**Supporting Information**

**Synthesis and isolation of trifluoromethylation products**

Ca. 45 mg of $C_{60}$ (99.98%, TermUSA) were placed into a thick-walled glass ampoule and ca. 0.4 mL $SbCl_5$ was added. The ampoule was cooled with liquid nitrogen, evacuated, sealed off, and heated at 440 °C for 5 d. After cooling and opening the ampoule, the reaction product was heated at 150 °C in vacuum for 1 h to remove excess of $SbCl_5$ and $SbCl_3$. The chlorination product was trifluoromethylated with gaseous $CF_3I$ in a quartz ampoule placed into in a tube gradient furnace at 450 °C for 3 h. The ampoule section with liquid $CF_3I$ was kept outside the furnace at room temperature, thus producing a $CF_3I$ gas pressure of ca. 6 bar. Trifluoromethylation products were sublimed into the less heated zone of the ampoule and deposited on the walls, forming an orange-colouled layer. The sublimate was dissolved in *n*-hexane and analyzed by MALDI TOF mass spectrometry, revealing the presence of $C_{60}(CF_3)_n$ compounds with *n* ranging form 10 to 18 and small amounts of $C_{60}(CF_3)_nF$ (*n* = 13 and 15), which are derivatives of non-IPR $C_{60}$ [S1] (Figure S1).

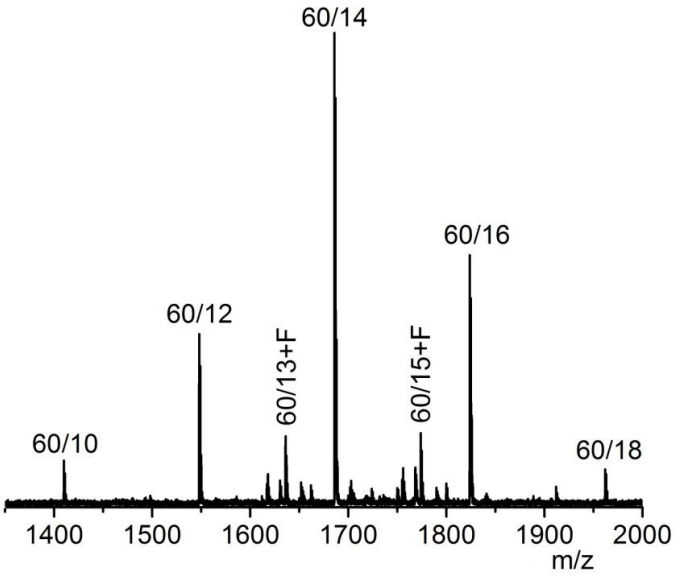


**Figure S1**. MALDI TOF mass spectrum of the trifluoromethylation product. Peak compositions $C_{60}(CF_3)_n$ and $C_{60}(CF_3)_nF$ are denoted as 60/n and 60/n+F, respectively.

The collected trifluoromethylation products were dissolved in *n*-hexane and subjected to HPLC separation in *n*-hexane using a semipreparative Cosmosil Buckyprep column (10 mm i.d. × 250 mm, Nacalai Tesque Inc.) (Figure S2) at a flow rate 3.5 mL $min^{-1}$. In the second HPLC step, several fractions of the first step were subjected to further HPLC separation in *n*-hexane using a semipreparative Cosmosil Buckyprep D column (10 mm i.d. × 250 mm, Nacalai Tesque Inc.), resulting in subfractions of much better purity. The HPLC traces and spectrometric data for three subfactions are given in Figures S3 – S5). Note that subfraction p8p2 ($C_{60}(CF_3)_{14}$) gave a mass spectrum which contains the main peak of $C_{60}(CF_3)_{13}$ (Figure S4). In fact, this phenomenon is known for $CF_3$ derivatives, featuring the presence of the addition motif of SPP (skewed-pentagonal pyramid), which results in an exceptionally easy detachment of one $CF_3$ group from a fullerene$(CF_3)_n$ molecule due to formation of anionic cyclopentadienyl structure.[S2,3] The presence of the SPP motif in the addition pattern of can be seen in Figure S6.

Several subfractions of the second HPLC step gave small yellow- or orange-coloured crystals after slow evaporation of *n*-hexane or recrystallization from toluene. An X-ray diffraction study with the use of synchrotron radiation revealed the crystal and molecular structures of three $CF_3$ derivatives $^{1809}C_{60}(CF_3)_n$ (*n* = 12, 14, and 16).

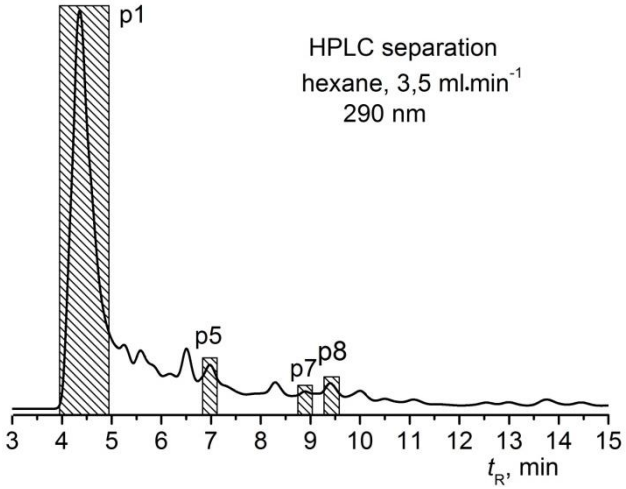


**Figure S2.** HPLC separation of the trifluoromethylation products (Cosmosil Buckyprep, 10 mm i.d. × 250 mm, *n*-hexane, 3.5 mL·min$^{-1}$; 290 nm). The fractions denoted as pN were further separated using another column.

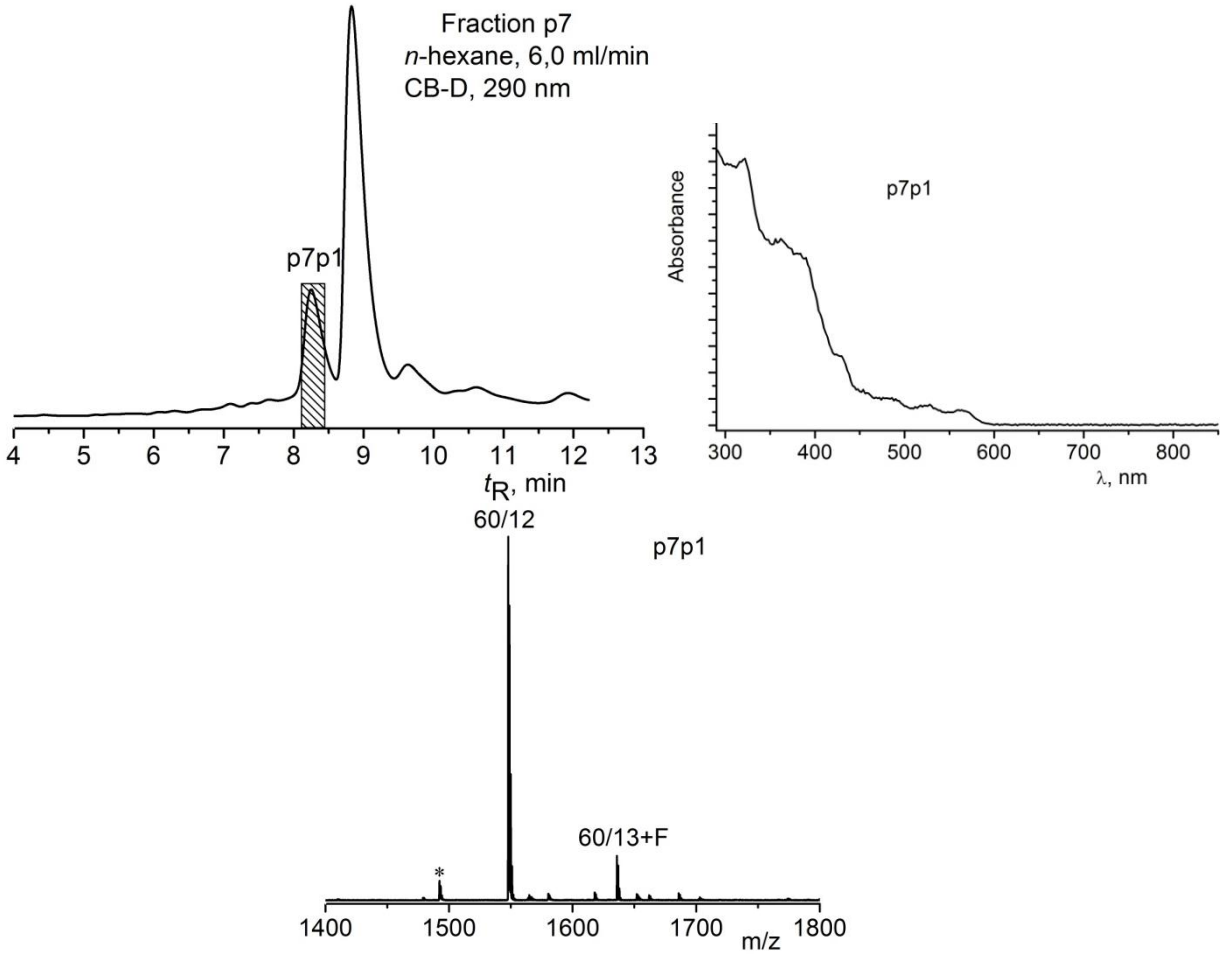


**Figure S3.** HPLC separation of fraction p7 on a Buckyprep D column and UV/Vis absorption spectrum of subfraction p7p1 (top panels). MALDI TOF mass spectrum shows a relatively good purity of $C_{60}(CF_3)_{12}$. The asterisk indicates a metastable peak.

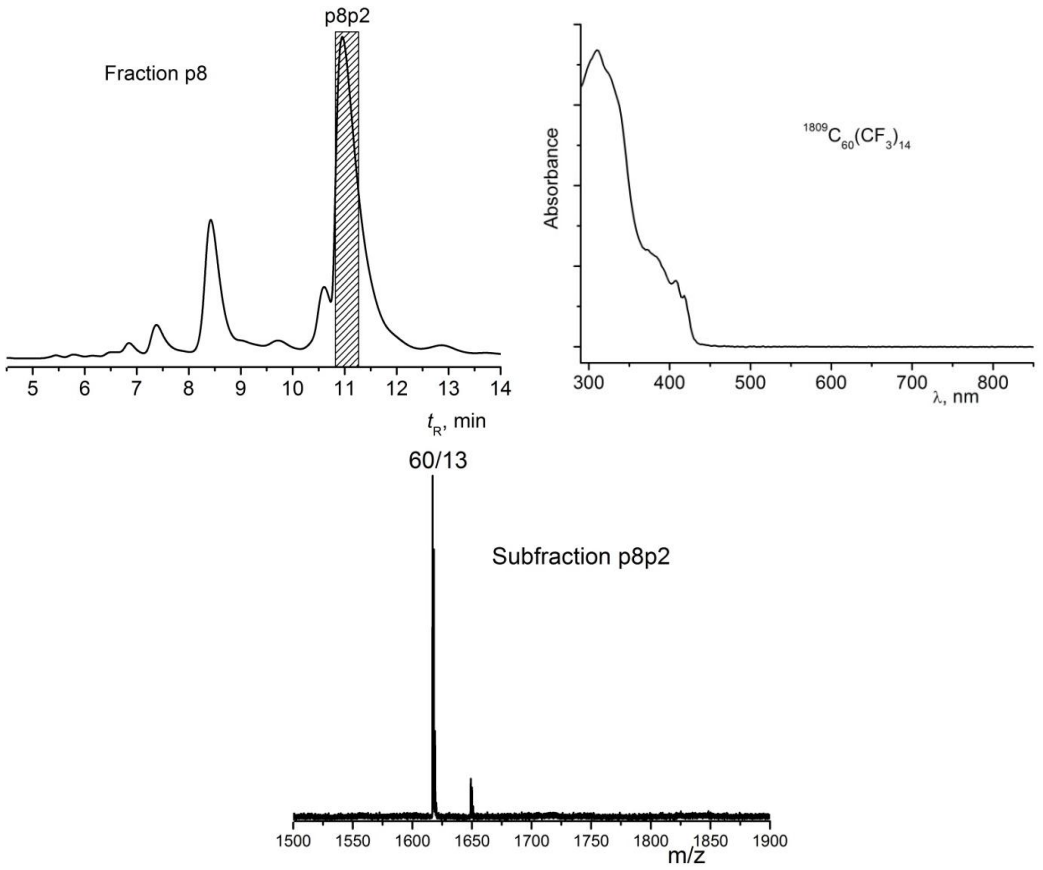


**Figure S4.** HPLC separation of fraction p8 on a Buckyprep D column and UV/Vis absorption spectrum of subfraction p8p2 (top panels). MALDI TOF mass spectrum with the prevailing peak of $C_{60}(CF_3)_{13}$ (denoted as 60/13) shows a good purity of $C_{60}(CF_3)_{14}$. This mass spectrum should replace the spectrum of $^{1809}C_{60}(CF_3)_{14}$ erroneously given in ref. S1. A small peak at 1649 mu corresponds to an admixture of $C_{60}(CF_3)_{14}$ dioxide.

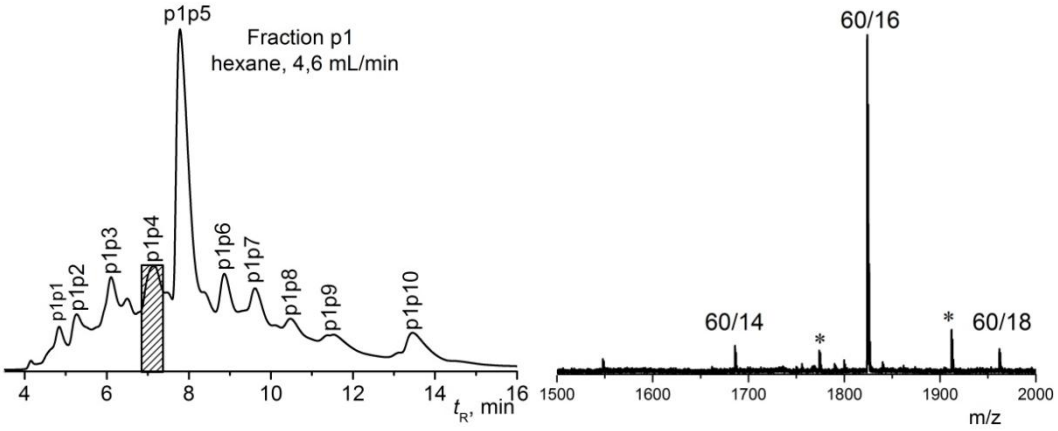


**Figure S5.** HPLC separation of fraction p1 on a Buckyprep D column and MALDI TOF mass spectrum with the prevailing peak of *C*1-$C_{60}(CF_3)_{16}$ (denoted as 60/16) demonstrating its relatively good purity. The asterisks indicate metastable peaks.

Note that nearly all (p1p1-p1p9) subfractions shown in Figure S5 (left) contained $C_{60}(CF_3)_{16}$ according to MALDI TOF analyses. It can be supposed that the hypothetic $C_s$-$C_{60}(CF_3)_{16}$ isomer (which is alternative to the experimental one) is probably present in the trifluoromethylation product but it was not isolated by HPLC in pure form.

**X-ray crystallography**

Synchrotron X-ray data were collected at 100 K on BL14.2 at the BESSY storage ring (Berlin, Germany) using a PILATUS 3S 2M pixel detector (λ = 0.8266 Å). All structures were solved and anisotropically refined using the SHELX package. Selected crystallographic data, some details of data collection and refinement, and CCDC deposition numbers are given in Table S1.

**Table S1**. Selected crystallographic data and some details of data collection and refinement.
+

| **Compound** | $^{1809}C_{60}(CF_3)_{12}$ | $^{1809}C_{60}(CF_3)_{14}$ * | $^{1809}C_{60}(CF_3)_{16}$ |
|---|---|---|---|
| Solvate molecule | PhMe | - | 0.5 PhMe |
| $M_r$ | 1640.85 | 1686.74 | 1870.83 |
| crystal system | monoclinic | orthorhombic | triclinic |
| space group | $P2_1/c$ | *Pbca* | $P\bar{1}$ |
| *a* [Å] | 18.161(1) | 20.135(1) | 12.484(1) |
| *b* [Å] | 12.380(1) | 20.793(1) | 13.298(1) |
| *c* [Å] | 24.509(2) | 25.050(2) | 20.898(2) |
| $\alpha$ [°] | 90 | 90 | 102.01(1) |
| $\beta$ [°] | 97.87(1) | 90 | 90.67(1) |
| $\gamma$ [°] | 90 | 90 | 115.74(1) |
| *V* [Å$^3$] | 5480.8(7) | 10487.6(11) | 3036.1(5) |
| *Z* | 4 | 8 | 2 |
| $D_c$ [g cm$^{-3}$] | 1.989 | 2.137 | 2.046 |
| refls collected / $R_{int}$ | 62085 / 0.189 | 158751 / 0.069 | 44837 / 0.093 |
| data / parameters | 12528 / 1025 | 15750 / 1050 | 14194 / 1154 |
| $R_1(I \geq 2\sigma(I))$ / $wR_2$(all) | 0.115 / 0.273 | 0.073 / 0.186 | 0.082 / 0.212 |
| $\Delta\rho_{max / min}$ [e Å$^{-3}$] | 0.79 /–0.49 | 0.91 /–0.44 | 0.59 /–0.49 |
| CCDC | 2061354 | 2061355 | 2061356 |

* The former structure determination of this compound (CCDC 1828801) was performed with much lower accuracy.

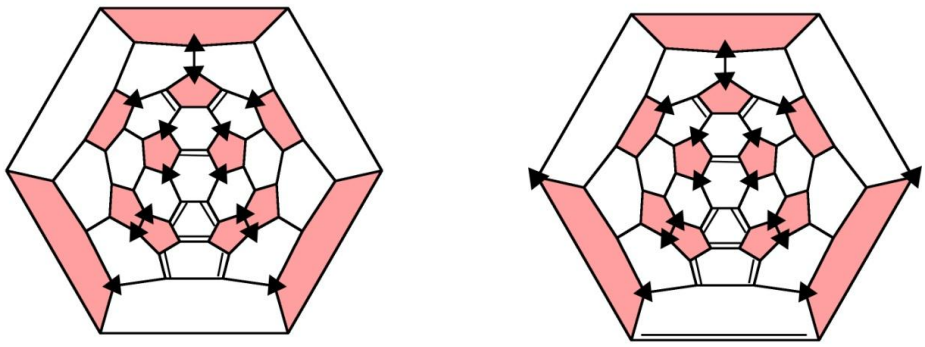

**Figure S6**. Schlegel diagrams of $C_s$-$^{1809}C_{60}(CF_3)_{14}$ and hypothetic $C_s$-$^{1809}C_{60}(CF_3)_{16}$ given parallel to the molecular mirror planes.

**Quantum-chemical calculations**

Formation energies of isomers $C_{60}Cl_n$ were calculated at the level of density functional theory (DFT) with the PBE exchange–correlation functional [S4] and the TZ2P-quality basis set [S5] implemented in the quantum-chemical PRIRODA package.[S6] The calculated values of HOMO-LUMO gaps demonstrate relatively high kinetic stabilities of $^{1809}C_{60}(CF_3)_n$ derivatives (in eV): 1.81 ($^{1809}C_{60}(CF_3)_{10}$), 1.45 ($^{1809}C_{60}(CF_3)_{12}$), 2.18 ($^{1809}C_{60}(CF_3)_{14}$), 1.99 (expt. $C_1$-$^{1809}C_{60}(CF_3)_{16}$), and 1.77 (hypot. $C_s$-$^{1809}C_{60}(CF_3)_{16}$).

**Cartesian coordinates DFT optimized molecules**

**$^{1809}C_{60}(CF_3)_{10}$**

Atomic Coordinates:

| Atom | x | y | z |
|---|---|---|---|
| C | 1.93735362 | 2.77371380 | 1.80533466 |
| C | 2.40550449 | 1.58805293 | 2.33937679 |
| C | 1.52496973 | 0.77912117 | 3.13872650 |
| C | 0.23008316 | 1.20537017 | 3.46455997 |
| C | -0.25730675 | 2.43680843 | 2.90762142 |
| C | 0.57893239 | 3.17420667 | 2.05876789 |
| C | 2.38463048 | 3.32264019 | 0.43241081 |
| C | 2.98980215 | 2.20144962 | -0.38039382 |
| C | 3.45451705 | 1.01722760 | 0.15196714 |
| C | 3.42802397 | 0.67698291 | 1.62376307 |
| C | 2.75704494 | -0.69957212 | 1.81100885 |
| C | 1.74145987 | -0.61270841 | 2.79043364 |
| C | 0.65643777 | -1.51107419 | 2.75784387 |
| C | -0.66631784 | -1.07682312 | 3.12440977 |
| C | -0.87707556 | 0.26095531 | 3.48891870 |
| C | -2.04539556 | 0.92668046 | 2.98527509 |
| C | -1.66544904 | 2.25272491 | 2.58573515 |
| C | -2.18499625 | 2.76592415 | 1.38705683 |
| C | -1.32131154 | 3.49955677 | 0.49930171 |
| C | 0.02876778 | 3.72647601 | 0.83493544 |
| C | 1.01851572 | 3.70541840 | -0.17415177 |
| C | 0.64084578 | 3.37835070 | -1.46798064 |
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| C | 2.93785714 | 0.60739675 | -2.09239142 |
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| C | 2.97423591 | -1.30091938 | -0.58725510 |
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| C | 1.51319713 | -2.53344936 | 0.74687210 |
| C | 0.54905467 | -2.48050287 | 1.72262910 |
| C | -0.90864513 | -2.90167371 | 1.51636480 |

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| C | -0.83996913 | 2.28359067 | -3.07325515 |
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| C | -0.51619139 | -2.21268040 | -2.27927836 |
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| C | -2.60334139 | -1.28606349 | -1.44481634 |
| C | 3.30387145 | 4.57127903 | 0.52909242 |
| F | 4.48343162 | 4.28269977 | 1.12369498 |
| F | 3.56928066 | 5.06130076 | -0.71149058 |
| F | 2.70824919 | 5.56096134 | 1.24597346 |
| C | 4.83715201 | 0.68643968 | 2.27790142 |
| F | 5.42351596 | 1.90186440 | 2.19263991 |

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$^{1809}C_{60}(CF_3)_{12}$

Atomic Coordinates:

| Atom | x | y | z |
|---|---|---|---|
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| C | 2.26018048 | 0.24597893 | -3.03499011 |
| C | 1.75622876 | -1.17591175 | -2.75224350 |
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| C | -2.96844542 | 2.35684862 | 1.19484520 |
| C | 3.43387708 | 0.18352177 | -4.05566382 |
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| F | 3.03470074 | -0.43365788 | -5.19826115 |
| F | 3.89619684 | 1.40791335 | -4.38665169 |
| C | 3.76110318 | -2.71006746 | 1.30063097 |
| F | 4.72858469 | -2.63212943 | 0.34709108 |
| F | 4.27193413 | -2.19523593 | 2.44349527 |

F 3.52571485 -4.03117238 1.48960557
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F 0.33310838 -3.41959452 4.86354848
F 0.46067252 -4.98273960 3.31634252
C 2.28471312 3.68748668 3.14063918
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F 3.53865397 3.58207125 2.63255075
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C -3.31383337 -4.08645430 -2.03125554
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F -4.66151136 0.42436638 -4.49471680
F -5.33923689 -1.35209170 -3.41015523
F -5.75936632 0.64013607 -2.60331724
C -4.96643525 -0.74395843 2.10973304
F -4.84048268 -0.70209535 3.45532229

| | | | |
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| F | -5.78095298 | 0.28850354 | 1.76520067 |
| F | -5.60579287 | -1.88910282 | 1.76862019 |
| C | -4.16636597 | 3.17313083 | 1.83634758 |
| F | -3.90821939 | 4.50265503 | 1.88192912 |
| F | -5.29437807 | 3.03335905 | 1.08836275 |
| F | -4.45155501 | 2.74618391 | 3.08873805 |

**$^{1809}C_{60}(CF_3)_{14}$**

Atomic Coordinates:

| Atom | x | y | z |
|---|---|---|---|
| C | 2.48738653 | 0.25632527 | 3.18471574 |
| C | 2.49770162 | -1.13222968 | 2.86439982 |
| C | 1.40091302 | -1.92342408 | 3.23143736 |
| C | 0.26881365 | -1.36262348 | 3.90717213 |
| C | 0.25777154 | -0.03024732 | 4.21254034 |
| C | 1.37932475 | 0.78772216 | 3.85668912 |
| C | 3.16711433 | 0.98538947 | 2.14613732 |
| C | 3.92459161 | -0.01537470 | 1.24017068 |
| C | 3.18011168 | -1.31912552 | 1.61218886 |
| C | 2.73614115 | -2.29062585 | 0.75627439 |
| C | 1.60630876 | -3.10992166 | 1.12162260 |
| C | 0.94940025 | -2.95209437 | 2.35137005 |
| C | -0.47608128 | -3.09882971 | 2.47952854 |
| C | -0.99668642 | -2.17768957 | 3.62497186 |
| C | -2.07363910 | -1.22181934 | 3.04784880 |
| C | -2.08630954 | 0.19550338 | 3.37762287 |
| C | -1.01405110 | 0.81645972 | 4.32002928 |
| C | -0.51451261 | 2.14742841 | 3.69425057 |
| C | 0.91195855 | 2.09320175 | 3.51853249 |
| C | 1.56175072 | 2.78508325 | 2.48725691 |
| C | 2.70076178 | 2.22652184 | 1.80257177 |
| C | 2.77284296 | 2.80234430 | 0.37767350 |
| C | 2.90847097 | 1.62240103 | -0.55272201 |
| C | 3.75211509 | 0.34561424 | -0.31076301 |
| C | 2.93382514 | -0.70818096 | -1.10135733 |

| | | | |
|---|---|---|---|
| C | 2.81360309 | -2.17828345 | -0.77722269 |
| C | 1.38668991 | -2.64416785 | -1.14922286 |
| C | 0.81709360 | -3.34284338 | -0.05058567 |
| C | -0.57796855 | -3.47322552 | 0.07242447 |
| C | -1.20640778 | -3.42345718 | 1.36402926 |
| C | -2.66025581 | -3.02764374 | 1.23753600 |
| C | -2.80144367 | -1.67243527 | 1.94331253 |
| C | -3.27055689 | -0.72867091 | 0.99723710 |
| C | -3.28085780 | 0.62354986 | 1.30635346 |
| C | -2.82132558 | 1.06473507 | 2.56830234 |
| C | -2.71321451 | 2.58873076 | 2.53674410 |
| C | -1.26416388 | 2.91861220 | 2.84250867 |
| C | -0.63599140 | 3.53586878 | 1.70240064 |
| C | 0.76088874 | 3.49464597 | 1.53454774 |
| C | 1.33352770 | 3.36034865 | 0.24159947 |
| C | 0.48660587 | 3.12146916 | -0.82652567 |
| C | 0.91849349 | 2.27710239 | -2.01184509 |
| C | 2.02754730 | 1.36754222 | -1.54886541 |
| C | 2.04353976 | -0.05270210 | -1.88805685 |
| C | 0.93919666 | -0.68393777 | -2.69928518 |
| C | 0.53501405 | -1.97095016 | -2.00222744 |
| C | -0.87993382 | -2.05676432 | -1.86635823 |
| C | -1.42934000 | -2.88157168 | -0.89931694 |
| C | -2.81904651 | -2.65682639 | -0.33490842 |
| C | -3.02058630 | -1.14639716 | -0.33045701 |
| C | -2.48253447 | -0.23664071 | -1.24350427 |
| C | -2.48962508 | 1.16922845 | -0.91575457 |
| C | -3.04352221 | 1.58696125 | 0.29584885 |
| C | -2.86109690 | 2.95112582 | 0.96140605 |
| C | -1.47672811 | 3.41470890 | 0.56749030 |
| C | -0.92733182 | 3.11235233 | -0.66847803 |
| C | -1.60351999 | 2.16985676 | -1.69229336 |
| C | -0.35938790 | 1.44882688 | -2.24102779 |
| C | -0.34916963 | 0.13974853 | -2.53313490 |
| C | -1.57281645 | -0.77456860 | -2.37507068 |

| | | | |
|---|---|---|---|
| C | 5.38320839 | -0.16730988 | 1.82733330 |
| F | 6.01603202 | -1.26159612 | 1.35092327 |
| F | 6.15485836 | 0.91608685 | 1.60076366 |
| F | 5.30953473 | -0.32159012 | 3.18097526 |
| C | -1.45775376 | -2.92858874 | 4.93532090 |
| F | -0.98380356 | -4.19932443 | 4.95937229 |
| F | -0.97632153 | -2.30158290 | 6.04230959 |
| F | -2.80259225 | -2.96683870 | 5.06695329 |
| C | -1.43266081 | 0.96679236 | 5.84105619 |
| F | -2.57892464 | 0.30036076 | 6.11342191 |
| F | -0.46376862 | 0.46758049 | 6.65617834 |
| F | -1.59434602 | 2.26326901 | 6.19821321 |
| C | 3.84248760 | 3.94340066 | 0.29209529 |
| F | 4.16541759 | 4.24379871 | -0.98309744 |
| F | 3.36745186 | 5.07604062 | 0.88133361 |
| F | 4.97768420 | 3.60367900 | 0.95040229 |
| C | 5.07072048 | 0.59693138 | -1.18263186 |
| F | 5.71060001 | 1.72972886 | -0.81722207 |
| F | 5.94792916 | -0.42401741 | -1.10124919 |
| F | 4.74961061 | 0.74021635 | -2.49304607 |
| C | 3.88286650 | -3.15405209 | -1.35992802 |
| F | 5.09664750 | -2.95580716 | -0.79701706 |
| F | 3.52621407 | -4.44384262 | -1.10437449 |
| F | 4.00897453 | -3.01847119 | -2.69823386 |
| C | -3.59687372 | -4.11259735 | 1.85500054 |
| F | -3.71473877 | -5.19875669 | 1.05529384 |
| F | -3.07654292 | -4.55765700 | 3.02768699 |
| F | -4.83247045 | -3.63034621 | 2.12378970 |
| C | -3.71497260 | 3.22273683 | 3.55197216 |
| F | -3.70650480 | 2.51466100 | 4.71110723 |
| F | -3.38987566 | 4.49861020 | 3.86228478 |
| F | -4.99043240 | 3.19208579 | 3.09775812 |
| C | 1.38821739 | 3.15226714 | -3.22672146 |
| F | 2.18475889 | 2.45128779 | -4.06747419 |
| F | 0.34146204 | 3.62567858 | -3.93976103 |

| | | | |
|---|---|---|---|
| F | 2.10081664 | 4.21915084 | -2.78682195 |
| C | 1.33784151 | -0.93600558 | -4.20037258 |
| F | 0.58206683 | -1.93301666 | -4.73115444 |
| F | 1.16323816 | 0.16517444 | -4.96192605 |
| F | 2.63321057 | -1.31134288 | -4.30089757 |
| C | -3.93532660 | -3.37321098 | -1.15491430 |
| F | -4.17036401 | -2.69846073 | -2.30765687 |
| F | -3.58391677 | -4.63467328 | -1.49676575 |
| F | -5.11280672 | -3.41102545 | -0.48655434 |
| C | -3.95251737 | 3.98257295 | 0.53704106 |
| F | -3.98691513 | 5.05134940 | 1.36898939 |
| F | -3.67619276 | 4.47152655 | -0.69775237 |
| F | -5.18623670 | 3.42954953 | 0.48280354 |
| C | -2.42647703 | 2.88284926 | -2.84987362 |
| F | -2.15056712 | 4.20540025 | -2.91629188 |
| F | -2.13673494 | 2.33933909 | -4.05720654 |
| F | -3.76344824 | 2.73820690 | -2.67354281 |
| C | -2.32435493 | -0.94371968 | -3.76931498 |
| F | -3.58683190 | -0.45431770 | -3.71380037 |
| F | -1.68264498 | -0.27340208 | -4.75878847 |
| F | -2.38151512 | -2.24074635 | -4.15044470 |

## $^{1809}C_{60}(CF_3)_{16}$

Atomic Coordinates:

| Atom | x | y | z |
|---|---|---|---|
| C | -2.45433128 | -0.58681552 | 2.80828303 |
| C | -2.23774867 | 0.77418922 | 2.94081774 |
| C | -0.95651216 | 1.23265740 | 3.34965433 |
| C | 0.08305278 | 0.33427554 | 3.64193241 |
| C | -0.16719835 | -1.05623542 | 3.51707269 |
| C | -1.42813276 | -1.50139241 | 3.13842438 |
| C | -3.45331343 | -1.18737870 | 1.82121515 |
| C | -3.52716118 | -0.21608708 | 0.61051975 |
| C | -3.28524459 | 1.18556724 | 0.72435882 |
| C | -2.92893157 | 1.83784482 | 2.08147557 |

| | | | |
|---|---|---|---|
| C | -1.75914361 | 2.83792168 | 1.87581357 |
| C | -0.65057336 | 2.46003204 | 2.68746680 |
| C | 0.68069204 | 2.69814282 | 2.27217692 |
| C | 1.73687508 | 1.78337662 | 2.59612693 |
| C | 1.44489727 | 0.63057007 | 3.28023836 |
| C | 2.21371744 | -0.68409578 | 3.09308870 |
| C | 1.05828579 | -1.69609266 | 3.05007263 |
| C | 0.95064893 | -2.70812786 | 2.15595213 |
| C | -0.34485855 | -3.21175105 | 1.74141331 |
| C | -1.62834807 | -2.84632328 | 2.45820167 |
| C | -2.70902431 | -2.49659536 | 1.42523181 |
| C | -2.68879570 | -2.98587391 | 0.17682633 |
| C | -3.41922675 | -2.26736817 | -0.93987607 |
| C | -3.50100755 | -0.78132561 | -0.66825187 |
| C | -3.07218879 | -0.06977807 | -1.80468947 |
| C | -2.84051107 | 1.28265599 | -1.69959738 |
| C | -3.03829144 | 1.92015886 | -0.45628958 |
| C | -2.41851543 | 3.30771016 | -0.49909627 |
| C | -1.50120113 | 3.47043786 | 0.68773065 |
| C | -0.15243545 | 3.63222747 | 0.22109445 |
| C | 0.93200790 | 3.31771308 | 1.02695938 |
| C | 2.34137989 | 3.00394974 | 0.49443602 |
| C | 2.93137427 | 1.94263302 | 1.62569444 |
| C | 3.18368311 | 0.54159139 | 1.06886724 |
| C | 2.83741974 | -0.60404141 | 1.71548744 |
| C | 2.68680964 | -1.69653854 | 0.74192851 |
| C | 1.95566816 | -2.97402456 | 1.04247222 |
| C | 1.01551772 | -3.31188491 | -0.12451577 |
| C | -0.29636385 | -3.60215993 | 0.43463624 |
| C | -1.51125887 | -3.79418780 | -0.42192377 |
| C | -1.28895401 | -3.00481593 | -1.71970741 |
| C | -2.34626554 | -2.24381119 | -2.01991630 |
| C | -2.34295753 | -0.95637808 | -2.82171310 |
| C | -0.90608530 | -0.39889244 | -2.90883110 |
| C | -0.67015551 | 1.01319249 | -2.80875204 |

| | | | |
|---|---|---|---|
| C | -1.84247558 | 2.01220709 | -2.60866982 |
| C | -1.42429715 | 3.10486537 | -1.63990031 |
| C | -0.16672950 | 3.36207764 | -1.21920147 |
| C | 1.03241399 | 2.78482414 | -1.89593241 |
| C | 2.12197484 | 2.34560456 | -0.87099181 |
| C | 2.52348122 | 1.09828442 | -1.20994706 |
| C | 3.41003782 | 0.20682061 | -0.40547137 |
| C | 2.92241106 | -1.25088256 | -0.50817836 |
| C | 2.34412824 | -1.90651657 | -1.75114216 |
| C | 1.22002097 | -2.89601105 | -1.39167533 |
| C | 0.04591616 | -2.78003413 | -2.38894585 |
| C | 0.16776993 | -1.28753883 | -2.74245418 |
| C | 1.46476959 | -0.84024568 | -2.42290926 |
| C | 1.65071753 | 0.51708137 | -2.22891410 |
| C | 0.62059246 | 1.43094594 | -2.50014333 |
| C | -4.86904578 | -1.48514822 | 2.47933554 |
| F | -4.86832799 | -1.18391462 | 3.80101007 |
| F | -5.85147716 | -0.76315417 | 1.88643970 |
| F | -5.20049825 | -2.79371191 | 2.37409681 |
| C | -4.14636771 | 2.45691613 | 2.83341636 |
| F | -3.71516304 | 3.25587609 | 3.84484258 |
| F | -4.93270211 | 3.19326868 | 2.01888252 |
| F | -4.92498958 | 1.49072807 | 3.37791316 |
| C | 3.21639630 | -1.01921361 | 4.27171692 |
| F | 2.75531859 | -2.06855470 | 5.00390346 |
| F | 4.44224056 | -1.35348820 | 3.80887200 |
| F | 3.35183409 | 0.02538675 | 5.12412943 |
| C | -2.02640155 | -3.93859128 | 3.49712362 |
| F | -1.00999480 | -4.12185297 | 4.38245895 |
| F | -3.12375843 | -3.57036342 | 4.20104782 |
| F | -2.28234863 | -5.12572355 | 2.90658540 |
| C | -4.80237283 | -2.85624464 | -1.33795992 |
| F | -5.39595517 | -2.09221995 | -2.29165162 |
| F | -4.69504471 | -4.11509544 | -1.81623156 |
| F | -5.63496674 | -2.88393925 | -0.26915384 |

| | | | |
|---|---|---|---|
| C | -3.35728714 | 4.52449898 | -0.74913936 |
| F | -2.62854906 | 5.57410119 | -1.21334363 |
| F | -4.30406318 | 4.23011591 | -1.67381975 |
| F | -3.98342175 | 4.93934750 | 0.37385686 |
| C | 3.10384697 | 4.36630931 | 0.32144365 |
| F | 3.38751755 | 4.96587363 | 1.49885404 |
| F | 4.24309584 | 4.23325250 | -0.39031591 |
| F | 2.30350821 | 5.23155558 | -0.35925192 |
| C | 4.17206374 | 2.42077843 | 2.48290504 |
| F | 3.80842701 | 3.31680121 | 3.43372250 |
| F | 4.69659474 | 1.35195308 | 3.13844900 |
| F | 5.16828512 | 2.95500699 | 1.74992590 |
| C | 2.91142500 | -4.15594788 | 1.36314704 |
| F | 3.68597498 | -3.86482468 | 2.43845535 |
| F | 2.21544561 | -5.28528234 | 1.64197183 |
| F | 3.72860643 | -4.41478292 | 0.31429174 |
| C | -1.77685390 | -5.32502348 | -0.67253635 |
| F | -2.55559186 | -5.85150228 | 0.29848833 |
| F | -2.38470809 | -5.53875189 | -1.86082934 |
| F | -0.60330997 | -6.01159821 | -0.68678069 |
| C | -3.02607068 | -1.12446787 | -4.23643583 |
| F | -2.11791889 | -1.01558163 | -5.23605268 |
| F | -3.61020632 | -2.34222360 | -4.35677682 |
| F | -3.98581118 | -0.19013754 | -4.43673993 |
| C | -2.42507540 | 2.58009149 | -3.95999453 |
| F | -2.01717907 | 1.85093220 | -5.02754587 |
| F | -3.77885871 | 2.58806424 | -3.95104136 |
| F | -2.01325164 | 3.85703292 | -4.15886600 |
| C | 1.58154994 | 3.67971099 | -3.07543098 |
| F | 1.57747231 | 4.99618795 | -2.79050221 |
| F | 2.84381946 | 3.31575020 | -3.40614549 |
| F | 0.80385983 | 3.51229089 | -4.17907896 |
| C | 4.89943300 | 0.36361359 | -0.84674145 |
| F | 5.34743076 | 1.61762151 | -0.60334401 |
| F | 5.70432374 | -0.50102941 | -0.19327236 |

| | | | |
|---|---|---|---|
| F | 5.02073878 | 0.14721191 | -2.18210605 |
| C | 3.47113283 | -2.56332166 | -2.65529938 |
| F | 4.66756974 | -2.56286864 | -2.01616426 |
| F | 3.18908240 | -3.85928956 | -2.93590741 |
| F | 3.62344013 | -1.89846452 | -3.82517373 |
| C | 0.16482012 | -3.69322027 | -3.65832739 |
| F | 0.43212848 | -4.97288629 | -3.30989717 |
| F | -0.99687906 | -3.68428767 | -4.36031738 |
| F | 1.13473558 | -3.26149476 | -4.49842915 |

**$^{1809}C_{60}(CF_3)_{16}$** (hypothetic)

Atomic Coordinates:

| Atom | x | y | z |
|---|---|---|---|
| C | -1.45119049 | 2.78531248 | 1.34347276 |
| C | -0.21926856 | 2.83508691 | 1.86294936 |
| C | 0.22176509 | 1.96215522 | 3.05188438 |
| C | -0.66329407 | 0.74406566 | 3.14794521 |
| C | -1.92006734 | 0.69330855 | 2.62129519 |
| C | -2.54894109 | 1.85073867 | 1.88413218 |
| C | -1.78795594 | 3.27656171 | -0.07580608 |
| C | -0.53983837 | 3.16494207 | -0.99018251 |
| C | 0.78981032 | 3.22019302 | -0.42924292 |
| C | 0.99634671 | 3.38941627 | 1.09887505 |
| C | 2.07631675 | 2.37046735 | 1.53638687 |
| C | 1.59722124 | 1.53701407 | 2.57606151 |
| C | 2.03917071 | 0.23178850 | 2.72645146 |
| C | 1.16302593 | -0.86203326 | 3.15069916 |
| C | -0.15483959 | -0.60421707 | 3.32759679 |
| C | -1.32119001 | -1.59463773 | 3.18232342 |
| C | -2.31285030 | -0.69308497 | 2.42700940 |
| C | -3.07773542 | -1.03094782 | 1.36125365 |
| C | -3.45935625 | 0.01054256 | 0.40756639 |
| C | -3.13550365 | 1.34646556 | 0.58027100 |
| C | -2.78350790 | 2.17551325 | -0.51245381 |
| C | -2.85717544 | 1.66810777 | -1.80018807 |

| | | | |
|---|---|---|---|
| C | -2.02458730 | 2.22810125 | -2.93150809 |
| C | -0.71160961 | 2.67035085 | -2.28848884 |
| C | 0.34341174 | 1.94915202 | -2.89462014 |
| C | 1.61854848 | 2.00098311 | -2.35544155 |
| C | 1.87176574 | 2.77713147 | -1.19941555 |
| C | 3.27533558 | 2.44166380 | -0.69617520 |
| C | 3.08248243 | 1.90538142 | 0.70398410 |
| C | 3.48275203 | 0.54083906 | 0.77993824 |
| C | 2.97821399 | -0.29198729 | 1.79791702 |
| C | 2.69323369 | -1.66275114 | 1.54459666 |
| C | 1.71016260 | -2.19527710 | 2.61110514 |
| C | 0.57050283 | -2.88185400 | 1.89511424 |
| C | -0.91494280 | -2.88680952 | 2.33365161 |
| C | -1.63384471 | -2.96125095 | 0.96553650 |
| C | -2.98843322 | -2.38336615 | 0.63432636 |
| C | -2.94321720 | -1.89163545 | -0.83312444 |
| C | -3.41385714 | -0.55091536 | -0.89684509 |
| C | -3.09363579 | 0.27590304 | -1.99122317 |
| C | -2.26750813 | -0.22639968 | -3.03384460 |
| C | -1.61138811 | 0.90953173 | -3.78747888 |
| C | -0.11415685 | 0.76395426 | -3.52029307 |
| C | 0.58517956 | -0.42609189 | -3.30956153 |
| C | 1.91777329 | -0.37351280 | -2.75417448 |
| C | 2.46333149 | 0.86820242 | -2.42891431 |
| C | 3.68699525 | 1.12590640 | -1.55538676 |
| C | 3.68982719 | 0.01278129 | -0.52631911 |
| C | 3.22777325 | -1.25923376 | -0.81175788 |
| C | 2.76663369 | -2.10592438 | 0.24121998 |
| C | 1.85473927 | -3.19780712 | -0.29222393 |
| C | 0.62843576 | -3.23756681 | 0.58623661 |
| C | -0.71649151 | -3.28249806 | 0.02120435 |
| C | -0.94703735 | -3.31187133 | -1.46841766 |
| C | -2.03255102 | -2.30015959 | -1.78807382 |
| C | -1.65585563 | -1.45692483 | -2.87581948 |
| C | -0.20987766 | -1.75350618 | -3.33971378 |

| | | | |
|---|---|---|---|
| C | 0.25226434 | -2.66495242 | -2.18798686 |
| C | 1.48505399 | -2.60383081 | -1.66146984 |
| C | 2.57648722 | -1.64345124 | -2.15892597 |
| C | 0.34854284 | 2.67277066 | 4.44103573 |
| F | 0.72847760 | 1.75890705 | 5.37595009 |
| F | 1.29479835 | 3.64192999 | 4.41242807 |
| F | -0.80857226 | 3.22836281 | 4.84764241 |
| C | -3.68112830 | 2.51499961 | 2.73811832 |
| F | -3.20481707 | 3.16348193 | 3.81750764 |
| F | -4.39915671 | 3.39533796 | 1.99921329 |
| F | -4.53960768 | 1.55084368 | 3.16990008 |
| C | -2.38494072 | 4.75129365 | -0.00394262 |
| F | -1.64754561 | 5.62444962 | -0.73068906 |
| F | -3.66325326 | 4.79767401 | -0.44255505 |
| F | -2.38463045 | 5.21170538 | 1.27455451 |
| C | 1.25525245 | 4.89984952 | 1.53453157 |
| F | 0.28269793 | 5.33071881 | 2.38086275 |
| F | 2.43477368 | 5.04234573 | 2.17969676 |
| F | 1.24156278 | 5.73756464 | 0.47049661 |
| C | -1.89480571 | -1.80091573 | 4.64485748 |
| F | -2.33440821 | -0.60997183 | 5.13902739 |
| F | -2.94537746 | -2.64646972 | 4.67317232 |
| F | -0.94955270 | -2.24772520 | 5.49955682 |
| C | -2.73873582 | 3.40165420 | -3.66830903 |
| F | -4.03853630 | 3.11899546 | -3.92067083 |
| F | -2.72011478 | 4.51234143 | -2.89013433 |
| F | -2.12676063 | 3.73280487 | -4.82881101 |
| C | 4.23007252 | 3.67321888 | -0.71310592 |
| F | 3.61050493 | 4.73909021 | -0.14924542 |
| F | 5.35388702 | 3.44194772 | 0.00752342 |
| F | 4.58414353 | 4.04795544 | -1.96315913 |
| C | 2.47200562 | -2.98496874 | 3.71940938 |
| F | 3.54234547 | -2.26126215 | 4.15232447 |
| F | 1.68511529 | -3.22111538 | 4.79276114 |
| F | 2.93319743 | -4.16998315 | 3.26199638 |

| | | | |
|---|---|---|---|
| C | -1.17065194 | -4.33300954 | 2.96991635 |
| F | -0.62583781 | -4.46512253 | 4.19610696 |
| F | -2.48874193 | -4.61757311 | 3.06272136 |
| F | -0.62189157 | -5.29510939 | 2.18604685 |
| C | -4.26463035 | -3.24707734 | 0.92114677 |
| F | -4.09410790 | -4.54328160 | 0.59163425 |
| F | -4.61271646 | -3.18422991 | 2.22951191 |
| F | -5.32037917 | -2.76771846 | 0.20534414 |
| C | -1.93911041 | 0.88173571 | -5.31150644 |
| F | -1.07685451 | 1.64083050 | -6.02789403 |
| F | -1.84392445 | -0.38595837 | -5.78236803 |
| F | -3.20290081 | 1.29101075 | -5.57144322 |
| C | 4.97777978 | 1.18587589 | -2.42469277 |
| F | 4.81528789 | 1.98245090 | -3.50862643 |
| F | 6.05324067 | 1.61387847 | -1.72476166 |
| F | 5.27904393 | -0.05046084 | -2.88916554 |
| C | 2.59417539 | -4.58384330 | -0.39157048 |
| F | 2.54811928 | -5.24420646 | 0.78728238 |
| F | 2.05005241 | -5.37934881 | -1.33695242 |
| F | 3.90227075 | -4.40241585 | -0.70939888 |
| C | -1.33512174 | -4.75419079 | -1.94329494 |
| F | -2.62199338 | -5.02178556 | -1.61014365 |
| F | -1.22676049 | -4.88686217 | -3.28468973 |
| F | -0.56035974 | -5.69826394 | -1.36254617 |
| C | -0.07745052 | -2.47930854 | -4.75124608 |
| F | -1.27700665 | -2.90582839 | -5.20785079 |
| F | 0.46416365 | -1.65591512 | -5.68342269 |
| F | 0.73600510 | -3.55872308 | -4.67261517 |
| C | 3.55488429 | -2.39160896 | -3.17327406 |
| F | 3.10365624 | -3.63832280 | -3.45762852 |
| F | 3.65165340 | -1.72275519 | -4.34805683 |
| F | 4.79652960 | -2.53865153 | -2.65937081 |

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