

Supporting Information for:

## Why are nH-perfluoroalkanoate ions more mobile than expected? Implications for identifying an emerging environmental pollutant

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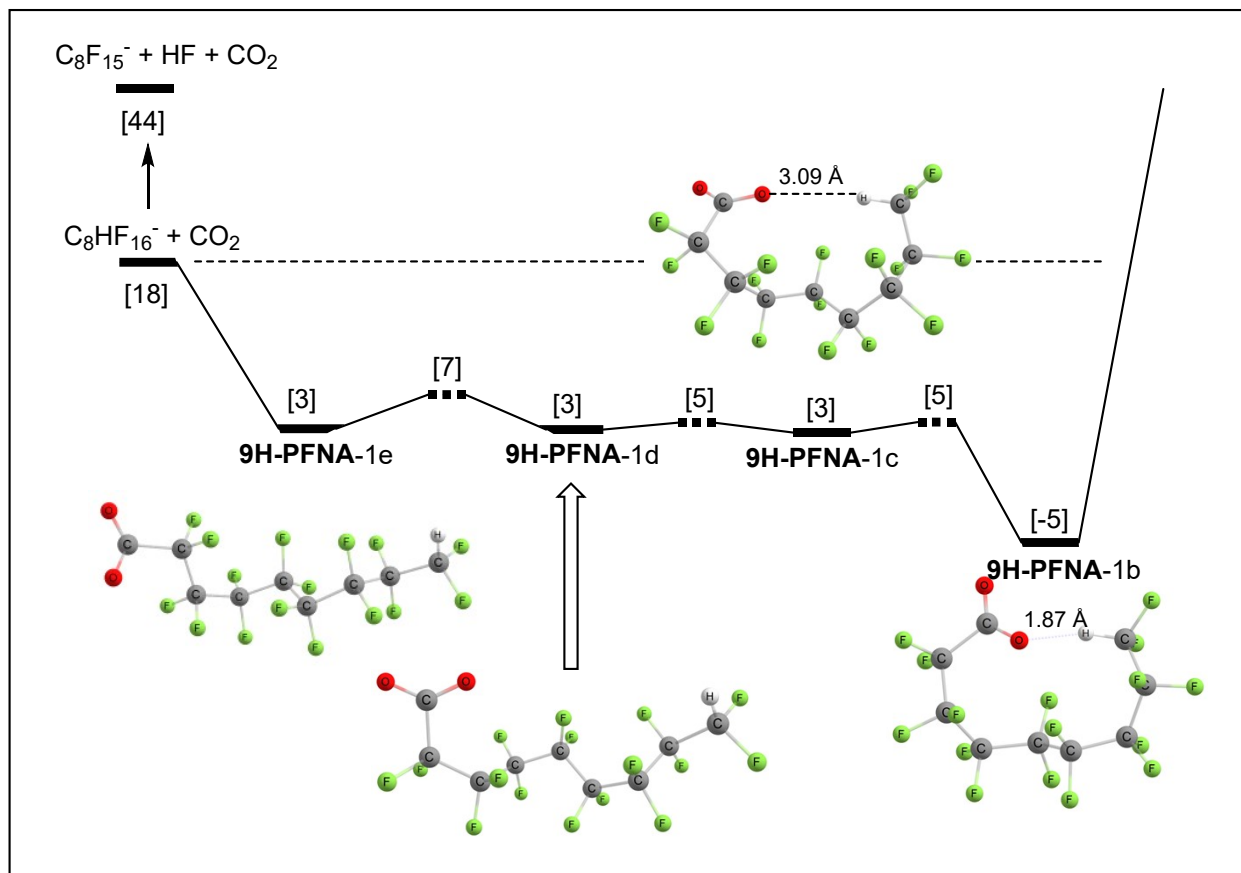
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**Table S1.** Total and free energies obtained using the B3LYP-D3BJ/ ma-def2-TZVPP level of theory [a]. Relative energies are given in kcal/mol. The collision-cross section (CCS) values were computed using MobCal-MPI 2.0 [b].

| Ion  | Total energy [0K]<br>(Hartree) | Total free energy<br>[298K] (Hartree) | Rel. free<br>energy<br>(kcal/mol) | MobCal<br>CCS (Å <sup>2</sup> ) |
|--|--------------------------------|---------------------------------------|-----------------------------------|---------------------------------|
| <b>9H-PFNA-1a</b>  | -2092.4881267                  | -2092.426969                          | 0                                 | 170.3                           |
| <b>9H-PFNA-1b</b>  | -2092.4991642                  | -2092.434630                          | -5                                | 146.2                           |
| <b>9H-PFNA-1c</b>  | -2092.4856507                  | -2092.422006                          | 3                                 | 154.7                           |
| <b>9H-PFNA-1d</b>  | -2092.4844611                  | -2092.422952                          | 3                                 | 159.8                           |
| <b>9H-PFNA-1e</b>  | -2092.4836251                  | -2092.422010                          | 3                                 | 165.9                           |
| <b>9H-PFNA-2</b>   | -2092.4172083                  | -2092.352671                          | 45                                | 141.6                           |
| <b>9H-PFNA-3</b>   | -2092.4371884                  | -2092.368136                          | 37                                | 136.1                           |
| <b>TS 9H-PFNA-1b → 1c</b>  | -2092.4852550                  | -2092.419508                          | 5                                 | -                               |
| <b>TS 9H-PFNA-1c → 1d</b>  | -2092.4843990                  | -2092.419291                          | 5                                 | -                               |
| <b>TS 9H-PFNA-1d → 1e</b>  | -2092.4785999                  | -2092.414771                          | 7                                 | -                               |
|  |                                |                                       |                                   |                                 |
| <b>C<sub>8</sub>F<sub>15</sub><sup>-</sup> + HF + CO<sub>2</sub></b> |                                | 2092.355437                           | 44                                | -                               |
| C <sub>8</sub> F <sub>15</sub> <sup>-</sup>                          | -1803.2307835                  | -1803.196776                          | -                                 | -                               |
| HF   | -100.4697273                   | -100.476758                           | -                                 | -                               |
| CO <sub>2</sub>  | -188.6722573                   | -188.681903                           | -                                 | -                               |
|  |                                |                                       |                                   |                                 |
| <b>C<sub>8</sub>HF<sub>16</sub><sup>-</sup> + CO<sub>2</sub></b>     |                                | 2092.399267                           | 18                                | -                               |
| C <sub>8</sub> HF <sub>16</sub> <sup>-</sup>                         | -1903.7662979                  | -1903.717364                          | -                                 | -                               |
| CO <sub>2</sub>  | -188.6722573                   | -188.681903                           | -                                 | -                               |
|  |                                |                                       |                                   |                                 |
| <b>PFNA-1a</b>   | -2191.7783046                  | -2191.726379                          | 0                                 | 169.6                           |
| <b>PFNA-1b</b>   | -2191.7689435                  | -2191.715526                          | 7                                 | 150.8                           |
|  |                                |                                       |                                   |                                 |
| <b>Nonanoate (1a)</b>  | -503.9722631                   | -503.768823                           | 0                                 | -                               |
| <b>Nonanoate (1b)</b>  | -503.9754017                   | -503.767121                           | 1                                 | -                               |

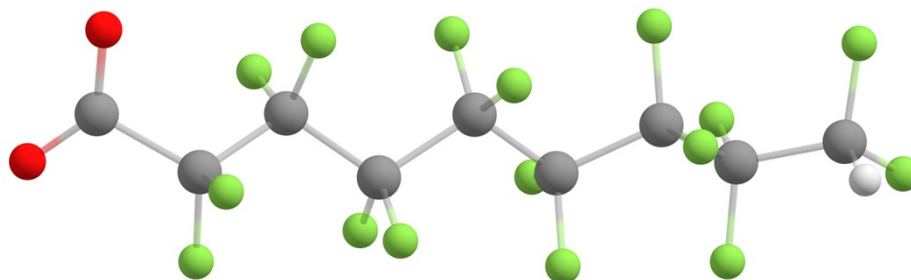
Notes: [a] The B3LYP-D3BJ method<sup>1</sup> is built into Gaussian 16<sup>2</sup>, whereas the basis set ma-def2-TZVPP<sup>3</sup> is not. Instead, the “gen” keyword was employed along with the basis set input provided by University of Minnesota<sup>4</sup>; [b] MobCal-MPI 2.0<sup>5,6</sup> was employed for CCS prediction using the trajectory method. MobCal-MPI 2.0 computes CCSs based on the ion’s geometry (computed using the B3LYP-D3BJ/ma-def2-TZVPP level of theory), partial charges (computed according to the Merz-Singh-Kollman scheme<sup>7</sup>), and atom classes defined by the MMFF94 force field<sup>8,9</sup>.

**Figure S1.** Energy diagram depicting the rotation of 9H-perfluorononanoate anions 9H-PFNA-1a to its H-bridged analogue 9H-PFNA-1b. The numbers in square brackets refer to relative energies computed at the B3LYP/ma-def2-TZVPP level of theory (in kcal/mol).



## Optimized geometries

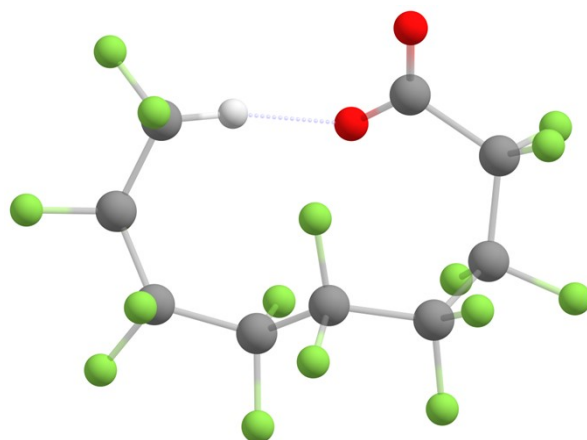
### 9H-PFNA-1a



### Cartesian coordinates (Å)

|   |                 |                 |                 |
|---|-----------------|-----------------|-----------------|
| C | -7.886982000000 | -1.515171000000 | -0.279000000000 |
| C | -6.508918000000 | -1.602135000000 | 0.416428000000  |
| F | -8.422744000000 | -0.285619000000 | -0.097620000000 |
| F | -8.707821000000 | -2.427209000000 | 0.297494000000  |
| H | -7.810753000000 | -1.726340000000 | -1.344118000000 |
| C | -5.487460000000 | -0.558357000000 | -0.138512000000 |
| F | -6.039985000000 | -2.854322000000 | 0.191725000000  |
| F | -6.665231000000 | -1.429316000000 | 1.741444000000  |
| C | -3.989042000000 | -0.895847000000 | 0.174553000000  |
| F | -5.801799000000 | 0.646173000000  | 0.370826000000  |
| F | -5.657144000000 | -0.516647000000 | -1.484687000000 |
| C | -3.022562000000 | 0.328233000000  | -0.007627000000 |
| F | -3.614886000000 | -1.896543000000 | -0.647095000000 |
| F | -3.923099000000 | -1.329407000000 | 1.449815000000  |
| C | -1.512631000000 | -0.083708000000 | -0.135551000000 |
| F | -3.193900000000 | 1.138972000000  | 1.053827000000  |
| C | -0.511511000000 | 1.098079000000  | 0.115917000000  |
| F | -1.342937000000 | -0.578688000000 | -1.380094000000 |
| F | -1.289338000000 | -1.075188000000 | 0.756670000000  |
| C | 0.940071000000  | 0.841988000000  | -0.381462000000 |
| F | -0.489961000000 | 1.304893000000  | 1.455709000000  |
| F | -1.040221000000 | 2.187761000000  | -0.482821000000 |
| C | 2.012304000000  | 1.836201000000  | 0.260428000000  |
| F | 1.209643000000  | -0.473669000000 | -0.127339000000 |
| O | 1.691262000000  | 3.023735000000  | 0.106983000000  |
| O | 2.981953000000  | 1.277209000000  | 0.781285000000  |
| F | -3.403807000000 | 0.985169000000  | -1.124837000000 |
| F | 0.933391000000  | 0.974330000000  | -1.747431000000 |

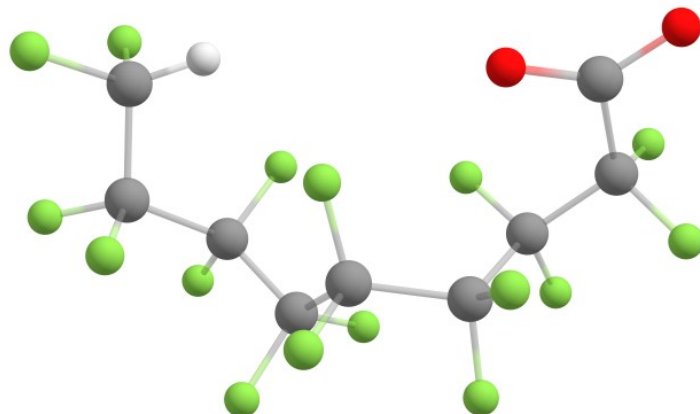
### 9H-PFNA-1b



### Cartesian coordinates

|   |                |                |                |
|---|----------------|----------------|----------------|
| O | 1.45856000000  | 2.94490100000  | 0.89790800000  |
| C | 1.44687600000  | 2.09326300000  | 0.01319000000  |
| C | 2.73738300000  | 1.19505100000  | -0.08465200000 |
| F | 3.57407800000  | 1.73883800000  | -1.02968000000 |
| F | 3.43544000000  | 1.16657500000  | 1.08132500000  |
| C | 2.56270700000  | -0.28984400000 | -0.52915000000 |
| F | 2.10352100000  | -0.37360900000 | -1.78772600000 |
| F | 3.81184000000  | -0.85584200000 | -0.53687600000 |
| C | 1.73915600000  | -1.26975400000 | 0.38329600000  |
| F | 1.84957300000  | -2.49870300000 | -0.18524800000 |
| F | 2.36217800000  | -1.31248000000 | 1.58281800000  |
| C | 0.21423400000  | -1.08599700000 | 0.73322800000  |
| F | -0.03878600000 | -2.03887800000 | 1.66932300000  |
| F | 0.02355200000  | 0.10630200000  | 1.31433400000  |
| C | -0.83439800000 | -1.32145200000 | -0.41090000000 |
| F | -0.49132000000 | -0.69548100000 | -1.53939300000 |
| F | -0.83508800000 | -2.65428000000 | -0.65965800000 |
| C | -2.32301700000 | -0.92918300000 | -0.04167700000 |
| F | -3.11570600000 | -1.78295000000 | -0.73747300000 |
| F | -2.53585300000 | -1.15653300000 | 1.27111900000  |
| C | -2.85779500000 | 0.50022600000  | -0.40341700000 |
| F | -2.82220700000 | 0.62855500000  | -1.74920200000 |
| F | -4.16700700000 | 0.48194900000  | -0.02810900000 |
| C | -2.18338200000 | 1.73847900000  | 0.21967800000  |
| F | -2.91310600000 | 2.81551700000  | -0.19112600000 |
| F | -2.29962900000 | 1.65660300000  | 1.57260500000  |
| O | 0.59360000000  | 1.80293100000  | -0.85516000000 |
| H | -1.13828700000 | 1.86550300000  | -0.09073000000 |

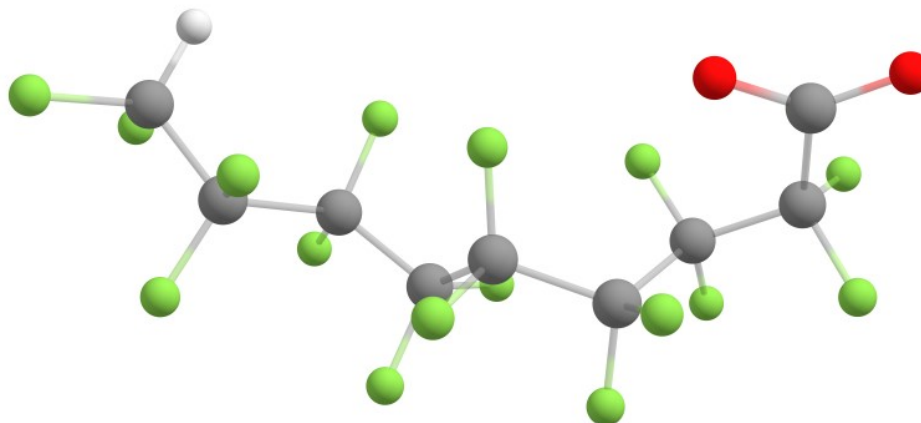
### 9H-PFNA-1c



Cartesian coordinates

|   |                |                |                |
|---|----------------|----------------|----------------|
| O | 1.66064000000  | 2.36784800000  | 0.67604100000  |
| C | 2.85933400000  | 2.37141400000  | 0.33383900000  |
| C | 3.30118000000  | 1.04647100000  | -0.41677000000 |
| F | 3.75980700000  | 1.33380600000  | -1.68076400000 |
| F | 4.33453600000  | 0.39966800000  | 0.22518900000  |
| C | 2.20622900000  | -0.03252300000 | -0.63511100000 |
| F | 1.18618700000  | 0.48247900000  | -1.37293500000 |
| F | 2.73845600000  | -1.04472300000 | -1.38561200000 |
| C | 1.61845400000  | -0.69927900000 | 0.66926300000  |
| F | 1.94392100000  | -2.02805800000 | 0.68502400000  |
| F | 2.15158500000  | -0.16440200000 | 1.78115900000  |
| C | 0.05892800000  | -0.67397300000 | 0.86049300000  |
| F | -0.16807000000 | -1.18262000000 | 2.09601000000  |
| F | -0.42042600000 | 0.58678000000  | 0.85219700000  |
| C | -0.78167000000 | -1.53402200000 | -0.16557400000 |
| F | -0.00058800000 | -1.94585200000 | -1.19029900000 |
| F | -1.25301600000 | -2.64140400000 | 0.45292900000  |
| C | -2.01037300000 | -0.81541400000 | -0.83042600000 |
| F | -1.55733900000 | 0.16001200000  | -1.64993900000 |
| F | -2.60493800000 | -1.75465000000 | -1.60507400000 |
| C | -3.09744200000 | -0.21190100000 | 0.13713800000  |
| F | -4.30882600000 | -0.71105100000 | -0.20524200000 |
| F | -2.84162400000 | -0.60814800000 | 1.41090900000  |
| C | -3.18774800000 | 1.33406700000  | 0.10970100000  |
| F | -3.74534200000 | 1.70773300000  | -1.07235400000 |
| F | -4.03103800000 | 1.71094800000  | 1.10849100000  |
| O | 3.77244900000  | 3.19136000000  | 0.45105400000  |
| H | -2.22615100000 | 1.82514000000  | 0.23931300000  |

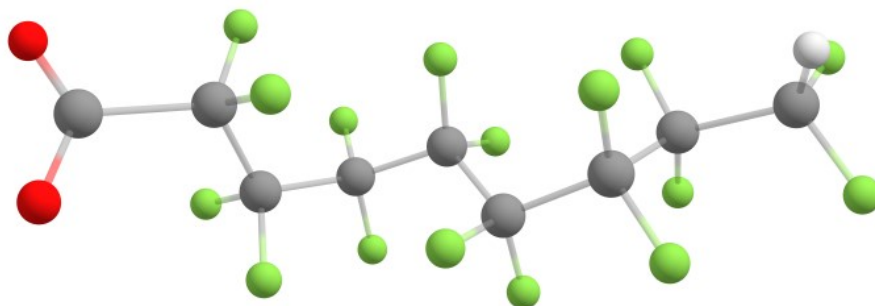
9H-PFNA-1d



Cartesian coordinates

|   |                 |                 |                 |
|---|-----------------|-----------------|-----------------|
| O | 2.449405000000  | 2.276997000000  | 0.897225000000  |
| C | 3.623238000000  | 2.060610000000  | 0.539855000000  |
| C | 3.782700000000  | 0.731380000000  | -0.308780000000 |
| F | 4.365021000000  | 0.991113000000  | -1.526677000000 |
| F | 4.598807000000  | -0.190030000000 | 0.312900000000  |
| C | 2.475427000000  | -0.031408000000 | -0.653791000000 |
| F | 1.650274000000  | 0.770444000000  | -1.376585000000 |
| F | 2.790747000000  | -1.080163000000 | -1.476561000000 |
| C | 1.688229000000  | -0.646583000000 | 0.572445000000  |
| F | 1.719230000000  | -2.014421000000 | 0.478593000000  |
| F | 2.269541000000  | -0.339460000000 | 1.742172000000  |
| C | 0.158850000000  | -0.293610000000 | 0.706081000000  |
| F | -0.216932000000 | -0.702541000000 | 1.948379000000  |
| F | -0.074259000000 | 1.021113000000  | 0.617735000000  |
| C | -0.764145000000 | -1.062890000000 | -0.312355000000 |
| F | -0.104338000000 | -1.256759000000 | -1.476907000000 |
| F | -1.078810000000 | -2.277563000000 | 0.197162000000  |
| C | -2.116423000000 | -0.381478000000 | -0.721535000000 |
| F | -1.863661000000 | 0.811447000000  | -1.316019000000 |
| F | -2.675931000000 | -1.194864000000 | -1.653469000000 |
| C | -3.188391000000 | -0.150705000000 | 0.381343000000  |
| F | -3.697042000000 | -1.344587000000 | 0.762797000000  |
| F | -2.626567000000 | 0.442540000000  | 1.461976000000  |
| C | -4.334022000000 | 0.777654000000  | -0.079226000000 |
| F | -4.969781000000 | 0.243122000000  | -1.152673000000 |
| F | -5.228457000000 | 0.875355000000  | 0.938124000000  |
| O | 4.686416000000  | 2.663763000000  | 0.706194000000  |
| H | -3.962009000000 | 1.771229000000  | -0.329755000000 |

9H-PFNA-1e

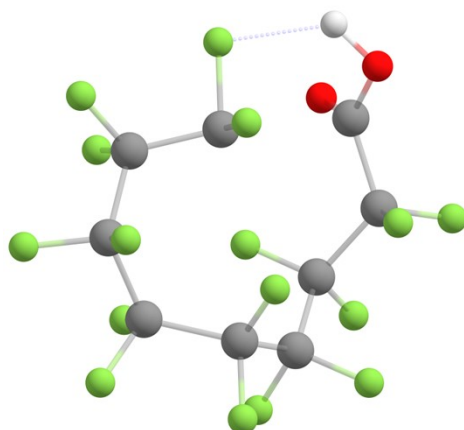


**Cartesian coordinates**

|   |                 |                 |                 |
|---|-----------------|-----------------|-----------------|
| O | 5.251561000000  | -1.194695000000 | -1.215369000000 |
| C | 4.479709000000  | -1.271976000000 | -0.255745000000 |
| C | 3.024585000000  | -0.665546000000 | -0.531047000000 |
| F | 2.886517000000  | -0.172734000000 | -1.797485000000 |
| F | 2.066514000000  | -1.642169000000 | -0.395539000000 |
| C | 2.640471000000  | 0.485206000000  | 0.434094000000  |
| F | 2.418301000000  | 0.025592000000  | 1.680216000000  |
| F | 3.678386000000  | 1.360559000000  | 0.490163000000  |
| C | 1.406299000000  | 1.392884000000  | 0.062900000000  |
| F | 1.206356000000  | 2.237441000000  | 1.110142000000  |
| F | 1.726956000000  | 2.148010000000  | -1.008703000000 |
| C | -0.002109000000 | 0.786545000000  | -0.284062000000 |
| F | -0.786670000000 | 1.855012000000  | -0.592571000000 |
| F | 0.089684000000  | 0.011676000000  | -1.375565000000 |
| C | -0.762757000000 | 0.006293000000  | 0.832093000000  |
| F | 0.013081000000  | -0.957877000000 | 1.344754000000  |
| F | -1.092892000000 | 0.867622000000  | 1.818151000000  |
| C | -2.083907000000 | -0.732200000000 | 0.393520000000  |
| F | -1.766044000000 | -1.777498000000 | -0.401999000000 |
| F | -2.610975000000 | -1.231959000000 | 1.538362000000  |
| C | -3.208412000000 | 0.061044000000  | -0.331213000000 |
| F | -3.492682000000 | 1.194143000000  | 0.339732000000  |
| F | -2.790303000000 | 0.375954000000  | -1.576348000000 |
| C | -4.502958000000 | -0.778648000000 | -0.495921000000 |
| F | -5.146897000000 | -0.893403000000 | 0.687385000000  |
| F | -5.323469000000 | -0.123114000000 | -1.354616000000 |
| O | 4.581027000000  | -1.733648000000 | 0.889336000000  |
| H | -4.288994000000 | -1.770163000000 | -0.894163000000 |



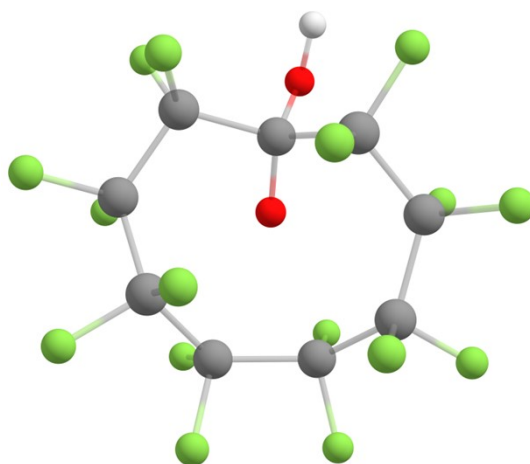
### 9H-PFNA-2



### Cartesian coordinates

|   |                 |                 |                 |
|---|-----------------|-----------------|-----------------|
| O | 2.350762000000  | 2.048964000000  | -1.316501000000 |
| C | 2.234400000000  | 1.707974000000  | -0.165877000000 |
| C | 2.377349000000  | 0.246520000000  | 0.265634000000  |
| F | 3.726936000000  | -0.032191000000 | 0.255852000000  |
| F | 1.980461000000  | 0.038767000000  | 1.534345000000  |
| C | 1.684393000000  | -0.793520000000 | -0.709750000000 |
| F | 0.922295000000  | -0.211073000000 | -1.638875000000 |
| F | 2.668147000000  | -1.463359000000 | -1.370939000000 |
| C | 0.845988000000  | -1.926516000000 | -0.021604000000 |
| F | 0.605753000000  | -2.862364000000 | -0.975160000000 |
| F | 1.635410000000  | -2.507295000000 | 0.913731000000  |
| C | -0.543020000000 | -1.660418000000 | 0.673952000000  |
| F | -0.877299000000 | -2.886336000000 | 1.164453000000  |
| F | -0.407431000000 | -0.848239000000 | 1.724037000000  |
| C | -1.756330000000 | -1.179668000000 | -0.235386000000 |
| F | -1.448472000000 | -1.295432000000 | -1.540001000000 |
| F | -2.775673000000 | -2.045888000000 | 0.005903000000  |
| C | -2.376134000000 | 0.240286000000  | 0.021666000000  |
| F | -3.505466000000 | 0.234877000000  | -0.745078000000 |
| F | -2.775134000000 | 0.283701000000  | 1.310916000000  |
| C | -1.607502000000 | 1.545931000000  | -0.356479000000 |
| F | -1.418494000000 | 1.512033000000  | -1.705939000000 |
| F | -2.556246000000 | 2.532115000000  | -0.137015000000 |
| C | -0.273649000000 | 1.828316000000  | 0.321779000000  |
| F | -0.051513000000 | 3.185465000000  | -0.044227000000 |
| F | -0.557010000000 | 1.914147000000  | 1.690632000000  |
| O | 2.384716000000  | 2.526524000000  | 0.898385000000  |
| H | 2.106834000000  | 3.402322000000  | 0.597597000000  |

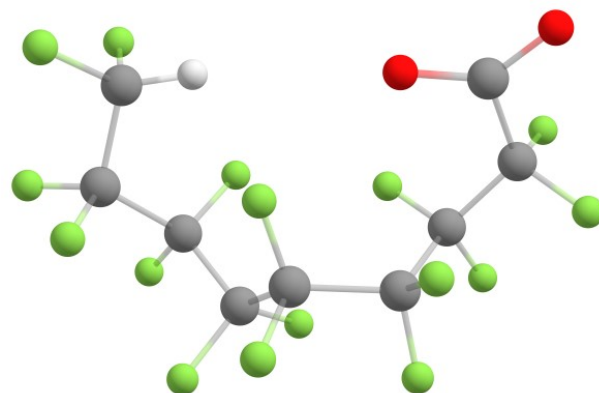
### 9H-PFNA-3



#### Cartesian coordinates

|   |                 |                 |                 |
|---|-----------------|-----------------|-----------------|
| C | -2.300342000000 | 0.264931000000  | 0.044292000000  |
| C | -1.293279000000 | 1.299794000000  | -0.582475000000 |
| C | -0.104612000000 | 2.024949000000  | 0.189396000000  |
| F | -2.108602000000 | 2.351476000000  | -0.918401000000 |
| F | -0.815667000000 | 0.794665000000  | -1.737394000000 |
| C | 1.388263000000  | 1.489419000000  | 0.535255000000  |
| F | -0.597315000000 | 2.505336000000  | 1.345144000000  |
| F | 0.114999000000  | 3.107241000000  | -0.624370000000 |
| C | 2.104889000000  | 0.347969000000  | -0.278581000000 |
| F | 1.539591000000  | 1.308331000000  | 1.847820000000  |
| F | 2.181748000000  | 2.584337000000  | 0.255722000000  |
| C | 1.934006000000  | -1.198409000000 | -0.043870000000 |
| F | 3.436456000000  | 0.542144000000  | -0.036478000000 |
| F | 1.897553000000  | 0.612562000000  | -1.590374000000 |
| C | 0.580980000000  | -1.893358000000 | -0.373386000000 |
| F | 2.342439000000  | -1.507749000000 | 1.197532000000  |
| F | 2.849822000000  | -1.752542000000 | -0.906392000000 |
| C | -0.502001000000 | -1.465369000000 | 0.694342000000  |
| F | 0.816032000000  | -3.248172000000 | -0.391009000000 |
| F | 0.286853000000  | -1.562244000000 | -1.656656000000 |
| C | -1.950439000000 | -1.264574000000 | 0.110969000000  |
| O | -0.148153000000 | -0.317547000000 | 1.189743000000  |
| O | -0.535883000000 | -2.502372000000 | 1.690750000000  |
| F | -2.890880000000 | -1.806177000000 | 0.932401000000  |
| F | -2.174439000000 | -1.829597000000 | -1.112772000000 |
| F | -3.416116000000 | 0.331766000000  | -0.756482000000 |
| F | -2.685646000000 | 0.711224000000  | 1.253580000000  |
| H | -0.663947000000 | -3.356167000000 | 1.263583000000  |

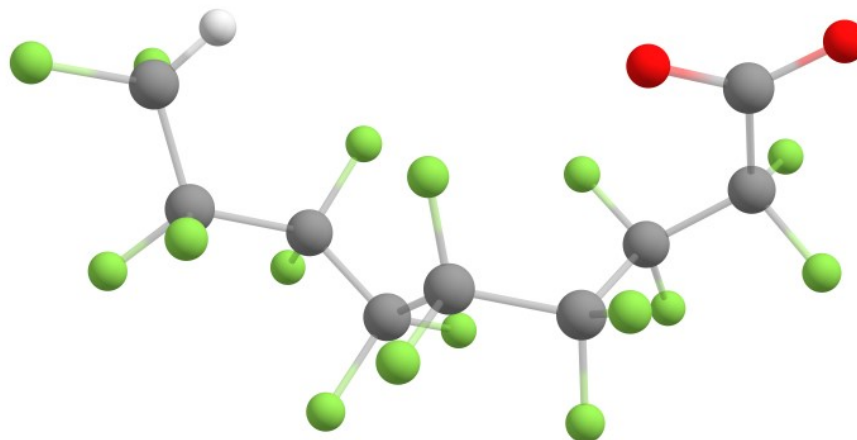
TS PFNA-1b → 1c



Cartesian coordinates

|   |                |                |                |
|---|----------------|----------------|----------------|
| O | 1.20380000000  | 2.32283800000  | 0.47518200000  |
| C | 2.43769600000  | 2.41461800000  | 0.31044000000  |
| C | 3.06286200000  | 1.16419100000  | -0.43790500000 |
| F | 3.44250500000  | 1.52456600000  | -1.71230400000 |
| F | 4.19532200000  | 0.68518800000  | 0.17508800000  |
| C | 2.14260300000  | -0.07051300000 | -0.64691600000 |
| F | 1.07234400000  | 0.27108100000  | -1.40793100000 |
| F | 2.83251500000  | -1.00693000000 | -1.36610900000 |
| C | 1.63888800000  | -0.79040100000 | 0.66355800000  |
| F | 2.07403300000  | -2.08274100000 | 0.66082400000  |
| F | 2.16516000000  | -0.20191000000 | 1.75794100000  |
| C | 0.09248900000  | -0.88566600000 | 0.94115600000  |
| F | -0.01048300000 | -1.55615500000 | 2.11742700000  |
| F | -0.42572300000 | 0.33857500000  | 1.13980600000  |
| C | -0.80560600000 | -1.65611700000 | -0.10988100000 |
| F | -0.03335500000 | -2.16572000000 | -1.09851400000 |
| F | -1.39771100000 | -2.70169600000 | 0.51406200000  |
| C | -1.96552800000 | -0.85703600000 | -0.82170200000 |
| F | -1.44802600000 | 0.00215400000  | -1.72317500000 |
| F | -2.65592900000 | -1.79965200000 | -1.51329600000 |
| C | -2.98215200000 | -0.07295200000 | 0.08659200000  |
| F | -4.23537800000 | -0.33706500000 | -0.35909700000 |
| F | -2.90620700000 | -0.54063300000 | 1.35959000000  |
| C | -2.79240800000 | 1.47161900000  | 0.08168400000  |
| F | -3.29827400000 | 1.94613900000  | -1.08859400000 |
| F | -3.55015300000 | 1.97011000000  | 1.09678700000  |
| O | 3.26554600000  | 3.28281500000  | 0.58877500000  |
| H | -1.76171300000 | 1.80099900000  | 0.19516100000  |

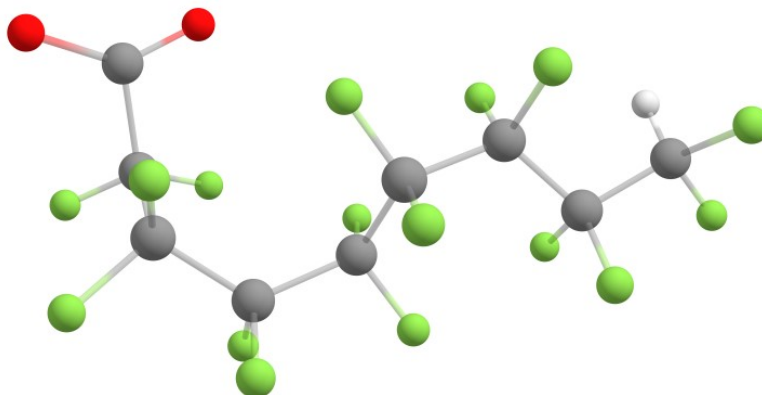
TS 9H-PFNA-1c → 1d



Cartesian coordinates

|   |                 |                 |                 |
|---|-----------------|-----------------|-----------------|
| O | 2.042751000000  | 2.363052000000  | 0.757565000000  |
| C | 3.225006000000  | 2.251505000000  | 0.381572000000  |
| C | 3.504251000000  | 0.914064000000  | -0.423363000000 |
| F | 3.961451000000  | 1.194650000000  | -1.689779000000 |
| F | 4.478193000000  | 0.139520000000  | 0.169804000000  |
| C | 2.298320000000  | -0.038168000000 | -0.645986000000 |
| F | 1.315935000000  | 0.602267000000  | -1.335751000000 |
| F | 2.706509000000  | -1.070068000000 | -1.447060000000 |
| C | 1.681335000000  | -0.691046000000 | 0.652178000000  |
| F | 1.906529000000  | -2.041100000000 | 0.630177000000  |
| F | 2.268763000000  | -0.227502000000 | 1.768064000000  |
| C | 0.129884000000  | -0.549260000000 | 0.866559000000  |
| F | -0.118488000000 | -1.072273000000 | 2.094815000000  |
| F | -0.252511000000 | 0.737979000000  | 0.890695000000  |
| C | -0.768409000000 | -1.347664000000 | -0.167364000000 |
| F | -0.027272000000 | -1.742848000000 | -1.225812000000 |
| F | -1.260203000000 | -2.464478000000 | 0.424915000000  |
| C | -1.995937000000 | -0.582338000000 | -0.767818000000 |
| F | -1.569323000000 | 0.553391000000  | -1.368504000000 |
| F | -2.514957000000 | -1.378968000000 | -1.732144000000 |
| C | -3.151502000000 | -0.233279000000 | 0.236763000000  |
| F | -4.111414000000 | -1.182933000000 | 0.155037000000  |
| F | -2.684043000000 | -0.230372000000 | 1.510476000000  |
| C | -3.779695000000 | 1.149617000000  | -0.026162000000 |
| F | -4.329532000000 | 1.157805000000  | -1.269211000000 |
| F | -4.774963000000 | 1.341039000000  | 0.878516000000  |
| O | 4.224631000000  | 2.964962000000  | 0.497529000000  |
| H | -3.048195000000 | 1.952153000000  | 0.062937000000  |

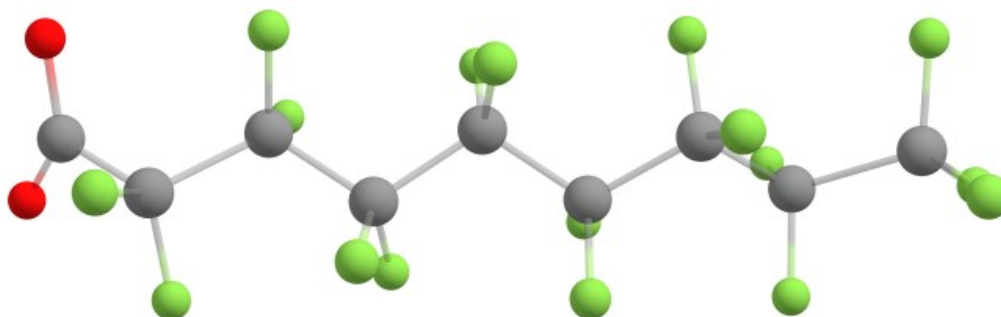
TS 9H-PFNA-1d → 1e



Cartesian coordinates

|   |                 |                 |                 |
|---|-----------------|-----------------|-----------------|
| O | -4.408438000000 | 2.169595000000  | 0.491883000000  |
| C | -3.412733000000 | 1.904499000000  | -0.191352000000 |
| C | -3.340826000000 | 0.365880000000  | -0.610906000000 |
| F | -4.575297000000 | -0.139127000000 | -0.885222000000 |
| F | -2.611175000000 | 0.178690000000  | -1.755317000000 |
| C | -2.702833000000 | -0.536731000000 | 0.510338000000  |
| F | -2.349293000000 | 0.202011000000  | 1.586690000000  |
| F | -3.617100000000 | -1.443431000000 | 0.943863000000  |
| C | -1.455105000000 | -1.420301000000 | 0.142477000000  |
| F | -1.185740000000 | -2.158282000000 | 1.252700000000  |
| F | -1.813823000000 | -2.280611000000 | -0.837228000000 |
| C | -0.057723000000 | -0.835427000000 | -0.309635000000 |
| F | 0.770973000000  | -1.917942000000 | -0.321500000000 |
| F | -0.114072000000 | -0.356526000000 | -1.557594000000 |
| C | 0.611846000000  | 0.235883000000  | 0.598754000000  |
| F | -0.174228000000 | 1.310615000000  | 0.683746000000  |
| F | 0.793352000000  | -0.287583000000 | 1.832764000000  |
| C | 2.005582000000  | 0.794163000000  | 0.117947000000  |
| F | 1.826982000000  | 1.546478000000  | -0.988773000000 |
| F | 2.420169000000  | 1.617473000000  | 1.113645000000  |
| C | 3.178023000000  | -0.181084000000 | -0.191341000000 |
| F | 3.302873000000  | -1.104200000000 | 0.781970000000  |
| F | 2.932449000000  | -0.804665000000 | -1.364634000000 |
| C | 4.524989000000  | 0.572971000000  | -0.359300000000 |
| F | 5.017067000000  | 0.935785000000  | 0.846416000000  |
| F | 5.417279000000  | -0.274128000000 | -0.933235000000 |
| O | -2.452324000000 | 2.571075000000  | -0.596392000000 |
| H | 4.415032000000  | 1.454515000000  | -0.990442000000 |

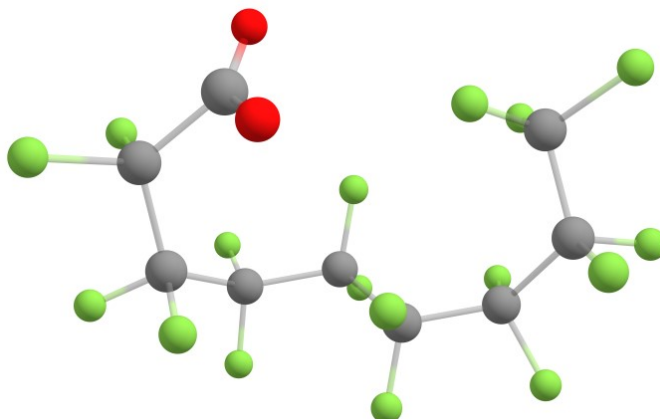
PFNA-1a



Cartesian coordinates

|   |                 |                 |                 |
|---|-----------------|-----------------|-----------------|
| C | -4.945562000000 | 0.196885000000  | -0.188551000000 |
| C | -3.612262000000 | -0.376268000000 | 0.391218000000  |
| F | -5.001801000000 | 1.522250000000  | -0.037267000000 |
| F | -5.972184000000 | -0.349687000000 | 0.473771000000  |
| F | -5.079409000000 | -0.098783000000 | -1.481176000000 |
| C | -2.325106000000 | 0.356416000000  | -0.118631000000 |
| F | -3.565607000000 | -1.681810000000 | 0.057749000000  |
| F | -3.681814000000 | -0.269017000000 | 1.730960000000  |
| C | -1.007781000000 | -0.462056000000 | 0.121090000000  |
| F | -2.251893000000 | 1.540528000000  | 0.519370000000  |
| F | -2.467263000000 | 0.584650000000  | -1.440550000000 |
| C | 0.291706000000  | 0.415068000000  | 0.036341000000  |
| F | -0.963750000000 | -1.439307000000 | -0.805023000000 |
| F | -1.084727000000 | -1.024167000000 | 1.345008000000  |
| C | 1.599993000000  | -0.428308000000 | -0.170466000000 |
| F | 0.372526000000  | 1.123940000000  | 1.178541000000  |
| C | 2.916558000000  | 0.352800000000  | 0.175445000000  |
| F | 1.617709000000  | -0.818406000000 | -1.462211000000 |
| F | 1.496798000000  | -1.526877000000 | 0.611275000000  |
| C | 4.220590000000  | -0.282484000000 | -0.384885000000 |
| F | 2.992794000000  | 0.399926000000  | 1.527491000000  |
| F | 2.755027000000  | 1.610108000000  | -0.293170000000 |
| C | 5.544270000000  | 0.263969000000  | 0.325513000000  |
| F | 4.071484000000  | -1.637015000000 | -0.267475000000 |
| O | 5.619572000000  | 1.499917000000  | 0.273631000000  |
| O | 6.274749000000  | -0.615448000000 | 0.790022000000  |
| F | 0.140931000000  | 1.270147000000  | -0.998089000000 |
| F | 4.260178000000  | -0.016688000000 | -1.729390000000 |

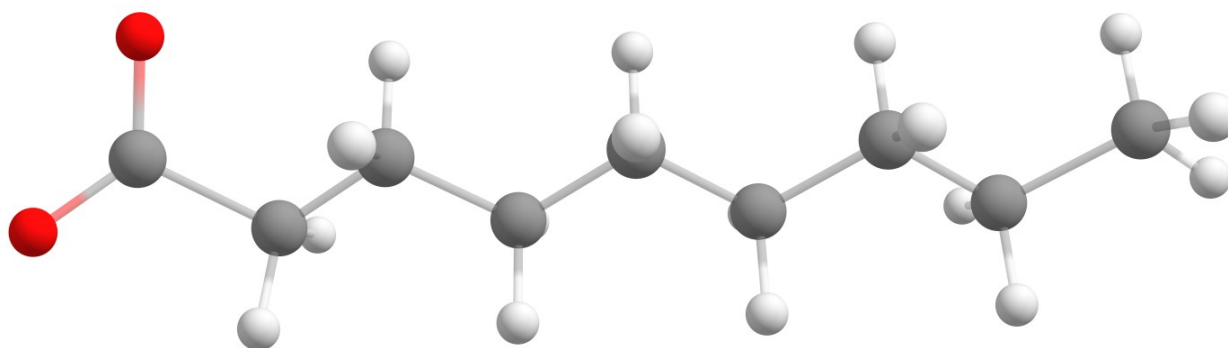
### PFNA-1b



### Cartesian coordinates

|   |                 |                 |                 |
|---|-----------------|-----------------|-----------------|
| O | 1.487623000000  | 2.755265000000  | 0.935150000000  |
| C | 1.670466000000  | 2.138999000000  | -0.118730000000 |
| C | 2.934746000000  | 1.175190000000  | -0.121470000000 |
| F | 3.825447000000  | 1.615576000000  | -1.071431000000 |
| F | 3.610412000000  | 1.182232000000  | 1.062245000000  |
| C | 2.711454000000  | -0.325999000000 | -0.475062000000 |
| F | 2.217300000000  | -0.475459000000 | -1.718202000000 |
| F | 3.939709000000  | -0.934078000000 | -0.466420000000 |
| C | 1.861472000000  | -1.222702000000 | 0.490337000000  |
| F | 2.015205000000  | -2.500402000000 | 0.053550000000  |
| F | 2.403751000000  | -1.146910000000 | 1.724818000000  |
| C | 0.313023000000  | -1.031109000000 | 0.726772000000  |
| F | 0.002800000000  | -2.004369000000 | 1.626660000000  |
| F | 0.084596000000  | 0.157448000000  | 1.296206000000  |
| C | -0.661635000000 | -1.213767000000 | -0.483970000000 |
| F | -0.412308000000 | -0.313555000000 | -1.436606000000 |
| F | -0.445140000000 | -2.449892000000 | -0.988818000000 |
| C | -2.213405000000 | -1.133909000000 | -0.127752000000 |
| F | -2.830828000000 | -2.049236000000 | -0.912989000000 |
| F | -2.437423000000 | -1.481176000000 | 1.154075000000  |
| C | -3.004098000000 | 0.197397000000  | -0.404090000000 |
| F | -2.971159000000 | 0.466091000000  | -1.720569000000 |
| F | -4.289056000000 | -0.087489000000 | -0.066471000000 |
| C | -2.622169000000 | 1.494263000000  | 0.371195000000  |
| F | -3.580657000000 | 2.408408000000  | 0.132104000000  |
| F | -2.602752000000 | 1.253307000000  | 1.689170000000  |
| O | 1.073516000000  | 2.122194000000  | -1.206012000000 |
| F | -1.466366000000 | 1.971743000000  | -0.021375000000 |

### Nonanoate (1a)

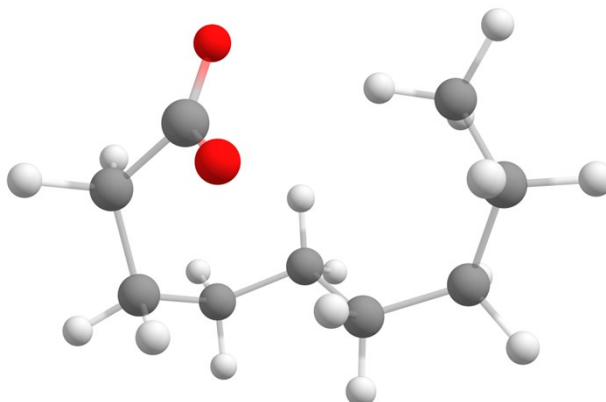


**Cartesian coordinates**

|   |                 |                 |                 |
|---|-----------------|-----------------|-----------------|
| C | -5.946745000000 | 0.432586000000  | -0.112577000000 |
| C | -4.701396000000 | -0.411224000000 | 0.147516000000  |
| H | -5.956139000000 | 1.321937000000  | 0.521552000000  |
| H | -6.863363000000 | -0.126682000000 | 0.084903000000  |
| H | -5.980272000000 | 0.771084000000  | -1.150603000000 |
| C | -3.398522000000 | 0.339203000000  | -0.118121000000 |
| H | -4.731533000000 | -1.309849000000 | -0.476434000000 |
| H | -4.707881000000 | -0.762980000000 | 1.183819000000  |
| C | -2.145439000000 | -0.493862000000 | 0.138004000000  |
| H | -3.367975000000 | 1.238970000000  | 0.505937000000  |
| H | -3.391942000000 | 0.692421000000  | -1.155091000000 |
| C | -0.842410000000 | 0.256236000000  | -0.126702000000 |
| H | -2.177361000000 | -1.393562000000 | -0.486445000000 |
| H | -2.153865000000 | -0.847130000000 | 1.175024000000  |
| C | 0.412912000000  | -0.575715000000 | 0.127124000000  |
| H | -0.809323000000 | 1.155020000000  | 0.498276000000  |
| C | 1.714443000000  | 0.181118000000  | -0.130476000000 |
| H | 0.378349000000  | -1.475344000000 | -0.498896000000 |
| H | 0.402882000000  | -0.932114000000 | 1.164004000000  |
| C | 2.969291000000  | -0.647754000000 | 0.111343000000  |
| H | 1.766382000000  | 1.071738000000  | 0.498857000000  |
| H | 1.718968000000  | 0.548248000000  | -1.162778000000 |
| C | 4.312356000000  | 0.146269000000  | 0.003632000000  |
| H | 2.936594000000  | -1.068941000000 | 1.124130000000  |
| O | 4.252656000000  | 1.368149000000  | 0.278177000000  |
| O | 5.311011000000  | -0.537808000000 | -0.319103000000 |
| H | -0.835157000000 | 0.611142000000  | -1.163130000000 |
| H | 3.015355000000  | -1.497828000000 | -0.574178000000 |



### Nonanoate (1b)



### Cartesian coordinates

|   |                 |                 |                 |
|---|-----------------|-----------------|-----------------|
| O | -0.956283000000 | -2.186545000000 | 0.695897000000  |
| C | -1.256240000000 | -1.384741000000 | -0.220291000000 |
| C | -2.460598000000 | -0.436436000000 | 0.060872000000  |
| H | -3.303127000000 | -0.836076000000 | -0.513517000000 |
| H | -2.727864000000 | -0.507382000000 | 1.118212000000  |
| C | -2.235118000000 | 1.021440000000  | -0.343212000000 |
| H | -1.799387000000 | 1.029243000000  | -1.343995000000 |
| H | -3.199777000000 | 1.538446000000  | -0.413096000000 |
| C | -1.351840000000 | 1.816745000000  | 0.627962000000  |
| H | -1.328041000000 | 2.866122000000  | 0.306579000000  |
| H | -1.830981000000 | 1.809482000000  | 1.613759000000  |
| C | 0.089236000000  | 1.319281000000  | 0.783239000000  |
| H | 0.577300000000  | 1.907932000000  | 1.570218000000  |
| H | 0.077435000000  | 0.289191000000  | 1.133642000000  |
| C | 0.911697000000  | 1.431660000000  | -0.500182000000 |
| H | 0.459759000000  | 0.795239000000  | -1.262335000000 |
| H | 0.843730000000  | 2.468496000000  | -0.854280000000 |
| C | 2.394669000000  | 1.062150000000  | -0.366713000000 |
| H | 2.933749000000  | 1.538224000000  | -1.193351000000 |
| H | 2.805189000000  | 1.502591000000  | 0.551862000000  |
| C | 2.730252000000  | -0.435569000000 | -0.404251000000 |
| H | 2.239180000000  | -0.881522000000 | -1.272515000000 |
| H | 3.811233000000  | -0.525915000000 | -0.566042000000 |
| C | 2.344959000000  | -1.241905000000 | 0.836329000000  |
| H | 2.838717000000  | -2.216939000000 | 0.822208000000  |
| H | 2.655273000000  | -0.727565000000 | 1.751710000000  |
| O | -0.709882000000 | -1.254162000000 | -1.342703000000 |
| H | 1.274825000000  | -1.439671000000 | 0.882870000000  |

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