Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Supporting Information: Quantum Chemistry Meets High-Resolution Spectroscopy for Characterizing the Molecular Bricks of Life in the Gas-Phase

Vincenzo Barone*

*Scuola Normale Superiore di Pisa, piazza dei Cavalieri 7, 56126 Pisa, Italy*

E-mail: vincenzo.barone@sns.it

# PCS/BONDS

Beta version.

The Pisa Composite Scheme (PCS) in its BONDS variant applies a set of linear corrections to covalent bonds starting from an initial geometry provided as input. The tool is used in three sequential steps:

- Select or deselect the optional valence corrections (on by default).
- Upload the starting geometry using an XYZ or Gaussian LOG file.
- Visualize the refined molecular structure, view its properties and download the refined XYZ geometry file.

The tool employs the redundant internal coordinates and penality function approach to determine improved Cartesian coordinates.

**PCS/BONDS**

$$r_{PCS/Bonds} = r(rDSD/3F12) + \Delta r_B$$

$$\Delta r_B = \Delta r_{CVB} + \Delta r_{VB}$$

$$\Delta r_{ij}^{CVB} = -k\sqrt{N_i N_j - 1}\left(r_i^{cov} + r_j^{cov}\right), N_i = min(n_i, 3)$$

$$\Delta r_{ij}^{VB} = \Delta r_{ij}^{CVB}\left\{\left(\sqrt{|P_{ij} - 2|} - 1\right)[1 - \delta(i,O) - \delta(j,O) + \delta(i,O)\delta(j,O)]\right\} - 0.25\left(1 - P_{ij}\right)^2[\delta(i,C)\delta(j,F) + \delta(i,F)\delta(j,C)]$$

☑ DVB correction

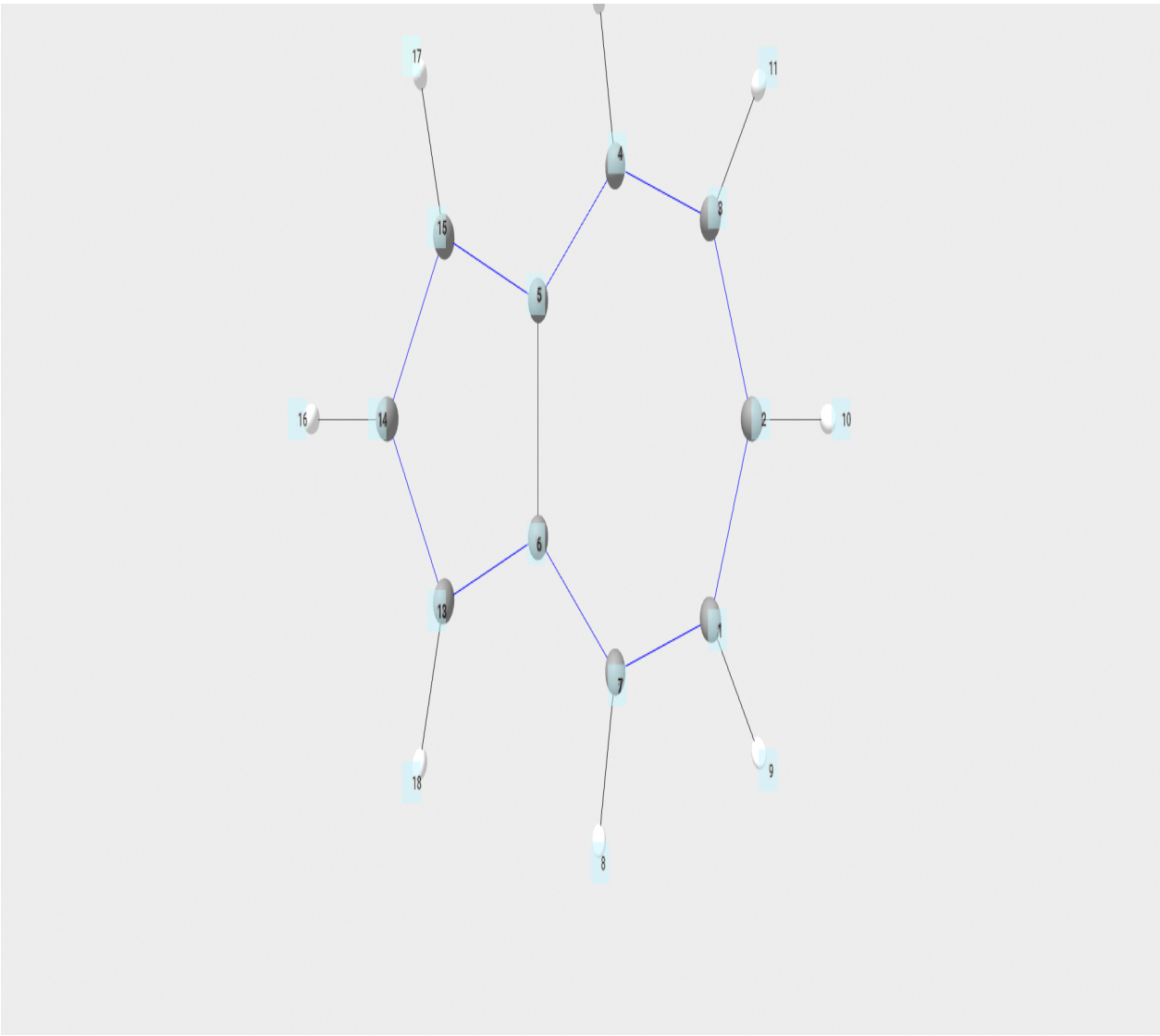
**2. Upload a molecular structure (XYZ or Gaussian LOG file).**

Scegli file azulene_revDSD_3F12-.xyz

**3. Download refined structure and view its properties.**


https://www.skies-village.it/proxima/pcsbonds/

PCS/BONDS




https://www.skies-village.it/proxima/pcsbonds/

Download refined structure

Converged! RMSD(R): 9.997845754158337e-7, MAX(R): 0.000002420441375328153

### Input Structure

```
6 1.913854 -1.263969 0.000000
6 2.504017 -0.000000 0.000000
6 1.913854 1.263969 0.000000
6 0.558209 1.593153 0.000000
6 -0.541981 0.746273 0.000000
6 -0.541981 -0.746273 0.000000
6 0.558209 -1.593153 0.000000
1 0.327070 -2.655939 0.000000
1 2.602115 -2.102763 0.000000
1 3.590234 -0.000000 0.000000
1 2.602115 2.102763 0.000000
1 0.327070 2.655939 0.000000
6 -1.886709 -1.148371 0.000000
6 -2.692789 -0.000000 0.000000
6 -1.886709 1.148371 0.000000
1 -3.775137 -0.000000 0.000000
1 -2.229330 2.173795 0.000000
1 -2.229330 -2.173795 0.000000
```

### Refined structure

```
18
 refined
6 1.911114 -1.262078 0.000000
6 2.500568 -0.000000 0.000000
6 1.911114 1.262078 0.000000
6 0.557375 1.590580 0.000000
6 -0.541288 0.744897 0.000000
6 -0.541288 -0.744897 0.000000
6 0.557375 -1.590580 0.000000
1 0.326449 -2.652174 0.000000
1 2.598504 -2.100028 0.000000
1 3.585578 -0.000000 0.000000
1 2.598504 2.100028 0.000000
1 0.326449 2.652174 0.000000
6 -1.883953 -1.146571 0.000000
6 -2.688948 -0.000000 0.000000
6 -1.883953 1.146571 0.000000
1 -3.770096 -0.000000 0.000000
1 -2.226138 2.170877 0.000000
1 -2.226138 -2.170877 0.000000
```

### Bond distances

(i, j) | Old dist | New dist | Convergence Err (%) | Original Bond Order

| | | | | |
|---|---|---|---|---|
| (1, 2) | 1.394959 | 1.392945 | 0.000067 | 1.517 |
| (1, 7) | 1.395040 | 1.393027 | 0.000029 | 1.517 |
| (1, 9) | 1.085025 | 1.083819 | 0.000001 | 0.951 |
| (2, 3) | 1.394959 | 1.392945 | 0.000067 | 1.517 |
| (2, 10) | 1.086217 | 1.085010 | 0.000027 | 0.947 |
| (3, 4) | 1.395040 | 1.393027 | 0.000029 | 1.517 |
| (3, 11) | 1.085025 | 1.083819 | 0.000001 | 0.951 |
| (4, 5) | 1.388389 | 1.386449 | 0.000081 | 1.551 |
| (4, 12) | 1.087630 | 1.086420 | 0.000021 | 0.943 |
| (5, 6) | 1.492546 | 1.489795 | 0.000162 | 1.096 |
| (5, 15) | 1.403558 | 1.401460 | 0.000102 | 1.474 |
| (6, 7) | 1.388389 | 1.386449 | 0.000081 | 1.551 |
| (6, 13) | 1.403558 | 1.401460 | 0.000102 | 1.474 |
| (7, 8) | 1.087630 | 1.086420 | 0.000021 | 0.943 |
| (13, 14) | 1.403040 | 1.400944 | 0.000103 | 1.477 |
| (13, 18) | 1.081149 | 1.079951 | 0.000002 | 0.964 |
| (14, 15) | 1.403040 | 1.400944 | 0.000103 | 1.477 |
| (14, 16) | 1.082348 | 1.081148 | 0.000013 | 0.960 |
| (15, 17) | 1.081149 | 1.079951 | 0.000002 | 0.964 |

### Parent rotational constants

Asymmetric top, nearly oblate

| MHz | A | B | C |
|---|---|---|---|
| Before correcting | 2856.3788184 | 1259.1727793 | 873.9228194 |
| After correcting | 2865.2631869 | 1262.7460638 | 876.4757032 |

Cartesian Coordinates of all the structures optimized at the rDSD/3F12$^-$ level.

```
 H2CS 4 atoms
 1     1.669324     0.923620     0.000000
 6     1.093395    -0.000000     0.000000
16    -0.515622     0.000000    -0.000000
 1     1.669324    -0.923620    -0.000000

 CH2F2 5 atoms
 1    -0.000000    -1.155015     0.911123
 6    -0.000000    -0.557145     0.000000
 1    -0.000000    -1.155015    -0.911123
 9    -1.101211     0.237226     0.000000
 9     1.101211     0.237226    -0.000000

 Pyrrole 10 atoms
 6     0.982406     0.711702     0.000000
 6     0.982406    -0.711702     0.000000
 6    -0.331306     1.122466     0.000000
 1     1.844094     1.359972     0.000000
 6    -0.331306    -1.122466     0.000000
 1     1.844094    -1.359972     0.000000
 7    -1.118521     0.000000     0.000000
 1    -0.764995     2.108829     0.000000
 1    -2.122136     0.000000     0.000000
 1    -0.764995    -2.108829     0.000000

 Furan 9 atoms
 8    -1.131052     0.000000    -0.000000
 6    -0.318717    -1.092247    -0.000000
 6    -0.318717     1.092247     0.000000
 6     0.986442    -0.717189    -0.000000
 6     0.986442     0.717189     0.000000
 1    -0.815186    -2.047362    -0.000000
 1    -0.815186     2.047362     0.000000
 1     1.840004    -1.375105    -0.000000
 1     1.840004     1.375105     0.000000

 Thiophene 9 atoms
16     1.142271     0.000000     0.000000
 6    -0.045367     1.233319    -0.000000
 6    -0.045367    -1.233319     0.000000
 6    -1.311854     0.711532    -0.000000
 6    -1.311854    -0.711532    -0.000000
 1     0.247564     2.271804    -0.000000
 1     0.247564    -2.271804     0.000000
 1    -2.205967     1.319792    -0.000000
 1    -2.205967    -1.319792    -0.000000

 Pyridine 11 atoms
 1    -2.494015     0.000000     0.000000
 6    -1.410500     0.000000     0.000000
 6    -0.699065     1.194769     0.000000
 1    -1.206310     2.151475     0.000000
```

```
 6     0.692105     1.140055     0.000000
 1     1.275926     2.054914     0.000000
 7     1.390142     0.000000     0.000000
 6     0.692105    -1.140055     0.000000
 1     1.275926    -2.054914     0.000000
 6    -0.699065    -1.194769     0.000000
 1    -1.206310    -2.151475     0.000000

2-Fluoropyridine 11 atoms
 1     1.812293     2.101399     0.000000
 6     1.236690     1.183763     0.000000
 6    -0.148775     1.232038     0.000000
 1    -0.704004     2.159663     0.000000
 6    -0.814701     0.009847    -0.000000
 9    -2.152682     0.024394    -0.000000
 7    -0.254329    -1.173276    -0.000000
 6     1.087539    -1.200333    -0.000000
 1     1.539397    -2.185942    -0.000000
 6     1.873803    -0.057630     0.000000
 1     2.952727    -0.136474     0.000000

3-Fluoropyridine 11 atoms
 1    -0.773478     2.157973     0.000000
 6    -0.207334     1.235405     0.000000
 6    -0.856033     0.014395    -0.000000
 9    -2.198537    -0.029040    -0.000000
 6    -0.139563    -1.174483    -0.000000
 1    -0.663495    -2.124114    -0.000000
 7     1.194277    -1.194259    -0.000000
 6     1.834746    -0.020983     0.000000
 1     2.917973    -0.068996     0.000000
 6     1.183628     1.209327     0.000000
 1     1.753501     2.129830     0.000000

3-Furonitrile 10 atoms
  8    1.786767     0.675360     0.000000
  6    1.792980    -0.689207    -0.000000
  6    0.527857    -1.173935    -0.000000
  6   -0.328036    -0.017802    -0.000000
  6    0.496231     1.070208     0.000000
  6   -1.749721     0.004155     0.000000
  7   -2.911573     0.008394     0.000000
  1    2.763298    -1.154381    -0.000000
  1    0.223033    -2.206961    -0.000000
  1    0.307953     2.130091     0.000000

Azulene 18 atoms
 6     1.913854    -1.263969     0.000000
 6     2.504017     0.000000     0.000000
 6     1.913854     1.263969     0.000000
 6     0.558209     1.593153     0.000000
 6    -0.541981     0.746273     0.000000
 6    -0.541981    -0.746273     0.000000
```

```
 6     0.558209    -1.593153     0.000000
 1     0.327070    -2.655939     0.000000
 1     2.602115    -2.102763     0.000000
 1     3.590234    -0.000000     0.000000
 1     2.602115     2.102763     0.000000
 1     0.327070     2.655939     0.000000
 6    -1.886709    -1.148371     0.000000
 6    -2.692789     0.000000     0.000000
 6    -1.886709     1.148371     0.000000
 1    -3.775137     0.000000     0.000000
 1    -2.229330     2.173795     0.000000
 1    -2.229330    -2.173795     0.000000

Quinoline 17 atoms
 6    -2.318629     0.717891    -0.000000
 6    -2.399293    -0.695563    -0.000000
 6    -1.237182    -1.422056     0.000000
 6     0.002486    -0.738885     0.000000
 6    -0.027074     0.682872     0.000000
 7    -1.191920     1.395742    -0.000000
 6     1.196445     1.397679     0.000000
 6     2.392992     0.724101     0.000000
 6     2.422604    -0.691177     0.000000
 6     1.252191    -1.408420     0.000000
 1    -3.368357    -1.179084     0.000000
 1    -1.250775    -2.506983     0.000000
 1    -3.232327     1.305726    -0.000000
 1     1.149795     2.479843    -0.000000
 1     3.325110     1.276830     0.000000
 1     3.375596    -1.206887     0.000000
 1     1.267100    -2.493256     0.000000

Glycine 10 atoms
Conformer I
  6   -0.768058    -0.744960     0.000000
  7   -2.003394     0.006849    -0.000000
  1   -2.035495     0.617509    -0.807580
  6    0.500998     0.087190    -0.000000
  8    0.552240     1.291109    -0.000000
  8    1.601457    -0.698022     0.000000
  1    2.366332    -0.106134     0.000000
  1   -0.730192    -1.402411    -0.872200
  1   -0.730192    -1.402411     0.872200
  1   -2.035495     0.617509     0.807580
Conformer II
 6   -0.713544    -0.816435     0.100305
 7   -1.864313     0.072570    -0.070529
 1   -2.211014     0.053183    -1.020456
 6    0.605346    -0.048453     0.007689
 8    1.672407    -0.597322    -0.065279
 8    0.465896     1.282729     0.040831
 1   -0.499012     1.437866     0.085972
 1   -0.737843    -1.262751     1.095965
```

```
 1   -0.667773    -1.636619    -0.618397
 1   -2.629059    -0.179822     0.539006

Cycloserine 13 atoms
Form I
 6    0.298849     0.804473     0.066192
 7   -1.022624     0.934730    -0.305205
 8   -1.763154    -0.207122     0.118095
 6   -0.818084    -1.269466    -0.064072
 6    0.508260    -0.678693     0.393902
 8    1.129690     1.685634     0.054996
 1   -1.171435    -2.111704     0.524734
 1   -0.765474    -1.543138    -1.124664
 7    1.662420    -1.308618    -0.211290
 1    0.597107    -0.750805     1.482086
 1   -1.531945     1.781474    -0.095389
 1    1.657497    -1.152110    -1.213705
 1    2.508895    -0.876180     0.140856
Form II
 6   -0.843767    -0.291795     0.130509
 7   -0.031817    -1.366246    -0.178155
 8    1.305383    -0.926741    -0.391650
 6    1.427602     0.137622     0.568795
 6    0.096116     0.863849     0.496216
 8   -2.054784    -0.292060     0.100125
 1    1.589848    -0.292924     1.561284
 1    2.276561     0.745397     0.264458
 7    0.096395     1.898727    -0.533771
 1   -0.197481     1.305303     1.447865
 1   -0.307976    -2.012795    -0.903903
 1   -0.846968     2.248530    -0.664171
 1    0.386219     1.501290    -1.421927

Creatinine 15 atoms
ZI
 6    1.441029    -0.052101    -0.011880
 7   -0.810398    -0.624488     0.210997
 7    0.632698     1.052359     0.003593
 1    0.962457     2.002816    -0.029974
 6   -0.730072     0.746014     0.044533
 7   -1.620592     1.651853    -0.049418
 1   -2.556438     1.262085    -0.007033
 8    2.649067    -0.079683    -0.043199
 6   -2.018254    -1.348555    -0.107632
 1   -2.877407    -0.862776     0.354474
 1   -2.189839    -1.420155    -1.188698
 1   -1.945540    -2.354666     0.305057
 6    0.487582    -1.239970     0.001275
 1    0.555943    -1.761383    -0.961767
 1    0.754519    -1.938877     0.796167
EI
 6    1.448984    -0.051336    -0.011451
 7   -0.799904    -0.618945     0.183328
```

```
 7    0.639717    1.058476   -0.000334
 1    0.997813    1.998662   -0.008118
 6   -0.729455    0.745841    0.038758
 7   -1.737935    1.522529   -0.034474
 1   -1.453597    2.493253   -0.112591
 8    2.656790   -0.071192   -0.033189
 6   -2.023579   -1.337058   -0.088085
 1   -2.863303   -0.696329    0.169766
 1   -2.102658   -1.616300   -1.145493
 1   -2.057364   -2.241890    0.520338
 6    0.494411   -1.236341   -0.005758
 1    0.574148   -1.765567   -0.964098
 1    0.753193   -1.931864    0.795571
A1
 6    1.436770    0.002731    0.020972
 7   -0.781374   -0.649157   -0.239025
 7    0.626976    1.133486    0.042349
 6   -0.605869    0.695326   -0.055109
 8    2.644523   -0.031383    0.059916
 6    0.535908   -1.242280   -0.069184
 1    0.601563   -1.818504    0.859486
 1    0.819581   -1.878858   -0.907708
 6   -1.968638   -1.369395    0.173382
 1   -2.034816   -1.466755    1.263251
 1   -2.868670   -0.873376   -0.189018
 1   -1.945155   -2.365091   -0.268183
 7   -1.672882    1.525945    0.041574
 1   -1.442993    2.504071   -0.015318
 1   -2.545291    1.250266   -0.372579

Isoamilacetate 23 atoms
 6   -2.879984   -1.412198   -0.135426
 6   -2.170973   -0.089169   -0.041055
 8   -2.663044    0.988208   -0.275078
 8   -0.891342   -0.255895    0.345330
 6   -0.118969    0.956059    0.470305
 6    1.287601    0.565816    0.871158
 6    2.019657   -0.344877   -0.118962
 6    2.153998    0.295458   -1.499168
 6    3.394868   -0.708333    0.436852
 1   -3.904711   -1.251686   -0.459056
 1   -2.867341   -1.906695    0.836709
 1   -2.360138   -2.060462   -0.841924
 1   -0.149035    1.491074   -0.479629
 1   -0.586183    1.592783    1.223812
 1    1.251257    0.078295    1.850669
 1    1.861443    1.491801    1.000046
 1    1.435867   -1.265643   -0.221446
 1    2.683646    1.251220   -1.430991
 1    2.722532   -0.352600   -2.170202
 1    1.183867    0.479794   -1.964653
 1    4.013146    0.187804    0.550018
 1    3.314193   -1.185520    1.416666
```

```
 1    3.921221    -1.394269    -0.230920

Aspirine 21 atoms
 6    0.816147     0.483394     0.095362
 6    0.272125    -0.784803     0.344563
 6    1.069970    -1.919825     0.315036
 6    2.426295    -1.810221     0.031260
 6    2.984695    -0.561263    -0.227568
 6    2.183543     0.571906    -0.194629
 6   -0.014614     1.713537     0.157677
 8   -1.052149    -0.957517     0.697346
 8   -1.185717     1.773170     0.452315
 8    0.694546     2.825489    -0.147992
 6   -1.989419    -0.744217    -0.285396
 1    0.069227     3.559540    -0.079755
 8   -1.702114    -0.597266    -1.440092
 6   -3.361578    -0.734030     0.311090
 1    0.610135    -2.879265     0.514640
 1    3.043239    -2.700384     0.008514
 1    4.039605    -0.469622    -0.453068
 1    2.611100     1.544996    -0.391204
 1   -3.479601    -1.554962     1.017576
 1   -4.102909    -0.796272    -0.480961
 1   -3.478057     0.204315     0.855967

Vitamin C 20 atoms
 Conformer I
 6    0.361557    -0.374769    -0.480370
 8   -0.659862    -1.385265    -0.421282
 6   -1.842013    -0.793486    -0.061274
 6   -1.635216     0.646180     0.068822
 6   -0.349283     0.920076    -0.204278
 8   -2.870133    -1.400843     0.094757
 8   -2.652728     1.475705     0.374709
 8    0.249621     2.116363    -0.272016
 6    1.450598    -0.773456     0.521109
 6    2.434598     0.343501     0.810708
 8    2.812314     1.060933    -0.368028
 8    2.197916    -1.864537     0.002548
 1    0.785399    -0.389656    -1.488531
 1   -3.440328     0.922962     0.469817
 1    1.179945     1.987437    -0.527794
 1    0.955511    -1.051598     1.460020
 1    1.589377    -2.587842    -0.180791
 1    3.283106     0.459146    -0.952921
 1    1.978121     1.080273     1.470569
 1    3.311794    -0.077657     1.306832
Conformer  II
 6    0.209039    -0.011489    -1.031064
 8   -0.621413    -1.173079    -0.957605
 6   -1.728824    -0.873287    -0.206881
 6   -1.629945     0.504507     0.267960
 6   -0.479122     1.024723    -0.184674
```

```
 8   -2.613271    -1.659755     0.015698
 8   -2.585939     1.047668     1.049464
 8    0.035890     2.245000     0.018098
 6    1.624487    -0.338738    -0.570297
 6    1.705858    -0.804530     0.869284
 8    3.101093    -0.940872     1.135981
 8    2.349943     0.880973    -0.739797
 1    0.258208     0.314408    -2.075013
 1   -3.267589     0.371070     1.160693
 1    0.965576     2.213037    -0.260538
 1    2.043776    -1.116187    -1.218149
 1    3.190813     0.765862    -0.281124
 1    3.225109    -1.139192     2.066605
 1    1.253655    -0.059971     1.532458
 1    1.180730    -1.756995     0.981466
Conformer III
 6   -0.353523    -0.455218    -0.795416
 8   -0.187153     0.973250    -0.674366
 6    1.050089     1.243861    -0.151022
 6    1.756946    -0.015629     0.041818
 6    0.953230    -1.016293    -0.336282
 8    1.443537     2.355889     0.088508
 8    3.012417    -0.082494     0.539732
 8    1.127952    -2.347772    -0.340571
 6   -1.551292    -0.920408     0.039729
 6   -2.837349    -0.191994    -0.356439
 8   -2.889482     1.108773     0.209467
 8   -1.303870    -0.765066     1.417476
 1   -0.538958    -0.679427    -1.851161
 1    3.293491     0.822550     0.727825
 1    1.987361    -2.555719     0.044222
 1   -1.669683    -1.990513    -0.160708
 1   -1.679419     0.090272     1.663781
 1   -2.169332     1.625754    -0.169356
 1   -2.939181    -0.162787    -1.447360
 1   -3.691815    -0.728894     0.055350

Uracil 12 atoms
    6    1.284614     0.312086     0.000000
    7    0.034976     0.949478     0.000000
    6   -1.216052     0.368704     0.000000
    7   -1.174808    -1.015698     0.000000
    6   -0.007792    -1.738244     0.000000
    6    1.199306    -1.142530     0.000000
    1   -2.071601    -1.472056     0.000000
    8   -2.253526     0.996013     0.000000
    1    0.046777     1.959872     0.000000
    8    2.308378     0.966836     0.000000
    1   -0.127684    -2.813517     0.000000
    1    2.115688    -1.711219     0.000000

2-Thiouracil 12 atoms
    7   -0.203123    -0.840560     0.000000
```

```
   6    0.853886    0.023739   -0.000000
   7    0.482671    1.343113   -0.000000
   6   -0.821831    1.767434   -0.000000
   6   -1.849858    0.897442   -0.000000
   6   -1.576225   -0.531295    0.000000
   1    0.029895   -1.824485    0.000000
  16    2.433402   -0.452163    0.000000
   1    1.243623    2.002945   -0.000000
   1   -0.959315    2.840475   -0.000000
   1   -2.877078    1.226543   -0.000000
   8   -2.401025   -1.422156    0.000000

Adenine 15 atoms
   6   -1.205420    0.658807    0.001521
   7   -1.960115   -0.446863    0.008249
   6   -1.344580   -1.640655    0.003494
   7   -0.039091   -1.906864   -0.003885
   6    0.681750   -0.780285   -0.003989
   6    0.193216    0.523057   -0.000919
   7    1.223441    1.448968    0.005143
   6    2.306667    0.710960    0.003696
   7    2.048144   -0.639212   -0.002473
   1    2.719412   -1.388386   -0.004172
   7   -1.811445    1.867317   -0.029754
   1   -1.259166    2.691264    0.127990
   1   -2.802419    1.900989    0.131467
   1   -2.004979   -2.500805    0.007858
   1    3.316393    1.092447    0.007252

Thymine 15 atoms
   6   -0.749894   -0.831627    0.000000
   7    0.636961   -1.011959    0.000000
   6    1.619268   -0.042395    0.000000
   7    1.108431    1.239721    0.000000
   6   -0.239179    1.524483    0.000000
   6   -1.186003    0.565450    0.000000
   1    1.793851    1.976113    0.000000
   8    2.808206   -0.285808    0.000000
   1    0.965435   -1.967353    0.000000
   8   -1.496246   -1.793478    0.000000
   1   -0.486848    2.578436    0.000000
   6   -2.655540    0.844137    0.000000
   1   -3.130839    0.400664    0.876877
   1   -2.846631    1.918004    0.000000
   1   -3.130839    0.400664   -0.876877

 Cytosine 13 atoms
 EA
 7    -0.072320   -0.985054   -0.005931
 6     1.069531   -0.307915   -0.000084
 7     1.247982    1.010842    0.001600
 6     0.113202    1.728021   -0.000783
 6    -1.141130    1.159679   -0.002004
```

```
 6     -1.185667    -0.247580    -0.003516
 8      2.176292    -1.067341     0.000327
 1      2.919491    -0.451343     0.002477
 1      0.231631     2.806435    -0.000780
 1     -2.039711     1.761387     0.003823
 7     -2.363616    -0.930686     0.035936
 1     -3.210484    -0.456004    -0.219233
 1     -2.312238    -1.917188    -0.154552
EAc
 7    -0.056705    -0.970551    -0.006664
 6     1.084978    -0.279393    -0.000307
 7     1.249360     1.035013     0.000923
 6     0.103169     1.731782    -0.000943
 6    -1.148741     1.152933    -0.001252
 6    -1.182852    -0.251730    -0.003630
 8     2.214852    -1.004400     0.001076
 1     1.943694    -1.930224     0.003748
 1     0.207132     2.811951    -0.001191
 1    -2.052323     1.747133     0.005301
 7    -2.354210    -0.949669     0.037900
 1    -3.201658    -0.480939    -0.227564
 1    -2.294255    -1.931830    -0.171188
 KA
  7    -0.078153    -1.021898    -0.007797
  6     1.162980    -0.435742     0.000144
  7     1.189456     0.978788     0.001013
  6     0.075602     1.745762    -0.000459
  6    -1.146405     1.162871    -0.001493
  6    -1.157926    -0.274770    -0.003988
  8     2.219195    -1.036845     0.001531
  1     2.108847     1.390779     0.002658
  1     0.220501     2.818340     0.001231
  1    -2.053492     1.748415     0.006904
  7    -2.354243    -0.917082     0.030356
  1    -3.198719    -0.420226    -0.184526
  1    -2.337836    -1.913240    -0.109058
 KI
  7    -0.047844    -0.952003     0.000000
  6     1.197538    -0.374345     0.000000
  7     1.167512     1.011885    -0.000000
  6     0.000712     1.739369    -0.000000
  6    -1.204221     1.142841    -0.000000
  6    -1.290952    -0.310696    -0.000000
  8     2.235531    -1.003688     0.000000
  1     2.066867     1.461764    -0.000000
  1     0.119952     2.814523    -0.000000
  1    -2.111965     1.727271    -0.000000
  7    -2.334375    -1.052842    -0.000000
  1    -3.171872    -0.477402    -0.000000
  1    -0.062679    -1.961678     0.000000
 KIc
   7    -0.038678    -0.957464     0.000000
   6     1.208083    -0.366506     0.000000
```

```
   7    1.168739    1.012893   -0.000000
   6   -0.007757    1.734546   -0.000000
   6   -1.206713    1.130660   -0.000000
   6   -1.291013   -0.321052   -0.000000
   8    2.244060   -1.000102    0.000000
   1    2.064378    1.470034   -0.000000
   1    0.106078    2.809864   -0.000000
   1   -2.126922    1.692995   -0.000000
   7   -2.418154   -0.927915   -0.000000
   1   -2.303251   -1.940703    0.000000
   1   -0.010002   -1.966096    0.000000

Guanine 16 atom
KA17 (I)
 6   -1.686287   -0.572285    0.007409
 7   -0.735486   -1.455361    0.016198
 6    0.521220   -0.916073    0.002602
 6    0.789164    0.445450    0.010178
 6   -0.237689    1.433680    0.004622
 7   -1.489574    0.789940    0.002665
 7    2.157365    0.557746    0.002798
 7    1.690830   -1.630740   -0.006218
 6    2.639256   -0.714039   -0.006816
 8   -0.143645    2.651152   -0.006296
 7   -3.002852   -0.977490   -0.057483
 1   -3.098243   -1.969038    0.101227
 1   -3.668447   -0.425209    0.460142
 1    3.698290   -0.921269   -0.013705
 1   -2.283670    1.408736   -0.079668
 1    2.682834    1.415899    0.001795
KA19 (II)
 6  -1.694293   -0.570665    0.006620
 7  -0.737344   -1.457438    0.014927
 6   0.494134   -0.881330    0.002088
 6   0.835213    0.462866    0.006387
 6  -0.218020    1.441259    0.003908
 7  -1.482136    0.777790    0.003438
 7   2.206993    0.623381    0.001102
 7   1.683671   -1.551458   -0.004045
 6   2.677146   -0.596391   -0.004932
 8  -0.180891    2.653668   -0.004209
 7  -3.003306   -0.984245   -0.054801
 1  -3.111575   -1.969239    0.128405
 1  -3.688432   -0.404500    0.402024
 1   3.722148   -0.864880   -0.009981
 1  -2.270308    1.406056   -0.064754
 1   1.792973   -2.551622   -0.009295
EA9 (III)
 6  -1.680812   -0.558482    0.003176
 7  -0.709874   -1.473463    0.010230
 6   0.499260   -0.910884    0.002876
 6   0.802277    0.453772   -0.004352
 6  -0.316203    1.293684    0.000692
```

```
 7   -1.538621    0.787263    0.005097
 7    2.173283    0.662266   -0.007613
 7    1.715960   -1.537619    0.004704
 6    2.674333   -0.543409   -0.002822
 8   -0.178930    2.621928    0.004404
 7   -2.968738   -1.014501   -0.047689
 1   -3.107299   -1.977537    0.204332
 1   -3.683356   -0.360020    0.217736
 1    3.727949   -0.777912   -0.004371
 1   -1.074297    2.987373    0.002539
 1    1.866427   -2.532094    0.005071
EAc9 (III')
 6   -1.697514   -0.518212    0.002985
 7   -0.750882   -1.464717    0.010465
 6    0.470773   -0.933525    0.002415
 6    0.789443    0.421274   -0.006175
 6   -0.302291    1.296683    0.000127
 7   -1.532032    0.826458    0.004974
 7    2.159789    0.623945   -0.008469
 7    1.685561   -1.570812    0.005341
 6    2.653620   -0.587597   -0.002379
 8   -0.149836    2.627021    0.005897
 7   -2.993854   -0.942200   -0.045186
 1   -3.163670   -1.902351    0.196671
 1   -3.694775   -0.263966    0.195614
 1    3.704906   -0.831367   -0.003131
 1    1.831418   -2.566167    0.007263
 1    0.798714    2.813248    0.002806

Ac3C 14 Atoms
Conformer I
  6    0.544662    0.232349    0.000000
  7    1.008550    1.588555    0.000000
  1    0.645112    2.077239    0.810520
  6   -0.930612    0.023536   -0.000000
  8   -1.746475    0.914634   -0.000000
  8   -1.288409   -1.283850   -0.000000
  1   -2.254846   -1.295790   -0.000000
  6    1.402632   -0.767953    0.746898
  6    1.402632   -0.767953   -0.746898
  1    0.899306   -1.578224    1.254102
  1    2.256153   -0.336735    1.250652
  1    0.899306   -1.578224   -1.254102
  1    2.256153   -0.336735   -1.250652
  1    0.645112    2.077239   -0.810520
Conformer II
  6    0.525765    0.228899    0.000000
  7    0.690989    1.664127    0.000000
  1    1.172691    1.999719    0.822265
  6   -0.911761   -0.224776   -0.000000
  8   -1.242786   -1.383427    0.000000
  8   -1.796443    0.781405    0.000000
  1   -1.257670    1.596154    0.000000
```

```
  6     1.487448    -0.665055     0.747431
  6     1.487448    -0.665055    -0.747431
  1     1.056502    -1.519700     1.249634
  1     2.303806    -0.167664     1.255120
  1     1.056502    -1.519700    -1.249634
  1     2.303806    -0.167664    -1.255120
  1     1.172691     1.999719    -0.822265
Conformer III
  6     0.533472     0.238660    -0.000000
  7     0.869772     1.632996    -0.000000
  1     0.482139     2.094298     0.814088
  6    -0.891874    -0.202522     0.000000
  8    -1.267651    -1.351184     0.000000
  8    -1.756077     0.840740    -0.000000
  1    -2.640356     0.448930     0.000000
  6     1.478053    -0.681763     0.745743
  6     1.478053    -0.681763    -0.745743
  1     1.034110    -1.529963     1.247413
  1     2.290637    -0.180463     1.252230
  1     1.034110    -1.529963    -1.247413
  1     2.290637    -0.180463    -1.252230
  1     0.482139     2.094298    -0.814088

Aib 16 Atoms
Conformer I
 6   -0.646141     0.003632     0.000000
 7   -1.294731    -1.299159    -0.000000
 1   -0.989882    -1.832684     0.807288
 6    0.880532    -0.127681    -0.000000
 8    1.492097    -1.167725    -0.000000
 8    1.503310     1.074188     0.000000
 1    2.452674     0.888840    -0.000000
 6   -1.077605     0.761717     1.257699
 6   -1.077605     0.761717    -1.257699
 1   -0.637593     1.758022     1.286961
 1   -2.164989     0.844383     1.258735
 1   -2.164989     0.844383    -1.258735
 1   -0.637593     1.758022    -1.286961
 1   -0.989882    -1.832684    -0.807288
 1   -0.773360     0.222471     2.158814
 1   -0.773360     0.222471    -2.158814
Conformer II
 6   -0.635028    -0.013951     0.011193
 7   -1.018466     1.362030     0.374497
 1   -1.867222     1.638879    -0.102213
 6    0.905933    -0.108175     0.024946
 8    1.496560    -1.156703    -0.011983
 8    1.532007     1.075064     0.035359
 1    0.812159     1.737093     0.089777
 6   -1.076707    -0.280366    -1.428864
 6   -1.212640    -1.061792     0.958505
 1   -0.709641    -1.252056    -1.757585
 1   -2.168384    -0.279503    -1.488481
```

```
 1   -2.303465    -1.051657     0.900390
 1   -0.848046    -2.054162     0.696412
 1   -1.193179     1.438334     1.370046
 1   -0.687402     0.485783    -2.103050
 1   -0.916223    -0.856573     1.990512
 Conformer III
 6    0.646395     0.000577     0.003112
 7    1.102061     0.769722    -1.158949
 1    0.638542     1.670689    -1.189748
 6   -0.877583    -0.145745     0.009791
 8   -1.497793    -1.179946     0.034381
 8   -1.496555     1.061808    -0.028200
 1   -2.446017     0.880179    -0.028679
 6    1.071493     0.747070     1.268498
 6    1.282245    -1.381113    -0.047269
 1    0.736286     0.217850     2.163078
 1    2.159627     0.818471     1.284002
 1    2.366762    -1.269475    -0.049805
 1    0.979802    -1.979758     0.811540
 1    0.869454     0.283141    -2.018024
 1    0.653391     1.754505     1.286246
 1    0.979389    -1.917504    -0.948475

Proline 17 Atoms
 IIE-
  7     0.833190    -1.005463     0.596960
  6    -0.034580     0.179585     0.769422
  6     0.750955     1.359540     0.179235
  6     1.657457     0.672026    -0.842447
  6     2.070124    -0.596795    -0.103972
  6    -1.363696    -0.020591     0.026167
  8    -2.219780     0.825652    -0.011480
  8    -1.478834    -1.210859    -0.570357
  1     1.031229    -1.456431     1.478790
  1    -0.292547     0.348352     1.816897
  1    -0.625419    -1.657281    -0.366674
  1     1.356293     1.826534     0.960064
  1     0.088544     2.114201    -0.241604
  1     2.512513     1.278930    -1.139738
  1     1.089990     0.416588    -1.741564
  1     2.875540    -0.372782     0.604904
  1     2.410800    -1.391043    -0.769486
 IIE+
  6     1.908154    -0.797418    -0.343434
  7     0.737806    -1.048239     0.522388
  6    -0.026047     0.216741     0.614953
  6     0.784098     1.282100    -0.160251
  6     2.195716     0.695214    -0.199466
  6    -1.430437     0.055839     0.033972
  8    -1.696074    -1.176615    -0.414543
  8    -2.218863     0.964029    -0.022152
  1     1.047587    -1.331363     1.442053
  1    -0.152217     0.512487     1.658660
```

```
  1    0.388482    1.383885   -1.173569
  1    0.723311    2.259674    0.314571
  1    2.800962    1.097740   -1.013149
  1    2.717628    0.884795    0.743246
  1    1.641580   -1.030361   -1.378562
  1    2.735161   -1.446746   -0.055749
  1   -0.879026   -1.686000   -0.219406
 IE-
  7   -0.902296   -0.967653   -0.726092
  6    0.023941    0.167403   -0.720616
  6   -0.714731    1.337355   -0.016682
  6   -1.741842    0.617042    0.856045
  6   -2.141467   -0.546845   -0.049379
  6    1.300716   -0.176417    0.015928
  8    1.472005   -1.146707    0.713727
  8    2.258021    0.753123   -0.188833
  1    0.311374    0.458681   -1.734418
  1    3.030189    0.472657    0.321557
  1   -1.221663    1.942004   -0.771852
  1   -0.035117    1.989065    0.532410
  1   -2.578991    1.256807    1.140372
  1   -1.269361    0.238300    1.766703
  1   -2.867529   -0.208121   -0.795615
  1   -2.581876   -1.390088    0.483746
  1   -0.472821   -1.720112   -0.200390
 IE+
  6    1.910286   -0.791364   -0.319725
  7    0.876798   -0.955180    0.708533
  6   -0.016985    0.198347    0.638102
  6    0.739793    1.269425   -0.192563
  6    2.162075    0.709343   -0.284893
  6   -1.349964   -0.130991    0.001914
  8   -2.202212    0.915249    0.072486
  8   -1.646461   -1.182061   -0.511822
  1   -0.234004    0.577843    1.641541
  1    0.305954    1.344128   -1.192864
  1    0.682182    2.255381    0.266185
  1    2.701468    1.074896   -1.159385
  1    2.733381    0.964382    0.610364
  1    1.566234   -1.090330   -1.320719
  1    2.791889   -1.382936   -0.068072
  1   -3.022631    0.634409   -0.355919
  1    0.352743   -1.811875    0.578188

Fluorothreonine 17 atoms
I'gg-g-
   9   -2.538320    0.752291   -0.821330
   6   -2.190131   -0.079927    0.242850
   6   -0.740385    0.156021    0.633215
   6    0.205286   -0.118658   -0.548050
   6    1.622358    0.287052   -0.192512
   1   -2.844947    0.146786    1.084251
   1   -2.342376   -1.114712   -0.071662
```

```
   1   -0.617921    1.185501    0.970468
   8   -0.417354   -0.691305    1.715731
   1   -0.251696   -1.558527    1.316768
   1   -0.102566    0.514059   -1.387911
   7    0.180087   -1.544209   -0.855328
   1    1.122899   -1.870098   -1.034620
   1   -0.385492   -1.737020   -1.669958
   8    2.584717   -0.435625   -0.270060
   8    1.693789    1.571063    0.201333
   1    2.621956    1.748645    0.407131
IItg-g-
   9    1.800798    1.288504    0.795299
   6    1.607549   -0.100280    0.759360
   6    1.013226   -0.521313   -0.578676
   6   -0.352959    0.117504   -0.890921
   6   -1.371783   -0.215473    0.207086
   1    2.577523   -0.577618    0.892862
   1    0.948436   -0.364434    1.588100
   1    1.703039   -0.227291   -1.374819
   8    0.932469   -1.930584   -0.601672
   1    0.167782   -2.166551   -0.053523
   1   -0.725151   -0.387181   -1.787315
   7   -0.348137    1.560151   -1.136445
   1    0.394310    2.013917   -0.618315
   1   -0.223535    1.768637   -2.117063
   8   -1.425405   -1.302190    0.739765
   8   -2.198896    0.776287    0.511292
   1   -1.899513    1.527720   -0.047160
IIggg-
   9    2.631116    0.647173   -0.087282
   6    2.108725   -0.536220   -0.605405
   6    0.687139   -0.779319   -0.155732
   6   -0.273120    0.373752   -0.464916
   6   -1.716257   -0.105458   -0.227311
   1    2.148204   -0.461769   -1.694817
   1    2.746833   -1.352124   -0.264711
   1    0.338705   -1.657197   -0.710856
   8    0.689472   -1.045045    1.241427
   1   -0.096419   -1.563923    1.440213
   1   -0.213692    0.613523   -1.532398
   7   -0.061704    1.602081    0.299692
   1    0.682582    2.151210   -0.108702
   1    0.248481    1.350806    1.234062
   8   -2.070417   -1.245200   -0.403170
   8   -2.540687    0.859370    0.176426
   1   -1.959812    1.638210    0.319741
I'gg-g
   9    2.596473    0.492016   -0.495533
   6    2.041542   -0.787989   -0.423346
   6    0.663483   -0.759388    0.209622
   6   -0.248571    0.299467   -0.452340
   6   -1.715526   -0.001697   -0.204462
   1    1.987709   -1.174802   -1.444594
```

```
   1    2.711629   -1.403768    0.177302
   1    0.235392   -1.752565    0.050414
   8    0.715000   -0.532555    1.597249
   1    0.656953    0.432177    1.693419
   1   -0.115006    0.239608   -1.541939
   7    0.049514    1.606214    0.109528
   1   -0.768613    2.200636    0.080874
   1    0.824342    2.045292   -0.366563
   8   -2.523037    0.794212    0.203010
   8   -2.035808   -1.265731   -0.545336
   1   -2.983683   -1.364592   -0.380820
Igtt
   9   -3.080182    0.454049   -0.048341
   6   -2.029971   -0.333280   -0.533971
   6   -0.734371    0.294179   -0.067661
   6    0.478345   -0.486774   -0.568980
   6    1.763171    0.213383   -0.129443
   1   -2.151544   -1.338220   -0.135625
   1   -2.096523   -0.344957   -1.623713
   1   -0.681729    1.317946   -0.452473
   8   -0.656971    0.299012    1.351119
   1   -1.455106    0.717124    1.688151
   1    0.466959   -0.444648   -1.663860
   7    0.399375   -1.869283   -0.143182
   1    0.373988   -1.892124    0.871030
   1    1.245328   -2.357704   -0.411416
   8    2.656843   -0.306295    0.486116
   8    1.805466    1.495210   -0.554718
   1    2.645481    1.862140   -0.246341
IIg-tt
   9   -2.740496   -0.856704   -0.387571
   6   -1.491056   -0.878085    0.242369
   6   -0.753422    0.370688   -0.196768
   6    0.597954    0.540872    0.501097
   6    1.528853   -0.605400    0.086317
   1   -1.666390   -0.868578    1.319287
   1   -0.974837   -1.789602   -0.049368
   1   -0.593919    0.327729   -1.283090
   8   -1.514065    1.526191    0.130393
   1   -2.400521    1.395739   -0.221840
   1    0.438551    0.458719    1.580904
   7    1.180970    1.820263    0.094621
   1    1.786107    2.183807    0.820843
   1    0.441538    2.498479   -0.048181
   8    1.424861   -1.722450    0.524950
   8    2.440419   -0.259934   -0.825418
   1    2.307077    0.701914   -0.965188
IIggg
   9    2.631116    0.647173   -0.087282
   6    2.108725   -0.536220   -0.605405
   6    0.687139   -0.779319   -0.155732
   6   -0.273120    0.373752   -0.464916
   6   -1.716257   -0.105458   -0.227311
```

```
   1    2.148204   -0.461769   -1.694817
   1    2.746833   -1.352124   -0.264711
   1    0.338705   -1.657197   -0.710856
   8    0.689472   -1.045045    1.241427
   1   -0.096419   -1.563923    1.440213
   1   -0.213692    0.613523   -1.532398
   7   -0.061704    1.602081    0.299692
   1    0.682582    2.151210   -0.108702
   1    0.248481    1.350806    1.234062
   8   -2.070417   -1.245200   -0.403170
   8   -2.540687    0.859370    0.176426
   1   -1.959812    1.638210    0.319741
IIg-g-g
   9    2.269409    0.959194    0.595909
   6    1.514515    0.911340   -0.583160
   6    0.739408   -0.390773   -0.582917
   6   -0.373687   -0.418395    0.489056
   6   -1.482924    0.550516    0.061390
   1    0.857940    1.778749   -0.599396
   1    2.217783    0.930803   -1.416082
   1    0.282657   -0.529582   -1.567640
   8    1.626118   -1.485064   -0.407763
   1    2.253587   -1.235916    0.280512
   1    0.040297   -0.050211    1.432491
   7   -0.914578   -1.774389    0.572269
   1   -1.263166   -1.970777    1.502145
   1   -0.179248   -2.442371    0.370499
   8   -1.387838    1.747815    0.159384
   8   -2.547647   -0.052750   -0.474298
   1   -2.362190   -1.012689   -0.387603
IIgtt
   9    3.118369    0.397680    0.061490
   6    2.019458   -0.197604    0.678740
   6    0.762568    0.286218   -0.010856
   6   -0.489293   -0.378745    0.558782
   6   -1.730967    0.443492    0.159571
   1    2.139723   -1.278769    0.581781
   1    2.028625    0.092877    1.731706
   1    0.666752    1.367393    0.125800
   8    0.791821   -0.044104   -1.392346
   1    1.559981    0.380900   -1.784685
   1   -0.452909   -0.319408    1.650734
   7   -0.659443   -1.775276    0.158968
   1   -0.194285   -1.937476   -0.727637
   1   -0.287561   -2.419137    0.842448
   8   -1.768457    1.642227    0.252762
   8   -2.762033   -0.295335   -0.250614
   1   -2.435313   -1.218939   -0.230274
III'ggg-
   9    2.515192    1.009004   -0.702051
   6    2.221186   -0.137062    0.032729
   6    0.799369   -0.563564   -0.274985
   6   -0.215577    0.498737    0.149818
```

```
   6   -1.609170    0.082035   -0.294588
   1    2.915491   -0.923267   -0.264096
   1    2.337227    0.096012    1.090267
   1    0.708544   -0.715553   -1.357106
   8    0.598402   -1.781876    0.422257
   1   -0.252954   -2.125005    0.125406
   1    0.032544    1.441478   -0.343407
   7   -0.155473    0.702161    1.593887
   1   -0.343410   -0.171199    2.073088
   1   -0.834772    1.389578    1.893808
   8   -1.951529   -1.042154   -0.590044
   8   -2.472284    1.116127   -0.273974
   1   -3.342338    0.763989   -0.510377
Ig-gg-
   9    0.372784   -2.109470    0.433759
   6    1.325902   -1.308971   -0.187985
   6    1.139978    0.131159    0.248539
   6   -0.056930    0.844697   -0.405411
   6   -1.361176    0.153117   -0.050600
   1    2.314179   -1.652925    0.117443
   1    1.212353   -1.421238   -1.268152
   1    0.990754    0.143461    1.337845
   8    2.323685    0.808843   -0.111488
   1    2.104487    1.749640   -0.057315
   1    0.087034    0.814001   -1.487084
   7   -0.017834    2.233803    0.041545
   1   -0.432058    2.294773    0.967000
   1   -0.572137    2.822280   -0.567893
   8   -1.964814    0.337710    0.977075
   8   -1.770439   -0.688843   -1.017086
   1   -2.557195   -1.142827   -0.682790
Ig-gg
   9    1.868069    1.341207    0.548522
   6    1.485758    0.862735   -0.697044
   6    0.820866   -0.489726   -0.572917
   6   -0.328524   -0.520643    0.461367
   6   -1.485174    0.337567   -0.019437
   1    0.808230    1.594157   -1.141455
   1    2.383531    0.766652   -1.309304
   1    0.397160   -0.734600   -1.561176
   8    1.797361   -1.432915   -0.205802
   1    1.303747   -2.180107    0.163125
   1    0.058649   -0.123201    1.399616
   7   -0.716628   -1.913859    0.644195
   1   -1.381461   -2.174969   -0.077450
   1   -1.178976   -2.043437    1.534780
   8   -2.392079   -0.070457   -0.704113
   8   -1.382264    1.620047    0.377812
   1   -2.141614    2.091183    0.005132

GlyDA. 16 atoms
C5
 6    0.528249    0.648633   -0.000000
```

```
 7   -0.543601    -0.307055     0.000000
 6   -1.838102     0.096007    -0.000000
 6   -2.872182    -1.006332     0.000000
 8   -2.143659     1.281127    -0.000000
 1   -0.275765    -1.278847     0.000000
 1   -2.434606    -2.004752     0.000000
 1   -3.504539    -0.889187     0.880304
 1   -3.504539    -0.889187    -0.880304
 6    1.851809    -0.099548     0.000000
 7    2.950520     0.694531    -0.000000
 1    3.858188     0.263449     0.000000
 1    2.882249     1.695516    -0.000000
 8    1.912862    -1.317676     0.000000
 1    0.472476     1.300283     0.877962
 1    0.472476     1.300283    -0.877962
C7
 6   -0.647267     0.712694    -0.828782
 7    0.605240     0.943333    -0.128387
 6    1.567924    -0.007045    -0.036292
 6    2.827616     0.388666     0.694829
 8    1.427325    -1.124181    -0.525449
 1    0.729848     1.813250     0.358476
 1    2.804342     1.410789     1.072890
 1    2.979230    -0.300994     1.525323
 1    3.670665     0.276842     0.012631
 6   -1.684260    -0.016520     0.028793
 7   -1.370101    -1.305676     0.297256
 1   -1.971352    -1.826956     0.911544
 1   -0.477883    -1.679287     0.005949
 8   -2.698701     0.538547     0.417535
 1   -0.431422     0.129986    -1.726114
 1   -1.074377     1.672206    -1.110106

AlaDA
C5
 1   -3.703750     0.245172     0.717712
 7   -2.837357    -0.261690     0.665841
 6   -1.755065     0.354082     0.129618
 8   -1.792553     1.492588    -0.309079
 1   -2.776369    -1.171800     1.083135
 6   -0.490838    -0.497712     0.069577
 7    0.617090     0.395274    -0.169628
 6    1.889729     0.044875     0.144024
 6    2.943239     1.097453    -0.116009
 1    2.529834     2.036596    -0.484073
 1    3.488198     1.278820     0.810460
 1    3.652055     0.705968    -0.846404
 1    0.380822     1.324946    -0.480547
 8    2.168298    -1.056246     0.601478
 1   -0.331703    -0.993556     1.031986
 6   -0.609696    -1.564153    -1.024383
 1   -0.796951    -1.090812    -1.990042
C7eq
```

```
 1   -1.424182    -2.259848    -0.812407
 1    0.323673    -2.123836    -1.073158
 1   -1.422824     2.540620     0.327536
 7   -0.996981     1.760328    -0.143139
 6   -1.472392     0.520384     0.126140
 8   -2.466280     0.300508     0.797925
 1   -0.087357     1.861343    -0.572917
 6   -0.636713    -0.609382    -0.502608
 7    0.617615    -0.765410     0.227019
 6    1.709199     0.002081    -0.010536
 6    2.939585    -0.322055     0.802293
 1    2.789201    -1.142157     1.504520
 1    3.747125    -0.579530     0.116462
 1    3.240929     0.571692     1.348856
 1    0.648761    -1.445246     0.968061
 8    1.705740     0.905597    -0.842529
 1   -0.367857    -0.311968    -1.518787
 6   -1.398954    -1.920130    -0.508018
 1   -1.663022    -2.214508     0.508968
 1   -0.796778    -2.702827    -0.972099
 1   -2.329233    -1.810700    -1.064066

Uridine 29 atoms
 1    -1.019815     2.796757     1.874773
 8    -1.194013     2.011397     1.351085
 6    -2.199282     2.309258     0.389296
 1    -1.880631     3.123227    -0.271186
 1    -3.138554     2.601389     0.873697
 6    -2.453269     1.074168    -0.446479
 1    -3.254255     1.289860    -1.156363
 8    -1.283198     0.735987    -1.218716
 6    -0.663717    -0.411790    -0.714547
 1    -0.671959    -1.206855    -1.464770
 7     0.759524    -0.105005    -0.426761
 6     1.294389     1.150521    -0.583831
 1     0.585195     1.897573    -0.901672
 6     2.597647     1.420783    -0.364745
 1     2.993576     2.415553    -0.497294
 6     3.499506     0.365643     0.051414
 8     4.688284     0.468258     0.285128
 7     2.860213    -0.879569     0.176613
 1     3.435630    -1.655791     0.472831
 6     1.537473    -1.169884    -0.030752
 8     1.080961    -2.297628     0.127823
 6    -2.802906    -0.182303     0.339834
 1    -3.283894     0.052137     1.294926
 6    -1.443961    -0.856054     0.541140
 1    -0.955048    -0.448653     1.429277
 8    -1.629439    -2.246896     0.634256
 1    -0.749274    -2.641251     0.534153
 8    -3.640718    -0.983702    -0.467278
 1    -3.410262    -1.900874    -0.269659
```

Testosterone 49 atoms

| | | | |
|---|---|---|---|
| 6 | -0.486311 | -1.728081 | 0.052236 |
| 6 | 0.267171 | -0.400468 | -0.138413 |
| 6 | -0.561218 | 0.812748 | 0.333261 |
| 6 | -1.929253 | 0.756427 | -0.330789 |
| 6 | -2.705760 | -0.533725 | -0.031853 |
| 6 | -1.893619 | -1.711434 | -0.558970 |
| 6 | -4.000629 | -0.225306 | -0.804095 |
| 6 | -4.304809 | 1.242992 | -0.460177 |
| 6 | -2.946633 | 1.873586 | -0.058610 |
| 6 | 0.168513 | 2.108117 | -0.004907 |
| 6 | 1.565367 | 2.127851 | 0.610438 |
| 6 | -3.027714 | -0.713862 | 1.455235 |
| 8 | -5.128424 | -1.028639 | -0.484059 |
| 1 | -4.990553 | -1.905469 | -0.851893 |
| 6 | 3.607308 | 1.058000 | -0.278984 |
| 6 | 4.512759 | -0.068323 | -0.550256 |
| 8 | 5.609315 | 0.095027 | -1.060334 |
| 6 | 2.365086 | 0.916280 | 0.222136 |
| 1 | -1.743845 | 0.752103 | -1.417260 |
| 1 | -0.695480 | 0.768308 | 1.421675 |
| 1 | 0.398408 | -0.260226 | -1.223238 |
| 1 | -2.939528 | 2.149697 | 0.999448 |
| 1 | -2.726235 | 2.778256 | -0.627186 |
| 1 | 0.247696 | 2.198517 | -1.095466 |
| 1 | -0.403628 | 2.970695 | 0.347885 |
| 1 | -2.393414 | -2.664141 | -0.347047 |
| 1 | -1.811269 | -1.625151 | -1.650013 |
| 1 | -3.781134 | -0.316308 | -1.877288 |
| 1 | -3.613062 | 0.117926 | 1.849638 |
| 1 | -3.620007 | -1.619655 | 1.597360 |
| 1 | -2.125753 | -0.801104 | 2.061451 |
| 1 | -4.769951 | 1.755493 | -1.302939 |
| 1 | -5.021643 | 1.263254 | 0.362666 |
| 1 | -0.562400 | -1.961032 | 1.117247 |
| 1 | 2.108656 | 3.032494 | 0.328328 |
| 1 | 1.465686 | 2.145263 | 1.702935 |
| 1 | 4.020657 | 2.046484 | -0.455275 |
| 1 | 0.082303 | -2.542822 | -0.401354 |
| 6 | 4.018610 | -1.421989 | -0.099300 |
| 1 | 4.552025 | -2.192946 | -0.657125 |
| 1 | 4.296208 | -1.534438 | 0.954853 |
| 6 | 2.508572 | -1.538427 | -0.274371 |
| 1 | 2.278274 | -1.482567 | -1.344641 |
| 1 | 2.177683 | -2.520112 | 0.071299 |
| 6 | 1.712016 | -0.438399 | 0.452001 |
| 6 | 1.703004 | -0.718430 | 1.967541 |
| 1 | 2.714636 | -0.653994 | 2.373730 |
| 1 | 1.085827 | -0.002379 | 2.511900 |
| 1 | 1.321574 | -1.719558 | 2.175416 |

Triptamine 24 atoms
Conformer I

```
6    0.781625    1.734814   -0.361576
6    0.908288    0.387864   -0.585959
6   -0.380584   -0.189070   -0.301297
6   -1.241155    0.867433    0.086036
7   -0.506040    2.028551    0.043181
6   -2.579609    0.655126    0.425341
6   -3.052382   -0.646814    0.370865
6   -2.216127   -1.713162   -0.013828
6   -0.889472   -1.496946   -0.349187
1   -3.226519    1.474200    0.718786
1   -4.085655   -0.848210    0.627557
1   -2.622174   -2.717171   -0.047238
1   -0.255895   -2.325302   -0.646313
1    1.520022    2.515772   -0.461490
1   -0.854136    2.947165    0.248189
6    2.147172   -0.345378   -0.993875
6    2.777707   -1.115026    0.168260
1    2.883674    0.363613   -1.380864
1    1.912486   -1.049481   -1.798965
7    3.210022   -0.180124    1.206792
1    3.658902   -1.650933   -0.194152
1    2.060872   -1.866028    0.529512
1    2.402634    0.315152    1.569947
1    3.621276   -0.680960    1.985207
Conformer II
6    0.755357    1.765651   -0.345189
6    0.901697    0.423658   -0.587386
6   -0.377984   -0.175421   -0.306339
6   -1.252685    0.862977    0.096634
7   -0.535373    2.035616    0.066220
6   -2.586866    0.626701    0.437028
6   -3.040291   -0.681178    0.366883
6   -2.189552   -1.730058   -0.033811
6   -0.867337   -1.490096   -0.369700
1   -3.244760    1.432159    0.743298
1   -4.069519   -0.901317    0.624281
1   -2.580568   -2.739516   -0.078259
1   -0.222791   -2.305559   -0.678568
1    1.477576    2.561905   -0.444521
1   -0.896460    2.945986    0.284913
6    2.145980   -0.291343   -1.004702
6    2.776542   -1.101311    0.141788
1    2.880069    0.432448   -1.374592
1    1.923544   -0.970373   -1.836200
7    3.209999   -0.323024    1.296790
1    3.640910   -1.650643   -0.240962
1    2.057137   -1.845613    0.493228
1    3.917241    0.348916    1.019613
1    2.429082    0.214478    1.657651

Serotonine 25 atoms
Conformer I
6    2.092327   -0.927100   -0.136307
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6    2.746661    0.253261    0.269133
6    2.044499    1.435751    0.421804
6    0.672353    1.419407    0.160457
6    0.001846    0.242609   -0.245895
6    0.733550   -0.950671   -0.394729
6   -1.384148    0.580945   -0.436520
6   -1.492634    1.919901   -0.145242
7   -0.265310    2.427131    0.219427
1    3.811833    0.211553    0.459024
1    0.236264   -1.870048   -0.687075
1    2.552439    2.341236    0.733706
8    2.884941   -2.042619   -0.252377
1    2.336035   -2.782185   -0.527250
1   -2.362472    2.558546   -0.180344
1   -0.079013    3.385213    0.451955
6   -2.496439   -0.331825   -0.855518
6   -3.109568   -1.120497    0.302511
1   -2.129810   -1.041672   -1.603339
1   -3.287229    0.257867   -1.328967
7   -2.123992   -2.029151    0.890331
1   -3.530128   -0.407211    1.026212
1   -3.936230   -1.726189   -0.079333
1   -1.371812   -1.494524    1.311941
1   -2.547395   -2.570833    1.634393
Conformer II
6    2.264968   -0.887211    0.003885
6    2.804267    0.357932    0.382389
6    2.010734    1.490907    0.425273
6    0.662862    1.358733    0.084234
6    0.106341    0.115914   -0.295537
6    0.930025   -1.023986   -0.334194
6   -1.284500    0.338496   -0.586983
6   -1.510817    1.676493   -0.372966
7   -0.347462    2.294448    0.031524
1    3.855477    0.406274    0.637130
1    0.530848   -1.991184   -0.625321
1    2.432317    2.446787    0.714579
8    3.143764   -1.942636   -0.005901
1    2.674278   -2.733987   -0.282792
1   -2.426176    2.238151   -0.481632
1   -0.247941    3.273479    0.227153
6   -2.291115   -0.692080   -0.991492
6   -2.710621   -1.587498    0.175927
1   -1.879473   -1.319507   -1.789318
1   -3.182691   -0.199820   -1.388520
7   -3.375166   -0.785477    1.202378
1   -3.421828   -2.335708   -0.184001
1   -1.827031   -2.125526    0.548644
1   -3.646595   -1.366451    1.986358
1   -2.725733   -0.093106    1.560056
Conformer III
6    2.247396   -0.902946   -0.005152
6    2.802472    0.331520    0.385947
```

| | | | |
|---|---|---|---|
| 6 | 2.024303 | 1.474362 | 0.438811 |
| 6 | 0.675216 | 1.363157 | 0.094716 |
| 6 | 0.103076 | 0.131830 | -0.297716 |
| 6 | 0.911412 | -1.018633 | -0.346626 |
| 6 | -1.284457 | 0.375238 | -0.589165 |
| 6 | -1.492958 | 1.714067 | -0.361962 |
| 7 | -0.322149 | 2.313046 | 0.049438 |
| 1 | 3.853641 | 0.363135 | 0.643382 |
| 1 | 0.500481 | -1.977711 | -0.647880 |
| 1 | 2.457929 | 2.421588 | 0.738439 |
| 8 | 3.112283 | -1.968959 | -0.023644 |
| 1 | 2.630920 | -2.754627 | -0.296365 |
| 1 | -2.397373 | 2.292945 | -0.473554 |
| 1 | -0.209912 | 3.288361 | 0.256260 |
| 6 | -2.298701 | -0.641630 | -1.002819 |
| 6 | -2.704140 | -1.577738 | 0.149187 |
| 1 | -1.904464 | -1.246816 | -1.828045 |
| 1 | -3.193396 | -0.136222 | -1.381808 |
| 7 | -3.328794 | -0.928568 | 1.296203 |
| 1 | -1.818380 | -2.107756 | 0.509793 |
| 1 | -3.395272 | -2.335384 | -0.230099 |
| 1 | -2.716299 | -0.201695 | 1.650571 |
| 1 | -4.186387 | -0.467768 | 1.012110 |