

Supplementary Material (ESI) for Dalton Transactions
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Fluoride Ion Complexation by a B₂/Hg Heteronuclear Tridentate Lewis Acid

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[Supplementary information](#)

Titration of **1** in CHCl₃

A solution of **1** (3.0 mL, 5.1896×10^{-5} M, in chloroform) was titrated with incremental amounts of fluoride anions by addition of a solution of TBAF in chloroform (1.90×10^{-3} M). The absorption was monitored at $\lambda_{\max} = 362$ nm ($\epsilon = 13,000$). The experimental data obtained was fitted by hand to a 1:1 binding isotherm to afford a stability constant for **1**-F of $K = 5.00 \times 10^5 \pm (0.2) \text{ M}^{-1}$. (See Table S1, Figure S1).

Table S1. Absorbance of a solution of **1** after successive additions of fluoride ions in chloroform

| C _{Fluoride} | Abs _{exp} | Abs _{calc} | C _{Fluoride} | Abs _{exp} | Abs _{calc} |
|-----------------------|--------------------|---------------------|-----------------------|--------------------|---------------------|
| 0.0000E 00 | 0.67664 | 6.7464E-01 | 8.4713E-05 | 0.03337 | 3.9303E-02 |
| 1.2583E-05 | 0.53519 | 5.1547E-01 | 9.6203E-05 | 0.02990 | 3.2877E-02 |
| 2.5000E-05 | 0.40319 | 3.6452E-01 | --- | --- | --- |
| 3.7255E-05 | 0.23099 | 2.2987E-01 | --- | --- | --- |
| 4.9351E-05 | 0.13563 | 1.2954E-01 | --- | --- | --- |
| 6.1290E-05 | 0.07752 | 7.5490E-02 | --- | --- | --- |
| 7.3077E-05 | 0.04419 | 5.1115E-02 | --- | --- | --- |

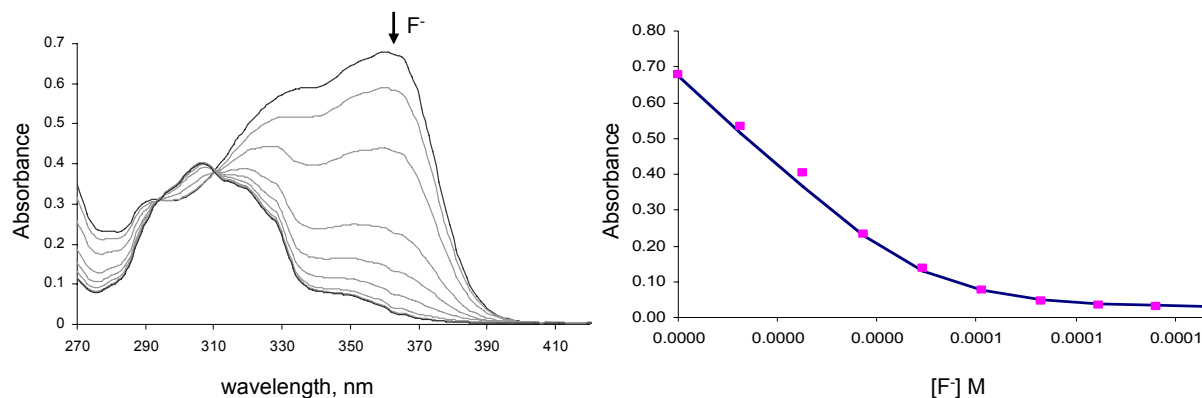


Figure S1. (left): Changes in the UV-vis absorption spectrum of **1** (3.0 mL, 5.1896×10^{-5} M, in chloroform) upon addition of a TBAF solution (1.90×10^{-2} M, in chloroform). (right): 1:1 binding isotherm for the formation of **1**-F.

Titration of **2** in CHCl₃

A solution of **2** (3.0 mL, 5.00×10^{-5} M, in chloroform) was titrated with incremental amounts of fluoride anions by addition of a solution of TBAF in chloroform (3.02×10^{-2} M). The absorption was monitored at $\lambda_{\max} = 365$ nm ($\epsilon = 8350$). The experimental data obtained was fitted by hand to a 1:1 binding isotherm to afford a stability constant for **2**-F of $K = 1.00 \times 10^3 \pm (0.2) \text{ M}^{-1}$. (See Table S2, Figure S2).

Table S2. Absorbance of a solution of **2** after successive additions of fluoride ions in chloroform

| C_{Fluoride} | Abs_{exp} | Abs_{calc} | C_{Fluoride} | Abs_{exp} | Abs_{calc} |
|-----------------------|--------------------|---------------------|-----------------------|--------------------|---------------------|
| 0.0000E 00 | 0.421 | 4.1750E-01 | 3.4827E-04 | 0.342 | 3.3604E-01 |
| 5.0250E-05 | 0.384 | 4.0157E-01 | 3.9737E-04 | 0.336 | 3.2875E-01 |
| 1.0033E-04 | 0.373 | 3.8738E-01 | 4.4631E-04 | 0.330 | 3.2221E-01 |
| 1.5025E-04 | 0.367 | 3.7472E-01 | 4.9508E-04 | 0.325 | 3.1636E-01 |
| 2.0000E-04 | 0.360 | 3.6339E-01 | 5.4370E-04 | 0.320 | 3.1112E-01 |
| 2.4959E-04 | 0.354 | 3.5326E-01 | --- | --- | --- |
| 2.9901E-04 | 0.348 | 3.4418E-01 | --- | --- | --- |

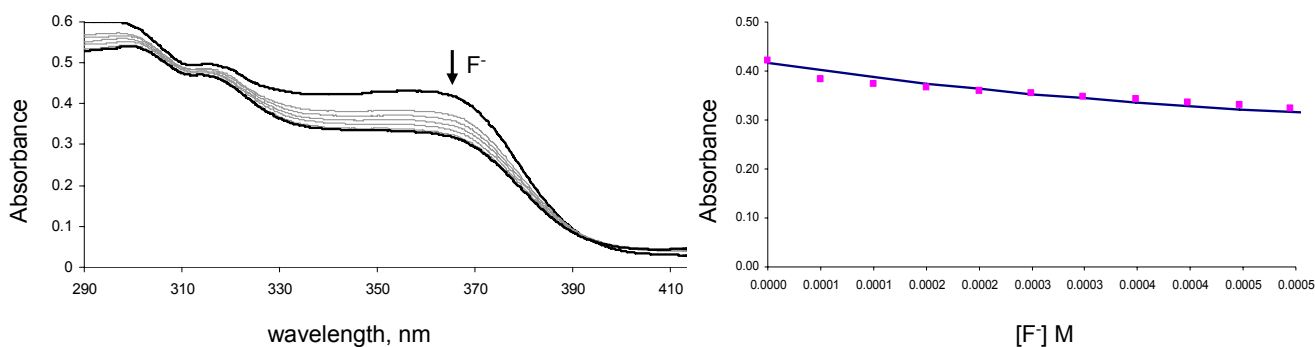


Figure S2. (left): Changes in the UV-vis absorption spectrum of **2** (3.0 mL, 5.00×10^{-5} M, in chloroform) upon addition of a TBAF solution (3.02×10^{-2} M, in chloroform). (right): 1:1 binding isotherm for the formation of **2-F**.

Titration of **3** in CHCl_3

A solution of **3** (3.0 mL, 2.525×10^{-5} M, in chloroform) was titrated with incremental amounts of fluoride anions by addition of a solution of TABF in chloroform (3.02×10^{-2} M). The absorption was monitored at $\lambda_{\text{max}} = 360$ nm ($\epsilon = 27,800$). The experimental data obtained was fitted by hand to a 1:1 binding isotherm to afford a stability constant for **3-F** of $K = 1.7 \times 10^3 \pm (0.1) \text{ M}^{-1}$. (See Table S3, Figure S3).

Table S3. Absorbance of a solution of **3** after successive additions of fluoride ions in chloroform

| C_{Fluoride} | Abs_{exp} | Abs_{calc} | C_{Fluoride} | Abs_{exp} | Abs_{calc} |
|-----------------------|--------------------|---------------------|-----------------------|--------------------|---------------------|
| 0.0000E 00 | 0.704 | 7.0195E-01 | 3.4827E-04 | 0.597 | 6.0181E-01 |
| 5.0250E-05 | 0.677 | 6.7920E-01 | 3.9737E-04 | 0.586 | 5.9491E-01 |
| 1.0033E-04 | 0.655 | 6.6023E-01 | 4.4631E-04 | 0.578 | 5.8906E-01 |
| 1.5025E-04 | 0.644 | 6.4432E-01 | --- | --- | --- |
| 2.0000E-04 | 0.631 | 6.3091E-01 | --- | --- | --- |
| 2.4959E-04 | 0.619 | 6.1957E-01 | --- | --- | --- |
| 2.9901E-04 | 0.609 | 6.0996E-01 | --- | --- | --- |

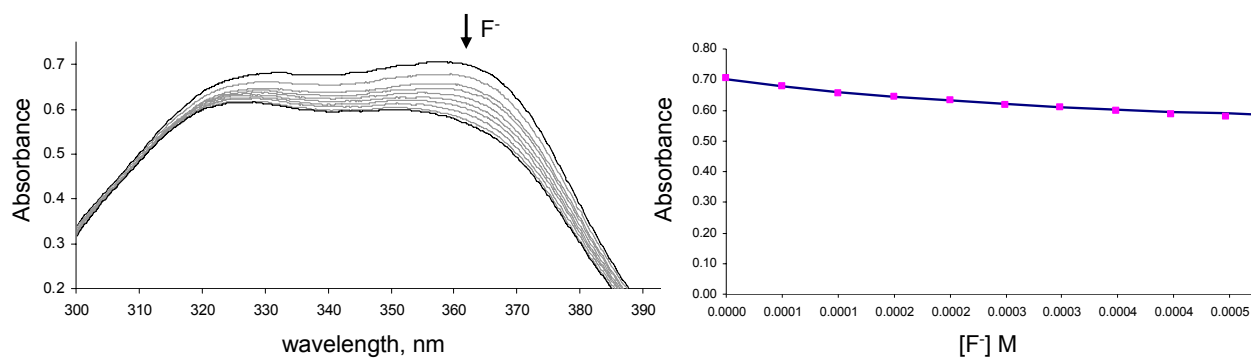
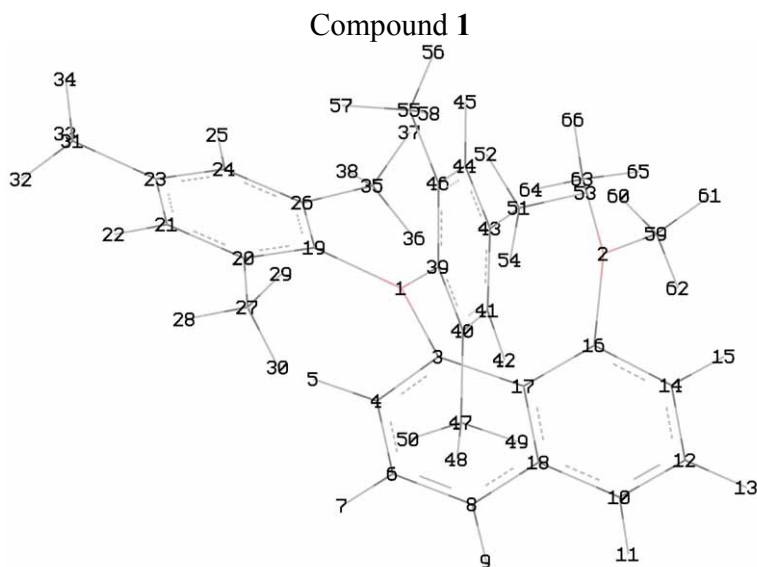


Figure S3. (left): Changes in the UV-vis absorption spectrum of **3** (3.0 mL, 2.525×10^{-5} M, in chloroform) upon addition of a TBAF solution (3.02×10^{-2} M, in chloroform). (right): 1:1 binding isotherm for the formation of **3-F**.

Computational details:

All energies, expressed in hartrees, are reported for standard conditions, 298 K and 1 atm., and include the vibrational and thermodynamic correction. For each structure, the numbering of the atoms follows their order of appearance in the Cartesian coordinate list. The energy corrected to enthalpy for the fluoride anion was found to be equal to -99.886333 hartrees.



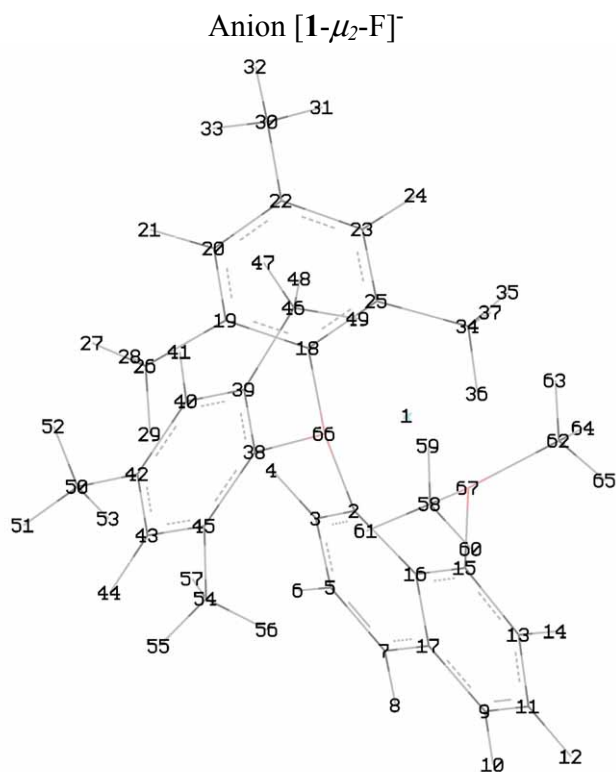
Energy Corrected for Enthalpy: -1213.167739

Cartesian Coordinates:

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| B | 0.452371 | -0.213231 | -0.111461 | H | 4.904264 | 0.365913 | -1.713443 |
| B | -2.258687 | 0.421831 | 1.669921 | C | 4.879929 | -0.77624 | 0.109101 |
| C | -0.437183 | -1.508975 | -0.2889 | C | 4.041709 | -1.333813 | 1.079518 |
| C | 0.238233 | -2.548892 | -0.950522 | H | 4.480176 | -1.913965 | 1.888457 |
| H | 1.302188 | -2.443827 | -1.12787 | C | 2.647073 | -1.17724 | 1.041034 |
| C | -0.399526 | -3.71331 | -1.428566 | C | 2.361071 | 0.92887 | -2.183086 |
| H | 0.178311 | -4.473969 | -1.943871 | H | 3.14989 | 1.066304 | -2.929912 |
| C | -1.75563 | -3.856289 | -1.250587 | H | 2.004718 | 1.921864 | -1.888337 |
| H | -2.278387 | -4.729396 | -1.632012 | H | 1.525116 | 0.423934 | -2.679639 |
| C | -3.914458 | -3.045128 | -0.429363 | C | 6.381845 | -0.93842 | 0.182149 |
| H | -4.36049 | -3.947763 | -0.837837 | H | 6.829765 | -0.982281 | -0.816748 |
| C | -4.689424 | -2.091815 | 0.187771 | H | 6.6601 | -1.851581 | 0.719186 |
| H | -5.7645 | -2.215986 | 0.272046 | H | 6.848508 | -0.095131 | 0.710059 |
| C | -4.066608 | -0.94341 | 0.725979 | C | 1.856484 | -1.801718 | 2.174975 |
| H | -4.694345 | -0.209676 | 1.222625 | H | 0.902366 | -2.213874 | 1.839678 |
| C | -2.681827 | -0.731884 | 0.684901 | H | 1.639303 | -1.067369 | 2.962734 |
| C | -1.860768 | -1.683865 | -0.033281 | H | 2.427593 | -2.610673 | 2.642697 |
| C | -2.509176 | -2.861675 | -0.566042 | C | -0.10388 | 1.26864 | -0.243574 |
| C | 2.03302 | -0.41763 | 0.000964 | C | -0.996784 | 1.645311 | -1.299603 |
| C | 2.891196 | 0.140787 | -0.996877 | C | -1.364907 | 2.988959 | -1.46896 |
| C | 4.278392 | -0.053627 | -0.929051 | H | -2.026684 | 3.249124 | -2.291529 |

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| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|----------|
| C | -0.902909 | 4.002953 | -0.623289 | C | 1.407455 | 2.080487 | 1.70448 |
| C | -0.01932 | 3.641837 | 0.402501 | H | 1.393779 | 2.916537 | 2.412018 |
| H | 0.367288 | 4.414206 | 1.063348 | H | 2.425083 | 1.999198 | 1.305687 |
| C | 0.399224 | 2.317999 | 0.593459 | H | 1.21133 | 1.166709 | 2.268062 |
| C | -1.547918 | 0.665143 | -2.320149 | C | -3.042402 | 1.799316 | 1.691494 |
| H | -1.839689 | 1.196781 | -3.231858 | H | -2.322871 | 2.624766 | 1.605977 |
| H | -2.437038 | 0.150234 | -1.939623 | H | -3.540906 | 1.934532 | 2.664993 |
| H | -0.827721 | -0.107886 | -2.598636 | H | -3.786702 | 1.919287 | 0.896671 |
| C | -1.348607 | 5.436642 | -0.800548 | C | -1.34445 | 0.08114 | 2.917557 |
| H | -0.553452 | 6.139874 | -0.529451 | H | -0.594586 | -0.695479 | 2.748187 |
| H | -2.214104 | 5.66375 | -0.163046 | H | -2.040804 | -0.322008 | 3.675004 |
| H | -1.644431 | 5.638755 | -1.835313 | H | -0.870615 | 0.961179 | 3.368482 |



Energy Corrected for Enthalpy: -1313.173708

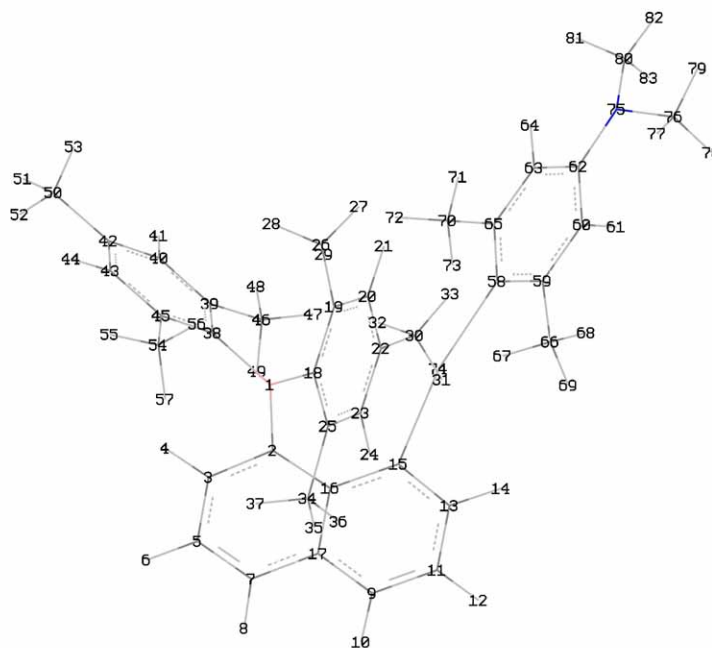
Cartesian Coordinates:

| | | | | | | | |
|---|-----------|-----------|-----------|---|----------|-----------|-----------|
| F | -0.264756 | -0.165315 | 1.573713 | C | 4.387653 | -2.029565 | 0.050203 |
| C | -0.75392 | -1.040275 | -0.754381 | C | 3.352906 | -2.503442 | 0.86037 |
| C | -0.291609 | -1.676371 | -1.906355 | H | 3.530617 | -3.372736 | 1.4918 |
| H | 0.757457 | -1.584126 | -2.171099 | C | 2.077537 | -1.912191 | 0.874877 |
| C | -1.13363 | -2.422841 | -2.764995 | C | 2.678196 | 0.815831 | -1.791918 |
| H | -0.71809 | -2.88676 | -3.65686 | H | 3.511334 | 0.804273 | -2.505618 |
| C | -2.474915 | -2.54148 | -2.47674 | H | 2.66615 | 1.795625 | -1.304015 |
| H | -3.144313 | -3.088391 | -3.137957 | H | 1.748884 | 0.74018 | -2.363021 |
| C | -4.395711 | -2.097026 | -0.996078 | C | 5.76377 | -2.660197 | 0.074778 |
| H | -5.027742 | -2.639987 | -1.695984 | H | 5.722305 | -3.692615 | 0.441848 |
| C | -4.918578 | -1.549847 | 0.155805 | H | 6.451994 | -2.109098 | 0.732749 |
| H | -5.979019 | -1.645623 | 0.379322 | H | 6.217703 | -2.674943 | -0.92409 |
| C | -4.065931 | -0.884406 | 1.066813 | C | 1.043403 | -2.582233 | 1.761652 |
| H | -4.4973 | -0.501223 | 1.98895 | H | 1.397739 | -3.572767 | 2.071818 |
| C | -2.695538 | -0.723515 | 0.846895 | H | 0.089018 | -2.707548 | 1.243312 |
| C | -2.143942 | -1.232282 | -0.389075 | H | 0.834248 | -1.998598 | 2.662706 |
| C | -3.01069 | -1.961349 | -1.291732 | C | 0.237803 | 1.554268 | -0.179954 |
| C | 1.786903 | -0.765383 | 0.070562 | C | 0.929843 | 2.396407 | 0.750626 |
| C | 2.836944 | -0.322462 | -0.794393 | C | 0.928756 | 3.793791 | 0.608049 |
| C | 4.096095 | -0.949315 | -0.786381 | H | 1.47396 | 4.393379 | 1.33554 |
| H | 4.865733 | -0.58165 | -1.463766 | C | 0.248378 | 4.436226 | -0.429778 |

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|---|-----------|----------|-----------|---|-----------|-----------|-----------|
| C | -0.427775 | 3.625913 | -1.343675 | H | -2.071866 | 0.945021 | -1.937319 |
| H | -0.960276 | 4.093656 | -2.17032 | H | -0.60545 | 0.78263 | -2.880346 |
| C | -0.4466 | 2.221907 | -1.241481 | C | -2.159515 | 1.505462 | 2.316406 |
| C | 1.687497 | 1.858388 | 1.954073 | H | -1.49364 | 1.927958 | 3.084504 |
| H | 2.361668 | 2.626341 | 2.352543 | H | -3.191829 | 1.603189 | 2.691501 |
| H | 2.279603 | 0.97401 | 1.710852 | H | -2.075816 | 2.125322 | 1.415892 |
| H | 0.997387 | 1.566368 | 2.753084 | C | -1.854144 | -0.954294 | 3.406466 |
| C | 0.221609 | 5.945816 | -0.540821 | H | -1.133168 | -0.560266 | 4.140318 |
| H | 0.142712 | 6.270391 | -1.58557 | H | -1.61752 | -2.012356 | 3.227944 |
| H | 1.127151 | 6.394823 | -0.114985 | H | -2.850961 | -0.914951 | 3.874572 |
| H | -0.636132 | 6.375975 | -0.002893 | B | 0.278942 | -0.082246 | 0.061597 |
| C | -1.220429 | 1.504526 | -2.335051 | B | -1.857041 | -0.061872 | 2.050736 |
| H | -1.60545 | 2.232543 | -3.059088 | | | | |

Compound 2



Energy Corrected for Enthalpy: -1705.702492

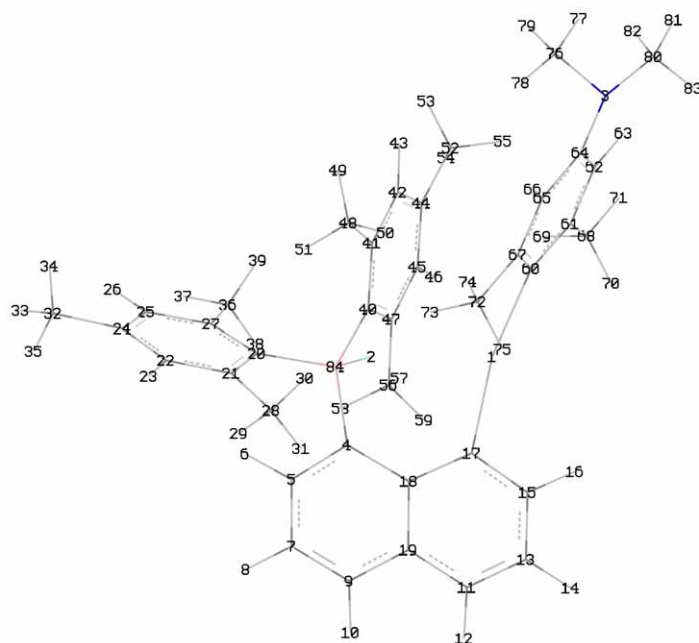
Cartesian Coordinates:

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| B | -2.194834 | 0.470399 | 0.40143 | C | 0.264023 | 2.344876 | 0.612248 |
| C | -2.978994 | -0.768143 | -0.19239 | H | 1.327433 | 2.602082 | 0.641831 |
| C | -4.362961 | -0.542324 | -0.214385 | H | -0.312066 | 3.264028 | 0.773067 |
| H | -4.734252 | 0.45227 | 0.009392 | H | 0.037402 | 2.005368 | -0.399373 |
| C | -5.307537 | -1.557621 | -0.487559 | C | 1.523515 | 0.447527 | 5.071122 |
| H | -6.368577 | -1.329543 | -0.462633 | H | 1.566352 | -0.527047 | 5.568826 |
| C | -4.865578 | -2.824645 | -0.787101 | H | 1.165437 | 1.176391 | 5.811291 |
| H | -5.570087 | -3.624198 | -1.000976 | H | 2.543898 | 0.737272 | 4.798054 |
| C | -3.058427 | -4.428216 | -1.207021 | C | -2.458214 | -1.532702 | 2.763102 |
| H | -3.821745 | -5.174944 | -1.409106 | H | -2.516201 | -1.953795 | 3.771867 |
| C | -1.722584 | -4.741401 | -1.303373 | H | -2.308893 | -2.361715 | 2.064084 |
| H | -1.404101 | -5.743099 | -1.576516 | H | -3.431941 | -1.093494 | 2.52818 |
| C | -0.7573 | -3.734722 | -1.059613 | C | -2.669993 | 1.894757 | -0.12373 |
| H | 0.28893 | -4.012363 | -1.167991 | C | -2.606379 | 2.220539 | -1.511214 |
| C | -1.097906 | -2.425286 | -0.705078 | C | -3.02267 | 3.479937 | -1.961323 |
| C | -2.493126 | -2.085545 | -0.565822 | H | -2.943741 | 3.712176 | -3.021191 |
| C | -3.472626 | -3.11486 | -0.849569 | C | -3.546836 | 4.44301 | -1.087195 |
| C | -1.145451 | 0.384256 | 1.587917 | C | -3.636624 | 4.112489 | 0.269324 |
| C | -0.048659 | 1.306475 | 1.677127 | H | -4.052946 | 4.838179 | 0.964201 |
| C | 0.809201 | 1.287345 | 2.786875 | C | -3.202149 | 2.871775 | 0.764499 |
| H | 1.649114 | 1.977208 | 2.808808 | C | -2.074457 | 1.238695 | -2.540042 |
| C | 0.617537 | 0.411461 | 3.861241 | H | -1.099609 | 0.823091 | -2.25796 |
| C | -0.457586 | -0.482984 | 3.787055 | H | -1.951205 | 1.726783 | -3.512461 |
| H | -0.630061 | -1.169009 | 4.612772 | H | -2.751457 | 0.38768 | -2.672793 |
| C | -1.32615 | -0.523851 | 2.686388 | C | -4.017312 | 5.785125 | -1.602678 |

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|---|-----------|-----------|-----------|----|----------|-----------|-----------|
| H | -4.243874 | 6.471214 | -0.780369 | H | 4.004908 | -1.754952 | 2.28081 |
| H | -4.926757 | 5.683336 | -2.209903 | H | 2.94034 | -2.625894 | 1.171132 |
| H | -3.258909 | 6.25891 | -2.237715 | C | 2.128597 | 0.912987 | -2.73544 |
| C | -3.343693 | 2.621257 | 2.25668 | H | 2.670382 | 1.430033 | -3.534738 |
| H | -3.972703 | 3.391419 | 2.715049 | H | 1.332285 | 1.586393 | -2.39211 |
| H | -2.373516 | 2.636673 | 2.766301 | H | 1.645241 | 0.033175 | -3.178784 |
| H | -3.801595 | 1.649733 | 2.474714 | Hg | 0.667916 | -1.204906 | -0.54413 |
| C | 2.627287 | -0.337387 | -0.562612 | N | 6.560511 | 1.327969 | -0.548229 |
| C | 3.555834 | -0.668447 | 0.454122 | C | 7.573223 | 0.712098 | 0.312621 |
| C | 4.850089 | -0.132174 | 0.443872 | H | 7.267616 | 0.759923 | 1.362014 |
| H | 5.528488 | -0.419251 | 1.237238 | H | 7.77245 | -0.342952 | 0.059567 |
| C | 5.277033 | 0.755479 | -0.570028 | H | 8.504806 | 1.274344 | 0.217339 |
| C | 4.35489 | 1.05477 | -1.59746 | C | 7.066073 | 1.929393 | -1.784526 |
| H | 4.641056 | 1.706083 | -2.413476 | H | 6.428613 | 2.761964 | -2.096327 |
| C | 3.055969 | 0.526692 | -1.597632 | H | 8.063263 | 2.333733 | -1.596818 |
| C | 3.182485 | -1.630342 | 1.567903 | H | 7.129465 | 1.212085 | -2.620213 |
| H | 2.308796 | -1.276365 | 2.127983 | | | | |

Anion [$2-\mu_2-F$]⁻



Energy Corrected for Enthalpy: -1805.697313

Cartesian Coordinates:

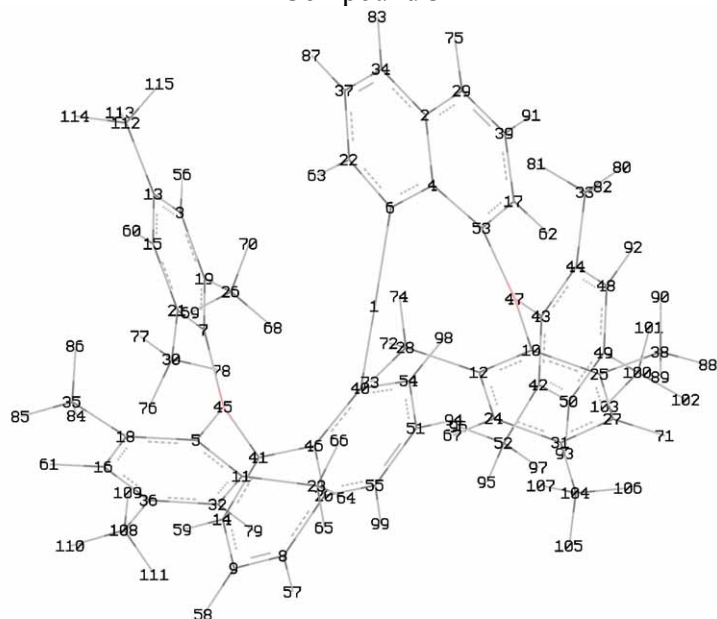
| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Hg | -0.825323 | -1.39764 | -0.381896 | H | 4.507289 | 4.441887 | 1.055355 |
| F | 0.834118 | 0.384519 | -1.103119 | C | 3.364657 | 2.664314 | 0.639491 |
| N | -6.586519 | 1.424274 | -1.066661 | C | 2.650579 | 1.265144 | -2.882322 |
| C | 2.783095 | -0.927177 | -0.134709 | H | 3.228857 | 1.533523 | -3.775833 |
| C | 4.1687 | -0.75011 | -0.074867 | H | 1.586764 | 1.381726 | -3.11337 |
| H | 4.55341 | 0.25507 | 0.054695 | H | 2.806295 | 0.203444 | -2.675495 |
| C | 5.111775 | -1.798441 | -0.181418 | C | 5.052776 | 5.4223 | -1.443291 |
| H | 6.174649 | -1.574085 | -0.12546 | H | 5.748898 | 5.727307 | -0.652442 |
| C | 4.67503 | -3.088339 | -0.361084 | H | 4.367091 | 6.265636 | -1.614051 |
| H | 5.375997 | -3.916252 | -0.448501 | H | 5.629747 | 5.285673 | -2.36647 |
| C | 2.869115 | -4.720066 | -0.591078 | C | 3.26641 | 2.403868 | 2.134555 |
| H | 3.638997 | -5.485019 | -0.673697 | H | 3.993764 | 3.025676 | 2.671559 |
| C | 1.53626 | -5.053849 | -0.626172 | H | 3.473242 | 1.359785 | 2.384039 |
| H | 1.221851 | -6.088962 | -0.740036 | H | 2.271971 | 2.632197 | 2.53108 |
| C | 0.568541 | -4.025821 | -0.512085 | C | 0.931336 | 0.622086 | 1.385505 |
| H | -0.478974 | -4.318855 | -0.5403 | C | -0.089801 | 1.632504 | 1.390312 |
| C | 0.904235 | -2.675436 | -0.374078 | C | -0.899473 | 1.84767 | 2.519621 |
| C | 2.302862 | -2.295065 | -0.322702 | H | -1.653224 | 2.632525 | 2.478506 |
| C | 3.281478 | -3.365923 | -0.431211 | C | -0.764689 | 1.093851 | 3.688945 |
| C | 2.791139 | 1.801101 | -0.343903 | C | 0.234734 | 0.117428 | 3.704713 |
| C | 3.074633 | 2.135138 | -1.708726 | H | 0.38447 | -0.468681 | 4.610431 |
| C | 3.804219 | 3.290623 | -2.037498 | C | 1.073493 | -0.124755 | 2.600052 |
| H | 3.99496 | 3.504944 | -3.088553 | C | -0.367231 | 2.541073 | 0.202704 |
| C | 4.306101 | 4.160646 | -1.064992 | H | -0.877483 | 3.452629 | 0.538956 |
| C | 4.091615 | 3.811664 | 0.269967 | H | -1.017439 | 2.045474 | -0.52609 |

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| | | | |
|---|-----------|-----------|-----------|
| H | 0.545357 | 2.825976 | -0.321761 |
| C | -1.670207 | 1.318284 | 4.881551 |
| H | -1.947446 | 2.375006 | 4.9804 |
| H | -1.186771 | 1.006239 | 5.815111 |
| H | -2.605438 | 0.746369 | 4.791904 |
| C | 2.137207 | -1.188508 | 2.819763 |
| H | 2.177369 | -1.462166 | 3.881255 |
| H | 3.133529 | -0.85491 | 2.518908 |
| H | 1.929421 | -2.097866 | 2.247801 |
| C | -2.766079 | -0.470179 | -0.575392 |
| C | -3.723427 | -0.514015 | 0.461122 |
| C | -4.974416 | 0.115854 | 0.313835 |
| H | -5.671083 | 0.079971 | 1.144024 |
| C | -5.312507 | 0.794575 | -0.86809 |
| C | -4.366553 | 0.816989 | -1.910068 |
| H | -4.62252 | 1.297471 | -2.850402 |
| C | -3.115012 | 0.202424 | -1.775961 |
| C | -3.416324 | -1.217279 | 1.770298 |
| H | -2.566641 | -0.746793 | 2.279748 |
| H | -3.153576 | -2.270424 | 1.604212 |
| H | -4.2756 | -1.190638 | 2.451532 |
| C | -2.146623 | 0.251355 | -2.944 |
| H | -1.171499 | 0.647144 | -2.637568 |
| H | -2.531485 | 0.879242 | -3.756263 |
| H | -1.970243 | -0.752545 | -3.35483 |
| C | -6.523617 | 2.854728 | -1.410151 |
| H | -7.506601 | 3.182677 | -1.767669 |
| H | -5.797382 | 3.022763 | -2.205727 |
| H | -6.237589 | 3.4823 | -0.545353 |
| C | -7.598902 | 1.174238 | -0.04233 |
| H | -8.556752 | 1.572884 | -0.394408 |
| H | -7.371034 | 1.646176 | 0.932639 |
| H | -7.711521 | 0.098144 | 0.114178 |
| B | 1.864009 | 0.452118 | 0.007298 |

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Compound 3



Energy Corrected for Enthalpy: -2370.078437

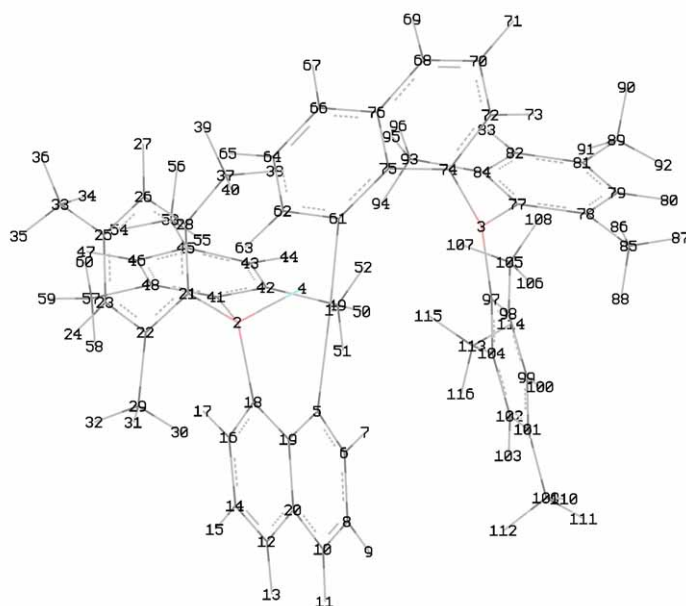
Cartesian Coordinates:

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Hg | -0.000053 | -1.234561 | -0.000031 | C | -4.963022 | 3.6886 | -0.855631 |
| C | -2.36277 | -1.26148 | 3.930943 | C | -1.347057 | 2.743858 | 1.288369 |
| C | 2.951438 | -1.202299 | 3.144671 | C | -3.405387 | -0.615021 | 4.655408 |
| C | -2.081819 | -0.896805 | 2.555306 | C | 4.505728 | -2.327189 | -0.720954 |
| C | 3.48648 | 1.969339 | -0.082593 | C | -4.084713 | 4.713575 | -0.482898 |
| C | -0.952063 | -1.526324 | 1.914453 | C | 2.916672 | 4.353745 | -0.199846 |
| C | 3.222883 | -0.622163 | 0.766901 | C | -4.506475 | -2.326091 | 0.721387 |
| C | 3.405773 | -0.615998 | -4.655326 | C | -1.605051 | -2.272413 | 4.584315 |
| C | 4.16096 | 0.372395 | -4.0715 | C | 5.715215 | 1.313981 | 1.048229 |
| C | -3.485914 | 1.969915 | 0.082396 | C | 4.085727 | 4.712891 | 0.482769 |
| C | 2.616823 | 3.018094 | -0.502509 | C | -0.581442 | -2.914307 | 3.927815 |
| C | -2.615835 | 3.01855 | 0.501986 | C | -5.715058 | 1.315028 | -1.047843 |
| C | 3.640168 | -2.409987 | 2.97961 | C | -4.160256 | 0.37364 | 4.071623 |
| C | 3.91907 | 0.716743 | -2.722689 | C | 0.951833 | -1.526314 | -1.914587 |
| C | 4.107252 | -2.720968 | 1.697632 | C | 2.949011 | 0.08711 | -1.927913 |
| C | 4.963794 | 3.687701 | 0.855762 | C | -2.747378 | -0.310646 | -2.083063 |
| C | -3.91842 | 0.717807 | 2.722755 | C | -3.223143 | -0.621725 | -0.766802 |
| C | 4.68397 | 2.336349 | 0.599841 | C | -3.911174 | -1.868772 | -0.598492 |
| C | 2.747177 | -0.310728 | 2.083162 | B | 3.140891 | 0.44782 | -0.402018 |
| C | 2.36282 | -1.262013 | -3.930957 | C | 2.081876 | -0.897209 | -2.55535 |
| C | 3.910418 | -1.869457 | 0.598782 | B | -3.140654 | 0.448354 | 0.40199 |
| C | -0.256701 | -2.523662 | 2.606854 | C | -4.108491 | -2.720265 | -1.69721 |
| C | 1.348235 | 2.743846 | -1.289373 | C | -3.641427 | -2.40955 | -2.979314 |
| C | -2.915442 | 4.354192 | 0.199379 | C | -2.952103 | -1.202269 | -3.1445 |
| C | -4.68343 | 2.337125 | -0.599718 | C | 0.580747 | -2.914042 | -3.928049 |
| C | 2.002082 | 0.971212 | 2.415656 | C | -2.001732 | 0.970922 | -2.415765 |

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| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -2.948687 | 0.087772 | 1.927903 | H | 6.657835 | 1.811172 | 1.300116 |
| C | 0.256077 | -2.523302 | -2.607099 | H | 5.383707 | 0.760748 | 1.934169 |
| C | 1.604732 | -2.272615 | -4.584414 | H | -0.008794 | -3.697 | 4.416655 |
| H | 2.55505 | -0.947861 | 4.12458 | H | -6.657627 | 1.812466 | -1.299439 |
| H | 3.580751 | -0.91636 | -5.685187 | H | -5.383948 | 0.76175 | -1.933905 |
| H | 4.941252 | 0.881417 | -4.628629 | H | -5.930987 | 0.572551 | -0.272035 |
| H | 4.537393 | 1.487588 | -2.275727 | H | -4.940283 | 0.882994 | 4.628819 |
| H | 4.65076 | -3.650463 | 1.546009 | H | -4.652304 | -3.649562 | -1.545418 |
| H | 5.892531 | 3.944204 | 1.360501 | H | -2.555587 | -0.948154 | -4.124432 |
| H | -4.536538 | 1.488828 | 2.275812 | H | 0.007754 | -3.696425 | -4.416973 |
| H | 0.591486 | -3.017336 | 2.140871 | H | -1.352206 | 0.81332 | -3.283004 |
| H | 0.65231 | 3.585637 | -1.213742 | H | -1.374626 | 1.324885 | -1.595795 |
| H | 1.564911 | 2.583003 | -2.352293 | H | -2.694643 | 1.786071 | -2.65689 |
| H | 0.824917 | 1.849289 | -0.940595 | H | -0.592388 | -3.016609 | -2.141237 |
| H | -2.224666 | 5.132982 | 0.515346 | H | 1.854851 | -2.524733 | -5.611548 |
| H | 1.375039 | 1.325237 | 1.595665 | C | -3.884423 | -3.334936 | -4.15013 |
| H | 2.695341 | 1.786145 | 2.656504 | H | -4.17091 | -4.337199 | -3.815347 |
| H | 1.352598 | 0.814067 | 3.28301 | H | -4.691823 | -2.958898 | -4.793139 |
| H | -5.891796 | 3.945297 | -1.360183 | H | -2.990541 | -3.427328 | -4.778147 |
| H | -0.82342 | 1.849964 | 0.938314 | C | -4.381317 | 6.158429 | -0.817759 |
| H | -0.651475 | 3.586016 | 1.213703 | H | -3.940147 | 6.441976 | -1.783437 |
| H | -1.563507 | 2.581521 | 2.351095 | H | -5.459196 | 6.340136 | -0.887544 |
| H | -3.580369 | -0.915274 | 5.6853 | H | -3.97054 | 6.837191 | -0.062229 |
| H | 5.095932 | -1.546763 | -1.210705 | C | 4.382649 | 6.157583 | 0.818039 |
| H | 5.161791 | -3.188309 | -0.557443 | H | 3.955698 | 6.436209 | 1.791516 |
| H | 3.730207 | -2.630351 | -1.431689 | H | 5.460899 | 6.342763 | 0.871885 |
| H | 2.226185 | 5.132684 | -0.516052 | H | 3.957987 | 6.837473 | 0.071335 |
| H | -5.162713 | -3.187124 | 0.558125 | C | 3.881868 | -3.335621 | 4.150503 |
| H | -3.730967 | -2.629218 | 1.432145 | H | 4.181482 | -4.334107 | 3.816039 |
| H | -5.096511 | -1.545434 | 1.210985 | H | 4.679223 | -2.952842 | 4.801957 |
| H | -1.855168 | -2.524432 | 5.611472 | H | 2.983147 | -3.438649 | 4.770007 |
| H | 5.931173 | 0.571479 | 0.272451 | | | | |

Anion [**3**- μ_2 -F]⁻



Energy Corrected for Enthalpy: -2470.078687

Cartesian Coordinates:

| | | | | | | | |
|----|-----------|-----------|-----------|---|----------|-----------|-----------|
| Hg | -0.148775 | -1.344393 | 0.076629 | C | 2.823757 | -1.503711 | -3.25141 |
| B | 2.661006 | 0.453085 | 0.221158 | H | 2.536413 | -1.27823 | -4.277339 |
| B | -3.137988 | 0.542236 | -0.365585 | C | 2.582432 | -0.538569 | -2.258245 |
| F | 1.200042 | 0.818737 | -0.025685 | C | 4.132914 | -2.421919 | 0.743046 |
| C | 0.782789 | -1.577837 | 2.006576 | H | 3.33071 | -2.693992 | 1.435613 |
| C | 0.11686 | -2.530217 | 2.783571 | H | 4.700663 | -1.622549 | 1.224833 |
| H | -0.718922 | -3.081314 | 2.360359 | H | 4.793002 | -3.291778 | 0.638233 |
| C | 0.46064 | -2.803401 | 4.130144 | C | 3.636678 | -3.776576 | -4.0433 |
| H | -0.091138 | -3.55424 | 4.691741 | H | 2.736094 | -4.387166 | -4.205553 |
| C | 1.488388 | -2.099396 | 4.711824 | H | 4.449955 | -4.46229 | -3.777046 |
| H | 1.769207 | -2.273245 | 5.74893 | H | 3.88668 | -3.311969 | -5.005141 |
| C | 3.313581 | -0.476997 | 4.608541 | C | 1.920793 | 0.74167 | -2.742086 |
| H | 3.513784 | -0.701246 | 5.654488 | H | 0.84002 | 0.715581 | -2.567441 |
| C | 4.088681 | 0.414172 | 3.907785 | H | 2.079953 | 0.862043 | -3.821221 |
| H | 4.918872 | 0.927211 | 4.387952 | H | 2.306108 | 1.626053 | -2.233887 |
| C | 3.810356 | 0.65809 | 2.542702 | C | 3.520686 | 1.854974 | -0.092884 |
| H | 4.455679 | 1.35462 | 2.019935 | C | 2.96855 | 3.128542 | 0.264486 |
| C | 2.766053 | 0.059355 | 1.831305 | C | 3.63304 | 4.325664 | -0.052887 |
| C | 1.911112 | -0.865537 | 2.572509 | H | 3.173068 | 5.269853 | 0.236943 |
| C | 2.230653 | -1.139692 | 3.965741 | C | 4.869544 | 4.343789 | -0.704963 |
| C | 2.952377 | -0.764373 | -0.889043 | C | 5.454786 | 3.107992 | -0.987488 |
| C | 3.590704 | -2.018482 | -0.618921 | H | 6.442642 | 3.083311 | -1.446027 |
| C | 3.798023 | -2.964661 | -1.641429 | C | 4.819409 | 1.887826 | -0.688974 |
| H | 4.294837 | -3.900867 | -1.390099 | C | 1.670685 | 3.282223 | 1.041569 |
| C | 3.418393 | -2.735586 | -2.96591 | H | 1.634235 | 4.271178 | 1.516453 |

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| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 1.573408 | 2.522404 | 1.819989 | H | -4.708879 | -3.014711 | 2.408064 |
| H | 0.792478 | 3.185459 | 0.396337 | C | -3.508934 | -1.611339 | 3.506533 |
| C | 5.548726 | 5.645077 | -1.075664 | C | -2.728282 | -0.454926 | 3.392398 |
| H | 6.632879 | 5.514722 | -1.177731 | H | -2.225504 | -0.065448 | 4.273919 |
| H | 5.372038 | 6.420764 | -0.319798 | C | -2.54755 | 0.204016 | 2.170506 |
| H | 5.177764 | 6.039247 | -2.033412 | C | -4.636145 | -2.161941 | -0.081397 |
| C | 5.625514 | 0.637771 | -1.007936 | H | -5.268351 | -2.982885 | 0.274493 |
| H | 5.601778 | -0.085802 | -0.188755 | H | -3.917603 | -2.576912 | -0.795282 |
| H | 6.674628 | 0.906001 | -1.185131 | H | -5.271454 | -1.468637 | -0.641994 |
| H | 5.257038 | 0.118978 | -1.898482 | C | -3.671158 | -2.306742 | 4.839253 |
| C | -1.186897 | -1.714955 | -1.797545 | H | -4.402836 | -3.119735 | 4.780333 |
| C | -0.527016 | -2.746676 | -2.475788 | H | -4.000917 | -1.608739 | 5.619243 |
| H | 0.363659 | -3.190783 | -2.040781 | H | -2.716901 | -2.734779 | 5.173931 |
| C | -0.940327 | -3.23487 | -3.738159 | C | -1.654104 | 1.431929 | 2.183809 |
| H | -0.379579 | -4.032395 | -4.218319 | H | -2.234647 | 2.360519 | 2.154012 |
| C | -2.039068 | -2.678126 | -4.3497 | H | -0.955624 | 1.452537 | 1.343816 |
| H | -2.370529 | -3.019428 | -5.327705 | H | -1.04723 | 1.440511 | 3.094715 |
| C | -3.878546 | -1.065641 | -4.397939 | | | | |
| H | -4.144697 | -1.469258 | -5.372376 | | | | |
| C | -4.586538 | -0.023655 | -3.849046 | | | | |
| H | -5.424773 | 0.422309 | -4.376886 | | | | |
| C | -4.203866 | 0.476327 | -2.58429 | | | | |
| H | -4.763753 | 1.311765 | -2.177485 | | | | |
| C | -3.154024 | -0.064811 | -1.82698 | | | | |
| C | -2.360326 | -1.13603 | -2.411222 | | | | |
| C | -2.76117 | -1.628806 | -3.717617 | | | | |
| C | -3.381029 | 2.117685 | -0.276124 | | | | |
| C | -4.508843 | 2.655345 | 0.408919 | | | | |
| C | -4.712314 | 4.044401 | 0.454646 | | | | |
| H | -5.586574 | 4.430224 | 0.975553 | | | | |
| C | -3.823366 | 4.943605 | -0.144328 | | | | |
| C | -2.717613 | 4.414858 | -0.822021 | | | | |
| H | -2.010689 | 5.092016 | -1.29629 | | | | |
| C | -2.491531 | 3.03392 | -0.913169 | | | | |
| C | -5.541265 | 1.778878 | 1.099678 | | | | |
| H | -5.859348 | 0.936787 | 0.474857 | | | | |
| H | -6.434232 | 2.365279 | 1.344064 | | | | |
| H | -5.154285 | 1.352601 | 2.032028 | | | | |
| C | -4.063518 | 6.437029 | -0.09082 | | | | |
| H | -4.516841 | 6.804977 | -1.022367 | | | | |
| H | -3.126054 | 6.987564 | 0.050248 | | | | |
| H | -4.739298 | 6.703631 | 0.729451 | | | | |
| C | -1.271345 | 2.561328 | -1.677584 | | | | |
| H | -0.59769 | 1.954123 | -1.063958 | | | | |
| H | -0.688585 | 3.414404 | -2.040752 | | | | |
| H | -1.551888 | 1.952689 | -2.543887 | | | | |
| C | -3.159873 | -0.301571 | 0.975079 | | | | |
| C | -3.933334 | -1.501642 | 1.09158 | | | | |
| C | -4.100191 | -2.115246 | 2.343936 | | | | |

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