# Oxidative dehydrogenation of an amine group of a macrocyclic ligand in the coordination sphere of a $Cu^{II}$ complex

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# Supporting information

**Table 1** Calculated bond angles for $[Fe^{II}L^{2'}]Cl_2$. Experimental values from Sosa-Torres and co-workers.[1]

| | Calculated bond angles | Experimental bond angles |
|---|---|---|
| $N_6$-Fe-$N_5$ | 81.5 | 82.9 |
| $N_6$-Fe-$N_3$ | 98.2 | 97.5 |
| $N_5$-Fe-$N_3$ | 85.5 | 86.8 |
| $N_6$-Fe-$N_2$ | 170.7 | 173.2 |
| $N_5$-Fe-$N_2$ | 90.1 | 90.8 |
| $N_3$-Fe-$N_2$ | 84.9 | 84.8 |
| $N_6$-Fe-$N_1$ | 95.7 | 95.4 |
| $N_2$-Fe-$N_1$ | 81.1 | 82.3 |
| $N_6$-Fe-$N_4$ | 93.8 | 93.0 |
| $N_5$-Fe-$N_4$ | 166.0 | 167.8 |
| $N_3$-Fe-$N_4$ | 82.1 | 82.4 |
| $N_2$-Fe-$N_4$ | 95.3 | 93.6 |
| $N_1$-Fe-$N_4$ | 98.6 | 97.1 |
| $C_9$-$N_2$-Fe | 117.2 | 118.1 |
| $C_7$-$N_2$-Fe | 116.9 | 118.2 |

([1] J. P. Saucedo-Vázquez, V. M. Ugalde-Saldívar, A. R. Toscano, P. M. H. Kroneck and M. E. Sosa-Torres, *Inorg. Chem.*, 2009, **48**, 1214-1222.)

## 1. Calculated structures for the copper system

### 1.1 Reactant $[Cu^{II}(H_2L')][CF_3SO_3]_2$

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| | | | |
|---|---|---|---|
| C | -0.753155 | 2.454023 | -0.147059 |
| N | -0.116595 | 1.468528 | 0.760643 |
| C | -0.924010 | 1.214748 | 1.984773 |
| C | -0.220418 | 0.284266 | 2.988377 |
| C | -0.433760 | -1.216753 | 2.746311 |
| N | 0.280365 | -1.788739 | 1.575093 |
| C | -0.452573 | -2.979933 | 1.057091 |
| C | -1.614116 | -2.644335 | 0.122673 |
| C | -1.217232 | -2.152246 | -1.274425 |
| N | -0.743492 | -0.738280 | -1.335191 |
| C | -0.442965 | -0.354623 | -2.736411 |
| C | 1.670332 | -2.158223 | 1.890699 |
| C | 2.442326 | -2.475698 | 0.622406 |
| N | 2.125068 | -1.758603 | -0.477870 |
| C | 2.799118 | -1.961674 | -1.622672 |
| C | 3.812072 | -2.911776 | -1.731762 |
| C | 4.140775 | -3.665097 | -0.605211 |
| C | 3.446099 | -3.444480 | 0.585098 |

| | | | |
|---|---|---|---|
| Cu | 0.767730 | -0.208168 | -0.061821 |
| H | -1.571181 | -0.160416 | -1.072940 |
| H | -0.926359 | 3.401703 | 0.385717 |
| H | -1.897188 | 0.804314 | 1.684578 |
| H | -1.113592 | 2.188211 | 2.466780 |
| H | 0.849869 | 0.532475 | 3.059730 |
| H | -0.644261 | 0.497699 | 3.979844 |
| H | -0.160065 | -1.784685 | 3.654621 |
| H | -1.505217 | -1.375624 | 2.582207 |
| H | 1.721200 | -3.019809 | 2.582110 |
| H | 2.156672 | -1.306706 | 2.384989 |
| H | 2.532648 | -1.313654 | -2.452890 |
| H | 4.334566 | -3.039997 | -2.675756 |
| H | 4.928988 | -4.413928 | -0.649637 |
| H | 3.676049 | -4.015132 | 1.482148 |
| H | -0.815912 | -3.577787 | 1.912009 |
| H | 0.265154 | -3.612654 | 0.519950 |
| H | -2.195622 | -3.565438 | -0.022974 |
| H | -2.309629 | -1.941441 | 0.597536 |
| H | -0.427835 | -2.789755 | -1.697521 |
| H | -2.101570 | -2.228790 | -1.923894 |
| H | -1.344873 | -0.451892 | -3.356817 |
| H | 0.340927 | -1.004222 | -3.141501 |
| H | -0.081465 | 2.638452 | -0.991674 |
| H | -0.091061 | 0.680154 | -2.769492 |
| H | 0.782632 | 1.855807 | 1.060280 |
| H | -1.712258 | 2.063544 | -0.501514 |
| S | 3.349410 | 1.235413 | -0.439088 |
| O | 2.442255 | 1.280143 | -1.702139 |
| O | 4.740559 | 0.604617 | -0.551357 |
| O | 2.468058 | 0.695889 | 0.805073 |
| C | 3.616764 | 3.100468 | 0.087736 |
| F | 4.204986 | 3.755040 | -0.904744 |
| F | 2.415728 | 3.638209 | 0.337940 |
| F | 4.366087 | 3.140688 | 1.183033 |
| S | -4.213478 | -0.162831 | -0.266724 |
| O | -3.176001 | 0.649535 | -1.136293 |
| O | -4.672925 | -1.485430 | -0.912566 |
| O | -3.798615 | -0.240081 | 1.234988 |
| C | -5.774521 | 1.000420 | -0.271711 |
| F | -6.187198 | 1.187354 | -1.525313 |
| F | -6.746859 | 0.432782 | 0.442223 |
| F | -5.446321 | 2.175133 | 0.272869 |

## 1.2 $[Cu^{I}(H_2L')][CF_3SO_3]$

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| | | | |
|---|---|---|---|
| C | -0.410902 | -3.344052 | 0.882757 |
| N | -0.534418 | -2.432668 | -0.274156 |
| C | -1.444066 | -2.992403 | -1.296111 |
| C | -1.758952 | -2.002027 | -2.417562 |
| C | -2.781141 | -0.937055 | -2.009108 |
| N | -2.270129 | 0.131146 | -1.111354 |
| C | -3.403771 | 0.722934 | -0.340553 |
| C | -3.824235 | -0.029618 | 0.928930 |
| C | -2.960271 | 0.245108 | 2.167779 |
| N | -1.699348 | -0.517156 | 2.175781 |

| | | | |
|---|---|---|---|
| C | -0.852372 | -0.163032 | 3.331482 |
| C | -1.607627 | 1.222891 | -1.919316 |
| C | -0.949348 | 2.187299 | -0.994859 |
| N | -0.268477 | 1.547690 | 0.051575 |
| C | 0.461616 | 2.356325 | 0.914827 |
| C | 0.497557 | 3.721296 | 0.790650 |
| C | -0.226692 | 4.380838 | -0.251568 |
| C | -0.947260 | 3.558439 | -1.143972 |
| Cu | -0.552421 | -0.366881 | 0.178124 |
| H | -1.933129 | -1.509600 | 2.248362 |
| H | -0.081688 | -4.346852 | 0.569531 |
| H | -2.378638 | -3.292923 | -0.798442 |
| H | -0.999062 | -3.910179 | -1.714576 |
| H | -0.830887 | -1.545392 | -2.789998 |
| H | -2.186127 | -2.563410 | -3.260790 |
| H | -3.212388 | -0.460898 | -2.906989 |
| H | -3.610849 | -1.440332 | -1.495092 |
| H | -2.349950 | 1.714668 | -2.569956 |
| H | -0.876148 | 0.708822 | -2.566120 |
| H | 1.031272 | 1.828423 | 1.674079 |
| H | 1.096872 | 4.293774 | 1.497087 |
| H | -0.214347 | 5.461081 | -0.358980 |
| H | -1.500799 | 3.993565 | -1.977253 |
| H | -4.267967 | 0.810651 | -1.021728 |
| H | -3.104813 | 1.743687 | -0.074361 |
| H | -4.848838 | 0.292426 | 1.164318 |
| H | -3.889774 | -1.114823 | 0.746234 |
| H | -2.695121 | 1.310199 | 2.199287 |
| H | -3.546173 | 0.033539 | 3.081359 |
| H | -1.376627 | -0.298959 | 4.293220 |
| H | -0.556240 | 0.887398 | 3.239557 |
| H | 0.317605 | -2.932992 | 1.586124 |
| H | 0.056872 | -0.770770 | 3.315121 |
| H | 0.410324 | -2.372299 | -0.702232 |
| H | -1.384609 | -3.450255 | 1.379724 |
| S | 2.568034 | -1.158641 | 0.181565 |
| O | 2.101218 | -1.870737 | -1.128101 |
| O | 3.635797 | -1.847486 | 1.035212 |
| O | 1.297941 | -0.692136 | 1.056214 |
| C | 3.372510 | 0.515248 | -0.441843 |
| F | 4.547479 | 0.223325 | -0.994313 |
| F | 2.573784 | 1.078708 | -1.341854 |
| F | 3.545358 | 1.324178 | 0.598738 |

## 1.3 [Cu(HL')][$CF_3SO_3$]

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| | | | |
|---|---|---|---|
| C | 0.324911 | -3.141288 | -0.820214 |
| N | -0.732788 | -2.167179 | -1.044965 |
| C | -1.954402 | -2.832363 | -1.456309 |
| C | -3.035855 | -1.922533 | -2.051821 |
| C | -3.839315 | -1.091187 | -1.046546 |
| N | -3.097165 | 0.009847 | -0.405835 |
| C | -3.770003 | 0.452109 | 0.830835 |
| C | -3.473591 | -0.408824 | 2.065445 |
| C | -2.074340 | -0.254974 | 2.677818 |
| N | -1.008439 | -1.004639 | 1.976863 |

| | | | |
|---|---|---|---|
| C | 0.231920 | -1.044460 | 2.789145 |
| C | -2.903583 | 1.137166 | -1.324730 |
| C | -1.864166 | 2.111910 | -0.809264 |
| N | -0.771631 | 1.577626 | -0.222252 |
| C | 0.192855 | 2.400160 | 0.235790 |
| C | 0.103060 | 3.788486 | 0.119229 |
| C | -1.017720 | 4.344828 | -0.494247 |
| C | -2.019281 | 3.491119 | -0.960623 |
| Cu | -0.643925 | -0.516236 | -0.113257 |
| H | -1.332595 | -1.968032 | 1.863775 |
| H | 0.560477 | -3.673308 | -1.759838 |
| H | -2.392824 | -3.415716 | -0.615012 |
| H | -1.697240 | -3.590077 | -2.219736 |
| H | -2.577108 | -1.286509 | -2.821634 |
| H | -3.760403 | -2.562729 | -2.577229 |
| H | -4.754636 | -0.695274 | -1.532476 |
| H | -4.183310 | -1.763043 | -0.248956 |
| H | -3.850856 | 1.675275 | -1.526063 |
| H | -2.555719 | 0.736544 | -2.286033 |
| H | 1.056836 | 1.925239 | 0.700145 |
| H | 0.907890 | 4.408574 | 0.505872 |
| H | -1.118171 | 5.423295 | -0.603237 |
| H | -2.915713 | 3.883495 | -1.436587 |
| H | -4.865195 | 0.499333 | 0.669096 |
| H | -3.445880 | 1.478151 | 1.046042 |
| H | -4.200240 | -0.119446 | 2.838663 |
| H | -3.673247 | -1.471879 | 1.858103 |
| H | -1.779469 | 0.803558 | 2.692261 |
| H | -2.115230 | -0.585709 | 3.731111 |
| H | 0.026563 | -1.398733 | 3.813415 |
| H | 0.671032 | -0.043154 | 2.840663 |
| H | 1.231324 | -2.651377 | -0.459571 |
| H | 0.970696 | -1.697563 | 2.315798 |
| H | 0.021527 | -3.918395 | -0.088600 |
| S | 2.772170 | -0.264067 | 0.502961 |
| O | 1.564419 | -0.226925 | -0.517096 |
| O | 2.746939 | 0.925772 | 1.503619 |
| O | 3.050149 | -1.667217 | 1.090708 |
| C | 4.295588 | 0.106898 | -0.655690 |
| F | 4.382110 | -0.838362 | -1.592575 |
| F | 5.412785 | 0.119846 | 0.072815 |
| F | 4.126463 | 1.298348 | -1.235829 |

## 1.4 $[Cu(HL')][CF_3SO_3]_2$

0 3

| | | | |
|---|---|---|---|
| C | 0.321843 | -1.234691 | -3.109302 |
| N | -0.726674 | -0.566929 | -2.377895 |
| C | -1.544981 | 0.303329 | -3.207231 |
| C | -2.516447 | 1.265291 | -2.516003 |
| C | -3.655224 | 0.614615 | -1.724593 |
| N | -3.266227 | 0.050133 | -0.415192 |
| C | -4.234432 | -0.980777 | 0.006619 |
| C | -3.924784 | -2.376626 | -0.536418 |
| C | -2.735035 | -3.073445 | 0.132743 |
| N | -1.395866 | -2.698881 | -0.386916 |
| C | -0.376814 | -3.633156 | 0.159824 |

| | | | |
|---|---|---|---|
| C | -3.135946 | 1.082161 | 0.623908 |
| C | -2.363648 | 0.568908 | 1.825469 |
| N | -1.283976 | -0.209433 | 1.588995 |
| C | -0.505070 | -0.608344 | 2.610278 |
| C | -0.795870 | -0.280758 | 3.931980 |
| C | -1.917680 | 0.504302 | 4.194125 |
| C | -2.708507 | 0.933627 | 3.128028 |
| Cu | -0.755806 | -0.567998 | -0.349115 |
| H | -1.419438 | -2.831639 | -1.401112 |
| H | 0.081386 | -1.353656 | -4.176137 |
| H | -2.099464 | -0.353867 | -3.907439 |
| H | -0.859229 | 0.889480 | -3.843516 |
| H | -1.952245 | 1.966438 | -1.894769 |
| H | -2.978954 | 1.854560 | -3.321955 |
| H | -4.473529 | 1.348026 | -1.589084 |
| H | -4.077298 | -0.205935 | -2.321981 |
| H | -4.123106 | 1.456044 | 0.955337 |
| H | -2.588460 | 1.944375 | 0.219678 |
| H | 0.380722 | -1.170464 | 2.326879 |
| H | -0.139627 | -0.620465 | 4.728745 |
| H | -2.171254 | 0.787774 | 5.213831 |
| H | -3.582096 | 1.559875 | 3.293911 |
| H | -5.260491 | -0.680347 | -0.278728 |
| H | -4.224569 | -1.033782 | 1.102951 |
| H | -4.810645 | -3.005247 | -0.364678 |
| H | -3.784791 | -2.350320 | -1.628439 |
| H | -2.734250 | -2.869153 | 1.211968 |
| H | -2.855079 | -4.164335 | 0.020468 |
| H | -0.707545 | -4.676796 | 0.032287 |
| H | -0.251513 | -3.433379 | 1.228662 |
| H | 1.244946 | -0.629299 | -3.004690 |
| H | 0.586278 | -3.482918 | -0.332697 |
| H | 0.573438 | -2.201631 | -2.656751 |
| O | -0.123611 | 1.325744 | -0.685055 |
| S | 0.206638 | 2.532019 | 0.341439 |
| O | -0.920723 | 3.590615 | 0.271928 |
| O | 0.701554 | 2.100921 | 1.730963 |
| C | 1.755304 | 3.310002 | -0.563415 |
| F | 1.475387 | 3.452163 | -1.858426 |
| F | 2.796855 | 2.511741 | -0.397336 |
| F | 1.996477 | 4.504135 | -0.020752 |
| O | 1.278224 | -1.155622 | 0.313062 |
| S | 2.561735 | -1.450386 | -0.570183 |
| O | 2.549229 | -2.893416 | -1.144432 |
| O | 2.942553 | -0.325416 | -1.557416 |
| C | 3.951826 | -1.433321 | 0.796136 |
| F | 3.593550 | -2.258706 | 1.785179 |
| F | 4.087630 | -0.197894 | 1.269056 |
| F | 5.100700 | -1.846002 | 0.262644 |

## 1.5 Imine product $[Cu^{I}(L')]^{+}$

1 1

| | | | |
|---|---|---|---|
| C | 1.919573 | -0.895408 | -2.912497 |
| N | 1.850922 | -0.697201 | -1.649244 |
| C | 2.882786 | -1.327865 | -0.804133 |
| C | 2.298288 | -2.241934 | 0.287306 |

| | | | |
|---|---|---|---|
| C | 1.697985 | -1.551296 | 1.521713 |
| N | 0.446489 | -0.788151 | 1.293198 |
| C | 0.178502 | 0.136525 | 2.427462 |
| C | 0.963696 | 1.457462 | 2.406101 |
| C | 0.473979 | 2.520251 | 1.411971 |
| N | 0.901206 | 2.281102 | 0.007932 |
| C | 0.408293 | 3.353266 | -0.888897 |
| C | -0.704567 | -1.692565 | 1.097551 |
| C | -1.859399 | -1.027084 | 0.369373 |
| N | -1.537006 | -0.144681 | -0.605286 |
| C | -2.531451 | 0.404884 | -1.331087 |
| C | -3.876831 | 0.110007 | -1.121234 |
| C | -4.211076 | -0.789884 | -0.108104 |
| C | -3.185995 | -1.362750 | 0.647149 |
| Cu | 0.470443 | 0.341131 | -0.649359 |
| H | 1.923503 | 2.326696 | -0.004490 |
| H | 2.710597 | -1.505119 | -3.365161 |
| H | 3.464126 | -0.519177 | -0.337867 |
| H | 3.574119 | -1.910332 | -1.432500 |
| H | 1.585384 | -2.940058 | -0.172862 |
| H | 3.125820 | -2.864491 | 0.655710 |
| H | 1.536797 | -2.307714 | 2.312165 |
| H | 2.440458 | -0.846244 | 1.915581 |
| H | -1.056513 | -2.114637 | 2.055384 |
| H | -0.370571 | -2.541114 | 0.486243 |
| H | -2.226127 | 1.103458 | -2.107336 |
| H | -4.638589 | 0.580378 | -1.737486 |
| H | -5.250212 | -1.041163 | 0.092587 |
| H | -3.409055 | -2.068587 | 1.444328 |
| H | 0.369502 | -0.389194 | 3.380519 |
| H | -0.893035 | 0.373778 | 2.411494 |
| H | 0.872721 | 1.893428 | 3.410793 |
| H | 2.040570 | 1.277165 | 2.265168 |
| H | -0.624045 | 2.558343 | 1.415831 |
| H | 0.828624 | 3.512568 | 1.737806 |
| H | 0.679678 | 4.355541 | -0.521759 |
| H | -0.683516 | 3.292249 | -0.954863 |
| H | 1.173961 | -0.450173 | -3.570444 |
| H | 0.828974 | 3.212455 | -1.889674 |

## 1.6 Protonated product $[Cu^{I}(H_4L')][CF_3SO_3]_3$

0 1

| | | | |
|---|---|---|---|
| C | 4.677323 | 3.028418 | 1.478951 |
| N | 3.754362 | 1.864778 | 1.550626 |
| C | 3.320971 | 1.507966 | 2.940999 |
| C | 2.259267 | 0.398715 | 2.959462 |
| C | 0.825518 | 0.908894 | 2.688612 |
| N | -0.014434 | -0.038882 | 1.939757 |
| C | -1.304660 | 0.540589 | 1.509494 |
| C | -2.144143 | 1.234511 | 2.604611 |
| C | -3.569065 | 1.585500 | 2.162654 |
| N | -3.614463 | 2.312876 | 0.843356 |
| C | -4.879089 | 3.073366 | 0.623200 |
| C | -0.139551 | -1.374454 | 2.514791 |
| C | -0.483440 | -2.438707 | 1.477163 |
| N | -0.104310 | -2.234456 | 0.194807 |

| | | | |
|---|---|---|---|
| C | -0.363885 | -3.197550 | -0.716340 |
| C | -0.984508 | -4.399479 | -0.392876 |
| C | -1.370560 | -4.616496 | 0.930549 |
| C | -1.122649 | -3.616628 | 1.869541 |
| Cu | 0.896553 | -0.609818 | -0.290128 |
| H | -2.805124 | 2.932656 | 0.729920 |
| H | 5.577508 | 2.818271 | 2.064392 |
| H | 2.952789 | 2.425010 | 3.419040 |
| H | 4.224057 | 1.185552 | 3.471618 |
| H | 2.534465 | -0.377746 | 2.236216 |
| H | 2.313178 | -0.079034 | 3.946798 |
| H | 0.372596 | 1.190945 | 3.659073 |
| H | 0.863763 | 1.816680 | 2.073274 |
| H | -0.881517 | -1.431135 | 3.335047 |
| H | 0.827666 | -1.651311 | 2.954052 |
| H | -0.057749 | -2.978939 | -1.735985 |
| H | -1.166398 | -5.138776 | -1.168580 |
| H | -1.864511 | -5.540521 | 1.223928 |
| H | -1.423768 | -3.740113 | 2.908156 |
| H | -1.890191 | -0.259958 | 1.045419 |
| H | -1.079726 | 1.251065 | 0.707188 |
| H | -2.242841 | 0.589769 | 3.490385 |
| H | -1.636167 | 2.149478 | 2.943607 |
| H | -4.196340 | 0.699766 | 2.012301 |
| H | -4.050368 | 2.227392 | 2.911051 |
| H | -4.994483 | 3.839624 | 1.396540 |
| H | -5.699758 | 2.351055 | 0.654792 |
| H | 4.943129 | 3.188571 | 0.430886 |
| H | -4.835768 | 3.536782 | -0.366655 |
| H | 2.919338 | 2.089044 | 0.939219 |
| H | 4.170333 | 3.916930 | 1.866109 |
| H | 4.243590 | 1.022678 | 1.137481 |
| H | -3.564461 | 1.558406 | 0.036971 |
| O | 0.290636 | 1.142661 | -1.203156 |
| S | 1.109763 | 2.493891 | -1.220492 |
| O | 1.658007 | 2.900755 | 0.202990 |
| O | 2.057324 | 2.736881 | -2.396258 |
| C | -0.361060 | 3.774762 | -1.409352 |
| F | -1.055955 | 3.801333 | -0.242574 |
| F | -1.173991 | 3.404929 | -2.387377 |
| F | 0.123046 | 4.989988 | -1.641703 |
| O | -3.616467 | 0.505874 | -1.034157 |
| S | -4.966370 | -0.337787 | -0.927610 |
| O | -5.716143 | 0.000204 | 0.396609 |
| O | -5.782690 | -0.429926 | -2.218494 |
| C | -4.258359 | -2.122904 | -0.615286 |
| F | -3.623982 | -2.125261 | 0.570390 |
| F | -3.396414 | -2.448746 | -1.578043 |
| F | -5.252237 | -3.007976 | -0.580830 |
| O | 2.871160 | -0.250189 | -0.612054 |
| S | 3.990996 | -1.227281 | -0.039241 |
| O | 5.093871 | -0.374940 | 0.683306 |
| O | 3.455124 | -2.442467 | 0.736931 |
| C | 4.838285 | -1.923634 | -1.653466 |
| F | 5.370239 | -0.913275 | -2.329222 |
| F | 3.899761 | -2.524089 | -2.380930 |

| | | | |
|---|---|---|---|
| F | 5.778362 | -2.797664 | -1.306694 |

## 1.7 Product $[Cu^{I}(NCMe)_4][CF_3SO_3]$

0 1

| | | | |
|---|---|---|---|
| S | 2.860465 | 0.751482 | -0.171012 |
| F | 1.527875 | -1.583147 | 0.344309 |
| O | 2.122774 | 1.372128 | 1.060971 |
| F | 3.431625 | -1.419539 | 1.391443 |
| O | 4.360503 | 1.057171 | -0.292273 |
| F | 3.392311 | -1.866874 | -0.746684 |
| O | 2.023911 | 0.838740 | -1.488164 |
| C | 2.807590 | -1.166618 | 0.233991 |
| Cu | -2.278727 | -0.026861 | 0.012093 |
| N | -4.241279 | -0.196057 | 0.049312 |
| N | -1.283619 | -0.427187 | 1.743284 |
| N | -1.313810 | -1.110920 | -1.418816 |
| N | -1.502964 | 1.822023 | -0.384165 |
| C | -5.397571 | -0.289667 | 0.059114 |
| C | -6.850436 | -0.407099 | 0.070106 |
| H | -7.148778 | -1.360750 | 0.522119 |
| H | -7.239965 | -0.364103 | -0.954194 |
| H | -7.290960 | 0.412544 | 0.650518 |
| C | -0.354339 | -0.416899 | 2.439411 |
| C | 0.839102 | -0.374871 | 3.270428 |
| H | 1.273149 | -1.377804 | 3.355686 |
| H | 0.597347 | 0.004380 | 4.270171 |
| H | 1.562920 | 0.288921 | 2.769673 |
| C | -0.385772 | -1.370793 | -2.066708 |
| C | 0.806139 | -1.649684 | -2.852652 |
| H | 1.248662 | -2.602985 | -2.541451 |
| H | 1.523225 | -0.836530 | -2.652935 |
| H | 0.560658 | -1.692435 | -3.920213 |
| C | -0.619935 | 2.564821 | -0.514709 |
| C | 0.494439 | 3.488032 | -0.658223 |
| H | 1.052876 | 3.231379 | -1.565395 |
| H | 1.171227 | 3.332001 | 0.192032 |
| H | 0.137896 | 4.524021 | -0.698260 |

## 1.8 Protonated free ligand $[H_4L'][CF_3SO_3]_2$

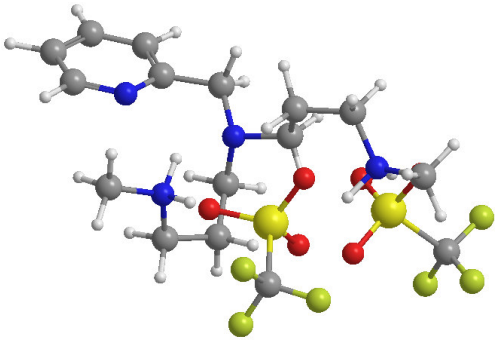

**Figure 1 Chem3D figure of the optimised structure of $[H_4L'][CF_3SO_3]_2$**

0 1

| | | | |
|---|---|---|---|
| C | -3.283208 | 1.125021 | 2.339065 |

| | | | |
|---|---|---|---|
| N | -2.075899 | 0.462120 | 1.777833 |
| C | -0.954149 | 0.326306 | 2.768683 |
| C | 0.411121 | 0.112169 | 2.100114 |
| C | 0.395742 | -0.975523 | 1.021080 |
| N | 1.688723 | -1.125387 | 0.313379 |
| C | 1.457984 | -1.615912 | -1.075525 |
| C | 0.986946 | -0.490425 | -2.010538 |
| C | 2.044805 | 0.585856 | -2.264306 |
| N | 2.452260 | 1.281269 | -0.995397 |
| C | 3.654111 | 2.141638 | -1.128809 |
| C | 2.580579 | -2.016113 | 1.059199 |
| C | 4.036549 | -1.962052 | 0.627854 |
| N | 4.532580 | -0.781027 | 0.214041 |
| C | 5.840306 | -0.717960 | -0.082367 |
| C | 6.714189 | -1.801279 | 0.010466 |
| C | 6.193244 | -3.028340 | 0.425006 |
| C | 4.836293 | -3.109469 | 0.733171 |
| H | 1.681016 | 1.914499 | -0.647195 |
| H | -3.033201 | 2.162188 | 2.578604 |
| H | -1.221693 | -0.517694 | 3.415622 |
| H | -0.929187 | 1.244293 | 3.363652 |
| H | 0.753738 | 1.059964 | 1.666064 |
| H | 1.122699 | -0.131745 | 2.902911 |
| H | 0.068843 | -1.942329 | 1.437468 |
| H | -0.346170 | -0.711077 | 0.263673 |
| H | 2.229142 | -3.064414 | 1.023695 |
| H | 2.540868 | -1.715125 | 2.116796 |
| H | 6.210580 | 0.255648 | -0.407889 |
| H | 7.765730 | -1.684286 | -0.241205 |
| H | 6.830665 | -3.907311 | 0.502562 |
| H | 4.392367 | -4.049911 | 1.053846 |
| H | 0.721511 | -2.435090 | -1.079132 |
| H | 2.410590 | -2.019069 | -1.447167 |
| H | 0.732134 | -0.936364 | -2.981499 |
| H | 0.057282 | -0.035695 | -1.646915 |
| H | 2.959035 | 0.145835 | -2.683749 |
| H | 1.681513 | 1.355854 | -2.955180 |
| H | 3.446612 | 2.928821 | -1.859702 |
| H | 4.501361 | 1.532723 | -1.451309 |
| H | -4.074546 | 1.089466 | 1.585313 |
| H | 3.862667 | 2.597713 | -0.158085 |
| H | -2.358539 | -0.516119 | 1.446680 |
| H | -3.607892 | 0.584414 | 3.233238 |
| H | -1.762123 | 1.015620 | 0.941839 |
| H | 2.590575 | 0.527380 | -0.276393 |
| O | 1.000968 | 3.359063 | -0.063749 |
| S | -0.525429 | 3.298154 | 0.294447 |
| O | -1.233825 | 2.063605 | -0.365353 |
| O | -0.873135 | 3.501083 | 1.786979 |
| C | -1.257688 | 4.843829 | -0.633324 |
| F | -1.018118 | 4.719170 | -1.937443 |
| F | -0.673071 | 5.943756 | -0.165471 |
| F | -2.569204 | 4.895922 | -0.413347 |
| O | -1.334273 | -3.701448 | -0.155121 |
| S | -2.401982 | -2.583838 | -0.195806 |
| O | -2.841429 | -2.052574 | 1.229541 |

| | | | |
|---|---|---|---|
| O | -2.151368 | -1.424841 | -1.197616 |
| C | -4.024024 | -3.460600 | -0.822352 |
| F | -4.370058 | -4.420250 | 0.036135 |
| F | -3.797906 | -3.993688 | -2.024437 |
| F | -5.005304 | -2.560248 | -0.909409 |

# 2. Calculated structures for the iron system

## 2.1 Reactant $[Fe^{III}H_2L^{2'}]Cl_3$

0 2

| | | | |
|---|---|---|---|
| Fe | -0.300401 | 0.011830 | -0.276478 |
| N | -0.404391 | -0.474361 | 1.662424 |
| C | 0.373059 | -1.361530 | 2.328390 |
| H | 1.197760 | -1.813458 | 1.780038 |
| C | 0.208008 | -1.598964 | 3.689198 |
| H | 0.873420 | -2.301479 | 4.183020 |
| C | -0.780768 | -0.902764 | 4.386550 |
| H | -0.930231 | -1.068742 | 5.451572 |
| C | -1.562124 | 0.029148 | 3.705140 |
| H | -2.328234 | 0.607158 | 4.215781 |
| C | -1.353775 | 0.228375 | 2.340299 |
| C | -2.169944 | 1.190036 | 1.526837 |
| H | -2.335892 | 2.130536 | 2.070265 |
| N | -1.442017 | 1.479213 | 0.266555 |
| C | -2.288484 | 1.943934 | -0.859803 |
| H | -2.661673 | 2.952317 | -0.634407 |
| H | -3.139692 | 1.265375 | -0.975599 |
| C | -1.344136 | 2.028497 | -2.053577 |
| H | -0.689310 | 2.889926 | -1.875947 |
| H | -1.877568 | 2.169919 | -3.003479 |
| N | -0.455148 | 0.801900 | -2.148854 |
| C | -1.028726 | -0.265556 | -3.018616 |
| H | -0.223076 | -0.974287 | -3.235689 |
| H | -1.376551 | 0.155913 | -3.974403 |
| C | -2.162618 | -0.974539 | -2.287345 |
| H | -2.385116 | -1.928447 | -2.782718 |
| H | -3.094266 | -0.399394 | -2.288605 |
| N | -1.809113 | -1.204113 | -0.848672 |
| H | -2.729158 | -1.017221 | -0.334496 |
| C | -1.430115 | -2.599118 | -0.531982 |
| H | -2.085742 | -3.313742 | -1.047124 |
| H | -1.585942 | -2.737447 | 0.546455 |
| C | 0.018977 | -2.808036 | -0.870567 |
| C | 0.568801 | -4.035305 | -1.211629 |
| H | -0.070826 | -4.911824 | -1.284108 |
| C | 1.949039 | -4.118671 | -1.450712 |
| H | 2.402498 | -5.070968 | -1.717760 |
| C | 2.723381 | -2.974582 | -1.324236 |
| H | 3.801941 | -2.991211 | -1.446629 |
| C | 2.105472 | -1.765788 | -0.983554 |
| H | 2.688859 | -0.864888 | -0.858435 |
| N | 0.773283 | -1.676729 | -0.788903 |
| C | 0.912120 | 1.205341 | -2.584534 |
| H | 1.403283 | 0.318894 | -3.007453 |
| C | 1.700038 | 1.687626 | -1.393020 |

| | | | |
|---|---|---|---|
| N | 1.356470 | 1.108025 | -0.208226 |
| C | 2.084025 | 1.380404 | 0.892128 |
| H | 1.790006 | 0.893062 | 1.809977 |
| C | 3.167678 | 2.260886 | 0.857261 |
| H | 3.728248 | 2.437496 | 1.769428 |
| C | 3.498356 | 2.877128 | -0.339253 |
| H | 4.324396 | 3.582699 | -0.390782 |
| C | 2.753356 | 2.580224 | -1.489378 |
| H | 2.987136 | 3.040958 | -2.446100 |
| H | 0.867364 | 1.965985 | -3.376541 |
| H | -3.147247 | 0.732954 | 1.283426 |
| H | -0.802307 | 2.330569 | 0.466255 |
| Cl | 3.560141 | -1.235698 | 1.554200 |
| Cl | -0.147393 | 4.139442 | 0.544404 |
| Cl | -4.623039 | -0.707641 | 0.065316 |

## 2.2 Intermediate $[Fe(HL)]Cl_2$

0 2

| | | | |
|---|---|---|---|
| Fe | -0.337630 | -0.324912 | -0.116855 |
| N | -0.392858 | 1.609804 | -0.639883 |
| C | 0.372866 | 2.622821 | -0.172993 |
| H | 1.165062 | 2.363423 | 0.524133 |
| C | 0.231287 | 3.926652 | -0.640365 |
| H | 0.888006 | 4.699851 | -0.251574 |
| C | -0.728499 | 4.197147 | -1.616887 |
| H | -0.865095 | 5.208030 | -1.996537 |
| C | -1.498528 | 3.147827 | -2.117394 |
| H | -2.245892 | 3.313256 | -2.889994 |
| C | -1.304449 | 1.859958 | -1.617319 |
| C | -2.073459 | 0.660877 | -2.087956 |
| H | -2.110925 | 0.632640 | -3.192566 |
| N | -1.435773 | -0.523544 | -1.550160 |
| C | -2.161975 | -1.769313 | -1.682821 |
| H | -2.363105 | -2.006890 | -2.742957 |
| H | -3.146138 | -1.688376 | -1.188268 |
| C | -1.266007 | -2.861255 | -1.091233 |
| H | -0.525713 | -3.152667 | -1.843637 |
| H | -1.831391 | -3.760052 | -0.806091 |
| N | -0.484554 | -2.352023 | 0.098761 |
| C | -1.157760 | -2.602744 | 1.402253 |
| H | -0.403194 | -2.467314 | 2.184759 |
| H | -1.525998 | -3.639561 | 1.465217 |
| C | -2.299147 | -1.609976 | 1.598956 |
| H | -2.632190 | -1.632554 | 2.646061 |
| H | -3.176305 | -1.849255 | 0.988079 |
| N | -1.892982 | -0.226794 | 1.203894 |
| H | -2.768425 | 0.164177 | 0.759380 |
| C | -1.518374 | 0.648670 | 2.331265 |
| H | -2.173650 | 0.490503 | 3.200189 |
| H | -1.671959 | 1.685375 | 1.999206 |
| C | -0.068143 | 0.453362 | 2.684430 |
| C | 0.455862 | 0.734112 | 3.941921 |
| H | -0.206843 | 1.053940 | 4.743098 |
| C | 1.836224 | 0.614924 | 4.145156 |
| H | 2.269479 | 0.836675 | 5.118585 |
| C | 2.640015 | 0.230679 | 3.078464 |

| | | | |
|---|---|---|---|
| H | 3.721372 | 0.174975 | 3.161829 |
| C | 2.044591 | -0.055866 | 1.847077 |
| H | 2.655336 | -0.307881 | 0.989344 |
| N | 0.711276 | 0.030341 | 1.654252 |
| C | 0.898553 | -2.895662 | 0.063276 |
| H | 1.337660 | -2.752700 | 1.059143 |
| C | 1.716343 | -2.126691 | -0.947183 |
| N | 1.361570 | -0.820928 | -1.092082 |
| C | 2.112821 | -0.022788 | -1.872085 |
| H | 1.816983 | 1.014407 | -1.940395 |
| C | 3.213776 | -0.511751 | -2.586700 |
| H | 3.797957 | 0.179035 | -3.186764 |
| C | 3.546224 | -1.853940 | -2.480724 |
| H | 4.391692 | -2.262940 | -3.030100 |
| C | 2.785996 | -2.679406 | -1.636927 |
| H | 3.027661 | -3.732719 | -1.512347 |
| H | 0.905901 | -3.976143 | -0.147985 |
| H | -3.122817 | 0.722945 | -1.719143 |
| Cl | 3.609366 | 1.815482 | -0.043653 |
| Cl | -4.677903 | 0.212384 | 0.024290 |

## 2.3 Imine product $[Fe^{II}L^{2'}]Cl_2$

0 1

| | | | |
|---|---|---|---|
| Fe | -0.274143 | -0.359206 | -0.029896 |
| N | -0.602691 | 1.542259 | -0.578505 |
| C | 0.041115 | 2.665171 | -0.206513 |
| H | 0.938987 | 2.542445 | 0.395963 |
| C | -0.355865 | 3.928697 | -0.656656 |
| H | 0.213401 | 4.798955 | -0.341274 |
| C | -1.453878 | 4.042676 | -1.508312 |
| H | -1.789294 | 5.016978 | -1.857794 |
| C | -2.107242 | 2.880509 | -1.923283 |
| H | -2.962463 | 2.914541 | -2.593509 |
| C | -1.649214 | 1.648943 | -1.456921 |
| C | -2.204710 | 0.362680 | -1.861443 |
| H | -3.079816 | 0.296876 | -2.504142 |
| N | -1.563561 | -0.669045 | -1.416082 |
| C | -2.093638 | -2.016693 | -1.541198 |
| H | -2.328339 | -2.275054 | -2.584721 |
| H | -3.042038 | -2.035939 | -0.981105 |
| C | -1.031663 | -2.981221 | -0.998430 |
| H | -0.301353 | -3.178223 | -1.790581 |
| H | -1.474061 | -3.945311 | -0.707278 |
| N | -0.257122 | -2.401856 | 0.160409 |
| C | -0.851625 | -2.714680 | 1.486966 |
| H | -0.078341 | -2.520412 | 2.238459 |
| H | -1.131194 | -3.778957 | 1.560296 |
| C | -2.062503 | -1.817408 | 1.747340 |
| H | -2.358811 | -1.902346 | 2.803607 |
| H | -2.931650 | -2.119908 | 1.153603 |
| N | -1.777638 | -0.403068 | 1.381931 |
| H | -2.675330 | -0.040223 | 0.975622 |
| C | -1.376284 | 0.459255 | 2.507895 |
| H | -1.918877 | 0.209585 | 3.432728 |
| H | -1.660017 | 1.486864 | 2.238665 |
| C | 0.116223 | 0.409158 | 2.719565 |

| | | | |
|---|---|---|---|
| C | 0.716550 | 0.729761 | 3.933451 |
| H | 0.095491 | 0.958835 | 4.796986 |
| C | 2.113142 | 0.773510 | 4.012860 |
| H | 2.603594 | 1.031029 | 4.949699 |
| C | 2.855876 | 0.506002 | 2.867936 |
| H | 3.939407 | 0.580003 | 2.853961 |
| C | 2.189232 | 0.168753 | 1.687831 |
| H | 2.742113 | 0.013987 | 0.769396 |
| N | 0.842000 | 0.094541 | 1.613414 |
| C | 1.169093 | -2.804757 | 0.054014 |
| H | 1.646127 | -2.580852 | 1.016646 |
| C | 1.831888 | -1.985811 | -1.030367 |
| N | 1.325348 | -0.730540 | -1.180417 |
| C | 1.924753 | 0.107436 | -2.047624 |
| H | 1.521493 | 1.108367 | -2.114756 |
| C | 3.017182 | -0.287033 | -2.828933 |
| H | 3.475394 | 0.438507 | -3.494225 |
| C | 3.505931 | -1.580274 | -2.706647 |
| H | 4.350557 | -1.916172 | -3.304746 |
| C | 2.902338 | -2.448198 | -1.784159 |
| H | 3.264255 | -3.465035 | -1.646900 |
| H | 1.282290 | -3.885368 | -0.129705 |
| Cl | 3.306083 | 2.235478 | -0.371887 |
| Cl | -4.491870 | 0.075185 | -0.041471 |

## 2.4 Product $[Fe^{II}H_2L^{2'}]Cl_2$

0 1

| | | | |
|---|---|---|---|
| Fe | 0.141354 | 0.133578 | -0.187919 |
| N | 0.245869 | -0.960560 | 1.493729 |
| C | 0.410791 | -0.518552 | 2.760707 |
| H | 0.518493 | 0.557025 | 2.876663 |
| C | 0.439730 | -1.365399 | 3.861353 |
| H | 0.575626 | -0.953486 | 4.858258 |
| C | 0.282710 | -2.739509 | 3.651157 |
| H | 0.292959 | -3.434444 | 4.488334 |
| C | 0.100380 | -3.202184 | 2.352308 |
| H | -0.041749 | -4.259729 | 2.145427 |
| C | 0.086876 | -2.295724 | 1.287003 |
| C | -0.065766 | -2.730421 | -0.141222 |
| H | -0.770398 | -3.570294 | -0.205835 |
| N | -0.579079 | -1.577849 | -0.916029 |
| C | -0.335024 | -1.633618 | -2.369853 |
| H | -0.984752 | -2.379823 | -2.853174 |
| H | 0.704345 | -1.934341 | -2.544991 |
| C | -0.680082 | -0.247900 | -2.920941 |
| H | -1.769059 | -0.126528 | -2.885678 |
| H | -0.363612 | -0.133916 | -3.968486 |
| N | -0.093037 | 0.866491 | -2.084037 |
| C | 1.246458 | 1.308650 | -2.555334 |
| H | 1.448667 | 2.275562 | -2.080451 |
| H | 1.252403 | 1.466986 | -3.646607 |
| C | 2.317327 | 0.296412 | -2.152795 |
| H | 3.310624 | 0.759274 | -2.249328 |
| H | 2.328382 | -0.585695 | -2.802119 |
| N | 2.097224 | -0.213342 | -0.766668 |
| H | 2.385584 | -1.227092 | -0.835324 |

| | | | |
|---|---|---|---|
| C | 2.960505 | 0.414187 | 0.247088 |
| H | 3.989277 | 0.562633 | -0.115419 |
| H | 3.019508 | -0.281590 | 1.096767 |
| C | 2.360467 | 1.711765 | 0.721287 |
| C | 3.119422 | 2.750829 | 1.262971 |
| H | 4.201897 | 2.652031 | 1.309386 |
| C | 2.479999 | 3.895194 | 1.739642 |
| H | 3.054575 | 4.714487 | 2.166582 |
| C | 1.087197 | 3.962871 | 1.656380 |
| H | 0.538035 | 4.829007 | 2.017320 |
| C | 0.395222 | 2.893819 | 1.094764 |
| H | -0.687997 | 2.904619 | 1.015361 |
| N | 1.006119 | 1.782854 | 0.623803 |
| C | -1.052619 | 1.996511 | -1.989103 |
| H | -0.490767 | 2.879260 | -1.654964 |
| C | -2.127737 | 1.670883 | -0.977170 |
| N | -1.736375 | 0.846420 | 0.033793 |
| C | -2.648455 | 0.499439 | 0.962925 |
| H | -2.322918 | -0.204759 | 1.717437 |
| C | -3.938426 | 1.040921 | 0.985789 |
| H | -4.629736 | 0.725348 | 1.761431 |
| C | -4.321510 | 1.913722 | -0.022653 |
| H | -5.325460 | 2.332398 | -0.046127 |
| C | -3.404232 | 2.215187 | -1.039335 |
| H | -3.677349 | 2.863696 | -1.869201 |
| H | -1.492834 | 2.245266 | -2.967844 |
| H | 0.916760 | -3.042036 | -0.544509 |
| H | -1.617556 | -1.603742 | -0.747063 |
| Cl | 3.054103 | -2.974838 | -1.628711 |
| Cl | -3.460138 | -2.185971 | -0.002578 |

## 2.5 Protonated ligand $[H_4L^{2'}]Cl_2$

0 1

| | | | |
|---|---|---|---|
| N | 2.405823 | -0.507713 | 0.158600 |
| H | 1.959520 | -1.380531 | 0.491510 |
| N | -0.562960 | 1.712442 | 0.704815 |
| N | -2.376137 | -0.945586 | -0.092557 |
| C | -1.496497 | 5.522993 | -1.027898 |
| C | -0.216941 | 4.133314 | 0.286037 |
| C | -0.371016 | 6.141189 | -1.577893 |
| H | -2.498412 | 5.833851 | -1.330640 |
| C | 0.970879 | 4.689022 | -0.211345 |
| C | 0.889534 | 5.711805 | -1.157137 |
| H | -0.484377 | 6.937625 | -2.310697 |
| H | 1.929505 | 4.313356 | 0.145785 |
| H | 1.794602 | 6.166370 | -1.557177 |
| C | 4.279800 | -1.958489 | -0.635330 |
| C | 6.457690 | -2.614748 | -0.331209 |
| C | 3.800211 | -3.250371 | -0.369188 |
| C | 6.082747 | -3.927411 | -0.034269 |
| H | 7.509416 | -2.325183 | -0.331978 |
| C | 4.724215 | -4.248236 | -0.057075 |
| H | 2.731278 | -3.461848 | -0.409642 |
| H | 6.837299 | -4.674231 | 0.204158 |
| H | 4.386601 | -5.260442 | 0.159047 |
| C | -4.524910 | -2.120039 | -0.432582 |

| | | | |
|---|---|---|---|
| C | -5.822429 | -2.180026 | 1.471757 |
| C | -5.561003 | -2.641303 | -1.214527 |
| C | -6.909401 | -2.711649 | 0.778349 |
| H | -5.883136 | -1.975857 | 2.540273 |
| C | -6.772316 | -2.944060 | -0.592974 |
| H | -5.418512 | -2.808801 | -2.280399 |
| H | -7.837668 | -2.932653 | 1.299281 |
| H | -7.598654 | -3.353075 | -1.170888 |
| N | -1.436145 | 4.545019 | -0.113449 |
| N | -4.653447 | -1.890213 | 0.881696 |
| N | 5.584440 | -1.642391 | -0.624837 |
| C | 3.328838 | -0.829741 | -0.978042 |
| H | 3.900809 | 0.077768 | -1.188908 |
| H | 2.696885 | -1.093647 | -1.834273 |
| C | 1.305055 | 0.436519 | -0.205425 |
| H | 1.785116 | 1.388125 | -0.446456 |
| H | 0.778041 | 0.026837 | -1.071977 |
| C | 0.367395 | 0.623054 | 0.993955 |
| H | 0.984842 | 0.845345 | 1.875636 |
| H | -0.164833 | -0.314959 | 1.195068 |
| C | -2.529268 | 0.532444 | -0.342338 |
| H | -3.607254 | 0.701915 | -0.450098 |
| C | -1.981768 | 1.431492 | 0.777830 |
| H | -2.493695 | 2.393868 | 0.658138 |
| C | -0.167072 | 3.006812 | 1.298532 |
| H | -0.811406 | 3.257965 | 2.159279 |
| H | 0.860298 | 2.906858 | 1.668251 |
| H | -2.033277 | 0.761687 | -1.290963 |
| H | -2.305658 | 1.015088 | 1.759220 |
| C | -3.155088 | -1.824750 | -1.017664 |
| H | -3.218636 | -1.342503 | -1.998826 |
| H | -2.556011 | -2.740326 | -1.126493 |
| H | -1.370701 | -1.317087 | -0.127095 |
| H | 2.954468 | 0.029667 | 0.921085 |
| H | -2.756898 | -1.157421 | 0.850086 |
| Cl | 3.504068 | 1.793247 | 1.726018 |
| Cl | 0.084609 | -2.692398 | -0.310110 |

## 2.6 $[Fe^{II}(MeOH)_6]Cl_2$

0 1

| | | | |
|---|---|---|---|
| Fe | 0.000313 | 0.000364 | -0.000666 |
| O | -1.213215 | -0.301641 | 1.616304 |
| O | -1.214063 | 1.553940 | -0.543301 |
| O | -1.213513 | -1.249229 | -1.072185 |
| O | 1.214112 | 0.301981 | -1.617252 |
| O | 1.211829 | -1.554065 | 0.542878 |
| O | 1.210753 | 1.251917 | 1.071976 |
| C | -1.212953 | -2.676334 | -0.879213 |
| H | -1.536343 | -2.936451 | 0.136815 |
| H | -1.888856 | -3.137621 | -1.609089 |
| H | -0.192737 | -3.028396 | -1.038070 |
| C | 1.212796 | -0.584035 | -2.752706 |
| H | 1.548543 | -1.589063 | -2.467129 |
| H | 0.189621 | -0.634614 | -3.127646 |
| H | 1.878560 | -0.179886 | -3.524639 |
| C | 1.205171 | -2.103024 | 1.874282 |

| | | | |
|---|---|---|---|
| H | 0.182465 | -2.410741 | 2.095937 |
| H | 1.876344 | -2.969406 | 1.908939 |
| H | 1.530282 | -1.356132 | 2.609948 |
| C | 1.211821 | 2.677618 | 0.868486 |
| H | 0.192730 | 3.032520 | 1.027340 |
| H | 1.890785 | 3.143127 | 1.592556 |
| H | 1.532969 | 2.929874 | -0.150458 |
| C | -1.202989 | 0.574561 | 2.759054 |
| H | -1.508798 | 1.590448 | 2.478724 |
| H | -1.888305 | 0.181221 | 3.519166 |
| H | -0.184016 | 0.595329 | 3.147528 |
| C | -1.208037 | 2.104686 | -1.873931 |
| H | -1.545103 | 1.362085 | -2.608433 |
| H | -1.870312 | 2.978083 | -1.904148 |
| H | -0.183359 | 2.402407 | -2.100380 |
| H | -2.149678 | -0.928398 | -0.909334 |
| H | -2.151284 | -0.316352 | 1.261004 |
| H | -2.151937 | 1.255231 | -0.350488 |
| H | 2.147558 | 0.930041 | 0.913761 |
| H | 2.150505 | 0.322397 | -1.258141 |
| H | 2.149895 | -1.256136 | 0.349196 |
| Cl | 3.756578 | 0.000195 | 0.003466 |
| Cl | -3.758327 | 0.001389 | 0.000132 |