

Supplementary Information for:

**Quantum Mechanical Investigation of G-Quartet Systems of DNA**

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**Optimized coordinates of the monomeric structure of Fig. 1**

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 7                | 0              | 4.908621                | -5.173767 | 0.055141  |
| 2                | 6                | 0              | 3.817089                | -5.960343 | -0.257634 |
| 3                | 7                | 0              | 2.709757                | -5.276380 | -0.351681 |
| 4                | 6                | 0              | 3.093580                | -3.977436 | -0.086504 |
| 5                | 6                | 0              | 2.319714                | -2.777294 | -0.051981 |
| 6                | 8                | 0              | 1.111217                | -2.657250 | -0.261919 |
| 7                | 7                | 0              | 3.105273                | -1.670115 | 0.255409  |
| 8                | 6                | 0              | 4.462317                | -1.696199 | 0.497631  |
| 9                | 7                | 0              | 5.029954                | -0.520132 | 0.810310  |
| 10               | 7                | 0              | 5.194464                | -2.797898 | 0.460815  |
| 11               | 6                | 0              | 4.457365                | -3.887128 | 0.167940  |
| 12               | 1                | 0              | 3.913068                | -7.033429 | -0.401995 |
| 13               | 1                | 0              | 2.634134                | -0.758517 | 0.274315  |
| 14               | 1                | 0              | 4.512995                | 0.349748  | 0.689755  |
| 15               | 1                | 0              | 6.039228                | -0.495528 | 0.842592  |
| 16               | 7                | 0              | 5.195382                | 4.877374  | -0.148573 |
| 17               | 6                | 0              | 5.981417                | 3.787156  | 0.170011  |
| 18               | 7                | 0              | 5.290853                | 2.689401  | 0.315183  |
| 19               | 6                | 0              | 3.987808                | 3.078544  | 0.078657  |
| 20               | 6                | 0              | 2.779910                | 2.315810  | 0.099564  |
| 21               | 8                | 0              | 2.653616                | 1.115270  | 0.347529  |
| 22               | 7                | 0              | 1.671844                | 3.103055  | -0.200467 |
| 23               | 6                | 0              | 1.702859                | 4.452837  | -0.478855 |
| 24               | 7                | 0              | 0.523590                | 5.024147  | -0.769577 |
| 25               | 7                | 0              | 2.811641                | 5.175484  | -0.491689 |
| 26               | 6                | 0              | 3.902059                | 4.435836  | -0.210407 |
| 27               | 1                | 0              | 7.059389                | 3.876323  | 0.277790  |
| 28               | 1                | 0              | 0.756790                | 2.638081  | -0.189126 |
| 29               | 1                | 0              | -0.347960               | 4.514977  | -0.631479 |
| 30               | 1                | 0              | 0.507580                | 6.031279  | -0.841913 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 31 | 7 | 0 | -4.896731 | 5.178441  | 0.086300  |
| 32 | 6 | 0 | -3.804161 | 5.965763  | -0.221048 |
| 33 | 7 | 0 | -2.699777 | 5.279484  | -0.331072 |
| 34 | 6 | 0 | -3.086672 | 3.978147  | -0.082235 |
| 35 | 6 | 0 | -2.316520 | 2.775328  | -0.066019 |
| 36 | 8 | 0 | -1.109285 | 2.653480  | -0.282616 |
| 37 | 7 | 0 | -3.103890 | 1.666971  | 0.231243  |
| 38 | 6 | 0 | -4.460138 | 1.693797  | 0.478726  |
| 39 | 7 | 0 | -5.030681 | 0.515531  | 0.772952  |
| 40 | 7 | 0 | -5.188983 | 2.798495  | 0.459881  |
| 41 | 6 | 0 | -4.449542 | 3.888796  | 0.178224  |
| 42 | 1 | 0 | -3.897062 | 7.041243  | -0.348787 |
| 43 | 1 | 0 | -2.634341 | 0.754412  | 0.242700  |
| 44 | 1 | 0 | -4.512717 | -0.354394 | 0.658593  |
| 45 | 1 | 0 | -6.038918 | 0.493278  | 0.823892  |
| 46 | 7 | 0 | -5.200957 | -4.877023 | -0.159355 |
| 47 | 6 | 0 | -5.990474 | -3.785882 | 0.147801  |
| 48 | 7 | 0 | -5.301378 | -2.688016 | 0.298109  |
| 49 | 6 | 0 | -3.995824 | -3.078049 | 0.077220  |
| 50 | 6 | 0 | -2.788585 | -2.315502 | 0.108534  |
| 51 | 8 | 0 | -2.665850 | -1.113571 | 0.352096  |
| 52 | 7 | 0 | -1.676409 | -3.102941 | -0.173477 |
| 53 | 6 | 0 | -1.703841 | -4.454062 | -0.447040 |
| 54 | 7 | 0 | -0.521065 | -5.027899 | -0.712140 |
| 55 | 7 | 0 | -2.813199 | -5.176237 | -0.473372 |
| 56 | 6 | 0 | -3.906806 | -4.436093 | -0.207314 |
| 57 | 1 | 0 | -7.069581 | -3.874526 | 0.244161  |
| 58 | 1 | 0 | -0.762180 | -2.636794 | -0.155451 |
| 59 | 1 | 0 | 0.350340  | -4.513113 | -0.595842 |
| 60 | 1 | 0 | -0.505544 | -6.032627 | -0.809087 |
| 61 | 1 | 0 | 5.498039  | 5.828890  | -0.311573 |
| 62 | 1 | 0 | 5.866962  | -5.471891 | 0.181490  |
| 63 | 1 | 0 | -5.502101 | -5.828888 | -0.322891 |
| 64 | 1 | 0 | -5.853195 | 5.478071  | 0.222943  |

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# Optimized coordinates of the monomeric structure of Fig. 2

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 7                | 0              | 7.253258                | 1.348726  | -0.219839 |
| 2                | 6                | 0              | 6.761853                | 2.610860  | 0.049661  |
| 3                | 7                | 0              | 5.475494                | 2.618054  | 0.269665  |
| 4                | 6                | 0              | 5.104140                | 1.294997  | 0.137872  |
| 5                | 6                | 0              | 3.817742                | 0.680952  | 0.256897  |
| 6                | 8                | 0              | 2.751218                | 1.234897  | 0.527168  |
| 7                | 7                | 0              | 3.876804                | -0.691272 | 0.023169  |
| 8                | 6                | 0              | 5.020184                | -1.391120 | -0.275657 |
| 9                | 7                | 0              | 4.878142                | -2.711764 | -0.507403 |
| 10               | 7                | 0              | 6.221641                | -0.844560 | -0.375316 |
| 11               | 6                | 0              | 6.191340                | 0.486840  | -0.169781 |
| 12               | 1                | 0              | 7.411239                | 3.482192  | 0.066872  |
| 13               | 1                | 0              | 2.965280                | -1.186176 | 0.005979  |
| 14               | 1                | 0              | 4.064181                | -3.245794 | -0.184035 |
| 15               | 1                | 0              | 5.751732                | -3.211418 | -0.609300 |
| 16               | 7                | 0              | 1.382587                | -6.404994 | 0.425208  |
| 17               | 6                | 0              | 2.665422                | -5.908677 | 0.478385  |
| 18               | 7                | 0              | 2.709664                | -4.618003 | 0.279602  |
| 19               | 6                | 0              | 1.393586                | -4.249545 | 0.086916  |
| 20               | 6                | 0              | 0.814579                | -2.962309 | -0.162075 |
| 21               | 8                | 0              | 1.376012                | -1.875459 | -0.259511 |
| 22               | 7                | 0              | -0.572637               | -3.053775 | -0.295568 |
| 23               | 6                | 0              | -1.313709               | -4.212931 | -0.215447 |
| 24               | 7                | 0              | -2.630807               | -4.090808 | -0.421679 |
| 25               | 7                | 0              | -0.789237               | -5.405309 | 0.030310  |
| 26               | 6                | 0              | 0.547655                | -5.348809 | 0.170189  |
| 27               | 1                | 0              | 3.521618                | -6.550464 | 0.667620  |
| 28               | 1                | 0              | -1.075884               | -2.170444 | -0.436077 |
| 29               | 1                | 0              | -3.058045               | -3.171738 | -0.532304 |
| 30               | 1                | 0              | -3.206514               | -4.906732 | -0.274447 |
| 31               | 7                | 0              | -7.254504               | -1.348600 | 0.213292  |
| 32               | 6                | 0              | -6.762956               | -2.611188 | -0.053901 |
| 33               | 7                | 0              | -5.476266               | -2.618933 | -0.271897 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 34 | 6 | 0 | -5.104809 | -1.295806 | -0.141050 |
| 35 | 6 | 0 | -3.818071 | -0.682273 | -0.258706 |
| 36 | 8 | 0 | -2.751316 | -1.236762 | -0.526858 |
| 37 | 7 | 0 | -3.877081 | 0.690187  | -0.026329 |
| 38 | 6 | 0 | -5.020737 | 1.390669  | 0.269984  |
| 39 | 7 | 0 | -4.878732 | 2.711423  | 0.500516  |
| 40 | 7 | 0 | -6.222558 | 0.844570  | 0.368143  |
| 41 | 6 | 0 | -6.192285 | -0.487034 | 0.163998  |
| 42 | 1 | 0 | -7.412542 | -3.482372 | -0.071133 |
| 43 | 1 | 0 | -2.965535 | 1.184872  | -0.007802 |
| 44 | 1 | 0 | -4.063361 | 3.245101  | 0.180273  |
| 45 | 1 | 0 | -5.752095 | 3.211622  | 0.601489  |
| 46 | 7 | 0 | -1.380613 | 6.407055  | -0.417048 |
| 47 | 6 | 0 | -2.663725 | 5.911581  | -0.471664 |
| 48 | 7 | 0 | -2.708774 | 4.620546  | -0.275503 |
| 49 | 6 | 0 | -1.392948 | 4.250911  | -0.083244 |
| 50 | 6 | 0 | -0.814741 | 2.962797  | 0.163028  |
| 51 | 8 | 0 | -1.376894 | 1.876083  | 0.257623  |
| 52 | 7 | 0 | 0.572475  | 3.053199  | 0.297458  |
| 53 | 6 | 0 | 1.314217  | 4.212141  | 0.220088  |
| 54 | 7 | 0 | 2.631144  | 4.088857  | 0.426697  |
| 55 | 7 | 0 | 0.790502  | 5.405319  | -0.023437 |
| 56 | 6 | 0 | -0.546372 | 5.349879  | -0.163904 |
| 57 | 1 | 0 | -3.519507 | 6.554285  | -0.659676 |
| 58 | 1 | 0 | 1.075217  | 2.169340  | 0.436472  |
| 59 | 1 | 0 | 3.057742  | 3.169264  | 0.535500  |
| 60 | 1 | 0 | 3.207437  | 4.904620  | 0.280882  |
| 61 | 1 | 0 | 1.090012  | -7.365929 | 0.545051  |
| 62 | 1 | 0 | 8.209817  | 1.091501  | -0.425057 |
| 63 | 1 | 0 | -1.087415 | 7.368096  | -0.534502 |
| 64 | 1 | 0 | -8.211263 | -1.090933 | 0.416992  |

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**Partially optimized (only Guanines) coordinates of the dimeric structure of Fig. 8**

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 9.111195                | -4.580840 | 2.682474  |
| 2                | 8                | 0              | 7.753694                | -4.191166 | 2.977222  |
| 3                | 6                | 0              | 9.391850                | -4.146339 | 1.248035  |
| 4                | 8                | 0              | 10.192810               | -5.107829 | 0.535042  |
| 5                | 6                | 0              | 8.028394                | -3.981939 | 0.623141  |
| 6                | 6                | 0              | 7.011085                | -4.150741 | 1.740608  |
| 7                | 7                | 0              | 6.040663                | -3.099489 | 1.830557  |
| 8                | 6                | 0              | 6.324317                | -1.776322 | 1.984207  |
| 9                | 7                | 0              | 5.247333                | -1.031309 | 1.947192  |
| 10               | 6                | 0              | 4.204815                | -1.916613 | 1.762451  |
| 11               | 6                | 0              | 2.804453                | -1.701205 | 1.669883  |
| 12               | 8                | 0              | 2.209581                | -0.615264 | 1.685999  |
| 13               | 7                | 0              | 2.109236                | -2.895723 | 1.548643  |
| 14               | 6                | 0              | 2.692466                | -4.140638 | 1.457191  |
| 15               | 7                | 0              | 1.879973                | -5.188139 | 1.256852  |
| 16               | 7                | 0              | 3.995900                | -4.354161 | 1.540168  |
| 17               | 6                | 0              | 4.684630                | -3.217296 | 1.697820  |
| 18               | 1                | 0              | 9.214544                | -5.642214 | 2.770246  |
| 19               | 1                | 0              | 9.897048                | -3.175252 | 1.258267  |
| 20               | 1                | 0              | 7.938786                | -2.974855 | 0.194133  |
| 21               | 1                | 0              | 7.875678                | -4.757113 | -0.138127 |
| 22               | 1                | 0              | 6.489433                | -5.099324 | 1.608131  |
| 23               | 1                | 0              | 7.341201                | -1.424046 | 2.137802  |
| 24               | 1                | 0              | 1.094649                | -2.805578 | 1.387626  |
| 25               | 1                | 0              | 0.859991                | -5.153511 | 1.299953  |
| 26               | 1                | 0              | 2.336371                | -6.090254 | 1.208207  |
| 27               | 15               | 0              | 9.970386                | -6.697674 | 0.694351  |
| 28               | 8                | 0              | 9.881317                | -7.018800 | 2.136948  |
| 29               | 8                | 0              | 10.969898               | -7.388593 | -0.151151 |
| 30               | 8                | 0              | 8.519783                | -6.923165 | 0.038076  |
| 31               | 6                | 0              | 8.394282                | -7.147338 | -1.370178 |
| 32               | 6                | 0              | 7.121108                | -7.902375 | -1.724592 |
| 33               | 8                | 0              | 5.948373                | -7.252554 | -1.170517 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 34 | 6 | 0 | 6.940469  | -7.991243 | -3.236621 |
| 35 | 8 | 0 | 6.982815  | -9.358103 | -3.695084 |
| 36 | 6 | 0 | 5.595653  | -7.359136 | -3.527572 |
| 37 | 6 | 0 | 4.955440  | -7.023926 | -2.201691 |
| 38 | 7 | 0 | 4.554864  | -5.644606 | -2.039855 |
| 39 | 6 | 0 | 5.411512  | -4.575274 | -1.880588 |
| 40 | 7 | 0 | 4.785374  | -3.446601 | -1.663965 |
| 41 | 6 | 0 | 3.451570  | -3.797391 | -1.665572 |
| 42 | 6 | 0 | 2.291717  | -2.998794 | -1.470430 |
| 43 | 8 | 0 | 2.238060  | -1.783681 | -1.279140 |
| 44 | 7 | 0 | 1.128426  | -3.776842 | -1.497941 |
| 45 | 6 | 0 | 1.097296  | -5.141208 | -1.681101 |
| 46 | 7 | 0 | -0.098287 | -5.753933 | -1.587391 |
| 47 | 7 | 0 | 2.162419  | -5.882979 | -1.906103 |
| 48 | 6 | 0 | 3.293987  | -5.160613 | -1.877791 |
| 49 | 1 | 0 | 9.224654  | -7.757305 | -1.711236 |
| 50 | 1 | 0 | 8.416528  | -6.176650 | -1.881488 |
| 51 | 1 | 0 | 7.196299  | -8.906355 | -1.314676 |
| 52 | 1 | 0 | 7.735491  | -7.421159 | -3.727093 |
| 53 | 1 | 0 | 5.725197  | -6.434299 | -4.109743 |
| 54 | 1 | 0 | 4.966151  | -8.079375 | -4.059130 |
| 55 | 1 | 0 | 4.111102  | -7.690261 | -2.048705 |
| 56 | 1 | 0 | 6.489058  | -4.708201 | -1.927641 |
| 57 | 1 | 0 | 0.261491  | -3.244601 | -1.366885 |
| 58 | 1 | 0 | -0.958131 | -5.210588 | -1.660056 |
| 59 | 1 | 0 | -0.094206 | -6.717288 | -1.897964 |
| 60 | 6 | 0 | -8.053521 | -4.379331 | -3.038398 |
| 61 | 8 | 0 | -6.749374 | -5.003127 | -2.984023 |
| 62 | 6 | 0 | -8.388937 | -3.887941 | -1.626134 |
| 63 | 8 | 0 | -9.345644 | -4.751509 | -0.997787 |
| 64 | 6 | 0 | -7.088496 | -3.929921 | -0.884486 |
| 65 | 6 | 0 | -6.188938 | -4.869410 | -1.658820 |
| 66 | 7 | 0 | -4.821329 | -4.338723 | -1.764610 |
| 67 | 6 | 0 | -3.711301 | -5.062805 | -1.681061 |
| 68 | 7 | 0 | -2.566168 | -4.320766 | -1.723988 |
| 69 | 6 | 0 | -2.976635 | -3.069350 | -1.802841 |
| 70 | 6 | 0 | -2.207801 | -1.814620 | -1.811071 |
| 71 | 8 | 0 | -1.006667 | -1.736690 | -1.877290 |
| 72 | 7 | 0 | -3.040366 | -0.694393 | -1.709895 |
| 73 | 6 | 0 | -4.394566 | -0.743421 | -1.740674 |

|     |    |   |            |           |           |
|-----|----|---|------------|-----------|-----------|
| 74  | 7  | 0 | -5.113449  | 0.345330  | -1.654149 |
| 75  | 7  | 0 | -5.121875  | -1.921373 | -1.861739 |
| 76  | 6  | 0 | -4.403688  | -2.999666 | -1.831874 |
| 77  | 1  | 0 | -8.784398  | -5.092356 | -3.358264 |
| 78  | 1  | 0 | -8.360733  | -3.022796 | -0.997143 |
| 79  | 1  | 0 | -6.650599  | -2.925399 | -0.864517 |
| 80  | 1  | 0 | -7.245837  | -4.317712 | 0.128767  |
| 81  | 1  | 0 | -6.193094  | -5.847391 | -1.174658 |
| 82  | 1  | 0 | -3.747449  | -6.145493 | -1.565617 |
| 83  | 1  | 0 | -2.528999  | 0.245109  | -1.570090 |
| 84  | 1  | 0 | -4.754514  | 1.370592  | -1.518871 |
| 85  | 1  | 0 | -6.118671  | 0.193080  | -1.697571 |
| 86  | 15 | 0 | -9.143629  | -6.355456 | -0.998720 |
| 87  | 8  | 0 | -9.004413  | -6.802104 | -2.402696 |
| 88  | 8  | 0 | -10.190791 | -6.950984 | -0.140057 |
| 89  | 8  | 0 | -7.719749  | -6.552127 | -0.264425 |
| 90  | 6  | 0 | -7.645804  | -6.742140 | 1.157782  |
| 91  | 6  | 0 | -6.485240  | -7.636655 | 1.576900  |
| 92  | 8  | 0 | -5.230362  | -7.169569 | 1.021125  |
| 93  | 6  | 0 | -6.330666  | -7.658388 | 3.100591  |
| 94  | 8  | 0 | -6.562569  | -8.970762 | 3.634240  |
| 95  | 6  | 0 | -4.917724  | -7.229259 | 3.352568  |
| 96  | 6  | 0 | -4.211293  | -7.311599 | 2.024324  |
| 97  | 7  | 0 | -3.157902  | -6.379922 | 1.743724  |
| 98  | 6  | 0 | -1.820177  | -6.685751 | 1.713670  |
| 99  | 7  | 0 | -1.059763  | -5.644799 | 1.472990  |
| 100 | 6  | 0 | -1.940996  | -4.614697 | 1.328830  |
| 101 | 6  | 0 | -1.686099  | -3.222640 | 1.107929  |
| 102 | 8  | 0 | -0.596473  | -2.704817 | 0.900655  |
| 103 | 7  | 0 | -2.861788  | -2.476704 | 1.125708  |
| 104 | 6  | 0 | -4.122948  | -3.004557 | 1.280801  |
| 105 | 7  | 0 | -5.154942  | -2.157760 | 1.226137  |
| 106 | 7  | 0 | -4.383102  | -4.304298 | 1.447675  |
| 107 | 6  | 0 | -3.266257  | -5.036631 | 1.494610  |
| 108 | 1  | 0 | -8.550980  | -7.223527 | 1.502032  |
| 109 | 1  | 0 | -7.549304  | -5.757638 | 1.635953  |
| 110 | 1  | 0 | -6.665365  | -8.650208 | 1.224032  |
| 111 | 1  | 0 | -7.018781  | -6.941317 | 3.555849  |
| 112 | 1  | 0 | -4.905910  | -6.191944 | 3.712038  |
| 113 | 1  | 0 | -4.446937  | -7.907739 | 4.068756  |

|     |    |   |            |           |           |
|-----|----|---|------------|-----------|-----------|
| 114 | 1  | 0 | -3.752415  | -8.297400 | 1.925535  |
| 115 | 1  | 0 | -1.470783  | -7.702424 | 1.882196  |
| 116 | 1  | 0 | -2.681654  | -1.421245 | 1.119810  |
| 117 | 1  | 0 | -5.043434  | -1.124694 | 1.426599  |
| 118 | 1  | 0 | -6.045017  | -2.594395 | 1.446263  |
| 119 | 6  | 0 | -8.633804  | 3.945885  | 3.251402  |
| 120 | 8  | 0 | -7.286207  | 3.553889  | 3.581354  |
| 121 | 6  | 0 | -8.779028  | 3.817606  | 1.736817  |
| 122 | 8  | 0 | -9.476404  | 4.933529  | 1.180762  |
| 123 | 6  | 0 | -7.364475  | 3.746178  | 1.211712  |
| 124 | 6  | 0 | -6.451765  | 3.689920  | 2.411128  |
| 125 | 7  | 0 | -5.552712  | 2.564197  | 2.349312  |
| 126 | 6  | 0 | -5.955307  | 1.273002  | 2.151920  |
| 127 | 7  | 0 | -4.963848  | 0.481390  | 1.825058  |
| 128 | 6  | 0 | -3.853858  | 1.297704  | 1.807943  |
| 129 | 6  | 0 | -2.485689  | 1.006588  | 1.557371  |
| 130 | 8  | 0 | -1.974549  | -0.060899 | 1.210175  |
| 131 | 7  | 0 | -1.687907  | 2.126155  | 1.752246  |
| 132 | 6  | 0 | -2.150318  | 3.383311  | 2.060035  |
| 133 | 7  | 0 | -1.224576  | 4.367772  | 2.132728  |
| 134 | 7  | 0 | -3.418883  | 3.681977  | 2.231764  |
| 135 | 6  | 0 | -4.209882  | 2.600610  | 2.129771  |
| 136 | 1  | 0 | -8.802542  | 4.959501  | 3.549747  |
| 137 | 1  | 0 | -9.313186  | 2.890169  | 1.500112  |
| 138 | 1  | 0 | -7.225040  | 2.839422  | 0.604276  |
| 139 | 1  | 0 | -7.141769  | 4.649566  | 0.629873  |
| 140 | 1  | 0 | -5.891699  | 4.623727  | 2.476319  |
| 141 | 1  | 0 | -6.995558  | 0.981002  | 2.273344  |
| 142 | 1  | 0 | -0.681135  | 1.959538  | 1.671287  |
| 143 | 1  | 0 | -0.307363  | 4.131053  | 2.500107  |
| 144 | 1  | 0 | -1.600738  | 5.232277  | 2.508522  |
| 145 | 15 | 0 | -9.389675  | 5.243944  | -0.398662 |
| 146 | 8  | 0 | -10.765058 | 5.297580  | -0.942568 |
| 147 | 8  | 0 | -8.396060  | 4.334411  | -1.010633 |
| 148 | 8  | 0 | -8.781230  | 6.733552  | -0.407963 |
| 149 | 6  | 0 | -8.327110  | 7.308896  | -1.631741 |
| 150 | 6  | 0 | -6.821372  | 7.576748  | -1.628338 |
| 151 | 8  | 0 | -6.105812  | 6.561460  | -0.903322 |
| 152 | 6  | 0 | -6.229749  | 7.616932  | -3.037960 |
| 153 | 8  | 0 | -6.064358  | 8.961489  | -3.514852 |

|     |   |   |           |           |           |
|-----|---|---|-----------|-----------|-----------|
| 154 | 6 | 0 | -4.907845 | 6.902306  | -2.914071 |
| 155 | 6 | 0 | -4.789833 | 6.464281  | -1.466445 |
| 156 | 7 | 0 | -4.358548 | 5.109840  | -1.254057 |
| 157 | 6 | 0 | -5.128681 | 3.979030  | -1.374386 |
| 158 | 7 | 0 | -4.380759 | 2.894376  | -1.338882 |
| 159 | 6 | 0 | -3.081272 | 3.341768  | -1.188649 |
| 160 | 6 | 0 | -1.834929 | 2.658593  | -1.179791 |
| 161 | 8 | 0 | -1.610046 | 1.453173  | -1.335813 |
| 162 | 7 | 0 | -0.772069 | 3.532485  | -0.955308 |
| 163 | 6 | 0 | -0.874707 | 4.895807  | -0.832799 |
| 164 | 7 | 0 | 0.262977  | 5.572129  | -0.545418 |
| 165 | 7 | 0 | -2.008830 | 5.554251  | -0.957135 |
| 166 | 6 | 0 | -3.058418 | 4.726736  | -1.117026 |
| 167 | 1 | 0 | -8.808751 | 8.258247  | -1.774653 |
| 168 | 1 | 0 | -8.604907 | 6.625711  | -2.445145 |
| 169 | 1 | 0 | -6.633014 | 8.533485  | -1.149193 |
| 170 | 1 | 0 | -6.869372 | 7.059691  | -3.722165 |
| 171 | 1 | 0 | -4.909739 | 6.013715  | -3.561848 |
| 172 | 1 | 0 | -4.083400 | 7.579623  | -3.167942 |
| 173 | 1 | 0 | -4.131886 | 7.146954  | -0.933445 |
| 174 | 1 | 0 | -6.224893 | 4.038007  | -1.444144 |
| 175 | 1 | 0 | 0.133120  | 3.061882  | -0.805716 |
| 176 | 1 | 0 | 1.167434  | 5.146894  | -0.773223 |
| 177 | 1 | 0 | 0.173473  | 6.573814  | -0.672404 |
| 178 | 6 | 0 | 4.680519  | 8.983795  | 2.508146  |
| 179 | 8 | 0 | 4.476593  | 7.623609  | 2.933503  |
| 180 | 6 | 0 | 4.060359  | 9.100942  | 1.119368  |
| 181 | 8 | 0 | 4.784725  | 10.005575 | 0.266169  |
| 182 | 6 | 0 | 4.084360  | 7.695913  | 0.584442  |
| 183 | 6 | 0 | 4.423545  | 6.786827  | 1.755860  |
| 184 | 7 | 0 | 3.428214  | 5.783016  | 2.046704  |
| 185 | 6 | 0 | 2.224337  | 6.068923  | 2.578574  |
| 186 | 7 | 0 | 1.496477  | 4.978621  | 2.860010  |
| 187 | 6 | 0 | 2.273822  | 3.961903  | 2.492559  |
| 188 | 6 | 0 | 2.009997  | 2.530599  | 2.533188  |
| 189 | 8 | 0 | 0.949570  | 2.031823  | 2.846549  |
| 190 | 7 | 0 | 3.131114  | 1.791964  | 2.163924  |
| 191 | 6 | 0 | 4.312078  | 2.342290  | 1.746694  |
| 192 | 7 | 0 | 5.326678  | 1.553045  | 1.482744  |
| 193 | 7 | 0 | 4.533303  | 3.685833  | 1.585378  |

|     |    |   |          |           |           |
|-----|----|---|----------|-----------|-----------|
| 194 | 6  | 0 | 3.522451 | 4.414887  | 1.984395  |
| 195 | 1  | 0 | 5.727280 | 9.200732  | 2.461990  |
| 196 | 1  | 0 | 3.021337 | 9.424074  | 1.209297  |
| 197 | 1  | 0 | 3.094099 | 7.433933  | 0.189960  |
| 198 | 1  | 0 | 4.855933 | 7.608605  | -0.184152 |
| 199 | 1  | 0 | 5.402344 | 6.334680  | 1.591926  |
| 200 | 1  | 0 | 1.917907 | 7.093154  | 2.774770  |
| 201 | 1  | 0 | 2.919031 | 0.744773  | 2.026413  |
| 202 | 1  | 0 | 5.294178 | 0.480487  | 1.693242  |
| 203 | 1  | 0 | 6.165032 | 2.023775  | 1.155436  |
| 204 | 15 | 0 | 6.396956 | 10.049357 | 0.246198  |
| 205 | 8  | 0 | 6.868778 | 10.312829 | 1.624038  |
| 206 | 8  | 0 | 6.821160 | 10.934629 | -0.860226 |
| 207 | 8  | 0 | 6.788006 | 8.538714  | -0.138312 |
| 208 | 6  | 0 | 6.957180 | 8.150727  | -1.508607 |
| 209 | 6  | 0 | 7.467896 | 6.727708  | -1.633093 |
| 210 | 8  | 0 | 6.568875 | 5.799455  | -0.986272 |
| 211 | 6  | 0 | 7.599657 | 6.308467  | -3.095809 |
| 212 | 8  | 0 | 8.976411 | 6.161751  | -3.469322 |
| 213 | 6  | 0 | 6.868060 | 4.992959  | -3.199298 |
| 214 | 6  | 0 | 6.429451 | 4.619864  | -1.800128 |
| 215 | 7  | 0 | 5.064723 | 4.171203  | -1.611212 |
| 216 | 6  | 0 | 3.992928 | 4.994838  | -1.425308 |
| 217 | 7  | 0 | 2.891041 | 4.345824  | -1.092302 |
| 218 | 6  | 0 | 3.266758 | 3.037337  | -1.058523 |
| 219 | 6  | 0 | 2.505104 | 1.863955  | -0.724168 |
| 220 | 8  | 0 | 1.346696 | 1.838960  | -0.333959 |
| 221 | 7  | 0 | 3.265677 | 0.702626  | -0.851987 |
| 222 | 6  | 0 | 4.583569 | 0.665103  | -1.218622 |
| 223 | 7  | 0 | 5.169200 | -0.519752 | -1.338466 |
| 224 | 7  | 0 | 5.331601 | 1.766264  | -1.450893 |
| 225 | 6  | 0 | 4.624318 | 2.887801  | -1.378807 |
| 226 | 1  | 0 | 7.690191 | 8.789418  | -1.978350 |
| 227 | 1  | 0 | 5.994820 | 8.249897  | -2.024436 |
| 228 | 1  | 0 | 8.441731 | 6.663114  | -1.157286 |
| 229 | 1  | 0 | 7.118009 | 7.054299  | -3.738438 |
| 230 | 1  | 0 | 5.982965 | 5.106672  | -3.837304 |
| 231 | 1  | 0 | 7.543589 | 4.224987  | -3.587385 |
| 232 | 1  | 0 | 7.089252 | 3.842579  | -1.414760 |
| 233 | 1  | 0 | 4.085652 | 6.071115  | -1.534573 |

|     |   |   |           |           |           |
|-----|---|---|-----------|-----------|-----------|
| 234 | 1 | 0 | 2.755015  | -0.195413 | -0.758639 |
| 235 | 1 | 0 | 4.684901  | -1.422093 | -1.284223 |
| 236 | 1 | 0 | 6.119794  | -0.521682 | -1.687760 |
| 237 | 1 | 0 | 9.786356  | -4.090385 | 3.352183  |
| 238 | 1 | 0 | 4.195490  | 9.656309  | 3.184440  |
| 239 | 1 | 0 | -6.561970 | -8.930882 | 4.593411  |
| 240 | 1 | 0 | 9.512169  | 6.052571  | -2.680245 |
| 241 | 1 | 0 | 6.984595  | -9.949385 | -2.938789 |
| 242 | 1 | 0 | -5.999832 | 9.560462  | -2.767411 |
| 243 | 1 | 0 | -9.332167 | 3.299829  | 3.741097  |
| 244 | 1 | 0 | -8.032410 | -3.551370 | -3.715845 |

-----

**Partially optimized (only Guanines) coordinates of the dimeric structure of Fig. 9**

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 8.483164                | 5.365499  | -1.913746 |
| 2                | 8                | 0              | 7.150564                | 5.528658  | -2.467902 |
| 3                | 6                | 0              | 8.366470                | 5.477838  | -0.388826 |
| 4                | 8                | 0              | 8.942314                | 6.708661  | 0.067941  |
| 5                | 6                | 0              | 6.886649                | 5.469913  | -0.115365 |
| 6                | 6                | 0              | 6.227397                | 5.871317  | -1.412663 |
| 7                | 7                | 0              | 4.959413                | 5.189441  | -1.634898 |
| 8                | 6                | 0              | 3.762651                | 5.765173  | -1.597386 |
| 9                | 7                | 0              | 2.725534                | 4.893891  | -1.780101 |
| 10               | 6                | 0              | 3.301877                | 3.717782  | -1.909241 |
| 11               | 6                | 0              | 2.706299                | 2.397058  | -2.158249 |
| 12               | 8                | 0              | 1.533139                | 2.215412  | -2.385543 |
| 13               | 7                | 0              | 3.661025                | 1.383152  | -2.129000 |
| 14               | 6                | 0              | 4.994912                | 1.592650  | -1.993051 |
| 15               | 7                | 0              | 5.832430                | 0.592999  | -2.055747 |
| 16               | 7                | 0              | 5.586447                | 2.850756  | -1.824107 |
| 17               | 6                | 0              | 4.733755                | 3.819575  | -1.800794 |
| 18               | 1                | 0              | 9.128189                | 6.133609  | -2.286371 |
| 19               | 1                | 0              | 8.860182                | 4.632450  | 0.104486  |
| 20               | 1                | 0              | 6.554735                | 4.456240  | 0.161499  |
| 21               | 1                | 0              | 6.645804                | 6.200948  | 0.666625  |
| 22               | 1                | 0              | 6.071138                | 6.949647  | -1.414884 |
| 23               | 1                | 0              | 3.642234                | 6.831546  | -1.408124 |
| 24               | 1                | 0              | 3.251437                | 0.356957  | -2.224442 |
| 25               | 1                | 0              | 5.561010                | -0.472862 | -2.045751 |
| 26               | 1                | 0              | 6.803676                | 0.856264  | -1.906765 |
| 27               | 15               | 0              | 8.220197                | 8.114371  | -0.247969 |
| 28               | 8                | 0              | 8.001627                | 8.205024  | -1.709236 |
| 29               | 8                | 0              | 8.963095                | 9.184822  | 0.453787  |
| 30               | 8                | 0              | 6.783782                | 7.944518  | 0.466724  |
| 31               | 6                | 0              | 5.805802                | 8.987885  | 0.387753  |
| 32               | 6                | 0              | 4.654660                | 8.797135  | 1.368132  |
| 33               | 8                | 0              | 3.794281                | 7.699091  | 1.001205  |

|    |   |   |            |           |           |
|----|---|---|------------|-----------|-----------|
| 34 | 6 | 0 | 5.156449   | 8.501241  | 2.774652  |
| 35 | 6 | 0 | 4.121447   | 7.568733  | 3.354221  |
| 36 | 6 | 0 | 3.203621   | 7.167256  | 2.209183  |
| 37 | 7 | 0 | 3.091485   | 5.753070  | 1.990181  |
| 38 | 6 | 0 | 4.192328   | 4.958860  | 1.769633  |
| 39 | 7 | 0 | 3.879110   | 3.772188  | 1.321452  |
| 40 | 6 | 0 | 2.502984   | 3.783714  | 1.253815  |
| 41 | 6 | 0 | 1.610113   | 2.758221  | 0.833285  |
| 42 | 8 | 0 | 1.894705   | 1.634414  | 0.424648  |
| 43 | 7 | 0 | 0.289340   | 3.184079  | 0.906837  |
| 44 | 6 | 0 | -0.118625  | 4.442994  | 1.292235  |
| 45 | 7 | 0 | -1.438538  | 4.678143  | 1.240098  |
| 46 | 7 | 0 | 0.707361   | 5.410930  | 1.658315  |
| 47 | 6 | 0 | 1.989526   | 5.014057  | 1.634409  |
| 48 | 1 | 0 | 5.374615   | 9.005486  | -0.603539 |
| 49 | 1 | 0 | 6.308830   | 9.946360  | 0.587229  |
| 50 | 1 | 0 | 4.058792   | 9.706102  | 1.387599  |
| 51 | 1 | 0 | 6.112279   | 8.021774  | 2.737258  |
| 52 | 1 | 0 | 4.615866   | 6.675286  | 3.758886  |
| 53 | 1 | 0 | 3.544554   | 8.093017  | 4.127552  |
| 54 | 1 | 0 | 2.224910   | 7.627033  | 2.356701  |
| 55 | 1 | 0 | 5.199026   | 5.324131  | 1.951912  |
| 56 | 1 | 0 | -0.421713  | 2.471512  | 0.711681  |
| 57 | 1 | 0 | -2.088225  | 3.897233  | 1.241768  |
| 58 | 1 | 0 | -1.759365  | 5.539750  | 1.663855  |
| 59 | 6 | 0 | -9.857673  | 2.357591  | 2.471734  |
| 60 | 8 | 0 | -8.553327  | 2.713200  | 2.993116  |
| 61 | 6 | 0 | -9.748897  | 2.339894  | 0.942182  |
| 62 | 8 | 0 | -10.672435 | 3.257348  | 0.338474  |
| 63 | 6 | 0 | -8.332775  | 2.744131  | 0.653003  |
| 64 | 6 | 0 | -7.797085  | 3.327258  | 1.936275  |
| 65 | 7 | 0 | -6.370738  | 3.167113  | 2.087148  |
| 66 | 6 | 0 | -5.482020  | 4.191882  | 2.120901  |
| 67 | 7 | 0 | -4.213431  | 3.805994  | 1.954631  |
| 68 | 6 | 0 | -4.298556  | 2.473535  | 1.799045  |
| 69 | 6 | 0 | -3.278058  | 1.505383  | 1.467803  |
| 70 | 8 | 0 | -2.100883  | 1.758182  | 1.265426  |
| 71 | 7 | 0 | -3.788380  | 0.214876  | 1.372692  |
| 72 | 6 | 0 | -5.117939  | -0.096431 | 1.462557  |
| 73 | 7 | 0 | -5.497649  | -1.357437 | 1.337225  |

|     |    |   |            |           |           |
|-----|----|---|------------|-----------|-----------|
| 74  | 7  | 0 | -6.096183  | 0.809655  | 1.674290  |
| 75  | 6  | 0 | -5.639381  | 2.029197  | 1.860345  |
| 76  | 1  | 0 | -10.582017 | 3.083637  | 2.776830  |
| 77  | 1  | 0 | -9.925577  | 1.328518  | 0.565133  |
| 78  | 1  | 0 | -7.745397  | 1.857712  | 0.379911  |
| 79  | 1  | 0 | -8.313199  | 3.497735  | -0.138770 |
| 80  | 1  | 0 | -7.984399  | 4.402151  | 1.944588  |
| 81  | 1  | 0 | -5.817172  | 5.221489  | 2.231440  |
| 82  | 1  | 0 | -3.053837  | -0.527711 | 1.193495  |
| 83  | 1  | 0 | -4.815150  | -2.161102 | 1.490100  |
| 84  | 1  | 0 | -6.493677  | -1.505080 | 1.474019  |
| 85  | 15 | 0 | -10.545608 | 4.847982  | 0.581898  |
| 86  | 8  | 0 | -10.695770 | 5.106296  | 2.031293  |
| 87  | 8  | 0 | -11.430445 | 5.535299  | -0.385577 |
| 88  | 8  | 0 | -9.016727  | 5.157317  | 0.172434  |
| 89  | 6  | 0 | -8.693377  | 5.827330  | -1.057965 |
| 90  | 6  | 0 | -7.564120  | 6.830622  | -0.873126 |
| 91  | 8  | 0 | -6.410647  | 6.199043  | -0.274829 |
| 92  | 6  | 0 | -7.136423  | 7.444956  | -2.199139 |
| 93  | 6  | 0 | -5.712532  | 6.997525  | -2.413492 |
| 94  | 6  | 0 | -5.257343  | 6.332098  | -1.130966 |
| 95  | 7  | 0 | -4.698529  | 4.993200  | -1.263657 |
| 96  | 6  | 0 | -5.367406  | 3.795949  | -1.158412 |
| 97  | 7  | 0 | -4.569698  | 2.757827  | -1.282772 |
| 98  | 6  | 0 | -3.318200  | 3.306384  | -1.474803 |
| 99  | 6  | 0 | -2.054243  | 2.685398  | -1.709984 |
| 100 | 8  | 0 | -1.782834  | 1.490573  | -1.782609 |
| 101 | 7  | 0 | -1.044684  | 3.643444  | -1.868483 |
| 102 | 6  | 0 | -1.221742  | 5.006651  | -1.806489 |
| 103 | 7  | 0 | -0.124064  | 5.769220  | -1.952926 |
| 104 | 7  | 0 | -2.392976  | 5.590149  | -1.634233 |
| 105 | 6  | 0 | -3.381636  | 4.694555  | -1.469666 |
| 106 | 1  | 0 | -9.553871  | 6.382679  | -1.405437 |
| 107 | 1  | 0 | -8.411173  | 5.071561  | -1.805006 |
| 108 | 1  | 0 | -7.908420  | 7.617963  | -0.218586 |
| 109 | 1  | 0 | -7.759984  | 7.086066  | -2.991143 |
| 110 | 1  | 0 | -5.666885  | 6.282743  | -3.236786 |
| 111 | 1  | 0 | -5.084433  | 7.869771  | -2.613475 |
| 112 | 1  | 0 | -4.529075  | 6.973308  | -0.649567 |
| 113 | 1  | 0 | -6.435196  | 3.763583  | -0.962587 |

|     |    |   |           |           |           |
|-----|----|---|-----------|-----------|-----------|
| 114 | 1  | 0 | -0.115759 | 3.252458  | -2.064240 |
| 115 | 1  | 0 | 0.814726  | 5.379474  | -1.892476 |
| 116 | 1  | 0 | -0.258642 | 6.757891  | -1.786182 |
| 117 | 6  | 0 | -7.570056 | -4.805635 | -2.531383 |
| 118 | 8  | 0 | -6.174311 | -5.123167 | -2.757551 |
| 119 | 6  | 0 | -7.805923 | -4.815765 | -1.020922 |
| 120 | 8  | 0 | -8.583554 | -5.959519 | -0.628739 |
| 121 | 6  | 0 | -6.433783 | -4.877528 | -0.417146 |
| 122 | 6  | 0 | -5.530737 | -5.414097 | -1.497542 |
| 123 | 7  | 0 | -4.218806 | -4.772706 | -1.504283 |
| 124 | 6  | 0 | -3.023039 | -5.396894 | -1.623484 |
| 125 | 7  | 0 | -1.991539 | -4.560662 | -1.764883 |
| 126 | 6  | 0 | -2.554501 | -3.335932 | -1.734290 |
| 127 | 6  | 0 | -1.942537 | -2.028106 | -1.870420 |
| 128 | 8  | 0 | -0.764389 | -1.793019 | -2.056024 |
| 129 | 7  | 0 | -2.887150 | -1.000543 | -1.771003 |
| 130 | 6  | 0 | -4.223151 | -1.188798 | -1.599626 |
| 131 | 7  | 0 | -5.019595 | -0.123501 | -1.550589 |
| 132 | 7  | 0 | -4.814647 | -2.405484 | -1.499010 |
| 133 | 6  | 0 | -3.956571 | -3.415357 | -1.574114 |
| 134 | 1  | 0 | -8.311621 | -3.895204 | -0.711848 |
| 135 | 1  | 0 | -6.109707 | -3.867102 | -0.136772 |
| 136 | 1  | 0 | -6.430749 | -5.552041 | 0.441259  |
| 137 | 1  | 0 | -5.445620 | -6.494869 | -1.382059 |
| 138 | 1  | 0 | -2.954497 | -6.482638 | -1.598094 |
| 139 | 1  | 0 | -2.499660 | -0.029593 | -1.790271 |
| 140 | 1  | 0 | -4.710906 | 0.864759  | -1.538811 |
| 141 | 1  | 0 | -6.008454 | -0.320068 | -1.441009 |
| 142 | 15 | 0 | -8.206842 | -7.448541 | -1.133925 |
| 143 | 8  | 0 | -7.935496 | -7.394963 | -2.588445 |
| 144 | 8  | 0 | -9.229932 | -8.381000 | -0.613574 |
| 145 | 8  | 0 | -6.817225 | -7.755505 | -0.375606 |
| 146 | 6  | 0 | -6.806380 | -8.035382 | 1.030913  |
| 147 | 6  | 0 | -5.397129 | -8.241750 | 1.579134  |
| 148 | 8  | 0 | -4.489781 | -7.237138 | 1.085801  |
| 149 | 6  | 0 | -5.376677 | -8.148974 | 3.103344  |
| 150 | 6  | 0 | -4.070998 | -7.463522 | 3.424930  |
| 151 | 6  | 0 | -3.530298 | -6.913709 | 2.116070  |
| 152 | 7  | 0 | -3.287243 | -5.500486 | 2.049181  |
| 153 | 6  | 0 | -4.268677 | -4.556933 | 2.156657  |

|     |   |   |           |           |           |
|-----|---|---|-----------|-----------|-----------|
| 154 | 7 | 0 | -3.842480 | -3.362814 | 1.843066  |
| 155 | 6 | 0 | -2.516829 | -3.526986 | 1.507602  |
| 156 | 6 | 0 | -1.540339 | -2.570159 | 1.107690  |
| 157 | 8 | 0 | -1.695734 | -1.356803 | 0.940017  |
| 158 | 7 | 0 | -0.307044 | -3.159477 | 0.884668  |
| 159 | 6 | 0 | -0.028868 | -4.497705 | 1.050857  |
| 160 | 7 | 0 | 1.242527  | -4.867421 | 0.830470  |
| 161 | 7 | 0 | -0.937299 | -5.403461 | 1.396950  |
| 162 | 6 | 0 | -2.144857 | -4.859154 | 1.619434  |
| 163 | 1 | 0 | -7.351825 | -8.949092 | 1.218873  |
| 164 | 1 | 0 | -7.296854 | -7.201328 | 1.551644  |
| 165 | 1 | 0 | -5.027816 | -9.218863 | 1.266769  |
| 166 | 1 | 0 | -4.238758 | -6.632350 | 4.123895  |
| 167 | 1 | 0 | -3.365270 | -8.196414 | 3.836891  |
| 168 | 1 | 0 | -2.585198 | -7.391661 | 1.884881  |
| 169 | 1 | 0 | -5.276894 | -4.824159 | 2.466524  |
| 170 | 1 | 0 | 0.464287  | -2.523633 | 0.636261  |
| 171 | 1 | 0 | 1.992737  | -4.175799 | 0.807457  |
| 172 | 1 | 0 | 1.489487  | -5.815173 | 1.087127  |
| 173 | 6 | 0 | 6.091721  | -7.570890 | -3.052026 |
| 174 | 8 | 0 | 5.882788  | -6.146865 | -3.242856 |
| 175 | 6 | 0 | 6.337311  | -7.800629 | -1.559039 |
| 176 | 8 | 0 | 7.690039  | -8.217419 | -1.328613 |
| 177 | 6 | 0 | 6.075714  | -6.463626 | -0.932858 |
| 178 | 6 | 0 | 6.275611  | -5.475826 | -2.036894 |
| 179 | 7 | 0 | 5.556577  | -4.220800 | -1.942043 |
| 180 | 6 | 0 | 6.155059  | -2.995608 | -1.877407 |
| 181 | 7 | 0 | 5.296988  | -2.004790 | -1.943923 |
| 182 | 6 | 0 | 4.064909  | -2.616379 | -2.057522 |
| 183 | 6 | 0 | 2.769847  | -2.053319 | -2.209426 |
| 184 | 8 | 0 | 2.458844  | -0.854405 | -2.297431 |
| 185 | 7 | 0 | 1.789684  | -3.025793 | -2.274705 |
| 186 | 6 | 0 | 2.022875  | -4.382217 | -2.226031 |
| 187 | 7 | 0 | 0.946821  | -5.181395 | -2.352544 |
| 188 | 7 | 0 | 3.224477  | -4.921132 | -2.110717 |
| 189 | 6 | 0 | 4.201238  | -4.000909 | -2.044859 |
| 190 | 1 | 0 | 6.943211  | -7.892394 | -3.614609 |
| 191 | 1 | 0 | 5.637708  | -8.544024 | -1.168060 |
| 192 | 1 | 0 | 5.034961  | -6.416451 | -0.588522 |
| 193 | 1 | 0 | 6.783749  | -6.266949 | -0.121785 |

|     |    |   |           |           |           |
|-----|----|---|-----------|-----------|-----------|
| 194 | 1  | 0 | 7.333238  | -5.237853 | -2.099756 |
| 195 | 1  | 0 | 7.232461  | -2.898860 | -1.765914 |
| 196 | 1  | 0 | 0.824482  | -2.669644 | -2.319683 |
| 197 | 1  | 0 | 0.000031  | -4.845457 | -2.164103 |
| 198 | 1  | 0 | 1.132352  | -6.162974 | -2.187141 |
| 199 | 15 | 0 | 8.304181  | -8.246054 | 0.160382  |
| 200 | 8  | 0 | 9.751533  | -8.540852 | 0.056615  |
| 201 | 8  | 0 | 7.437707  | -9.098854 | 1.003041  |
| 202 | 8  | 0 | 8.135698  | -6.715147 | 0.643378  |
| 203 | 6  | 0 | 9.241934  | -5.804578 | 0.564362  |
| 204 | 6  | 0 | 9.175723  | -4.699683 | 1.608137  |
| 205 | 8  | 0 | 8.213329  | -3.685084 | 1.267449  |
| 206 | 6  | 0 | 8.788099  | -5.236590 | 2.975447  |
| 207 | 6  | 0 | 8.013115  | -4.112787 | 3.609058  |
| 208 | 6  | 0 | 7.649155  | -3.153839 | 2.487748  |
| 209 | 7  | 0 | 6.231481  | -3.065101 | 2.220822  |
| 210 | 6  | 0 | 5.408257  | -4.164836 | 2.062887  |
| 211 | 7  | 0 | 4.238948  | -3.869571 | 1.549024  |
| 212 | 6  | 0 | 4.310554  | -2.519084 | 1.326812  |
| 213 | 6  | 0 | 3.313554  | -1.625886 | 0.835184  |
| 214 | 8  | 0 | 2.157459  | -1.910075 | 0.530109  |
| 215 | 7  | 0 | 3.802530  | -0.321602 | 0.723721  |
| 216 | 6  | 0 | 5.063653  | 0.073861  | 1.095523  |
| 217 | 7  | 0 | 5.380320  | 1.384355  | 0.931144  |
| 218 | 7  | 0 | 5.989968  | -0.738780 | 1.575289  |
| 219 | 6  | 0 | 5.551157  | -2.002951 | 1.694349  |
| 220 | 1  | 0 | 9.255285  | -5.326047 | -0.396904 |
| 221 | 1  | 0 | 10.162647 | -6.373598 | 0.689524  |
| 222 | 1  | 0 | 10.156168 | -4.234717 | 1.680630  |
| 223 | 1  | 0 | 8.172285  | -6.105863 | 2.875267  |
| 224 | 1  | 0 | 7.096636  | -4.505534 | 4.069488  |
| 225 | 1  | 0 | 8.641246  | -3.593281 | 4.342730  |
| 226 | 1  | 0 | 8.092057  | -2.180117 | 2.694491  |
| 227 | 1  | 0 | 5.740563  | -5.166171 | 2.333266  |
| 228 | 1  | 0 | 3.104545  | 0.400638  | 0.474646  |
| 229 | 1  | 0 | 4.665591  | 2.121169  | 1.019264  |
| 230 | 1  | 0 | 6.258734  | 1.620897  | 1.383803  |
| 231 | 1  | 0 | -7.790944 | -3.836367 | -2.927146 |
| 232 | 1  | 0 | 8.871653  | 4.404343  | -2.178610 |
| 233 | 1  | 0 | -5.401492 | -9.126818 | 3.537057  |

|     |   |   |            |           |           |
|-----|---|---|------------|-----------|-----------|
| 234 | 1 | 0 | 5.223037   | -8.111371 | -3.365343 |
| 235 | 8 | 0 | -6.478856  | -7.366547 | 3.570153  |
| 236 | 1 | 0 | -6.966304  | -7.020263 | 2.819099  |
| 237 | 1 | 0 | -10.140393 | 1.389007  | 2.827845  |
| 238 | 8 | 0 | -7.200445  | 8.871662  | -2.126272 |
| 239 | 1 | 0 | -7.232498  | 9.236288  | -3.013751 |
| 240 | 1 | 0 | -8.190504  | -5.540098 | -3.000966 |
| 241 | 8 | 0 | 9.955885   | -5.534832 | 3.745011  |
| 242 | 1 | 0 | 10.691313  | -5.713513 | 3.154401  |
| 243 | 8 | 0 | 5.229555   | 9.705414  | 3.542456  |
| 244 | 1 | 0 | 5.255524   | 10.461043 | 2.950890  |

-----

**Partially optimized (only Guanines) coordinates of the dimeric structure of Fig. 10**

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 8.860371                | -5.090613 | 3.294347  |
| 2                | 1                | 0              | 9.173343                | -6.012214 | 3.738870  |
| 3                | 8                | 0              | 7.451744                | -4.854588 | 3.573584  |
| 4                | 6                | 0              | 6.730775                | -4.698589 | 2.361189  |
| 5                | 1                | 0              | 6.227856                | -5.674267 | 2.182025  |
| 6                | 7                | 0              | 5.742774                | -3.622429 | 2.453031  |
| 7                | 6                | 0              | 4.406836                | -3.652338 | 2.123206  |
| 8                | 7                | 0              | 1.551249                | -5.420613 | 1.210271  |
| 9                | 1                | 0              | 0.536343                | -5.323423 | 1.289699  |
| 10               | 1                | 0              | 1.934666                | -6.355696 | 1.276687  |
| 11               | 7                | 0              | 3.671248                | -4.730953 | 1.800505  |
| 12               | 6                | 0              | 2.402459                | -4.438725 | 1.563881  |
| 13               | 7                | 0              | 1.881809                | -3.163829 | 1.622448  |
| 14               | 1                | 0              | 0.895615                | -3.007943 | 1.360031  |
| 15               | 6                | 0              | 2.626430                | -2.022821 | 1.886180  |
| 16               | 8                | 0              | 2.078603                | -0.910912 | 1.828734  |
| 17               | 6                | 0              | 3.984395                | -2.325627 | 2.185446  |
| 18               | 7                | 0              | 5.030792                | -1.489782 | 2.525406  |
| 19               | 6                | 0              | 6.051778                | -2.298931 | 2.675174  |
| 20               | 1                | 0              | 7.055645                | -2.003651 | 2.969837  |
| 21               | 6                | 0              | 7.762194                | -4.439334 | 1.257864  |
| 22               | 1                | 0              | 8.022363                | -3.357954 | 1.181876  |
| 23               | 1                | 0              | 7.399657                | -4.765155 | 0.262410  |
| 24               | 6                | 0              | 8.992967                | -5.171110 | 1.762830  |
| 25               | 1                | 0              | 9.918091                | -4.618827 | 1.464206  |
| 26               | 8                | 0              | 9.029183                | -6.519774 | 1.278299  |
| 27               | 15               | 0              | 9.578905                | -6.814144 | -0.190250 |
| 28               | 8                | 0              | 9.555410                | -5.572718 | -0.999591 |
| 29               | 8                | 0              | 10.884238               | -7.495713 | -0.065212 |
| 30               | 8                | 0              | 8.516414                | -7.856447 | -0.781493 |
| 31               | 6                | 0              | 7.259326                | -7.292156 | -1.169802 |
| 32               | 1                | 0              | 7.437034                | -6.451240 | -1.880440 |
| 33               | 1                | 0              | 6.745471                | -6.877059 | -0.266951 |
| 34               | 6                | 0              | 6.300121                | -8.327594 | -1.829411 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 35 | 1 | 0 | 6.431633  | -9.339245 | -1.391438 |
| 36 | 8 | 0 | 4.928546  | -7.914888 | -1.583323 |
| 37 | 6 | 0 | 4.762465  | -6.863600 | -2.503662 |
| 38 | 1 | 0 | 5.584974  | -6.161893 | -2.322190 |
| 39 | 7 | 0 | 3.557881  | -6.112350 | -2.301521 |
| 40 | 6 | 0 | 3.562952  | -4.802205 | -1.878855 |
| 41 | 7 | 0 | 5.347947  | -1.989530 | -0.853936 |
| 42 | 1 | 0 | 5.207133  | -0.979269 | -0.884606 |
| 43 | 1 | 0 | 6.276205  | -2.324292 | -1.088981 |
| 44 | 7 | 0 | 4.653788  | -4.063529 | -1.589252 |
| 45 | 6 | 0 | 4.354634  | -2.831140 | -1.232483 |
| 46 | 7 | 0 | 3.070219  | -2.342658 | -1.180581 |
| 47 | 1 | 0 | 2.901621  | -1.358867 | -0.937678 |
| 48 | 6 | 0 | 1.913402  | -3.090114 | -1.441937 |
| 49 | 8 | 0 | 0.811276  | -2.564617 | -1.314435 |
| 50 | 6 | 0 | 2.230456  | -4.430110 | -1.826152 |
| 51 | 7 | 0 | 1.410482  | -5.486955 | -2.168940 |
| 52 | 6 | 0 | 2.233203  | -6.467720 | -2.445673 |
| 53 | 1 | 0 | 1.947289  | -7.470802 | -2.752239 |
| 54 | 6 | 0 | 5.085310  | -7.540832 | -3.820512 |
| 55 | 1 | 0 | 5.339122  | -6.808791 | -4.618666 |
| 56 | 1 | 0 | 4.245855  | -8.179004 | -4.151811 |
| 57 | 6 | 0 | 6.322808  | -8.376732 | -3.399468 |
| 58 | 1 | 0 | 7.264977  | -7.867803 | -3.711797 |
| 59 | 8 | 0 | 6.218262  | -9.718914 | -3.862221 |
| 60 | 6 | 0 | -4.441605 | 9.180834  | -2.702599 |
| 61 | 1 | 0 | -5.234373 | 9.245569  | -3.418300 |
| 62 | 8 | 0 | -3.745767 | 7.913737  | -2.838692 |
| 63 | 6 | 0 | -4.021069 | 7.068755  | -1.714515 |
| 64 | 1 | 0 | -4.976985 | 6.552575  | -1.952276 |
| 65 | 7 | 0 | -2.912320 | 6.156787  | -1.575264 |
| 66 | 6 | 0 | -2.925615 | 4.786687  | -1.636617 |
| 67 | 7 | 0 | -4.700491 | 1.834510  | -1.935576 |
| 68 | 1 | 0 | -4.589188 | 0.820274  | -1.931353 |
| 69 | 1 | 0 | -5.633023 | 2.230829  | -1.931850 |
| 70 | 7 | 0 | -4.005858 | 4.008175  | -1.757868 |
| 71 | 6 | 0 | -3.705163 | 2.718360  | -1.790371 |
| 72 | 7 | 0 | -2.419633 | 2.229674  | -1.688649 |
| 73 | 1 | 0 | -2.265388 | 1.210223  | -1.679302 |
| 74 | 6 | 0 | -1.284047 | 3.015102  | -1.518600 |

|     |    |   |           |           |           |
|-----|----|---|-----------|-----------|-----------|
| 75  | 8  | 0 | -0.177742 | 2.479593  | -1.363448 |
| 76  | 6  | 0 | -1.589637 | 4.405294  | -1.534967 |
| 77  | 7  | 0 | -0.765074 | 5.513056  | -1.444845 |
| 78  | 6  | 0 | -1.589805 | 6.532301  | -1.480231 |
| 79  | 1  | 0 | -1.308232 | 7.582290  | -1.486254 |
| 80  | 6  | 0 | -4.248350 | 8.056020  | -0.562736 |
| 81  | 1  | 0 | -3.275863 | 8.444278  | -0.186213 |
| 82  | 1  | 0 | -4.809470 | 7.616569  | 0.280398  |
| 83  | 6  | 0 | -5.010512 | 9.192060  | -1.281444 |
| 84  | 1  | 0 | -4.778593 | 10.174628 | -0.810000 |
| 85  | 8  | 0 | -6.411560 | 8.982934  | -1.334551 |
| 86  | 15 | 0 | -7.428743 | 9.276145  | -0.173593 |
| 87  | 8  | 0 | -6.702049 | 9.425081  | 1.106617  |
| 88  | 8  | 0 | -8.317209 | 10.383377 | -0.591605 |
| 89  | 8  | 0 | -8.269631 | 7.924748  | -0.143133 |
| 90  | 6  | 0 | -7.503404 | 6.720851  | -0.302804 |
| 91  | 1  | 0 | -6.666141 | 6.691543  | 0.438350  |
| 92  | 1  | 0 | -7.086328 | 6.645781  | -1.336008 |
| 93  | 6  | 0 | -8.355490 | 5.490927  | -0.084615 |
| 94  | 1  | 0 | -9.095937 | 5.350047  | -0.906491 |
| 95  | 8  | 0 | -7.442465 | 4.377751  | -0.088335 |
| 96  | 6  | 0 | -7.613962 | 3.634729  | 1.089997  |
| 97  | 1  | 0 | -8.504212 | 2.995063  | 0.869320  |
| 98  | 7  | 0 | -6.548981 | 2.672779  | 1.261127  |
| 99  | 6  | 0 | -5.178352 | 2.782160  | 1.362467  |
| 100 | 7  | 0 | -2.280766 | 4.699805  | 1.677384  |
| 101 | 1  | 0 | -1.324611 | 4.607677  | 1.338544  |
| 102 | 1  | 0 | -2.709358 | 5.611998  | 1.564728  |
| 103 | 7  | 0 | -4.444473 | 3.908128  | 1.497314  |
| 104 | 6  | 0 | -3.149748 | 3.666816  | 1.505674  |
| 105 | 7  | 0 | -2.588977 | 2.415525  | 1.385501  |
| 106 | 1  | 0 | -1.569215 | 2.309888  | 1.386652  |
| 107 | 6  | 0 | -3.307958 | 1.225013  | 1.213097  |
| 108 | 8  | 0 | -2.733771 | 0.156527  | 1.023762  |
| 109 | 6  | 0 | -4.712470 | 1.474352  | 1.260227  |
| 110 | 7  | 0 | -5.742124 | 0.578384  | 1.084968  |
| 111 | 6  | 0 | -6.810062 | 1.326592  | 1.085138  |
| 112 | 1  | 0 | -7.833556 | 0.975238  | 0.974712  |
| 113 | 6  | 0 | -8.096376 | 4.612848  | 2.160658  |
| 114 | 1  | 0 | -7.269556 | 5.258621  | 2.521748  |

|     |    |   |            |           |           |
|-----|----|---|------------|-----------|-----------|
| 115 | 1  | 0 | -8.622588  | 4.128880  | 3.012996  |
| 116 | 6  | 0 | -9.050643  | 5.441383  | 1.287837  |
| 117 | 1  | 0 | -9.162464  | 6.427795  | 1.687070  |
| 118 | 6  | 0 | -8.678609  | -5.170081 | -3.247414 |
| 119 | 1  | 0 | -8.713106  | -6.172844 | -3.619133 |
| 120 | 8  | 0 | -7.355105  | -4.599902 | -3.462769 |
| 121 | 6  | 0 | -6.732441  | -4.357627 | -2.215672 |
| 122 | 1  | 0 | -6.174977  | -5.287446 | -1.965141 |
| 123 | 7  | 0 | -5.785512  | -3.262817 | -2.247919 |
| 124 | 6  | 0 | -4.416858  | -3.342265 | -2.074556 |
| 125 | 7  | 0 | -1.511748  | -5.187171 | -1.797919 |
| 126 | 1  | 0 | -0.482814  | -5.129737 | -1.857645 |
| 127 | 1  | 0 | -1.947593  | -6.101865 | -1.818987 |
| 128 | 7  | 0 | -3.669012  | -4.429608 | -1.960352 |
| 129 | 6  | 0 | -2.346695  | -4.154249 | -1.862542 |
| 130 | 7  | 0 | -1.824008  | -2.895206 | -1.848786 |
| 131 | 1  | 0 | -0.799835  | -2.779696 | -1.671520 |
| 132 | 6  | 0 | -2.572906  | -1.717121 | -1.908109 |
| 133 | 8  | 0 | -2.049537  | -0.619339 | -1.874515 |
| 134 | 6  | 0 | -3.987860  | -1.997513 | -2.034184 |
| 135 | 7  | 0 | -5.027347  | -1.144979 | -2.143871 |
| 136 | 6  | 0 | -6.089532  | -1.933798 | -2.266484 |
| 137 | 1  | 0 | -7.108517  | -1.582825 | -2.405971 |
| 138 | 6  | 0 | -7.859857  | -4.177640 | -1.203251 |
| 139 | 1  | 0 | -8.274135  | -3.149626 | -1.260588 |
| 140 | 1  | 0 | -7.510121  | -4.373931 | -0.167095 |
| 141 | 6  | 0 | -8.899620  | -5.161066 | -1.722693 |
| 142 | 1  | 0 | -9.930538  | -4.773670 | -1.528382 |
| 143 | 8  | 0 | -8.710973  | -6.454238 | -1.150083 |
| 144 | 15 | 0 | -9.294295  | -6.710367 | 0.311294  |
| 145 | 8  | 0 | -10.257549 | -7.834596 | 0.233715  |
| 146 | 8  | 0 | -9.788328  | -5.451093 | 0.913169  |
| 147 | 8  | 0 | -8.014890  | -7.178394 | 1.117424  |
| 148 | 6  | 0 | -7.594965  | -8.543120 | 0.941940  |
| 149 | 1  | 0 | -7.407192  | -8.763378 | -0.138499 |
| 150 | 1  | 0 | -8.376160  | -9.248738 | 1.311069  |
| 151 | 6  | 0 | -6.297692  | -8.810205 | 1.712380  |
| 152 | 1  | 0 | -5.970416  | -9.848572 | 1.509354  |
| 153 | 8  | 0 | -5.246485  | -7.892993 | 1.249649  |
| 154 | 6  | 0 | -4.519640  | -7.564821 | 2.409924  |

|     |   |   |           |           |          |
|-----|---|---|-----------|-----------|----------|
| 155 | 1 | 0 | -3.985865 | -8.499262 | 2.688938 |
| 156 | 7 | 0 | -3.535976 | -6.551770 | 2.081437 |
| 157 | 6 | 0 | -3.667634 | -5.218628 | 1.724070 |
| 158 | 7 | 0 | -5.577351 | -2.377011 | 1.144174 |
| 159 | 1 | 0 | -5.490539 | -1.349988 | 1.069223 |
| 160 | 1 | 0 | -6.469949 | -2.757092 | 1.442785 |
| 161 | 7 | 0 | -4.776263 | -4.475831 | 1.637954 |
| 162 | 6 | 0 | -4.532353 | -3.201894 | 1.308942 |
| 163 | 7 | 0 | -3.275205 | -2.675684 | 1.109606 |
| 164 | 1 | 0 | -3.159515 | -1.649857 | 0.998867 |
| 165 | 6 | 0 | -2.086422 | -3.414071 | 1.188181 |
| 166 | 8 | 0 | -0.992591 | -2.894931 | 1.021795 |
| 167 | 6 | 0 | -2.351383 | -4.796481 | 1.478521 |
| 168 | 7 | 0 | -1.454481 | -5.812598 | 1.631496 |
| 169 | 6 | 0 | -2.197045 | -6.838334 | 1.981952 |
| 170 | 1 | 0 | -1.828406 | -7.840708 | 2.190247 |
| 171 | 6 | 0 | -5.628779 | -7.255208 | 3.383928 |
| 172 | 1 | 0 | -6.276925 | -6.438598 | 2.990834 |
| 173 | 1 | 0 | -5.298635 | -6.976740 | 4.399597 |
| 174 | 6 | 0 | -6.339938 | -8.599609 | 3.270372 |
| 175 | 1 | 0 | -7.347642 | -8.534683 | 3.624229 |
| 176 | 6 | 0 | 4.683073  | 7.915763  | 3.531320 |
| 177 | 8 | 0 | 4.362755  | 6.584735  | 3.084925 |
| 178 | 6 | 0 | 4.123013  | 6.544762  | 1.671986 |
| 179 | 1 | 0 | 5.018045  | 6.074713  | 1.203018 |
| 180 | 7 | 0 | 3.011871  | 5.631701  | 1.413163 |
| 181 | 6 | 0 | 3.089044  | 4.237594  | 1.544044 |
| 182 | 7 | 0 | 4.855072  | 1.340169  | 2.102492 |
| 183 | 1 | 0 | 4.809867  | 0.300390  | 2.277495 |
| 184 | 1 | 0 | 5.760922  | 1.798483  | 2.133850 |
| 185 | 7 | 0 | 4.134779  | 3.481933  | 1.717675 |
| 186 | 6 | 0 | 3.830778  | 2.135047  | 1.871928 |
| 187 | 7 | 0 | 2.577294  | 1.623915  | 1.839361 |
| 188 | 1 | 0 | 2.440224  | 0.546727  | 1.888563 |
| 189 | 6 | 0 | 1.421753  | 2.374268  | 1.607680 |
| 190 | 8 | 0 | 0.315554  | 1.895457  | 1.602809 |
| 191 | 6 | 0 | 1.723916  | 3.805051  | 1.421518 |
| 192 | 7 | 0 | 0.910907  | 4.812269  | 1.175591 |
| 193 | 6 | 0 | 1.725656  | 5.906252  | 1.163966 |
| 194 | 1 | 0 | 1.363480  | 6.921155  | 1.015772 |

|     |    |   |           |           |           |
|-----|----|---|-----------|-----------|-----------|
| 195 | 6  | 0 | 4.092551  | 8.011809  | 1.190014  |
| 196 | 1  | 0 | 3.075124  | 8.453516  | 1.222446  |
| 197 | 1  | 0 | 4.492394  | 8.124052  | 0.165025  |
| 198 | 6  | 0 | 4.981503  | 8.697930  | 2.246710  |
| 199 | 1  | 0 | 4.678615  | 9.758836  | 2.399355  |
| 200 | 8  | 0 | 6.377180  | 8.651735  | 1.960344  |
| 201 | 15 | 0 | 7.105336  | 9.169816  | 0.668269  |
| 202 | 8  | 0 | 6.162412  | 9.953608  | -0.160106 |
| 203 | 8  | 0 | 8.352668  | 9.851615  | 1.079667  |
| 204 | 8  | 0 | 7.465747  | 7.817493  | -0.092002 |
| 205 | 6  | 0 | 8.455368  | 6.955505  | 0.496684  |
| 206 | 1  | 0 | 8.172654  | 6.671156  | 1.539648  |
| 207 | 1  | 0 | 9.446501  | 7.466626  | 0.535890  |
| 208 | 6  | 0 | 8.626170  | 5.662050  | -0.309148 |
| 209 | 1  | 0 | 9.374746  | 5.008378  | 0.192018  |
| 210 | 8  | 0 | 7.397749  | 4.890655  | -0.359737 |
| 211 | 6  | 0 | 7.542603  | 4.090565  | -1.513035 |
| 212 | 1  | 0 | 8.457209  | 3.474201  | -1.348333 |
| 213 | 7  | 0 | 6.415108  | 3.168022  | -1.539899 |
| 214 | 6  | 0 | 5.036314  | 3.346014  | -1.446507 |
| 215 | 7  | 0 | 2.155479  | 5.268734  | -1.587150 |
| 216 | 1  | 0 | 1.113536  | 5.222604  | -1.591671 |
| 217 | 1  | 0 | 2.605705  | 6.145308  | -1.835277 |
| 218 | 7  | 0 | 4.304324  | 4.451969  | -1.559694 |
| 219 | 6  | 0 | 2.975717  | 4.215342  | -1.493917 |
| 220 | 7  | 0 | 2.400465  | 2.979912  | -1.333284 |
| 221 | 1  | 0 | 1.338256  | 2.879692  | -1.366486 |
| 222 | 6  | 0 | 3.119060  | 1.789332  | -1.175525 |
| 223 | 8  | 0 | 2.582476  | 0.711301  | -1.003028 |
| 224 | 6  | 0 | 4.541576  | 2.037915  | -1.218949 |
| 225 | 7  | 0 | 5.535880  | 1.122809  | -1.138348 |
| 226 | 6  | 0 | 6.630144  | 1.834815  | -1.322819 |
| 227 | 1  | 0 | 7.641802  | 1.432519  | -1.316790 |
| 228 | 6  | 0 | 7.844352  | 5.140620  | -2.565931 |
| 229 | 1  | 0 | 6.999974  | 5.853820  | -2.697504 |
| 230 | 1  | 0 | 8.158258  | 4.711102  | -3.536297 |
| 231 | 6  | 0 | 9.014241  | 5.799699  | -1.815091 |
| 232 | 1  | 0 | 9.108045  | 6.877732  | -2.074518 |
| 233 | 8  | 0 | 10.199033 | 5.061667  | -2.091448 |
| 234 | 1  | 0 | 5.503977  | -9.782633 | -4.500449 |

|     |   |   |            |           |           |
|-----|---|---|------------|-----------|-----------|
| 235 | 1 | 0 | 10.938637  | 5.666664  | -2.183993 |
| 236 | 1 | 0 | 9.450052   | -4.281503 | 3.671860  |
| 237 | 1 | 0 | -9.421462  | -4.570965 | -3.731282 |
| 238 | 1 | 0 | -3.757941  | 9.993517  | -2.833173 |
| 239 | 1 | 0 | 3.849396   | 8.347139  | 4.044932  |
| 240 | 1 | 0 | 5.544573   | 7.898686  | 4.165690  |
| 241 | 8 | 0 | -5.613617  | -9.626910 | 3.950086  |
| 242 | 1 | 0 | -5.191333  | -9.258164 | 4.729383  |
| 243 | 8 | 0 | -10.321685 | 4.794677  | 1.182364  |
| 244 | 1 | 0 | -11.020270 | 5.450520  | 1.241093  |

---

**Partially optimized (only Guanines) coordinates of the dimeric structure of Fig. 11**

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 1.811832                | 10.481825 | 2.393779  |
| 2                | 8                | 0              | 1.888305                | 9.113878  | 2.890802  |
| 3                | 6                | 0              | 2.306461                | 8.229128  | 1.842416  |
| 4                | 1                | 0              | 3.401648                | 8.074006  | 1.938956  |
| 5                | 7                | 0              | 1.601640                | 6.962779  | 1.984356  |
| 6                | 6                | 0              | 2.061812                | 5.661963  | 1.869473  |
| 7                | 7                | 0              | 4.630745                | 3.369693  | 1.674682  |
| 8                | 1                | 0              | 4.876170                | 2.361359  | 1.658327  |
| 9                | 1                | 0              | 5.371634                | 4.055083  | 1.555764  |
| 10               | 7                | 0              | 3.304942                | 5.231423  | 1.743901  |
| 11               | 6                | 0              | 3.405573                | 3.881381  | 1.738627  |
| 12               | 7                | 0              | 2.335780                | 3.029314  | 1.826408  |
| 13               | 1                | 0              | 2.502225                | 1.994985  | 1.804616  |
| 14               | 6                | 0              | 1.000104                | 3.431763  | 1.896115  |
| 15               | 8                | 0              | 0.077707                | 2.635551  | 1.919847  |
| 16               | 6                | 0              | 0.887540                | 4.873458  | 1.956029  |
| 17               | 7                | 0              | -0.210315               | 5.633073  | 2.125721  |
| 18               | 6                | 0              | 0.252810                | 6.878810  | 2.139385  |
| 19               | 1                | 0              | -0.348575               | 7.772300  | 2.286003  |
| 20               | 6                | 0              | 1.977348                | 8.958442  | 0.542811  |
| 21               | 1                | 0              | 0.895122                | 8.861430  | 0.300701  |
| 22               | 1                | 0              | 2.534863                | 8.534041  | -0.311400 |
| 23               | 6                | 0              | 2.241468                | 10.407927 | 0.909836  |
| 24               | 1                | 0              | 1.593898                | 11.089270 | 0.307885  |
| 25               | 8                | 0              | 3.614293                | 10.780518 | 0.727697  |
| 26               | 15               | 0              | 4.294020                | 10.664120 | -0.708736 |
| 27               | 8                | 0              | 3.243295                | 10.699209 | -1.753614 |
| 28               | 8                | 0              | 5.384138                | 11.661274 | -0.815909 |
| 29               | 8                | 0              | 4.908852                | 9.206686  | -0.678371 |
| 30               | 6                | 0              | 6.093078                | 8.914404  | 0.076068  |
| 31               | 1                | 0              | 5.838418                | 8.762178  | 1.149955  |
| 32               | 1                | 0              | 6.836062                | 9.747307  | 0.008961  |
| 33               | 6                | 0              | 6.753448                | 7.651122  | -0.496586 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 34 | 1 | 0 | 7.711558  | 7.444006  | 0.026458  |
| 35 | 8 | 0 | 5.914517  | 6.476980  | -0.305659 |
| 36 | 6 | 0 | 5.750990  | 5.808480  | -1.557088 |
| 37 | 1 | 0 | 6.596132  | 5.092138  | -1.637399 |
| 38 | 7 | 0 | 4.471929  | 5.148329  | -1.525823 |
| 39 | 6 | 0 | 4.193854  | 3.811693  | -1.394075 |
| 40 | 7 | 0 | 5.222756  | 0.525202  | -1.495960 |
| 41 | 1 | 0 | 4.908327  | -0.454146 | -1.475855 |
| 42 | 1 | 0 | 6.213811  | 0.699374  | -1.611322 |
| 43 | 7 | 0 | 5.062974  | 2.805936  | -1.411352 |
| 44 | 6 | 0 | 4.462206  | 1.602522  | -1.337781 |
| 45 | 7 | 0 | 3.117159  | 1.431984  | -1.143695 |
| 46 | 1 | 0 | 2.747494  | 0.466989  | -1.060064 |
| 47 | 6 | 0 | 2.174164  | 2.466389  | -1.125445 |
| 48 | 8 | 0 | 0.981074  | 2.249074  | -0.981570 |
| 49 | 6 | 0 | 2.799265  | 3.754201  | -1.268182 |
| 50 | 7 | 0 | 2.239967  | 4.997807  | -1.313457 |
| 51 | 6 | 0 | 3.269793  | 5.808515  | -1.459219 |
| 52 | 1 | 0 | 3.228490  | 6.894498  | -1.506191 |
| 53 | 6 | 0 | 5.884872  | 6.885685  | -2.623085 |
| 54 | 1 | 0 | 4.948398  | 7.480304  | -2.694756 |
| 55 | 1 | 0 | 6.128459  | 6.477437  | -3.625786 |
| 56 | 6 | 0 | 6.979513  | 7.743825  | -2.026525 |
| 57 | 1 | 0 | 6.817262  | 8.792097  | -2.378927 |
| 58 | 8 | 0 | 8.240268  | 7.226949  | -2.436288 |
| 59 | 6 | 0 | 10.369492 | -1.823647 | 2.102771  |
| 60 | 8 | 0 | 8.969185  | -1.661405 | 2.469773  |
| 61 | 6 | 0 | 8.116810  | -2.039932 | 1.379807  |
| 62 | 1 | 0 | 7.860144  | -3.108827 | 1.549576  |
| 63 | 7 | 0 | 6.924137  | -1.221566 | 1.422526  |
| 64 | 6 | 0 | 5.622257  | -1.636397 | 1.538319  |
| 65 | 7 | 0 | 3.291340  | -4.205521 | 1.769340  |
| 66 | 1 | 0 | 2.334304  | -4.342282 | 2.084561  |
| 67 | 1 | 0 | 3.932868  | -4.989187 | 1.775640  |
| 68 | 7 | 0 | 5.182100  | -2.908881 | 1.586330  |
| 69 | 6 | 0 | 3.877294  | -2.988198 | 1.744970  |
| 70 | 7 | 0 | 3.045431  | -1.896816 | 1.856254  |
| 71 | 1 | 0 | 2.035683  | -2.023640 | 1.975129  |
| 72 | 6 | 0 | 3.454972  | -0.563712 | 1.742819  |
| 73 | 8 | 0 | 2.620515  | 0.339060  | 1.780120  |

|     |    |   |           |           |           |
|-----|----|---|-----------|-----------|-----------|
| 74  | 6  | 0 | 4.872815  | -0.466969 | 1.605400  |
| 75  | 7  | 0 | 5.689245  | 0.645558  | 1.561435  |
| 76  | 6  | 0 | 6.899761  | 0.154968  | 1.457556  |
| 77  | 1  | 0 | 7.821153  | 0.731197  | 1.433925  |
| 78  | 6  | 0 | 8.984719  | -1.937852 | 0.117374  |
| 79  | 1  | 0 | 9.026616  | -0.889095 | -0.248809 |
| 80  | 1  | 0 | 8.611136  | -2.586039 | -0.697732 |
| 81  | 6  | 0 | 10.367966 | -2.333170 | 0.645230  |
| 82  | 1  | 0 | 11.172457 | -1.793389 | 0.092235  |
| 83  | 8  | 0 | 10.596478 | -3.739959 | 0.590063  |
| 84  | 15 | 0 | 10.847497 | -4.491454 | -0.782228 |
| 85  | 8  | 0 | 11.867667 | -5.543277 | -0.565686 |
| 86  | 8  | 0 | 11.113519 | -3.510918 | -1.861674 |
| 87  | 8  | 0 | 9.438896  | -5.172269 | -1.057185 |
| 88  | 6  | 0 | 9.098379  | -6.298213 | -0.229159 |
| 89  | 1  | 0 | 9.062350  | -6.004858 | 0.846830  |
| 90  | 1  | 0 | 9.853208  | -7.116675 | -0.338208 |
| 91  | 6  | 0 | 7.731734  | -6.871456 | -0.621479 |
| 92  | 1  | 0 | 7.482219  | -7.675497 | 0.096477  |
| 93  | 8  | 0 | 6.675461  | -5.883393 | -0.499601 |
| 94  | 6  | 0 | 5.823653  | -5.929290 | -1.650880 |
| 95  | 1  | 0 | 5.075804  | -6.728463 | -1.455701 |
| 96  | 7  | 0 | 5.190348  | -4.648506 | -1.745935 |
| 97  | 6  | 0 | 3.880818  | -4.381570 | -1.473902 |
| 98  | 7  | 0 | 0.675077  | -5.554066 | -0.766256 |
| 99  | 1  | 0 | -0.260954 | -5.182196 | -0.935315 |
| 100 | 1  | 0 | 0.810369  | -6.482562 | -1.158105 |
| 101 | 7  | 0 | 2.908339  | -5.297764 | -1.288221 |
| 102 | 6  | 0 | 1.752617  | -4.741358 | -1.013353 |
| 103 | 7  | 0 | 1.558163  | -3.388770 | -0.919607 |
| 104 | 1  | 0 | 0.619636  | -3.038248 | -0.707915 |
| 105 | 6  | 0 | 2.532777  | -2.404656 | -1.132929 |
| 106 | 8  | 0 | 2.241139  | -1.215399 | -1.030279 |
| 107 | 6  | 0 | 3.794265  | -2.996596 | -1.432571 |
| 108 | 7  | 0 | 5.026663  | -2.418815 | -1.644517 |
| 109 | 6  | 0 | 5.837711  | -3.433862 | -1.811663 |
| 110 | 1  | 0 | 6.911499  | -3.384127 | -1.977723 |
| 111 | 6  | 0 | 6.751764  | -6.371453 | -2.788306 |
| 112 | 1  | 0 | 7.381657  | -5.524593 | -3.141065 |
| 113 | 1  | 0 | 6.196054  | -6.797858 | -3.646720 |

|     |    |   |           |            |           |
|-----|----|---|-----------|------------|-----------|
| 114 | 6  | 0 | 7.629293  | -7.409532  | -2.069796 |
| 115 | 1  | 0 | 8.635808  | -7.413055  | -2.549039 |
| 116 | 8  | 0 | 7.017409  | -8.699783  | -2.132383 |
| 117 | 6  | 0 | -2.298621 | -9.683748  | 3.044149  |
| 118 | 1  | 0 | -3.213665 | -9.938572  | 3.536753  |
| 119 | 8  | 0 | -2.054554 | -8.263175  | 3.147389  |
| 120 | 6  | 0 | -2.122914 | -7.693157  | 1.849996  |
| 121 | 1  | 0 | -3.194556 | -7.430664  | 1.687016  |
| 122 | 7  | 0 | -1.373060 | -6.440330  | 1.838788  |
| 123 | 6  | 0 | -1.892485 | -5.142841  | 1.876357  |
| 124 | 7  | 0 | -4.536447 | -2.947617  | 1.808357  |
| 125 | 1  | 0 | -4.848752 | -1.945995  | 1.967292  |
| 126 | 1  | 0 | -5.229538 | -3.656162  | 1.579628  |
| 127 | 7  | 0 | -3.123118 | -4.751079  | 1.740161  |
| 128 | 6  | 0 | -3.297639 | -3.383070  | 1.941442  |
| 129 | 7  | 0 | -2.305884 | -2.526627  | 2.262162  |
| 130 | 1  | 0 | -2.485916 | -1.435968  | 2.217284  |
| 131 | 6  | 0 | -0.945082 | -2.871750  | 2.312441  |
| 132 | 8  | 0 | -0.063606 | -2.077795  | 2.525383  |
| 133 | 6  | 0 | -0.743045 | -4.313961  | 2.113313  |
| 134 | 7  | 0 | 0.360702  | -5.031335  | 2.203840  |
| 135 | 6  | 0 | -0.054249 | -6.310670  | 2.022616  |
| 136 | 1  | 0 | 0.606052  | -7.173877  | 2.069638  |
| 137 | 6  | 0 | -1.706330 | -8.789752  | 0.885907  |
| 138 | 1  | 0 | -0.604606 | -8.944807  | 0.911126  |
| 139 | 1  | 0 | -1.996079 | -8.548822  | -0.152794 |
| 140 | 6  | 0 | -2.406880 | -9.978094  | 1.529264  |
| 141 | 1  | 0 | -1.865806 | -10.927186 | 1.303710  |
| 142 | 8  | 0 | -3.767088 | -10.077947 | 1.131298  |
| 143 | 15 | 0 | -4.180552 | -10.458548 | -0.342216 |
| 144 | 8  | 0 | -5.138954 | -11.583115 | -0.279264 |
| 145 | 8  | 0 | -2.977707 | -10.643981 | -1.187121 |
| 146 | 8  | 0 | -4.940246 | -9.153784  | -0.820241 |
| 147 | 6  | 0 | -6.274528 | -8.943797  | -0.327058 |
| 148 | 1  | 0 | -6.273514 | -8.876072  | 0.787297  |
| 149 | 1  | 0 | -6.930474 | -9.796853  | -0.621786 |
| 150 | 6  | 0 | -6.889566 | -7.662444  | -0.905525 |
| 151 | 1  | 0 | -7.794389 | -7.384029  | -0.337514 |
| 152 | 8  | 0 | -5.993283 | -6.540138  | -0.803198 |
| 153 | 6  | 0 | -5.880041 | -5.924149  | -2.074975 |

|     |   |   |            |           |           |
|-----|---|---|------------|-----------|-----------|
| 154 | 1 | 0 | -6.715718  | -5.193621 | -2.144065 |
| 155 | 7 | 0 | -4.562433  | -5.320284 | -2.023104 |
| 156 | 6 | 0 | -4.246562  | -4.060067 | -1.575523 |
| 157 | 7 | 0 | -5.020984  | -0.731264 | -1.095411 |
| 158 | 1 | 0 | -4.536744  | 0.154596  | -0.915339 |
| 159 | 1 | 0 | -5.975597  | -0.712912 | -1.436278 |
| 160 | 7 | 0 | -5.016496  | -2.992695 | -1.515147 |
| 161 | 6 | 0 | -4.361971  | -1.872028 | -1.121339 |
| 162 | 7 | 0 | -3.036558  | -1.856865 | -0.750147 |
| 163 | 1 | 0 | -2.611348  | -0.942196 | -0.519853 |
| 164 | 6 | 0 | -2.228046  | -2.984648 | -0.725212 |
| 165 | 8 | 0 | -1.072059  | -2.960326 | -0.289211 |
| 166 | 6 | 0 | -2.890202  | -4.158068 | -1.180708 |
| 167 | 7 | 0 | -2.414572  | -5.427154 | -1.316417 |
| 168 | 6 | 0 | -3.446537  | -6.099131 | -1.788192 |
| 169 | 1 | 0 | -3.472760  | -7.178980 | -1.944968 |
| 170 | 6 | 0 | -6.088132  | -7.049515 | -3.079738 |
| 171 | 1 | 0 | -5.191611  | -7.705550 | -3.121093 |
| 172 | 1 | 0 | -6.322933  | -6.677050 | -4.094566 |
| 173 | 6 | 0 | -7.236335  | -7.782717 | -2.404242 |
| 174 | 1 | 0 | -7.232072  | -8.857066 | -2.708085 |
| 175 | 8 | 0 | -8.471230  | -7.137526 | -2.717595 |
| 176 | 6 | 0 | -10.061055 | 1.922025  | 2.506504  |
| 177 | 8 | 0 | -8.811433  | 1.756258  | 3.224487  |
| 178 | 6 | 0 | -7.772700  | 2.516347  | 2.601518  |
| 179 | 1 | 0 | -7.488662  | 3.292075  | 3.343876  |
| 180 | 7 | 0 | -6.658216  | 1.614440  | 2.316825  |
| 181 | 6 | 0 | -5.360236  | 1.994587  | 2.111604  |
| 182 | 7 | 0 | -2.993101  | 4.500844  | 1.744805  |
| 183 | 1 | 0 | -1.989649  | 4.654996  | 1.855386  |
| 184 | 1 | 0 | -3.607469  | 5.304661  | 1.782121  |
| 185 | 7 | 0 | -4.906478  | 3.255349  | 2.043499  |
| 186 | 6 | 0 | -3.590665  | 3.311819  | 1.918086  |
| 187 | 7 | 0 | -2.776209  | 2.200795  | 1.933487  |
| 188 | 1 | 0 | -1.754581  | 2.322255  | 1.879172  |
| 189 | 6 | 0 | -3.225102  | 0.893056  | 1.957275  |
| 190 | 8 | 0 | -2.391593  | -0.032145 | 1.941617  |
| 191 | 6 | 0 | -4.639634  | 0.805992  | 2.019884  |
| 192 | 7 | 0 | -5.481000  | -0.285923 | 2.149826  |
| 193 | 6 | 0 | -6.672554  | 0.241084  | 2.329349  |

|     |    |   |            |           |           |
|-----|----|---|------------|-----------|-----------|
| 194 | 1  | 0 | -7.597369  | -0.301604 | 2.500474  |
| 195 | 6  | 0 | -8.406859  | 3.227782  | 1.401283  |
| 196 | 1  | 0 | -7.727879  | 3.321653  | 0.532454  |
| 197 | 1  | 0 | -8.710745  | 4.239060  | 1.748586  |
| 198 | 6  | 0 | -9.648695  | 2.395613  | 1.095688  |
| 199 | 1  | 0 | -9.411021  | 1.510656  | 0.460148  |
| 200 | 8  | 0 | -10.700904 | 3.193786  | 0.549886  |
| 201 | 6  | 0 | -8.065912  | 6.850040  | -2.614259 |
| 202 | 1  | 0 | -9.054408  | 6.585702  | -3.056586 |
| 203 | 8  | 0 | -7.770563  | 8.206174  | -2.939265 |
| 204 | 1  | 0 | -7.536210  | 8.263033  | -3.867924 |
| 205 | 15 | 0 | -10.725941 | 3.602010  | -0.982540 |
| 206 | 8  | 0 | -10.618313 | 2.380298  | -1.809566 |
| 207 | 8  | 0 | -11.910594 | 4.461368  | -1.211436 |
| 208 | 8  | 0 | -9.411366  | 4.473045  | -1.199412 |
| 209 | 6  | 0 | -9.384669  | 5.803510  | -0.655913 |
| 210 | 1  | 0 | -9.406930  | 5.774211  | 0.455718  |
| 211 | 1  | 0 | -10.277740 | 6.389557  | -0.978340 |
| 212 | 6  | 0 | -8.125621  | 6.572211  | -1.105771 |
| 213 | 1  | 0 | -8.096723  | 7.546901  | -0.568561 |
| 214 | 8  | 0 | -6.882581  | 5.853555  | -0.788244 |
| 215 | 6  | 0 | -6.031958  | 5.751329  | -1.947121 |
| 216 | 1  | 0 | -5.334194  | 6.614223  | -1.905534 |
| 217 | 7  | 0 | -5.391169  | 4.464785  | -1.835637 |
| 218 | 6  | 0 | -4.089089  | 4.148980  | -1.557508 |
| 219 | 7  | 0 | -0.777693  | 5.086130  | -1.040770 |
| 220 | 1  | 0 | 0.139478   | 4.648435  | -1.112476 |
| 221 | 1  | 0 | -0.833339  | 6.033154  | -1.397775 |
| 222 | 7  | 0 | -3.032648  | 4.984297  | -1.519747 |
| 223 | 6  | 0 | -1.909970  | 4.364638  | -1.211368 |
| 224 | 7  | 0 | -1.805713  | 3.007047  | -1.001563 |
| 225 | 1  | 0 | -0.876565  | 2.604626  | -0.829513 |
| 226 | 6  | 0 | -2.872822  | 2.116211  | -1.057433 |
| 227 | 8  | 0 | -2.704609  | 0.902660  | -0.862472 |
| 228 | 6  | 0 | -4.100649  | 2.776467  | -1.323324 |
| 229 | 7  | 0 | -5.377824  | 2.257062  | -1.405883 |
| 230 | 6  | 0 | -6.120678  | 3.290550  | -1.699220 |
| 231 | 1  | 0 | -7.207409  | 3.292456  | -1.806598 |
| 232 | 6  | 0 | -6.988743  | 5.908501  | -3.144776 |
| 233 | 1  | 0 | -7.466328  | 4.942849  | -3.417531 |

|     |   |   |            |            |           |
|-----|---|---|------------|------------|-----------|
| 234 | 1 | 0 | -6.466068  | 6.319328   | -4.031042 |
| 235 | 1 | 0 | 8.209077   | 6.267462   | -2.433134 |
| 236 | 1 | 0 | -9.191313  | -7.766890  | -2.634045 |
| 237 | 1 | 0 | 6.473694   | -8.834254  | -1.352709 |
| 238 | 1 | 0 | -1.483647  | -10.230948 | 3.469931  |
| 239 | 1 | 0 | -10.583242 | 0.989913   | 2.448288  |
| 240 | 1 | 0 | -10.669419 | 2.661361   | 2.984179  |
| 241 | 1 | 0 | 10.838163  | -2.540822  | 2.743793  |
| 242 | 1 | 0 | 10.878307  | -0.884407  | 2.164707  |
| 243 | 1 | 0 | 0.809458   | 10.848129  | 2.471025  |
| 244 | 1 | 0 | 2.480391   | 11.112527  | 2.941633  |

-----

**Totally Optimized Coordinates of the dimeric structure of Fig.9**

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 8.236021                | 5.429572  | -2.824446 |
| 2                | 8                | 0              | 6.819902                | 5.327673  | -3.009715 |
| 3                | 6                | 0              | 8.504592                | 5.452572  | -1.299537 |
| 4                | 8                | 0              | 9.045025                | 6.648987  | -0.782076 |
| 5                | 6                | 0              | 7.128714                | 5.105669  | -0.715182 |
| 6                | 6                | 0              | 6.192825                | 5.638450  | -1.797893 |
| 7                | 7                | 0              | 4.869037                | 5.016777  | -1.809346 |
| 8                | 6                | 0              | 3.688874                | 5.702546  | -1.735302 |
| 9                | 7                | 0              | 2.631763                | 4.920646  | -1.774997 |
| 10               | 6                | 0              | 3.155996                | 3.651106  | -1.891636 |
| 11               | 6                | 0              | 2.498339                | 2.389629  | -1.915476 |
| 12               | 8                | 0              | 1.287413                | 2.155287  | -1.888150 |
| 13               | 7                | 0              | 3.409307                | 1.332713  | -1.955710 |
| 14               | 6                | 0              | 4.775635                | 1.482825  | -1.980474 |
| 15               | 7                | 0              | 5.519861                | 0.345068  | -1.981548 |
| 16               | 7                | 0              | 5.395246                | 2.640570  | -1.952995 |
| 17               | 6                | 0              | 4.545500                | 3.691638  | -1.908213 |
| 18               | 1                | 0              | 8.609213                | 6.352759  | -3.282566 |
| 19               | 1                | 0              | 9.243276                | 4.684940  | -1.030605 |
| 20               | 1                | 0              | 7.001878                | 4.016086  | -0.637955 |
| 21               | 1                | 0              | 7.002195                | 5.607985  | 0.247276  |
| 22               | 1                | 0              | 6.024167                | 6.719567  | -1.695815 |
| 23               | 1                | 0              | 3.682063                | 6.784613  | -1.623760 |
| 24               | 1                | 0              | 2.980396                | 0.399275  | -1.992617 |
| 25               | 1                | 0              | 5.089954                | -0.557293 | -2.164774 |
| 26               | 1                | 0              | 6.483567                | 0.478998  | -2.264422 |
| 27               | 15               | 0              | 8.309699                | 8.136522  | -0.968432 |
| 28               | 8                | 0              | 7.592086                | 8.181560  | -2.299290 |
| 29               | 8                | 0              | 9.221325                | 9.182727  | -0.418584 |
| 30               | 8                | 0              | 7.053366                | 7.884323  | 0.184455  |
| 31               | 6                | 0              | 6.162280                | 8.972067  | 0.200830  |
| 32               | 6                | 0              | 5.047803                | 8.706673  | 1.180828  |
| 33               | 8                | 0              | 4.178250                | 7.666859  | 0.699981  |

|    |   |   |            |           |           |
|----|---|---|------------|-----------|-----------|
| 34 | 6 | 0 | 5.491121   | 8.191306  | 2.548902  |
| 35 | 6 | 0 | 4.186894   | 7.602260  | 3.075740  |
| 36 | 6 | 0 | 3.468319   | 7.136216  | 1.796239  |
| 37 | 7 | 0 | 3.438579   | 5.682573  | 1.638269  |
| 38 | 6 | 0 | 4.524148   | 4.856886  | 1.503629  |
| 39 | 7 | 0 | 4.189868   | 3.602738  | 1.307190  |
| 40 | 6 | 0 | 2.809670   | 3.607039  | 1.311782  |
| 41 | 6 | 0 | 1.877812   | 2.548656  | 1.114861  |
| 42 | 8 | 0 | 2.104833   | 1.348784  | 0.930708  |
| 43 | 7 | 0 | 0.561589   | 3.011784  | 1.151219  |
| 44 | 6 | 0 | 0.190262   | 4.320819  | 1.371366  |
| 45 | 7 | 0 | -1.137457  | 4.588999  | 1.363250  |
| 46 | 7 | 0 | 1.044682   | 5.306313  | 1.544906  |
| 47 | 6 | 0 | 2.328015   | 4.895345  | 1.500355  |
| 48 | 1 | 0 | 5.748162   | 9.158433  | -0.807031 |
| 49 | 1 | 0 | 6.685352   | 9.895515  | 0.514834  |
| 50 | 1 | 0 | 4.466944   | 9.636250  | 1.330215  |
| 51 | 1 | 0 | 6.252817   | 7.409900  | 2.383464  |
| 52 | 1 | 0 | 4.308963   | 6.792073  | 3.804515  |
| 53 | 1 | 0 | 3.622250   | 8.415391  | 3.552778  |
| 54 | 1 | 0 | 2.410039   | 7.436170  | 1.772886  |
| 55 | 1 | 0 | 5.537027   | 5.247969  | 1.547194  |
| 56 | 1 | 0 | -0.159999  | 2.302147  | 1.002264  |
| 57 | 1 | 0 | -1.799181  | 3.834579  | 1.522185  |
| 58 | 1 | 0 | -1.387100  | 5.512299  | 1.696791  |
| 59 | 6 | 0 | -10.066023 | 2.615268  | 2.011444  |
| 60 | 8 | 0 | -8.681785  | 2.545606  | 2.434872  |
| 61 | 6 | 0 | -10.091696 | 3.351555  | 0.639098  |
| 62 | 8 | 0 | -10.727798 | 4.603226  | 0.600831  |
| 63 | 6 | 0 | -8.592938  | 3.437341  | 0.310661  |
| 64 | 6 | 0 | -8.029738  | 3.542333  | 1.720287  |
| 65 | 7 | 0 | -6.574079  | 3.320245  | 1.746830  |
| 66 | 6 | 0 | -5.688015  | 4.288365  | 1.962434  |
| 67 | 7 | 0 | -4.376915  | 3.901733  | 1.818231  |
| 68 | 6 | 0 | -4.471727  | 2.626108  | 1.510303  |
| 69 | 6 | 0 | -3.410444  | 1.644430  | 1.295603  |
| 70 | 8 | 0 | -2.232864  | 1.940094  | 1.221371  |
| 71 | 7 | 0 | -3.882739  | 0.351001  | 1.186855  |
| 72 | 6 | 0 | -5.207572  | 0.017561  | 1.249695  |
| 73 | 7 | 0 | -5.552180  | -1.237684 | 1.307973  |

|     |    |   |            |           |           |
|-----|----|---|------------|-----------|-----------|
| 74  | 7  | 0 | -6.243019  | 0.944943  | 1.322121  |
| 75  | 6  | 0 | -5.838968  | 2.161149  | 1.467575  |
| 76  | 1  | 0 | -10.645672 | 3.182124  | 2.748420  |
| 77  | 1  | 0 | -10.616809 | 2.743153  | -0.109230 |
| 78  | 1  | 0 | -8.246778  | 2.487167  | -0.130351 |
| 79  | 1  | 0 | -8.353081  | 4.294705  | -0.325943 |
| 80  | 1  | 0 | -8.175096  | 4.530609  | 2.172268  |
| 81  | 1  | 0 | -6.011321  | 5.301065  | 2.200029  |
| 82  | 1  | 0 | -3.093240  | -0.390703 | 1.145781  |
| 83  | 1  | 0 | -4.843754  | -2.058120 | 1.336963  |
| 84  | 1  | 0 | -6.553587  | -1.415171 | 1.326265  |
| 85  | 15 | 0 | -10.307420 | 5.900110  | 1.600789  |
| 86  | 8  | 0 | -10.005508 | 5.348599  | 2.970253  |
| 87  | 8  | 0 | -11.186599 | 7.033315  | 1.194285  |
| 88  | 8  | 0 | -8.737847  | 6.214443  | 0.997163  |
| 89  | 6  | 0 | -8.603541  | 6.896439  | -0.214009 |
| 90  | 6  | 0 | -7.153751  | 7.317059  | -0.307074 |
| 91  | 8  | 0 | -6.309598  | 6.147875  | -0.095279 |
| 92  | 6  | 0 | -6.730321  | 7.901098  | -1.664928 |
| 93  | 6  | 0 | -5.907774  | 6.764770  | -2.286568 |
| 94  | 6  | 0 | -5.259104  | 6.216966  | -1.021561 |
| 95  | 7  | 0 | -4.685191  | 4.880718  | -1.128119 |
| 96  | 6  | 0 | -5.334574  | 3.695826  | -1.143401 |
| 97  | 7  | 0 | -4.501212  | 2.652097  | -1.291746 |
| 98  | 6  | 0 | -3.275125  | 3.197182  | -1.402907 |
| 99  | 6  | 0 | -1.997474  | 2.561655  | -1.627263 |
| 100 | 8  | 0 | -1.796913  | 1.368453  | -1.763758 |
| 101 | 7  | 0 | -0.969188  | 3.507155  | -1.680714 |
| 102 | 6  | 0 | -1.135454  | 4.856760  | -1.544466 |
| 103 | 7  | 0 | -0.070392  | 5.633315  | -1.591718 |
| 104 | 7  | 0 | -2.346189  | 5.463380  | -1.373551 |
| 105 | 6  | 0 | -3.329801  | 4.598262  | -1.293159 |
| 106 | 1  | 0 | -9.261299  | 7.781078  | -0.248423 |
| 107 | 1  | 0 | -8.865695  | 6.247496  | -1.077374 |
| 108 | 1  | 0 | -6.922702  | 8.047446  | 0.482075  |
| 109 | 1  | 0 | -7.608692  | 8.169717  | -2.272711 |
| 110 | 1  | 0 | -6.559896  | 5.992816  | -2.725702 |
| 111 | 1  | 0 | -5.186663  | 7.118821  | -3.034173 |
| 112 | 1  | 0 | -4.438202  | 6.872177  | -0.686473 |
| 113 | 1  | 0 | -6.415687  | 3.627894  | -1.043884 |

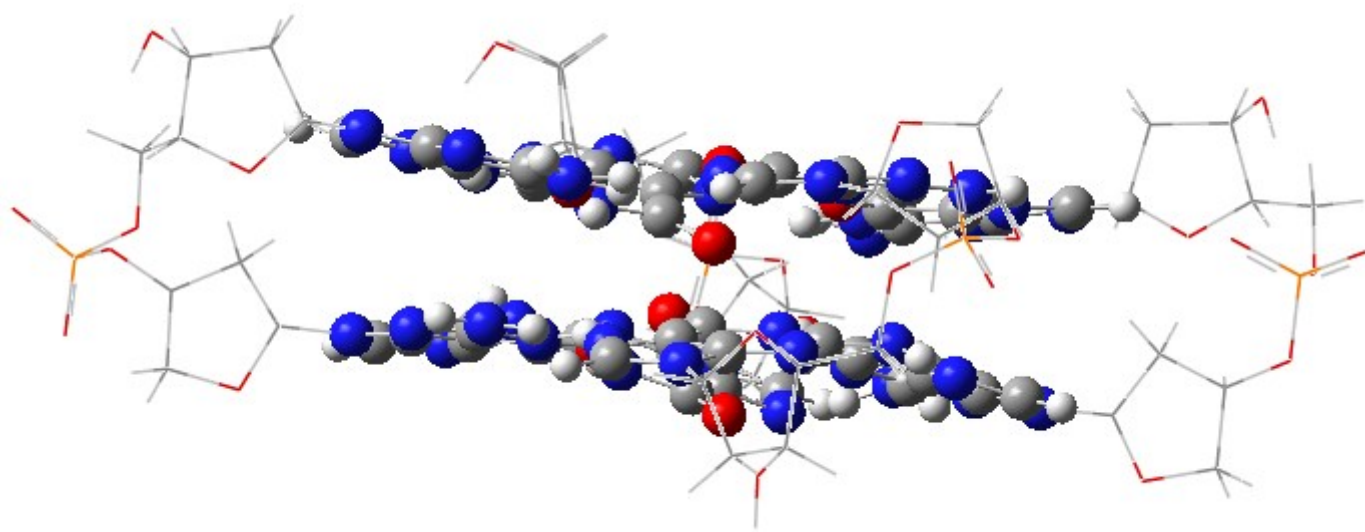
|     |    |   |           |           |           |
|-----|----|---|-----------|-----------|-----------|
| 114 | 1  | 0 | 0.000057  | 3.096458  | -1.813824 |
| 115 | 1  | 0 | 0.927304  | 5.299863  | -1.678857 |
| 116 | 1  | 0 | -0.247393 | 6.622534  | -1.457133 |
| 117 | 6  | 0 | -8.172832 | -5.098088 | -2.627418 |
| 118 | 8  | 0 | -6.788834 | -4.900142 | -2.960547 |
| 119 | 6  | 0 | -8.244109 | -5.453097 | -1.117596 |
| 120 | 8  | 0 | -8.665721 | -6.756466 | -0.793303 |
| 121 | 6  | 0 | -6.813837 | -5.146504 | -0.657467 |
| 122 | 6  | 0 | -6.024627 | -5.442668 | -1.925043 |
| 123 | 7  | 0 | -4.703551 | -4.812333 | -1.926588 |
| 124 | 6  | 0 | -3.529557 | -5.503544 | -1.940591 |
| 125 | 7  | 0 | -2.468296 | -4.724116 | -1.878472 |
| 126 | 6  | 0 | -2.989967 | -3.449496 | -1.824886 |
| 127 | 6  | 0 | -2.334329 | -2.191532 | -1.724235 |
| 128 | 8  | 0 | -1.119304 | -1.963100 | -1.696247 |
| 129 | 7  | 0 | -3.234629 | -1.134605 | -1.639947 |
| 130 | 6  | 0 | -4.601818 | -1.278564 | -1.683320 |
| 131 | 7  | 0 | -5.341222 | -0.141956 | -1.594539 |
| 132 | 7  | 0 | -5.225451 | -2.433959 | -1.758842 |
| 133 | 6  | 0 | -4.380608 | -3.485625 | -1.842034 |
| 134 | 1  | 0 | -8.963910 | -4.795210 | -0.609576 |
| 135 | 1  | 0 | -6.705661 | -4.074656 | -0.425935 |
| 136 | 1  | 0 | -6.504028 | -5.767706 | 0.186755  |
| 137 | 1  | 0 | -5.849043 | -6.517965 | -2.064533 |
| 138 | 1  | 0 | -3.530560 | -6.590818 | -1.979933 |
| 139 | 1  | 0 | -2.799676 | -0.197175 | -1.622806 |
| 140 | 1  | 0 | -4.918595 | 0.777987  | -1.726705 |
| 141 | 1  | 0 | -6.307581 | -0.260328 | -1.878728 |
| 142 | 15 | 0 | -7.946102 | -8.156854 | -1.412225 |
| 143 | 8  | 0 | -7.542839 | -7.898527 | -2.838447 |
| 144 | 8  | 0 | -8.723979 | -9.290140 | -0.829158 |
| 145 | 8  | 0 | -6.456880 | -8.072478 | -0.583269 |
| 146 | 6  | 0 | -6.500841 | -8.224506 | 0.801636  |
| 147 | 6  | 0 | -5.069857 | -8.242360 | 1.304188  |
| 148 | 8  | 0 | -4.308221 | -7.200897 | 0.656910  |
| 149 | 6  | 0 | -4.868368 | -7.941268 | 2.791369  |
| 150 | 6  | 0 | -3.392971 | -7.564159 | 2.814147  |
| 151 | 6  | 0 | -3.197650 | -6.880975 | 1.446750  |
| 152 | 7  | 0 | -3.130313 | -5.415492 | 1.507245  |
| 153 | 6  | 0 | -4.199524 | -4.563248 | 1.511318  |

|     |   |   |           |           |           |
|-----|---|---|-----------|-----------|-----------|
| 154 | 7 | 0 | -3.835202 | -3.302207 | 1.440161  |
| 155 | 6 | 0 | -2.455556 | -3.332574 | 1.391475  |
| 156 | 6 | 0 | -1.504481 | -2.285781 | 1.256289  |
| 157 | 8 | 0 | -1.716130 | -1.068912 | 1.173732  |
| 158 | 7 | 0 | -0.200211 | -2.772658 | 1.218218  |
| 159 | 6 | 0 | 0.145802  | -4.105171 | 1.293941  |
| 160 | 7 | 0 | 1.462103  | -4.399617 | 1.232924  |
| 161 | 7 | 0 | -0.731112 | -5.087075 | 1.382928  |
| 162 | 6 | 0 | -2.003318 | -4.644714 | 1.425041  |
| 163 | 1 | 0 | -7.009611 | -9.162158 | 1.086555  |
| 164 | 1 | 0 | -7.062223 | -7.387286 | 1.263068  |
| 165 | 1 | 0 | -4.609313 | -9.214281 | 1.053568  |
| 166 | 1 | 0 | -3.146931 | -6.904613 | 3.654785  |
| 167 | 1 | 0 | -2.768520 | -8.465892 | 2.865995  |
| 168 | 1 | 0 | -2.252268 | -7.181368 | 0.967639  |
| 169 | 1 | 0 | -5.211430 | -4.947488 | 1.588561  |
| 170 | 1 | 0 | 0.536617  | -2.072112 | 1.094135  |
| 171 | 1 | 0 | 2.159044  | -3.669396 | 1.360715  |
| 172 | 1 | 0 | 1.715334  | -5.347524 | 1.486944  |
| 173 | 6 | 0 | 6.468868  | -7.649634 | -2.218578 |
| 174 | 8 | 0 | 6.157918  | -6.247929 | -2.227579 |
| 175 | 6 | 0 | 5.813020  | -8.266127 | -0.962635 |
| 176 | 8 | 0 | 6.768097  | -8.694802 | -0.000157 |
| 177 | 6 | 0 | 4.817932  | -7.160493 | -0.545631 |
| 178 | 6 | 0 | 5.573222  | -5.919502 | -0.998351 |
| 179 | 7 | 0 | 4.804156  | -4.678368 | -1.225621 |
| 180 | 6 | 0 | 5.424337  | -3.493567 | -1.290945 |
| 181 | 7 | 0 | 4.592000  | -2.454121 | -1.581744 |
| 182 | 6 | 0 | 3.396423  | -3.006480 | -1.673715 |
| 183 | 6 | 0 | 2.109482  | -2.380012 | -1.948083 |
| 184 | 8 | 0 | 1.928781  | -1.209434 | -2.195521 |
| 185 | 7 | 0 | 1.071334  | -3.313793 | -1.893312 |
| 186 | 6 | 0 | 1.236916  | -4.644853 | -1.681684 |
| 187 | 7 | 0 | 0.187277  | -5.429683 | -1.656843 |
| 188 | 7 | 0 | 2.461982  | -5.260943 | -1.494997 |
| 189 | 6 | 0 | 3.453506  | -4.426395 | -1.459590 |
| 190 | 1 | 0 | 7.555996  | -7.791899 | -2.175708 |
| 191 | 1 | 0 | 5.266909  | -9.181361 | -1.221158 |
| 192 | 1 | 0 | 3.909099  | -7.275160 | -1.150917 |
| 193 | 1 | 0 | 4.600181  | -7.170862 | 0.525828  |

|     |    |   |           |           |           |
|-----|----|---|-----------|-----------|-----------|
| 194 | 1  | 0 | 6.333095  | -5.620738 | -0.268230 |
| 195 | 1  | 0 | 6.505426  | -3.414288 | -1.157417 |
| 196 | 1  | 0 | 0.088501  | -2.883148 | -1.917241 |
| 197 | 1  | 0 | -0.826413 | -5.109166 | -1.763326 |
| 198 | 1  | 0 | 0.380569  | -6.406196 | -1.456719 |
| 199 | 15 | 0 | 7.498627  | -7.665644 | 1.064499  |
| 200 | 8  | 0 | 8.657886  | -8.305842 | 1.772431  |
| 201 | 8  | 0 | 6.394410  | -6.923746 | 1.811315  |
| 202 | 8  | 0 | 8.117305  | -6.566459 | -0.055162 |
| 203 | 6  | 0 | 9.463974  | -6.148646 | 0.023048  |
| 204 | 6  | 0 | 9.621334  | -4.997057 | 0.990574  |
| 205 | 8  | 0 | 8.825283  | -3.869404 | 0.569812  |
| 206 | 6  | 0 | 9.145100  | -5.284370 | 2.415228  |
| 207 | 6  | 0 | 8.949472  | -3.865154 | 2.939567  |
| 208 | 6  | 0 | 8.383486  | -3.164516 | 1.700475  |
| 209 | 7  | 0 | 6.896125  | -3.121757 | 1.655502  |
| 210 | 6  | 0 | 5.991534  | -4.130444 | 1.845533  |
| 211 | 7  | 0 | 4.719132  | -3.756304 | 1.614827  |
| 212 | 6  | 0 | 4.818797  | -2.470510 | 1.246951  |
| 213 | 6  | 0 | 3.775774  | -1.504593 | 0.985272  |
| 214 | 8  | 0 | 2.594104  | -1.802813 | 0.843205  |
| 215 | 7  | 0 | 4.245558  | -0.206766 | 0.888912  |
| 216 | 6  | 0 | 5.567892  | 0.135730  | 0.992956  |
| 217 | 7  | 0 | 5.896447  | 1.408073  | 0.993247  |
| 218 | 7  | 0 | 6.581782  | -0.772199 | 1.144851  |
| 219 | 6  | 0 | 6.167820  | -2.003407 | 1.293013  |
| 220 | 1  | 0 | 9.767411  | -5.839598 | -0.987988 |
| 221 | 1  | 0 | 10.110115 | -6.971805 | 0.366158  |
| 222 | 1  | 0 | 10.685723 | -4.702508 | 1.029244  |
| 223 | 1  | 0 | 8.155500  | -5.756227 | 2.376489  |
| 224 | 1  | 0 | 8.290948  | -3.788105 | 3.813305  |
| 225 | 1  | 0 | 9.925522  | -3.423285 | 3.188990  |
| 226 | 1  | 0 | 8.668262  | -2.105884 | 1.625519  |
| 227 | 1  | 0 | 6.266049  | -5.179614 | 2.080670  |
| 228 | 1  | 0 | 3.488498  | 0.538587  | 0.835173  |
| 229 | 1  | 0 | 5.210677  | 2.209120  | 1.018221  |
| 230 | 1  | 0 | 6.889778  | 1.607159  | 1.059024  |
| 231 | 1  | 0 | -8.687878 | -4.149703 | -2.839813 |
| 232 | 1  | 0 | 8.684502  | 4.543309  | -3.297118 |
| 233 | 1  | 0 | -5.096315 | -8.809286 | 3.429272  |

|     |   |   |            |           |           |
|-----|---|---|------------|-----------|-----------|
| 234 | 1 | 0 | 6.065571   | -8.080098 | -3.146203 |
| 235 | 8 | 0 | -5.584040  | -6.787509 | 3.203208  |
| 236 | 1 | 0 | -6.527327  | -7.001198 | 3.208715  |
| 237 | 1 | 0 | -10.416388 | 1.578408  | 1.927490  |
| 238 | 8 | 0 | -5.912030  | 9.022143  | -1.397905 |
| 239 | 1 | 0 | -5.777190  | 9.507896  | -2.221730 |
| 240 | 1 | 0 | -8.585294  | -5.919182 | -3.224072 |
| 241 | 8 | 0 | 10.030902  | -6.071497 | 3.145310  |
| 242 | 1 | 0 | 9.772819   | -6.992996 | 2.938082  |
| 243 | 8 | 0 | 5.958999   | 9.197537  | 3.406118  |
| 244 | 1 | 0 | 6.845947   | 9.444446  | 3.107658  |

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**Figure SI\_1.** Three-dimensional graphical representation of Fig. 7(a).

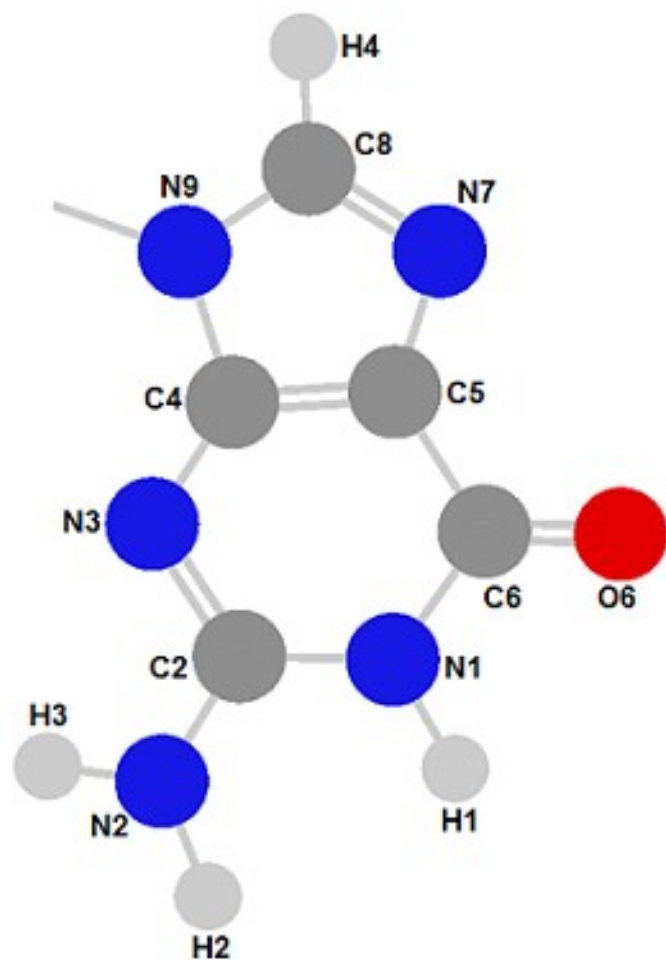
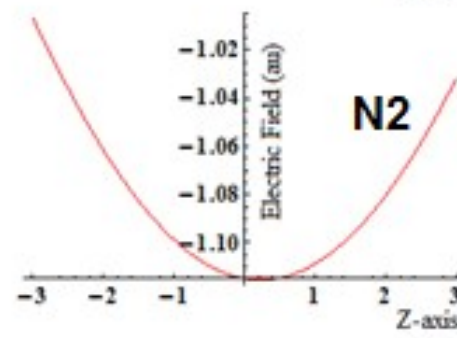
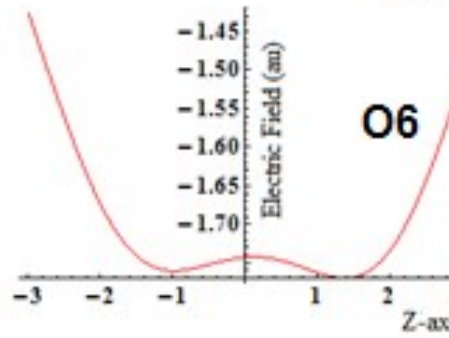
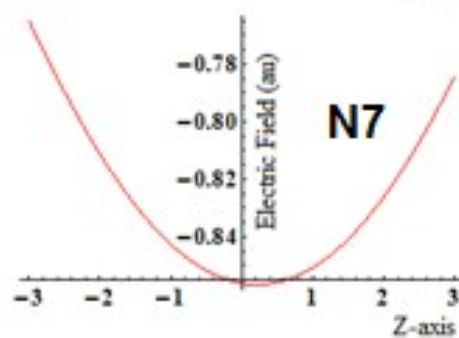
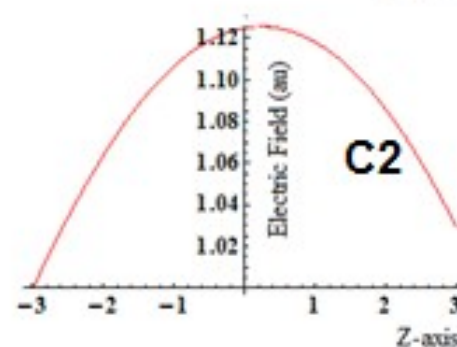
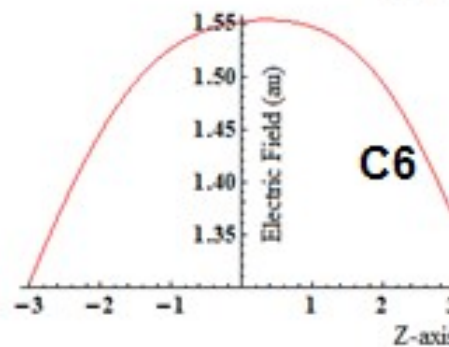
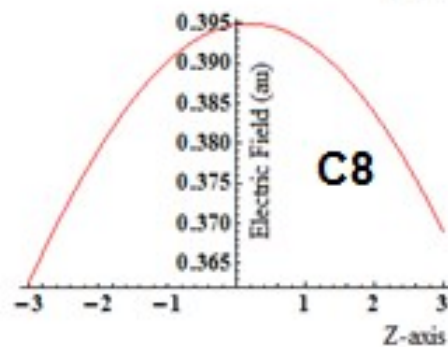
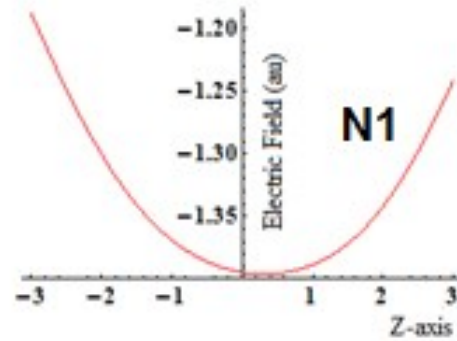
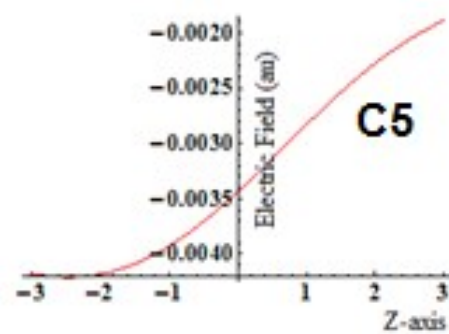
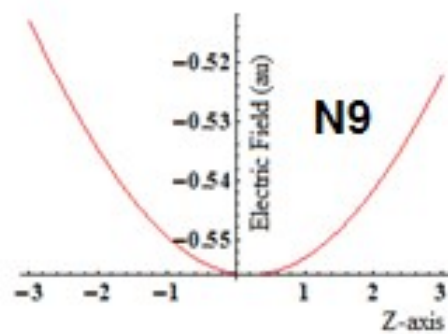
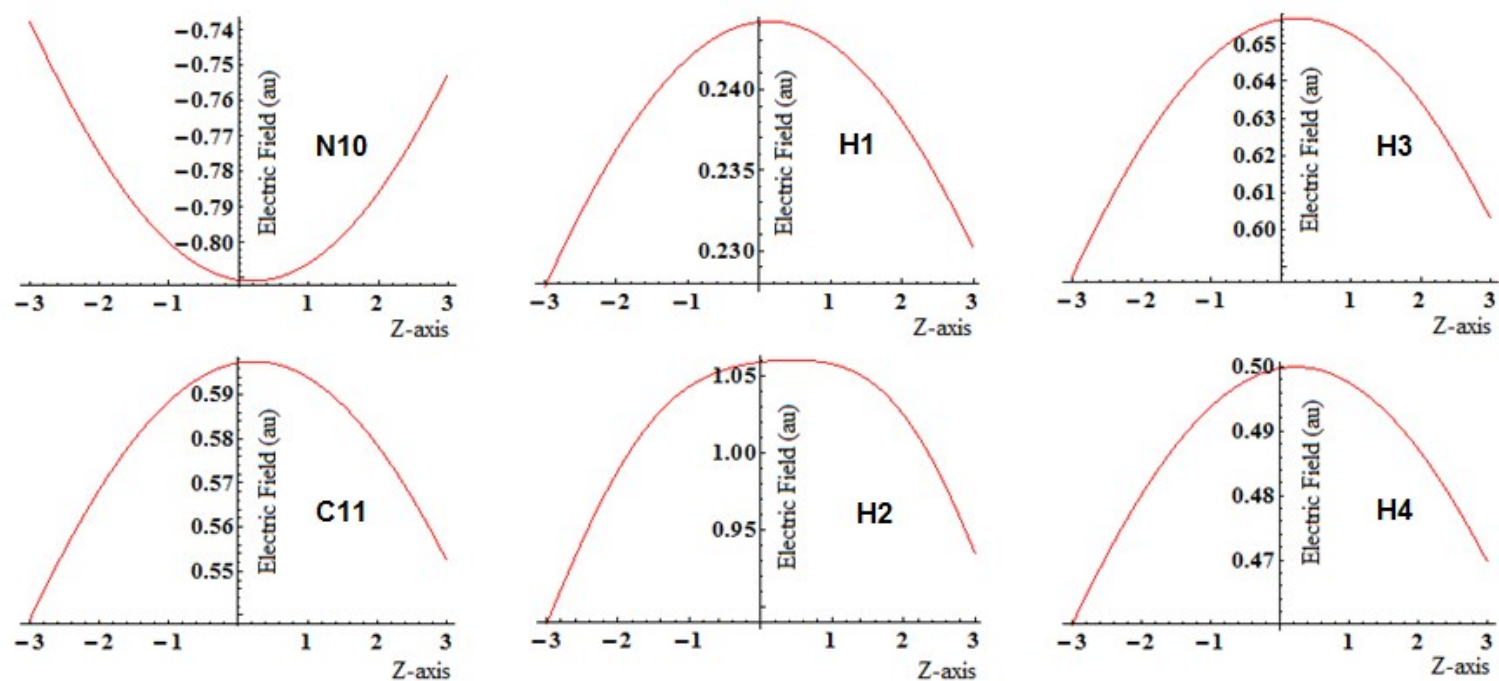
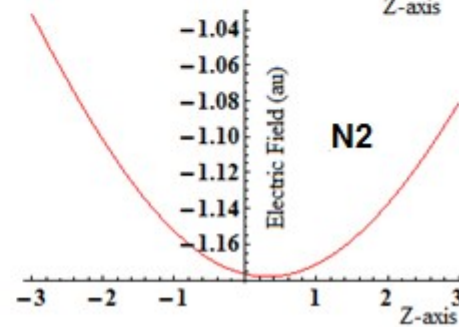
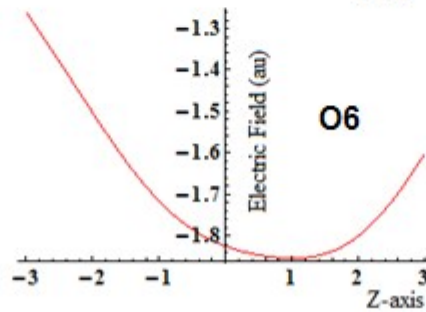
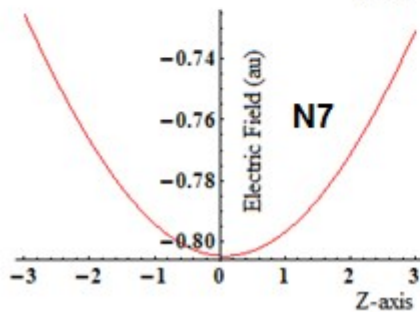
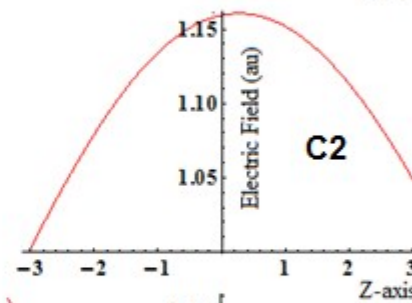
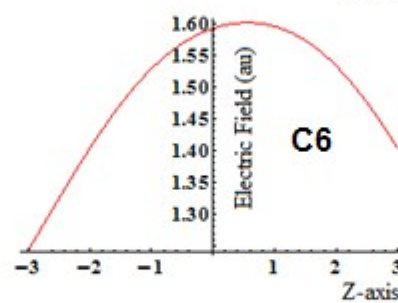
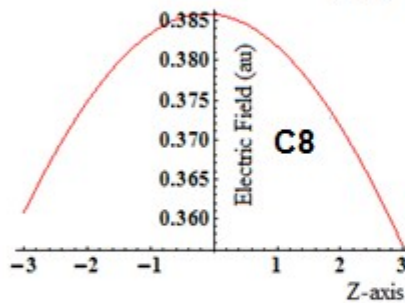
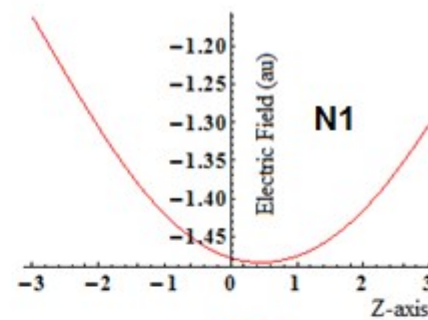
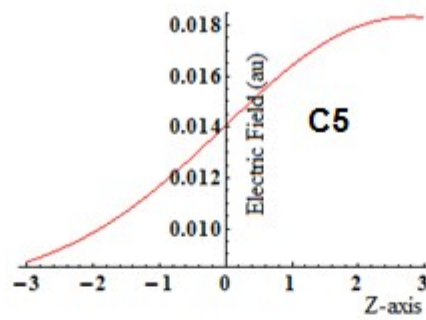
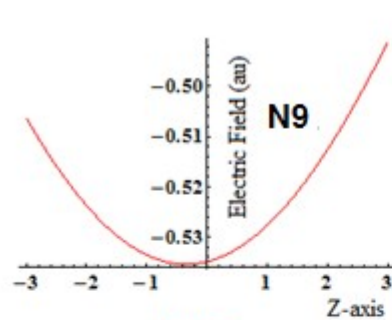


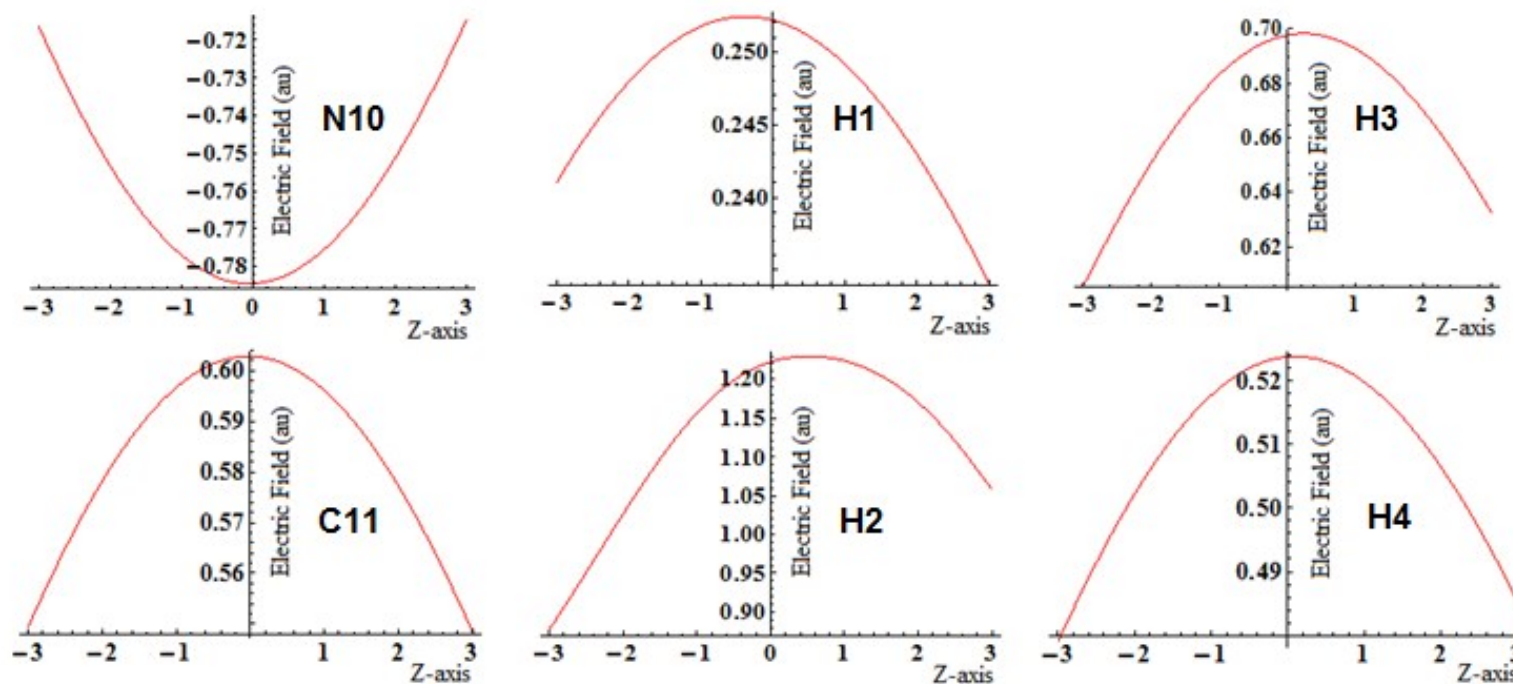
Figure SI\_2. Numbering of atoms of Guanine.



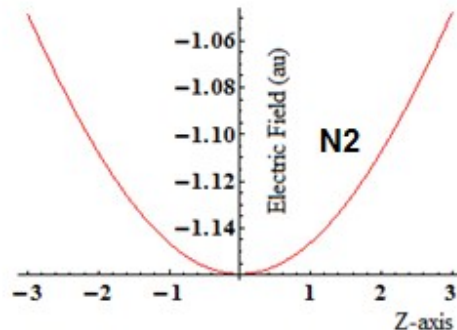
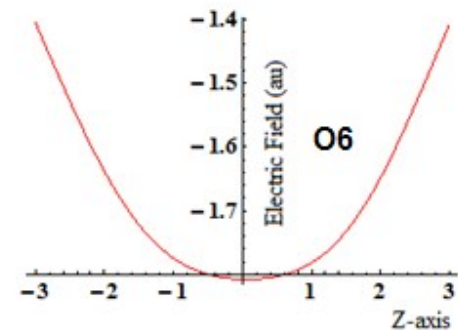
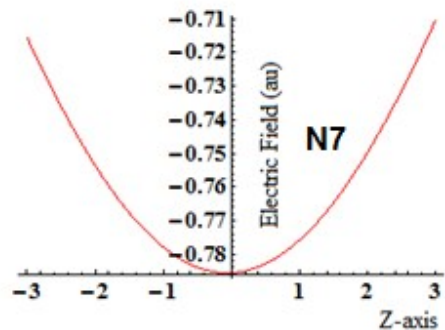
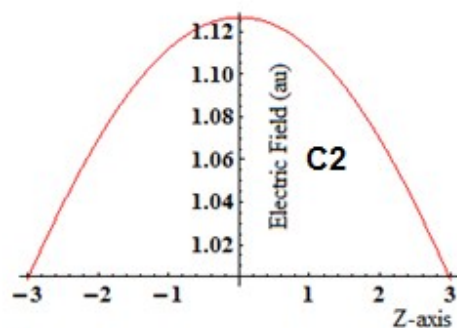
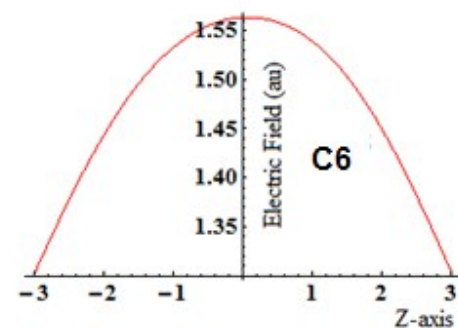
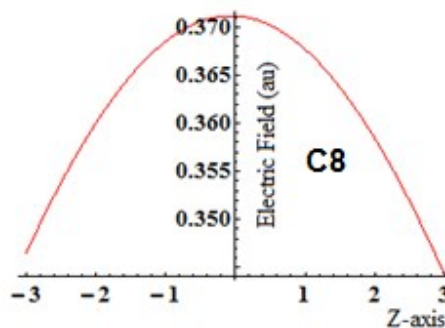
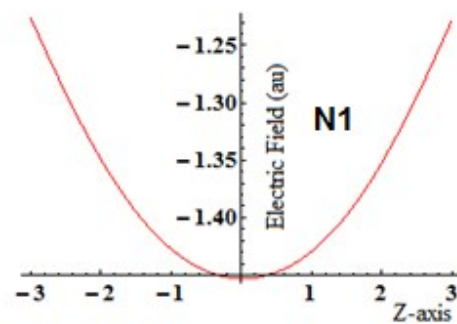
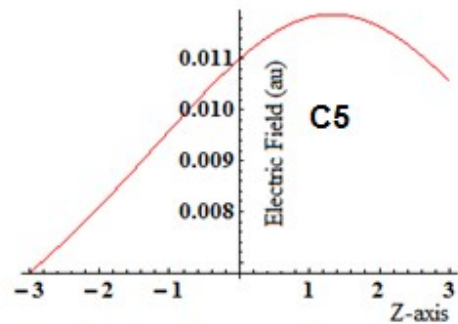
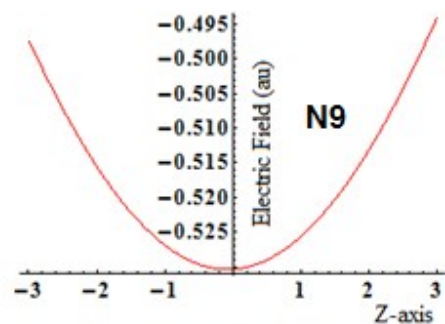


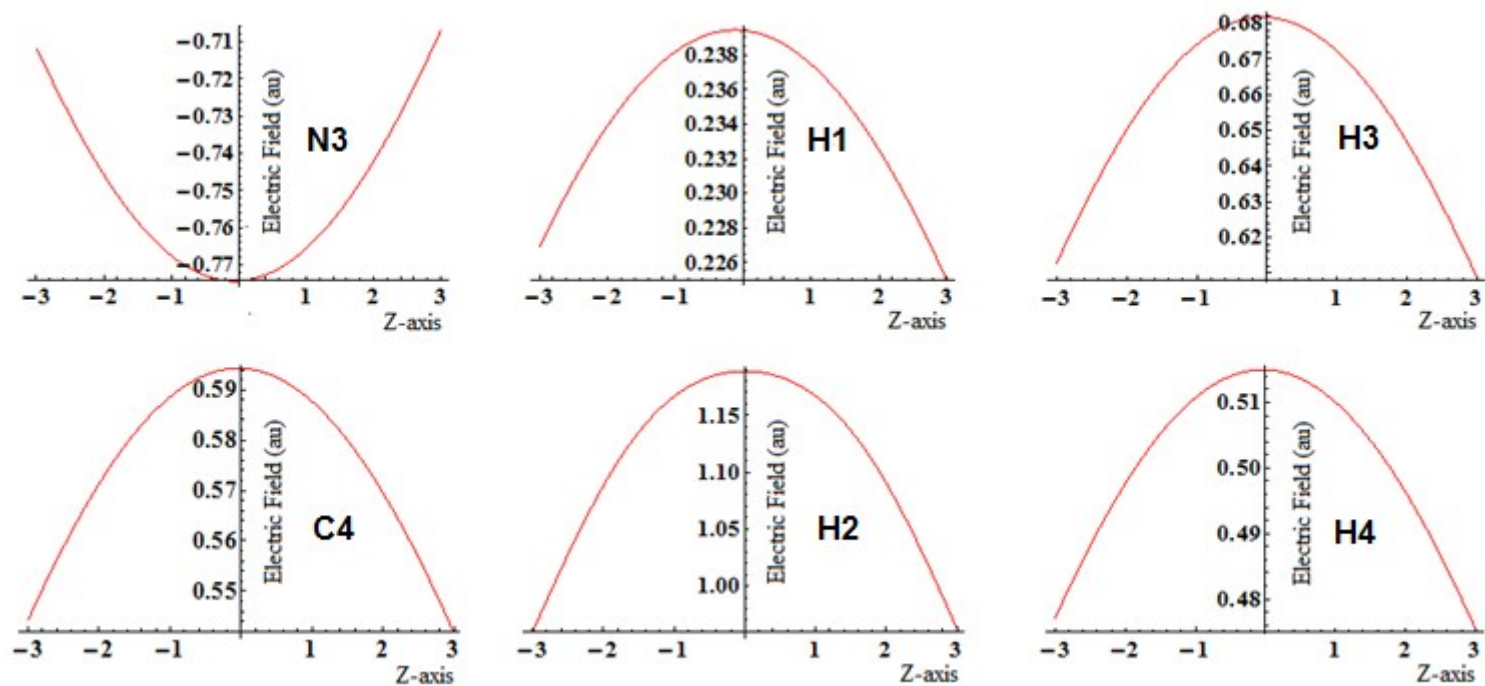
**Figure SI\_3.** Atomic decomposition in the atomic types of the Guanines (for the numeration see Fig. SI\_2) of the Z-component of the electric field of Fig. 12(a) of the system of Fig. 7(a).



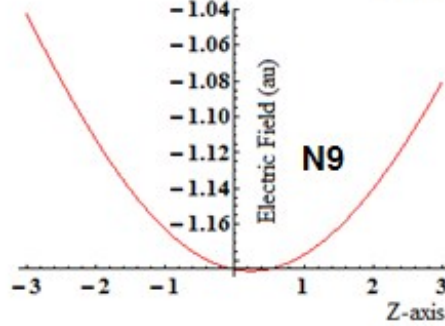
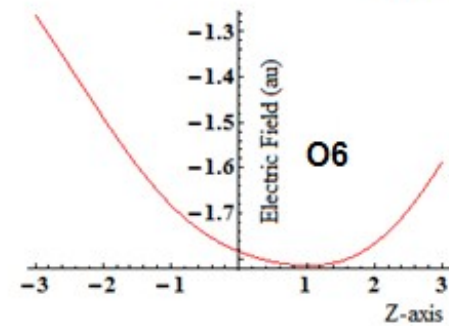
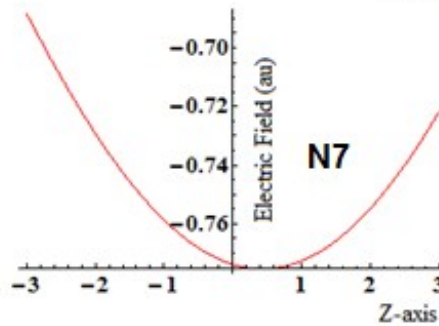
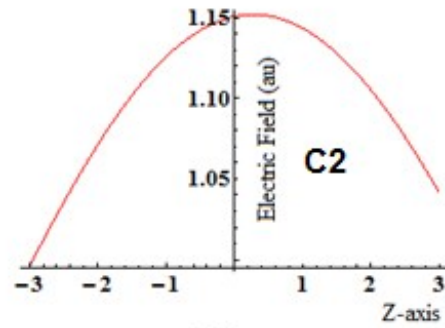
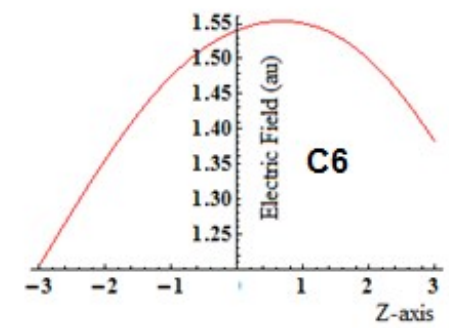
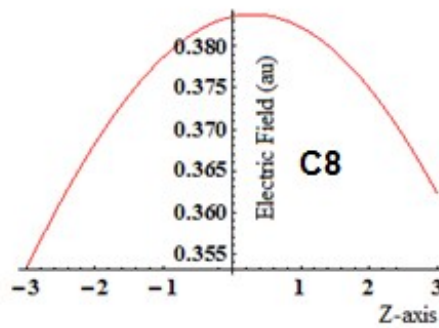
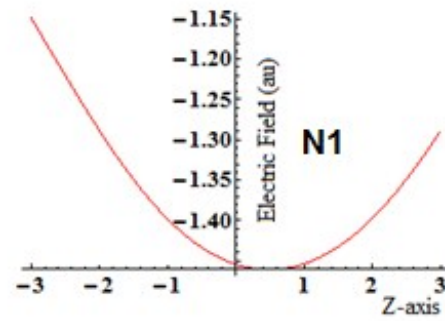
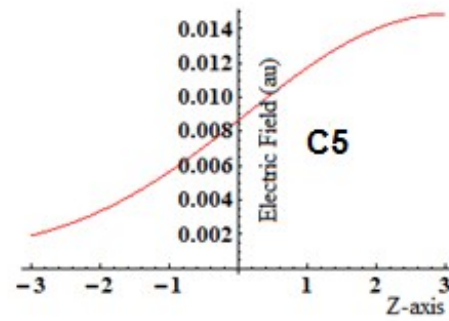
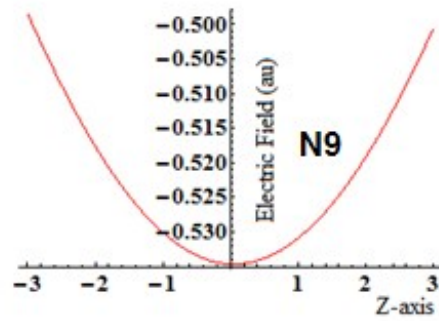


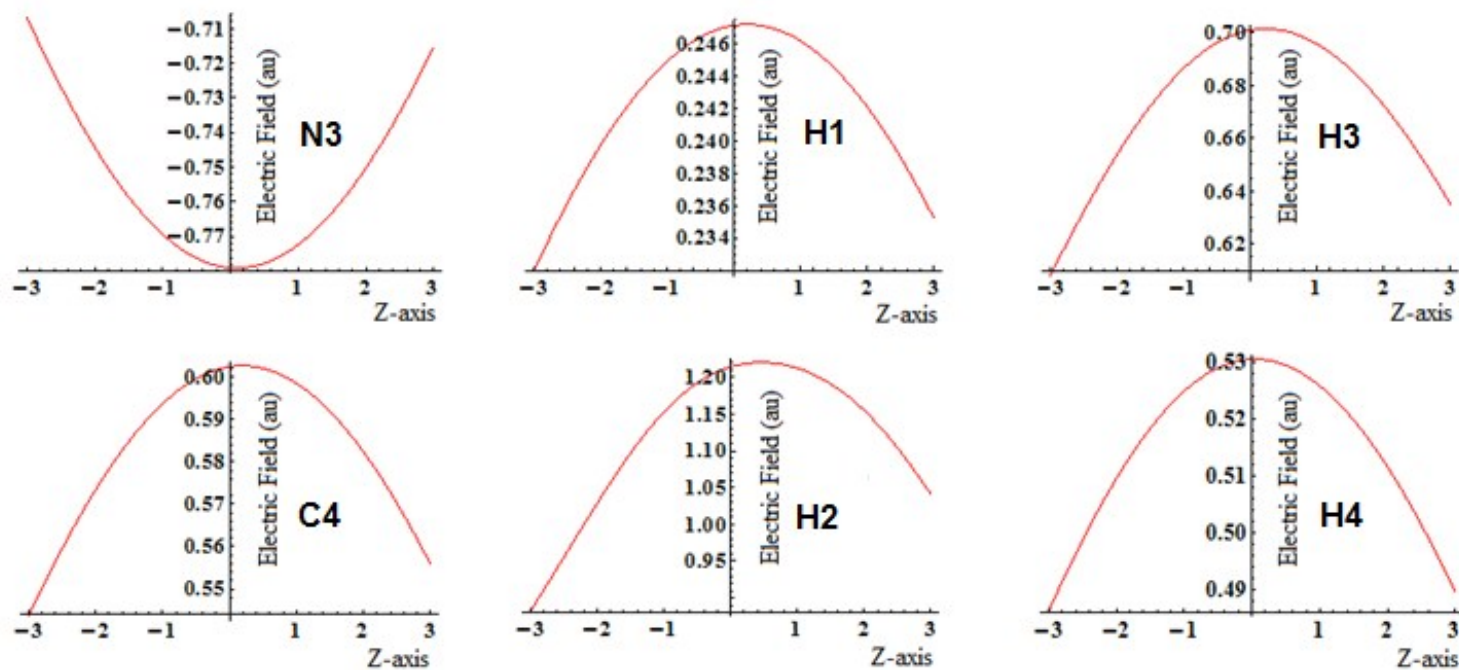
**Figure SI\_4.** Atomic decomposition in the atomic types of the Guanines (for the numeration see Fig. SI\_2) of the Z-component of the electric field of Fig. 12(a) of the system of Fig. 7(b) .





**Figure SI\_5.** Atomic decomposition in the atomic types of the Guanines (for the numeration see Fig. SI\_2) of the Z-component of the electric field of Fig. 12(a) of the system of Fig. 7(c).





**Figure SI\_6.** Atomic decomposition in the atomic types of the Guanines (for the numeration see Fig. SI\_2) of the Z-component of the electric field of Fig. 12(a) of the system of Fig. 7(d).