

**Supplementary Data 1.** The optimized atomic coordinates of the Fmoc-F-F molecule.

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.36164705 | -2.69779039 | 0.71974451  |
| C | -4.53431549 | 1.83646845  | 2.42016564  |
| C | -3.35229200 | 1.09481717  | 2.39061476  |
| C | -3.28363954 | -0.10783142 | 1.68574401  |
| C | -4.40824248 | -0.55083639 | 1.00371282  |
| C | -5.60284198 | 0.18859974  | 1.04628963  |
| C | -5.67077405 | 1.38631610  | 1.75300101  |
| H | -4.56966795 | 2.77066023  | 2.97422696  |
| H | -2.47668380 | 1.45512085  | 2.92430999  |
| H | -2.36148330 | -0.68175735 | 1.67140353  |
| H | -6.59322567 | 1.96054729  | 1.78684789  |
| C | -4.58868733 | -1.78592898 | 0.15040048  |
| C | -6.05040692 | -1.70963676 | -0.22614158 |
| C | -6.80623952 | -2.59058867 | -0.98510052 |
| C | -8.14685277 | -2.28965756 | -1.23284876 |
| C | -8.71564174 | -1.11952064 | -0.72804013 |
| C | -7.95928944 | -0.23135520 | 0.03339551  |
| C | -6.62276144 | -0.53078184 | 0.28224984  |
| H | -6.36904650 | -3.50587141 | -1.37780824 |
| H | -8.75272965 | -2.97265393 | -1.82203312 |
| H | -9.76070648 | -0.90007004 | -0.92990525 |
| H | -8.40771747 | 0.67787338  | 0.42566572  |
| C | -3.71848236 | -1.78057823 | -1.10981697 |
| H | -3.92716267 | -2.66747123 | -1.71587641 |
| H | -3.90396020 | -0.88246491 | -1.70392855 |
| O | -2.33979346 | -1.84205480 | -0.75476926 |
| C | -1.61742677 | -0.71308133 | -0.95736929 |
| O | -2.00781123 | 0.27444541  | -1.55232062 |
| N | -0.39980461 | -0.83166372 | -0.38597657 |
| H | -0.07545639 | -1.70601946 | 0.00768476  |
| C | 0.55043902  | 0.24007405  | -0.48354464 |
| H | 0.57855280  | 0.60463103  | -1.51895384 |
| C | 0.16644382  | 1.43531602  | 0.43018488  |
| H | -0.92768374 | 1.47354030  | 0.43685711  |
| H | 0.49529216  | 1.23326664  | 1.45661624  |
| C | 0.70165640  | 2.74925555  | -0.06961823 |
| C | 0.14054407  | 3.31554778  | -1.22168221 |
| C | 1.76385101  | 3.40596298  | 0.55401496  |
| C | 0.63465545  | 4.50919660  | -1.73406911 |
| H | -0.69089846 | 2.80537385  | -1.70508714 |

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 2.26546250 | 4.59897903  | 0.03662828  |
| H | 2.21286116 | 2.97340634  | 1.44530520  |
| C | 1.70118245 | 5.15336708  | -1.10704312 |
| H | 0.18685868 | 4.93977290  | -2.62595277 |
| H | 3.10465037 | 5.08560189  | 0.52525994  |
| H | 2.09113089 | 6.08332815  | -1.51204306 |
| C | 1.91226810 | -0.34643606 | -0.12056673 |
| O | 2.02349077 | -1.49219515 | 0.31020713  |
| N | 2.97439392 | 0.46771693  | -0.28686319 |
| H | 2.86807304 | 1.43428017  | -0.57602281 |
| C | 4.28801435 | 0.01602231  | 0.09901031  |
| H | 4.21236692 | -0.52258575 | 1.05061446  |
| C | 5.16319533 | 1.23207307  | 0.29400405  |
| O | 4.87418467 | 2.35269295  | -0.05906705 |
| O | 6.32272529 | 0.91870668  | 0.88124898  |
| H | 6.83956699 | 1.74138323  | 0.93111818  |
| C | 4.89841744 | -0.95596222 | -0.94660225 |
| H | 4.05677582 | -1.54689655 | -1.32087702 |
| H | 5.29615688 | -0.38289143 | -1.79225714 |
| C | 5.93490176 | -1.88082659 | -0.37046188 |
| C | 7.29071542 | -1.74932893 | -0.66884876 |
| C | 5.52863191 | -2.90073107 | 0.49625361  |
| C | 8.22656115 | -2.61912638 | -0.11493936 |
| H | 7.61605073 | -0.95708229 | -1.33954686 |
| C | 6.46155177 | -3.76743235 | 1.05470278  |
| H | 4.46927554 | -3.00770665 | 0.72409059  |
| C | 7.81445066 | -3.62902584 | 0.74970297  |
| H | 9.27970590 | -2.50694862 | -0.35939906 |
| H | 6.13199425 | -4.55725528 | 1.72469735  |
| H | 8.54397145 | -4.30843080 | 1.18244168  |

### The optimized atomic coordinates of the Dimer 1

|   |            |             |            |
|---|------------|-------------|------------|
| H | 6.45874014 | 2.38753700  | 0.29694367 |
| C | 5.64414744 | -1.70768855 | 2.75797563 |
| C | 4.70341026 | -0.67934482 | 2.68241947 |
| C | 4.87098983 | 0.37431058  | 1.78235346 |
| C | 5.98486472 | 0.37826396  | 0.95456119 |
| C | 6.94116516 | -0.64778094 | 1.04331407 |
| C | 6.77371893 | -1.69682804 | 1.94348173 |
| H | 5.49788877 | -2.51997199 | 3.46489490 |
| H | 3.83380123 | -0.69569458 | 3.33433475 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.13664779  | 1.17313341  | 1.73190969  |
| H | 7.51132179  | -2.49234163 | 2.01374297  |
| C | 6.38183910  | 1.37159240  | -0.11378687 |
| C | 7.72322368  | 0.84216146  | -0.56710400 |
| C | 8.59190978  | 1.35598007  | -1.51829196 |
| C | 9.76893582  | 0.66098117  | -1.80282720 |
| C | 10.06434415 | -0.53273723 | -1.14322992 |
| C | 9.19370607  | -1.05265851 | -0.18800876 |
| C | 8.02021727  | -0.36048638 | 0.09737946  |
| H | 8.36857597  | 2.28795923  | -2.03271057 |
| H | 10.46154190 | 1.05381419  | -2.54217075 |
| H | 10.98498514 | -1.06113581 | -1.37606300 |
| H | 9.42983126  | -1.98185628 | 0.32432370  |
| C | 5.40858286  | 1.40125452  | -1.29650128 |
| H | 5.75026150  | 2.11718327  | -2.04983079 |
| H | 5.32325182  | 0.41004028  | -1.74788335 |
| O | 4.12133808  | 1.84173320  | -0.86907484 |
| C | 3.15417830  | 0.89694377  | -0.81978244 |
| O | 3.25658510  | -0.23641313 | -1.25407446 |
| N | 2.05719383  | 1.37806391  | -0.19211757 |
| H | 1.93217241  | 2.37299672  | -0.04514955 |
| C | 0.87780787  | 0.56207732  | -0.11052175 |
| H | 0.68901205  | 0.10164675  | -1.09190548 |
| C | 1.03441883  | -0.58305760 | 0.92543310  |
| H | 2.10764668  | -0.78373425 | 1.00291306  |
| H | 0.69681402  | -0.24256847 | 1.91141647  |
| C | 0.33921165  | -1.86260628 | 0.53308464  |
| C | 0.83399771  | -2.60297355 | -0.54974076 |
| C | -0.77290558 | -2.34685854 | 1.22672097  |
| C | 0.24372918  | -3.81288271 | -0.90552527 |
| H | 1.70472847  | -2.22825888 | -1.08467699 |
| C | -1.38017299 | -3.54644526 | 0.85666480  |
| H | -1.17497195 | -1.77903768 | 2.06239405  |
| C | -0.86356652 | -4.29022822 | -0.19948869 |
| H | 0.66063169  | -4.39474966 | -1.72439919 |
| H | -2.26003718 | -3.89269981 | 1.39112835  |
| H | -1.32202016 | -5.23643934 | -0.47593092 |
| C | -0.28966638 | 1.50410588  | 0.19256233  |
| O | -0.14867301 | 2.72299347  | 0.20945891  |
| N | -1.47301719 | 0.89754066  | 0.40311524  |
| H | -1.53042447 | -0.10930970 | 0.50024187  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.67728872 | 1.65574674  | 0.65442401  |
| H | -2.45279585 | 2.43831060  | 1.39236857  |
| C | -3.68261611 | 0.70109824  | 1.26755968  |
| O | -3.33827044 | -0.39095432 | 1.71134634  |
| O | -4.90924295 | 1.14573032  | 1.25718550  |
| H | -5.53492520 | 0.39001309  | 1.45552875  |
| C | -3.22043609 | 2.33586205  | -0.62591397 |
| H | -2.34341369 | 2.57890713  | -1.23503801 |
| H | -3.83355062 | 1.61853229  | -1.18239478 |
| C | -3.98231575 | 3.60383021  | -0.34767779 |
| C | -5.36334223 | 3.68371981  | -0.52562617 |
| C | -3.29011054 | 4.73465152  | 0.09807303  |
| C | -6.04239978 | 4.87109215  | -0.26544203 |
| H | -5.90650294 | 2.80398724  | -0.86078711 |
| C | -3.96737363 | 5.92017645  | 0.36352951  |
| H | -2.21061567 | 4.67452476  | 0.22906400  |
| C | -5.34710760 | 5.99165481  | 0.18105702  |
| H | -7.11873620 | 4.91975143  | -0.40946270 |
| H | -3.41685849 | 6.79218637  | 0.70736356  |
| H | -5.87763420 | 6.91808282  | 0.38510308  |
| N | -8.14511453 | -2.95679918 | -0.03779905 |
| H | -8.47444439 | -1.99493500 | 0.02521817  |
| C | -6.70182343 | -2.93024658 | -0.16194675 |
| H | -6.30577252 | -3.94576492 | -0.05655180 |
| C | -6.32836574 | -2.38869429 | -1.56316562 |
| C | -6.00643070 | -2.04086985 | 0.84877913  |
| H | -6.75221422 | -3.08518114 | -2.29356655 |
| H | -6.83375975 | -1.42481445 | -1.69389967 |
| C | -4.86524097 | -2.17473070 | -1.77793734 |
| O | -6.48633774 | -0.96682666 | 1.19669273  |
| N | -4.29826391 | -0.92730243 | -1.63173129 |
| C | -3.88790780 | -3.09838425 | -2.05743937 |
| C | -3.00998243 | -1.10088100 | -1.82749344 |
| N | -2.71382088 | -2.39324470 | -2.09587774 |
| H | -3.92277881 | -4.16481658 | -2.22355688 |
| H | -2.25600316 | -0.32591725 | -1.80262204 |
| H | -1.78440372 | -2.78617018 | -2.15924353 |
| O | -4.83871317 | -2.49957209 | 1.24753113  |
| H | -8.40723867 | -3.39800967 | 0.84012785  |
| H | -4.32315371 | -1.75125195 | 1.65564559  |

## The optimized atomic coordinates of the Dimer 2

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.18075956  | 1.30749344  | -1.54079386 |
| C | 4.17529025  | -0.21226804 | 3.03470882  |
| C | 2.98916788  | -0.00769818 | 2.32860627  |
| C | 3.01088055  | 0.17221604  | 0.94430222  |
| C | 4.22897391  | 0.14696053  | 0.27836590  |
| C | 5.42306412  | -0.05748977 | 0.99103218  |
| C | 5.40042110  | -0.23953580 | 2.37165133  |
| H | 4.14357114  | -0.34929921 | 4.11221620  |
| H | 2.03806319  | 0.01785564  | 2.85395872  |
| H | 2.08729689  | 0.31948579  | 0.39662542  |
| H | 6.32221866  | -0.39625794 | 2.92609798  |
| C | 4.52027365  | 0.32036289  | -1.19485082 |
| C | 6.02675720  | 0.21420671  | -1.24174141 |
| C | 6.87624332  | 0.30141138  | -2.33449449 |
| C | 8.24951262  | 0.14985857  | -2.13505273 |
| C | 8.75921430  | -0.08467027 | -0.85718367 |
| C | 7.90954064  | -0.17153682 | 0.24322087  |
| C | 6.53969013  | -0.02247037 | 0.04554298  |
| H | 6.48512651  | 0.48984271  | -3.33166135 |
| H | 8.92762152  | 0.21738118  | -2.98133786 |
| H | 9.83106790  | -0.19899124 | -0.71930406 |
| H | 8.31186129  | -0.35258547 | 1.23671182  |
| C | 3.85525185  | -0.73570139 | -2.07875989 |
| H | 4.14596075  | -0.59387675 | -3.12455512 |
| H | 4.12925243  | -1.74603392 | -1.76511321 |
| O | 2.44207206  | -0.57386617 | -2.00189520 |
| C | 1.74041506  | -1.61032846 | -1.48725167 |
| O | 2.16902007  | -2.73638468 | -1.32223675 |
| N | 0.47938691  | -1.20907955 | -1.18628449 |
| H | 0.26974661  | -0.20835850 | -1.19268617 |
| C | -0.37278930 | -2.11927128 | -0.45696822 |
| H | -0.34730789 | -3.09057319 | -0.96375034 |
| C | 0.06544973  | -2.32896448 | 1.00703172  |
| H | 1.10202259  | -2.67802370 | 0.98419571  |
| H | 0.04705874  | -1.35917685 | 1.51557048  |
| C | -0.83357308 | -3.31783250 | 1.69525647  |
| C | -0.62487007 | -4.69055729 | 1.53219705  |
| C | -1.93984475 | -2.88962446 | 2.43472374  |
| C | -1.49876788 | -5.61413182 | 2.09787958  |
| H | 0.23491140  | -5.03203409 | 0.95879859  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.81449989 | -3.81149085 | 3.00313893  |
| H | -2.11753630 | -1.82317377 | 2.55459479  |
| C | -2.59679555 | -5.17660669 | 2.83513039  |
| H | -1.32050188 | -6.67802807 | 1.96537255  |
| H | -3.66694213 | -3.46232492 | 3.58027907  |
| H | -3.27815585 | -5.89742924 | 3.27909412  |
| C | -1.77567862 | -1.54266403 | -0.47737645 |
| O | -2.03250381 | -0.45330863 | 0.05150381  |
| N | -2.72702136 | -2.25121433 | -1.08819489 |
| H | -2.54898603 | -3.18181549 | -1.44591987 |
| C | -4.08720432 | -1.77161785 | -1.15179377 |
| H | -4.37805113 | -1.39665459 | -0.16338369 |
| C | -4.95569934 | -2.96282985 | -1.48519692 |
| O | -4.54092411 | -4.05290287 | -1.80289015 |
| O | -6.25703058 | -2.65851722 | -1.40746041 |
| H | -6.74778490 | -3.46015210 | -1.65806660 |
| C | -4.27532419 | -0.62159602 | -2.19247692 |
| H | -3.33244226 | -0.52529320 | -2.73897601 |
| H | -5.03552410 | -0.91774024 | -2.92418926 |
| C | -4.66375974 | 0.70035675  | -1.58326064 |
| C | -5.97823439 | 0.91543987  | -1.16030552 |
| C | -3.72748444 | 1.72524447  | -1.43225608 |
| C | -6.35206288 | 2.13520004  | -0.60332651 |
| H | -6.71233368 | 0.12004852  | -1.27401857 |
| C | -4.10001077 | 2.94961313  | -0.88560944 |
| H | -2.69489472 | 1.56155329  | -1.73044488 |
| C | -5.41401074 | 3.15618822  | -0.47200384 |
| H | -7.37978219 | 2.29137836  | -0.28481941 |
| H | -3.36539289 | 3.74324128  | -0.78310262 |
| H | -5.70482423 | 4.11710084  | -0.05493274 |
| N | 2.14868039  | 3.43115683  | 0.23866327  |
| H | 2.12806498  | 3.25877971  | -0.76523593 |
| C | 0.78769665  | 3.32116437  | 0.74278859  |
| H | 0.82080996  | 3.30433378  | 1.83759410  |
| C | -0.00550653 | 4.54395539  | 0.27290138  |
| C | 0.10662075  | 2.04738970  | 0.25967661  |
| H | 0.60853167  | 5.42239741  | 0.50270141  |
| H | -0.08845211 | 4.50495247  | -0.82158118 |
| C | -1.36824061 | 4.71204884  | 0.86446266  |
| O | 0.14141936  | 1.70006304  | -0.91204259 |
| N | -2.16320506 | 5.76564855  | 0.46940932  |

|   |             |            |            |
|---|-------------|------------|------------|
| C | -2.01801485 | 3.96655558 | 1.81844195 |
| C | -3.26561656 | 5.65910114 | 1.17160785 |
| N | -3.22694274 | 4.58896607 | 2.00605893 |
| H | -1.74834960 | 3.06172527 | 2.33987378 |
| H | -4.11658284 | 6.32582918 | 1.11928655 |
| H | -3.97012001 | 4.26622120 | 2.60512382 |
| O | -0.48730477 | 1.34282862 | 1.21230601 |
| H | 2.72614953  | 2.69662033 | 0.64205356 |
| H | -1.01925468 | 0.60961822 | 0.78133047 |

### The optimized atomic coordinates of the Dimer 3

|   |              |             |             |
|---|--------------|-------------|-------------|
| H | -6.20644145  | -2.28096201 | -1.96053191 |
| C | -5.32543885  | -1.78236253 | 2.78014828  |
| C | -4.31069209  | -1.74171044 | 1.82274940  |
| C | -4.61677522  | -1.65481760 | 0.46377903  |
| C | -5.94872922  | -1.59718599 | 0.07870543  |
| C | -6.97070161  | -1.65472156 | 1.04202438  |
| C | -6.66382157  | -1.74563468 | 2.39712357  |
| H | -5.06848872  | -1.84914646 | 3.83399336  |
| H | -3.27080470  | -1.77865403 | 2.13672015  |
| H | -3.82190174  | -1.62556115 | -0.27589897 |
| H | -7.45244246  | -1.78842261 | 3.14419129  |
| C | -6.54205931  | -1.46553314 | -1.30518307 |
| C | -8.02626708  | -1.53928746 | -1.03052859 |
| C | -9.08571402  | -1.49975615 | -1.92468262 |
| C | -10.38994998 | -1.54522575 | -1.42857025 |
| C | -10.62376531 | -1.62549843 | -0.05509701 |
| C | -9.56240339  | -1.66353690 | 0.84649561  |
| C | -8.26139207  | -1.61892009 | 0.35318722  |
| H | -8.90960520  | -1.44055290 | -2.99639678 |
| H | -11.22990223 | -1.51944742 | -2.11747756 |
| H | -11.64518334 | -1.66008815 | 0.31454452  |
| H | -9.74964128  | -1.72754054 | 1.91541542  |
| C | -6.19898402  | -0.13402924 | -1.98200646 |
| H | -6.68603452  | -0.07290755 | -2.96007291 |
| H | -6.52074950  | 0.70645823  | -1.36219765 |
| O | -4.79704390  | -0.04485033 | -2.21446043 |
| C | -4.11849613  | 0.84033015  | -1.44058478 |
| O | -4.63015249  | 1.65226835  | -0.69131730 |
| N | -2.78988897  | 0.68493305  | -1.60980118 |
| H | -2.40138904  | 0.02787268  | -2.27491025 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.86389022 | 1.48283158  | -0.85911327 |
| H | -2.16795869 | 2.53595670  | -0.91077322 |
| C | -1.81437290 | 1.06164182  | 0.63760571  |
| H | -2.83352472 | 0.76660032  | 0.90761200  |
| H | -1.16712256 | 0.18344874  | 0.74201599  |
| C | -1.36740083 | 2.17425251  | 1.54673272  |
| C | -2.23506102 | 3.24614550  | 1.78900354  |
| C | -0.09445047 | 2.18888832  | 2.12742716  |
| C | -1.84004392 | 4.30862591  | 2.59474392  |
| H | -3.22509888 | 3.23078509  | 1.33630123  |
| C | 0.30012162  | 3.25641918  | 2.93400599  |
| H | 0.59159879  | 1.37025082  | 1.91965325  |
| C | -0.56981195 | 4.31736229  | 3.16972969  |
| H | -2.52558805 | 5.13226044  | 2.77672510  |
| H | 1.29182219  | 3.25566877  | 3.38035073  |
| H | -0.26115039 | 5.14808878  | 3.79891480  |
| C | -0.49340318 | 1.29708606  | -1.50190768 |
| O | -0.27930989 | 0.41646953  | -2.32432078 |
| N | 0.46640657  | 2.14691506  | -1.06458635 |
| H | 0.25569739  | 2.69778426  | -0.24124501 |
| C | 1.85633182  | 1.84093024  | -1.30784004 |
| H | 2.04408745  | 1.80830051  | -2.38469377 |
| C | 2.24438839  | 0.48315604  | -0.72305434 |
| O | 1.79332056  | 0.06836069  | 0.33302829  |
| O | 3.16652448  | -0.11022435 | -1.44215409 |
| H | 3.59369895  | -0.84798710 | -0.88853835 |
| C | 2.71908964  | 2.93495074  | -0.64738307 |
| H | 2.49029068  | 3.88601305  | -1.14309468 |
| H | 2.39882433  | 3.02843661  | 0.39879451  |
| C | 4.19455966  | 2.64299004  | -0.69882480 |
| C | 4.83165833  | 2.03904536  | 0.38739767  |
| C | 4.93719833  | 2.90303344  | -1.85209837 |
| C | 6.17696754  | 1.68990376  | 0.31834778  |
| H | 4.25693069  | 1.81498858  | 1.28365739  |
| C | 6.28095167  | 2.55114424  | -1.92603009 |
| H | 4.45168222  | 3.37184781  | -2.70567585 |
| C | 6.90670636  | 1.93849768  | -0.84203522 |
| H | 6.65218126  | 1.20637021  | 1.16857168  |
| H | 6.84175461  | 2.74786179  | -2.83593379 |
| H | 7.94493958  | 1.62653969  | -0.91384459 |
| N | 8.97441719  | -1.06479467 | -1.23457980 |



|   |            |             |             |
|---|------------|-------------|-------------|
| H | 8.94267629 | -1.63110825 | -2.08081038 |
| C | 8.18142080 | -1.72946770 | -0.20886602 |
| H | 8.28121108 | -1.16711974 | 0.72575017  |
| C | 6.71453659 | -1.73620669 | -0.64596226 |
| C | 8.66452459 | -3.15748548 | 0.01057134  |
| H | 6.49608894 | -0.74217821 | -1.05136365 |
| H | 6.59707496 | -2.45048628 | -1.47260477 |
| C | 5.72918495 | -2.03084052 | 0.43697026  |
| O | 8.83203512 | -3.95606908 | -0.88013709 |
| N | 4.39365499 | -1.76525884 | 0.24141671  |
| C | 5.90468394 | -2.51678443 | 1.70773775  |
| C | 3.77306156 | -2.06949182 | 1.35807346  |
| N | 4.64962270 | -2.53502237 | 2.27351263  |
| H | 6.78453066 | -2.84290731 | 2.24043834  |
| H | 2.71717217 | -1.92166929 | 1.53484815  |
| H | 4.42629129 | -2.83196932 | 3.21032994  |
| O | 8.92667551 | -3.44567113 | 1.30245553  |
| H | 9.95139010 | -1.03683984 | -0.95243249 |
| H | 9.22663275 | -4.37208937 | 1.31642954  |

### The optimized atomic coordinates of the Trimer 1

|   |             |            |             |
|---|-------------|------------|-------------|
| H | 10.47909386 | 4.44370658 | -2.18134784 |
| C | 9.40557277  | 4.28213002 | 2.54119447  |
| C | 8.77846037  | 3.45917081 | 1.60448410  |
| C | 9.26858450  | 3.36097594 | 0.30129097  |
| C | 10.39895933 | 4.08701409 | -0.04668577 |
| C | 11.02126299 | 4.92727778 | 0.89273906  |
| C | 10.52865189 | 5.02744962 | 2.19113173  |
| H | 9.01015168  | 4.34620652 | 3.55144152  |
| H | 7.89830488  | 2.88921286 | 1.89052737  |
| H | 8.77310679  | 2.72067110 | -0.42277342 |
| H | 11.00901450 | 5.67583320 | 2.91965236  |
| C | 11.14237859 | 4.13385834 | -1.36205323 |
| C | 12.21755563 | 5.16064889 | -1.09142729 |
| C | 13.19838842 | 5.64708866 | -1.94278996 |
| C | 14.11687359 | 6.57735517 | -1.45272964 |
| C | 14.05094440 | 7.00808582 | -0.12698012 |
| C | 13.06802671 | 6.52097096 | 0.73174124  |
| C | 12.15110791 | 5.59388243 | 0.24420869  |
| H | 13.25218738 | 5.31767699 | -2.97798927 |
| H | 14.88833348 | 6.97060721 | -2.10920533 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 14.77358938 | 7.73284761  | 0.23859503  |
| H | 13.01982676 | 6.86101206  | 1.76313951  |
| C | 11.77671992 | 2.79218936  | -1.74202971 |
| H | 12.34377182 | 2.89348534  | -2.67255346 |
| H | 12.44080340 | 2.44099369  | -0.94841234 |
| O | 10.76314472 | 1.82084406  | -1.98072232 |
| C | 10.65219102 | 0.83154178  | -1.05827617 |
| O | 11.43723769 | 0.62741702  | -0.15035629 |
| N | 9.53588240  | 0.10955396  | -1.28387071 |
| H | 8.92647855  | 0.28874993  | -2.07221818 |
| C | 9.17642542  | -0.96908988 | -0.40960801 |
| H | 10.04951745 | -1.61465784 | -0.25070904 |
| C | 8.68723280  | -0.45764777 | 0.97585718  |
| H | 9.28507736  | 0.43058095  | 1.20497869  |
| H | 7.63833238  | -0.15063437 | 0.89419990  |
| C | 8.86823217  | -1.47055848 | 2.07421118  |
| C | 10.15985001 | -1.75887275 | 2.53154588  |
| C | 7.78451214  | -2.15992350 | 2.62919534  |
| C | 10.36358817 | -2.71459089 | 3.52124046  |
| H | 11.00111885 | -1.21808013 | 2.10118461  |
| C | 7.99115199  | -3.11907610 | 3.62060449  |
| H | 6.78228176  | -1.95577534 | 2.25837751  |
| C | 9.27912343  | -3.39902145 | 4.06863236  |
| H | 11.37168189 | -2.92519823 | 3.86883243  |
| H | 7.14008988  | -3.64709034 | 4.04438323  |
| H | 9.43906620  | -4.14610443 | 4.84161020  |
| C | 8.06134545  | -1.74714463 | -1.10033739 |
| O | 7.47702724  | -1.30605284 | -2.08099269 |
| N | 7.74075310  | -2.92970200 | -0.52189422 |
| H | 8.12575209  | -3.11199195 | 0.39709281  |
| C | 6.47695389  | -3.55458201 | -0.83458779 |
| H | 6.44235528  | -3.80953488 | -1.89747055 |
| C | 5.30260141  | -2.62354683 | -0.53722781 |
| O | 5.28916090  | -1.86511644 | 0.41936539  |
| O | 4.30609105  | -2.81497474 | -1.36898471 |
| H | 3.46700130  | -2.40752746 | -0.97054087 |
| C | 6.33478736  | -4.82653057 | 0.02605907  |
| H | 7.12972758  | -5.52123279 | -0.27042907 |
| H | 6.52135366  | -4.54616819 | 1.07115338  |
| C | 4.98291765  | -5.47860280 | -0.08707489 |
| C | 3.98946642  | -5.21272249 | 0.85773911  |

|   |              |             |             |
|---|--------------|-------------|-------------|
| C | 4.67491470   | -6.30661618 | -1.16839552 |
| C | 2.71429283   | -5.75328834 | 0.72089191  |
| H | 4.21346116   | -4.55439102 | 1.69447324  |
| C | 3.39993672   | -6.84397409 | -1.31169771 |
| H | 5.43951169   | -6.52024684 | -1.91262498 |
| C | 2.41183538   | -6.56698864 | -0.36882472 |
| H | 1.95057338   | -5.52429493 | 1.46031443  |
| H | 3.17286746   | -7.47641573 | -2.16576915 |
| H | 1.40691632   | -6.95918360 | -0.49947062 |
| N | -0.99535444  | -5.40755092 | -1.54233750 |
| H | -1.14209972  | -5.01546551 | -2.47068098 |
| C | -0.85019605  | -4.31324803 | -0.59549751 |
| H | -0.76616439  | -4.72980513 | 0.41412646  |
| C | 0.42526246   | -3.53490799 | -0.93753246 |
| C | -2.03000960  | -3.35544586 | -0.63306627 |
| H | 1.21135224   | -4.27561897 | -1.12163733 |
| H | 0.26430120   | -3.00018743 | -1.88378694 |
| C | 0.90753884   | -2.58046068 | 0.10608323  |
| O | -2.44589166  | -2.91411157 | -1.70094802 |
| N | 2.15379083   | -2.00989381 | -0.01986143 |
| C | 0.33695248   | -2.14596480 | 1.27654350  |
| C | 2.34518990   | -1.26096553 | 1.04343335  |
| N | 1.26560145   | -1.30812555 | 1.85254010  |
| H | -0.61947717  | -2.34968542 | 1.73196759  |
| H | 3.25490283   | -0.71846623 | 1.25752841  |
| H | 1.15827238   | -0.81744109 | 2.72651133  |
| O | -2.53739884  | -3.05312242 | 0.54122082  |
| H | -1.83111491  | -5.94544059 | -1.32665991 |
| H | -3.19327150  | -2.29320157 | 0.44420857  |
| H | -13.41112191 | 3.71815699  | -0.76679873 |
| C | -13.54242602 | -1.10111472 | -1.27065453 |
| C | -12.42066000 | -0.34447682 | -1.61243887 |
| C | -12.32718269 | 0.99736705  | -1.24003562 |
| C | -13.36349749 | 1.56663136  | -0.51381874 |
| C | -14.50006317 | 0.80835702  | -0.18335144 |
| C | -14.59367335 | -0.52916330 | -0.55830804 |
| H | -13.59897210 | -2.14439226 | -1.56951033 |
| H | -11.61307159 | -0.80317440 | -2.17705956 |
| H | -11.45439568 | 1.58285340  | -1.51494170 |
| H | -15.47124153 | -1.11802382 | -0.30357859 |
| C | -13.49494580 | 2.96966399  | 0.03302892  |

|   |              |             |             |
|---|--------------|-------------|-------------|
| C | -14.87704549 | 2.95183851  | 0.64439919  |
| C | -15.56668098 | 3.97436425  | 1.27852255  |
| C | -16.83188033 | 3.70922304  | 1.80573428  |
| C | -17.39134996 | 2.43516250  | 1.69916806  |
| C | -16.70115434 | 1.40516284  | 1.06394428  |
| C | -15.43991181 | 1.66839396  | 0.53685935  |
| H | -15.13676770 | 4.97006426  | 1.36109460  |
| H | -17.38630600 | 4.50139590  | 2.30144555  |
| H | -18.37741694 | 2.24534041  | 2.11470565  |
| H | -17.14255707 | 0.41513218  | 0.98213648  |
| C | -12.45264649 | 3.29547685  | 1.10658993  |
| H | -12.62289107 | 4.30000861  | 1.50596400  |
| H | -12.49760613 | 2.56812686  | 1.92070887  |
| O | -11.14498580 | 3.29504729  | 0.53924895  |
| C | -10.32683152 | 2.28447567  | 0.92096491  |
| O | -10.56896932 | 1.46961572  | 1.79005902  |
| N | -9.18536100  | 2.31394093  | 0.19526652  |
| H | -9.06674740  | 2.96493059  | -0.56994775 |
| C | -8.22769142  | 1.24953846  | 0.30346374  |
| H | -8.05034285  | 1.04118659  | 1.36485690  |
| C | -8.74061605  | -0.04633975 | -0.37661109 |
| H | -9.71809512  | -0.25925723 | 0.07053657  |
| H | -8.89869733  | 0.17487074  | -1.43870467 |
| C | -7.81578895  | -1.21996740 | -0.20891677 |
| C | -7.67681764  | -1.83031389 | 1.04299166  |
| C | -7.04945250  | -1.70013941 | -1.27467743 |
| C | -6.79120702  | -2.88879933 | 1.22383412  |
| H | -8.28029328  | -1.47576177 | 1.87681724  |
| C | -6.17326711  | -2.76878189 | -1.10022697 |
| H | -7.13830729  | -1.22754830 | -2.25050549 |
| C | -6.03849847  | -3.36298230 | 0.15141163  |
| H | -6.69494677  | -3.35055311 | 2.20295499  |
| H | -5.58184640  | -3.12585292 | -1.93936455 |
| H | -5.34548631  | -4.18776936 | 0.29430055  |
| C | -6.95155434  | 1.71500282  | -0.38356905 |
| O | -6.98544407  | 2.48491883  | -1.33428401 |
| N | -5.81283999  | 1.17345422  | 0.10870494  |
| H | -5.87936562  | 0.46685342  | 0.83096306  |
| C | -4.56309105  | 1.22253435  | -0.61781650 |
| H | -4.76508324  | 1.60131863  | -1.62190839 |
| C | -4.03254286  | -0.19251690 | -0.69080138 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -3.91637730 | -0.84771745 | 0.34422887  |
| O | -3.70993463 | -0.59808479 | -1.88565168 |
| H | -3.29169519 | -1.50905092 | -1.83595030 |
| C | -3.51318027 | 2.10510670  | 0.08770860  |
| H | -3.90204367 | 3.12880909  | 0.09727406  |
| H | -3.43921078 | 1.76584850  | 1.12727737  |
| C | -2.16917397 | 2.03375303  | -0.58966725 |
| C | -1.23502913 | 1.06151608  | -0.21674231 |
| C | -1.86088331 | 2.88539457  | -1.65301943 |
| C | -0.02566701 | 0.93663841  | -0.89412727 |
| H | -1.46567104 | 0.38432852  | 0.60309334  |
| C | -0.64874640 | 2.77000605  | -2.32707898 |
| H | -2.57936335 | 3.64528994  | -1.95389602 |
| C | 0.27018314  | 1.79308923  | -1.95140628 |
| H | 0.68344686  | 0.16690725  | -0.60319447 |
| H | -0.42268155 | 3.44313962  | -3.14976660 |
| H | 1.21448177  | 1.69821659  | -2.48047377 |

## The optimized atomic coordinates of the Trimer 2

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.72358800 | -1.50531400 | -0.38872800 |
| C | -7.15889800 | 1.92507500  | 2.00031400  |
| C | -5.79300500 | 1.74321000  | 2.15067500  |
| C | -5.07930700 | 0.92017400  | 1.28751400  |
| C | -5.76392700 | 0.28792200  | 0.27062000  |
| C | -7.14057300 | 0.46387100  | 0.12215100  |
| C | -7.84618400 | 1.28325500  | 0.98214700  |
| H | -7.68892500 | 2.56383600  | 2.67942300  |
| H | -5.27735800 | 2.24639200  | 2.94517700  |
| H | -4.02527700 | 0.78863000  | 1.41547100  |
| H | -8.90410600 | 1.41978700  | 0.87117400  |
| C | -5.23228000 | -0.64710500 | -0.81029900 |
| C | -6.50530900 | -1.02624300 | -1.55651900 |
| C | -6.66761700 | -1.88169000 | -2.62335400 |
| C | -7.93721700 | -2.05795800 | -3.16036500 |
| C | -9.02405600 | -1.38377100 | -2.62839400 |
| C | -8.86463600 | -0.52574800 | -1.54979600 |
| C | -7.60256000 | -0.35218700 | -1.01725100 |
| H | -5.83097000 | -2.41091700 | -3.03771500 |
| H | -8.07657200 | -2.72189100 | -3.99054500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -9.99820700 | -1.52904100 | -3.05199300 |
| H | -9.71046100 | -0.01063300 | -1.13866500 |
| C | -4.27913000 | 0.10137200  | -1.76393900 |
| H | -3.98752900 | -0.51782200 | -2.61809500 |
| H | -4.74039600 | 1.02083000  | -2.12755200 |
| O | -3.10555900 | 0.41026200  | -0.98748800 |
| C | -2.21818300 | 1.27893700  | -1.52600500 |
| O | -2.32967500 | 1.77801300  | -2.63869700 |
| N | -1.17380100 | 1.47772800  | -0.66479700 |
| H | -1.31571200 | 1.20174800  | 0.31083500  |
| C | -0.26162200 | 2.57565900  | -0.91938300 |
| H | -0.23789500 | 2.74285000  | -1.99828000 |
| C | -0.74201200 | 3.87388000  | -0.20079200 |
| H | -1.73942300 | 4.08807700  | -0.56343500 |
| H | -0.80025500 | 3.65753700  | 0.85732900  |
| C | 0.18149600  | 5.04253400  | -0.47236900 |
| C | 0.03659600  | 5.79610400  | -1.62952000 |
| C | 1.20353600  | 5.36141400  | 0.41205700  |
| C | 0.89464400  | 6.84787800  | -1.89872500 |
| H | -0.75601500 | 5.56454700  | -2.31577100 |
| C | 2.06154200  | 6.41545700  | 0.14575100  |
| H | 1.32894400  | 4.77662400  | 1.30174100  |
| C | 1.90973300  | 7.16063000  | -1.01076500 |
| H | 0.76686100  | 7.42463600  | -2.79353500 |
| H | 2.84012900  | 6.65676700  | 0.84251300  |
| H | 2.57073600  | 7.97954600  | -1.21492700 |
| C | 1.12199200  | 2.20792600  | -0.37817500 |
| O | 1.31101900  | 2.05668800  | 0.83641100  |
| N | 2.10228900  | 2.10986600  | -1.30637400 |
| H | 1.82555000  | 2.29717200  | -2.26012700 |
| C | 3.53181700  | 1.84475000  | -1.09944600 |
| H | 4.03361500  | 2.18729600  | -2.00581800 |
| C | 3.81080500  | 0.33873800  | -0.97766300 |
| O | 3.72320400  | -0.27258600 | 0.08968500  |
| O | 4.11310900  | -0.22485500 | -2.12834400 |
| H | 4.31070600  | -1.21260100 | -2.00900600 |
| C | 4.11676800  | 2.58850800  | 0.13541300  |
| H | 3.81970300  | 3.62682600  | 0.06529200  |
| H | 3.67338700  | 2.16523300  | 1.02061300  |
| C | 5.62730000  | 2.46982100  | 0.15478700  |
| C | 6.25350600  | 1.49231200  | 0.91480100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 6.40905600  | 3.33489400  | -0.60017500 |
| C | 7.63408600  | 1.38356200  | 0.92122900  |
| H | 5.65616000  | 0.81724500  | 1.49405900  |
| C | 7.78745700  | 3.22619400  | -0.59764200 |
| H | 5.93668600  | 4.10313400  | -1.18311000 |
| C | 8.40418900  | 2.24844600  | 0.16488700  |
| H | 8.10543600  | 0.62811000  | 1.51856600  |
| H | 8.37803700  | 3.90333700  | -1.18260000 |
| H | 9.47287700  | 2.16546800  | 0.17142300  |
| N | 6.18508000  | -5.06229300 | 0.22198100  |
| H | 6.02249600  | -4.67804500 | 1.14923800  |
| C | 5.02339800  | -4.86421600 | -0.64198500 |
| H | 5.29632200  | -5.20075100 | -1.64689300 |
| C | 3.83161600  | -5.68376800 | -0.11341300 |
| C | 4.61948500  | -3.39303100 | -0.76923800 |
| H | 4.18301600  | -6.71202800 | 0.03073200  |
| H | 3.54334200  | -5.30691600 | 0.87397100  |
| C | 2.62709500  | -5.65638300 | -1.01274000 |
| O | 4.65322200  | -2.77394400 | -1.83714300 |
| N | 1.33844300  | -5.77976000 | -0.51299700 |
| C | 2.57818900  | -5.55982600 | -2.38623300 |
| C | 0.54233800  | -5.77464800 | -1.56490900 |
| N | 1.24241000  | -5.63789700 | -2.72324400 |
| H | 3.34482000  | -5.42957800 | -3.13395800 |
| H | -0.53532800 | -5.85990000 | -1.54004500 |
| H | 0.85668800  | -5.56650200 | -3.65325100 |
| O | 4.27900700  | -2.84175800 | 0.38123200  |
| H | 7.01643100  | -4.62197900 | -0.16210200 |
| H | 4.06662900  | -1.86005200 | 0.26982900  |
| N | -2.77238700 | -0.45615200 | 4.37934800  |
| H | -3.04400100 | -1.19276000 | 3.72992600  |
| C | -1.34879700 | -0.19923500 | 4.28049000  |
| H | -1.05953300 | 0.46704200  | 5.10661000  |
| C | -0.54256700 | -1.51072700 | 4.46927100  |
| C | -0.90932700 | 0.54804200  | 3.01172300  |
| H | 0.51163300  | -1.26583500 | 4.62358800  |
| H | -0.91753900 | -1.96494800 | 5.39432900  |
| C | -0.65575100 | -2.48591200 | 3.33110700  |
| O | -1.67341200 | 0.91629600  | 2.12422600  |
| N | -1.87281000 | -2.90379600 | 2.82101200  |
| C | 0.36639900  | -3.10345300 | 2.64416100  |

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -1.58502600 | -3.74453800 | 1.84514600 |
| N | -0.24036200 | -3.90474400 | 1.69972900 |
| H | 1.43969900  | -3.01731000 | 2.71848200 |
| H | -2.30619600 | -4.25702000 | 1.22357900 |
| H | 0.24387300  | -4.48129700 | 1.01702300 |
| O | 0.39849700  | 0.80195200  | 2.99009500 |
| H | -3.31722800 | 0.37330300  | 4.16495200 |
| H | 0.64104700  | 1.29521300  | 2.16698700 |