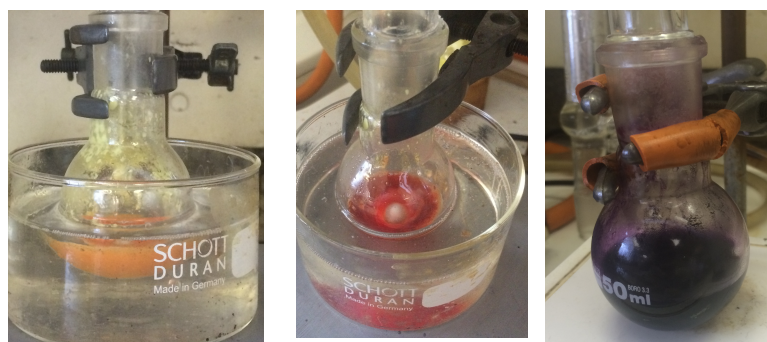


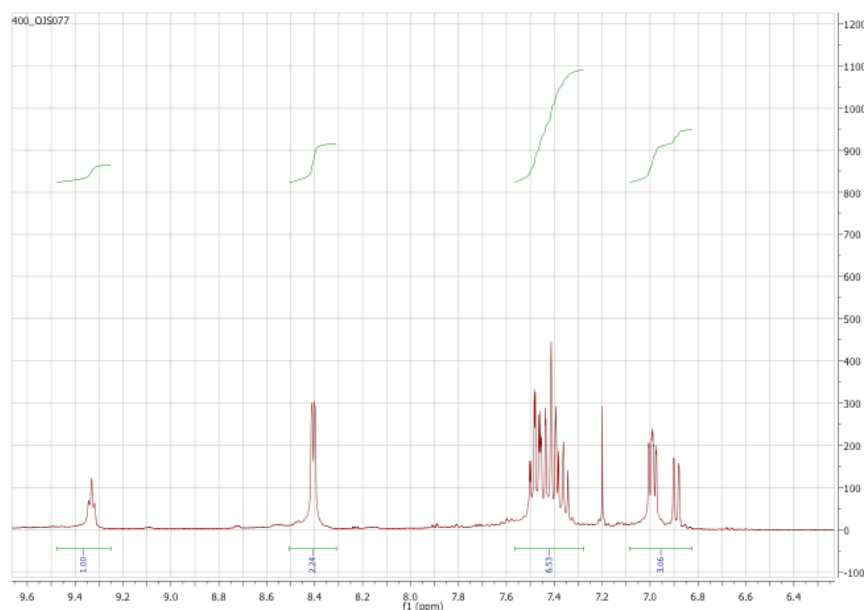
## Near-IR luminescent lanthanide complexes of 1,8-diaminoanthraquinone-based chromophoric ligands

Oliver J. Stacey, Benjamin D. Ward, Angelo J. Amoroso and Simon J.A. Pope

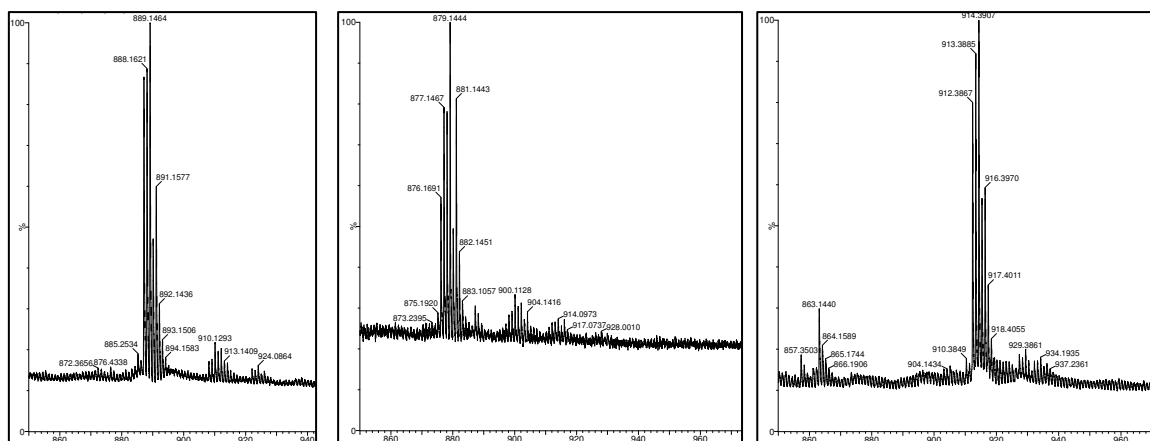
### Electronic Supplementary Information



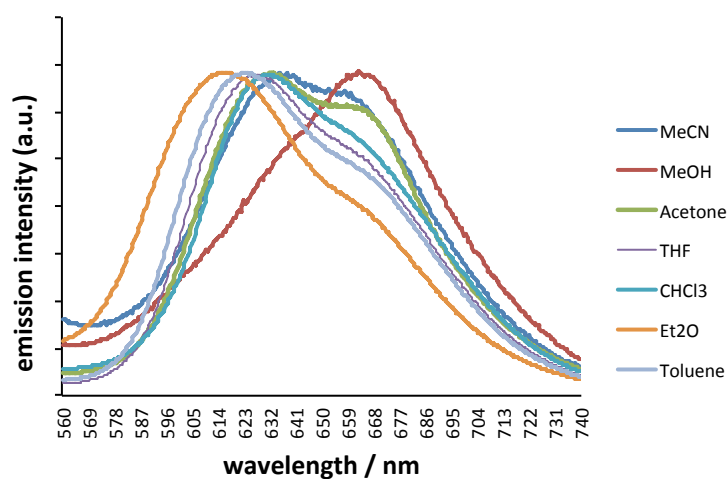
**Figure S1.** Photographic evidence for the reaction progress showing the colour changes of the reaction medium (left: initial colour; centre: after 2 hours; right: after 12 hrs).



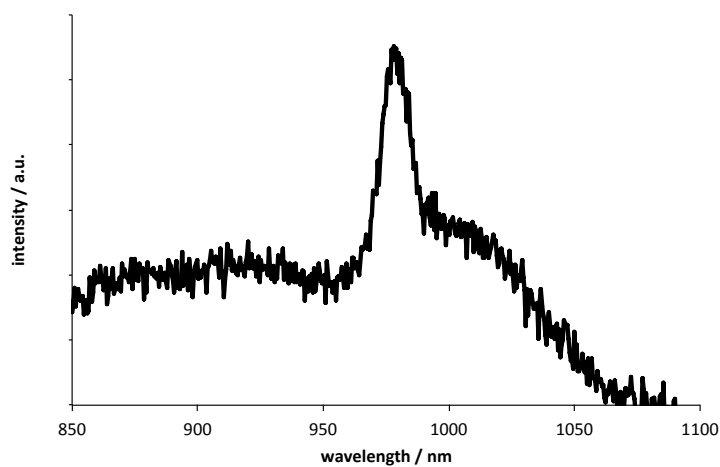
**Figure S2.**  $^1\text{H}$  NMR spectrum for  $\text{L}^2$  (400 MHz,  $\text{CDCl}_3$ , 295K) showing the aromatic region. Note the NH resonance at ca. 9.3 ppm.



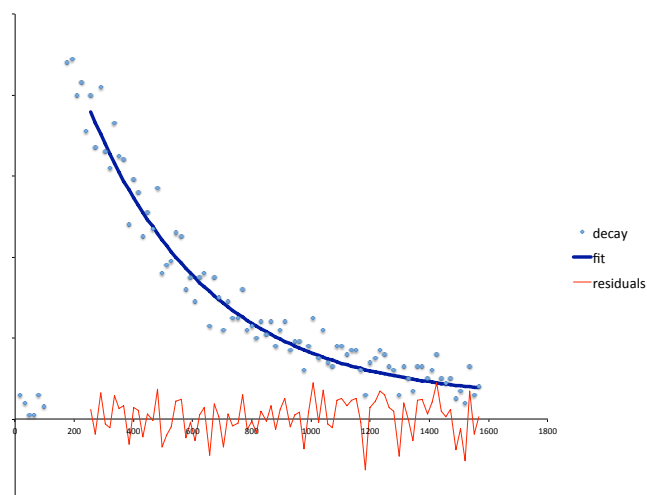
**Figure S3.** Selected examples of MALDI MS data for (l-to-r)  $[\text{Er}(\text{L}^2)](\text{OTf})_3$ ,  $[\text{Gd}(\text{L}^2)](\text{OTf})_3$  and  $[\text{Er}(\text{L}^3)](\text{OTf})_3$ .



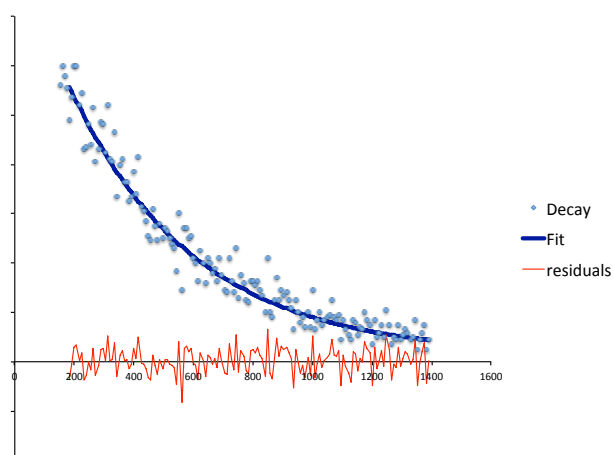
**Figure S4.** Solvent dependent emission spectra for  $\text{L}^1$  ( $\lambda_{\text{ex}} = 525 \text{ nm}$ ).



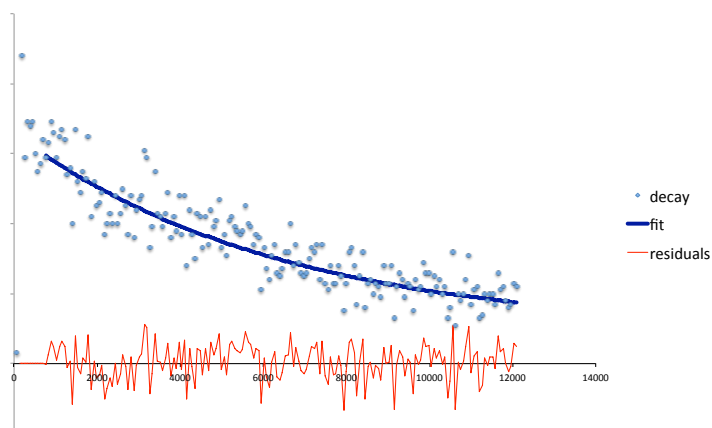
**Figure S5.** Steady state emission spectrum for  $\text{Yb-L}^1$  ( $\text{CD}_3\text{OD}$ ,  $\lambda_{\text{ex}} = 525 \text{ nm}$ ).



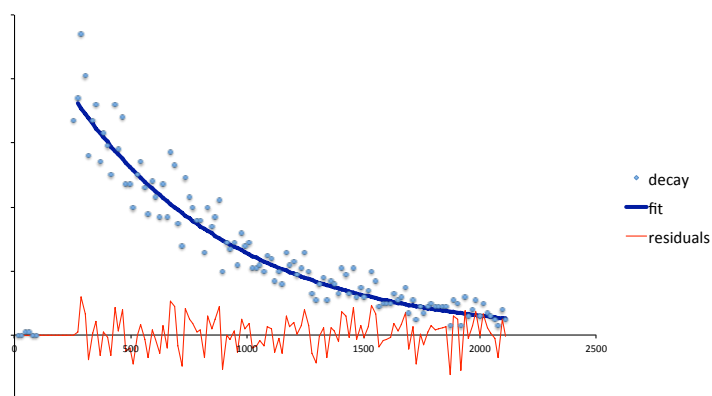
**Figure S6.** Fitted decay ( $\tau = 378$  ns) profile (intensity vs. ns) for Nd-L<sup>2</sup> (CD<sub>3</sub>OD,  $\lambda_{\text{em}} = 1055$  nm,  $\lambda_{\text{ex}} = 355$  nm).



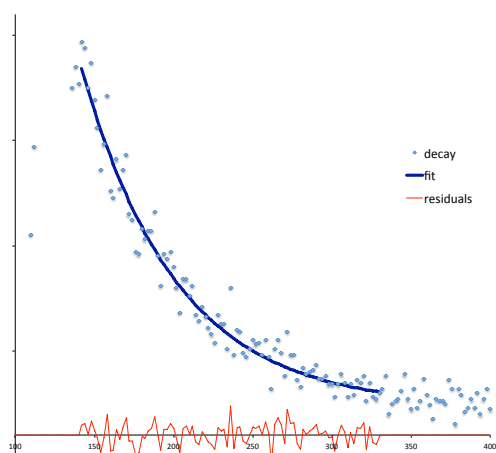
**Figure S7.** Fitted decay ( $\tau = 415$  ns) profile (intensity vs. ns) for Nd-L<sup>3</sup> (CD<sub>3</sub>OD,  $\lambda_{\text{em}} = 1055$  nm,  $\lambda_{\text{ex}} = 355$  nm).



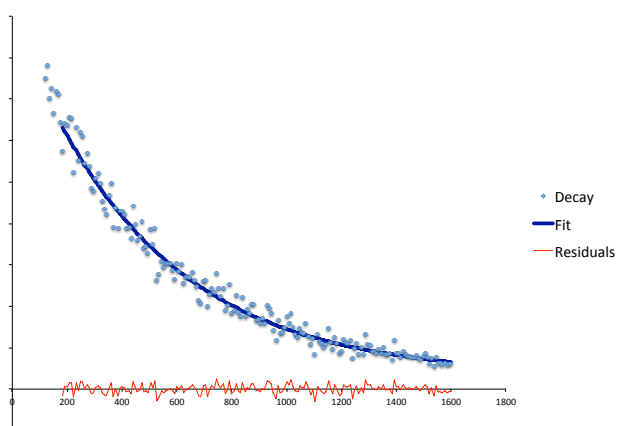
**Figure S8.** Fitted decay ( $\tau = 5680$  ns) profile (intensity vs. ns) for Yb-L<sup>1</sup> (CD<sub>3</sub>OD,  $\lambda_{\text{em}} = 980$  nm,  $\lambda_{\text{ex}} = 355$  nm).



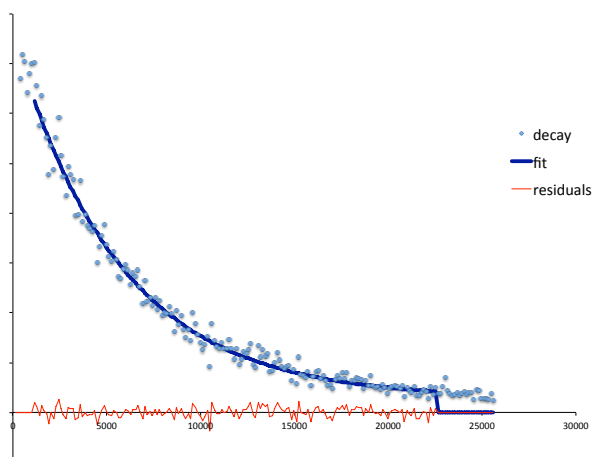
**Figure S9.** Fitted decay ( $\tau = 441$  ns) profile (intensity vs. ns) for Yb-L<sup>2</sup> (CH<sub>3</sub>OH,  $\lambda_{\text{em}} = 980$  nm,  $\lambda_{\text{ex}} = 355$  nm).



**Figure S10.** Fitted decay ( $\tau = 48$  ns) profile (intensity vs. ns) for Nd-L<sup>2</sup> (CH<sub>3</sub>OH,  $\lambda_{\text{em}} = 1055$  nm,  $\lambda_{\text{ex}} = 355$  nm).



**Figure S11.** Fitted decay ( $\tau = 597$  ns) profile (intensity vs. ns) for Er-L<sup>2</sup> complexes (CD<sub>3</sub>OD,  $\lambda_{\text{em}} = 1535$  nm,  $\lambda_{\text{ex}} = 355$  nm).

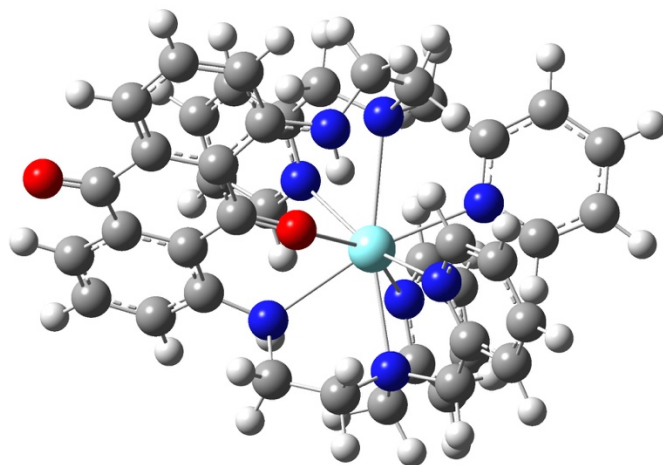


**Figure S12.** Fitted decay ( $\tau = 6350$  ns) profile (intensity vs. ns) for Yb-L<sup>2</sup> (CD<sub>3</sub>OD,  $\lambda_{\text{em}} = 980$  nm,  $\lambda_{\text{ex}} = 355$  nm).

## DFT Studies

Atomic coordinates for calculated complexes

$[\text{Y}(\text{L}^1)]^{3+}$

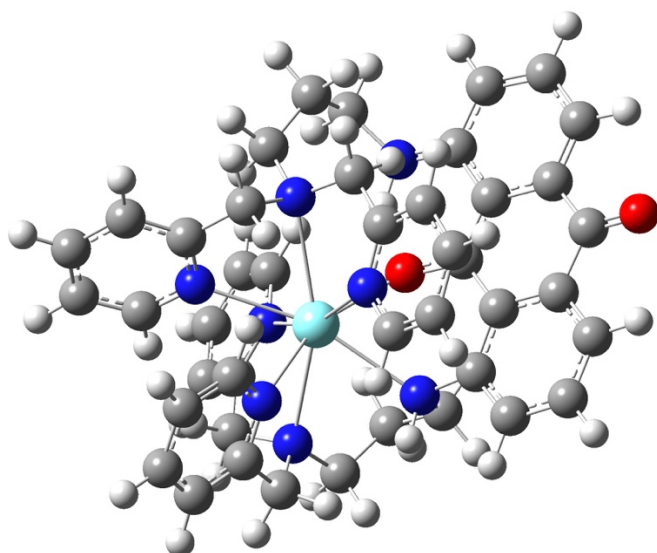


|   |         |          |          |
|---|---------|----------|----------|
| C | 5.31573 | -3.26056 | -0.14358 |
| C | 5.72776 | -1.97014 | 0.23177  |
| C | 4.78475 | -1.01065 | 0.52632  |
| C | 3.38698 | -1.30497 | 0.5116   |
| C | 2.98522 | -2.62236 | 0.1019   |
| C | 3.97501 | -3.56822 | -0.23623 |
| C | 5.26602 | 0.37373  | 0.75562  |
| C | 2.43308 | -0.26543 | 0.78124  |
| C | 2.86018 | 1.13623  | 0.89781  |
| C | 4.23472 | 1.45022  | 0.81422  |
| C | 4.68663 | 2.76543  | 0.80808  |
| H | 5.76324 | 2.94015  | 0.75392  |
| C | 3.77301 | 3.8096   | 0.87291  |
| C | 2.41714 | 3.52261  | 1.00863  |
| C | 1.95054 | 2.21088  | 1.04022  |
| H | 6.06269 | -4.02494 | -0.36892 |
| H | 6.7841  | -1.69705 | 0.27013  |
| H | 3.66205 | -4.57478 | -0.52368 |
| H | 4.11269 | 4.84721  | 0.8543   |
| H | 1.70078 | 4.34502  | 1.11948  |
| O | 1.18123 | -0.53728 | 0.8498   |
| O | 6.44442 | 0.64172  | 0.8378   |
| N | 0.542   | 2.013    | 1.32715  |
| H | 0.09166 | 2.88734  | 1.04056  |
| N | 1.6657  | -2.96836 | -0.02987 |
| H | 1.05644 | -2.25553 | 0.34973  |

|   |          |          |          |
|---|----------|----------|----------|
| C | 0.37167  | 1.94288  | 2.81686  |
| H | 0.34085  | 2.96953  | 3.22161  |
| H | 1.27659  | 1.48677  | 3.24527  |
| C | 1.16677  | -3.66061 | -1.20654 |
| H | 1.95583  | -3.67756 | -1.9786  |
| H | 0.9258   | -4.71948 | -1.00299 |
| C | -0.10004 | -3.02127 | -1.76429 |
| H | -0.27533 | -3.49567 | -2.75032 |
| H | -0.97745 | -3.28169 | -1.14753 |
| C | -0.8356  | 1.12413  | 3.24997  |
| H | -0.54196 | 0.07628  | 3.42023  |
| H | -1.21941 | 1.5052   | 4.21653  |
| N | -1.91296 | 1.11395  | 2.23757  |
| N | -0.11364 | -1.53198 | -1.9279  |
| C | -1.18842 | -1.23071 | -2.90283 |
| H | -1.0516  | -1.82959 | -3.82313 |
| H | -1.09842 | -0.17419 | -3.21127 |
| C | 1.15192  | -1.04584 | -2.49776 |
| H | 1.99073  | -1.41585 | -1.88702 |
| H | 1.31024  | -1.4579  | -3.51601 |
| C | -2.48147 | 2.46163  | 2.03549  |
| H | -3.22418 | 2.69803  | 2.82022  |
| H | -1.68599 | 3.21524  | 2.16282  |
| C | -2.99463 | 0.22383  | 2.69387  |
| H | -3.31745 | 0.50228  | 3.71635  |
| H | -3.87233 | 0.40328  | 2.04485  |
| C | -2.61208 | -1.22611 | 2.65676  |
| C | -3.20824 | -2.12359 | 3.53567  |
| C | -1.38399 | -2.91587 | 1.68767  |
| C | -2.87865 | -3.4724  | 3.4617   |
| H | -3.92304 | -1.76146 | 4.27862  |
| C | -1.9409  | -3.87646 | 2.5165   |
| H | -0.62243 | -3.21409 | 0.96304  |
| H | -3.33496 | -4.19395 | 4.1429   |
| H | -1.63193 | -4.91889 | 2.4293   |
| C | -3.08631 | 2.61646  | 0.66873  |
| C | -4.21289 | 3.40733  | 0.46853  |
| C | -2.93138 | 2.18327  | -1.59675 |
| C | -4.69689 | 3.5885   | -0.82338 |
| H | -4.70407 | 3.8813   | 1.32181  |
| C | -4.03744 | 2.9671   | -1.88107 |
| H | -2.40015 | 1.67106  | -2.40694 |
| H | -5.57949 | 4.20656  | -1.00231 |

|   |          |          |          |
|---|----------|----------|----------|
| H | -4.37688 | 3.08256  | -2.91141 |
| C | -2.55448 | -1.45599 | -2.33507 |
| C | -3.54326 | -2.10346 | -3.06769 |
| C | -4.81752 | -2.23116 | -2.52516 |
| H | -3.31292 | -2.50112 | -4.05881 |
| C | -4.0104  | -1.09297 | -0.58891 |
| C | -5.05628 | -1.7109  | -1.25628 |
| H | -5.61082 | -2.7349  | -3.08197 |
| H | -4.17739 | -0.68634 | 0.41286  |
| H | -6.03685 | -1.78845 | -0.78437 |
| C | 1.25059  | 0.45441  | -2.5562  |
| C | 2.19454  | 1.03152  | -3.40291 |
| C | 2.32243  | 2.41335  | -3.44908 |
| H | 2.82066  | 0.3908   | -4.02899 |
| C | 0.56105  | 2.54144  | -1.84938 |
| C | 1.47323  | 3.18929  | -2.66241 |
| H | 3.05954  | 2.88056  | -4.10581 |
| H | -0.13265 | 3.12588  | -1.23496 |
| H | 1.51276  | 4.2793   | -2.68281 |
| N | -2.77375 | -0.95397 | -1.10146 |
| N | 0.44558  | 1.19807  | -1.76574 |
| N | -1.70507 | -1.60827 | 1.73051  |
| N | -2.44998 | 1.99644  | -0.35093 |
| Y | -0.83378 | 0.15119  | 0.12841  |

$[\text{Y}(\text{L}^2)]^{3+}$



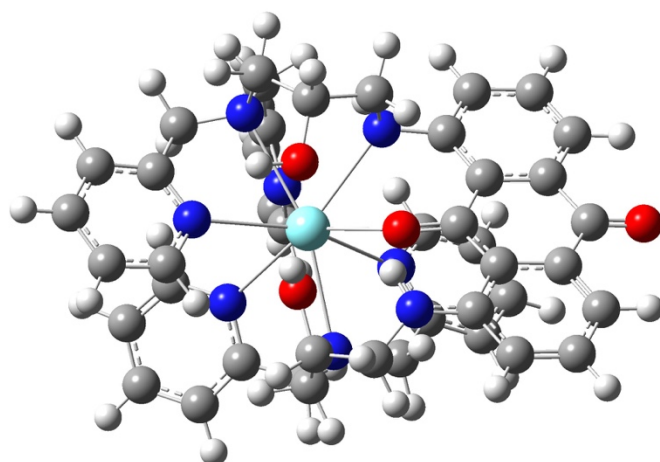
|   |         |         |          |
|---|---------|---------|----------|
| C | 5.57286 | 2.9132  | 0.03493  |
| C | 5.85122 | 1.53414 | -0.04498 |
| C | 4.83999 | 0.64997 | -0.33209 |
| C | 3.49843 | 1.09617 | -0.57145 |

|   |          |          |          |
|---|----------|----------|----------|
| C | 3.22995  | 2.50997  | -0.47172 |
| C | 4.29582  | 3.38583  | -0.14909 |
| C | 5.17815  | -0.7954  | -0.29824 |
| C | 2.46034  | 0.13532  | -0.77988 |
| C | 2.77264  | -1.3028  | -0.84815 |
| C | 4.07837  | -1.75956 | -0.57153 |
| C | 4.39505  | -3.11511 | -0.56591 |
| H | 5.42575  | -3.402   | -0.34672 |
| C | 3.41477  | -4.05604 | -0.85258 |
| C | 2.13062  | -3.62589 | -1.17788 |
| C | 1.801    | -2.27391 | -1.18111 |
| H | 6.37984  | 3.61713  | 0.25036  |
| H | 6.85409  | 1.14147  | 0.13375  |
| H | 4.10908  | 4.45863  | -0.08672 |
| H | 3.65194  | -5.12192 | -0.85853 |
| H | 1.3697   | -4.36136 | -1.46282 |
| O | 1.22596  | 0.50019  | -0.86583 |
| O | 6.2978   | -1.18498 | -0.0431  |
| N | 0.48946  | -1.89095 | -1.65315 |
| H | -0.05614 | -2.75885 | -1.66778 |
| N | 1.98146  | 3.00022  | -0.67804 |
| H | 1.31007  | 2.28244  | -0.92911 |
| C | -0.54778 | -0.85857 | -3.73584 |
| H | -0.38201 | -0.85566 | -4.8251  |
| C | -1.83131 | -1.60359 | -3.44667 |
| H | -2.6081  | -1.34871 | -4.18851 |
| H | -1.65802 | -2.6869  | -3.56927 |
| N | -2.38058 | -1.36266 | -2.06928 |
| N | -0.03742 | 1.57087  | 1.79981  |
| C | -0.95783 | 1.16637  | 2.88555  |
| H | -0.74243 | 1.74361  | 3.80564  |
| H | -0.76363 | 0.11243  | 3.14452  |
| C | 1.31176  | 1.17527  | 2.22022  |
| H | 2.04745  | 1.5776   | 1.50878  |
| H | 1.5677   | 1.614    | 3.20683  |
| C | -2.91434 | -2.63118 | -1.53755 |
| H | -3.78535 | -2.97325 | -2.12955 |
| H | -2.14142 | -3.41112 | -1.66156 |
| C | -3.4944  | -0.40191 | -2.17486 |
| H | -4.20243 | -0.70654 | -2.96912 |
| H | -4.0701  | -0.44351 | -1.23293 |
| C | -3.01176 | 0.99764  | -2.42655 |
| C | -3.66696 | 1.83364  | -3.32294 |

|   |          |          |          |
|---|----------|----------|----------|
| C | -1.48387 | 2.65757  | -1.93069 |
| C | -3.19959 | 3.13187  | -3.51554 |
| H | -4.53523 | 1.46533  | -3.8743  |
| C | -2.08114 | 3.55396  | -2.80417 |
| H | -0.60013 | 2.95523  | -1.35797 |
| H | -3.69795 | 3.80085  | -4.22046 |
| H | -1.67176 | 4.55789  | -2.92771 |
| C | -3.26691 | -2.55755 | -0.08363 |
| C | -4.43666 | -3.13652 | 0.39676  |
| C | -2.61762 | -1.98917 | 2.05551  |
| C | -4.69211 | -3.12959 | 1.7647   |
| H | -5.13857 | -3.59787 | -0.30178 |
| C | -3.75377 | -2.55159 | 2.61467  |
| H | -1.85934 | -1.53882 | 2.70286  |
| H | -5.60634 | -3.57722 | 2.16112  |
| H | -3.89373 | -2.53882 | 3.69654  |
| C | -2.3914  | 1.33736  | 2.50089  |
| C | -3.32477 | 1.7729   | 3.43686  |
| C | -4.65277 | 1.92506  | 3.05682  |
| H | -3.0032  | 2.0021   | 4.45576  |
| C | -3.99342 | 1.25286  | 0.863    |
| C | -4.98956 | 1.67436  | 1.73066  |
| H | -5.40405 | 2.26233  | 3.77418  |
| H | -4.2413  | 1.09976  | -0.18869 |
| H | -6.00696 | 1.81756  | 1.36342  |
| C | 1.4956   | -0.31687 | 2.30531  |
| C | 2.54652  | -0.82481 | 3.06429  |
| C | 2.72365  | -2.20011 | 3.15897  |
| H | 3.21431  | -0.13697 | 3.58923  |
| C | 0.80907  | -2.45798 | 1.76275  |
| C | 1.82387  | -3.03836 | 2.50483  |
| H | 3.5418   | -2.61332 | 3.75305  |
| H | 0.07965  | -3.0887  | 1.24146  |
| H | 1.90419  | -4.1245  | 2.56846  |
| N | -2.71265 | 1.04548  | 1.2233   |
| N | 0.63934  | -1.12449 | 1.63963  |
| N | -1.92458 | 1.40432  | -1.73092 |
| N | -2.36508 | -1.96299 | 0.73146  |
| H | -0.63028 | 0.20338  | -3.45262 |
| C | 0.66174  | -1.5047  | -3.10387 |
| H | 1.52666  | -0.83052 | -3.16867 |
| H | 0.94197  | -2.42072 | -3.65666 |
| C | 1.44121  | 4.19601  | -0.06363 |

|   |          |          |          |
|---|----------|----------|----------|
| H | 0.58393  | 4.53362  | -0.6713  |
| H | 2.16584  | 5.02016  | -0.1185  |
| C | 1.01056  | 3.98555  | 1.38379  |
| H | 0.70423  | 4.97402  | 1.76654  |
| H | 1.88452  | 3.7119   | 1.99938  |
| C | -0.18925 | 3.07571  | 1.66552  |
| H | -0.60512 | 3.43228  | 2.62533  |
| H | -0.98469 | 3.2596   | 0.92029  |
| Y | -0.82231 | -0.18881 | -0.17596 |

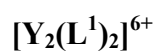
$[\text{Y}(\text{L}^3)]^{3+}$

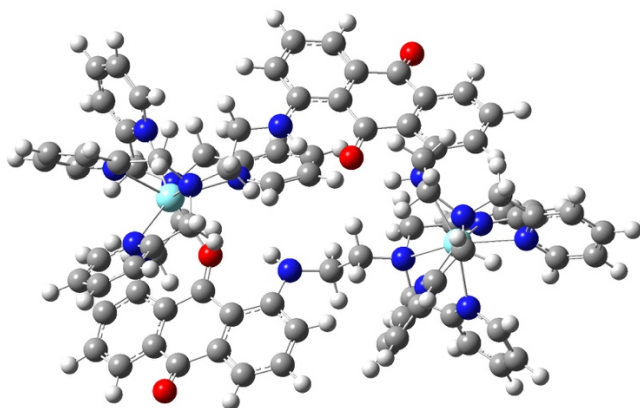


|   |          |          |          |
|---|----------|----------|----------|
| C | -5.66578 | -3.07367 | -0.27725 |
| C | -5.97822 | -1.70271 | -0.21758 |
| C | -4.99915 | -0.76559 | -0.46816 |
| C | -3.66979 | -1.16423 | -0.79373 |
| C | -3.37461 | -2.56715 | -0.87543 |
| C | -4.39189 | -3.50169 | -0.58972 |
| C | -5.34762 | 0.67099  | -0.30237 |
| C | -2.63194 | -0.17373 | -0.89155 |
| C | -2.95598 | 1.25564  | -0.84205 |
| C | -4.26455 | 1.67298  | -0.5317  |
| C | -4.58386 | 3.02275  | -0.41251 |
| H | -5.61366 | 3.29287  | -0.16858 |
| C | -3.59929 | 3.98307  | -0.6116  |
| C | -2.30583 | 3.58663  | -0.94541 |
| C | -1.96949 | 2.23955  | -1.06088 |
| H | -6.44664 | -3.81296 | -0.08439 |
| H | -6.98204 | -1.35846 | 0.03872  |
| H | -4.17414 | -4.56988 | -0.66499 |
| H | -3.83791 | 5.04544  | -0.52881 |
| H | -1.5406  | 4.34922  | -1.13339 |
| O | -1.40827 | -0.50872 | -0.98028 |

|   |          |          |          |
|---|----------|----------|----------|
| O | -6.4586  | 1.02618  | 0.02862  |
| N | -0.61748 | 1.90816  | -1.46236 |
| H | -0.10027 | 2.77637  | -1.32288 |
| N | -2.1218  | -2.95636 | -1.22991 |
| H | -1.52761 | -2.16875 | -1.46858 |
| C | 0.65176  | 0.96809  | -3.42781 |
| H | 0.50799  | 0.79441  | -4.50966 |
| C | 1.9598   | 1.71226  | -3.23307 |
| H | 2.73894  | 1.1828   | -3.80909 |
| H | 1.90184  | 2.72079  | -3.68189 |
| N | 2.37077  | 1.76411  | -1.81033 |
| N | 0.04099  | -2.00149 | 1.52142  |
| C | 0.7689   | -1.8198  | 2.79328  |
| H | 0.59104  | -2.68176 | 3.46491  |
| H | 0.3433   | -0.94351 | 3.31282  |
| C | -1.38215 | -1.81204 | 1.82723  |
| H | -1.98122 | -2.17399 | 0.98161  |
| H | -1.67383 | -2.43368 | 2.69848  |
| C | 2.26851  | 3.12052  | -1.26036 |
| H | 3.10091  | 3.75845  | -1.62039 |
| H | 1.3683   | 3.62385  | -1.65414 |
| C | 3.78198  | 1.3714   | -1.68421 |
| H | 4.40902  | 1.93793  | -2.40069 |
| H | 4.12562  | 1.68884  | -0.68179 |
| C | 4.04805  | -0.09695 | -1.82108 |
| C | 5.27571  | -0.50994 | -2.33577 |
| C | 3.48885  | -2.26186 | -1.29375 |
| C | 5.61288  | -1.85773 | -2.30712 |
| H | 5.96871  | 0.23096  | -2.74226 |
| C | 4.69993  | -2.75256 | -1.75831 |
| H | 2.75506  | -2.94484 | -0.86183 |
| H | 6.57251  | -2.20156 | -2.69962 |
| H | 4.91557  | -3.82033 | -1.69621 |
| C | 2.25928  | 3.12451  | 0.24385  |
| C | 2.73461  | 4.24739  | 0.91856  |
| C | 1.8078   | 2.06689  | 2.23598  |
| C | 2.72946  | 4.2665   | 2.30723  |
| H | 3.11617  | 5.09805  | 0.34832  |
| C | 2.25922  | 3.14304  | 2.98168  |
| H | 1.42367  | 1.17914  | 2.74423  |
| H | 3.09768  | 5.13741  | 2.8539   |
| H | 2.24373  | 3.09663  | 4.07142  |
| C | 2.23192  | -1.58896 | 2.61048  |

|   |          |          |          |
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| C | 3.14035  | -2.10357 | 3.53276  |
| C | 4.48335  | -1.76645 | 3.42633  |
| H | 2.78621  | -2.75565 | 4.33469  |
| C | 3.89837  | -0.46811 | 1.51067  |
| C | 4.86707  | -0.91363 | 2.3953   |
| H | 5.21505  | -2.15549 | 4.13787  |
| H | 4.19023  | 0.19987  | 0.69877  |
| H | 5.90398  | -0.59709 | 2.27319  |
| C | -1.72144 | -0.37686 | 2.11116  |
| C | -2.85249 | -0.08922 | 2.87226  |
| C | -3.1887  | 1.23426  | 3.12864  |
| H | -3.45771 | -0.90893 | 3.26817  |
| C | -1.26248 | 1.86399  | 1.86845  |
| C | -2.36939 | 2.23532  | 2.6155   |
| H | -4.06924 | 1.47982  | 3.72671  |
| H | -0.60446 | 2.63555  | 1.45736  |
| H | -2.57895 | 3.29183  | 2.79066  |
| N | 2.59418  | -0.79776 | 1.58164  |
| N | -0.92256 | 0.58665  | 1.6028   |
| N | 3.13606  | -0.96069 | -1.32315 |
| N | 1.78714  | 2.03422  | 0.88688  |
| C | -0.60474 | 1.63757  | -2.92973 |
| H | -1.45219 | 0.97577  | -3.15913 |
| H | -0.77314 | 2.57123  | -3.49807 |
| C | -1.3836  | -4.12495 | -0.83225 |
| C | 0.03955  | -3.72596 | -0.37819 |
| H | 0.68442  | -4.60001 | -0.5904  |
| C | 0.30441  | -3.39046 | 1.08354  |
| H | -0.23389 | -4.10885 | 1.73341  |
| H | 1.37999  | -3.5637  | 1.25505  |
| O | 0.74714  | -0.30166 | -2.75466 |
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| O | 0.53749  | -2.59305 | -1.11686 |
| H | 0.55029  | -2.80253 | -2.06341 |
| H | -1.29706 | -4.84746 | -1.66438 |
| H | -1.89098 | -4.66406 | -0.01221 |
| Y | 0.78787  | -0.08004 | -0.26869 |





|   |          |          |          |
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| C | -0.07759 | -5.1919  | -0.47733 |
| C | -1.38542 | -5.66916 | -0.4976  |
| C | -2.41458 | -4.78041 | -0.73318 |
| C | -2.21676 | -3.379   | -0.90869 |
| C | -0.86039 | -2.89983 | -0.85366 |
| C | 0.16712  | -3.84561 | -0.65622 |
| C | -3.76562 | -5.38638 | -0.82249 |
| C | -3.39396 | -2.53496 | -1.13304 |
| C | -4.68302 | -3.15772 | -1.52946 |
| C | -4.83306 | -4.56135 | -1.42926 |
| C | -5.98632 | -5.236   | -1.81657 |
| H | -6.01889 | -6.3207  | -1.69322 |
| C | -7.05138 | -4.52656 | -2.35232 |
| C | -6.96104 | -3.14014 | -2.40606 |
| C | -5.82744 | -2.4518  | -1.97479 |
| H | 0.75328  | -5.88454 | -0.32777 |
| H | -1.6233  | -6.72518 | -0.35854 |
| H | 1.20116  | -3.5045  | -0.62467 |
| H | -7.95157 | -5.03719 | -2.70092 |
| H | -7.81576 | -2.56731 | -2.78411 |
| O | -3.30705 | -1.27434 | -0.98339 |
| O | -3.98147 | -6.51412 | -0.43866 |
| N | -5.93843 | -0.99679 | -2.00851 |
| H | -6.92957 | -0.84256 | -1.78792 |
| N | -0.48875 | -1.57338 | -1.0144  |
| H | -1.26149 | -0.9773  | -1.29992 |
| C | -5.80189 | -0.50606 | -3.42833 |
| H | -6.80492 | -0.44327 | -3.88213 |
| H | -5.2611  | -1.26785 | -4.0095  |
| C | 0.79269  | -1.22941 | -1.63592 |
| H | 1.05276  | -2.00784 | -2.3745  |
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| C | 1.96345  | -1.00673 | -0.64938 |

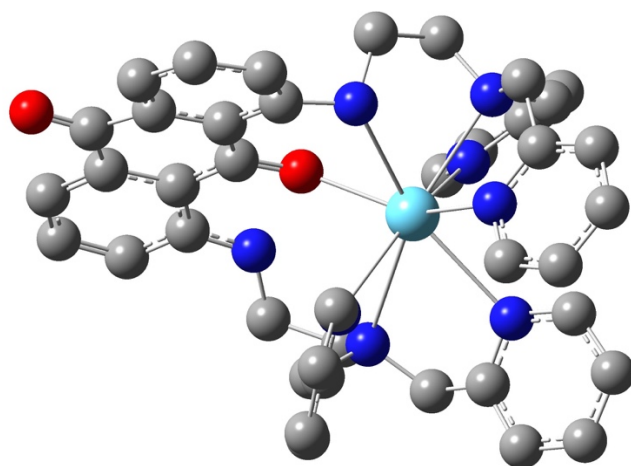
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| H | -3.97024 | 0.61999  | -3.55089 |
| H | -5.31487 | 1.3031   | -4.48152 |
| N | -5.30758 | 1.70322  | -2.38316 |
| N | 3.29502  | -0.71158 | -1.27857 |
| C | 3.26722  | 0.65079  | -1.86344 |
| H | 2.94761  | 1.34804  | -1.06623 |
| H | 2.51447  | 0.71803  | -2.67165 |
| C | 3.60123  | -1.70846 | -2.34217 |
| H | 3.03772  | -2.63063 | -2.11083 |
| H | 3.21611  | -1.36715 | -3.32154 |
| C | -6.7033  | 2.17032  | -2.3015  |
| H | -6.97744 | 2.78201  | -3.1842  |
| H | -7.39109 | 1.30535  | -2.32083 |
| C | -4.44183 | 2.88687  | -2.54807 |
| H | -4.48046 | 3.24942  | -3.59285 |
| H | -4.82048 | 3.71435  | -1.9275  |
| C | -3.03276 | 2.61145  | -2.14776 |
| C | -1.99757 | 3.32157  | -2.75398 |
| C | -1.54413 | 1.43893  | -0.85151 |
| C | -0.68823 | 3.07615  | -2.36956 |
| H | -2.22984 | 4.05875  | -3.52598 |
| C | -0.45945 | 2.09707  | -1.40789 |
| H | -1.37817 | 0.66613  | -0.09781 |
| H | 0.13525  | 3.63441  | -2.82233 |
| H | 0.54483  | 1.85123  | -1.05899 |
| C | -6.88403 | 2.96604  | -1.03453 |
| C | -7.8698  | 3.94185  | -0.92842 |
| C | -6.10012 | 3.44157  | 1.08033  |
| C | -7.9593  | 4.6856   | 0.24437  |
| H | -8.55174 | 4.12721  | -1.76232 |
| C | -7.03828 | 4.4445   | 1.26344  |
| H | -5.37972 | 3.21452  | 1.87461  |
| H | -8.72467 | 5.4578   | 0.35455  |
| H | -7.05218 | 5.02532  | 2.18734  |
| C | 4.58727  | 1.11849  | -2.40567 |
| C | 4.64387  | 1.79236  | -3.62004 |
| C | 5.8611   | 2.29566  | -4.07426 |
| H | 3.73501  | 1.92639  | -4.21131 |
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| C | 6.99151  | 2.10549  | -3.28764 |

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| H | 5.92475  | 2.8273   | -5.02663 |
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| H | 7.96894  | 2.4833   | -3.59277 |
| C | 5.02985  | -2.15986 | -2.50099 |
| C | 5.45968  | -2.65666 | -3.72653 |
| C | 6.68237  | -3.3205  | -3.80315 |
| H | 4.82772  | -2.55394 | -4.61217 |
| C | 6.95739  | -2.92383 | -1.46807 |
| C | 7.43177  | -3.4906  | -2.64005 |
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| H | -4.21137 | -3.63699 | 3.57943  |
| C | -7.03224 | -3.56772 | 1.69898  |
| H | -6.35684 | -4.89686 | 3.26908  |
| H | -8.00306 | -4.04706 | 1.55907  |
| C | -6.05657 | 0.35377  | 2.9437   |
| C | -6.95568 | 0.13608  | 3.98404  |
| C | -7.79059 | 0.62425  | 1.44339  |
| C | -8.3221  | 0.1674   | 3.72195  |
| H | -6.58861 | -0.04516 | 4.99749  |
| C | -8.75222 | 0.4221   | 2.42037  |
| H | -8.09724 | 0.84408  | 0.41082  |
| H | -9.04503 | 0.00238  | 4.52448  |
| H | -9.8136  | 0.46723  | 2.1708   |
| N | -6.46592 | 0.5859   | 1.683    |
| N | -5.5029  | -1.82646 | 1.03241  |
| C | -6.67801 | -2.46941 | 0.92788  |

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| H | -7.38635 | -2.08572 | 0.18555  |
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| H | -2.03051 | 0.41611  | 3.45497  |
| H | -1.60647 | 0.17156  | 1.75826  |
| C | -2.2883  | 2.17022  | 2.19707  |
| H | -2.97244 | 2.44251  | 1.36126  |
| H | -2.64845 | 2.72409  | 3.08528  |
| N | -0.94226 | 2.54652  | 1.86213  |
| H | -0.19221 | 1.86012  | 1.90362  |
| C | -0.58743 | 3.76719  | 1.37448  |
| C | 0.74045  | 4.02813  | 0.90098  |
| C | -1.54719 | 4.80244  | 1.30723  |
| C | 1.78728  | 3.02776  | 0.96221  |
| C | 1.00335  | 5.30096  | 0.31816  |
| C | -1.23891 | 6.03206  | 0.75908  |
| H | -2.54431 | 4.64269  | 1.72268  |
| C | 3.18485  | 3.41174  | 0.62528  |
| C | 2.33104  | 5.60646  | -0.27339 |
| C | 0.03545  | 6.28135  | 0.23344  |
| H | -1.9959  | 6.81941  | 0.73925  |
| C | 4.29194  | 2.57894  | 0.90617  |
| C | 3.44358  | 4.65957  | 0.02172  |
| H | 0.28919  | 7.23807  | -0.227   |
| C | 5.58267  | 3.02832  | 0.63047  |
| C | 4.73462  | 5.07052  | -0.29813 |
| C | 5.815    | 4.25993  | 0.02744  |
| H | 6.44026  | 2.39724  | 0.89975  |
| H | 4.86644  | 6.04772  | -0.76944 |
| H | 6.83605  | 4.59063  | -0.17641 |
| O | 2.51701  | 6.58584  | -0.96116 |
| O | 1.54713  | 1.83101  | 1.28232  |
| C | 4.93087  | 0.03268  | 3.53858  |
| H | 4.12662  | -0.72339 | 3.49043  |
| H | 5.19592  | 0.14402  | 4.60777  |
| C | 4.44861  | 1.35215  | 2.99119  |
| H | 5.1866   | 2.152    | 3.15337  |
| H | 3.54093  | 1.67187  | 3.53184  |
| N | 4.16084  | 1.26742  | 1.52145  |
| H | 3.1467   | 1.06523  | 1.46225  |
| C | 7.29342  | 0.33052  | 2.95948  |
| H | 7.70475  | 0.20623  | 3.97939  |
| H | 7.01347  | 1.3937   | 2.87728  |
| C | 6.39323  | -1.86794 | 3.26038  |

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| H | 6.40858  | -1.88963 | 4.36642  |
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| C | 5.46188  | -2.90974 | 2.72167  |
| C | 5.26446  | -4.09819 | 3.41919  |
| C | 4.50438  | -5.1075  | 2.84209  |
| H | 5.72379  | -4.2352  | 4.40147  |
| C | 4.1779   | -3.67658 | 0.9592   |
| C | 3.95044  | -4.89059 | 1.57987  |
| H | 4.35383  | -6.05509 | 3.36495  |
| H | 3.77616  | -3.4837  | -0.04086 |
| H | 3.36591  | -5.66384 | 1.07936  |
| C | 8.33879  | 0.01936  | 1.92686  |
| C | 9.68928  | 0.14502  | 2.23004  |
| C | 10.63967 | -0.09466 | 1.24154  |
| H | 9.9949   | 0.42953  | 3.24009  |
| C | 8.84236  | -0.5853  | -0.25178 |
| C | 10.20285 | -0.46938 | -0.0286  |
| H | 11.70612 | -0.00054 | 1.46103  |
| H | 8.47758  | -0.89021 | -1.23861 |
| H | 10.91002 | -0.67716 | -0.83342 |
| N | 7.89961  | -0.34441 | 0.693    |
| N | 4.91516  | -2.683   | 1.50432  |
| Y | 5.47168  | -0.57588 | 0.34999  |
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$[\text{La}(\text{L}^1)]^{3+}$



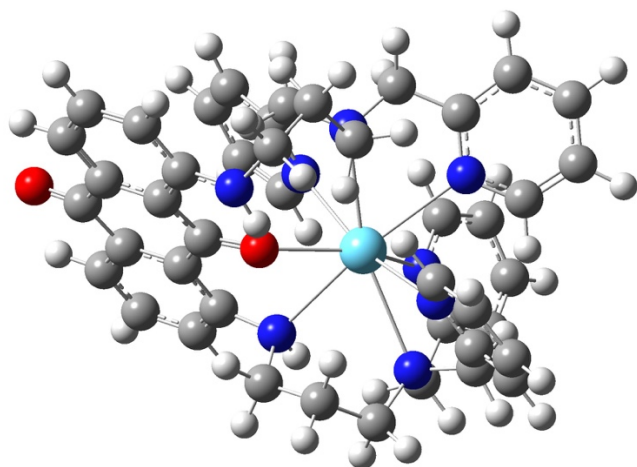
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| C | -2.86485 | 1.80939  | -0.27537 |
| C | -4.13339 | 2.31557  | 0.08622  |
| C | -4.32227 | 3.64722  | 0.44082  |
| H | -5.33221 | 3.9713   | 0.70102  |
| C | -3.2399  | 4.51553  | 0.46465  |
| C | -1.98707 | 4.05048  | 0.07445  |
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| H | -6.8847  | -2.90223 | 0.16496  |
| H | -7.171   | -0.40071 | 0.32209  |
| H | -4.6754  | -3.86442 | -0.30552 |
| H | -3.36882 | 5.55886  | 0.7592   |
| H | -1.1414  | 4.74663  | 0.04365  |
| O | -1.5542  | -0.07444 | -0.87184 |
| O | -6.43948 | 1.90132  | 0.30272  |
| N | -0.46645 | 2.38545  | -0.81174 |
| H | 0.1652   | 3.05764  | -0.36797 |
| N | -2.45706 | -2.53862 | -0.70116 |
| H | -1.72683 | -1.88294 | -0.94346 |
| C | -0.40753 | 2.66995  | -2.282   |
| H | -0.304   | 3.75941  | -2.43168 |
| H | -1.38455 | 2.40619  | -2.71385 |
| C | -2.06415 | -3.81087 | -0.13901 |
| H | -2.62531 | -3.98869 | 0.79639  |
| H | -2.3124  | -4.66057 | -0.80111 |
| C | -0.57055 | -3.8794  | 0.11547  |
| H | -0.39849 | -4.81393 | 0.68582  |
| H | -0.01875 | -4.00282 | -0.83034 |
| C | 0.67323  | 1.88803  | -3.02951 |
| H | 0.24886  | 0.94522  | -3.40733 |
| H | 0.99384  | 2.4632   | -3.92037 |
| N | 1.8332   | 1.54467  | -2.17956 |
| N | 0.07713  | -2.73826 | 0.84555  |
| C | 1.38938  | -3.29359 | 1.24907  |
| H | 1.74926  | -3.90236 | 0.39881  |
| H | 1.2522   | -4.00732 | 2.08557  |
| C | -0.73389 | -2.43391 | 2.0408   |
| H | -1.75987 | -2.20618 | 1.70082  |
| H | -0.80596 | -3.32731 | 2.69385  |
| C | 2.5421   | 2.75634  | -1.72994 |
| H | 3.3074   | 3.06108  | -2.46798 |
| H | 1.83092  | 3.59998  | -1.70741 |

|   |          |          |          |
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| C | 2.79102  | 0.67217  | -2.89022 |
| H | 3.229    | 1.20182  | -3.75934 |
| H | 3.63466  | 0.47576  | -2.19901 |
| C | 2.19257  | -0.6264  | -3.3535  |
| C | 2.59735  | -1.20283 | -4.55171 |
| C | 0.66211  | -2.31891 | -3.00259 |
| C | 2.01345  | -2.39721 | -4.96488 |
| H | 3.35805  | -0.71227 | -5.16327 |
| C | 1.01209  | -2.96137 | -4.17997 |
| H | -0.14933 | -2.71377 | -2.38279 |
| H | 2.3193   | -2.86743 | -5.90199 |
| H | 0.49895  | -3.8758  | -4.48083 |
| C | 3.16054  | 2.62859  | -0.36541 |
| C | 4.33156  | 3.31983  | -0.0652  |
| C | 3.00303  | 1.86688  | 1.80703  |
| C | 4.82765  | 3.29216  | 1.23434  |
| H | 4.84316  | 3.88759  | -0.84623 |
| C | 4.14076  | 2.55697  | 2.19598  |
| H | 2.47039  | 1.24287  | 2.53474  |
| H | 5.73887  | 3.83752  | 1.49075  |
| H | 4.48645  | 2.50627  | 3.2297   |
| C | 2.5414   | -2.38139 | 1.55637  |
| C | 3.41724  | -2.72197 | 2.58427  |
| C | 4.65766  | -2.09561 | 2.66314  |
| H | 3.14601  | -3.50954 | 3.29127  |
| C | 4.03175  | -0.81498 | 0.75427  |
| C | 4.98898  | -1.14718 | 1.70086  |
| H | 5.36539  | -2.36539 | 3.45009  |
| H | 4.25009  | -0.04002 | 0.01028  |
| H | 5.96646  | -0.66232 | 1.6876   |
| C | -0.31612 | -1.24951 | 2.86419  |
| C | -0.28656 | -1.3391  | 4.2527   |
| C | -0.12737 | -0.18345 | 5.0129   |
| H | -0.4209  | -2.30889 | 4.73781  |
| C | -0.00068 | 1.03849  | 2.97237  |
| C | -0.00569 | 1.03897  | 4.35941  |
| H | -0.11679 | -0.23606 | 6.10377  |
| H | 0.11701  | 1.98442  | 2.42945  |
| H | 0.08691  | 1.97557  | 4.91128  |
| N | 2.81734  | -1.38994 | 0.67999  |
| N | -0.13545 | -0.07147 | 2.22436  |
| N | 1.24675  | -1.18796 | -2.5701  |
| N | 2.50104  | 1.89117  | 0.55694  |

|    |         |         |          |
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| La | 0.71714 | 0.00723 | -0.27902 |
|----|---------|---------|----------|

[La(L<sup>2</sup>)]<sup>3+</sup>

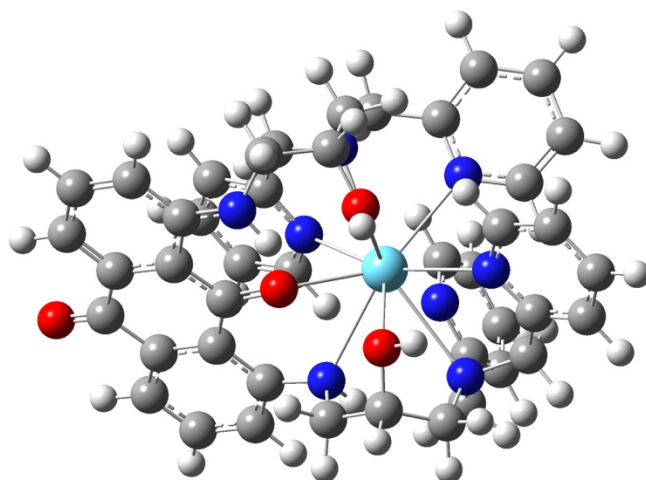


|   |          |          |          |
|---|----------|----------|----------|
| C | -5.7253  | -2.86819 | -0.13967 |
| C | -5.96437 | -1.48236 | -0.17103 |
| C | -4.94423 | -0.62084 | -0.49939 |
| C | -3.6323  | -1.09502 | -0.82655 |
| C | -3.41496 | -2.52148 | -0.81627 |
| C | -4.48066 | -3.37143 | -0.4355  |
| C | -5.24111 | 0.83084  | -0.41364 |
| C | -2.56323 | -0.14984 | -0.99974 |
| C | -2.83104 | 1.30267  | -0.99163 |
| C | -4.12531 | 1.77645  | -0.68882 |
| C | -4.4193  | 3.13559  | -0.62842 |
| H | -5.44356 | 3.42996  | -0.39012 |
| C | -3.42386 | 4.06918  | -0.87994 |
| C | -2.14558 | 3.62743  | -1.20826 |
| C | -1.83434 | 2.27084  | -1.26881 |
| H | -6.53617 | -3.55398 | 0.11623  |
| H | -6.9418  | -1.06452 | 0.07729  |
| H | -4.32494 | -4.45127 | -0.42998 |
| H | -3.64189 | 5.13864  | -0.84678 |
| H | -1.36786 | 4.3608   | -1.44937 |
| O | -1.34395 | -0.5408  | -1.09988 |
| O | -6.34    | 1.24157  | -0.10598 |
| N | -0.49819 | 1.91448  | -1.6793  |
| H | 0.03888  | 2.78383  | -1.61961 |
| N | -2.21902 | -3.06539 | -1.16703 |
| H | -1.55159 | -2.38664 | -1.51278 |
| C | 0.75299  | 0.81101  | -3.57942 |
| H | 0.65657  | 0.65276  | -4.66602 |
| C | 2.05244  | 1.55379  | -3.32418 |

|   |          |          |          |
|---|----------|----------|----------|
| H | 2.8418   | 1.1476   | -3.97809 |
| H | 1.94277  | 2.61104  | -3.62422 |
| N | 2.52271  | 1.49002  | -1.90178 |
| N | -0.16867 | -1.75662 | 1.63594  |
| C | 0.59439  | -1.86816 | 2.88653  |
| H | 0.3252   | -2.79461 | 3.43246  |
| H | 0.28706  | -1.03234 | 3.54291  |
| C | -1.55493 | -1.40736 | 1.96362  |
| H | -2.20655 | -1.66704 | 1.11746  |
| H | -1.92944 | -1.99627 | 2.82368  |
| C | 2.76327  | 2.84459  | -1.37084 |
| H | 3.62257  | 3.32425  | -1.8797  |
| H | 1.89115  | 3.47841  | -1.61393 |
| C | 3.7952   | 0.74613  | -1.84193 |
| H | 4.54397  | 1.20433  | -2.51747 |
| H | 4.21164  | 0.85927  | -0.82375 |
| C | 3.64733  | -0.71268 | -2.16945 |
| C | 4.59485  | -1.35013 | -2.96355 |
| C | 2.47888  | -2.6828  | -1.90948 |
| C | 4.46811  | -2.71166 | -3.22365 |
| H | 5.42905  | -0.77936 | -3.3787  |
| C | 3.38311  | -3.39366 | -2.68488 |
| H | 1.6135   | -3.20025 | -1.48292 |
| H | 5.20218  | -3.22864 | -3.8456  |
| H | 3.23283  | -4.45906 | -2.86505 |
| C | 2.96995  | 2.87313  | 0.11744  |
| C | 3.92487  | 3.70785  | 0.68871  |
| C | 2.28479  | 2.15542  | 2.20697  |
| C | 4.04174  | 3.76235  | 2.07493  |
| H | 4.56961  | 4.31598  | 0.04977  |
| C | 3.20054  | 2.97159  | 2.85251  |
| H | 1.61262  | 1.51146  | 2.78566  |
| H | 4.78383  | 4.41407  | 2.54175  |
| H | 3.25367  | 2.98294  | 3.94209  |
| C | 2.07879  | -1.793   | 2.68893  |
| C | 2.93462  | -2.43778 | 3.57876  |
| C | 4.30841  | -2.2904  | 3.43121  |
| H | 2.52066  | -3.04798 | 4.38521  |
| C | 3.86479  | -0.91369 | 1.53672  |
| C | 4.78605  | -1.50505 | 2.38517  |
| H | 4.99728  | -2.78456 | 4.11992  |
| H | 4.21546  | -0.29608 | 0.70386  |
| H | 5.855    | -1.35848 | 2.22421  |

|    |          |          |          |
|----|----------|----------|----------|
| C  | -1.74367 | 0.05817  | 2.25232  |
| C  | -2.83389 | 0.47149  | 3.01518  |
| C  | -3.06241 | 1.8303   | 3.1985   |
| H  | -3.49975 | -0.27304 | 3.4591   |
| C  | -1.11094 | 2.25004  | 1.8939   |
| C  | -2.17928 | 2.74278  | 2.62518  |
| H  | -3.91457 | 2.17381  | 3.78932  |
| H  | -0.38812 | 2.9384   | 1.43996  |
| H  | -2.31135 | 3.81888  | 2.74859  |
| N  | 2.53123  | -1.04061 | 1.66522  |
| N  | -0.88463 | 0.93657  | 1.69569  |
| N  | 2.58928  | -1.36942 | -1.64055 |
| N  | 2.1582   | 2.0944   | 0.86739  |
| La | 0.81919  | 0.06422  | -0.16398 |
| H  | 0.80767  | -0.21176 | -3.15747 |
| C  | -0.50113 | 1.52748  | -3.12847 |
| H  | -1.37552 | 0.88387  | -3.29837 |
| H  | -0.66475 | 2.43774  | -3.73543 |
| C  | -1.65509 | -4.28699 | -0.6182  |
| H  | -0.87278 | -4.62819 | -1.31659 |
| H  | -2.39993 | -5.09447 | -0.59916 |
| C  | -1.0616  | -4.06808 | 0.77938  |
| H  | -0.62025 | -5.01429 | 1.12856  |
| H  | -1.87656 | -3.84434 | 1.48705  |
| C  | 0.00429  | -2.95746 | 0.77758  |
| H  | 0.99294  | -3.37876 | 1.02122  |
| H  | 0.09612  | -2.59948 | -0.27172 |

$[\text{La}(\text{L}^3)]^{3+}$

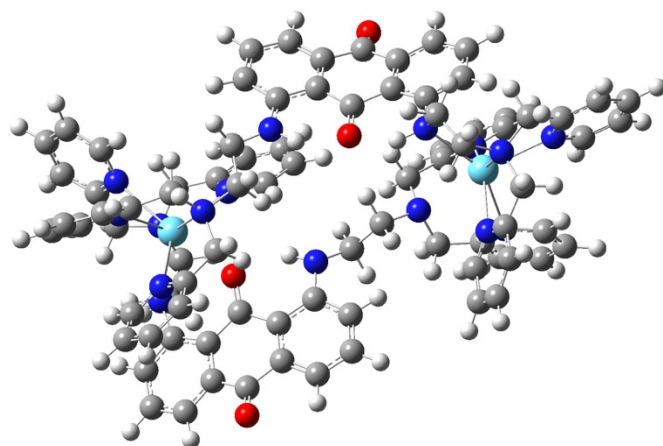
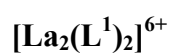


|   |          |          |          |
|---|----------|----------|----------|
| C | -5.75434 | -2.94963 | -0.48163 |
| C | -6.05082 | -1.58063 | -0.35476 |
| C | -5.06092 | -0.64529 | -0.56496 |

|   |          |          |          |
|---|----------|----------|----------|
| C | -3.73619 | -1.03833 | -0.91406 |
| C | -3.45167 | -2.44059 | -1.04718 |
| C | -4.48367 | -3.37409 | -0.80965 |
| C | -5.39433 | 0.78393  | -0.32855 |
| C | -2.69377 | -0.04979 | -0.98845 |
| C | -2.99308 | 1.38034  | -0.82857 |
| C | -4.29885 | 1.78564  | -0.48848 |
| C | -4.61083 | 3.12364  | -0.2647  |
| H | -5.64041 | 3.37828  | -0.00394 |
| C | -3.62037 | 4.08985  | -0.38279 |
| C | -2.32854 | 3.70987  | -0.73903 |
| C | -1.99628 | 2.3745   | -0.96197 |
| H | -6.54247 | -3.6899  | -0.32555 |
| H | -7.04976 | -1.23575 | -0.08096 |
| H | -4.27941 | -4.44042 | -0.93225 |
| H | -3.85164 | 5.14415  | -0.21725 |
| H | -1.55727 | 4.47907  | -0.86195 |
| O | -1.4805  | -0.3901  | -1.1472  |
| O | -6.50397 | 1.13221  | 0.01498  |
| N | -0.63384 | 2.08227  | -1.3567  |
| H | -0.1093  | 2.91934  | -1.09936 |
| N | -2.19654 | -2.84508 | -1.37647 |
| H | -1.57516 | -2.07973 | -1.61653 |
| C | 0.72448  | 1.34646  | -3.36781 |
| H | 0.61346  | 1.33217  | -4.46766 |
| C | 2.04232  | 2.03472  | -3.04982 |
| H | 2.822    | 1.55445  | -3.66664 |
| H | 2.01411  | 3.0869   | -3.38828 |
| N | 2.43612  | 1.93106  | -1.62332 |
| N | -0.08135 | -2.16668 | 1.45266  |
| C | 0.62679  | -2.06584 | 2.74605  |
| H | 0.40371  | -2.95231 | 3.37214  |
| H | 0.21216  | -1.20069 | 3.29277  |
| C | -1.51088 | -1.97985 | 1.73362  |
| H | -2.08228 | -2.2673  | 0.8416   |
| H | -1.83768 | -2.66202 | 2.54564  |
| C | 2.34944  | 3.23744  | -0.95241 |
| H | 3.17019  | 3.90449  | -1.28519 |
| H | 1.43318  | 3.76171  | -1.27685 |
| C | 3.84212  | 1.49732  | -1.51641 |
| H | 4.49542  | 2.14771  | -2.13154 |
| H | 4.16179  | 1.66314  | -0.46984 |
| C | 4.09838  | 0.05688  | -1.85114 |

|    |          |          |          |
|----|----------|----------|----------|
| C  | 5.2853   | -0.30007 | -2.4878  |
| C  | 3.53393  | -2.15799 | -1.5622  |
| C  | 5.59725  | -1.6464  | -2.64748 |
| H  | 5.96741  | 0.47631  | -2.84294 |
| C  | 4.70707  | -2.59723 | -2.15952 |
| H  | 2.80919  | -2.87903 | -1.17035 |
| H  | 6.52483  | -1.94644 | -3.13995 |
| H  | 4.91283  | -3.66545 | -2.2434  |
| C  | 2.37504  | 3.13004  | 0.5481   |
| C  | 2.95746  | 4.14717  | 1.3005   |
| C  | 1.8288   | 1.96821  | 2.4612   |
| C  | 2.95508  | 4.05797  | 2.68784  |
| H  | 3.41545  | 5.00192  | 0.79655  |
| C  | 2.37896  | 2.93938  | 3.28291  |
| H  | 1.36846  | 1.07627  | 2.89851  |
| H  | 3.40632  | 4.84557  | 3.29519  |
| H  | 2.35969  | 2.81643  | 4.3666   |
| C  | 2.10743  | -1.87844 | 2.62621  |
| C  | 2.96062  | -2.46277 | 3.55956  |
| C  | 4.32004  | -2.17896 | 3.51078  |
| H  | 2.55482  | -3.12928 | 4.32435  |
| C  | 3.86789  | -0.79826 | 1.61902  |
| C  | 4.78315  | -1.31612 | 2.52172  |
| H  | 5.00744  | -2.62226 | 4.23461  |
| H  | 4.21271  | -0.12723 | 0.82672  |
| H  | 5.83881  | -1.05204 | 2.44474  |
| C  | -1.86841 | -0.567   | 2.10481  |
| C  | -3.03669 | -0.3305  | 2.82705  |
| C  | -3.38961 | 0.9746   | 3.14811  |
| H  | -3.66013 | -1.17279 | 3.13915  |
| C  | -1.40691 | 1.68927  | 2.03176  |
| C  | -2.55179 | 2.01069  | 2.74369  |
| H  | -4.3006  | 1.17986  | 3.71491  |
| H  | -0.72363 | 2.48108  | 1.70419  |
| H  | -2.77606 | 3.05225  | 2.97975  |
| N  | 2.54938  | -1.0661  | 1.64546  |
| N  | -1.05628 | 0.43119  | 1.7015   |
| N  | 3.21009  | -0.85998 | -1.4118  |
| N  | 1.80839  | 2.04479  | 1.11649  |
| La | 0.79216  | -0.08466 | -0.2638  |
| C  | -0.55151 | 1.96204  | -2.83895 |
| H  | -1.38501 | 1.32565  | -3.17001 |
| H  | -0.7     | 2.94859  | -3.31742 |

|   |          |          |          |
|---|----------|----------|----------|
| C | -1.52577 | -4.07203 | -1.04323 |
| C | -0.08997 | -3.78284 | -0.556   |
| H | 0.49711  | -4.69242 | -0.78338 |
| C | 0.18191  | -3.52029 | 0.91999  |
| H | -0.34653 | -4.28475 | 1.52549  |
| H | 1.26055  | -3.69998 | 1.06771  |
| O | 0.78115  | -0.00957 | -2.88608 |
| H | 1.52239  | -0.45194 | -3.32671 |
| O | 0.49099  | -2.66868 | -1.26707 |
| H | 0.55645  | -2.89181 | -2.20794 |
| H | -1.4714  | -4.75124 | -1.91438 |
| H | -2.06746 | -4.62805 | -0.25757 |



|   |          |         |         |
|---|----------|---------|---------|
| C | -0.15377 | 5.12261 | 0.73934 |
| C | -1.45911 | 5.61203 | 0.72755 |
| C | -2.50255 | 4.72468 | 0.89179 |
| C | -2.31595 | 3.31729 | 1.01332 |
| C | -0.96518 | 2.82391 | 0.96708 |
| C | 0.07802  | 3.76744 | 0.86428 |
| C | -3.85783 | 5.32475 | 0.95473 |
| C | -3.49358 | 2.4715  | 1.20141 |
| C | -4.78564 | 3.08044 | 1.61099 |
| C | -4.93718 | 4.48462 | 1.52435 |
| C | -6.09554 | 5.15059 | 1.91285 |
| H | -6.13225 | 6.2363  | 1.80003 |
| C | -7.15646 | 4.43221 | 2.4448  |
| C | -7.05759 | 3.04593 | 2.50035 |
| C | -5.92247 | 2.36295 | 2.06442 |
| H | 0.6872   | 5.81371 | 0.65156 |
| H | -1.68206 | 6.67512 | 0.62103 |
| H | 1.11117  | 3.41999 | 0.86225 |

|   |          |          |          |
|---|----------|----------|----------|
| H | -8.05841 | 4.93712  | 2.79711  |
| H | -7.90419 | 2.46759  | 2.888    |
| O | -3.4082  | 1.21655  | 1.01595  |
| O | -4.0677  | 6.45914  | 0.5876   |
| N | -6.02149 | 0.91004  | 2.09309  |
| H | -7.01881 | 0.74066  | 1.91915  |
| N | -0.629   | 1.48192  | 1.04872  |
| H | -1.43463 | 0.90289  | 1.27313  |
| C | -5.79527 | 0.37038  | 3.4783   |
| H | -6.76169 | 0.3338   | 4.00894  |
| H | -5.18253 | 1.09452  | 4.03622  |
| C | 0.61611  | 1.06361  | 1.69934  |
| H | 0.85575  | 1.77568  | 2.50984  |
| H | 0.40005  | 0.10075  | 2.19146  |
| C | 1.82948  | 0.89076  | 0.75921  |
| H | 1.59078  | 0.15178  | -0.02534 |
| H | 2.0371   | 1.83767  | 0.23122  |
| C | -5.093   | -0.97406 | 3.50232  |
| H | -4.00191 | -0.82163 | 3.45621  |
| H | -5.30029 | -1.46726 | 4.47299  |
| N | -5.43859 | -1.86919 | 2.38055  |
| N | 3.10003  | 0.46067  | 1.4184   |
| C | 2.99773  | -0.95562 | 1.82837  |
| H | 2.70106  | -1.53417 | 0.93007  |
| H | 2.20055  | -1.09613 | 2.58549  |
| C | 3.39975  | 1.31962  | 2.58897  |
| H | 3.02042  | 2.33434  | 2.3623   |
| H | 2.84157  | 0.98193  | 3.4837   |
| C | -6.86097 | -2.25418 | 2.35826  |
| H | -7.14171 | -2.8289  | 3.26346  |
| H | -7.48614 | -1.34219 | 2.38337  |
| C | -4.61774 | -3.08858 | 2.49399  |
| H | -4.68555 | -3.50755 | 3.51699  |
| H | -5.02361 | -3.86264 | 1.82271  |
| C | -3.18455 | -2.85644 | 2.13134  |
| C | -2.18624 | -3.62268 | 2.7324   |
| C | -1.62356 | -1.68168 | 0.91488  |
| C | -0.86016 | -3.40392 | 2.38682  |
| H | -2.45661 | -4.38096 | 3.47101  |
| C | -0.57341 | -2.39437 | 1.47224  |
| H | -1.41834 | -0.89133 | 0.18456  |
| H | -0.06516 | -4.00795 | 2.83117  |
| H | 0.45255  | -2.17348 | 1.17085  |

|    |          |          |          |
|----|----------|----------|----------|
| C  | -7.16214 | -3.0565  | 1.1173   |
| C  | -8.14444 | -4.03915 | 1.11446  |
| C  | -6.59418 | -3.536   | -1.07034 |
| C  | -8.34927 | -4.78742 | -0.04316 |
| H  | -8.73617 | -4.22849 | 2.01363  |
| C  | -7.54097 | -4.54557 | -1.15222 |
| H  | -5.96044 | -3.30174 | -1.9334  |
| H  | -9.11712 | -5.56408 | -0.07141 |
| H  | -7.64623 | -5.12931 | -2.06814 |
| C  | 4.26699  | -1.55177 | 2.37365  |
| C  | 4.24691  | -2.32484 | 3.52931  |
| C  | 5.42285  | -2.92403 | 3.9781   |
| H  | 3.31338  | -2.45941 | 4.08121  |
| C  | 6.52656  | -1.94504 | 2.10659  |
| C  | 6.59194  | -2.73055 | 3.24962  |
| H  | 5.42598  | -3.53493 | 4.88396  |
| H  | 7.42682  | -1.78952 | 1.49813  |
| H  | 7.53679  | -3.18185 | 3.55706  |
| C  | 4.85169  | 1.48975  | 2.95596  |
| C  | 5.25235  | 1.57097  | 4.28578  |
| C  | 6.57473  | 1.89696  | 4.58353  |
| H  | 4.53082  | 1.39758  | 5.08823  |
| C  | 6.99063  | 2.02429  | 2.24287  |
| C  | 7.46401  | 2.14833  | 3.54039  |
| H  | 6.90498  | 1.96931  | 5.62265  |
| H  | 7.65342  | 2.21986  | 1.38718  |
| H  | 8.4983   | 2.4403   | 3.73055  |
| N  | 5.3996   | -1.36022 | 1.66551  |
| N  | 5.72175  | 1.68743  | 1.9468   |
| N  | -2.91568 | -1.90948 | 1.20653  |
| N  | -6.4075  | -2.77933 | 0.02873  |
| La | -4.9827  | -0.49607 | 0.08197  |
| La | 5.59531  | 0.42352  | -0.2797  |
| N  | 6.43651  | 1.09117  | -2.76152 |
| N  | -3.74249 | 0.17414  | -2.31316 |
| C  | -4.564   | -0.23774 | -3.48124 |
| H  | -4.29053 | 0.36635  | -4.36855 |
| H  | -4.29785 | -1.27917 | -3.73222 |
| C  | -3.61417 | 1.653    | -2.25928 |
| H  | -2.90405 | 1.88437  | -1.44357 |
| H  | -3.1503  | 2.02148  | -3.19509 |
| C  | -4.90827 | 2.3773   | -2.02419 |
| C  | -5.21721 | 3.52618  | -2.74639 |

|   |          |          |          |
|---|----------|----------|----------|
| C | -6.42704 | 4.17546  | -2.51188 |
| H | -4.51792 | 3.90671  | -3.49489 |
| C | -7.30623 | 3.62853  | -1.58282 |
| H | -6.6887  | 5.08059  | -3.06499 |
| H | -8.28072 | 4.07952  | -1.38664 |
| C | -6.05237 | -0.20379 | -3.26554 |
| C | -6.90944 | 0.19758  | -4.28479 |
| C | -7.84115 | -0.70345 | -1.89467 |
| C | -8.28619 | 0.13274  | -4.08277 |
| H | -6.50347 | 0.55171  | -5.23586 |
| C | -8.7652  | -0.32646 | -2.85784 |
| H | -8.18814 | -1.07634 | -0.92029 |
| H | -8.97692 | 0.43695  | -4.87272 |
| H | -9.83524 | -0.39676 | -2.6559  |
| N | -6.50895 | -0.65255 | -2.0798  |
| N | -5.73514 | 1.86913  | -1.08723 |
| C | -6.91611 | 2.48025  | -0.90645 |
| H | -7.60233 | 2.02862  | -0.17979 |
| C | -2.37602 | -0.35847 | -2.45966 |
| H | -1.93499 | -0.02223 | -3.42133 |
| H | -1.76743 | 0.10753  | -1.66097 |
| C | -2.26879 | -1.8723  | -2.33834 |
| H | -2.92261 | -2.22925 | -1.50721 |
| H | -2.62716 | -2.38697 | -3.25    |
| N | -0.89917 | -2.19886 | -2.0518  |
| H | -0.17581 | -1.48953 | -2.17257 |
| C | -0.45717 | -3.40354 | -1.59837 |
| C | 0.91107  | -3.5947  | -1.21912 |
| C | -1.35165 | -4.48985 | -1.45768 |
| C | 1.90156  | -2.55201 | -1.4002  |
| C | 1.27816  | -4.83058 | -0.61667 |
| C | -0.94506 | -5.68575 | -0.89967 |
| H | -2.37685 | -4.39626 | -1.82256 |
| C | 3.34137  | -2.87697 | -1.2013  |
| C | 2.65612  | -5.03733 | -0.10942 |
| C | 0.36801  | -5.85337 | -0.43702 |
| H | -1.65566 | -6.51175 | -0.82047 |
| C | 4.37842  | -2.02572 | -1.65997 |
| C | 3.70698  | -4.09571 | -0.59969 |
| H | 0.69628  | -6.78211 | 0.03373  |
| C | 5.71096  | -2.44611 | -1.53241 |
| C | 5.0376   | -4.48083 | -0.44471 |
| C | 6.04412  | -3.66432 | -0.94038 |

|   |          |          |          |
|---|----------|----------|----------|
| H | 6.51527  | -1.84341 | -1.96839 |
| H | 5.25059  | -5.44126 | 0.03067  |
| H | 7.09     | -3.97548 | -0.88329 |
| O | 2.93918  | -5.92728 | 0.66262  |
| O | 1.58414  | -1.38176 | -1.72992 |
| C | 5.30481  | 0.89426  | -3.70056 |
| H | 4.5636   | 1.68521  | -3.49218 |
| H | 5.63996  | 1.04577  | -4.74566 |
| C | 4.65006  | -0.46231 | -3.57334 |
| H | 5.3334   | -1.27677 | -3.85731 |
| H | 3.81529  | -0.52265 | -4.28946 |
| N | 4.13811  | -0.7184  | -2.19314 |
| H | 3.11732  | -0.57297 | -2.16389 |
| C | 7.61206  | 0.29245  | -3.16612 |
| H | 8.09444  | 0.73392  | -4.05974 |
| H | 7.28019  | -0.70976 | -3.48826 |
| C | 6.84109  | 2.51365  | -2.77884 |
| H | 6.95951  | 2.86463  | -3.82227 |
| H | 7.84595  | 2.59188  | -2.32407 |
| C | 5.92197  | 3.42973  | -2.02724 |
| C | 5.83182  | 4.77022  | -2.39336 |
| C | 5.07741  | 5.64001  | -1.6153  |
| H | 6.3682   | 5.13077  | -3.27456 |
| C | 4.53957  | 3.78806  | -0.20971 |
| C | 4.41475  | 5.1353   | -0.49639 |
| H | 5.01255  | 6.69936  | -1.87432 |
| H | 4.04771  | 3.35957  | 0.67075  |
| H | 3.8255   | 5.78491  | 0.15259  |
| C | 8.61712  | 0.15577  | -2.05456 |
| C | 9.96922  | 0.00973  | -2.34631 |
| C | 10.88217 | -0.15935 | -1.30938 |
| H | 10.30668 | 0.03199  | -3.38567 |
| C | 9.05494  | 0.00284  | 0.2143   |
| C | 10.41329 | -0.15918 | 0.00354  |
| H | 11.94776 | -0.27586 | -1.52159 |
| H | 8.66208  | 0.03176  | 1.23849  |
| H | 11.09379 | -0.27224 | 0.849    |
| N | 8.15019  | 0.14947  | -0.78071 |
| N | 5.27761  | 2.93163  | -0.94756 |