Optimized Structure of 3**




| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | C | -1.354969 | 9.220790 | 1.554189 |
| 2 | H | -1.797537 | 10.224230 | 1.564031 |
| 3 | H | -2.175621 | 8.495306 | 1.597691 |
| 4 | H | -0.763406 | 9.109356 | 2.469968 |
| 5 | C | -1.354969 | 9.220790 | -1.554189 |
| 6 | H | -1.797537 | 10.224230 | -1.564031 |
| 7 | H | -0.763406 | 9.109356 | -2.469968 |
| 8 | H | -2.175621 | 8.495306 | -1.597691 |
| 9 | C | 2.059964 | 6.973209 | -1.546593 |
| 10 | H | 2.767513 | 6.135936 | -1.545845 |
| 11 | H | 1.479102 | 6.915561 | -2.474261 |
| 12 | H | 2.645055 | 7.900438 | -1.577870 |
| 13 | C | 2.059964 | 6.973209 | 1.546593 |
| 14 | H | 1.479102 | 6.915561 | 2.474261 |
| 15 | H | 2.767513 | 6.135936 | 1.545845 |
| 16 | H | 2.645055 | 7.900438 | 1.577870 |
| 17 | C | -1.595202 | 5.089238 | 1.546001 |
| 18 | H | -1.015331 | 5.022181 | 2.473702 |
| 19 | H | -2.159610 | 6.028858 | 1.576085 |
| 20 | H | -2.322375 | 4.269025 | 1.550636 |
| 21 | C | -1.595202 | 5.089238 | -1.546001 |
| 22 | H | -2.159610 | 6.028858 | -1.576085 |
| 23 | H | -1.015331 | 5.022181 | -2.473702 |
| 24 | H | -2.322375 | 4.269025 | -1.550636 |
| 25 | C | 1.900476 | 2.943881 | -1.546903 |
| 26 | H | 1.315311 | 2.932353 | -2.473647 |
| 27 | H | 2.547487 | 3.828120 | -1.575843 |
| 28 | H | 2.549341 | 2.060629 | -1.554467 |
| 29 | C | 1.900476 | 2.943881 | 1.546903 |
| 30 | H | 2.547487 | 3.828120 | 1.575843 |
| 31 | H | 1.315311 | 2.932353 | 2.473647 |
| 32 | H | 2.549341 | 2.060629 | 1.554467 |
| 33 | C | -1.750598 | 1.066195 | 1.546722 |
| 34 | H | -1.166200 | 1.041616 | 2.473702 |
| 35 | H | -2.363086 | 1.974914 | 1.565985 |
| 36 | H | -2.433208 | 0.208924 | 1.563802 |
| 37 | C | -1.750598 | 1.066195 | -1.546722 |

| | | | | |
|---|---|---|---|---|
| 38 | H | -2.363086 | 1.974914 | -1.565985 |
| 39 | H | -1.166200 | 1.041616 | -2.473702 |
| 40 | H | -2.433208 | 0.208924 | -1.563802 |
| 41 | C | 1.750974 | -1.066394 | 1.546741 |
| 42 | H | 2.433789 | -0.209291 | 1.563761 |
| 43 | H | 1.166573 | -1.041605 | 2.473714 |
| 44 | H | 2.363240 | -1.975260 | 1.566078 |
| 45 | C | 1.750974 | -1.066394 | -1.546741 |
| 46 | H | 1.166573 | -1.041605 | -2.473714 |
| 47 | H | 2.433789 | -0.209291 | -1.563761 |
| 48 | H | 2.363240 | -1.975260 | -1.566078 |
| 49 | C | -1.900244 | -2.943649 | -1.546896 |
| 50 | H | -2.548932 | -2.060261 | -1.554493 |
| 51 | H | -1.315085 | -2.932277 | -2.473646 |
| 52 | H | -2.547425 | -3.827765 | -1.575781 |
| 53 | C | -1.900244 | -2.943649 | 1.546896 |
| 54 | H | -1.315085 | -2.932277 | 2.473646 |
| 55 | H | -2.548932 | -2.060261 | 1.554493 |
| 56 | H | -2.547425 | -3.827765 | 1.575781 |
| 57 | C | 1.595207 | -5.089463 | 1.546006 |
| 58 | H | 2.322579 | -4.269426 | 1.550621 |
| 59 | H | 1.015349 | -5.022241 | 2.473702 |
| 60 | H | 2.159385 | -6.029219 | 1.576118 |
| 61 | C | 1.595207 | -5.089463 | -1.546006 |
| 62 | H | 1.015349 | -5.022241 | -2.473702 |
| 63 | H | 2.322579 | -4.269426 | -1.550621 |
| 64 | H | 2.159385 | -6.029219 | -1.576118 |
| 65 | C | -2.060185 | -6.972979 | -1.546578 |
| 66 | H | -2.767716 | -6.135689 | -1.545764 |
| 67 | H | -1.479351 | -6.915295 | -2.474262 |
| 68 | H | -2.645301 | -7.900191 | -1.577887 |
| 69 | C | -2.060185 | -6.972979 | 1.546578 |
| 70 | H | -1.479351 | -6.915295 | 2.474262 |
| 71 | H | -2.767716 | -6.135689 | 1.545764 |
| 72 | H | -2.645301 | -7.900191 | 1.577887 |
| 73 | C | 1.354554 | -9.220931 | 1.554177 |
| 74 | H | 2.175424 | -8.495686 | 1.597547 |
| 75 | H | 0.763076 | -9.109219 | 2.469976 |
| 76 | H | 1.796827 | -10.224500 | 1.564106 |
| 77 | C | 1.354554 | -9.220931 | -1.554177 |
| 78 | H | 0.763076 | -9.109219 | -2.469976 |
| 79 | H | 2.175424 | -8.495686 | -1.597547 |
| 80 | H | 1.796827 | -10.224500 | -1.564106 |
| 81 | Si | -0.285248 | 8.976114 | 0.000000 |
| 82 | Si | 0.934099 | 6.939323 | 0.000000 |
| 83 | Si | -0.469255 | 5.009422 | 0.000000 |
| 84 | Si | 0.774118 | 2.965305 | 0.000000 |
| 85 | Si | -0.624484 | 1.022095 | 0.000000 |
| 86 | Si | 0.624894 | -1.022149 | 0.000000 |
| 87 | Si | -0.773884 | -2.965210 | 0.000000 |
| 88 | Si | 0.469282 | -5.009450 | 0.000000 |
| 89 | Si | -0.934294 | -6.939191 | 0.000000 |
| 90 | Si | 0.284849 | -8.976112 | 0.000000 |
| 91 | H | -0.748534 | -10.066003 | 0.000000 |
| 92 | H | 0.748002 | 10.066132 | 0.000000 |

---

**Table S6. Magnetic Shielding Tensors of $^{29}$Si and $^{13}$C Nuclei of 3 Calculated by the GIAO Method**

```
SCF GIAO Magnetic shielding tensor (ppm):
  1  C    Isotropic =   185.3507   Anisotropy =     3.5399
   XX=   184.5045   YX=     0.6311   ZX=    -1.9901
```

```
  XY=    -0.6536   YY=   185.8021   ZY=     2.1326
  XZ=     2.8465   YZ=     1.6869   ZZ=   185.7454
  Eigenvalues:   183.7332   184.6082   187.7106
  Eigenvectors:
     (1)  -0.385061  -0.627105   0.677102
     (2)   0.918336  -0.333162   0.213687
     (3)   0.091580   0.704090   0.704180
 5  C    Isotropic =   185.3507   Anisotropy =     3.5399
  XX=   184.5045   YX=     0.6311   ZX=     1.9901
  XY=    -0.6536   YY=   185.8021   ZY=    -2.1326
  XZ=    -2.8465   YZ=    -1.6869   ZZ=   185.7454
  Eigenvalues:   183.7332   184.6082   187.7106
  Eigenvectors:
     (1)   0.385059   0.627105   0.677103
     (2)   0.918337  -0.333161  -0.213685
     (3)  -0.091581  -0.704090   0.704180
 9  C    Isotropic =   184.1259   Anisotropy =     1.6696
  XX=   184.7096   YX=    -0.7749   ZX=    -3.1598
  XY=     0.5125   YY=   184.2662   ZY=    -0.5688
  XZ=     1.2487   YZ=     0.7452   ZZ=   183.4019
  Eigenvalues:   182.8977   184.2410   185.2390
  Eigenvectors:
     (1)   0.465743  -0.012376   0.884834
     (2)   0.146891   0.987112  -0.063511
     (3)   0.872644  -0.159553  -0.461558
13  C    Isotropic =   184.1259   Anisotropy =     1.6696
  XX=   184.7096   YX=    -0.7749   ZX=     3.1598
  XY=     0.5125   YY=   184.2662   ZY=     0.5688
  XZ=    -1.2487   YZ=    -0.7452   ZZ=   183.4019
  Eigenvalues:   182.8977   184.2410   185.2390
  Eigenvectors:
     (1)  -0.465742   0.012376   0.884834
     (2)   0.146893   0.987111   0.063513
     (3)   0.872643  -0.159557   0.461557
17  C    Isotropic =   183.2777   Anisotropy =     3.4074
  XX=   183.1869   YX=     0.4210   ZX=    -3.9185
  XY=    -0.3380   YY=   185.5476   ZY=     0.3867
  XZ=     1.4758   YZ=    -0.2196   ZZ=   181.0987
  Eigenvalues:   180.5342   183.7496   185.5493
  Eigenvectors:
     (1)   0.418400  -0.018603   0.908072
     (2)   0.908217  -0.001502  -0.418497
     (3)   0.009149   0.999826   0.016267
21  C    Isotropic =   183.2777   Anisotropy =     3.4074
  XX=   183.1869   YX=     0.4210   ZX=     3.9185
  XY=    -0.3380   YY=   185.5476   ZY=    -0.3867
  XZ=    -1.4758   YZ=     0.2196   ZZ=   181.0987
  Eigenvalues:   180.5342   183.7496   185.5493
  Eigenvectors:
     (1)  -0.418400   0.018603   0.908072
     (2)   0.908217  -0.001504   0.418497
     (3)   0.009151   0.999826  -0.016266
25  C    Isotropic =   182.8897   Anisotropy =     4.4488
  XX=   182.5809   YX=    -0.3625   ZX=    -4.0437
  XY=     0.1922   YY=   185.8507   ZY=     0.0595
  XZ=     1.2319   YZ=     0.0967   ZZ=   180.2374
  Eigenvalues:   179.5788   183.2347   185.8555
  Eigenvectors:
     (1)   0.423973  -0.005525   0.905658
     (2)   0.904967   0.042097  -0.423393
     (3)  -0.035786   0.999098   0.022848
29  C    Isotropic =   182.8897   Anisotropy =     4.4488
  XX=   182.5809   YX=    -0.3625   ZX=     4.0437
  XY=     0.1922   YY=   185.8507   ZY=    -0.0595
  XZ=    -1.2319   YZ=    -0.0967   ZZ=   180.2374
  Eigenvalues:   179.5788   183.2347   185.8555
```

```
  Eigenvectors:
     (1)  -0.423973   0.005525   0.905658
     (2)   0.904967   0.042097   0.423393
     (3)  -0.035786   0.999098  -0.022848
33  C    Isotropic =   182.8297   Anisotropy =     4.7915
  XX=   182.4564   YX=     0.1079   ZX=    -4.1322
  XY=     0.0716   YY=   186.0199   ZY=     0.2396
  XZ=     1.2579   YZ=     0.0349   ZZ=   180.0128
  Eigenvalues:   179.3443   183.1208   186.0240
  Eigenvectors:
     (1)   0.419703  -0.024300   0.907336
     (2)   0.907490  -0.008208  -0.419994
     (3)   0.017653   0.999671   0.018607
37  C    Isotropic =   182.8297   Anisotropy =     4.7915
  XX=   182.4564   YX=     0.1079   ZX=     4.1322
  XY=     0.0716   YY=   186.0199   ZY=    -0.2396
  XZ=    -1.2579   YZ=    -0.0349   ZZ=   180.0128
  Eigenvalues:   179.3443   183.1208   186.0240
  Eigenvectors:
     (1)  -0.419703   0.024300   0.907336
     (2)   0.907490  -0.008209   0.419994
     (3)   0.017654   0.999671  -0.018606
41  C    Isotropic =   182.8320   Anisotropy =     4.7880
  XX=   182.4607   YX=     0.1083   ZX=     4.1320
  XY=     0.0715   YY=   186.0199   ZY=    -0.2401
  XZ=    -1.2572   YZ=    -0.0344   ZZ=   180.0154
  Eigenvalues:   179.3471   183.1249   186.0240
  Eigenvectors:
     (1)  -0.419594   0.024323   0.907386
     (2)   0.907539  -0.008271   0.419887
     (3)   0.017718   0.999670  -0.018604
45  C    Isotropic =   182.8320   Anisotropy =     4.7880
  XX=   182.4607   YX=     0.1083   ZX=    -4.1320
  XY=     0.0715   YY=   186.0199   ZY=     0.2401
  XZ=     1.2572   YZ=     0.0344   ZZ=   180.0154
  Eigenvalues:   179.3471   183.1249   186.0240
  Eigenvectors:
     (1)   0.419594  -0.024323   0.907386
     (2)   0.907539  -0.008271  -0.419887
     (3)   0.017718   0.999670   0.018604
49  C    Isotropic =   182.8876   Anisotropy =     4.4519
  XX=   182.5779   YX=    -0.3623   ZX=     4.0437
  XY=     0.1927   YY=   185.8507   ZY=    -0.0599
  XZ=    -1.2324   YZ=    -0.0964   ZZ=   180.2342
  Eigenvalues:   179.5759   183.2315   185.8555
  Eigenvectors:
     (1)  -0.423907   0.005551   0.905689
     (2)   0.905004   0.041942   0.423330
     (3)  -0.035636   0.999105  -0.022803
53  C    Isotropic =   182.8876   Anisotropy =     4.4519
  XX=   182.5779   YX=    -0.3623   ZX=    -4.0437
  XY=     0.1927   YY=   185.8507   ZY=     0.0599
  XZ=     1.2324   YZ=     0.0964   ZZ=   180.2342
  Eigenvalues:   179.5759   183.2315   185.8555
  Eigenvectors:
     (1)   0.423907  -0.005551   0.905689
     (2)   0.905004   0.041942  -0.423330
     (3)  -0.035637   0.999105   0.022803
57  C    Isotropic =   183.2783   Anisotropy =     3.4070
  XX=   183.1875   YX=     0.4219   ZX=     3.9192
  XY=    -0.3377   YY=   185.5478   ZY=    -0.3874
  XZ=    -1.4754   YZ=     0.2196   ZZ=   181.0995
  Eigenvalues:   180.5346   183.7506   185.5496
  Eigenvectors:
     (1)  -0.418509   0.018704   0.908020
     (2)   0.908164  -0.001735   0.418611
```

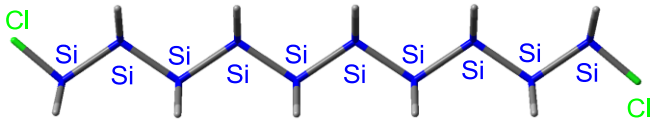
```
     (3)    0.009405    0.999824   -0.016260
61  C    Isotropic =    183.2783    Anisotropy =      3.4070
  XX=    183.1875    YX=      0.4219    ZX=     -3.9192
  XY=     -0.3377    YY=    185.5478    ZY=      0.3874
  XZ=      1.4754    YZ=     -0.2196    ZZ=    181.0995
  Eigenvalues:    180.5346    183.7506    185.5496
  Eigenvectors:
     (1)    0.418509   -0.018704    0.908020
     (2)    0.908164   -0.001737   -0.418611
     (3)    0.009407    0.999824    0.016260
65  C    Isotropic =    184.1254    Anisotropy =      1.6700
  XX=    184.7088    YX=     -0.7757    ZX=      3.1599
  XY=      0.5118    YY=    184.2656    ZY=      0.5690
  XZ=     -1.2481    YZ=     -0.7448    ZZ=    183.4019
  Eigenvalues:    182.8973    184.2402    185.2388
  Eigenvectors:
     (1)   -0.465972    0.011891    0.884720
     (2)    0.147016    0.987051    0.064165
     (3)    0.872500   -0.159967    0.461686
69  C    Isotropic =    184.1254    Anisotropy =      1.6700
  XX=    184.7088    YX=     -0.7757    ZX=     -3.1599
  XY=      0.5118    YY=    184.2656    ZY=     -0.5690
  XZ=      1.2481    YZ=      0.7448    ZZ=    183.4019
  Eigenvalues:    182.8973    184.2402    185.2388
  Eigenvectors:
     (1)    0.465971   -0.011890    0.884720
     (2)    0.147019    0.987050   -0.064168
     (3)    0.872500   -0.159971   -0.461685
73  C    Isotropic =    185.3507    Anisotropy =      3.5399
  XX=    184.5052    YX=      0.6331    ZX=      1.9893
  XY=     -0.6527    YY=    185.8012    ZY=     -2.1336
  XZ=     -2.8471    YZ=     -1.6858    ZZ=    185.7457
  Eigenvalues:    183.7334    184.6081    187.7106
  Eigenvectors:
     (1)    0.384356    0.627338    0.677287
     (2)    0.918580   -0.333067   -0.212784
     (3)   -0.092094   -0.703927    0.704276
77  C    Isotropic =    185.3507    Anisotropy =      3.5399
  XX=    184.5052    YX=      0.6331    ZX=     -1.9893
  XY=     -0.6527    YY=    185.8012    ZY=      2.1336
  XZ=      2.8471    YZ=      1.6858    ZZ=    185.7457
  Eigenvalues:    183.7334    184.6081    187.7106
  Eigenvectors:
     (1)   -0.384354   -0.627339    0.677288
     (2)    0.918581   -0.333066    0.212782
     (3)    0.092095    0.703927    0.704276
81  Si   Isotropic =    358.4121    Anisotropy =     24.2578
  XX=    362.9993    YX=    -17.4186    ZX=      0.0000
  XY=    -21.2835    YY=    342.2602    ZY=      0.0000
  XZ=      0.0000    YZ=      0.0000    ZZ=    369.9769
  Eigenvalues:    330.6754    369.9769    374.5840
  Eigenvectors:
     (1)    0.513651    0.857999    0.000000
     (2)    0.000000    0.000000    1.000000
     (3)    0.857999   -0.513651    0.000000
82  Si   Isotropic =    356.7629    Anisotropy =     21.9678
  XX=    369.9136    YX=      6.3850    ZX=      0.0000
  XY=      6.7433    YY=    342.5761    ZY=      0.0000
  XZ=      0.0000    YZ=      0.0000    ZZ=    357.7991
  Eigenvalues:    341.0816    357.7991    371.4081
  Eigenvectors:
     (1)   -0.221989    0.975049    0.000000
     (2)    0.000000    0.000000    1.000000
     (3)    0.975049    0.221989    0.000000
83  Si   Isotropic =    354.6636    Anisotropy =     19.1698
  XX=    366.6597    YX=     -4.6579    ZX=      0.0000
```

```
  XY=    -4.1310   YY=   342.8041   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   354.5271
  Eigenvalues:   342.0203   354.5271   367.4435
  Eigenvectors:
     (1)   0.175581   0.984465   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.984465  -0.175581   0.000000
84  Si   Isotropic =   351.8937   Anisotropy =    19.5089
  XX=   364.8987   YX=     0.1119   ZX=     0.0000
  XY=     0.1793   YY=   341.6887   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   349.0936
  Eigenvalues:   341.6878   349.0936   364.8996
  Eigenvectors:
     (1)  -0.006274   0.999980   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.999980   0.006274   0.000000
85  Si   Isotropic =   352.2530   Anisotropy =    19.3997
  XX=   365.1013   YX=    -1.2881   ZX=     0.0000
  XY=    -1.5286   YY=   341.7849   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   349.8727
  Eigenvalues:   341.7002   349.8727   365.1861
  Eigenvectors:
     (1)   0.060075   0.998194   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.998194  -0.060075   0.000000
86  Si   Isotropic =   352.2556   Anisotropy =    19.4016
  XX=   365.1043   YX=    -1.2984   ZX=     0.0000
  XY=    -1.5360   YY=   341.7808   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   349.8819
  Eigenvalues:   341.6950   349.8819   365.1901
  Eigenvectors:
     (1)   0.060431   0.998172   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.998172  -0.060431   0.000000
87  Si   Isotropic =   351.8919   Anisotropy =    19.5056
  XX=   364.8949   YX=     0.1055   ZX=     0.0000
  XY=     0.1749   YY=   341.6914   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   349.0895
  Eigenvalues:   341.6906   349.0895   364.8957
  Eigenvectors:
     (1)  -0.006042   0.999982   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.999982   0.006042   0.000000
88  Si   Isotropic =   354.6737   Anisotropy =    19.1681
  XX=   366.6656   YX=    -4.6707   ZX=     0.0000
  XY=    -4.1367   YY=   342.8062   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   354.5493
  Eigenvalues:   342.0193   354.5493   367.4524
  Eigenvectors:
     (1)   0.175892   0.984410   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.984410  -0.175892   0.000000
89  Si   Isotropic =   356.7571   Anisotropy =    21.9562
  XX=   369.9001   YX=     6.3835   ZX=     0.0000
  XY=     6.7413   YY=   342.5784   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   357.7928
  Eigenvalues:   341.0839   357.7928   371.3946
  Eigenvectors:
     (1)  -0.222048   0.975036   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.975036   0.222048   0.000000
90  Si   Isotropic =   358.4118   Anisotropy =    24.2635
  XX=   362.9959   YX=   -17.4261   ZX=     0.0000
  XY=   -21.2852   YY=   342.2670   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   369.9723
  Eigenvalues:   330.6755   369.9723   374.5874
```

Eigenvectors:

| | | | |
|---|---|---|---|
| (1) | 0.513781 | 0.857921 | 0.000000 |
| (2) | 0.000000 | 0.000000 | 1.000000 |
| (3) | 0.857921 | -0.513781 | 0.000001 |

**Table S7. Atomic Coordinates of the Optimized Structure of 4**




| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | C | -1.619186 | 9.164062 | 1.546122 |
| 2 | H | -2.087131 | 10.155261 | 1.541674 |
| 3 | H | -2.417807 | 8.412836 | 1.588540 |
| 4 | H | -1.023428 | 9.075801 | 2.460666 |
| 5 | C | -1.619186 | 9.164062 | -1.546122 |
| 6 | H | -2.087131 | 10.155261 | -1.541674 |
| 7 | H | -1.023428 | 9.075801 | -2.460666 |
| 8 | H | -2.417807 | 8.412836 | -1.588540 |
| 9 | C | 1.865465 | 7.024614 | -1.549711 |
| 10 | H | 2.611843 | 6.221855 | -1.540698 |
| 11 | H | 1.286535 | 6.929684 | -2.475337 |
| 12 | H | 2.403178 | 7.979085 | -1.586281 |
| 13 | C | 1.865465 | 7.024614 | 1.549711 |
| 14 | H | 1.286535 | 6.929684 | 2.475337 |
| 15 | H | 2.611843 | 6.221855 | 1.540698 |
| 16 | H | 2.403178 | 7.979085 | 1.586281 |
| 17 | C | -1.737088 | 5.039564 | 1.547000 |
| 18 | H | -1.153813 | 4.993551 | 2.473724 |
| 19 | H | -2.331567 | 5.960543 | 1.575700 |
| 20 | H | -2.437923 | 4.196967 | 1.555373 |
| 21 | C | -1.737088 | 5.039564 | -1.547000 |
| 22 | H | -2.331567 | 5.960543 | -1.575700 |
| 23 | H | -1.153813 | 4.993551 | -2.473724 |
| 24 | H | -2.437923 | 4.196967 | -1.555373 |
| 25 | C | 1.818553 | 2.993701 | -1.547655 |
| 26 | H | 1.233203 | 2.968096 | -2.473945 |
| 27 | H | 2.443256 | 3.893766 | -1.575951 |
| 28 | H | 2.489275 | 2.127006 | -1.556385 |
| 29 | C | 1.818553 | 2.993701 | 1.547655 |
| 30 | H | 2.443256 | 3.893766 | 1.575951 |
| 31 | H | 1.233203 | 2.968096 | 2.473945 |
| 32 | H | 2.489275 | 2.127006 | 1.556385 |
| 33 | C | -1.780489 | 1.018620 | 1.546987 |
| 34 | H | -1.195538 | 1.010419 | 2.473845 |
| 35 | H | -2.416739 | 1.910840 | 1.565241 |
| 36 | H | -2.440544 | 0.143953 | 1.564962 |
| 37 | C | -1.780489 | 1.018620 | -1.546987 |
| 38 | H | -2.416739 | 1.910840 | -1.565241 |
| 39 | H | -1.195538 | 1.010419 | -2.473845 |
| 40 | H | -2.440544 | 0.143953 | -1.564962 |
| 41 | C | 1.781155 | -1.018820 | 1.547009 |
| 42 | H | 2.441460 | -0.144343 | 1.564932 |
| 43 | H | 1.196178 | -1.010375 | 2.473849 |
| 44 | H | 2.417146 | -1.911221 | 1.565357 |

| | | | | |
|---|---|---|---|---|
| 45 | C | 1.781155 | -1.018820 | -1.547009 |
| 46 | H | 1.196178 | -1.010375 | -2.473849 |
| 47 | H | 2.441460 | -0.144343 | -1.564932 |
| 48 | H | 2.417146 | -1.911221 | -1.565357 |
| 49 | C | -1.818065 | -2.993489 | -1.547633 |
| 50 | H | -2.488675 | -2.126701 | -1.556366 |
| 51 | H | -1.232751 | -2.967992 | -2.473947 |
| 52 | H | -2.442885 | -3.893476 | -1.575865 |
| 53 | C | -1.818065 | -2.993489 | 1.547633 |
| 54 | H | -1.232751 | -2.967992 | 2.473947 |
| 55 | H | -2.488675 | -2.126701 | 1.556366 |
| 56 | H | -2.442885 | -3.893476 | 1.575865 |
| 57 | C | 1.737274 | -5.039916 | 1.547020 |
| 58 | H | 2.438426 | -4.197582 | 1.555355 |
| 59 | H | 1.153988 | -4.993618 | 2.473724 |
| 60 | H | 2.331409 | -5.961112 | 1.575809 |
| 61 | C | 1.737274 | -5.039916 | -1.547020 |
| 62 | H | 1.153988 | -4.993618 | -2.473724 |
| 63 | H | 2.438426 | -4.197582 | -1.555355 |
| 64 | H | 2.331409 | -5.961112 | -1.575809 |
| 65 | C | -1.865724 | -7.024183 | -1.549673 |
| 66 | H | -2.611948 | -6.221280 | -1.540546 |
| 67 | H | -1.286855 | -6.929304 | -2.475341 |
| 68 | H | -2.403623 | -7.978549 | -1.586256 |
| 69 | C | -1.865724 | -7.024183 | 1.549673 |
| 70 | H | -1.286855 | -6.929304 | 2.475341 |
| 71 | H | -2.611948 | -6.221280 | 1.540546 |
| 72 | H | -2.403623 | -7.978549 | 1.586256 |
| 73 | C | 1.618545 | -9.164426 | 1.546106 |
| 74 | H | 2.417512 | -8.413561 | 1.588375 |
| 75 | H | 1.022891 | -9.075792 | 2.460682 |
| 76 | H | 2.086042 | -10.155837 | 1.541741 |
| 77 | C | 1.618545 | -9.164426 | -1.546106 |
| 78 | H | 1.022891 | -9.075792 | -2.460682 |
| 79 | H | 2.417512 | -8.413561 | -1.588375 |
| 80 | H | 2.086042 | -10.155837 | -1.541741 |
| 81 | Si | -0.556807 | 8.924441 | 0.000000 |
| 82 | Si | 0.753344 | 6.945024 | 0.000000 |
| 83 | Si | -0.612513 | 4.986544 | 0.000000 |
| 84 | Si | 0.694697 | 2.982205 | 0.000000 |
| 85 | Si | -0.655085 | 1.003135 | 0.000000 |
| 86 | Si | 0.655785 | -1.003160 | 0.000000 |
| 87 | Si | -0.694178 | -2.982091 | 0.000000 |
| 88 | Si | 0.612731 | -4.986615 | 0.000000 |
| 89 | Si | -0.753537 | -6.944841 | 0.000000 |
| 90 | Si | 0.556206 | -8.924531 | 0.000000 |
| 91 | Cl | -0.836040 | -10.538803 | 0.000000 |
| 92 | Cl | 0.835069 | 10.539030 | 0.000000 |

---

**Table S8. Magnetic Shielding Tensors of $^{29}$Si and $^{13}$C Nuclei of 4 Calculated by the GIAO Method**

```
SCF GIAO Magnetic shielding tensor (ppm):
  1  C    Isotropic =   176.1428   Anisotropy =    15.0425
   XX=   175.8114   YX=     7.9405   ZX=   -10.1961
   XY=     4.3883   YY=   177.0808   ZY=     4.9803
   XZ=    -9.7288   YZ=     2.0934   ZZ=   175.5362
   Eigenvalues:   162.4676   179.7896   186.1711
   Eigenvectors:
      (1)   0.659279  -0.427772   0.618355
      (2)   0.094505   0.863013   0.496264
      (3)   0.745936   0.268738  -0.609393
```

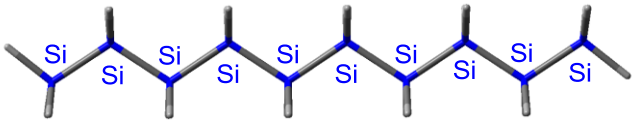
```
 5  C    Isotropic =   176.1428   Anisotropy =    15.0425
  XX=   175.8114   YX=     7.9405   ZX=    10.1961
  XY=     4.3883   YY=   177.0808   ZY=    -4.9803
  XZ=     9.7288   YZ=    -2.0934   ZZ=   175.5362
  Eigenvalues:   162.4676   179.7896   186.1711
  Eigenvectors:
     (1)   0.659279  -0.427772  -0.618355
     (2)   0.094505   0.863013  -0.496264
     (3)   0.745936   0.268739   0.609393
 9  C    Isotropic =   185.9177   Anisotropy =     3.8369
  XX=   185.1216   YX=    -2.1559   ZX=    -1.5868
  XY=    -1.1242   YY=   185.5217   ZY=    -1.2311
  XZ=     3.2765   YZ=    -1.0931   ZZ=   187.1098
  Eigenvalues:   183.6627   185.6147   188.4756
  Eigenvectors:
     (1)   0.733710   0.677718   0.048663
     (2)  -0.516469   0.509733   0.688064
     (3)   0.441508  -0.529973   0.724016
13  C    Isotropic =   185.9177   Anisotropy =     3.8369
  XX=   185.1216   YX=    -2.1559   ZX=     1.5868
  XY=    -1.1242   YY=   185.5217   ZY=     1.2311
  XZ=    -3.2765   YZ=     1.0931   ZZ=   187.1098
  Eigenvalues:   183.6627   185.6147   188.4756
  Eigenvectors:
     (1)   0.733710   0.677718  -0.048663
     (2)   0.516468  -0.509733   0.688065
     (3)  -0.441509   0.529973   0.724016
17  C    Isotropic =   183.5893   Anisotropy =     3.3578
  XX=   183.2054   YX=     0.3603   ZX=    -3.5261
  XY=    -0.4277   YY=   185.8253   ZY=     0.2054
  XZ=     1.5761   YZ=    -0.4049   ZZ=   181.7371
  Eigenvalues:   181.2484   183.6916   185.8278
  Eigenvectors:
     (1)   0.446120   0.022792   0.894683
     (2)   0.894964  -0.006722  -0.446088
     (3)  -0.004153   0.999718  -0.023396
21  C    Isotropic =   183.5893   Anisotropy =     3.3578
  XX=   183.2054   YX=     0.3603   ZX=     3.5261
  XY=    -0.4277   YY=   185.8253   ZY=    -0.2054
  XZ=    -1.5761   YZ=     0.4050   ZZ=   181.7371
  Eigenvalues:   181.2484   183.6916   185.8278
  Eigenvectors:
     (1)  -0.446120  -0.022791   0.894683
     (2)   0.894964  -0.006723   0.446088
     (3)  -0.004152   0.999718   0.023397
25  C    Isotropic =   182.9938   Anisotropy =     4.5865
  XX=   182.6460   YX=    -0.4307   ZX=    -4.0199
  XY=     0.0538   YY=   186.0382   ZY=    -0.1024
  XZ=     1.1994   YZ=     0.1875   ZZ=   180.2971
  Eigenvalues:   179.6360   183.2938   186.0514
  Eigenvectors:
     (1)   0.424582   0.006484   0.905366
     (2)   0.903064   0.068595  -0.423994
     (3)  -0.064853   0.997624   0.023268
29  C    Isotropic =   182.9938   Anisotropy =     4.5865
  XX=   182.6460   YX=    -0.4307   ZX=     4.0199
  XY=     0.0538   YY=   186.0382   ZY=     0.1024
  XZ=    -1.1994   YZ=    -0.1875   ZZ=   180.2971
  Eigenvalues:   179.6360   183.2938   186.0514
  Eigenvectors:
     (1)  -0.424583  -0.006484   0.905366
     (2)   0.903064   0.068595   0.423994
     (3)  -0.064853   0.997624  -0.023268
33  C    Isotropic =   182.8815   Anisotropy =     4.8761
  XX=   182.4393   YX=     0.0284   ZX=    -4.0657
  XY=    -0.0671   YY=   186.1320   ZY=     0.0650
```

```
  XZ=     1.2832   YZ=    -0.0119   ZZ=   180.0733
  Eigenvalues:   179.4301   183.0823   186.1323
  Eigenvectors:
     (1)   0.419628  -0.002388   0.907693
     (2)   0.907665   0.009401  -0.419591
     (3)  -0.007531   0.999953   0.006113
37  C    Isotropic =   182.8816   Anisotropy =     4.8761
  XX=   182.4393   YX=     0.0285   ZX=     4.0657
  XY=    -0.0671   YY=   186.1320   ZY=    -0.0650
  XZ=    -1.2832   YZ=     0.0119   ZZ=   180.0733
  Eigenvalues:   179.4301   183.0823   186.1323
  Eigenvectors:
     (1)  -0.419628   0.002388   0.907693
     (2)   0.907665   0.009401   0.419590
     (3)  -0.007531   0.999953  -0.006113
41  C    Isotropic =   182.8840   Anisotropy =     4.8726
  XX=   182.4435   YX=     0.0300   ZX=     4.0653
  XY=    -0.0667   YY=   186.1321   ZY=    -0.0658
  XZ=    -1.2823   YZ=     0.0122   ZZ=   180.0763
  Eigenvalues:   179.4331   183.0864   186.1324
  Eigenvectors:
     (1)  -0.419564   0.002485   0.907722
     (2)   0.907697   0.009158   0.419527
     (3)  -0.007270   0.999955  -0.006097
45  C    Isotropic =   182.8840   Anisotropy =     4.8726
  XX=   182.4435   YX=     0.0300   ZX=    -4.0653
  XY=    -0.0667   YY=   186.1321   ZY=     0.0658
  XZ=     1.2823   YZ=    -0.0122   ZZ=   180.0763
  Eigenvalues:   179.4331   183.0865   186.1324
  Eigenvectors:
     (1)   0.419564  -0.002485   0.907722
     (2)   0.907697   0.009158  -0.419527
     (3)  -0.007271   0.999955   0.006098
49  C    Isotropic =   182.9909   Anisotropy =     4.5902
  XX=   182.6416   YX=    -0.4303   ZX=     4.0200
  XY=     0.0545   YY=   186.0379   ZY=     0.1020
  XZ=    -1.1998   YZ=    -0.1879   ZZ=   180.2932
  Eigenvalues:   179.6322   183.2894   186.0510
  Eigenvectors:
     (1)  -0.424610  -0.006379   0.905354
     (2)   0.903068   0.068375   0.424019
     (3)  -0.064608   0.997639  -0.023272
53  C    Isotropic =   182.9909   Anisotropy =     4.5902
  XX=   182.6416   YX=    -0.4303   ZX=    -4.0200
  XY=     0.0545   YY=   186.0379   ZY=    -0.1020
  XZ=     1.1998   YZ=     0.1880   ZZ=   180.2932
  Eigenvalues:   179.6322   183.2894   186.0510
  Eigenvectors:
     (1)   0.424609   0.006379   0.905354
     (2)   0.903068   0.068375  -0.424019
     (3)  -0.064608   0.997639   0.023272
57  C    Isotropic =   183.5899   Anisotropy =     3.3571
  XX=   183.2063   YX=     0.3622   ZX=     3.5271
  XY=    -0.4267   YY=   185.8256   ZY=    -0.2066
  XZ=    -1.5747   YZ=     0.4043   ZZ=   181.7378
  Eigenvalues:   181.2482   183.6935   185.8280
  Eigenvectors:
     (1)  -0.446355  -0.022462   0.894574
     (2)   0.894849  -0.007168   0.446312
     (3)  -0.003613   0.999722   0.023299
61  C    Isotropic =   183.5899   Anisotropy =     3.3571
  XX=   183.2063   YX=     0.3622   ZX=    -3.5271
  XY=    -0.4267   YY=   185.8256   ZY=     0.2066
  XZ=     1.5747   YZ=    -0.4043   ZZ=   181.7378
  Eigenvalues:   181.2482   183.6935   185.8280
  Eigenvectors:
```

```
     (1)    0.446355    0.022462    0.894574
     (2)    0.894849   -0.007169   -0.446312
     (3)   -0.003612    0.999722   -0.023300
65  C    Isotropic =   185.9153   Anisotropy =     3.8372
  XX=   185.1177   YX=    -2.1573   ZX=     1.5871
  XY=    -1.1247   YY=   185.5206   ZY=     1.2314
  XZ=    -3.2757   YZ=     1.0925   ZZ=   187.1077
  Eigenvalues:   183.6591   185.6134   188.4735
  Eigenvectors:
     (1)    0.734030    0.677382   -0.048517
     (2)    0.516098   -0.509969    0.688167
     (3)   -0.441410    0.530175    0.723928
69  C    Isotropic =   185.9153   Anisotropy =     3.8372
  XX=   185.1177   YX=    -2.1573   ZX=    -1.5871
  XY=    -1.1247   YY=   185.5206   ZY=    -1.2314
  XZ=     3.2757   YZ=    -1.0925   ZZ=   187.1077
  Eigenvalues:   183.6591   185.6134   188.4735
  Eigenvectors:
     (1)    0.734030    0.677382    0.048516
     (2)   -0.516097    0.509969    0.688168
     (3)    0.441411   -0.530175    0.723927
73  C    Isotropic =   176.1432   Anisotropy =    15.0431
  XX=   175.8155   YX=     7.9414   ZX=    10.1946
  XY=     4.3896   YY=   177.0778   ZY=    -4.9835
  XZ=     9.7281   YZ=    -2.0943   ZZ=   175.5363
  Eigenvalues:   162.4681   179.7895   186.1719
  Eigenvectors:
     (1)    0.659164   -0.427959   -0.618347
     (2)    0.094639    0.862944   -0.496359
     (3)    0.746020    0.268662    0.609323
77  C    Isotropic =   176.1432   Anisotropy =    15.0431
  XX=   175.8155   YX=     7.9414   ZX=   -10.1946
  XY=     4.3896   YY=   177.0778   ZY=     4.9835
  XZ=    -9.7281   YZ=     2.0943   ZZ=   175.5363
  Eigenvalues:   162.4681   179.7895   186.1719
  Eigenvectors:
     (1)    0.659164   -0.427959    0.618347
     (2)    0.094639    0.862943    0.496359
     (3)    0.746020    0.268662   -0.609323
81  Si   Isotropic =   289.6117   Anisotropy =    52.6036
  XX=   302.9764   YX=    27.6850   ZX=     0.0000
  XY=    20.8325   YY=   297.5669   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   268.2918
  Eigenvalues:   268.2918   275.8626   324.6808
  Eigenvectors:
     (1)    0.000000    0.000000    1.000000
     (2)   -0.666780    0.745255    0.000000
     (3)    0.745255    0.666780    0.000000
82  Si   Isotropic =   356.3525   Anisotropy =    23.5405
  XX=   369.3400   YX=     8.1181   ZX=     0.0000
  XY=    10.1868   YY=   341.0914   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   358.6260
  Eigenvalues:   338.3853   358.6260   372.0461
  Eigenvectors:
     (1)   -0.283538    0.958961    0.000000
     (2)    0.000000    0.000000    1.000000
     (3)    0.958961    0.283538    0.000000
83  Si   Isotropic =   356.6207   Anisotropy =    20.6844
  XX=   369.7339   YX=    -5.5644   ZX=     0.0000
  XY=    -3.1828   YY=   342.1286   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   357.9994
  Eigenvalues:   341.4523   357.9994   370.4103
  Eigenvectors:
     (1)    0.152829    0.988253    0.000000
     (2)    0.000000    0.000000    1.000000
     (3)    0.988253   -0.152829    0.000000
```

```
84  Si   Isotropic =   352.1289   Anisotropy =    18.6401
  XX=   364.4961   YX=     1.2065   ZX=     0.0000
  XY=     1.1604   YY=   341.0261   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   350.8644
  Eigenvalues:   340.9666   350.8644   364.5556
  Eigenvectors:
     (1)  -0.050231   0.998738   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.998738   0.050231   0.000000
85  Si   Isotropic =   351.6754   Anisotropy =    18.7393
  XX=   364.1536   YX=    -0.4548   ZX=     0.0000
  XY=    -0.7004   YY=   341.3920   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   349.4806
  Eigenvalues:   341.3773   349.4806   364.1682
  Eigenvectors:
     (1)   0.025351   0.999679   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.999679  -0.025351   0.000000
86  Si   Isotropic =   351.6758   Anisotropy =    18.7415
  XX=   364.1549   YX=    -0.4672   ZX=     0.0000
  XY=    -0.7087   YY=   341.3867   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   349.4857
  Eigenvalues:   341.3715   349.4857   364.1701
  Eigenvectors:
     (1)   0.025797   0.999667   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.999667  -0.025797   0.000000
87  Si   Isotropic =   352.1287   Anisotropy =    18.6407
  XX=   364.4965   YX=     1.2030   ZX=     0.0000
  XY=     1.1587   YY=   341.0316   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   350.8579
  Eigenvalues:   340.9723   350.8579   364.5558
  Eigenvectors:
     (1)  -0.050134   0.998743   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.998743   0.050134   0.000000
88  Si   Isotropic =   356.6295   Anisotropy =    20.6834
  XX=   369.7383   YX=    -5.5815   ZX=     0.0000
  XY=    -3.1909   YY=   342.1285   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   358.0216
  Eigenvalues:   341.4485   358.0216   370.4184
  Eigenvectors:
     (1)   0.153215   0.988193   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.988193  -0.153215   0.000000
89  Si   Isotropic =   356.3356   Anisotropy =    23.5290
  XX=   369.3190   YX=     8.1049   ZX=     0.0000
  XY=    10.1805   YY=   341.0929   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   358.5950
  Eigenvalues:   338.3902   358.5950   372.0217
  Eigenvectors:
     (1)  -0.283480   0.958978   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.958978   0.283480   0.000000
90  Si   Isotropic =   289.6177   Anisotropy =    52.6041
  XX=   302.9961   YX=    27.6846   ZX=     0.0000
  XY=    20.8319   YY=   297.5577   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   268.2992
  Eigenvalues:   268.2992   275.8667   324.6870
  Eigenvectors:
     (1)   0.000000   0.000000   1.000000
     (2)  -0.666560   0.745451   0.000000
     (3)   0.745451   0.666560   0.000000
```

**Table S9. Atomic Coordinates of the Optimized Structure of 5**




| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | C | -1.520083 | 9.150326 | 1.545060 |
| 2 | H | -1.997419 | 10.138432 | 1.571748 |
| 3 | H | -2.317814 | 8.398670 | 1.561903 |
| 4 | H | -0.940719 | 9.038761 | 2.469138 |
| 5 | C | -1.520083 | 9.150326 | -1.545060 |
| 6 | H | -1.997419 | 10.138432 | -1.571748 |
| 7 | H | -0.940719 | 9.038761 | -2.469138 |
| 8 | H | -2.317814 | 8.398670 | -1.561903 |
| 9 | C | 1.962181 | 6.992886 | -1.545317 |
| 10 | H | 2.672195 | 6.157793 | -1.541351 |
| 11 | H | 1.383018 | 6.930543 | -2.473860 |
| 12 | H | 2.546368 | 7.920671 | -1.580556 |
| 13 | C | 1.962181 | 6.992886 | 1.545317 |
| 14 | H | 1.383018 | 6.930543 | 2.473860 |
| 15 | H | 2.672195 | 6.157793 | 1.541351 |
| 16 | H | 2.546368 | 7.920671 | 1.580556 |
| 17 | C | -1.665424 | 5.060858 | 1.545888 |
| 18 | H | -1.084660 | 5.000875 | 2.473546 |
| 19 | H | -2.243919 | 5.991622 | 1.577801 |
| 20 | H | -2.379320 | 4.229134 | 1.548350 |
| 21 | C | -1.665424 | 5.060858 | -1.545888 |
| 22 | H | -2.243919 | 5.991622 | -1.577801 |
| 23 | H | -1.084660 | 5.000875 | -2.473546 |
| 24 | H | -2.379320 | 4.229134 | -1.548350 |
| 25 | C | 1.861783 | 2.966552 | -1.546676 |
| 26 | H | 1.276826 | 2.951963 | -2.473518 |
| 27 | H | 2.501994 | 3.855749 | -1.574117 |
| 28 | H | 2.517147 | 2.088146 | -1.555403 |
| 29 | C | 1.861783 | 2.966552 | 1.546676 |
| 30 | H | 2.501994 | 3.855749 | 1.574117 |
| 31 | H | 1.276826 | 2.951963 | 2.473518 |
| 32 | H | 2.517147 | 2.088146 | 1.555403 |
| 33 | C | -1.765016 | 1.043224 | 1.546578 |
| 34 | H | -1.180410 | 1.025292 | 2.473585 |
| 35 | H | -2.388310 | 1.944498 | 1.566219 |
| 36 | H | -2.437082 | 0.177673 | 1.563058 |
| 37 | C | -1.765016 | 1.043224 | -1.546578 |
| 38 | H | -2.388310 | 1.944498 | -1.566219 |
| 39 | H | -1.180410 | 1.025292 | -2.473585 |
| 40 | H | -2.437082 | 0.177673 | -1.563058 |
| 41 | C | 1.765213 | -1.043359 | 1.546589 |
| 42 | H | 2.437377 | -0.177887 | 1.563065 |
| 43 | H | 1.180601 | -1.025351 | 2.473591 |
| 44 | H | 2.388403 | -1.944704 | 1.566243 |
| 45 | C | 1.765213 | -1.043359 | -1.546589 |
| 46 | H | 1.180601 | -1.025351 | -2.473591 |
| 47 | H | 2.437377 | -0.177887 | -1.563065 |
| 48 | H | 2.388403 | -1.944704 | -1.566243 |
| 49 | C | -1.861677 | -2.966404 | -1.546673 |
| 50 | H | -2.517028 | -2.087984 | -1.555358 |
| 51 | H | -1.276726 | -2.951783 | -2.473518 |

| | | | | |
|---|---|---|---|---|
| 52 | H | -2.501900 | -3.855589 | -1.574147 |
| 53 | C | -1.861677 | -2.966404 | 1.546673 |
| 54 | H | -1.276726 | -2.951783 | 2.473518 |
| 55 | H | -2.517028 | -2.087984 | 1.555358 |
| 56 | H | -2.501900 | -3.855589 | 1.574147 |
| 57 | C | 1.665420 | -5.060960 | 1.545883 |
| 58 | H | 2.379445 | -4.229346 | 1.548305 |
| 59 | H | 1.084669 | -5.000845 | 2.473541 |
| 60 | H | 2.243775 | -5.991810 | 1.577838 |
| 61 | C | 1.665420 | -5.060960 | -1.545883 |
| 62 | H | 1.084669 | -5.000845 | -2.473541 |
| 63 | H | 2.379445 | -4.229346 | -1.548305 |
| 64 | H | 2.243775 | -5.991810 | -1.577838 |
| 65 | C | -1.962283 | -6.992842 | -1.545310 |
| 66 | H | -2.672306 | -6.157757 | -1.541308 |
| 67 | H | -1.383142 | -6.930470 | -2.473863 |
| 68 | H | -2.546462 | -7.920632 | -1.580558 |
| 69 | C | -1.962283 | -6.992842 | 1.545310 |
| 70 | H | -1.383142 | -6.930470 | 2.473863 |
| 71 | H | -2.672306 | -6.157757 | 1.541308 |
| 72 | H | -2.546462 | -7.920632 | 1.580558 |
| 73 | C | 1.519941 | -9.150358 | 1.545051 |
| 74 | H | 2.317726 | -8.398759 | 1.561852 |
| 75 | H | 0.940608 | -9.038725 | 2.469139 |
| 76 | H | 1.997201 | -10.138501 | 1.571749 |
| 77 | C | 1.519941 | -9.150358 | -1.545051 |
| 78 | H | 0.940608 | -9.038725 | -2.469139 |
| 79 | H | 2.317726 | -8.398759 | -1.561852 |
| 80 | H | 1.997201 | -10.138501 | -1.571749 |
| 81 | Si | -0.419764 | 8.985149 | 0.000000 |
| 82 | Si | 0.831801 | 6.959670 | 0.000000 |
| 83 | Si | -0.538228 | 5.003888 | 0.000000 |
| 84 | Si | 0.734940 | 2.976915 | 0.000000 |
| 85 | Si | -0.638326 | 1.014084 | 0.000000 |
| 86 | Si | 0.638538 | -1.014112 | 0.000000 |
| 87 | Si | -0.734835 | -2.976849 | 0.000000 |
| 88 | Si | 0.538219 | -5.003897 | 0.000000 |
| 89 | Si | -0.831894 | -6.959633 | 0.000000 |
| 90 | Si | 0.419614 | -8.985139 | 0.000000 |
| 91 | C | -0.809646 | -10.443470 | 0.000000 |
| 92 | H | -1.457012 | -10.429457 | -0.884847 |
| 93 | H | -0.271422 | -11.400315 | 0.000000 |
| 94 | H | -1.457012 | -10.429457 | 0.884847 |
| 95 | C | 0.809446 | 10.443522 | 0.000000 |
| 96 | H | 0.271192 | 11.400348 | 0.000000 |
| 97 | H | 1.456813 | 10.429529 | 0.884847 |
| 98 | H | 1.456813 | 10.429529 | -0.884847 |

---

**Table S10. Magnetic Shielding Tensors of $^{29}$Si and $^{13}$C Nuclei of 5 Calculated by the GIAO Method**

```
SCF GIAO Magnetic shielding tensor (ppm):
  1  C    Isotropic =   181.7994   Anisotropy =     6.3587
   XX=   181.3241   YX=     3.3758   ZX=    -5.2135
   XY=     0.2789   YY=   182.6386   ZY=     2.5178
   XZ=    -4.0252   YZ=     0.1534   ZZ=   181.4354
   Eigenvalues:   176.0035   183.3562   186.0385
   Eigenvectors:
      (1)   0.681392  -0.320154   0.658184
      (2)   0.143439   0.940232   0.308851
      (3)   0.717726   0.116040  -0.686589
  5  C    Isotropic =   181.7994   Anisotropy =     6.3587
```

```
  XX=   181.3242   YX=     3.3758   ZX=     5.2135
  XY=     0.2789   YY=   182.6386   ZY=    -2.5178
  XZ=     4.0252   YZ=    -0.1534   ZZ=   181.4354
  Eigenvalues:   176.0035   183.3562   186.0385
  Eigenvectors:
     (1)   0.681392  -0.320154  -0.658184
     (2)   0.143438   0.940232  -0.308852
     (3)   0.717726   0.116041   0.686588
 9  C    Isotropic =   185.0150   Anisotropy =     1.2139
  XX=   184.8197   YX=    -1.2729   ZX=    -2.2897
  XY=     0.0084   YY=   184.9425   ZY=    -0.3368
  XZ=     2.9951   YZ=    -0.1182   ZZ=   185.2829
  Eigenvalues:   184.2331   184.9877   185.8243
  Eigenvectors:
     (1)   0.759696   0.639733  -0.116638
     (2)  -0.321120   0.525038   0.788173
     (3)   0.565460  -0.561317   0.604300
13  C    Isotropic =   185.0150   Anisotropy =     1.2139
  XX=   184.8197   YX=    -1.2729   ZX=     2.2897
  XY=     0.0084   YY=   184.9425   ZY=     0.3368
  XZ=    -2.9951   YZ=     0.1182   ZZ=   185.2829
  Eigenvalues:   184.2331   184.9877   185.8243
  Eigenvectors:
     (1)   0.759696   0.639733   0.116639
     (2)   0.321118  -0.525037   0.788175
     (3)  -0.565461   0.561318   0.604298
17  C    Isotropic =   183.2452   Anisotropy =     3.7406
  XX=   182.9736   YX=     0.4999   ZX=    -3.7592
  XY=    -0.1397   YY=   185.7271   ZY=     0.3471
  XZ=     1.3914   YZ=    -0.2507   ZZ=   181.0350
  Eigenvalues:   180.4715   183.5252   185.7390
  Eigenvectors:
     (1)   0.428937  -0.022982   0.903042
     (2)   0.900779  -0.064258  -0.429497
     (3)   0.067898   0.997669  -0.006861
21  C    Isotropic =   183.2452   Anisotropy =     3.7406
  XX=   182.9736   YX=     0.4999   ZX=     3.7592
  XY=    -0.1397   YY=   185.7271   ZY=    -0.3471
  XZ=    -1.3914   YZ=     0.2507   ZZ=   181.0350
  Eigenvalues:   180.4715   183.5252   185.7390
  Eigenvectors:
     (1)  -0.428937   0.022982   0.903042
     (2)   0.900779  -0.064259   0.429497
     (3)   0.067899   0.997669   0.006862
25  C    Isotropic =   182.8255   Anisotropy =     4.7314
  XX=   182.4743   YX=    -0.3417   ZX=    -4.1009
  XY=     0.1367   YY=   185.9738   ZY=     0.0177
  XZ=     1.1785   YZ=     0.1523   ZZ=   180.0285
  Eigenvalues:   179.3458   183.1509   185.9798
  Eigenvectors:
     (1)   0.423043  -0.005075   0.906095
     (2)   0.905263   0.045589  -0.422399
     (3)  -0.039164   0.998947   0.023881
29  C    Isotropic =   182.8255   Anisotropy =     4.7314
  XX=   182.4743   YX=    -0.3417   ZX=     4.1009
  XY=     0.1367   YY=   185.9738   ZY=    -0.0177
  XZ=    -1.1785   YZ=    -0.1523   ZZ=   180.0285
  Eigenvalues:   179.3458   183.1509   185.9798
  Eigenvectors:
     (1)  -0.423043   0.005075   0.906095
     (2)   0.905263   0.045589   0.422399
     (3)  -0.039164   0.998947  -0.023881
33  C    Isotropic =   182.8133   Anisotropy =     4.9358
  XX=   182.3893   YX=     0.1091   ZX=    -4.0982
  XY=     0.0658   YY=   186.1011   ZY=     0.1704
  XZ=     1.2412   YZ=     0.0192   ZZ=   179.9494
```

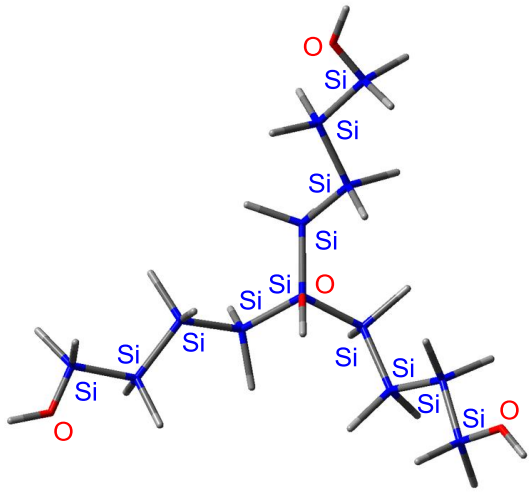
```
  Eigenvalues:   179.2887   183.0474   186.1038
  Eigenvectors:
     (1)   0.418776  -0.018009   0.907911
     (2)   0.907884  -0.012986  -0.419021
     (3)   0.019336   0.999753   0.010911
37  C    Isotropic =   182.8133   Anisotropy =     4.9358
  XX=   182.3893   YX=     0.1091   ZX=     4.0982
  XY=     0.0658   YY=   186.1011   ZY=    -0.1704
  XZ=    -1.2412   YZ=    -0.0192   ZZ=   179.9494
  Eigenvalues:   179.2887   183.0474   186.1038
  Eigenvectors:
     (1)  -0.418776   0.018009   0.907911
     (2)   0.907884  -0.012986   0.419021
     (3)   0.019337   0.999753  -0.010911
41  C    Isotropic =   182.8146   Anisotropy =     4.9344
  XX=   182.3914   YX=     0.1082   ZX=     4.0981
  XY=     0.0652   YY=   186.1015   ZY=    -0.1705
  XZ=    -1.2411   YZ=    -0.0186   ZZ=   179.9509
  Eigenvalues:   179.2903   183.0494   186.1042
  Eigenvectors:
     (1)  -0.418726   0.017932   0.907936
     (2)   0.907911  -0.012822   0.418968
     (3)   0.019155   0.999757  -0.010912
45  C    Isotropic =   182.8146   Anisotropy =     4.9344
  XX=   182.3914   YX=     0.1082   ZX=    -4.0981
  XY=     0.0652   YY=   186.1015   ZY=     0.1705
  XZ=     1.2411   YZ=     0.0186   ZZ=   179.9509
  Eigenvalues:   179.2903   183.0494   186.1042
  Eigenvectors:
     (1)   0.418726  -0.017932   0.907935
     (2)   0.907911  -0.012822  -0.418968
     (3)   0.019155   0.999757   0.010912
49  C    Isotropic =   182.8249   Anisotropy =     4.7329
  XX=   182.4733   YX=    -0.3441   ZX=     4.1008
  XY=     0.1359   YY=   185.9740   ZY=    -0.0173
  XZ=    -1.1786   YZ=    -0.1516   ZZ=   180.0273
  Eigenvalues:   179.3448   183.1497   185.9801
  Eigenvectors:
     (1)  -0.423011   0.004901   0.906111
     (2)   0.905258   0.046006   0.422364
     (3)  -0.039616   0.998929  -0.023897
53  C    Isotropic =   182.8249   Anisotropy =     4.7329
  XX=   182.4733   YX=    -0.3441   ZX=    -4.1008
  XY=     0.1359   YY=   185.9740   ZY=     0.0173
  XZ=     1.1786   YZ=     0.1516   ZZ=   180.0273
  Eigenvalues:   179.3448   183.1497   185.9801
  Eigenvectors:
     (1)   0.423011  -0.004901   0.906111
     (2)   0.905258   0.046006  -0.422364
     (3)  -0.039617   0.998929   0.023898
57  C    Isotropic =   183.2446   Anisotropy =     3.7410
  XX=   182.9724   YX=     0.5010   ZX=     3.7598
  XY=    -0.1392   YY=   185.7265   ZY=    -0.3478
  XZ=    -1.3911   YZ=     0.2506   ZZ=   181.0349
  Eigenvalues:   180.4707   183.5245   185.7386
  Eigenvectors:
     (1)  -0.429151   0.023125   0.902937
     (2)   0.900656  -0.064511   0.429719
     (3)   0.068186   0.997649   0.006857
61  C    Isotropic =   183.2446   Anisotropy =     3.7410
  XX=   182.9724   YX=     0.5010   ZX=    -3.7598
  XY=    -0.1392   YY=   185.7266   ZY=     0.3478
  XZ=     1.3911   YZ=    -0.2506   ZZ=   181.0349
  Eigenvalues:   180.4707   183.5245   185.7386
  Eigenvectors:
     (1)   0.429151  -0.023126   0.902937
```

```
     (2)    0.900655  -0.064512  -0.429719
     (3)    0.068188   0.997649  -0.006857
65  C    Isotropic =   185.0150   Anisotropy =     1.2131
  XX=   184.8199   YX=    -1.2726   ZX=     2.2898
  XY=     0.0086   YY=   184.9420   ZY=     0.3368
  XZ=    -2.9947   YZ=     0.1177   ZZ=   185.2832
  Eigenvalues:   184.2333   184.9880   185.8238
  Eigenvectors:
     (1)    0.759525   0.639965   0.116476
     (2)    0.321532  -0.525023   0.788015
     (3)   -0.565454   0.561067   0.604538
69  C    Isotropic =   185.0150   Anisotropy =     1.2131
  XX=   184.8199   YX=    -1.2726   ZX=    -2.2898
  XY=     0.0086   YY=   184.9420   ZY=    -0.3368
  XZ=     2.9947   YZ=    -0.1177   ZZ=   185.2832
  Eigenvalues:   184.2333   184.9880   185.8238
  Eigenvectors:
     (1)    0.759525   0.639965  -0.116477
     (2)   -0.321530   0.525022   0.788017
     (3)    0.565456  -0.561068   0.604535
73  C    Isotropic =   181.7991   Anisotropy =     6.3587
  XX=   181.3241   YX=     3.3761   ZX=     5.2136
  XY=     0.2792   YY=   182.6383   ZY=    -2.5183
  XZ=     4.0250   YZ=    -0.1535   ZZ=   181.4349
  Eigenvalues:   176.0030   183.3560   186.0382
  Eigenvectors:
     (1)    0.681366  -0.320199  -0.658190
     (2)    0.143434   0.940212  -0.308914
     (3)    0.717752   0.116076   0.686556
77  C    Isotropic =   181.7991   Anisotropy =     6.3587
  XX=   181.3241   YX=     3.3761   ZX=    -5.2136
  XY=     0.2792   YY=   182.6383   ZY=     2.5183
  XZ=    -4.0250   YZ=     0.1535   ZZ=   181.4349
  Eigenvalues:   176.0030   183.3560   186.0382
  Eigenvectors:
     (1)    0.681366  -0.320199   0.658190
     (2)    0.143433   0.940212   0.308915
     (3)    0.717752   0.116078  -0.686555
81  Si   Isotropic =   340.1348   Anisotropy =     6.4999
  XX=   342.4299   YX=     2.0663   ZX=     0.0000
  XY=     2.7618   YY=   333.5065   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   344.4681
  Eigenvalues:   332.8953   343.0411   344.4681
  Eigenvectors:
     (1)   -0.245446   0.969410   0.000000
     (2)    0.969410   0.245446   0.000000
     (3)    0.000000   0.000000   1.000000
82  Si   Isotropic =   359.3533   Anisotropy =    21.5502
  XX=   371.9720   YX=     6.9910   ZX=     0.0000
  XY=     7.0098   YY=   345.6868   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   360.4012
  Eigenvalues:   343.9386   360.4012   373.7202
  Eigenvectors:
     (1)   -0.242277   0.970207   0.000000
     (2)    0.000000   0.000000   1.000000
     (3)    0.970207   0.242277   0.000000
83  Si   Isotropic =   354.8584   Anisotropy =    20.2050
  XX=   367.8008   YX=    -4.0464   ZX=     0.0000
  XY=    -3.2873   YY=   342.8422   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   353.9321
  Eigenvalues:   342.3146   353.9321   368.3283
  Eigenvectors:
     (1)    0.142409   0.989808   0.000000
     (2)    0.000000   0.000000   1.000000
     (3)    0.989808  -0.142409   0.000000
84  Si   Isotropic =   351.8858   Anisotropy =    19.1567
```

```
  XX=   364.6543   YX=     0.1334   ZX=     0.0000
  XY=     0.3668   YY=   341.7750   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   349.2282
  Eigenvalues:   341.7723   349.2282   364.6570
  Eigenvectors:
     (1)  -0.010930   0.999940   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.999940   0.010930   0.000000
85  Si   Isotropic =   351.9563   Anisotropy =    19.3710
  XX=   364.8321   YX=    -0.8270   ZX=     0.0000
  XY=    -1.0539   YY=   341.7695   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   349.2674
  Eigenvalues:   341.7312   349.2674   364.8703
  Eigenvectors:
     (1)   0.040677   0.999172   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.999172  -0.040677   0.000000
86  Si   Isotropic =   351.9579   Anisotropy =    19.3710
  XX=   364.8330   YX=    -0.8338   ZX=     0.0000
  XY=    -1.0602   YY=   341.7676   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   349.2730
  Eigenvalues:   341.7288   349.2730   364.8719
  Eigenvectors:
     (1)   0.040953   0.999161   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.999161  -0.040953   0.000000
87  Si   Isotropic =   351.8846   Anisotropy =    19.1576
  XX=   364.6537   YX=     0.1312   ZX=     0.0000
  XY=     0.3622   YY=   341.7761   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   349.2240
  Eigenvalues:   341.7735   349.2240   364.6564
  Eigenvectors:
     (1)  -0.010783   0.999942   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.999942   0.010783   0.000000
88  Si   Isotropic =   354.8609   Anisotropy =    20.2031
  XX=   367.8009   YX=    -4.0522   ZX=     0.0000
  XY=    -3.2892   YY=   342.8450   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   353.9367
  Eigenvalues:   342.3163   353.9367   368.3296
  Eigenvectors:
     (1)   0.142564   0.989786   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.989786  -0.142564   0.000000
89  Si   Isotropic =   359.3512   Anisotropy =    21.5512
  XX=   371.9696   YX=     6.9929   ZX=     0.0000
  XY=     7.0115   YY=   345.6872   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   360.3969
  Eigenvalues:   343.9381   360.3969   373.7187
  Eigenvectors:
     (1)  -0.242350   0.970189   0.000000
     (2)   0.000000   0.000000   1.000000
     (3)   0.970189   0.242350   0.000000
90  Si   Isotropic =   340.1364   Anisotropy =     6.5012
  XX=   342.4310   YX=     2.0642   ZX=     0.0000
  XY=     2.7619   YY=   333.5077   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   344.4705
  Eigenvalues:   332.8969   343.0417   344.4705
  Eigenvectors:
     (1)  -0.245360   0.969432   0.000000
     (2)   0.969432   0.245360  -0.000004
     (3)   0.000004   0.000001   1.000000
91  C    Isotropic =   183.8052   Anisotropy =     7.4967
  XX=   184.9656   YX=     1.4409   ZX=     0.0000
  XY=     6.2412   YY=   184.9582   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   181.4918
```

```
  Eigenvalues:   181.1208   181.4918   188.8030
  Eigenvectors:
     (1)  -0.706766   0.707447   0.000004
     (2)   0.000003  -0.000003   1.000000
     (3)   0.707447   0.706766   0.000000
95  C    Isotropic =   183.8050   Anisotropy =     7.4969
  XX=   184.9648   YX=     1.4413   ZX=     0.0000
  XY=     6.2417   YY=   184.9581   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   181.4921
  Eigenvalues:   181.1199   181.4921   188.8029
  Eigenvectors:
     (1)  -0.706795   0.707419  -0.000001
     (2)  -0.000001   0.000001   1.000000
     (3)   0.707419   0.706795   0.000000
```

**Table S11. Atomic Coordinates of the Optimized Structure of 8a**




| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | Si | -0.090446 | 0.050454 | 0.992370 |
| 2 | O | 0.104673 | 0.040120 | -0.699216 |
| 3 | C | -0.353252 | 1.064380 | -1.560457 |
| 4 | H | -0.304762 | 0.694338 | -2.590250 |
| 5 | H | -1.393205 | 1.353995 | -1.348877 |
| 6 | H | 0.276348 | 1.961274 | -1.485762 |
| 7 | Si | -2.443298 | 0.041878 | 1.535784 |
| 8 | Si | 0.994050 | 1.915730 | 2.067552 |
| 9 | Si | 0.985388 | -2.005005 | 1.587532 |
| 10 | Si | 3.067359 | -2.379223 | 0.460364 |
| 11 | Si | 0.892563 | 4.126606 | 1.146824 |
| 12 | Si | -3.843034 | -1.219138 | 0.052786 |
| 13 | C | 2.858495 | 1.532294 | 2.276153 |
| 14 | H | 3.006458 | 0.605578 | 2.841139 |
| 15 | H | 3.367488 | 1.421920 | 1.312398 |
| 16 | H | 3.360464 | 2.337221 | 2.827127 |
| 17 | C | 0.295706 | 2.003074 | 3.852088 |
| 18 | H | 0.853575 | 2.741581 | 4.440416 |
| 19 | H | -0.761243 | 2.288867 | 3.881591 |

| | | | | |
|---|---|---|---|---|
| 20 | H | 0.394191 | 1.035568 | 4.359279 |
| 21 | C | 1.046740 | 5.310128 | 2.648148 |
| 22 | H | 1.045357 | 6.358248 | 2.324187 |
| 23 | H | 0.207310 | 5.176236 | 3.340865 |
| 24 | H | 1.972097 | 5.139651 | 3.209951 |
| 25 | C | −0.765936 | 4.559738 | 0.300129 |
| 26 | H | −0.940209 | 3.973094 | −0.607927 |
| 27 | H | −1.612391 | 4.389010 | 0.974264 |
| 28 | H | −0.779764 | 5.620058 | 0.018820 |
| 29 | C | 1.278996 | −2.100640 | 3.477105 |
| 30 | H | 1.703115 | −3.076837 | 3.743365 |
| 31 | H | 1.973501 | −1.333143 | 3.835175 |
| 32 | H | 0.340069 | −1.989385 | 4.032820 |
| 33 | C | −0.221587 | −3.426325 | 1.166237 |
| 34 | H | −1.117011 | −3.371730 | 1.795415 |
| 35 | H | −0.540190 | −3.389398 | 0.118668 |
| 36 | H | 0.244201 | −4.402832 | 1.339710 |
| 37 | C | 3.242206 | −1.280462 | −1.090916 |
| 38 | H | 2.392027 | −1.407348 | −1.768063 |
| 39 | H | 3.278429 | −0.219861 | −0.816762 |
| 40 | H | 4.161227 | −1.517066 | −1.640367 |
| 41 | C | 4.509224 | −1.964595 | 1.650797 |
| 42 | H | 4.483003 | −0.917050 | 1.969997 |
| 43 | H | 4.482146 | −2.588446 | 2.551610 |
| 44 | H | 5.475806 | −2.133204 | 1.160152 |
| 45 | C | −2.663015 | −0.661770 | 3.303128 |
| 46 | H | −3.717622 | −0.618909 | 3.602356 |
| 47 | H | −2.342644 | −1.707165 | 3.371524 |
| 48 | H | −2.088293 | −0.084800 | 4.037119 |
| 49 | C | −3.089368 | 1.843944 | 1.590071 |
| 50 | H | −2.492775 | 2.456522 | 2.275291 |
| 51 | H | −3.057552 | 2.322370 | 0.605233 |
| 52 | H | −4.128242 | 1.872860 | 1.939279 |
| 53 | C | −3.097446 | −1.307668 | −1.705421 |
| 54 | H | −3.124417 | −0.334130 | −2.207611 |
| 55 | H | −2.050970 | −1.630332 | −1.671905 |
| 56 | H | −3.653936 | −2.016380 | −2.330234 |
| 57 | C | −4.024972 | −3.014715 | 0.691068 |
| 58 | H | −4.694577 | −3.584653 | 0.034849 |
| 59 | H | −3.063791 | −3.538231 | 0.709975 |
| 60 | H | −4.445258 | −3.050020 | 1.702739 |
| 61 | Si | 3.294077 | −4.659847 | −0.183959 |
| 62 | Si | 2.721228 | 4.613044 | −0.303178 |
| 63 | Si | −6.025582 | −0.273044 | −0.083155 |
| 64 | C | −6.768234 | 0.002539 | 1.658151 |
| 65 | H | −6.785790 | −0.925911 | 2.240873 |
| 66 | H | −6.197721 | 0.743416 | 2.230512 |
| 67 | H | −7.799542 | 0.366489 | 1.579553 |
| 68 | C | −5.986797 | 1.400078 | −1.006156 |
| 69 | H | −5.424583 | 2.155865 | −0.446041 |
| 70 | H | −5.524772 | 1.303784 | −1.995842 |
| 71 | H | −7.007068 | 1.772499 | −1.152880 |
| 72 | C | 3.073030 | −5.826004 | 1.317196 |
| 73 | H | 2.058198 | −5.777418 | 1.729261 |
| 74 | H | 3.261765 | −6.863996 | 1.018688 |
| 75 | H | 3.771433 | −5.579935 | 2.125718 |
| 76 | C | 2.013286 | −5.127074 | −1.522594 |
| 77 | H | 0.990191 | −5.098875 | −1.131131 |
| 78 | H | 2.061969 | −4.445164 | −2.379576 |
| 79 | H | 2.210693 | −6.139957 | −1.891604 |
| 80 | C | 3.040481 | 3.253273 | −1.606697 |
| 81 | H | 3.230535 | 2.277860 | −1.143619 |
| 82 | H | 2.196187 | 3.134663 | −2.295012 |
| 83 | H | 3.919755 | 3.517055 | −2.206385 |
| 84 | C | 4.312392 | 4.826648 | 0.734205 |
| 85 | H | 4.179629 | 5.567632 | 1.530817 |

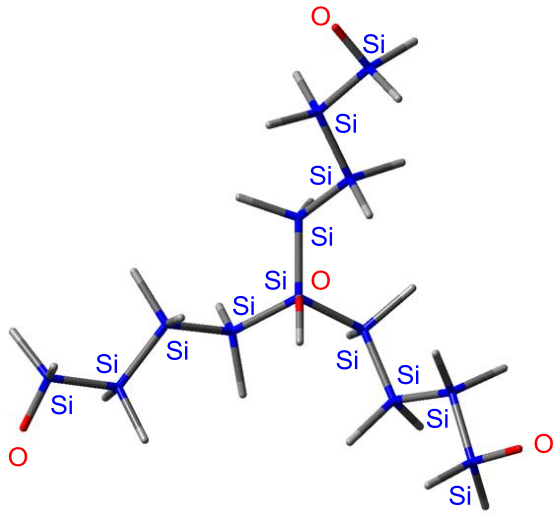
| | | | | |
|---|---|---|---|---|
| 86 | H | 4.621001 | 3.884318 | 1.201176 |
| 87 | H | 5.130840 | 5.172165 | 0.092291 |
| 88 | Si | 2.384261 | 6.635828 | -1.484961 |
| 89 | Si | -7.517832 | -1.691690 | -1.254074 |
| 90 | Si | 5.427449 | -5.156732 | -1.085578 |
| 91 | C | 1.037131 | 6.504137 | -2.815899 |
| 92 | H | 1.243896 | 5.685448 | -3.514820 |
| 93 | H | 0.055698 | 6.316573 | -2.363280 |
| 94 | H | 0.954229 | 7.428817 | -3.401218 |
| 95 | C | 1.958852 | 8.105239 | -0.359929 |
| 96 | H | 1.001860 | 7.939479 | 0.150818 |
| 97 | H | 2.724608 | 8.257295 | 0.409458 |
| 98 | H | 1.866175 | 9.040050 | -0.927391 |
| 99 | C | -8.058932 | -3.193511 | -0.225984 |
| 100 | H | -8.804189 | -3.800326 | -0.755933 |
| 101 | H | -7.204811 | -3.845932 | -0.006717 |
| 102 | H | -8.497343 | -2.887397 | 0.730736 |
| 103 | C | -6.825328 | -2.331219 | -2.902008 |
| 104 | H | -6.495457 | -1.509536 | -3.547866 |
| 105 | H | -5.962793 | -2.987375 | -2.730744 |
| 106 | H | -7.570473 | -2.914695 | -3.457650 |
| 107 | C | 5.958257 | -4.035589 | -2.522733 |
| 108 | H | 5.203235 | -4.011024 | -3.316751 |
| 109 | H | 6.114599 | -3.005644 | -2.178563 |
| 110 | H | 6.901473 | -4.374256 | -2.970387 |
| 111 | C | 6.813318 | -5.136525 | 0.212427 |
| 112 | H | 6.963720 | -4.125348 | 0.610135 |
| 113 | H | 6.580430 | -5.794467 | 1.057386 |
| 114 | H | 7.770664 | -5.465114 | -0.212095 |
| 115 | O | 5.202279 | -6.733955 | -1.647226 |
| 116 | O | 3.885011 | 6.886539 | -2.215465 |
| 117 | O | -8.847223 | -0.691250 | -1.540054 |
| 118 | C | -10.030024 | -1.115740 | -2.195843 |
| 119 | H | -10.535495 | -1.922834 | -1.646311 |
| 120 | H | -10.713360 | -0.262068 | -2.255904 |
| 121 | H | -9.827491 | -1.466170 | -3.218091 |
| 122 | C | 6.215024 | -7.510277 | -2.263607 |
| 123 | H | 7.071795 | -7.672082 | -1.593758 |
| 124 | H | 5.790556 | -8.487155 | -2.518536 |
| 125 | H | 6.582046 | -7.043485 | -3.189005 |
| 126 | C | 4.186690 | 7.987222 | -3.056249 |
| 127 | H | 4.096838 | 8.944900 | -2.523681 |
| 128 | H | 5.221371 | 7.882258 | -3.399250 |
| 129 | H | 3.533410 | 8.018952 | -3.940019 |

**Table S12. Magnetic Shielding Tensors of $^{29}$Si Nuclei of 8a Calculated by the GIAO Method**

```
SCF GIAO Magnetic shielding tensor (ppm):
      1  Si   Isotropic =   292.9949   Anisotropy =   155.5017
   XX=   243.3344   YX=    -2.1812   ZX=   -10.3374
   XY=    -0.2356   YY=   242.2260   ZY=   -19.4329
   XZ=   -20.0553   YZ=   -13.5185   ZZ=   393.4243
   Eigenvalues:   238.2575   244.0645   396.6627
      7  Si   Isotropic =   353.6035   Anisotropy =    14.3029
   XX=   351.1943   YX=    -3.2570   ZX=    -0.6680
   XY=    -4.9839   YY=   354.8180   ZY=     4.4659
   XZ=    -7.1704   YZ=     6.7832   ZZ=   354.7983
   Eigenvalues:   348.4670   349.2048   363.1388
      8  Si   Isotropic =   360.4757   Anisotropy =    18.8016
   XX=   370.2572   YX=    -7.2877   ZX=     0.3422
   XY=    -9.4183   YY=   347.6580   ZY=     4.6623
```

```
XZ=     2.6316   YZ=     4.8605   ZZ=   363.5118
Eigenvalues:   343.6532   364.7638   373.0101
   9  Si   Isotropic =   353.4580   Anisotropy =    16.0470
XX=   347.8926   YX=     7.0220   ZX=    -4.2395
XY=     7.3382   YY=   355.4643   ZY=    -4.6399
XZ=    -3.1347   YZ=    -3.9034   ZZ=   357.0170
Eigenvalues:   343.4837   352.7342   364.1560
  10  Si   Isotropic =   358.7647   Anisotropy =    22.4263
XX=   358.7831   YX=    11.2270   ZX=     0.9881
XY=    10.5099   YY=   355.3798   ZY=   -12.9926
XZ=     2.1428   YZ=   -11.1090   ZZ=   362.1313
Eigenvalues:   340.8229   361.7557   373.7156
  11  Si   Isotropic =   361.2584   Anisotropy =    13.4159
XX=   366.4067   YX=    -5.2744   ZX=     4.6994
XY=    -6.6960   YY=   359.4393   ZY=     0.6553
XZ=     5.1563   YZ=     9.3043   ZZ=   357.9292
Eigenvalues:   350.0516   363.5212   370.2023
  12  Si   Isotropic =   355.8741   Anisotropy =    23.4484
XX=   343.8949   YX=    -0.7489   ZX=    -8.5766
XY=    -5.9149   YY=   360.8579   ZY=     6.1269
XZ=    -4.1270   YZ=     9.4895   ZZ=   362.8695
Eigenvalues:   341.9117   354.2042   371.5064
  61  Si   Isotropic =   364.4544   Anisotropy =    25.6191
XX=   354.8548   YX=    15.8186   ZX=    10.1366
XY=    15.9030   YY=   370.4224   ZY=    -2.5542
XZ=    13.0479   YZ=    -3.7066   ZZ=   368.0858
Eigenvalues:   340.1843   371.6450   381.5337
  62  Si   Isotropic =   366.7060   Anisotropy =    21.2592
XX=   377.4232   YX=    -3.5985   ZX=     5.9895
XY=    -0.2640   YY=   357.3319   ZY=    17.2815
XZ=     5.9227   YZ=    11.0973   ZZ=   365.3627
Eigenvalues:   345.7574   373.4817   380.8787
  63  Si   Isotropic =   362.4711   Anisotropy =    22.1422
XX=   350.5890   YX=   -13.7706   ZX=   -10.0283
XY=    -8.4108   YY=   372.0885   ZY=    -5.9791
XZ=    -9.2917   YZ=    -6.4193   ZZ=   364.7358
Eigenvalues:   340.5740   369.6067   377.2325
  88  Si   Isotropic =   308.2238   Anisotropy =    67.5440
XX=   333.9608   YX=     7.7087   ZX=   -27.8400
XY=    14.8082   YY=   293.6106   ZY=   -13.6783
XZ=   -27.9594   YZ=   -11.6846   ZZ=   297.1001
Eigenvalues:   278.9954   292.4229   353.2532
  89  Si   Isotropic =   307.7927   Anisotropy =    65.6609
XX=   331.8774   YX=   -29.3388   ZX=    15.4779
XY=   -23.0738   YY=   305.2037   ZY=    -0.1652
XZ=    17.1817   YZ=    -5.1070   ZZ=   286.2971
Eigenvalues:   279.0005   292.8110   351.5667
  90  Si   Isotropic =   307.1649   Anisotropy =    64.7144
XX=   291.9465   YX=    -4.2479   ZX=    -5.5976
XY=     4.7428   YY=   339.4647   ZY=    23.0661
XZ=    -1.9394   YZ=    27.9684   ZZ=   290.0833
Eigenvalues:   278.3313   292.8555   350.3078
```

**Table S13. Atomic Coordinates of the Optimized Structure of 8b**




| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | Si | -0.071905 | 0.025208 | 0.841370 |
| 2 | O | 0.108799 | -0.011461 | -0.850701 |
| 3 | C | -0.369191 | 0.984714 | -1.733900 |
| 4 | H | -0.374541 | 0.570808 | -2.748024 |
| 5 | H | -1.392850 | 1.304669 | -1.489256 |
| 6 | H | 0.279955 | 1.870999 | -1.727045 |
| 7 | Si | -2.419049 | 0.008282 | 1.409344 |
| 8 | Si | 1.007247 | 1.911146 | 1.884901 |
| 9 | Si | 1.020995 | -2.016119 | 1.453247 |
| 10 | Si | 3.103209 | -2.384077 | 0.324604 |
| 11 | Si | 0.867598 | 4.110983 | 0.940929 |
| 12 | Si | -3.834810 | -1.270247 | -0.044156 |
| 13 | C | 2.876375 | 1.544324 | 2.079228 |
| 14 | H | 3.035551 | 0.621433 | 2.647385 |
| 15 | H | 3.378613 | 1.433082 | 1.112110 |
| 16 | H | 3.376815 | 2.355328 | 2.622522 |
| 17 | C | 0.327952 | 2.009620 | 3.676271 |
| 18 | H | 0.885971 | 2.758784 | 4.250774 |
| 19 | H | -0.730942 | 2.286656 | 3.715146 |
| 20 | H | 0.440855 | 1.048255 | 4.192107 |
| 21 | C | 0.967259 | 5.314359 | 2.430613 |
| 22 | H | 0.944684 | 6.358477 | 2.094943 |
| 23 | H | 0.120147 | 5.166591 | 3.111042 |
| 24 | H | 1.887020 | 5.173344 | 3.009450 |
| 25 | C | -0.784859 | 4.494995 | 0.059560 |
| 26 | H | -0.931324 | 3.890673 | -0.841766 |
| 27 | H | -1.638904 | 4.317386 | 0.722062 |
| 28 | H | -0.815797 | 5.550038 | -0.239617 |
| 29 | C | 1.320103 | -2.093411 | 3.342711 |
| 30 | H | 1.747230 | -3.066033 | 3.617127 |
| 31 | H | 2.013787 | -1.321000 | 3.691811 |
| 32 | H | 0.382312 | -1.979088 | 3.899650 |
| 33 | C | -0.178158 | -3.448159 | 1.046328 |
| 34 | H | -1.070205 | -3.396355 | 1.680464 |
| 35 | H | -0.503042 | -3.418120 | 0.000453 |

| | | | | |
|---|---|---|---|---|
| 36 | H | 0.295079 | -4.420751 | 1.221619 |
| 37 | C | 3.271949 | -1.285268 | -1.227219 |
| 38 | H | 2.422561 | -1.417658 | -1.904266 |
| 39 | H | 3.301753 | -0.224391 | -0.953195 |
| 40 | H | 4.192566 | -1.516042 | -1.776466 |
| 41 | C | 4.542996 | -1.961569 | 1.514721 |
| 42 | H | 4.513327 | -0.913016 | 1.830373 |
| 43 | H | 4.516968 | -2.582442 | 2.417597 |
| 44 | H | 5.510520 | -2.128803 | 1.025570 |
| 45 | C | -2.614849 | -0.685477 | 3.183470 |
| 46 | H | -3.665981 | -0.644136 | 3.494848 |
| 47 | H | -2.290127 | -1.729294 | 3.254505 |
| 48 | H | -2.033488 | -0.101974 | 3.906994 |
| 49 | C | -3.071217 | 1.808080 | 1.462917 |
| 50 | H | -2.465796 | 2.426958 | 2.134609 |
| 51 | H | -3.056248 | 2.279847 | 0.474534 |
| 52 | H | -4.104569 | 1.836319 | 1.828224 |
| 53 | C | -3.119110 | -1.375246 | -1.813675 |
| 54 | H | -3.144772 | -0.405007 | -2.322144 |
| 55 | H | -2.075679 | -1.709046 | -1.795838 |
| 56 | H | -3.693562 | -2.082802 | -2.423921 |
| 57 | C | -3.993189 | -3.058901 | 0.617143 |
| 58 | H | -4.674087 | -3.640286 | -0.016366 |
| 59 | H | -3.027886 | -3.575179 | 0.619481 |
| 60 | H | -4.389550 | -3.086016 | 1.638573 |
| 61 | Si | 3.337284 | -4.664851 | -0.315168 |
| 62 | Si | 2.703559 | 4.618466 | -0.490559 |
| 63 | Si | -6.018801 | -0.325653 | -0.147602 |
| 64 | C | -6.741410 | -0.086978 | 1.606845 |
| 65 | H | -6.753323 | -1.027642 | 2.169798 |
| 66 | H | -6.164104 | 0.641255 | 2.188736 |
| 67 | H | -7.773355 | 0.277728 | 1.545281 |
| 68 | C | -5.988585 | 1.366912 | -1.035955 |
| 69 | H | -5.410913 | 2.108355 | -0.472946 |
| 70 | H | -5.548331 | 1.289109 | -2.037168 |
| 71 | H | -7.009478 | 1.748941 | -1.151794 |
| 72 | C | 3.137368 | -5.823915 | 1.193937 |
| 73 | H | 2.129550 | -5.771201 | 1.622413 |
| 74 | H | 3.319409 | -6.863725 | 0.897754 |
| 75 | H | 3.849345 | -5.574820 | 1.989575 |
| 76 | C | 2.047495 | -5.142887 | -1.641071 |
| 77 | H | 1.027132 | -5.109995 | -1.243022 |
| 78 | H | 2.091267 | -4.468290 | -2.504046 |
| 79 | H | 2.240501 | -6.159251 | -2.002901 |
| 80 | C | 3.031674 | 3.263709 | -1.797226 |
| 81 | H | 3.218900 | 2.286630 | -1.336424 |
| 82 | H | 2.190071 | 3.148190 | -2.489572 |
| 83 | H | 3.913776 | 3.528435 | -2.392299 |
| 84 | C | 4.286960 | 4.840971 | 0.556206 |
| 85 | H | 4.142061 | 5.577192 | 1.355175 |
| 86 | H | 4.600976 | 3.899458 | 1.020975 |
| 87 | H | 5.106513 | 5.196891 | -0.078543 |
| 88 | Si | 2.358859 | 6.643732 | -1.663243 |
| 89 | Si | -7.546666 | -1.685639 | -1.339542 |
| 90 | Si | 5.464413 | -5.151777 | -1.233027 |
| 91 | C | 1.032518 | 6.510648 | -3.012876 |
| 92 | H | 1.259593 | 5.704236 | -3.719463 |
| 93 | H | 0.043697 | 6.310080 | -2.582100 |
| 94 | H | 0.954210 | 7.443718 | -3.587022 |
| 95 | C | 1.894912 | 8.101369 | -0.540554 |
| 96 | H | 0.925090 | 7.934344 | -0.054859 |
| 97 | H | 2.640842 | 8.256260 | 0.247273 |
| 98 | H | 1.814815 | 9.036378 | -1.111287 |
| 99 | C | -7.911507 | -3.346702 | -0.499081 |
| 100 | H | -8.702836 | -3.893917 | -1.029209 |
| 101 | H | -7.023913 | -3.991103 | -0.486949 |

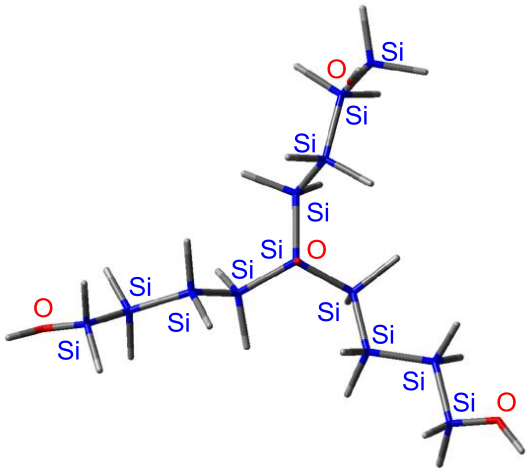
| | | | | |
|---|---|---|---|---|
| 102 | H | -8.239407 | -3.210067 | 0.537519 |
| 103 | C | -7.006894 | -2.049051 | -3.121397 |
| 104 | H | -6.803441 | -1.126281 | -3.676325 |
| 105 | H | -6.095558 | -2.659898 | -3.142266 |
| 106 | H | -7.781981 | -2.602623 | -3.668324 |
| 107 | C | 5.968089 | -4.050340 | -2.693171 |
| 108 | H | 5.206702 | -4.048963 | -3.481271 |
| 109 | H | 6.122122 | -3.011881 | -2.374081 |
| 110 | H | 6.910001 | -4.394330 | -3.141764 |
| 111 | C | 6.868137 | -5.085496 | 0.041996 |
| 112 | H | 7.018057 | -4.065166 | 0.416150 |
| 113 | H | 6.659375 | -5.729414 | 0.903688 |
| 114 | H | 7.820198 | -5.414015 | -0.396411 |
| 115 | O | 5.257844 | -6.746394 | -1.767875 |
| 116 | H | 6.038134 | -7.154967 | -2.171397 |
| 117 | O | 3.870352 | 6.924917 | -2.373309 |
| 118 | H | 3.935900 | 7.726374 | -2.913632 |
| 119 | O | -8.948860 | -0.735355 | -1.347437 |
| 120 | H | -9.719012 | -1.132073 | -1.781049 |

**Table S14. Magnetic Shielding Tensors of $^{29}$Si Nuclei of 8b Calculated by the GIAO Method**

```
SCF GIAO Magnetic shielding tensor (ppm):
      1  Si   Isotropic =   293.1289   Anisotropy =   155.3557
   XX=   242.9990   YX=    -2.9778   ZX=    -8.8401
   XY=    -1.1050   YY=   242.2378   ZY=   -17.4251
   XZ=   -18.5868   YZ=   -11.5589   ZZ=   394.1499
   Eigenvalues:   237.9991   244.6883   396.6994
      7  Si   Isotropic =   353.7665   Anisotropy =    14.0184
   XX=   350.7947   YX=    -2.6906   ZX=    -0.6031
   XY=    -4.3165   YY=   355.4714   ZY=     4.2479
   XZ=    -6.9931   YZ=     7.1406   ZZ=   355.0333
   Eigenvalues:   348.5540   349.6334   363.1121
      8  Si   Isotropic =   360.1307   Anisotropy =    17.4681
   XX=   369.3461   YX=    -6.6377   ZX=     0.6347
   XY=    -8.4869   YY=   348.2248   ZY=     4.5408
   XZ=     1.9825   YZ=     4.3757   ZZ=   362.8214
   Eigenvalues:   344.6115   364.0045   371.7761
      9  Si   Isotropic =   352.3263   Anisotropy =    17.3612
   XX=   347.1478   YX=     6.2445   ZX=    -4.3003
   XY=     6.9115   YY=   353.9260   ZY=    -5.8208
   XZ=    -3.7109   YZ=    -5.4584   ZZ=   355.9052
   Eigenvalues:   343.1127   349.9658   363.9005
     10  Si   Isotropic =   358.2189   Anisotropy =    23.8261
   XX=   358.2539   YX=    11.7254   ZX=     0.0847
   XY=    10.1326   YY=   356.1179   ZY=   -14.4391
   XZ=     1.6167   YZ=   -10.7261   ZZ=   360.2850
   Eigenvalues:   340.6019   359.9518   374.1030
     11  Si   Isotropic =   360.8839   Anisotropy =    13.1399
   XX=   366.6518   YX=    -4.6196   ZX=     4.2902
   XY=    -5.9692   YY=   359.1010   ZY=     2.1055
   XZ=     5.2651   YZ=     9.9000   ZZ=   356.8989
   Eigenvalues:   349.0540   363.9538   369.6438
     12  Si   Isotropic =   355.5229   Anisotropy =    24.3669
   XX=   344.3616   YX=     0.2058   ZX=    -9.8274
   XY=    -6.6963   YY=   360.5270   ZY=     7.8911
   XZ=    -4.4372   YZ=     9.3260   ZZ=   361.6799
   Eigenvalues:   341.8010   353.0001   371.7675
     61  Si   Isotropic =   364.3930   Anisotropy =    26.4569
   XX=   355.1025   YX=    16.2873   ZX=    10.3602
   XY=    16.4569   YY=   370.7182   ZY=    -2.9294
```

```
XZ=    12.9697   YZ=    -4.0239   ZZ=   367.3584
Eigenvalues:   339.7488   371.3993   382.0310
  62  Si   Isotropic =   365.5613   Anisotropy =    20.7492
XX=   376.6860   YX=    -3.5340   ZX=     5.3326
XY=    -0.7336   YY=   355.7904   ZY=    17.6106
XZ=     5.0361   YZ=    12.0395   ZZ=   364.2076
Eigenvalues:   343.8722   373.4177   379.3941
  63  Si   Isotropic =   361.0836   Anisotropy =    25.5027
XX=   350.6482   YX=   -14.2804   ZX=   -11.6363
XY=    -8.7514   YY=   373.0616   ZY=    -1.7981
XZ=    -9.8812   YZ=    -3.9301   ZZ=   359.5411
Eigenvalues:   339.6541   365.5113   378.0854
  88  Si   Isotropic =   308.1611   Anisotropy =    60.4305
XX=   331.2465   YX=     6.7963   ZX=   -23.4227
XY=    16.2335   YY=   294.9402   ZY=   -11.5256
XZ=   -25.4894   YZ=    -8.8156   ZZ=   298.2964
Eigenvalues:   283.6162   292.4190   348.4481
  89  Si   Isotropic =   308.2097   Anisotropy =    56.9495
XX=   333.2007   YX=   -27.7935   ZX=     4.1582
XY=   -18.6823   YY=   303.2059   ZY=     3.1181
XZ=     6.7701   YZ=    -0.8985   ZZ=   288.2226
Eigenvalues:   285.4126   293.0405   346.1760
  90  Si   Isotropic =   306.5508   Anisotropy =    56.8513
XX=   292.3618   YX=    -7.2204   ZX=    -5.8739
XY=     5.3752   YY=   335.9749   ZY=    17.9431
XZ=    -2.3508   YZ=    24.1868   ZZ=   291.3156
Eigenvalues:   281.7913   293.4094   344.4517
```

**Table S15. Atomic Coordinates of the Optimized Structure of 9a**




| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | Si | 0.076043 | 0.066254 | 0.865368 |
| 2 | Si | -1.724173 | -1.347372 | 1.600680 |
| 3 | Si | 2.233214 | -0.798815 | 1.483847 |
| 4 | Si | -0.252329 | 2.339216 | 1.553134 |
| 5 | Si | -1.917786 | -3.358828 | 0.311513 |
| 6 | Si | 3.808729 | -0.367251 | -0.249581 |

| | | | | |
|---|---|---|---|---|
| 7 | Si | −1.432705 | 3.529234 | −0.143815 |
| 8 | C | −1.484834 | −1.809000 | 3.442280 |
| 9 | H | −2.322431 | −2.421667 | 3.797853 |
| 10 | H | −0.564026 | −2.377237 | 3.612492 |
| 11 | H | −1.445724 | −0.910020 | 4.069136 |
| 12 | C | 2.797919 | −0.095594 | 3.171753 |
| 13 | H | 2.021745 | −0.219588 | 3.936895 |
| 14 | H | 3.690516 | −0.628710 | 3.522092 |
| 15 | H | 3.047172 | 0.968541 | 3.118161 |
| 16 | C | −1.100991 | 2.377057 | 3.269069 |
| 17 | H | −1.139593 | 3.405823 | 3.647635 |
| 18 | H | −2.126308 | 1.993733 | 3.250249 |
| 19 | H | −0.536074 | 1.784113 | 3.999256 |
| 20 | C | −3.378480 | −0.393808 | 1.482251 |
| 21 | H | −3.356007 | 0.516564 | 2.091597 |
| 22 | H | −3.605803 | −0.098541 | 0.453126 |
| 23 | H | −4.207599 | −1.013002 | 1.844444 |
| 24 | C | 2.193944 | −2.701770 | 1.706477 |
| 25 | H | 1.503763 | −2.996378 | 2.505555 |
| 26 | H | 1.888400 | −3.219853 | 0.790703 |
| 27 | H | 3.189089 | −3.074758 | 1.977783 |
| 28 | C | 1.414645 | 3.250232 | 1.786711 |
| 29 | H | 1.988326 | 2.829051 | 2.619548 |
| 30 | H | 2.035084 | 3.199368 | 0.886705 |
| 31 | H | 1.240388 | 4.309939 | 2.011279 |
| 32 | C | −1.016259 | −4.797086 | 1.195035 |
| 33 | H | −1.499137 | −5.041253 | 2.148349 |
| 34 | H | −1.029410 | −5.703176 | 0.576711 |
| 35 | H | 0.030592 | −4.556950 | 1.405869 |
| 36 | C | 3.700415 | 1.429283 | −0.888404 |
| 37 | H | 3.950035 | 2.155016 | −0.106561 |
| 38 | H | 4.395429 | 1.590428 | −1.721707 |
| 39 | H | 2.688596 | 1.649874 | −1.247223 |
| 40 | C | −2.866876 | 2.519426 | −0.894629 |
| 41 | H | −3.662158 | 2.314991 | −0.169598 |
| 42 | H | −3.307338 | 3.066759 | −1.736914 |
| 43 | H | −2.490785 | 1.561644 | −1.270576 |
| 44 | C | −1.092226 | −3.114122 | −1.402408 |
| 45 | H | −0.015843 | −2.922854 | −1.296001 |
| 46 | H | −1.195980 | −4.004730 | −2.033185 |
| 47 | H | −1.541820 | −2.274908 | −1.947188 |
| 48 | C | 3.356758 | −1.515554 | −1.715165 |
| 49 | H | 2.332342 | −1.318486 | −2.053224 |
| 50 | H | 4.019359 | −1.343592 | −2.572205 |
| 51 | H | 3.427700 | −2.576035 | −1.447850 |
| 52 | C | −0.179944 | 3.891764 | −1.534814 |
| 53 | H | 0.683054 | 4.461440 | −1.171782 |
| 54 | H | 0.187104 | 2.951429 | −1.962116 |
| 55 | H | −0.662256 | 4.477597 | −2.324724 |
| 56 | O | 0.004734 | 0.191270 | −0.847021 |
| 57 | H | 0.002239 | −0.660309 | −1.307694 |
| 58 | Si | −4.185966 | −4.011456 | 0.001811 |
| 59 | Si | 6.044922 | −0.774159 | 0.452475 |
| 60 | Si | −2.314104 | 5.583928 | 0.664867 |
| 61 | Si | −4.400998 | −6.131966 | −1.029925 |
| 62 | Si | −3.483856 | 6.680056 | −1.079954 |
| 63 | Si | 7.554108 | −0.856775 | −1.369806 |
| 64 | C | −5.121631 | −2.758456 | −1.094874 |
| 65 | H | −5.192407 | −1.776824 | −0.613127 |
| 66 | H | −4.628332 | −2.620636 | −2.064103 |
| 67 | H | −6.138748 | −3.117765 | −1.288758 |
| 68 | C | −5.071728 | −4.131964 | 1.692373 |
| 69 | H | −4.558686 | −4.824642 | 2.369719 |
| 70 | H | −5.126071 | −3.157661 | 2.191731 |
| 71 | H | −6.096991 | −4.496022 | 1.557392 |
| 72 | C | −3.832640 | −7.567644 | 0.074275 |

| | | | | |
|---|---|---|---|---|
| 73 | H | -2.755585 | -7.506904 | 0.272509 |
| 74 | H | -4.349160 | -7.558245 | 1.040932 |
| 75 | H | -4.023571 | -8.540595 | -0.396343 |
| 76 | C | -3.489506 | -6.270842 | -2.689259 |
| 77 | H | -3.767512 | -5.459725 | -3.371808 |
| 78 | H | -2.403061 | -6.226891 | -2.542082 |
| 79 | H | -3.709889 | -7.220848 | -3.192541 |
| 80 | C | 6.207704 | -2.435378 | 1.385042 |
| 81 | H | 5.647278 | -2.422974 | 2.327603 |
| 82 | H | 5.837638 | -3.276476 | 0.787340 |
| 83 | H | 7.258968 | -2.633432 | 1.625374 |
| 84 | C | 6.616570 | 0.627187 | 1.618375 |
| 85 | H | 6.524558 | 1.610338 | 1.142805 |
| 86 | H | 6.026286 | 0.646689 | 2.542374 |
| 87 | H | 7.669164 | 0.486264 | 1.889130 |
| 88 | C | 7.439145 | 0.641334 | -2.530459 |
| 89 | H | 6.464831 | 0.669875 | -3.034616 |
| 90 | H | 7.559540 | 1.584702 | -1.985605 |
| 91 | H | 8.207701 | 0.608286 | -3.313332 |
| 92 | C | 7.344817 | -2.426659 | -2.417303 |
| 93 | H | 7.451464 | -3.331778 | -1.808426 |
| 94 | H | 6.350896 | -2.453608 | -2.880880 |
| 95 | H | 8.084339 | -2.478948 | -3.226454 |
| 96 | C | -0.923749 | 6.728475 | 1.310017 |
| 97 | H | -0.395084 | 6.269204 | 2.154244 |
| 98 | H | -0.183099 | 6.941951 | 0.530965 |
| 99 | H | -1.327834 | 7.687263 | 1.657211 |
| 100 | C | -3.552915 | 5.301079 | 2.097269 |
| 101 | H | -4.378381 | 4.648484 | 1.790238 |
| 102 | H | -3.064946 | 4.833672 | 2.960320 |
| 103 | H | -3.988433 | 6.248732 | 2.438170 |
| 104 | C | -3.474119 | 8.570024 | -0.884310 |
| 105 | H | -4.015867 | 9.070770 | -1.696933 |
| 106 | H | -3.957897 | 8.861713 | 0.056594 |
| 107 | H | -2.452267 | 8.966061 | -0.867749 |
| 108 | C | -5.292610 | 6.110219 | -1.183966 |
| 109 | H | -5.362890 | 5.024027 | -1.313108 |
| 110 | H | -5.835141 | 6.372240 | -0.267064 |
| 111 | H | -5.821448 | 6.581922 | -2.021922 |
| 112 | O | -2.674299 | 6.248877 | -2.499033 |
| 113 | O | -6.067197 | -6.234217 | -1.279770 |
| 114 | O | 9.058516 | -0.874149 | -0.603521 |
| 115 | C | -6.720480 | -7.357118 | -1.846703 |
| 116 | H | -6.566045 | -8.265882 | -1.247566 |
| 117 | H | -7.794755 | -7.147245 | -1.879848 |
| 118 | H | -6.377681 | -7.555190 | -2.872426 |
| 119 | C | 10.297645 | -0.944413 | -1.287963 |
| 120 | H | 11.100960 | -0.935582 | -0.543679 |
| 121 | H | 10.386897 | -1.867189 | -1.878987 |
| 122 | H | 10.442898 | -0.086511 | -1.960083 |
| 123 | C | -3.039867 | 6.719205 | -3.785585 |
| 124 | H | -2.932407 | 7.810232 | -3.866813 |
| 125 | H | -2.375826 | 6.253508 | -4.521066 |
| 126 | H | -4.075714 | 6.452959 | -4.040545 |

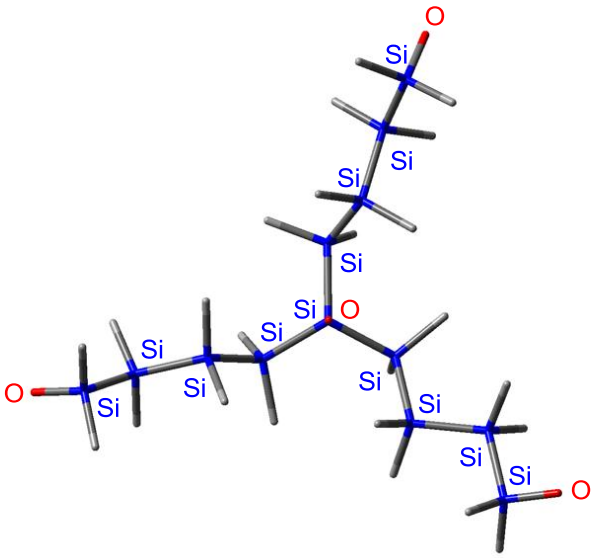
---

**Table S16. Magnetic Shielding Tensors of $^{29}$Si Nuclei of 9a Calculated by the GIAO Method**

```
SCF GIAO Magnetic shielding tensor (ppm):
      1  Si   Isotropic =   292.0001   Anisotropy =   168.0473
   XX=   238.4920   YX=    -0.8255   ZX=     2.0688
   XY=    -6.4726   YY=   233.4802   ZY=     3.5549
```

```
XZ=    -0.5717   YZ=    -3.2854   ZZ=   404.0282
Eigenvalues:   231.5582   240.4105   404.0317
   2  Si   Isotropic =   352.8671   Anisotropy =    15.1177
XX=   354.8343   YX=    -6.5729   ZX=    -8.0658
XY=    -7.1543   YY=   349.3352   ZY=    -0.0852
XZ=    -5.6860   YZ=    -2.3970   ZZ=   354.4317
Eigenvalues:   342.4295   353.2261   362.9455
   3  Si   Isotropic =   347.1554   Anisotropy =    18.6429
XX=   348.3296   YX=     2.6887   ZX=     6.7370
XY=     5.1642   YY=   343.3189   ZY=    -1.2831
XZ=    12.4733   YZ=     4.2488   ZZ=   349.8177
Eigenvalues:   338.5716   343.3107   359.5840
   4  Si   Isotropic =   346.4299   Anisotropy =    17.0571
XX=   349.4462   YX=    -9.1624   ZX=     3.2802
XY=   -11.6130   YY=   337.6964   ZY=     4.9045
XZ=    -3.7798   YZ=     7.2180   ZZ=   352.1470
Eigenvalues:   330.4120   351.0763   357.8013
   5  Si   Isotropic =   359.1471   Anisotropy =    22.0259
XX=   359.2595   YX=    -9.6103   ZX=    -9.6570
XY=   -12.7866   YY=   353.5296   ZY=     1.0812
XZ=    -7.0277   YZ=     0.4479   ZZ=   364.6523
Eigenvalues:   343.7548   359.8556   373.8311
   6  Si   Isotropic =   354.3625   Anisotropy =    19.8137
XX=   341.2366   YX=    -6.8107   ZX=     2.4198
XY=    -1.1574   YY=   357.3861   ZY=    -2.9912
XZ=     5.9905   YZ=    -5.3982   ZZ=   364.4649
Eigenvalues:   339.8818   355.6342   367.5717
   7  Si   Isotropic =   349.0909   Anisotropy =    19.1734
XX=   343.4047   YX=     4.2921   ZX=    -6.1794
XY=    13.0851   YY=   343.1604   ZY=     0.3322
XZ=     1.6977   YZ=     9.0068   ZZ=   360.7076
Eigenvalues:   333.6996   351.7000   361.8732
  58  Si   Isotropic =   361.7561   Anisotropy =    24.1165
XX=   371.4573   YX=   -13.7159   ZX=    -3.1312
XY=   -11.5548   YY=   352.5232   ZY=    -8.8971
XZ=    -3.6247   YZ=    -8.5009   ZZ=   361.2877
Eigenvalues:   341.7733   365.6612   377.8337
  59  Si   Isotropic =   361.6868   Anisotropy =    18.1957
XX=   352.6053   YX=     2.1031   ZX=    14.8790
XY=     3.7644   YY=   368.3233   ZY=    -0.2404
XZ=    13.4581   YZ=    -1.5557   ZZ=   364.1319
Eigenvalues:   342.7357   368.5076   373.8173
  60  Si   Isotropic =   365.2074   Anisotropy =    22.1056
XX=   363.0938   YX=    13.8067   ZX=    -8.3154
XY=    12.6357   YY=   365.6643   ZY=    12.7097
XZ=    -6.2707   YZ=    11.1877   ZZ=   366.8641
Eigenvalues:   343.2929   372.3849   379.9445
  61  Si   Isotropic =   307.7491   Anisotropy =    66.9746
XX=   348.1399   YX=     8.2760   ZX=    11.0609
XY=    12.5288   YY=   290.6829   ZY=     8.9991
XZ=    12.2910   YZ=     6.2345   ZZ=   284.4245
Eigenvalues:   279.0436   291.8049   352.3988
  62  Si   Isotropic =   302.4693   Anisotropy =    78.4172
XX=   288.8624   YX=   -21.0394   ZX=   -20.7817
XY=   -16.3213   YY=   276.5557   ZY=     5.6130
XZ=   -27.9023   YZ=    13.7134   ZZ=   341.9897
Eigenvalues:   262.3883   290.2721   354.7474
  63  Si   Isotropic =   308.3641   Anisotropy =    68.0985
XX=   346.4666   YX=    -1.5839   ZX=    22.1802
XY=    -3.6111   YY=   279.1761   ZY=    -2.3364
XZ=    17.2095   YZ=    -2.0696   ZZ=   299.4495
Eigenvalues:   278.9348   292.3944   353.7631
```

**Table S17. Atomic Coordinates of the Optimized Structure of 9b**




| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | Si | -0.078734 | -0.035805 | 0.720133 |
| 2 | Si | 1.162261 | 1.852815 | 1.535343 |
| 3 | Si | -2.383268 | 0.030487 | 1.396989 |
| 4 | Si | 0.996894 | -2.105329 | 1.254243 |
| 5 | Si | 0.653753 | 3.855714 | 0.319463 |
| 6 | Si | -3.761188 | -0.786365 | -0.367349 |
| 7 | Si | 2.563730 | -2.716735 | -0.439728 |
| 8 | C | 0.798900 | 2.136670 | 3.393175 |
| 9 | H | 1.408479 | 2.962944 | 3.779271 |
| 10 | H | -0.250735 | 2.384105 | 3.584272 |
| 11 | H | 1.046010 | 1.244132 | 3.980759 |
| 12 | C | -2.631735 | -0.919855 | 3.038883 |
| 13 | H | -1.954062 | -0.547094 | 3.816834 |
| 14 | H | -3.656672 | -0.782882 | 3.404787 |
| 15 | H | -2.457834 | -1.995045 | 2.932143 |
| 16 | C | 1.765850 | -1.985071 | 3.002738 |
| 17 | H | 2.189249 | -2.951229 | 3.302855 |
| 18 | H | 2.565468 | -1.239496 | 3.065370 |
| 19 | H | 1.003326 | -1.720264 | 3.745931 |
| 20 | C | 3.037388 | 1.505313 | 1.398962 |
| 21 | H | 3.318894 | 0.613476 | 1.970206 |
| 22 | H | 3.344636 | 1.346711 | 0.361025 |
| 23 | H | 3.616671 | 2.347257 | 1.796063 |
| 24 | C | -2.968365 | 1.822317 | 1.745648 |
| 25 | H | -2.394164 | 2.277610 | 2.560924 |
| 26 | H | -2.871895 | 2.468833 | 0.866198 |
| 27 | H | -4.024038 | 1.828321 | 2.044390 |
| 28 | C | -0.255018 | -3.551601 | 1.328227 |
| 29 | H | -0.972729 | -3.422608 | 2.145761 |
| 30 | H | -0.817831 | -3.649693 | 0.394736 |
| 31 | H | 0.271900 | -4.498243 | 1.499864 |
| 32 | C | -0.569232 | 4.927121 | 1.327865 |
| 33 | H | -0.114025 | 5.278445 | 2.260896 |

| | | | | |
|---|---|---|---|---|
| 34 | H | −0.877373 | 5.811397 | 0.756333 |
| 35 | H | −1.475905 | 4.371026 | 1.589569 |
| 36 | C | −2.975202 | −2.277682 | −1.263628 |
| 37 | H | −2.893413 | −3.150259 | −0.606329 |
| 38 | H | −3.575810 | −2.573855 | −2.132476 |
| 39 | H | −1.969955 | −2.021094 | −1.616763 |
| 40 | C | 3.519945 | −1.233545 | −1.166441 |
| 41 | H | 4.166071 | −0.753251 | −0.424484 |
| 42 | H | 4.155330 | −1.558614 | −1.999412 |
| 43 | H | 2.818198 | −0.483726 | −1.548656 |
| 44 | C | −0.198887 | 3.413444 | −1.342138 |
| 45 | H | −1.145205 | 2.882086 | −1.173675 |
| 46 | H | −0.438015 | 4.311763 | −1.923150 |
| 47 | H | 0.447967 | 2.786060 | −1.967502 |
| 48 | C | −3.908823 | 0.629624 | −1.650502 |
| 49 | H | −2.918711 | 0.938125 | −2.008495 |
| 50 | H | −4.482835 | 0.308101 | −2.528260 |
| 51 | H | −4.404872 | 1.513459 | −1.233525 |
| 52 | C | 1.542398 | −3.481239 | −1.863977 |
| 53 | H | 1.000408 | −4.379361 | −1.547319 |
| 54 | H | 0.807842 | −2.753922 | −2.228932 |
| 55 | H | 2.185109 | −3.759258 | −2.708557 |
| 56 | O | −0.015703 | −0.032767 | −0.995647 |
| 57 | H | −0.352414 | 0.777212 | −1.405618 |
| 58 | Si | 2.585720 | 5.161615 | −0.156244 |
| 59 | Si | −5.917331 | −1.406658 | 0.423853 |
| 60 | Si | 4.123786 | −4.294505 | 0.426645 |
| 61 | Si | 2.048967 | 7.218489 | −1.196652 |
| 62 | Si | 5.483658 | −5.251131 | −1.254758 |
| 63 | Si | −7.470462 | −1.669981 | −1.338771 |
| 64 | C | 3.770054 | 4.221101 | −1.322208 |
| 65 | H | 4.183110 | 3.328047 | −0.839811 |
| 66 | H | 3.263737 | 3.901740 | −2.240520 |
| 67 | H | 4.605525 | 4.868671 | −1.611614 |
| 68 | C | 3.514344 | 5.591118 | 1.459350 |
| 69 | H | 2.871772 | 6.131957 | 2.164009 |
| 70 | H | 3.881848 | 4.691541 | 1.966606 |
| 71 | H | 4.379281 | 6.228548 | 1.241165 |
| 72 | C | 1.185803 | 8.436099 | −0.025678 |
| 73 | H | 0.207126 | 8.056648 | 0.293485 |
| 74 | H | 1.783302 | 8.615657 | 0.875246 |
| 75 | H | 1.016179 | 9.406107 | −0.512176 |
| 76 | C | 0.968614 | 7.049741 | −2.747272 |
| 77 | H | 1.407831 | 6.356147 | −3.472985 |
| 78 | H | −0.034972 | 6.683325 | −2.496538 |
| 79 | H | 0.842971 | 8.019048 | −3.248416 |
| 80 | C | −6.614869 | −0.093793 | 1.626628 |
| 81 | H | −5.991127 | −0.006333 | 2.524539 |
| 82 | H | −6.670693 | 0.897415 | 1.161761 |
| 83 | H | −7.625962 | −0.368825 | 1.949206 |
| 84 | C | −5.796371 | −3.070661 | 1.355161 |
| 85 | H | −5.382206 | −3.860534 | 0.718211 |
| 86 | H | −5.156823 | −2.987169 | 2.241994 |
| 87 | H | −6.790614 | −3.395323 | 1.682797 |
| 88 | C | −6.856515 | −2.825731 | −2.711989 |
| 89 | H | −5.992262 | −2.398711 | −3.236450 |
| 90 | H | −6.556379 | −3.800752 | −2.311941 |
| 91 | H | −7.637478 | −3.000791 | −3.464316 |
| 92 | C | −7.956493 | −0.022981 | −2.145152 |
| 93 | H | −8.384924 | 0.670806 | −1.412921 |
| 94 | H | −7.086385 | 0.466733 | −2.599832 |
| 95 | H | −8.700594 | −0.170825 | −2.939320 |
| 96 | C | 3.225552 | −5.722002 | 1.327414 |
| 97 | H | 2.666859 | −5.354737 | 2.196826 |
| 98 | H | 2.515673 | −6.237143 | 0.669821 |
| 99 | H | 3.949327 | −6.463878 | 1.684618 |

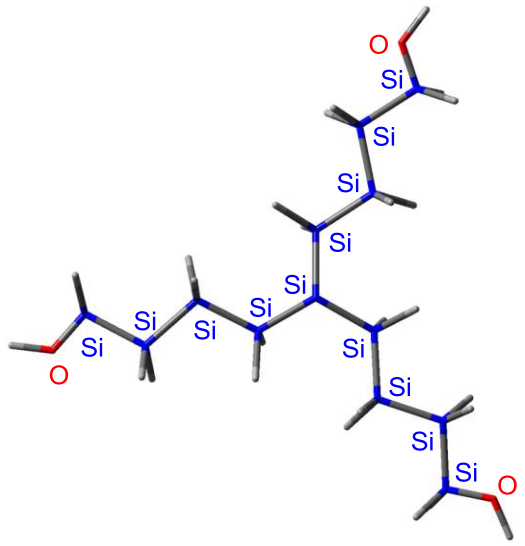
| | | | | |
|---|---|---|---|---|
| 100 | C | 5.281068 | -3.429702 | 1.678551 |
| 101 | H | 5.797460 | -2.574155 | 1.228125 |
| 102 | H | 4.724724 | -3.062179 | 2.548820 |
| 103 | H | 6.045701 | -4.129670 | 2.034519 |
| 104 | C | 6.393321 | -3.967238 | -2.314408 |
| 105 | H | 7.070177 | -4.450207 | -3.032167 |
| 106 | H | 5.686639 | -3.359911 | -2.893945 |
| 107 | H | 6.992995 | -3.286510 | -1.699782 |
| 108 | C | 4.519231 | -6.383754 | -2.431736 |
| 109 | H | 4.016091 | -7.192119 | -1.889361 |
| 110 | H | 3.752266 | -5.820398 | -2.977604 |
| 111 | H | 5.180492 | -6.844202 | -3.178125 |
| 112 | O | 6.606284 | -6.161365 | -0.371459 |
| 113 | H | 7.259117 | -6.643961 | -0.900128 |
| 114 | O | 3.572231 | 7.821131 | -1.624553 |
| 115 | H | 3.573631 | 8.693857 | -2.045106 |
| 116 | O | -8.817799 | -2.355088 | -0.575973 |
| 117 | H | -9.575311 | -2.537064 | -1.151857 |

**Table S18. Magnetic Shielding Tensors of $^{29}$Si Nuclei of 9b Calculated by the GIAO Method**

```
SCF GIAO Magnetic shielding tensor (ppm):
      1  Si   Isotropic =   292.0361   Anisotropy =   167.0416
   XX=   239.8576   YX=     4.2705   ZX=     4.8780
   XY=    -3.2306   YY=   233.7839   ZY=   -17.2621
   XZ=     1.4200   YZ=    -7.0495   ZZ=   402.4668
   Eigenvalues:   232.8331   239.8781   403.3972
      2  Si   Isotropic =   355.2337   Anisotropy =    10.0053
   XX=   361.4251   YX=    -2.7538   ZX=     0.8858
   XY=    -2.2344   YY=   346.3594   ZY=     2.4523
   XZ=    -1.0542   YZ=     3.0391   ZZ=   357.9167
   Eigenvalues:   345.3763   358.4209   361.9039
      3  Si   Isotropic =   350.6110   Anisotropy =    17.0666
   XX=   347.9200   YX=     7.5936   ZX=    -4.1603
   XY=     6.8932   YY=   351.1507   ZY=     0.5297
   XZ=    -4.8143   YZ=   -10.7972   ZZ=   352.7623
   Eigenvalues:   342.1028   347.7414   361.9887
      4  Si   Isotropic =   348.2993   Anisotropy =    21.4310
   XX=   357.8312   YX=    -0.8797   ZX=    -2.6250
   XY=    -4.7127   YY=   334.3537   ZY=   -13.7176
   XZ=     9.3199   YZ=   -10.6212   ZZ=   352.7130
   Eigenvalues:   328.2548   354.0564   362.5866
      5  Si   Isotropic =   360.8009   Anisotropy =    18.8080
   XX=   364.2398   YX=    -6.5650   ZX=    11.5774
   XY=    -7.6308   YY=   353.5087   ZY=     5.3791
   XZ=     6.1968   YZ=     7.9061   ZZ=   364.6543
   Eigenvalues:   344.7593   364.3039   373.3396
      6  Si   Isotropic =   356.7237   Anisotropy =    20.8725
   XX=   348.7512   YX=   -10.3148   ZX=    -5.6789
   XY=    -6.7186   YY=   356.5725   ZY=     2.7197
   XZ=    -7.8843   YZ=     4.6006   ZZ=   364.8472
   Eigenvalues:   342.5905   356.9418   370.6386
      7  Si   Isotropic =   363.3851   Anisotropy =    25.8009
   XX=   354.3330   YX=    14.5792   ZX=     6.0297
   XY=    20.2104   YY=   368.6001   ZY=     1.5223
   XZ=     2.8753   YZ=    -2.6066   ZZ=   367.2222
   Eigenvalues:   342.0281   367.5415   380.5857
     58  Si   Isotropic =   364.9498   Anisotropy =    19.1430
   XX=   377.2814   YX=    -2.7674   ZX=     1.5174
   XY=    -3.4719   YY=   346.5875   ZY=    10.8689
   XZ=    -0.0484   YZ=    13.4362   ZZ=   370.9805
```

```
 Eigenvalues:   341.2885   375.8491   377.7118
   59  Si   Isotropic =   362.4902   Anisotropy =    16.7892
XX=   350.5117   YX=    -2.9366   ZX=   -13.7883
XY=    -5.4463   YY=   371.1997   ZY=    -5.1139
XZ=   -13.2292   YZ=    -0.3510   ZZ=   365.7591
 Eigenvalues:   341.7751   372.0124   373.6830
   60  Si   Isotropic =   365.3176   Anisotropy =    20.9828
XX=   359.4542   YX=    14.1335   ZX=    15.0265
XY=    11.9338   YY=   368.2696   ZY=    -5.2918
XZ=    13.5038   YZ=   -10.5762   ZZ=   368.2289
 Eigenvalues:   340.5654   376.0812   379.3061
   61  Si   Isotropic =   306.7817   Anisotropy =    58.9800
XX=   327.9914   YX=    13.6905   ZX=   -12.1665
XY=    25.9049   YY=   302.6992   ZY=   -11.8972
XZ=   -20.2209   YZ=   -13.1367   ZZ=   289.6545
 Eigenvalues:   281.5323   292.7111   346.1017
   62  Si   Isotropic =   305.9433   Anisotropy =    62.0056
XX=   315.6485   YX=   -29.4644   ZX=    20.4196
XY=   -28.7707   YY=   303.3572   ZY=   -16.0954
XZ=     9.9703   YZ=    -9.0192   ZZ=   298.8242
 Eigenvalues:   279.7412   290.8084   347.2804
   63  Si   Isotropic =   309.1671   Anisotropy =    59.6295
XX=   331.2434   YX=    22.3666   ZX=   -19.7471
XY=    21.2198   YY=   296.2377   ZY=   -12.3959
XZ=   -12.4839   YZ=    -7.2991   ZZ=   300.0202
 Eigenvalues:   285.3536   293.2277   348.9201
```

**Table S19. Atomic Coordinates of the Optimized Structure of 10a**




| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | Si | 0.000000 | 0.000000 | 0.534495 |
| 2 | H | 0.000000 | 0.000000 | 2.038510 |
| 3 | Si | -1.603607 | 1.660598 | -0.118940 |
| 4 | Si | 2.239923 | 0.558465 | -0.118940 |
| 5 | Si | -0.636318 | -2.219063 | -0.118940 |

| | | | | |
|---|---|---|---|---|
| 6 | Si | −1.070290 | 3.950344 | 0.279650 |
| 7 | Si | 3.956244 | −1.048273 | 0.279650 |
| 8 | Si | −2.885954 | −2.902071 | 0.279650 |
| 9 | Si | −3.026202 | 5.304282 | 0.094561 |
| 10 | Si | 6.106744 | −0.031373 | 0.094561 |
| 11 | Si | −3.080542 | −5.272908 | 0.094561 |
| 12 | Si | −2.467938 | 7.591307 | −0.154692 |
| 13 | Si | 7.808234 | −1.658357 | −0.154692 |
| 14 | Si | −5.340296 | −5.932950 | −0.154692 |
| 15 | C | −1.987890 | 1.439190 | −1.980323 |
| 16 | H | −2.759209 | 2.145291 | −2.309938 |
| 17 | H | −1.097163 | 1.607486 | −2.596503 |
| 18 | H | −2.351203 | 0.427005 | −2.194473 |
| 19 | C | 2.240321 | 1.001969 | −1.980323 |
| 20 | H | 1.940705 | 0.146427 | −2.596503 |
| 21 | H | 1.545399 | 1.822699 | −2.194473 |
| 22 | H | 3.237481 | 1.316900 | −2.309938 |
| 23 | C | −0.252431 | −2.441159 | −1.980323 |
| 24 | H | −0.478272 | −3.462190 | −2.309938 |
| 25 | H | −0.843543 | −1.753914 | −2.596503 |
| 26 | H | 0.805805 | −2.249704 | −2.194473 |
| 27 | C | −3.205391 | 1.339146 | 0.877978 |
| 28 | H | −3.566830 | 0.313876 | 0.759970 |
| 29 | H | −3.041799 | 1.512415 | 1.948076 |
| 30 | H | −4.006459 | 2.012995 | 0.550876 |
| 31 | C | 2.762430 | 2.106377 | 0.877978 |
| 32 | H | 2.055239 | 2.932028 | 0.759970 |
| 33 | H | 2.830690 | 1.878068 | 1.948076 |
| 34 | H | 3.746534 | 2.463198 | 0.550876 |
| 35 | C | 0.442962 | −3.445524 | 0.877978 |
| 36 | H | 1.511590 | −3.245903 | 0.759970 |
| 37 | H | 0.211110 | −3.390483 | 1.948076 |
| 38 | H | 0.259925 | −4.476193 | 0.550876 |
| 39 | C | 0.222879 | 4.593361 | −0.977483 |
| 40 | H | 0.501670 | 5.630283 | −0.752255 |
| 41 | H | 1.143391 | 4.000230 | −0.976598 |
| 42 | H | −0.181458 | 4.575132 | −1.996555 |
| 43 | C | 3.866528 | −2.489699 | −0.977483 |
| 44 | H | 4.625133 | −3.249600 | −0.752255 |
| 45 | H | 2.892605 | −2.990321 | −0.976598 |
| 46 | H | 4.052909 | −2.130418 | −1.996555 |
| 47 | C | −4.089408 | −2.103662 | −0.977483 |
| 48 | H | −5.126803 | −2.380683 | −0.752255 |
| 49 | H | −4.035996 | −1.009909 | −0.976598 |
| 50 | H | −3.871452 | −2.444713 | −1.996555 |
| 51 | C | −0.411714 | 4.188612 | 2.059559 |
| 52 | H | −0.189094 | 5.244179 | 2.257966 |
| 53 | H | −1.156965 | 3.865419 | 2.795543 |
| 54 | H | 0.502333 | 3.614047 | 2.242576 |
| 55 | C | 3.833301 | −1.737752 | 2.059559 |
| 56 | H | 4.636139 | −2.458329 | 2.257966 |
| 57 | H | 3.926033 | −0.930748 | 2.795543 |
| 58 | H | 2.878690 | −2.242056 | 2.242576 |
| 59 | C | −3.421587 | −2.450860 | 2.059559 |
| 60 | H | −4.447045 | −2.785850 | 2.257966 |
| 61 | H | −2.769068 | −2.934671 | 2.795543 |
| 62 | H | −3.381023 | −1.371991 | 2.242576 |
| 63 | C | −4.079785 | 5.150193 | 1.681094 |
| 64 | H | −4.474712 | 4.135831 | 1.809383 |
| 65 | H | −3.496624 | 5.395675 | 2.576067 |
| 66 | H | −4.927494 | 5.843416 | 1.636674 |
| 67 | C | 6.500091 | 0.958101 | 1.681094 |
| 68 | H | 5.819090 | 1.807299 | 1.809383 |
| 69 | H | 6.421104 | 0.330327 | 2.576067 |
| 70 | H | 7.524293 | 1.345627 | 1.636674 |
| 71 | C | −2.420305 | −6.108295 | 1.681094 |

| | | | | |
|---|---|---|---|---|
| 72 | H | -1.344378 | -5.943129 | 1.809383 |
| 73 | H | -2.924481 | -5.726003 | 2.576067 |
| 74 | H | -2.596799 | -7.189043 | 1.636674 |
| 75 | C | -4.113748 | 4.818902 | -1.402053 |
| 76 | H | -3.558176 | 4.872699 | -2.345665 |
| 77 | H | -4.505174 | 3.799276 | -1.302894 |
| 78 | H | -4.970684 | 5.498241 | -1.481916 |
| 79 | C | 6.230166 | 1.153159 | -1.402053 |
| 80 | H | 5.998969 | 0.645122 | -2.345665 |
| 81 | H | 5.542857 | 2.001956 | -1.302894 |
| 82 | H | 7.246960 | 1.555618 | -1.481916 |
| 83 | C | -2.116418 | -5.972061 | -1.402053 |
| 84 | H | -2.440793 | -5.517820 | -2.345665 |
| 85 | H | -1.037683 | -5.801233 | -1.302894 |
| 86 | H | -2.276274 | -7.053860 | -1.481916 |
| 87 | C | -1.755553 | 8.001401 | -1.866387 |
| 88 | H | -0.795955 | 7.494744 | -2.025493 |
| 89 | H | -2.434746 | 7.688264 | -2.667708 |
| 90 | H | -1.578222 | 9.078347 | -1.981918 |
| 91 | C | 7.807193 | -2.480347 | -1.866387 |
| 92 | H | 6.888617 | -3.058055 | -2.025493 |
| 93 | H | 7.875605 | -1.735580 | -2.667708 |
| 94 | H | 8.651189 | -3.172393 | -1.981918 |
| 95 | C | -6.051640 | -5.521054 | -1.866387 |
| 96 | H | -6.092661 | -4.436690 | -2.025493 |
| 97 | H | -5.440859 | -5.952684 | -2.667708 |
| 98 | H | -7.072967 | -5.905953 | -1.981918 |
| 99 | C | -1.243142 | 8.214661 | 1.155717 |
| 100 | H | -1.614249 | 8.035800 | 2.171494 |
| 101 | H | -0.275195 | 7.706669 | 1.059705 |
| 102 | H | -1.055090 | 9.291218 | 1.054727 |
| 103 | C | 7.735676 | -3.030738 | 1.155717 |
| 104 | H | 7.766331 | -2.619920 | 2.171494 |
| 105 | H | 6.811768 | -3.615009 | 1.059705 |
| 106 | H | 8.573975 | -3.731873 | 1.054727 |
| 107 | C | -6.492534 | -5.183922 | 1.155717 |
| 108 | H | -6.152082 | -5.415880 | 2.171494 |
| 109 | H | -6.536574 | -4.091660 | 1.059705 |
| 110 | H | -7.518885 | -5.559343 | 1.054727 |
| 111 | O | -3.955324 | 8.366075 | 0.038256 |
| 112 | O | 9.222896 | -0.757627 | 0.038256 |
| 113 | O | -5.267572 | -7.608449 | 0.038256 |
| 114 | C | -4.131199 | 9.770488 | -0.039166 |
| 115 | H | -3.816147 | 10.169876 | -1.013888 |
| 116 | H | -5.195889 | 9.990116 | 0.092964 |
| 117 | H | -3.571722 | 10.295658 | 0.748210 |
| 118 | C | 10.527090 | -1.307520 | -0.039166 |
| 119 | H | 10.715445 | -1.780058 | -1.013888 |
| 120 | H | 11.249638 | -0.495286 | 0.092964 |
| 121 | H | 10.702163 | -2.054627 | 0.748210 |
| 122 | C | -6.395891 | -8.462968 | -0.039166 |
| 123 | H | -6.899298 | -8.389819 | -1.013888 |
| 124 | H | -6.053749 | -9.494830 | 0.092964 |
| 125 | H | -7.130440 | -8.241031 | 0.748210 |

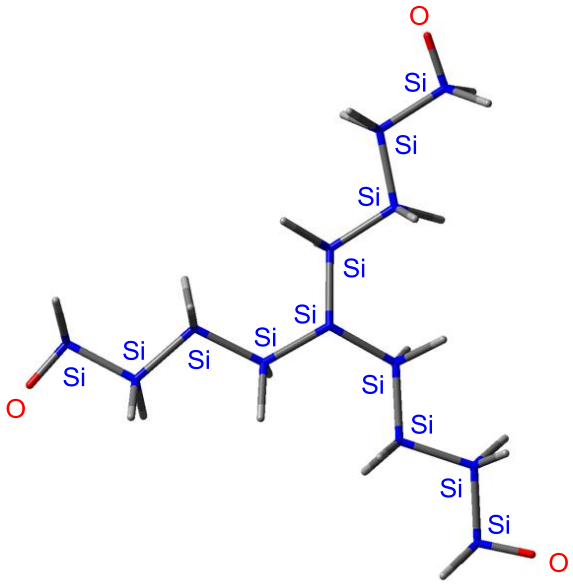
---

**Table S20. Magnetic Shielding Tensors of $^{29}$Si Nuclei of 10a Calculated by the GIAO Method**

```
SCF GIAO Magnetic shielding tensor (ppm):
      1  Si   Isotropic =   413.8787   Anisotropy =    29.3959
   XX=   432.6934   YX=    10.8303   ZX=    -1.1338
   XY=    -8.7158   YY=   432.0317   ZY=     0.6995
```

```
XZ=     0.1305   YZ=    -1.2442   ZZ=   376.9111
Eigenvalues:   376.9053   431.2549   433.4760
   3  Si   Isotropic =   351.2994   Anisotropy =    27.8939
XX=   363.1513   YX=     5.9260   ZX=    11.6065
XY=     6.0373   YY=   338.4784   ZY=    -0.5856
XZ=     8.5027   YZ=    -0.6564   ZZ=   352.2684
Eigenvalues:   336.4518   347.5510   369.8953
   4  Si   Isotropic =   349.3024   Anisotropy =    31.0630
XX=   337.8042   YX=     8.1896   ZX=    -6.3005
XY=     7.3851   YY=   361.7630   ZY=   -12.7720
XZ=    -6.3967   YZ=    -6.9591   ZZ=   348.3402
Eigenvalues:   334.3829   343.5134   370.0111
   5  Si   Isotropic =   350.1386   Anisotropy =    28.4575
XX=   348.8216   YX=   -14.0032   ZX=    -6.9037
XY=   -13.9369   YY=   350.8195   ZY=    10.9257
XZ=    -2.8765   YZ=     6.7347   ZZ=   350.7749
Eigenvalues:   335.3230   345.9827   369.1103
   6  Si   Isotropic =   354.9873   Anisotropy =    30.3719
XX=   365.6527   YX=    11.7132   ZX=     6.3032
XY=    16.4902   YY=   348.9333   ZY=    -2.0959
XZ=     8.0558   YZ=     1.7611   ZZ=   350.3760
Eigenvalues:   339.4988   350.2279   375.2353
   7  Si   Isotropic =   358.9511   Anisotropy =    29.8190
XX=   338.3007   YX=    -1.7149   ZX=    -4.4189
XY=    -0.0435   YY=   377.8006   ZY=    -3.2837
XZ=    -2.5114   YZ=    -5.3455   ZZ=   360.7520
Eigenvalues:   337.7199   360.3030   378.8304
   8  Si   Isotropic =   358.4751   Anisotropy =    28.5524
XX=   367.1265   YX=   -17.1340   ZX=    -0.4737
XY=   -13.9779   YY=   349.7990   ZY=     4.2321
XZ=    -4.4221   YZ=     6.4582   ZZ=   358.4999
Eigenvalues:   340.0211   357.8943   377.5101
   9  Si   Isotropic =   362.4173   Anisotropy =    23.3082
XX=   375.2686   YX=     2.4379   ZX=    -2.5554
XY=    -0.4607   YY=   341.6353   ZY=     7.1101
XZ=    -6.4737   YZ=    -1.9120   ZZ=   370.3479
Eigenvalues:   341.3440   367.9518   377.9561
  10  Si   Isotropic =   363.8767   Anisotropy =    22.0183
XX=   349.1973   YX=    15.2760   ZX=     6.5782
XY=    13.2709   YY=   366.9205   ZY=    -0.9779
XZ=     2.7727   YZ=     3.0023   ZZ=   375.5124
Eigenvalues:   340.8821   372.1924   378.5556
  11  Si   Isotropic =   364.8868   Anisotropy =    18.5302
XX=   351.2219   YX=   -15.5713   ZX=    -6.3085
XY=   -16.0214   YY=   367.5931   ZY=    -2.2937
XZ=    -0.7736   YZ=    -2.4612   ZZ=   375.8453
Eigenvalues:   341.0938   376.3263   377.2402
  12  Si   Isotropic =   307.9380   Anisotropy =    68.8246
XX=   332.7624   YX=   -24.8809   ZX=    -7.9072
XY=   -32.1439   YY=   312.1802   ZY=     2.8509
XZ=   -10.5374   YZ=     1.5238   ZZ=   278.8713
Eigenvalues:   277.0336   292.9593   353.8210
  13  Si   Isotropic =   307.3185   Anisotropy =    67.9830
XX=   341.5358   YX=    26.2484   ZX=     6.2388
XY=    18.4831   YY=   301.8289   ZY=     4.5279
XZ=     7.3199   YZ=     8.3153   ZZ=   278.5907
Eigenvalues:   276.9125   292.4024   352.6405
  14  Si   Isotropic =   307.7221   Anisotropy =    69.1268
XX=   292.3343   YX=    10.3889   ZX=     0.7539
XY=     1.9482   YY=   352.0671   ZY=    -8.1496
XZ=     2.5053   YZ=   -10.5116   ZZ=   278.7648
Eigenvalues:   277.2083   292.1513   353.8066
```

**Table S21. Atomic Coordinates of the Optimized Structure of 10b**




| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | Si | 0.000000 | 0.000000 | 0.538080 |
| 2 | H | 0.000000 | 0.000000 | 2.042095 |
| 3 | Si | 0.120568 | 2.304679 | -0.116520 |
| 4 | Si | 1.935627 | -1.256755 | -0.116520 |
| 5 | Si | -2.056195 | -1.047925 | -0.116520 |
| 6 | Si | 2.156273 | 3.481579 | 0.279145 |
| 7 | Si | 1.936999 | -3.608177 | 0.279145 |
| 8 | Si | -4.093273 | 0.126598 | 0.279145 |
| 9 | Si | 1.804582 | 5.832715 | 0.086518 |
| 10 | Si | 4.148989 | -4.479172 | 0.086518 |
| 11 | Si | -5.953571 | -1.353544 | 0.086518 |
| 12 | Si | 3.853048 | 6.991524 | -0.156800 |
| 13 | Si | 4.128313 | -6.832599 | -0.156800 |
| 14 | Si | -7.981361 | -0.158924 | -0.156800 |
| 15 | C | -0.303850 | 2.431549 | -1.978070 |
| 16 | H | -0.313799 | 3.476458 | -2.309908 |
| 17 | H | 0.426779 | 1.893846 | -2.593243 |
| 18 | H | -1.291818 | 2.006294 | -2.191295 |
| 19 | C | 2.257708 | -0.952633 | -1.978070 |
| 20 | H | 1.426728 | -1.316524 | -2.593243 |
| 21 | H | 2.383410 | 0.115600 | -2.191295 |
| 22 | H | 3.167601 | -1.466472 | -2.309908 |
| 23 | C | -1.953858 | -1.478916 | -1.978070 |
| 24 | H | -2.853802 | -2.009987 | -2.309908 |
| 25 | H | -1.853508 | -0.577320 | -2.593243 |
| 26 | H | -1.091592 | -2.121894 | -2.191295 |
| 27 | C | -1.210504 | 3.252912 | 0.879623 |
| 28 | H | -2.203904 | 2.810289 | 0.765363 |
| 29 | H | -0.970042 | 3.256725 | 1.949236 |
| 30 | H | -1.272613 | 4.296844 | 0.549229 |
| 31 | C | 3.422356 | -0.578129 | 0.879623 |
| 32 | H | 3.535734 | 0.503492 | 0.765363 |
| 33 | H | 3.305427 | -0.788282 | 1.949236 |

| | | | | |
|---|---|---|---|---|
| 34 | H | 4.357482 | −1.046307 | 0.549229 |
| 35 | C | −2.211852 | −2.674783 | 0.879623 |
| 36 | H | −1.331830 | −3.313782 | 0.765363 |
| 37 | H | −2.335385 | −2.468443 | 1.949236 |
| 38 | H | −3.084869 | −3.250537 | 0.549229 |
| 39 | C | 3.508771 | 2.975226 | −0.977970 |
| 40 | H | 4.454692 | 3.485368 | −0.757372 |
| 41 | H | 3.709312 | 1.898671 | −0.971728 |
| 42 | H | 3.215881 | 3.251370 | −1.997928 |
| 43 | C | 0.822235 | −4.526298 | −0.977970 |
| 44 | H | 0.791073 | −5.600561 | −0.757372 |
| 45 | H | −0.210359 | −4.161695 | −0.971728 |
| 46 | H | 1.207829 | −4.410719 | −1.997928 |
| 47 | C | −4.331007 | 1.551072 | −0.977970 |
| 48 | H | −5.245763 | 2.115192 | −0.757372 |
| 49 | H | −3.498954 | 2.263023 | −0.971728 |
| 50 | H | −4.423709 | 1.159350 | −1.997928 |
| 51 | C | 2.781811 | 3.169030 | 2.059261 |
| 52 | H | 3.703633 | 3.730157 | 2.255454 |
| 53 | H | 2.036547 | 3.492574 | 2.795062 |
| 54 | H | 2.989496 | 2.110011 | 2.245053 |
| 55 | C | 1.353555 | −3.993634 | 2.059261 |
| 56 | H | 1.378594 | −5.072518 | 2.255454 |
| 57 | H | 2.006384 | −3.509988 | 2.795062 |
| 58 | H | 0.332574 | −3.643985 | 2.245053 |
| 59 | C | −4.135365 | 0.824604 | 2.059261 |
| 60 | H | −5.082227 | 1.342361 | 2.255454 |
| 61 | H | −4.042930 | 0.017415 | 2.795062 |
| 62 | H | −3.322071 | 1.533974 | 2.245053 |
| 63 | C | 0.966208 | 6.499236 | 1.668526 |
| 64 | H | −0.042148 | 6.089479 | 1.797585 |
| 65 | H | 1.544634 | 6.248255 | 2.565042 |
| 66 | H | 0.886956 | 7.591253 | 1.619765 |
| 67 | C | 5.145399 | −4.086379 | 1.668526 |
| 68 | H | 5.294717 | −3.008238 | 1.797585 |
| 69 | H | 4.638830 | −4.461820 | 2.565042 |
| 70 | H | 6.130740 | −4.563753 | 1.619765 |
| 71 | C | −6.111608 | −2.412857 | 1.668526 |
| 72 | H | −5.252569 | −3.081241 | 1.797585 |
| 73 | H | −6.183464 | −1.786435 | 2.565042 |
| 74 | H | −7.017696 | −3.027500 | 1.619765 |
| 75 | C | 0.713161 | 6.285686 | −1.417133 |
| 76 | H | 1.139365 | 5.915587 | −2.356995 |
| 77 | H | −0.297031 | 5.869589 | −1.322171 |
| 78 | H | 0.618139 | 7.374766 | −1.501134 |
| 79 | C | 5.086983 | −3.760459 | −1.417133 |
| 80 | H | 4.553366 | −3.944512 | −2.356995 |
| 81 | H | 5.231729 | −2.677558 | −1.322171 |
| 82 | H | 6.077665 | −4.222707 | −1.501134 |
| 83 | C | −5.800145 | −2.525227 | −1.417133 |
| 84 | H | −5.692731 | −1.971075 | −2.356995 |
| 85 | H | −4.934698 | −3.192030 | −1.322171 |
| 86 | H | −6.695804 | −3.152059 | −1.501134 |
| 87 | C | 4.642055 | 6.764614 | −1.867429 |
| 88 | H | 4.935517 | 5.721399 | −2.037357 |
| 89 | H | 3.951676 | 7.052535 | −2.668403 |
| 90 | H | 5.547127 | 7.378222 | −1.971667 |
| 91 | C | 3.537301 | −7.402444 | −1.867429 |
| 92 | H | 2.487117 | −7.134983 | −2.037357 |
| 93 | H | 4.131836 | −6.948519 | −2.668403 |
| 94 | H | 3.616164 | −8.493063 | −1.971667 |
| 95 | C | −8.179355 | 0.637830 | −1.867429 |
| 96 | H | −7.422636 | 1.413585 | −2.037357 |
| 97 | H | −8.083513 | −0.104015 | −2.668403 |
| 98 | H | −9.163291 | 1.114841 | −1.971667 |
| 99 | C | 5.150978 | 6.517317 | 1.143477 |

| | | | | |
|---|---|---|---|---|
| 100 | H | 4.771831 | 6.660153 | 2.161798 |
| 101 | H | 5.450890 | 5.466506 | 1.041656 |
| 102 | H | 6.059984 | 7.125022 | 1.039236 |
| 103 | C | 3.068674 | -7.719536 | 1.143477 |
| 104 | H | 3.381946 | -7.462603 | 2.161798 |
| 105 | H | 2.008688 | -7.453862 | 1.041656 |
| 106 | H | 3.140459 | -8.810612 | 1.039236 |
| 107 | C | -8.219651 | 1.202219 | 1.143477 |
| 108 | H | -8.153777 | 0.802451 | 2.161798 |
| 109 | H | -7.459577 | 1.987356 | 1.041656 |
| 110 | H | -9.200443 | 1.685589 | 1.039236 |
| 111 | O | 3.402000 | 8.610786 | 0.048951 |
| 112 | H | 4.117875 | 9.257039 | -0.043129 |
| 113 | O | 5.756160 | -7.251611 | 0.048951 |
| 114 | H | 5.957893 | -8.194704 | -0.043129 |
| 115 | O | -9.158159 | -1.359175 | 0.048951 |
| 116 | H | -10.075769 | -1.062335 | -0.043129 |

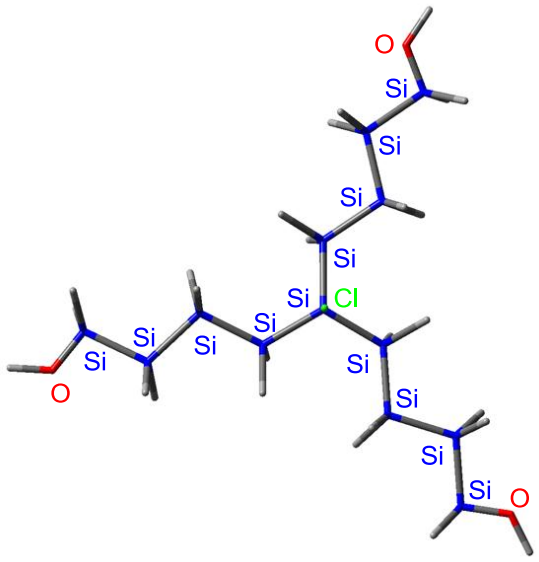
---

**Table S22. Magnetic Shielding Tensors of $^{29}$Si Nuclei of 10b Calculated by the GIAO Method**

```
SCF GIAO Magnetic shielding tensor (ppm):
      1  Si   Isotropic =   414.8223   Anisotropy =    28.8058
   XX=   433.5305   YX=     8.7563   ZX=     0.3319
   XY=   -10.9062   YY=   431.6921   ZY=     0.7742
   XZ=     0.5727   YZ=     0.4319   ZZ=   379.2443
   Eigenvalues:   379.2334   431.2074   434.0261
      3  Si   Isotropic =   353.0965   Anisotropy =    28.0877
   XX=   357.8087   YX=   -14.9805   ZX=     7.3580
   XY=   -12.9812   YY=   345.6608   ZY=    -8.2587
   XZ=     3.7179   YZ=    -6.6665   ZZ=   355.8200
   Eigenvalues:   335.9040   351.5638   371.8216
      4  Si   Isotropic =   351.0935   Anisotropy =    29.0504
   XX=   358.8154   YX=    11.7545   ZX=   -12.7285
   XY=    11.0631   YY=   342.3362   ZY=    -2.7808
   XZ=    -8.6055   YZ=    -0.4074   ZZ=   352.1290
   Eigenvalues:   335.5901   347.2300   370.4605
      5  Si   Isotropic =   349.3884   Anisotropy =    29.7525
   XX=   336.6449   YX=     2.1566   ZX=     2.0823
   XY=     0.2607   YY=   363.9206   ZY=    12.4074
   XZ=     2.6585   YZ=     8.6571   ZZ=   347.5998
   Eigenvalues:   336.1050   342.8369   369.2234
      6  Si   Isotropic =   358.0951   Anisotropy =    28.2920
   XX=   373.0712   YX=    -9.7458   ZX=     1.4126
   XY=    -8.4636   YY=   343.9674   ZY=    -3.8836
   XZ=     6.7957   YZ=    -3.6502   ZZ=   357.2466
   Eigenvalues:   340.9563   356.3725   376.9564
      7  Si   Isotropic =   359.3991   Anisotropy =    28.2176
   XX=   359.0227   YX=    18.4033   ZX=    -1.7822
   XY=    19.5076   YY=   357.5787   ZY=     0.4173
   XZ=    -6.6416   YZ=    -3.0338   ZZ=   361.5957
   Eigenvalues:   339.1539   360.8326   378.2108
      8  Si   Isotropic =   362.3987   Anisotropy =    26.8694
   XX=   341.7617   YX=    -9.4975   ZX=     1.0554
   XY=    -7.4200   YY=   377.1972   ZY=     1.6929
   XZ=    -0.2175   YZ=     6.2856   ZZ=   368.2373
   Eigenvalues:   339.7868   367.0977   380.3117
      9  Si   Isotropic =   362.3994   Anisotropy =    20.3948
   XX=   357.0741   YX=   -16.1408   ZX=     3.2123
   XY=   -17.7145   YY=   358.3195   ZY=     4.6089
   XZ=     0.5858   YZ=     5.1554   ZZ=   371.8047
   Eigenvalues:   340.0426   371.1597   375.9960
```

```
  10  Si   Isotropic =   361.8712   Anisotropy =    19.8779
XX=   372.8716   YX=     8.6982   ZX=     1.4989
XY=     7.6366   YY=   342.4914   ZY=    -4.8463
XZ=     2.4252   YZ=    -3.2244   ZZ=   370.2504
Eigenvalues:   339.8009   370.6895   375.1231
  11  Si   Isotropic =   361.9111   Anisotropy =    19.3673
XX=   342.9044   YX=     9.5468   ZX=    -5.2846
XY=     9.4186   YY=   371.4285   ZY=     2.5229
XZ=    -5.4064   YZ=     3.0681   ZZ=   371.4004
Eigenvalues:   338.9562   371.9544   374.8226
  12  Si   Isotropic =   307.8146   Anisotropy =    61.8772
XX=   292.9005   YX=    -4.4883   ZX=     0.1373
XY=   -12.5993   YY=   347.1124   ZY=     7.0973
XZ=    -2.7550   YZ=     5.6050   ZZ=   283.4309
Eigenvalues:   282.7798   291.5979   349.0661
  13  Si   Isotropic =   307.6681   Anisotropy =    61.1643
XX=   340.2380   YX=   -14.1887   ZX=     6.7097
XY=   -23.9287   YY=   299.7123   ZY=    -3.1671
XZ=     6.1382   YZ=     0.1562   ZZ=   283.0541
Eigenvalues:   282.3085   292.2515   348.4443
  14  Si   Isotropic =   307.5154   Anisotropy =    60.4443
XX=   326.3274   YX=    31.8049   ZX=    -6.1062
XY=    20.7709   YY=   313.0828   ZY=    -5.2425
XZ=    -4.6111   YZ=    -7.1274   ZZ=   283.1360
Eigenvalues:   281.9080   292.8265   347.8116
```

**Table S23. Atomic Coordinates of the Optimized Structure of 11a**




| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | Si | 0.000000 | 0.000000 | 0.481905 |
| 2 | Si | 2.311469 | -0.167539 | -0.151082 |
| 3 | Si | -1.300828 | -1.918022 | -0.151082 |
| 4 | Si | -1.010642 | 2.085561 | -0.151082 |
| 5 | Si | 3.472566 | -2.218724 | 0.211064 |

| | | | | |
|---|---|---|---|---|
| 6 | Si | −3.657753 | −1.897968 | 0.211064 |
| 7 | Si | 0.185188 | 4.116692 | 0.211064 |
| 8 | Si | 5.819611 | −1.853629 | 0.003523 |
| 9 | Si | −4.515095 | −4.113117 | 0.003523 |
| 10 | Si | −1.304515 | 5.966745 | 0.003523 |
| 11 | Si | 6.999708 | −3.887432 | −0.276125 |
| 12 | Si | −6.866470 | −4.118209 | −0.276125 |
| 13 | Si | −0.133239 | 8.005641 | −0.276125 |
| 14 | C | 2.404668 | 0.249152 | −2.018430 |
| 15 | H | 3.446373 | 0.270973 | −2.359967 |
| 16 | H | 1.873735 | −0.492977 | −2.625570 |
| 17 | H | 1.967556 | 1.230711 | −2.236257 |
| 18 | C | −0.986563 | −2.207079 | −2.018430 |
| 19 | H | −1.363798 | −1.376214 | −2.625570 |
| 20 | H | 0.082049 | −2.319309 | −2.236257 |
| 21 | H | −1.488517 | −3.120133 | −2.359967 |
| 22 | C | −1.418105 | 1.957928 | −2.018430 |
| 23 | H | −1.957856 | 2.849160 | −2.359967 |
| 24 | H | −0.509937 | 1.869191 | −2.625570 |
| 25 | H | −2.049605 | 1.088598 | −2.236257 |
| 26 | C | 3.253793 | 1.173857 | 0.827922 |
| 27 | H | 2.837884 | 2.170766 | 0.657774 |
| 28 | H | 3.209687 | 0.973684 | 1.904133 |
| 29 | H | 4.309274 | 1.197423 | 0.531890 |
| 30 | C | −0.610306 | −3.404796 | 0.827922 |
| 31 | H | 0.460996 | −3.543062 | 0.657774 |
| 32 | H | −0.761609 | −3.266513 | 1.904133 |
| 33 | H | −1.117638 | −4.330653 | 0.531890 |
| 34 | C | −2.643487 | 2.230939 | 0.827922 |
| 35 | H | −3.298880 | 1.372297 | 0.657774 |
| 36 | H | −2.448079 | 2.292829 | 1.904133 |
| 37 | H | −3.191636 | 3.133229 | 0.531890 |
| 38 | C | 2.947070 | −3.522172 | −1.089765 |
| 39 | H | 3.427381 | −4.487317 | −0.886316 |
| 40 | H | 1.865311 | −3.692754 | −1.099935 |
| 41 | H | 3.242507 | −3.213786 | −2.099704 |
| 42 | C | −4.523826 | −0.791151 | −1.089765 |
| 43 | H | −5.599821 | −0.724540 | −0.886316 |
| 44 | H | −4.130675 | 0.230970 | −1.099935 |
| 45 | H | −4.404474 | −1.201201 | −2.099704 |
| 46 | C | 1.576756 | 4.313324 | −1.089765 |
| 47 | H | 2.172440 | 5.211857 | −0.886316 |
| 48 | H | 2.265363 | 3.461783 | −1.099935 |
| 49 | H | 1.161966 | 4.414987 | −2.099704 |
| 50 | C | 3.166988 | −2.905037 | 1.968250 |
| 51 | H | 3.740046 | −3.826443 | 2.130805 |
| 52 | H | 3.480114 | −2.181905 | 2.729742 |
| 53 | H | 2.111405 | −3.132086 | 2.148932 |
| 54 | C | −4.099330 | −1.290173 | 1.968250 |
| 55 | H | −5.183821 | −1.325754 | 2.130805 |
| 56 | H | −3.629641 | −1.922914 | 2.729742 |
| 57 | H | −3.768169 | −0.262488 | 2.148932 |
| 58 | C | 0.932342 | 4.195210 | 1.968250 |
| 59 | H | 1.443774 | 5.152197 | 2.130805 |
| 60 | H | 0.149528 | 4.104819 | 2.729742 |
| 61 | H | 1.656763 | 3.394573 | 2.148932 |
| 62 | C | 6.504201 | −1.025561 | 1.582821 |
| 63 | H | 6.105628 | −0.013899 | 1.720665 |
| 64 | H | 6.257097 | −1.605778 | 2.479152 |
| 65 | H | 7.596289 | −0.956935 | 1.522197 |
| 66 | C | −4.140263 | −5.120023 | 1.582821 |
| 67 | H | −3.064850 | −5.280680 | 1.720665 |
| 68 | H | −4.519193 | −4.615915 | 2.479152 |
| 69 | H | −4.626874 | −6.100112 | 1.522197 |
| 70 | C | −2.363938 | 6.145584 | 1.582821 |
| 71 | H | −3.040778 | 5.294579 | 1.720665 |

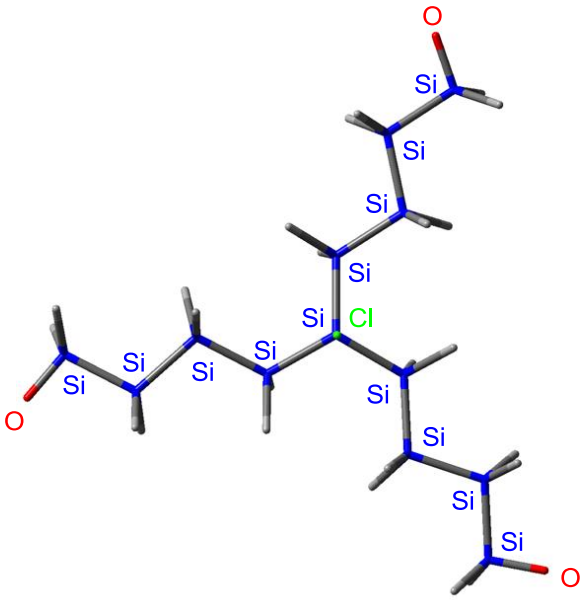
| | | | | |
|---|---|---|---|---|
| 72 | H | -1.737904 | 6.221694 | 2.479152 |
| 73 | H | -2.969415 | 7.057046 | 1.522197 |
| 74 | C | 6.245886 | -0.746698 | -1.496404 |
| 75 | H | 5.861451 | -1.165133 | -2.433908 |
| 76 | H | 5.829877 | 0.261736 | -1.385468 |
| 77 | H | 7.333299 | -0.648736 | -1.596301 |
| 78 | C | -3.769602 | -5.035747 | -1.496404 |
| 79 | H | -3.939760 | -4.493598 | -2.433908 |
| 80 | H | -2.688269 | -5.179689 | -1.385468 |
| 81 | H | -4.228472 | -6.026455 | -1.596301 |
| 82 | C | -2.476285 | 5.782445 | -1.496404 |
| 83 | H | -1.921691 | 5.658731 | -2.433908 |
| 84 | H | -3.141608 | 4.917955 | -1.385468 |
| 85 | H | -3.104827 | 6.675191 | -1.596301 |
| 86 | C | 6.743746 | -4.665794 | -1.988701 |
| 87 | H | 5.694684 | -4.950632 | -2.135131 |
| 88 | H | 7.014197 | -3.968331 | -2.789978 |
| 89 | H | 7.349402 | -5.571994 | -2.116437 |
| 90 | C | -7.412569 | -3.507359 | -1.988701 |
| 91 | H | -7.134715 | -2.456425 | -2.135131 |
| 92 | H | -6.943774 | -4.090307 | -2.789978 |
| 93 | H | -8.500189 | -3.578771 | -2.116437 |
| 94 | C | 0.668822 | 8.173153 | -1.988701 |
| 95 | H | 1.440032 | 7.407057 | -2.135131 |
| 96 | H | -0.070423 | 8.058638 | -2.789978 |
| 97 | H | 1.150787 | 9.150765 | -2.116437 |
| 98 | C | 6.582279 | -5.193636 | 1.036160 |
| 99 | H | 6.712775 | -4.800224 | 2.050818 |
| 100 | H | 5.541660 | -5.527870 | 0.938802 |
| 101 | H | 7.218761 | -6.082435 | 0.939162 |
| 102 | C | -7.788960 | -3.103603 | 1.036160 |
| 103 | H | -7.513505 | -3.413322 | 2.050818 |
| 104 | H | -7.558106 | -2.035283 | 0.938802 |
| 105 | H | -8.876923 | -3.210413 | 0.939162 |
| 106 | C | 1.206681 | 8.297238 | 1.036160 |
| 107 | H | 0.800729 | 8.213546 | 2.050818 |
| 108 | H | 2.016445 | 7.563153 | 0.938802 |
| 109 | H | 1.658162 | 9.292848 | 0.939162 |
| 110 | Cl | 0.000000 | 0.000000 | 2.638774 |
| 111 | O | -1.361398 | 9.150584 | -0.105798 |
| 112 | O | 8.605337 | -3.396288 | -0.105798 |
| 113 | O | -7.243940 | -5.754297 | -0.105798 |
| 114 | C | -8.548757 | -6.291016 | -0.243885 |
| 115 | H | -8.963126 | -6.106555 | -1.245472 |
| 116 | H | -8.490995 | -7.373870 | -0.091252 |
| 117 | H | -9.242975 | -5.876044 | 0.500938 |
| 118 | C | -1.173800 | 10.548949 | -0.243885 |
| 119 | H | -0.806868 | 10.815571 | -1.245472 |
| 120 | H | -2.140461 | 11.040352 | -0.091252 |
| 121 | H | -0.467317 | 10.942674 | 0.500938 |
| 122 | C | 9.722558 | -4.257933 | -0.243885 |
| 123 | H | 9.769994 | -4.709017 | -1.245472 |
| 124 | H | 10.631456 | -3.666482 | -0.091252 |
| 125 | H | 9.710292 | -5.066628 | 0.500938 |

**Table S24. Magnetic Shielding Tensors of $^{29}$Si Nuclei of 11a Calculated by the GIAO Method**

```
SCF GIAO Magnetic shielding tensor (ppm):
      1  Si   Isotropic =   294.8570   Anisotropy =   103.1075
   XX=   260.7765   YX=    -0.2019   ZX=    -0.2735
   XY=     1.0477   YY=   260.1999   ZY=     0.0294
```

```
XZ=     0.1300   YZ=     0.5382   ZZ=   363.5945
Eigenvalues:   259.9756   261.0000   363.5953
   2  Si   Isotropic =   352.3290   Anisotropy =    35.8742
XX=   343.9536   YX=    16.6253   ZX=   -13.8322
XY=    17.4464   YY=   360.9207   ZY=    -8.4917
XZ=    -7.1187   YZ=    -3.3807   ZZ=   352.1125
Eigenvalues:   331.5272   349.2145   376.2451
   3  Si   Isotropic =   350.2834   Anisotropy =    36.9079
XX=   341.4129   YX=   -14.6242   ZX=    -1.1157
XY=   -15.9236   YY=   361.4773   ZY=    17.3962
XZ=     1.1286   YZ=     8.9523   ZZ=   347.9600
Eigenvalues:   330.3990   345.5626   374.8887
   4  Si   Isotropic =   347.7864   Anisotropy =    38.2523
XX=   368.3226   YX=     0.8414   ZX=    16.2123
XY=    -1.7745   YY=   333.4112   ZY=    -6.6607
XZ=     8.3915   YZ=    -4.7655   ZZ=   341.6255
Eigenvalues:   329.5937   340.4775   373.2880
   5  Si   Isotropic =   356.4498   Anisotropy =    25.4500
XX=   342.9663   YX=     7.3687   ZX=    -3.7662
XY=     9.4830   YY=   369.9325   ZY=    -1.2555
XZ=    -2.5851   YZ=    -5.7442   ZZ=   356.4506
Eigenvalues:   340.2710   355.6619   373.4165
   6  Si   Isotropic =   357.6926   Anisotropy =    25.2838
XX=   355.5515   YX=   -18.4486   ZX=     0.5272
XY=   -16.1821   YY=   356.8150   ZY=     3.1105
XZ=    -2.5026   YZ=     5.4611   ZZ=   360.7113
Eigenvalues:   338.6201   359.9092   374.5485
   7  Si   Isotropic =   360.6148   Anisotropy =    24.2931
XX=   374.0297   YX=     6.8075   ZX=     1.4106
XY=     9.3309   YY=   340.6512   ZY=    -1.2663
XZ=     5.1021   YZ=    -0.3927   ZZ=   367.1634
Eigenvalues:   338.7192   366.3149   376.8102
   8  Si   Isotropic =   363.9702   Anisotropy =    21.8510
XX=   358.9207   YX=    18.0089   ZX=     4.8118
XY=    16.3109   YY=   358.3931   ZY=    -2.5525
XZ=     6.5491   YZ=    -0.5192   ZZ=   374.5968
Eigenvalues:   340.7273   372.6457   378.5375
   9  Si   Isotropic =   362.2339   Anisotropy =    20.4836
XX=   343.2663   YX=    -7.6287   ZX=    -4.3795
XY=    -9.0706   YY=   373.1452   ZY=    -1.7769
XZ=    -4.0704   YZ=    -3.8894   ZZ=   370.2902
Eigenvalues:   340.3196   370.4924   375.8896
  10  Si   Isotropic =   363.0438   Anisotropy =    18.3512
XX=   371.8621   YX=    -9.3968   ZX=     1.8464
XY=    -9.6446   YY=   343.1149   ZY=     4.7701
XZ=     2.0658   YZ=     6.4096   ZZ=   374.1543
Eigenvalues:   339.2449   374.6085   375.2779
  11  Si   Isotropic =   307.2898   Anisotropy =    68.6243
XX=   351.0237   YX=    12.4672   ZX=     6.4994
XY=     6.6528   YY=   292.0510   ZY=     0.9830
XZ=     5.2350   YZ=     3.1704   ZZ=   278.7946
Eigenvalues:   278.1866   290.6434   353.0393
  12  Si   Isotropic =   308.6275   Anisotropy =    67.4465
XX=   299.4201   YX=    23.0157   ZX=    -2.0978
XY=    16.2161   YY=   345.9959   ZY=    -6.5083
XZ=     0.5106   YZ=    -4.9233   ZZ=   280.4666
Eigenvalues:   279.9126   292.3781   353.5918
  13  Si   Isotropic =   307.4784   Anisotropy =    67.0774
XX=   315.0958   YX=   -25.3232   ZX=    -4.8538
XY=   -33.3135   YY=   327.9735   ZY=     5.1721
XZ=    -6.5267   YZ=     3.2587   ZZ=   279.3658
Eigenvalues:   278.4771   291.7614   352.1966
```

**Table S25. Atomic Coordinates of the Optimized Structure of 11b**




| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | Si | 0.000000 | 0.000000 | 0.341120 |
| 2 | Si | -0.560852 | 2.255305 | -0.281034 |
| 3 | Si | 2.233577 | -0.641940 | -0.281034 |
| 4 | Si | -1.672725 | -1.613365 | -0.281034 |
| 5 | Si | 1.041901 | 3.969799 | 0.142257 |
| 6 | Si | 2.916996 | -2.887212 | 0.142257 |
| 7 | Si | -3.958897 | -1.082587 | 0.142257 |
| 8 | Si | 0.000000 | 6.110544 | 0.015600 |
| 9 | Si | 5.291886 | -3.055272 | 0.015600 |
| 10 | Si | -5.291886 | -3.055272 | 0.015600 |
| 11 | Si | 1.605926 | 7.838874 | -0.166664 |
| 12 | Si | 5.985701 | -5.310210 | -0.166664 |
| 13 | Si | -7.591627 | -2.528664 | -0.166664 |
| 14 | C | -0.977563 | 2.239727 | -2.149474 |
| 15 | H | -1.271896 | 3.240382 | -2.487735 |
| 16 | H | -0.121634 | 1.923600 | -2.756562 |
| 17 | H | -1.809875 | 1.560001 | -2.367537 |
| 18 | C | 2.428442 | -0.273269 | -2.149474 |
| 19 | H | 1.726703 | -0.856462 | -2.756562 |
| 20 | H | 2.255938 | 0.787397 | -2.367537 |
| 21 | H | 3.442201 | -0.518697 | -2.487735 |
| 22 | C | -1.450879 | -1.966458 | -2.149474 |
| 23 | H | -2.170305 | -2.721685 | -2.487735 |
| 24 | H | -1.605069 | -1.067138 | -2.756562 |
| 25 | H | -0.446063 | -2.347398 | -2.367537 |
| 26 | C | -2.130647 | 2.735639 | 0.694139 |
| 27 | H | -2.951919 | 2.035193 | 0.521279 |
| 28 | H | -1.929756 | 2.755386 | 1.771045 |
| 29 | H | -2.475775 | 3.733277 | 0.397994 |
| 30 | C | 3.434456 | 0.477375 | 0.694139 |
| 31 | H | 3.238488 | 1.538840 | 0.521279 |
| 32 | H | 3.351112 | 0.293525 | 1.771045 |
| 33 | H | 4.471000 | 0.277446 | 0.397994 |

| | | | | |
|---|---|---|---|---|
| 34 | C | −1.303809 | −3.213014 | 0.694139 |
| 35 | H | −0.286569 | −3.574033 | 0.521279 |
| 36 | H | −1.421356 | −3.048911 | 1.771045 |
| 37 | H | −1.995225 | −4.010723 | 0.397994 |
| 38 | C | 2.445738 | 3.904441 | −1.157638 |
| 39 | H | 3.225183 | 4.641376 | −0.928002 |
| 40 | H | 2.929346 | 2.923038 | −1.206592 |
| 41 | H | 2.059689 | 4.133358 | −2.158109 |
| 42 | C | 2.158476 | −4.070292 | −1.157638 |
| 43 | H | 2.406958 | −5.113778 | −0.928002 |
| 44 | H | 1.066752 | −3.998407 | −1.206592 |
| 45 | H | 2.549748 | −3.850422 | −2.158109 |
| 46 | C | −4.604214 | 0.165851 | −1.157638 |
| 47 | H | −5.632141 | 0.472402 | −0.928002 |
| 48 | H | −3.996098 | 1.075369 | −1.206592 |
| 49 | H | −4.609438 | −0.282936 | −2.158109 |
| 50 | C | 1.765558 | 3.813599 | 1.904216 |
| 51 | H | 2.496581 | 4.607997 | 2.099476 |
| 52 | H | 0.972373 | 3.901546 | 2.655213 |
| 53 | H | 2.261891 | 2.852074 | 2.067419 |
| 54 | C | 2.419895 | −3.435818 | 1.904216 |
| 55 | H | 2.742352 | −4.466101 | 2.099476 |
| 56 | H | 2.892651 | −2.792873 | 2.655213 |
| 57 | H | 1.339023 | −3.384892 | 2.067419 |
| 58 | C | −4.185453 | −0.377781 | 1.904216 |
| 59 | H | −5.238933 | −0.141896 | 2.099476 |
| 60 | H | −3.865024 | −1.108673 | 2.655213 |
| 61 | H | −3.600914 | 0.532818 | 2.067419 |
| 62 | C | −1.006053 | 6.444274 | 1.604339 |
| 63 | H | −1.842727 | 5.744447 | 1.710968 |
| 64 | H | −0.382054 | 6.355442 | 2.500900 |
| 65 | H | −1.412032 | 7.461996 | 1.581921 |
| 66 | C | 6.083931 | −2.350870 | 1.604339 |
| 67 | H | 5.896200 | −1.276375 | 1.710968 |
| 68 | H | 5.695001 | −2.846853 | 2.500900 |
| 69 | H | 7.168294 | −2.508142 | 1.581921 |
| 70 | C | −5.077878 | −4.093404 | 1.604339 |
| 71 | H | −4.053474 | −4.468072 | 1.710968 |
| 72 | H | −5.312947 | −3.508589 | 2.500900 |
| 73 | H | −5.756262 | −4.953854 | 1.581921 |
| 74 | C | −1.172368 | 6.253754 | −1.488608 |
| 75 | H | −0.656994 | 6.036226 | −2.431472 |
| 76 | H | −2.020381 | 5.563554 | −1.404855 |
| 77 | H | −1.578229 | 7.269944 | −1.557906 |
| 78 | C | 6.002094 | −2.111577 | −1.488608 |
| 79 | H | 5.556022 | −2.449140 | −2.431472 |
| 80 | H | 5.828370 | −1.032076 | −1.404855 |
| 81 | H | 7.085071 | −2.268186 | −1.557906 |
| 82 | C | −4.829726 | −4.142177 | −1.488608 |
| 83 | H | −4.899028 | −3.587086 | −2.431472 |
| 84 | H | −3.807989 | −4.531478 | −1.404855 |
| 85 | H | −5.506842 | −5.001758 | −1.557906 |
| 86 | C | 2.437411 | 7.912853 | −1.870275 |
| 87 | H | 3.018291 | 7.004118 | −2.070380 |
| 88 | H | 1.698332 | 8.020432 | −2.672282 |
| 89 | H | 3.129008 | 8.763369 | −1.938915 |
| 90 | C | 5.634026 | −6.067286 | −1.870275 |
| 91 | H | 4.556599 | −6.115976 | −2.070380 |
| 92 | H | 6.096732 | −5.481015 | −2.672282 |
| 93 | H | 6.024796 | −7.091485 | −1.938915 |
| 94 | C | −8.071437 | −1.845567 | −1.870275 |
| 95 | H | −7.574890 | −0.888142 | −2.070380 |
| 96 | H | −7.795064 | −2.539417 | −2.672282 |
| 97 | H | −9.153804 | −1.671884 | −1.938915 |
| 98 | C | 2.974925 | 7.734759 | 1.142184 |
| 99 | H | 2.560992 | 7.717367 | 2.156745 |

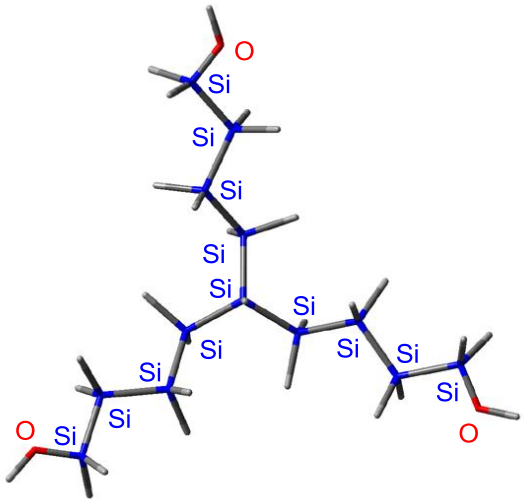
| | | | | |
|---|---|---|---|---|
| 100 | H | 3.580547 | 6.828857 | 1.012357 |
| 101 | H | 3.657046 | 8.593011 | 1.075831 |
| 102 | C | 5.211035 | -6.443740 | 1.142184 |
| 103 | H | 5.402940 | -6.076568 | 2.156745 |
| 104 | H | 4.123690 | -6.515273 | 1.012357 |
| 105 | H | 5.613243 | -7.463600 | 1.075831 |
| 106 | C | -8.185960 | -1.291019 | 1.142184 |
| 107 | H | -7.963932 | -1.640799 | 2.156745 |
| 108 | H | -7.704237 | -0.313584 | 1.012357 |
| 109 | H | -9.270289 | -1.129411 | 1.075831 |
| 110 | Cl | 0.000000 | 0.000000 | 2.498909 |
| 111 | O | -8.340764 | -4.027180 | 0.078073 |
| 112 | H | -9.308646 | -4.022876 | 0.036708 |
| 113 | O | 0.682742 | 9.236903 | 0.078073 |
| 114 | H | 1.170410 | 10.072962 | 0.036708 |
| 115 | O | 7.658022 | -5.209723 | 0.078073 |
| 116 | H | 8.138236 | -6.050086 | 0.036708 |

**Table S26. Magnetic Shielding Tensors of $^{29}$Si Nuclei of 11b Calculated by the GIAO Method**

```
SCF GIAO Magnetic shielding tensor (ppm):
      1  Si   Isotropic =   295.6340   Anisotropy =   110.0908
   XX=   258.9245   YX=    -4.0742   ZX=    -0.0212
   XY=     3.9483   YY=   258.9528   ZY=     0.2820
   XZ=     1.1648   YZ=    -0.1468   ZZ=   369.0248
   Eigenvalues:   258.8719   259.0023   369.0279
      2  Si   Isotropic =   346.0471   Anisotropy =    38.9640
   XX=   363.3687   YX=    -8.1010   ZX=    15.4504
   XY=    -8.5920   YY=   333.7584   ZY=   -11.5747
   XZ=     7.7659   YZ=    -9.2318   ZZ=   341.0142
   Eigenvalues:   326.3684   339.7499   372.0231
      3  Si   Isotropic =   347.0210   Anisotropy =    36.3190
   XX=   348.3933   YX=    16.3340   ZX=   -17.5937
   XY=    16.5331   YY=   349.5995   ZY=    -6.2564
   XZ=   -10.3876   YZ=    -1.3399   ZZ=   343.0702
   Eigenvalues:   327.6617   342.1676   371.2337
      4  Si   Isotropic =   349.6466   Anisotropy =    34.9135
   XX=   336.2842   YX=    -9.4108   ZX=     4.1489
   XY=    -8.6575   YY=   364.7937   ZY=    16.0813
   XZ=     2.7162   YZ=     9.7761   ZZ=   347.8620
   Eigenvalues:   330.2746   345.7431   372.9223
      5  Si   Isotropic =   357.9587   Anisotropy =    31.2497
   XX=   377.2320   YX=    -1.7885   ZX=     5.0467
   XY=     0.9004   YY=   337.8145   ZY=    -6.4206
   XZ=     5.8823   YZ=    -2.0266   ZZ=   358.8295
   Eigenvalues:   336.9881   358.0962   378.7918
      6  Si   Isotropic =   359.2710   Anisotropy =    29.4978
   XX=   350.3563   YX=    15.0594   ZX=    -7.1431
   XY=    18.3704   YY=   366.6660   ZY=    -0.4146
   XZ=    -7.3743   YZ=    -3.8491   ZZ=   360.7908
   Eigenvalues:   338.7233   360.1536   378.9363
      7  Si   Isotropic =   351.3469   Anisotropy =    33.8301
   XX=   346.3350   YX=   -16.0188   ZX=     2.7078
   XY=   -10.8096   YY=   364.2289   ZY=     8.9809
   XZ=    -3.7139   YZ=    10.0853   ZZ=   343.4766
   Eigenvalues:   336.0594   344.0809   373.9003
      8  Si   Isotropic =   366.5049   Anisotropy =    26.0500
   XX=   369.8466   YX=   -14.8178   ZX=    -0.1383
   XY=   -15.5899   YY=   347.9545   ZY=     4.8802
   XZ=    -3.9236   YZ=     2.7539   ZZ=   381.7136
   Eigenvalues:   340.0186   375.6245   383.8716
```

```
    9  Si   Isotropic =   363.4534   Anisotropy =    20.2515
 XX=   365.9277   YX=    16.7671   ZX=     2.1018
 XY=    16.1714   YY=   350.7562   ZY=    -4.3046
 XZ=     2.4881   YZ=     1.6830   ZZ=   373.6764
 Eigenvalues:   340.0464   373.3594   376.9544
   10  Si   Isotropic =   361.5904   Anisotropy =    25.0743
 XX=   340.2602   YX=    -0.3891   ZX=    -4.0262
 XY=    -4.5742   YY=   375.5715   ZY=    -3.0328
 XZ=     2.8012   YZ=    -6.8609   ZZ=   368.9394
 Eigenvalues:   340.0542   366.4103   378.3065
   11  Si   Isotropic =   306.0130   Anisotropy =    60.6980
 XX=   299.6215   YX=   -13.5640   ZX=    -4.3756
 XY=   -26.3665   YY=   336.1752   ZY=     7.6932
 XZ=    -8.0492   YZ=     8.3570   ZZ=   282.2422
 Eigenvalues:   280.1807   291.3798   346.4783
   12  Si   Isotropic =   307.4716   Anisotropy =    60.9457
 XX=   346.2679   YX=     1.1006   ZX=     9.1976
 XY=    -9.7338   YY=   292.0651   ZY=    -0.6015
 XZ=    10.4941   YZ=     1.6804   ZZ=   284.0817
 Eigenvalues:   282.4086   291.9041   348.1020
   13  Si   Isotropic =   308.6731   Anisotropy =    59.8787
 XX=   308.9655   YX=    30.0341   ZX=    -4.6902
 XY=    20.1258   YY=   330.8570   ZY=    -7.1617
 XZ=    -3.3228   YZ=    -9.2539   ZZ=   286.1967
 Eigenvalues:   284.7171   292.7099   348.5922
```

**Table S27. Atomic Coordinates of the Optimized Structure of 12a**




| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | Si | 0.000000 | 0.000000 | 0.407628 |
| 2 | Si | 1.802083 | -1.391195 | 1.176347 |
| 3 | Si | -2.105851 | -0.865051 | 1.176347 |
| 4 | Si | 0.303769 | 2.256246 | 1.176347 |
| 5 | Si | 2.144792 | -3.480785 | 0.046210 |
| 6 | Si | -4.086844 | -0.117052 | 0.046210 |

| | | | | |
|---|---|---|---|---|
| 7 | Si | 1.942052 | 3.597837 | 0.046210 |
| 8 | Si | 4.459770 | -4.044041 | -0.003867 |
| 9 | Si | -5.732128 | -1.840254 | -0.003867 |
| 10 | Si | 1.272357 | 5.884295 | -0.003867 |
| 11 | C | 0.000000 | 0.000000 | -1.517012 |
| 12 | H | -0.365669 | -0.952720 | -1.914694 |
| 13 | H | -0.642245 | 0.793038 | -1.914694 |
| 14 | H | 1.007914 | 0.159681 | -1.914694 |
| 15 | C | 3.405252 | -0.359072 | 1.011854 |
| 16 | H | 3.584045 | -0.040563 | -0.021756 |
| 17 | H | 3.341665 | 0.540773 | 1.633105 |
| 18 | H | 4.282323 | -0.927426 | 1.341611 |
| 19 | C | 1.600985 | -1.774437 | 3.041062 |
| 20 | H | 0.716632 | -2.388645 | 3.243939 |
| 21 | H | 2.475350 | -2.320495 | 3.416447 |
| 22 | H | 1.509430 | -0.851870 | 3.626793 |
| 23 | C | 1.482302 | -3.453304 | -1.747317 |
| 24 | H | 0.397428 | -3.295507 | -1.758954 |
| 25 | H | 1.940687 | -2.657104 | -2.344168 |
| 26 | H | 1.683466 | -4.405199 | -2.252979 |
| 27 | C | 1.235755 | -4.892285 | 0.965385 |
| 28 | H | 1.568238 | -4.980969 | 2.005989 |
| 29 | H | 0.151115 | -4.742913 | 0.971910 |
| 30 | H | 1.430310 | -5.853450 | 0.473573 |
| 31 | C | 5.426604 | -2.872056 | -1.163444 |
| 32 | H | 5.426890 | -1.841705 | -0.790168 |
| 33 | H | 6.467555 | -3.204097 | -1.249007 |
| 34 | H | 4.997679 | -2.862110 | -2.172461 |
| 35 | C | 5.227368 | -3.951268 | 1.745861 |
| 36 | H | 4.707187 | -4.610129 | 2.451111 |
| 37 | H | 6.278182 | -4.262816 | 1.713699 |
| 38 | H | 5.193716 | -2.934656 | 2.154856 |
| 39 | C | 0.736214 | 2.273713 | 3.041062 |
| 40 | H | 1.710312 | 1.814944 | 3.243939 |
| 41 | H | 0.771932 | 3.303964 | 3.416447 |
| 42 | H | -0.016974 | 1.733140 | 3.626793 |
| 43 | C | -1.391661 | 3.128571 | 1.011854 |
| 44 | H | -1.756894 | 3.124156 | -0.021756 |
| 45 | H | -2.139155 | 2.623580 | 1.633105 |
| 46 | H | -1.337987 | 4.172313 | 1.341611 |
| 47 | C | 2.249498 | 3.010363 | -1.747317 |
| 48 | H | 2.655278 | 1.991935 | -1.758954 |
| 49 | H | 1.330776 | 3.009236 | -2.344168 |
| 50 | H | 2.973281 | 3.660524 | -2.252979 |
| 51 | C | 3.618966 | 3.516337 | 0.965385 |
| 52 | H | 3.529526 | 3.848618 | 2.005989 |
| 53 | H | 4.031926 | 2.502326 | 0.971910 |
| 54 | H | 4.354081 | 4.165410 | 0.473573 |
| 55 | C | 0.808215 | 6.502667 | 1.745861 |
| 56 | H | -0.055372 | 5.965217 | 2.154856 |
| 57 | H | 1.638895 | 6.381609 | 2.451111 |
| 58 | H | 0.552615 | 7.568473 | 1.713699 |
| 59 | C | -0.226029 | 6.135606 | -1.163444 |
| 60 | H | -0.020179 | 5.759171 | -2.172461 |
| 61 | H | -1.118482 | 5.620677 | -0.790168 |
| 62 | H | -0.458948 | 7.203116 | -1.249007 |
| 63 | C | -2.337200 | -0.499275 | 3.041062 |
| 64 | H | -2.426943 | 0.573702 | 3.243939 |
| 65 | H | -3.247282 | -0.983469 | 3.416447 |
| 66 | H | -1.492456 | -0.881270 | 3.626793 |
| 67 | C | -2.013592 | -2.769499 | 1.011854 |
| 68 | H | -1.827152 | -3.083592 | -0.021756 |
| 69 | H | -1.202510 | -3.164352 | 1.633105 |
| 70 | H | -2.944336 | -3.244888 | 1.341611 |
| 71 | C | -4.854720 | 1.375947 | 0.965385 |
| 72 | H | -5.097765 | 1.132351 | 2.005989 |

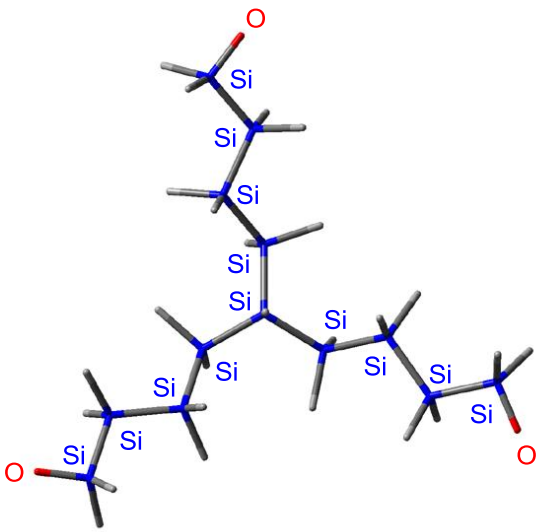
| | | | | |
|---|---|---|---|---|
| 73 | H | -4.183041 | 2.240587 | 0.971910 |
| 74 | H | -5.784391 | 1.688040 | 0.473573 |
| 75 | C | -3.731800 | 0.442941 | -1.747317 |
| 76 | H | -3.052706 | 1.303571 | -1.758954 |
| 77 | H | -3.271463 | -0.352131 | -2.344168 |
| 78 | H | -4.656747 | 0.744675 | -2.252979 |
| 79 | C | -5.200576 | -3.263550 | -1.163444 |
| 80 | H | -4.308408 | -3.778972 | -0.790168 |
| 81 | H | -6.008607 | -3.999018 | -1.249007 |
| 82 | H | -4.977499 | -2.897061 | -2.172461 |
| 83 | C | -6.035582 | -2.551399 | 1.745861 |
| 84 | H | -5.138344 | -3.030562 | 2.154856 |
| 85 | H | -6.346084 | -1.771480 | 2.451111 |
| 86 | H | -6.830799 | -3.305657 | 1.713699 |
| 87 | Si | -7.832063 | -1.068228 | -0.782380 |
| 88 | Si | 4.841143 | -6.248650 | -0.782380 |
| 89 | Si | 2.990918 | 7.316879 | -0.782380 |
| 90 | C | 3.745897 | 6.796093 | -2.444929 |
| 91 | H | 4.302677 | 5.855877 | -2.345151 |
| 92 | H | 2.976479 | 6.649691 | -3.211447 |
| 93 | H | 4.450191 | 7.549962 | -2.819437 |
| 94 | C | 4.411229 | 7.528271 | 0.459978 |
| 95 | H | 4.044681 | 7.873084 | 1.433670 |
| 96 | H | 4.937550 | 6.579289 | 0.620253 |
| 97 | H | 5.152300 | 8.256270 | 0.105681 |
| 98 | C | 4.012641 | -6.642089 | -2.444929 |
| 99 | H | 2.920001 | -6.654166 | -2.345151 |
| 100 | H | 4.270561 | -5.902552 | -3.211447 |
| 101 | H | 4.313364 | -7.628960 | -2.819437 |
| 102 | C | 4.314060 | -7.584372 | 0.459978 |
| 103 | H | 4.795950 | -7.439338 | 1.433670 |
| 104 | H | 3.229057 | -7.565688 | 0.620253 |
| 105 | H | 4.573989 | -8.590158 | 0.105681 |
| 106 | C | -7.758538 | -0.154005 | -2.444929 |
| 107 | H | -7.222677 | 0.798289 | -2.345151 |
| 108 | H | -7.247041 | -0.747138 | -3.211447 |
| 109 | H | -8.763555 | 0.078997 | -2.819437 |
| 110 | C | -8.725288 | 0.056101 | 0.459978 |
| 111 | H | -8.840631 | -0.433746 | 1.433670 |
| 112 | H | -8.166607 | 0.986399 | 0.620253 |
| 113 | H | -9.726289 | 0.333888 | 0.105681 |
| 114 | O | -8.692529 | -2.509509 | -0.962113 |
| 115 | O | 6.519563 | -6.273196 | -0.962113 |
| 116 | O | 2.172966 | 8.782706 | -0.962113 |
| 117 | C | 7.260870 | -7.404754 | -1.384381 |
| 118 | H | 8.318698 | -7.124425 | -1.426958 |
| 119 | H | 7.156583 | -8.246736 | -0.685034 |
| 120 | H | 6.955688 | -7.744713 | -2.384503 |
| 121 | C | 2.782269 | 9.990475 | -1.384381 |
| 122 | H | 2.010584 | 10.766416 | -1.426958 |
| 123 | H | 3.563591 | 10.321151 | -0.685034 |
| 124 | H | 3.229274 | 9.896159 | -2.384503 |
| 125 | C | -10.043139 | -2.585721 | -1.384381 |
| 126 | H | -10.329282 | -3.641991 | -1.426958 |
| 127 | H | -10.720175 | -2.074415 | -0.685034 |
| 128 | H | -10.184963 | -2.151446 | -2.384503 |

**Table S28. Magnetic Shielding Tensors of $^{29}$Si Nuclei of 12a Calculated by the GIAO Method**

```
SCF GIAO Magnetic shielding tensor (ppm):
      1  Si    Isotropic =   370.4709   Anisotropy =    14.6761
```

```
XX=   365.9327   YX=     1.3296   ZX=     0.6105
XY=    -0.9310   YY=   365.2787   ZY=    -0.0193
XZ=     0.2269   YZ=     1.5823   ZZ=   380.2013
Eigenvalues:   365.1946   365.9631   380.2550
   2  Si   Isotropic =   351.1461   Anisotropy =    18.7587
XX=   354.8724   YX=     2.0127   ZX=     6.2246
XY=     0.7425   YY=   339.6745   ZY=    -0.0855
XZ=     6.1433   YZ=     4.3472   ZZ=   358.8914
Eigenvalues:   339.4051   350.3813   363.6519
   3  Si   Isotropic =   350.9535   Anisotropy =    20.8952
XX=   341.9361   YX=     8.9611   ZX=    -2.9225
XY=     6.4099   YY=   351.6970   ZY=    -5.2929
XZ=    -0.8994   YZ=    -8.7030   ZZ=   359.2273
Eigenvalues:   337.5607   350.4161   364.8836
   4  Si   Isotropic =   352.7351   Anisotropy =    21.3597
XX=   345.9444   YX=    -6.2664   ZX=    -4.5090
XY=    -7.1955   YY=   351.4172   ZY=     5.5086
XZ=    -9.5143   YZ=     4.2646   ZZ=   360.8436
Eigenvalues:   340.8123   350.4179   366.9749
   5  Si   Isotropic =   358.4543   Anisotropy =    22.5416
XX=   349.9651   YX=     8.1894   ZX=     9.9867
XY=    10.8583   YY=   356.2818   ZY=     2.5436
XZ=     4.7325   YZ=     1.9887   ZZ=   369.1158
Eigenvalues:   342.2309   359.6498   373.4820
   6  Si   Isotropic =   360.6244   Anisotropy =    20.0032
XX=   348.0978   YX=    -8.1433   ZX=    -2.7854
XY=    -7.8491   YY=   362.0576   ZY=    -6.5225
XZ=    -2.2277   YZ=    -3.7111   ZZ=   371.7178
Eigenvalues:   343.7564   364.1570   373.9599
   7  Si   Isotropic =   355.9486   Anisotropy =    22.5016
XX=   359.9815   YX=    -4.1717   ZX=    -8.1658
XY=    -0.2234   YY=   342.9481   ZY=     7.5854
XZ=    -6.0638   YZ=     2.0681   ZZ=   364.9162
Eigenvalues:   341.9044   354.9917   370.9496
   8  Si   Isotropic =   363.9783   Anisotropy =    22.8129
XX=   371.3512   YX=    15.0943   ZX=     1.7742
XY=    13.5104   YY=   349.6122   ZY=    -6.2450
XZ=     1.2297   YZ=    -9.7259   ZZ=   370.9714
Eigenvalues:   340.5017   372.2462   379.1869
   9  Si   Isotropic =   358.2791   Anisotropy =    24.2901
XX=   343.8386   YX=     2.8989   ZX=    -6.6292
XY=    -0.3126   YY=   374.3390   ZY=     2.7004
XZ=    -6.0858   YZ=     0.1186   ZZ=   356.6598
Eigenvalues:   341.1302   359.2346   374.4725
  10  Si   Isotropic =   361.2144   Anisotropy =    25.6498
XX=   367.1876   YX=   -15.0861   ZX=     5.0120
XY=   -18.3068   YY=   352.2221   ZY=     5.0370
XZ=     6.8000   YZ=     5.9462   ZZ=   364.2336
Eigenvalues:   338.9775   366.3515   378.3143
  87  Si   Isotropic =   307.9705   Anisotropy =    65.4317
XX=   313.4026   YX=    31.3884   ZX=    10.5251
XY=    25.4514   YY=   328.6424   ZY=     1.4596
XZ=     9.6100   YZ=     5.5285   ZZ=   281.8666
Eigenvalues:   278.2055   294.1145   351.5917
  88  Si   Isotropic =   306.6778   Anisotropy =    64.0845
XX=   346.1843   YX=    -4.1801   ZX=    -9.3585
XY=   -12.3097   YY=   293.0105   ZY=     6.2161
XZ=   -12.4631   YZ=     4.5534   ZZ=   280.8386
Eigenvalues:   277.9211   292.7114   349.4008
  89  Si   Isotropic =   308.3302   Anisotropy =    68.0806
XX=   299.4727   YX=   -19.6700   ZX=    -2.1828
XY=   -23.6784   YY=   343.4448   ZY=   -10.4733
XZ=     0.6835   YZ=   -11.6187   ZZ=   282.0730
Eigenvalues:   278.7211   292.5521   353.7173
```

**Table S29. Atomic Coordinates of the Optimized Structure of 12b**




| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | Si | 0.000000 | 0.000000 | 0.406904 |
| 2 | Si | 1.535639 | -1.684178 | 1.167897 |
| 3 | Si | -2.226360 | -0.487813 | 1.167897 |
| 4 | Si | 0.690721 | 2.171991 | 1.167897 |
| 5 | Si | 1.550186 | -3.765387 | -0.024544 |
| 6 | Si | -4.036014 | 0.540193 | -0.024544 |
| 7 | Si | 2.485828 | 3.225194 | -0.024544 |
| 8 | Si | 3.734522 | -4.714424 | -0.059917 |
| 9 | Si | -5.950072 | -0.876979 | -0.059917 |
| 10 | Si | 2.215550 | 5.591403 | -0.059917 |
| 11 | C | 0.000000 | 0.000000 | -1.516936 |
| 12 | H | -0.506507 | -0.885899 | -1.913993 |
| 13 | H | -0.513958 | 0.881598 | -1.913993 |
| 14 | H | 1.020465 | 0.004302 | -1.913993 |
| 15 | C | 3.293403 | -0.932927 | 1.068853 |
| 16 | H | 3.551948 | -0.625821 | 0.048857 |
| 17 | H | 3.370939 | -0.051079 | 1.714215 |
| 18 | H | 4.051027 | -1.652167 | 1.400103 |
| 19 | C | 1.230202 | -2.087420 | 3.014265 |
| 20 | H | 0.262717 | -2.575221 | 3.175608 |
| 21 | H | 2.007610 | -2.762298 | 3.393672 |
| 22 | H | 1.253483 | -1.178778 | 3.627584 |
| 23 | C | 0.960158 | -3.580390 | -1.834627 |
| 24 | H | -0.090195 | -3.269618 | -1.881376 |
| 25 | H | 1.549491 | -2.839297 | -2.385930 |
| 26 | H | 1.046071 | -4.534780 | -2.367419 |
| 27 | C | 0.381943 | -5.015819 | 0.833715 |
| 28 | H | 0.681910 | -5.204296 | 1.870970 |
| 29 | H | -0.653752 | -4.660764 | 0.844850 |
| 30 | H | 0.392189 | -5.977966 | 0.306960 |
| 31 | C | 4.913172 | -3.673409 | -1.145359 |
| 32 | H | 5.080452 | -2.676618 | -0.722124 |
| 33 | H | 5.883945 | -4.174645 | -1.232226 |

| | | | | |
|---|---|---|---|---|
| 34 | H | 4.515259 | -3.544320 | -2.158608 |
| 35 | C | 4.463573 | -4.840949 | 1.703710 |
| 36 | H | 3.821743 | -5.438569 | 2.361543 |
| 37 | H | 5.447806 | -5.323039 | 1.672643 |
| 38 | H | 4.589094 | -3.855537 | 2.167813 |
| 39 | C | 1.192658 | 2.109096 | 3.014265 |
| 40 | H | 2.098848 | 1.515129 | 3.175608 |
| 41 | H | 1.388415 | 3.119791 | 3.393672 |
| 42 | H | 0.394110 | 1.674938 | 3.627584 |
| 43 | C | -0.838762 | 3.318635 | 1.068853 |
| 44 | H | -1.233997 | 3.388988 | 0.048857 |
| 45 | H | -1.641234 | 2.944859 | 1.714215 |
| 46 | H | -0.594696 | 4.334375 | 1.400103 |
| 47 | C | 2.620630 | 2.621717 | -1.834627 |
| 48 | H | 2.876671 | 1.556698 | -1.881376 |
| 49 | H | 1.684158 | 2.761546 | -2.385930 |
| 50 | H | 3.404199 | 3.173314 | -2.367419 |
| 51 | C | 4.152856 | 2.838682 | 0.833715 |
| 52 | H | 4.166099 | 3.192699 | 1.870970 |
| 53 | H | 4.363216 | 1.764216 | 0.844850 |
| 54 | H | 4.980976 | 3.328628 | 0.306960 |
| 55 | C | 1.960599 | 6.286042 | 1.703710 |
| 56 | H | 1.044446 | 5.902041 | 2.167813 |
| 57 | H | 2.799068 | 6.029011 | 2.361543 |
| 58 | H | 1.885983 | 7.379457 | 1.672643 |
| 59 | C | 0.724679 | 6.091636 | -1.145359 |
| 60 | H | 0.811841 | 5.682490 | -2.158608 |
| 61 | H | -0.222206 | 5.738109 | -0.722124 |
| 62 | H | 0.673376 | 7.182969 | -1.232226 |
| 63 | C | -2.422860 | -0.021676 | 3.014265 |
| 64 | H | -2.361564 | 1.060091 | 3.175608 |
| 65 | H | -3.396026 | -0.357492 | 3.393672 |
| 66 | H | -1.647594 | -0.496160 | 3.627584 |
| 67 | C | -2.454640 | -2.385706 | 1.068853 |
| 68 | H | -2.317951 | -2.763167 | 0.048857 |
| 69 | H | -1.729705 | -2.893780 | 1.714215 |
| 70 | H | -3.456331 | -2.682209 | 1.400103 |
| 71 | C | -4.534798 | 2.177138 | 0.833715 |
| 72 | H | -4.848008 | 2.011598 | 1.870970 |
| 73 | H | -3.709464 | 2.896548 | 0.844850 |
| 74 | H | -5.373165 | 2.649338 | 0.306960 |
| 75 | C | -3.580788 | 0.958673 | -1.834627 |
| 76 | H | -2.786476 | 1.712921 | -1.881376 |
| 77 | H | -3.233649 | 0.077750 | -2.385930 |
| 78 | H | -4.450270 | 1.361466 | -2.367419 |
| 79 | C | -5.637851 | -2.418228 | -1.145359 |
| 80 | H | -4.858246 | -3.061491 | -0.722124 |
| 81 | H | -6.557322 | -3.008324 | -1.232226 |
| 82 | H | -5.327101 | -2.138170 | -2.158608 |
| 83 | C | -6.424172 | -1.445093 | 1.703710 |
| 84 | H | -5.633540 | -2.046504 | 2.167813 |
| 85 | H | -6.620811 | -0.590442 | 2.361543 |
| 86 | H | -7.333790 | -2.056420 | 1.672643 |
| 87 | Si | -7.858640 | 0.208462 | -0.948718 |
| 88 | Si | 3.748787 | -6.910013 | -0.948718 |
| 89 | Si | 4.109853 | 6.701551 | -0.948718 |
| 90 | C | 4.661417 | 6.068438 | -2.650362 |
| 91 | H | 5.036697 | 5.039026 | -2.589512 |
| 92 | H | 3.839070 | 6.083184 | -3.374585 |
| 93 | H | 5.473867 | 6.685377 | -3.057690 |
| 94 | C | 5.620134 | 6.643795 | 0.198402 |
| 95 | H | 5.382596 | 7.032346 | 1.195163 |
| 96 | H | 5.990397 | 5.618273 | 0.319564 |
| 97 | H | 6.448052 | 7.243081 | -0.204123 |
| 98 | C | 2.924714 | -7.071125 | -2.650362 |
| 99 | H | 1.845576 | -6.881420 | -2.589512 |

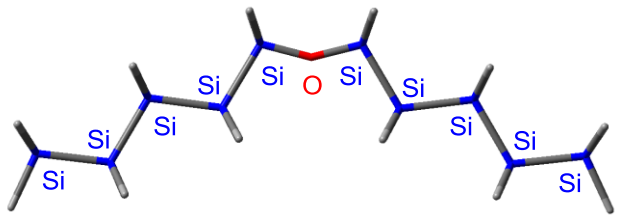
| | | | | |
|---|---|---|---|---|
| 100 | H | 3.348656 | -6.366324 | -3.374585 |
| 101 | H | 3.052773 | -8.083197 | -3.057690 |
| 102 | C | 2.943629 | -8.189076 | 0.198402 |
| 103 | H | 3.398893 | -8.177637 | 1.195163 |
| 104 | H | 1.870368 | -7.996973 | 0.319564 |
| 105 | H | 3.048665 | -9.205718 | -0.204123 |
| 106 | C | -7.586131 | 1.002685 | -2.650362 |
| 107 | H | -6.882273 | 1.842395 | -2.589512 |
| 108 | H | -7.187728 | 0.283141 | -3.374585 |
| 109 | H | -8.526640 | 1.397820 | -3.057690 |
| 110 | C | -8.563762 | 1.545281 | 0.198402 |
| 111 | H | -8.781488 | 1.145291 | 1.195163 |
| 112 | H | -7.860766 | 2.378700 | 0.319564 |
| 113 | H | -9.496718 | 1.962637 | -0.204123 |
| 114 | O | -8.968423 | -1.063976 | -1.085312 |
| 115 | H | -9.846674 | -0.818080 | -1.412116 |
| 116 | O | 5.405641 | -7.234894 | -1.085312 |
| 117 | H | 5.631815 | -8.118431 | -1.412116 |
| 118 | O | 3.562781 | 8.298870 | -1.085312 |
| 119 | H | 4.214859 | 8.936510 | -1.412116 |

**Table S30. Magnetic Shielding Tensors of $^{29}$Si Nuclei of 12b Calculated by the GIAO Method**

```
SCF GIAO Magnetic shielding tensor (ppm):
      1  Si   Isotropic =   370.5428   Anisotropy =    19.2702
   XX=   363.7372   YX=     0.7787   ZX=     0.0809
   XY=     0.1214   YY=   364.5061   ZY=     0.2273
   XZ=     0.3949   YZ=    -0.5839   ZZ=   383.3852
   Eigenvalues:   363.5255   364.7133   383.3896
      2  Si   Isotropic =   349.1612   Anisotropy =    21.2328
   XX=   352.3904   YX=    -0.8871   ZX=     7.1792
   XY=    -1.8193   YY=   340.4341   ZY=    -1.8631
   XZ=    12.2631   YZ=     3.4066   ZZ=   354.6590
   Eigenvalues:   339.8347   344.3324   363.3163
      3  Si   Isotropic =   350.2405   Anisotropy =    19.5955
   XX=   343.6713   YX=     7.2743   ZX=    -4.8380
   XY=     6.0245   YY=   349.1914   ZY=    -3.7989
   XZ=    -3.5045   YZ=    -8.0828   ZZ=   357.8587
   Eigenvalues:   339.2299   348.1874   363.3042
      4  Si   Isotropic =   349.8453   Anisotropy =    19.9632
   XX=   340.9200   YX=    -3.5488   ZX=    -1.1155
   XY=    -5.8633   YY=   352.1172   ZY=     5.8754
   XZ=    -6.3429   YZ=     8.1082   ZZ=   356.4988
   Eigenvalues:   339.1116   347.2702   363.1542
      5  Si   Isotropic =   357.6760   Anisotropy =    22.9389
   XX=   354.5729   YX=    10.3858   ZX=    10.2340
   XY=    12.3434   YY=   352.9233   ZY=     0.7933
   XZ=     7.5681   YZ=     0.9779   ZZ=   365.5320
   Eigenvalues:   341.0443   359.0152   372.9686
      6  Si   Isotropic =   361.6428   Anisotropy =    22.3165
   XX=   345.7243   YX=    -6.4576   ZX=    -4.9399
   XY=    -8.5275   YY=   366.1500   ZY=    -7.5557
   XZ=    -6.3836   YZ=    -4.3058   ZZ=   373.0540
   Eigenvalues:   341.5816   366.8263   376.5205
      7  Si   Isotropic =   360.0893   Anisotropy =    19.9250
   XX=   364.4413   YX=    -7.6936   ZX=    -4.5358
   XY=    -4.9884   YY=   347.1028   ZY=     8.6617
   XZ=    -2.1535   YZ=     3.7858   ZZ=   368.7238
   Eigenvalues:   344.0208   362.8745   373.3727
      8  Si   Isotropic =   362.0036   Anisotropy =    27.1747
   XX=   376.5083   YX=    12.4009   ZX=     3.8990
```

```
XY=     9.5412   YY=   346.7912   ZY=    -7.1377
XZ=     2.2744   YZ=   -12.1008   ZZ=   362.7115
Eigenvalues:   338.8948   366.9960   380.1201
   9  Si   Isotropic =   362.1778   Anisotropy =    21.6720
XX=   345.5209   YX=     7.3154   ZX=    -8.2702
XY=     8.0572   YY=   374.7263   ZY=     1.0914
XZ=   -10.0136   YZ=     3.3552   ZZ=   366.2862
Eigenvalues:   340.2250   369.6825   376.6258
  10  Si   Isotropic =   358.8444   Anisotropy =    23.0517
XX=   359.9140   YX=   -13.4525   ZX=     3.5924
XY=   -17.4112   YY=   357.4215   ZY=     6.5349
XZ=     6.2893   YZ=     6.8144   ZZ=   359.1977
Eigenvalues:   339.6877   362.6333   374.2122
  87  Si   Isotropic =   306.7400   Anisotropy =    57.2667
XX=   321.2920   YX=    31.5027   ZX=     7.7900
XY=    21.5055   YY=   313.6912   ZY=    -0.6673
XZ=     6.8308   YZ=     2.7862   ZZ=   285.2368
Eigenvalues:   282.6404   292.6618   344.9178
  88  Si   Isotropic =   307.1764   Anisotropy =    58.6337
XX=   339.5509   YX=   -11.8968   ZX=    -3.3670
XY=   -22.2006   YY=   296.6005   ZY=     6.8636
XZ=    -7.1644   YZ=     4.4488   ZZ=   285.3779
Eigenvalues:   282.9440   292.3198   346.2655
  89  Si   Isotropic =   307.7876   Anisotropy =    55.4393
XX=   294.5533   YX=    -5.4226   ZX=    -5.0832
XY=   -15.7122   YY=   341.8572   ZY=    -5.8791
XZ=     0.0636   YZ=    -7.5652   ZZ=   286.9523
Eigenvalues:   284.4452   294.1705   344.7471
```

**Table S31. Atomic Coordinates of the Optimized Structure of 13**




| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | C | -3.289897 | 1.984998 | 1.535407 |
| 2 | H | -4.196482 | 1.366598 | 1.542255 |
| 3 | H | -2.740623 | 1.779572 | 2.461257 |
| 4 | H | -3.606169 | 3.035143 | 1.561721 |
| 5 | C | -3.289897 | 1.984998 | -1.535407 |
| 6 | H | -2.740623 | 1.779572 | -2.461257 |
| 7 | H | -4.196482 | 1.366598 | -1.542255 |
| 8 | H | -3.606169 | 3.035143 | -1.561721 |
| 9 | C | 0.794290 | 2.301092 | -1.547391 |
| 10 | H | 0.899148 | 1.210048 | -1.578257 |
| 11 | H | 0.300500 | 2.613844 | -2.474652 |
| 12 | H | 1.801727 | 2.732751 | -1.546441 |
| 13 | C | 0.794290 | 2.301092 | 1.547391 |
| 14 | H | 0.300500 | 2.613844 | 2.474652 |
| 15 | H | 0.899148 | 1.210048 | 1.578257 |
| 16 | H | 1.801727 | 2.732751 | 1.546441 |

| | | | | |
|---|---|---|---|---|
| 17 | C | −1.506358 | 5.700171 | 1.546837 |
| 18 | H | −2.479295 | 5.194762 | 1.565655 |
| 19 | H | −0.981802 | 5.440740 | 2.473699 |
| 20 | H | −1.695450 | 6.780054 | 1.564798 |
| 21 | C | −1.506358 | 5.700171 | −1.546837 |
| 22 | H | −0.981802 | 5.440740 | −2.473699 |
| 23 | H | −2.479295 | 5.194762 | −1.565655 |
| 24 | H | −1.695450 | 6.780054 | −1.564798 |
| 25 | C | 2.594927 | 5.942218 | −1.546304 |
| 26 | H | 2.865454 | 4.879898 | −1.547813 |
| 27 | H | 2.048065 | 6.146049 | −2.474221 |
| 28 | H | 3.527712 | 6.518597 | −1.577810 |
| 29 | C | 2.594927 | 5.942218 | 1.546304 |
| 30 | H | 2.048065 | 6.146049 | 2.474221 |
| 31 | H | 2.865454 | 4.879898 | 1.547813 |
| 32 | H | 3.527712 | 6.518597 | 1.577810 |
| 33 | C | 0.365412 | 9.377144 | 1.545539 |
| 34 | H | −0.664158 | 9.002830 | 1.580515 |
| 35 | H | 0.864623 | 9.058608 | 2.468235 |
| 36 | H | 0.318681 | 10.473783 | 1.556879 |
| 37 | C | 0.365412 | 9.377144 | −1.545539 |
| 38 | H | 0.864623 | 9.058608 | −2.468235 |
| 39 | H | −0.664158 | 9.002830 | −1.580515 |
| 40 | H | 0.318681 | 10.473783 | −1.556879 |
| 41 | Si | −2.237542 | 1.621604 | 0.000000 |
| 42 | Si | −0.194876 | 2.835667 | 0.000000 |
| 43 | Si | −0.495369 | 5.199331 | 0.000000 |
| 44 | Si | 1.562367 | 6.401462 | 0.000000 |
| 45 | Si | 1.292942 | 8.765085 | 0.000000 |
| 46 | C | 3.022234 | 9.569323 | 0.000000 |
| 47 | H | 3.603404 | 9.283750 | −0.884820 |
| 48 | H | 2.937151 | 10.663829 | 0.000000 |
| 49 | H | 3.603404 | 9.283750 | 0.884820 |
| 50 | O | −1.822319 | 0.000000 | 0.000000 |
| 51 | Si | −2.237476 | −1.621575 | 0.000000 |
| 52 | Si | −0.194823 | −2.835644 | 0.000000 |
| 53 | Si | −0.495319 | −5.199326 | 0.000000 |
| 54 | Si | 1.562408 | −6.401466 | 0.000000 |
| 55 | Si | 1.292840 | −8.765083 | 0.000000 |
| 56 | C | 3.022093 | −9.569399 | 0.000000 |
| 57 | H | 3.603270 | −9.283834 | 0.884819 |
| 58 | H | 2.936994 | −10.663903 | 0.000000 |
| 59 | H | 3.603270 | −9.283834 | −0.884819 |
| 60 | C | 0.365223 | −9.377106 | 1.545504 |
| 61 | H | −0.664348 | −9.002782 | 1.580364 |
| 62 | H | 0.318476 | −10.473744 | 1.556848 |
| 63 | H | 0.864337 | −9.058567 | 2.468250 |
| 64 | C | 0.365223 | −9.377106 | −1.545504 |
| 65 | H | −0.664348 | −9.002782 | −1.580364 |
| 66 | H | 0.864337 | −9.058567 | −2.468250 |
| 67 | H | 0.318476 | −10.473744 | −1.556848 |
| 68 | C | 2.594984 | −5.942327 | 1.546318 |
| 69 | H | 2.865424 | −4.879987 | 1.548011 |
| 70 | H | 2.048175 | −6.146370 | 2.474220 |
| 71 | H | 3.527814 | −6.518642 | 1.577681 |
| 72 | C | 2.594984 | −5.942327 | −1.546318 |
| 73 | H | 2.048175 | −6.146370 | −2.474220 |
| 74 | H | 2.865424 | −4.879987 | −1.548011 |
| 75 | H | 3.527814 | −6.518642 | −1.577681 |
| 76 | C | −1.506262 | −5.700000 | 1.546917 |
| 77 | H | −1.695187 | −6.779903 | 1.565253 |
| 78 | H | −0.981728 | −5.440179 | 2.473686 |
| 79 | H | −2.479272 | −5.194728 | 1.565589 |
| 80 | C | −1.506262 | −5.700000 | −1.546917 |
| 81 | H | −0.981728 | −5.440179 | −2.473686 |
| 82 | H | −1.695187 | −6.779903 | −1.565253 |

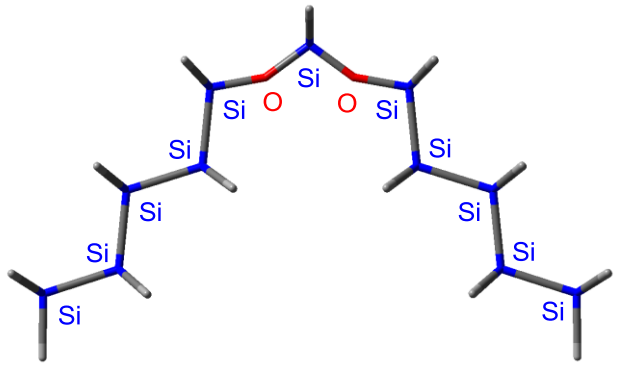
```
  83          H          -2.479272   -5.194728   -1.565589
  84          C           0.794407   -2.301248    1.547416
  85          H           0.300821   -2.614429    2.474643
  86          H           1.801922   -2.732731    1.546153
  87          H           0.899086   -1.210200    1.578675
  88          C           0.794407   -2.301248   -1.547416
  89          H           1.801922   -2.732731   -1.546153
  90          H           0.300821   -2.614429   -2.474643
  91          H           0.899086   -1.210200   -1.578675
  92          C          -3.289758   -1.984951    1.535458
  93          H          -2.740390   -1.779483    2.461245
  94          H          -4.196326   -1.366528    1.542360
  95          H          -3.606046   -3.035087    1.561861
  96          C          -3.289758   -1.984951   -1.535458
  97          H          -4.196326   -1.366528   -1.542360
  98          H          -2.740390   -1.779483   -2.461245
  99          H          -3.606046   -3.035087   -1.561861
 ---------------------------------------------------------------
```

**Table S32. Magnetic Shielding Tensors of $^{29}$Si Nuclei of 13 Calculated by the GIAO Method**

```
SCF GIAO Magnetic shielding tensor (ppm):
 41  Si   Isotropic =   314.6354   Anisotropy =    58.0414
   XX=   304.5682   YX=    -8.8456   ZX=     0.0000
   XY=   -13.3620   YY=   350.8011   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=   288.5368
   Eigenvalues:   288.5368   302.0396   353.3296
   Eigenvectors:
      (1)   0.000000   0.000000   1.000000
      (2)   0.975039   0.222033   0.000000
      (3)  -0.222033   0.975039   0.000000
 42  Si   Isotropic =   365.7691   Anisotropy =    18.6508
   XX=   362.7304   YX=   -19.8187   ZX=     0.0000
   XY=   -16.8403   YY=   356.4890   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=   378.0880
   Eigenvalues:   341.0164   378.0880   378.2030
   Eigenvectors:
      (1)   0.645042   0.764147   0.000000
      (2)  -0.000006   0.000005   1.000000
      (3)   0.764147  -0.645042   0.000008
 43  Si   Isotropic =   359.8401   Anisotropy =    19.6675
   XX=   367.6972   YX=    -9.5569   ZX=     0.0000
   XY=   -13.6022   YY=   347.4336   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=   364.3894
   Eigenvalues:   342.1791   364.3894   372.9518
   Eigenvectors:
      (1)   0.413222   0.910630   0.000000
      (2)   0.000000   0.000000   1.000000
      (3)   0.910630  -0.413222   0.000000
 44  Si   Isotropic =   363.1194   Anisotropy =    18.3257
   XX=   373.9876   YX=    -7.9675   ZX=     0.0000
   XY=    -5.2416   YY=   343.0001   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=   372.3705
   Eigenvalues:   341.6512   372.3705   375.3365
   Eigenvectors:
      (1)   0.200115   0.979773   0.000000
      (2)   0.000000   0.000000   1.000000
      (3)   0.979773  -0.200115   0.000000
 45  Si   Isotropic =   337.8778   Anisotropy =     5.2705
   XX=   339.8403   YX=    -0.4863   ZX=     0.0000
   XY=    -1.8481   YY=   332.4016   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=   341.3915
```

```
  Eigenvalues:   332.2228   340.0191   341.3915
  Eigenvectors:
     (1)   0.151456   0.988464   0.000000
     (2)   0.988464  -0.151456   0.000000
     (3)   0.000000   0.000000   1.000000
51  Si   Isotropic =   314.6408   Anisotropy =    58.0404
  XX=   304.5753   YX=     8.8487   ZX=     0.0000
  XY=    13.3675   YY=   350.8038   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   288.5433
  Eigenvalues:   288.5433   302.0447   353.3344
  Eigenvectors:
     (1)   0.000000   0.000000   1.000000
     (2)   0.975018  -0.222124   0.000000
     (3)   0.222124   0.975018   0.000000
52  Si   Isotropic =   365.7739   Anisotropy =    18.6509
  XX=   362.7477   YX=    19.8210   ZX=     0.0000
  XY=    16.8377   YY=   356.4767   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   378.0973
  Eigenvalues:   341.0166   378.0973   378.2078
  Eigenvectors:
     (1)  -0.644742   0.764401   0.000000
     (2)   0.000010   0.000009   1.000000
     (3)   0.764401   0.644742  -0.000014
53  Si   Isotropic =   359.8309   Anisotropy =    19.6952
  XX=   367.7044   YX=     9.5601   ZX=     0.0000
  XY=    13.6141   YY=   347.4198   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   364.3685
  Eigenvalues:   342.1632   364.3685   372.9611
  Eigenvectors:
     (1)  -0.413137   0.910669   0.000000
     (2)   0.000001   0.000000   1.000000
     (3)   0.910669   0.413137  -0.000001
54  Si   Isotropic =   363.1226   Anisotropy =    18.3275
  XX=   373.9929   YX=     7.9693   ZX=     0.0000
  XY=     5.2380   YY=   342.9930   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   372.3819
  Eigenvalues:   341.6450   372.3819   375.3409
  Eigenvectors:
     (1)  -0.200018   0.979792   0.000000
     (2)   0.000001   0.000000   1.000000
     (3)   0.979792   0.200018  -0.000001
55  Si   Isotropic =   337.8754   Anisotropy =     5.2756
  XX=   339.8299   YX=     0.4864   ZX=     0.0000
  XY=     1.8384   YY=   332.4038   ZY=     0.0000
  XZ=     0.0000   YZ=     0.0000   ZZ=   341.3925
  Eigenvalues:   332.2261   340.0076   341.3925
  Eigenvectors:
     (1)  -0.151117   0.988516   0.000000
     (2)   0.988516   0.151117  -0.000003
     (3)   0.000003   0.000000   1.000000
```

**Table S33. Atomic Coordinates of the Optimized Structure of 14**




| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | O | 3.267614 | -1.329228 | 0.000000 |
| 2 | O | 3.267462 | 1.329061 | 0.000000 |
| 3 | C | -5.114141 | 8.007291 | 0.000000 |
| 4 | H | -5.526563 | 7.508075 | 0.884899 |
| 5 | H | -5.487008 | 9.039777 | 0.000000 |
| 6 | H | -5.526563 | 7.508075 | -0.884899 |
| 7 | C | -2.610083 | 8.922928 | 1.545428 |
| 8 | H | -2.922692 | 8.422254 | 2.469509 |
| 9 | H | -1.517862 | 9.013097 | 1.572120 |
| 10 | H | -3.025833 | 9.938674 | 1.563537 |
| 11 | C | -2.610083 | 8.922928 | -1.545428 |
| 12 | H | -2.922692 | 8.422254 | -2.469509 |
| 13 | H | -3.025833 | 9.938674 | -1.563537 |
| 14 | H | -1.517862 | 9.013097 | -1.572120 |
| 15 | C | -3.221271 | 4.874430 | -1.546826 |
| 16 | H | -2.825729 | 5.304732 | -2.474248 |
| 17 | H | -3.002293 | 3.800444 | -1.560248 |
| 18 | H | -4.312091 | 4.989555 | -1.567172 |
| 19 | C | -3.221271 | 4.874430 | 1.546826 |
| 20 | H | -3.002293 | 3.800444 | 1.560248 |
| 21 | H | -2.825729 | 5.304732 | 2.474248 |
| 22 | H | -4.312091 | 4.989555 | 1.567172 |
| 23 | C | 0.604594 | 6.361392 | 1.545827 |
| 24 | H | 0.317559 | 7.419389 | 1.566832 |
| 25 | H | 0.243602 | 5.902230 | 2.473408 |
| 26 | H | 1.700234 | 6.317067 | 1.559830 |
| 27 | C | 0.604594 | 6.361392 | -1.545827 |
| 28 | H | 0.243602 | 5.902230 | -2.473408 |
| 29 | H | 0.317559 | 7.419389 | -1.566832 |
| 30 | H | 1.700234 | 6.317067 | -1.559830 |
| 31 | C | -0.052567 | 2.302977 | -1.548316 |
| 32 | H | -1.147279 | 2.243496 | -1.542303 |
| 33 | H | 0.247377 | 2.805945 | -2.474963 |
| 34 | H | 0.336584 | 1.278279 | -1.584337 |
| 35 | C | -0.052567 | 2.302977 | 1.548316 |
| 36 | H | 0.247377 | 2.805945 | 2.474963 |
| 37 | H | -1.147279 | 2.243496 | 1.542303 |
| 38 | H | 0.336584 | 1.278279 | 1.584337 |
| 39 | C | 3.781760 | 3.734089 | 1.535346 |
| 40 | H | 3.638969 | 4.821255 | 1.563919 |

| | | | | |
|---|---|---|---|---|
| 41 | H | 3.365983 | 3.319311 | 2.460615 |
| 42 | H | 4.862505 | 3.542647 | 1.540902 |
| 43 | C | 3.781760 | 3.734089 | -1.535346 |
| 44 | H | 3.365983 | 3.319311 | -2.460615 |
| 45 | H | 3.638969 | 4.821255 | -1.563919 |
| 46 | H | 4.862505 | 3.542647 | -1.540902 |
| 47 | C | 5.304015 | 0.000000 | -1.553877 |
| 48 | H | 4.677520 | 0.000000 | -2.453249 |
| 49 | H | 5.950024 | 0.885274 | -1.597855 |
| 50 | H | 5.950090 | -0.885189 | -1.597857 |
| 51 | C | 5.304015 | 0.000000 | 1.553877 |
| 52 | H | 5.950024 | 0.885274 | 1.597855 |
| 53 | H | 4.677520 | 0.000000 | 2.453249 |
| 54 | H | 5.950090 | -0.885189 | 1.597857 |
| 55 | C | 3.781811 | -3.734261 | 1.535346 |
| 56 | H | 4.862563 | -3.542854 | 1.540895 |
| 57 | H | 3.366052 | -3.319463 | 2.460615 |
| 58 | H | 3.638984 | -4.821422 | 1.563926 |
| 59 | C | 3.781811 | -3.734261 | -1.535346 |
| 60 | H | 3.366052 | -3.319463 | -2.460615 |
| 61 | H | 4.862563 | -3.542854 | -1.540895 |
| 62 | H | 3.638984 | -4.821422 | -1.563926 |
| 63 | C | -0.052455 | -2.302985 | -1.548314 |
| 64 | H | 0.247482 | -2.805952 | -2.474964 |
| 65 | H | -1.147165 | -2.243465 | -1.542313 |
| 66 | H | 0.336733 | -1.278301 | -1.584317 |
| 67 | C | -0.052455 | -2.302985 | 1.548314 |
| 68 | H | -1.147165 | -2.243465 | 1.542313 |
| 69 | H | 0.247482 | -2.805952 | 2.474964 |
| 70 | H | 0.336733 | -1.278301 | 1.584317 |
| 71 | C | 0.604529 | -6.361434 | 1.545826 |
| 72 | H | 1.700172 | -6.317176 | 1.559809 |
| 73 | H | 0.243582 | -5.902238 | 2.473408 |
| 74 | H | 0.317428 | -7.419412 | 1.566848 |
| 75 | C | 0.604529 | -6.361434 | -1.545826 |
| 76 | H | 0.243582 | -5.902238 | -2.473408 |
| 77 | H | 1.700172 | -6.317176 | -1.559809 |
| 78 | H | 0.317428 | -7.419412 | -1.566848 |
| 79 | C | -3.221271 | -4.874311 | -1.546826 |
| 80 | H | -3.002236 | -3.800337 | -1.560250 |
| 81 | H | -2.825752 | -5.304635 | -2.474248 |
| 82 | H | -4.312098 | -4.989378 | -1.567172 |
| 83 | C | -3.221271 | -4.874311 | 1.546826 |
| 84 | H | -2.825752 | -5.304635 | 2.474248 |
| 85 | H | -3.002236 | -3.800337 | 1.560250 |
| 86 | H | -4.312098 | -4.989378 | 1.567172 |
| 87 | C | -2.610255 | -8.922836 | 1.545428 |
| 88 | H | -1.518041 | -9.013089 | 1.572091 |
| 89 | H | -2.922800 | -8.422123 | 2.469510 |
| 90 | H | -3.026084 | -9.938549 | 1.563564 |
| 91 | C | -2.610255 | -8.922836 | -1.545428 |
| 92 | H | -2.922800 | -8.422123 | -2.469510 |
| 93 | H | -1.518041 | -9.013089 | -1.572091 |
| 94 | H | -3.026084 | -9.938549 | -1.563564 |
| 95 | C | -5.114280 | -8.007106 | 0.000000 |
| 96 | H | -5.526684 | -7.507876 | -0.884899 |
| 97 | H | -5.487180 | -9.039579 | 0.000000 |
| 98 | H | -5.526684 | -7.507876 | 0.884899 |
| 99 | Si | -3.207751 | -7.983874 | 0.000000 |
| 100 | Si | -2.475955 | -5.722016 | 0.000000 |
| 101 | Si | -0.106301 | -5.483639 | 0.000000 |
| 102 | Si | 0.608161 | -3.210788 | 0.000000 |
| 103 | Si | 2.969415 | -2.975135 | 0.000000 |
| 104 | Si | 4.244356 | 0.000000 | 0.000000 |
| 105 | Si | 2.969339 | 2.974987 | 0.000000 |
| 106 | Si | 0.608095 | 3.210742 | 0.000000 |

```
  107          Si          -0.106266     5.483624     0.000000
  108          Si          -2.475913     5.722099     0.000000
  109          Si          -3.207614     7.983989     0.000000
 ---------------------------------------------------------------
```

**Table S34. Magnetic Shielding Tensors of $^{29}$Si Nuclei of 14 Calculated by the GIAO Method**

```
SCF GIAO Magnetic shielding tensor (ppm):
 99  Si    Isotropic =   340.5795   Anisotropy =     7.1781
   XX=   340.3860   YX=    -6.1928   ZX=     0.0000
   XY=    -5.2102   YY=   335.9875   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=   345.3648
   Eigenvalues:   332.0758   344.2977   345.3648
   Eigenvectors:
      (1)   0.565736   0.824586   0.000000
      (2)   0.824586  -0.565736   0.000000
      (3)   0.000000   0.000000   1.000000
100  Si    Isotropic =   360.0235   Anisotropy =    18.5700
   XX=   361.5220   YX=   -14.4702   ZX=     0.0000
   XY=   -14.5251   YY=   353.0878   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=   365.4605
   Eigenvalues:   342.2064   365.4605   372.4034
   Eigenvectors:
      (1)   0.600289   0.799783   0.000000
      (2)   0.000000   0.000000   1.000000
      (3)   0.799783  -0.600289   0.000000
101  Si    Isotropic =   363.9988   Anisotropy =    19.2272
   XX=   357.8166   YX=   -17.0724   ZX=     0.0000
   XY=   -16.9133   YY=   361.6194   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=   372.5602
   Eigenvalues:   342.6192   372.5602   376.8169
   Eigenvectors:
      (1)   0.745385   0.666634   0.000000
      (2)   0.000000   0.000000   1.000000
      (3)  -0.666634   0.745385   0.000000
102  Si    Isotropic =   362.5925   Anisotropy =    21.1069
   XX=   342.5244   YX=   -12.6885   ZX=     0.0000
   XY=   -12.2338   YY=   372.1153   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=   373.1378
   Eigenvalues:   337.9760   373.1378   376.6637
   Eigenvectors:
      (1)   0.939379   0.342881   0.000000
      (2)   0.000000   0.000000   1.000000
      (3)  -0.342881   0.939379   0.000000
103  Si    Isotropic =   318.1557   Anisotropy =    50.6205
   XX=   310.2774   YX=     8.3354   ZX=     0.0000
   XY=     5.7922   YY=   350.7040   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=   293.4857
   Eigenvalues:   293.4857   309.0787   351.9027
   Eigenvectors:
      (1)   0.000000   0.000000   1.000000
      (2)   0.985905  -0.167307   0.000000
      (3)   0.167307   0.985905   0.000000
104  Si    Isotropic =   351.5625   Anisotropy =    30.0066
   XX=   341.1496   YX=    -0.0027   ZX=     0.0000
   XY=    -0.0058   YY=   341.9709   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=   371.5669
   Eigenvalues:   341.1495   341.9709   371.5669
   Eigenvectors:
      (1)   0.999987   0.005140   0.000000
      (2)  -0.005140   0.999987   0.000000
      (3)   0.000000   0.000000   1.000000
```

```
105  Si   Isotropic =   318.1539   Anisotropy =    50.6173
   XX=   310.2761   YX=    -8.3348   ZX=     0.0000
   XY=    -5.7896   YY=   350.7005   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=   293.4851
   Eigenvalues:   293.4851   309.0779   351.8988
   Eigenvectors:
      (1)   0.000000   0.000000   1.000000
      (2)   0.985909   0.167282   0.000000
      (3)  -0.167282   0.985909   0.000000
106  Si   Isotropic =   362.5910   Anisotropy =    21.1087
   XX=   342.5251   YX=    12.6909   ZX=     0.0000
   XY=    12.2352   YY=   372.1136   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=   373.1344
   Eigenvalues:   337.9752   373.1344   376.6635
   Eigenvectors:
      (1)   0.939359  -0.342935   0.000000
      (2)   0.000000   0.000001   1.000000
      (3)   0.342935   0.939359  -0.000001
107  Si   Isotropic =   363.9992   Anisotropy =    19.2280
   XX=   357.8183   YX=    17.0730   ZX=     0.0000
   XY=    16.9141   YY=   361.6184   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=   372.5608
   Eigenvalues:   342.6189   372.5608   376.8178
   Eigenvectors:
      (1)   0.745358  -0.666665   0.000000
      (2)  -0.000001  -0.000002   1.000000
      (3)   0.666665   0.745358   0.000002
108  Si   Isotropic =   360.0219   Anisotropy =    18.5711
   XX=   361.5235   YX=    14.4690   ZX=     0.0000
   XY=    14.5244   YY=   353.0855   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=   365.4567
   Eigenvalues:   342.2063   365.4567   372.4026
   Eigenvectors:
      (1)  -0.600234   0.799824   0.000000
      (2)   0.000001   0.000001   1.000000
      (3)   0.799824   0.600234  -0.000002
109  Si   Isotropic =   340.5806   Anisotropy =     7.1803
   XX=   340.3879   YX=     6.1920   ZX=     0.0000
   XY=     5.2108   YY=   335.9864   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=   345.3674
   Eigenvalues:   332.0757   344.2986   345.3674
   Eigenvectors:
      (1)  -0.565637   0.824654   0.000000
      (2)   0.824654   0.565637  -0.000003
      (3)   0.000002   0.000002   1.000000
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